



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:06 PM EDT

PDB ID : 7RF7 / pdb_00007rf7
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 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 : 2.09 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)

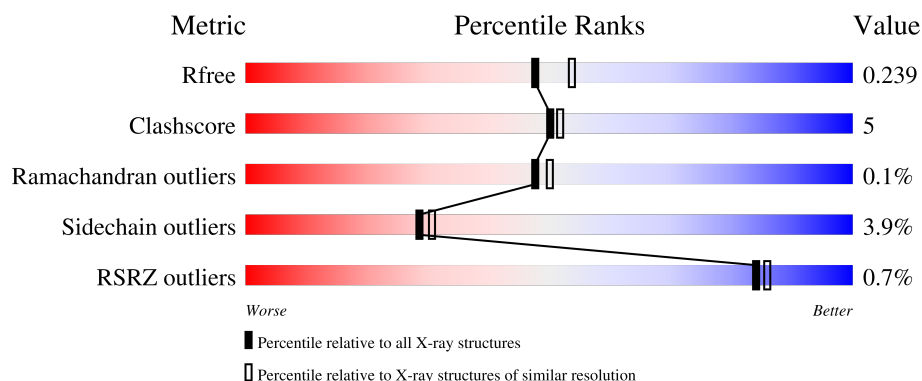
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	 88% 9% .
1	a	344	 83% 13% . .

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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 106082 atoms, of which 52760 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

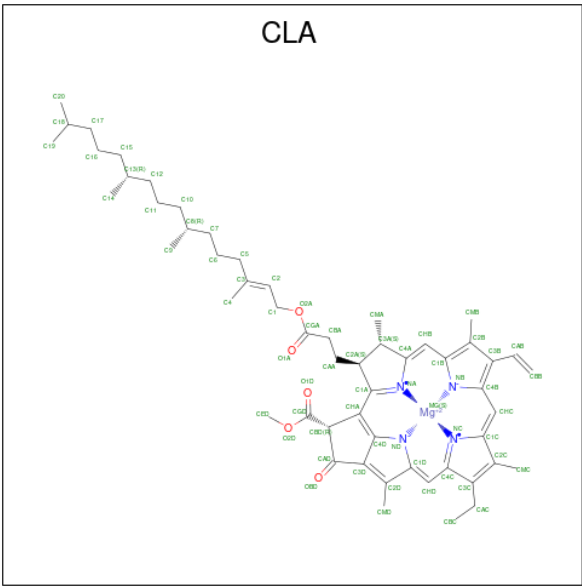
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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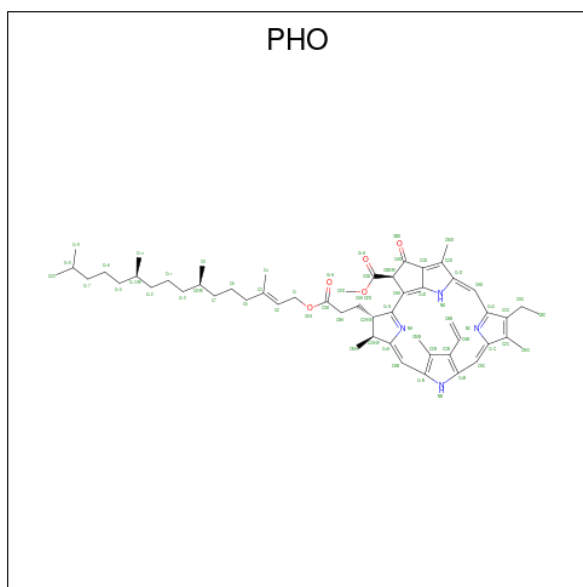
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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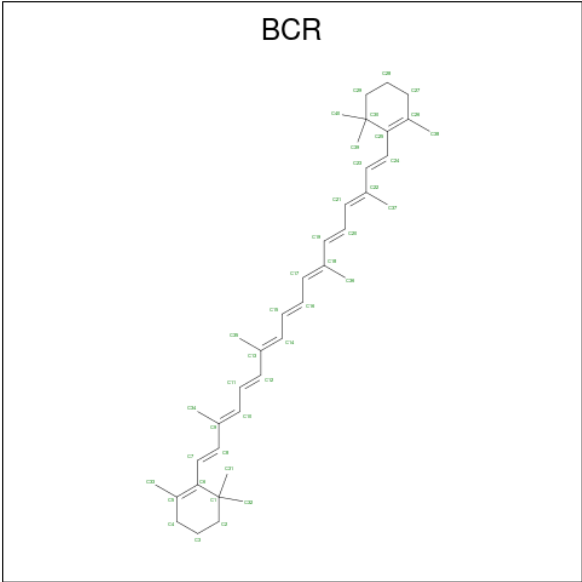
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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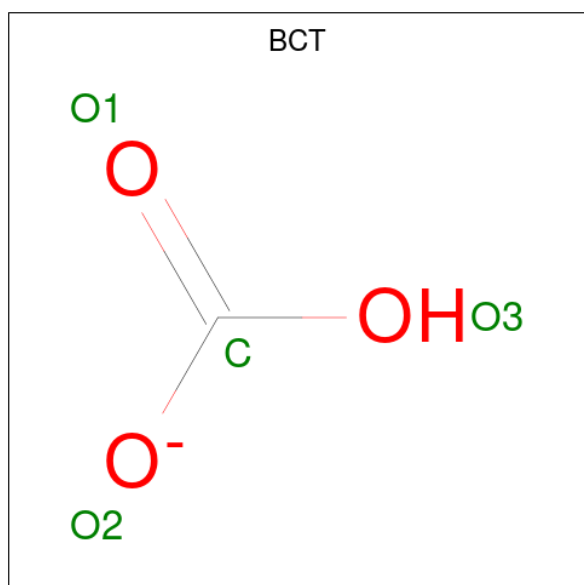
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

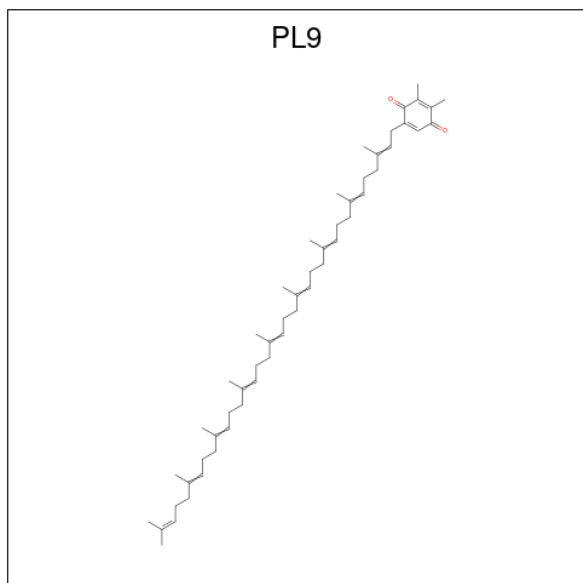
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



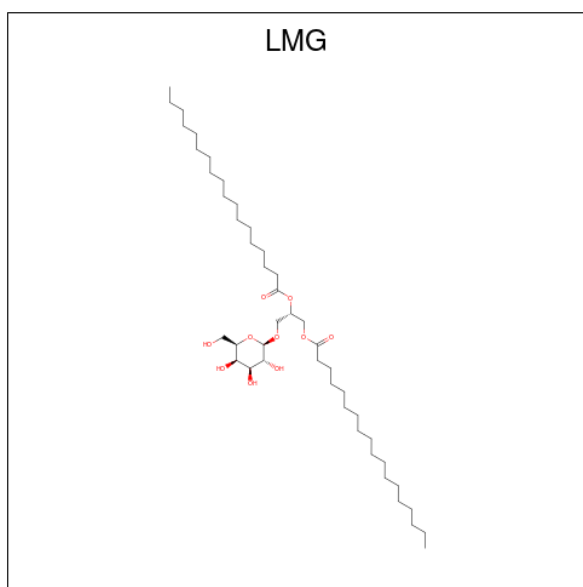
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 27 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
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

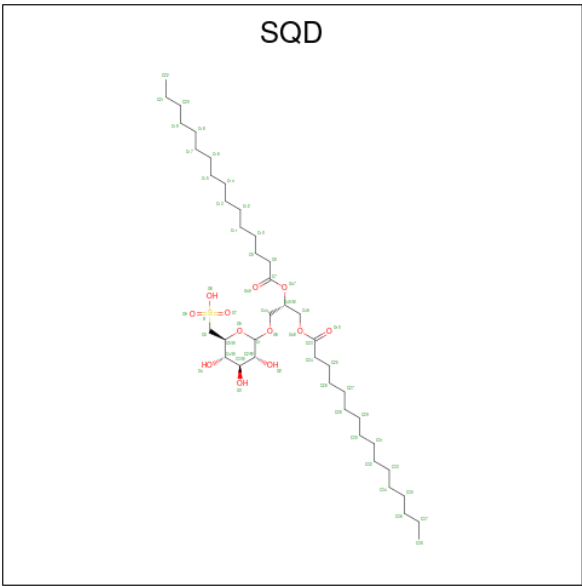
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

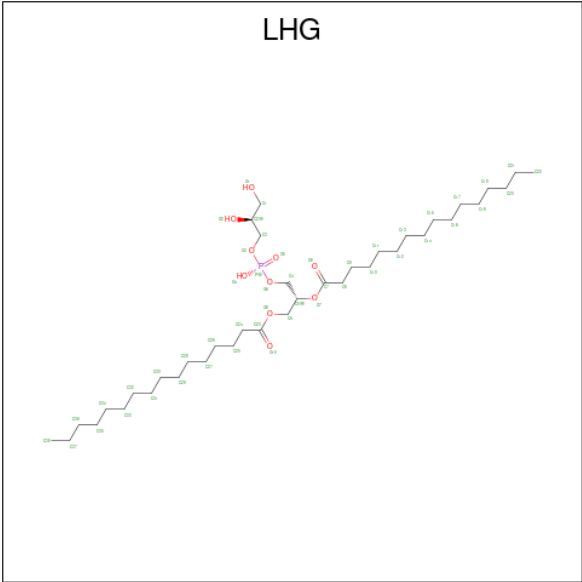
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



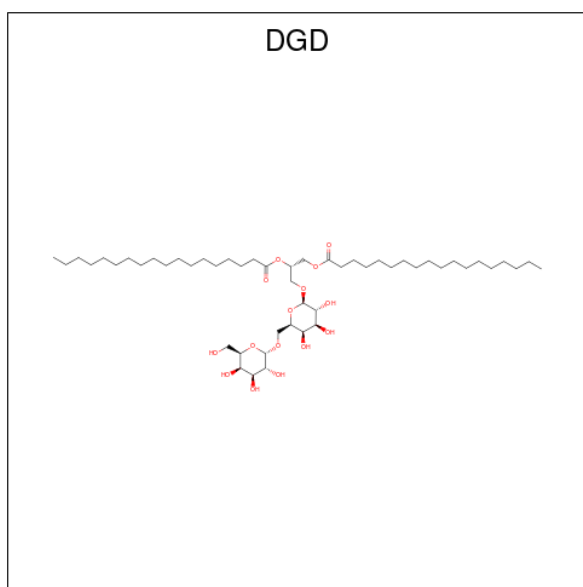
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

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



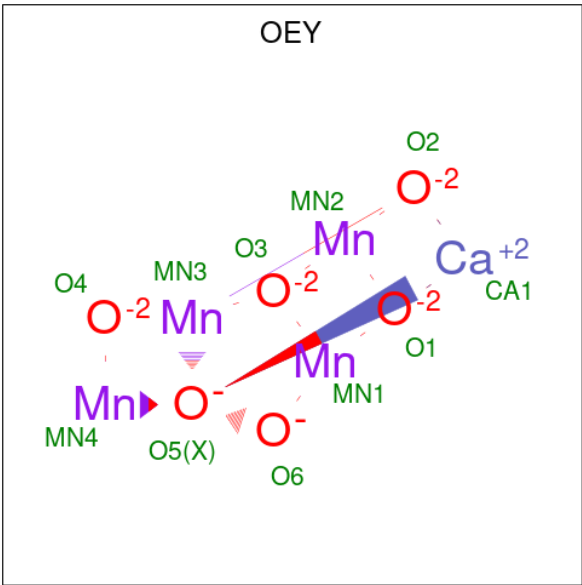
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



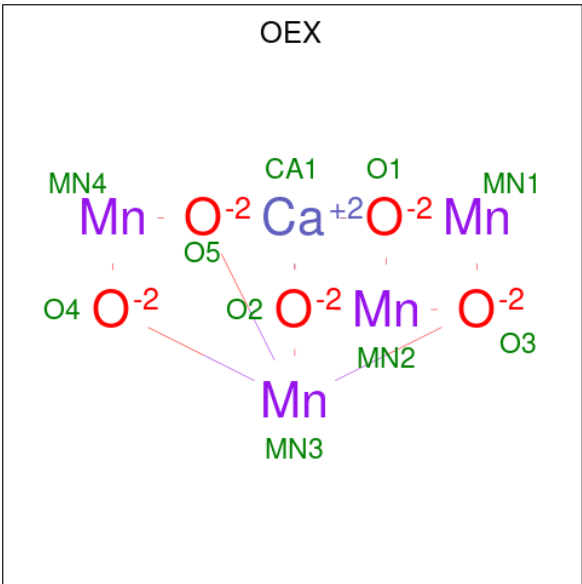
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total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

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



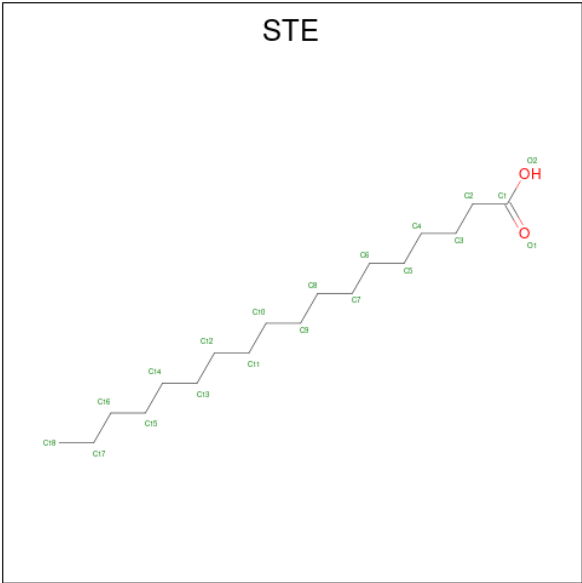
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 34 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



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

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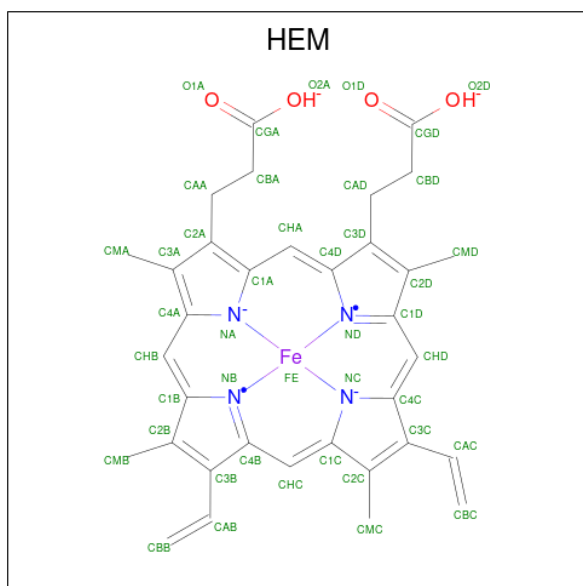
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	1	Total C H O 28 10 16 2	0	0
34	L	1	Total C H O 28 10 16 2	0	0
34	M	1	Total C H O 37 13 22 2	0	0
34	M	1	Total C H 26 10 16	0	0
34	R	1	Total C H O 28 10 16 2	0	0
34	T	1	Total C H 44 15 29	0	0
34	X	1	Total C H O 55 18 35 2	0	0
34	Z	1	Total C H 20 8 12	0	0
34	a	1	Total C H 26 10 16	0	0
34	a	1	Total C H O 28 10 16 2	0	0
34	a	1	Total C H 41 15 26	0	0
34	b	1	Total C H 47 16 31	0	0
34	b	1	Total C H O 55 18 35 2	0	0
34	b	1	Total C H O 40 14 24 2	0	0
34	b	1	Total C H O 55 18 35 2	0	0
34	b	1	Total C H 26 10 16	0	0
34	c	1	Total C H O 55 18 35 2	0	0
34	c	1	Total C H O 28 10 16 2	0	0
34	d	1	Total C H O 43 15 26 2	0	0
34	d	1	Total C H O 55 18 35 2	0	0
34	d	1	Total C H O 55 18 35 2	0	0

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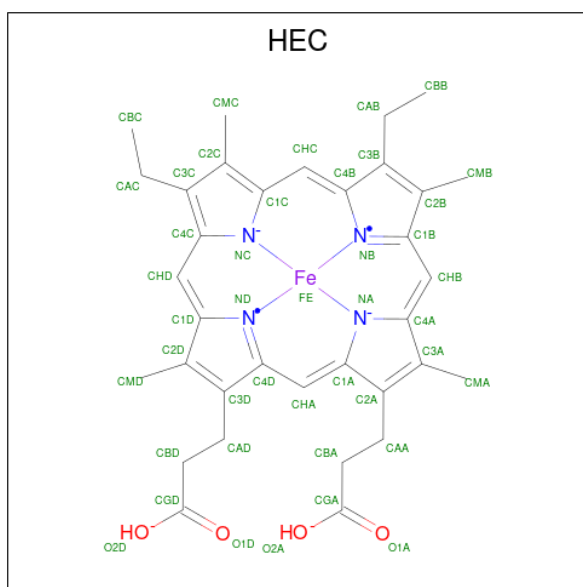
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	h	1	Total	C	H	0	0
			41	14	27		
34	j	1	Total	C	H	O	0
			28	10	16	2	
34	l	1	Total	C	H	0	0
			53	18	35		
34	t	1	Total	C	H	O	0
			34	12	20	2	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	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: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	151	Total O 151 151	0	8
37	B	204	Total O 204 204	0	0
37	C	173	Total O 173 173	0	0
37	D	131	Total O 131 131	0	0
37	E	33	Total O 33 33	0	0
37	F	8	Total O 8 8	0	0
37	H	34	Total O 34 34	0	0
37	I	17	Total O 17 17	0	0
37	J	24	Total O 24 24	0	0
37	K	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	10	Total 10	O 10	0	0
37	M	8	Total 8	O 8	0	0
37	O	86	Total 86	O 86	0	0
37	R	4	Total 4	O 4	0	0
37	T	8	Total 8	O 8	0	0
37	U	34	Total 34	O 34	0	0
37	V	64	Total 64	O 64	0	0
37	X	15	Total 15	O 15	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	10	Total 10	O 10	0	0
37	a	132	Total 132	O 132	0	8
37	b	172	Total 172	O 172	0	0
37	c	157	Total 157	O 157	0	0
37	d	110	Total 110	O 110	0	0
37	e	28	Total 28	O 28	0	0
37	f	6	Total 6	O 6	0	0
37	h	20	Total 20	O 20	0	0
37	i	11	Total 11	O 11	0	0
37	j	8	Total 8	O 8	0	0
37	k	5	Total 5	O 5	0	0
37	l	8	Total 8	O 8	0	0

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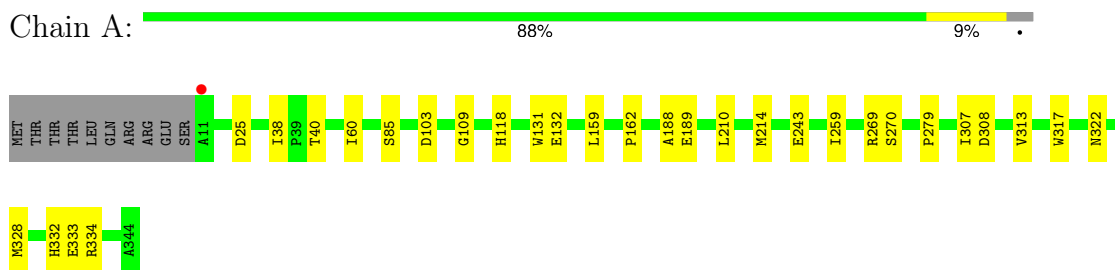
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	7	Total 7	O 7	0	0
37	o	100	Total 100	O 100	0	0
37	r	7	Total 7	O 7	0	0
37	t	8	Total 8	O 8	0	0
37	u	48	Total 48	O 48	0	0
37	v	59	Total 59	O 59	0	0
37	x	11	Total 11	O 11	0	0
37	y	4	Total 4	O 4	0	0
37	z	12	Total 12	O 12	0	0

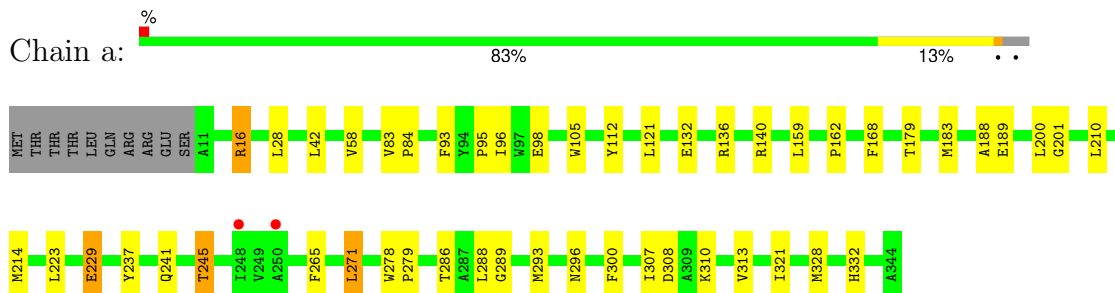
3 Residue-property plots

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.

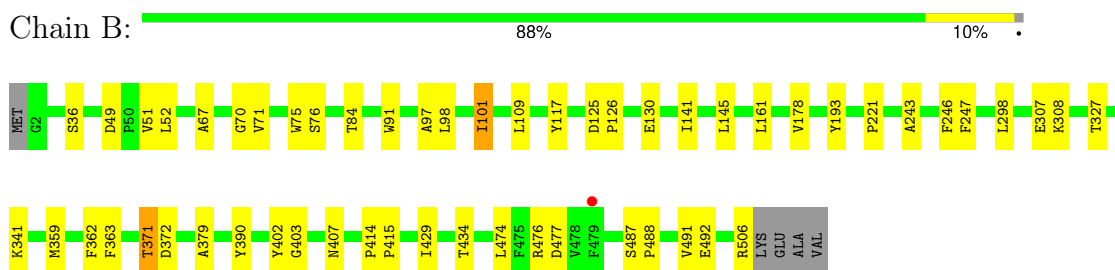
- Molecule 1: Photosystem II protein D1 1



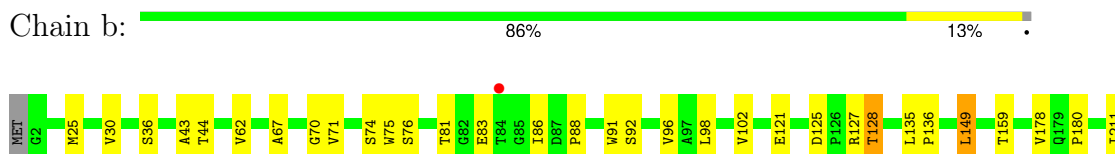
- Molecule 1: Photosystem II protein D1 1

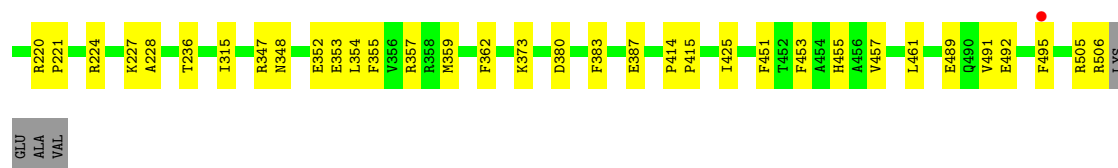


- Molecule 2: Photosystem II CP47 reaction center protein



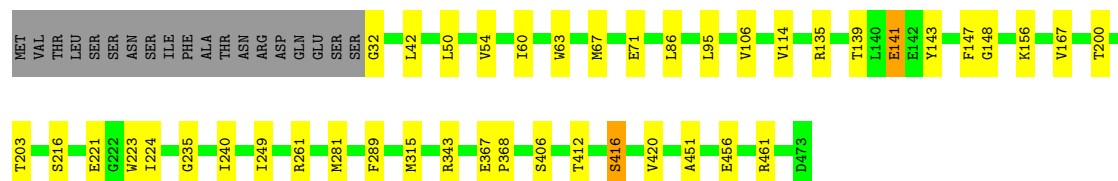
- Molecule 2: Photosystem II CP47 reaction center protein





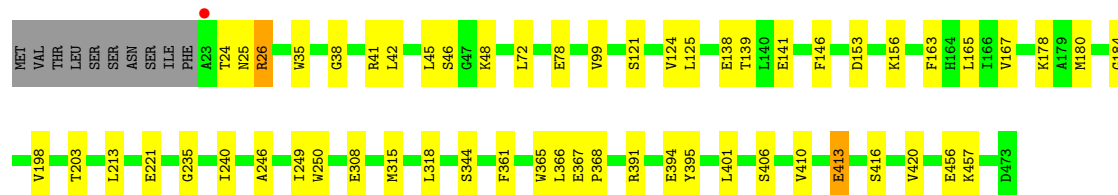
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 9% .



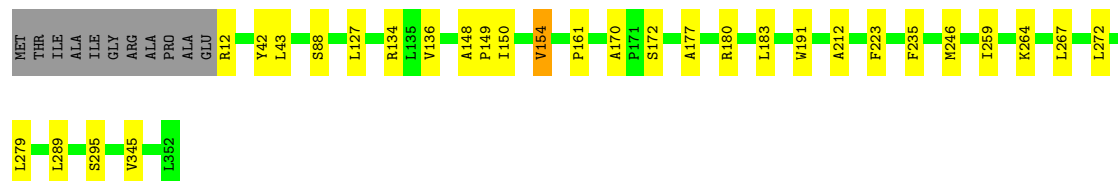
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12% .



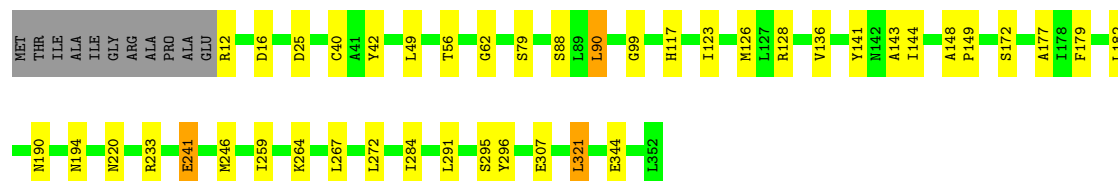
- Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .



- Molecule 4: Photosystem II D2 protein

Chain d: 85% 11% . .

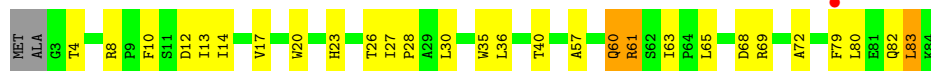


- Molecule 5: Cytochrome b559 subunit alpha

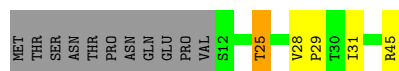
Chain E: 81% 17% .



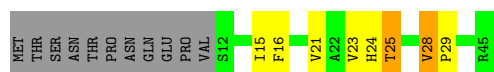
- Molecule 5: Cytochrome b559 subunit alpha



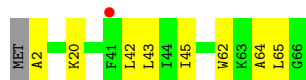
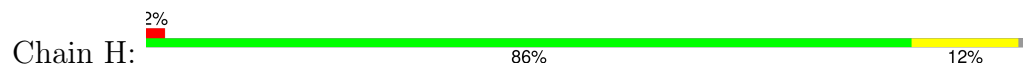
- Molecule 6: Cytochrome b559 subunit beta



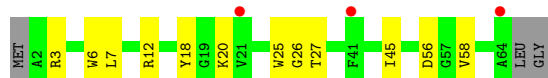
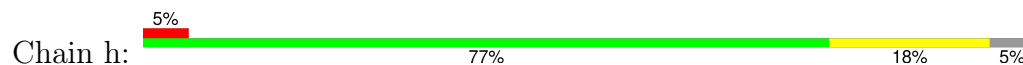
- Molecule 6: Cytochrome b559 subunit beta



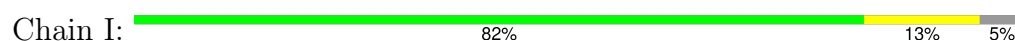
- Molecule 7: Photosystem II reaction center protein H



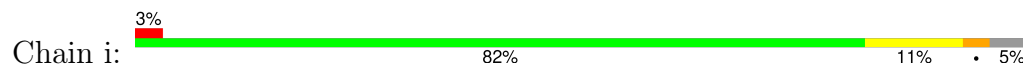
- Molecule 7: Photosystem II reaction center protein H

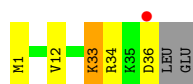


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 80% 10% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 65% 25% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 67% 11% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 48% 33% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 81% 14% 5% 2%



- Molecule 12: Photosystem II reaction center protein M

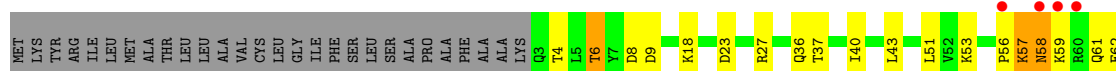
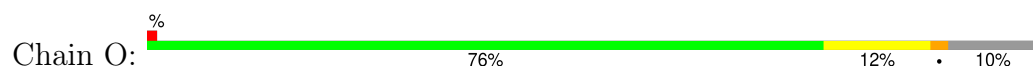
Chain M: 69% 22% 8%



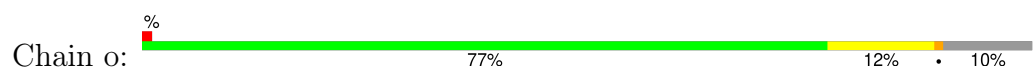
- Molecule 12: Photosystem II reaction center protein M



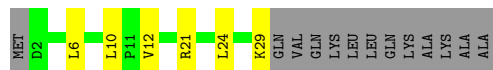
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



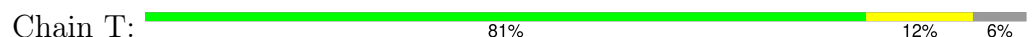
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y

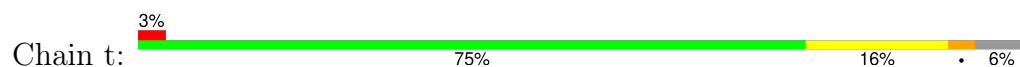


- Molecule 15: Photosystem II reaction center protein T

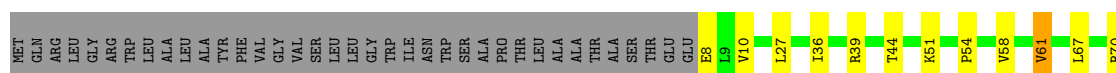




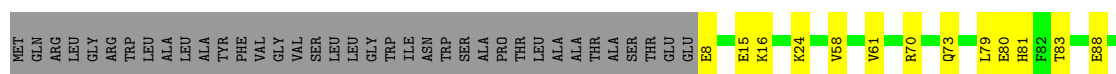
- Molecule 15: Photosystem II reaction center protein T



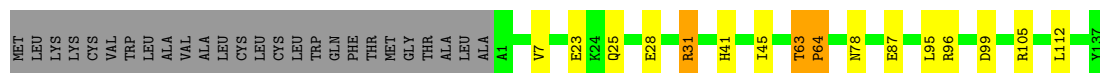
- Molecule 16: Photosystem II 12 kDa extrinsic protein



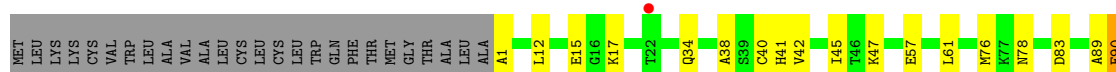
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 17: Cytochrome c-550

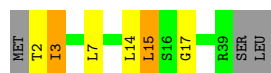


- Molecule 17: Cytochrome c-550



- Molecule 18: Photosystem II reaction center X protein

Chain X:  78% 10% 5% 7%

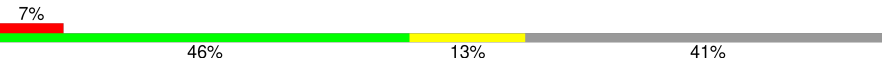


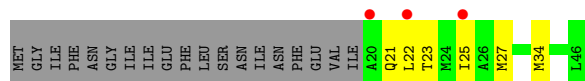
- Molecule 18: Photosystem II reaction center X protein

Chain x:  2% 71% 22% 5%

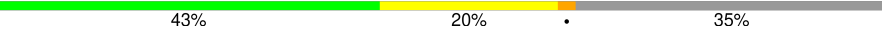


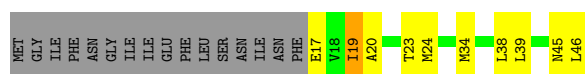
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  7% 46% 13% 41%



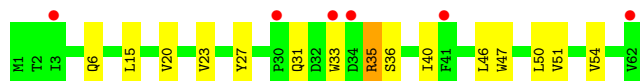
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  43% 20% 35%



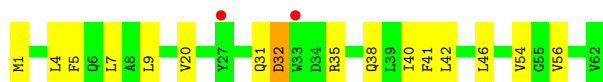
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  10% 76% 23%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  3% 74% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 85.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 0.239	Depositor DCC
R_{free} test set	4171 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	106082	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, BCR, LMG, LHG, OEY, HEM, FME, OEX, PL9, FE2, DGD, SQD, BCT, HEC, CL, PHO, CLA

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	0.55	1/3227 (0.0%)	0.61	0/4397
1	a	0.48	0/3224	0.57	0/4393
2	B	0.59	2/4161 (0.0%)	0.65	4/5669 (0.1%)
2	b	0.53	0/4118	0.60	0/5611
3	C	0.52	0/3647	0.61	0/4965
3	c	0.48	0/3719	0.58	0/5061
4	D	0.58	0/2825	0.64	0/3847
4	d	0.54	0/2834	0.62	0/3859
5	E	0.47	0/688	0.57	0/940
5	e	0.43	0/683	0.57	0/932
6	F	0.46	0/284	0.50	0/387
6	f	0.39	0/284	0.57	0/387
7	H	0.54	0/523	0.63	0/713
7	h	0.48	0/511	0.59	0/697
8	I	0.50	0/293	0.56	0/396
8	i	0.51	0/293	0.53	0/396
9	J	0.44	0/263	0.56	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.43	0/303	0.54	0/416
10	k	0.39	0/303	0.49	0/416
11	L	0.57	0/311	0.61	0/422
11	l	0.57	0/303	0.54	0/412
12	M	0.52	0/249	0.62	0/341
12	m	0.61	0/244	0.61	0/334
13	O	0.51	0/1904	0.65	0/2585
13	o	0.52	0/1905	0.61	0/2583
14	R	0.31	0/227	0.42	0/313
14	r	0.30	0/227	0.39	0/313
15	T	0.57	0/257	0.69	0/349
15	t	0.55	0/255	0.53	0/346
16	U	0.47	0/785	0.57	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.55	0/785	0.60	0/1064
17	V	0.53	0/1085	0.59	0/1473
17	v	0.50	0/1085	0.58	0/1473
18	X	0.46	0/284	0.61	0/384
18	x	0.40	0/289	0.50	0/391
19	Y	0.41	0/197	0.48	0/264
19	y	0.35	0/219	0.48	0/294
20	Z	0.39	0/490	0.49	0/669
20	z	0.34	0/488	0.44	0/666
All	All	0.52	3/44035 (0.0%)	0.60	4/59934 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PRO	CA-C	-14.99	1.42	1.52
1	A	38	ILE	CA-CB	12.88	1.61	1.54
2	B	221	PRO	C-O	5.72	1.29	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	PRO	O-C-N	-14.12	114.51	121.15
2	B	221	PRO	CA-C-O	5.14	124.79	120.73
2	B	221	PRO	CA-C-N	5.03	124.94	119.76
2	B	221	PRO	C-N-CA	5.03	124.94	119.76

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	21	0
1	a	3110	2976	2954	31	0
2	B	4005	3873	3867	33	0
2	b	3978	3836	3836	49	0
3	C	3509	3432	3409	28	0
3	c	3583	3503	3492	39	0
4	D	2731	2637	2637	21	0
4	d	2737	2643	2643	30	0
5	E	666	651	651	8	0
5	e	664	648	648	24	0
6	F	275	282	282	4	0
6	f	275	282	282	6	0
7	H	510	532	532	7	0
7	h	498	518	518	9	0
8	I	296	311	311	1	0
8	i	296	311	311	3	0
9	J	257	268	268	3	0
9	j	257	268	268	6	0
10	K	293	305	305	6	0
10	k	293	305	305	8	0
11	L	304	316	316	3	0
11	l	296	304	304	3	0
12	M	256	269	269	7	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	28	0
13	o	1874	1846	1846	20	0
14	R	221	238	238	1	0
14	r	221	238	238	3	0
15	T	258	261	261	2	0
15	t	256	256	256	5	0
16	U	774	773	773	7	0
16	u	774	773	773	5	0
17	V	1064	1071	1073	11	0
17	v	1064	1071	1073	19	0
18	X	281	312	312	4	0
18	x	286	316	314	10	0
19	Y	196	217	217	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	7	0
20	Z	479	516	516	7	0
20	z	477	509	509	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	249	264	264	1	0
22	B	1035	1139	1139	15	0
22	C	839	922	922	14	0
22	D	130	144	144	2	0
22	a	260	288	288	4	0
22	b	1035	1139	1139	20	0
22	c	839	919	919	7	0
22	d	130	144	144	0	0
23	A	64	74	74	1	0
23	D	64	74	74	1	0
23	d	128	148	148	1	0
24	A	40	56	56	0	0
24	B	120	168	168	2	0
24	C	40	56	56	2	0
24	D	40	56	56	1	0
24	H	40	56	56	1	0
24	K	80	112	112	0	0
24	T	40	56	56	1	0
24	Y	40	56	56	0	0
24	a	40	56	56	0	0
24	b	120	168	168	4	0
24	c	80	112	112	1	0
24	d	40	56	56	2	0
24	k	80	112	112	1	0
24	t	40	56	56	4	0
24	x	40	56	56	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	4	1	1	0	0
26	a	4	1	1	0	0
27	A	55	80	80	4	0
27	D	55	80	80	0	0
27	a	55	80	80	2	0
27	d	55	80	80	0	0
28	A	48	66	66	2	0
28	C	48	66	66	1	0
28	D	112	157	157	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	M	51	72	71	1	0
28	a	55	86	86	3	0
28	b	106	158	158	1	0
28	c	134	181	181	7	0
28	d	44	58	58	0	0
29	A	91	135	134	4	0
29	B	54	78	78	1	0
29	D	36	46	46	1	0
29	a	90	133	133	1	0
29	b	49	65	65	1	0
29	f	41	48	48	2	0
30	A	49	74	74	0	0
30	B	98	148	148	1	0
30	D	96	141	141	4	0
30	d	137	199	199	5	0
30	e	42	57	57	1	0
30	l	49	74	74	0	0
31	A	66	96	96	4	0
31	C	186	246	244	1	0
31	H	62	82	82	0	0
31	c	186	246	244	4	0
31	h	62	82	80	1	0
32	A	11	0	0	2	0
32	a	11	0	0	2	0
33	A	10	0	0	0	0
33	a	10	0	0	0	0
34	B	75	117	117	4	0
34	C	40	63	63	1	0
34	H	18	35	35	1	0
34	I	15	26	26	2	0
34	J	12	16	16	0	0
34	L	12	16	16	1	0
34	M	25	38	38	2	0
34	R	12	16	16	1	0
34	T	15	29	29	1	0
34	X	20	35	35	2	0
34	Z	8	12	12	1	0
34	a	37	58	58	4	0
34	b	82	141	141	8	0
34	c	32	51	51	2	0
34	d	57	96	96	4	0
34	h	14	27	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	j	12	16	16	2	0
34	l	18	35	35	2	0
34	t	14	20	20	0	0
35	F	43	30	30	3	0
35	e	43	30	30	6	0
36	V	43	30	30	0	0
36	v	43	30	30	3	0
37	A	151	0	0	7	0
37	B	204	0	0	5	0
37	C	173	0	0	4	0
37	D	131	0	0	2	0
37	E	33	0	0	1	0
37	F	8	0	0	0	0
37	H	34	0	0	2	0
37	I	17	0	0	0	0
37	J	24	0	0	1	0
37	K	15	0	0	1	0
37	L	10	0	0	1	0
37	M	8	0	0	3	0
37	O	86	0	0	10	0
37	R	4	0	0	1	0
37	T	8	0	0	0	0
37	U	34	0	0	3	0
37	V	64	0	0	5	1
37	X	15	0	0	1	0
37	Y	3	0	0	0	0
37	Z	10	0	0	1	0
37	a	132	0	0	5	0
37	b	172	0	0	11	0
37	c	157	0	0	16	0
37	d	110	0	0	3	0
37	e	28	0	0	6	0
37	f	6	0	0	0	0
37	h	20	0	0	3	0
37	i	11	0	0	0	0
37	j	8	0	0	2	0
37	k	5	0	0	1	0
37	l	8	0	0	0	0
37	m	7	0	0	3	0
37	o	100	0	0	5	0
37	r	7	0	0	1	0
37	t	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	u	48	0	0	0	1
37	v	59	0	0	7	0
37	x	11	0	0	7	0
37	y	4	0	0	3	0
37	z	12	0	0	0	0
All	All	53322	52760	52670	552	1

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

All (552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:40:CYS:SG	36:v:201:HEC:CAC	2.03	1.47
19:y:17:GLU:N	37:y:101:HOH:O	1.87	1.07
2:b:353:GLU:HA	37:b:701:HOH:O	1.55	1.05
5:e:36:LEU:C	37:e:201:HOH:O	2.00	1.03
2:b:352:GLU:C	37:b:701:HOH:O	1.98	1.03
2:b:353:GLU:CA	37:b:701:HOH:O	2.09	0.99
34:R:101:STE:O1	37:R:201:HOH:O	1.82	0.98
5:e:36:LEU:HA	37:e:201:HOH:O	1.64	0.97
4:d:25:ASP:OD1	37:d:501:HOH:O	1.84	0.95
18:x:21:LEU:HA	37:x:202:HOH:O	1.66	0.95
3:c:246:ALA:O	37:c:601:HOH:O	1.85	0.94
5:e:36:LEU:O	37:e:201:HOH:O	1.85	0.93
2:b:353:GLU:N	37:b:701:HOH:O	2.01	0.93
5:e:36:LEU:CA	37:e:201:HOH:O	2.13	0.88
12:M:5:GLN:O	37:M:201:HOH:O	1.93	0.87
17:v:17:LYS:NZ	37:v:301:HOH:O	2.07	0.86
4:D:12:ARG:O	37:D:501:HOH:O	1.93	0.85
18:x:35:ASP:OD2	37:x:201:HOH:O	1.94	0.85
2:b:352:GLU:O	37:b:701:HOH:O	1.93	0.83
13:O:53:LYS:O	37:O:301:HOH:O	1.95	0.83
3:C:32:GLY:N	37:C:602:HOH:O	2.10	0.82
17:V:105:ARG:O	37:V:301:HOH:O	1.98	0.82
17:v:40:CYS:SG	36:v:201:HEC:C3C	2.68	0.81
34:M:102:STE:O1	37:M:202:HOH:O	1.97	0.81
13:O:57:LYS:NZ	37:O:305:HOH:O	2.14	0.81
16:U:36:ILE:O	37:U:201:HOH:O	1.98	0.81
34:a:414:STE:C2	37:a:502:HOH:O	2.28	0.81
13:O:23:ASP:OD1	37:O:302:HOH:O	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:189:ARG:NE	37:o:301:HOH:O	2.03	0.79
3:c:221:GLU:OE1	37:c:602:HOH:O	2.01	0.78
32:a:418[B]:OEY:O6	32:a:418[B]:OEY:O5	2.01	0.78
34:a:414:STE:H22	37:a:502:HOH:O	1.83	0.78
5:E:61:ARG:NH1	37:E:102:HOH:O	2.04	0.77
34:X:101:STE:O1	37:X:201:HOH:O	2.01	0.77
12:m:5:GLN:O	37:m:101:HOH:O	2.02	0.76
13:O:111:ALA:O	37:O:303:HOH:O	2.02	0.76
13:o:23:ASP:OD2	37:o:302:HOH:O	2.04	0.76
16:U:54:PRO:O	37:U:202:HOH:O	2.03	0.75
2:b:387:GLU:O	37:b:702:HOH:O	2.05	0.74
28:c:522:LMG:O2	37:c:603:HOH:O	2.05	0.73
3:C:343:ARG:O	37:C:601:HOH:O	2.07	0.72
2:B:506:ARG:HD2	37:B:720:HOH:O	1.89	0.72
17:V:28:GLU:HG2	37:V:354:HOH:O	1.88	0.72
18:X:17:GLY:HA2	34:X:101:STE:H142	1.71	0.72
9:j:36:LEU:O	37:j:201:HOH:O	2.07	0.72
5:e:35:TRP:O	37:e:201:HOH:O	2.08	0.71
7:h:56:ASP:O	37:h:201:HOH:O	2.09	0.71
2:b:353:GLU:O	37:b:704:HOH:O	2.10	0.70
34:B:624:STE:O1	37:B:701:HOH:O	2.10	0.69
3:c:394:GLU:OE1	37:c:604:HOH:O	2.09	0.69
4:d:241:GLU:OE1	37:d:502:HOH:O	2.10	0.69
18:x:20:VAL:O	37:x:202:HOH:O	2.09	0.69
11:L:8:GLN:OE1	37:L:201:HOH:O	2.11	0.68
9:J:36:LEU:O	37:J:201:HOH:O	2.10	0.68
10:K:23:ASP:OD2	37:K:201:HOH:O	2.12	0.68
3:c:249:ILE:N	37:c:601:HOH:O	2.27	0.67
32:A:417[B]:OEY:O5	32:A:417[B]:OEY:O6	2.11	0.67
3:C:114:VAL:HG22	34:C:520:STE:H102	1.76	0.67
24:t:101:BCR:HC8	24:t:101:BCR:H311	1.74	0.67
1:A:269:ARG:HD2	4:D:235:PHE:HB2	1.76	0.67
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.27	0.67
16:U:70:ARG:NH2	37:U:203:HOH:O	2.28	0.67
2:b:127:ARG:NH2	7:h:18:TYR:O	2.28	0.67
13:O:244:GLU:OE1	37:O:304:HOH:O	2.12	0.66
9:j:34:ALA:O	37:j:201:HOH:O	2.13	0.66
27:A:410:PL9:H361	6:F:25:THR:HG21	1.77	0.66
34:d:413:STE:H92	34:h:102:STE:H61	1.78	0.66
17:v:83:ASP:OD2	37:v:302:HOH:O	2.15	0.65
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD1	37:A:501:HOH:O	2.15	0.64
6:f:21:VAL:O	6:f:25:THR:OG1	2.14	0.64
2:b:227:LYS:NZ	37:b:710:HOH:O	2.25	0.64
20:z:1:MET:HB3	20:z:4:LEU:HB3	1.79	0.63
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.80	0.63
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.63
13:O:27:ARG:NH1	37:O:307:HOH:O	2.22	0.63
28:D:406:LMG:H112	37:D:508:HOH:O	1.98	0.62
13:o:27:ARG:NH1	37:o:304:HOH:O	2.19	0.62
12:m:5:GLN:NE2	37:m:103:HOH:O	2.31	0.62
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.82	0.62
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.82	0.61
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	1.81	0.61
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.36	0.61
34:B:624:STE:C1	37:B:701:HOH:O	2.49	0.60
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.25	0.60
16:u:70:ARG:NH1	16:u:73:GLN:OE1	2.34	0.60
3:c:413[A]:GLU:OE2	17:v:47:LYS:NZ	2.30	0.60
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.84	0.60
19:y:17:GLU:HB3	37:y:101:HOH:O	2.02	0.60
19:y:17:GLU:CB	37:y:101:HOH:O	2.49	0.59
28:A:412:LMG:H391	3:C:281:MET:HG3	1.83	0.59
15:t:28:ARG:N	37:t:201:HOH:O	2.30	0.59
17:v:61:LEU:O	37:v:303:HOH:O	2.17	0.59
2:b:91:TRP:HE1	34:b:623:STE:H141	1.66	0.58
18:x:24:THR:HB	37:x:202:HOH:O	2.03	0.58
9:J:15:THR:HG22	9:J:19:MET:HE2	1.83	0.58
28:c:522:LMG:C3	37:c:603:HOH:O	2.51	0.58
5:e:61:ARG:NH1	17:v:125:ILE:O	2.36	0.58
22:b:604:CLA:H143	22:b:615:CLA:HMA3	1.85	0.58
20:Z:35:ARG:HB2	37:Z:202:HOH:O	2.03	0.58
35:e:101:HEM:HMC1	35:e:101:HEM:HBC2	1.86	0.58
29:A:413:SQD:H291	30:D:409:LHG:H151	1.86	0.57
3:C:148:GLY:O	3:C:156:LYS:NZ	2.36	0.57
3:c:315:MET:HE3	3:c:365:TRP:HZ3	1.70	0.57
5:e:30:LEU:HD11	35:e:101:HEM:HBB2	1.87	0.57
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.20	0.56
31:c:517:DGD:HA42	34:j:101:STE:H72	1.87	0.56
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.86	0.56
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.87	0.56
35:e:101:HEM:HBB2	35:e:101:HEM:HHC	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:153:ASP:OD2	37:c:605:HOH:O	2.18	0.56
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.40	0.56
3:c:406:SER:HA	3:c:420:VAL:HG23	1.88	0.56
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.88	0.56
13:o:178:LYS:NZ	37:o:309:HOH:O	2.38	0.55
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.42	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.42	0.55
37:A:561:HOH:O	13:O:107:THR:HG22	2.07	0.55
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.55
37:c:708:HOH:O	8:i:33:LYS:HE2	2.07	0.55
34:d:412:STE:H71	18:x:16:SER:HB3	1.89	0.55
16:U:58:VAL:O	16:U:61:VAL:HG22	2.07	0.55
1:a:189[B]:GLU:OE1	32:a:418[B]:OEY:O6	2.25	0.54
12:m:30:GLU:OE2	37:m:102:HOH:O	2.18	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.07	0.54
22:C:509:CLA:H91	22:C:512:CLA:HAA2	1.90	0.54
4:d:12:ARG:HH11	4:d:16:ASP:HB3	1.73	0.54
7:h:58:VAL:HB	37:h:208:HOH:O	2.08	0.54
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	1.90	0.54
2:b:102:VAL:HG11	22:b:606:CLA:H142	1.89	0.54
1:a:229:GLU:CD	1:a:229:GLU:H	2.16	0.53
31:A:416:DGD:HD5	2:b:75:TRP:HB3	1.90	0.53
2:B:117:TYR:HA	11:L:1:MET:HE1	1.90	0.53
6:f:24:HIS:O	6:f:28:VAL:HG13	2.08	0.53
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.73	0.53
18:x:21:LEU:CA	37:x:202:HOH:O	2.36	0.53
22:C:506:CLA:H8	24:C:514:BCR:H12C	1.90	0.53
10:K:13:GLU:N	10:K:13:GLU:OE1	2.42	0.53
4:d:79:SER:HA	4:d:172:SER:HB3	1.91	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
1:a:201:GLY:HA3	1:a:286:THR:HB	1.89	0.53
17:v:78:ASN:OD1	17:v:96:ARG:NH1	2.41	0.53
24:T:101:BCR:H321	24:T:101:BCR:HC8	1.91	0.53
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.90	0.53
28:c:522:LMG:HC4	37:c:603:HOH:O	2.09	0.53
22:C:502:CLA:H61	22:C:512:CLA:H42	1.91	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.52
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.90	0.52
2:b:347:ARG:NH2	37:b:706:HOH:O	2.23	0.52
17:v:41:HIS:HA	17:v:45:ILE:O	2.10	0.52
13:O:189:ARG:NE	37:O:306:HOH:O	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:220:ARG:HG3	7:h:20:LYS:HD3	1.91	0.52
34:c:520:STE:O1	37:c:606:HOH:O	2.19	0.52
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.09	0.52
31:A:416:DGD:HB41	34:I:101:STE:H62	1.92	0.52
20:Z:51:VAL:O	20:Z:54:VAL:O	2.26	0.52
2:b:25:MET:HG2	24:b:617:BCR:H23C	1.92	0.52
5:e:30:LEU:HD11	35:e:101:HEM:CBB	2.40	0.52
1:A:322:ASN:OD1	37:A:502:HOH:O	2.19	0.51
2:B:371:THR:HG23	2:B:372:ASP:O	2.10	0.51
2:b:36:SER:OG	24:b:618:BCR:H362	2.09	0.51
12:M:28:GLN:HB3	12:m:27:VAL:HG12	1.91	0.51
16:u:24:LYS:HB2	16:u:83:THR:HG22	1.93	0.51
36:v:201:HEC:HMC1	36:v:201:HEC:HBC3	1.92	0.51
18:x:24:THR:CB	37:x:202:HOH:O	2.58	0.51
5:e:68:ASP:O	5:e:72:ALA:HB2	2.11	0.51
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.92	0.51
10:K:24:VAL:HG13	19:Y:25:ILE:HD13	1.92	0.51
17:V:63:THR:HG22	17:V:64:PRO:CD	2.41	0.51
3:c:315:MET:HE3	3:c:365:TRP:CZ3	2.46	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.92	0.51
28:c:522:LMG:HC3	37:c:603:HOH:O	2.11	0.51
7:H:20:LYS:NZ	37:H:201:HOH:O	2.43	0.51
13:o:111:ALA:O	37:o:305:HOH:O	2.19	0.51
3:C:261:ARG:NE	37:C:604:HOH:O	2.23	0.51
10:K:26:PRO:O	10:K:29:PRO:HD2	2.11	0.50
34:a:414:STE:O1	37:a:502:HOH:O	2.19	0.50
4:d:12:ARG:NH1	4:d:16:ASP:HB3	2.26	0.50
20:z:32:ASP:N	20:z:32:ASP:OD1	2.45	0.50
2:b:92:SER:O	2:b:96:VAL:HG23	2.11	0.50
37:A:601:HOH:O	13:O:107:THR:HG21	2.12	0.50
1:A:243:GLU:OE1	37:A:503:HOH:O	2.19	0.49
27:A:410:PL9:H452	29:D:407:SQD:H351	1.94	0.49
37:A:633:HOH:O	34:b:626:STE:H62	2.12	0.49
7:H:2:ALA:N	37:H:202:HOH:O	2.44	0.49
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.44	0.49
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.13	0.49
2:B:414:PRO:N	2:B:415:PRO:HD2	2.25	0.49
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.42	0.49
2:B:506:ARG:NH1	37:B:720:HOH:O	2.45	0.49
12:M:5:GLN:HG2	37:M:203:HOH:O	2.10	0.49
2:B:91:TRP:HE1	34:B:620:STE:H32	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:LEU:HD23	14:R:12:VAL:HG22	1.93	0.49
22:b:602:CLA:H43	7:h:45:ILE:HG22	1.94	0.49
22:b:614:CLA:H122	22:b:614:CLA:H91	1.95	0.49
3:c:78:GLU:OE1	17:v:106:ASN:ND2	2.45	0.49
30:d:408:LHG:HC62	11:l:15:THR:HG23	1.95	0.49
13:o:205:ASP:OD1	13:o:207:ARG:NE	2.45	0.49
22:B:602:CLA:H43	7:H:45:ILE:HG22	1.94	0.49
34:B:627:STE:H92	34:H:103:STE:H62	1.95	0.49
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.95	0.49
18:X:3:ILE:HD12	18:X:7:LEU:HD23	1.95	0.49
2:b:44:THR:HG22	34:b:621:STE:H61	1.95	0.49
3:c:456:GLU:OE2	3:c:457:LYS:NZ	2.44	0.49
4:d:194:ASN:HA	4:d:295:SER:OG	2.13	0.49
11:l:22:LEU:HB2	15:t:16:LEU:HD21	1.94	0.49
1:A:103:ASP:OD1	13:O:69:LYS:HE2	2.13	0.49
2:b:211:ILE:HG23	34:b:627:STE:H22	1.95	0.49
10:k:24:VAL:O	10:k:27:VAL:HG22	2.13	0.49
13:o:84:GLU:OE1	13:o:86:LYS:NZ	2.36	0.49
2:B:193:TYR:O	7:H:65:LEU:HD23	2.14	0.48
4:d:56:THR:HG22	37:e:213:HOH:O	2.13	0.48
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
22:D:403:CLA:H142	18:X:14:LEU:HG	1.95	0.48
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.96	0.48
30:d:408:LHG:H281	15:t:17:PHE:CD1	2.49	0.48
22:B:606:CLA:H72	24:B:619:BCR:H311	1.94	0.48
17:V:25:GLN:HG2	37:V:332:HOH:O	2.13	0.48
24:d:405:BCR:H331	24:d:405:BCR:C8	2.43	0.48
3:C:139:THR:HB	3:C:141:GLU:OE2	2.13	0.48
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.96	0.48
10:k:26:PRO:O	10:k:29:PRO:HD2	2.13	0.48
10:k:25:LEU:HB2	37:k:202:HOH:O	2.14	0.48
29:A:413:SQD:H272	30:D:409:LHG:H142	1.96	0.48
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.95	0.48
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.96	0.48
13:O:189:ARG:NH2	37:O:306:HOH:O	2.44	0.48
17:V:31:ARG:HH11	17:V:31:ARG:HB3	1.79	0.48
2:b:91:TRP:CD1	34:b:623:STE:H162	2.49	0.48
22:b:610:CLA:H152	22:b:612:CLA:O1A	2.14	0.48
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.96	0.47
5:e:8:ARG:HG2	5:e:13:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.29	0.47
2:b:221:PRO:HA	22:b:609:CLA:HED3	1.96	0.47
17:V:99:ASP:OD1	17:V:99:ASP:N	2.47	0.47
22:b:607:CLA:H191	30:d:407:LHG:H141	1.95	0.47
22:C:508:CLA:H203	31:C:516:DGD:HAE1	1.97	0.47
28:C:518:LMG:H192	10:K:27:VAL:HG11	1.95	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.47
22:b:615:CLA:HHC	22:b:615:CLA:HBB1	1.96	0.47
10:k:25:LEU:N	10:k:26:PRO:CD	2.77	0.47
1:a:16:ARG:HH11	1:a:16:ARG:HB3	1.78	0.47
2:b:414:PRO:HB2	2:b:415:PRO:HD3	1.97	0.47
2:B:141:ILE:O	2:B:145:LEU:HG	2.13	0.47
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.97	0.47
13:O:69:LYS:NZ	37:O:309:HOH:O	2.48	0.47
20:Z:27:TYR:HE1	20:Z:33:TRP:CH2	2.33	0.47
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.50	0.47
1:a:307:ILE:HG22	1:a:313:VAL:HA	1.96	0.47
17:v:57:GLU:OE2	37:v:304:HOH:O	2.20	0.47
1:A:308:ASP:C	1:A:308:ASP:OD1	2.58	0.47
27:A:410:PL9:H33	4:D:42:TYR:HB2	1.96	0.47
3:C:95:LEU:HD21	22:C:501:CLA:OBD	2.15	0.47
3:c:250:TRP:N	37:c:601:HOH:O	2.04	0.47
28:c:522:LMG:C4	37:c:603:HOH:O	2.62	0.47
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.45	0.47
17:v:34:GLN:HA	17:v:38:ALA:HB2	1.97	0.47
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	1.96	0.46
2:B:341:LYS:HD2	2:B:429:ILE:HG22	1.97	0.46
22:B:603:CLA:CMD	22:B:606:CLA:HMB1	2.45	0.46
3:c:213:LEU:HD21	24:c:515:BCR:C20	2.44	0.46
22:c:501:CLA:H192	22:c:507:CLA:HBB1	1.96	0.46
20:Z:47:TRP:CE3	34:Z:101:STE:H142	2.50	0.46
2:b:228:ALA:HB2	34:h:102:STE:H62	1.97	0.46
7:h:25:TRP:O	7:h:26:GLY:C	2.59	0.46
17:v:104:MET:HA	17:v:107:LEU:HD22	1.96	0.46
20:z:9:LEU:HD13	20:z:54:VAL:HG11	1.96	0.46
17:V:87:GLU:CD	17:V:96:ARG:HH12	2.22	0.46
1:a:332[A]:HIS:HA	4:d:321:LEU:HD11	1.97	0.46
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.46
17:V:95:LEU:HD11	17:V:112:LEU:HD11	1.96	0.46
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.51	0.46
3:c:45:LEU:HA	3:c:139:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:48:LYS:HG3	3:c:138:GLU:HA	1.96	0.46
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.98	0.46
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.46	0.46
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.97	0.46
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.97	0.46
2:B:434:THR:OG1	13:O:178:LYS:NZ	2.39	0.46
3:c:25:ASN:ND2	3:c:41:ARG:O	2.49	0.46
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	1.98	0.45
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.51	0.45
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.50	0.45
4:D:272:LEU:C	4:D:272:LEU:HD23	2.41	0.45
31:c:517:DGD:HA51	34:j:101:STE:H92	1.98	0.45
4:d:141:TYR:OH	30:d:407:LHG:O4	2.26	0.45
12:M:29:THR:HA	12:M:32:GLN:HE21	1.82	0.45
1:a:289:GLY:O	1:a:293:MET:HE3	2.16	0.45
3:c:198:VAL:HB	37:c:672:HOH:O	2.17	0.45
3:c:246:ALA:C	37:c:601:HOH:O	2.47	0.45
24:k:101:BCR:H321	24:k:101:BCR:HC8	1.97	0.45
2:B:247:PHE:CE1	22:B:602:CLA:H102	2.52	0.45
4:D:267:LEU:C	4:D:267:LEU:HD23	2.41	0.45
28:b:622:LMG:H391	12:m:13:LEU:HB3	1.98	0.45
34:d:413:STE:H62	34:h:102:STE:H71	1.98	0.45
10:k:28:ILE:HA	10:k:31:LEU:HD12	1.99	0.45
2:B:67:ALA:HA	2:B:71:VAL:O	2.16	0.45
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.99	0.45
22:c:512:CLA:H121	22:c:513:CLA:H151	1.98	0.45
5:e:26:THR:HA	14:r:15:ALA:HB1	1.97	0.45
10:k:17:ILE:HG13	10:k:18:PHE:CD1	2.51	0.45
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.17	0.45
4:d:267:LEU:C	4:d:267:LEU:HD23	2.42	0.45
24:H:101:BCR:C8	24:H:101:BCR:H331	2.46	0.45
13:O:56:PRO:O	13:O:58:ASN:N	2.42	0.45
28:c:521:LMG:H292	28:c:521:LMG:H112	1.98	0.45
13:O:27:ARG:O	13:O:27:ARG:HG2	2.16	0.45
13:O:189:ARG:NH2	13:O:226:GLY:O	2.50	0.45
1:a:93:PHE:HZ	22:a:404:CLA:HAA1	1.82	0.45
28:a:416:LMG:O10	28:a:416:LMG:C10	2.64	0.45
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.99	0.45
22:C:511:CLA:H171	20:Z:20:VAL:HA	1.98	0.45
23:d:402:PHO:HHD	23:d:402:PHO:HBC2	1.99	0.45
22:B:607:CLA:H142	22:B:613:CLA:H172	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:VAL:HG13	22:C:512:CLA:H93	1.98	0.45
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.05	0.45
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.98	0.45
22:D:403:CLA:H18	18:X:15:LEU:HD21	2.00	0.44
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.99	0.44
4:d:123:ILE:HD11	31:h:101:DGD:HAH2	1.99	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.44
15:T:8:PHE:CE2	34:T:102:STE:H183	2.53	0.44
5:e:14:ILE:O	5:e:20:TRP:NE1	2.46	0.44
14:r:20:VAL:O	14:r:24:LEU:HB2	2.18	0.44
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.52	0.44
22:B:614:CLA:H42	34:L:101:STE:H22	1.98	0.44
5:E:60:GLN:NE2	5:E:62:SER:O	2.51	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.52	0.44
22:a:410:CLA:O1A	22:a:410:CLA:H43	2.17	0.44
3:C:451:ALA:HA	3:C:456:GLU:OE1	2.17	0.44
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.98	0.44
22:c:506:CLA:O1A	22:c:506:CLA:C2	2.65	0.44
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.98	0.44
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.00	0.44
4:d:241:GLU:CD	4:d:241:GLU:H	2.26	0.44
31:A:416:DGD:HBN1	8:I:7:THR:HG21	1.99	0.44
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.00	0.44
35:e:101:HEM:HBC2	35:e:101:HEM:CMC	2.46	0.44
2:B:403:GLY:C	2:B:407:ASN:HB2	2.43	0.44
30:D:408:LHG:H322	15:T:21:ILE:HD11	1.99	0.44
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	2.00	0.44
9:j:19:MET:O	9:j:23:VAL:HG23	2.18	0.44
22:B:603:CLA:H171	22:B:609:CLA:H111	1.99	0.44
16:U:73:GLN:O	16:U:77:GLU:HG3	2.18	0.44
2:b:81:THR:OG1	2:b:83:GLU:HG3	2.17	0.44
2:b:86:ILE:HD12	2:b:88:PRO:HD3	2.00	0.44
3:C:141:GLU:H	3:C:141:GLU:CD	2.25	0.44
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.52	0.44
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.84	0.44
2:B:474:LEU:O	4:D:134:ARG:NH1	2.49	0.43
8:i:34:ARG:C	8:i:36:ASP:H	2.24	0.43
20:z:40:ILE:HG13	20:z:41:PHE:N	2.33	0.43
1:A:332[B]:HIS:O	1:A:333[B]:GLU:C	2.60	0.43
2:b:67:ALA:HA	2:b:71:VAL:O	2.18	0.43
13:o:24:ASP:HA	13:o:203:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:12:LEU:HD23	17:v:17:LYS:HD3	1.99	0.43
1:A:322:ASN:OD1	3:C:412:THR:HA	2.18	0.43
1:a:310:LYS:HD2	17:v:1:ALA:HB1	2.00	0.43
1:a:321:ILE:HD11	4:d:179:PHE:HB2	2.00	0.43
37:a:620:HOH:O	3:c:410:VAL:HB	2.18	0.43
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.35	0.43
4:d:99:GLY:HA3	34:d:412:STE:H142	2.00	0.43
4:d:128:ARG:NH1	37:d:504:HOH:O	2.30	0.43
1:A:210:LEU:HD23	1:A:214:MET:HG2	2.01	0.43
1:a:308:ASP:OD1	1:a:308:ASP:C	2.62	0.43
22:b:615:CLA:H112	22:b:615:CLA:H152	1.84	0.43
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.49	0.43
28:D:406:LMG:H212	28:D:406:LMG:H182	1.87	0.43
22:b:614:CLA:H62	22:b:614:CLA:H41	1.71	0.43
2:B:36:SER:OG	24:B:618:BCR:H362	2.19	0.43
1:a:296:ASN:HB3	3:c:401:LEU:HA	1.99	0.43
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.43
3:c:318:LEU:C	3:c:318:LEU:HD23	2.44	0.43
1:A:189[B]:GLU:OE1	32:A:417[B]:OEY:O6	2.36	0.43
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.99	0.43
27:A:410:PL9:H271	27:A:410:PL9:H251	1.91	0.43
22:B:611:CLA:H72	22:B:611:CLA:H112	1.82	0.43
3:C:461:ARG:HG2	4:D:223:PHE:CD1	2.54	0.43
30:d:409:LHG:H272	30:d:409:LHG:H242	1.73	0.43
19:y:19:ILE:O	19:y:23:THR:HG22	2.19	0.43
29:A:413:SQD:H251	30:D:409:LHG:H142	2.00	0.43
34:M:103:STE:H61	29:b:620:SQD:H262	2.00	0.43
17:v:127:GLY:HA3	37:v:309:HOH:O	2.18	0.43
2:B:51:VAL:HG13	2:B:308:LYS:HB2	2.00	0.43
3:C:216:SER:O	3:C:221:GLU:HB2	2.19	0.43
3:c:46:SER:OG	3:c:141:GLU:OE2	2.35	0.43
3:c:180:MET:HE2	3:c:180:MET:HB3	1.90	0.43
16:u:80:GLU:HG3	16:u:81:HIS:CD2	2.54	0.43
22:C:505:CLA:HBC2	24:C:514:BCR:H341	2.01	0.42
1:a:300:PHE:HZ	31:c:518:DGD:HB61	1.83	0.42
2:B:75:TRP:HB3	28:a:416:LMG:HC92	2.00	0.42
22:B:608:CLA:C1A	22:B:608:CLA:CGA	2.98	0.42
34:a:414:STE:C1	37:a:502:HOH:O	2.59	0.42
2:b:453:PHE:O	2:b:457:VAL:HG23	2.19	0.42
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.01	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
22:B:604:CLA:H91	22:B:604:CLA:H111	1.86	0.42
6:F:45:ARG:NH2	9:J:40:LEU:OXT	2.42	0.42
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.48	0.42
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.01	0.42
22:b:614:CLA:H93	22:b:614:CLA:H61	1.81	0.42
4:d:49:LEU:HD13	24:d:405:BCR:C15	2.49	0.42
5:e:23:HIS:HA	5:e:26:THR:OG1	2.20	0.42
7:h:3:ARG:NH2	37:h:202:HOH:O	2.17	0.42
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.42
18:x:21:LEU:C	37:x:202:HOH:O	2.57	0.42
4:D:295:SER:O	4:D:295:SER:OG	2.37	0.42
4:d:62:GLY:HA2	5:e:63:ILE:HG21	2.02	0.42
20:z:38:GLN:O	20:z:42:LEU:HD13	2.19	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.01	0.42
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.20	0.42
13:O:27:ARG:HG3	37:O:307:HOH:O	2.18	0.42
2:b:357:ARG:NH2	37:b:705:HOH:O	2.51	0.42
3:c:344:SER:O	13:o:75:THR:HG22	2.19	0.42
3:c:367:GLU:N	3:c:368:PRO:CD	2.82	0.42
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.54	0.42
22:C:509:CLA:H93	22:C:509:CLA:H112	1.79	0.42
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.02	0.42
22:a:404:CLA:H111	22:a:404:CLA:H52	2.02	0.42
2:b:357:ARG:NE	37:b:705:HOH:O	2.19	0.42
24:t:101:BCR:C23	24:t:101:BCR:C38	2.96	0.42
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.42
22:A:411:CLA:C4A	22:A:411:CLA:HBA1	2.49	0.42
2:B:477:ASP:OD1	2:B:477:ASP:N	2.52	0.42
29:B:623:SQD:H442	15:t:23:PHE:CD1	2.55	0.42
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.52	0.42
22:c:505:CLA:C1A	22:c:505:CLA:CGA	2.98	0.42
4:d:40:CYS:HB3	4:d:117:HIS:O	2.20	0.42
19:y:20:ALA:O	19:y:24:MET:HG2	2.19	0.42
5:E:68:ASP:O	5:E:72:ALA:HB2	2.20	0.42
3:c:121:SER:HB3	34:c:520:STE:H182	2.02	0.42
29:A:415:SQD:H383	22:b:606:CLA:H93	2.01	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.42
4:D:150:ILE:O	4:D:154:VAL:HG13	2.19	0.42
35:e:101:HEM:HAA1	6:f:15:ILE:HG23	2.02	0.42
16:u:16:LYS:HE2	16:u:88:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ARG:O	3:C:135:ARG:HD3	2.20	0.42
13:O:72:THR:CG2	13:O:107:THR:HG23	2.50	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.19	0.42
5:e:10:PHE:N	30:e:102:LHG:O4	2.53	0.42
19:Y:23:THR:HG22	19:Y:27:MET:HE3	2.02	0.41
2:b:355:PHE:HE2	2:b:373:LYS:HG2	1.85	0.41
3:c:42:LEU:HD21	22:c:511:CLA:H2A	2.01	0.41
2:B:97:ALA:O	2:B:101:ILE:HD12	2.20	0.41
3:C:143:TYR:CE1	22:C:513:CLA:HED3	2.55	0.41
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.41
7:H:62:TRP:C	7:H:64:ALA:H	2.28	0.41
10:K:24:VAL:CG1	19:Y:25:ILE:HD13	2.50	0.41
13:O:6:THR:HG23	13:O:8:ASP:H	1.85	0.41
16:U:44:THR:HB	37:V:311:HOH:O	2.19	0.41
2:b:91:TRP:HD1	34:b:623:STE:H162	1.85	0.41
22:b:601:CLA:H91	22:b:601:CLA:H111	1.89	0.41
22:b:601:CLA:HMB3	22:b:601:CLA:H193	2.01	0.41
28:c:522:LMG:HC5	37:c:706:HOH:O	2.20	0.41
13:o:33:ASP:HB3	13:o:36:GLN:HE21	1.85	0.41
2:B:487:SER:OG	2:B:488:PRO:HD2	2.20	0.41
22:B:601:CLA:H93	22:B:601:CLA:H62	1.86	0.41
22:B:614:CLA:H161	22:B:614:CLA:H141	1.81	0.41
3:C:50:LEU:O	3:C:54:VAL:HG23	2.20	0.41
17:V:87:GLU:HB3	37:V:331:HOH:O	2.20	0.41
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.41
1:a:210:LEU:HD23	1:a:214:MET:HG2	2.01	0.41
22:b:614:CLA:H111	22:b:614:CLA:H152	1.85	0.41
9:j:9:PRO:HG2	9:j:12:ILE:HD12	2.02	0.41
17:v:89:ALA:HB2	37:v:327:HOH:O	2.18	0.41
31:A:416:DGD:HB62	34:I:101:STE:H51	2.01	0.41
2:B:49:ASP:OD2	13:o:57:LYS:HD2	2.20	0.41
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.55	0.41
3:c:146:PHE:O	3:c:156:LYS:NZ	2.31	0.41
3:c:315:MET:CE	3:c:366:LEU:HD13	2.50	0.41
5:e:17:VAL:HG23	9:j:7:ARG:HD3	2.02	0.41
24:t:101:BCR:H382	24:t:101:BCR:C23	2.49	0.41
1:A:328[B]:MET:HE1	4:D:183:LEU:HD22	2.01	0.41
22:B:608:CLA:H43	22:B:609:CLA:H101	2.03	0.41
3:C:60:ILE:HG22	22:C:503:CLA:HMD3	2.03	0.41
3:C:147:PHE:CD2	22:C:513:CLA:H3A	2.55	0.41
3:C:367:GLU:N	3:C:368:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LEU:HD13	28:D:411:LMG:H341	2.01	0.41
1:a:265:PHE:CD1	1:a:271:LEU:HD23	2.56	0.41
28:a:416:LMG:O10	28:a:416:LMG:C11	2.69	0.41
24:b:617:BCR:H24C	24:b:617:BCR:H371	1.92	0.41
24:b:618:BCR:C8	24:b:618:BCR:H331	2.51	0.41
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.02	0.41
22:b:612:CLA:H122	22:b:612:CLA:H162	1.90	0.41
6:f:16:PHE:HB2	29:f:101:SQD:H82	2.02	0.41
13:o:56:PRO:HB3	13:o:61:GLN:HB2	2.02	0.41
2:B:52:LEU:HD12	13:o:59:LYS:HE2	2.02	0.41
13:O:36:GLN:HE21	13:O:37:THR:H	1.69	0.41
2:b:135:LEU:N	2:b:136:PRO:CD	2.84	0.41
2:b:149:LEU:HD11	22:b:604:CLA:H111	2.02	0.41
5:e:79:PHE:HA	5:e:82:GLN:HE21	1.85	0.41
1:A:40:THR:O	1:A:118:HIS:HB3	2.20	0.41
3:C:63:TRP:CZ2	3:C:67:MET:HG2	2.56	0.41
22:C:509:CLA:H92	22:C:509:CLA:H62	1.91	0.41
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.41
5:E:65:LEU:O	5:E:67:THR:HG23	2.21	0.41
13:O:36:GLN:HG3	13:O:37:THR:N	2.36	0.41
16:U:27:LEU:HD13	16:U:61:VAL:CG1	2.51	0.41
27:a:409:PL9:H371	27:a:409:PL9:H351	1.82	0.41
34:b:621:STE:H52	34:b:621:STE:H82	1.91	0.41
3:c:163:PHE:O	3:c:167:VAL:HG23	2.21	0.41
20:z:31:GLN:HG3	20:z:32:ASP:OD1	2.21	0.41
22:B:603:CLA:H203	7:H:42:LEU:HD12	2.02	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.21	0.41
17:V:41:HIS:HA	17:V:45:ILE:O	2.21	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.21	0.41
3:c:38:GLY:HA3	22:c:511:CLA:HMD2	2.02	0.41
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.21	0.41
17:v:90:GLU:HB2	37:v:345:HOH:O	2.22	0.41
2:B:492:GLU:O	37:B:703:HOH:O	2.22	0.40
30:B:622:LHG:H171	30:B:622:LHG:H142	1.91	0.40
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.56	0.40
34:l:102:STE:H52	34:l:102:STE:C1	2.51	0.40
24:D:404:BCR:C8	24:D:404:BCR:H331	2.51	0.40
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.40
1:a:58[A]:VAL:HB	1:a:83:VAL:HB	2.02	0.40
3:c:25:ASN:HB3	3:c:26:ARG:H	1.80	0.40
31:c:517:DGD:HA82	31:c:518:DGD:HB81	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:y:34:MET:O	19:y:38:LEU:HG	2.21	0.40
20:z:32:ASP:HB2	20:z:35:ARG:HB2	2.03	0.40
1:A:334[B]:ARG:HA	37:A:506:HOH:O	2.20	0.40
23:A:404:PHO:HBB1	23:A:404:PHO:HMB3	2.03	0.40
2:B:109:LEU:HD13	29:a:412:SQD:H132	2.03	0.40
22:B:608:CLA:H193	7:H:43:LEU:HD21	2.02	0.40
3:C:261:ARG:NH2	37:C:604:HOH:O	2.51	0.40
2:b:30:VAL:HG12	22:b:605:CLA:HHD	2.03	0.40
2:b:43:ALA:CB	34:b:621:STE:H92	2.51	0.40
3:c:178:LYS:NZ	3:c:184:GLY:O	2.50	0.40
5:e:36:LEU:HA	5:e:36:LEU:HD23	1.87	0.40
5:e:80:LEU:HA	5:e:83:LEU:HD22	2.02	0.40
15:t:29:ILE:HD12	15:t:29:ILE:H	1.85	0.40
2:B:327:THR:HG21	28:M:101:LMG:H291	2.02	0.40
2:B:359:MET:HE2	2:B:363:PHE:O	2.22	0.40
6:F:31:ILE:HG13	35:F:101:HEM:HMC2	2.03	0.40
22:a:404:CLA:H2	8:i:12:VAL:HG11	2.03	0.40
29:f:101:SQD:H312	18:x:27:VAL:HG11	2.03	0.40
11:l:7:ARG:HH11	34:l:102:STE:C1	2.34	0.40
14:r:21:ARG:HD2	37:r:102:HOH:O	2.21	0.40
19:y:39:LEU:HD23	19:y:39:LEU:HA	1.95	0.40
1:A:85:SER:HA	1:A:109:GLY:HA3	2.04	0.40
28:A:412:LMG:HC72	3:C:216:SER:HB2	2.04	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.03	0.40
5:E:26:THR:O	5:E:30:LEU:HG	2.22	0.40
20:Z:36:SER:O	20:Z:40:ILE:HG12	2.21	0.40
27:a:409:PL9:H322	27:a:409:PL9:H301	1.93	0.40
2:b:62:VAL:HB	22:b:605:CLA:HED3	2.04	0.40
2:b:380:ASP:OD1	4:d:344:GLU:OE2	2.39	0.40
5:e:36:LEU:O	5:e:40:THR:HG23	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:V:332:HOH:O	37:u:244:HOH:O[3_457]	2.12	0.08

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%)	390 (98%)	6 (2%)	1 (0%)	36	36
1	a	397/344 (115%)	388 (98%)	9 (2%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	454/461 (98%)	444 (98%)	9 (2%)	1 (0%)	43	44
3	c	463/461 (100%)	452 (98%)	10 (2%)	1 (0%)	43	44
4	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	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%)	231 (95%)	9 (4%)	3 (1%)	10	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
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%)	27 (96%)	1 (4%)	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%)	130 (96%)	4 (3%)	1 (1%)	18	15
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
All	All	5387/5700 (94%)	5241 (97%)	139 (3%)	7 (0%)	48	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	O	62	GLU
13	O	58	ASN
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	321 (99%)	3 (1%)	70	78
1	a	323/280 (115%)	311 (96%)	12 (4%)	30	33
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	53
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	45
3	C	356/362 (98%)	348 (98%)	8 (2%)	45	53
3	c	364/362 (101%)	354 (97%)	10 (3%)	39	45
4	D	277/283 (98%)	273 (99%)	4 (1%)	59	67
4	d	278/283 (98%)	268 (96%)	10 (4%)	31	34
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	11
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	17
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	6
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	28
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	37
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	34
13	O	206/228 (90%)	194 (94%)	12 (6%)	18	16
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	0
14	r	22/33 (67%)	18 (82%)	4 (18%)	2	1
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
16	U	84/112 (75%)	78 (93%)	6 (7%)	13	11
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	46
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4451/4654 (96%)	4280 (96%)	171 (4%)	28	32

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

Mol	Chain	Res	Type
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	270	SER
2	B	76	SER
2	B	84	THR
2	B	98	LEU
2	B	101	ILE
2	B	130	GLU
2	B	161	LEU
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	106	VAL
3	C	141	GLU
3	C	200	THR
3	C	240	ILE
3	C	249	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	43	LEU
4	D	154	VAL
4	D	259	ILE
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE

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Mol	Chain	Res	Type
5	E	81	GLU
6	F	25	THR
8	I	4	LEU
8	I	6	ILE
8	I	34	ARG
10	K	13	GLU
11	L	10	VAL
12	M	16	LEU
12	M	25	LEU
13	O	4	THR
13	O	6	THR
13	O	18	LYS
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	24	LEU
14	R	29	LYS
15	T	25	GLU
16	U	8	GLU
16	U	10	VAL
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	7	VAL
17	V	23	GLU
17	V	31	ARG
18	X	2	THR
18	X	3	ILE
18	X	15	LEU
19	Y	21	GLN
19	Y	34	MET
20	Z	6	GLN

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Mol	Chain	Res	Type
20	Z	15	LEU
20	Z	31	GLN
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	74	SER
2	b	76	SER
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	315	ILE
2	b	362	PHE
2	b	492	GLU
2	b	495	PHE
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
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	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	144	ILE
4	d	182	LEU
4	d	233	ARG

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Mol	Chain	Res	Type
4	d	241	GLU
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	60	GLN
5	e	61	ARG
5	e	65	LEU
5	e	83	LEU
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	6	TRP
7	h	7	LEU
7	h	27	THR
8	i	33	LYS
9	j	21	VAL
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	24	ASP
13	o	49	THR
13	o	64	GLU
13	o	87	VAL
13	o	89	SER
13	o	115	ARG
13	o	118	LEU
13	o	130	GLN
13	o	199	LEU
13	o	234	LYS
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	14	LEU

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Mol	Chain	Res	Type
15	t	29	ILE
16	u	8	GLU
16	u	15	GLU
16	u	61	VAL
17	v	15	GLU
17	v	42	VAL
17	v	90	GLU
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
18	x	21	LEU
19	y	19	ILE
19	y	45	ASN
19	y	46	LEU
20	z	7	LEU
20	z	20	VAL
20	z	32	ASP
20	z	46	LEU
20	z	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
2	B	394	GLN
2	B	409	GLN
3	C	155	ASN
3	C	385	GLN
4	D	301	GLN
5	E	82	GLN
11	L	8	GLN
12	M	32	GLN
13	O	3	GLN
13	O	36	GLN
13	O	88	ASN
14	R	22	ASN
16	U	37	GLN
16	U	78	ASN
17	V	86	GLN
18	X	38	GLN
19	Y	45	ASN
1	a	234	ASN

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Mol	Chain	Res	Type
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
3	c	28	GLN
3	c	201	ASN
3	c	378	ASN
3	c	382	ASN
3	c	415	ASN
4	d	350	ASN
5	e	82	GLN
6	f	44	GLN
7	h	59	ASN
13	o	36	GLN
13	o	61	GLN
13	o	132	ASN
13	o	155	ASN
16	u	37	GLN
17	v	25	GLN
17	v	106	ASN
18	x	33	GLN
20	z	31	GLN
20	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.00	1 (12%)	8,9,11	1.28	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.92	0	8,9,11	1.44	1 (12%)
15	FME	T	1	15	8,9,10	1.04	0	8,9,11	1.13	1 (12%)
15	FME	t	1	15	8,9,10	1.11	1 (12%)	8,9,11	1.11	0
12	FME	M	1	12	8,9,10	0.87	0	8,9,11	0.80	0
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.13	1 (12%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.79	1.42	1.46
15	t	1	FME	CA-N	-2.46	1.43	1.46
12	m	1	FME	CA-N	-2.06	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.15	117.98	122.82
12	m	1	FME	CB-CA-N	2.22	114.56	110.52
8	I	1	FME	CA-N-CN	-2.05	119.67	122.82
15	T	1	FME	O1-CN-N	-2.00	120.14	125.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	N-CA-CB-CG
15	t	1	FME	O-C-CA-CB

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
22	CLA	C	505	3	69,73,73	1.28	8 (11%)	82,113,113	1.24	8 (9%)
28	LMG	D	411	-	26,26,55	0.64	0	26,26,63	1.23	2 (7%)
22	CLA	C	511	3	69,73,73	1.60	10 (14%)	82,113,113	1.32	3 (3%)
24	BCR	C	514	-	41,41,41	1.31	4 (9%)	56,56,56	1.36	6 (10%)
22	CLA	b	602	2	69,73,73	1.11	9 (13%)	82,113,113	1.54	8 (9%)
24	BCR	k	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
31	DGD	C	515	-	63,63,67	1.11	3 (4%)	77,77,81	1.39	12 (15%)
22	CLA	B	607	37	69,73,73	1.25	10 (14%)	82,113,113	1.43	11 (13%)
34	STE	H	103	-	17,17,19	0.45	0	16,16,19	0.68	0
34	STE	b	621	-	15,15,19	0.41	0	14,14,19	0.78	0
28	LMG	a	416	-	55,55,55	1.21	5 (9%)	63,63,63	1.49	7 (11%)
34	STE	d	412	-	19,19,19	0.77	0	19,19,19	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HEC	V	201	17	50,50,50	1.60	4 (8%)	68,82,82	1.48	13 (19%)
31	DGD	c	518	-	63,63,67	1.02	3 (4%)	77,77,81	1.38	11 (14%)
23	PHO	A	404	-	58,69,69	1.80	10 (17%)	55,99,99	1.76	11 (20%)
24	BCR	H	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.33	9 (16%)
34	STE	d	413	-	19,19,19	0.60	0	19,19,19	1.09	1 (5%)
30	LHG	e	102	-	41,41,48	1.06	4 (9%)	44,47,54	1.38	5 (11%)
34	STE	d	411	-	16,16,19	0.53	0	16,16,19	1.43	4 (25%)
23	PHO	d	402	-	58,69,69	2.03	10 (17%)	55,99,99	1.52	9 (16%)
28	LMG	b	624	-	55,55,55	0.88	2 (3%)	63,63,63	1.50	10 (15%)
28	LMG	c	519	-	37,37,55	1.22	5 (13%)	45,45,63	1.35	7 (15%)
29	SQD	D	407	-	34,36,54	0.96	2 (5%)	42,45,65	2.21	12 (28%)
34	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.21	1 (9%)
24	BCR	K	102	-	41,41,41	1.13	4 (9%)	56,56,56	1.19	7 (12%)
22	CLA	d	404	4	69,73,73	1.42	11 (15%)	82,113,113	1.24	11 (13%)
30	LHG	A	414	-	48,48,48	0.87	3 (6%)	51,54,54	1.21	4 (7%)
24	BCR	b	618	-	41,41,41	1.29	4 (9%)	56,56,56	1.26	7 (12%)
22	CLA	B	606	2	69,73,73	1.38	6 (8%)	82,113,113	1.22	6 (7%)
34	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.62	0
24	BCR	x	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	7 (12%)
29	SQD	a	411	-	52,54,54	1.01	4 (7%)	62,65,65	1.75	11 (17%)
34	STE	h	102	-	13,13,19	0.44	0	12,12,19	0.64	0
22	CLA	b	601	37	69,73,73	1.37	8 (11%)	82,113,113	1.60	8 (9%)
22	CLA	c	504	37	64,68,73	1.28	6 (9%)	76,107,113	1.22	11 (14%)
28	LMG	A	412	-	48,48,55	1.06	3 (6%)	56,56,63	1.35	7 (12%)
22	CLA	B	615	2	69,73,73	1.23	12 (17%)	82,113,113	1.30	10 (12%)
22	CLA	D	403	4	69,73,73	1.52	11 (15%)	82,113,113	1.31	12 (14%)
22	CLA	B	611	2	69,73,73	1.41	10 (14%)	82,113,113	1.48	13 (15%)
28	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.32	7 (12%)
24	BCR	B	618	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	C	504	37	63,67,73	1.25	9 (14%)	74,105,113	1.28	11 (14%)
22	CLA	b	604	2	69,73,73	1.04	6 (8%)	82,113,113	1.51	11 (13%)
22	CLA	B	603	2	69,73,73	1.24	7 (10%)	82,113,113	1.44	12 (14%)
22	CLA	b	612	2	69,73,73	1.10	6 (8%)	82,113,113	1.30	9 (10%)
31	DGD	A	416	-	67,67,67	1.27	9 (13%)	81,81,81	1.44	11 (13%)
34	STE	Z	101	-	7,7,19	0.34	0	6,6,19	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	OEX	a	417[A]	37,3,1	0,14,14	-	-	-		
24	BCR	A	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)
27	PL9	a	409	-	55,55,55	1.24	7 (12%)	68,69,69	1.54	12 (17%)
30	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	4 (7%)
22	CLA	c	513	3	69,73,73	1.36	9 (13%)	82,113,113	1.15	8 (9%)
24	BCR	T	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.27	4 (7%)
22	CLA	d	403	4	69,73,73	1.39	9 (13%)	82,113,113	1.31	8 (9%)
22	CLA	A	411	37	69,73,73	1.23	9 (13%)	82,113,113	1.28	7 (8%)
28	LMG	d	410	-	44,44,55	1.05	2 (4%)	52,52,63	1.36	8 (15%)
34	STE	X	101	-	19,19,19	0.67	0	19,19,19	1.32	3 (15%)
24	BCR	a	405	-	41,41,41	1.11	3 (7%)	56,56,56	1.39	9 (16%)
34	STE	B	627	-	11,11,19	0.81	0	11,11,19	0.84	0
34	STE	C	519	-	11,11,19	0.75	0	11,11,19	1.17	1 (9%)
31	DGD	C	516	-	63,63,67	1.25	8 (12%)	77,77,81	1.34	9 (11%)
34	STE	T	102	-	14,14,19	0.41	0	13,13,19	0.83	0
22	CLA	a	404	1	69,73,73	1.42	10 (14%)	82,113,113	1.40	6 (7%)
22	CLA	a	403	37	69,73,73	1.29	7 (10%)	82,113,113	1.30	11 (13%)
22	CLA	c	506	3	69,73,73	1.35	9 (13%)	82,113,113	1.37	11 (13%)
22	CLA	C	502	3	69,73,73	1.17	6 (8%)	82,113,113	1.48	10 (12%)
23	PHO	d	401	-	58,69,69	1.86	11 (18%)	55,99,99	1.58	10 (18%)
24	BCR	c	515	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	4 (7%)
22	CLA	C	507	37	69,73,73	1.37	7 (10%)	82,113,113	1.56	12 (14%)
22	CLA	b	603	2	69,73,73	1.34	8 (11%)	82,113,113	1.51	13 (15%)
22	CLA	c	508	3	68,72,73	1.32	9 (13%)	80,111,113	1.33	11 (13%)
24	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	7 (12%)
22	CLA	a	410	37	69,73,73	1.49	5 (7%)	82,113,113	1.33	5 (6%)
22	CLA	C	510	3	69,73,73	1.26	11 (15%)	82,113,113	1.21	4 (4%)
34	STE	B	625	-	17,17,19	0.66	0	17,17,19	1.12	1 (5%)
24	BCR	d	405	-	41,41,41	1.25	3 (7%)	56,56,56	1.21	6 (10%)
22	CLA	c	502	3	69,73,73	1.28	8 (11%)	82,113,113	1.46	8 (9%)
29	SQD	A	413	-	50,52,54	0.96	4 (8%)	60,63,65	1.83	12 (20%)
22	CLA	b	615	2	69,73,73	1.54	8 (11%)	82,113,113	1.45	8 (9%)
36	HEC	v	201	17	50,50,50	1.60	6 (12%)	68,82,82	1.40	9 (13%)
24	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.08	4 (7%)
22	CLA	c	507	37	69,73,73	1.26	3 (4%)	82,113,113	1.31	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HEM	e	101	5,6	50,50,50	1.47	10 (20%)	67,82,82	1.39	11 (16%)
22	CLA	c	505	3	69,73,73	1.16	6 (8%)	82,113,113	1.13	6 (7%)
26	BCT	a	408	21	3,3,3	1.33	0	2,3,3	2.71	1 (50%)
22	CLA	C	512	3	69,73,73	1.19	9 (13%)	82,113,113	1.24	9 (10%)
22	CLA	c	510	3	69,73,73	1.38	8 (11%)	82,113,113	1.30	8 (9%)
35	HEM	F	101	5,6	50,50,50	1.36	6 (12%)	67,82,82	1.25	7 (10%)
29	SQD	b	620	-	47,49,54	0.94	4 (8%)	57,60,65	2.11	16 (28%)
22	CLA	C	506	3	69,73,73	1.35	10 (14%)	82,113,113	1.17	8 (9%)
22	CLA	b	608	2	69,73,73	1.22	9 (13%)	82,113,113	1.25	6 (7%)
22	CLA	B	605	2	69,73,73	1.11	7 (10%)	82,113,113	1.22	8 (9%)
32	OEY	A	417[B]	37,3,1	0,16,16	-	-	-	-	-
31	DGD	C	517	-	63,63,67	0.92	4 (6%)	77,77,81	1.32	7 (9%)
30	LHG	d	409	-	38,38,48	0.73	1 (2%)	41,44,54	1.15	3 (7%)
28	LMG	C	518	-	48,48,55	1.16	5 (10%)	56,56,63	1.34	6 (10%)
22	CLA	B	613	2	69,73,73	1.41	13 (18%)	82,113,113	1.39	8 (9%)
24	BCR	t	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.37	8 (14%)
31	DGD	c	517	-	63,63,67	0.99	4 (6%)	77,77,81	1.42	10 (12%)
34	STE	b	625	-	15,15,19	0.76	0	15,15,19	0.98	1 (6%)
22	CLA	A	402	1	69,73,73	1.27	8 (11%)	82,113,113	1.40	10 (12%)
33	OEX	A	418[A]	37,3,1	0,14,14	-	-	-	-	-
31	DGD	h	101	-	63,63,67	1.04	4 (6%)	77,77,81	1.48	11 (14%)
30	LHG	B	622	-	48,48,48	0.91	3 (6%)	51,54,54	1.42	8 (15%)
34	STE	J	101	-	11,11,19	0.68	0	11,11,19	1.38	1 (9%)
22	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.52	11 (13%)
32	OEY	a	418[B]	37,3,1	0,16,16	-	-	-	-	-
24	BCR	D	404	-	41,41,41	1.24	2 (4%)	56,56,56	1.14	4 (7%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.33	8 (14%)
22	CLA	C	513	3	69,73,73	1.25	7 (10%)	82,113,113	1.22	6 (7%)
30	LHG	D	409	-	46,46,48	1.00	3 (6%)	49,52,54	1.35	3 (6%)
29	SQD	a	412	-	35,35,54	1.12	2 (5%)	37,37,65	1.46	4 (10%)
34	STE	I	101	-	14,14,19	0.48	0	13,13,19	0.60	0
22	CLA	A	405	1	58,62,73	1.25	8 (13%)	68,99,113	1.36	12 (17%)
22	CLA	c	512	3	69,73,73	1.24	9 (13%)	82,113,113	1.43	7 (8%)
22	CLA	b	611	2	69,73,73	1.07	4 (5%)	82,113,113	1.36	10 (12%)
30	LHG	B	621	-	48,48,48	1.02	2 (4%)	51,54,54	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	d	406	-	55,55,55	1.69	7 (12%)	68,69,69	1.64	14 (20%)
29	SQD	B	623	-	52,54,54	0.96	3 (5%)	62,65,65	1.73	11 (17%)
34	STE	C	521	-	11,11,19	0.61	0	11,11,19	1.58	2 (18%)
30	LHG	d	408	-	48,48,48	0.97	3 (6%)	51,54,54	1.21	4 (7%)
28	LMG	M	101	-	51,51,55	1.07	6 (11%)	59,59,63	1.43	9 (15%)
22	CLA	a	402	1	69,73,73	1.32	8 (11%)	82,113,113	1.40	10 (12%)
22	CLA	B	614	2	69,73,73	1.35	8 (11%)	82,113,113	1.41	11 (13%)
22	CLA	B	612	2	69,73,73	1.10	6 (8%)	82,113,113	1.44	9 (10%)
22	CLA	B	608	2	69,73,73	1.16	7 (10%)	82,113,113	1.45	13 (15%)
34	STE	c	520	-	19,19,19	0.69	0	19,19,19	1.04	1 (5%)
22	CLA	c	503	3	69,73,73	1.32	9 (13%)	82,113,113	1.37	5 (6%)
28	LMG	c	522	-	49,49,55	0.96	2 (4%)	57,57,63	1.32	4 (7%)
34	STE	a	414	-	11,11,19	0.86	0	11,11,19	1.00	0
24	BCR	b	617	-	41,41,41	1.20	4 (9%)	56,56,56	1.41	9 (16%)
22	CLA	c	509	3	69,73,73	1.30	6 (8%)	82,113,113	1.33	9 (10%)
26	BCT	A	409	21	3,3,3	1.19	0	2,3,3	3.30	1 (50%)
31	DGD	c	516	-	63,63,67	1.25	11 (17%)	77,77,81	1.44	14 (18%)
34	STE	B	624	-	11,11,19	0.96	1 (9%)	11,11,19	1.36	2 (18%)
34	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.27	1 (7%)
29	SQD	f	101	-	39,41,54	1.12	5 (12%)	49,52,65	1.94	10 (20%)
22	CLA	c	511	3	69,73,73	1.33	10 (14%)	82,113,113	1.38	5 (6%)
34	STE	L	101	-	11,11,19	0.76	0	11,11,19	1.58	2 (18%)
22	CLA	C	503	3	69,73,73	1.38	11 (15%)	82,113,113	1.55	9 (10%)
24	BCR	K	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.31	8 (14%)
27	PL9	D	405	-	55,55,55	1.69	10 (18%)	68,69,69	1.69	14 (20%)
22	CLA	C	509	3	69,73,73	1.08	7 (10%)	82,113,113	1.54	7 (8%)
24	BCR	B	617	-	41,41,41	1.22	3 (7%)	56,56,56	1.29	6 (10%)
22	CLA	B	601	37	69,73,73	1.30	7 (10%)	82,113,113	1.65	10 (12%)
34	STE	M	102	-	14,14,19	0.80	0	14,14,19	1.02	1 (7%)
22	CLA	B	616	2	64,68,73	1.32	8 (12%)	76,107,113	1.73	14 (18%)
22	CLA	b	614	2	69,73,73	1.13	5 (7%)	82,113,113	1.27	8 (9%)
22	CLA	D	402	4	69,73,73	1.20	5 (7%)	82,113,113	1.31	10 (12%)
22	CLA	B	609	2	69,73,73	1.24	7 (10%)	82,113,113	1.38	7 (8%)
34	STE	a	415	-	14,14,19	0.42	0	13,13,19	0.86	0
22	CLA	b	605	2	69,73,73	1.15	7 (10%)	82,113,113	1.49	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	d	407	-	48,48,48	0.98	3 (6%)	51,54,54	1.37	7 (13%)
34	STE	b	626	-	19,19,19	0.69	0	19,19,19	0.84	0
22	CLA	b	606	2	69,73,73	1.58	9 (13%)	82,113,113	1.82	17 (20%)
28	LMG	b	622	-	51,51,55	1.02	5 (9%)	59,59,63	1.47	7 (11%)
22	CLA	A	403	37	69,73,73	1.27	10 (14%)	82,113,113	1.15	6 (7%)
22	CLA	b	607	37	69,73,73	1.25	7 (10%)	82,113,113	1.49	8 (9%)
22	CLA	B	610	37	69,73,73	1.16	6 (8%)	82,113,113	1.54	10 (12%)
31	DGD	H	102	-	63,63,67	1.23	7 (11%)	77,77,81	1.47	12 (15%)
22	CLA	c	501	3	69,73,73	1.03	5 (7%)	82,113,113	1.44	9 (10%)
28	LMG	D	406	-	51,51,55	0.88	2 (3%)	59,59,63	1.43	9 (15%)
22	CLA	b	609	2	69,73,73	1.23	8 (11%)	82,113,113	1.32	8 (9%)
34	STE	b	627	-	9,9,19	0.51	0	8,8,19	0.56	0
22	CLA	B	602	2	69,73,73	1.28	9 (13%)	82,113,113	1.39	11 (13%)
34	STE	l	102	-	17,17,19	0.32	0	16,16,19	1.00	0
34	STE	C	520	-	15,15,19	0.40	0	14,14,19	0.80	0
22	CLA	b	613	2	69,73,73	1.20	8 (11%)	82,113,113	1.53	10 (12%)
24	BCR	Y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	4 (7%)
34	STE	a	413	-	9,9,19	0.52	0	8,8,19	0.52	0
30	LHG	D	408	-	48,48,48	1.09	4 (8%)	51,54,54	1.30	7 (13%)
22	CLA	B	604	2	69,73,73	1.46	6 (8%)	82,113,113	1.57	9 (10%)
28	LMG	D	410	-	31,31,55	0.91	2 (6%)	33,33,63	1.17	2 (6%)
34	STE	B	620	-	16,16,19	0.66	0	16,16,19	1.10	0
22	CLA	b	616	2	64,68,73	1.42	9 (14%)	76,107,113	1.40	9 (11%)
34	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.69	0
27	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	1.81	15 (22%)
23	PHO	D	401	-	58,69,69	1.93	8 (13%)	55,99,99	1.48	11 (20%)
34	STE	b	623	-	19,19,19	0.65	0	19,19,19	1.11	2 (10%)
34	STE	c	523	-	11,11,19	0.80	0	11,11,19	0.91	0
34	STE	R	101	-	11,11,19	0.89	0	11,11,19	0.77	0
29	SQD	A	415	-	38,38,54	1.01	3 (7%)	40,40,65	1.28	5 (12%)
22	CLA	C	501	3	69,73,73	1.31	7 (10%)	82,113,113	1.49	8 (9%)
24	BCR	c	514	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	6 (10%)
22	CLA	b	610	37	69,73,73	1.31	6 (8%)	82,113,113	1.44	13 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	505	3	-	12/39/115/115	-
28	LMG	D	411	-	-	10/22/22/70	-
22	CLA	C	511	3	-	12/39/115/115	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
22	CLA	b	602	2	-	7/39/115/115	-
24	BCR	k	102	-	-	7/29/63/63	0/2/2/2
31	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	B	607	37	-	8/39/115/115	-
34	STE	H	103	-	-	11/15/15/17	-
34	STE	b	621	-	-	5/13/13/17	-
28	LMG	a	416	-	-	25/50/70/70	0/1/1/1
34	STE	d	412	-	-	10/17/17/17	-
36	HEC	V	201	17	1/1/7/7	5/14/54/54	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
34	STE	d	413	-	-	9/17/17/17	-
30	LHG	e	102	-	-	26/46/46/53	-
34	STE	d	411	-	-	9/14/14/17	-
23	PHO	d	402	-	-	7/37/103/103	0/5/6/6
28	LMG	b	624	-	-	28/50/70/70	0/1/1/1
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
34	STE	j	101	-	-	4/9/9/17	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	d	404	4	-	8/39/115/115	-
30	LHG	A	414	-	-	29/53/53/53	-
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
22	CLA	B	606	2	-	10/39/115/115	-
34	STE	B	626	-	-	10/13/13/17	-
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2
29	SQD	a	411	-	-	25/49/69/69	0/1/1/1
34	STE	h	102	-	-	5/11/11/17	-
22	CLA	b	601	37	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	504	37	-	8/33/109/115	-
28	LMG	A	412	-	-	18/43/63/70	0/1/1/1
22	CLA	B	615	2	-	7/39/115/115	-
22	CLA	D	403	4	-	9/39/115/115	-
22	CLA	B	611	2	-	6/39/115/115	-
28	LMG	c	521	-	-	24/43/63/70	0/1/1/1
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
22	CLA	C	504	37	-	8/32/108/115	-
22	CLA	b	604	2	-	4/39/115/115	-
22	CLA	B	603	2	-	10/39/115/115	-
22	CLA	b	612	2	-	6/39/115/115	-
31	DGD	A	416	-	-	24/55/95/95	0/2/2/2
34	STE	Z	101	-	-	3/5/5/17	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
27	PL9	a	409	-	-	23/53/73/73	0/1/1/1
30	LHG	l	101	-	-	18/53/53/53	-
22	CLA	c	513	3	-	7/39/115/115	-
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
22	CLA	d	403	4	-	8/39/115/115	-
22	CLA	A	411	37	-	10/39/115/115	-
28	LMG	d	410	-	-	12/39/59/70	0/1/1/1
34	STE	X	101	-	-	9/17/17/17	-
24	BCR	a	405	-	-	2/29/63/63	0/2/2/2
34	STE	B	627	-	-	6/9/9/17	-
34	STE	C	519	-	-	5/9/9/17	-
31	DGD	C	516	-	-	19/51/91/95	0/2/2/2
34	STE	T	102	-	-	7/12/12/17	-
22	CLA	a	404	1	-	6/39/115/115	-
22	CLA	a	403	37	-	13/39/115/115	-
22	CLA	c	506	3	-	14/39/115/115	-
22	CLA	C	502	3	-	5/39/115/115	-
23	PHO	d	401	-	-	4/37/103/103	0/5/6/6
24	BCR	c	515	-	-	7/29/63/63	0/2/2/2
22	CLA	C	507	37	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	603	2	-	6/39/115/115	-
22	CLA	c	508	3	-	14/38/114/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	a	410	37	-	3/39/115/115	-
22	CLA	C	510	3	-	9/39/115/115	-
34	STE	B	625	-	-	9/15/15/17	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
22	CLA	c	502	3	-	5/39/115/115	-
29	SQD	A	413	-	-	15/47/67/69	0/1/1/1
22	CLA	b	615	2	-	10/39/115/115	-
36	HEC	v	201	17	1/1/7/7	4/14/54/54	-
24	BCR	k	101	-	-	8/29/63/63	0/2/2/2
22	CLA	c	507	37	-	7/39/115/115	-
35	HEM	e	101	5,6	-	5/14/54/54	-
22	CLA	c	505	3	-	7/39/115/115	-
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	c	510	3	-	12/39/115/115	-
35	HEM	F	101	5,6	-	3/14/54/54	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
22	CLA	C	506	3	-	9/39/115/115	-
22	CLA	b	608	2	-	7/39/115/115	-
22	CLA	B	605	2	-	11/39/115/115	-
31	DGD	C	517	-	-	15/51/91/95	0/2/2/2
30	LHG	d	409	-	-	18/43/43/53	-
28	LMG	C	518	-	-	21/43/63/70	0/1/1/1
22	CLA	B	613	2	-	10/39/115/115	-
24	BCR	t	101	-	-	5/29/63/63	0/2/2/2
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
34	STE	b	625	-	-	4/13/13/17	-
22	CLA	A	402	1	-	3/39/115/115	-
31	DGD	h	101	-	-	16/51/91/95	0/2/2/2
30	LHG	B	622	-	-	22/53/53/53	-
34	STE	J	101	-	-	2/9/9/17	-
22	CLA	C	508	3	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	BCR	b	619	-	-	3/29/63/63	0/2/2/2
22	CLA	C	513	3	-	10/39/115/115	-
30	LHG	D	409	-	-	26/51/51/53	-
29	SQD	a	412	-	-	14/37/37/69	-
34	STE	I	101	-	-	6/12/12/17	-
22	CLA	A	405	1	-	6/26/102/115	-
22	CLA	c	512	3	-	22/39/115/115	-
22	CLA	b	611	2	-	6/39/115/115	-
30	LHG	B	621	-	-	26/53/53/53	-
27	PL9	d	406	-	-	12/53/73/73	0/1/1/1
29	SQD	B	623	-	-	22/49/69/69	0/1/1/1
34	STE	C	521	-	-	5/9/9/17	-
30	LHG	d	408	-	-	22/53/53/53	-
28	LMG	M	101	-	-	18/46/66/70	0/1/1/1
22	CLA	a	402	1	-	6/39/115/115	-
22	CLA	B	614	2	-	11/39/115/115	-
22	CLA	B	612	2	-	9/39/115/115	-
22	CLA	B	608	2	-	1/39/115/115	-
34	STE	c	520	-	-	10/17/17/17	-
22	CLA	c	503	3	-	3/39/115/115	-
28	LMG	c	522	-	-	19/44/64/70	0/1/1/1
34	STE	a	414	-	-	5/9/9/17	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	c	509	3	-	11/39/115/115	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
34	STE	B	624	-	-	3/9/9/17	-
34	STE	t	102	-	-	5/11/11/17	-
29	SQD	f	101	-	-	15/36/56/69	0/1/1/1
22	CLA	c	511	3	-	13/39/115/115	-
34	STE	L	101	-	-	4/9/9/17	-
22	CLA	C	503	3	-	3/39/115/115	-
24	BCR	K	101	-	-	14/29/63/63	0/2/2/2
27	PL9	D	405	-	-	10/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	509	3	-	9/39/115/115	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	B	601	37	-	21/39/115/115	-
34	STE	M	102	-	-	4/12/12/17	-
22	CLA	B	616	2	-	8/33/109/115	-
22	CLA	b	614	2	-	18/39/115/115	-
22	CLA	D	402	4	-	11/39/115/115	-
22	CLA	B	609	2	-	7/39/115/115	-
34	STE	a	415	-	-	7/12/12/17	-
22	CLA	b	605	2	-	12/39/115/115	-
30	LHG	d	407	-	-	22/53/53/53	-
34	STE	b	626	-	-	5/17/17/17	-
22	CLA	b	606	2	-	12/39/115/115	-
28	LMG	b	622	-	-	24/46/66/70	0/1/1/1
22	CLA	A	403	37	-	11/39/115/115	-
22	CLA	b	607	37	-	14/39/115/115	-
22	CLA	B	610	37	-	7/39/115/115	-
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	c	501	3	-	5/39/115/115	-
28	LMG	D	406	-	-	16/46/66/70	0/1/1/1
22	CLA	b	609	2	-	6/39/115/115	-
34	STE	b	627	-	-	5/7/7/17	-
22	CLA	B	602	2	-	6/39/115/115	-
34	STE	l	102	-	-	9/15/15/17	-
34	STE	C	520	-	-	5/13/13/17	-
22	CLA	b	613	2	-	4/39/115/115	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
34	STE	a	413	-	-	3/7/7/17	-
30	LHG	D	408	-	-	25/53/53/53	-
22	CLA	B	604	2	-	10/39/115/115	-
28	LMG	D	410	-	-	14/33/33/70	-
34	STE	B	620	-	-	8/14/14/17	-
22	CLA	b	616	2	-	13/33/109/115	-
34	STE	M	103	-	-	1/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	A	410	-	-	22/53/73/73	0/1/1/1
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
34	STE	b	623	-	-	11/17/17/17	-
34	STE	c	523	-	-	5/9/9/17	-
34	STE	R	101	-	-	4/9/9/17	-
29	SQD	A	415	-	-	12/39/39/69	-
22	CLA	C	501	3	-	1/39/115/115	-
24	BCR	c	514	-	-	6/29/63/63	0/2/2/2
22	CLA	b	610	37	-	7/39/115/115	-

All (862) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	9.23	1.49	1.39
22	b	606	CLA	MG-NA	8.45	2.26	2.06
22	C	511	CLA	MG-NA	8.43	2.26	2.06
23	d	402	PHO	C3B-C4B	8.34	1.49	1.41
23	D	401	PHO	C3B-C4B	8.24	1.49	1.41
23	d	401	PHO	C1B-C2B	8.04	1.48	1.39
22	a	410	CLA	MG-NA	7.99	2.25	2.06
23	D	401	PHO	C1B-C2B	7.83	1.48	1.39
36	v	201	HEC	C3D-C2D	7.03	1.51	1.36
23	A	404	PHO	C3B-C4B	6.91	1.48	1.41
23	d	401	PHO	C3B-C4B	6.85	1.48	1.41
36	V	201	HEC	C3D-C2D	6.81	1.51	1.36
22	b	615	CLA	MG-NB	6.79	2.19	2.05
22	B	604	CLA	MG-NA	6.75	2.22	2.06
22	C	503	CLA	MG-NA	6.54	2.21	2.06
22	C	507	CLA	MG-NA	6.49	2.21	2.06
27	d	406	PL9	C6-C1	-6.42	1.37	1.48
22	c	507	CLA	MG-NB	-6.13	1.93	2.05
23	A	404	PHO	C1B-C2B	6.01	1.46	1.39
22	c	513	CLA	MG-ND	-5.63	1.94	2.05
22	B	603	CLA	MG-NA	5.61	2.19	2.06
22	B	616	CLA	MG-NA	5.58	2.19	2.06
22	b	610	CLA	MG-NB	-5.53	1.94	2.05
22	b	603	CLA	MG-NA	5.50	2.19	2.06
22	B	606	CLA	MG-NA	5.49	2.19	2.06
22	b	615	CLA	MG-NA	5.44	2.19	2.06
22	b	616	CLA	MG-ND	-5.43	1.95	2.05
22	b	601	CLA	MG-NA	5.31	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	MG-ND	-5.28	1.95	2.05
22	a	403	CLA	MG-NC	5.25	2.18	2.06
22	c	510	CLA	MG-NA	5.08	2.18	2.06
27	D	405	PL9	C6-C1	-5.06	1.40	1.48
22	B	611	CLA	MG-NA	5.02	2.18	2.06
22	d	404	CLA	MG-ND	-4.99	1.95	2.05
22	c	503	CLA	MG-NC	4.96	2.18	2.06
22	a	404	CLA	MG-NA	4.95	2.18	2.06
22	D	403	CLA	MG-NB	-4.94	1.96	2.05
22	C	501	CLA	MG-NA	4.90	2.17	2.06
22	d	403	CLA	MG-ND	-4.87	1.96	2.05
27	A	410	PL9	C7-C3	-4.86	1.44	1.51
22	D	403	CLA	C1D-ND	4.80	1.44	1.37
22	B	604	CLA	MG-ND	-4.79	1.96	2.05
22	c	504	CLA	MG-ND	-4.75	1.96	2.05
22	c	506	CLA	MG-NB	4.74	2.15	2.05
22	c	508	CLA	MG-NA	4.72	2.17	2.06
22	c	511	CLA	MG-NA	4.72	2.17	2.06
28	a	416	LMG	C4-C5	4.69	1.63	1.53
22	b	613	CLA	MG-NA	4.67	2.17	2.06
27	d	406	PL9	C3-C4	-4.66	1.42	1.49
24	H	101	BCR	C30-C25	-4.66	1.47	1.53
22	b	607	CLA	MG-NA	4.62	2.17	2.06
24	C	514	BCR	C1-C6	-4.61	1.47	1.53
22	c	510	CLA	MG-ND	-4.61	1.96	2.05
24	Y	101	BCR	C30-C25	-4.53	1.48	1.53
22	C	513	CLA	MG-NA	4.53	2.17	2.06
36	V	201	HEC	FE-ND	4.52	2.08	1.94
22	A	405	CLA	MG-ND	-4.50	1.96	2.05
22	B	614	CLA	MG-ND	-4.48	1.96	2.05
30	B	621	LHG	O7-C5	-4.48	1.36	1.46
22	C	505	CLA	MG-NA	4.46	2.16	2.06
22	D	402	CLA	MG-ND	-4.41	1.97	2.05
24	b	618	BCR	C30-C25	-4.24	1.48	1.53
22	d	403	CLA	MG-NA	4.23	2.16	2.06
24	D	404	BCR	C30-C25	-4.22	1.48	1.53
22	a	402	CLA	MG-NA	4.21	2.16	2.06
22	b	606	CLA	C1D-ND	4.18	1.43	1.37
31	A	416	DGD	C4E-C5E	4.18	1.61	1.53
22	C	508	CLA	MG-NA	4.17	2.16	2.06
22	A	402	CLA	C1D-ND	4.15	1.43	1.37
22	c	509	CLA	MG-NC	4.15	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	MG-NC	-4.13	1.96	2.06
24	b	617	BCR	C1-C6	-4.13	1.48	1.53
22	A	403	CLA	MG-NB	-4.07	1.97	2.05
22	B	613	CLA	MG-NC	4.07	2.15	2.06
22	c	506	CLA	MG-ND	-4.06	1.97	2.05
22	d	404	CLA	MG-NB	-4.05	1.97	2.05
22	b	610	CLA	C1D-ND	4.04	1.43	1.37
27	D	405	PL9	C7-C3	-4.04	1.45	1.51
22	B	611	CLA	MG-NB	4.02	2.13	2.05
22	c	509	CLA	MG-NB	-3.98	1.97	2.05
22	C	506	CLA	MG-NA	3.98	2.15	2.06
24	d	405	BCR	C1-C6	-3.96	1.48	1.53
31	c	516	DGD	C4D-C3D	3.94	1.62	1.52
22	c	508	CLA	C1D-ND	3.94	1.43	1.37
22	C	502	CLA	MG-ND	3.94	2.13	2.05
22	B	611	CLA	MG-ND	-3.93	1.98	2.05
24	B	617	BCR	C1-C6	-3.92	1.48	1.53
36	V	201	HEC	FE-NB	3.92	2.07	1.94
22	c	509	CLA	C1D-ND	3.91	1.43	1.37
24	B	618	BCR	C30-C25	-3.90	1.48	1.53
22	a	404	CLA	MG-NB	-3.90	1.98	2.05
27	D	405	PL9	C52-C5	-3.87	1.42	1.50
36	v	201	HEC	FE-NA	3.86	2.07	1.95
27	a	409	PL9	C3-C4	-3.83	1.43	1.49
24	B	617	BCR	C30-C25	-3.83	1.48	1.53
24	c	514	BCR	C1-C6	-3.83	1.48	1.53
24	x	101	BCR	C30-C25	-3.82	1.48	1.53
23	A	404	PHO	C4D-ND	-3.81	1.32	1.38
29	a	411	SQD	O48-C23	3.80	1.44	1.33
30	D	408	LHG	O8-C6	-3.79	1.36	1.45
27	D	405	PL9	C11-C9	-3.76	1.43	1.51
22	b	616	CLA	C1D-ND	3.75	1.42	1.37
27	D	405	PL9	C41-C39	-3.75	1.43	1.51
24	b	619	BCR	C30-C25	-3.75	1.49	1.53
24	c	515	BCR	C1-C6	-3.71	1.49	1.53
22	d	404	CLA	C1D-ND	3.71	1.42	1.37
23	D	401	PHO	C4D-ND	-3.70	1.33	1.38
28	C	518	LMG	C4-C5	3.70	1.60	1.53
24	d	405	BCR	C30-C25	-3.69	1.49	1.53
22	A	411	CLA	MG-NA	3.69	2.15	2.06
22	B	613	CLA	C4B-NB	3.68	1.42	1.37
30	d	408	LHG	O7-C5	-3.68	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	LMG	O1-C7	-3.68	1.37	1.43
22	c	502	CLA	MG-NA	3.66	2.15	2.06
22	c	505	CLA	MG-NB	-3.66	1.98	2.05
24	K	101	BCR	C30-C25	-3.62	1.49	1.53
24	k	101	BCR	C30-C25	-3.61	1.49	1.53
22	b	616	CLA	MG-NB	3.61	2.12	2.05
24	Y	101	BCR	C1-C6	-3.61	1.49	1.53
31	H	102	DGD	C4E-C5E	3.60	1.60	1.53
27	d	406	PL9	C53-C6	-3.59	1.43	1.50
31	C	516	DGD	C4D-C3D	3.59	1.61	1.52
29	B	623	SQD	O47-C7	3.58	1.44	1.34
23	A	404	PHO	CMC-C2C	-3.58	1.45	1.50
22	c	511	CLA	MG-NB	3.57	2.12	2.05
27	a	409	PL9	C6-C1	-3.57	1.42	1.48
22	C	512	CLA	MG-NA	3.57	2.14	2.06
24	A	406	BCR	C1-C6	-3.56	1.49	1.53
24	c	514	BCR	C30-C25	-3.56	1.49	1.53
24	T	101	BCR	C30-C25	-3.56	1.49	1.53
22	B	601	CLA	C1D-ND	3.55	1.42	1.37
24	B	619	BCR	C30-C25	-3.53	1.49	1.53
22	C	510	CLA	MG-NC	3.52	2.14	2.06
28	d	410	LMG	O1-C7	-3.52	1.37	1.43
27	d	406	PL9	C46-C44	-3.52	1.44	1.51
23	D	401	PHO	CMB-C2B	-3.51	1.44	1.51
22	B	614	CLA	C4B-NB	3.51	1.42	1.37
22	d	403	CLA	MG-NB	-3.50	1.98	2.05
22	c	505	CLA	MG-NC	3.50	2.14	2.06
30	d	407	LHG	O7-C5	-3.49	1.38	1.46
22	a	402	CLA	C1D-ND	3.47	1.42	1.37
28	c	522	LMG	O7-C8	-3.47	1.38	1.46
29	a	412	SQD	O47-C7	3.46	1.44	1.34
22	D	402	CLA	C1D-ND	3.45	1.42	1.37
28	d	410	LMG	O7-C8	-3.45	1.38	1.46
24	B	619	BCR	C1-C6	-3.43	1.49	1.53
29	a	412	SQD	O48-C23	3.43	1.43	1.33
35	F	101	HEM	FE-NC	3.42	2.06	1.95
22	C	511	CLA	C1D-ND	3.40	1.42	1.37
22	B	601	CLA	MG-NC	3.40	2.14	2.06
22	B	614	CLA	MG-NB	3.40	2.12	2.05
35	e	101	HEM	FE-NB	3.40	2.05	1.94
24	b	618	BCR	C1-C6	-3.39	1.49	1.53
28	a	416	LMG	C4-C3	3.38	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C1B-C2B	3.38	1.51	1.43
22	D	403	CLA	MG-NA	3.38	2.14	2.06
29	A	415	SQD	O48-C23	3.38	1.43	1.33
22	C	506	CLA	MG-ND	-3.37	1.99	2.05
22	b	601	CLA	MG-NC	-3.37	1.98	2.06
22	C	513	CLA	C1D-ND	3.37	1.42	1.37
24	K	101	BCR	C1-C6	-3.37	1.49	1.53
22	b	610	CLA	MG-NC	3.36	2.14	2.06
22	B	613	CLA	MG-ND	-3.36	1.99	2.05
22	b	609	CLA	MG-NA	3.35	2.14	2.06
22	B	616	CLA	MG-NB	3.35	2.12	2.05
31	c	518	DGD	O2G-C2G	-3.35	1.38	1.46
22	B	606	CLA	MG-NC	-3.34	1.98	2.06
22	a	404	CLA	C1D-ND	3.34	1.42	1.37
24	b	619	BCR	C1-C6	-3.34	1.49	1.53
22	b	614	CLA	C4B-NB	3.32	1.42	1.37
22	B	615	CLA	C1D-ND	3.32	1.42	1.37
22	C	501	CLA	C1D-ND	3.31	1.42	1.37
28	c	521	LMG	O1-C1	3.31	1.45	1.40
22	C	506	CLA	C1B-NB	-3.31	1.33	1.37
22	c	513	CLA	MG-NB	3.30	2.12	2.05
22	c	502	CLA	CMD-C2D	-3.29	1.44	1.50
22	B	613	CLA	MG-NA	3.29	2.14	2.06
22	A	411	CLA	C1D-ND	3.29	1.42	1.37
31	C	515	DGD	C4D-C3D	3.27	1.60	1.52
28	a	416	LMG	O8-C9	-3.25	1.37	1.45
22	c	507	CLA	C1D-ND	3.24	1.42	1.37
22	c	504	CLA	C4B-NB	3.24	1.42	1.37
22	C	513	CLA	C4B-NB	3.24	1.42	1.37
22	d	404	CLA	CMD-C2D	-3.23	1.44	1.50
31	C	516	DGD	O3E-C3E	-3.21	1.35	1.43
24	C	514	BCR	C30-C25	-3.20	1.49	1.53
22	B	601	CLA	MG-NA	3.19	2.13	2.06
23	d	402	PHO	C1D-C2D	3.19	1.43	1.39
22	B	602	CLA	MG-NB	3.18	2.12	2.05
24	K	102	BCR	C30-C25	-3.18	1.49	1.53
22	C	504	CLA	MG-NA	3.18	2.13	2.06
22	B	604	CLA	C1D-ND	3.18	1.42	1.37
30	D	408	LHG	O7-C5	-3.17	1.39	1.46
31	H	102	DGD	O5D-C1E	3.17	1.45	1.40
22	B	614	CLA	C1D-ND	3.16	1.42	1.37
22	b	608	CLA	MG-ND	3.15	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	C1B-C2B	3.15	1.50	1.43
22	C	507	CLA	C1B-C2B	3.15	1.50	1.43
23	A	404	PHO	C1D-C2D	3.14	1.43	1.39
22	b	609	CLA	C1D-ND	3.14	1.42	1.37
29	D	407	SQD	O48-C23	3.14	1.42	1.33
30	B	622	LHG	O7-C5	-3.14	1.39	1.46
22	b	601	CLA	C1B-C2B	3.14	1.50	1.43
22	C	505	CLA	C1B-C2B	3.14	1.50	1.43
23	D	401	PHO	C1D-C2D	3.12	1.43	1.39
30	D	409	LHG	P-O6	3.12	1.71	1.59
24	k	102	BCR	C30-C25	-3.12	1.49	1.53
23	d	401	PHO	C3B-C2B	-3.12	1.36	1.40
23	A	404	PHO	C3D-C4D	3.11	1.45	1.41
22	C	504	CLA	C4B-NB	3.11	1.41	1.37
24	c	515	BCR	C30-C25	-3.11	1.49	1.53
22	c	512	CLA	C1D-ND	3.11	1.41	1.37
35	e	101	HEM	FE-ND	3.11	2.04	1.94
31	A	416	DGD	C3G-C2G	3.10	1.60	1.50
30	e	102	LHG	P-O6	3.10	1.71	1.59
22	C	507	CLA	MG-NB	-3.10	1.99	2.05
22	C	510	CLA	C1D-ND	3.09	1.41	1.37
22	B	602	CLA	C1D-ND	3.08	1.41	1.37
31	A	416	DGD	C4D-C3D	3.08	1.60	1.52
22	b	605	CLA	C1B-C2B	3.08	1.50	1.43
29	b	620	SQD	O47-C7	3.08	1.43	1.34
22	C	502	CLA	MG-NA	3.07	2.13	2.06
24	b	617	BCR	C30-C25	-3.07	1.49	1.53
22	c	502	CLA	C1D-ND	3.07	1.41	1.37
22	c	502	CLA	C4B-NB	3.06	1.41	1.37
24	k	101	BCR	C1-C6	-3.05	1.49	1.53
22	a	402	CLA	MG-NB	3.05	2.11	2.05
22	B	608	CLA	C1D-ND	3.05	1.41	1.37
22	a	410	CLA	C1D-ND	3.04	1.41	1.37
22	c	513	CLA	C1D-ND	3.04	1.41	1.37
29	b	620	SQD	O48-C23	3.03	1.42	1.33
22	c	512	CLA	C4B-NB	3.03	1.41	1.37
28	D	410	LMG	C7-C8	3.03	1.58	1.51
27	d	406	PL9	C11-C9	-3.02	1.45	1.51
29	A	415	SQD	O47-C7	3.02	1.42	1.34
22	b	615	CLA	CMD-C2D	-3.02	1.44	1.50
24	t	101	BCR	C30-C25	-3.02	1.49	1.53
31	C	515	DGD	O2E-C2E	-3.02	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C1D-ND	3.02	1.41	1.37
22	B	608	CLA	CMD-C2D	-3.01	1.44	1.50
22	B	607	CLA	C1D-ND	3.01	1.41	1.37
31	C	516	DGD	O5D-C6D	-3.01	1.38	1.43
28	c	519	LMG	O1-C1	3.00	1.45	1.40
23	d	401	PHO	C3D-C4D	2.99	1.45	1.41
22	a	402	CLA	C1B-C2B	2.99	1.50	1.43
22	B	607	CLA	MG-NC	2.99	2.13	2.06
27	d	406	PL9	C16-C14	-2.98	1.45	1.51
22	B	616	CLA	CMC-C2C	-2.98	1.44	1.50
22	b	601	CLA	C1D-ND	2.97	1.41	1.37
22	B	609	CLA	C1B-NB	-2.97	1.34	1.37
22	B	601	CLA	C1B-C2B	2.97	1.50	1.43
29	f	101	SQD	O48-C23	2.96	1.42	1.33
22	B	606	CLA	C1D-ND	2.96	1.41	1.37
22	b	609	CLA	C4B-NB	2.96	1.41	1.37
28	b	624	LMG	O1-C7	-2.95	1.38	1.43
22	c	508	CLA	C3B-C4B	2.94	1.51	1.42
24	a	405	BCR	C1-C6	-2.94	1.50	1.53
31	c	517	DGD	O2G-C2G	-2.94	1.39	1.46
22	b	607	CLA	C1D-ND	2.94	1.41	1.37
22	C	510	CLA	C1B-C2B	2.94	1.50	1.43
22	B	612	CLA	C4B-NB	2.93	1.41	1.37
22	A	402	CLA	C4B-NB	2.93	1.41	1.37
22	B	601	CLA	C4B-NB	2.92	1.41	1.37
22	b	609	CLA	CMB-C2B	-2.92	1.44	1.50
22	b	613	CLA	CMD-C2D	-2.92	1.44	1.50
31	c	516	DGD	O3G-C1D	-2.92	1.35	1.40
22	C	505	CLA	CHC-C1C	2.92	1.44	1.38
29	f	101	SQD	O47-C7	2.92	1.42	1.34
22	C	506	CLA	C1D-ND	2.91	1.41	1.37
28	c	521	LMG	C3-C2	2.91	1.59	1.52
22	B	609	CLA	CMD-C2D	-2.91	1.44	1.50
29	a	411	SQD	O47-C7	2.91	1.42	1.34
22	B	609	CLA	C1D-ND	2.91	1.41	1.37
24	K	102	BCR	C1-C6	-2.90	1.50	1.53
22	C	508	CLA	C1B-C2B	2.90	1.49	1.43
22	C	511	CLA	C1B-C2B	2.90	1.49	1.43
30	d	408	LHG	O8-C6	-2.89	1.38	1.45
22	c	506	CLA	CMD-C2D	-2.89	1.44	1.50
22	B	613	CLA	C1D-ND	2.89	1.41	1.37
35	e	101	HEM	C3B-C2B	-2.89	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CMC-C2C	-2.89	1.44	1.50
22	B	615	CLA	C1B-C2B	2.89	1.49	1.43
22	C	508	CLA	C3B-C4B	2.88	1.51	1.42
22	b	605	CLA	CMD-C2D	-2.88	1.44	1.50
28	C	518	LMG	O8-C9	-2.88	1.38	1.45
22	A	405	CLA	C4B-NB	2.88	1.41	1.37
22	a	410	CLA	C4B-NB	2.87	1.41	1.37
22	C	501	CLA	C3B-C4B	2.87	1.51	1.42
23	D	401	PHO	CAC-C3C	-2.87	1.46	1.51
22	c	503	CLA	C1D-ND	2.87	1.41	1.37
28	b	624	LMG	C3-C2	2.85	1.59	1.52
29	B	623	SQD	O48-C23	2.85	1.41	1.33
22	b	602	CLA	C1D-ND	2.85	1.41	1.37
22	b	614	CLA	CMC-C2C	-2.85	1.44	1.50
22	b	615	CLA	MG-ND	-2.84	2.00	2.05
28	c	519	LMG	C1-C2	2.84	1.60	1.52
22	C	503	CLA	CMD-C2D	-2.84	1.45	1.50
22	B	607	CLA	MG-ND	-2.83	2.00	2.05
22	C	501	CLA	C4B-NB	2.83	1.41	1.37
22	B	606	CLA	CMD-C2D	-2.83	1.45	1.50
22	a	402	CLA	C3B-C4B	2.83	1.51	1.42
22	a	403	CLA	C4B-NB	2.83	1.41	1.37
22	c	512	CLA	MG-NC	2.83	2.13	2.06
28	C	518	LMG	O7-C8	-2.82	1.40	1.46
22	C	507	CLA	C1B-NB	-2.82	1.34	1.37
24	T	101	BCR	C1-C6	-2.82	1.50	1.53
24	D	404	BCR	C1-C6	-2.81	1.50	1.53
22	c	510	CLA	CMB-C2B	-2.81	1.45	1.50
22	c	509	CLA	C4B-NB	2.81	1.41	1.37
27	a	409	PL9	C53-C6	-2.80	1.45	1.50
30	B	621	LHG	O8-C6	-2.80	1.38	1.45
28	A	412	LMG	C4-C3	2.80	1.59	1.52
22	c	505	CLA	C3B-C4B	2.80	1.50	1.42
22	B	615	CLA	C4B-NB	2.79	1.41	1.37
35	e	101	HEM	CAC-C3C	2.79	1.54	1.47
30	D	409	LHG	C8-C7	-2.79	1.42	1.50
22	A	403	CLA	C1D-ND	2.78	1.41	1.37
22	B	610	CLA	C4B-NB	2.78	1.41	1.37
22	C	505	CLA	C4B-NB	2.78	1.41	1.37
22	C	508	CLA	C4B-NB	2.78	1.41	1.37
22	a	410	CLA	CMB-C2B	-2.78	1.45	1.50
31	C	516	DGD	C6E-C5E	2.77	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1D-C2D	2.77	1.42	1.39
22	c	506	CLA	C1B-NB	-2.77	1.34	1.37
27	A	410	PL9	C3-C4	-2.77	1.45	1.49
27	D	405	PL9	C53-C6	-2.77	1.45	1.50
22	a	403	CLA	C1B-NB	-2.77	1.34	1.37
36	v	201	HEC	FE-NC	2.77	2.04	1.95
22	B	612	CLA	C1B-C2B	2.77	1.49	1.43
31	C	516	DGD	C1E-C2E	2.76	1.60	1.52
22	b	602	CLA	C1B-C2B	2.76	1.49	1.43
22	B	607	CLA	MG-NA	2.76	2.12	2.06
22	b	615	CLA	C3B-C4B	2.76	1.50	1.42
22	B	612	CLA	C1B-NB	-2.76	1.34	1.37
28	c	519	LMG	C3-C2	2.76	1.59	1.52
22	a	403	CLA	C1D-ND	2.76	1.41	1.37
27	D	405	PL9	C36-C34	-2.76	1.45	1.51
22	b	606	CLA	MG-NC	2.76	2.12	2.06
28	c	522	LMG	O1-C7	-2.75	1.39	1.43
22	b	608	CLA	C1B-C2B	2.75	1.49	1.43
23	d	402	PHO	C4D-ND	-2.75	1.34	1.38
27	A	410	PL9	C31-C29	-2.75	1.45	1.51
22	b	612	CLA	CMC-C2C	-2.75	1.45	1.50
22	a	410	CLA	C1B-C2B	2.75	1.49	1.43
22	C	507	CLA	C4B-NB	2.74	1.41	1.37
28	M	101	LMG	O4-C4	-2.74	1.36	1.43
22	C	506	CLA	C4B-NB	2.73	1.41	1.37
22	c	508	CLA	CHC-C1C	2.73	1.44	1.38
22	C	503	CLA	C1D-ND	2.73	1.41	1.37
22	c	502	CLA	C1B-C2B	2.73	1.49	1.43
22	A	411	CLA	C1B-NB	-2.73	1.34	1.37
22	c	513	CLA	C3B-C4B	2.73	1.50	1.42
22	B	610	CLA	C1D-ND	2.72	1.41	1.37
22	c	510	CLA	C1B-C2B	2.72	1.49	1.43
22	C	511	CLA	CMB-C2B	-2.72	1.45	1.50
22	C	510	CLA	CMC-C2C	-2.72	1.45	1.50
31	c	517	DGD	O3G-C3G	-2.71	1.39	1.43
22	b	602	CLA	C4B-NB	2.71	1.41	1.37
22	d	403	CLA	C1D-ND	2.71	1.41	1.37
22	B	602	CLA	MG-NC	-2.70	1.99	2.06
30	e	102	LHG	O8-C23	2.69	1.41	1.33
27	D	405	PL9	C3-C4	-2.68	1.45	1.49
23	d	401	PHO	C4D-CHA	2.68	1.43	1.39
22	b	608	CLA	CHC-C1C	2.68	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	CHC-C1C	2.68	1.43	1.38
31	c	518	DGD	C6D-C5D	2.68	1.59	1.51
22	A	402	CLA	O2D-CED	-2.68	1.39	1.45
31	C	517	DGD	O2G-C2G	-2.67	1.40	1.46
30	A	414	LHG	C24-C23	2.67	1.58	1.50
22	B	608	CLA	C1B-C2B	2.67	1.49	1.43
22	C	513	CLA	C1B-C2B	2.66	1.49	1.43
22	B	613	CLA	CHC-C1C	2.66	1.43	1.38
22	d	404	CLA	C4B-NB	2.66	1.41	1.37
22	b	608	CLA	C4B-NB	2.66	1.41	1.37
22	C	503	CLA	C1B-C2B	2.66	1.49	1.43
22	c	511	CLA	C1B-C2B	2.65	1.49	1.43
22	d	403	CLA	C4B-NB	2.65	1.41	1.37
29	A	413	SQD	O2-C2	-2.65	1.36	1.43
24	T	101	BCR	C27-C26	-2.65	1.46	1.51
22	B	610	CLA	CMB-C2B	-2.65	1.45	1.50
24	k	102	BCR	C1-C6	-2.65	1.50	1.53
35	F	101	HEM	CAB-C3B	2.65	1.54	1.47
27	D	405	PL9	C46-C44	-2.64	1.45	1.51
22	B	613	CLA	CMD-C2D	-2.63	1.45	1.50
31	h	101	DGD	C4D-C3D	2.63	1.59	1.52
22	A	405	CLA	CMD-C2D	-2.63	1.45	1.50
22	B	605	CLA	CMD-C2D	-2.63	1.45	1.50
31	A	416	DGD	C4D-C5D	2.62	1.58	1.53
22	b	613	CLA	C1B-NB	-2.62	1.34	1.37
22	b	615	CLA	C1B-C2B	2.62	1.49	1.43
31	h	101	DGD	C4E-C5E	2.62	1.58	1.53
29	A	415	SQD	O47-C45	-2.62	1.42	1.47
36	v	201	HEC	CMA-C3A	2.62	1.56	1.50
35	e	101	HEM	CAB-C3B	2.62	1.54	1.47
22	C	505	CLA	C1D-ND	2.61	1.41	1.37
22	A	411	CLA	CMD-C2D	-2.61	1.45	1.50
22	a	404	CLA	C1B-C2B	2.61	1.49	1.43
22	C	505	CLA	CMC-C2C	-2.61	1.45	1.50
22	B	611	CLA	C1B-NB	-2.61	1.34	1.37
22	c	512	CLA	CMB-C2B	-2.61	1.45	1.50
22	A	411	CLA	C1B-C2B	2.61	1.49	1.43
22	B	606	CLA	C1B-C2B	2.61	1.49	1.43
22	B	610	CLA	C3B-C4B	2.61	1.50	1.42
22	b	603	CLA	MG-NB	-2.60	2.00	2.05
22	C	510	CLA	C4B-NB	2.60	1.41	1.37
22	C	511	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	MG-NC	2.60	2.12	2.06
22	b	612	CLA	CMD-C2D	-2.59	1.45	1.50
30	A	414	LHG	P-O6	2.59	1.69	1.59
22	b	606	CLA	C3B-C4B	2.59	1.50	1.42
28	b	622	LMG	C4-C3	2.59	1.59	1.52
31	c	516	DGD	O6E-C5E	-2.59	1.38	1.44
24	C	514	BCR	C36-C18	-2.58	1.45	1.50
22	c	513	CLA	C4B-NB	2.58	1.41	1.37
22	b	612	CLA	C1B-C2B	2.58	1.49	1.43
35	e	101	HEM	FE-NA	2.58	2.03	1.95
22	B	610	CLA	CMC-C2C	-2.58	1.45	1.50
28	b	622	LMG	C4-C5	2.58	1.58	1.53
22	c	507	CLA	C1B-C2B	2.58	1.49	1.43
28	c	519	LMG	C7-C8	2.57	1.58	1.50
24	b	618	BCR	C38-C26	-2.57	1.46	1.50
22	B	609	CLA	MG-NA	2.57	2.12	2.06
22	B	605	CLA	C3B-C4B	2.57	1.50	1.42
22	c	511	CLA	MG-ND	-2.57	2.00	2.05
22	d	403	CLA	CMD-C2D	-2.57	1.45	1.50
22	c	506	CLA	C1B-C2B	2.57	1.49	1.43
22	C	509	CLA	CMC-C2C	-2.56	1.45	1.50
22	c	504	CLA	MG-NA	-2.56	2.00	2.06
22	b	608	CLA	C3B-C4B	2.56	1.50	1.42
28	c	519	LMG	C4-C5	2.56	1.58	1.53
22	c	501	CLA	C4B-NB	2.55	1.41	1.37
22	c	503	CLA	C4B-NB	2.55	1.41	1.37
22	b	604	CLA	CMC-C2C	-2.55	1.45	1.50
22	B	615	CLA	MG-NA	2.55	2.12	2.06
31	c	518	DGD	O3D-C3D	-2.55	1.36	1.43
22	A	403	CLA	C1B-C2B	2.55	1.49	1.43
22	C	504	CLA	C1D-ND	2.55	1.41	1.37
22	b	603	CLA	CMD-C2D	-2.55	1.45	1.50
22	d	403	CLA	CMB-C2B	-2.54	1.45	1.50
23	d	402	PHO	CAC-C3C	-2.54	1.47	1.51
23	d	402	PHO	CMD-C2D	-2.54	1.46	1.51
22	C	511	CLA	C3B-C4B	2.54	1.50	1.42
22	D	403	CLA	C1B-C2B	2.53	1.49	1.43
22	c	512	CLA	C1B-C2B	2.53	1.49	1.43
22	D	402	CLA	C4B-NB	2.52	1.41	1.37
31	h	101	DGD	O2G-C1B	2.52	1.41	1.34
22	c	509	CLA	C1B-C2B	2.52	1.49	1.43
22	c	512	CLA	C1B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	517	DGD	O3G-C3G	-2.52	1.39	1.43
22	a	402	CLA	CMB-C2B	-2.52	1.45	1.50
22	B	602	CLA	C4B-NB	2.51	1.41	1.37
29	A	413	SQD	O48-C23	2.51	1.40	1.33
31	A	416	DGD	C1E-C2E	2.51	1.59	1.52
22	c	503	CLA	MG-ND	-2.51	2.00	2.05
22	B	604	CLA	MG-NB	2.51	2.10	2.05
22	b	607	CLA	C1B-C2B	2.51	1.49	1.43
22	b	606	CLA	C1B-C2B	2.51	1.49	1.43
22	C	512	CLA	C3B-C4B	2.51	1.50	1.42
29	A	413	SQD	O47-C7	2.50	1.41	1.34
31	A	416	DGD	O2G-C1B	2.50	1.41	1.34
22	b	606	CLA	CMD-C2D	-2.50	1.45	1.50
22	b	614	CLA	CHC-C1C	2.50	1.43	1.38
31	h	101	DGD	O2D-C2D	-2.50	1.36	1.43
22	B	611	CLA	CMB-C2B	-2.50	1.45	1.50
28	M	101	LMG	O7-C8	-2.50	1.40	1.46
22	C	512	CLA	CMB-C2B	-2.50	1.45	1.50
22	C	507	CLA	C1D-ND	2.50	1.41	1.37
22	c	513	CLA	CMB-C2B	-2.50	1.45	1.50
22	B	611	CLA	C1B-C2B	2.50	1.49	1.43
22	C	506	CLA	C1B-C2B	2.50	1.49	1.43
22	c	503	CLA	CMC-C2C	-2.50	1.45	1.50
22	B	616	CLA	C1B-C2B	2.49	1.49	1.43
22	C	506	CLA	CMA-C3A	-2.49	1.47	1.53
22	C	512	CLA	C1B-C2B	2.49	1.49	1.43
22	b	611	CLA	C1B-C2B	2.49	1.49	1.43
31	A	416	DGD	O5D-C6D	-2.48	1.39	1.43
24	b	617	BCR	C33-C5	-2.48	1.47	1.50
22	C	510	CLA	C3B-C4B	2.48	1.50	1.42
22	b	607	CLA	CHD-C1D	-2.48	1.33	1.38
22	b	607	CLA	C1B-NB	-2.48	1.34	1.37
24	B	618	BCR	C1-C6	-2.48	1.50	1.53
22	C	512	CLA	CMD-C2D	-2.48	1.45	1.50
22	B	607	CLA	CMB-C2B	-2.48	1.45	1.50
22	C	508	CLA	CMD-C2D	-2.48	1.45	1.50
22	C	511	CLA	CHC-C1C	2.47	1.43	1.38
22	c	513	CLA	CHC-C1C	2.47	1.43	1.38
31	H	102	DGD	C6E-C5E	2.47	1.60	1.51
22	C	504	CLA	CHC-C1C	2.47	1.43	1.38
27	a	409	PL9	C25-C24	-2.47	1.44	1.50
22	C	503	CLA	C4B-NB	2.47	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	404	CLA	MG-NC	2.47	2.12	2.06
22	b	605	CLA	CHC-C1C	2.47	1.43	1.38
22	b	603	CLA	C1B-NB	-2.47	1.34	1.37
22	C	513	CLA	C3B-C4B	2.47	1.49	1.42
22	B	605	CLA	C1B-C2B	2.47	1.48	1.43
22	d	404	CLA	CMC-C2C	-2.46	1.45	1.50
22	B	607	CLA	CMC-C2C	-2.45	1.45	1.50
22	C	510	CLA	CMD-C2D	-2.45	1.45	1.50
22	b	604	CLA	C4B-NB	2.45	1.41	1.37
22	B	603	CLA	C1B-C2B	2.45	1.48	1.43
35	e	101	HEM	C2A-C3A	-2.45	1.32	1.38
22	b	611	CLA	C1D-ND	2.45	1.41	1.37
22	B	604	CLA	C3B-C4B	2.44	1.49	1.42
28	M	101	LMG	C4-C5	2.44	1.58	1.53
22	C	508	CLA	C1D-C2D	2.44	1.50	1.45
22	d	404	CLA	CMB-C2B	-2.43	1.45	1.50
22	B	602	CLA	CMB-C2B	-2.43	1.45	1.50
22	b	608	CLA	CMD-C2D	-2.43	1.45	1.50
22	b	602	CLA	CAC-C3C	-2.43	1.44	1.51
28	c	521	LMG	C4-C3	2.43	1.58	1.52
30	d	407	LHG	C24-C23	2.43	1.57	1.50
22	c	504	CLA	CAC-C3C	-2.43	1.44	1.51
29	B	623	SQD	O2-C2	-2.43	1.36	1.43
22	C	510	CLA	C1B-NB	-2.42	1.34	1.37
31	H	102	DGD	C4D-C5D	2.42	1.58	1.53
22	c	505	CLA	CMB-C2B	-2.42	1.45	1.50
22	b	616	CLA	CAB-C3B	-2.42	1.40	1.47
22	c	513	CLA	CMC-C2C	-2.42	1.45	1.50
35	F	101	HEM	CAC-C3C	2.42	1.53	1.47
22	c	509	CLA	CMB-C2B	-2.41	1.45	1.50
31	c	516	DGD	O4D-C4D	-2.41	1.37	1.43
28	D	410	LMG	C9-C8	2.41	1.58	1.50
22	c	508	CLA	CMC-C2C	-2.41	1.45	1.50
29	f	101	SQD	O3-C3	-2.40	1.37	1.43
22	C	509	CLA	CMD-C2D	-2.40	1.45	1.50
24	K	101	BCR	C33-C5	-2.40	1.47	1.50
35	F	101	HEM	FE-NB	2.40	2.02	1.94
36	V	201	HEC	CAC-C3C	2.40	1.57	1.51
22	c	502	CLA	CMC-C2C	-2.40	1.45	1.50
22	c	503	CLA	C1B-C2B	2.40	1.48	1.43
28	b	622	LMG	O6-C1	2.39	1.48	1.41
31	H	102	DGD	O6E-C1E	2.39	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C1B-C2B	2.39	1.48	1.43
22	C	513	CLA	CMB-C2B	-2.39	1.45	1.50
22	b	607	CLA	CMC-C2C	-2.39	1.45	1.50
22	B	614	CLA	MG-NA	2.39	2.11	2.06
31	C	517	DGD	C4D-C3D	2.38	1.58	1.52
22	B	609	CLA	C1B-C2B	2.38	1.48	1.43
22	b	609	CLA	CAC-C3C	-2.38	1.45	1.51
22	b	613	CLA	MG-NC	-2.38	2.00	2.06
22	a	403	CLA	CMD-C2D	-2.38	1.45	1.50
31	H	102	DGD	C4D-C3D	2.38	1.58	1.52
22	b	611	CLA	CMD-C2D	-2.38	1.45	1.50
31	c	516	DGD	O1G-C1A	2.37	1.40	1.33
22	c	510	CLA	MG-NB	2.37	2.10	2.05
22	b	601	CLA	CHC-C1C	2.37	1.43	1.38
31	C	515	DGD	C2A-C1A	-2.37	1.43	1.50
22	A	411	CLA	C3B-C4B	2.37	1.49	1.42
22	b	605	CLA	C3B-C4B	2.37	1.49	1.42
22	A	402	CLA	MG-ND	-2.37	2.01	2.05
29	f	101	SQD	O2-C2	-2.36	1.37	1.43
22	B	605	CLA	CHC-C1C	2.36	1.43	1.38
27	A	410	PL9	C53-C6	-2.36	1.45	1.50
23	d	402	PHO	CMC-C2C	-2.36	1.46	1.50
22	B	614	CLA	CHC-C1C	2.35	1.43	1.38
22	B	602	CLA	C1B-NB	-2.35	1.34	1.37
22	D	403	CLA	CMC-C2C	-2.35	1.46	1.50
22	b	605	CLA	MG-NA	2.35	2.11	2.06
22	c	501	CLA	CMD-C2D	-2.35	1.46	1.50
30	e	102	LHG	O7-C5	-2.34	1.41	1.46
22	C	510	CLA	CHC-C1C	2.34	1.43	1.38
22	B	613	CLA	C1B-C2B	2.34	1.48	1.43
22	B	612	CLA	C3B-C4B	2.34	1.49	1.42
30	d	408	LHG	C1-C2	-2.34	1.42	1.51
22	B	607	CLA	C4B-NB	2.34	1.40	1.37
24	a	405	BCR	C38-C26	-2.34	1.47	1.50
22	C	502	CLA	C1B-C2B	2.34	1.48	1.43
22	b	610	CLA	C1B-C2B	2.34	1.48	1.43
22	b	611	CLA	C3B-C4B	2.33	1.49	1.42
22	B	613	CLA	C1B-NB	-2.33	1.34	1.37
22	D	402	CLA	CAA-C2A	-2.33	1.49	1.54
22	d	404	CLA	C1B-C2B	2.33	1.48	1.43
35	e	101	HEM	CMC-C2C	2.33	1.55	1.50
24	B	617	BCR	C33-C5	-2.33	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	MG-ND	-2.33	2.01	2.05
27	a	409	PL9	C30-C29	-2.33	1.45	1.50
23	A	404	PHO	CMB-C2B	-2.33	1.47	1.51
22	C	504	CLA	CMD-C2D	-2.33	1.46	1.50
22	B	615	CLA	MG-ND	2.32	2.10	2.05
24	A	406	BCR	C33-C5	-2.32	1.47	1.50
22	b	612	CLA	CMB-C2B	-2.32	1.46	1.50
22	B	603	CLA	CMD-C2D	-2.32	1.46	1.50
22	B	611	CLA	CMD-C2D	-2.32	1.46	1.50
22	C	509	CLA	C1B-NB	-2.32	1.34	1.37
22	C	508	CLA	CMB-C2B	-2.31	1.46	1.50
22	B	611	CLA	C1D-ND	2.31	1.40	1.37
22	C	508	CLA	C1D-ND	2.31	1.40	1.37
29	D	407	SQD	O2-C2	-2.31	1.37	1.43
22	B	604	CLA	O2D-CGD	2.30	1.38	1.33
22	b	604	CLA	C1B-C2B	2.30	1.48	1.43
22	C	512	CLA	C1D-ND	2.30	1.40	1.37
22	A	405	CLA	CMB-C2B	-2.30	1.46	1.50
22	c	512	CLA	CMC-C2C	-2.30	1.46	1.50
30	D	408	LHG	C8-C7	-2.30	1.44	1.50
22	C	512	CLA	CMC-C2C	-2.30	1.46	1.50
22	B	608	CLA	C1B-NB	-2.30	1.34	1.37
22	c	502	CLA	C3B-C4B	2.30	1.49	1.42
22	a	403	CLA	CHC-C1C	2.30	1.43	1.38
22	b	607	CLA	C3B-C4B	2.30	1.49	1.42
22	C	508	CLA	CHC-C1C	2.30	1.43	1.38
22	c	511	CLA	C1D-ND	2.29	1.40	1.37
24	x	101	BCR	C33-C5	-2.29	1.47	1.50
22	b	613	CLA	CMB-C2B	-2.29	1.46	1.50
22	C	504	CLA	CMB-C2B	-2.29	1.46	1.50
22	c	512	CLA	CHC-C1C	2.29	1.43	1.38
23	d	401	PHO	O2D-CGD	2.29	1.38	1.33
22	C	504	CLA	C3B-C4B	2.29	1.49	1.42
28	C	518	LMG	O1-C7	-2.29	1.39	1.43
22	b	601	CLA	MG-NB	2.28	2.10	2.05
31	c	516	DGD	O2E-C2E	-2.28	1.37	1.43
22	B	613	CLA	MG-NB	-2.28	2.01	2.05
22	b	616	CLA	CMC-C2C	-2.28	1.46	1.50
22	C	502	CLA	CHC-C1C	2.28	1.43	1.38
23	d	402	PHO	C3D-C4D	2.28	1.44	1.41
22	b	608	CLA	CMB-C2B	-2.28	1.46	1.50
31	c	516	DGD	C3G-C2G	2.28	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	CAA-C2A	-2.28	1.49	1.54
22	B	603	CLA	C3B-C4B	2.28	1.49	1.42
22	A	402	CLA	CMC-C2C	-2.27	1.46	1.50
22	b	601	CLA	C3B-C4B	2.27	1.49	1.42
22	A	405	CLA	MG-NA	-2.27	2.00	2.06
22	c	511	CLA	C3B-C4B	2.26	1.49	1.42
24	K	102	BCR	C27-C26	-2.26	1.46	1.51
22	A	403	CLA	MG-NA	-2.26	2.00	2.06
29	a	411	SQD	O2-C2	-2.26	1.37	1.43
23	D	401	PHO	CMD-C2D	-2.26	1.47	1.51
22	a	404	CLA	CAC-C3C	-2.26	1.45	1.51
22	b	616	CLA	CMD-C2D	-2.26	1.46	1.50
22	B	612	CLA	C1D-ND	2.26	1.40	1.37
22	A	403	CLA	C4B-NB	2.25	1.40	1.37
22	C	513	CLA	CHC-C1C	2.25	1.43	1.38
22	B	603	CLA	MG-ND	2.25	2.10	2.05
22	C	503	CLA	C3B-C4B	2.25	1.49	1.42
22	C	503	CLA	CMC-C2C	-2.25	1.46	1.50
22	C	511	CLA	C1B-NB	-2.25	1.34	1.37
22	b	616	CLA	CMB-C2B	-2.25	1.46	1.50
22	c	503	CLA	MG-NA	2.25	2.11	2.06
27	d	406	PL9	C25-C24	-2.25	1.45	1.50
22	C	506	CLA	CHC-C1C	2.25	1.43	1.38
22	B	612	CLA	CMC-C2C	-2.25	1.46	1.50
22	b	613	CLA	C1D-ND	2.24	1.40	1.37
22	b	614	CLA	C3B-C4B	2.24	1.49	1.42
30	B	622	LHG	C24-C23	2.24	1.57	1.50
22	C	507	CLA	C3B-C4B	2.24	1.49	1.42
22	B	609	CLA	C4B-NB	2.24	1.40	1.37
22	B	603	CLA	CHC-C1C	2.24	1.43	1.38
22	b	609	CLA	C1B-C2B	2.23	1.48	1.43
31	c	516	DGD	O6D-C1D	2.23	1.47	1.41
31	C	516	DGD	C6D-C5D	2.23	1.58	1.51
22	B	615	CLA	C1B-NB	-2.23	1.34	1.37
31	C	516	DGD	O5D-C1E	2.23	1.43	1.40
22	B	605	CLA	MG-NB	2.23	2.10	2.05
22	C	503	CLA	CMB-C2B	-2.23	1.46	1.50
28	A	412	LMG	O7-C8	-2.23	1.41	1.46
22	b	601	CLA	C4B-NB	2.23	1.40	1.37
22	C	501	CLA	CMD-C2D	-2.23	1.46	1.50
23	D	401	PHO	CMC-C2C	-2.23	1.47	1.50
22	b	616	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	416	DGD	C3D-C2D	2.22	1.58	1.52
22	c	501	CLA	CAC-C3C	-2.22	1.45	1.51
22	B	605	CLA	C1B-NB	-2.22	1.34	1.37
22	c	508	CLA	C1B-C2B	2.22	1.48	1.43
23	A	404	PHO	C3B-C2B	-2.22	1.37	1.40
22	B	602	CLA	C1D-C2D	2.22	1.49	1.45
24	B	619	BCR	C38-C26	-2.22	1.47	1.50
22	b	603	CLA	C1D-ND	2.22	1.40	1.37
28	a	416	LMG	O7-C10	2.22	1.40	1.34
22	a	403	CLA	C1B-C2B	2.22	1.48	1.43
22	b	606	CLA	CHC-C4B	-2.21	1.34	1.39
22	B	613	CLA	CMB-C2B	-2.21	1.46	1.50
22	b	602	CLA	CMD-C2D	-2.21	1.46	1.50
22	C	504	CLA	C1B-NB	-2.21	1.35	1.37
22	B	614	CLA	C1B-C2B	2.21	1.48	1.43
22	C	504	CLA	C1B-C2B	2.21	1.48	1.43
22	D	403	CLA	C3B-C4B	2.21	1.49	1.42
23	d	401	PHO	CMC-C2C	-2.20	1.47	1.50
22	A	402	CLA	C3B-C4B	2.20	1.49	1.42
31	A	416	DGD	O1G-C1G	-2.20	1.40	1.45
29	b	620	SQD	O2-C2	-2.20	1.37	1.43
30	A	414	LHG	O7-C5	-2.20	1.41	1.46
22	B	608	CLA	C3B-C4B	2.20	1.49	1.42
31	c	516	DGD	O5D-C6D	2.20	1.47	1.43
22	B	613	CLA	C3B-C4B	2.20	1.49	1.42
22	d	403	CLA	CMC-C2C	-2.20	1.46	1.50
24	b	617	BCR	C4-C5	-2.19	1.46	1.51
22	B	611	CLA	MG-NC	-2.19	2.01	2.06
22	C	501	CLA	CHC-C1C	2.19	1.42	1.38
22	c	505	CLA	C1B-C2B	2.19	1.48	1.43
22	C	506	CLA	CMC-C2C	-2.19	1.46	1.50
22	b	615	CLA	CHC-C1C	2.19	1.42	1.38
28	M	101	LMG	O7-C10	2.19	1.40	1.34
22	c	510	CLA	C3B-C4B	2.19	1.49	1.42
22	c	511	CLA	C1B-NB	-2.19	1.35	1.37
22	C	502	CLA	CMB-C2B	-2.19	1.46	1.50
28	M	101	LMG	O1-C7	-2.19	1.40	1.43
22	b	605	CLA	MG-ND	2.18	2.10	2.05
22	A	403	CLA	C3B-C4B	2.18	1.49	1.42
22	D	403	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	612	CLA	C3B-C4B	2.18	1.49	1.42
22	A	403	CLA	C1B-NB	-2.18	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C1B-C2B	2.18	1.48	1.43
22	B	610	CLA	CHC-C1C	2.18	1.42	1.38
22	c	501	CLA	C1B-NB	-2.18	1.35	1.37
22	c	504	CLA	C3B-C4B	2.17	1.49	1.42
22	c	511	CLA	CHC-C1C	2.17	1.42	1.38
22	c	506	CLA	CAC-C3C	-2.17	1.45	1.51
35	F	101	HEM	C2A-C3A	-2.17	1.33	1.38
22	C	506	CLA	C3B-C4B	2.17	1.49	1.42
22	C	511	CLA	MG-NC	-2.17	2.01	2.06
28	D	406	LMG	O7-C8	-2.17	1.41	1.46
30	D	409	LHG	O3-C3	-2.17	1.36	1.44
29	a	411	SQD	O3-C3	-2.17	1.37	1.43
22	c	511	CLA	C4B-NB	2.17	1.40	1.37
31	c	517	DGD	O5D-C6D	-2.17	1.40	1.43
22	B	607	CLA	C3B-C4B	2.16	1.49	1.42
24	T	101	BCR	C38-C26	-2.16	1.47	1.50
22	C	510	CLA	CMB-C2B	-2.16	1.46	1.50
22	B	615	CLA	CMB-C2B	-2.16	1.46	1.50
22	C	511	CLA	CMC-C2C	-2.16	1.46	1.50
22	b	610	CLA	CMB-C2B	-2.16	1.46	1.50
28	D	406	LMG	C4-C3	2.16	1.57	1.52
22	B	616	CLA	CMD-C2D	-2.15	1.46	1.50
22	b	609	CLA	C1B-NB	-2.15	1.35	1.37
22	A	403	CLA	CMD-C2D	-2.15	1.46	1.50
22	b	602	CLA	CMC-C2C	-2.15	1.46	1.50
22	C	510	CLA	CAA-C2A	-2.15	1.50	1.54
23	d	401	PHO	C4D-ND	-2.15	1.35	1.38
22	b	602	CLA	CMB-C2B	-2.15	1.46	1.50
22	b	616	CLA	C3D-C4D	2.15	1.49	1.44
22	B	608	CLA	MG-NA	2.15	2.11	2.06
22	D	403	CLA	CHC-C4B	-2.15	1.34	1.39
23	d	402	PHO	CMB-C2B	-2.14	1.47	1.51
22	A	402	CLA	C1B-NB	-2.14	1.35	1.37
30	B	622	LHG	P-O4	-2.14	1.45	1.55
22	c	508	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	411	CLA	CMB-C2B	-2.14	1.46	1.50
22	B	616	CLA	C1D-ND	2.14	1.40	1.37
22	c	512	CLA	C3D-C4D	2.14	1.49	1.44
22	C	503	CLA	C1D-C2D	2.13	1.49	1.45
28	c	521	LMG	C7-C8	2.13	1.57	1.50
22	A	411	CLA	CAC-C3C	-2.13	1.45	1.51
22	c	501	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	O2D-CGD	2.13	1.38	1.33
24	k	101	BCR	C33-C5	-2.13	1.47	1.50
22	c	506	CLA	CHC-C1C	2.13	1.42	1.38
24	B	618	BCR	C27-C26	-2.13	1.47	1.51
22	A	405	CLA	MG-NB	-2.13	2.01	2.05
22	c	506	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	615	CLA	MG-NC	-2.12	2.01	2.06
22	A	405	CLA	C1B-NB	-2.12	1.35	1.37
28	b	622	LMG	C6-C5	2.12	1.58	1.51
30	e	102	LHG	C4-C5	2.12	1.57	1.50
22	d	403	CLA	C1B-C2B	2.12	1.48	1.43
22	B	614	CLA	CMC-C2C	-2.12	1.46	1.50
22	c	505	CLA	CMC-C2C	-2.12	1.46	1.50
22	a	404	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	611	CLA	C3B-C4B	2.12	1.48	1.42
28	C	518	LMG	C1-C2	2.11	1.58	1.52
22	b	602	CLA	MG-NC	2.11	2.11	2.06
22	b	613	CLA	CMC-C2C	-2.11	1.46	1.50
22	b	612	CLA	C1B-NB	-2.11	1.35	1.37
22	B	603	CLA	CAB-C3B	-2.11	1.41	1.47
22	b	606	CLA	O1D-CGD	2.11	1.26	1.21
22	b	605	CLA	C4B-NB	2.11	1.40	1.37
22	b	615	CLA	CMC-C2C	-2.11	1.46	1.50
31	H	102	DGD	O2D-C2D	-2.11	1.37	1.43
22	A	411	CLA	C4B-NB	2.10	1.40	1.37
22	B	608	CLA	CMC-C2C	-2.10	1.46	1.50
29	f	101	SQD	O4-C4	-2.10	1.37	1.43
22	B	601	CLA	CMB-C2B	-2.10	1.46	1.50
22	B	615	CLA	CAC-C3C	-2.10	1.45	1.51
22	B	607	CLA	C1B-C2B	2.10	1.48	1.43
22	B	609	CLA	CAB-C3B	-2.10	1.41	1.47
22	C	503	CLA	C3D-C4D	2.10	1.48	1.44
22	b	609	CLA	CMD-C2D	-2.09	1.46	1.50
22	a	404	CLA	C3B-C4B	2.09	1.48	1.42
22	B	601	CLA	CMC-C2C	-2.09	1.46	1.50
22	D	403	CLA	C3D-C4D	2.09	1.48	1.44
22	A	405	CLA	C1B-C2B	2.09	1.48	1.43
22	B	615	CLA	C3D-C4D	2.09	1.48	1.44
22	b	614	CLA	MG-NA	2.09	2.11	2.06
22	b	604	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	605	CLA	CMC-C2C	-2.09	1.46	1.50
22	C	512	CLA	C4B-NB	2.08	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	CMD-C2D	-2.08	1.47	1.51
22	C	503	CLA	CHC-C1C	2.08	1.42	1.38
24	t	101	BCR	C33-C5	-2.08	1.47	1.50
22	b	606	CLA	CAC-C3C	-2.08	1.45	1.51
22	A	403	CLA	CMC-C2C	-2.08	1.46	1.50
31	C	517	DGD	O1G-C1G	-2.07	1.40	1.45
23	A	404	PHO	CMD-C2D	-2.07	1.47	1.51
24	x	101	BCR	C1-C6	-2.07	1.51	1.53
22	b	602	CLA	CHC-C4B	-2.07	1.34	1.39
31	C	516	DGD	C1G-C2G	2.07	1.57	1.50
28	a	416	LMG	C14-C13	2.07	1.62	1.51
22	a	402	CLA	MG-ND	-2.07	2.01	2.05
29	A	413	SQD	O47-C45	-2.07	1.41	1.46
22	c	503	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	613	CLA	C5-C3	-2.07	1.47	1.51
22	D	402	CLA	C1B-C2B	2.06	1.48	1.43
24	C	514	BCR	C27-C26	-2.06	1.47	1.51
22	d	404	CLA	CHC-C4B	-2.06	1.34	1.39
22	c	508	CLA	MG-NB	2.06	2.09	2.05
22	B	606	CLA	CHC-C1C	2.06	1.42	1.38
28	M	101	LMG	C9-C8	2.06	1.57	1.50
22	B	616	CLA	C3B-C4B	2.06	1.48	1.42
31	c	517	DGD	C6E-C5E	2.05	1.58	1.51
22	b	604	CLA	C3B-C4B	2.05	1.48	1.42
22	C	509	CLA	C3B-C4B	2.05	1.48	1.42
24	a	405	BCR	C30-C25	-2.05	1.51	1.53
22	B	615	CLA	CHC-C4B	-2.05	1.34	1.39
35	e	101	HEM	CMB-C2B	2.05	1.55	1.50
22	c	503	CLA	CMD-C2D	-2.05	1.46	1.50
22	c	508	CLA	C4B-NB	2.05	1.40	1.37
22	B	615	CLA	CHC-C1C	2.05	1.42	1.38
30	d	409	LHG	P-O6	2.05	1.67	1.59
27	a	409	PL9	C40-C39	-2.05	1.45	1.50
22	c	506	CLA	C1D-ND	2.04	1.40	1.37
31	c	516	DGD	O3E-C3E	-2.04	1.37	1.43
24	c	515	BCR	C35-C13	-2.04	1.46	1.50
23	d	402	PHO	C1D-ND	2.04	1.42	1.38
35	e	101	HEM	CMA-C3A	2.04	1.54	1.50
22	B	616	CLA	CAB-C3B	-2.03	1.42	1.47
22	b	608	CLA	O2D-CED	-2.03	1.40	1.45
29	b	620	SQD	O3-C3	-2.03	1.37	1.43
23	A	404	PHO	CAC-C3C	-2.03	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	MG-NA	2.03	2.11	2.06
24	K	102	BCR	C33-C5	-2.03	1.47	1.50
22	c	510	CLA	CHC-C1C	2.03	1.42	1.38
34	B	624	STE	C2-C1	2.03	1.55	1.50
22	c	504	CLA	CMD-C2D	-2.03	1.46	1.50
36	v	201	HEC	CMB-C2B	2.03	1.54	1.50
22	b	608	CLA	CMC-C2C	-2.03	1.46	1.50
22	c	511	CLA	C3D-C4D	2.03	1.48	1.44
22	b	603	CLA	C1B-C2B	2.03	1.47	1.43
36	v	201	HEC	CAC-C3C	2.02	1.56	1.51
22	c	510	CLA	CMD-C2D	-2.02	1.46	1.50
28	b	622	LMG	O8-C28	2.02	1.39	1.33
27	a	409	PL9	C10-C9	-2.02	1.45	1.50
22	C	505	CLA	C3B-C4B	2.02	1.48	1.42
24	b	618	BCR	C36-C18	-2.02	1.46	1.50
31	c	516	DGD	O1A-C1A	2.02	1.28	1.22
22	b	603	CLA	CMC-C2C	-2.02	1.46	1.50
23	d	401	PHO	CMB-C2B	-2.02	1.47	1.51
22	C	505	CLA	MG-ND	-2.02	2.01	2.05
22	A	403	CLA	CHC-C1C	2.02	1.42	1.38
22	C	509	CLA	O2D-CGD	2.01	1.38	1.33
22	b	613	CLA	C4B-NB	2.01	1.40	1.37
30	l	101	LHG	P-O6	2.01	1.67	1.59
30	d	407	LHG	P-O6	2.01	1.67	1.59
24	d	405	BCR	C33-C5	-2.01	1.47	1.50
22	B	602	CLA	CHC-C1C	2.01	1.42	1.38
35	F	101	HEM	CMA-C3A	2.01	1.54	1.50
22	a	404	CLA	C4B-NB	2.01	1.40	1.37
22	C	502	CLA	C3B-C4B	2.01	1.48	1.42
24	A	406	BCR	C30-C25	-2.00	1.51	1.53
27	D	405	PL9	C26-C24	-2.00	1.47	1.51
22	D	403	CLA	CMB-C2B	-2.00	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.00	1.46	1.50
30	D	408	LHG	C3-C2	2.00	1.57	1.51
22	d	404	CLA	MG-NA	2.00	2.11	2.06
22	a	402	CLA	CMC-C2C	-2.00	1.46	1.50

All (1254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	10.58	111.51	106.68
22	B	601	CLA	C4A-NA-C1A	10.46	111.45	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O6-C1-C2	9.54	122.76	108.27
22	b	601	CLA	C4A-NA-C1A	9.38	110.96	106.68
22	B	604	CLA	C4A-NA-C1A	9.28	110.91	106.68
29	D	407	SQD	O6-C1-C2	9.20	122.24	108.27
22	b	607	CLA	C4A-NA-C1A	8.64	110.62	106.68
22	C	503	CLA	C4A-NA-C1A	8.61	110.61	106.68
22	B	616	CLA	C4A-NA-C1A	8.59	110.60	106.68
22	c	511	CLA	C4A-NA-C1A	8.37	110.50	106.68
22	C	507	CLA	C4A-NA-C1A	8.28	110.46	106.68
22	C	509	CLA	C4A-NA-C1A	8.13	110.39	106.68
22	C	508	CLA	C4A-NA-C1A	7.98	110.32	106.68
22	a	404	CLA	C4A-NA-C1A	7.75	110.21	106.68
29	a	411	SQD	O6-C1-C2	7.64	119.88	108.27
22	b	602	CLA	C4A-NA-C1A	7.47	110.09	106.68
29	B	623	SQD	O6-C1-C2	7.43	119.56	108.27
22	B	609	CLA	C4A-NA-C1A	7.43	110.07	106.68
22	C	501	CLA	C4A-NA-C1A	7.33	110.03	106.68
22	c	502	CLA	C4A-NA-C1A	7.33	110.03	106.68
29	A	413	SQD	O6-C1-C2	7.29	119.35	108.27
22	C	511	CLA	C4A-NA-C1A	7.22	109.97	106.68
22	a	410	CLA	C4A-NA-C1A	7.17	109.95	106.68
22	c	503	CLA	C4A-NA-C1A	7.10	109.92	106.68
22	C	502	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	b	615	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	B	607	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	c	510	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	B	612	CLA	C4A-NA-C1A	6.26	109.54	106.68
22	a	402	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	b	604	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	A	411	CLA	C4A-NA-C1A	6.23	109.52	106.68
27	D	405	PL9	C7-C3-C4	6.21	122.02	116.91
22	C	510	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	f	101	SQD	O7-S-C6	5.94	115.62	106.76
22	B	611	CLA	C4A-NA-C1A	5.92	109.38	106.68
27	A	410	PL9	C7-C3-C4	5.79	121.68	116.91
23	A	404	PHO	C4D-CHA-CBD	-5.77	105.69	108.45
22	B	610	CLA	O2D-CGD-O1D	-5.75	112.65	123.85
29	f	101	SQD	O6-C1-C2	5.68	116.90	108.27
22	D	403	CLA	C4A-NA-C1A	5.67	109.26	106.68
22	B	610	CLA	C4A-NA-C1A	5.53	109.20	106.68
22	c	509	CLA	C4A-NA-C1A	5.50	109.19	106.68
22	B	613	CLA	C4A-NA-C1A	5.49	109.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	C4A-NA-C1A	5.43	109.16	106.68
22	C	513	CLA	C4A-NA-C1A	5.39	109.14	106.68
22	B	603	CLA	C3B-C4B-NB	-5.39	105.72	110.53
22	c	501	CLA	C4A-NA-C1A	5.34	109.11	106.68
22	B	602	CLA	O2D-CGD-CBD	5.33	120.54	111.23
22	A	402	CLA	C4A-NA-C1A	5.29	109.09	106.68
27	d	406	PL9	C7-C3-C4	5.26	121.24	116.91
22	b	616	CLA	C4A-NA-C1A	5.20	109.05	106.68
28	b	624	LMG	C1-O6-C5	-5.20	103.57	113.72
22	c	501	CLA	O2D-CGD-O1D	-5.19	113.75	123.85
29	D	407	SQD	O9-S-C6	5.07	114.32	106.76
22	c	507	CLA	C4A-NA-C1A	5.01	108.97	106.68
22	b	605	CLA	C4A-NA-C1A	4.96	108.94	106.68
22	b	613	CLA	C1-C2-C3	-4.85	118.25	126.20
22	b	610	CLA	C4A-NA-C1A	4.85	108.89	106.68
30	D	409	LHG	O4-P-O5	4.83	134.93	112.44
27	A	410	PL9	C7-C3-C2	-4.82	117.70	123.39
22	B	602	CLA	O2D-CGD-O1D	-4.80	114.50	123.85
22	C	501	CLA	O2D-CGD-O1D	-4.78	114.55	123.85
22	B	606	CLA	C4A-NA-C1A	4.77	108.86	106.68
27	a	409	PL9	C7-C3-C4	4.75	120.82	116.91
22	b	614	CLA	C4A-NA-C1A	4.72	108.83	106.68
22	C	506	CLA	C4A-NA-C1A	4.64	108.80	106.68
23	d	401	PHO	C4D-CHA-CBD	-4.64	106.23	108.45
22	b	609	CLA	C4A-NA-C1A	4.64	108.79	106.68
28	a	416	LMG	C1-C2-C3	-4.61	100.30	110.01
22	c	506	CLA	C4A-NA-C1A	4.61	108.78	106.68
29	A	413	SQD	C1-C2-C3	-4.59	100.35	110.01
22	b	601	CLA	O2D-CGD-O1D	-4.57	114.95	123.85
22	c	508	CLA	C4A-NA-C1A	4.57	108.76	106.68
22	d	403	CLA	C4A-NA-C1A	4.56	108.76	106.68
22	b	613	CLA	C4A-NA-C1A	4.55	108.75	106.68
29	A	413	SQD	O47-C7-C8	4.53	121.29	111.48
29	b	620	SQD	O7-S-C6	4.53	113.52	106.76
22	B	615	CLA	C4A-NA-C1A	4.52	108.74	106.68
22	b	615	CLA	C3B-C4B-NB	-4.51	106.50	110.53
30	A	414	LHG	O4-P-O5	4.49	133.35	112.44
22	b	603	CLA	C4A-NA-C1A	4.44	108.70	106.68
22	b	603	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
31	C	516	DGD	O3G-C3G-C2G	-4.39	100.15	110.82
27	a	409	PL9	C35-C34-C36	4.37	122.81	115.23
22	b	611	CLA	O2D-CGD-CBD	4.36	118.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	O2D-CGD-CBD	4.35	118.83	111.23
22	C	508	CLA	O2D-CGD-O1D	-4.34	115.41	123.85
30	e	102	LHG	O4-P-O5	4.30	132.43	112.44
30	l	101	LHG	O4-P-O5	4.28	132.34	112.44
28	b	622	LMG	O3-C3-C2	-4.28	100.30	110.38
28	a	416	LMG	C1-O6-C5	-4.27	105.38	113.72
31	C	517	DGD	O3G-C3G-C2G	-4.27	100.43	110.82
22	B	610	CLA	C3B-C4B-NB	-4.25	106.73	110.53
31	H	102	DGD	O3G-C3G-C2G	-4.25	100.47	110.82
30	B	622	LHG	O4-P-O5	4.24	132.17	112.44
26	A	409	BCT	O2-C-O1	4.24	130.52	119.68
31	c	517	DGD	O2D-C2D-C1D	-4.23	99.99	110.08
22	b	605	CLA	O2D-CGD-O1D	-4.22	115.64	123.85
22	b	612	CLA	C4A-NA-C1A	4.21	108.60	106.68
31	c	518	DGD	O3G-C3G-C2G	-4.19	100.62	110.82
22	b	611	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
22	B	614	CLA	C4A-NA-C1A	4.18	108.59	106.68
27	D	405	PL9	C7-C3-C2	-4.18	118.46	123.39
30	B	621	LHG	O4-P-O5	4.16	131.81	112.44
22	C	507	CLA	C1-C2-C3	-4.16	119.38	126.20
22	B	614	CLA	C3B-C4B-NB	-4.15	106.82	110.53
30	d	409	LHG	O4-P-O5	4.15	131.75	112.44
29	a	412	SQD	O48-C23-C24	4.14	124.46	111.83
24	T	101	BCR	C7-C8-C9	-4.14	120.12	126.23
22	c	512	CLA	C1-C2-C3	-4.12	119.44	126.20
29	a	412	SQD	O48-C23-O10	-4.11	113.33	123.63
29	f	101	SQD	O9-S-O7	-4.11	100.45	113.82
23	D	401	PHO	C2B-C1B-NB	-4.10	106.47	109.43
22	c	502	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
22	B	603	CLA	C4A-NA-C1A	4.10	108.55	106.68
22	B	608	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
22	B	608	CLA	C4A-NA-C1A	4.07	108.53	106.68
29	a	411	SQD	O7-S-C6	4.06	112.81	106.76
22	B	613	CLA	C1-C2-C3	-4.05	119.55	126.20
30	D	408	LHG	O4-P-O5	4.05	131.27	112.44
23	d	402	PHO	O1D-CGD-CBD	4.04	130.86	124.72
30	d	407	LHG	O4-P-O5	4.04	131.23	112.44
29	B	623	SQD	O47-C7-C8	4.03	120.20	111.48
28	b	622	LMG	O1-C1-C2	-4.03	102.15	108.27
22	c	512	CLA	C3B-C4B-NB	-4.02	106.94	110.53
22	b	601	CLA	CHB-C4A-NA	4.02	130.20	124.40
29	A	413	SQD	C1-O5-C5	-4.02	105.88	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	C4A-NA-C1A	4.02	108.51	106.68
22	b	602	CLA	O2D-CGD-O1D	-4.01	116.04	123.85
22	C	502	CLA	C3B-C4B-NB	-4.01	106.95	110.53
22	C	504	CLA	O2D-CGD-O1D	-3.99	116.07	123.85
22	d	404	CLA	CMB-C2B-C1B	-3.99	119.34	125.42
36	v	201	HEC	C1D-ND-C4D	3.99	109.94	105.21
29	b	620	SQD	C1-C2-C3	-3.99	101.62	110.01
22	b	613	CLA	CMB-C2B-C1B	-3.99	119.35	125.42
36	V	201	HEC	C1D-ND-C4D	3.98	109.92	105.21
22	b	604	CLA	C1-C2-C3	-3.98	119.68	126.20
35	e	101	HEM	CBD-CAD-C3D	-3.98	101.54	112.53
22	b	610	CLA	O2D-CGD-O1D	-3.97	116.11	123.85
24	C	514	BCR	C15-C16-C17	-3.96	115.41	123.52
24	b	617	BCR	C2-C1-C6	3.95	116.18	110.44
24	B	619	BCR	C2-C1-C6	3.95	116.17	110.44
23	A	404	PHO	CMB-C2B-C3B	3.94	132.56	124.68
22	b	616	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
22	c	501	CLA	O2D-CGD-CBD	3.92	118.08	111.23
22	b	608	CLA	C3B-C4B-NB	-3.89	107.06	110.53
22	b	616	CLA	CHB-C4A-NA	3.89	130.01	124.40
22	C	501	CLA	O2D-CGD-CBD	3.87	118.00	111.23
23	A	404	PHO	C3B-C4B-NB	-3.87	104.94	107.46
30	d	408	LHG	O4-P-O5	3.86	130.41	112.44
22	c	502	CLA	C3B-C4B-NB	-3.84	107.10	110.53
23	d	402	PHO	CMB-C2B-C3B	3.84	132.35	124.68
27	d	406	PL9	C36-C34-C33	-3.77	112.70	121.17
22	C	509	CLA	CHB-C4A-NA	3.75	129.82	124.40
22	A	402	CLA	CHB-C4A-NA	3.74	129.79	124.40
28	b	624	LMG	O2-C2-C1	-3.73	101.18	110.08
30	D	408	LHG	O8-C23-O10	-3.71	114.35	123.63
30	e	102	LHG	O8-C23-C24	3.71	123.15	111.83
22	C	509	CLA	C3B-C4B-NB	-3.71	107.22	110.53
22	B	611	CLA	O2D-CGD-O1D	-3.71	116.64	123.85
22	c	509	CLA	O2A-CGA-O1A	-3.71	114.36	123.63
22	B	614	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
22	C	504	CLA	C4A-NA-C1A	3.70	108.37	106.68
23	d	401	PHO	OBD-CAD-CBD	-3.70	120.40	125.82
36	v	201	HEC	CHB-C1B-NB	3.69	128.39	124.42
31	h	101	DGD	O3G-C3G-C2G	-3.69	101.85	110.82
27	A	410	PL9	C27-C28-C29	-3.68	119.19	127.62
27	D	405	PL9	C42-C43-C44	-3.68	119.20	127.62
30	B	622	LHG	O8-C23-C24	3.68	123.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	C4A-NA-C1A	3.68	108.36	106.68
27	a	409	PL9	C22-C23-C24	-3.67	119.21	127.62
22	b	605	CLA	C4-C3-C5	3.67	121.60	115.23
22	C	512	CLA	C3B-C4B-NB	-3.66	107.27	110.53
22	C	507	CLA	C4-C3-C5	3.65	121.57	115.23
22	c	512	CLA	O2A-CGA-O1A	-3.65	114.51	123.63
22	c	512	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
22	A	402	CLA	C1D-ND-C4D	-3.61	103.78	106.31
22	C	509	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
22	a	403	CLA	C4A-NA-C1A	3.59	108.32	106.68
27	A	410	PL9	C40-C39-C41	3.59	121.46	115.23
23	D	401	PHO	O2D-CGD-O1D	-3.59	116.86	123.85
31	A	416	DGD	C3G-C2G-C1G	-3.59	103.42	111.78
29	A	413	SQD	O9-S-O7	-3.59	102.16	113.82
35	F	101	HEM	CBA-CAA-C2A	-3.58	102.63	112.53
23	d	402	PHO	C4D-CHA-CBD	-3.58	106.74	108.45
23	d	401	PHO	CBC-CAC-C3C	3.57	117.99	112.87
22	D	403	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
22	b	609	CLA	C3B-C4B-NB	-3.56	107.35	110.53
27	a	409	PL9	C7-C3-C2	-3.56	119.19	123.39
22	C	505	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
29	b	620	SQD	O47-C7-C8	3.53	119.11	111.48
23	A	404	PHO	O2D-CGD-CBD	3.52	114.81	110.95
22	c	513	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
22	b	611	CLA	CHB-C4A-NA	3.52	129.48	124.40
22	A	405	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
34	L	101	STE	O2-C1-C2	3.50	125.05	114.00
22	A	405	CLA	O2D-CGD-CBD	3.50	117.34	111.23
30	d	407	LHG	O8-C23-C24	3.49	122.48	111.83
22	b	603	CLA	C3B-C4B-NB	-3.47	107.43	110.53
22	a	402	CLA	CMB-C2B-C1B	-3.46	120.15	125.42
23	D	401	PHO	O1D-CGD-CBD	3.45	129.96	124.72
22	A	402	CLA	O1D-CGD-CBD	3.44	131.31	124.52
29	D	407	SQD	O5-C1-C2	-3.44	103.30	110.37
24	t	101	BCR	C15-C16-C17	-3.44	116.48	123.52
27	d	406	PL9	C7-C3-C2	-3.44	119.34	123.39
22	B	605	CLA	C3B-C4B-NB	-3.43	107.47	110.53
22	B	607	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
29	a	411	SQD	O9-S-O7	-3.43	102.68	113.82
22	c	506	CLA	C4-C3-C5	3.43	121.17	115.23
27	D	405	PL9	C22-C23-C24	-3.42	119.79	127.62
22	b	613	CLA	CHB-C4A-NA	3.42	129.34	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	CBD-CAD-C3D	-3.42	103.09	112.53
22	c	503	CLA	C3B-C4B-NB	-3.41	107.49	110.53
22	D	402	CLA	CED-O2D-CGD	3.40	123.63	115.92
22	B	613	CLA	CMB-C2B-C1B	-3.40	120.24	125.42
22	b	613	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
29	B	623	SQD	O7-S-C6	3.39	111.81	106.76
36	v	201	HEC	CHA-C4D-ND	3.39	128.07	124.42
22	B	602	CLA	CHB-C4A-NA	3.37	129.26	124.40
31	C	515	DGD	O3G-C3G-C2G	-3.36	102.64	110.82
22	A	405	CLA	C4A-NA-C1A	3.36	108.21	106.68
22	c	508	CLA	C3B-C4B-NB	-3.36	107.53	110.53
22	B	615	CLA	CHB-C4A-NA	3.34	129.23	124.40
23	A	404	PHO	C2B-C1B-NB	-3.34	107.01	109.43
26	a	408	BCT	O2-C-O1	3.34	128.22	119.68
22	a	403	CLA	C3B-C4B-NB	-3.34	107.55	110.53
31	c	517	DGD	O3G-C3G-C2G	-3.33	102.71	110.82
22	d	404	CLA	CMB-C2B-C3B	3.33	134.39	126.55
22	c	505	CLA	C3B-C4B-NB	-3.33	107.56	110.53
23	d	401	PHO	CMB-C2B-C3B	3.33	131.33	124.68
22	d	403	CLA	O2A-CGA-O1A	-3.33	115.31	123.63
22	B	616	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
22	C	508	CLA	CMB-C2B-C1B	-3.32	120.37	125.42
22	b	614	CLA	C3B-C4B-NB	-3.31	107.57	110.53
22	C	509	CLA	CMB-C2B-C3B	3.31	134.33	126.55
22	C	502	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
31	A	416	DGD	O2D-C2D-C1D	-3.30	102.22	110.08
22	B	608	CLA	O2D-CGD-CBD	3.29	116.99	111.23
36	V	201	HEC	CMC-C2C-C1C	-3.29	120.40	125.42
27	d	406	PL9	C37-C38-C39	-3.29	120.09	127.62
23	d	401	PHO	OBD-CAD-C3D	3.29	133.02	127.89
22	B	601	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
22	B	603	CLA	C2D-C1D-ND	-3.29	106.87	110.13
24	a	405	BCR	C27-C26-C25	3.28	127.14	122.70
27	d	406	PL9	C40-C39-C41	3.28	120.92	115.23
22	c	509	CLA	CMB-C2B-C1B	-3.28	120.43	125.42
22	B	607	CLA	C3B-C4B-NB	-3.27	107.61	110.53
22	c	504	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
29	a	411	SQD	O48-C23-C24	3.26	121.79	111.83
35	e	101	HEM	C3B-C2B-C1B	3.26	108.86	106.41
22	C	502	CLA	O1D-CGD-CBD	3.26	130.96	124.52
22	B	608	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
22	B	610	CLA	O1D-CGD-CBD	3.26	130.95	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	O2A-CGA-O1A	-3.26	115.48	123.63
24	H	101	BCR	C16-C15-C14	-3.26	116.85	123.52
31	C	517	DGD	O6D-C1D-O3G	-3.26	102.35	110.04
22	C	512	CLA	C4A-NA-C1A	3.25	108.16	106.68
22	c	508	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
24	b	619	BCR	C2-C1-C6	3.25	115.15	110.44
22	b	605	CLA	C1-C2-C3	-3.24	120.88	126.20
22	D	402	CLA	C3B-C4B-NB	-3.24	107.64	110.53
29	f	101	SQD	C1-C2-C3	-3.24	103.19	110.01
31	H	102	DGD	O2D-C2D-C1D	-3.24	102.37	110.08
22	c	508	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
31	A	416	DGD	O5D-C1E-C2E	3.23	113.18	108.27
22	C	503	CLA	C7-C6-C5	-3.23	104.66	113.26
22	C	505	CLA	CAC-C3C-C4C	3.22	128.98	124.79
23	D	401	PHO	CMB-C2B-C3B	3.22	131.12	124.68
22	a	403	CLA	CED-O2D-CGD	-3.22	108.61	115.92
22	a	402	CLA	CAC-C3C-C4C	3.22	128.98	124.79
27	D	405	PL9	C7-C8-C9	-3.22	121.28	126.83
27	A	410	PL9	O2-C1-C6	3.21	125.58	120.48
29	D	407	SQD	O8-S-C6	3.21	112.16	105.97
31	h	101	DGD	C1D-C2D-C3D	-3.20	103.27	110.01
22	b	614	CLA	CHD-C1D-ND	-3.20	120.30	124.80
22	C	502	CLA	C1-C2-C3	-3.20	120.95	126.20
22	c	510	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
22	B	611	CLA	O2D-CGD-CBD	3.20	116.82	111.23
29	a	411	SQD	O9-S-C6	3.20	111.53	106.76
22	B	612	CLA	CHB-C4A-NA	3.19	129.00	124.40
28	M	101	LMG	C1-O6-C5	-3.18	107.51	113.72
24	B	617	BCR	C2-C1-C6	3.18	115.05	110.44
22	a	404	CLA	C4-C3-C5	3.17	120.74	115.23
22	C	513	CLA	O2A-CGA-O1A	-3.17	115.70	123.63
22	B	607	CLA	CHB-C1B-NB	3.17	128.80	124.05
22	b	603	CLA	CHC-C4B-NB	3.17	128.80	124.05
31	C	516	DGD	O2D-C2D-C1D	-3.16	102.54	110.08
22	b	605	CLA	O1D-CGD-CBD	3.16	130.75	124.52
29	a	412	SQD	O47-C7-C8	3.15	118.31	111.48
30	D	409	LHG	O8-C23-C24	3.15	121.45	111.83
22	b	609	CLA	CED-O2D-CGD	3.15	123.05	115.92
34	C	521	STE	C3-C2-C1	-3.14	106.30	114.51
29	A	415	SQD	C45-O47-C7	3.14	122.31	117.78
24	Y	101	BCR	C27-C26-C25	3.14	126.95	122.70
22	B	614	CLA	C4-C3-C5	3.14	120.68	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	415	SQD	O48-C23-C24	3.14	121.41	111.83
22	c	502	CLA	C1-C2-C3	-3.14	121.06	126.20
27	A	410	PL9	C22-C23-C24	-3.13	120.45	127.62
22	b	606	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
23	d	401	PHO	C2B-C1B-NB	-3.13	107.17	109.43
29	D	407	SQD	C44-O6-C1	3.12	119.01	113.68
22	b	612	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
22	a	403	CLA	CHB-C4A-NA	3.12	128.90	124.40
24	H	101	BCR	C2-C1-C6	3.11	114.96	110.44
27	A	410	PL9	C35-C34-C36	3.11	120.63	115.23
24	C	514	BCR	C36-C18-C17	-3.11	117.78	122.82
24	b	617	BCR	C3-C4-C5	-3.11	108.51	114.06
27	d	406	PL9	C22-C23-C24	-3.11	120.52	127.62
22	b	606	CLA	CGD-CBD-CAD	-3.11	100.79	110.85
22	A	403	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
22	b	602	CLA	CHB-C4A-NA	3.10	128.87	124.40
28	d	410	LMG	O1-C1-C2	-3.08	103.59	108.27
29	B	623	SQD	O48-C23-C24	3.08	121.23	111.83
22	B	616	CLA	C1D-ND-C4D	3.08	108.47	106.31
30	d	407	LHG	O8-C23-O10	-3.08	115.94	123.63
28	C	518	LMG	O1-C7-C8	-3.07	103.34	110.82
22	b	604	CLA	C11-C12-C13	-3.07	105.76	115.97
31	C	516	DGD	O6D-C1D-O3G	-3.07	102.79	110.04
22	b	616	CLA	CMB-C2B-C3B	3.07	133.76	126.55
22	C	501	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	A	403	CLA	CMB-C2B-C3B	3.07	133.76	126.55
24	x	101	BCR	C38-C26-C25	-3.06	121.14	124.48
22	b	613	CLA	O2A-CGA-O1A	-3.06	115.97	123.63
28	d	410	LMG	O6-C1-O1	-3.05	102.83	110.04
31	h	101	DGD	C4D-C3D-C2D	-3.05	105.47	110.83
22	a	403	CLA	O2D-CGD-CBD	3.05	116.57	111.23
24	T	101	BCR	C27-C26-C25	3.05	126.83	122.70
22	C	513	CLA	C3B-C4B-NB	-3.05	107.81	110.53
24	x	101	BCR	C27-C26-C25	3.05	126.82	122.70
24	d	405	BCR	C27-C26-C25	3.05	126.82	122.70
22	b	601	CLA	O2D-CGD-CBD	3.05	116.56	111.23
28	D	406	LMG	O1-C7-C8	-3.04	103.42	110.82
31	H	102	DGD	C3D-C4D-C5D	-3.04	104.72	110.23
22	c	511	CLA	CHB-C4A-NA	3.04	128.78	124.40
22	B	605	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	t	101	BCR	C3-C4-C5	-3.03	108.65	114.06
31	C	515	DGD	O6D-C1D-O3G	-3.03	102.88	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	CAC-C3C-C4C	3.03	128.73	124.79
22	c	513	CLA	CHB-C4A-NA	3.02	128.76	124.40
28	A	412	LMG	C1-O6-C5	-3.02	107.83	113.72
22	b	614	CLA	C1-C2-C3	-3.01	121.26	126.20
22	c	512	CLA	CHB-C4A-NA	3.01	128.74	124.40
24	b	619	BCR	C29-C30-C25	3.00	114.80	110.44
22	C	503	CLA	C3B-C4B-NB	-3.00	107.85	110.53
22	B	602	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
22	B	608	CLA	CHD-C1D-ND	-3.00	120.58	124.80
24	t	101	BCR	C7-C8-C9	-3.00	121.80	126.23
23	A	404	PHO	O2D-CGD-O1D	-3.00	118.01	123.85
24	A	406	BCR	C38-C26-C25	-2.99	121.22	124.48
24	c	515	BCR	C27-C26-C25	2.99	126.74	122.70
22	B	616	CLA	CHB-C4A-NA	2.98	128.71	124.40
22	C	503	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	c	507	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	a	405	BCR	C29-C30-C25	2.98	114.77	110.44
23	d	402	PHO	O2D-CGD-O1D	-2.98	118.06	123.85
24	k	102	BCR	C27-C26-C25	2.98	126.72	122.70
22	b	611	CLA	C4A-NA-C1A	2.97	108.03	106.68
28	A	412	LMG	C38-C37-C36	-2.97	99.37	114.37
24	A	406	BCR	C27-C26-C25	2.97	126.71	122.70
22	b	606	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
27	D	405	PL9	C37-C38-C39	-2.96	120.84	127.62
22	B	612	CLA	O2A-CGA-O1A	-2.96	116.22	123.63
22	B	610	CLA	O2D-CGD-CBD	2.96	116.40	111.23
29	A	413	SQD	O47-C7-O49	-2.96	116.79	123.70
22	c	506	CLA	CBC-CAC-C3C	-2.96	104.41	112.42
22	A	402	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	B	601	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	c	507	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
23	d	402	PHO	C1-C2-C3	-2.94	121.37	126.20
22	b	610	CLA	C1-C2-C3	-2.94	121.39	126.20
24	b	618	BCR	C27-C26-C25	2.93	126.66	122.70
31	C	515	DGD	C3G-C2G-C1G	-2.92	104.97	111.78
22	C	501	CLA	O2A-CGA-O1A	-2.92	116.32	123.63
29	b	620	SQD	O9-S-O7	-2.92	104.33	113.82
29	a	411	SQD	C1-O5-C5	-2.92	108.02	113.72
22	C	503	CLA	CMB-C2B-C1B	-2.91	121.00	125.42
22	A	411	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	B	611	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
31	c	516	DGD	O2G-C1B-O1B	-2.90	116.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	LMG	O6-C1-O1	-2.89	103.20	110.04
22	a	404	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
22	c	504	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
28	b	622	LMG	C1-O6-C5	-2.88	108.10	113.72
22	C	513	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
24	D	404	BCR	C27-C26-C25	2.87	126.58	122.70
28	M	101	LMG	C1-C2-C3	-2.86	103.98	110.01
22	c	506	CLA	C3B-C4B-NB	-2.86	107.97	110.53
24	t	101	BCR	C2-C1-C6	2.86	114.60	110.44
22	b	605	CLA	C3B-C4B-NB	-2.86	107.97	110.53
22	c	503	CLA	C7-C6-C5	-2.86	105.64	113.26
24	B	617	BCR	C15-C16-C17	-2.86	117.66	123.52
22	c	513	CLA	CMB-C2B-C3B	2.86	133.27	126.55
31	h	101	DGD	C3D-C4D-C5D	-2.85	105.06	110.23
23	A	404	PHO	CBC-CAC-C3C	2.85	116.96	112.87
27	A	410	PL9	C36-C34-C33	-2.85	114.76	121.17
22	b	601	CLA	CHD-C1D-ND	-2.85	120.79	124.80
34	C	521	STE	C4-C3-C2	-2.85	102.66	113.13
28	a	416	LMG	O6-C1-C2	-2.85	104.52	110.37
24	B	619	BCR	C29-C30-C25	2.85	114.57	110.44
22	b	612	CLA	CHB-C4A-NA	2.85	128.51	124.40
24	K	101	BCR	C11-C10-C9	-2.84	123.29	127.28
23	A	404	PHO	C2D-C1D-ND	2.84	111.48	109.43
27	A	410	PL9	C25-C24-C26	2.84	120.15	115.23
22	c	513	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
29	a	412	SQD	O49-C7-C8	-2.84	112.69	123.78
28	c	521	LMG	O7-C10-O9	-2.83	117.08	123.70
22	A	411	CLA	CHB-C4A-NA	2.83	128.49	124.40
22	D	402	CLA	C4-C3-C5	2.83	120.14	115.23
31	C	515	DGD	O1G-C1A-C2A	-2.83	103.21	111.83
22	B	616	CLA	O1D-CGD-CBD	2.82	130.08	124.52
29	f	101	SQD	O48-C23-O10	-2.82	116.57	123.63
28	b	622	LMG	C38-C37-C36	-2.82	100.12	114.37
31	C	516	DGD	C4E-C3E-C2E	-2.82	105.89	110.83
34	j	101	STE	O2-C1-C2	2.82	122.90	114.00
24	a	405	BCR	C30-C25-C26	-2.82	118.79	122.64
22	c	509	CLA	CMB-C2B-C3B	2.81	133.17	126.55
22	B	612	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
35	F	101	HEM	CBD-CAD-C3D	-2.81	104.76	112.53
30	A	414	LHG	O8-C23-C24	2.81	120.40	111.83
28	b	624	LMG	O5-C6-C5	-2.81	101.77	111.33
22	C	507	CLA	C2A-C1A-CHA	2.81	128.74	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	101	BCR	C36-C18-C17	-2.81	118.27	122.82
28	d	410	LMG	O2-C2-C1	-2.81	103.39	110.08
23	d	402	PHO	C3D-C4D-ND	2.80	111.30	107.71
24	k	102	BCR	C11-C10-C9	-2.80	123.35	127.28
22	b	610	CLA	C2C-C1C-NC	2.80	112.92	109.98
22	b	614	CLA	CHB-C4A-NA	2.80	128.44	124.40
23	d	402	PHO	C2B-C1B-NB	-2.80	107.41	109.43
22	b	612	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
22	d	404	CLA	CAC-C3C-C4C	2.80	128.43	124.79
22	B	603	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
30	d	408	LHG	C20-C19-C18	-2.79	100.25	114.37
24	a	405	BCR	C7-C8-C9	-2.79	122.11	126.23
22	C	509	CLA	C1-C2-C3	-2.79	121.63	126.20
30	D	408	LHG	O8-C23-C24	2.78	120.31	111.83
23	d	402	PHO	CBC-CAC-C3C	2.78	116.85	112.87
36	V	201	HEC	CBD-CAD-C3D	-2.78	104.85	112.53
31	h	101	DGD	C3G-C2G-C1G	-2.78	105.31	111.78
22	B	605	CLA	C7-C6-C5	-2.78	105.86	113.26
22	B	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	B	616	CLA	C1-O2A-CGA	2.78	123.37	116.65
22	c	510	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
24	a	405	BCR	C37-C22-C23	2.77	122.33	118.09
22	B	611	CLA	CHB-C4A-NA	2.77	128.40	124.40
22	b	604	CLA	CHD-C1D-ND	-2.77	120.91	124.80
22	c	511	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	d	403	CLA	C3B-C4B-NB	-2.76	108.06	110.53
22	b	606	CLA	C6-C5-C3	-2.76	106.73	113.47
24	B	618	BCR	C2-C1-C6	2.76	114.45	110.44
29	B	623	SQD	O9-S-O7	-2.76	104.84	113.82
22	C	505	CLA	C3B-C4B-NB	-2.76	108.06	110.53
22	a	410	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
29	b	620	SQD	O48-C23-C24	2.76	120.25	111.83
35	e	101	HEM	C3B-C4B-NB	-2.76	107.49	109.47
31	c	516	DGD	O3E-C3E-C2E	-2.75	103.89	110.38
22	B	616	CLA	C2D-C1D-ND	-2.75	107.40	110.13
22	b	614	CLA	C4-C3-C5	2.75	120.00	115.23
22	B	604	CLA	O2D-CGD-CBD	2.75	116.03	111.23
22	B	613	CLA	OBD-CAD-C3D	2.75	134.84	128.42
28	c	521	LMG	O1-C1-C2	-2.75	104.10	108.27
31	H	102	DGD	O2G-C1B-O1B	-2.74	117.29	123.70
24	c	514	BCR	C27-C26-C25	2.74	126.41	122.70
22	c	506	CLA	CMB-C2B-C1B	-2.74	121.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	CHB-C4A-NA	2.74	128.35	124.40
22	b	606	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
28	D	406	LMG	O3-C3-C2	-2.74	103.92	110.38
22	A	402	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	C	512	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	d	405	BCR	C38-C26-C25	-2.73	121.50	124.48
22	b	605	CLA	C1D-ND-C4D	2.73	108.23	106.31
22	b	612	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
31	c	518	DGD	O3E-C3E-C2E	-2.73	103.95	110.38
24	c	515	BCR	C38-C26-C25	-2.73	121.51	124.48
31	h	101	DGD	C4E-C3E-C2E	-2.73	106.04	110.83
24	H	101	BCR	C27-C26-C25	2.72	126.38	122.70
24	k	101	BCR	C38-C26-C25	-2.72	121.52	124.48
24	B	617	BCR	C27-C26-C25	2.72	126.38	122.70
28	c	521	LMG	O3-C3-C2	-2.72	103.97	110.38
22	B	611	CLA	C1-C2-C3	-2.72	121.75	126.20
22	c	504	CLA	C3B-C4B-NB	-2.72	108.11	110.53
22	C	507	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	v	201	HEC	CMD-C2D-C1D	2.71	129.27	125.03
23	D	401	PHO	C3B-C4B-NB	-2.71	105.70	107.46
22	b	615	CLA	CHB-C1B-NB	2.71	128.11	124.05
28	A	412	LMG	O6-C1-O1	-2.71	103.65	110.04
31	c	517	DGD	O3D-C3D-C4D	-2.71	104.00	110.38
35	e	101	HEM	CBA-CAA-C2A	-2.70	105.06	112.53
31	H	102	DGD	C3E-C4E-C5E	-2.70	105.33	110.23
27	A	410	PL9	O2-C1-C2	-2.70	115.69	121.83
22	b	605	CLA	C2D-C1D-ND	-2.70	107.45	110.13
29	f	101	SQD	C3-C4-C5	2.70	115.13	110.23
29	D	407	SQD	O8-S-O9	-2.70	104.64	111.40
22	b	604	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	d	403	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
28	c	519	LMG	C40-C39-C38	-2.69	100.76	114.37
22	b	608	CLA	O2D-CGD-CBD	2.69	115.93	111.23
22	B	612	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
29	A	413	SQD	O48-C23-C24	2.68	120.02	111.83
22	b	613	CLA	CMB-C2B-C3B	2.68	132.86	126.55
31	c	516	DGD	O2D-C2D-C1D	-2.68	103.68	110.08
22	B	604	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
29	f	101	SQD	O47-C7-C8	2.68	120.78	110.93
34	d	412	STE	O2-C1-O1	-2.68	116.44	123.33
22	b	610	CLA	CHC-C4B-NB	2.68	128.07	124.05
30	l	101	LHG	O8-C23-C24	2.68	120.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	101	BCR	C2-C1-C6	2.67	114.32	110.44
22	b	606	CLA	CMB-C2B-C3B	2.67	132.84	126.55
22	b	610	CLA	CHB-C4A-NA	2.67	128.26	124.40
34	J	101	STE	O2-C1-C2	2.67	122.44	114.00
31	H	102	DGD	C4D-C3D-C2D	-2.67	106.14	110.83
30	B	622	LHG	O8-C23-O10	-2.67	116.95	123.63
22	C	512	CLA	CHB-C4A-NA	2.67	128.25	124.40
22	b	615	CLA	CHB-C4A-NA	2.67	128.25	124.40
28	c	522	LMG	O6-C1-O1	-2.67	103.74	110.04
22	b	606	CLA	O1D-CGD-CBD	2.66	129.77	124.52
27	D	405	PL9	C12-C13-C14	-2.66	121.53	127.62
24	B	618	BCR	C15-C16-C17	-2.66	118.07	123.52
24	D	404	BCR	C24-C23-C22	-2.66	122.30	126.23
31	c	516	DGD	O6E-C5E-C4E	2.66	114.49	109.70
35	e	101	HEM	CAB-C3B-C2B	-2.66	119.78	128.43
27	a	409	PL9	C27-C28-C29	-2.66	121.54	127.62
31	C	515	DGD	CDB-CCB-CBB	-2.66	100.94	114.37
22	C	504	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	b	620	SQD	O2-C2-C1	2.66	116.40	110.08
22	c	512	CLA	O1D-CGD-CBD	2.65	129.75	124.52
24	a	405	BCR	C37-C22-C21	-2.65	118.52	122.82
34	B	624	STE	O2-C1-O1	-2.65	116.51	123.33
24	A	406	BCR	C2-C1-C6	2.65	114.29	110.44
22	a	402	CLA	C7-C6-C5	-2.65	106.20	113.26
22	c	508	CLA	CMB-C2B-C3B	2.65	132.77	126.55
24	B	618	BCR	C37-C22-C21	-2.64	118.53	122.82
22	B	604	CLA	C11-C12-C13	-2.64	107.18	115.97
22	B	607	CLA	CMB-C2B-C3B	2.64	132.77	126.55
22	a	403	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	D	404	BCR	C38-C26-C25	-2.64	121.60	124.48
27	d	406	PL9	C7-C8-C9	-2.64	122.28	126.83
36	V	201	HEC	C4B-NB-C1B	2.64	108.33	105.21
22	b	603	CLA	O1D-CGD-CBD	2.64	129.72	124.52
24	x	101	BCR	C37-C22-C21	-2.64	118.55	122.82
29	a	411	SQD	O47-C7-C8	2.63	117.18	111.48
24	k	102	BCR	C16-C15-C14	-2.63	118.13	123.52
22	b	608	CLA	CHB-C4A-NA	2.63	128.20	124.40
22	B	612	CLA	C11-C12-C13	-2.63	107.23	115.97
36	V	201	HEC	CHD-C4C-NC	2.63	128.62	123.86
22	b	603	CLA	C7-C6-C5	-2.63	106.26	113.26
28	c	522	LMG	C40-C39-C38	-2.63	101.10	114.37
30	B	622	LHG	O3-P-O5	-2.62	98.54	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	DGD	O6D-C1D-C2D	2.62	115.75	110.37
31	c	518	DGD	O6D-C1D-O3G	-2.62	103.86	110.04
22	D	403	CLA	CHB-C1B-NB	2.62	127.97	124.05
27	A	410	PL9	C20-C19-C21	2.62	119.77	115.23
24	b	617	BCR	C15-C16-C17	-2.61	118.17	123.52
22	c	508	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	B	613	CLA	CMB-C2B-C3B	2.61	132.70	126.55
28	a	416	LMG	O5-C6-C5	-2.61	102.44	111.33
22	C	506	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
22	B	604	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	a	410	CLA	C2A-C1A-CHA	2.61	128.39	123.87
29	f	101	SQD	C1-O5-C5	-2.61	108.63	113.72
30	d	407	LHG	C11-C10-C9	-2.61	101.18	114.37
22	C	507	CLA	C4-C3-C2	-2.61	116.93	123.63
31	H	102	DGD	C1D-C2D-C3D	-2.61	104.53	110.01
22	b	603	CLA	CHB-C1B-NB	2.61	127.96	124.05
28	b	624	LMG	C3-C4-C5	-2.60	105.51	110.23
30	e	102	LHG	C20-C19-C18	-2.60	101.21	114.37
29	b	620	SQD	O5-C1-C2	-2.60	105.03	110.37
22	b	607	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	b	617	BCR	C29-C30-C25	2.60	114.22	110.44
31	c	518	DGD	C1D-C2D-C3D	-2.60	104.55	110.01
24	b	618	BCR	C38-C26-C25	-2.60	121.65	124.48
22	B	603	CLA	CHB-C1B-NB	2.60	127.94	124.05
29	b	620	SQD	C3-C4-C5	2.59	114.94	110.23
24	H	101	BCR	C37-C22-C23	2.59	122.05	118.09
24	B	619	BCR	C1-C6-C5	-2.59	119.09	122.64
22	A	403	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
29	b	620	SQD	O5-C5-C4	2.59	114.37	109.70
22	B	606	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
22	B	608	CLA	C1D-ND-C4D	-2.59	104.50	106.31
24	K	101	BCR	C35-C13-C14	-2.59	118.62	122.82
22	B	602	CLA	C4A-NA-C1A	2.59	107.86	106.68
31	A	416	DGD	O6D-C1D-O3G	-2.58	103.94	110.04
24	B	618	BCR	C40-C30-C25	2.58	114.29	110.24
34	d	413	STE	O2-C1-C2	2.58	122.16	114.00
22	B	601	CLA	CHC-C4B-NB	2.58	127.92	124.05
22	c	506	CLA	C4-C3-C2	-2.58	117.00	123.63
34	d	411	STE	O2-C1-C2	2.58	122.14	114.00
22	b	603	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
22	C	503	CLA	CHD-C1D-ND	-2.58	121.18	124.80
24	A	406	BCR	C36-C18-C19	2.57	122.02	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.37
22	B	614	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	c	501	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
22	B	614	CLA	CHA-C1A-NA	-2.57	120.57	126.39
22	b	612	CLA	C11-C12-C13	-2.57	107.43	115.97
22	B	609	CLA	CHC-C4B-NB	2.57	127.90	124.05
22	B	608	CLA	CHD-C4C-NC	2.56	128.21	124.23
24	b	618	BCR	C31-C1-C6	2.56	114.26	110.24
22	b	610	CLA	C11-C12-C13	-2.56	107.44	115.97
22	b	607	CLA	C6-C7-C8	-2.56	107.45	115.97
22	C	511	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
29	D	407	SQD	C46-C45-C44	-2.56	105.39	113.67
22	c	501	CLA	CHB-C4A-NA	2.56	128.10	124.40
31	c	517	DGD	O6D-C1D-O3G	-2.56	103.99	110.04
24	c	514	BCR	C15-C16-C17	-2.56	118.28	123.52
22	B	604	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	B	608	CLA	CMB-C2B-C3B	2.56	132.57	126.55
22	a	402	CLA	CMB-C2B-C3B	2.56	132.56	126.55
31	A	416	DGD	C4E-C3E-C2E	-2.55	106.35	110.83
27	D	405	PL9	C35-C34-C36	2.55	119.66	115.23
23	d	401	PHO	C3B-C4B-NB	-2.55	105.80	107.46
31	c	516	DGD	O5E-C6E-C5E	-2.55	102.65	111.33
22	C	510	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
22	B	606	CLA	C3B-C4B-NB	-2.55	108.26	110.53
35	e	101	HEM	CHD-C4C-NC	2.54	127.22	124.45
24	b	617	BCR	C8-C7-C6	-2.54	120.21	127.00
24	k	101	BCR	C27-C26-C25	2.54	126.14	122.70
22	C	506	CLA	CHB-C4A-NA	2.54	128.07	124.40
29	b	620	SQD	O8-S-C6	2.54	110.88	105.97
22	B	608	CLA	CHB-C4A-NA	2.54	128.06	124.40
22	C	508	CLA	O2D-CGD-CBD	2.54	115.66	111.23
28	b	622	LMG	C9-C8-C7	-2.54	105.87	111.78
22	c	509	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
29	D	407	SQD	O9-S-O7	-2.53	105.59	113.82
31	c	516	DGD	O3D-C3D-C4D	-2.53	104.41	110.38
29	D	407	SQD	O48-C23-O10	-2.53	117.30	123.63
22	d	404	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
31	C	517	DGD	O3E-C3E-C2E	-2.52	104.43	110.38
24	C	514	BCR	C15-C14-C13	-2.52	123.74	127.28
34	t	102	STE	C3-C2-C1	-2.52	107.93	114.51
22	b	606	CLA	CHB-C1B-NB	2.52	127.83	124.05
22	c	505	CLA	O2D-CGD-O1D	-2.52	118.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	404	CLA	O2D-CGD-CBD	2.52	115.64	111.23
22	B	611	CLA	C7-C6-C5	-2.52	106.55	113.26
22	d	404	CLA	CHA-C1A-NA	-2.52	120.69	126.39
36	V	201	HEC	CHB-C1B-NB	2.52	127.13	124.42
22	C	502	CLA	C4D-C3D-CAD	-2.52	105.37	108.11
22	c	508	CLA	C7-C6-C5	-2.52	106.56	113.26
31	c	518	DGD	CDB-CCB-CBB	-2.52	101.66	114.37
34	L	101	STE	O1-C1-C2	-2.51	115.12	123.09
24	t	101	BCR	C37-C22-C23	2.51	121.92	118.09
22	C	502	CLA	CHD-C1D-ND	-2.51	121.27	124.80
29	b	620	SQD	O48-C23-O10	-2.51	117.35	123.63
22	B	608	CLA	C3D-C4D-ND	2.51	114.06	109.99
22	C	512	CLA	C1-C2-C3	-2.51	122.09	126.20
22	b	612	CLA	CMB-C2B-C3B	2.51	132.44	126.55
22	B	605	CLA	O1D-CGD-CBD	2.51	129.46	124.52
31	c	516	DGD	O1G-C1A-C2A	-2.50	104.20	111.83
24	K	101	BCR	C27-C26-C25	2.50	126.09	122.70
22	b	616	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
22	B	616	CLA	C3B-C4B-NB	-2.50	108.30	110.53
22	C	510	CLA	CHB-C4A-NA	2.50	128.00	124.40
24	c	515	BCR	C7-C8-C9	-2.50	122.54	126.23
22	D	403	CLA	CMB-C2B-C1B	-2.50	121.62	125.42
36	V	201	HEC	CAC-C3C-C2C	2.49	130.84	126.89
31	c	517	DGD	O3G-C1D-C2D	-2.49	104.48	108.27
22	C	506	CLA	O1D-CGD-CBD	2.49	129.44	124.52
29	a	411	SQD	C1-C2-C3	-2.49	104.77	110.01
22	d	403	CLA	C4-C3-C5	2.49	119.55	115.23
22	D	403	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	C	506	CLA	CHA-C1A-NA	-2.49	120.75	126.39
22	B	614	CLA	C1-C2-C3	-2.49	122.12	126.20
22	D	402	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
22	B	616	CLA	C2A-C3A-C4A	2.49	105.88	101.87
22	c	508	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
27	d	406	PL9	C30-C29-C31	-2.48	110.92	115.23
24	d	405	BCR	C24-C23-C22	-2.48	122.56	126.23
22	B	612	CLA	O1D-CGD-CBD	2.48	129.41	124.52
22	B	615	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
22	B	607	CLA	CHD-C4C-NC	2.48	128.07	124.23
22	c	503	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
22	B	607	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
29	b	620	SQD	C1-O5-C5	-2.47	108.89	113.72
30	d	409	LHG	C26-C25-C24	2.47	122.21	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	406	PL9	C42-C43-C44	-2.47	121.97	127.62
22	B	616	CLA	CMB-C2B-C3B	2.47	132.36	126.55
22	c	502	CLA	O1D-CGD-CBD	2.47	129.38	124.52
22	a	410	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	b	607	CLA	CHD-C1D-ND	-2.46	121.34	124.80
34	M	102	STE	C3-C2-C1	-2.46	108.08	114.51
22	B	611	CLA	CHD-C4C-NC	2.46	128.05	124.23
30	B	621	LHG	C27-C26-C25	-2.46	101.93	114.37
27	a	409	PL9	C26-C24-C23	-2.46	115.64	121.17
22	c	506	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	A	416	DGD	O6E-C5E-C4E	2.46	114.12	109.70
24	b	619	BCR	C15-C16-C17	-2.46	118.50	123.52
22	b	611	CLA	CED-O2D-CGD	-2.45	110.35	115.92
22	b	610	CLA	CAA-CBA-CGA	-2.45	106.24	113.21
22	C	502	CLA	C4D-CHA-C1A	2.45	124.17	121.24
22	C	501	CLA	C2D-C1D-ND	-2.45	107.70	110.13
22	b	607	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
22	B	602	CLA	CMB-C2B-C3B	2.45	132.31	126.55
22	b	605	CLA	CHD-C1D-C2D	2.45	130.58	125.49
22	c	507	CLA	C2C-C1C-NC	2.44	112.55	109.98
30	B	622	LHG	C20-C19-C18	-2.44	102.01	114.37
27	a	409	PL9	C7-C8-C9	-2.44	122.62	126.83
22	c	506	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	H	101	BCR	C37-C22-C21	-2.44	118.86	122.82
22	A	402	CLA	CHD-C1D-ND	-2.44	121.37	124.80
28	D	406	LMG	C1-C2-C3	-2.44	104.88	110.01
28	C	518	LMG	C38-C37-C36	-2.44	102.05	114.37
22	B	614	CLA	CHC-C4B-NB	2.44	127.70	124.05
22	b	606	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
23	A	404	PHO	CMA-C3A-C4A	-2.43	109.37	114.61
24	t	101	BCR	C29-C30-C25	2.43	113.97	110.44
24	K	101	BCR	C24-C23-C22	-2.43	122.64	126.23
24	K	102	BCR	C37-C22-C21	-2.43	118.88	122.82
22	B	609	CLA	C2C-C1C-NC	2.43	112.53	109.98
31	c	518	DGD	O5D-C1E-C2E	2.43	111.96	108.27
31	H	102	DGD	C7B-C6B-C5B	-2.43	102.08	114.37
22	c	509	CLA	O1D-CGD-CBD	2.43	129.31	124.52
24	K	101	BCR	C7-C8-C9	-2.43	122.65	126.23
22	c	507	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	C	503	CLA	CMB-C2B-C3B	2.42	132.25	126.55
22	b	603	CLA	C4-C3-C5	2.42	119.43	115.23
29	A	413	SQD	O5-C1-O6	2.42	115.77	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	C4-C3-C5	2.42	119.43	115.23
31	h	101	DGD	O3E-C3E-C2E	-2.42	104.67	110.38
24	c	514	BCR	C20-C21-C22	-2.42	123.89	127.28
22	b	603	CLA	CMB-C2B-C3B	2.42	132.24	126.55
31	A	416	DGD	O1G-C1A-O1A	-2.42	117.58	123.63
22	B	601	CLA	O2D-CGD-CBD	2.42	115.46	111.23
31	c	516	DGD	O3G-C3G-C2G	-2.42	104.94	110.82
22	C	506	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
22	D	402	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
22	B	615	CLA	C2A-C3A-C4A	2.42	105.78	101.87
24	C	514	BCR	C7-C8-C9	-2.42	122.66	126.23
34	c	520	STE	C3-C2-C1	-2.42	108.20	114.51
28	c	519	LMG	O2-C2-C1	-2.41	104.34	110.08
22	C	502	CLA	CHD-C4C-NC	2.40	127.96	124.23
31	A	416	DGD	O3G-C3G-C2G	-2.40	104.97	110.82
22	c	505	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
22	b	609	CLA	CHC-C4B-NB	2.40	127.65	124.05
22	c	510	CLA	O1D-CGD-CBD	2.40	129.25	124.52
29	D	407	SQD	C1-C2-C3	-2.40	104.96	110.01
22	B	603	CLA	C1D-ND-C4D	2.40	108.00	106.31
34	X	101	STE	C3-C2-C1	-2.40	108.25	114.51
22	b	606	CLA	C2A-C1A-CHA	2.40	128.03	123.87
22	B	601	CLA	C1-C2-C3	-2.40	122.27	126.20
24	b	617	BCR	C36-C18-C17	-2.40	118.93	122.82
31	H	102	DGD	O3E-C3E-C2E	-2.40	104.73	110.38
29	B	623	SQD	C3-C4-C5	2.40	114.58	110.23
22	C	505	CLA	CGD-CBD-CAD	-2.39	103.10	110.85
28	c	521	LMG	O2-C2-C1	-2.39	104.38	110.08
22	b	615	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
30	l	101	LHG	C11-C10-C9	-2.39	102.30	114.37
36	v	201	HEC	C1D-C2D-C3D	-2.39	104.47	106.98
35	e	101	HEM	CHC-C4B-C3B	2.39	129.83	125.07
29	B	623	SQD	O8-S-C6	2.38	110.57	105.97
22	C	510	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
31	c	517	DGD	C3E-C4E-C5E	-2.38	105.91	110.23
22	A	402	CLA	CAA-CBA-CGA	-2.38	106.45	113.21
29	A	415	SQD	O47-C7-C8	2.38	116.62	111.48
31	c	518	DGD	C6B-C5B-C4B	-2.38	102.36	114.37
22	B	603	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	B	609	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	b	603	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
31	C	515	DGD	CCB-CBB-CAB	-2.37	102.37	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	O9-S-C6	2.37	110.30	106.76
22	B	602	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
27	D	405	PL9	C32-C33-C34	-2.37	122.20	127.62
22	d	404	CLA	C1-C2-C3	-2.37	122.31	126.20
24	b	619	BCR	C36-C18-C17	-2.37	118.98	122.82
22	c	504	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
24	d	405	BCR	C2-C1-C6	2.37	113.88	110.44
22	B	602	CLA	C3B-C4B-NB	-2.37	108.42	110.53
22	C	508	CLA	C3B-C4B-NB	-2.37	108.42	110.53
22	D	402	CLA	CMB-C2B-C3B	2.36	132.11	126.55
22	c	501	CLA	C3B-C4B-NB	-2.36	108.42	110.53
30	e	102	LHG	C11-C10-C9	-2.36	102.43	114.37
28	c	519	LMG	C1-O6-C5	-2.36	109.11	113.72
27	d	406	PL9	C20-C19-C21	2.36	119.32	115.23
22	d	403	CLA	CHC-C4B-NB	2.36	127.59	124.05
24	a	405	BCR	C15-C16-C17	-2.36	118.69	123.52
22	C	511	CLA	CHA-C4D-ND	2.36	137.41	132.55
22	b	616	CLA	O1D-CGD-CBD	2.36	129.17	124.52
31	C	516	DGD	CDB-CCB-CBB	-2.36	102.45	114.37
28	D	406	LMG	O2-C2-C1	-2.36	104.46	110.08
22	a	402	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
24	c	515	BCR	C15-C16-C17	-2.35	118.70	123.52
22	C	503	CLA	O1D-CGD-CBD	2.35	129.16	124.52
34	C	519	STE	O2-C1-C2	2.35	121.43	114.00
22	c	504	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
22	c	513	CLA	C3B-C4B-NB	-2.35	108.43	110.53
22	B	611	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	C	518	LMG	O6-C1-O1	-2.35	104.50	110.04
22	b	602	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
22	C	513	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	B	612	CLA	CMB-C2B-C3B	2.34	132.06	126.55
28	d	410	LMG	O1-C7-C8	-2.34	105.12	110.82
29	B	623	SQD	C1-O5-C5	-2.34	109.14	113.72
23	D	401	PHO	C3D-C4D-ND	2.34	110.71	107.71
22	b	606	CLA	CHB-C1B-C2B	-2.34	120.63	127.43
22	B	606	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
22	a	402	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	c	509	CLA	CHB-C4A-NA	2.34	127.77	124.40
28	b	622	LMG	O1-C7-C8	-2.34	105.14	110.82
22	B	610	CLA	CHB-C4A-NA	2.33	127.77	124.40
22	C	508	CLA	CHB-C4A-NA	2.33	127.77	124.40
27	d	406	PL9	C15-C14-C13	-2.33	117.64	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	101	BCR	C16-C15-C14	-2.33	118.75	123.52
22	B	605	CLA	CHB-C4A-NA	2.33	127.76	124.40
22	B	602	CLA	CHD-C1D-ND	-2.33	121.53	124.80
29	f	101	SQD	C46-C45-C44	-2.33	106.36	111.78
35	F	101	HEM	C1D-C2D-C3D	2.33	109.43	106.98
30	D	408	LHG	C29-C28-C27	-2.33	102.61	114.37
22	b	613	CLA	CHA-C1A-NA	-2.33	121.12	126.39
24	B	617	BCR	C37-C22-C23	2.33	121.64	118.09
29	a	411	SQD	O5-C5-C4	2.32	113.89	109.70
22	B	603	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	B	614	CLA	O1D-CGD-CBD	2.32	129.10	124.52
22	C	504	CLA	C4-C3-C5	2.32	119.26	115.23
22	b	603	CLA	CHA-C4D-ND	2.32	137.33	132.55
29	A	415	SQD	O47-C45-C44	2.32	113.15	107.96
28	c	519	LMG	O6-C1-O1	-2.32	104.57	110.04
24	b	619	BCR	C12-C13-C14	-2.32	115.37	119.01
22	A	403	CLA	CED-O2D-CGD	-2.32	110.66	115.92
27	D	405	PL9	C20-C19-C21	2.32	119.25	115.23
27	d	406	PL9	C12-C13-C14	-2.32	122.32	127.62
29	f	101	SQD	O5-C1-O6	2.32	115.52	110.04
22	a	410	CLA	O2D-CGD-CBD	2.32	115.28	111.23
30	A	414	LHG	C11-C10-C9	-2.31	102.68	114.37
22	B	613	CLA	CHA-C1A-NA	-2.31	121.16	126.39
24	t	101	BCR	C31-C1-C6	2.31	113.87	110.24
31	H	102	DGD	C3G-C2G-C1G	-2.31	106.40	111.78
22	b	614	CLA	CHD-C1D-C2D	2.31	130.29	125.49
22	d	404	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
24	d	405	BCR	C16-C15-C14	-2.31	118.79	123.52
22	B	601	CLA	C1-O2A-CGA	2.31	122.24	116.65
22	A	402	CLA	CMB-C2B-C3B	2.31	131.98	126.55
22	b	601	CLA	C3B-C4B-NB	-2.31	108.47	110.53
28	b	624	LMG	O6-C5-C6	2.30	112.15	106.44
34	X	101	STE	O2-C1-C2	2.30	121.28	114.00
22	A	405	CLA	C1D-ND-C4D	-2.30	104.70	106.31
22	b	610	CLA	O2D-CGD-CBD	2.30	115.25	111.23
22	b	616	CLA	C4-C3-C5	2.30	119.22	115.23
36	V	201	HEC	C2B-C1B-NB	-2.30	107.25	109.90
22	C	505	CLA	O1D-CGD-CBD	2.29	129.04	124.52
22	d	404	CLA	O1D-CGD-CBD	2.29	129.04	124.52
24	b	618	BCR	C30-C25-C26	-2.29	119.50	122.64
22	B	607	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	a	402	CLA	CGD-CBD-CAD	-2.29	103.44	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C16-C17-C18	-2.29	124.07	127.28
30	D	408	LHG	C27-C26-C25	-2.29	102.81	114.37
28	c	519	LMG	C9-C8-C7	-2.29	106.45	111.78
24	a	405	BCR	C38-C26-C27	-2.28	108.72	113.60
22	c	507	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
22	C	512	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
24	t	101	BCR	C1-C6-C5	-2.28	119.52	122.64
22	B	605	CLA	CHD-C4C-NC	2.28	127.77	124.23
36	v	201	HEC	CHD-C1D-ND	2.28	127.19	124.37
22	B	610	CLA	C1-C2-C3	-2.28	122.46	126.20
31	c	516	DGD	O6D-C1D-O3G	-2.28	104.65	110.04
22	B	615	CLA	CAC-C3C-C4C	2.28	127.76	124.79
29	b	620	SQD	O8-S-O7	-2.28	105.70	111.40
34	b	625	STE	O2-C1-C2	2.28	121.19	114.00
22	c	506	CLA	CMB-C2B-C3B	2.28	131.90	126.55
31	c	518	DGD	C3D-C4D-C5D	-2.28	106.11	110.23
28	D	406	LMG	O8-C28-O10	-2.27	117.94	123.63
31	C	516	DGD	C1D-C2D-C3D	-2.27	105.23	110.01
22	C	507	CLA	CHB-C4A-NA	2.27	127.68	124.40
24	x	101	BCR	C2-C1-C6	2.27	113.74	110.44
22	B	607	CLA	CED-O2D-CGD	2.27	121.06	115.92
22	c	510	CLA	CHB-C4A-NA	2.27	127.67	124.40
22	A	403	CLA	CHB-C4A-NA	2.27	127.67	124.40
22	C	507	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	b	617	BCR	C38-C26-C25	-2.26	122.01	124.48
22	C	512	CLA	O2D-CGD-CBD	2.26	115.19	111.23
24	A	406	BCR	C15-C16-C17	-2.26	118.89	123.52
24	c	514	BCR	C7-C8-C9	-2.26	122.89	126.23
30	d	409	LHG	O8-C23-O10	-2.26	117.97	123.63
28	C	518	LMG	O3-C3-C2	-2.26	105.04	110.38
22	c	502	CLA	CHB-C1B-NB	2.26	127.44	124.05
22	C	509	CLA	C2A-C1A-CHA	2.26	127.79	123.87
35	F	101	HEM	O2D-CGD-CBD	2.26	121.14	114.00
22	B	605	CLA	C3D-C4D-ND	2.26	113.66	109.99
22	C	504	CLA	O1D-CGD-CBD	2.26	128.97	124.52
22	c	504	CLA	CHB-C1B-NB	2.26	127.44	124.05
22	B	608	CLA	C6-C7-C8	-2.26	108.46	115.97
22	C	512	CLA	CAA-CBA-CGA	-2.26	106.80	113.21
31	h	101	DGD	O6D-C1D-O3G	-2.26	104.71	110.04
22	a	403	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
24	k	102	BCR	C8-C7-C6	-2.26	120.97	127.00
22	b	604	CLA	OBD-CAD-C3D	2.26	133.69	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
30	A	414	LHG	C20-C19-C18	-2.25	102.97	114.37
28	D	411	LMG	O7-C10-O9	-2.25	117.53	123.33
22	b	606	CLA	C2D-C1D-ND	-2.25	107.89	110.13
23	A	404	PHO	O2A-CGA-O1A	-2.25	117.99	123.63
30	d	408	LHG	O7-C7-C8	-2.25	106.61	111.48
22	A	405	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	b	608	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
29	D	407	SQD	O5-C5-C4	2.25	113.76	109.70
24	K	102	BCR	C7-C8-C9	-2.25	122.91	126.23
34	d	411	STE	C3-C2-C1	-2.25	108.64	114.51
24	C	514	BCR	C27-C26-C25	2.25	125.74	122.70
22	a	403	CLA	CHC-C4B-NB	2.25	127.42	124.05
28	M	101	LMG	O6-C1-O1	-2.24	104.74	110.04
31	A	416	DGD	CBB-CAB-C9B	-2.24	103.03	114.37
22	D	402	CLA	C1D-ND-C4D	-2.24	104.74	106.31
22	A	411	CLA	CHA-C1A-NA	-2.24	121.32	126.39
22	B	616	CLA	C5-C3-C2	2.24	126.19	121.17
23	D	401	PHO	C7-C6-C5	-2.24	107.30	113.26
36	V	201	HEC	C1D-C2D-C3D	-2.24	104.63	106.98
29	a	411	SQD	O10-C23-C24	-2.24	115.03	123.78
22	A	411	CLA	C2C-C1C-NC	2.24	112.33	109.98
28	c	521	LMG	C42-C41-C40	-2.24	103.06	114.37
22	B	615	CLA	C4-C3-C5	2.24	119.11	115.23
24	K	102	BCR	C38-C26-C25	-2.23	122.05	124.48
28	M	101	LMG	O1-C7-C8	-2.23	105.39	110.82
22	c	501	CLA	CED-O2D-CGD	-2.23	110.85	115.92
34	b	623	STE	O2-C1-C2	2.23	121.05	114.00
22	D	403	CLA	C6-C7-C8	-2.23	108.55	115.97
24	d	405	BCR	C7-C8-C9	-2.23	122.94	126.23
28	D	406	LMG	C3-C4-C5	-2.23	106.19	110.23
22	B	604	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
22	B	601	CLA	C4-C3-C5	2.23	119.10	115.23
22	c	507	CLA	CHC-C4B-NB	2.23	127.39	124.05
28	b	624	LMG	O7-C10-O9	-2.23	118.50	123.70
28	b	624	LMG	C40-C39-C38	-2.23	103.12	114.37
22	B	601	CLA	CHB-C4A-NA	2.23	127.61	124.40
28	M	101	LMG	O3-C3-C2	-2.22	105.13	110.38
22	A	405	CLA	C4-C3-C5	2.22	119.09	115.23
34	B	624	STE	O2-C1-C2	2.22	121.02	114.00
31	C	515	DGD	O3E-C3E-C2E	-2.22	105.14	110.38
22	C	508	CLA	O2A-CGA-O1A	-2.22	118.07	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	CMB-C2B-C3B	2.22	131.77	126.55
22	b	608	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
30	B	622	LHG	C11-C10-C9	-2.22	103.16	114.37
22	b	606	CLA	C1D-ND-C4D	2.22	107.87	106.31
27	d	406	PL9	C8-C7-C3	2.22	117.76	112.03
30	d	407	LHG	C20-C19-C18	-2.22	103.17	114.37
22	D	403	CLA	O1D-CGD-CBD	2.21	128.89	124.52
35	F	101	HEM	CHC-C4B-NB	2.21	126.81	124.42
29	a	411	SQD	C45-O47-C7	2.21	123.09	117.80
30	d	407	LHG	C27-C26-C25	-2.21	103.19	114.37
24	b	618	BCR	C8-C7-C6	-2.21	121.09	127.00
22	c	511	CLA	CHD-C1D-ND	-2.21	121.69	124.80
22	B	615	CLA	C2B-C1B-NB	-2.21	108.03	110.33
22	B	616	CLA	CHD-C1D-C2D	2.21	130.08	125.49
24	K	102	BCR	C27-C26-C25	2.21	125.69	122.70
27	d	406	PL9	C47-C48-C49	-2.21	120.28	127.64
22	B	603	CLA	CMB-C2B-C3B	2.20	131.74	126.55
22	c	508	CLA	CHD-C4C-NC	2.20	127.65	124.23
22	b	604	CLA	CHB-C1B-NB	2.20	127.36	124.05
23	D	401	PHO	O2A-CGA-O1A	-2.20	118.11	123.63
22	a	403	CLA	CMB-C2B-C3B	2.20	131.73	126.55
24	B	618	BCR	C29-C30-C25	2.20	113.64	110.44
22	c	505	CLA	O2D-CGD-CBD	2.20	115.08	111.23
22	d	404	CLA	CHB-C1B-NB	2.20	127.35	124.05
29	B	623	SQD	O5-C5-C4	2.20	113.67	109.70
24	Y	101	BCR	C30-C25-C26	-2.20	119.63	122.64
22	C	507	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
24	x	101	BCR	C15-C16-C17	-2.20	119.02	123.52
22	B	616	CLA	CAA-CBA-CGA	-2.20	106.96	113.21
22	b	602	CLA	C11-C12-C13	-2.20	108.66	115.97
22	A	403	CLA	C4A-NA-C1A	2.20	107.68	106.68
28	b	624	LMG	O8-C28-O10	-2.20	118.13	123.63
22	c	513	CLA	O2D-CGD-CBD	2.20	115.07	111.23
27	D	405	PL9	C36-C34-C33	-2.20	116.23	121.17
22	C	504	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
24	B	619	BCR	C27-C26-C25	2.19	125.67	122.70
22	B	614	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
22	C	508	CLA	CMB-C2B-C3B	2.19	131.71	126.55
22	c	513	CLA	C4A-NA-C1A	2.19	107.68	106.68
22	A	402	CLA	CMD-C2D-C1D	2.19	128.59	124.73
22	B	611	CLA	C2A-C3A-C4A	2.19	105.41	101.87
29	D	407	SQD	O48-C23-C24	2.19	118.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	CHB-C1B-NB	2.19	127.33	124.05
27	A	410	PL9	C7-C8-C9	-2.19	123.06	126.83
22	B	609	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
35	e	101	HEM	CHB-C1B-NB	2.19	127.07	124.37
36	V	201	HEC	C1B-C2B-C3B	2.18	109.28	106.98
22	b	604	CLA	CED-O2D-CGD	-2.18	110.96	115.92
35	e	101	HEM	O1A-CGA-CBA	-2.18	116.17	123.09
22	c	513	CLA	C11-C12-C13	-2.18	108.71	115.97
22	c	501	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
28	D	406	LMG	O1-C1-C2	-2.18	104.96	108.27
22	b	610	CLA	C3B-C4B-NB	-2.18	108.58	110.53
22	c	503	CLA	C3A-C2A-C1A	2.18	104.61	101.34
28	a	416	LMG	O6-C5-C4	2.18	113.63	109.70
22	c	506	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
30	D	408	LHG	C18-C17-C16	-2.18	103.35	114.37
24	A	406	BCR	C37-C22-C21	-2.18	119.28	122.82
34	d	411	STE	O1-C1-C2	-2.18	116.19	123.09
22	B	606	CLA	C4-C3-C5	2.18	119.01	115.23
31	C	516	DGD	CBB-CAB-C9B	-2.18	103.37	114.37
22	a	403	CLA	C2D-C1D-ND	-2.18	107.97	110.13
22	b	611	CLA	C7-C6-C5	-2.18	107.47	113.26
22	C	513	CLA	O1D-CGD-CBD	2.18	128.81	124.52
22	C	507	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
27	a	409	PL9	C42-C43-C44	-2.17	122.65	127.62
22	b	609	CLA	O1D-CGD-CBD	2.17	128.80	124.52
28	M	101	LMG	C38-C37-C36	-2.17	103.39	114.37
22	C	503	CLA	C1-O2A-CGA	2.17	121.91	116.65
22	c	508	CLA	CHD-C1D-ND	-2.17	121.75	124.80
22	B	603	CLA	CHD-C1D-C2D	2.17	130.00	125.49
34	b	623	STE	C3-C2-C1	-2.17	108.85	114.51
31	H	102	DGD	CAB-C9B-C8B	-2.17	103.41	114.37
22	d	404	CLA	CHD-C4C-C3C	2.17	127.94	124.77
28	A	412	LMG	O8-C28-O10	-2.17	118.21	123.63
28	D	406	LMG	C38-C37-C36	-2.17	103.42	114.37
22	B	610	CLA	CAA-C2A-C3A	-2.16	107.15	113.00
22	C	508	CLA	O1D-CGD-CBD	2.16	128.78	124.52
24	K	102	BCR	C40-C30-C39	-2.16	102.44	108.63
28	d	410	LMG	O3-C3-C2	-2.16	105.28	110.38
24	T	101	BCR	C31-C1-C6	2.16	113.63	110.24
28	a	416	LMG	C9-C8-C7	-2.16	106.75	111.78
28	D	410	LMG	O8-C28-O10	-2.16	118.23	123.63
22	b	616	CLA	C3B-C2B-C1B	-2.16	104.62	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	C6-C5-C3	2.16	118.73	113.47
22	c	510	CLA	CHB-C1B-NB	2.16	127.28	124.05
31	h	101	DGD	O6E-C5E-C6E	-2.16	101.09	106.44
24	T	101	BCR	C1-C6-C5	-2.16	119.69	122.64
24	c	514	BCR	C2-C1-C6	2.15	113.57	110.44
22	b	610	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	b	603	CLA	O2D-CGD-CBD	2.15	115.00	111.23
22	B	604	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
28	c	519	LMG	C38-C37-C36	-2.15	103.49	114.37
31	c	516	DGD	O4D-C4D-C5D	-2.15	104.02	109.32
28	c	522	LMG	O7-C10-O9	-2.15	118.67	123.70
28	D	411	LMG	O8-C28-O10	-2.15	117.80	123.33
22	B	602	CLA	CHC-C1C-NC	2.15	127.55	124.31
24	k	101	BCR	C1-C6-C5	-2.15	119.70	122.64
22	A	411	CLA	CMB-C2B-C3B	2.15	131.60	126.55
22	c	504	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	B	615	CLA	C6-C7-C8	-2.15	108.83	115.97
27	D	405	PL9	C41-C39-C38	-2.14	116.36	121.17
23	d	401	PHO	O2A-CGA-O1A	-2.14	118.27	123.63
29	A	413	SQD	O48-C23-O10	-2.14	118.27	123.63
29	b	620	SQD	C45-O47-C7	2.14	122.92	117.80
30	B	622	LHG	C27-C26-C25	-2.14	103.55	114.37
24	b	619	BCR	C37-C22-C21	-2.14	119.35	122.82
24	B	619	BCR	C38-C26-C25	-2.14	122.15	124.48
24	B	618	BCR	C28-C27-C26	-2.14	110.24	114.06
27	D	405	PL9	C50-C49-C48	-2.14	116.24	122.66
22	a	402	CLA	CHA-C4D-ND	2.14	136.96	132.55
24	H	101	BCR	C34-C9-C8	-2.14	114.82	118.09
28	A	412	LMG	C12-C11-C10	-2.14	105.87	113.69
31	C	517	DGD	CDB-CCB-CBB	-2.14	103.57	114.37
31	C	515	DGD	C6B-C5B-C4B	-2.14	103.58	114.37
22	B	605	CLA	CHA-C1A-NA	-2.13	121.56	126.39
29	A	413	SQD	O4-C4-C3	-2.13	105.35	110.38
22	c	505	CLA	CMB-C2B-C3B	2.13	131.57	126.55
22	C	502	CLA	CHB-C4A-NA	2.13	127.48	124.40
28	b	624	LMG	O1-C1-C2	-2.13	105.03	108.27
22	b	602	CLA	C1-C2-C3	-2.13	122.70	126.20
31	c	518	DGD	O3D-C3D-C4D	-2.13	105.35	110.38
30	D	408	LHG	C20-C19-C18	-2.13	103.60	114.37
27	A	410	PL9	C42-C43-C44	-2.13	122.75	127.62
27	a	409	PL9	C32-C33-C34	-2.13	122.75	127.62
22	c	509	CLA	O2A-CGA-CBA	2.13	118.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	C25-C24-C23	-2.13	105.90	113.69
31	C	515	DGD	C9B-C8B-C7B	-2.13	103.62	114.37
22	d	403	CLA	C1-C2-C3	-2.13	122.71	126.20
24	B	619	BCR	C2-C3-C4	-2.13	106.60	111.28
35	F	101	HEM	CAC-C3C-C4C	2.12	129.89	124.82
22	b	606	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
22	C	504	CLA	O2D-CGD-CBD	2.12	114.94	111.23
28	C	518	LMG	C40-C39-C38	-2.12	103.63	114.37
24	B	617	BCR	C8-C7-C6	-2.12	121.33	127.00
31	H	102	DGD	O6D-C1D-O3G	-2.12	105.03	110.04
28	M	101	LMG	O8-C28-O10	-2.12	118.32	123.63
27	a	409	PL9	C36-C34-C33	-2.12	116.41	121.17
34	B	625	STE	O2-C1-C2	2.12	120.70	114.00
22	b	602	CLA	C2D-C1D-ND	-2.12	108.03	110.13
24	b	617	BCR	C15-C14-C13	-2.12	124.31	127.28
31	C	516	DGD	O5D-C6D-C5D	-2.12	104.65	109.42
23	A	404	PHO	C4D-ND-C1D	-2.12	106.34	108.87
30	d	408	LHG	O8-C23-C24	2.11	118.28	111.83
36	V	201	HEC	CHB-C4A-NA	2.11	126.75	124.45
22	c	508	CLA	O2D-CGD-CBD	2.11	114.92	111.23
31	A	416	DGD	O5D-C6D-C5D	-2.11	104.66	109.42
22	A	405	CLA	C2C-C1C-NC	2.11	112.20	109.98
22	B	612	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
24	K	101	BCR	C36-C18-C17	-2.11	119.40	122.82
22	c	504	CLA	CMB-C2B-C3B	2.11	131.51	126.55
30	B	621	LHG	C20-C19-C18	-2.11	103.70	114.37
27	D	405	PL9	C8-C7-C3	2.11	117.48	112.03
27	a	409	PL9	C20-C19-C21	2.11	118.89	115.23
28	D	410	LMG	O1-C7-C8	-2.11	106.35	111.77
22	A	405	CLA	C3D-C4D-ND	2.11	113.41	109.99
24	b	618	BCR	C29-C30-C25	2.11	113.50	110.44
31	C	516	DGD	O3D-C3D-C4D	-2.11	105.41	110.38
22	b	615	CLA	C11-C10-C8	-2.11	108.96	115.97
29	b	620	SQD	O47-C45-C46	2.11	115.90	108.34
24	x	101	BCR	C36-C18-C19	2.11	121.30	118.09
27	A	410	PL9	C12-C13-C14	-2.10	122.81	127.62
31	c	516	DGD	C3G-C2G-C1G	-2.10	106.89	111.78
24	K	102	BCR	C15-C16-C17	-2.10	119.22	123.52
35	e	101	HEM	O1D-CGD-CBD	-2.10	116.43	123.09
22	b	607	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
30	e	102	LHG	C18-C17-C16	-2.10	103.77	114.37
31	C	515	DGD	O6E-C5E-C4E	2.10	113.48	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C8-C7-C6	-2.10	121.40	127.00
22	c	506	CLA	CMC-C2C-C1C	2.10	128.31	125.03
22	b	607	CLA	CHD-C4C-NC	2.10	127.48	124.23
22	C	506	CLA	C3B-C4B-NB	-2.09	108.66	110.53
28	C	518	LMG	O2-C2-C1	-2.09	105.08	110.08
24	C	514	BCR	C2-C1-C6	2.09	113.48	110.44
28	b	624	LMG	C38-C37-C36	-2.09	103.80	114.37
22	c	502	CLA	CHD-C4C-NC	2.09	127.47	124.23
22	a	402	CLA	C2A-C1A-CHA	2.09	127.50	123.87
22	b	609	CLA	CHB-C1B-NB	2.09	127.19	124.05
24	K	102	BCR	C29-C30-C25	2.09	113.47	110.44
22	a	404	CLA	CHB-C4A-NA	2.09	127.41	124.40
22	b	612	CLA	CHC-C1C-NC	2.09	127.46	124.31
27	a	409	PL9	C25-C24-C23	-2.08	118.28	123.63
22	C	508	CLA	CHD-C1D-ND	-2.08	121.87	124.80
22	b	616	CLA	C3B-C4B-NB	-2.08	108.67	110.53
22	D	402	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
22	D	403	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
31	A	416	DGD	O4D-C4D-C3D	2.08	115.29	110.38
36	v	201	HEC	CBB-CAB-C3B	-2.08	106.78	112.42
31	C	517	DGD	O3D-C3D-C4D	-2.08	105.47	110.38
24	H	101	BCR	C38-C26-C25	-2.08	122.21	124.48
22	C	512	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	b	604	CLA	C4D-CHA-C1A	2.08	123.72	121.24
22	C	504	CLA	CHD-C1D-ND	-2.08	121.88	124.80
30	B	622	LHG	C18-C17-C16	-2.08	103.86	114.37
22	B	601	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
22	c	509	CLA	C3B-C4B-NB	-2.08	108.67	110.53
30	d	407	LHG	O2-C2-C3	-2.08	102.52	109.70
28	d	410	LMG	C3-C4-C5	-2.08	106.47	110.23
36	v	201	HEC	CHA-C1A-C2A	2.08	128.14	124.86
31	C	515	DGD	C6D-O5D-C1E	2.08	118.25	113.80
31	h	101	DGD	O6E-C1E-O5D	-2.07	105.14	110.04
34	d	411	STE	C6-C5-C4	-2.07	103.88	114.37
22	c	510	CLA	CMB-C2B-C3B	2.07	131.43	126.55
35	F	101	HEM	CAC-C3C-C2C	-2.07	121.69	128.43
28	A	412	LMG	O7-C10-C11	2.07	115.97	111.48
22	c	507	CLA	O1D-CGD-CBD	2.07	128.61	124.52
22	b	604	CLA	C2A-C1A-CHA	2.07	127.47	123.87
31	c	517	DGD	O2E-C2E-C1E	-2.07	105.14	110.08
22	b	609	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	c	518	DGD	CAB-C9B-C8B	-2.07	103.91	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	PHO	C4D-ND-C1D	-2.07	106.39	108.87
22	B	609	CLA	CHA-C1A-NA	-2.07	121.71	126.39
28	b	622	LMG	O6-C5-C6	2.07	111.56	106.44
24	k	102	BCR	C37-C22-C21	-2.07	119.47	122.82
22	B	608	CLA	C2A-C3A-C4A	2.07	105.21	101.87
24	a	405	BCR	C2-C1-C6	2.07	113.44	110.44
28	A	412	LMG	C35-C34-C33	-2.06	103.93	114.37
22	B	615	CLA	C14-C13-C15	-2.06	103.92	111.27
22	C	505	CLA	C6-C7-C8	-2.06	109.11	115.97
22	B	611	CLA	C14-C13-C15	-2.06	103.92	111.27
22	C	507	CLA	CHC-C4B-NB	2.06	127.14	124.05
31	c	517	DGD	C3G-O3G-C1D	2.06	118.22	113.80
31	C	515	DGD	O2D-C2D-C1D	-2.06	105.17	110.08
22	b	613	CLA	C16-C15-C13	-2.06	109.12	115.97
24	b	618	BCR	C15-C16-C17	-2.06	119.31	123.52
22	B	606	CLA	CHB-C4A-NA	2.06	127.37	124.40
22	d	404	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
28	a	416	LMG	O8-C28-O10	-2.06	118.48	123.63
22	b	606	CLA	C2C-C1C-NC	2.06	112.14	109.98
22	B	603	CLA	O1A-CGA-CBA	2.06	131.82	123.78
22	B	603	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
24	H	101	BCR	C29-C30-C25	2.05	113.42	110.44
22	b	601	CLA	CHD-C1D-C2D	2.05	129.76	125.49
22	b	607	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
22	B	611	CLA	CHD-C4C-C3C	-2.05	121.78	124.77
22	c	504	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
22	D	403	CLA	C1-C2-C3	-2.05	122.84	126.20
22	C	505	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
29	A	413	SQD	O8-S-C6	2.05	109.93	105.97
22	A	405	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	c	518	DGD	CBB-CAB-C9B	-2.05	104.02	114.37
22	B	609	CLA	C3B-C4B-NB	-2.05	108.70	110.53
22	A	405	CLA	CHA-C1A-NA	-2.05	121.76	126.39
22	D	403	CLA	CHA-C1A-NA	-2.05	121.76	126.39
35	e	101	HEM	O2D-CGD-CBD	2.05	120.46	114.00
29	A	413	SQD	O7-S-C6	2.04	109.81	106.76
22	c	510	CLA	C3B-C4B-NB	-2.04	108.70	110.53
22	c	505	CLA	CMD-C2D-C3D	2.04	132.38	127.69
22	c	511	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
22	c	501	CLA	CMB-C2B-C3B	2.04	131.36	126.55
22	D	402	CLA	C3D-C4D-ND	2.04	113.31	109.99
28	M	101	LMG	C22-C21-C20	-2.04	104.05	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	519	LMG	O8-C28-O10	-2.04	118.52	123.63
24	B	617	BCR	C37-C22-C21	-2.04	119.51	122.82
22	b	606	CLA	CHB-C4A-NA	2.04	127.34	124.40
22	B	616	CLA	O2A-C1-C2	2.04	115.96	108.11
22	B	602	CLA	C1-C2-C3	-2.04	122.86	126.20
28	d	410	LMG	C9-C8-C7	-2.04	107.03	111.78
23	D	401	PHO	C1-C2-C3	-2.04	122.86	126.20
28	M	101	LMG	C37-C36-C35	-2.04	104.08	114.37
22	c	504	CLA	O2D-CGD-CBD	2.03	114.79	111.23
24	b	619	BCR	C16-C15-C14	-2.03	119.36	123.52
22	C	506	CLA	CHA-C4D-ND	2.03	136.74	132.55
22	b	609	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
31	c	516	DGD	O3G-C1D-C2D	-2.03	105.19	108.27
23	D	401	PHO	C4D-CHA-CBD	-2.03	107.48	108.45
22	C	504	CLA	CHB-C4A-NA	2.03	127.33	124.40
22	A	405	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
24	k	101	BCR	C4-C5-C6	2.03	125.45	122.70
22	b	610	CLA	O1D-CGD-CBD	2.03	128.52	124.52
31	c	517	DGD	O5D-C6D-C5D	-2.03	104.84	109.42
24	B	619	BCR	C28-C27-C26	-2.03	110.44	114.06
23	d	401	PHO	C1-C2-C3	-2.03	122.87	126.20
36	V	201	HEC	C2C-C1C-NC	-2.03	106.89	110.14
22	b	615	CLA	CHD-C4C-C3C	-2.03	121.81	124.77
23	D	401	PHO	O2D-CGD-CBD	2.03	113.18	110.95
22	A	411	CLA	C2A-C1A-CHA	2.03	127.39	123.87
22	b	611	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
31	c	517	DGD	C5B-C4B-C3B	-2.03	104.11	114.37
22	B	614	CLA	CMD-C2D-C3D	2.03	132.34	127.69
22	B	610	CLA	C11-C10-C8	-2.03	109.22	115.97
24	b	619	BCR	C27-C26-C25	2.03	125.44	122.70
22	B	604	CLA	CHA-C1A-NA	-2.03	121.80	126.39
36	V	201	HEC	C1C-C2C-C3C	2.03	109.14	106.82
30	D	409	LHG	O7-C7-C8	-2.03	107.10	111.48
30	l	101	LHG	C20-C19-C18	-2.02	104.14	114.37
22	b	612	CLA	C1-C2-C3	-2.02	122.88	126.20
22	b	604	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
29	A	415	SQD	O48-C23-O10	-2.02	118.57	123.63
22	b	615	CLA	C14-C13-C15	-2.02	104.06	111.27
24	K	101	BCR	C38-C26-C25	-2.02	122.28	124.48
22	C	507	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	C	517	DGD	C5B-C4B-C3B	-2.02	104.17	114.37
22	C	504	CLA	CHA-C1A-NA	-2.02	121.82	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	101	DGD	O2E-C2E-C1E	-2.02	105.27	110.08
34	X	101	STE	C12-C11-C10	-2.02	104.17	114.37
22	b	605	CLA	CHD-C1D-ND	-2.02	121.96	124.80
28	c	522	LMG	C38-C37-C36	-2.02	104.17	114.37
28	c	521	LMG	O6-C1-O1	-2.02	105.28	110.04
24	c	514	BCR	C37-C22-C21	-2.02	119.55	122.82
22	b	601	CLA	O1D-CGD-CBD	2.02	128.49	124.52
22	b	611	CLA	C1-C2-C3	-2.02	122.89	126.20
22	B	611	CLA	CMB-C2B-C3B	2.02	131.29	126.55
22	C	504	CLA	CHB-C1B-NB	2.02	127.07	124.05
22	a	404	CLA	C3B-C4B-NB	-2.01	108.73	110.53
22	C	508	CLA	CHD-C1D-C2D	2.01	129.68	125.49
27	A	410	PL9	C41-C39-C38	-2.01	116.65	121.17
22	B	613	CLA	O1D-CGD-CBD	2.01	128.49	124.52
22	b	611	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	C	505	CLA	CMB-C2B-C3B	2.01	131.29	126.55
22	C	501	CLA	CHD-C1D-C2D	2.01	129.67	125.49
24	Y	101	BCR	C8-C7-C6	-2.01	121.63	127.00
28	c	521	LMG	C40-C39-C38	-2.01	104.21	114.37
31	C	517	DGD	O3G-C1D-C2D	-2.01	105.22	108.27
22	B	615	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
22	B	607	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
24	k	102	BCR	C1-C6-C5	-2.01	119.89	122.64
24	D	404	BCR	C7-C8-C9	-2.01	123.27	126.23
22	D	403	CLA	C1D-ND-C4D	-2.01	104.90	106.31
22	c	502	CLA	O2D-CGD-CBD	2.01	114.74	111.23
22	B	608	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
22	a	403	CLA	CAC-C3C-C4C	2.01	127.40	124.79
24	b	617	BCR	C27-C26-C25	2.00	125.41	122.70
22	b	611	CLA	CHA-C1A-NA	-2.00	121.85	126.39
23	d	401	PHO	CMD-C2D-C3D	2.00	128.68	124.68
22	c	504	CLA	O1A-CGA-CBA	2.00	131.61	123.78
28	d	410	LMG	C6-C5-C4	-2.00	108.11	113.02
22	b	613	CLA	O1D-CGD-CBD	2.00	128.47	124.52

All (2) chirality outliers are listed below:

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

All (1837) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
22	B	601	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	C4-C3-C5-C6
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	402	CLA	C11-C10-C8-C9
22	a	403	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB
22	b	605	CLA	C4B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C2-C3-C5-C6
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
24	B	618	BCR	C11-C10-C9-C34
24	C	514	BCR	C11-C12-C13-C14
24	D	404	BCR	C37-C22-C23-C24
24	K	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C17-C18-C19-C20
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C18-C19-C20-C21
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	c	515	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	d	405	BCR	C21-C22-C23-C24
24	d	405	BCR	C37-C22-C23-C24
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C5-C6-C7-C8
24	t	101	BCR	C17-C18-C19-C20
24	x	101	BCR	C11-C10-C9-C8
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
27	A	410	PL9	C25-C24-C26-C27
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	A	410	PL9	C40-C39-C41-C42
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C32-C33-C34-C36
27	a	409	PL9	C22-C23-C24-C25
27	a	409	PL9	C22-C23-C24-C26
27	a	409	PL9	C39-C41-C42-C43
27	a	409	PL9	C42-C43-C44-C45
27	a	409	PL9	C42-C43-C44-C46
27	d	406	PL9	C27-C28-C29-C30
27	d	406	PL9	C32-C33-C34-C36
27	d	406	PL9	C33-C34-C36-C37
27	d	406	PL9	C42-C43-C44-C45
27	d	406	PL9	C42-C43-C44-C46
28	A	412	LMG	O9-C10-O7-C8
28	D	410	LMG	C11-C10-O7-C8
28	b	624	LMG	C11-C10-O7-C8
28	c	521	LMG	C11-C10-O7-C8
28	c	522	LMG	O6-C1-O1-C7
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	D	407	SQD	O5-C1-O6-C44
29	a	411	SQD	O6-C44-C45-O47
29	a	411	SQD	C5-C6-S-O7
29	a	411	SQD	C5-C6-S-O8
29	a	411	SQD	C5-C6-S-O9
29	a	412	SQD	C8-C7-O47-C45
29	b	620	SQD	O49-C7-O47-C45
29	b	620	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
30	A	414	LHG	O1-C1-C2-O2
30	A	414	LHG	O1-C1-C2-C3
30	A	414	LHG	C4-O6-P-O4
30	B	621	LHG	C3-O3-P-O4
30	B	621	LHG	C4-O6-P-O3
30	B	621	LHG	C4-O6-P-O4
30	B	621	LHG	C4-O6-P-O5
30	B	622	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	B	622	LHG	C3-O3-P-O4
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	O2-C2-C3-O3
30	D	408	LHG	C3-O3-P-O4
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	D	409	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
30	d	408	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O4
30	d	408	LHG	C4-O6-P-O5
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	O10-C23-O8-C6
30	e	102	LHG	C24-C23-O8-C6
30	l	101	LHG	C3-O3-P-O4
30	l	101	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O5
31	A	416	DGD	C2B-C1B-O2G-C2G
31	A	416	DGD	O1B-C1B-O2G-C2G
31	A	416	DGD	O2G-C2G-C3G-O3G
28	c	522	LMG	O10-C28-O8-C9
29	a	412	SQD	O10-C23-O48-C46
30	A	414	LHG	O10-C23-O8-C6
28	c	522	LMG	C29-C28-O8-C9
29	D	407	SQD	C24-C23-O48-C46
28	M	101	LMG	O10-C28-O8-C9
28	c	521	LMG	O10-C28-O8-C9
29	b	620	SQD	O10-C23-O48-C46
36	V	201	HEC	C4C-C3C-CAC-CBC
28	D	410	LMG	O9-C10-O7-C8
28	b	624	LMG	O9-C10-O7-C8
28	c	521	LMG	O9-C10-O7-C8
22	A	405	CLA	C3-C5-C6-C7
28	c	521	LMG	C29-C28-O8-C9
29	a	412	SQD	C24-C23-O48-C46
29	b	620	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
29	f	101	SQD	C24-C23-O48-C46
22	B	601	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
28	A	412	LMG	C11-C10-O7-C8
22	b	614	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
27	A	410	PL9	C20-C19-C21-C22
27	a	409	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
27	A	410	PL9	C13-C14-C16-C17
27	A	410	PL9	C43-C44-C46-C47
27	a	409	PL9	C33-C34-C36-C37
27	D	405	PL9	C47-C48-C49-C51
22	B	604	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
28	M	101	LMG	C29-C28-O8-C9
29	B	623	SQD	C24-C23-O48-C46
30	A	414	LHG	C24-C23-O8-C6
27	A	410	PL9	C12-C13-C14-C16
29	B	623	SQD	O10-C23-O48-C46
29	f	101	SQD	O10-C23-O48-C46
31	A	416	DGD	O6E-C5E-C6E-O5E
22	B	603	CLA	CBD-CGD-O2D-CED
30	d	407	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	e	102	LHG	O2-C2-C3-O3
29	D	407	SQD	O10-C23-O48-C46
31	H	102	DGD	C4E-C5E-C6E-O5E
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
28	b	624	LMG	O6-C5-C6-O5
36	V	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C2C-C3C-CAC-CBC
27	D	405	PL9	C47-C48-C49-C50
22	B	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
27	A	410	PL9	C23-C24-C26-C27
28	b	624	LMG	O10-C28-O8-C9
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C34-C36-C37-C38
27	A	410	PL9	C39-C41-C42-C43
27	A	410	PL9	C44-C46-C47-C48
27	a	409	PL9	C9-C11-C12-C13
27	a	409	PL9	C19-C21-C22-C23
27	d	406	PL9	C34-C36-C37-C38
22	B	614	CLA	C15-C16-C17-C18
28	b	622	LMG	C29-C28-O8-C9
31	H	102	DGD	O6E-C5E-C6E-O5E
27	a	409	PL9	C7-C8-C9-C10
31	A	416	DGD	C4E-C5E-C6E-O5E
22	b	607	CLA	CBD-CGD-O2D-CED
22	d	404	CLA	CBD-CGD-O2D-CED
30	D	408	LHG	C1-C2-C3-O3
30	d	407	LHG	C1-C2-C3-O3
30	d	408	LHG	C1-C2-C3-O3
22	b	601	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CBA-CGA-O2A-C1
34	C	521	STE	C4-C5-C6-C7
30	B	621	LHG	C7-C8-C9-C10
34	a	415	STE	C4-C5-C6-C7
22	b	605	CLA	C2-C3-C5-C6
27	a	409	PL9	C23-C24-C26-C27
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	B	609	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
22	b	611	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	510	CLA	C11-C10-C8-C9
22	c	512	CLA	C6-C7-C8-C9
28	d	410	LMG	C10-C11-C12-C13
22	B	601	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1A-CGA-O2A-C1
24	A	406	BCR	C37-C22-C23-C24
24	C	514	BCR	C36-C18-C19-C20
24	K	101	BCR	C7-C8-C9-C34
24	K	102	BCR	C36-C18-C19-C20
24	T	101	BCR	C7-C8-C9-C34
24	Y	101	BCR	C11-C12-C13-C35
24	b	619	BCR	C37-C22-C23-C24
24	c	515	BCR	C7-C8-C9-C34
24	k	101	BCR	C7-C8-C9-C34
24	k	102	BCR	C37-C22-C23-C24
24	t	101	BCR	C36-C18-C19-C20
28	D	406	LMG	C10-C11-C12-C13
22	b	601	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1A-CGA-O2A-C1
28	C	518	LMG	O10-C28-O8-C9
30	e	102	LHG	O6-C4-C5-O7
28	C	518	LMG	C11-C10-O7-C8
29	B	623	SQD	O6-C44-C45-O47
22	B	613	CLA	C8-C10-C11-C12
22	b	611	CLA	C15-C16-C17-C18
22	c	507	CLA	C5-C6-C7-C8
28	C	518	LMG	C28-C29-C30-C31
27	d	406	PL9	C12-C13-C14-C15
22	C	506	CLA	C13-C15-C16-C17
22	C	513	CLA	C5-C6-C7-C8
22	b	615	CLA	C11-C12-C13-C15
22	c	506	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
28	c	521	LMG	C28-C29-C30-C31
29	b	620	SQD	C23-C24-C25-C26
31	c	518	DGD	C1A-C2A-C3A-C4A
29	a	412	SQD	O49-C7-O47-C45
27	A	410	PL9	C29-C31-C32-C33
27	a	409	PL9	C14-C16-C17-C18
27	a	409	PL9	C24-C26-C27-C28
27	a	409	PL9	C34-C36-C37-C38
22	b	604	CLA	C15-C16-C17-C18
22	b	614	CLA	C10-C11-C12-C13
22	c	504	CLA	C5-C6-C7-C8
22	A	402	CLA	C2C-C3C-CAC-CBC
28	M	101	LMG	C28-C29-C30-C31
28	c	519	LMG	C28-C29-C30-C31
29	B	623	SQD	C23-C24-C25-C26
31	C	515	DGD	C1B-C2B-C3B-C4B
34	b	623	STE	C1-C2-C3-C4
34	d	413	STE	C1-C2-C3-C4
28	a	416	LMG	O10-C28-O8-C9
28	b	624	LMG	C29-C28-O8-C9
22	B	601	CLA	C5-C6-C7-C8
22	B	609	CLA	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
22	C	510	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
24	c	515	BCR	C18-C19-C20-C21
22	B	603	CLA	C8-C10-C11-C12
22	B	606	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
22	C	513	CLA	C15-C16-C17-C18
22	b	602	CLA	C8-C10-C11-C12
22	b	603	CLA	C5-C6-C7-C8
22	b	615	CLA	C10-C11-C12-C13
22	c	503	CLA	C8-C10-C11-C12
28	b	624	LMG	C4-C5-C6-O5
30	d	407	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
34	R	101	STE	C1-C2-C3-C4
34	d	412	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C8-C10-C11-C12
22	C	503	CLA	C5-C6-C7-C8
22	C	506	CLA	C8-C10-C11-C12
22	C	509	CLA	C10-C11-C12-C13
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C13-C15-C16-C17
22	c	509	CLA	C13-C15-C16-C17
22	c	511	CLA	C13-C15-C16-C17
28	C	518	LMG	C29-C28-O8-C9
30	A	414	LHG	C7-C8-C9-C10
30	D	409	LHG	C7-C8-C9-C10
34	b	625	STE	C1-C2-C3-C4
22	B	604	CLA	C13-C15-C16-C17
22	D	402	CLA	C15-C16-C17-C18
30	d	409	LHG	C30-C31-C32-C33
22	B	614	CLA	C8-C10-C11-C12
22	B	616	CLA	C5-C6-C7-C8
22	C	508	CLA	C15-C16-C17-C18
22	c	511	CLA	C15-C16-C17-C18
28	D	410	LMG	C10-C11-C12-C13
22	B	603	CLA	O1D-CGD-O2D-CED
30	d	408	LHG	C28-C29-C30-C31
22	b	601	CLA	C8-C10-C11-C12
30	d	409	LHG	C24-C25-C26-C27
28	D	410	LMG	C28-C29-C30-C31
29	A	413	SQD	C7-C8-C9-C10
34	j	101	STE	C1-C2-C3-C4
22	B	602	CLA	C13-C15-C16-C17
22	B	605	CLA	C13-C15-C16-C17
29	A	413	SQD	C11-C12-C13-C14
22	B	616	CLA	C3-C5-C6-C7
22	B	613	CLA	C13-C15-C16-C17
29	A	413	SQD	C30-C31-C32-C33
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	CBA-CGA-O2A-C1
28	a	416	LMG	C29-C28-O8-C9
22	B	601	CLA	C8-C10-C11-C12
22	B	607	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	a	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	505	CLA	C15-C16-C17-C18
22	c	509	CLA	C10-C11-C12-C13
28	D	411	LMG	C28-C29-C30-C31
28	d	410	LMG	C28-C29-C30-C31
22	A	411	CLA	C15-C16-C17-C18
22	B	615	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
28	c	519	LMG	O9-C10-O7-C8
22	B	601	CLA	C13-C15-C16-C17
22	B	607	CLA	C8-C10-C11-C12
22	B	615	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
22	b	613	CLA	C15-C16-C17-C18
22	b	615	CLA	C15-C16-C17-C18
22	B	607	CLA	C10-C11-C12-C13
22	b	607	CLA	C8-C10-C11-C12
22	b	616	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
27	a	409	PL9	C27-C28-C29-C30
29	B	623	SQD	C2-C1-O6-C44
31	C	516	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
22	B	611	CLA	C8-C10-C11-C12
22	B	612	CLA	C10-C11-C12-C13
34	B	626	STE	C11-C12-C13-C14
23	d	402	PHO	O1D-CGD-O2D-CED
22	C	513	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C14
22	d	404	CLA	C15-C16-C17-C18
24	A	406	BCR	C20-C21-C22-C37
24	B	617	BCR	C11-C10-C9-C34
24	B	617	BCR	C35-C13-C14-C15
24	B	617	BCR	C16-C17-C18-C36
24	B	619	BCR	C20-C21-C22-C37
24	C	514	BCR	C35-C13-C14-C15
24	C	514	BCR	C20-C21-C22-C37
24	D	404	BCR	C20-C21-C22-C37
24	a	405	BCR	C11-C10-C9-C34
24	a	405	BCR	C20-C21-C22-C37
24	b	618	BCR	C11-C10-C9-C34
24	b	619	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C35-C13-C14-C15
24	t	101	BCR	C20-C21-C22-C37
22	c	509	CLA	C3-C5-C6-C7
34	J	101	STE	C1-C2-C3-C4
24	B	618	BCR	C37-C22-C23-C24
28	b	622	LMG	C38-C39-C40-C41
28	D	406	LMG	O6-C5-C6-O5
24	k	101	BCR	C17-C18-C19-C20
22	c	512	CLA	O1A-CGA-O2A-C1
31	C	517	DGD	O1A-C1A-O1G-C1G
22	c	512	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C15-C16-C17-C18
30	D	409	LHG	O1-C1-C2-C3
30	d	407	LHG	O1-C1-C2-C3
30	d	409	LHG	O1-C1-C2-C3
29	b	620	SQD	C46-C45-O47-C7
22	B	612	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
22	B	605	CLA	C3-C5-C6-C7
24	B	619	BCR	C11-C10-C9-C8
24	C	514	BCR	C11-C10-C9-C8
24	K	101	BCR	C12-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C19
24	c	515	BCR	C12-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C23
24	t	101	BCR	C20-C21-C22-C23
28	C	518	LMG	O6-C1-O1-C7
28	b	622	LMG	O6-C1-O1-C7
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
28	b	624	LMG	C10-C11-C12-C13
22	B	603	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C19
22	B	616	CLA	C11-C12-C13-C15
22	c	511	CLA	C16-C17-C18-C19
29	D	407	SQD	C31-C32-C33-C34
29	a	412	SQD	C11-C10-C9-C8
30	B	621	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C11-C10-C9-C8
31	C	516	DGD	C7B-C8B-C9B-CAB
31	c	516	DGD	C4A-C5A-C6A-C7A
34	d	411	STE	C10-C11-C12-C13
34	d	412	STE	C3-C4-C5-C6
24	K	101	BCR	C14-C15-C16-C17
24	c	515	BCR	C14-C15-C16-C17
28	C	518	LMG	C32-C33-C34-C35
28	b	622	LMG	C33-C34-C35-C36
28	c	521	LMG	C16-C17-C18-C19
30	A	414	LHG	C24-C25-C26-C27
30	B	621	LHG	C34-C35-C36-C37
30	l	101	LHG	C17-C18-C19-C20
31	h	101	DGD	CBA-CCA-CDA-CEA
34	b	623	STE	C14-C15-C16-C17
34	d	412	STE	C10-C11-C12-C13
34	l	102	STE	C4-C5-C6-C7
28	c	522	LMG	C12-C13-C14-C15
28	c	522	LMG	C30-C31-C32-C33
28	d	410	LMG	C32-C33-C34-C35
29	f	101	SQD	C29-C30-C31-C32
30	A	414	LHG	C34-C35-C36-C37
30	d	407	LHG	C32-C33-C34-C35
31	A	416	DGD	C4B-C5B-C6B-C7B
34	B	626	STE	C4-C5-C6-C7
34	B	626	STE	C13-C14-C15-C16
34	c	520	STE	C2-C3-C4-C5
28	M	101	LMG	C13-C14-C15-C16
28	a	416	LMG	C36-C37-C38-C39
28	c	521	LMG	C30-C31-C32-C33
28	c	522	LMG	C39-C40-C41-C42
29	b	620	SQD	C27-C28-C29-C30
30	B	622	LHG	C29-C30-C31-C32
30	D	408	LHG	C12-C13-C14-C15
30	D	409	LHG	C9-C10-C11-C12
31	C	516	DGD	C5A-C6A-C7A-C8A
31	c	517	DGD	CAB-CBB-CCB-CDB
34	h	102	STE	C11-C12-C13-C14
30	B	622	LHG	O1-C1-C2-O2
30	D	408	LHG	O1-C1-C2-O2
30	D	409	LHG	O1-C1-C2-O2
28	D	410	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	D	409	LHG	C11-C10-C9-C8
30	d	408	LHG	C11-C12-C13-C14
31	c	516	DGD	C4B-C5B-C6B-C7B
34	B	620	STE	C6-C7-C8-C9
34	H	103	STE	C10-C11-C12-C13
34	b	621	STE	C6-C7-C8-C9
34	c	520	STE	C9-C10-C11-C12
22	b	609	CLA	C4B-C3B-CAB-CBB
22	c	505	CLA	C4B-C3B-CAB-CBB
22	d	403	CLA	C4B-C3B-CAB-CBB
30	B	622	LHG	C7-C8-C9-C10
28	a	416	LMG	C12-C13-C14-C15
34	b	623	STE	C7-C8-C9-C10
22	C	510	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
28	D	410	LMG	O10-C28-O8-C9
29	f	101	SQD	C31-C32-C33-C34
28	a	416	LMG	C11-C10-O7-C8
28	c	519	LMG	C33-C34-C35-C36
30	B	621	LHG	C31-C32-C33-C34
22	B	606	CLA	C6-C7-C8-C10
22	B	611	CLA	C12-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C10-C8-C7
31	c	516	DGD	O6D-C5D-C6D-O5D
30	D	408	LHG	C10-C11-C12-C13
30	d	407	LHG	C10-C11-C12-C13
31	c	517	DGD	C7A-C8A-C9A-CAA
22	A	411	CLA	C13-C15-C16-C17
28	c	521	LMG	C39-C40-C41-C42
30	d	409	LHG	C32-C33-C34-C35
30	e	102	LHG	C11-C10-C9-C8
31	H	102	DGD	C3B-C4B-C5B-C6B
31	c	516	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	CBB-CCB-CDB-CEB
34	b	626	STE	C12-C13-C14-C15
34	b	626	STE	C14-C15-C16-C17
34	d	413	STE	C14-C15-C16-C17
31	c	518	DGD	O1A-C1A-O1G-C1G
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
29	a	411	SQD	C17-C18-C19-C20
29	a	411	SQD	C25-C26-C27-C28
29	b	620	SQD	C25-C26-C27-C28
30	A	414	LHG	C26-C27-C28-C29
30	D	409	LHG	C25-C26-C27-C28
31	h	101	DGD	C9A-CAA-CBA-CCA
30	B	621	LHG	C12-C13-C14-C15
31	c	517	DGD	C5B-C6B-C7B-C8B
22	B	601	CLA	C15-C16-C17-C18
22	c	512	CLA	C5-C6-C7-C8
22	c	513	CLA	C5-C6-C7-C8
23	d	402	PHO	C5-C6-C7-C8
34	c	523	STE	C5-C6-C7-C8
22	B	601	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C15
30	D	408	LHG	C34-C35-C36-C37
30	e	102	LHG	C14-C15-C16-C17
30	l	101	LHG	C32-C33-C34-C35
22	A	403	CLA	C15-C16-C17-C18
22	c	511	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
28	M	101	LMG	C16-C17-C18-C19
29	b	620	SQD	C28-C29-C30-C31
31	c	517	DGD	C6A-C7A-C8A-C9A
28	a	416	LMG	O1-C7-C8-C9
28	b	622	LMG	C32-C33-C34-C35
29	A	415	SQD	C12-C13-C14-C15
29	a	412	SQD	C10-C11-C12-C13
30	D	408	LHG	C32-C33-C34-C35
30	d	408	LHG	C29-C30-C31-C32
31	c	517	DGD	C6B-C7B-C8B-C9B
34	H	103	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	Z	101	STE	C11-C12-C13-C14
34	a	415	STE	C7-C8-C9-C10
30	A	414	LHG	C23-C24-C25-C26
28	D	411	LMG	C14-C15-C16-C17
28	b	624	LMG	C17-C18-C19-C20
28	d	410	LMG	C33-C34-C35-C36
29	a	412	SQD	C15-C16-C17-C18
30	A	414	LHG	C15-C16-C17-C18
30	D	409	LHG	C10-C11-C12-C13
30	e	102	LHG	C16-C17-C18-C19
30	l	101	LHG	C27-C28-C29-C30
31	A	416	DGD	C6B-C7B-C8B-C9B
31	c	518	DGD	C5B-C6B-C7B-C8B
34	B	620	STE	C4-C5-C6-C7
34	B	626	STE	C5-C6-C7-C8
34	H	103	STE	C13-C14-C15-C16
34	T	102	STE	C12-C13-C14-C15
22	C	513	CLA	O1A-CGA-O2A-C1
29	B	623	SQD	C33-C34-C35-C36
30	A	414	LHG	C11-C12-C13-C14
30	e	102	LHG	C24-C25-C26-C27
31	H	102	DGD	C7A-C8A-C9A-CAA
31	c	518	DGD	C7A-C8A-C9A-CAA
34	d	411	STE	C5-C6-C7-C8
31	c	516	DGD	C6B-C7B-C8B-C9B
34	a	415	STE	C5-C6-C7-C8
34	l	102	STE	C13-C14-C15-C16
29	B	623	SQD	C11-C12-C13-C14
29	a	411	SQD	C24-C25-C26-C27
31	A	416	DGD	CBB-CCB-CDB-CEB
34	c	520	STE	C11-C12-C13-C14
22	c	512	CLA	C16-C17-C18-C19
28	b	622	LMG	C28-C29-C30-C31
28	b	622	LMG	O10-C28-O8-C9
22	B	601	CLA	C2B-C3B-CAB-CBB
22	b	605	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
24	D	404	BCR	C23-C24-C25-C26
24	D	404	BCR	C23-C24-C25-C30
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
28	D	411	LMG	C32-C33-C34-C35
28	c	521	LMG	C31-C32-C33-C34
29	b	620	SQD	C29-C30-C31-C32
34	R	101	STE	C3-C4-C5-C6
34	h	102	STE	C9-C10-C11-C12
28	D	406	LMG	C35-C36-C37-C38
28	A	412	LMG	C16-C17-C18-C19
28	D	411	LMG	C30-C31-C32-C33
28	b	622	LMG	C37-C38-C39-C40
31	c	517	DGD	C8A-C9A-CAA-CBA
31	C	516	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	C5B-C6B-C7B-C8B
28	b	622	LMG	C18-C19-C20-C21
34	t	102	STE	C4-C5-C6-C7
28	D	411	LMG	C31-C32-C33-C34
31	C	517	DGD	C6A-C7A-C8A-C9A
34	b	627	STE	C6-C7-C8-C9
24	B	619	BCR	C10-C11-C12-C13
22	b	609	CLA	C13-C15-C16-C17
22	c	506	CLA	C2-C3-C5-C6
29	B	623	SQD	C13-C14-C15-C16
30	D	408	LHG	C11-C12-C13-C14
31	c	518	DGD	C6A-C7A-C8A-C9A
31	h	101	DGD	C2B-C3B-C4B-C5B
34	j	101	STE	C4-C5-C6-C7
23	A	404	PHO	C14-C13-C15-C16
29	A	413	SQD	C13-C14-C15-C16
30	B	622	LHG	C10-C11-C12-C13
31	C	517	DGD	C5A-C6A-C7A-C8A
24	B	618	BCR	C22-C23-C24-C25
28	A	412	LMG	C34-C35-C36-C37
28	C	518	LMG	C31-C32-C33-C34
29	D	407	SQD	C30-C31-C32-C33
22	c	501	CLA	O1D-CGD-O2D-CED
29	D	407	SQD	C2-C1-O6-C44
28	c	522	LMG	C17-C18-C19-C20
34	I	101	STE	C11-C10-C9-C8
34	d	413	STE	C9-C10-C11-C12
34	l	102	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	M	101	LMG	C12-C13-C14-C15
28	b	624	LMG	C11-C12-C13-C14
28	b	624	LMG	C32-C33-C34-C35
34	a	415	STE	C9-C10-C11-C12
30	d	408	LHG	C12-C13-C14-C15
30	l	101	LHG	C26-C27-C28-C29
22	b	601	CLA	C3-C5-C6-C7
22	d	403	CLA	C3-C5-C6-C7
22	B	616	CLA	C11-C12-C13-C14
28	M	101	LMG	C36-C37-C38-C39
34	B	620	STE	C1-C2-C3-C4
34	C	519	STE	C1-C2-C3-C4
28	d	410	LMG	C38-C39-C40-C41
29	a	411	SQD	C27-C28-C29-C30
29	A	413	SQD	C16-C17-C18-C19
31	A	416	DGD	C5B-C6B-C7B-C8B
22	C	504	CLA	C11-C12-C13-C14
24	T	101	BCR	C36-C18-C19-C20
24	c	514	BCR	C7-C8-C9-C34
24	k	101	BCR	C36-C18-C19-C20
28	D	406	LMG	C39-C40-C41-C42
28	M	101	LMG	C29-C30-C31-C32
29	B	623	SQD	C34-C35-C36-C37
34	l	102	STE	C12-C13-C14-C15
36	v	201	HEC	C4C-C3C-CAC-CBC
28	c	521	LMG	C34-C35-C36-C37
30	d	407	LHG	C31-C32-C33-C34
28	a	416	LMG	C8-C7-O1-C1
28	c	522	LMG	C33-C34-C35-C36
30	D	408	LHG	C9-C10-C11-C12
34	B	626	STE	C11-C10-C9-C8
34	X	101	STE	C11-C10-C9-C8
22	B	601	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C20
22	a	403	CLA	C16-C17-C18-C19
22	a	403	CLA	C16-C17-C18-C20
29	a	412	SQD	C9-C10-C11-C12
31	A	416	DGD	C2B-C3B-C4B-C5B
34	H	103	STE	C5-C6-C7-C8
34	M	102	STE	C11-C10-C9-C8
34	b	623	STE	C13-C14-C15-C16
34	d	412	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	410	PL9	C45-C44-C46-C47
31	C	515	DGD	C2A-C3A-C4A-C5A
22	B	603	CLA	C5-C6-C7-C8
22	c	504	CLA	C8-C10-C11-C12
28	D	406	LMG	C21-C22-C23-C24
28	b	622	LMG	C14-C15-C16-C17
31	C	515	DGD	C6B-C7B-C8B-C9B
31	c	518	DGD	C9B-CAB-CBB-CCB
34	a	413	STE	C2-C3-C4-C5
30	d	409	LHG	O10-C23-O8-C6
23	d	402	PHO	C2C-C3C-CAC-CBC
22	B	605	CLA	C8-C10-C11-C12
22	C	504	CLA	C8-C10-C11-C12
28	A	412	LMG	C28-C29-C30-C31
31	c	518	DGD	C2A-C3A-C4A-C5A
30	d	407	LHG	C25-C26-C27-C28
22	B	606	CLA	C16-C17-C18-C20
30	A	414	LHG	C32-C33-C34-C35
30	d	407	LHG	C16-C17-C18-C19
34	B	626	STE	C12-C13-C14-C15
34	b	627	STE	C2-C3-C4-C5
31	c	516	DGD	O6E-C5E-C6E-O5E
28	a	416	LMG	C11-C12-C13-C14
29	b	620	SQD	C26-C27-C28-C29
30	D	409	LHG	C32-C33-C34-C35
31	A	416	DGD	C4A-C5A-C6A-C7A
30	d	407	LHG	C7-C8-C9-C10
22	C	509	CLA	C8-C10-C11-C12
29	a	411	SQD	C32-C33-C34-C35
28	c	521	LMG	O6-C5-C6-O5
28	c	521	LMG	O1-C7-C8-O7
28	a	416	LMG	C30-C31-C32-C33
29	f	101	SQD	C28-C29-C30-C31
31	C	515	DGD	C5A-C6A-C7A-C8A
31	H	102	DGD	C9A-CAA-CBA-CCA
34	H	103	STE	C14-C15-C16-C17
34	X	101	STE	C7-C8-C9-C10
34	b	623	STE	C10-C11-C12-C13
34	t	102	STE	C11-C10-C9-C8
28	c	519	LMG	O6-C5-C6-O5
28	C	518	LMG	C18-C19-C20-C21
29	a	411	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C30-C31-C32-C33
30	D	409	LHG	C31-C32-C33-C34
31	c	516	DGD	C3B-C4B-C5B-C6B
34	H	103	STE	C12-C13-C14-C15
34	X	101	STE	C4-C5-C6-C7
34	d	411	STE	C9-C10-C11-C12
22	B	612	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C20
22	b	606	CLA	C10-C11-C12-C13
28	b	624	LMG	C31-C32-C33-C34
34	d	411	STE	C4-C5-C6-C7
28	a	416	LMG	O6-C5-C6-O5
22	C	510	CLA	C4-C3-C5-C6
34	B	625	STE	C1-C2-C3-C4
22	C	510	CLA	C2-C3-C5-C6
28	C	518	LMG	C30-C31-C32-C33
28	c	522	LMG	C15-C16-C17-C18
29	b	620	SQD	C24-C25-C26-C27
31	H	102	DGD	CCA-CDA-CEA-CFA
24	B	618	BCR	C14-C15-C16-C17
31	h	101	DGD	C6B-C7B-C8B-C9B
34	C	521	STE	C5-C6-C7-C8
34	d	412	STE	C6-C7-C8-C9
30	d	407	LHG	C34-C35-C36-C37
34	B	625	STE	C9-C10-C11-C12
34	b	623	STE	C9-C10-C11-C12
22	b	613	CLA	C13-C15-C16-C17
22	b	614	CLA	C5-C6-C7-C8
31	C	516	DGD	C9A-CAA-CBA-CCA
34	X	101	STE	C12-C13-C14-C15
22	b	607	CLA	O1D-CGD-O2D-CED
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
28	a	416	LMG	C33-C34-C35-C36
30	d	407	LHG	C15-C16-C17-C18
30	d	407	LHG	C29-C30-C31-C32
34	H	103	STE	C11-C12-C13-C14
34	b	623	STE	C2-C3-C4-C5
22	A	402	CLA	C4C-C3C-CAC-CBC
30	D	409	LHG	C30-C31-C32-C33
31	C	516	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
34	M	102	STE	C9-C10-C11-C12
22	B	601	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
30	D	409	LHG	C24-C25-C26-C27
27	d	406	PL9	C47-C48-C49-C51
28	b	622	LMG	C11-C12-C13-C14
30	B	621	LHG	C18-C19-C20-C21
31	H	102	DGD	CAA-CBA-CCA-CDA
31	H	102	DGD	CAB-CBB-CCB-CDB
31	c	518	DGD	C5A-C6A-C7A-C8A
30	B	621	LHG	O9-C7-O7-C5
31	c	516	DGD	O1B-C1B-O2G-C2G
29	a	411	SQD	C15-C16-C17-C18
30	d	408	LHG	C14-C15-C16-C17
22	B	603	CLA	C12-C13-C15-C16
22	B	606	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	601	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C12-C13-C15
30	d	407	LHG	C33-C34-C35-C36
31	H	102	DGD	C5B-C6B-C7B-C8B
34	X	101	STE	C13-C14-C15-C16
31	c	518	DGD	CBA-CCA-CDA-CEA
30	B	621	LHG	C30-C31-C32-C33
31	c	518	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	C1A-C2A-C3A-C4A
27	D	405	PL9	C30-C29-C31-C32
22	c	510	CLA	C2-C3-C5-C6
27	A	410	PL9	C33-C34-C36-C37
30	D	409	LHG	C11-C12-C13-C14
22	c	509	CLA	C15-C16-C17-C18
22	B	603	CLA	C14-C13-C15-C16
22	B	604	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	c	506	CLA	C6-C7-C8-C9
22	c	510	CLA	C14-C13-C15-C16
30	l	101	LHG	C33-C34-C35-C36
34	X	101	STE	C2-C3-C4-C5
30	B	621	LHG	C32-C33-C34-C35
22	d	404	CLA	O1D-CGD-O2D-CED
30	e	102	LHG	C27-C28-C29-C30
28	d	410	LMG	O6-C5-C6-O5
31	C	515	DGD	O6E-C5E-C6E-O5E
29	B	623	SQD	C35-C36-C37-C38
28	C	518	LMG	O1-C7-C8-C9
28	c	522	LMG	O1-C7-C8-C9
29	B	623	SQD	O6-C44-C45-C46
29	a	411	SQD	O6-C44-C45-C46
30	d	409	LHG	C4-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-C3G
28	a	416	LMG	C39-C40-C41-C42
30	A	414	LHG	C30-C31-C32-C33
31	A	416	DGD	CAB-CBB-CCB-CDB
34	l	102	STE	C9-C10-C11-C12
34	B	625	STE	C13-C14-C15-C16
22	c	510	CLA	C16-C17-C18-C20
34	C	519	STE	C2-C3-C4-C5
31	c	516	DGD	C4D-C5D-C6D-O5D
28	a	416	LMG	C32-C33-C34-C35
30	A	414	LHG	C28-C29-C30-C31
24	B	617	BCR	C20-C21-C22-C37
22	C	506	CLA	C3-C5-C6-C7
31	h	101	DGD	O6E-C5E-C6E-O5E
29	A	413	SQD	C34-C35-C36-C37
30	d	407	LHG	C27-C28-C29-C30
34	d	411	STE	C6-C7-C8-C9
22	c	510	CLA	C4-C3-C5-C6
27	D	405	PL9	C13-C14-C16-C17
34	b	625	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	d	404	CLA	C8-C10-C11-C12
24	B	619	BCR	C37-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24
30	D	408	LHG	C33-C34-C35-C36
31	C	516	DGD	C3A-C4A-C5A-C6A
34	c	523	STE	C6-C7-C8-C9
22	C	513	CLA	C8-C10-C11-C12
22	a	404	CLA	C5-C6-C7-C8
28	d	410	LMG	C14-C15-C16-C17
31	h	101	DGD	CAB-CBB-CCB-CDB
28	a	416	LMG	C34-C35-C36-C37
30	D	409	LHG	C27-C28-C29-C30
22	C	505	CLA	C15-C16-C17-C18
22	C	506	CLA	C5-C6-C7-C8
34	h	102	STE	C7-C8-C9-C10
28	b	624	LMG	C16-C17-C18-C19
29	A	415	SQD	C18-C19-C20-C21
30	A	414	LHG	C16-C17-C18-C19
31	C	516	DGD	C9B-CAB-CBB-CCB
29	a	411	SQD	C35-C36-C37-C38
28	D	411	LMG	C16-C17-C18-C19
28	b	624	LMG	C30-C31-C32-C33
28	d	410	LMG	C30-C31-C32-C33
29	A	413	SQD	C9-C10-C11-C12
30	d	408	LHG	C16-C17-C18-C19
34	L	101	STE	C4-C5-C6-C7
34	d	411	STE	C7-C8-C9-C10
24	B	617	BCR	C10-C11-C12-C13
22	c	503	CLA	C5-C6-C7-C8
22	c	509	CLA	C8-C10-C11-C12
28	a	416	LMG	C18-C19-C20-C21
30	l	101	LHG	C15-C16-C17-C18
31	c	518	DGD	CBB-CCB-CDB-CEB
34	B	625	STE	C11-C12-C13-C14
24	k	101	BCR	C19-C20-C21-C22
31	c	516	DGD	C1A-C2A-C3A-C4A
28	c	519	LMG	C36-C37-C38-C39
31	c	518	DGD	C2A-C1A-O1G-C1G
30	l	101	LHG	C7-C8-C9-C10
34	C	520	STE	C4-C5-C6-C7
28	b	624	LMG	C34-C35-C36-C37
34	C	519	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	I	101	STE	C5-C6-C7-C8
34	B	627	STE	C7-C8-C9-C10
34	a	413	STE	C7-C8-C9-C10
28	c	521	LMG	C41-C42-C43-C44
34	B	626	STE	C6-C7-C8-C9
34	H	103	STE	C3-C4-C5-C6
34	a	415	STE	C6-C7-C8-C9
34	h	102	STE	C6-C7-C8-C9
28	D	406	LMG	C36-C37-C38-C39
31	C	517	DGD	C8B-C9B-CAB-CBB
34	M	103	STE	C4-C5-C6-C7
34	b	621	STE	C7-C8-C9-C10
30	A	414	LHG	C19-C20-C21-C22
30	d	407	LHG	C19-C20-C21-C22
28	a	416	LMG	C38-C39-C40-C41
29	B	623	SQD	C9-C10-C11-C12
30	D	408	LHG	C13-C14-C15-C16
34	d	411	STE	C11-C12-C13-C14
28	c	522	LMG	O1-C7-C8-O7
34	B	626	STE	C14-C15-C16-C17
34	b	623	STE	C5-C6-C7-C8
29	A	413	SQD	C17-C18-C19-C20
30	D	409	LHG	C35-C36-C37-C38
28	c	519	LMG	C34-C35-C36-C37
28	c	522	LMG	C31-C32-C33-C34
30	D	408	LHG	C25-C26-C27-C28
22	c	508	CLA	C16-C17-C18-C19
34	C	520	STE	C3-C4-C5-C6
34	I	101	STE	C1-C2-C3-C4
30	d	409	LHG	C26-C27-C28-C29
22	c	513	CLA	C3-C5-C6-C7
28	b	624	LMG	C42-C43-C44-C45
29	a	412	SQD	C31-C32-C33-C34
22	b	616	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	C2-C1-O2A-CGA
29	a	412	SQD	C28-C29-C30-C31
29	A	415	SQD	C19-C20-C21-C22
31	C	517	DGD	CDB-CEB-CFB-CGB
28	c	521	LMG	C12-C13-C14-C15
31	h	101	DGD	C7A-C8A-C9A-CAA
34	B	627	STE	C2-C3-C4-C5
28	D	410	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	B	621	LHG	C27-C28-C29-C30
34	c	520	STE	C3-C4-C5-C6
34	l	102	STE	C7-C8-C9-C10
30	d	409	LHG	C35-C36-C37-C38
27	D	405	PL9	C7-C8-C9-C10
27	D	405	PL9	C37-C38-C39-C40
27	a	409	PL9	C37-C38-C39-C40
31	h	101	DGD	C3B-C4B-C5B-C6B
30	B	622	LHG	C18-C19-C20-C21
31	C	517	DGD	C3A-C4A-C5A-C6A
22	B	610	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
29	A	413	SQD	C28-C29-C30-C31
28	b	624	LMG	C12-C13-C14-C15
31	C	515	DGD	CBA-CCA-CDA-CEA
31	C	516	DGD	C6B-C7B-C8B-C9B
34	C	519	STE	C3-C4-C5-C6
22	A	403	CLA	C11-C12-C13-C14
22	B	605	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	a	403	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
22	b	615	CLA	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C12-C13-C14
34	c	520	STE	C4-C5-C6-C7
22	C	511	CLA	C15-C16-C17-C18
22	b	605	CLA	C5-C6-C7-C8
22	C	512	CLA	C4B-C3B-CAB-CBB
30	d	407	LHG	C18-C19-C20-C21
22	C	508	CLA	C10-C11-C12-C13
29	f	101	SQD	C35-C36-C37-C38
34	B	626	STE	C3-C4-C5-C6
34	d	412	STE	C7-C8-C9-C10
34	d	411	STE	C12-C13-C14-C15
30	B	622	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	b	621	STE	C10-C11-C12-C13
28	c	522	LMG	C2-C1-O1-C7
22	B	608	CLA	C13-C15-C16-C17
28	A	412	LMG	C12-C13-C14-C15
28	A	412	LMG	C33-C34-C35-C36
28	b	622	LMG	C31-C32-C33-C34
30	B	622	LHG	C24-C25-C26-C27
30	B	622	LHG	C28-C29-C30-C31
30	e	102	LHG	C11-C12-C13-C14
34	X	101	STE	C10-C11-C12-C13
34	B	624	STE	C7-C8-C9-C10
30	d	408	LHG	O6-C4-C5-C6
30	e	102	LHG	O6-C4-C5-C6
30	D	409	LHG	C33-C34-C35-C36
34	d	413	STE	C2-C3-C4-C5
31	c	516	DGD	CDB-CEB-CFB-CGB
22	B	604	CLA	C12-C13-C15-C16
22	B	605	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
22	c	512	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	C	510	CLA	C10-C11-C12-C13
34	c	523	STE	C7-C8-C9-C10
28	D	406	LMG	C32-C33-C34-C35
22	B	611	CLA	C16-C17-C18-C20
31	C	516	DGD	CDA-CEA-CFA-CGA
22	B	601	CLA	C3A-C2A-CAA-CBA
27	A	410	PL9	C28-C29-C31-C32
31	A	416	DGD	CFA-CGA-CHA-CIA
31	C	515	DGD	C4B-C5B-C6B-C7B
34	b	623	STE	C6-C7-C8-C9
22	b	607	CLA	C13-C15-C16-C17
28	c	519	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	C	518	LMG	C19-C20-C21-C22
24	C	514	BCR	C11-C12-C13-C35
24	b	617	BCR	C36-C18-C19-C20
28	a	416	LMG	C23-C24-C25-C26
31	C	517	DGD	CBA-CCA-CDA-CEA
34	R	101	STE	C4-C5-C6-C7
28	C	518	LMG	C39-C40-C41-C42
31	A	416	DGD	CEB-CFB-CGB-CHB
34	R	101	STE	C6-C7-C8-C9
28	a	416	LMG	C37-C38-C39-C40
29	B	623	SQD	C27-C28-C29-C30
30	A	414	LHG	C9-C10-C11-C12
30	B	622	LHG	C1-C2-C3-O3
30	B	622	LHG	C31-C32-C33-C34
31	A	416	DGD	CCA-CDA-CEA-CFA
22	B	609	CLA	C13-C15-C16-C17
28	M	101	LMG	C7-C8-C9-O8
28	c	521	LMG	O1-C7-C8-C9
28	c	521	LMG	C7-C8-C9-O8
29	a	412	SQD	C44-C45-C46-O48
22	A	405	CLA	C6-C7-C8-C9
34	b	621	STE	C15-C16-C17-C18
22	C	505	CLA	C16-C17-C18-C20
31	C	516	DGD	C2A-C3A-C4A-C5A
34	C	521	STE	C6-C7-C8-C9
28	D	410	LMG	O1-C7-C8-C9
31	c	518	DGD	C6B-C7B-C8B-C9B
22	B	609	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
30	B	621	LHG	C23-C24-C25-C26
34	d	413	STE	C3-C4-C5-C6
27	d	406	PL9	C13-C14-C16-C17
28	D	406	LMG	C11-C12-C13-C14
22	B	610	CLA	C15-C16-C17-C18
34	B	626	STE	C15-C16-C17-C18
29	a	412	SQD	C14-C15-C16-C17
22	B	603	CLA	C16-C17-C18-C19
22	C	505	CLA	C16-C17-C18-C19
28	D	410	LMG	C35-C36-C37-C38
24	b	617	BCR	C1-C6-C7-C8
24	d	405	BCR	C23-C24-C25-C30
24	k	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	b	622	LMG	C34-C35-C36-C37
30	B	622	LHG	C25-C26-C27-C28
31	c	517	DGD	CAA-CBA-CCA-CDA
22	b	606	CLA	C5-C6-C7-C8
22	C	501	CLA	CBD-CGD-O2D-CED
22	a	402	CLA	CBD-CGD-O2D-CED
28	D	406	LMG	C30-C31-C32-C33
34	l	102	STE	C1-C2-C3-C4
27	a	409	PL9	C47-C48-C49-C50
30	l	101	LHG	C34-C35-C36-C37
34	C	520	STE	C12-C13-C14-C15
22	B	605	CLA	C16-C17-C18-C20
22	B	610	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
22	b	615	CLA	C8-C10-C11-C12
28	b	622	LMG	O7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-O47
29	a	411	SQD	O47-C45-C46-O48
29	a	412	SQD	O47-C45-C46-O48
30	A	414	LHG	O7-C5-C6-O8
30	B	621	LHG	C19-C20-C21-C22
27	a	409	PL9	C4-C3-C7-C8
28	c	519	LMG	C11-C10-O7-C8
30	l	101	LHG	C13-C14-C15-C16
34	L	101	STE	C7-C8-C9-C10
28	D	406	LMG	C12-C13-C14-C15
28	M	101	LMG	C15-C16-C17-C18
30	d	408	LHG	C17-C18-C19-C20
24	d	405	BCR	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
22	c	507	CLA	C8-C10-C11-C12
23	A	404	PHO	C2-C3-C5-C6
30	D	408	LHG	C14-C15-C16-C17
31	c	516	DGD	C8A-C9A-CAA-CBA
31	A	416	DGD	CBA-CCA-CDA-CEA
34	b	621	STE	C5-C6-C7-C8
34	c	520	STE	C7-C8-C9-C10
22	c	512	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
31	C	517	DGD	CAB-CBB-CCB-CDB
28	c	521	LMG	C29-C30-C31-C32
30	l	101	LHG	C31-C32-C33-C34
34	b	627	STE	C1-C2-C3-C4
34	b	627	STE	C4-C5-C6-C7
22	c	511	CLA	O1D-CGD-O2D-CED
24	A	406	BCR	C14-C15-C16-C17
28	C	518	LMG	C38-C39-C40-C41
28	a	416	LMG	C35-C36-C37-C38
30	l	101	LHG	C9-C10-C11-C12
30	e	102	LHG	C28-C29-C30-C31
28	c	521	LMG	C35-C36-C37-C38
28	c	519	LMG	C30-C31-C32-C33
28	D	410	LMG	O1-C7-C8-O7
30	d	407	LHG	C13-C14-C15-C16
34	d	413	STE	C12-C13-C14-C15
31	c	518	DGD	C8B-C9B-CAB-CBB
31	h	101	DGD	CDA-CEA-CFA-CGA
34	H	103	STE	C1-C2-C3-C4
22	D	403	CLA	C8-C10-C11-C12
22	A	405	CLA	CBA-CGA-O2A-C1
31	A	416	DGD	C2A-C1A-O1G-C1G
22	B	609	CLA	C2-C3-C5-C6
30	B	622	LHG	C12-C13-C14-C15
22	a	402	CLA	O1D-CGD-O2D-CED
30	B	622	LHG	C19-C20-C21-C22
29	a	411	SQD	C16-C17-C18-C19
31	c	516	DGD	C3A-C4A-C5A-C6A
34	l	102	STE	C14-C15-C16-C17
28	A	412	LMG	C40-C41-C42-C43
28	C	518	LMG	C37-C38-C39-C40
31	c	518	DGD	CCA-CDA-CEA-CFA
24	B	618	BCR	C16-C17-C18-C36
24	K	102	BCR	C16-C17-C18-C36
24	b	617	BCR	C16-C17-C18-C36
24	b	619	BCR	C20-C21-C22-C37
24	d	405	BCR	C20-C21-C22-C37
24	k	102	BCR	C20-C21-C22-C37
22	c	510	CLA	C13-C15-C16-C17
22	b	608	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C8-C10-C11-C12
22	c	512	CLA	C8-C10-C11-C12
34	B	620	STE	C7-C8-C9-C10
22	A	403	CLA	C11-C10-C8-C7
22	A	403	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C7
22	b	603	CLA	C11-C10-C8-C7
22	b	604	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	c	511	CLA	C12-C13-C15-C16
22	c	512	CLA	C12-C13-C15-C16
28	b	624	LMG	C28-C29-C30-C31
30	d	409	LHG	C7-C8-C9-C10
31	A	416	DGD	C1B-C2B-C3B-C4B
28	C	518	LMG	C15-C16-C17-C18
27	A	410	PL9	C17-C18-C19-C20
31	A	416	DGD	C7B-C8B-C9B-CAB
34	M	102	STE	C3-C4-C5-C6
22	b	616	CLA	C10-C11-C12-C13
24	K	101	BCR	C11-C12-C13-C14
24	K	101	BCR	C17-C18-C19-C20
30	d	407	LHG	C17-C18-C19-C20
34	h	102	STE	C10-C11-C12-C13
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C5D-C6D-O5D-C1E
31	C	515	DGD	C9A-CAA-CBA-CCA
22	b	614	CLA	C8-C10-C11-C12
22	c	513	CLA	C13-C15-C16-C17
22	c	501	CLA	C2A-CAA-CBA-CGA
29	a	411	SQD	C10-C11-C12-C13
29	A	415	SQD	C30-C31-C32-C33
30	D	409	LHG	C14-C15-C16-C17
28	D	410	LMG	C9-C8-O7-C10
28	a	416	LMG	C9-C8-O7-C10
28	b	624	LMG	C37-C38-C39-C40
30	A	414	LHG	C27-C28-C29-C30
22	c	505	CLA	C13-C15-C16-C17
28	M	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	a	413	STE	C4-C5-C6-C7
24	k	101	BCR	C11-C10-C9-C8
28	D	410	LMG	C13-C14-C15-C16
34	T	102	STE	C10-C11-C12-C13
34	a	414	STE	C3-C4-C5-C6
34	d	412	STE	C5-C6-C7-C8
34	d	412	STE	C11-C12-C13-C14
28	b	622	LMG	C7-C8-C9-O8
28	b	624	LMG	O1-C7-C8-C9
29	f	101	SQD	C44-C45-C46-O48
30	A	414	LHG	C4-C5-C6-O8
31	A	416	DGD	C1G-C2G-C3G-O3G
35	F	101	HEM	C4C-C3C-CAC-CBC
35	e	101	HEM	C4B-C3B-CAB-CBB
22	b	612	CLA	C16-C17-C18-C20
34	d	412	STE	C15-C16-C17-C18
31	C	516	DGD	CBA-CCA-CDA-CEA
29	a	411	SQD	C11-C10-C9-C8
28	c	521	LMG	C13-C14-C15-C16
28	C	518	LMG	O1-C7-C8-O7
28	M	101	LMG	O7-C8-C9-O8
28	c	521	LMG	O7-C8-C9-O8
22	B	610	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C10-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	A	411	CLA	C16-C17-C18-C19
28	b	622	LMG	C39-C40-C41-C42
29	f	101	SQD	C24-C25-C26-C27
31	c	516	DGD	C5A-C6A-C7A-C8A
34	H	103	STE	C2-C3-C4-C5
30	D	409	LHG	O9-C7-O7-C5
28	M	101	LMG	C14-C15-C16-C17
28	b	622	LMG	C13-C14-C15-C16
28	c	521	LMG	C15-C16-C17-C18
31	H	102	DGD	C5A-C6A-C7A-C8A
30	B	622	LHG	C26-C27-C28-C29
30	d	407	LHG	C28-C29-C30-C31
31	A	416	DGD	C8A-C9A-CAA-CBA
34	B	627	STE	C6-C7-C8-C9
34	c	520	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	d	413	STE	C11-C12-C13-C14
22	c	502	CLA	C13-C15-C16-C17
28	D	406	LMG	C17-C18-C19-C20
28	b	624	LMG	C40-C41-C42-C43
30	D	409	LHG	C26-C27-C28-C29
28	D	411	LMG	C12-C13-C14-C15
22	b	611	CLA	C10-C11-C12-C13
30	B	621	LHG	C16-C17-C18-C19
28	C	518	LMG	C2-C1-O1-C7
34	b	627	STE	C5-C6-C7-C8
27	a	409	PL9	C12-C13-C14-C16
30	B	622	LHG	C9-C10-C11-C12
22	C	506	CLA	C4-C3-C5-C6
29	D	407	SQD	C25-C26-C27-C28
30	B	622	LHG	O2-C2-C3-O3
34	X	101	STE	C5-C6-C7-C8
22	b	610	CLA	C2A-CAA-CBA-CGA
22	b	608	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C14
22	c	505	CLA	C5-C6-C7-C8
28	b	622	LMG	C19-C20-C21-C22
31	c	516	DGD	CBB-CCB-CDB-CEB
34	B	620	STE	C11-C10-C9-C8
34	C	520	STE	C7-C8-C9-C10
28	b	622	LMG	C12-C13-C14-C15
29	A	413	SQD	C10-C11-C12-C13
28	b	622	LMG	C16-C17-C18-C19
29	b	620	SQD	C12-C13-C14-C15
34	d	413	STE	C4-C5-C6-C7
34	d	411	STE	C1-C2-C3-C4
22	C	512	CLA	C3-C5-C6-C7
29	D	407	SQD	C44-C45-C46-O48
22	B	601	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
22	a	404	CLA	C10-C11-C12-C13
24	c	514	BCR	C17-C18-C19-C20
34	c	520	STE	C10-C11-C12-C13
34	a	415	STE	C1-C2-C3-C4
31	c	517	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	CBB-CCB-CDB-CEB
28	C	518	LMG	O9-C10-O7-C8
30	B	622	LHG	O9-C7-O7-C5
30	e	102	LHG	O9-C7-O7-C5
29	B	623	SQD	C19-C20-C21-C22
22	A	411	CLA	C11-C12-C13-C15
22	A	411	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	605	CLA	C11-C10-C8-C7
22	B	609	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C12-C13-C15
22	b	602	CLA	C11-C12-C13-C15
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	c	510	CLA	C16-C17-C18-C19
34	T	102	STE	C5-C6-C7-C8
29	b	620	SQD	C15-C16-C17-C18
30	B	621	LHG	C26-C27-C28-C29
30	d	408	LHG	C15-C16-C17-C18
22	c	510	CLA	C8-C10-C11-C12
28	D	406	LMG	C34-C35-C36-C37
34	a	414	STE	C2-C3-C4-C5
22	A	405	CLA	O1A-CGA-O2A-C1
30	D	409	LHG	C2-C3-O3-P
31	C	515	DGD	CCB-CDB-CEB-CFB
27	D	405	PL9	C28-C29-C31-C32
22	b	604	CLA	C5-C6-C7-C8
31	H	102	DGD	CDB-CEB-CFB-CGB
30	d	408	LHG	O6-C4-C5-O7
22	a	410	CLA	C2C-C3C-CAC-CBC
22	B	605	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C12-C13-C14
22	c	506	CLA	C14-C13-C15-C16
22	c	502	CLA	C16-C17-C18-C19
29	A	413	SQD	C26-C27-C28-C29
31	C	515	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
28	a	416	LMG	C29-C30-C31-C32
30	l	101	LHG	C14-C15-C16-C17
30	e	102	LHG	C17-C18-C19-C20
22	b	616	CLA	C3-C5-C6-C7
22	a	403	CLA	C13-C15-C16-C17
28	a	416	LMG	O1-C7-C8-O7
28	b	624	LMG	O1-C7-C8-O7
28	b	624	LMG	O7-C8-C9-O8
29	b	620	SQD	O47-C45-C46-O48
29	f	101	SQD	O47-C45-C46-O48
30	d	409	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
28	M	101	LMG	C39-C40-C41-C42
28	b	624	LMG	C7-C8-C9-O8
31	C	517	DGD	C4B-C5B-C6B-C7B
22	C	512	CLA	C8-C10-C11-C12
30	d	409	LHG	C29-C30-C31-C32
28	d	410	LMG	C15-C16-C17-C18
22	B	607	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
28	A	412	LMG	C17-C18-C19-C20
28	D	406	LMG	C38-C39-C40-C41
28	c	521	LMG	C38-C39-C40-C41
28	A	412	LMG	C14-C15-C16-C17
31	c	516	DGD	C7A-C8A-C9A-CAA
31	C	516	DGD	CAB-CBB-CCB-CDB
22	B	607	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
24	c	514	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	A	415	SQD	C46-C45-O47-C7
30	A	414	LHG	C3-O3-P-O4
30	A	414	LHG	C3-O3-P-O5
30	A	414	LHG	C4-O6-P-O3
30	D	408	LHG	C4-O6-P-O5
30	D	409	LHG	C3-O3-P-O5
30	e	102	LHG	C3-O3-P-O6
22	c	502	CLA	C16-C17-C18-C20
22	c	505	CLA	C2B-C3B-CAB-CBB
28	M	101	LMG	C22-C23-C24-C25
28	C	518	LMG	C11-C12-C13-C14
34	Z	101	STE	C14-C15-C16-C17
28	C	518	LMG	C16-C17-C18-C19
34	T	102	STE	C13-C14-C15-C16
29	a	411	SQD	C23-C24-C25-C26
22	C	507	CLA	C5-C6-C7-C8
27	A	410	PL9	C4-C3-C7-C8
22	b	612	CLA	C16-C17-C18-C19
28	D	406	LMG	C14-C15-C16-C17
22	d	403	CLA	C8-C10-C11-C12
29	f	101	SQD	C44-C45-O47-C7
29	f	101	SQD	C46-C45-O47-C7
31	C	515	DGD	O1G-C1A-C2A-C3A
22	B	603	CLA	C10-C11-C12-C13
22	C	505	CLA	C2-C3-C5-C6
31	h	101	DGD	C7B-C8B-C9B-CAB
34	j	101	STE	C5-C6-C7-C8
34	T	102	STE	C15-C16-C17-C18
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	b	605	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	c	513	CLA	C6-C7-C8-C9
22	c	513	CLA	C11-C12-C13-C14
34	t	102	STE	C7-C8-C9-C10
22	A	403	CLA	C6-C7-C8-C10
22	B	611	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C11-C12-C13-C15
24	x	101	BCR	C12-C13-C14-C15
28	c	519	LMG	C39-C40-C41-C42
28	c	522	LMG	C13-C14-C15-C16
22	b	616	CLA	C11-C12-C13-C15
31	c	516	DGD	C2A-C3A-C4A-C5A
29	a	411	SQD	C7-C8-C9-C10
34	B	627	STE	C3-C4-C5-C6
27	d	406	PL9	C7-C8-C9-C10
31	A	416	DGD	O1G-C1G-C2G-O2G
31	C	515	DGD	O1G-C1G-C2G-O2G
31	C	517	DGD	C2A-C1A-O1G-C1G
24	k	102	BCR	C19-C20-C21-C22
29	A	415	SQD	C11-C10-C9-C8
34	I	101	STE	C9-C10-C11-C12
22	C	512	CLA	C2A-CAA-CBA-CGA
34	b	626	STE	C3-C4-C5-C6
31	C	517	DGD	O6D-C5D-C6D-O5D
36	V	201	HEC	C2B-C3B-CAB-CBB
22	B	601	CLA	C4-C3-C5-C6
22	c	509	CLA	CAA-CBA-CGA-O2A
22	B	601	CLA	C3-C5-C6-C7
29	b	620	SQD	C19-C20-C21-C22
34	d	412	STE	C4-C5-C6-C7
27	D	405	PL9	C27-C28-C29-C30
31	H	102	DGD	O2G-C1B-C2B-C3B
31	C	516	DGD	C2G-C3G-O3G-C1D
31	H	102	DGD	CBA-CCA-CDA-CEA
31	c	516	DGD	O1G-C1A-C2A-C3A
22	C	506	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
27	a	409	PL9	C38-C39-C41-C42
31	H	102	DGD	CCB-CDB-CEB-CFB
30	e	102	LHG	C7-C8-C9-C10
30	d	408	LHG	C9-C10-C11-C12
22	A	411	CLA	C11-C12-C13-C14
22	B	604	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C10-C8-C9
22	b	613	CLA	C14-C13-C15-C16
29	B	623	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	D	409	LHG	C15-C16-C17-C18
35	e	101	HEM	C2A-CAA-CBA-CGA
22	b	610	CLA	C16-C17-C18-C20
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	601	CLA	C2A-CAA-CBA-CGA
31	H	102	DGD	C6B-C7B-C8B-C9B
24	Y	101	BCR	C13-C14-C15-C16
29	A	415	SQD	C31-C32-C33-C34
30	B	621	LHG	C24-C25-C26-C27
30	B	622	LHG	C30-C31-C32-C33
34	b	626	STE	C11-C10-C9-C8
22	D	402	CLA	C12-C13-C15-C16
22	b	616	CLA	C8-C10-C11-C12
28	c	521	LMG	C36-C37-C38-C39
29	A	413	SQD	C31-C32-C33-C34
31	C	517	DGD	CBB-CCB-CDB-CEB
34	Z	101	STE	C13-C14-C15-C16
22	D	403	CLA	C3A-C2A-CAA-CBA
29	B	623	SQD	C30-C31-C32-C33
31	C	515	DGD	C2B-C3B-C4B-C5B
31	c	517	DGD	C4B-C5B-C6B-C7B
29	D	407	SQD	C34-C35-C36-C37
22	D	402	CLA	C10-C11-C12-C13
23	d	401	PHO	C2C-C3C-CAC-CBC
30	e	102	LHG	C12-C13-C14-C15
22	b	616	CLA	C2-C1-O2A-CGA
28	b	622	LMG	C40-C41-C42-C43
34	b	625	STE	C9-C10-C11-C12
29	b	620	SQD	C11-C12-C13-C14
34	c	520	STE	O2-C1-C2-C3
22	A	411	CLA	C4C-C3C-CAC-CBC
34	T	102	STE	C9-C10-C11-C12
34	X	101	STE	C9-C10-C11-C12
34	c	520	STE	O1-C1-C2-C3
28	D	411	LMG	C10-C11-C12-C13
22	B	601	CLA	C11-C12-C13-C14
22	B	605	CLA	C6-C7-C8-C9
22	C	511	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C12-C13-C14
22	D	403	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	610	CLA	C14-C13-C15-C16
22	b	606	CLA	C16-C17-C18-C20
31	h	101	DGD	CCB-CDB-CEB-CFB
31	h	101	DGD	O2G-C1B-C2B-C3B
29	B	623	SQD	C46-C45-O47-C7
22	b	612	CLA	C13-C15-C16-C17
36	V	201	HEC	CAD-CBD-CGD-O2D
22	b	603	CLA	C4-C3-C5-C6
34	B	625	STE	C4-C5-C6-C7
30	d	409	LHG	O1-C1-C2-O2
34	B	620	STE	O2-C1-C2-C3
30	A	414	LHG	C18-C19-C20-C21
24	B	618	BCR	C11-C10-C9-C8
22	C	502	CLA	C16-C17-C18-C19
29	A	415	SQD	C10-C11-C12-C13
31	C	515	DGD	O6D-C5D-C6D-O5D
22	C	502	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C2B-C3B-CAB-CBB
22	D	402	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	504	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C1-C6-C7-C8
24	K	102	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C30
24	c	514	BCR	C1-C6-C7-C8
24	d	405	BCR	C23-C24-C25-C26
24	k	102	BCR	C5-C6-C7-C8
24	k	102	BCR	C23-C24-C25-C30
24	x	101	BCR	C23-C24-C25-C30
34	B	620	STE	O1-C1-C2-C3
22	b	605	CLA	C10-C11-C12-C13
34	B	625	STE	C11-C10-C9-C8
28	A	412	LMG	C31-C32-C33-C34
30	A	414	LHG	C11-C10-C9-C8
34	L	101	STE	C3-C4-C5-C6
34	c	523	STE	O2-C1-C2-C3
22	D	403	CLA	C4-C3-C5-C6
27	a	409	PL9	C40-C39-C41-C42
30	e	102	LHG	C19-C20-C21-C22
28	c	522	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	B	621	LHG	O6-C4-C5-C6
31	h	101	DGD	CCA-CDA-CEA-CFA
34	c	523	STE	O1-C1-C2-C3
35	e	101	HEM	CAD-CBD-CGD-O1D
22	A	403	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	B	616	CLA	C11-C10-C8-C7
22	D	402	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	b	611	CLA	C12-C13-C15-C16
22	b	614	CLA	C12-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C10
22	d	404	CLA	C6-C7-C8-C10
23	d	401	PHO	C6-C7-C8-C10
22	c	503	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
28	D	406	LMG	C33-C34-C35-C36
28	D	411	LMG	C33-C34-C35-C36
30	d	409	LHG	C25-C26-C27-C28
31	C	515	DGD	C5B-C6B-C7B-C8B
34	B	625	STE	C12-C13-C14-C15
34	B	625	STE	O1-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
30	D	408	LHG	C28-C29-C30-C31
30	d	409	LHG	C27-C28-C29-C30
22	B	601	CLA	C2-C3-C5-C6
22	b	603	CLA	C2-C3-C5-C6
22	A	411	CLA	C16-C17-C18-C20
22	b	608	CLA	C13-C15-C16-C17
31	C	517	DGD	C9B-CAB-CBB-CCB
22	B	604	CLA	C2C-C3C-CAC-CBC
28	d	410	LMG	C34-C35-C36-C37
22	c	511	CLA	C11-C10-C8-C9
31	C	516	DGD	C2B-C3B-C4B-C5B
29	B	623	SQD	C45-C46-O48-C23
29	D	407	SQD	C26-C27-C28-C29
29	A	415	SQD	C24-C25-C26-C27
27	A	410	PL9	C11-C12-C13-C14
34	H	103	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	C	516	DGD	O6D-C1D-O3G-C3G
30	e	102	LHG	C23-C24-C25-C26
22	D	402	CLA	C2C-C3C-CAC-CBC
22	b	608	CLA	C4-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
27	a	409	PL9	C25-C24-C26-C27
30	d	409	LHG	C2-C3-O3-P
22	C	511	CLA	O1A-CGA-O2A-C1
35	F	101	HEM	CAD-CBD-CGD-O2D
28	D	410	LMG	C33-C34-C35-C36
34	d	413	STE	C15-C16-C17-C18
28	A	412	LMG	C7-C8-C9-O8
28	M	101	LMG	O1-C7-C8-C9
29	A	413	SQD	O6-C44-C45-C46
31	C	515	DGD	O1G-C1G-C2G-C3G
35	e	101	HEM	CAD-CBD-CGD-O2D
36	V	201	HEC	CAD-CBD-CGD-O1D
29	a	412	SQD	C11-C12-C13-C14
22	b	614	CLA	C2A-CAA-CBA-CGA
31	c	516	DGD	C8B-C9B-CAB-CBB
34	B	625	STE	O2-C1-C2-C3
34	a	414	STE	C6-C7-C8-C9
30	B	621	LHG	O6-C4-C5-O7
23	d	402	PHO	C4-C3-C5-C6
28	a	416	LMG	O8-C28-C29-C30
22	b	606	CLA	C16-C17-C18-C19
31	C	517	DGD	CCA-CDA-CEA-CFA
28	c	521	LMG	C33-C34-C35-C36
22	C	502	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
22	C	505	CLA	O1A-CGA-O2A-C1
29	a	411	SQD	C11-C12-C13-C14
34	b	625	STE	C10-C11-C12-C13
34	B	627	STE	O2-C1-C2-C3
22	B	602	CLA	C16-C17-C18-C19
23	A	404	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
24	H	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C20-C21-C22-C37
24	x	101	BCR	C20-C21-C22-C37
22	b	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C10-C11-C12-C13
23	d	402	PHO	C8-C10-C11-C12
36	v	201	HEC	CAD-CBD-CGD-O1D
28	D	406	LMG	C37-C38-C39-C40
30	A	414	LHG	C14-C15-C16-C17
22	a	410	CLA	C4C-C3C-CAC-CBC
30	B	621	LHG	C9-C10-C11-C12
31	C	516	DGD	C8A-C9A-CAA-CBA
36	v	201	HEC	CAD-CBD-CGD-O2D
30	B	621	LHG	C11-C12-C13-C14
28	c	522	LMG	C32-C33-C34-C35
28	b	624	LMG	O6-C1-O1-C7
28	A	412	LMG	O6-C5-C6-O5
22	B	604	CLA	C6-C7-C8-C10
22	b	613	CLA	C12-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C10
28	c	522	LMG	C37-C38-C39-C40
29	a	411	SQD	C18-C19-C20-C21
30	B	622	LHG	C15-C16-C17-C18
31	c	516	DGD	CCB-CDB-CEB-CFB
34	b	623	STE	O1-C1-C2-C3
29	A	415	SQD	C15-C16-C17-C18
34	J	101	STE	C5-C6-C7-C8
34	M	102	STE	C7-C8-C9-C10
27	a	409	PL9	C44-C46-C47-C48
24	Y	101	BCR	C11-C12-C13-C14
22	a	404	CLA	C11-C10-C8-C9
22	a	404	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C12-C13-C14
22	d	404	CLA	C14-C13-C15-C16
34	j	101	STE	C3-C4-C5-C6
22	B	613	CLA	C2-C1-O2A-CGA
22	A	403	CLA	C16-C17-C18-C19
22	A	411	CLA	C2C-C3C-CAC-CBC
22	B	607	CLA	C3A-C2A-CAA-CBA
22	d	404	CLA	C3A-C2A-CAA-CBA
31	h	101	DGD	O1B-C1B-C2B-C3B
34	b	623	STE	O2-C1-C2-C3
22	c	508	CLA	C2-C3-C5-C6
30	d	409	LHG	C11-C10-C9-C8
31	C	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
34	a	415	STE	C11-C10-C9-C8
22	C	512	CLA	O2A-C1-C2-C3
22	b	601	CLA	O2A-C1-C2-C3
28	b	624	LMG	C9-C8-O7-C10
34	t	102	STE	O2-C1-C2-C3
28	A	412	LMG	C38-C39-C40-C41
31	c	517	DGD	C4A-C5A-C6A-C7A
22	b	601	CLA	CAA-CBA-CGA-O2A
22	C	513	CLA	C16-C17-C18-C19
28	A	412	LMG	C18-C19-C20-C21
30	d	407	LHG	C35-C36-C37-C38
29	f	101	SQD	C32-C33-C34-C35
34	B	620	STE	C2-C3-C4-C5
22	a	403	CLA	C8-C10-C11-C12
30	A	414	LHG	C2-C3-O3-P
28	b	624	LMG	C15-C16-C17-C18
24	D	404	BCR	C22-C23-C24-C25
29	a	411	SQD	C44-C45-C46-O48
30	e	102	LHG	C4-C5-C6-O8
31	A	416	DGD	O1G-C1G-C2G-C3G
31	C	515	DGD	CDB-CEB-CFB-CGB
30	B	621	LHG	C17-C18-C19-C20
22	B	601	CLA	C2A-CAA-CBA-CGA
34	t	102	STE	O1-C1-C2-C3
34	C	519	STE	C6-C7-C8-C9
29	A	413	SQD	C29-C30-C31-C32
30	A	414	LHG	C10-C11-C12-C13
30	d	408	LHG	C25-C26-C27-C28
22	c	511	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	CAA-CBA-CGA-O2A
29	b	620	SQD	O6-C44-C45-O47
29	B	623	SQD	C29-C30-C31-C32
31	c	517	DGD	C3A-C4A-C5A-C6A
34	B	627	STE	O1-C1-C2-C3
22	A	411	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	511	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	c	508	CLA	C6-C7-C8-C9
22	c	508	CLA	C14-C13-C15-C16
24	A	406	BCR	C17-C18-C19-C20
34	I	101	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	h	101	DGD	CBB-CCB-CDB-CEB
22	B	603	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C11-C12-C13-C15
22	D	403	CLA	C6-C7-C8-C10
22	a	404	CLA	C11-C10-C8-C7
22	b	603	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	b	616	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	K	101	BCR	C23-C24-C25-C30
24	K	102	BCR	C23-C24-C25-C26
24	b	617	BCR	C5-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	k	102	BCR	C23-C24-C25-C26
24	x	101	BCR	C23-C24-C25-C26
22	D	402	CLA	C2-C1-O2A-CGA
34	l	102	STE	C2-C3-C4-C5
22	B	606	CLA	C8-C10-C11-C12
30	B	621	LHG	O7-C7-C8-C9
30	D	409	LHG	O8-C23-C24-C25
31	c	516	DGD	O6E-C1E-O5D-C6D
34	C	520	STE	C11-C12-C13-C14
22	A	403	CLA	C16-C17-C18-C20
29	b	620	SQD	C17-C18-C19-C20
27	d	406	PL9	C28-C29-C31-C32
28	D	411	LMG	O8-C28-C29-C30
28	c	522	LMG	C35-C36-C37-C38
29	a	411	SQD	C8-C7-O47-C45
30	e	102	LHG	C8-C7-O7-C5
29	a	411	SQD	O47-C7-C8-C9
22	c	511	CLA	C3-C5-C6-C7
28	d	410	LMG	C37-C38-C39-C40
31	c	517	DGD	C1B-C2B-C3B-C4B
28	b	622	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	x	101	BCR	C11-C10-C9-C34
34	a	414	STE	C4-C5-C6-C7
30	D	408	LHG	C29-C30-C31-C32
30	B	621	LHG	C11-C10-C9-C8
22	A	403	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	D	403	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C10-C8-C9
23	d	401	PHO	C6-C7-C8-C9
23	D	401	PHO	C8-C10-C11-C12
22	b	612	CLA	CAA-CBA-CGA-O2A
22	c	510	CLA	CAA-CBA-CGA-O2A
30	e	102	LHG	O8-C23-C24-C25
31	c	518	DGD	CAB-CBB-CCB-CDB
29	b	620	SQD	C44-C45-C46-O48
31	c	516	DGD	C9A-CAA-CBA-CCA
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C4B-C3B-CAB-CBB
22	D	402	CLA	C4B-C3B-CAB-CBB
22	c	513	CLA	C1A-C2A-CAA-CBA
22	b	616	CLA	CBA-CGA-O2A-C1
31	A	416	DGD	CDA-CEA-CFA-CGA
27	d	406	PL9	C20-C19-C21-C22
28	A	412	LMG	O6-C1-O1-C7
31	C	515	DGD	O6E-C1E-O5D-C6D
28	A	412	LMG	O1-C7-C8-O7
24	K	101	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
24	K	101	BCR	C9-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O2A
28	b	624	LMG	C23-C24-C25-C26
31	C	515	DGD	C4D-C5D-C6D-O5D
22	B	613	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C15
22	D	402	CLA	C11-C10-C8-C7
22	b	610	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C10-C8-C7
22	d	403	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C2C-C3C-CAC-CBC
34	L	101	STE	C5-C6-C7-C8
23	d	401	PHO	O2A-C1-C2-C3
28	a	416	LMG	C22-C23-C24-C25
34	C	521	STE	C3-C4-C5-C6
28	d	410	LMG	O7-C10-C11-C12
30	D	409	LHG	C13-C14-C15-C16
34	I	101	STE	C7-C8-C9-C10
22	B	610	CLA	C10-C11-C12-C13
22	B	610	CLA	C2A-CAA-CBA-CGA
22	C	513	CLA	C10-C11-C12-C13
22	b	610	CLA	C5-C6-C7-C8
30	D	409	LHG	O10-C23-C24-C25
34	b	626	STE	O1-C1-C2-C3
22	B	602	CLA	C3A-C2A-CAA-CBA
30	D	408	LHG	O10-C23-O8-C6
22	c	506	CLA	C8-C10-C11-C12
30	l	101	LHG	C28-C29-C30-C31
29	f	101	SQD	O48-C23-C24-C25
29	a	411	SQD	C12-C13-C14-C15
24	C	514	BCR	C16-C17-C18-C19
28	D	410	LMG	C11-C12-C13-C14
22	B	612	CLA	CAA-CBA-CGA-O1A
31	C	515	DGD	C3A-C4A-C5A-C6A
31	C	515	DGD	O1B-C1B-C2B-C3B
22	c	511	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	D	402	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
28	b	622	LMG	C35-C36-C37-C38
29	A	415	SQD	O10-C23-C24-C25
28	c	522	LMG	C11-C12-C13-C14
28	b	624	LMG	C18-C19-C20-C21
24	t	101	BCR	C11-C12-C13-C35
22	B	605	CLA	C2-C3-C5-C6
28	b	622	LMG	O8-C28-C29-C30
30	e	102	LHG	O10-C23-C24-C25
30	D	409	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	C2B-C3B-C4B-C5B
28	M	101	LMG	C8-C7-O1-C1
31	c	516	DGD	C5D-C6D-O5D-C1E
28	A	412	LMG	O7-C8-C9-O8
30	e	102	LHG	O7-C5-C6-O8
22	c	510	CLA	CAA-CBA-CGA-O1A
31	c	516	DGD	O1B-C1B-C2B-C3B
34	T	102	STE	C4-C5-C6-C7
35	e	101	HEM	CAA-CBA-CGA-O2A
30	B	622	LHG	C32-C33-C34-C35
22	D	403	CLA	C10-C11-C12-C13
22	a	410	CLA	C8-C10-C11-C12
28	a	416	LMG	O7-C10-C11-C12
28	C	518	LMG	C4-C5-C6-O5
22	B	609	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
34	B	624	STE	C3-C4-C5-C6
29	A	415	SQD	O48-C23-C24-C25
34	a	414	STE	O2-C1-C2-C3
22	a	402	CLA	C2-C1-O2A-CGA
28	M	101	LMG	C17-C18-C19-C20
30	l	101	LHG	O7-C7-C8-C9
30	D	408	LHG	C7-C8-C9-C10
34	B	624	STE	C1-C2-C3-C4
30	D	408	LHG	C11-C10-C9-C8
31	C	515	DGD	O2G-C1B-C2B-C3B
22	b	612	CLA	CAA-CBA-CGA-O1A
22	B	604	CLA	C4C-C3C-CAC-CBC
22	C	505	CLA	CBA-CGA-O2A-C1
34	C	521	STE	O2-C1-C2-C3

There are no ring outliers.

119 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	505	CLA	1	0
28	D	411	LMG	1	0
22	C	511	CLA	2	0
24	C	514	BCR	2	0
22	b	602	CLA	1	0
22	B	607	CLA	1	0
34	H	103	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	621	STE	3	0
28	a	416	LMG	3	0
34	d	412	STE	2	0
31	c	518	DGD	2	0
23	A	404	PHO	1	0
24	H	101	BCR	1	0
34	d	413	STE	2	0
30	e	102	LHG	1	0
23	d	402	PHO	1	0
29	D	407	SQD	1	0
34	j	101	STE	2	0
24	b	618	BCR	2	0
22	B	606	CLA	2	0
34	h	102	STE	3	0
22	b	601	CLA	2	0
28	A	412	LMG	2	0
22	D	403	CLA	2	0
22	B	611	CLA	1	0
28	c	521	LMG	1	0
24	B	618	BCR	1	0
22	b	604	CLA	2	0
22	B	603	CLA	3	0
22	b	612	CLA	2	0
31	A	416	DGD	4	0
34	Z	101	STE	1	0
27	a	409	PL9	2	0
22	c	513	CLA	1	0
24	T	101	BCR	1	0
22	A	411	CLA	1	0
34	X	101	STE	2	0
34	B	627	STE	1	0
31	C	516	DGD	1	0
34	T	102	STE	1	0
22	a	404	CLA	3	0
22	c	506	CLA	1	0
22	C	502	CLA	1	0
24	c	515	BCR	1	0
24	B	619	BCR	1	0
22	a	410	CLA	1	0
24	d	405	BCR	2	0
29	A	413	SQD	3	0
22	b	615	CLA	4	0

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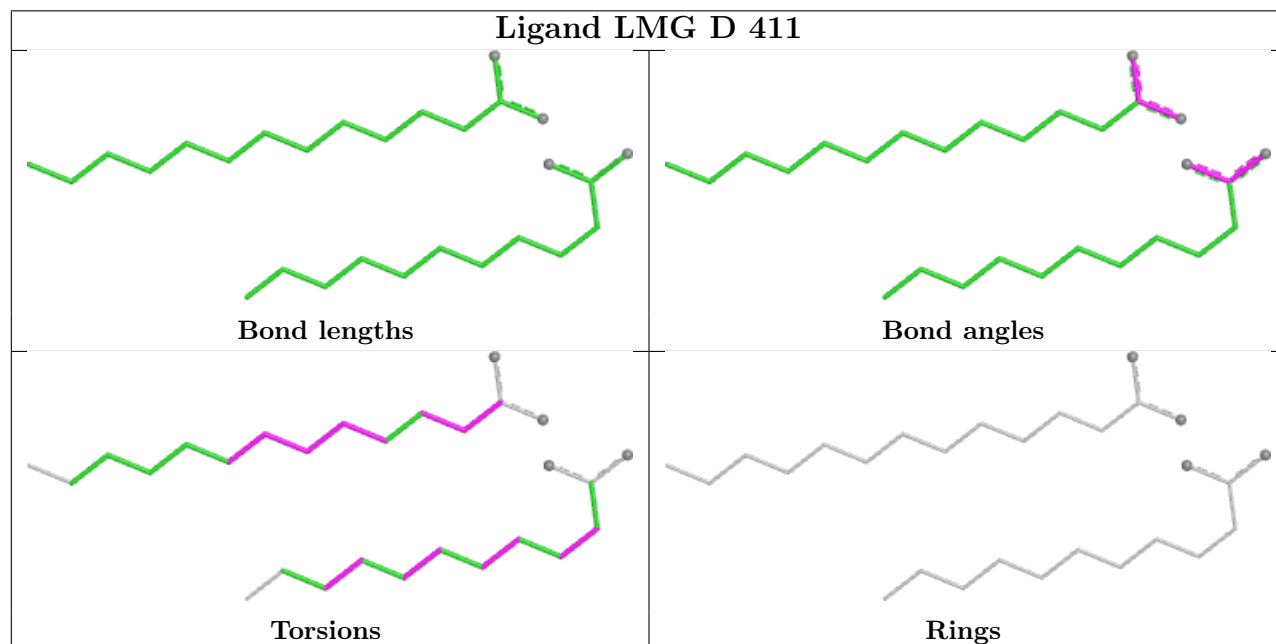
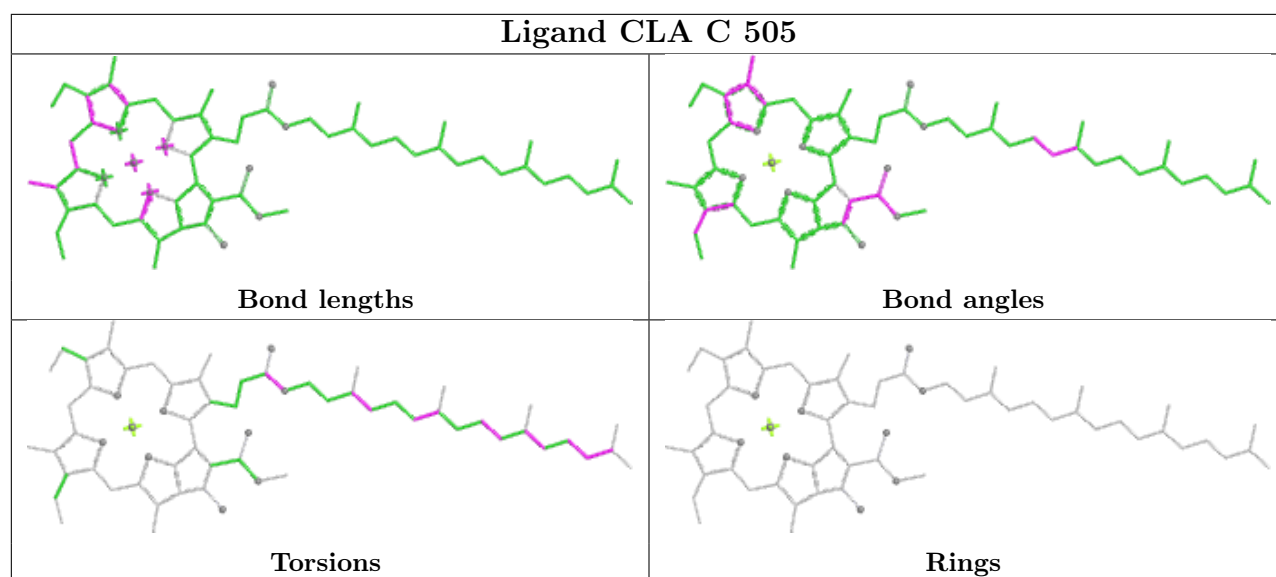
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	v	201	HEC	3	0
24	k	101	BCR	1	0
22	c	507	CLA	1	0
35	e	101	HEM	6	0
22	c	505	CLA	1	0
22	C	512	CLA	3	0
35	F	101	HEM	3	0
29	b	620	SQD	1	0
22	C	506	CLA	1	0
32	A	417[B]	OEY	2	0
30	d	409	LHG	1	0
28	C	518	LMG	1	0
22	B	613	CLA	1	0
24	t	101	BCR	4	0
31	c	517	DGD	3	0
31	h	101	DGD	1	0
30	B	622	LHG	1	0
22	C	508	CLA	1	0
32	a	418[B]	OEY	2	0
24	D	404	BCR	1	0
22	C	513	CLA	2	0
30	D	409	LHG	3	0
29	a	412	SQD	1	0
34	I	101	STE	2	0
22	c	512	CLA	1	0
29	B	623	SQD	1	0
30	d	408	LHG	2	0
28	M	101	LMG	1	0
22	B	614	CLA	2	0
22	B	608	CLA	3	0
34	c	520	STE	2	0
22	c	503	CLA	1	0
28	c	522	LMG	6	0
34	a	414	STE	4	0
24	b	617	BCR	2	0
34	B	624	STE	2	0
29	f	101	SQD	2	0
22	c	511	CLA	2	0
34	L	101	STE	1	0
22	C	503	CLA	1	0
22	C	509	CLA	3	0
22	B	601	CLA	1	0

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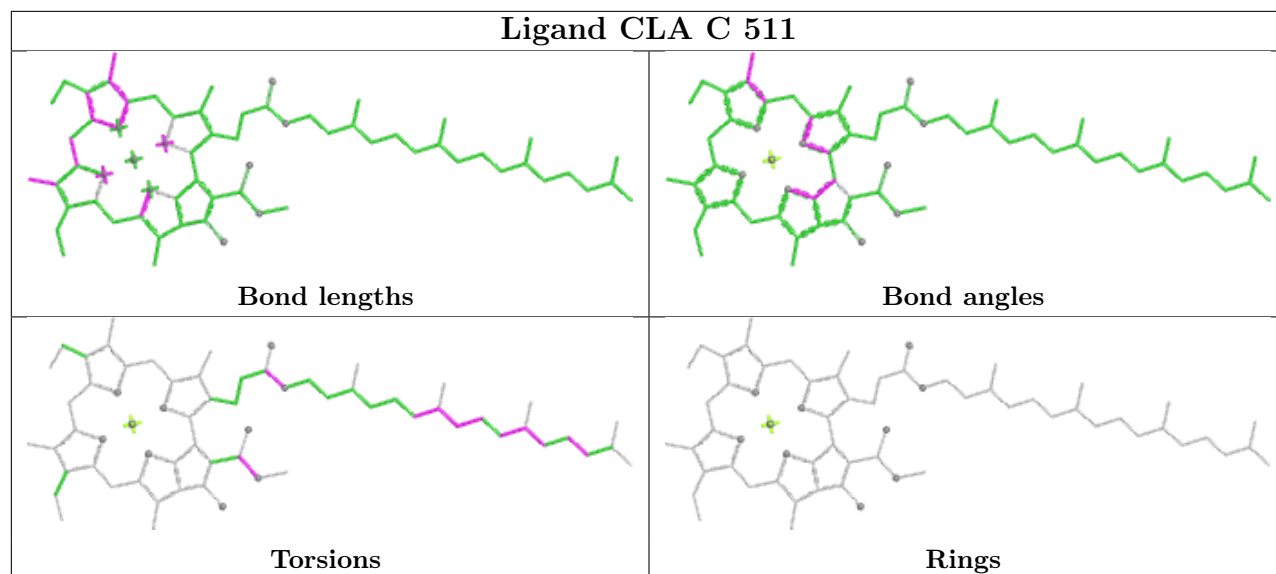
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	M	102	STE	1	0
22	b	614	CLA	4	0
22	B	609	CLA	2	0
22	b	605	CLA	2	0
30	d	407	LHG	2	0
34	b	626	STE	1	0
22	b	606	CLA	2	0
28	b	622	LMG	1	0
22	b	607	CLA	1	0
22	c	501	CLA	2	0
28	D	406	LMG	2	0
22	b	609	CLA	1	0
34	b	627	STE	1	0
22	B	602	CLA	2	0
34	l	102	STE	2	0
34	C	520	STE	1	0
30	D	408	LHG	1	0
22	B	604	CLA	1	0
34	B	620	STE	1	0
22	b	616	CLA	1	0
34	M	103	STE	1	0
27	A	410	PL9	4	0
23	D	401	PHO	1	0
34	b	623	STE	3	0
34	R	101	STE	1	0
29	A	415	SQD	1	0
22	C	501	CLA	1	0
22	b	610	CLA	1	0

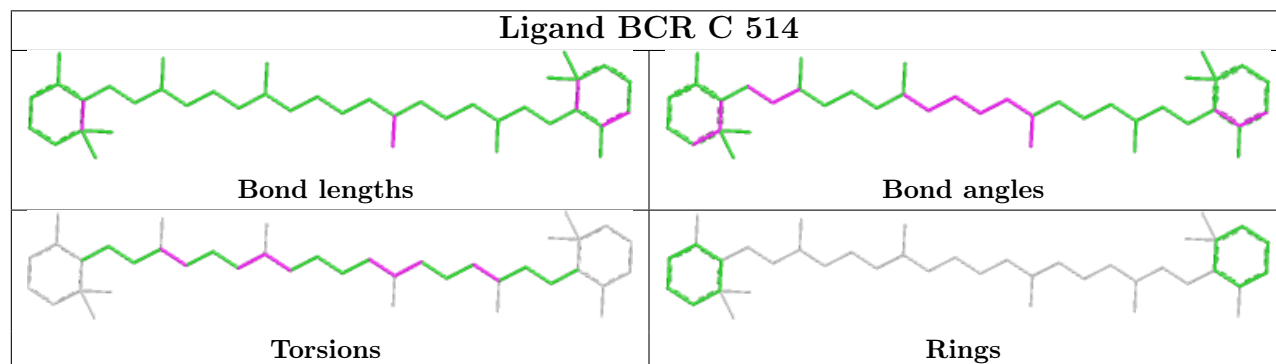
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



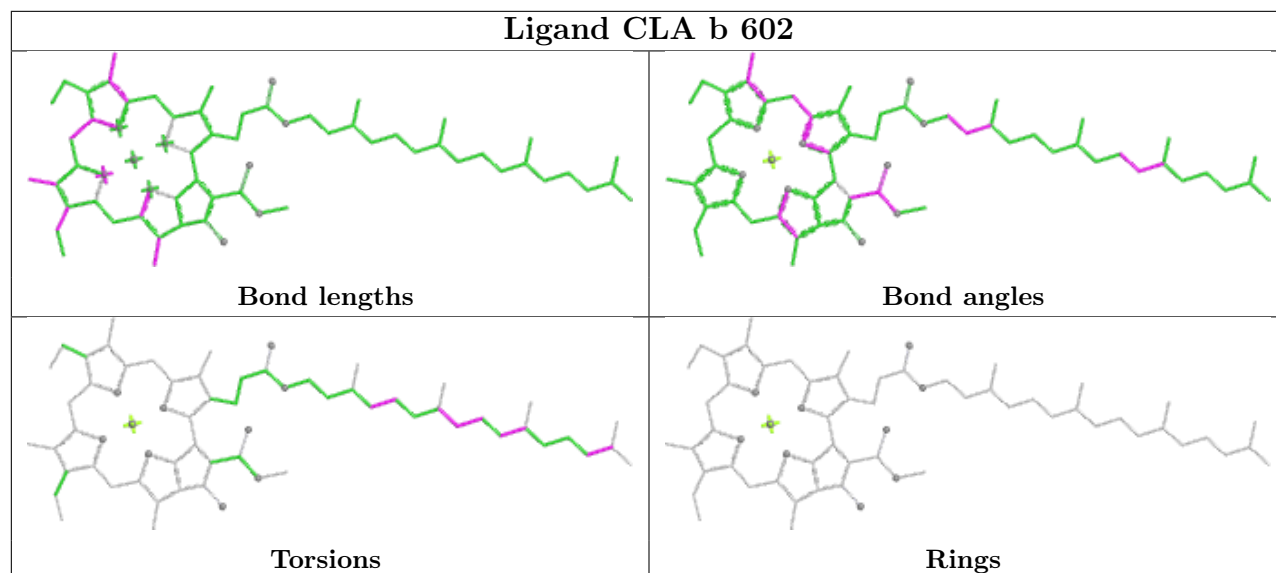
Ligand CLA C 511

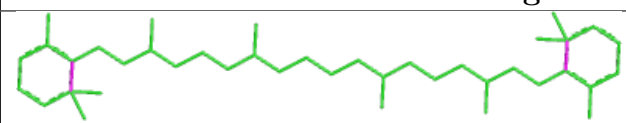
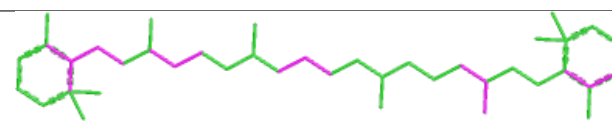
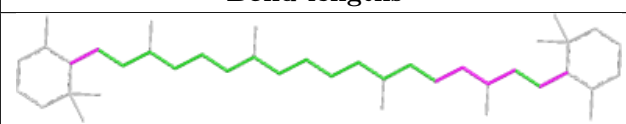
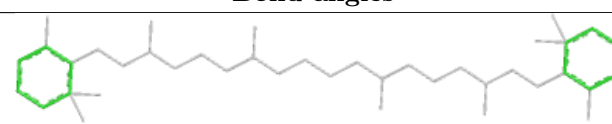


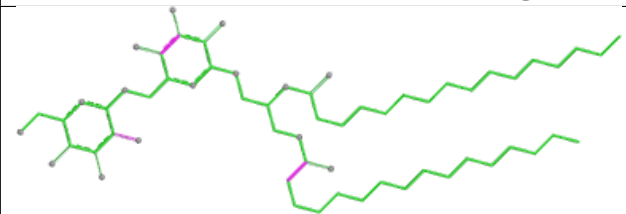
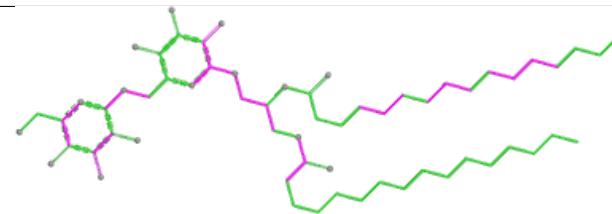
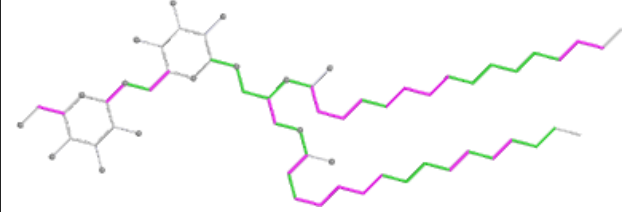
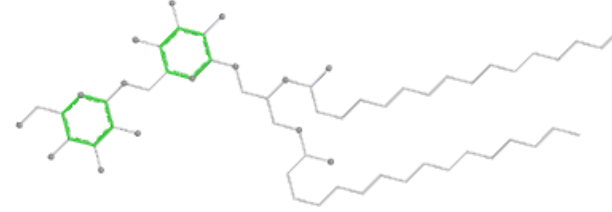
Ligand BCR C 514

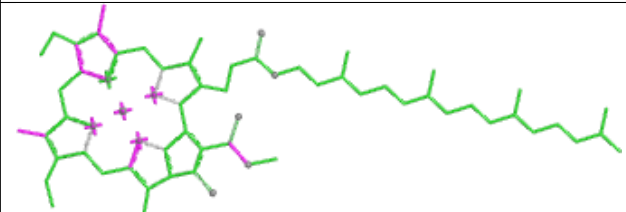
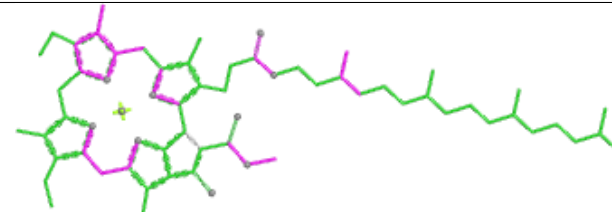
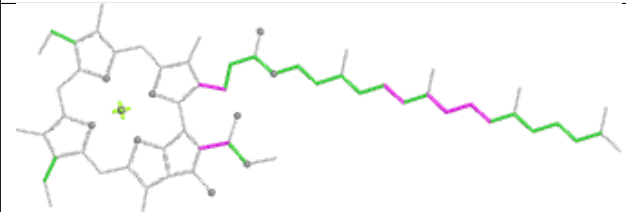
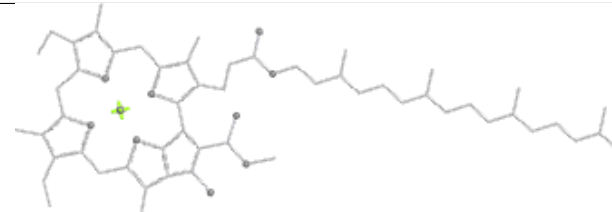


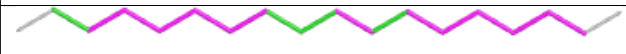
Ligand CLA b 602

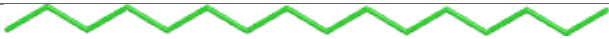
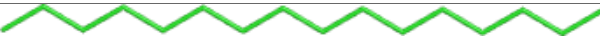
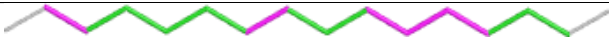


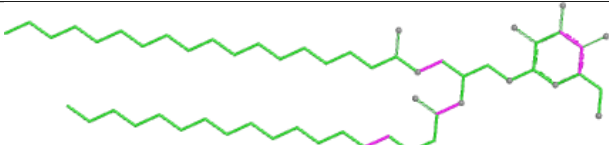
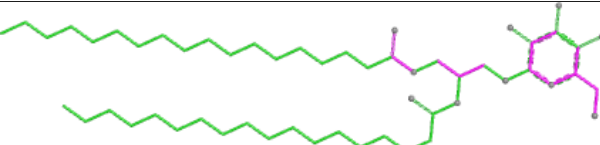
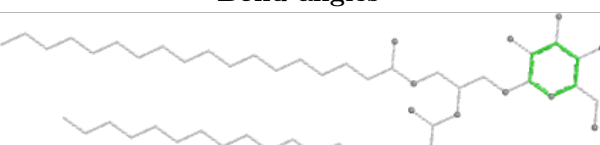
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

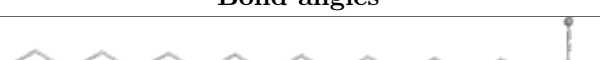
Ligand DGD C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

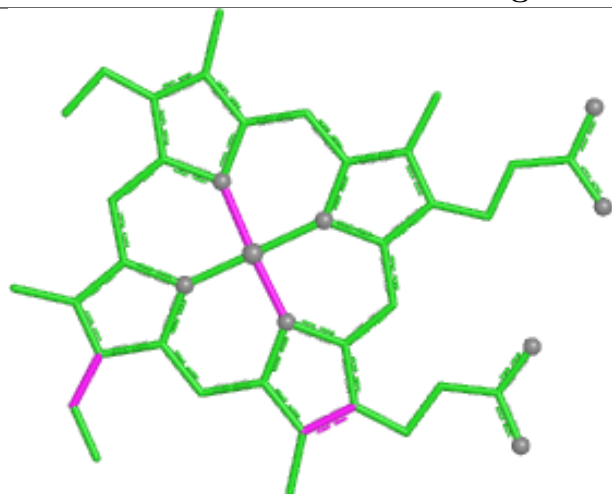
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

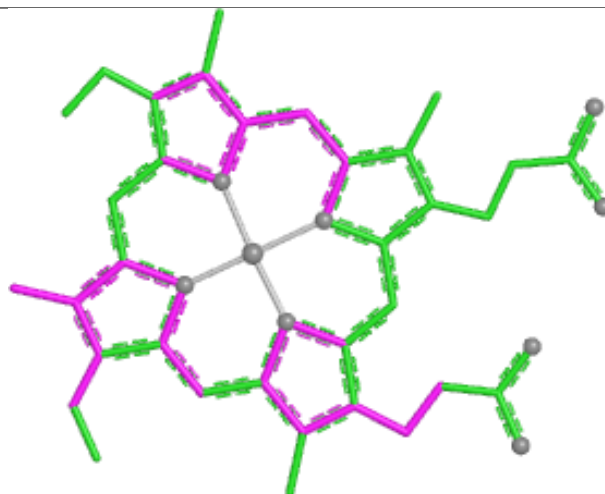
Ligand LMG a 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

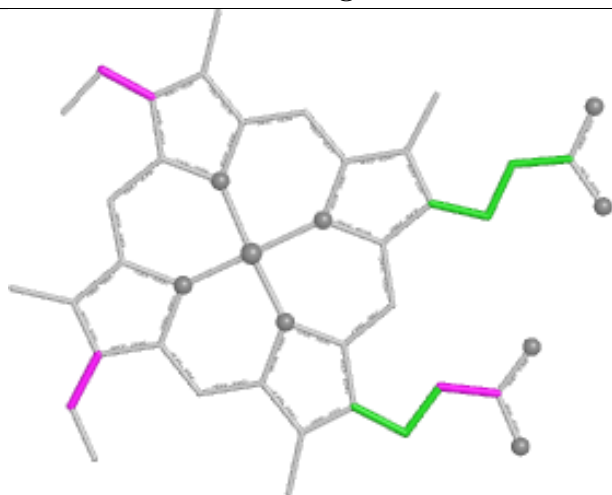
Ligand HEC V 201



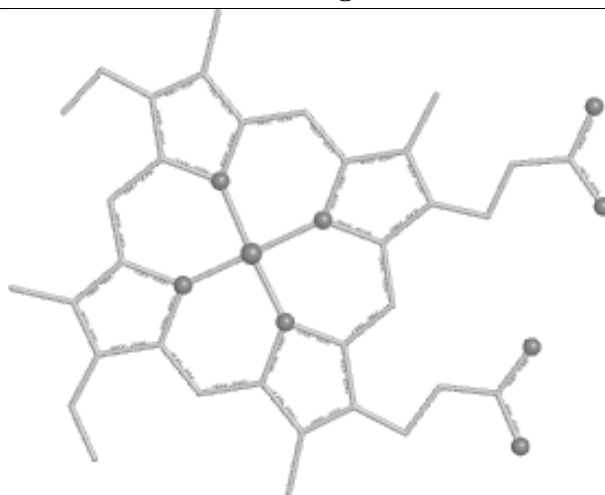
Bond lengths



Bond angles

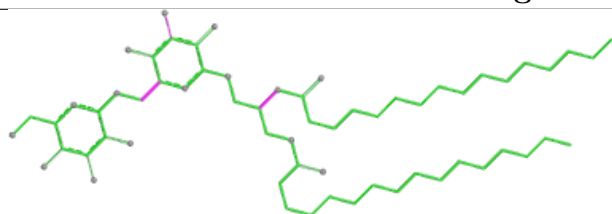


Torsions

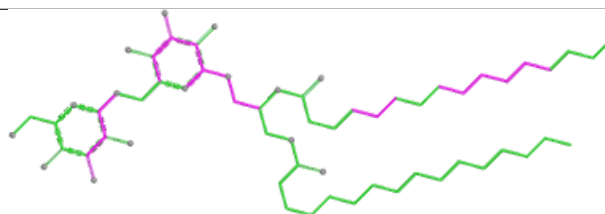


Rings

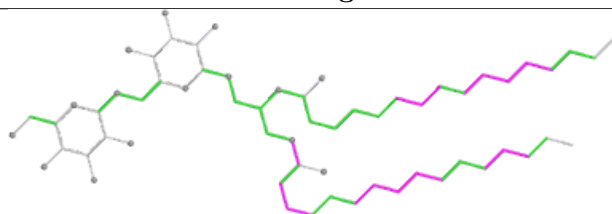
Ligand DGD c 518



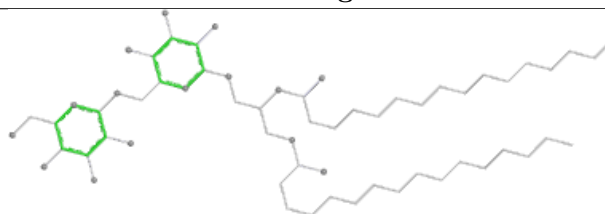
Bond lengths



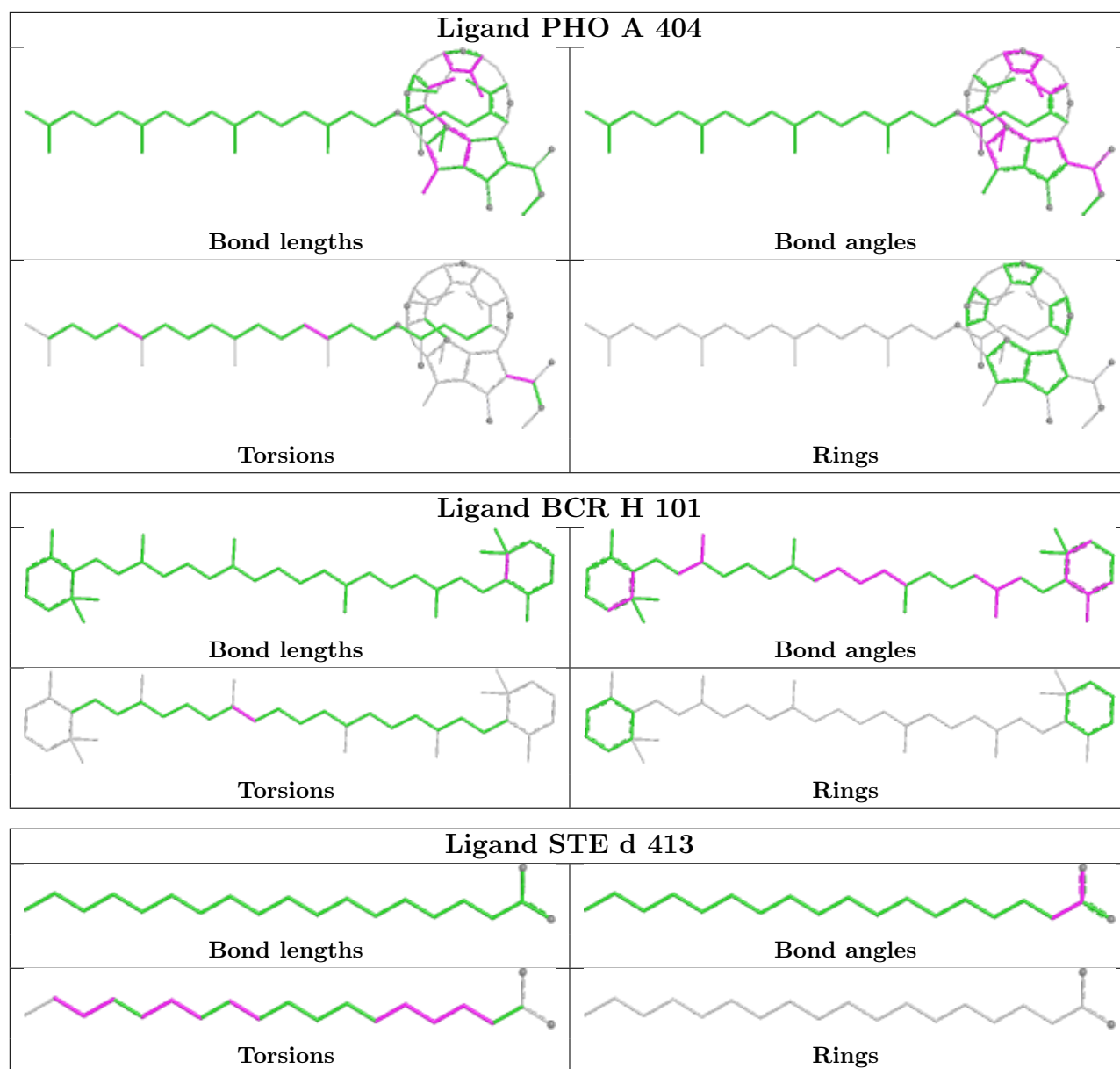
Bond angles

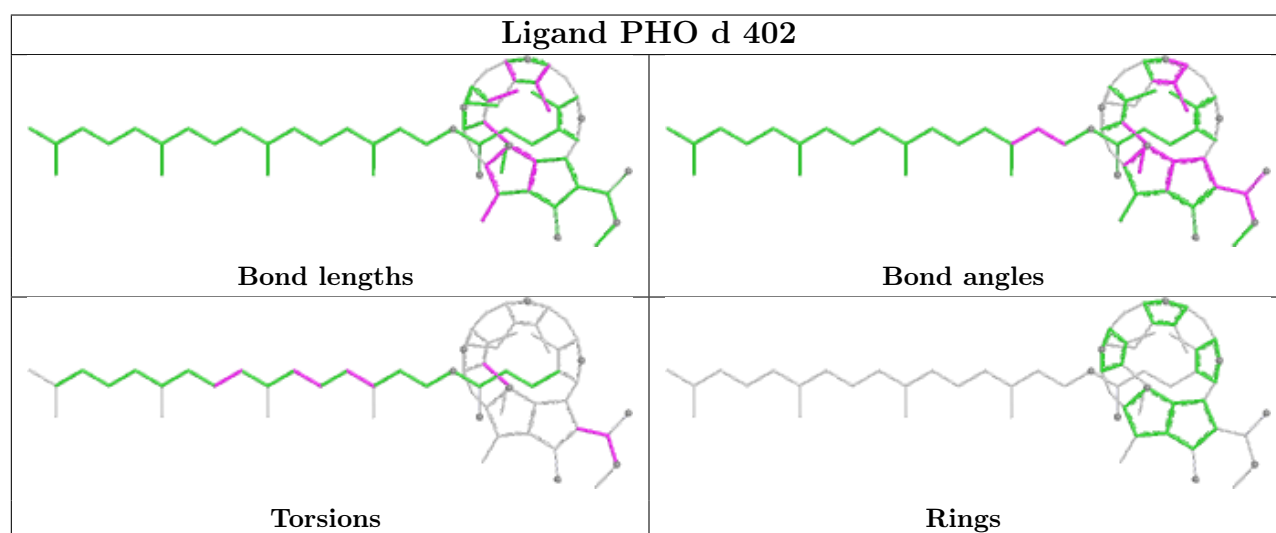
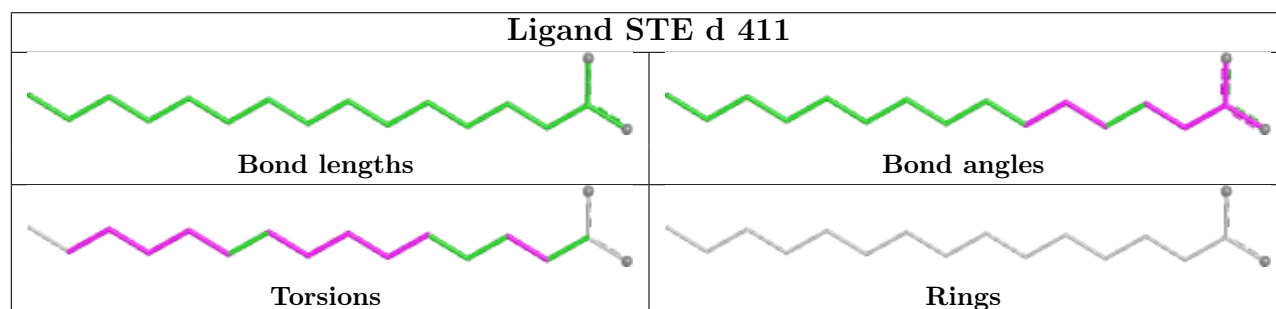
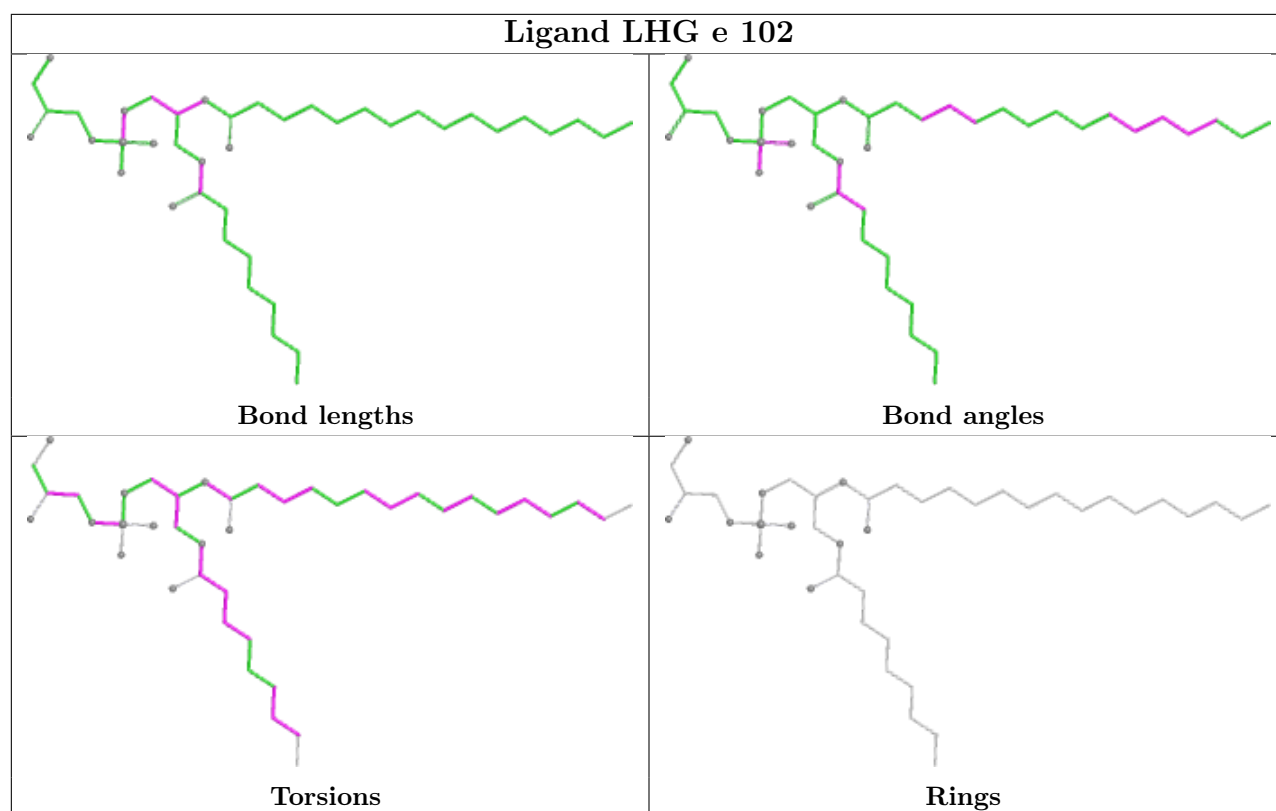


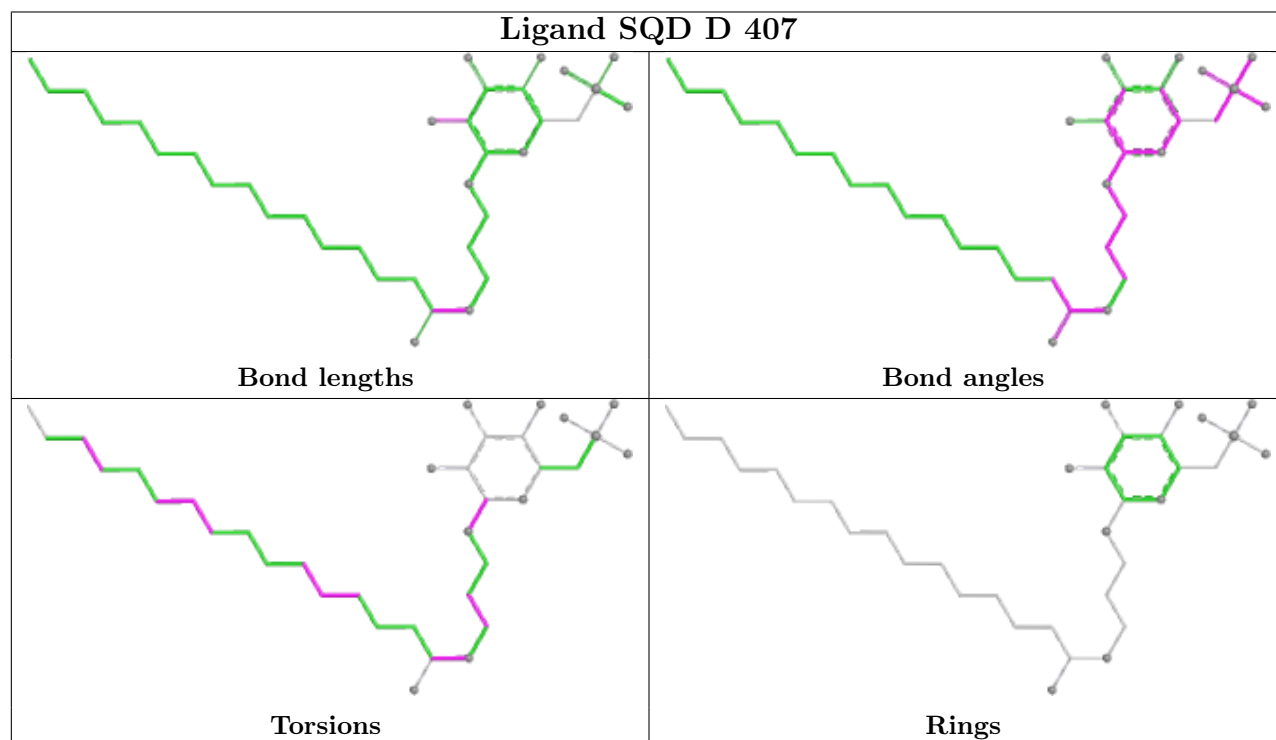
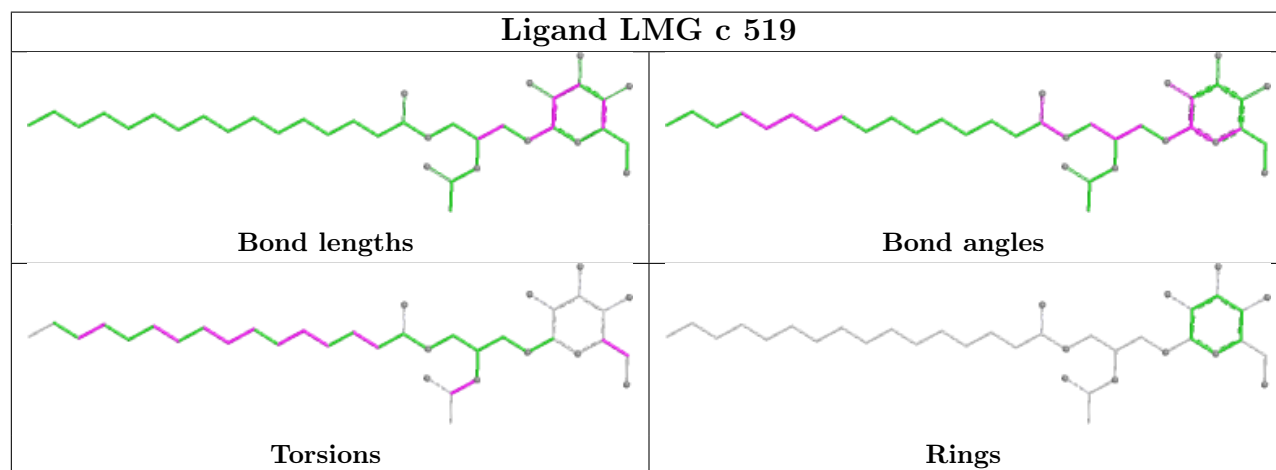
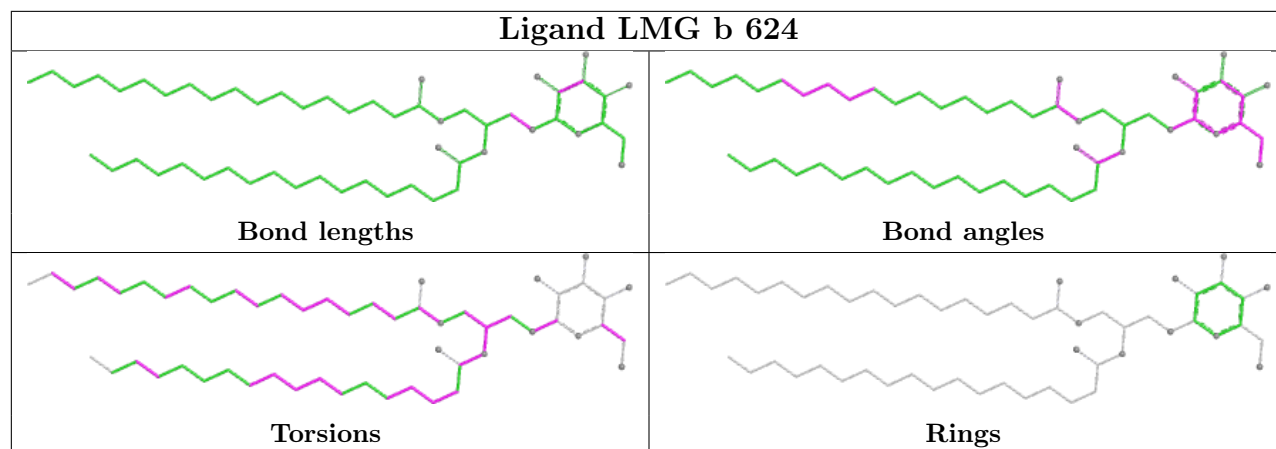
Torsions

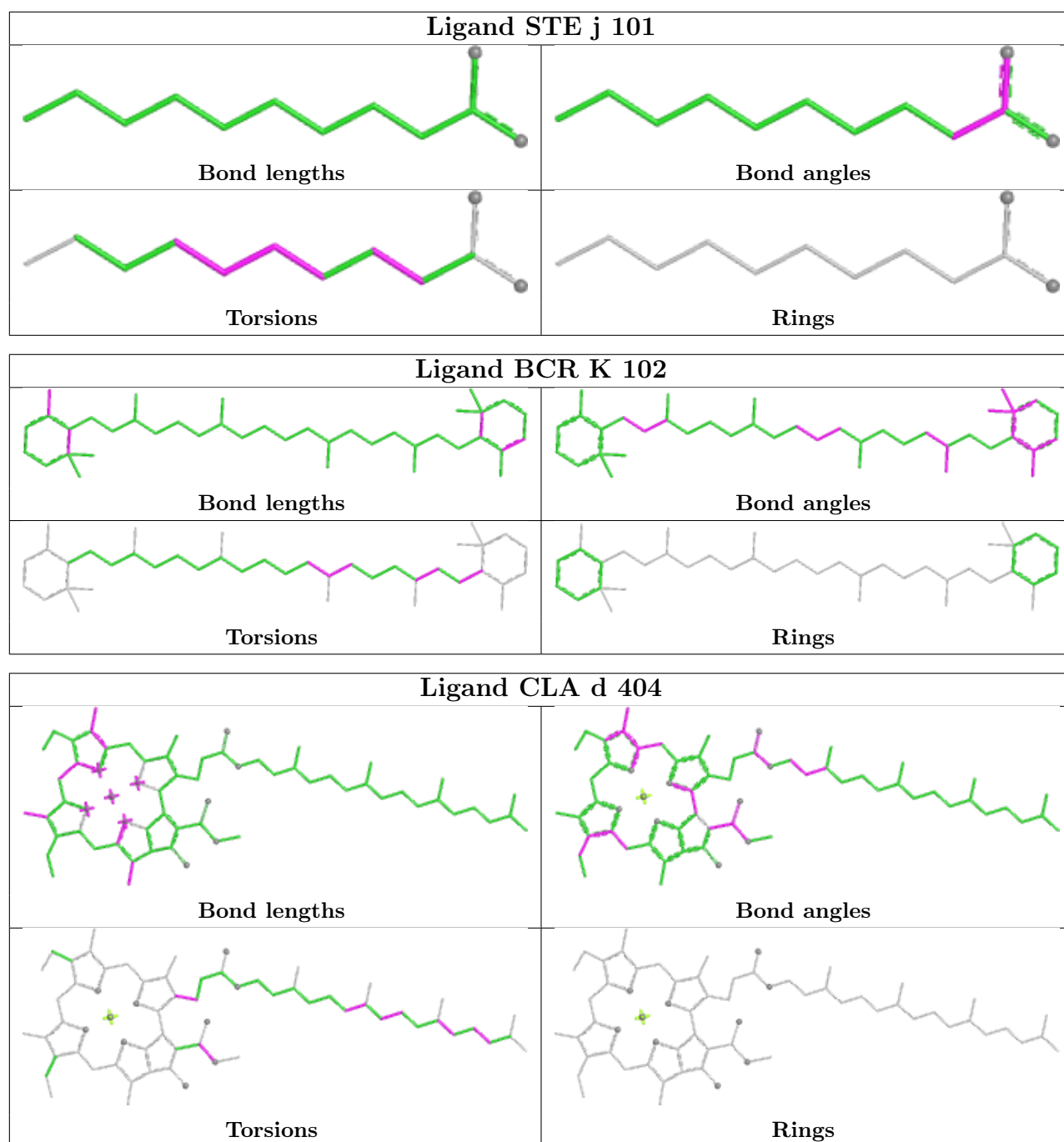


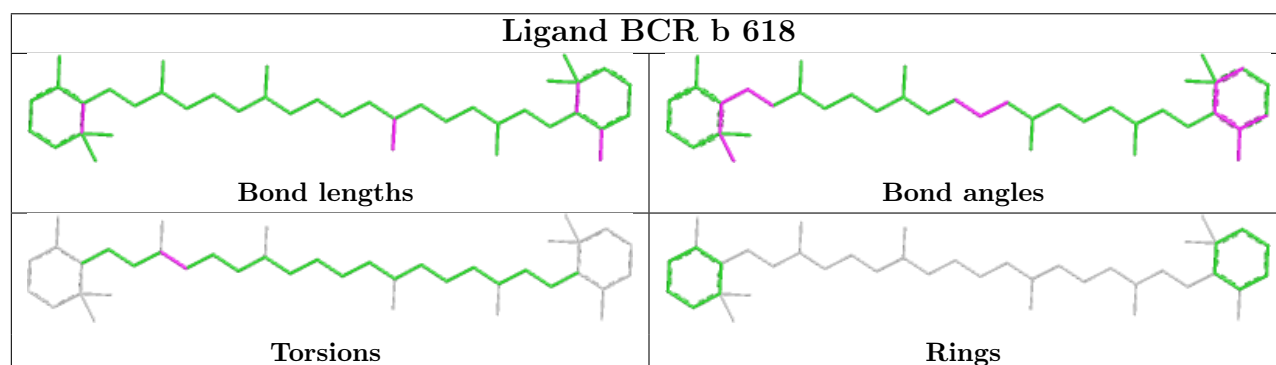
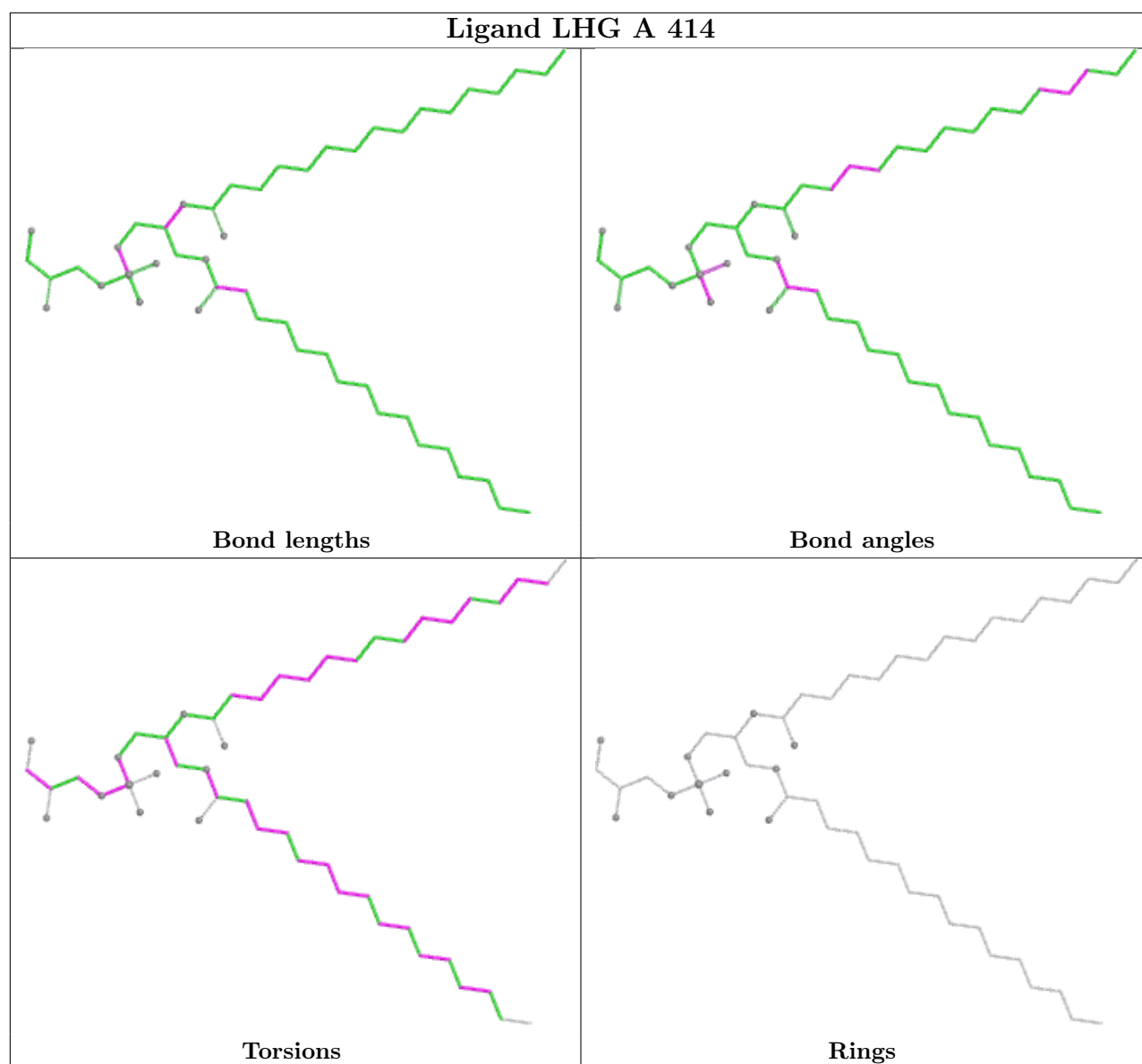
Rings

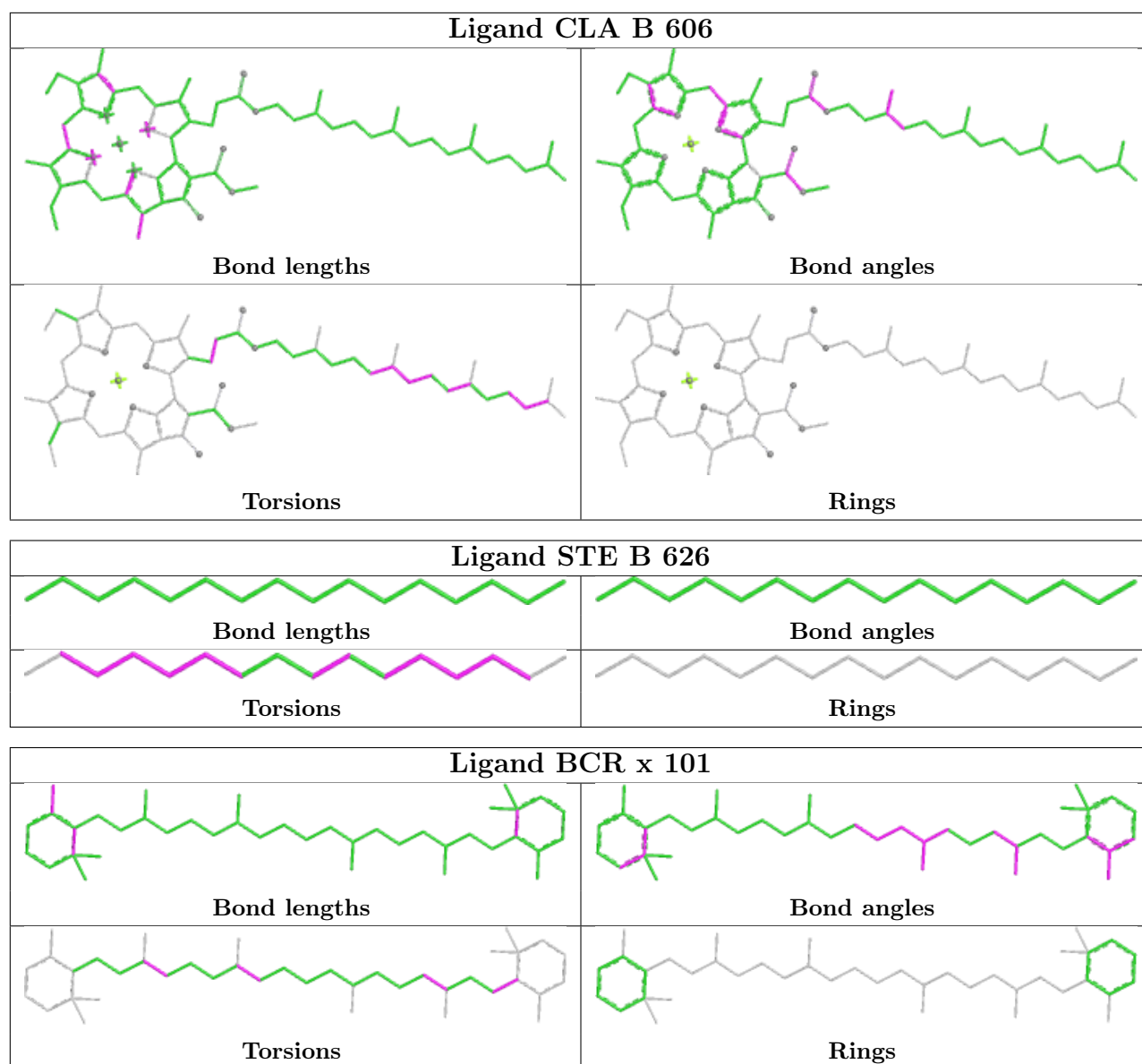


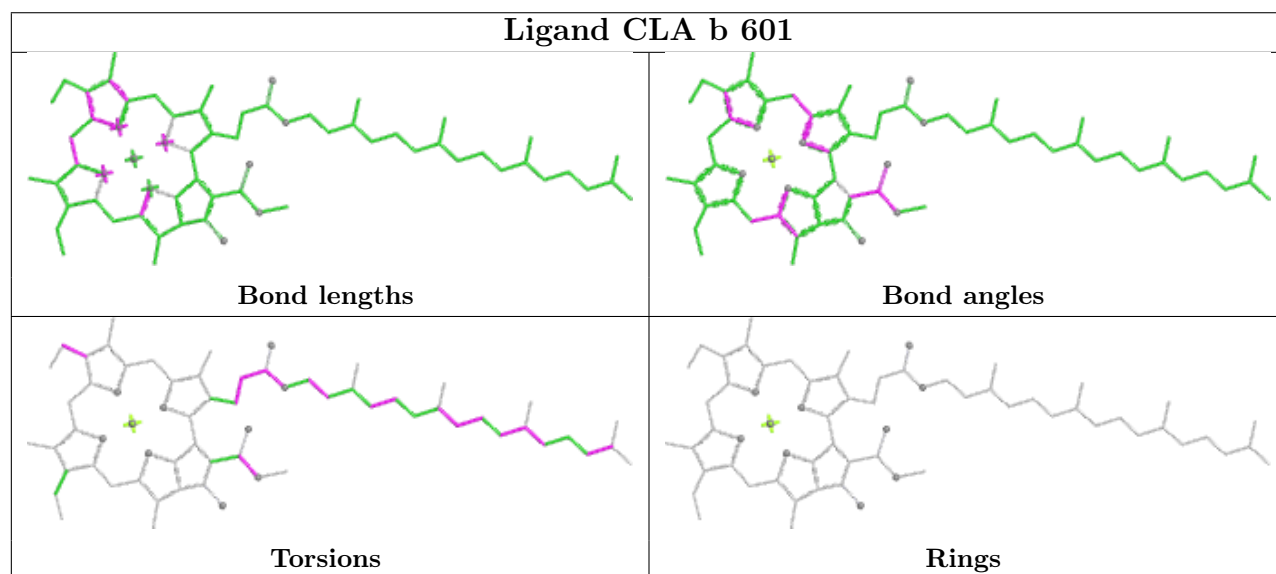
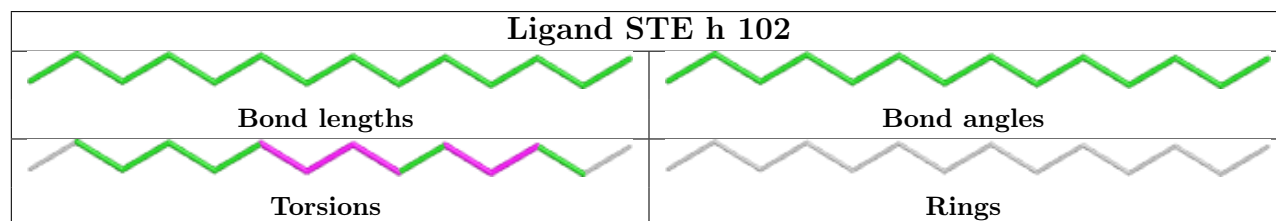
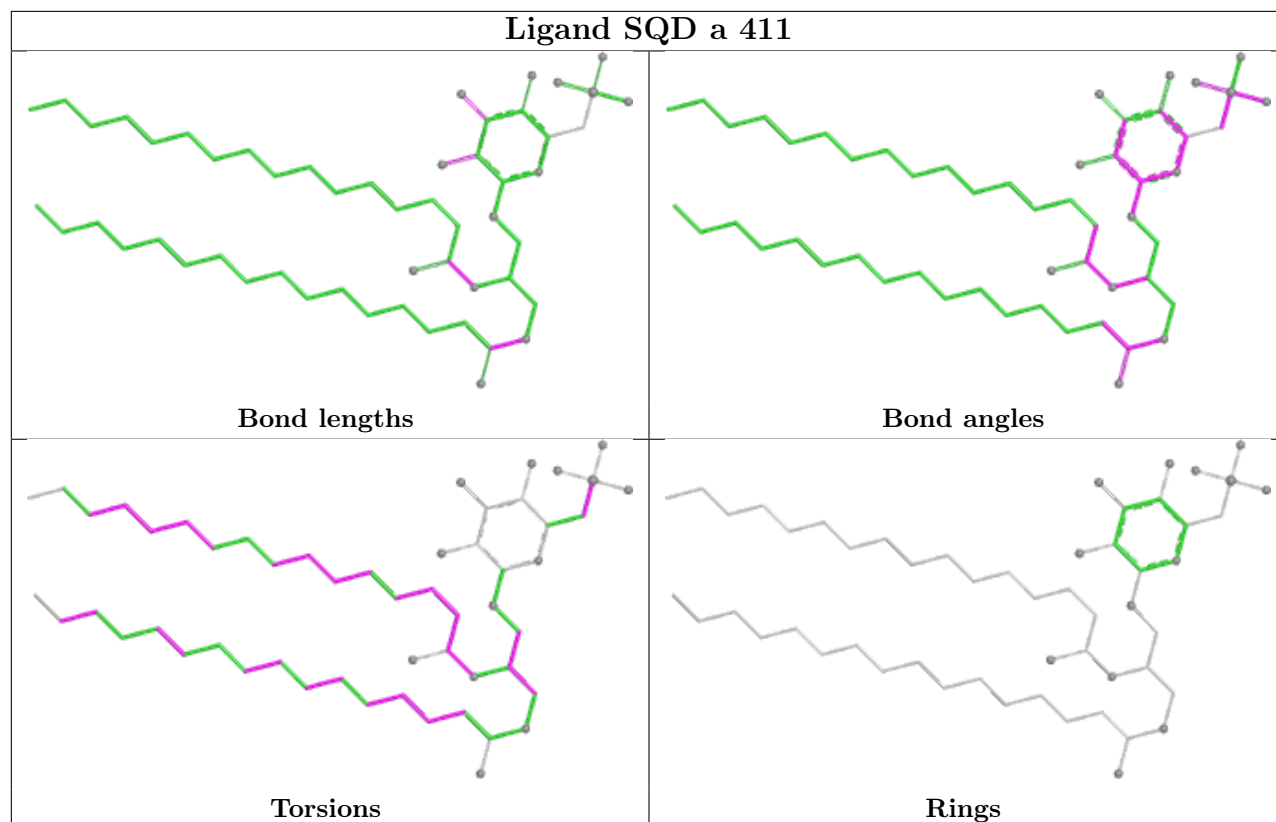


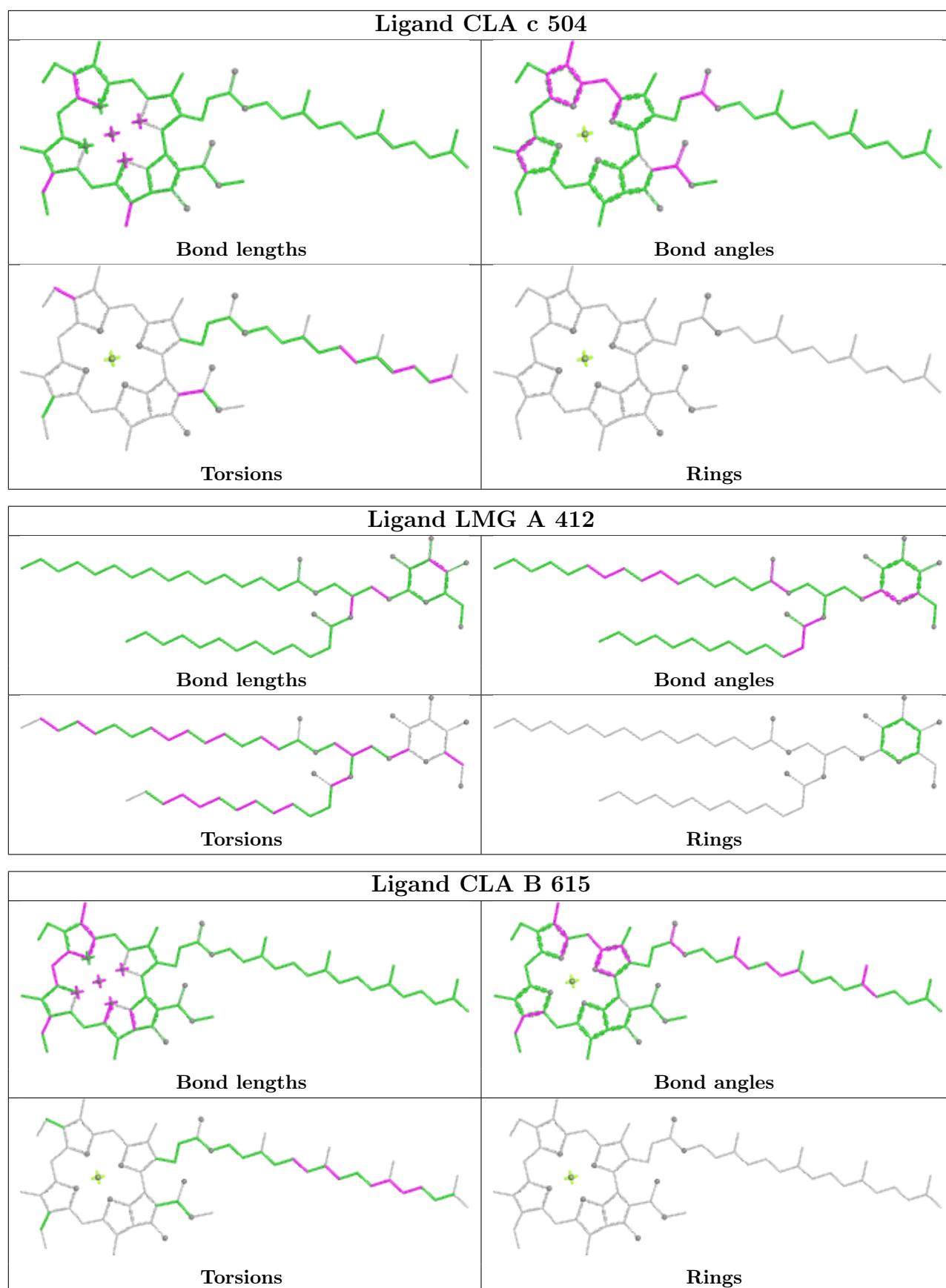




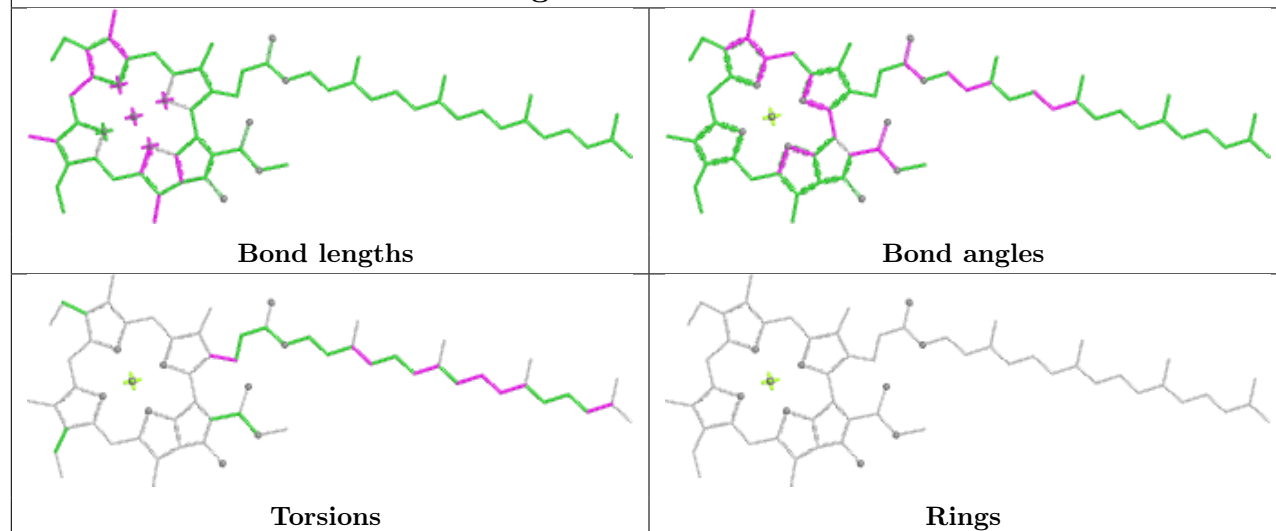




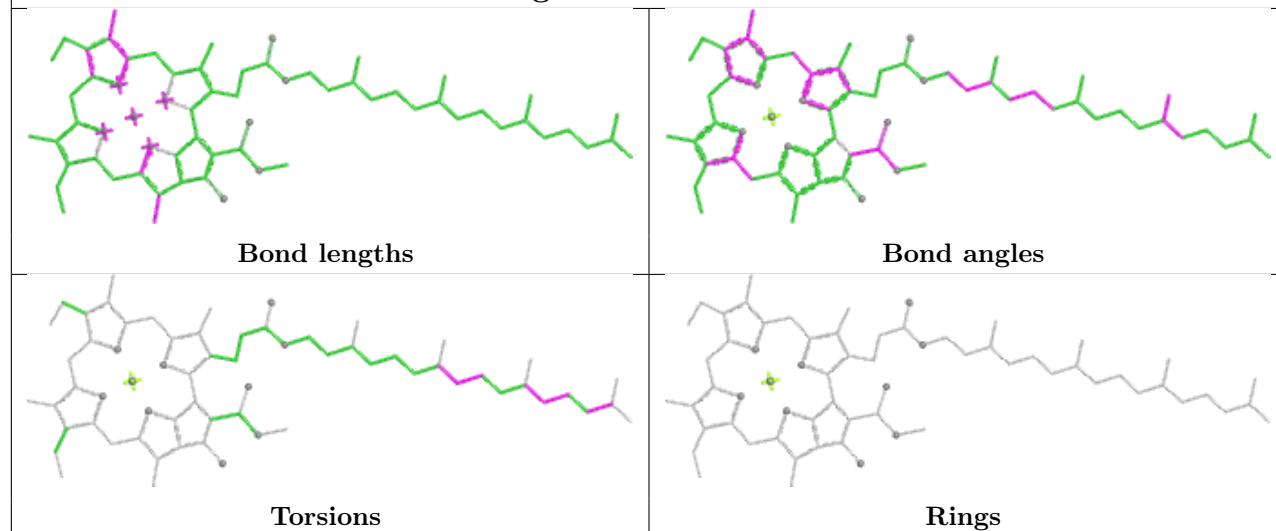




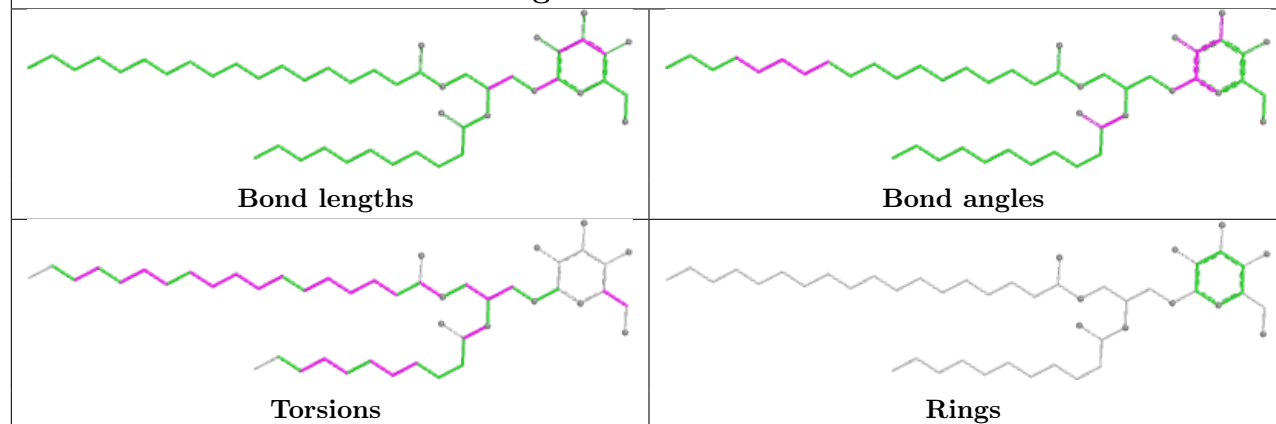
Ligand CLA D 403



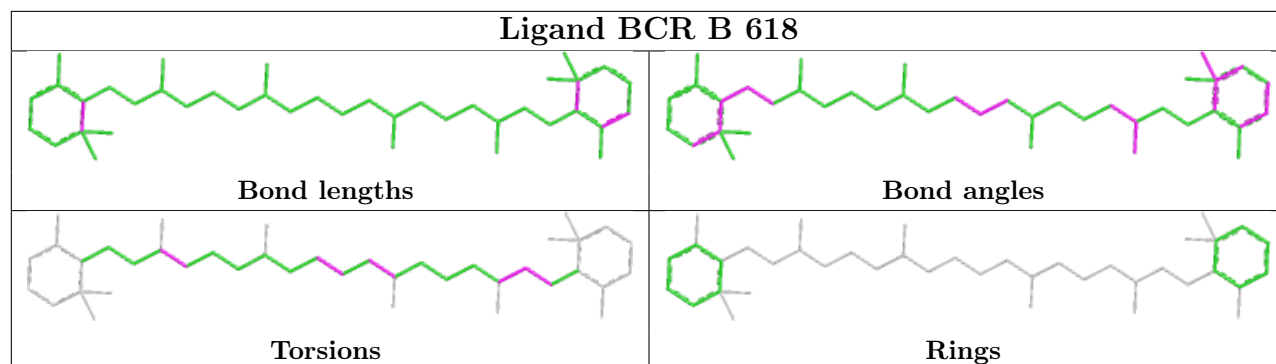
Ligand CLA B 611



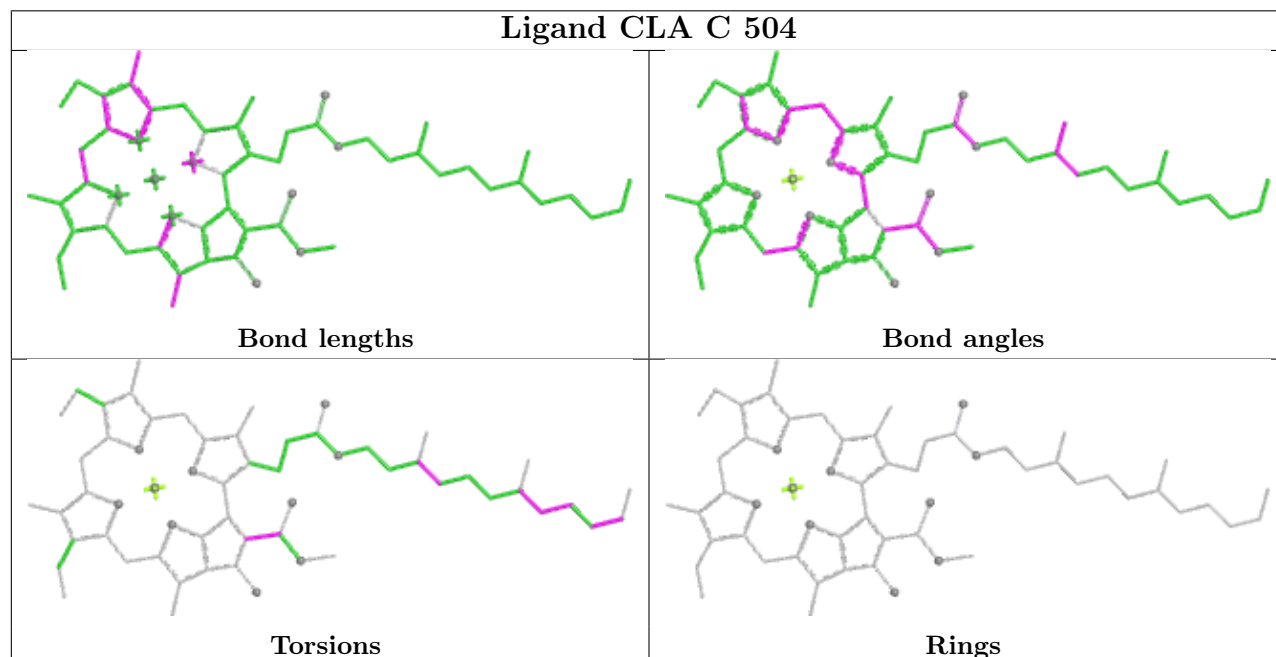
Ligand LMG c 521



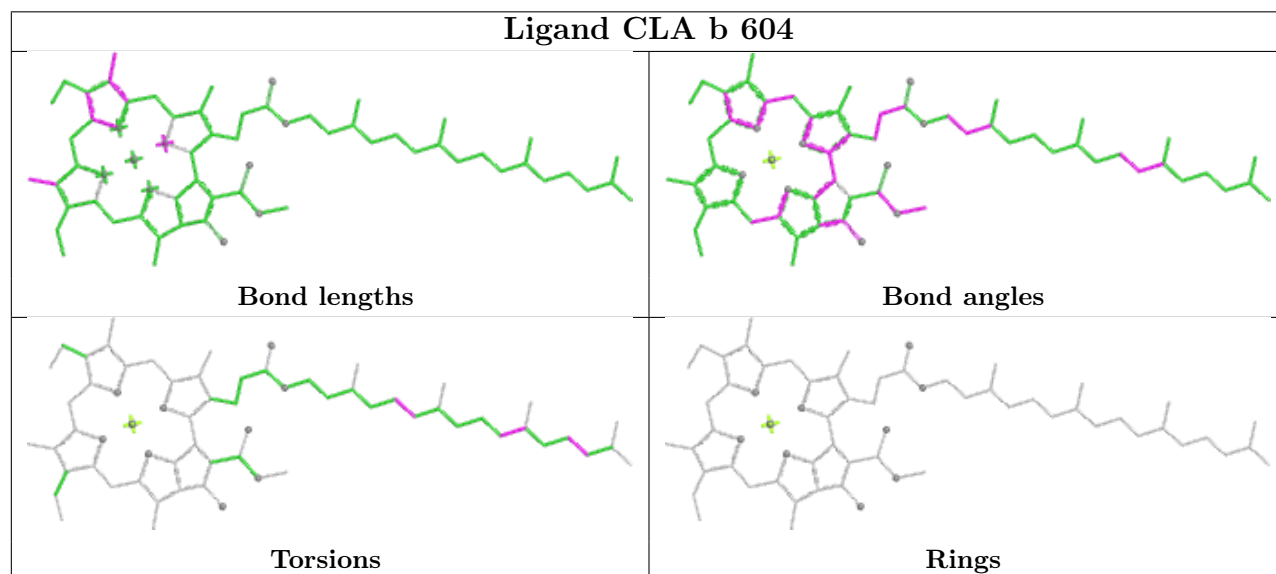
Ligand BCR B 618

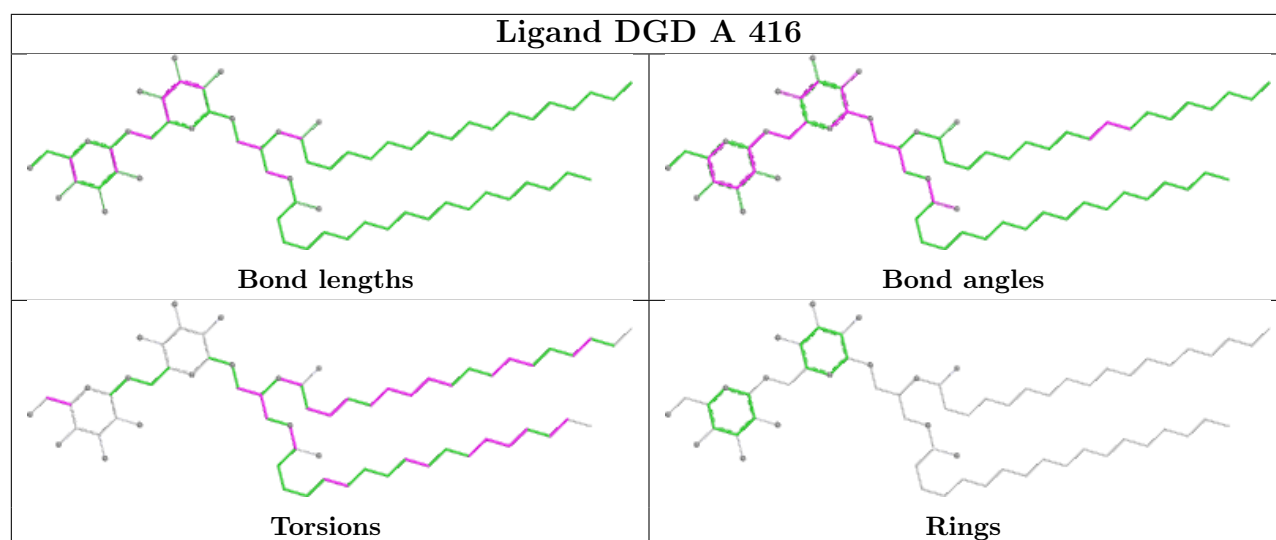
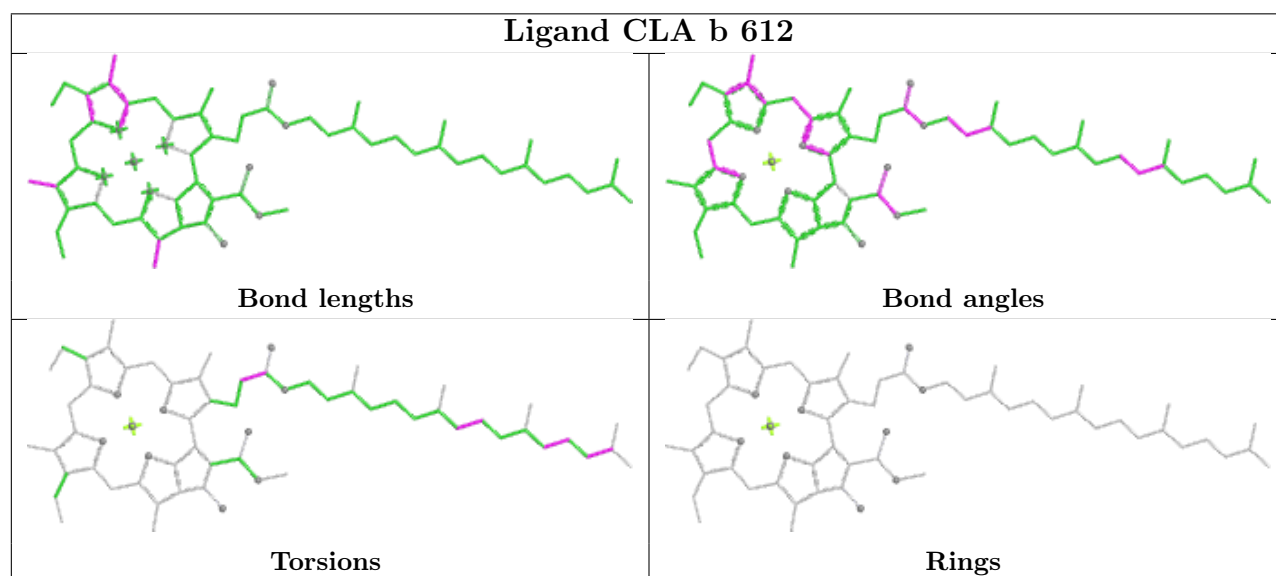
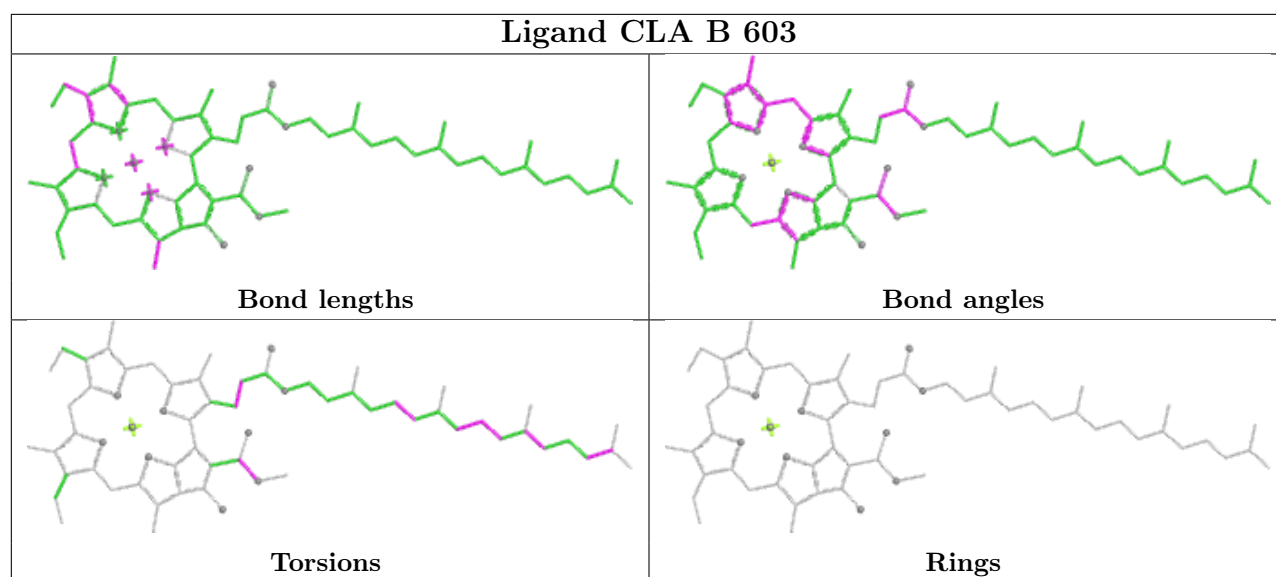


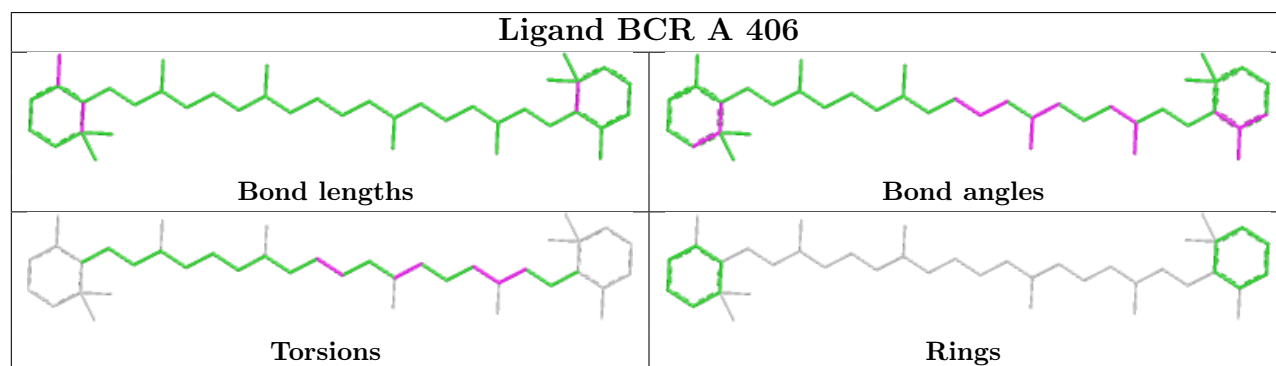
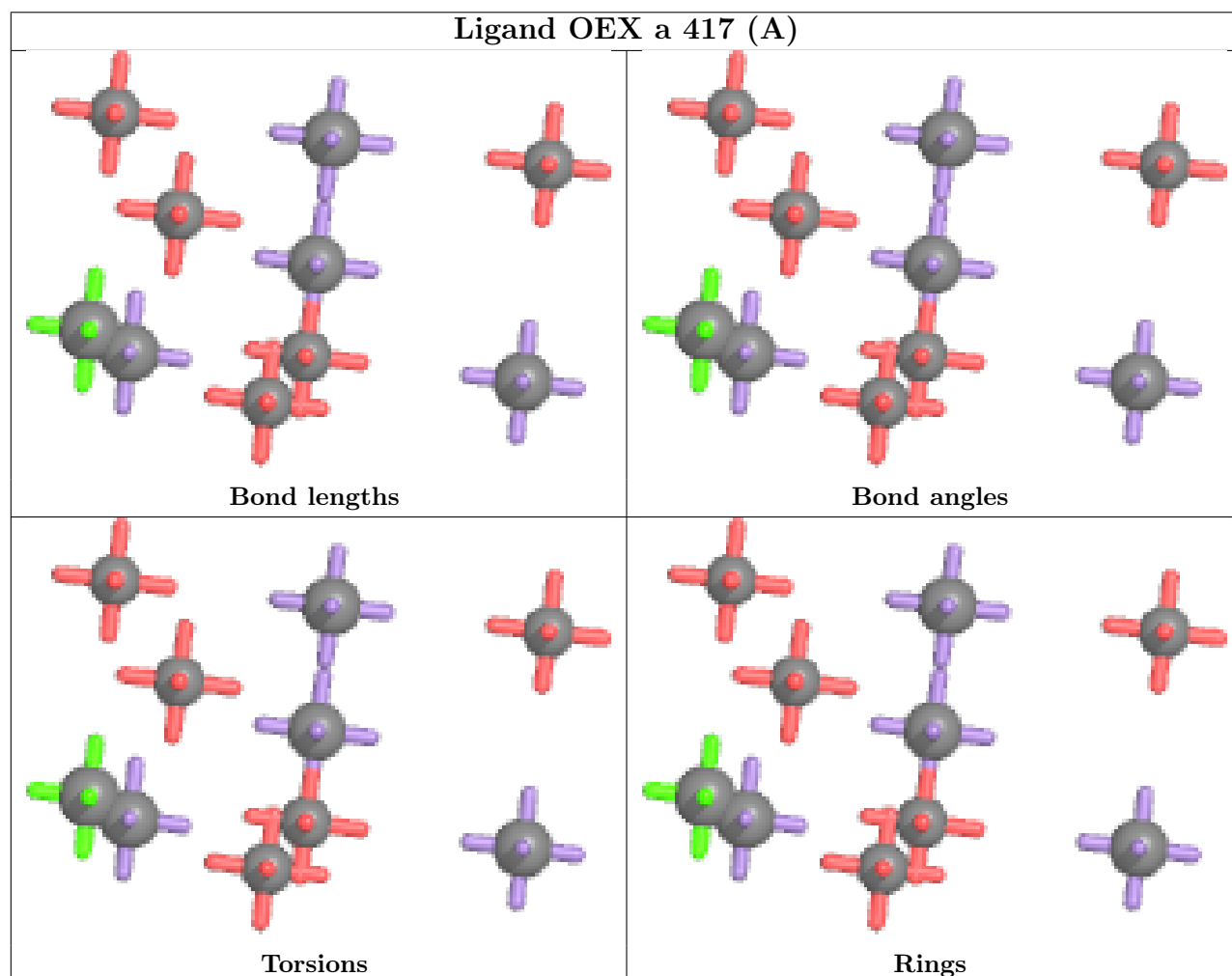
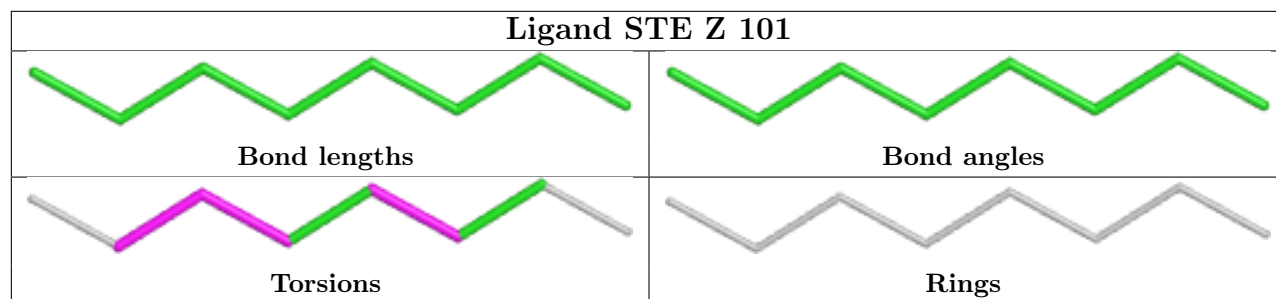
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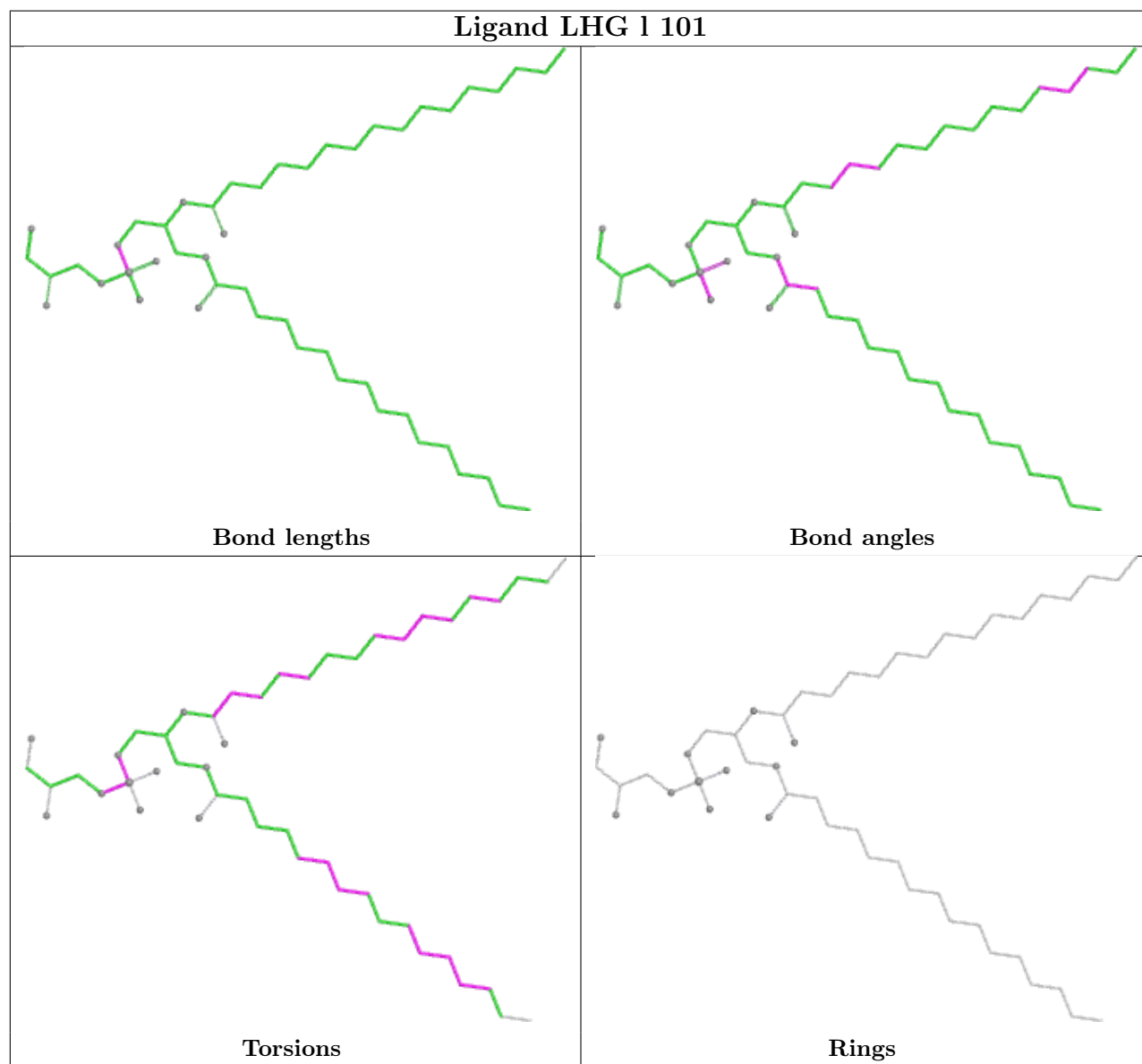
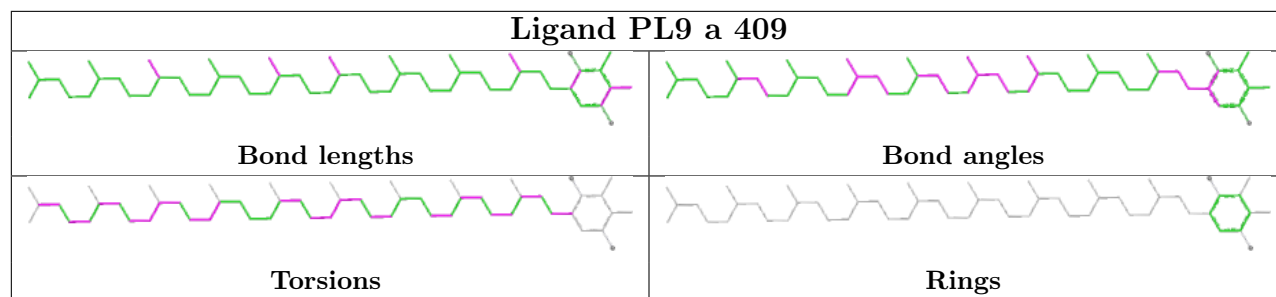


Ligand CLA b 604

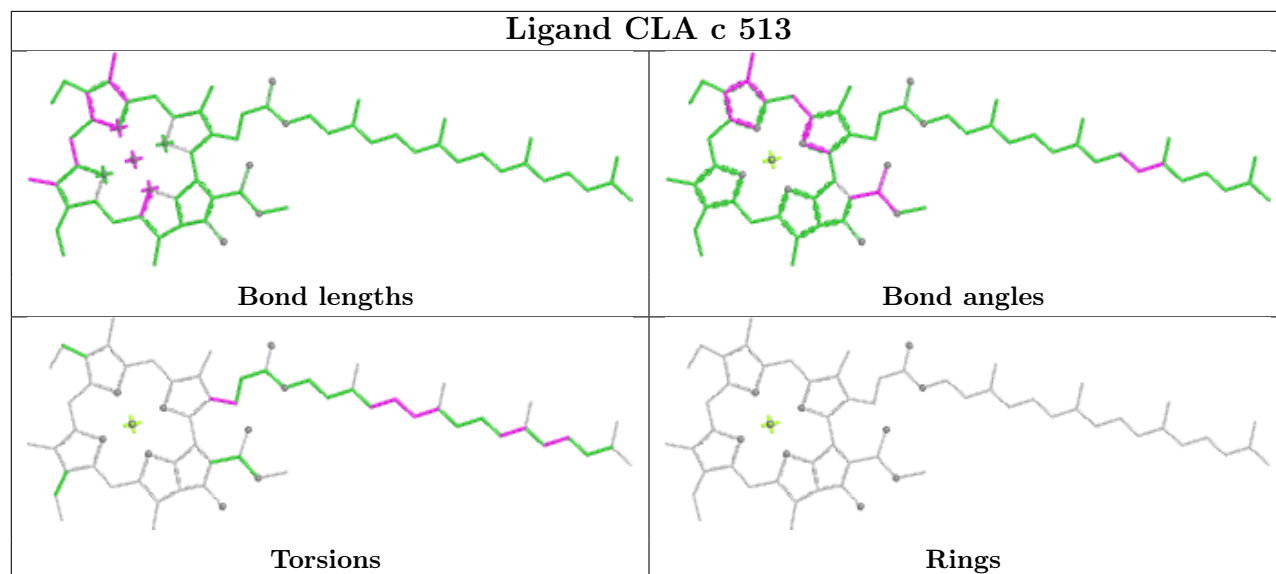




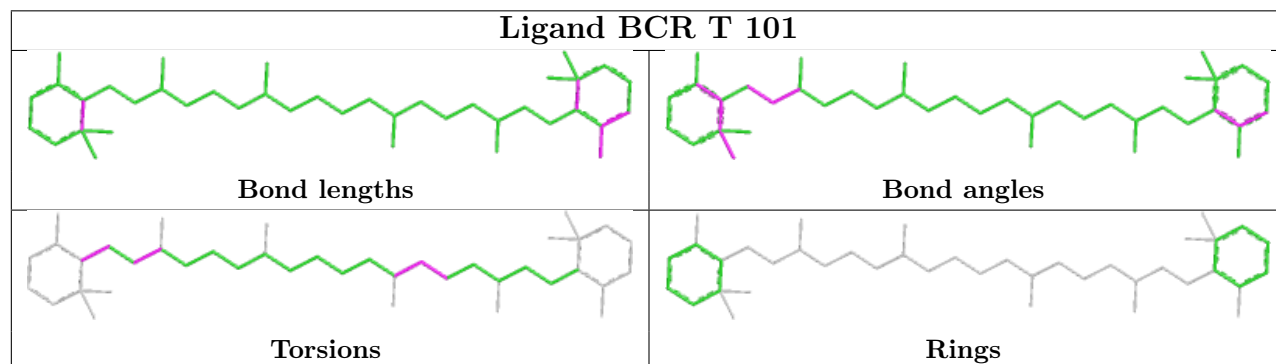




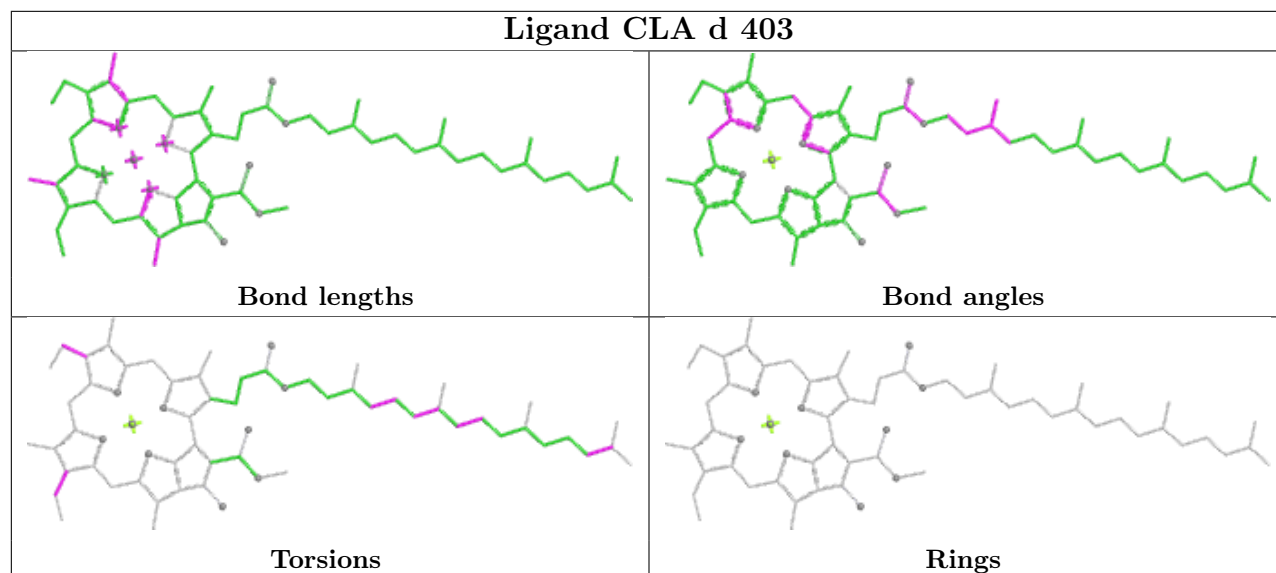
Ligand CLA c 513

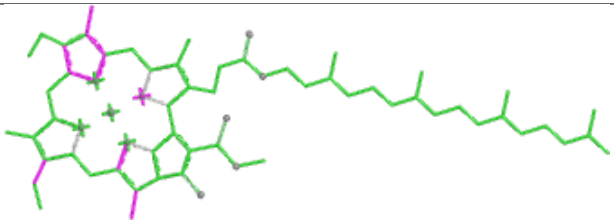
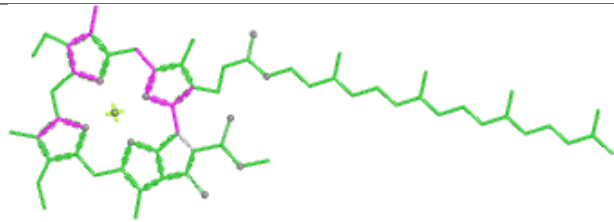
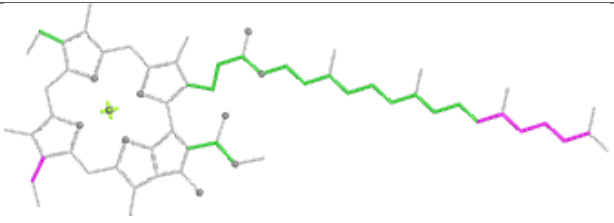
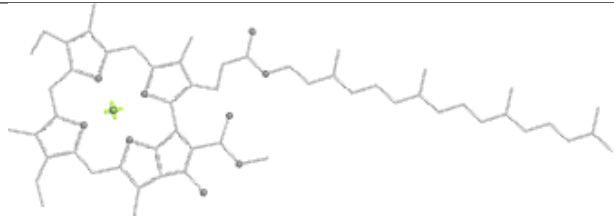


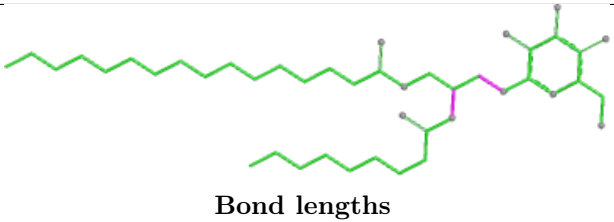
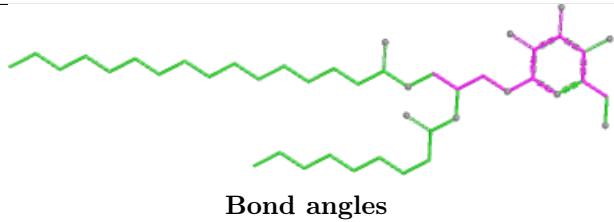
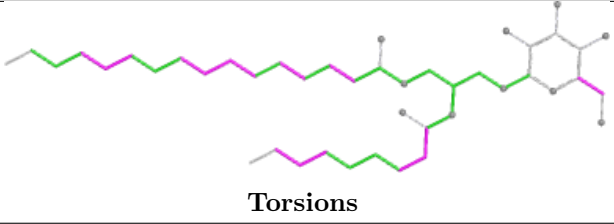
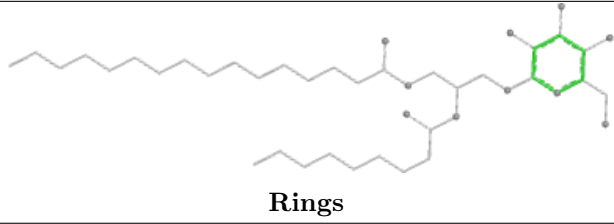
Ligand BCR T 101

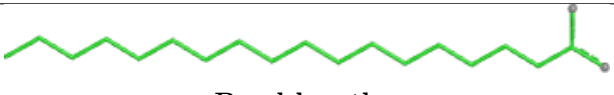
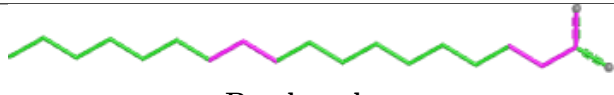
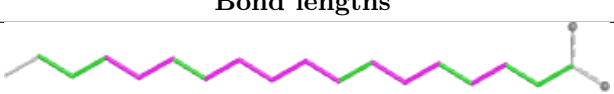
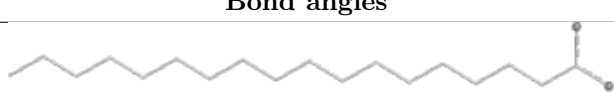


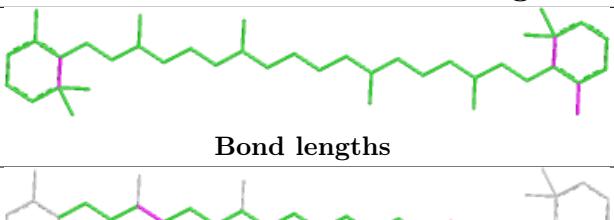
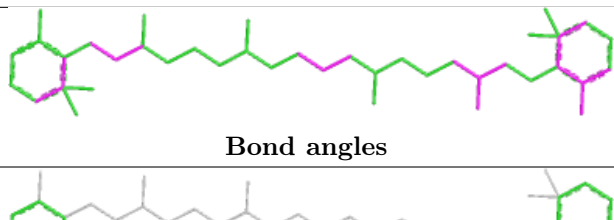
Ligand CLA d 403

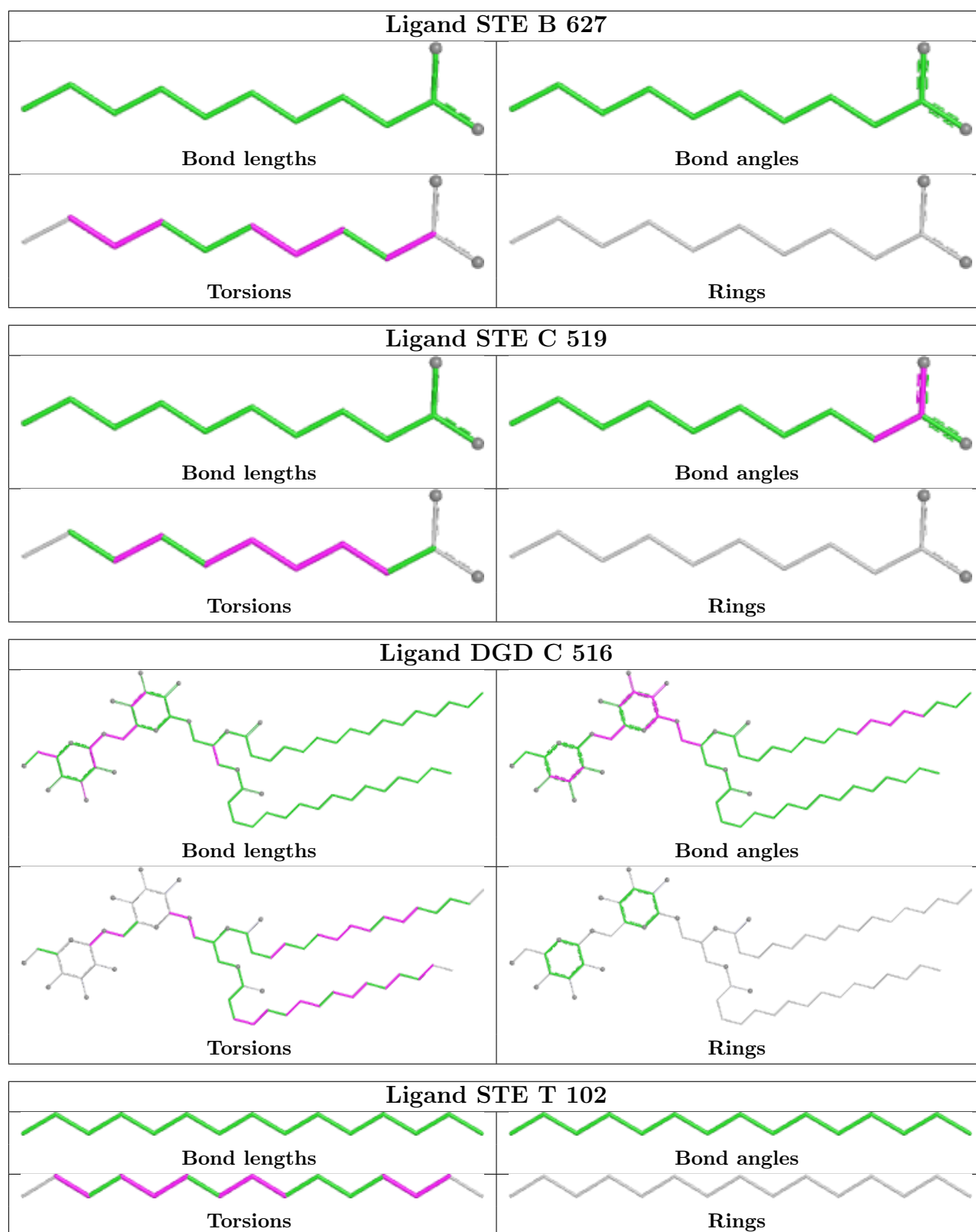


Ligand CLA A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

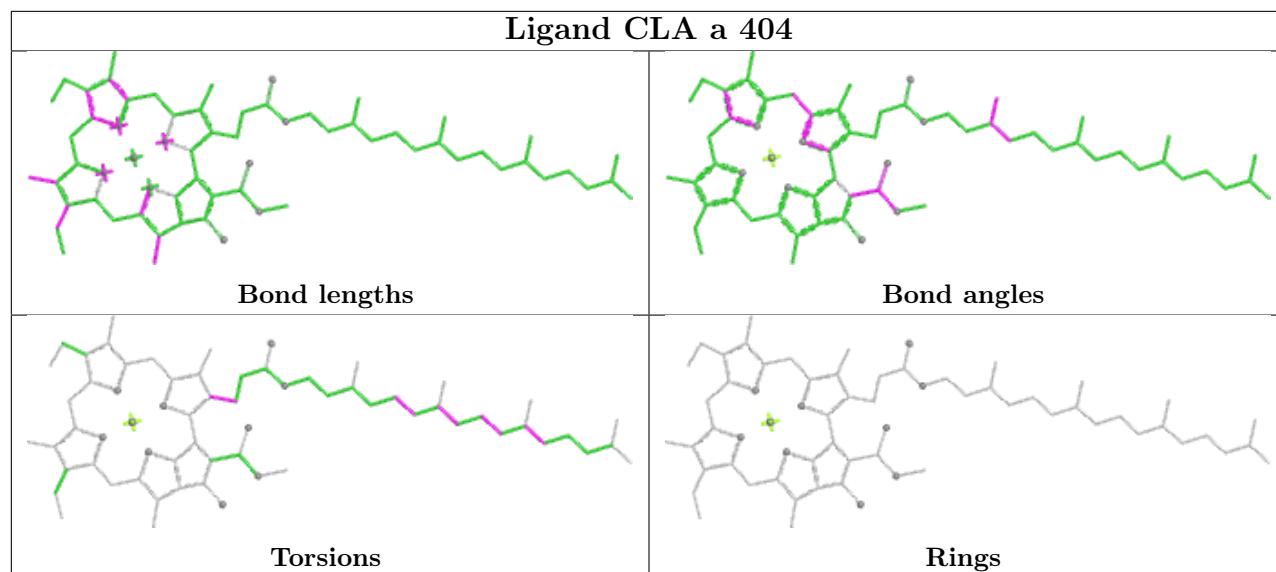
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

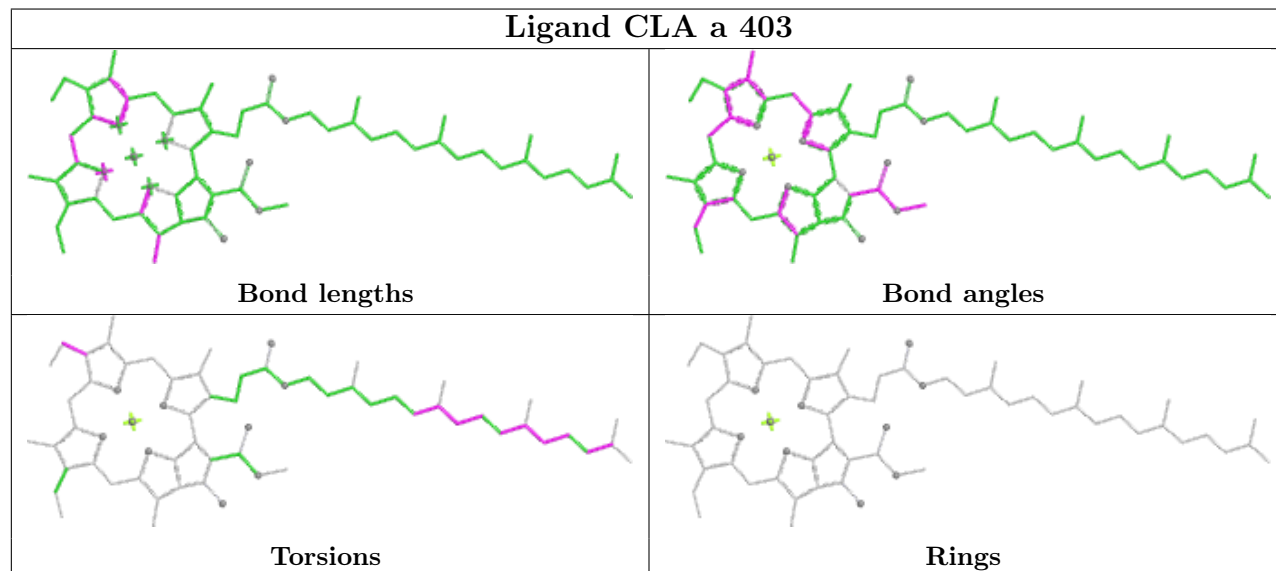
Ligand BCR a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



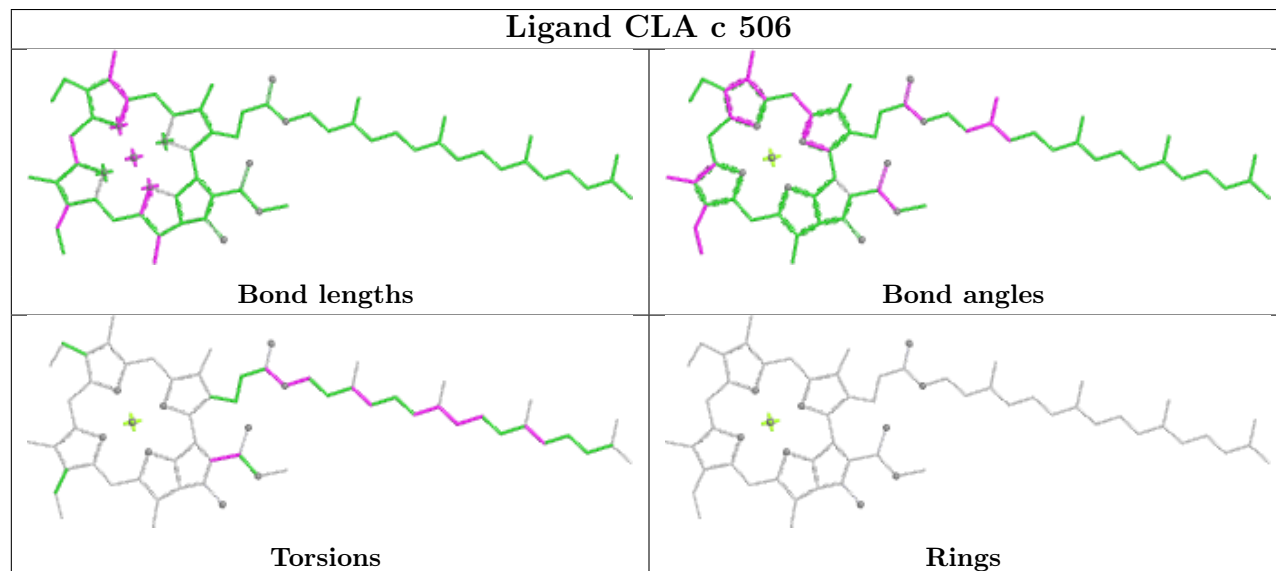
Ligand CLA a 404

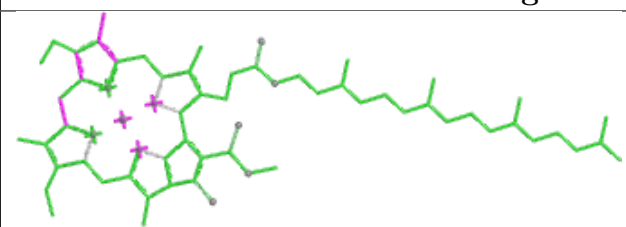
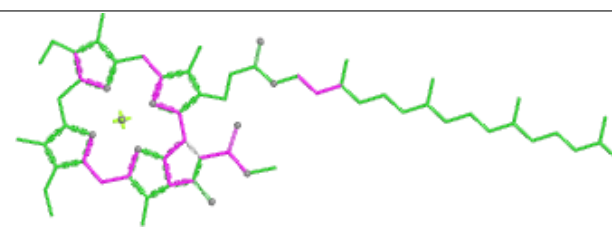
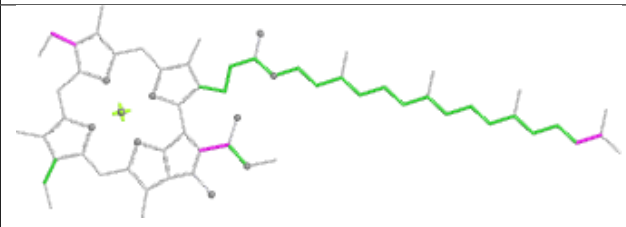
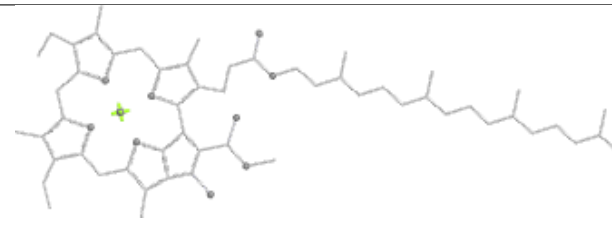


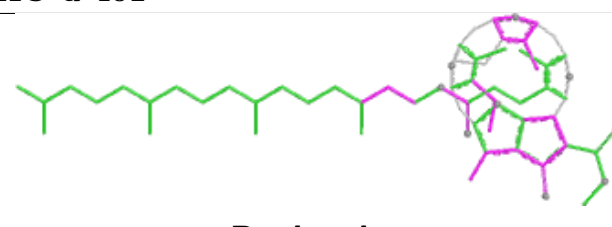
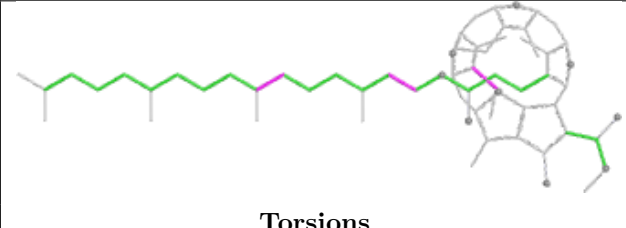
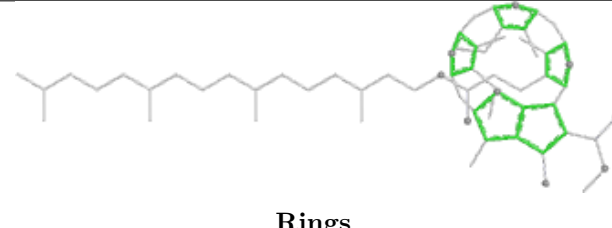
Ligand CLA a 403

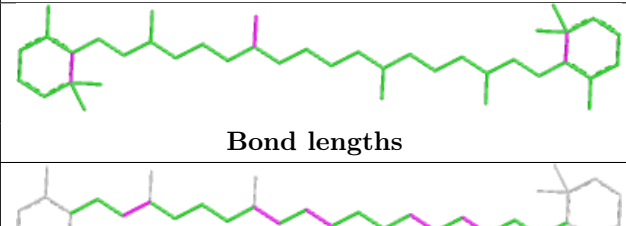
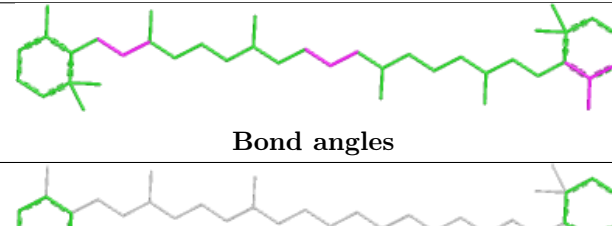
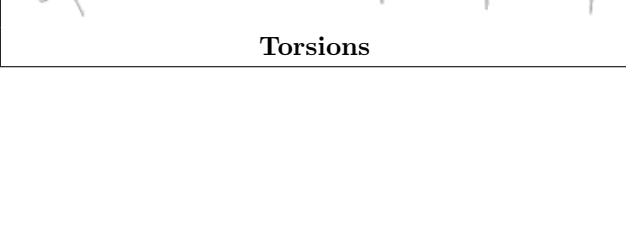
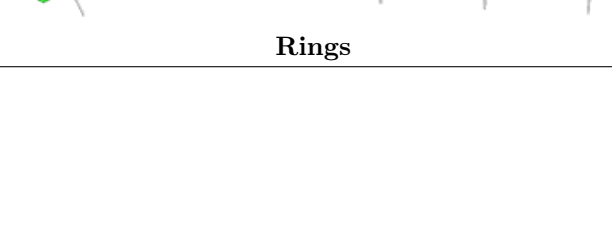


Ligand CLA c 506

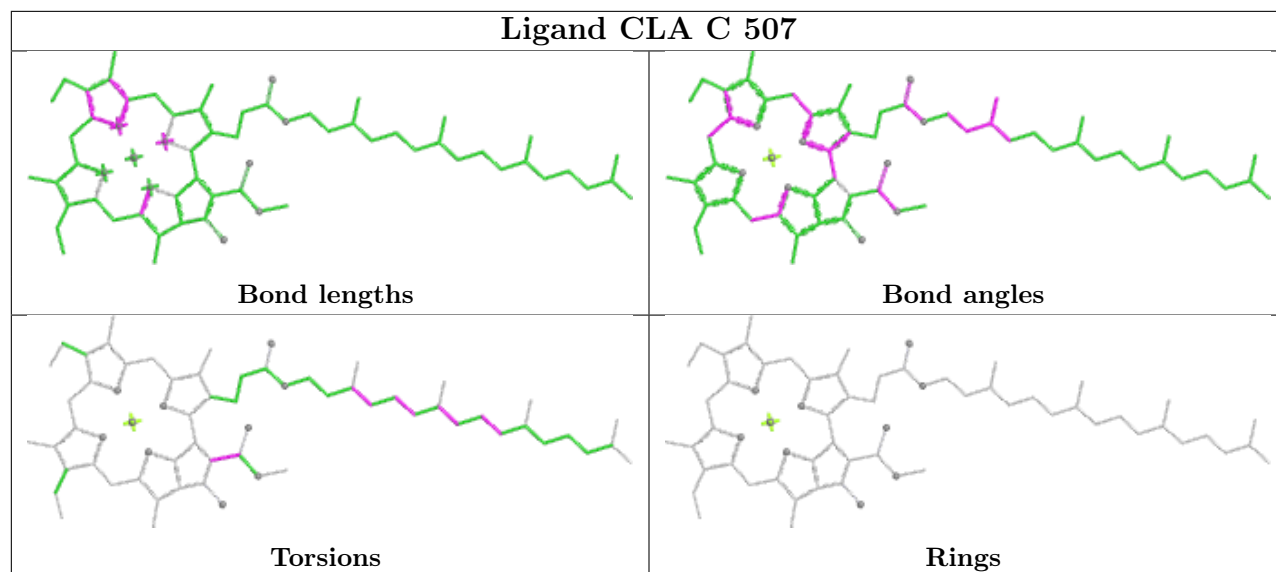


Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

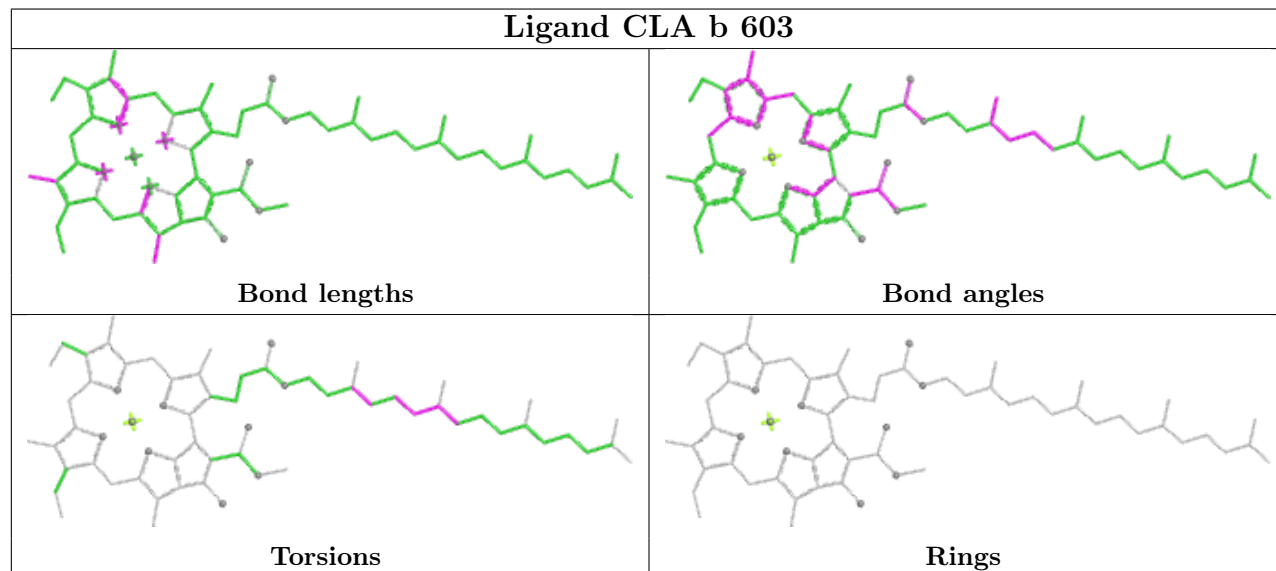
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

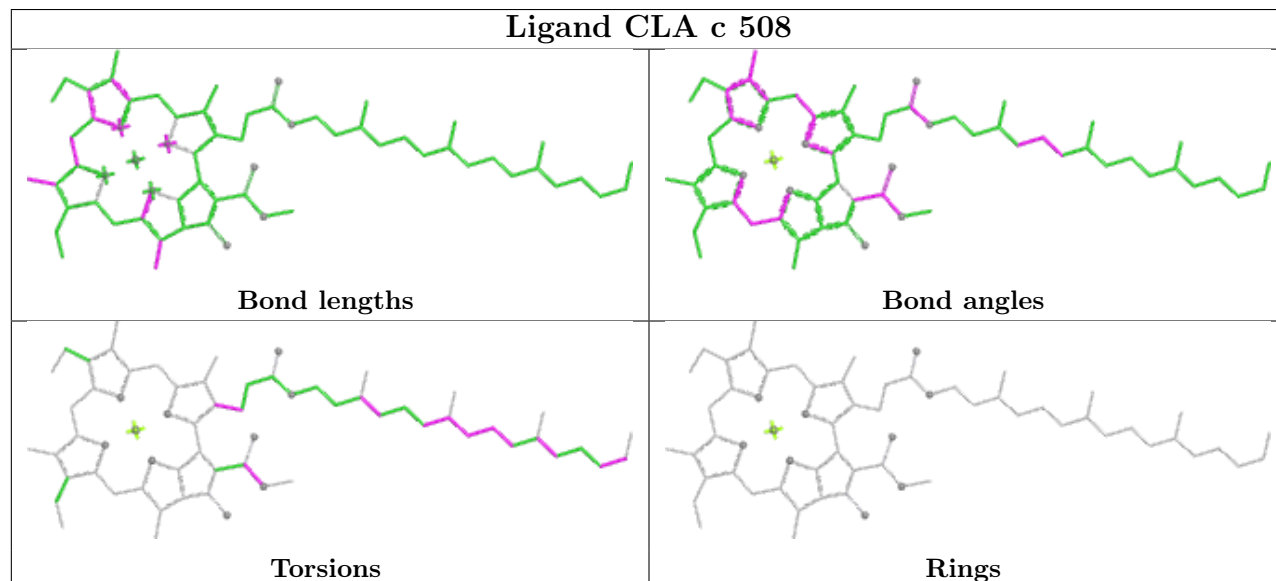
Ligand CLA C 507

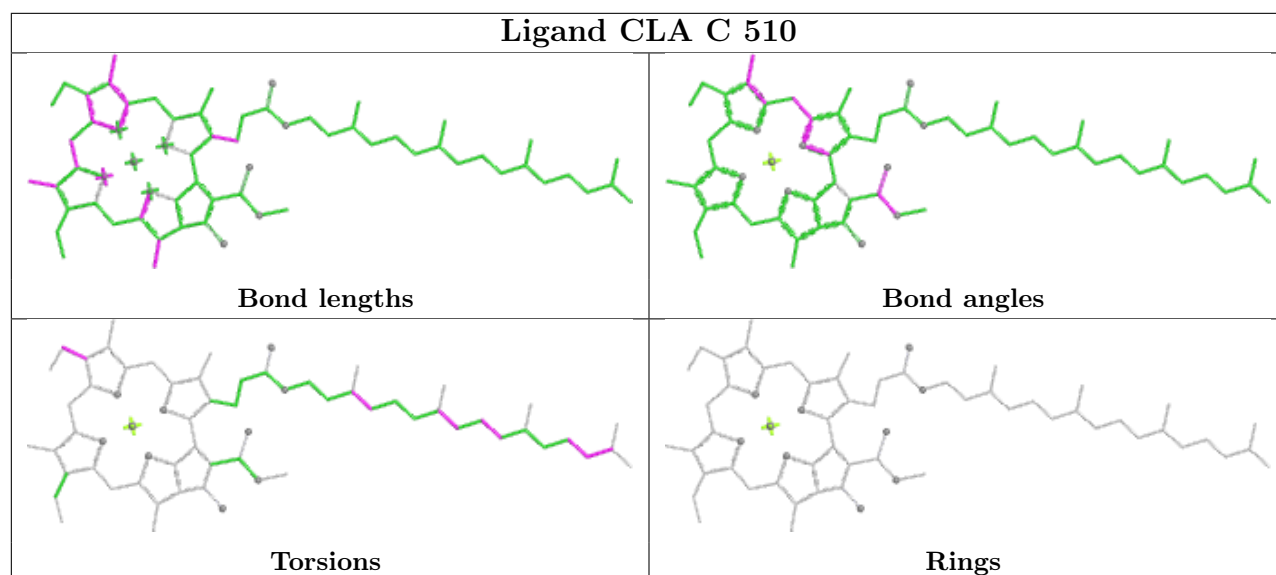
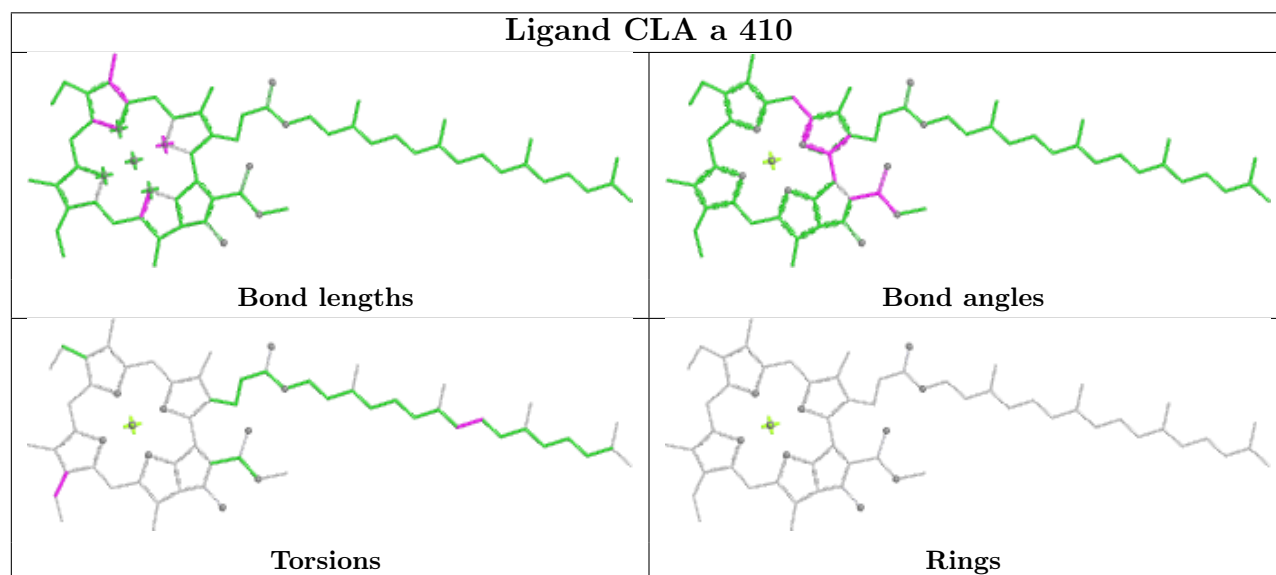
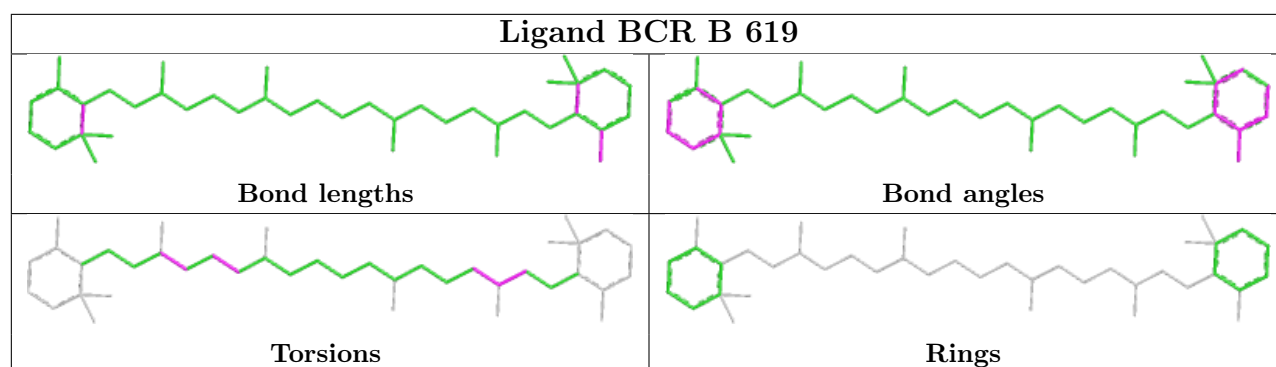


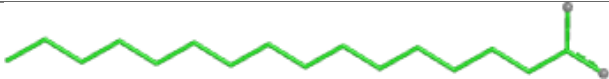
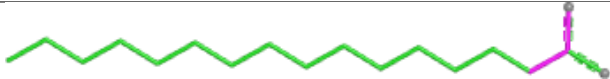
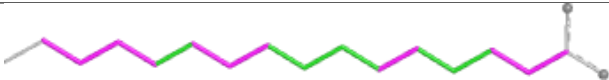
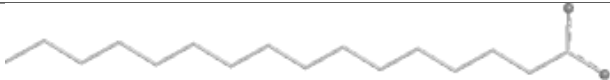
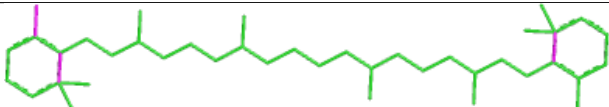
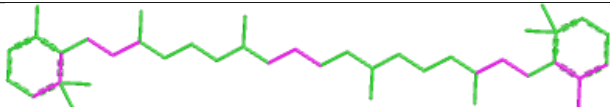
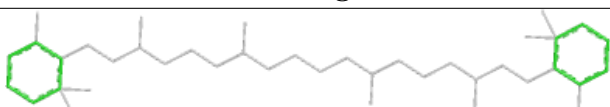
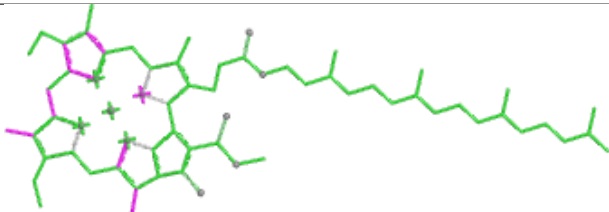
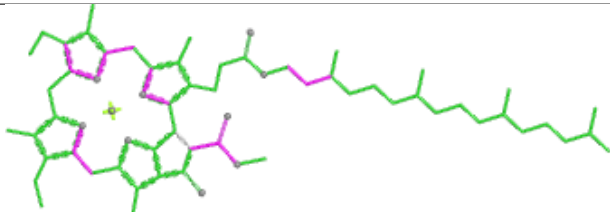
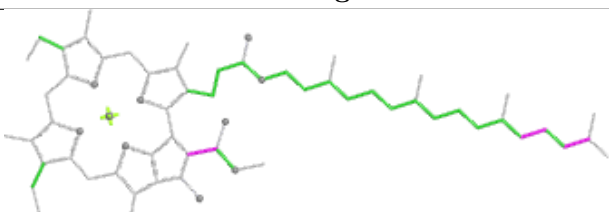
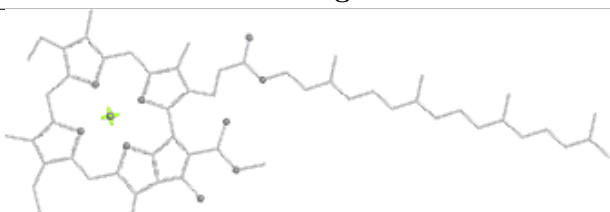
Ligand CLA b 603

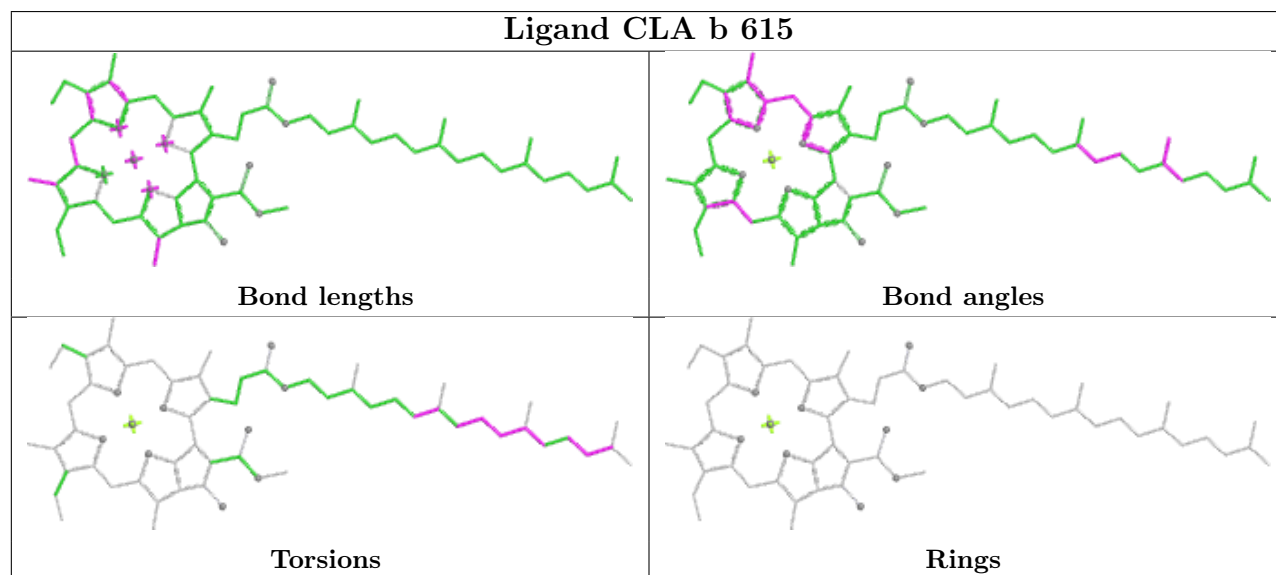
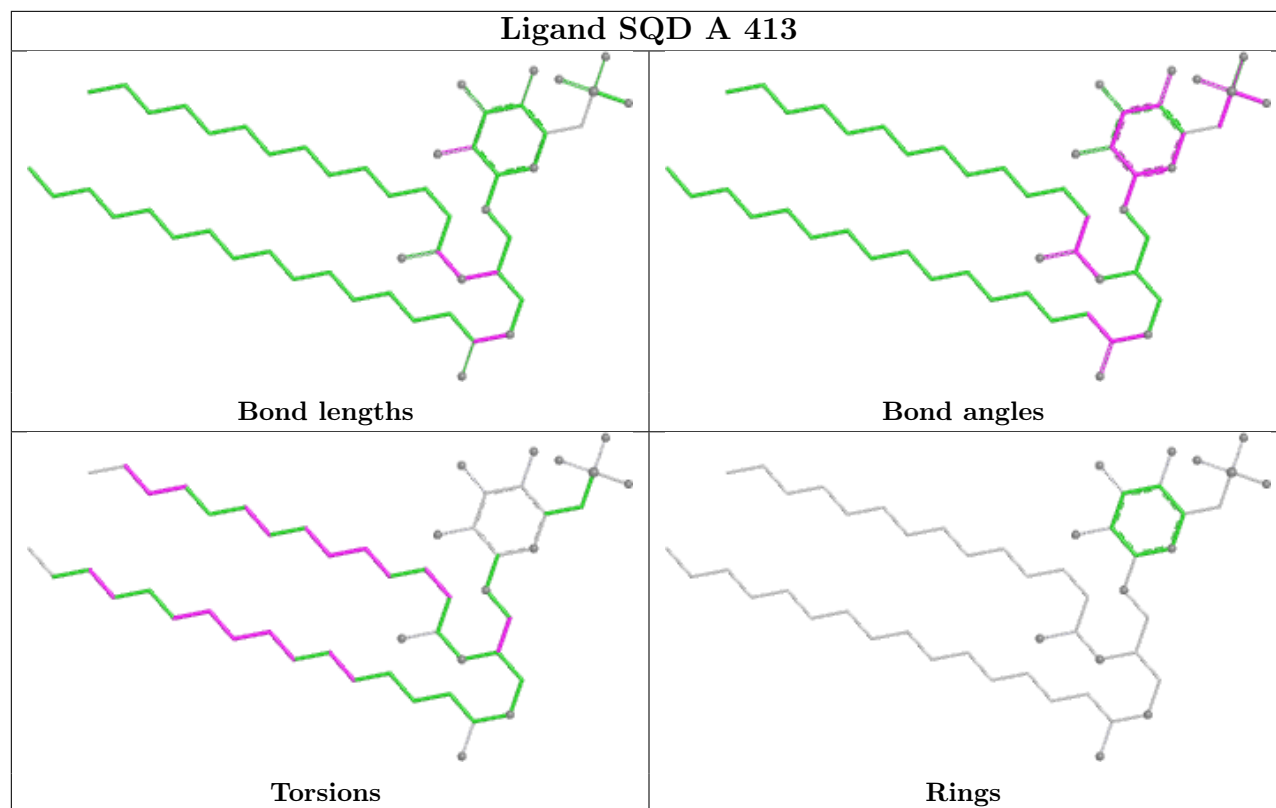


Ligand CLA c 508

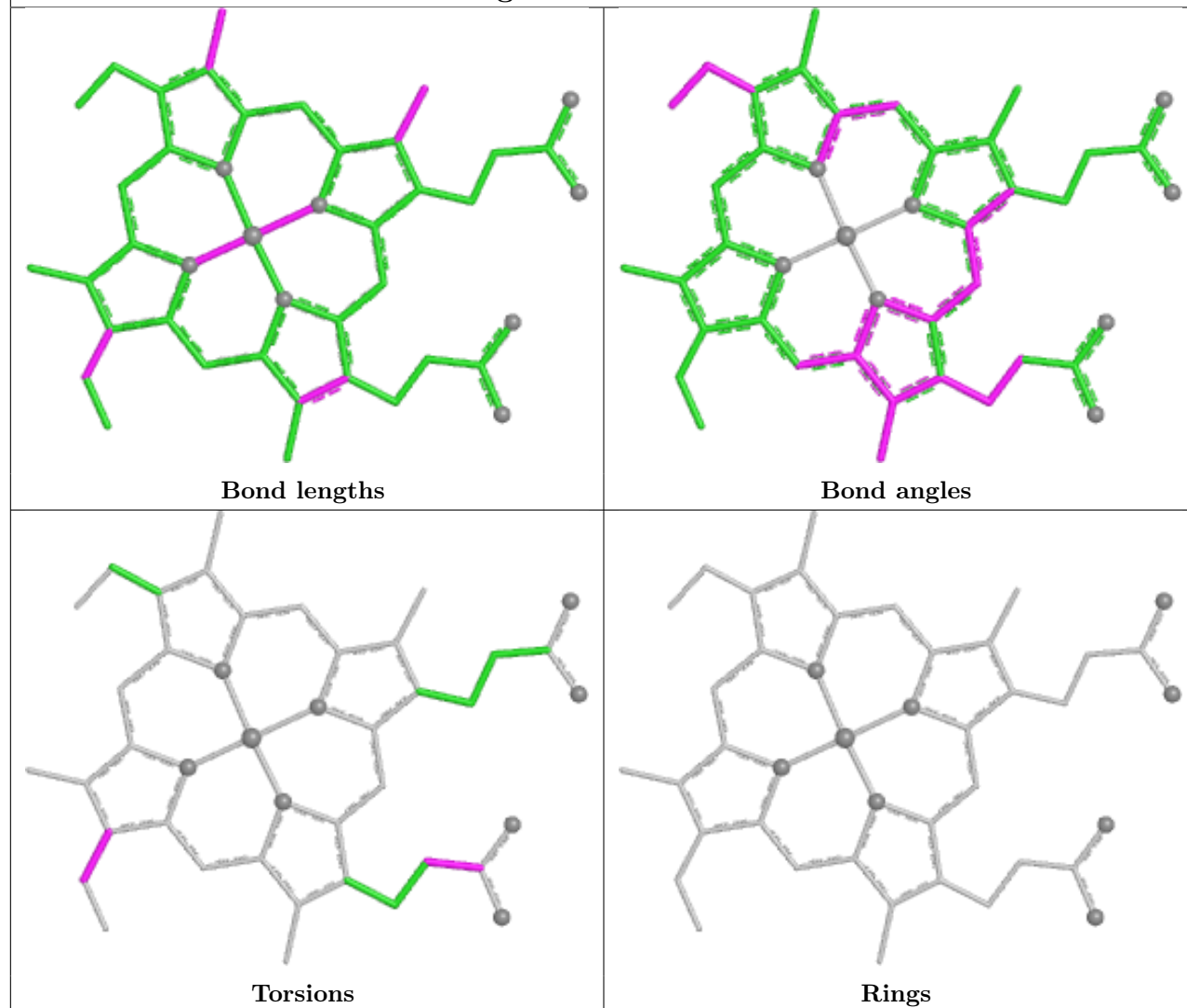




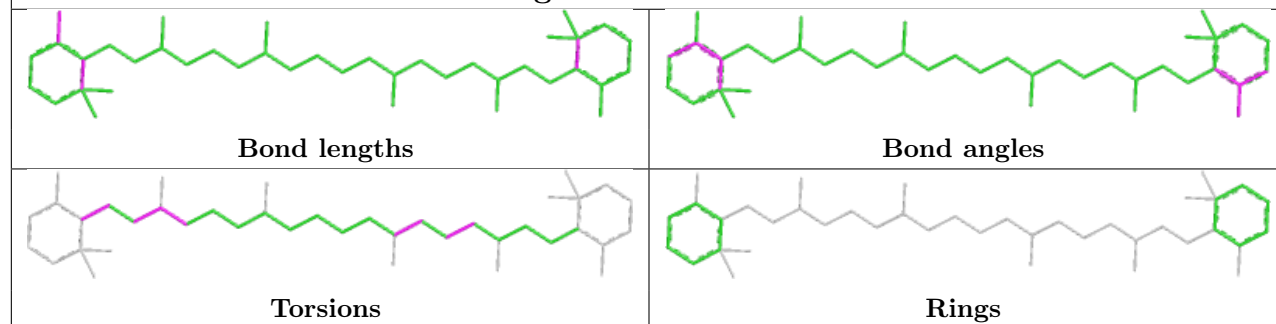
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings



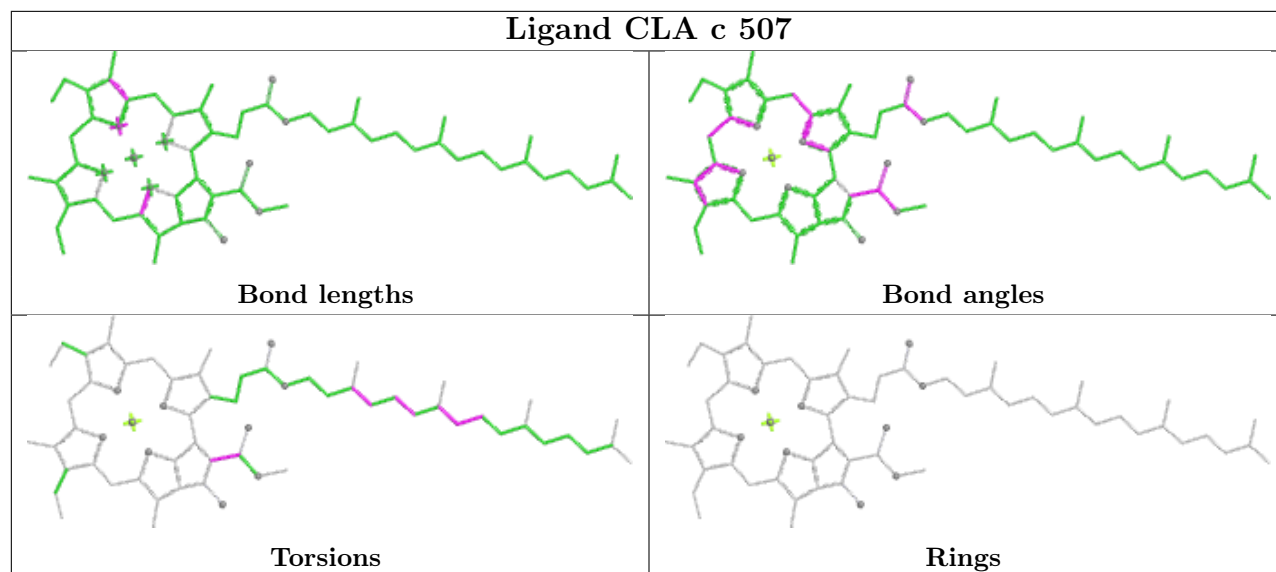
Ligand HEC v 201



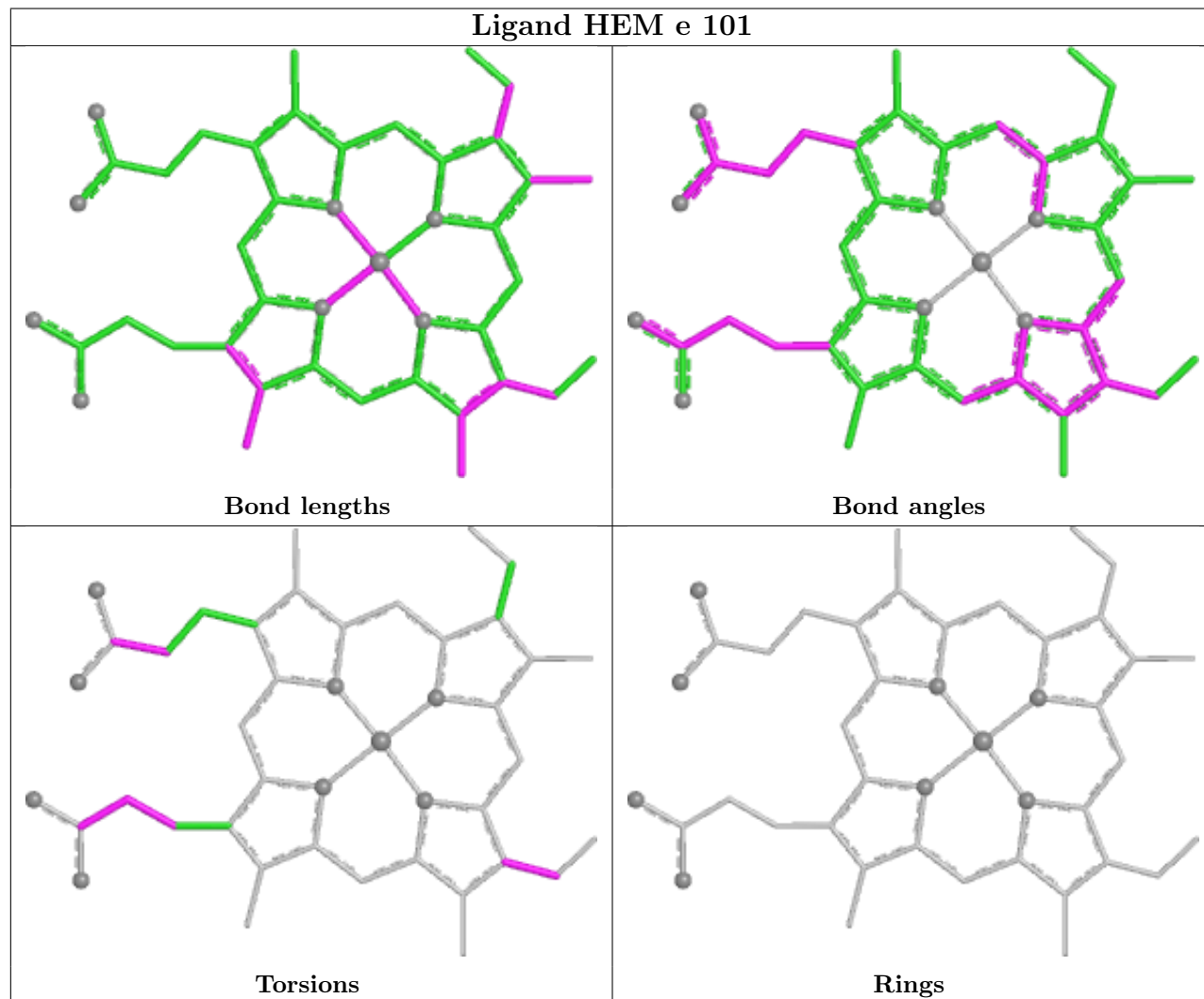
Ligand BCR k 101



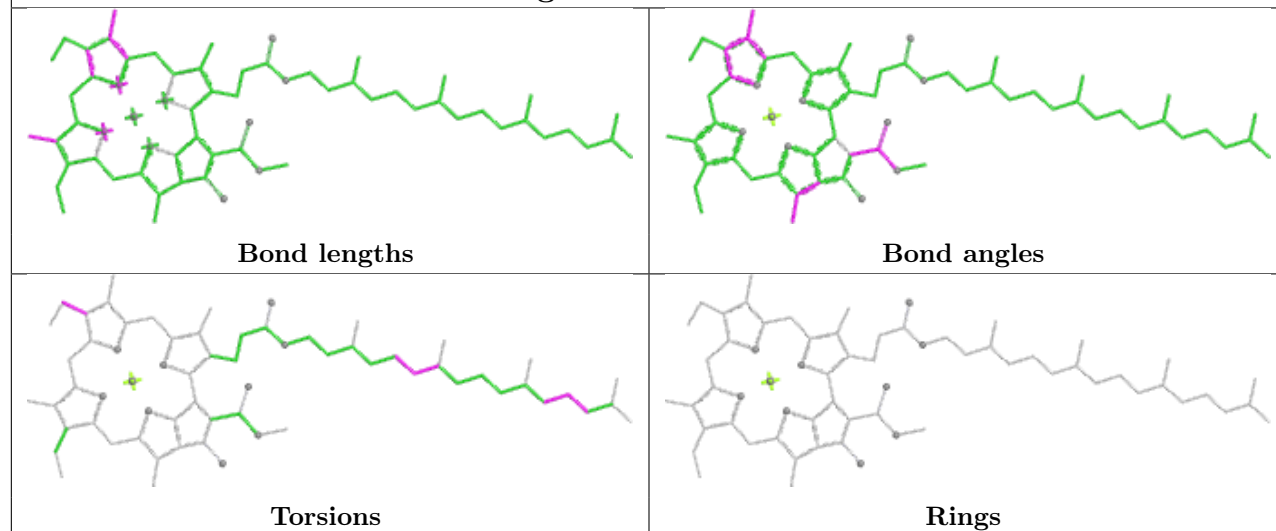
Ligand CLA c 507



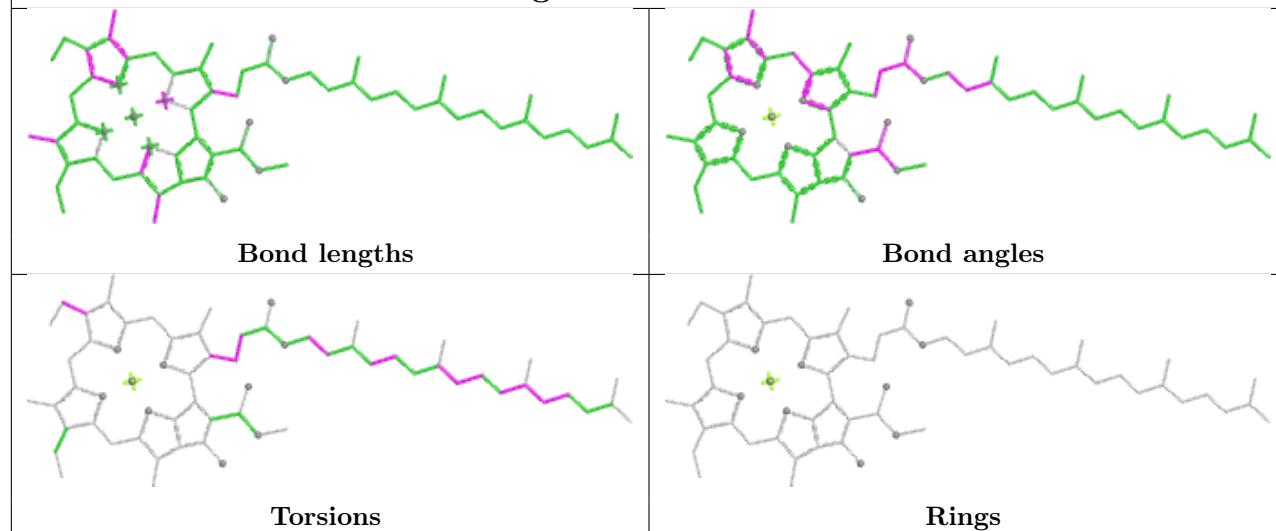
Ligand HEM e 101



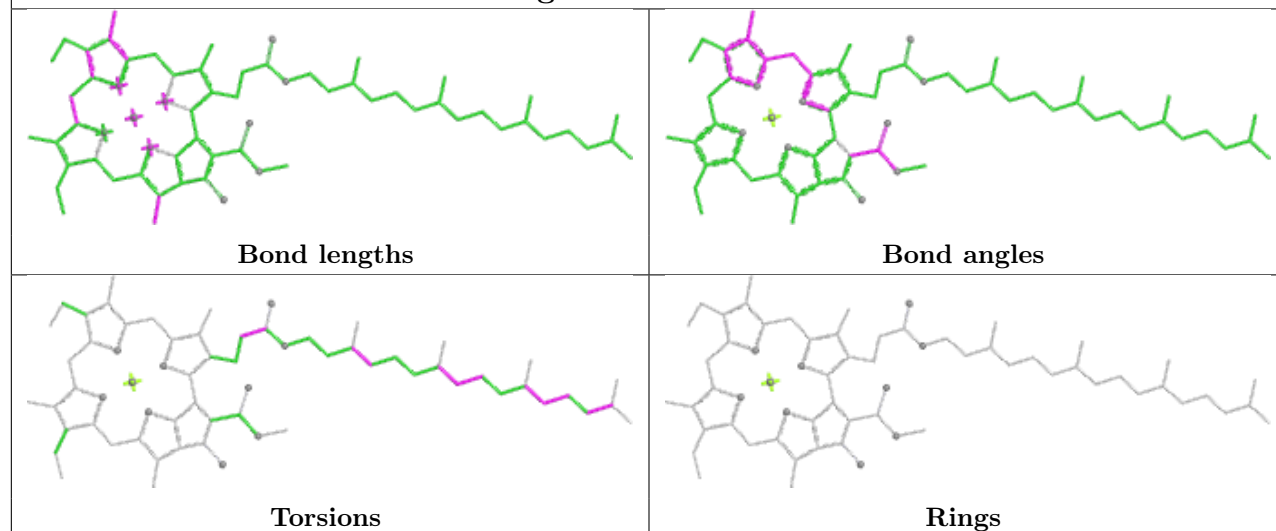
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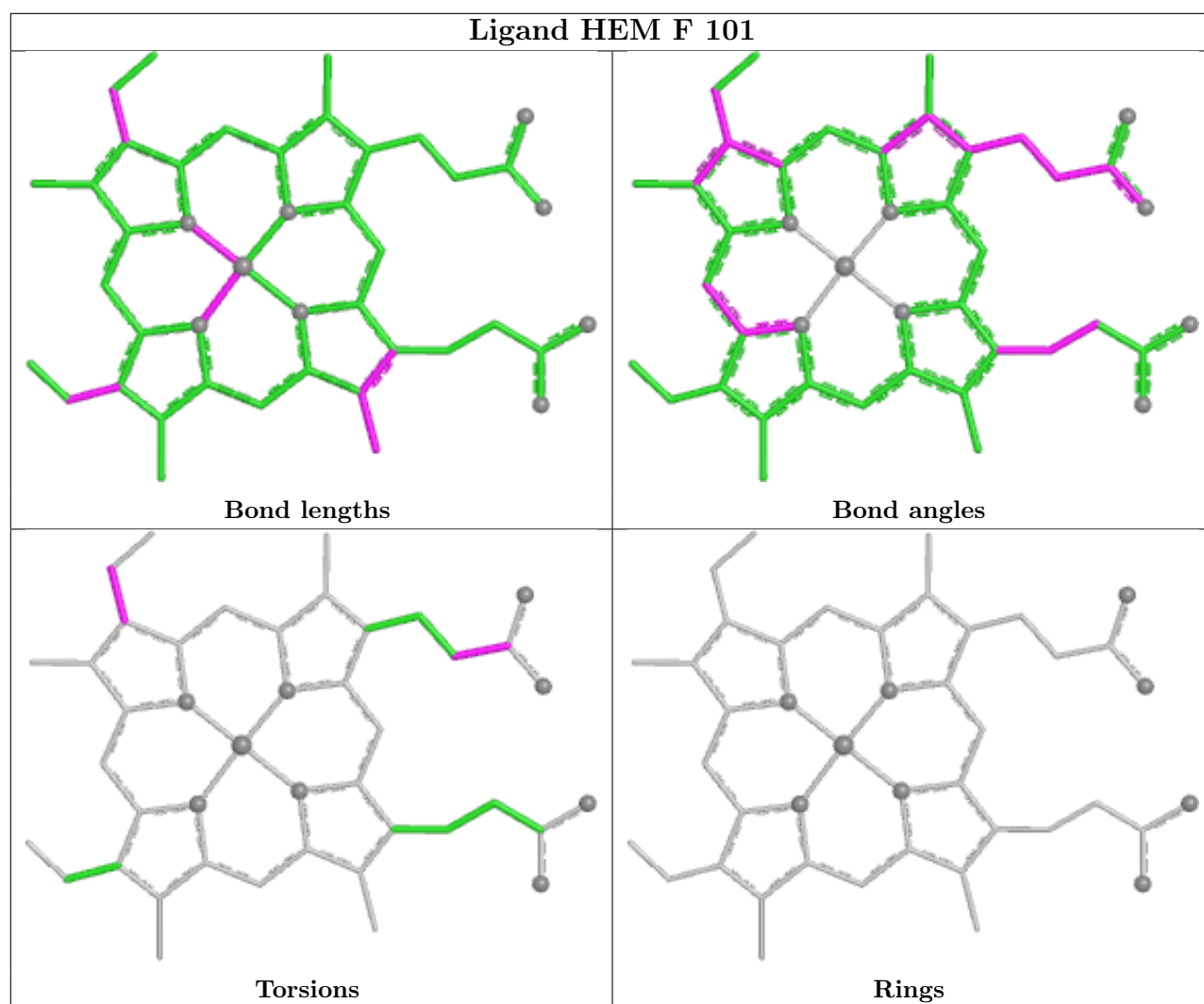


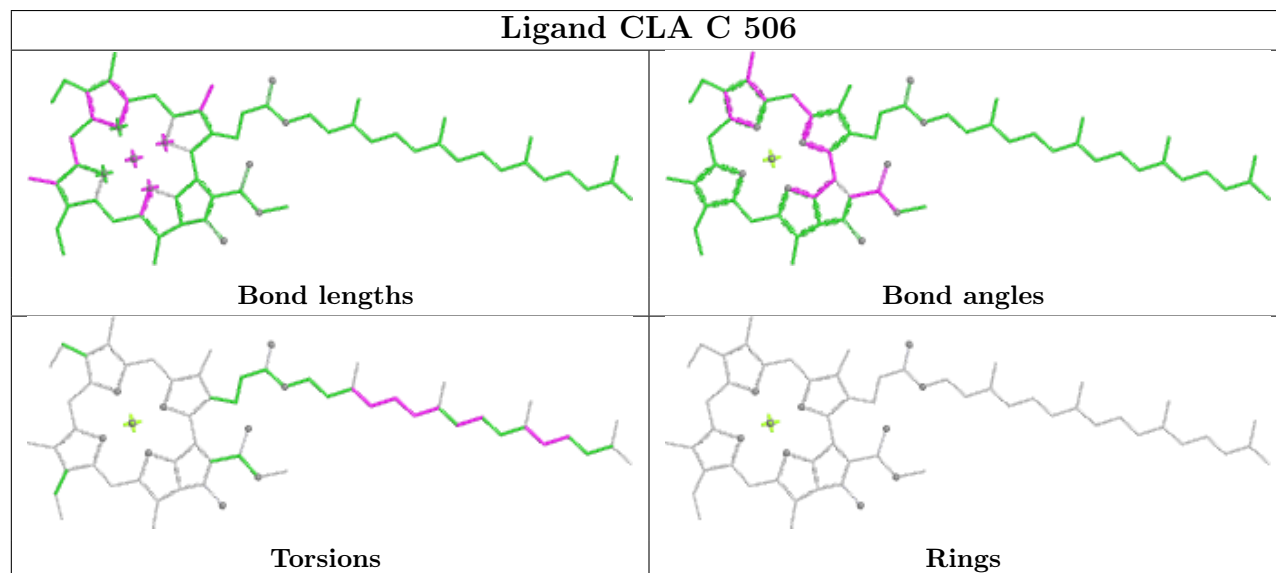
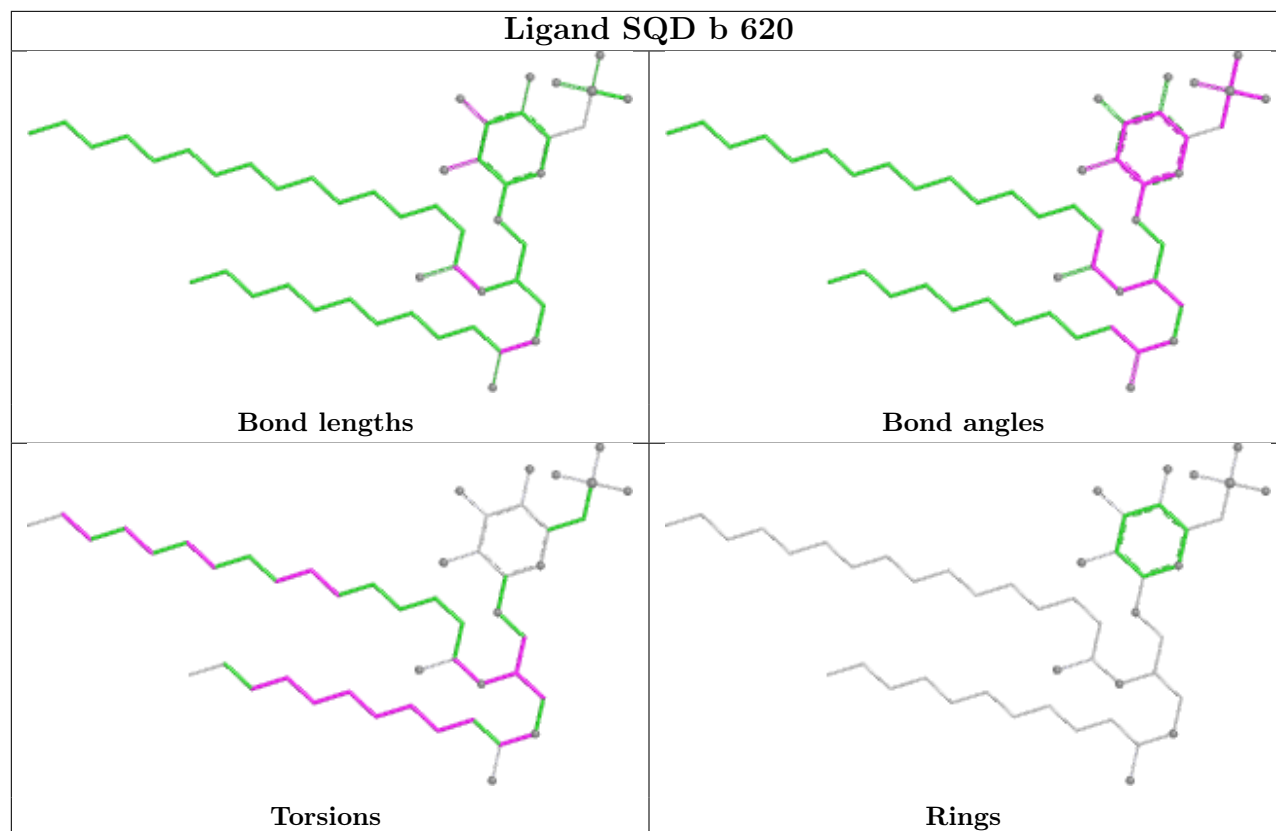
Ligand CLA C 512



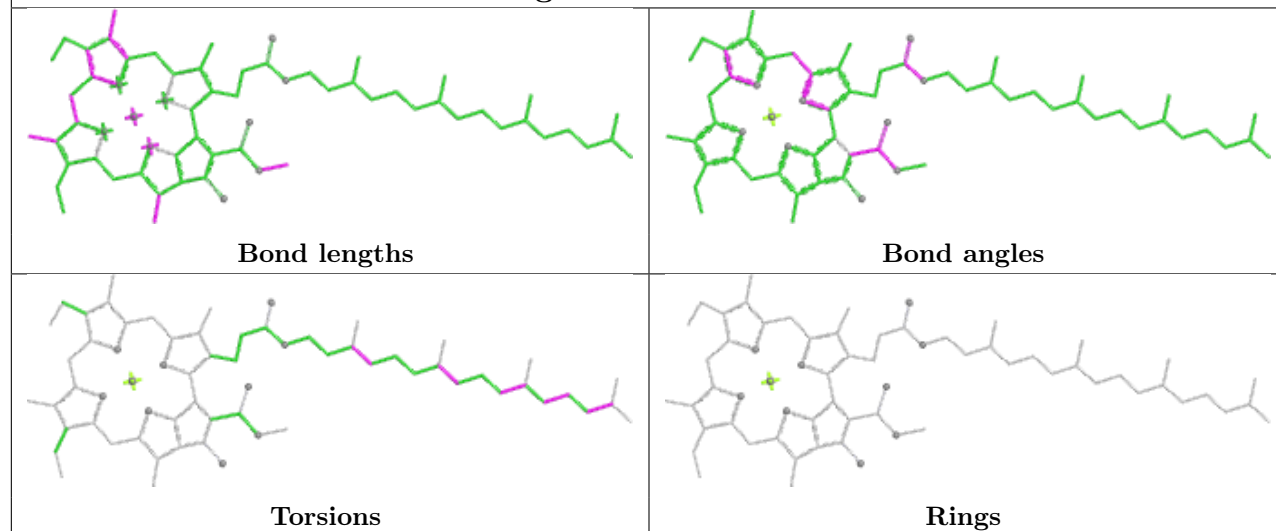
Ligand CLA c 510



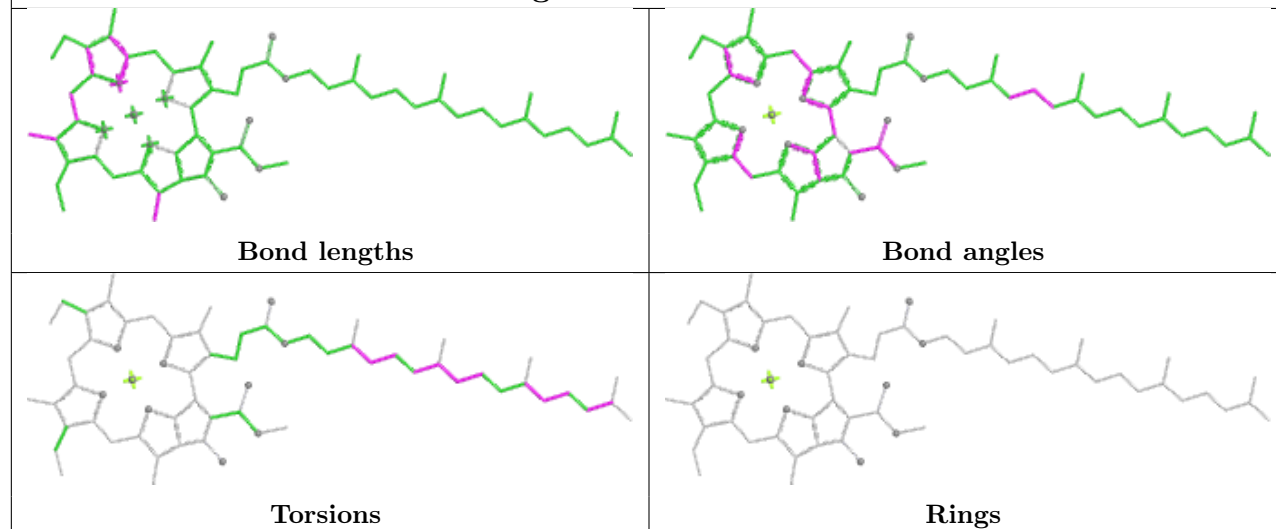




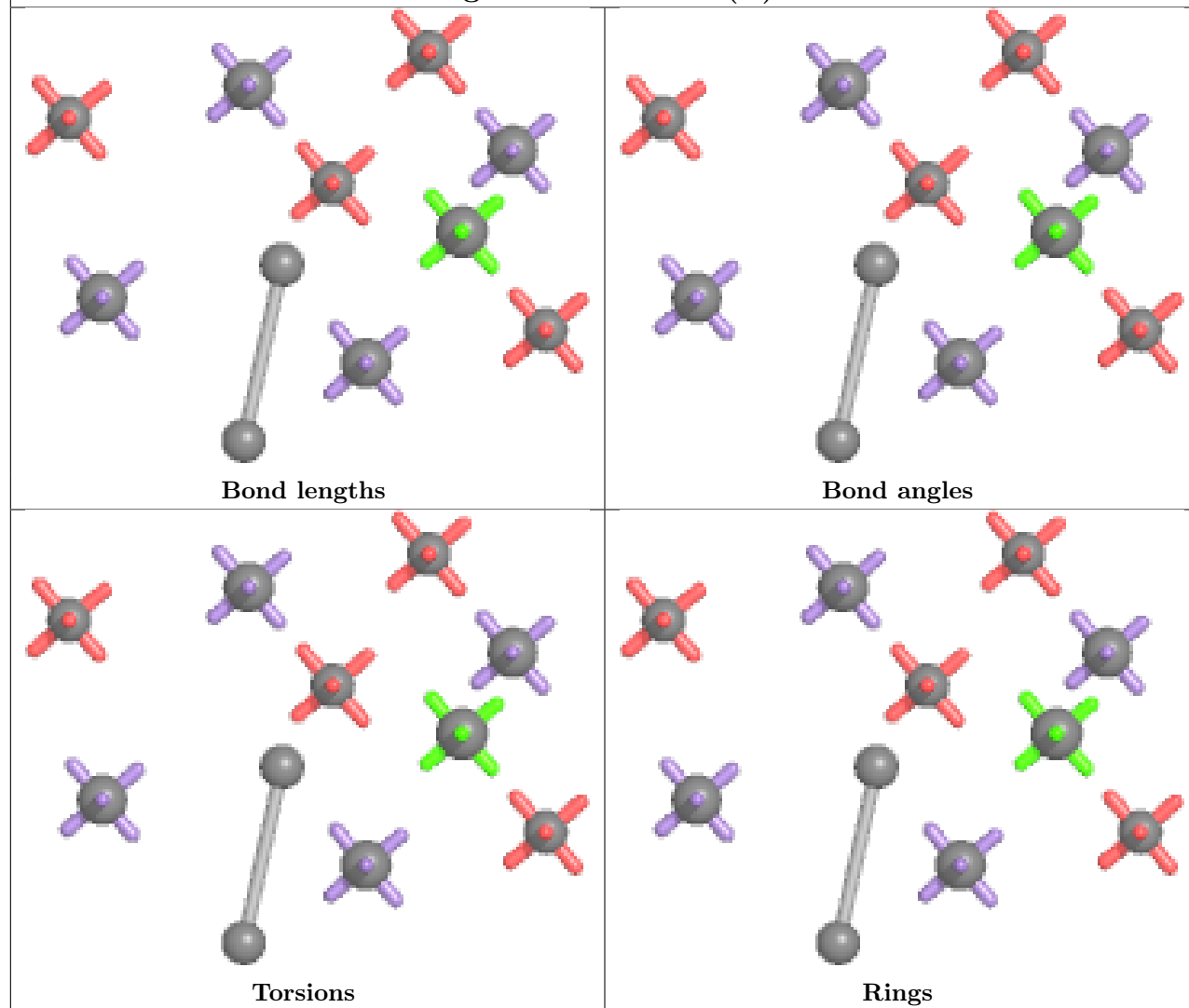
Ligand CLA b 608



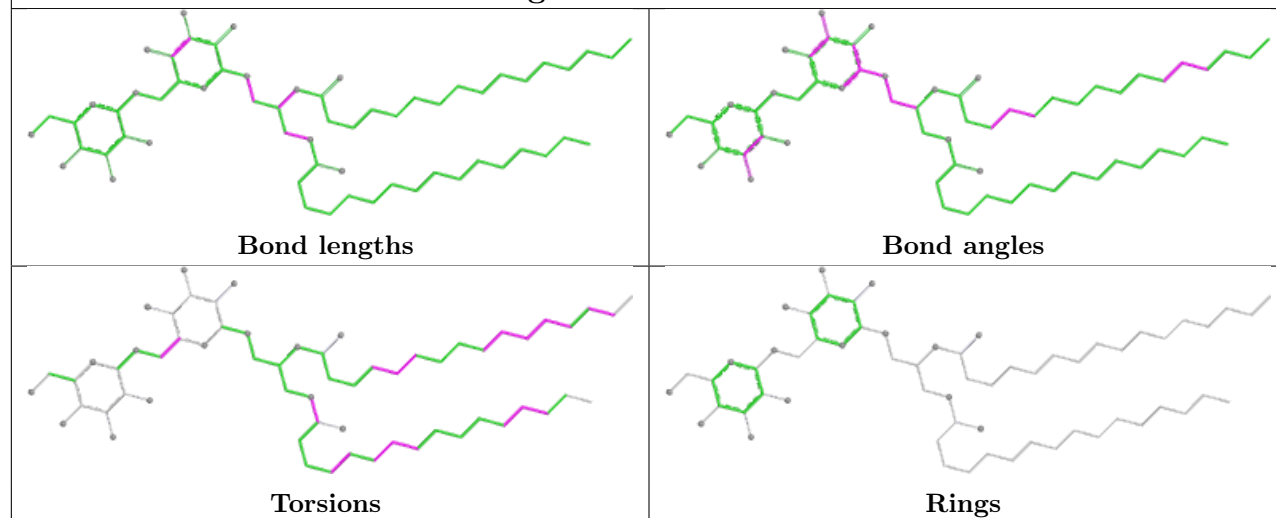
Ligand CLA B 605

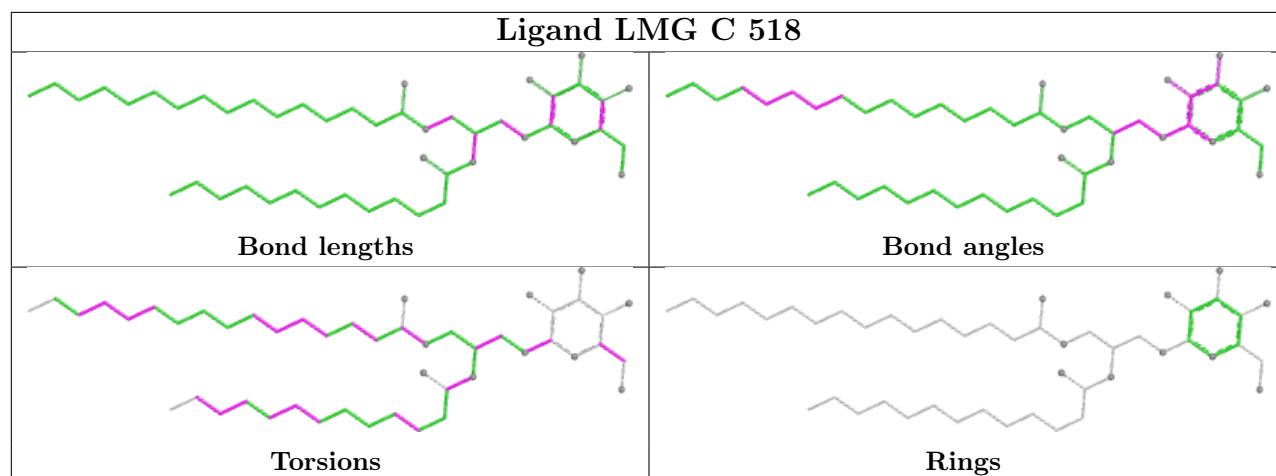
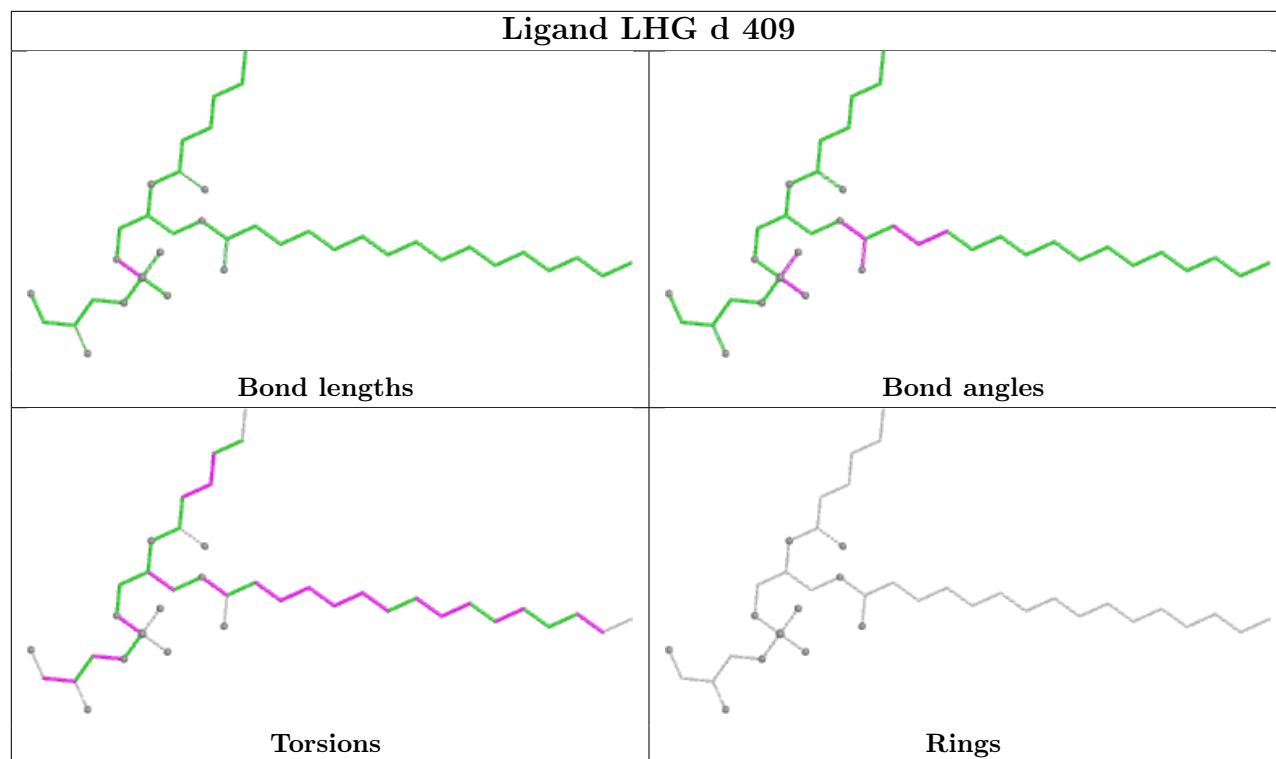


Ligand OEY A 417 (B)

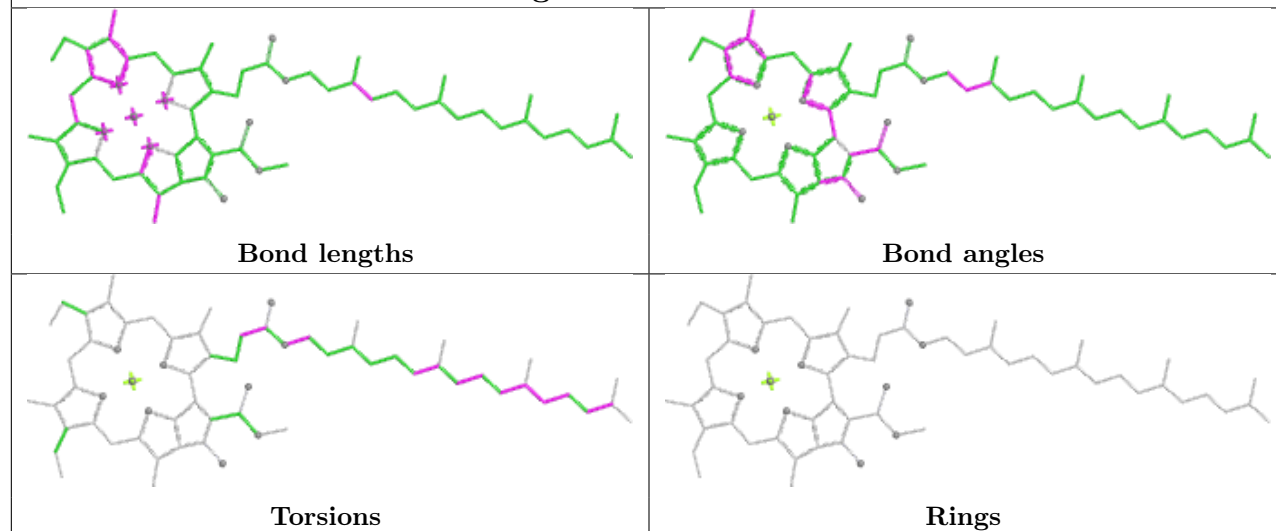


Ligand DGD C 517

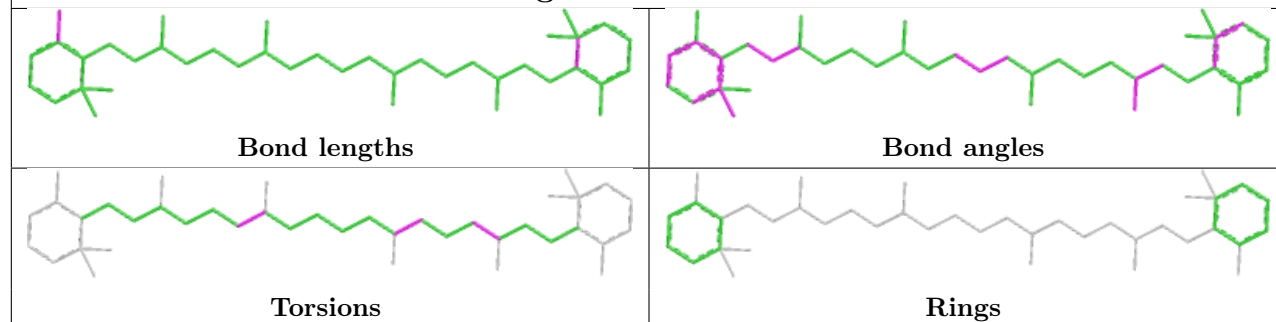




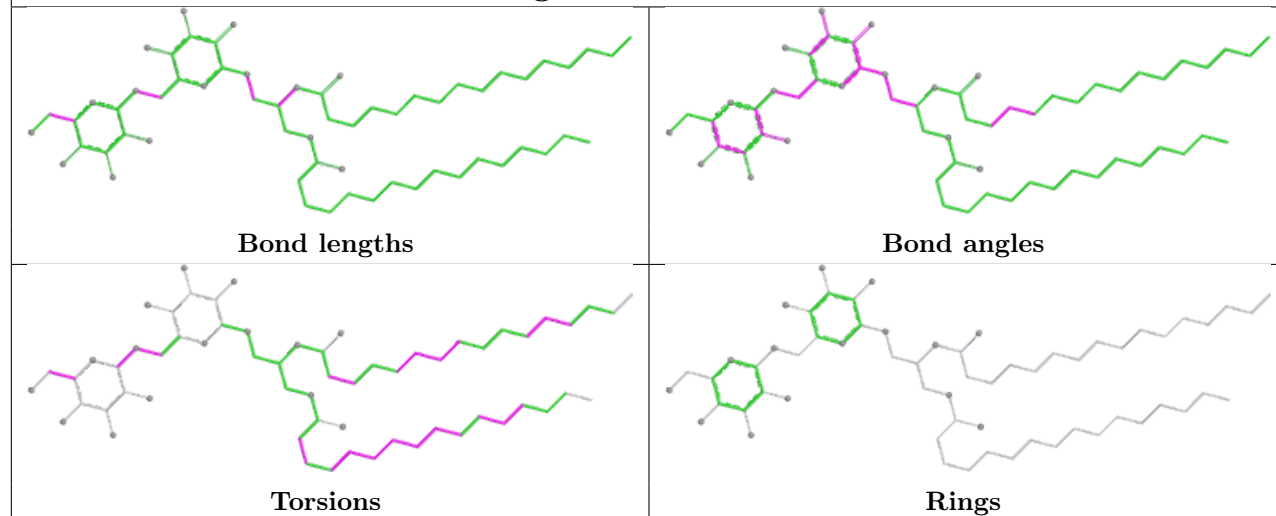
Ligand CLA B 613

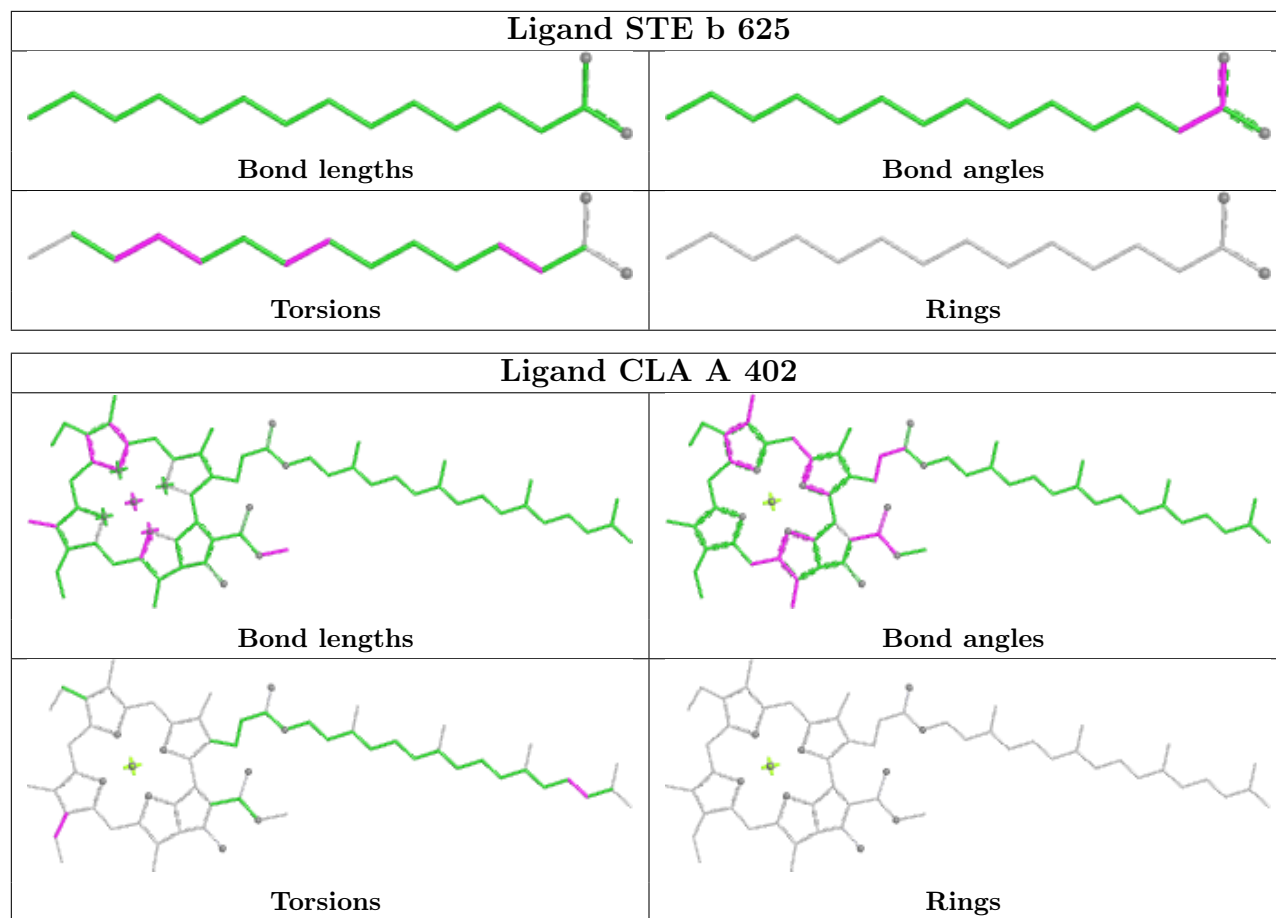


Ligand BCR t 101

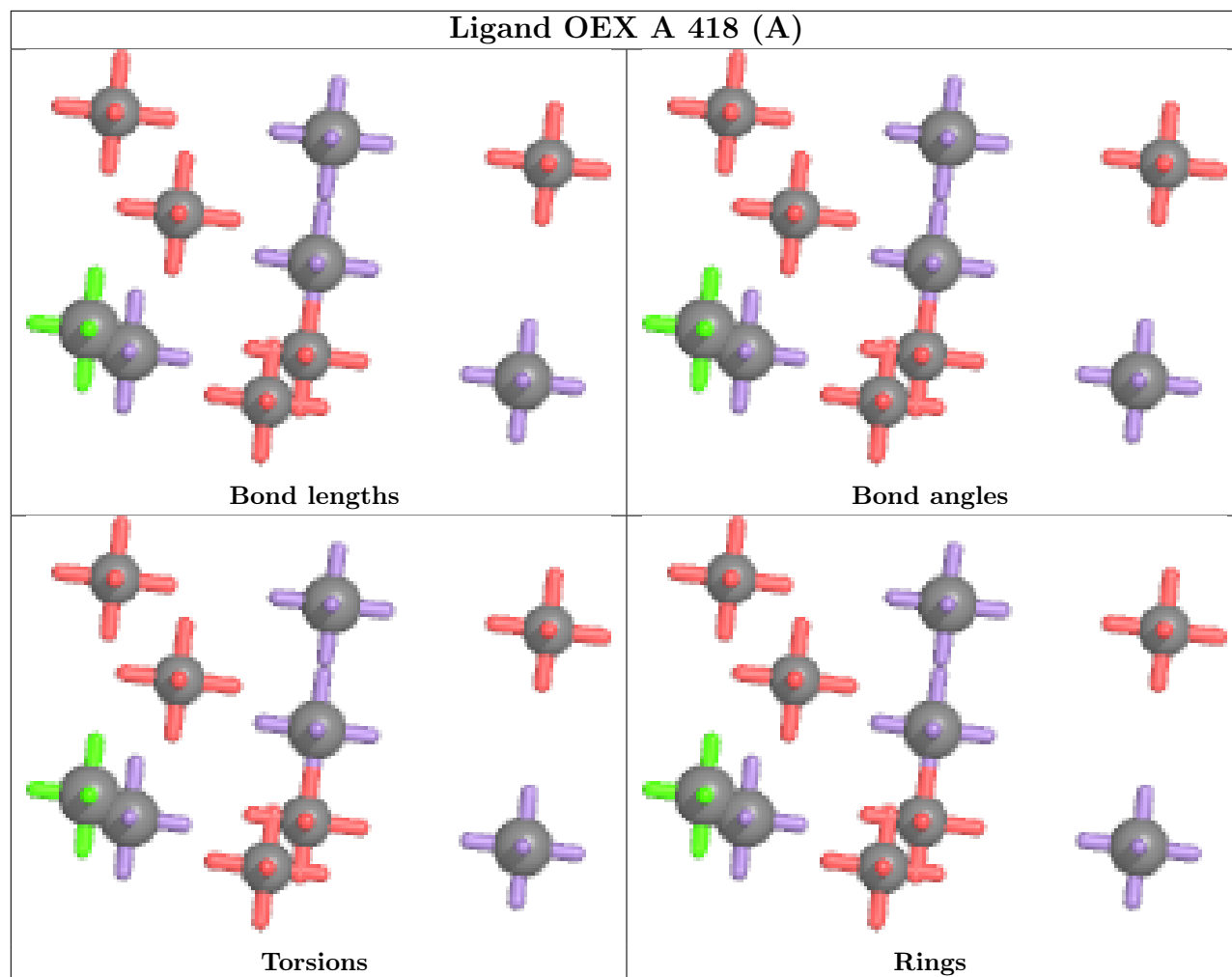


Ligand DGD c 517

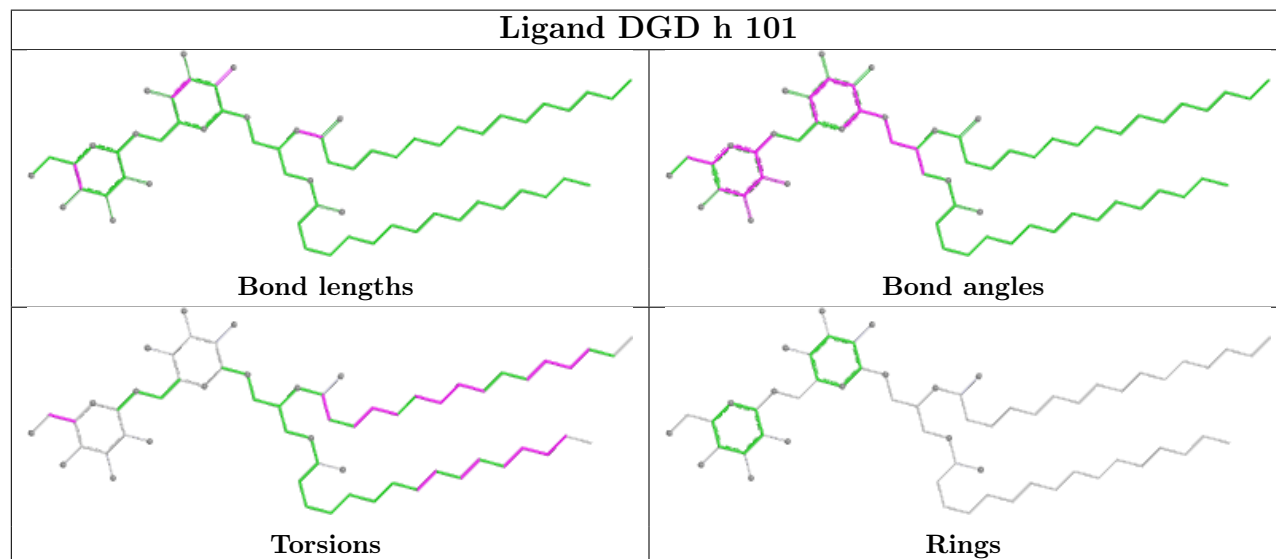


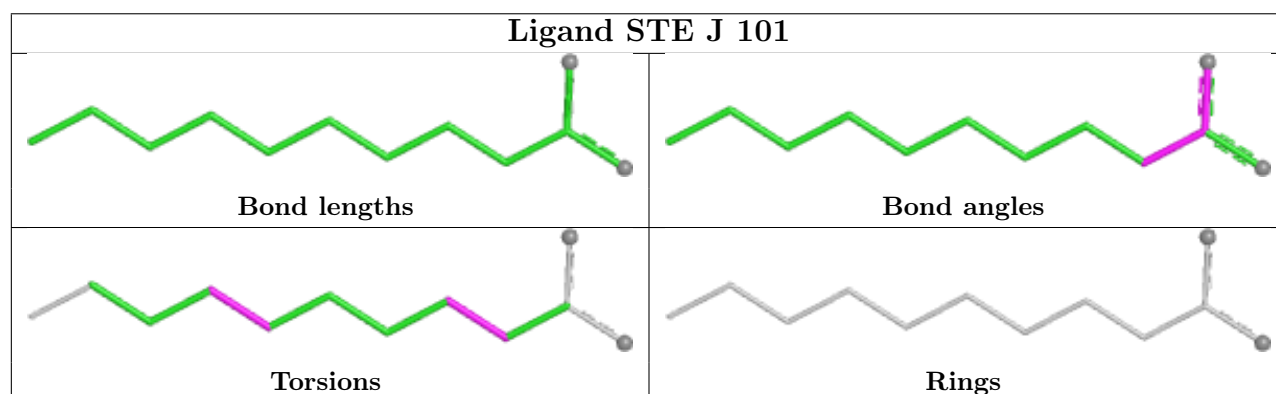
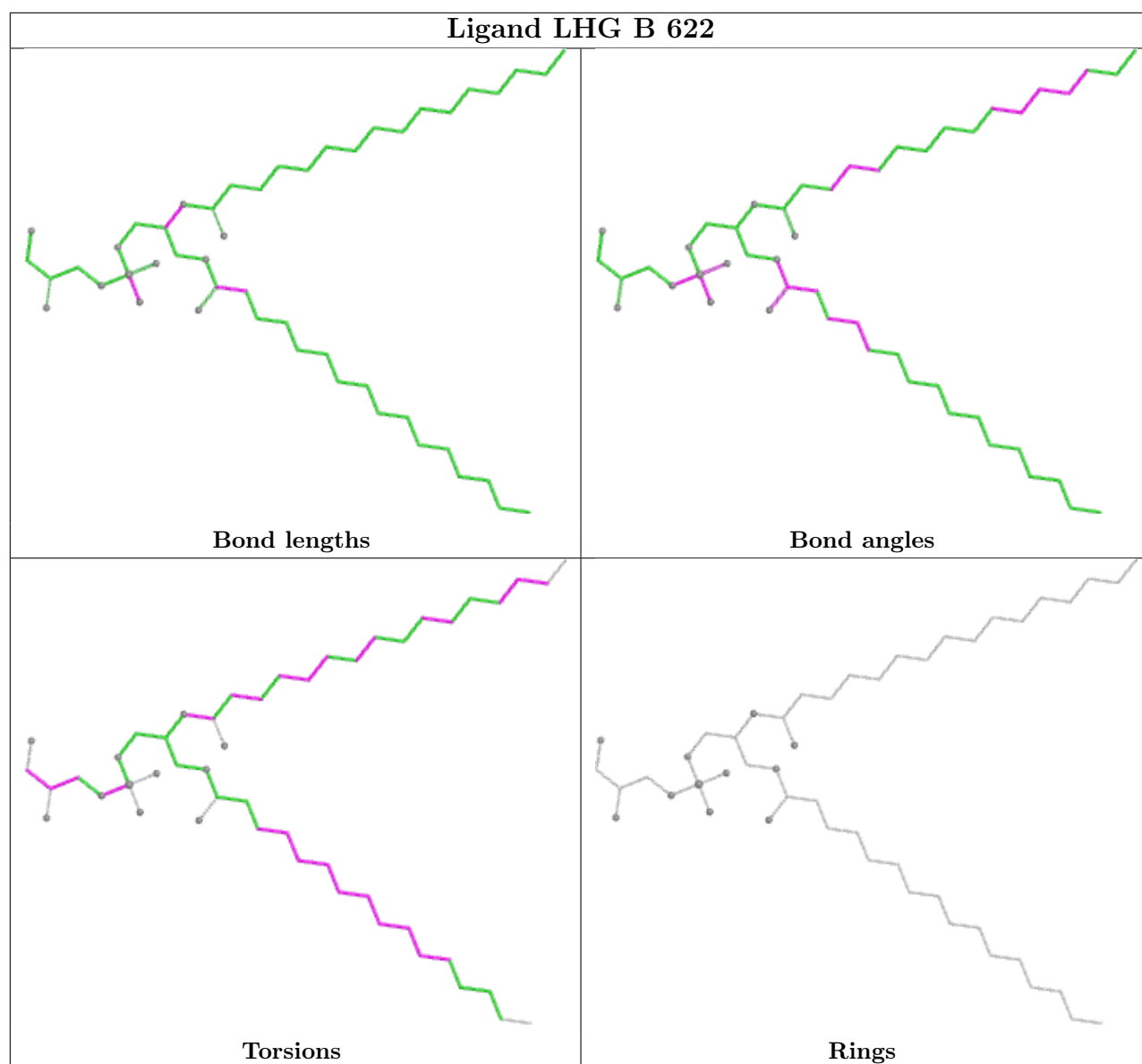


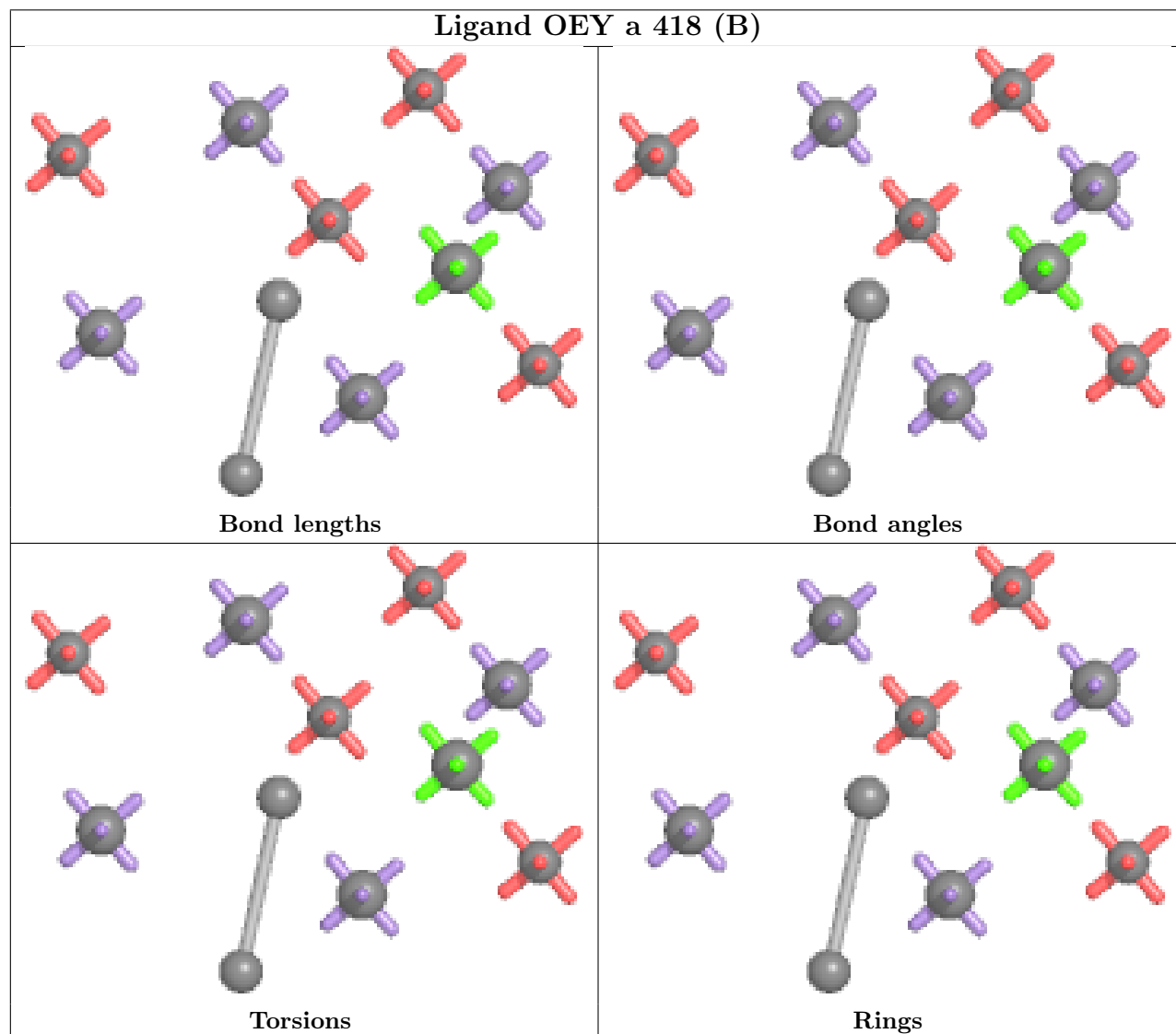
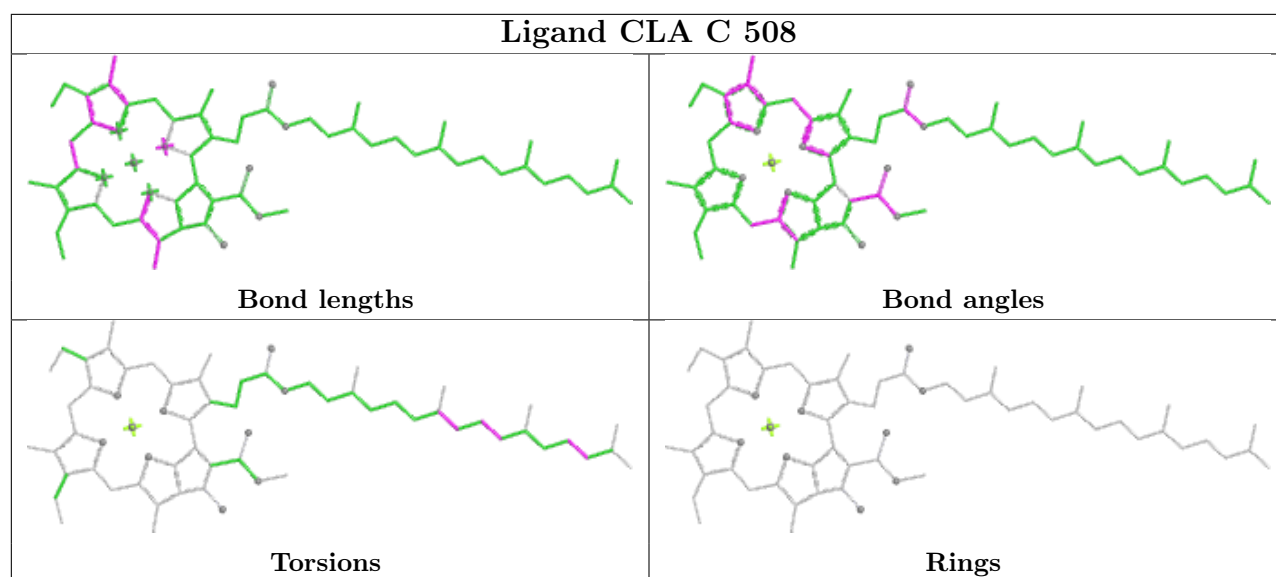
Ligand OEX A 418 (A)

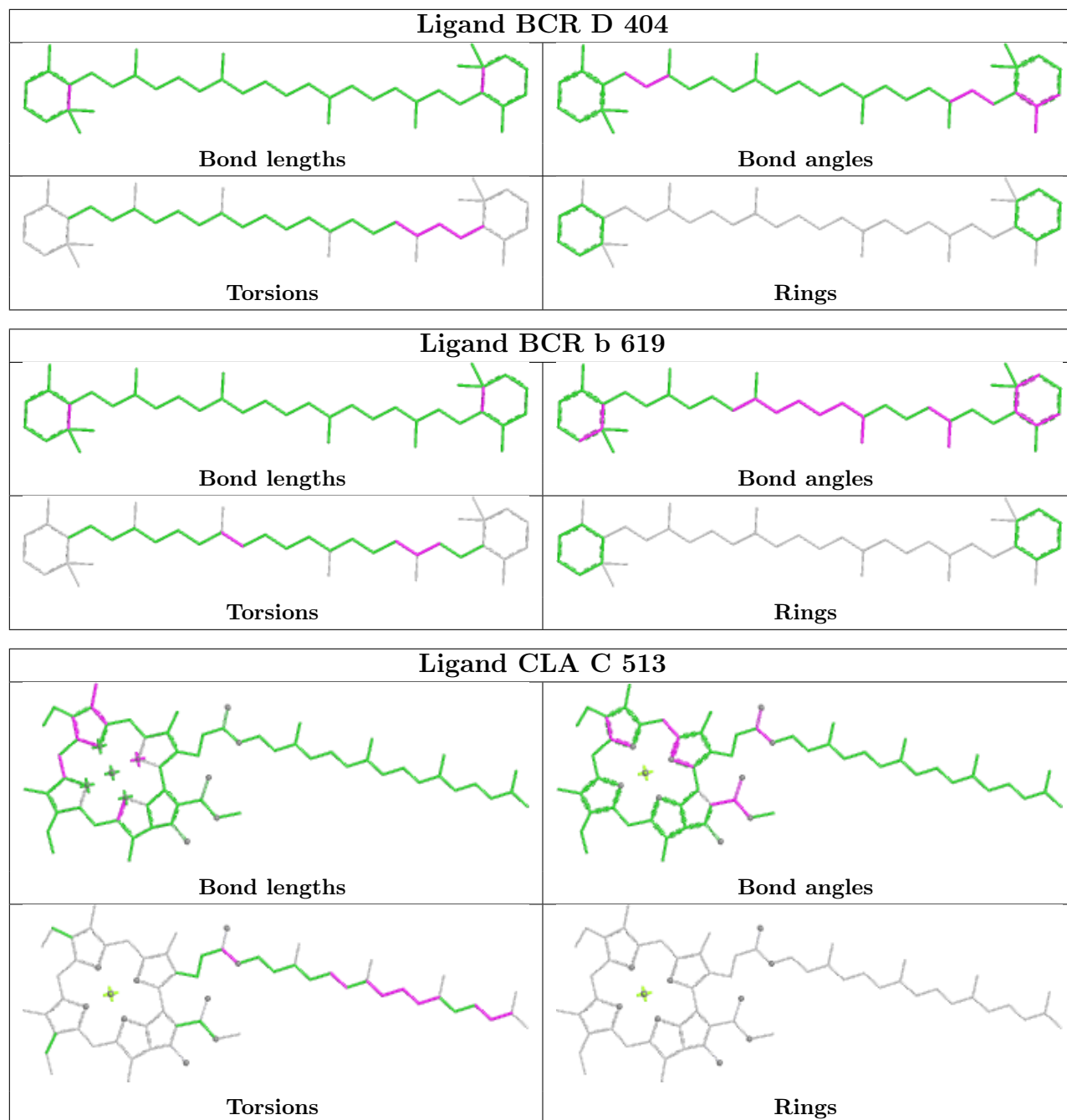


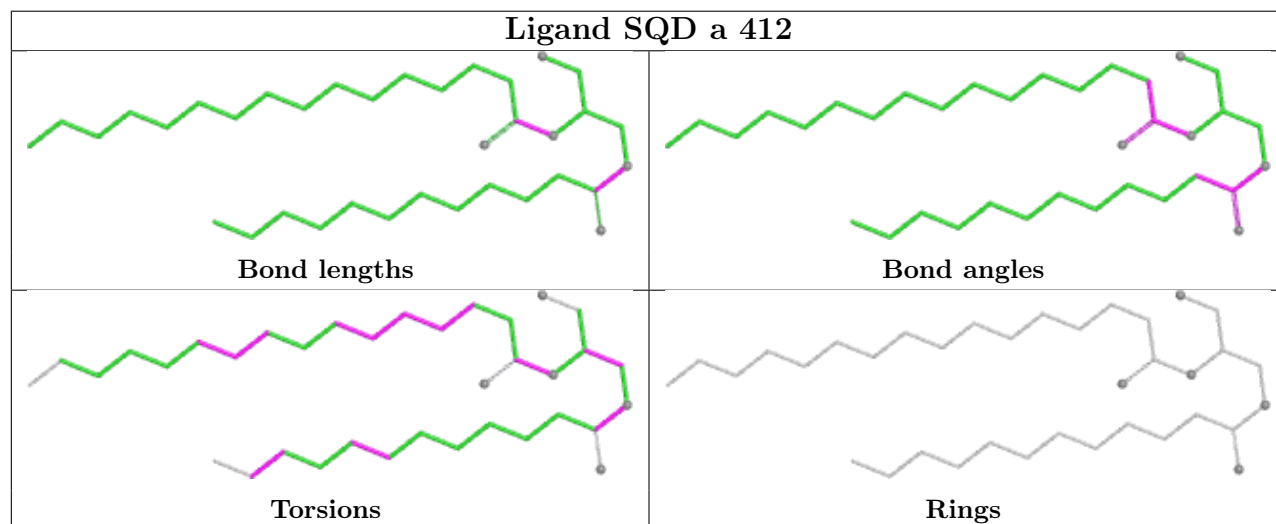
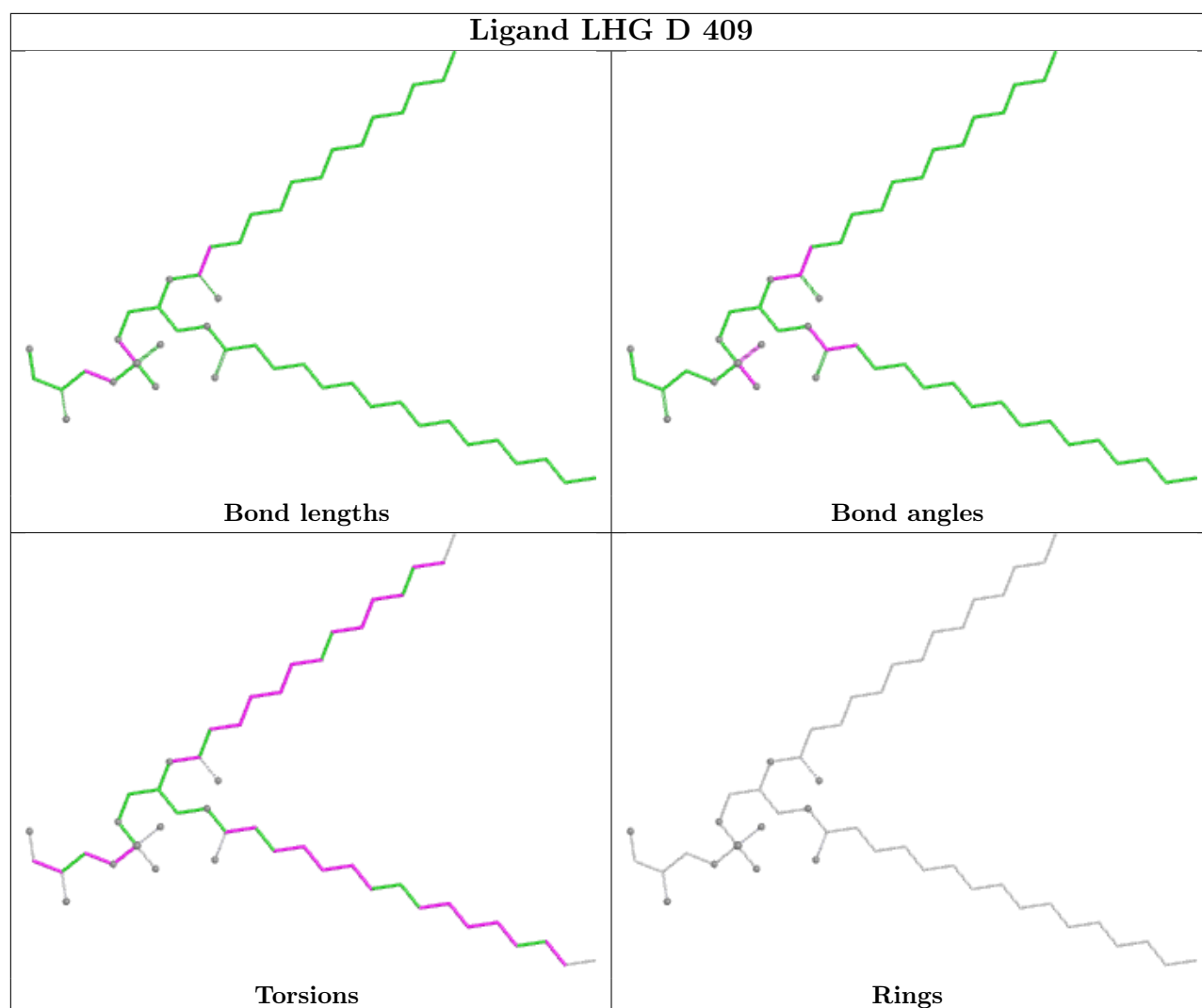
Ligand DGD h 101

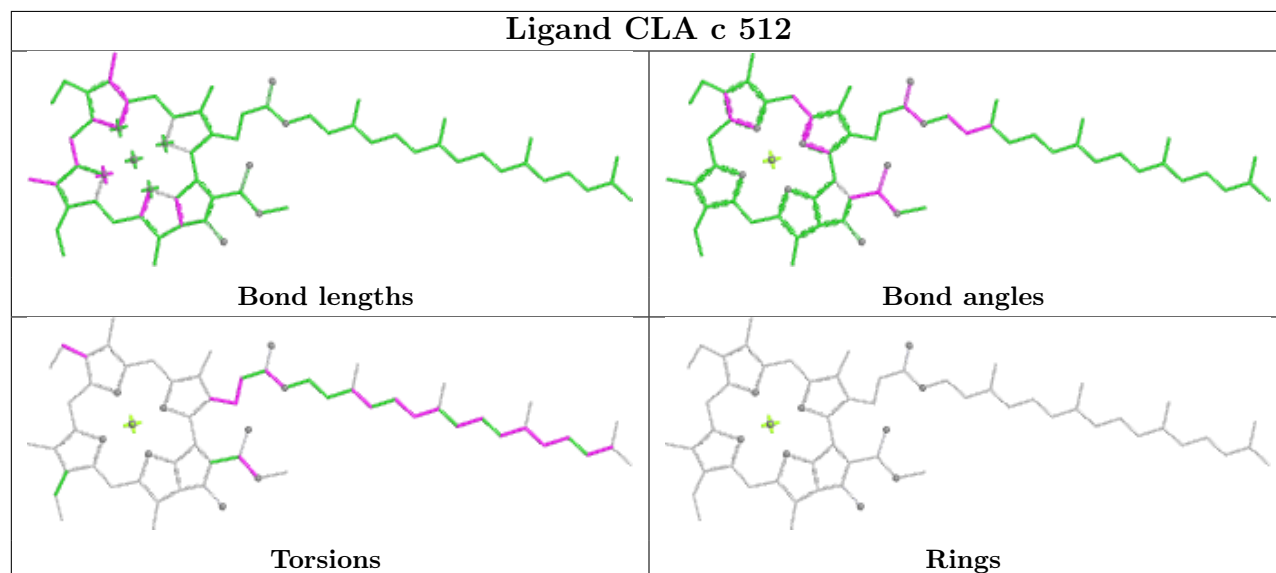
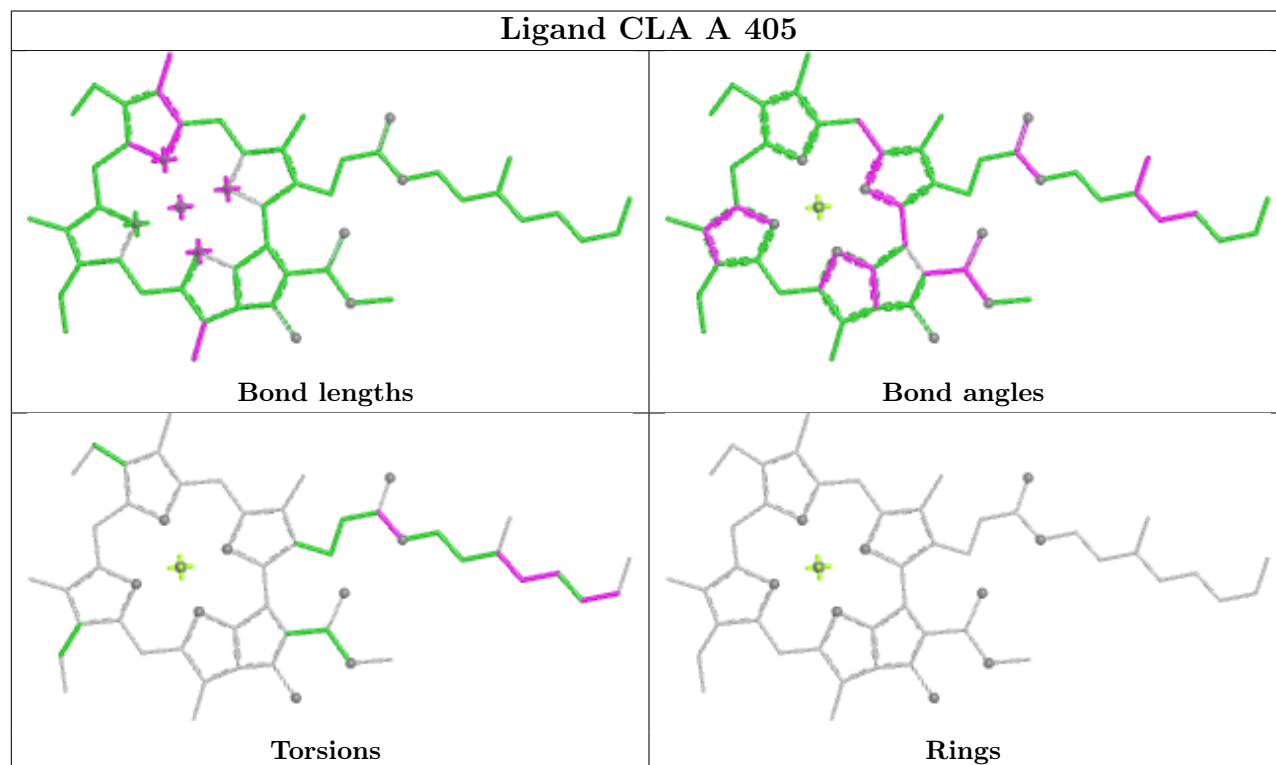
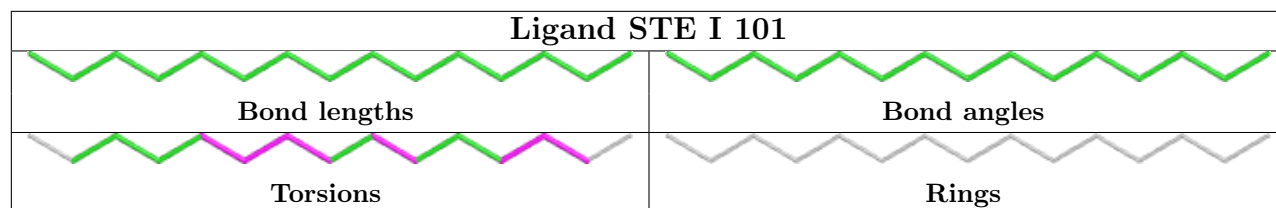


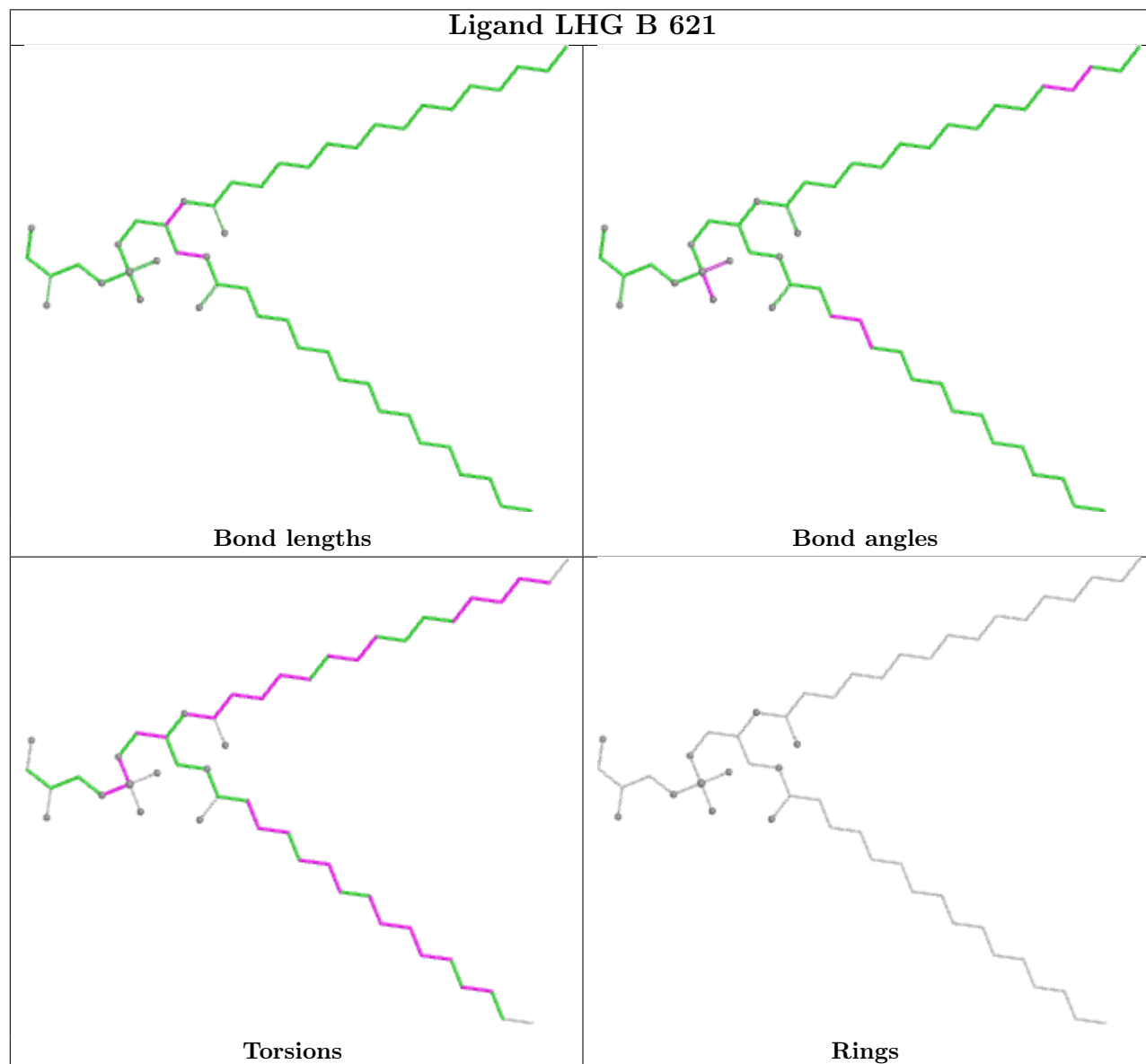
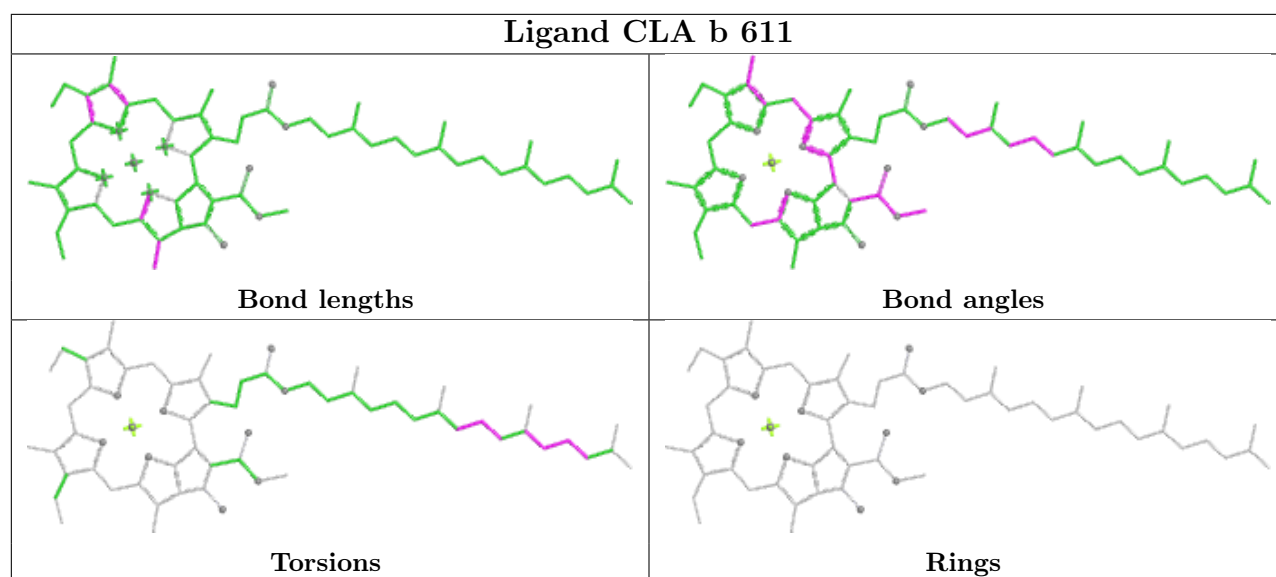


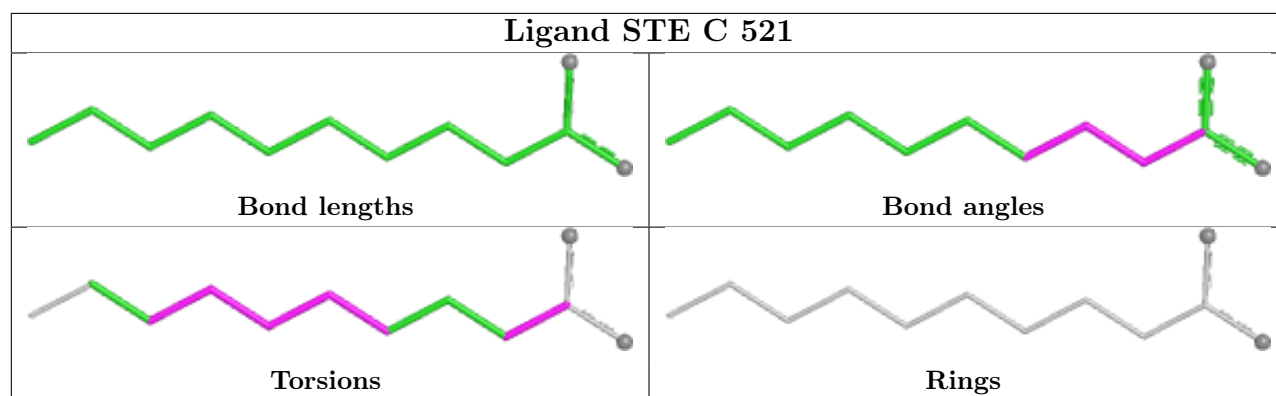
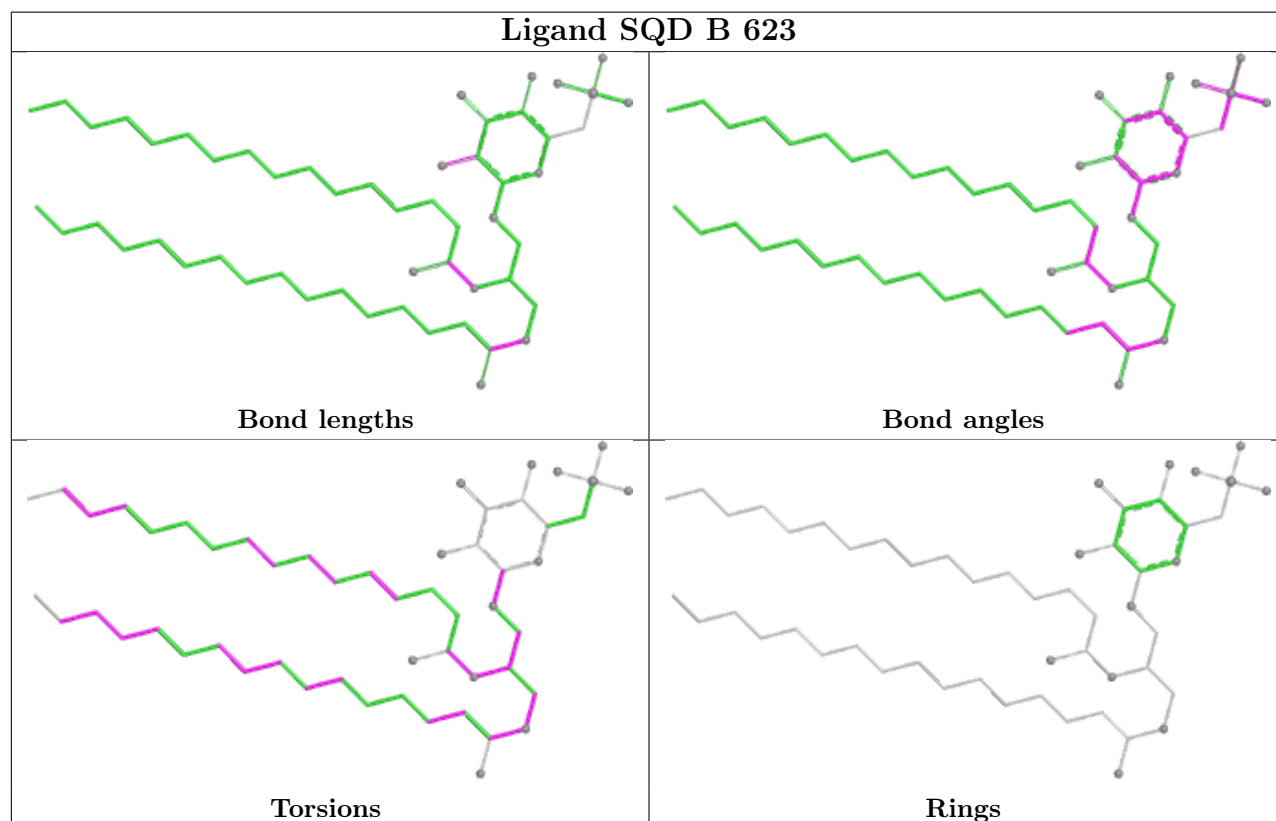
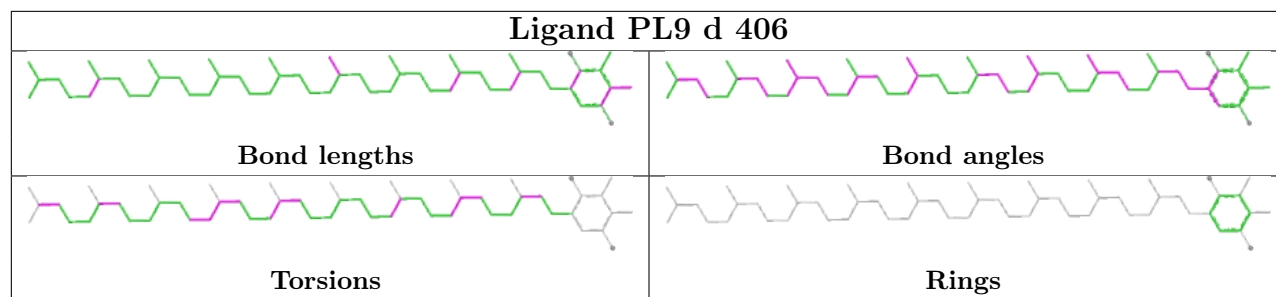


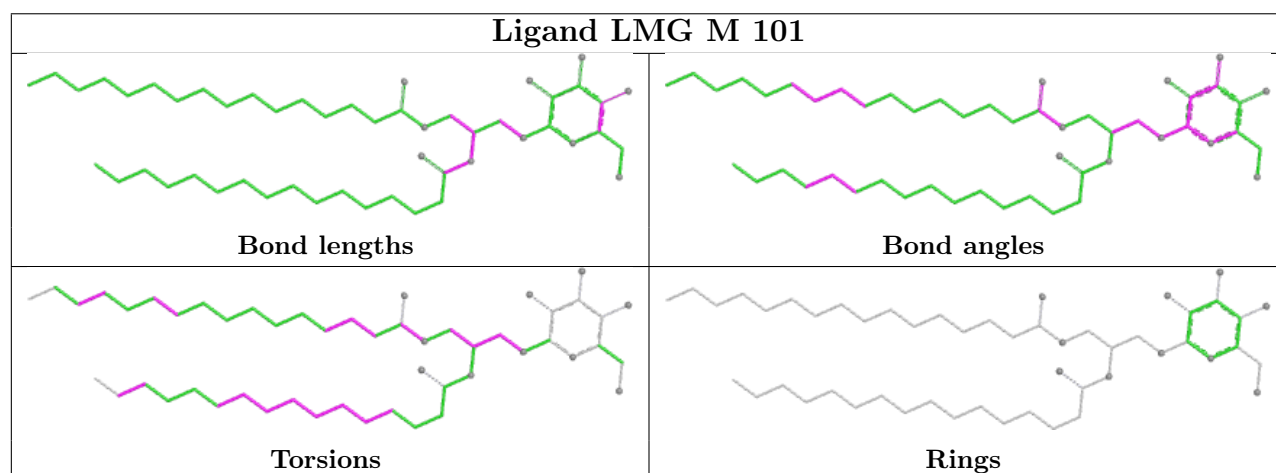
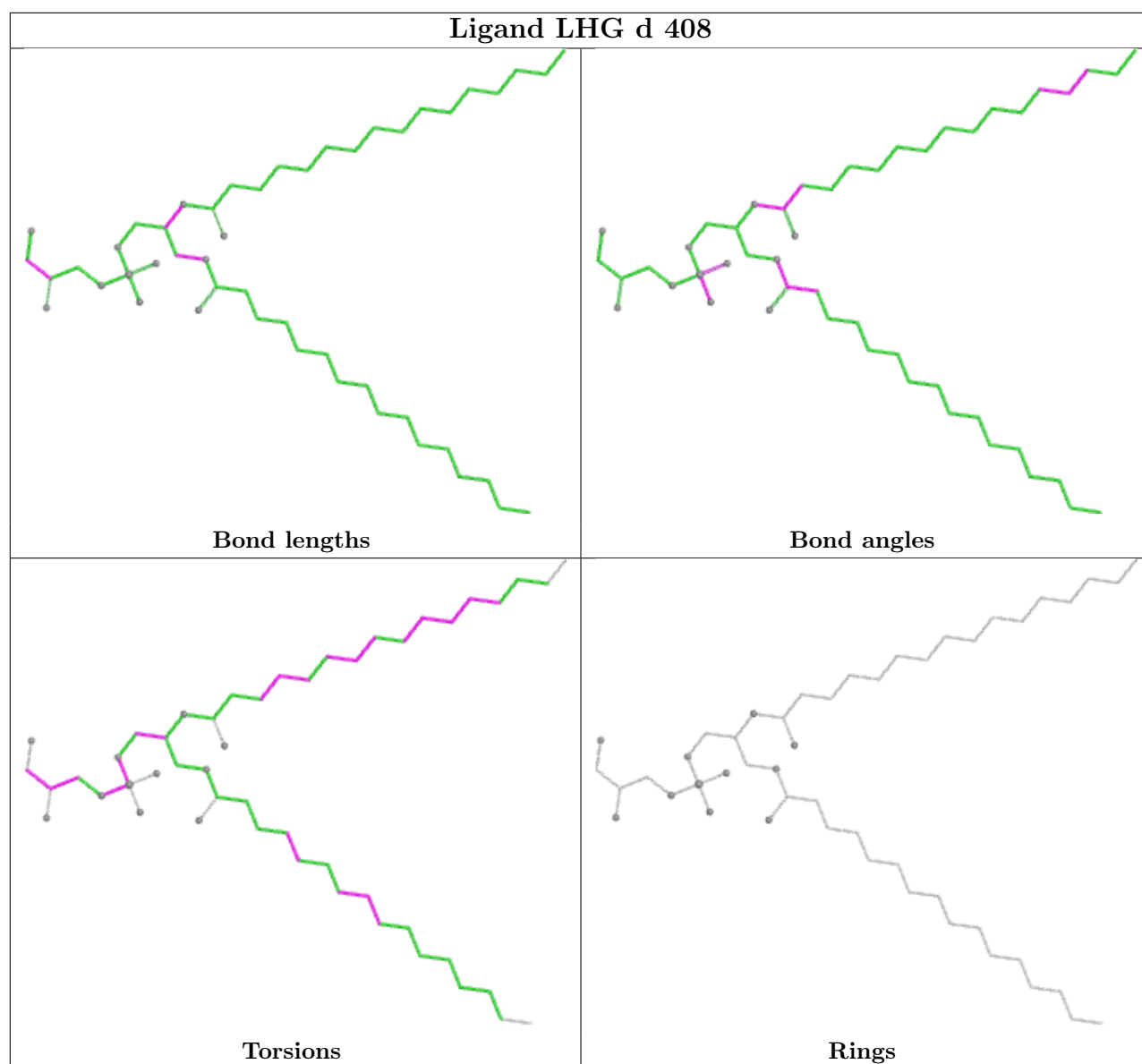




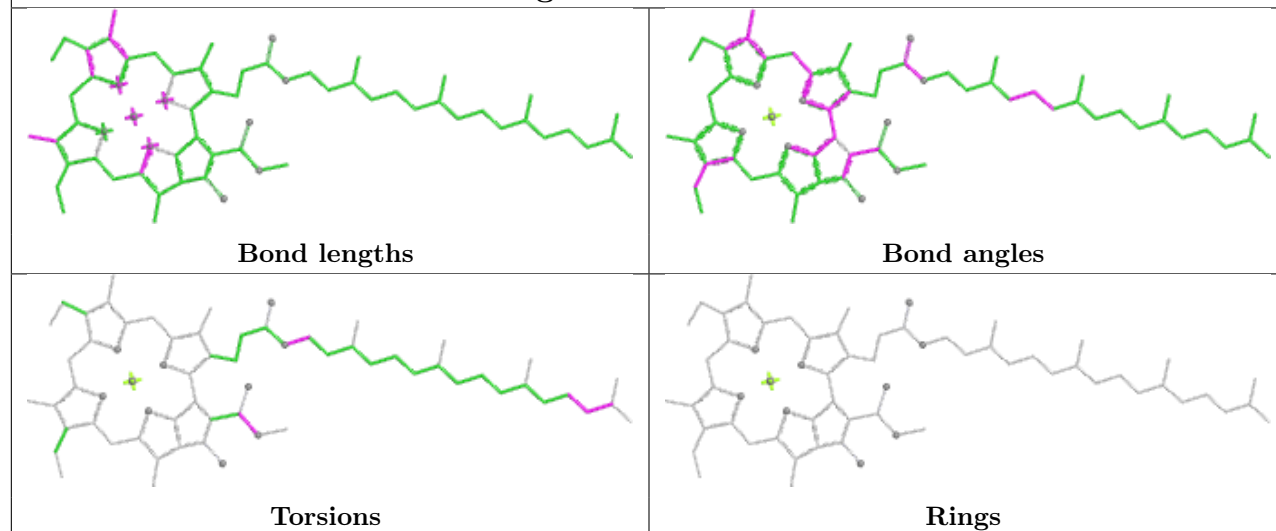




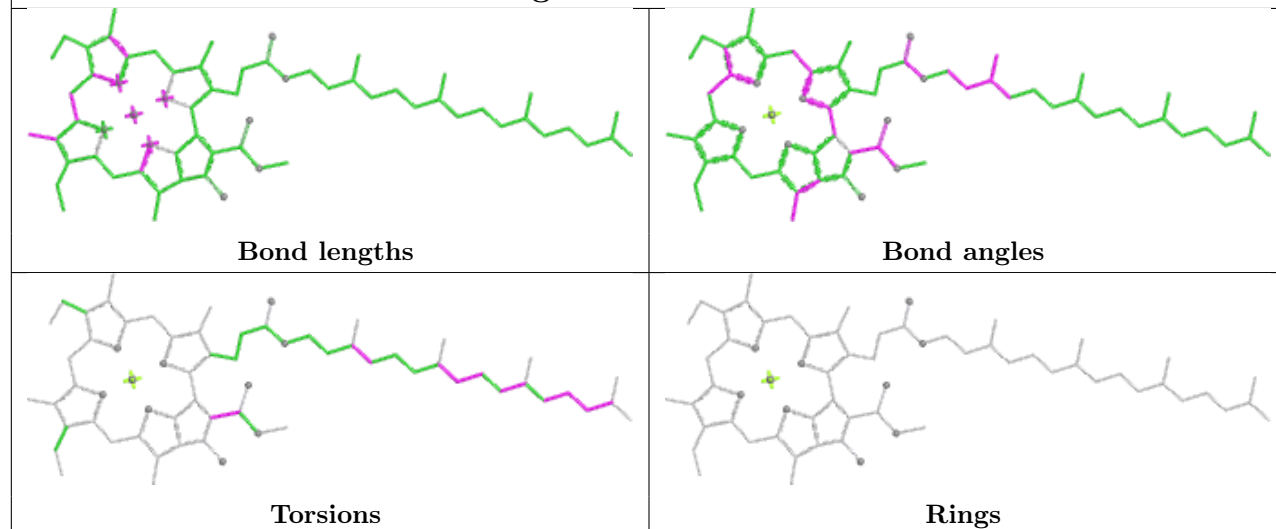




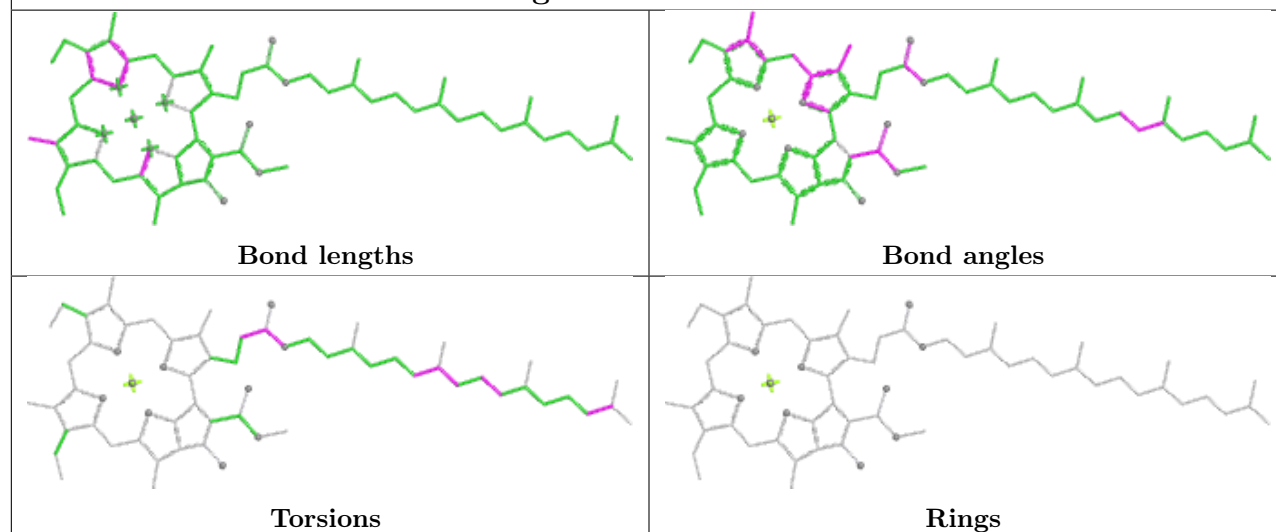
Ligand CLA a 402



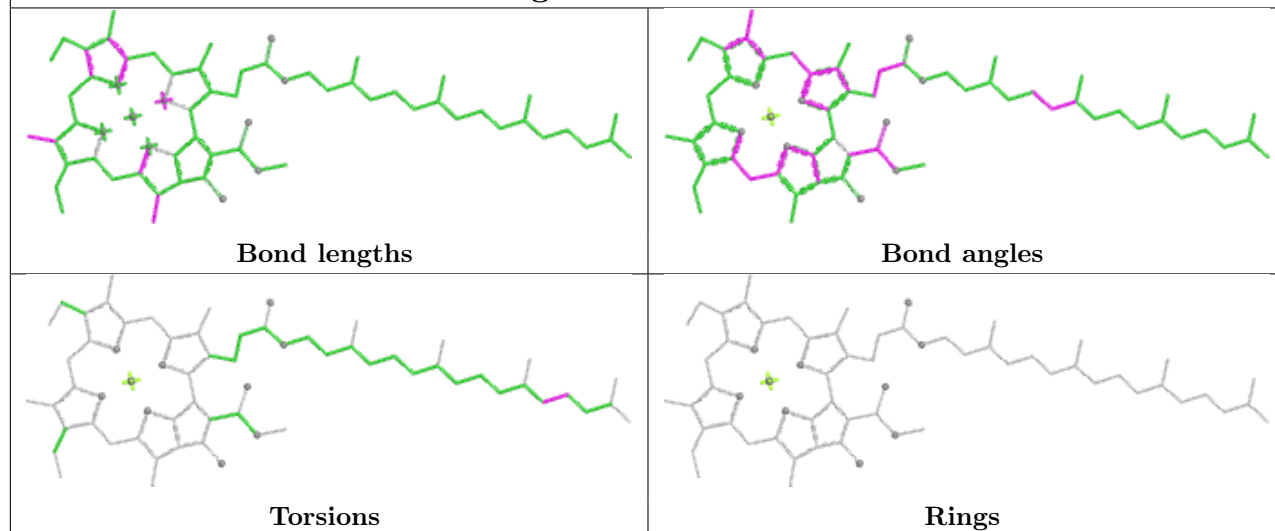
Ligand CLA B 614



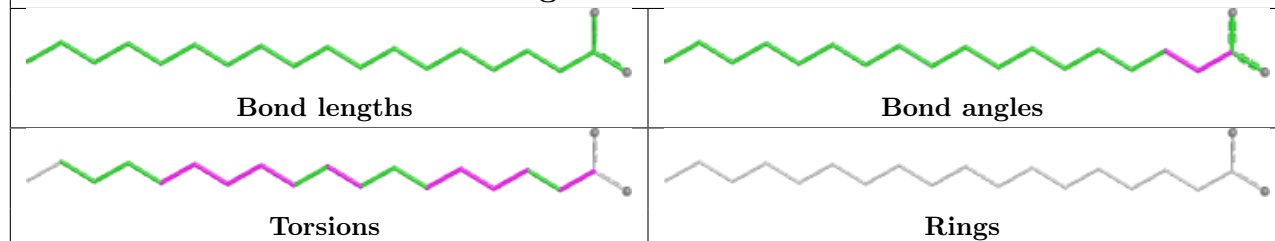
Ligand CLA B 612



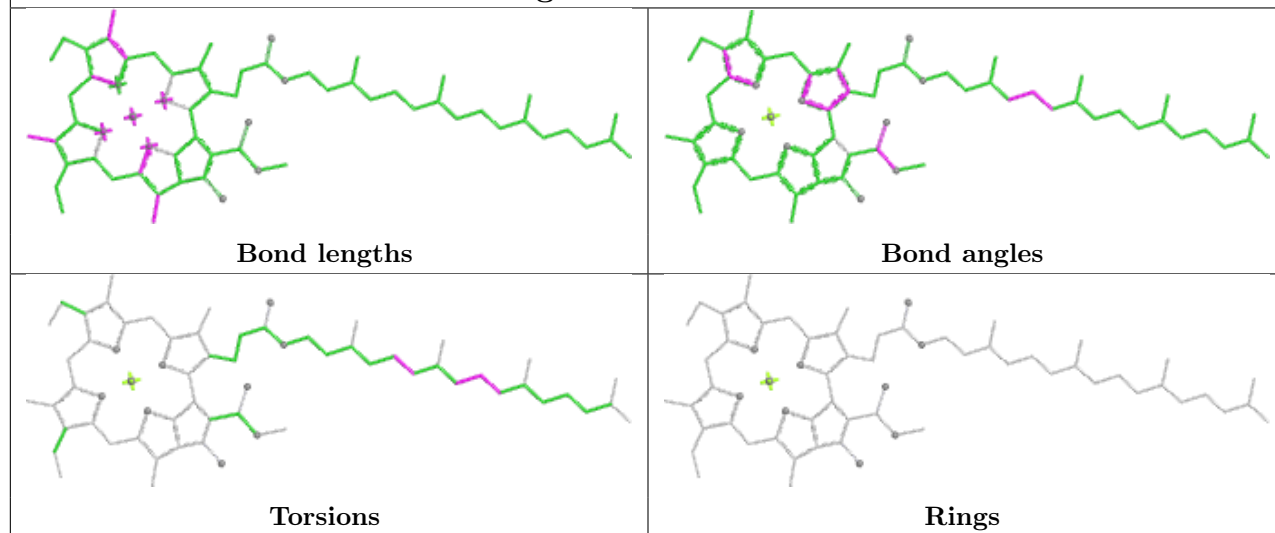
Ligand CLA B 608

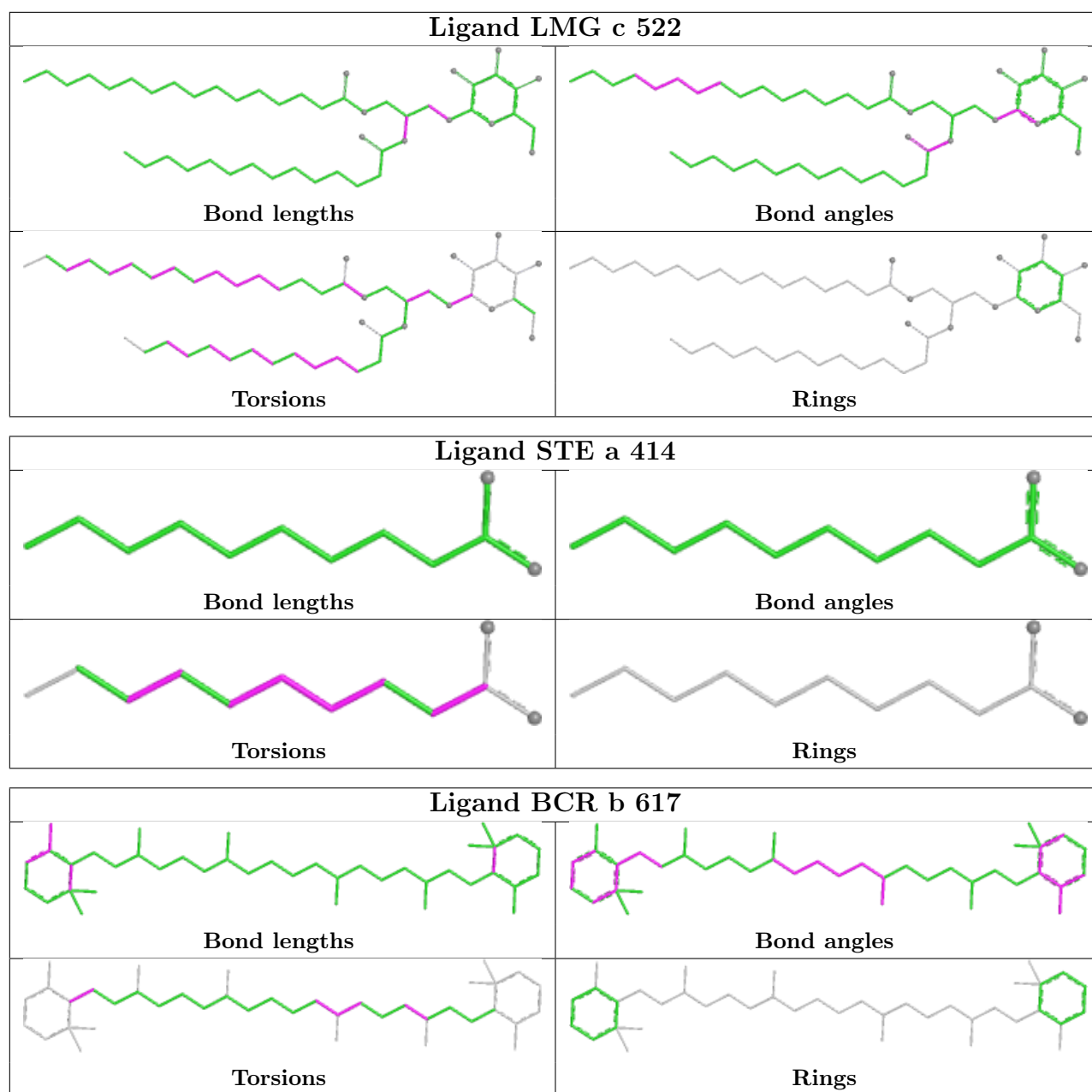


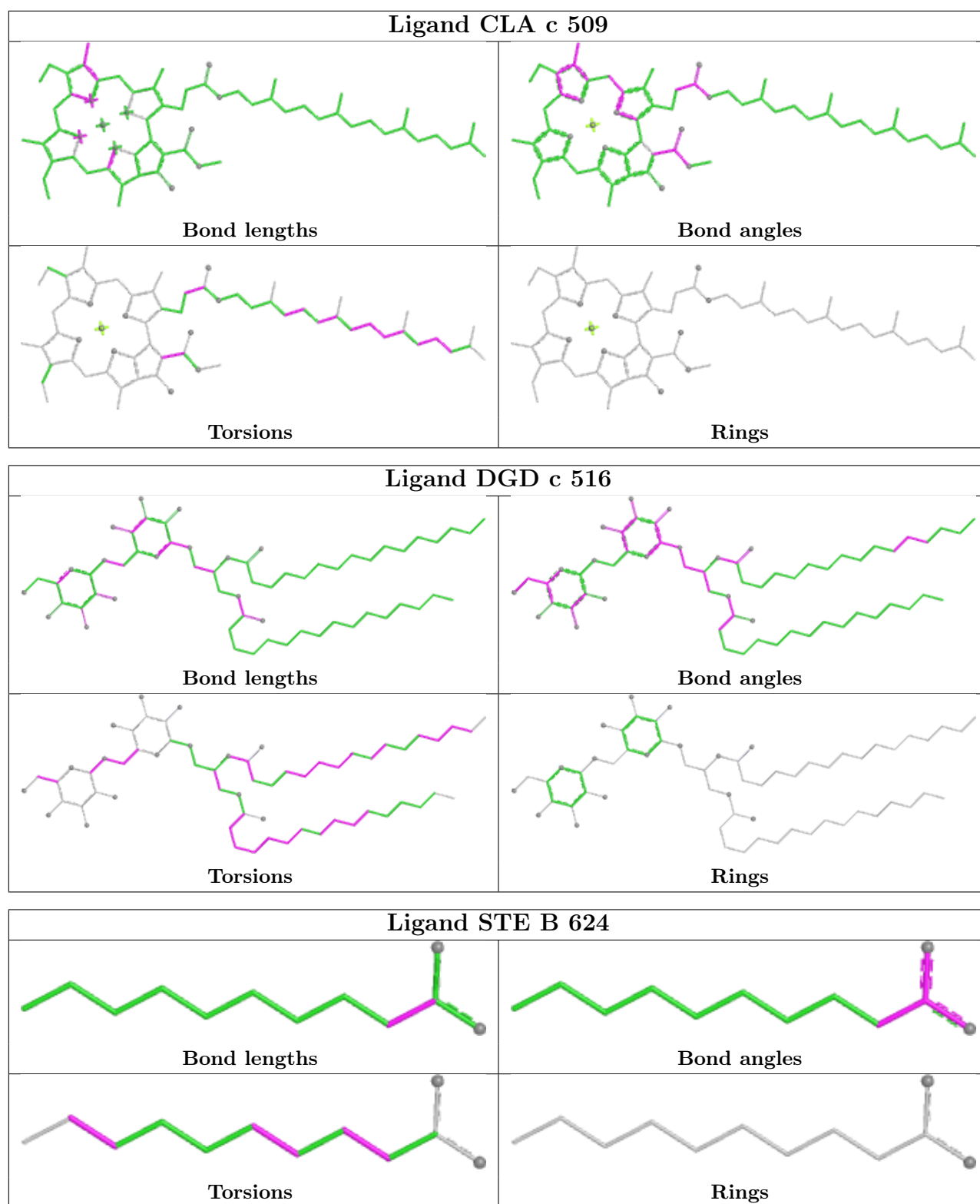
Ligand STE c 520

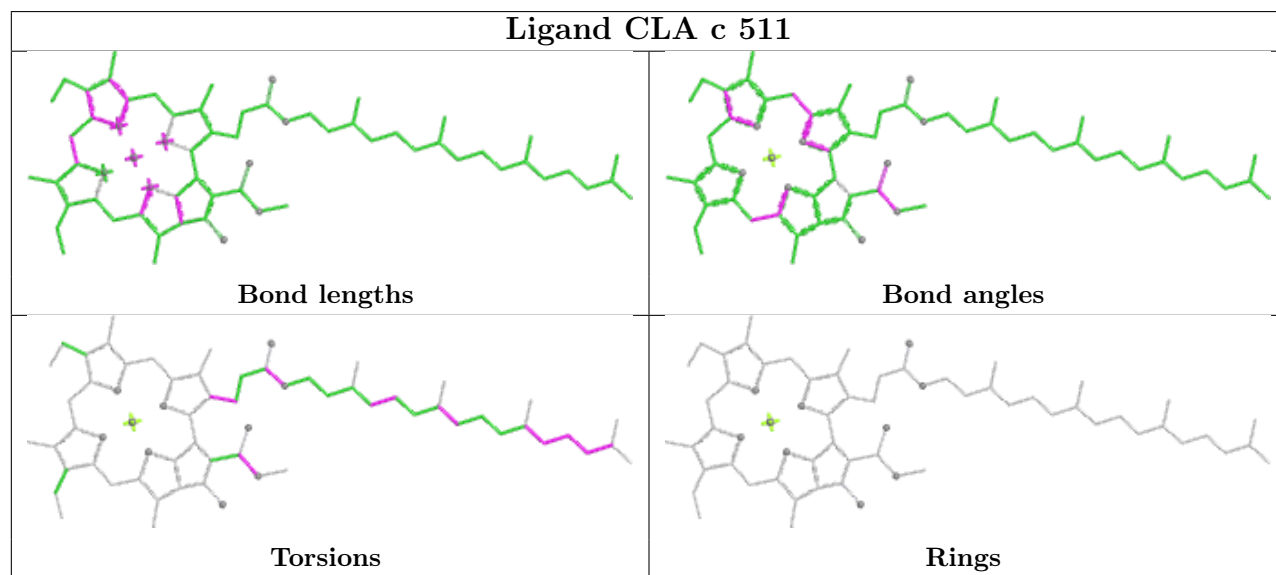
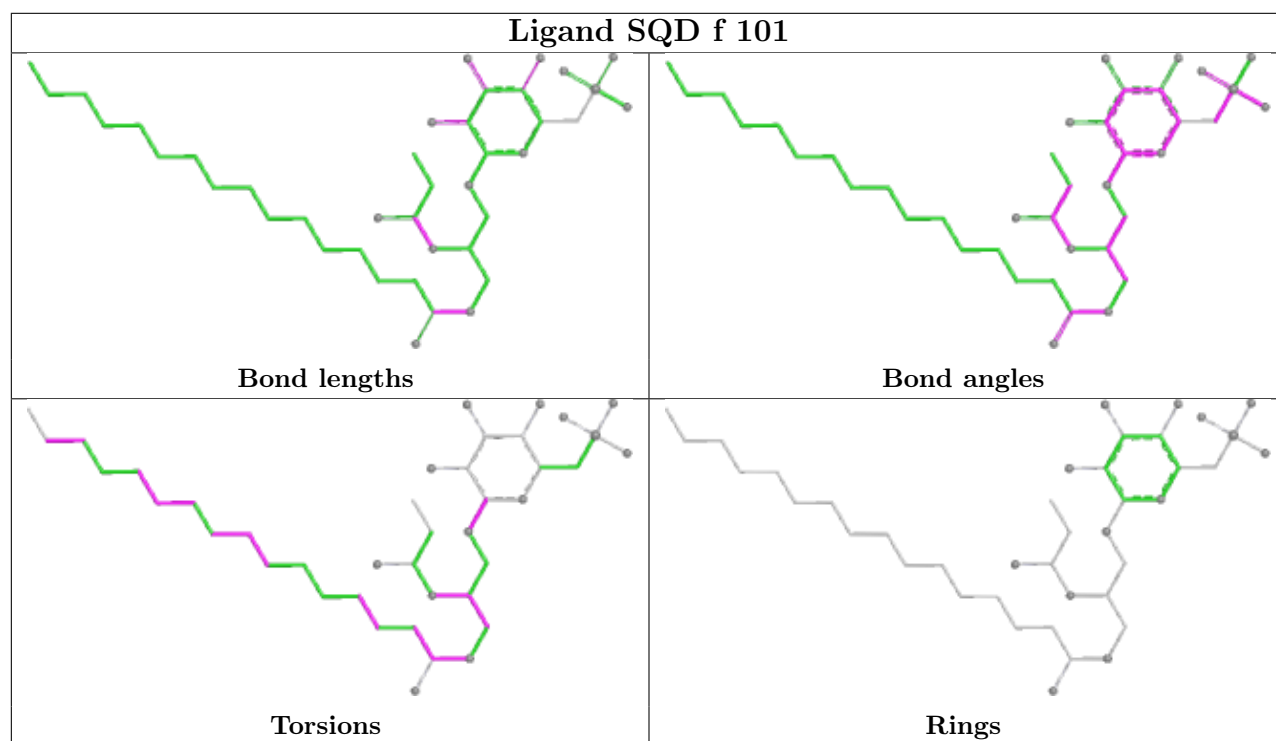
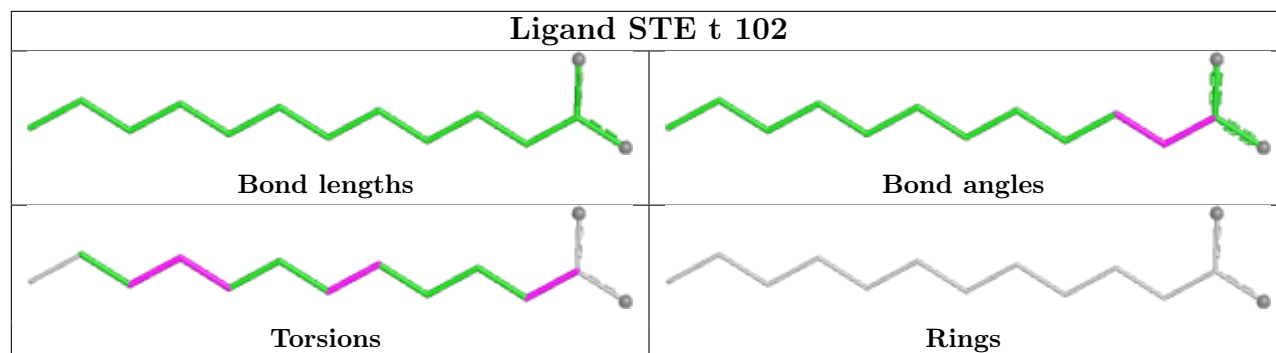


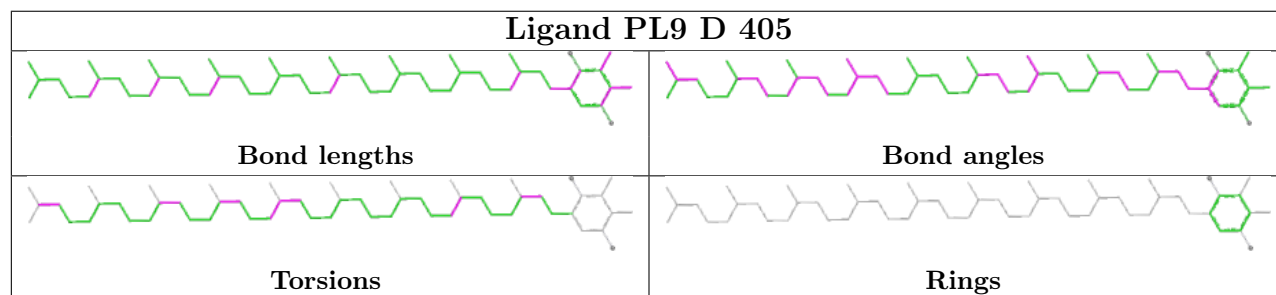
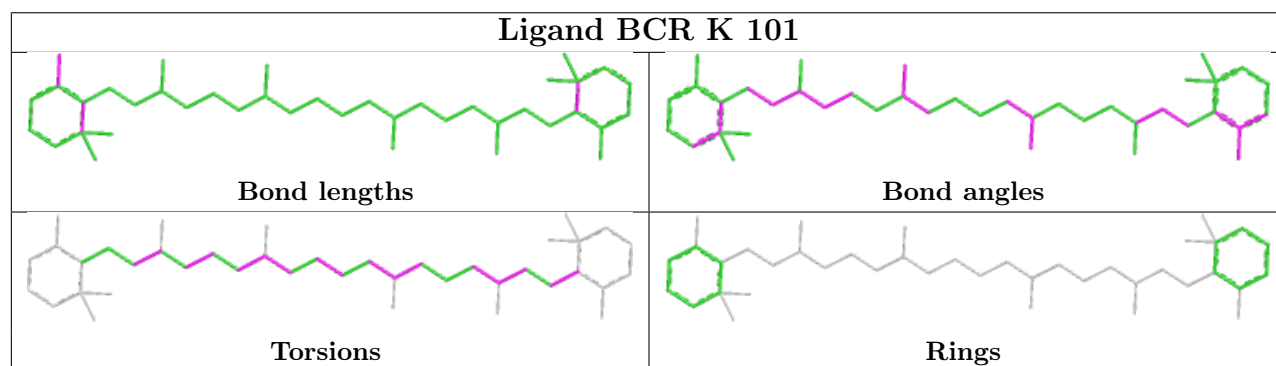
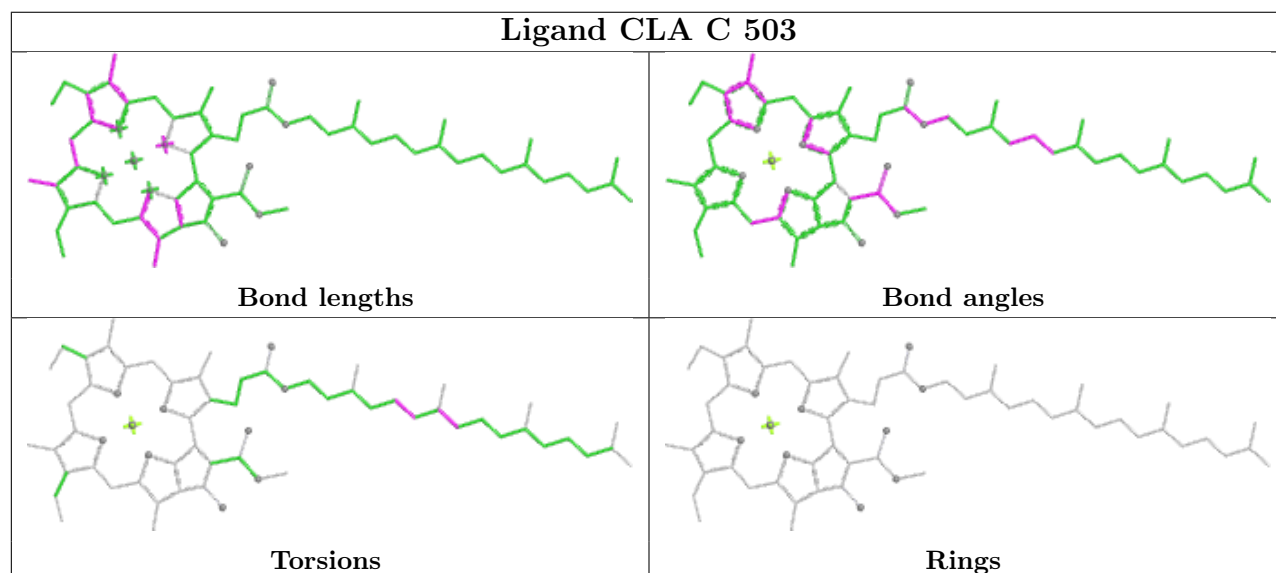
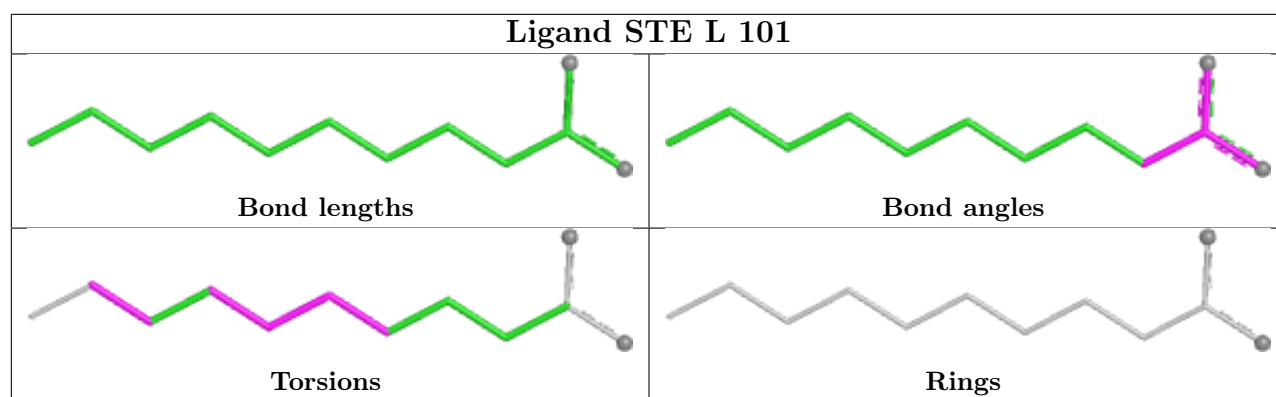
Ligand CLA c 503

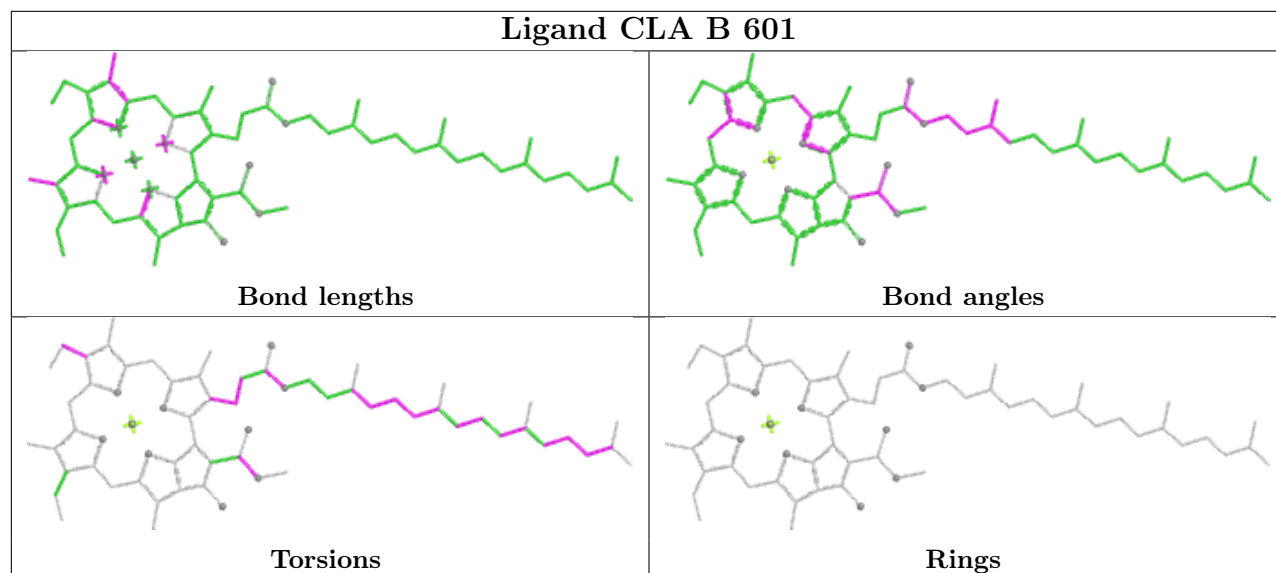
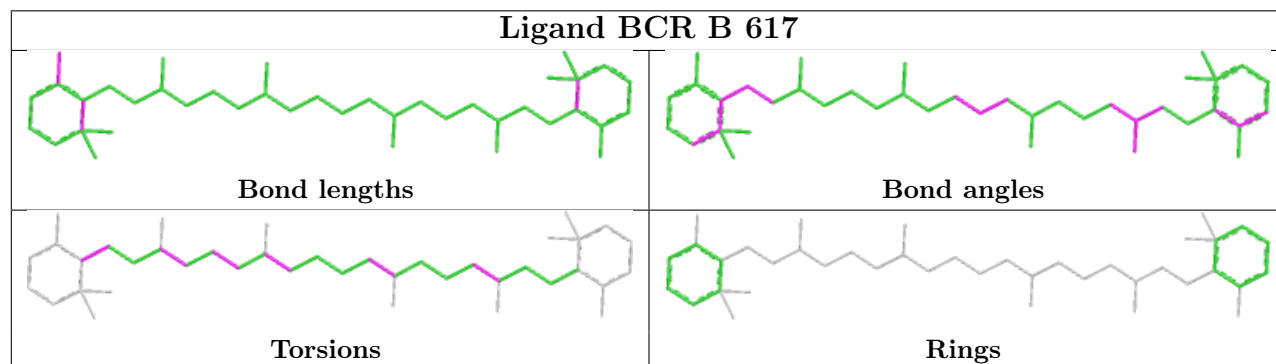
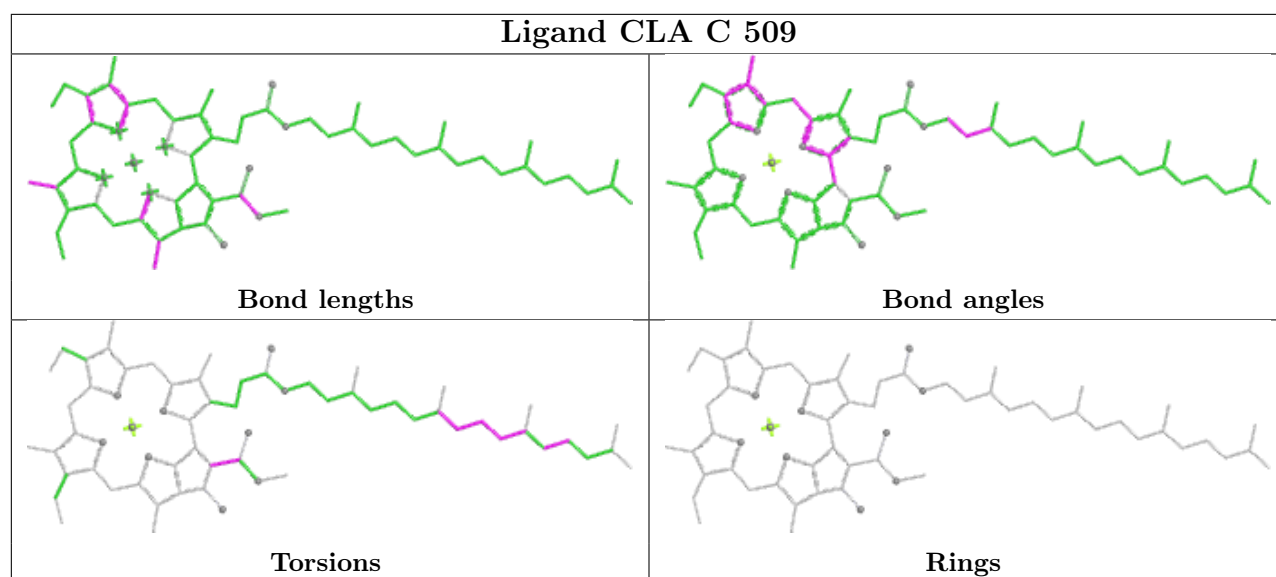


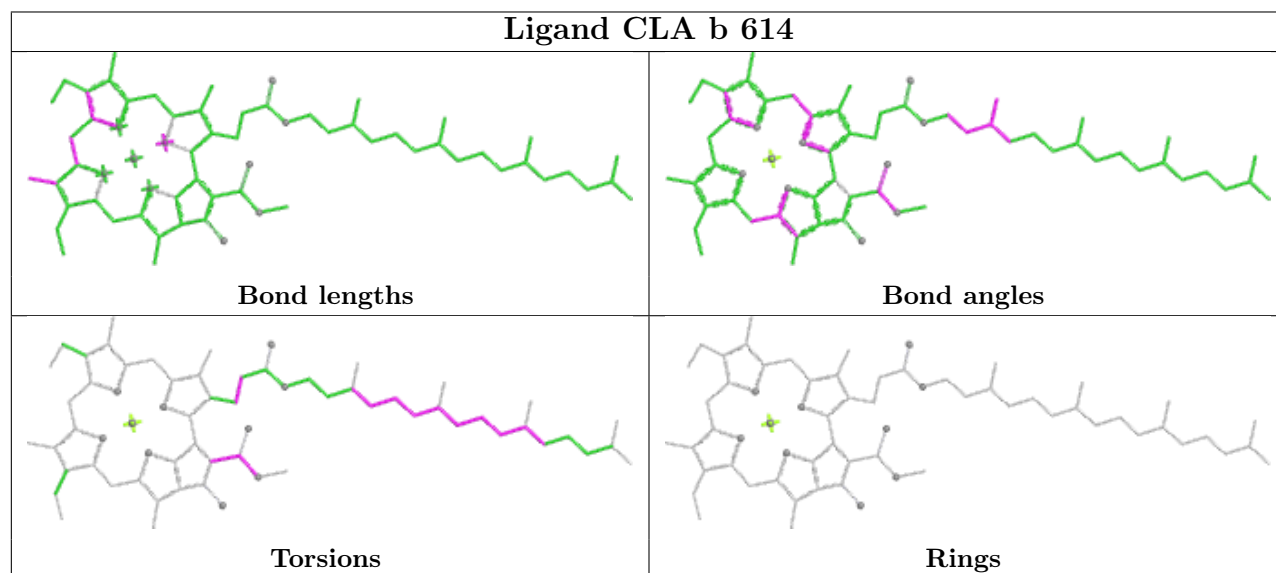
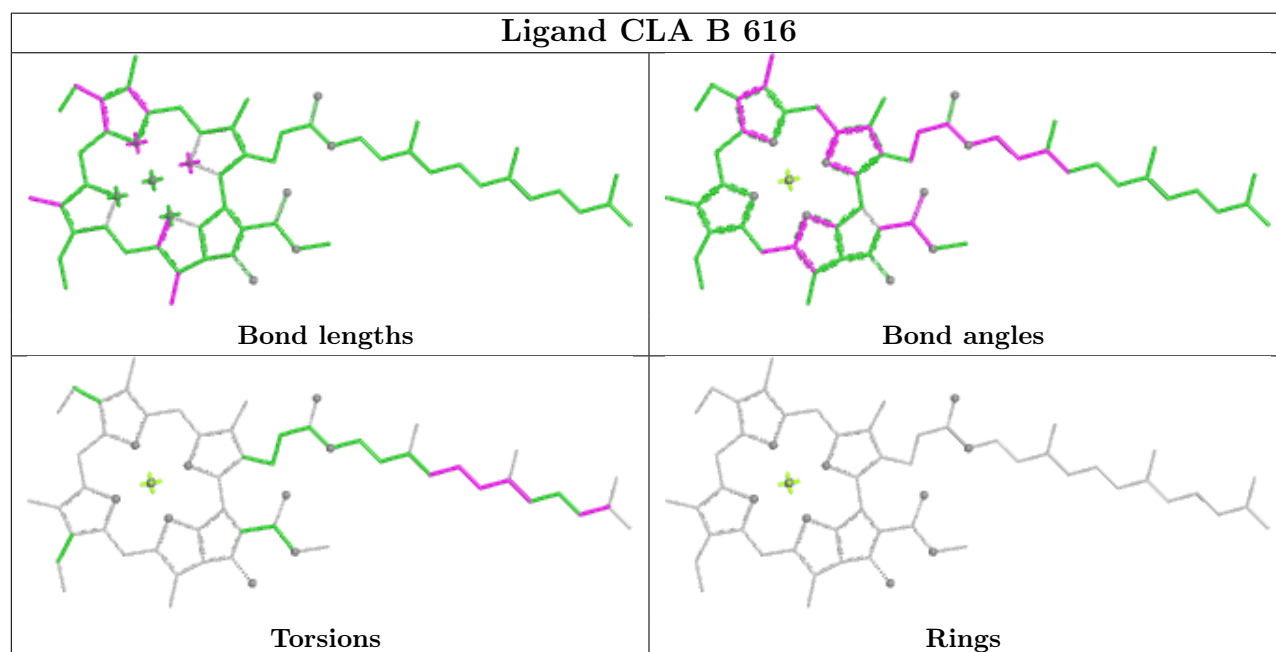
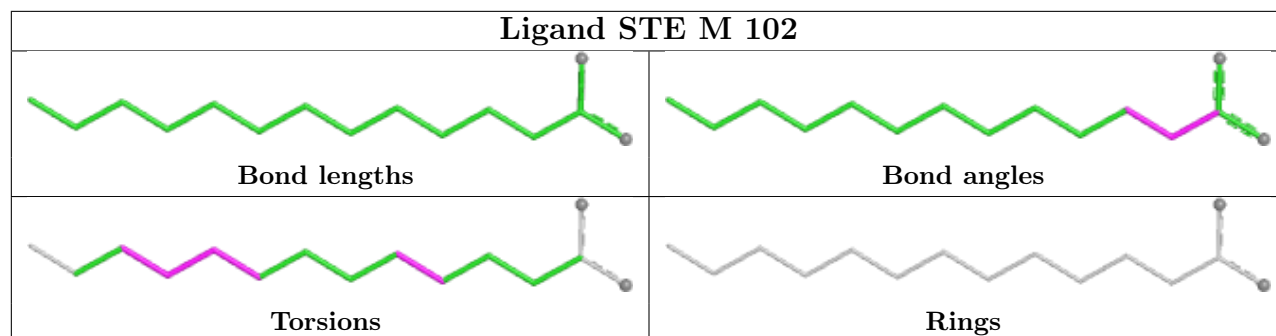


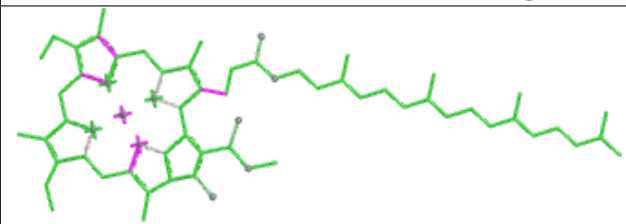
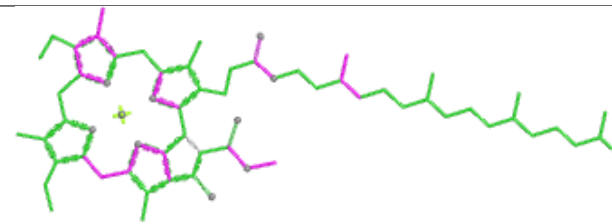
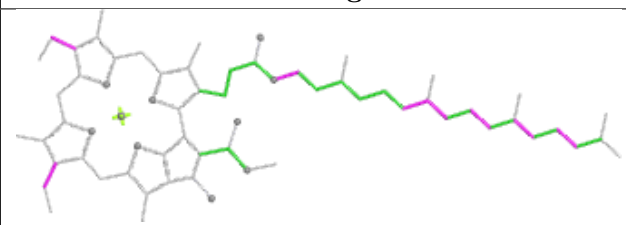
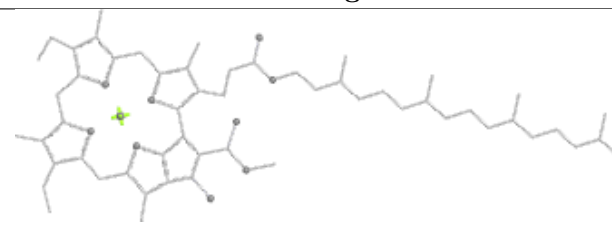


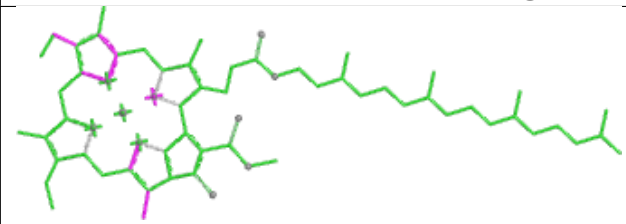
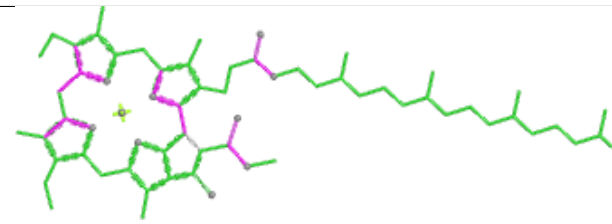
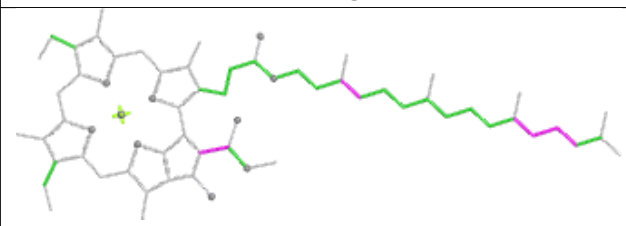
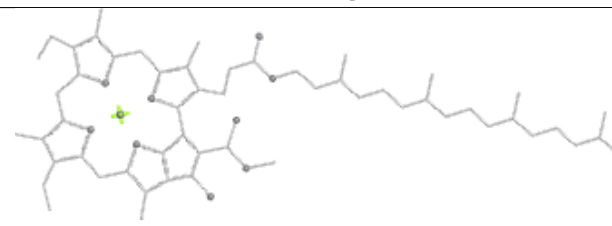


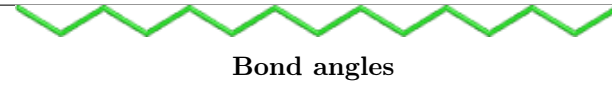


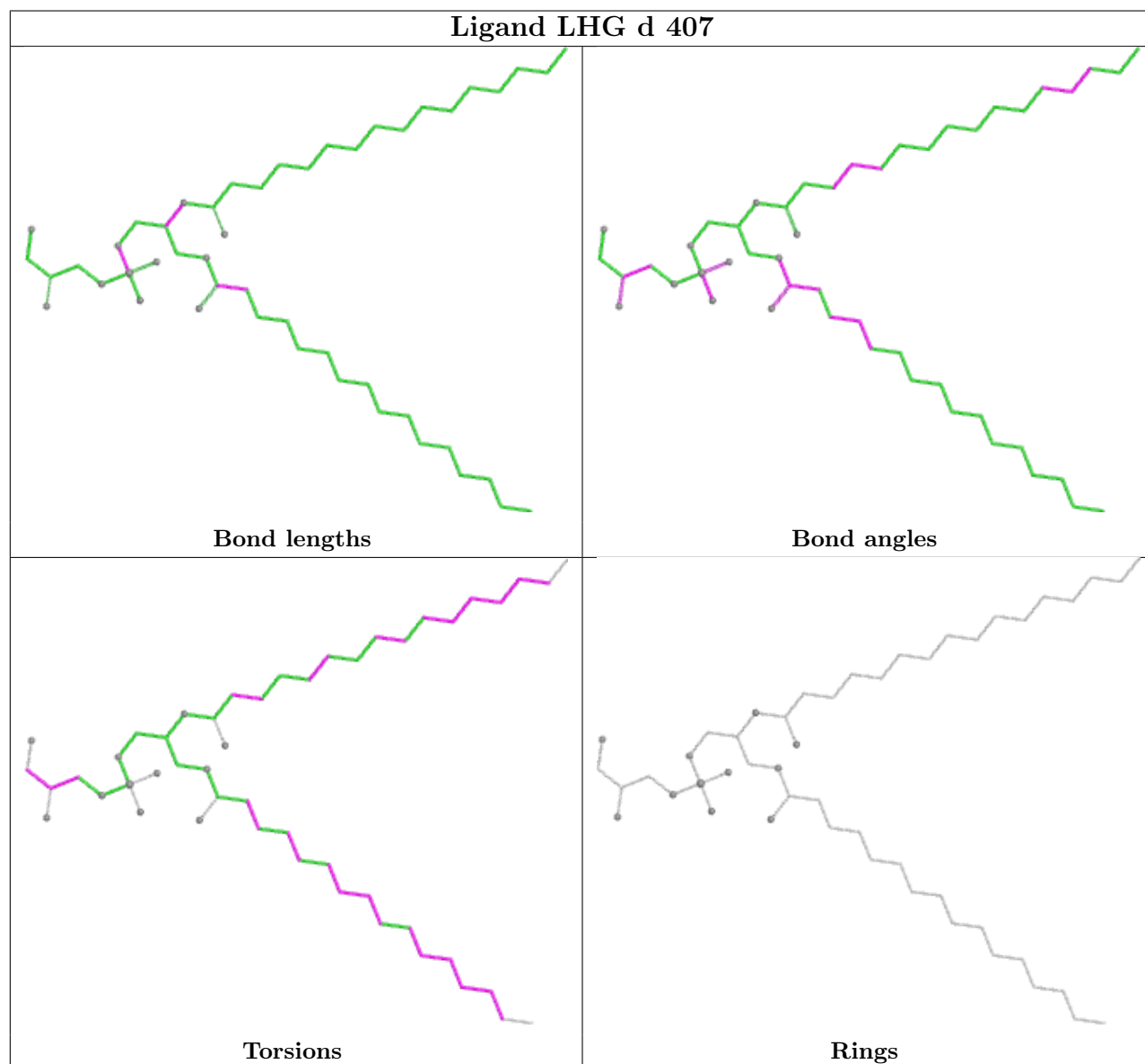
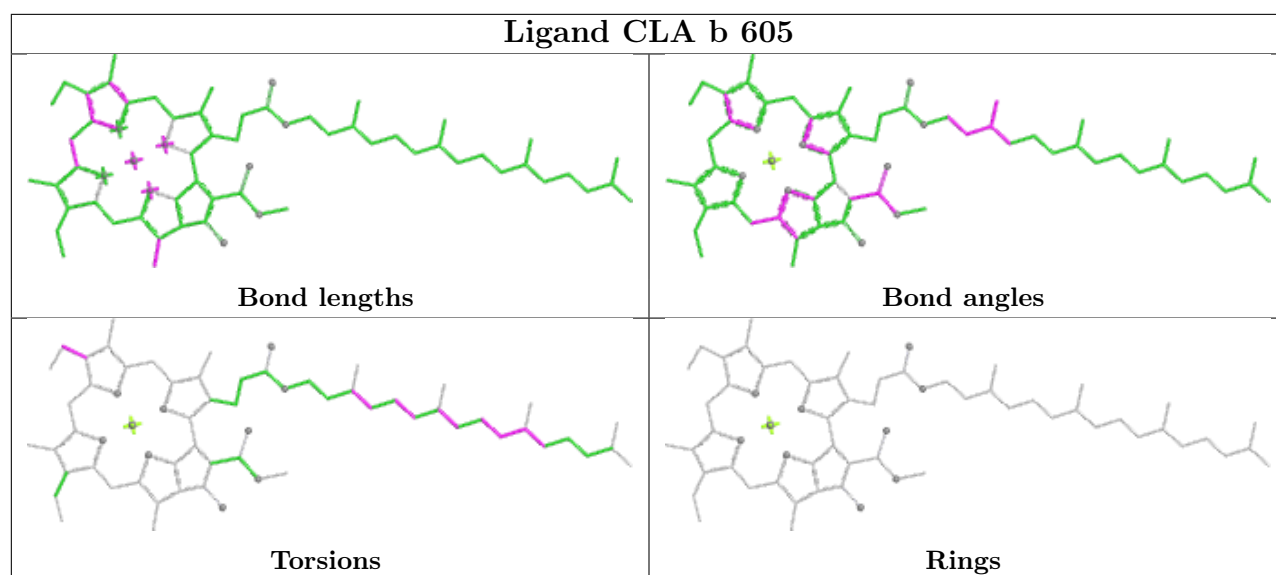


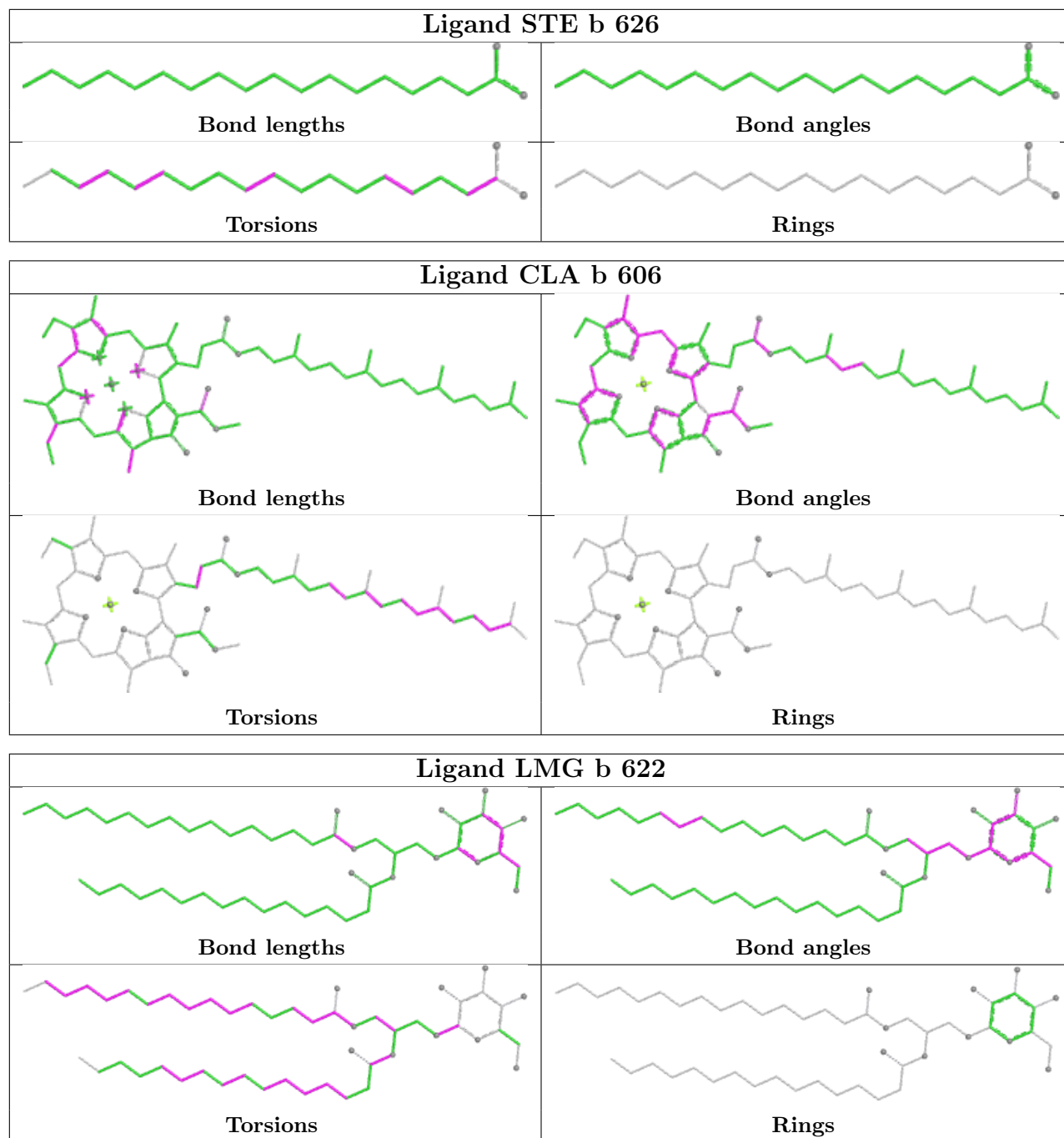


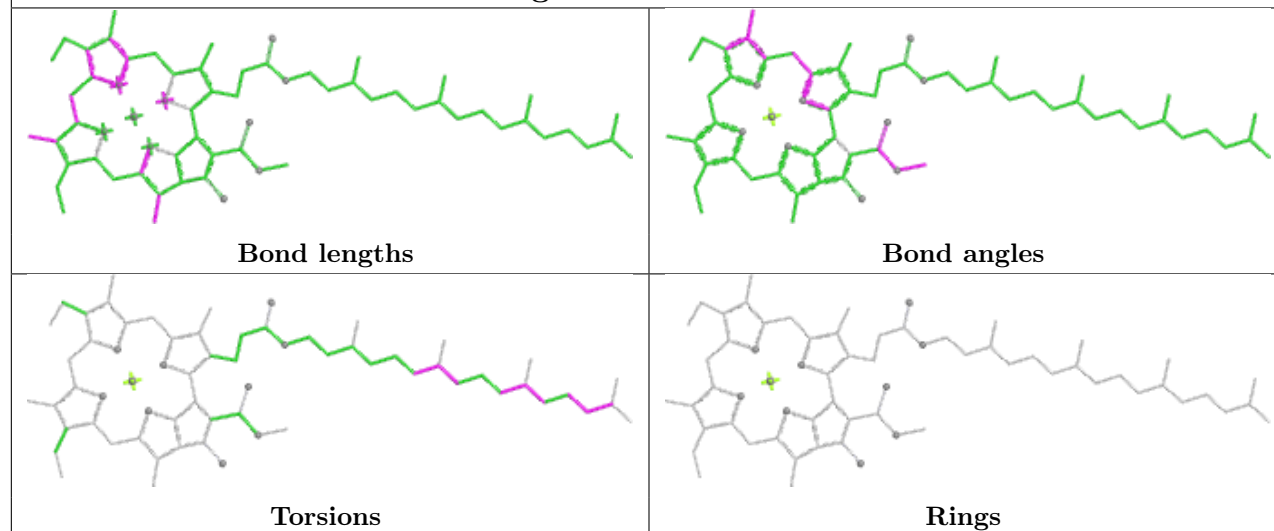
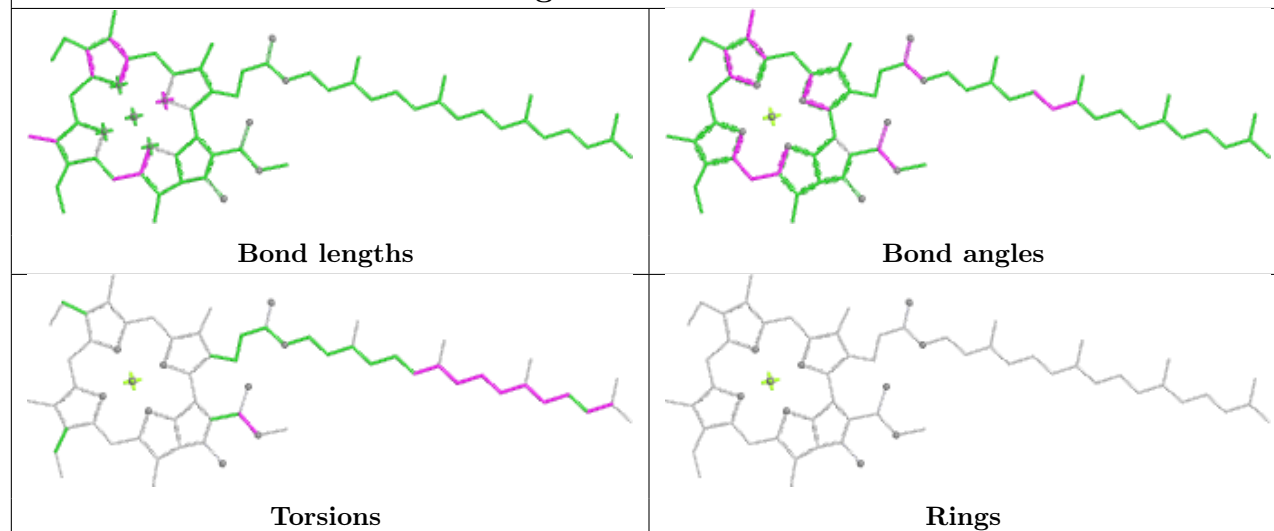
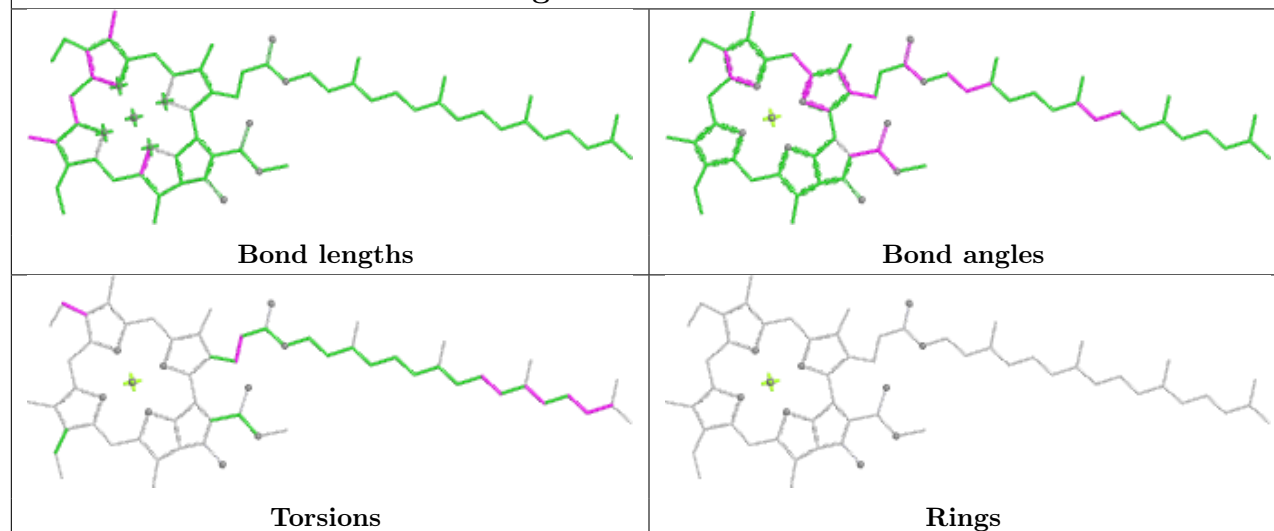
Ligand CLA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

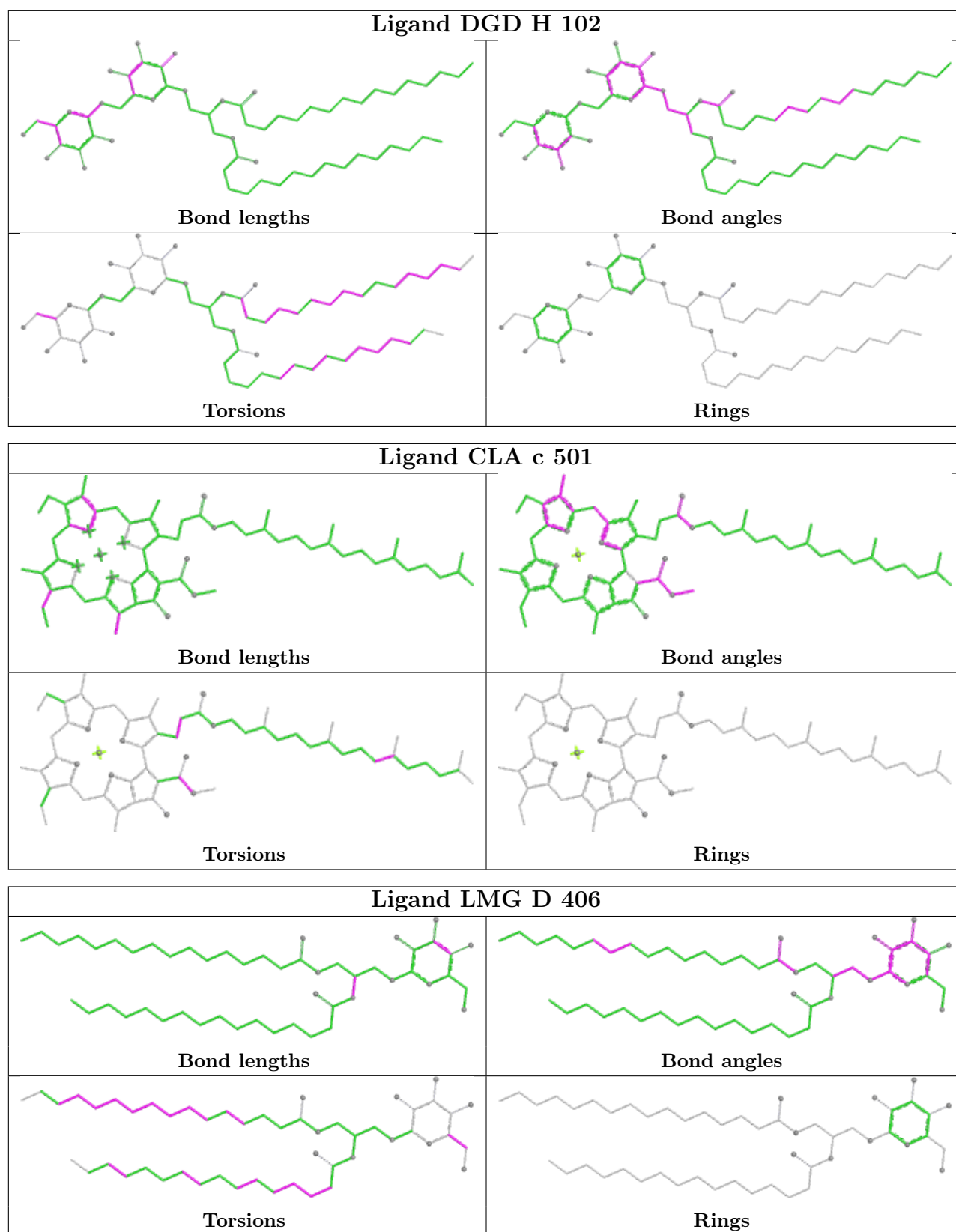
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

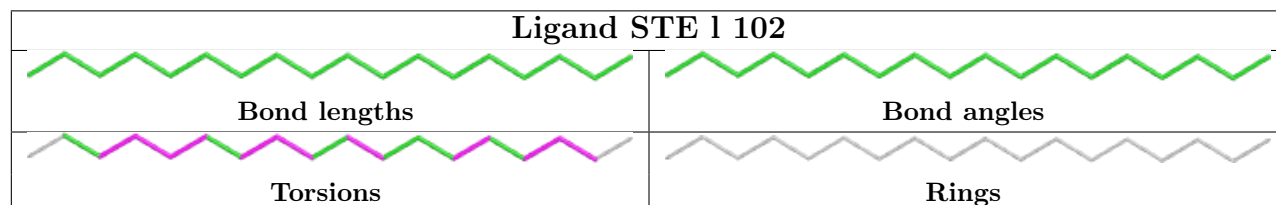
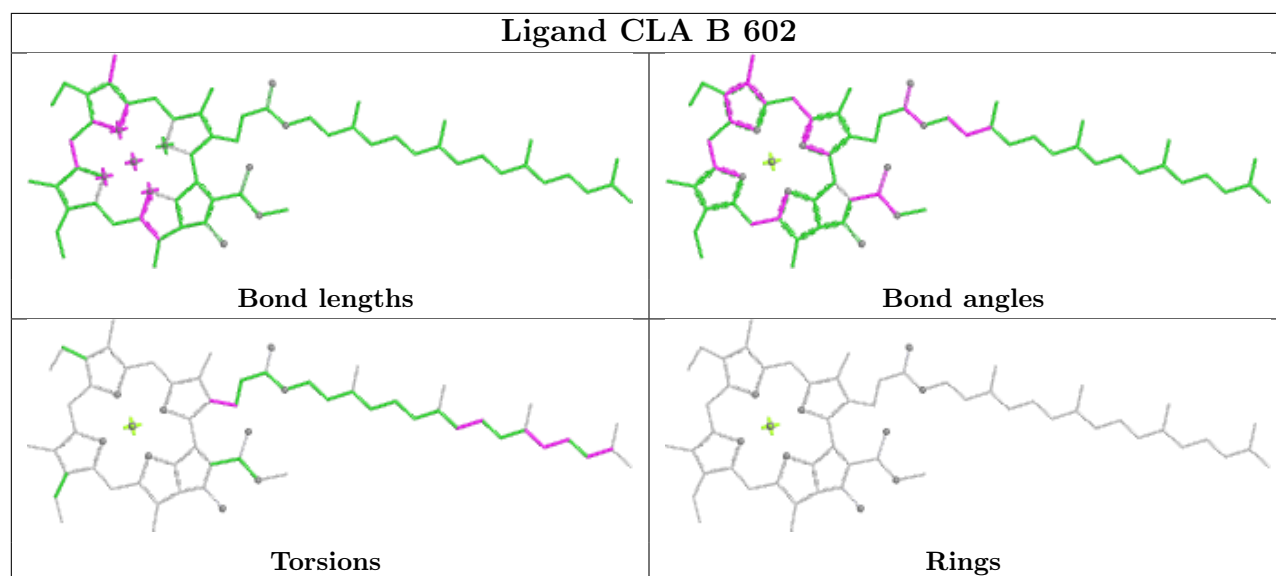
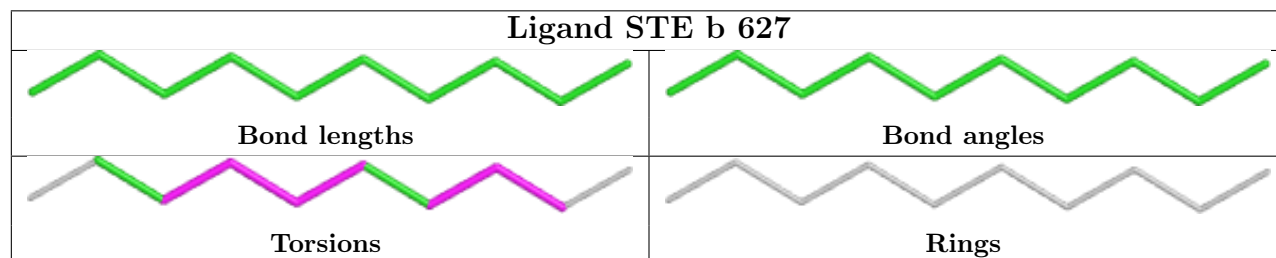
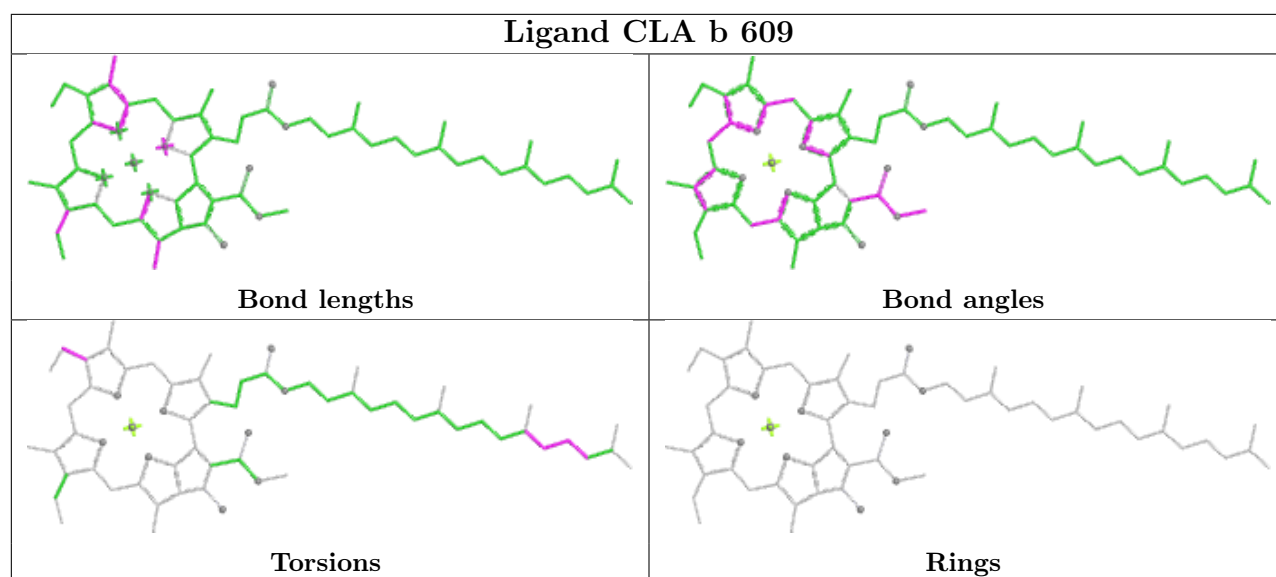
Ligand STE a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

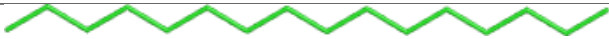
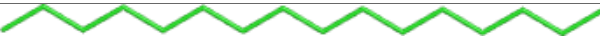
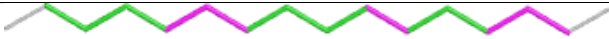


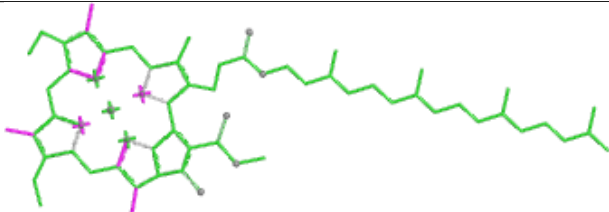
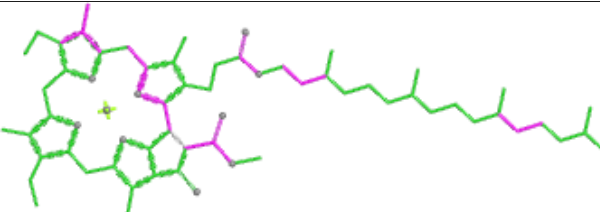
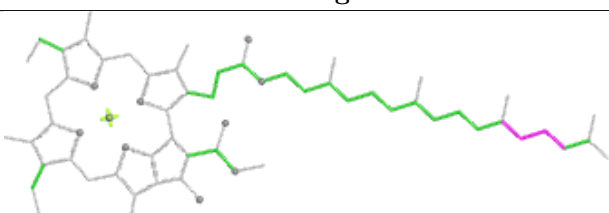
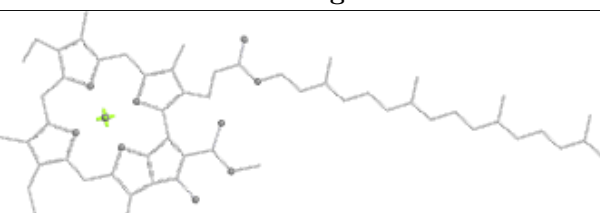


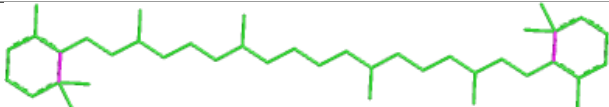
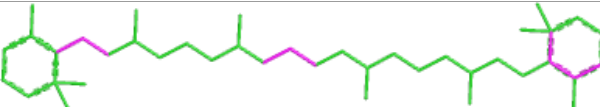
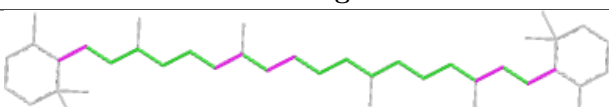
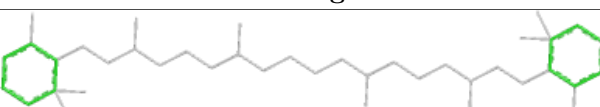
Ligand CLA A 403**Ligand CLA b 607****Ligand CLA B 610**

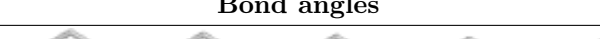


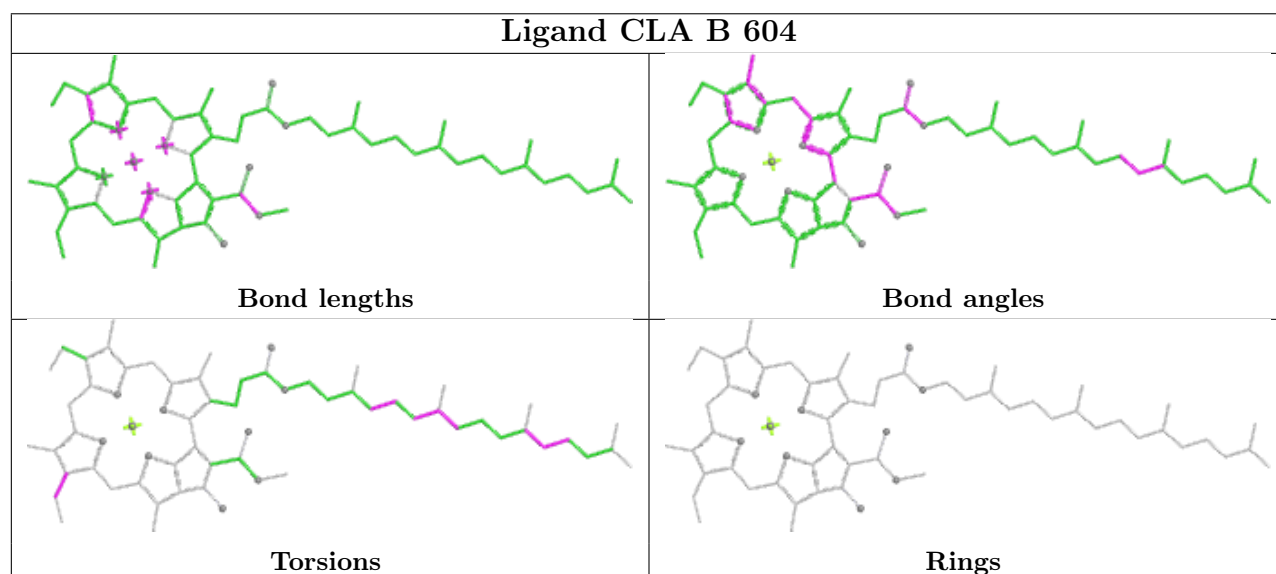
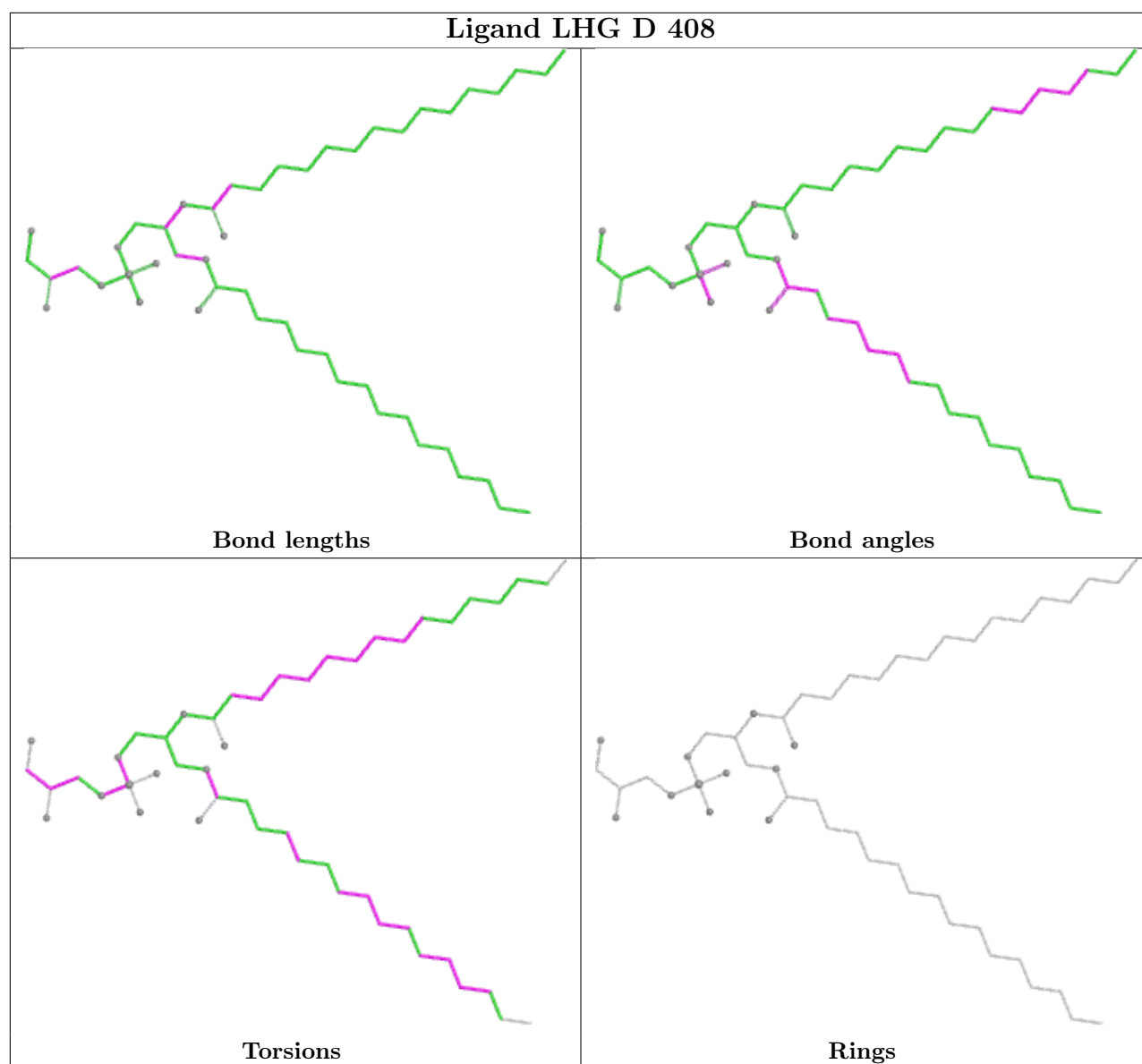


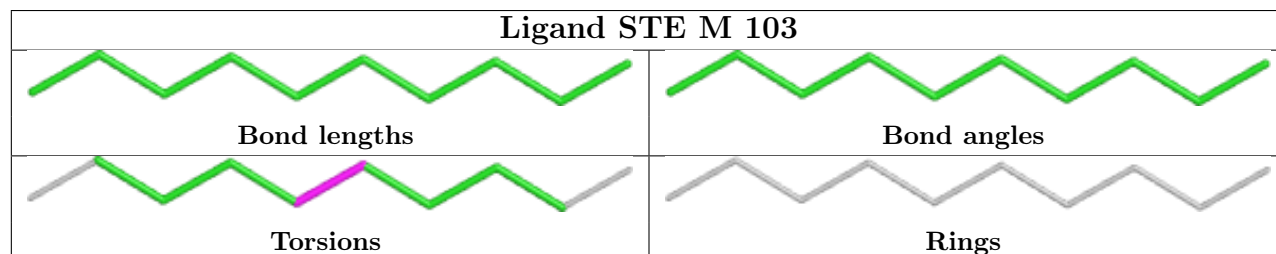
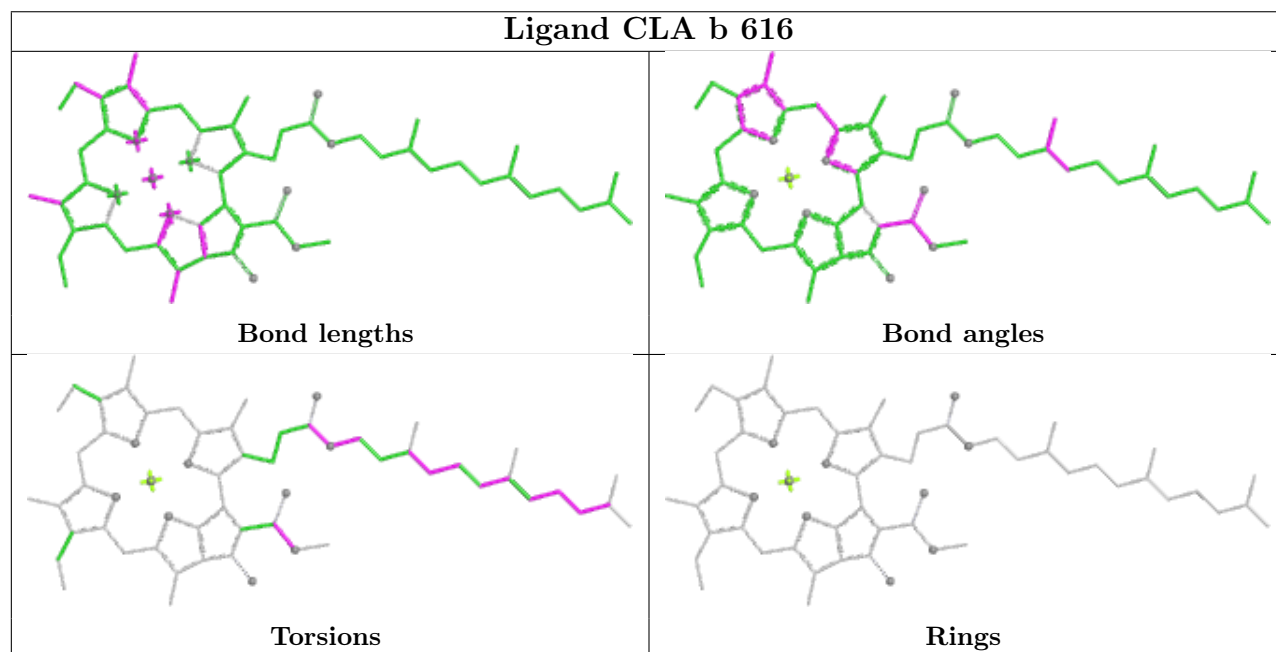
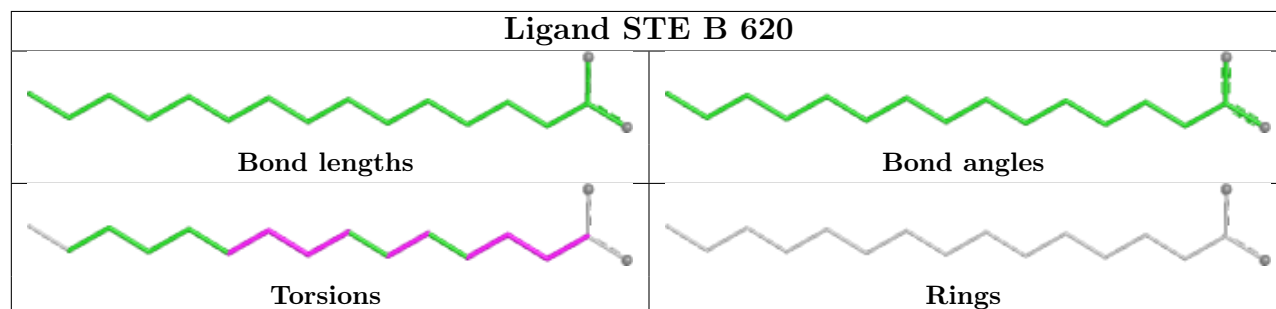
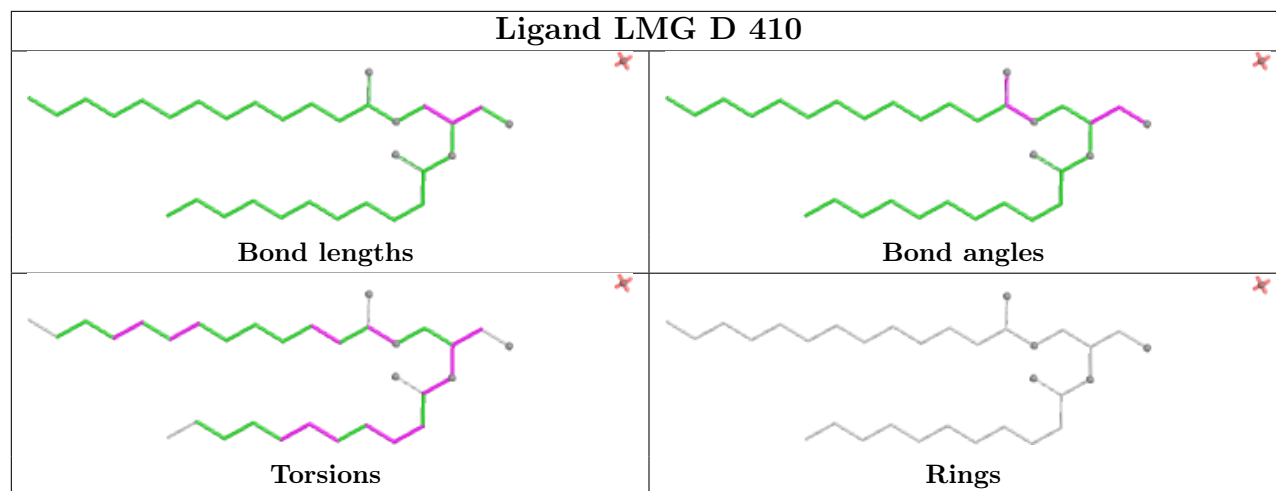
Ligand STE C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

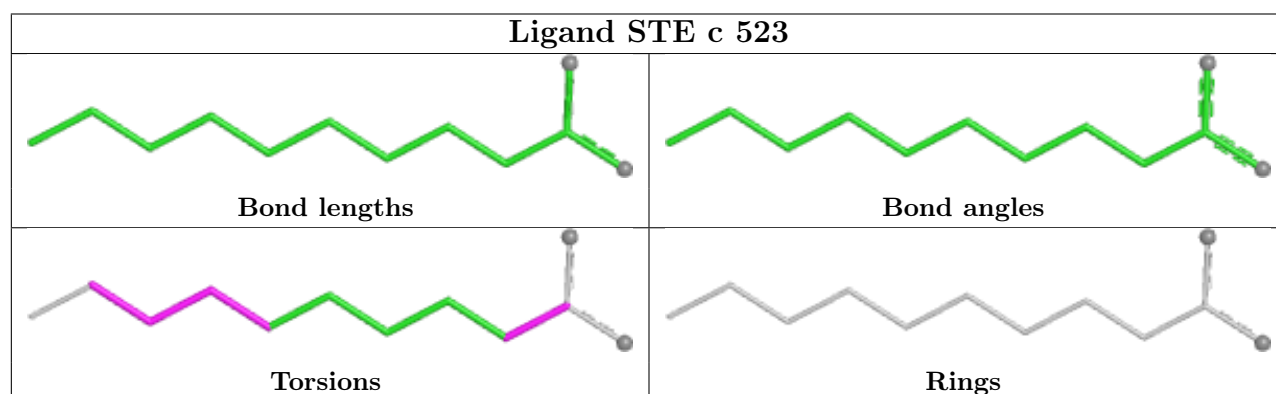
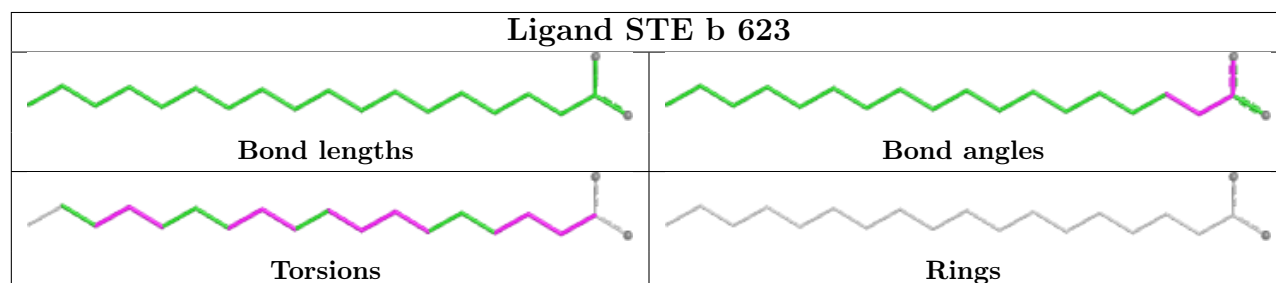
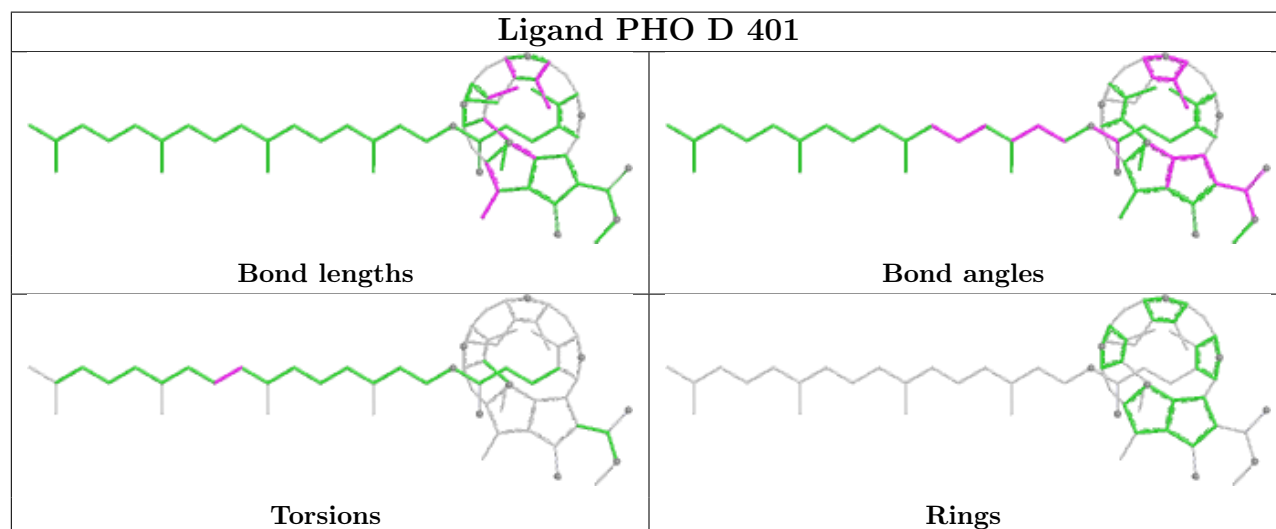
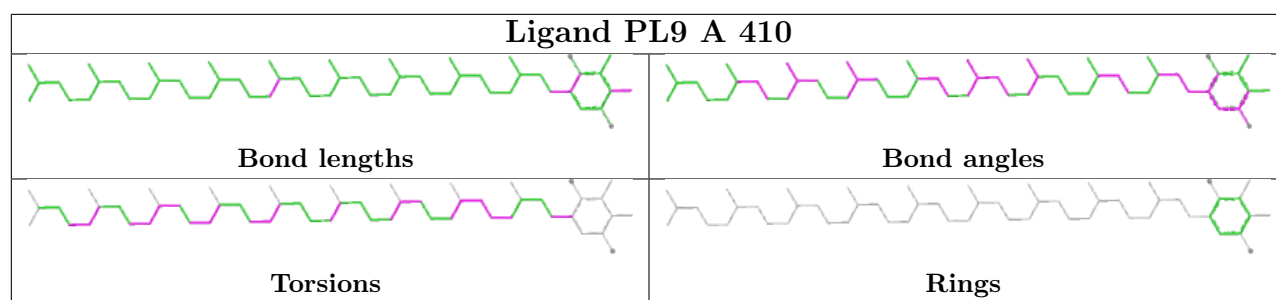
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

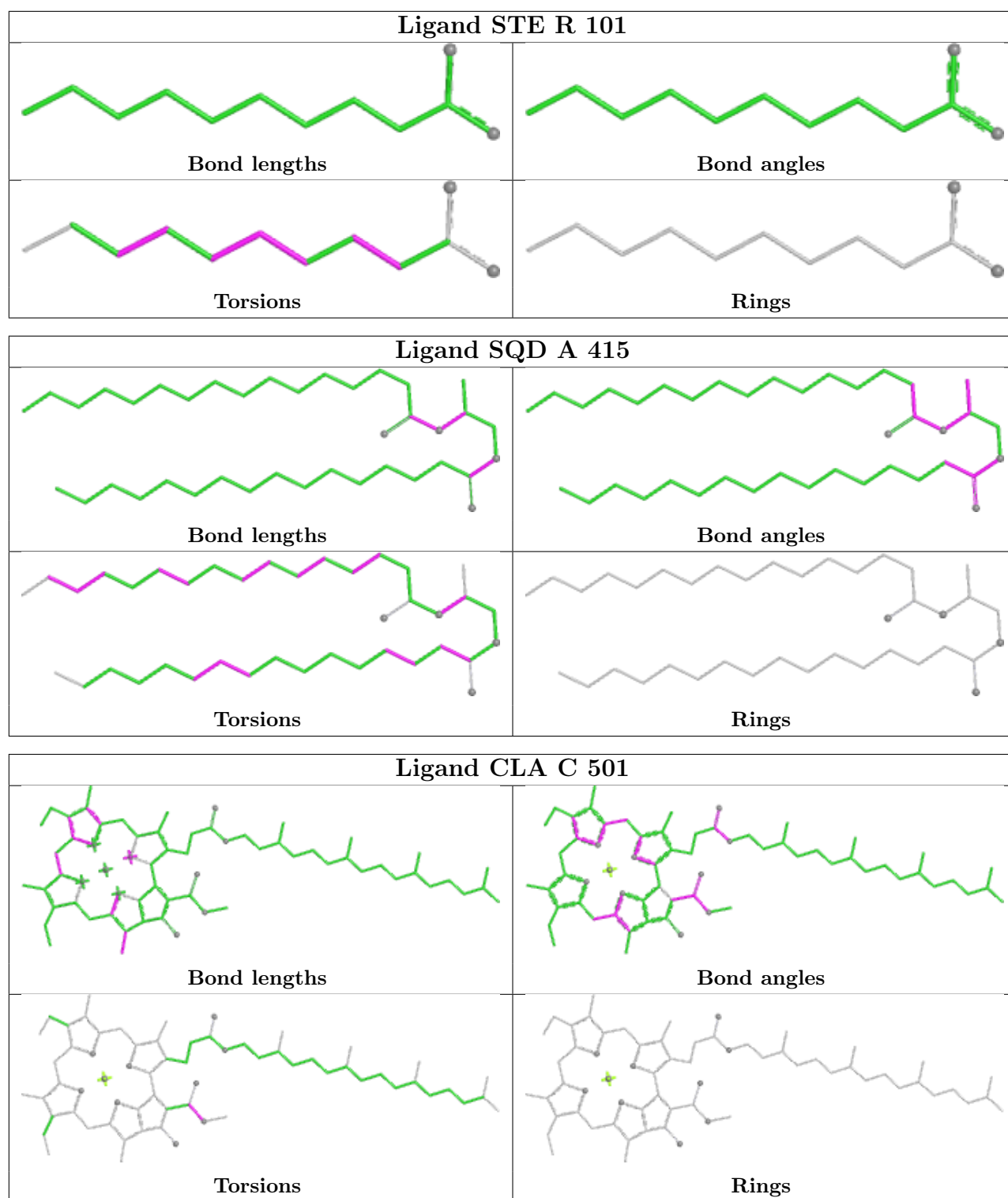
Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

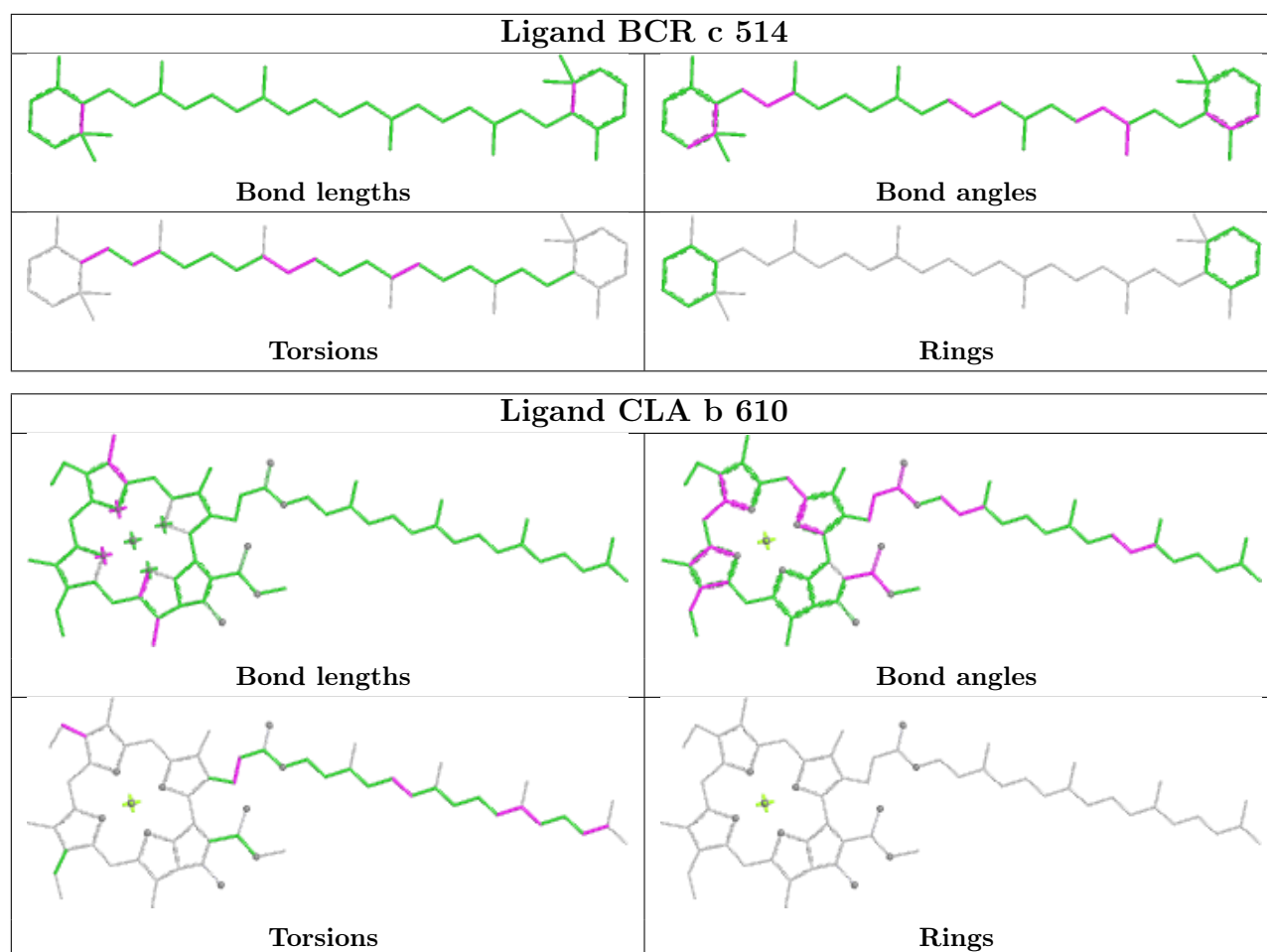
Ligand STE a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings











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%)	-0.50	1 (0%) 90 91	13, 30, 47, 79	64 (19%)
1	a	334/344 (97%)	-0.40	2 (0%) 85 87	13, 32, 57, 78	64 (19%)
2	B	505/510 (99%)	-0.43	1 (0%) 91 92	19, 35, 62, 87	4 (0%)
2	b	505/510 (99%)	-0.29	2 (0%) 88 90	25, 38, 70, 102	0
3	C	442/461 (95%)	-0.37	0 100 100	15, 38, 53, 76	11 (2%)
3	c	451/461 (97%)	-0.28	1 (0%) 91 92	14, 42, 62, 94	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	16, 33, 47, 78	2 (0%)
4	d	341/352 (96%)	-0.42	0 100 100	15, 36, 57, 81	3 (0%)
5	E	82/84 (97%)	0.14	0 100 100	31, 52, 66, 83	1 (1%)
5	e	82/84 (97%)	0.30	1 (1%) 76 78	41, 59, 76, 91	0
6	F	34/45 (75%)	-0.15	0 100 100	37, 44, 60, 80	0
6	f	34/45 (75%)	0.09	0 100 100	42, 52, 75, 88	0
7	H	65/66 (98%)	-0.21	1 (1%) 72 74	32, 43, 58, 70	0
7	h	63/66 (95%)	0.05	3 (4%) 35 38	39, 50, 64, 69	0
8	I	35/38 (92%)	-0.32	0 100 100	35, 41, 68, 82	0
8	i	35/38 (92%)	-0.02	1 (2%) 53 56	33, 43, 78, 87	0
9	J	36/40 (90%)	-0.15	0 100 100	36, 52, 72, 95	0
9	j	36/40 (90%)	0.04	0 100 100	37, 54, 84, 97	0
10	K	37/46 (80%)	-0.08	0 100 100	41, 53, 70, 74	0
10	k	37/46 (80%)	0.12	0 100 100	46, 56, 72, 76	0
11	L	37/37 (100%)	-0.53	0 100 100	27, 33, 64, 69	0
11	l	36/37 (97%)	-0.55	0 100 100	27, 34, 73, 87	0
12	M	32/36 (88%)	-0.47	0 100 100	29, 38, 59, 71	0
12	m	31/36 (86%)	-0.47	0 100 100	30, 38, 54, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.16	4 (1%) 70 73	26, 45, 85, 140	1 (0%)
13	o	244/272 (89%)	-0.15	2 (0%) 82 84	27, 44, 81, 124	0
14	R	28/41 (68%)	0.65	0 100 100	58, 68, 83, 92	0
14	r	28/41 (68%)	1.02	2 (7%) 22 23	65, 83, 103, 113	0
15	T	29/32 (90%)	-0.55	0 100 100	28, 34, 61, 81	0
15	t	29/32 (90%)	-0.32	1 (3%) 48 50	31, 35, 82, 95	0
16	U	97/134 (72%)	-0.21	0 100 100	34, 46, 70, 84	0
16	u	97/134 (72%)	-0.32	0 100 100	32, 42, 59, 80	0
17	V	137/163 (84%)	-0.33	0 100 100	32, 42, 57, 77	0
17	v	137/163 (84%)	-0.09	1 (0%) 84 86	34, 49, 68, 78	0
18	X	38/41 (92%)	-0.09	0 100 100	40, 51, 70, 76	0
18	x	39/41 (95%)	0.24	1 (2%) 57 60	48, 59, 84, 97	0
19	Y	27/46 (58%)	0.89	3 (11%) 10 10	52, 73, 94, 100	0
19	y	30/46 (65%)	0.63	0 100 100	62, 72, 87, 96	0
20	Z	62/62 (100%)	0.72	6 (9%) 13 14	54, 67, 108, 114	0
20	z	62/62 (100%)	0.68	2 (3%) 50 53	56, 73, 109, 124	0
All	All	5293/5700 (92%)	-0.26	35 (0%) 84 86	13, 40, 72, 140	162 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.4
15	t	30	THR	4.4
18	x	40	SER	3.5
13	O	60	ARG	3.4
2	b	495	PHE	3.3
20	z	33	TRP	3.3
20	Z	62	VAL	3.2
5	e	79	PHE	3.1
3	c	23	ALA	3.1
7	H	41	PHE	3.0
19	Y	20	ALA	2.8
14	r	20	VAL	2.8
13	O	59	LYS	2.8
19	Y	25	ILE	2.8
8	i	36	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
20	Z	33	TRP	2.4
1	A	11	ALA	2.4
20	Z	41	PHE	2.4
2	b	84	THR	2.4
20	Z	30	PRO	2.4
19	Y	22	LEU	2.3
13	O	56	PRO	2.3
17	v	22	THR	2.3
20	Z	3	ILE	2.2
1	a	250	ALA	2.2
20	z	27	TYR	2.2
20	Z	34	ASP	2.2
1	a	248	ILE	2.2
13	o	57	LYS	2.1
7	h	41	PHE	2.1
7	h	21	VAL	2.1
13	O	58	ASN	2.1
7	h	64	ALA	2.1
14	r	27	ALA	2.1
2	B	479[A]	PHE	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
15	FME	t	1	10/11	0.94	0.07	29,43,62,63	0
12	FME	M	1	10/11	0.95	0.07	40,49,68,70	0
12	FME	m	1	10/11	0.96	0.07	33,47,63,74	0
15	FME	T	1	10/11	0.96	0.07	29,41,62,62	0
8	FME	I	1	10/11	0.96	0.08	34,41,49,59	0
8	FME	i	1	10/11	0.97	0.07	35,44,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	STE	b	627	10/20	0.73	0.19	44,59,69,70	0
34	STE	L	101	12/20	0.77	0.18	46,59,75,80	0
34	STE	I	101	15/20	0.77	0.17	39,56,70,70	0
34	STE	h	102	14/20	0.77	0.17	47,62,75,78	0
34	STE	H	103	18/20	0.78	0.16	48,66,76,79	0
34	STE	j	101	12/20	0.78	0.13	42,56,70,73	0
34	STE	b	626	20/20	0.79	0.14	44,62,74,79	0
34	STE	d	413	20/20	0.80	0.14	42,62,76,76	0
30	LHG	A	414	49/49	0.80	0.13	47,70,98,111	0
28	LMG	b	624	55/55	0.80	0.16	50,72,91,96	0
28	LMG	a	416	55/55	0.81	0.13	38,56,75,80	0
29	SQD	a	412	36/54	0.81	0.14	33,59,78,86	0
34	STE	c	523	12/20	0.81	0.12	49,64,81,82	0
34	STE	a	413	10/20	0.82	0.14	37,60,68,72	0
34	STE	a	414	12/20	0.82	0.13	50,64,74,78	0
34	STE	B	626	16/20	0.82	0.13	45,63,72,75	0
28	LMG	c	521	48/55	0.82	0.14	47,69,94,103	0
29	SQD	A	415	39/54	0.83	0.14	37,59,88,94	0
30	LHG	e	102	42/49	0.83	0.14	57,79,100,109	0
34	STE	R	101	12/20	0.84	0.15	51,75,78,85	0
34	STE	b	621	16/20	0.84	0.13	35,49,65,75	0
31	DGD	A	416	66/66	0.85	0.11	41,61,75,79	0
34	STE	c	520	20/20	0.85	0.12	43,57,79,88	0
28	LMG	D	410	33/55	0.85	0.13	36,55,74,80	0
34	STE	a	415	15/20	0.85	0.16	42,58,69,74	0
34	STE	B	627	12/20	0.85	0.14	44,59,76,79	0
34	STE	C	520	16/20	0.85	0.12	36,52,62,69	0
34	STE	b	625	16/20	0.86	0.12	45,62,72,74	0
28	LMG	A	412	48/55	0.86	0.10	36,55,74,89	0
34	STE	B	625	18/20	0.86	0.12	38,57,69,74	0
34	STE	C	519	12/20	0.86	0.12	46,56,66,67	0
34	STE	B	620	17/20	0.87	0.10	36,50,62,62	0
34	STE	T	102	15/20	0.87	0.12	41,56,70,76	0
34	STE	Z	101	8/20	0.87	0.17	46,57,66,66	0
28	LMG	c	522	49/55	0.87	0.10	37,55,79,96	0
28	LMG	c	519	37/55	0.87	0.12	39,61,75,81	0
34	STE	B	624	12/20	0.88	0.12	44,55,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	PL9	A	410	55/55	0.88	0.12	34,63,84,90	0
34	STE	C	521	12/20	0.88	0.11	34,47,54,58	0
34	STE	d	412	20/20	0.88	0.11	36,55,71,73	0
34	STE	b	623	20/20	0.88	0.11	39,55,69,79	0
22	CLA	b	601	65/65	0.88	0.11	42,65,85,91	0
28	LMG	C	518	48/55	0.88	0.12	36,65,86,89	0
34	STE	l	102	18/20	0.88	0.12	34,47,72,80	0
29	SQD	b	620	49/54	0.89	0.09	38,57,85,89	0
27	PL9	a	409	55/55	0.89	0.12	37,66,80,89	0
34	STE	J	101	12/20	0.89	0.11	45,59,70,72	0
34	STE	X	101	20/20	0.89	0.10	31,48,62,64	0
34	STE	t	102	14/20	0.89	0.10	33,52,62,65	0
24	BCR	c	514	40/40	0.90	0.10	43,59,70,72	0
29	SQD	f	101	41/54	0.90	0.12	49,76,94,100	0
22	CLA	B	601	65/65	0.90	0.10	30,59,82,94	0
34	STE	M	103	10/20	0.90	0.10	35,48,55,58	0
24	BCR	K	101	40/40	0.90	0.11	41,55,70,71	0
28	LMG	b	622	51/55	0.90	0.10	29,50,68,80	0
29	SQD	B	623	54/54	0.90	0.09	40,57,86,96	0
24	BCR	Y	101	40/40	0.90	0.10	35,50,68,71	0
28	LMG	D	411	28/55	0.91	0.10	28,48,59,61	0
29	SQD	D	407	36/54	0.91	0.11	44,68,83,94	0
28	LMG	M	101	51/55	0.91	0.09	29,47,70,84	0
22	CLA	C	513	65/65	0.91	0.09	40,60,87,89	0
34	STE	M	102	15/20	0.91	0.10	34,48,63,63	0
34	STE	d	411	17/20	0.91	0.10	40,54,61,61	0
31	DGD	h	101	62/66	0.92	0.09	24,47,62,66	0
29	SQD	a	411	54/54	0.92	0.10	41,61,84,85	0
24	BCR	d	405	40/40	0.92	0.10	32,51,85,98	0
24	BCR	k	101	40/40	0.92	0.10	42,61,73,75	0
28	LMG	d	410	44/55	0.92	0.09	31,50,73,88	0
24	BCR	x	101	40/40	0.92	0.09	31,51,66,74	0
26	BCT	a	408	4/4	0.92	0.10	26,32,39,46	0
24	BCR	H	101	40/40	0.92	0.09	26,44,57,61	0
31	DGD	C	516	62/66	0.92	0.09	30,48,91,108	0
22	CLA	c	513	65/65	0.93	0.10	39,68,104,108	0
31	DGD	H	102	62/66	0.93	0.08	26,41,58,63	0
31	DGD	c	517	62/66	0.93	0.08	33,51,82,89	0
24	BCR	B	618	40/40	0.93	0.07	24,37,49,55	0
24	BCR	B	619	40/40	0.93	0.08	29,41,54,60	0
24	BCR	k	102	40/40	0.93	0.10	39,54,66,67	0
24	BCR	D	404	40/40	0.93	0.09	25,43,76,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	512	65/65	0.93	0.10	33,53,82,92	0
22	CLA	c	511	65/65	0.93	0.10	39,52,71,74	0
22	CLA	c	512	65/65	0.93	0.10	39,57,86,92	0
30	LHG	d	407	49/49	0.93	0.11	32,50,70,76	0
24	BCR	b	618	40/40	0.93	0.08	25,39,57,61	0
24	BCR	b	619	40/40	0.93	0.08	28,45,65,68	0
22	CLA	c	506	65/65	0.94	0.10	30,48,87,97	0
30	LHG	d	409	39/49	0.94	0.09	28,46,69,71	0
24	BCR	C	514	40/40	0.94	0.08	25,41,53,63	0
22	CLA	c	508	64/65	0.94	0.09	30,45,85,96	0
31	DGD	C	515	62/66	0.94	0.09	22,40,74,80	0
29	SQD	A	413	52/54	0.94	0.09	29,55,82,90	0
31	DGD	C	517	62/66	0.94	0.08	25,45,68,74	0
28	LMG	D	406	51/55	0.94	0.10	28,50,76,88	0
24	BCR	c	515	40/40	0.94	0.08	27,43,56,61	0
23	PHO	d	402	64/64	0.94	0.07	27,38,48,50	0
24	BCR	B	617	40/40	0.94	0.07	28,39,55,60	0
24	BCR	K	102	40/40	0.94	0.09	32,48,61,64	0
24	BCR	T	101	40/40	0.94	0.06	22,39,54,62	0
22	CLA	C	511	65/65	0.94	0.08	28,49,64,66	0
24	BCR	b	617	40/40	0.94	0.07	23,41,53,57	0
22	CLA	C	505	65/65	0.95	0.09	24,39,69,74	0
22	CLA	C	506	65/65	0.95	0.09	23,42,82,89	0
22	CLA	c	509	65/65	0.95	0.08	32,46,62,68	0
22	CLA	C	507	65/65	0.95	0.07	22,40,52,57	0
22	CLA	C	509	65/65	0.95	0.08	26,43,64,72	0
22	CLA	C	510	65/65	0.95	0.07	25,42,58,62	0
24	BCR	t	101	40/40	0.95	0.06	24,39,52,55	0
22	CLA	d	404	65/65	0.95	0.09	27,46,81,87	0
22	CLA	B	606	65/65	0.95	0.08	24,36,74,79	0
24	BCR	A	406	40/40	0.95	0.07	23,35,45,47	0
30	LHG	B	622	49/49	0.95	0.09	27,45,65,70	0
30	LHG	D	409	47/49	0.95	0.09	27,48,73,88	0
27	PL9	D	405	55/55	0.95	0.06	21,33,46,47	0
22	CLA	C	502	65/65	0.95	0.07	28,39,61,73	0
27	PL9	d	406	55/55	0.95	0.06	22,34,42,44	0
30	LHG	l	101	49/49	0.95	0.08	31,43,57,64	0
22	CLA	C	503	65/65	0.95	0.07	26,41,51,57	0
22	CLA	C	504	59/65	0.95	0.08	28,40,76,84	0
22	CLA	b	602	65/65	0.95	0.08	28,42,60,61	0
22	CLA	b	606	65/65	0.95	0.08	27,39,69,74	0
22	CLA	b	609	65/65	0.95	0.08	29,45,60,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DGD	c	516	62/66	0.95	0.08	22,41,70,78	0
22	CLA	b	614	65/65	0.95	0.08	24,41,73,77	0
31	DGD	c	518	62/66	0.95	0.08	30,49,77,88	0
22	CLA	b	616	60/65	0.95	0.08	26,42,85,88	0
22	CLA	c	502	65/65	0.95	0.07	29,41,61,65	0
22	CLA	c	503	65/65	0.95	0.07	30,43,53,62	0
24	BCR	a	405	40/40	0.95	0.06	22,33,46,49	0
22	CLA	c	504	60/65	0.95	0.08	29,42,80,83	0
22	CLA	c	505	65/65	0.95	0.07	26,39,64,73	0
22	CLA	a	404	65/65	0.96	0.08	20,37,74,79	0
23	PHO	A	404	64/64	0.96	0.05	18,28,36,40	0
23	PHO	D	401	64/64	0.96	0.06	22,34,43,48	0
23	PHO	d	401	64/64	0.96	0.06	18,32,39,48	0
22	CLA	a	410	65/65	0.96	0.06	20,29,47,54	0
22	CLA	B	616	60/65	0.96	0.09	22,38,79,86	0
22	CLA	C	501	65/65	0.96	0.07	22,36,50,53	0
22	CLA	b	603	65/65	0.96	0.07	23,36,68,70	0
22	CLA	b	605	65/65	0.96	0.06	21,35,49,52	0
22	CLA	B	603	65/65	0.96	0.07	16,34,59,61	0
22	CLA	b	607	65/65	0.96	0.08	20,36,67,71	0
22	CLA	b	608	65/65	0.96	0.07	25,41,58,61	0
22	CLA	B	604	65/65	0.96	0.07	20,34,66,70	0
22	CLA	b	610	65/65	0.96	0.07	24,39,48,56	0
22	CLA	b	611	65/65	0.96	0.07	22,34,54,60	0
22	CLA	b	612	65/65	0.96	0.07	20,34,51,54	0
22	CLA	A	402	65/65	0.96	0.07	16,27,41,55	0
22	CLA	b	615	65/65	0.96	0.07	26,40,56,60	0
22	CLA	B	607	65/65	0.96	0.07	18,34,60,69	0
22	CLA	c	501	65/65	0.96	0.07	23,41,52,56	0
22	CLA	B	609	65/65	0.96	0.07	23,37,61,73	0
30	LHG	B	621	49/49	0.96	0.07	27,42,59,64	0
22	CLA	B	610	65/65	0.96	0.07	20,34,46,47	0
30	LHG	D	408	49/49	0.96	0.07	21,40,51,57	0
22	CLA	C	508	65/65	0.96	0.08	27,43,95,106	0
22	CLA	B	611	65/65	0.96	0.06	22,32,51,54	0
30	LHG	d	408	49/49	0.96	0.07	26,42,52,57	0
22	CLA	B	612	65/65	0.96	0.07	19,34,46,50	0
22	CLA	c	507	65/65	0.96	0.07	27,44,59,61	0
22	CLA	B	613	65/65	0.96	0.07	19,32,63,67	0
26	BCT	A	409	4/4	0.96	0.08	31,32,33,40	0
22	CLA	B	614	65/65	0.96	0.08	21,37,73,79	0
22	CLA	c	510	65/65	0.96	0.07	32,47,64,67	0

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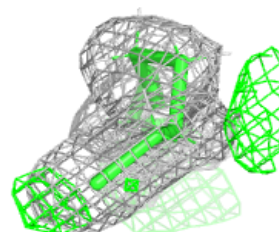
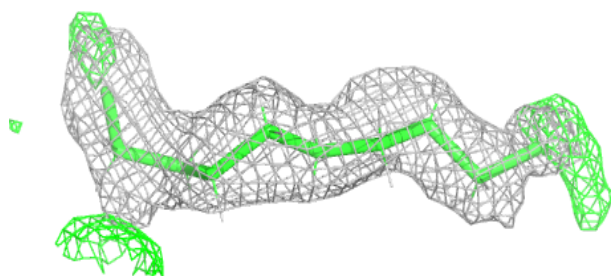
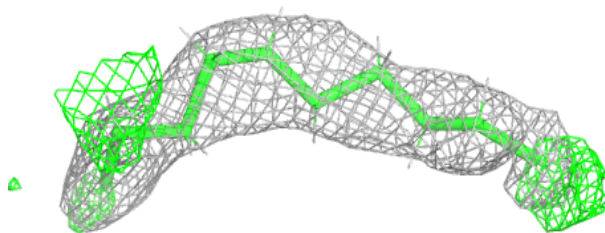
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	B	615	65/65	0.96	0.07	23,36,61,64	0
22	CLA	D	403	65/65	0.96	0.07	24,43,100,108	0
22	CLA	a	403	65/65	0.96	0.08	23,41,91,95	0
22	CLA	d	403	65/65	0.96	0.07	20,35,57,67	0
22	CLA	A	405	54/65	0.97	0.06	18,33,58,67	0
22	CLA	A	411	65/65	0.97	0.06	18,27,56,59	0
22	CLA	B	605	65/65	0.97	0.06	21,32,46,53	0
22	CLA	D	402	65/65	0.97	0.06	13,30,54,60	0
22	CLA	b	613	65/65	0.97	0.07	18,34,72,79	0
22	CLA	b	604	65/65	0.97	0.07	18,35,71,83	0
22	CLA	A	403	65/65	0.97	0.08	21,35,85,91	0
22	CLA	a	402	65/65	0.97	0.05	18,30,47,60	0
22	CLA	B	602	65/65	0.97	0.06	23,36,55,60	0
22	CLA	B	608	65/65	0.97	0.06	22,35,54,62	0
35	HEM	F	101	43/43	0.97	0.08	32,45,60,66	0
35	HEM	e	101	43/43	0.97	0.08	40,51,71,74	0
25	CL	a	406	1/1	0.98	0.04	28,28,28,28	0
36	HEC	V	201	43/43	0.98	0.06	23,33,44,47	0
36	HEC	v	201	43/43	0.98	0.07	25,37,47,49	0
32	OEY	A	417[B]	11/11	0.99	0.03	20,26,30,32	11
33	OEX	A	418[A]	10/10	0.99	0.03	29,31,35,35	10
33	OEX	a	417[A]	10/10	0.99	0.03	26,32,35,35	10
25	CL	A	407	1/1	0.99	0.03	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.07	28,28,28,28	0
25	CL	A	408	1/1	0.99	0.04	28,28,28,28	0
32	OEY	a	418[B]	11/11	1.00	0.02	22,25,29,31	11
21	FE2	a	401	1/1	1.00	0.02	32,32,32,32	0
21	FE2	A	401	1/1	1.00	0.01	27,27,27,27	0

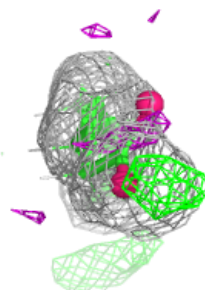
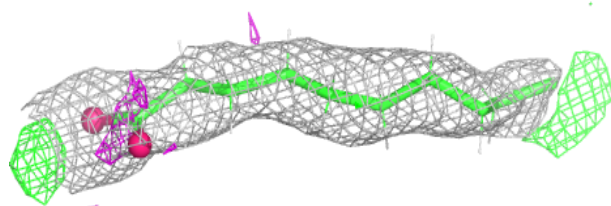
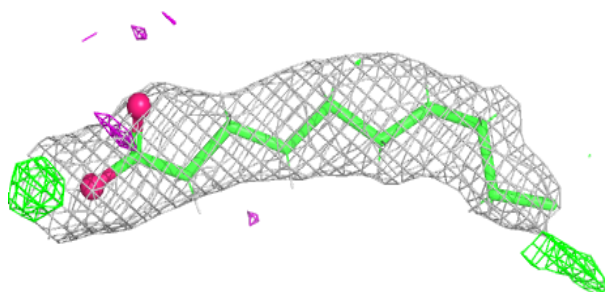
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE b 627:

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

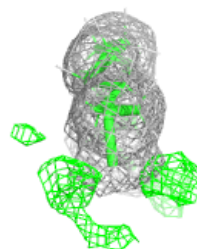
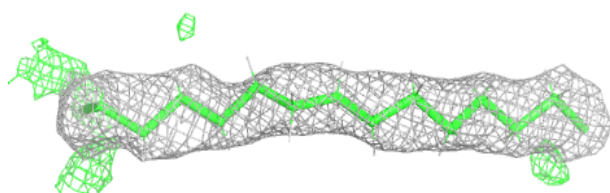
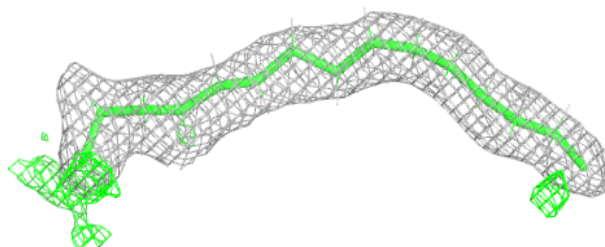
**Electron density around STE L 101:**

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

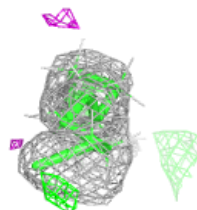
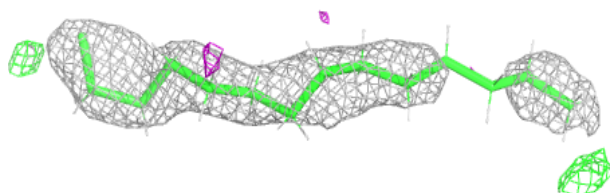
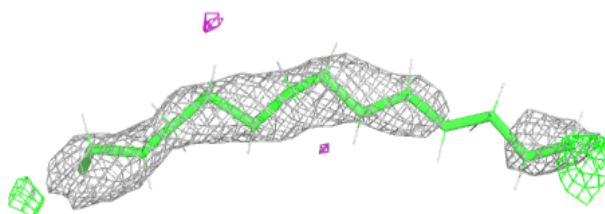


Electron density around STE I 101:

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

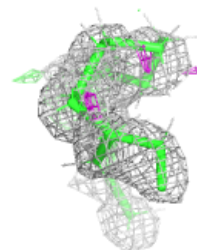
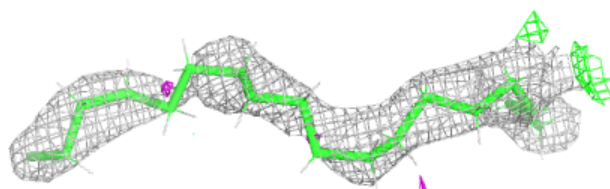
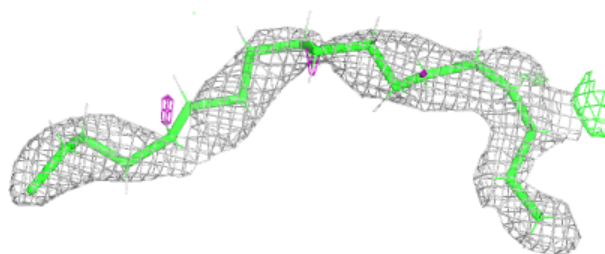
**Electron density around STE h 102:**

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

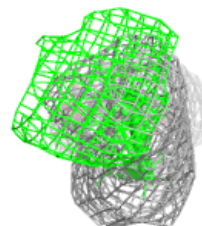
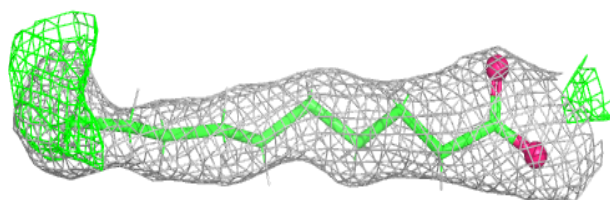
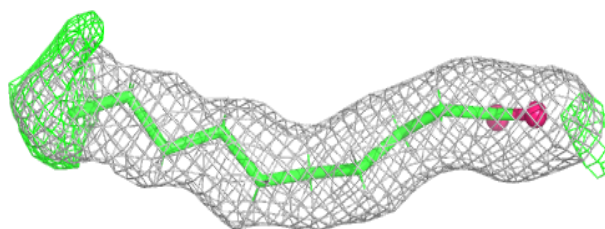


Electron density around STE H 103:

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

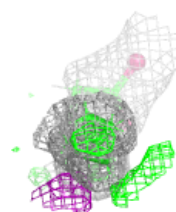
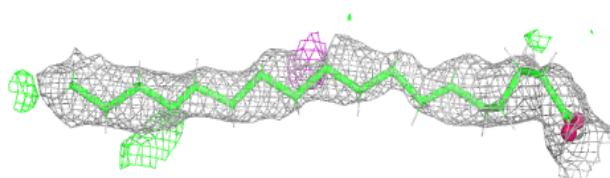
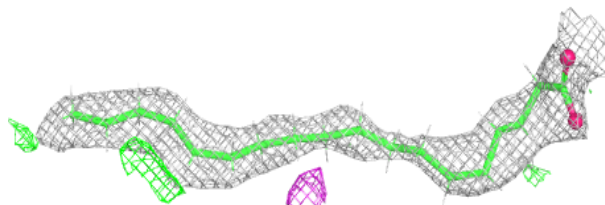
**Electron density around STE j 101:**

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

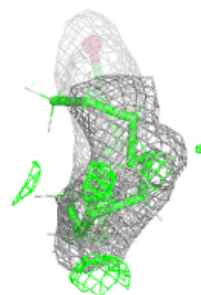
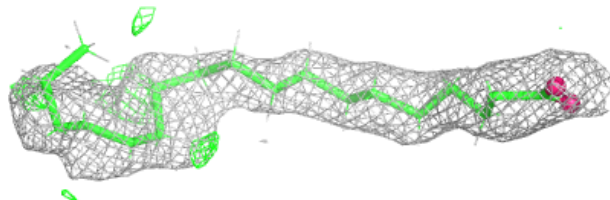
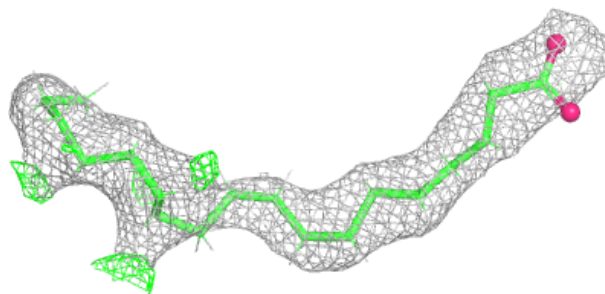


Electron density around STE b 626:

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

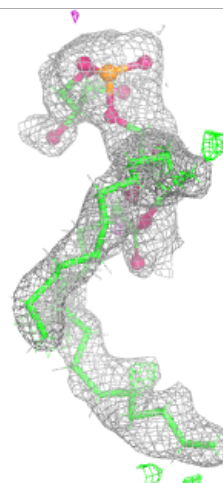
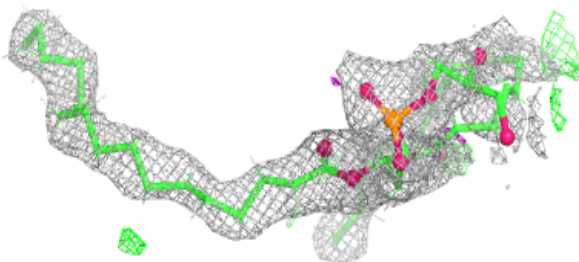
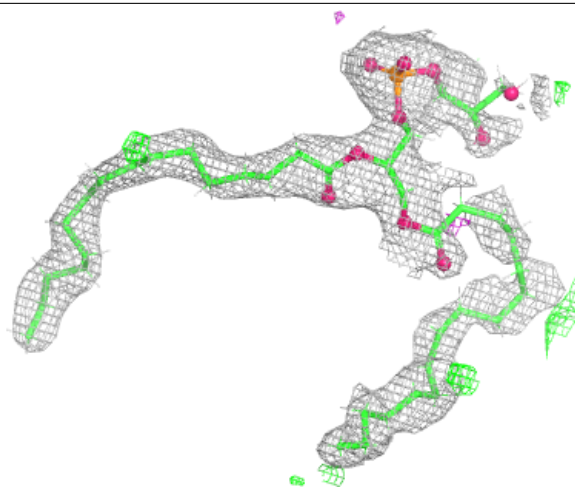
**Electron density around STE d 413:**

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



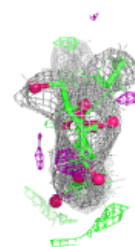
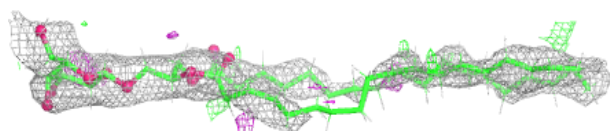
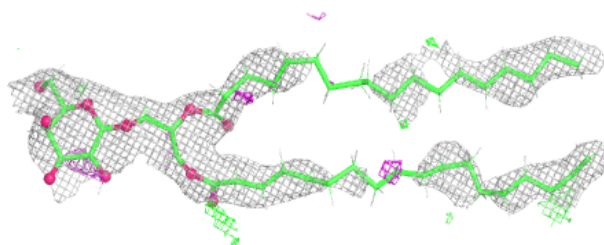
Electron density around LHG A 414:

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

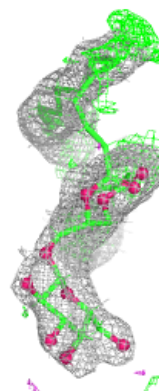
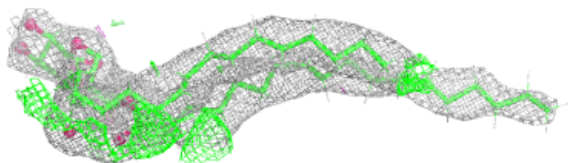
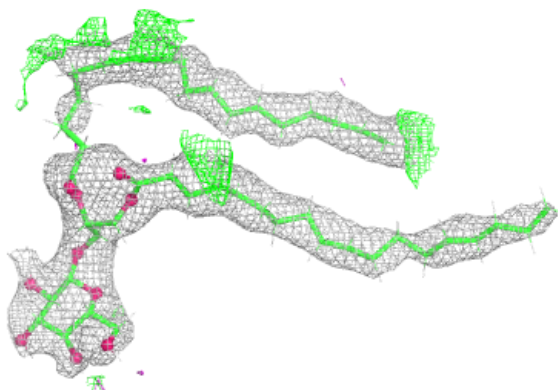


Electron density around LMG b 624:

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

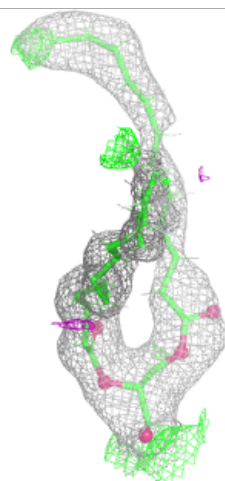
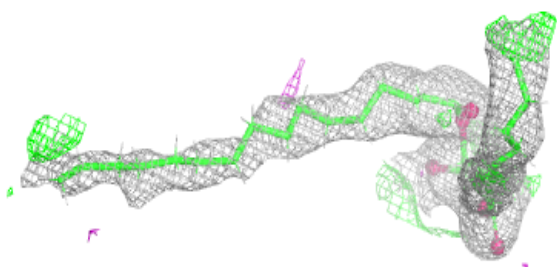
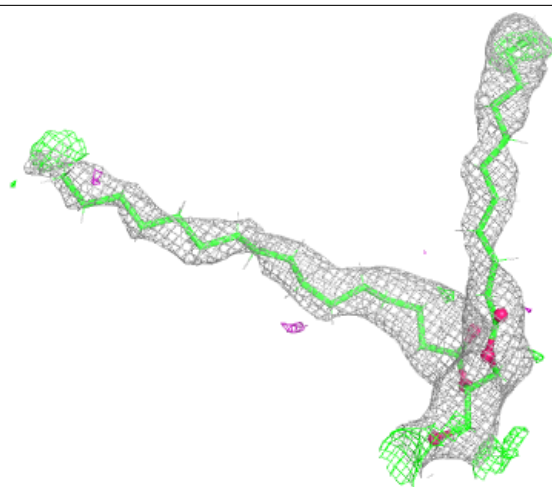
**Electron density around LMG a 416:**

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



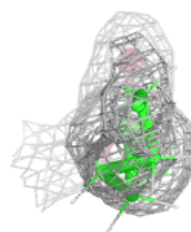
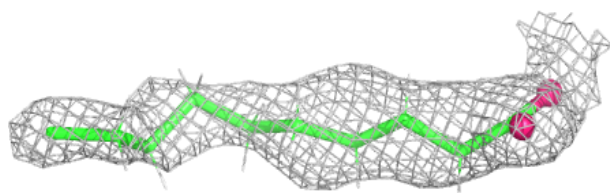
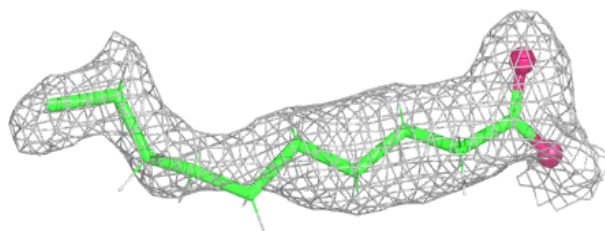
Electron density around SQD a 412:

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

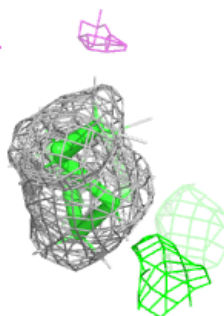
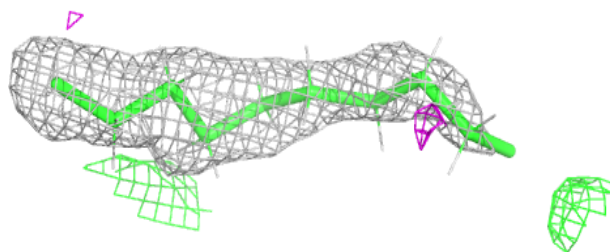
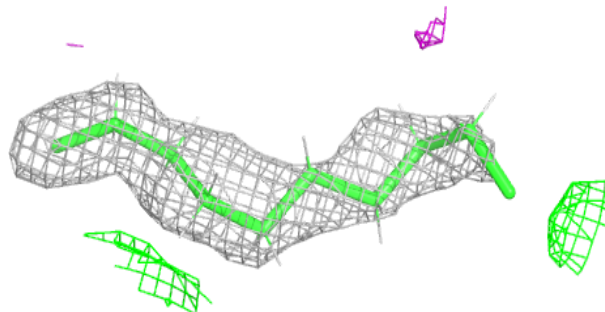


Electron density around STE c 523:

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

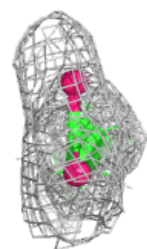
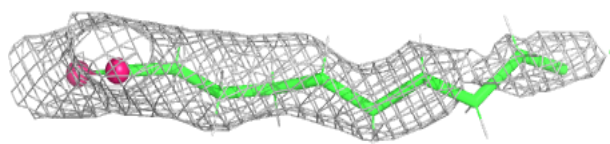
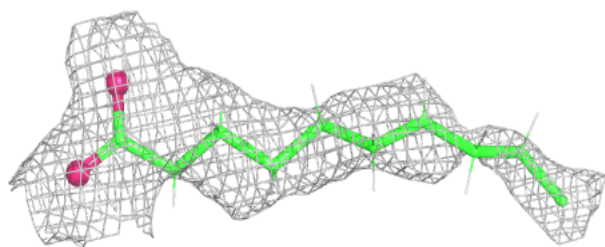
**Electron density around STE a 413:**

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

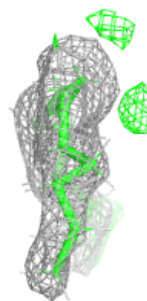
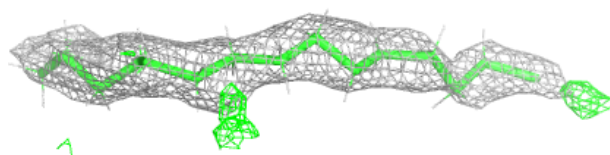
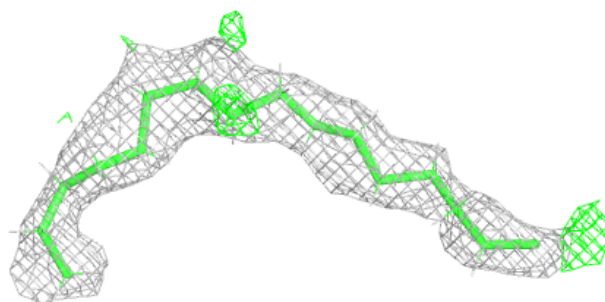


Electron density around STE a 414:

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

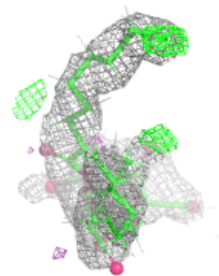
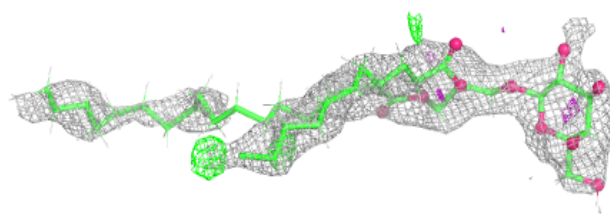
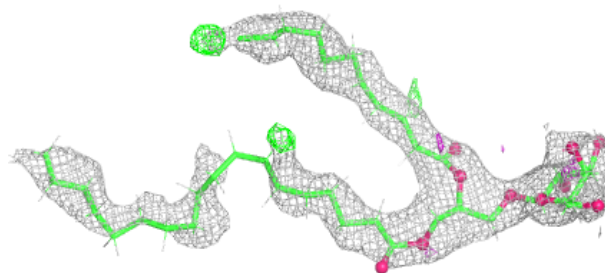
**Electron density around STE B 626:**

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



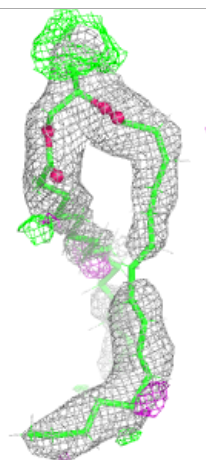
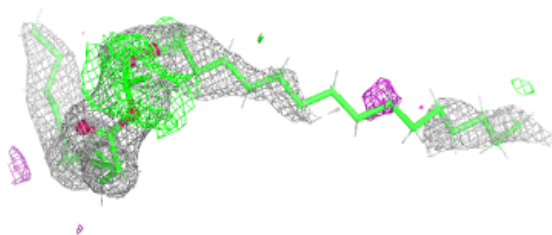
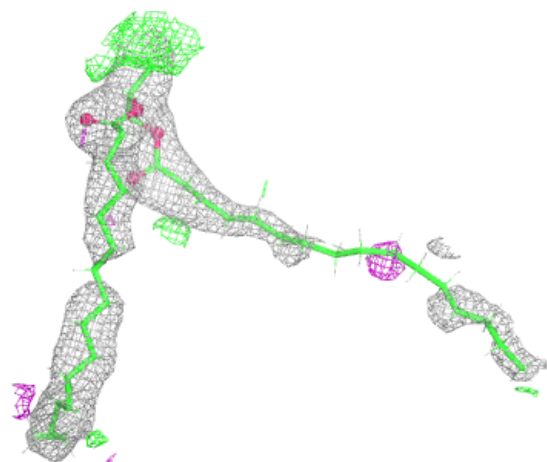
Electron density around LMG c 521:

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



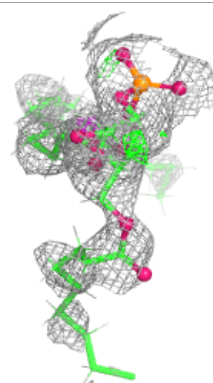
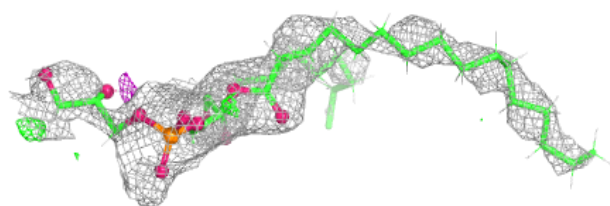
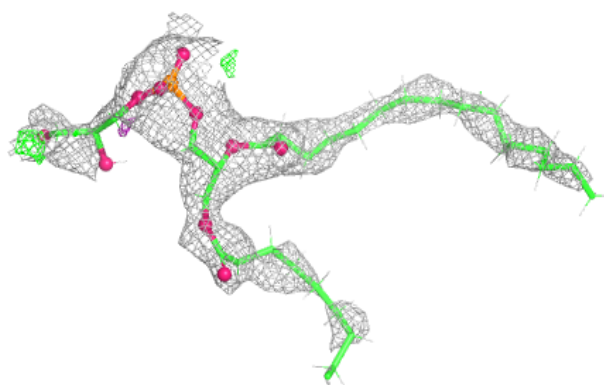
Electron density around SQD A 415:

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

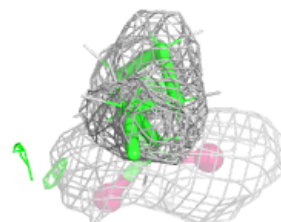
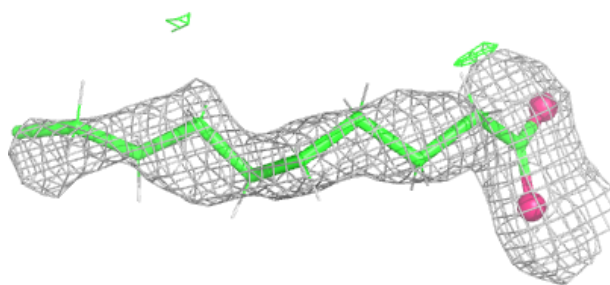
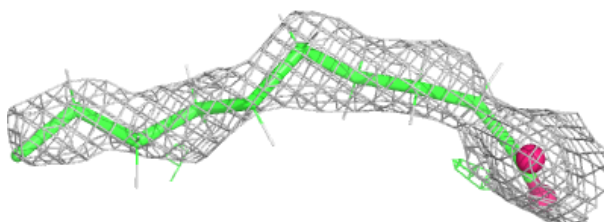


Electron density around LHG e 102:

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

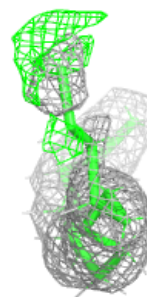
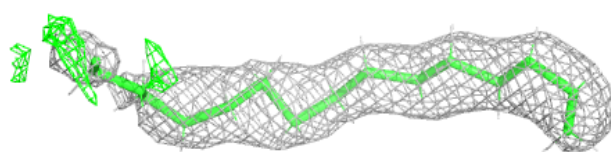
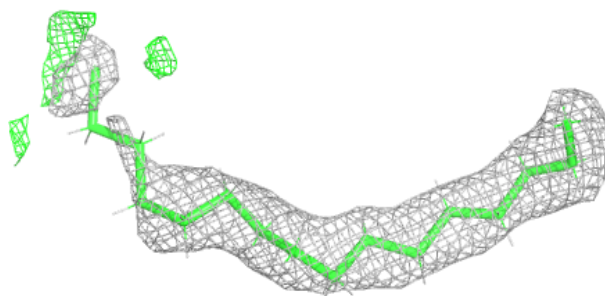
**Electron density around STE R 101:**

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

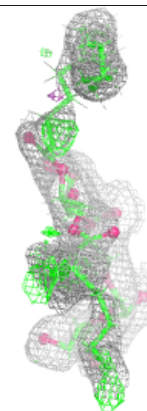
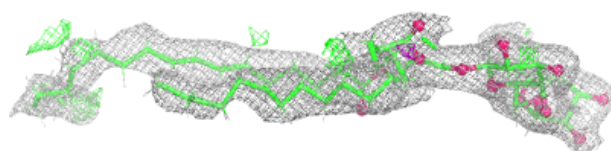
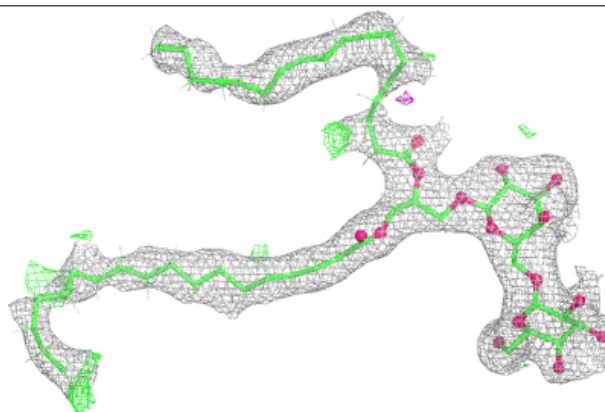


Electron density around STE b 621:

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

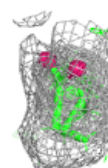
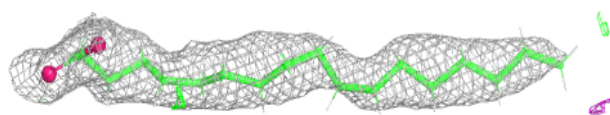
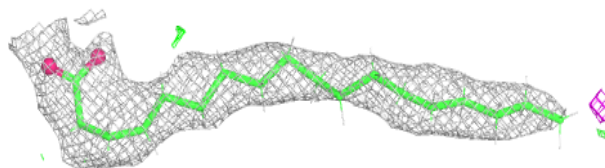
**Electron density around DGD A 416:**

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

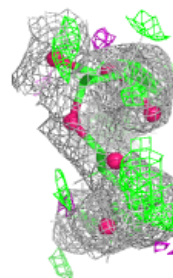
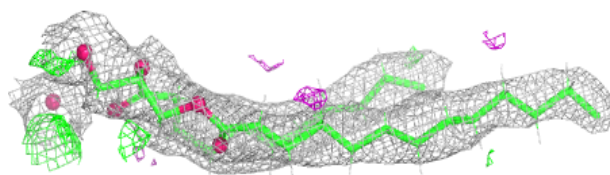
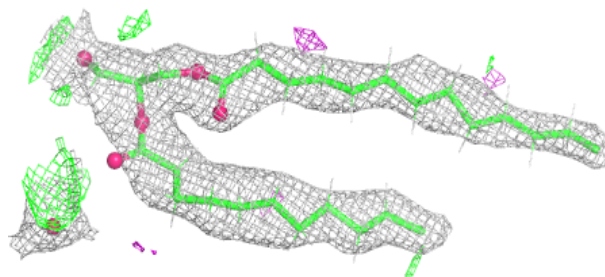


Electron density around STE c 520:

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

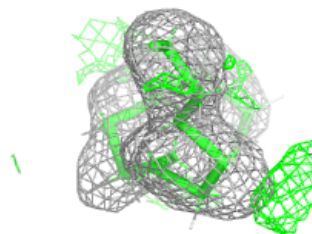
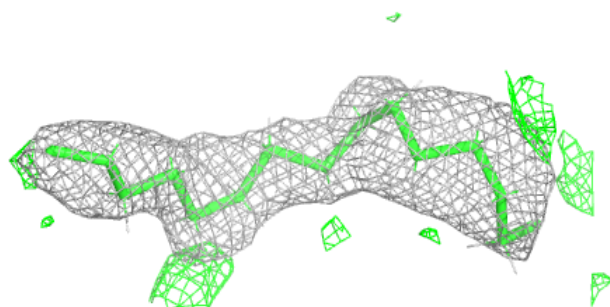
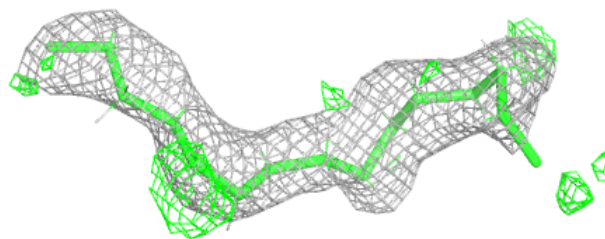
**Electron density around LMG D 410:**

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

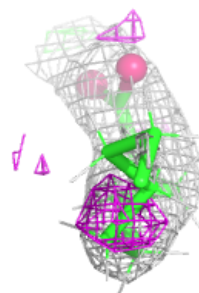
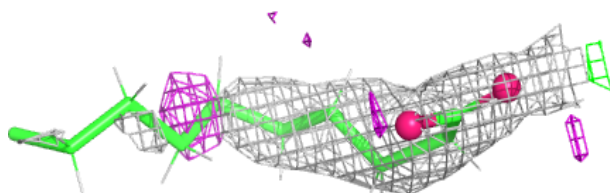
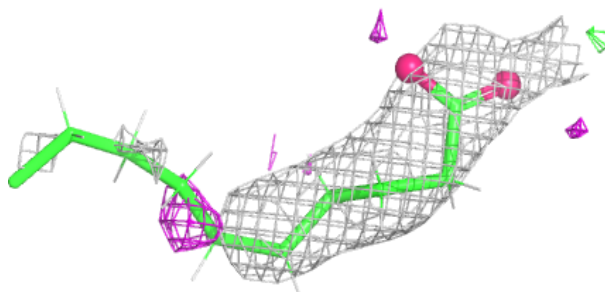


Electron density around STE a 415:

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

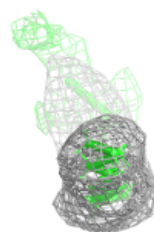
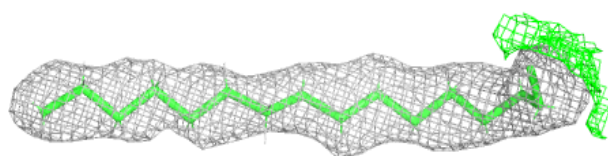
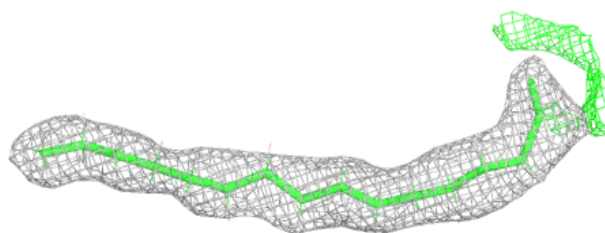
**Electron density around STE B 627:**

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

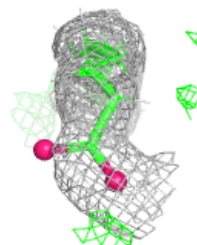
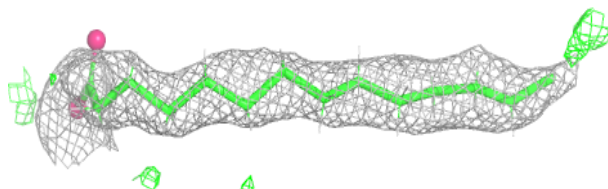
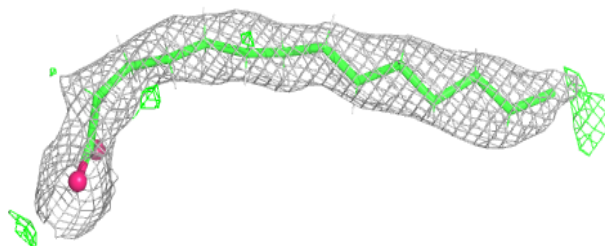


Electron density around STE C 520:

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

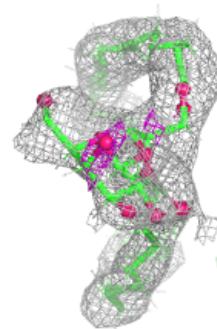
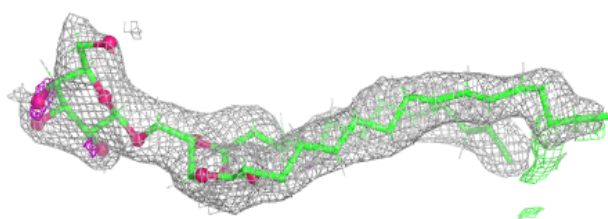
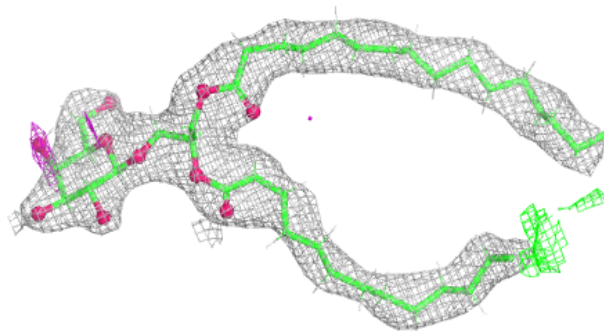
**Electron density around STE b 625:**

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

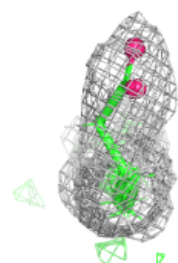
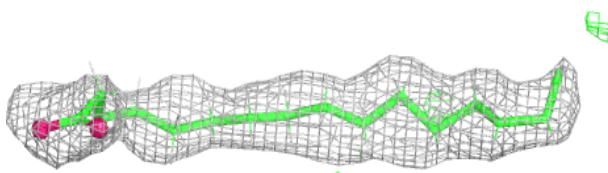
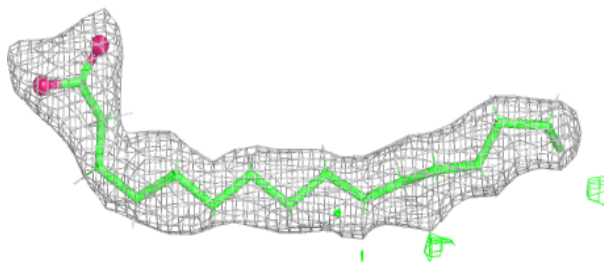


Electron density around LMG A 412:

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

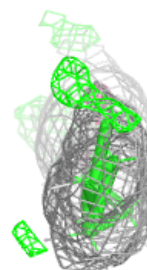
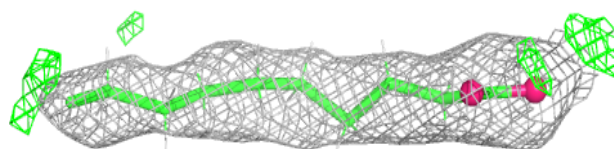
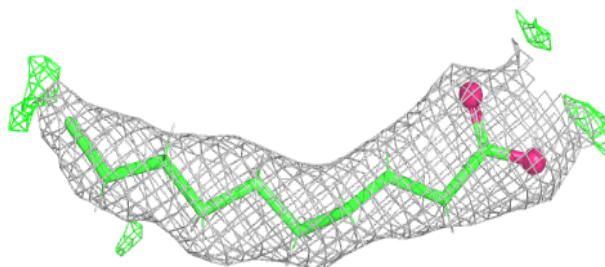
**Electron density around STE B 625:**

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

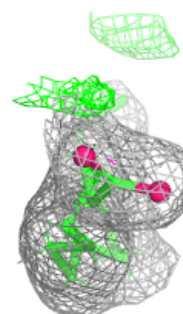
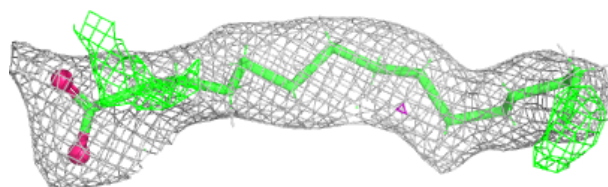
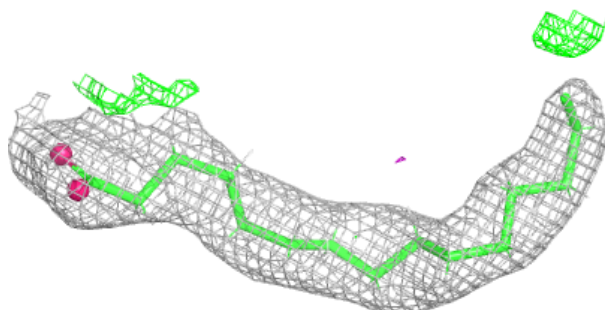


Electron density around STE C 519:

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

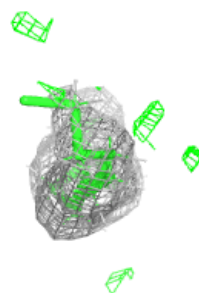
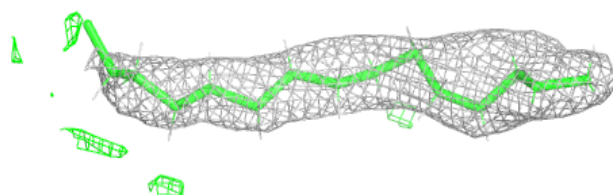
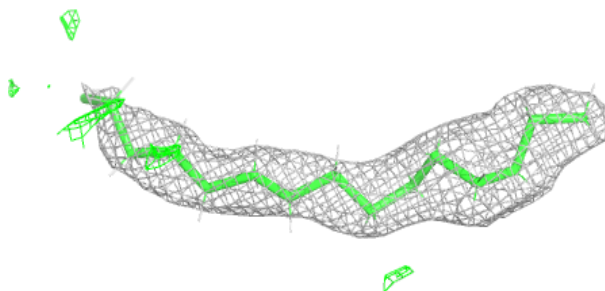
**Electron density around STE B 620:**

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

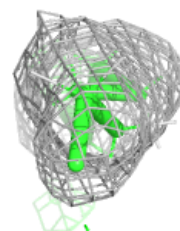
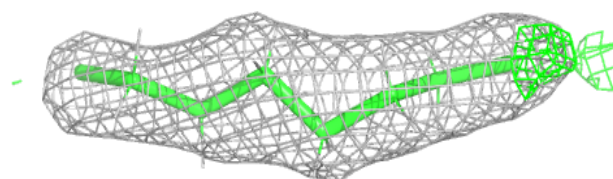
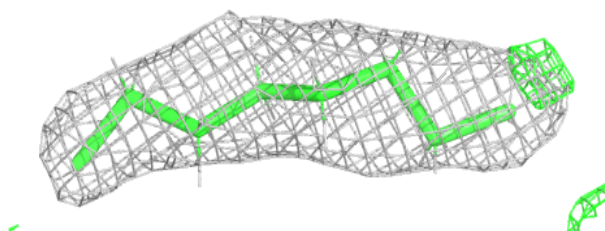


Electron density around STE T 102:

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

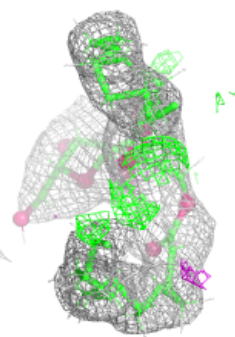
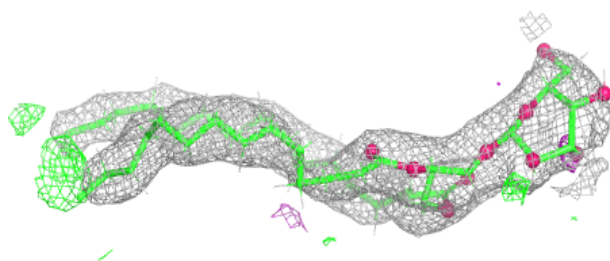
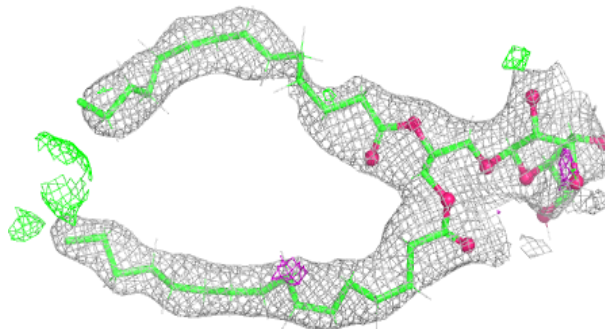
**Electron density around STE Z 101:**

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

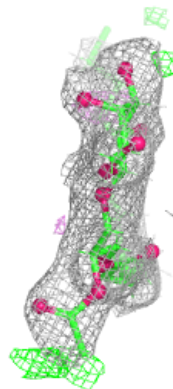
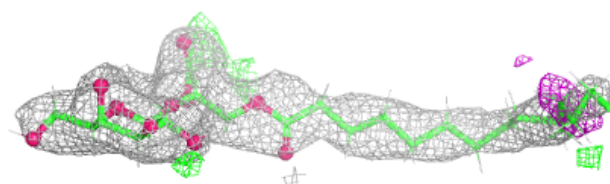
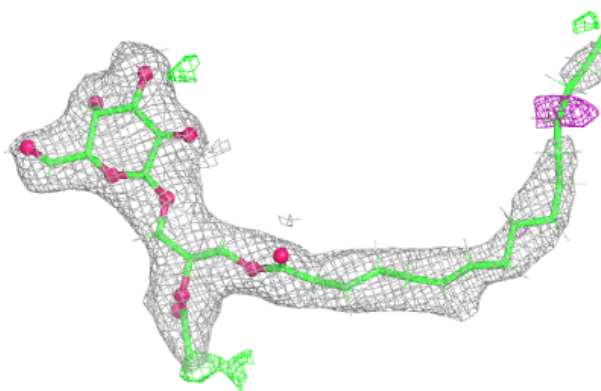


Electron density around LMG c 522:

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

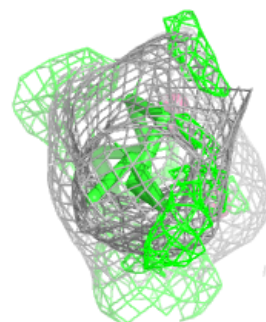
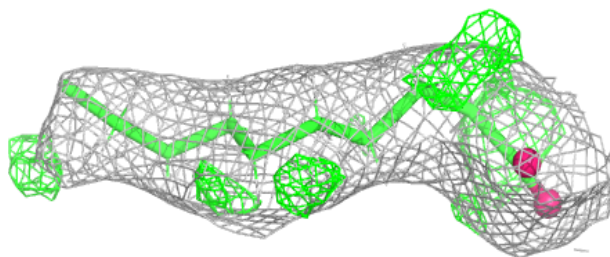
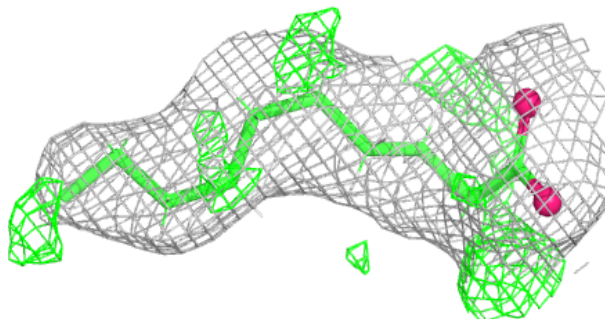
**Electron density around LMG c 519:**

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

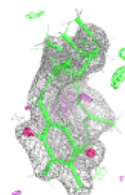
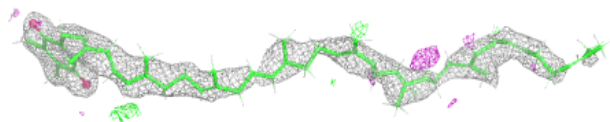
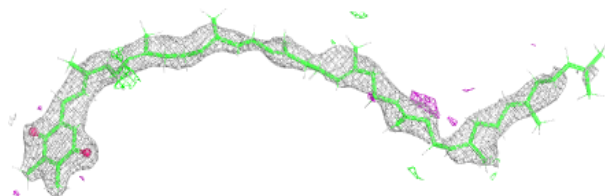


Electron density around STE B 624:

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

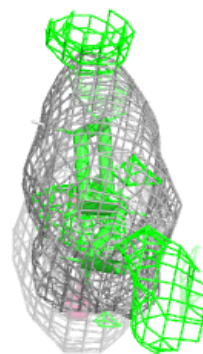
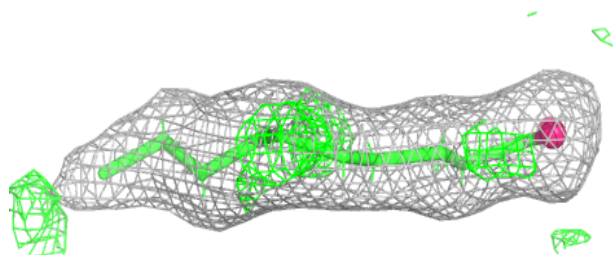
**Electron density around PL9 A 410:**

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

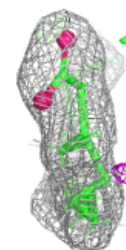
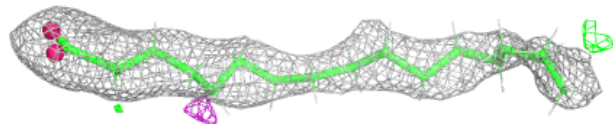
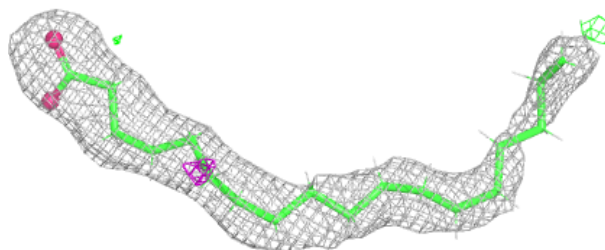


Electron density around STE C 521:

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

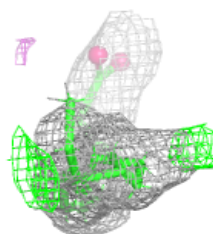
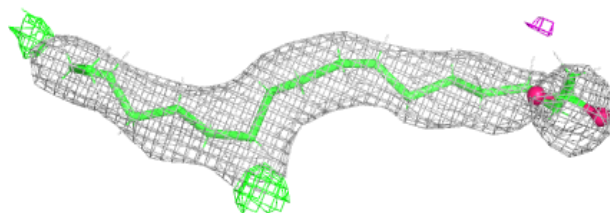
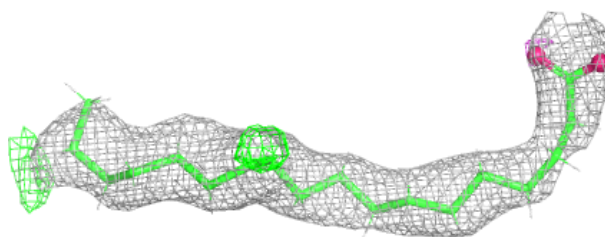
**Electron density around STE d 412:**

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

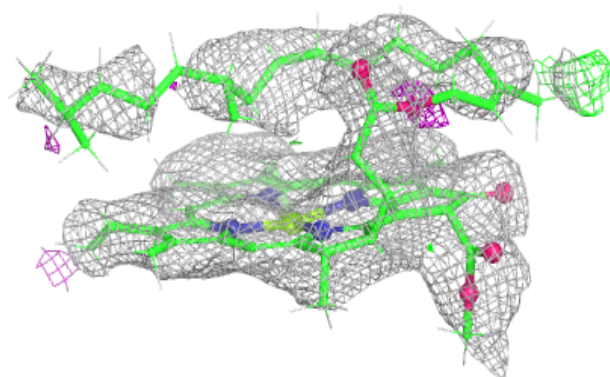
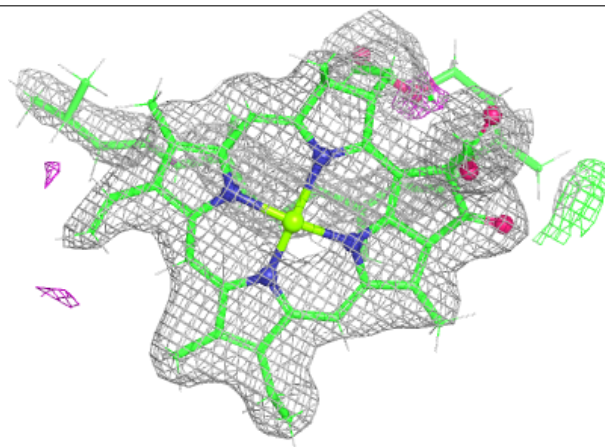


Electron density around STE b 623:

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

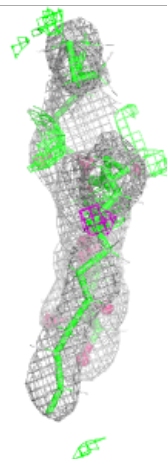
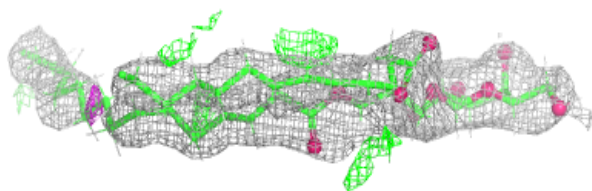
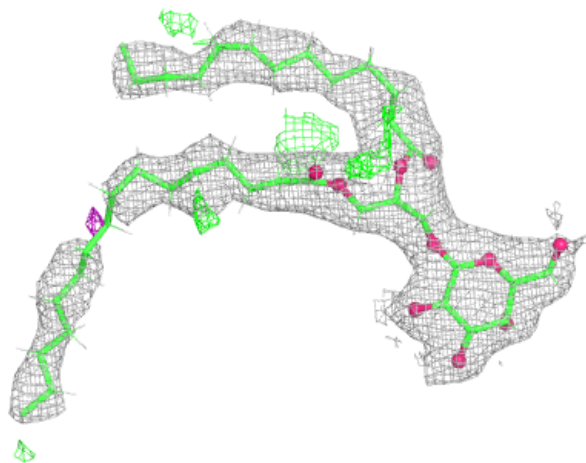
**Electron density around CLA b 601:**

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



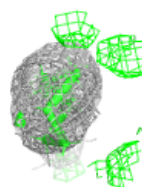
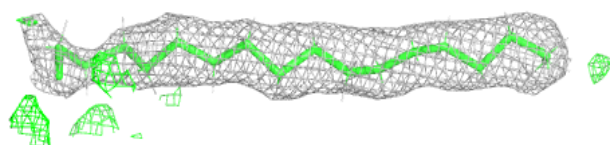
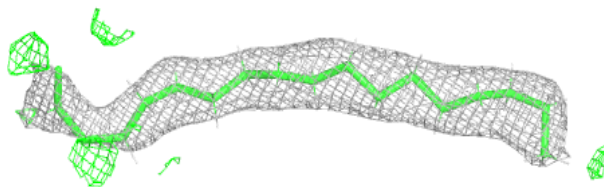
Electron density around LMG C 518:

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

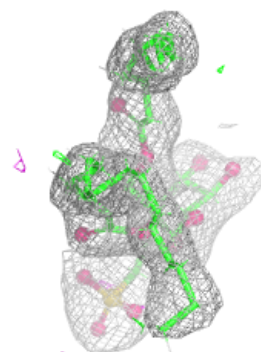
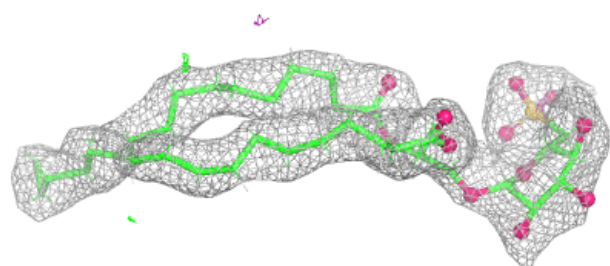
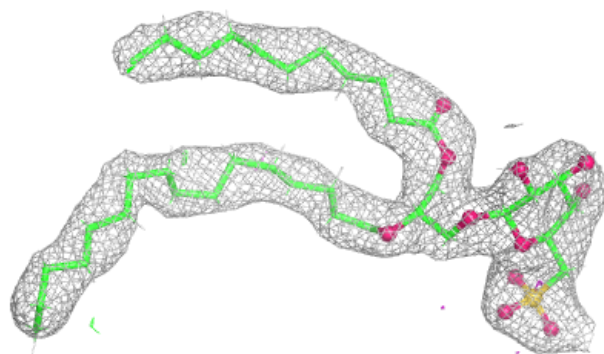


Electron density around STE l 102:

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

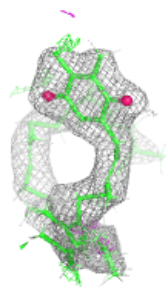
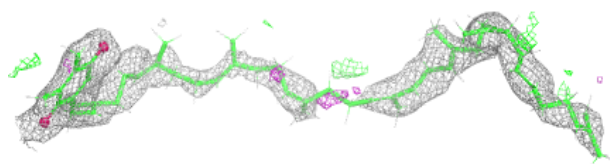
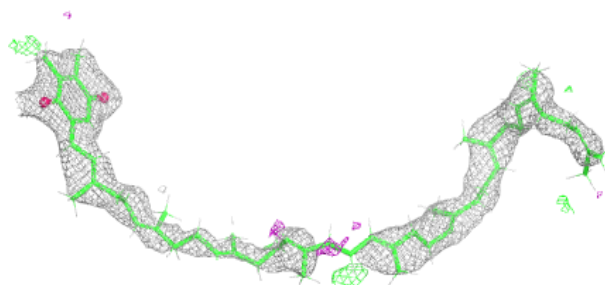
**Electron density around SQD b 620:**

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

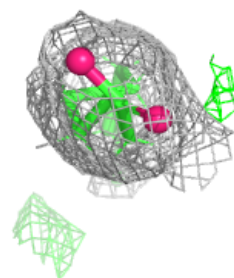
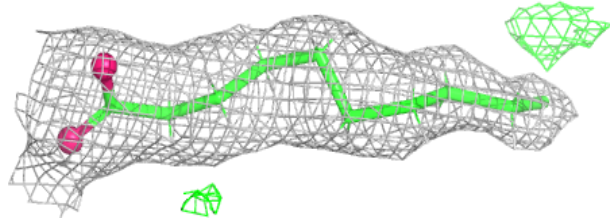
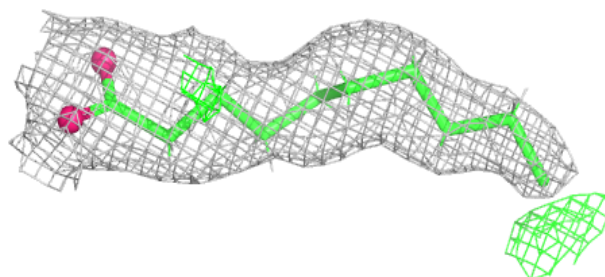


Electron density around PL9 a 409:

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

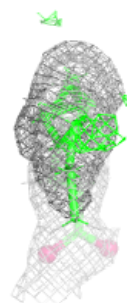
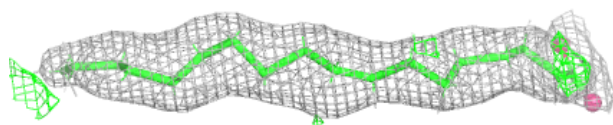
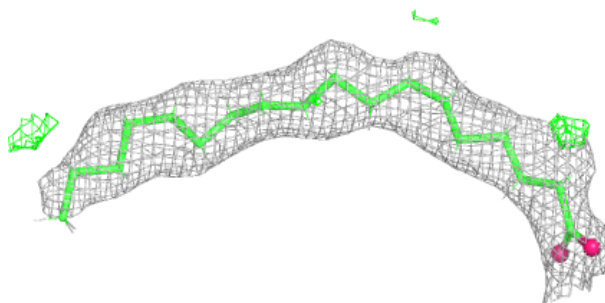
**Electron density around STE J 101:**

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

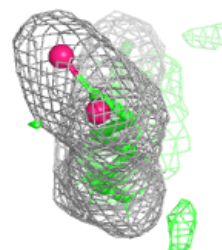
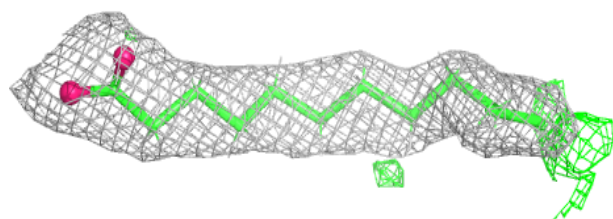
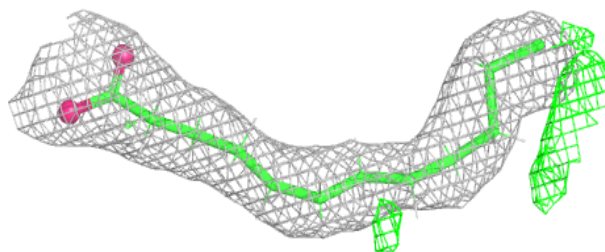


Electron density around STE X 101:

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

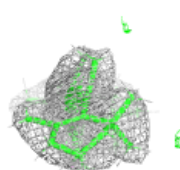
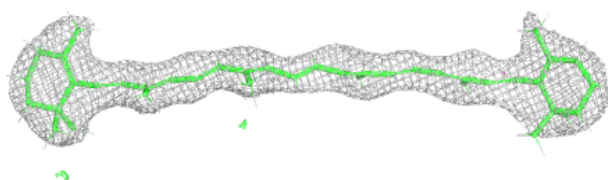
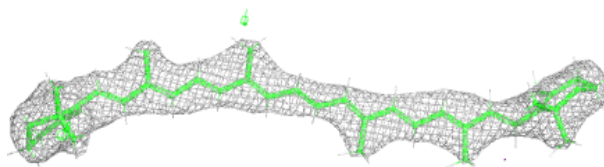
**Electron density around STE t 102:**

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

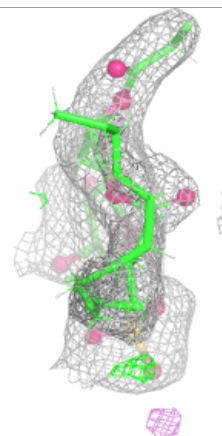
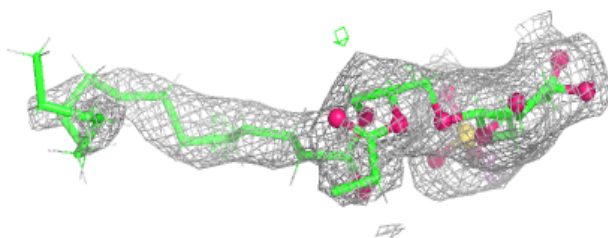
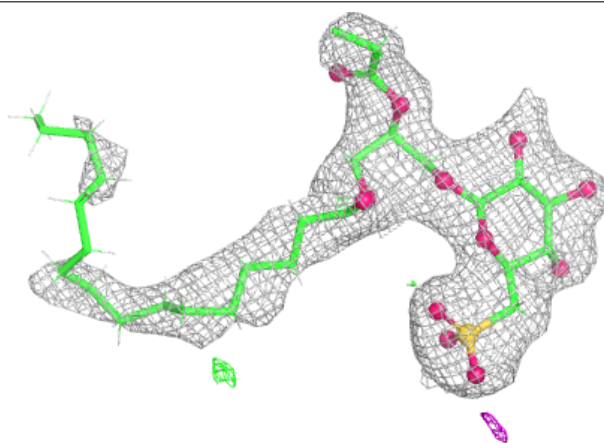


Electron density around BCR c 514:

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

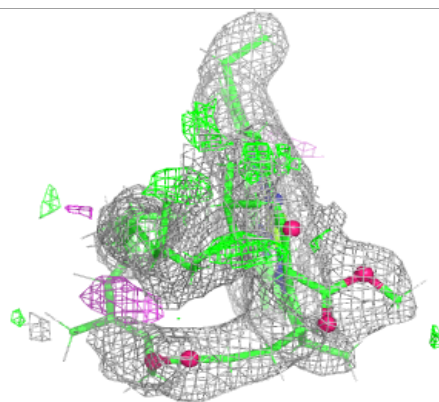
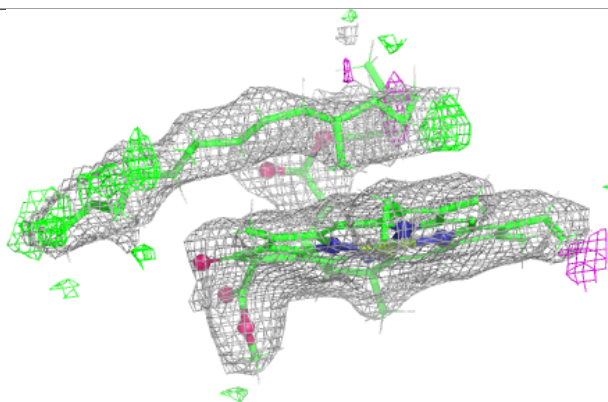
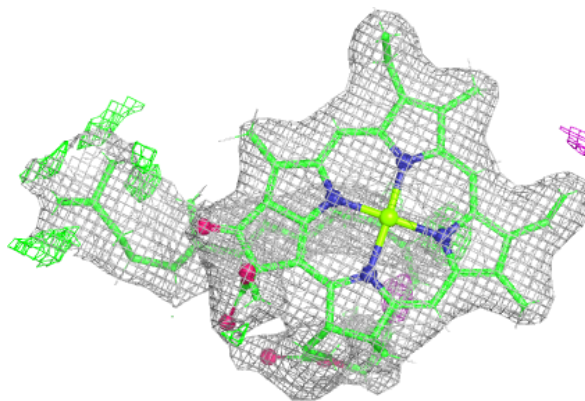
**Electron density around SQD f 101:**

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

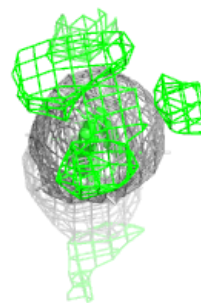
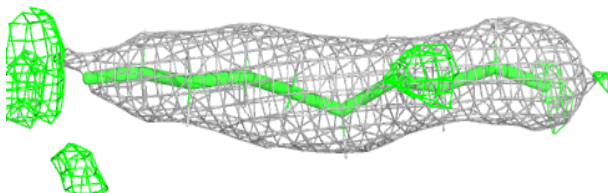
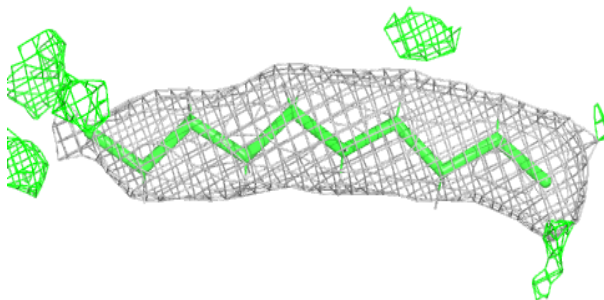


Electron density around CLA B 601:

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

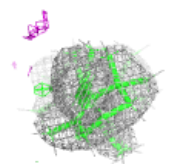
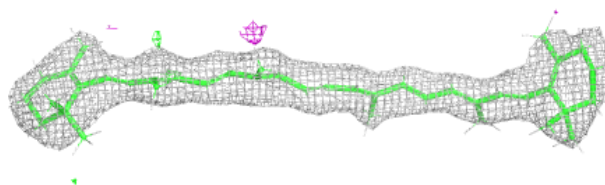
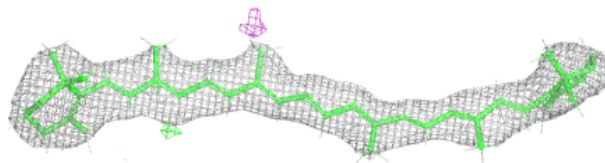
**Electron density around STE M 103:**

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

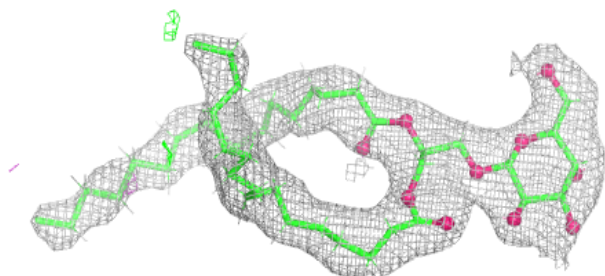
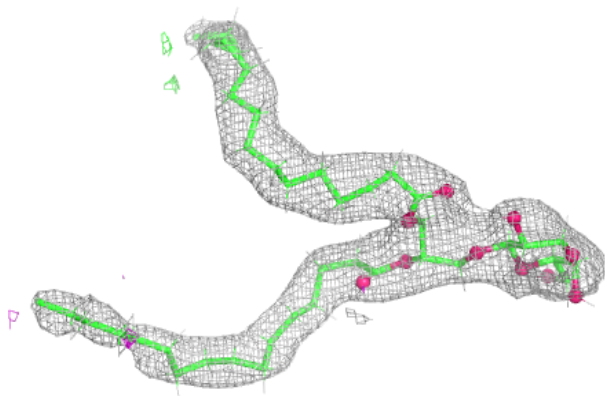


Electron density around BCR K 101:

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

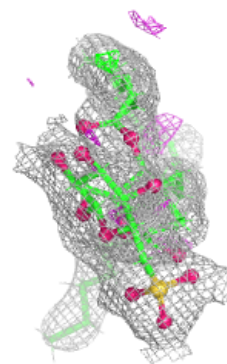
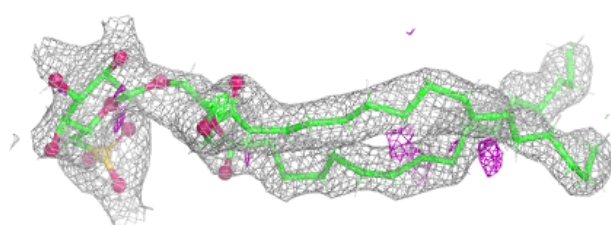
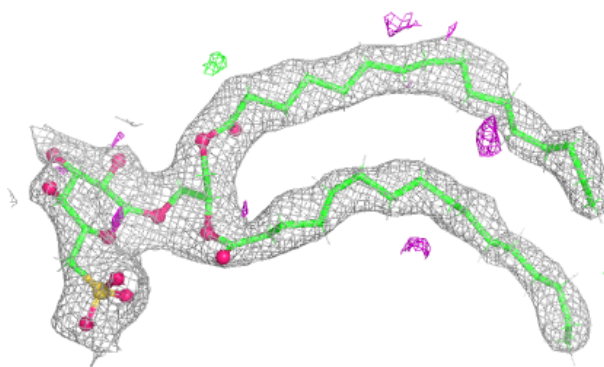
**Electron density around LMG b 622:**

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

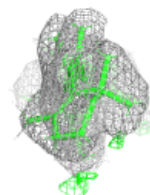
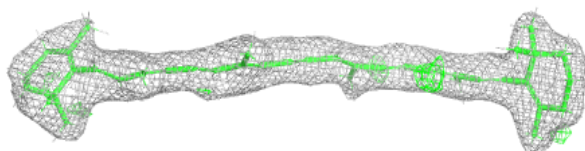
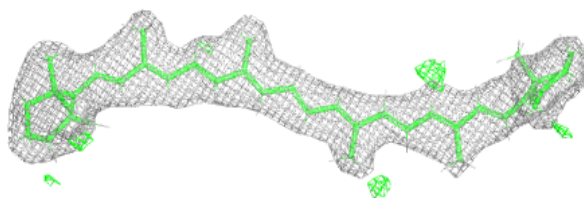


Electron density around SQD B 623:

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

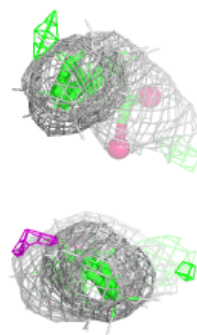
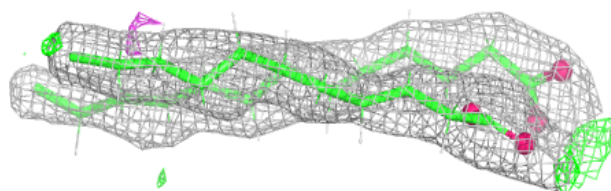
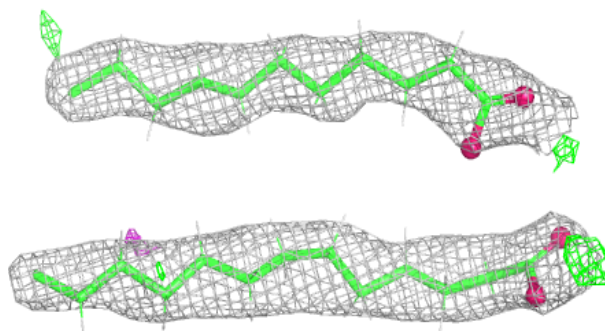
**Electron density around BCR Y 101:**

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

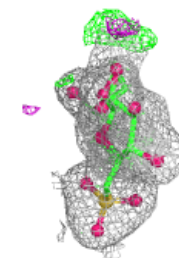
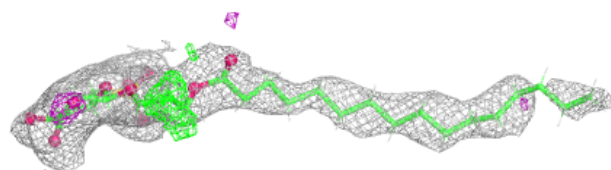
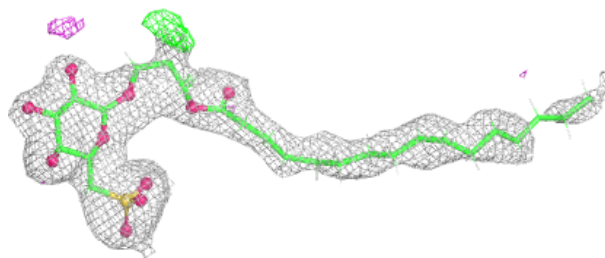


Electron density around LMG D 411:

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

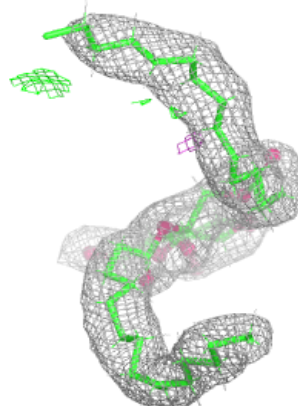
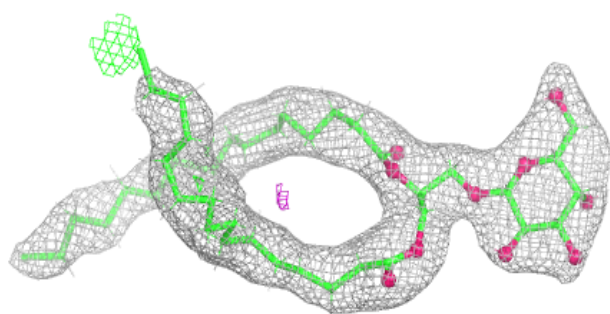
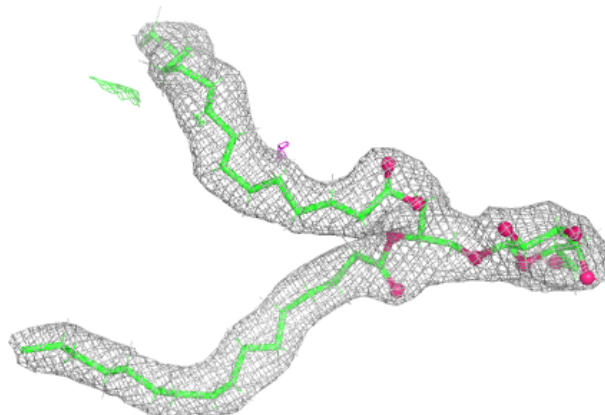
**Electron density around SQD D 407:**

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

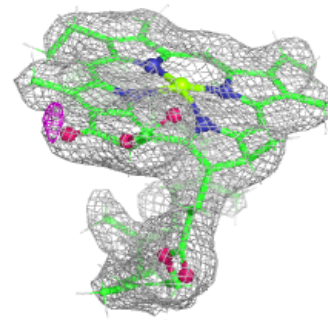
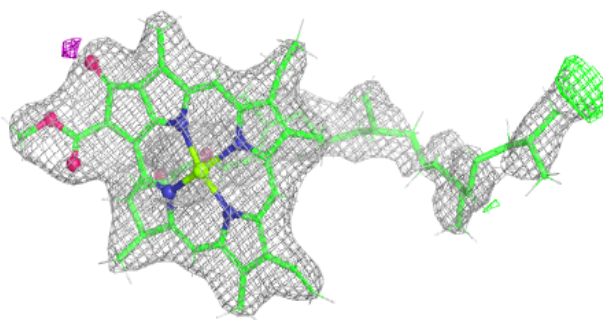
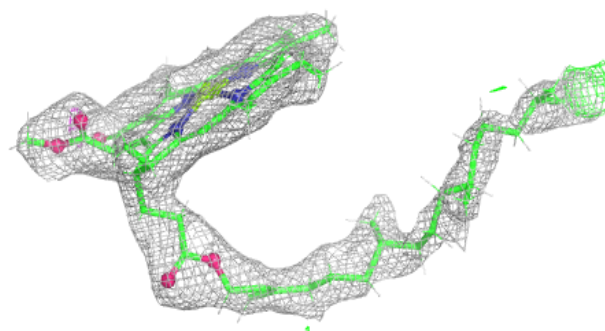


Electron density around LMG M 101:

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

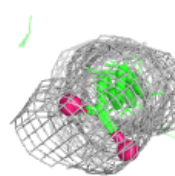
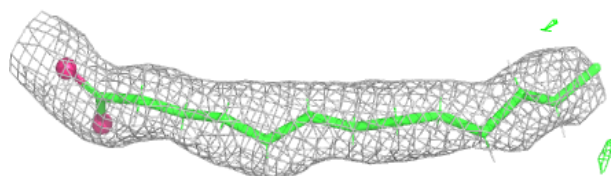
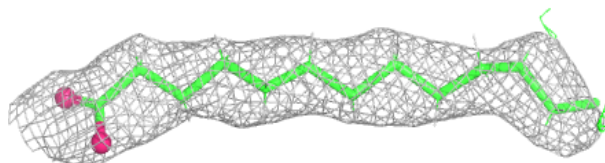
**Electron density around CLA C 513:**

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

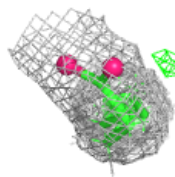
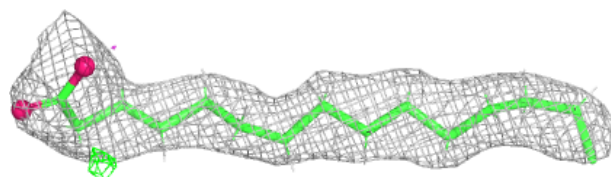
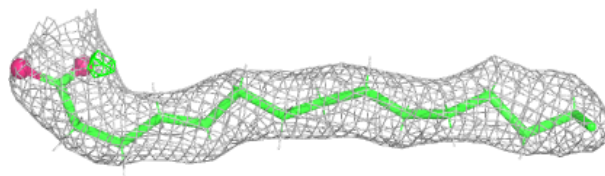


Electron density around STE M 102:

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

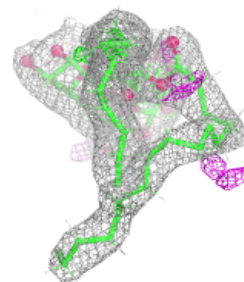
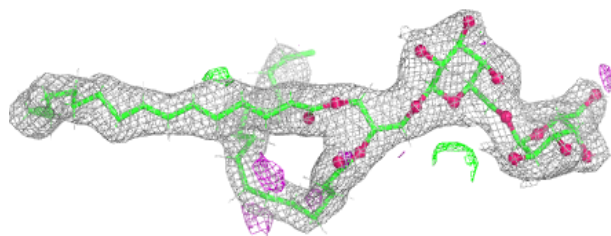
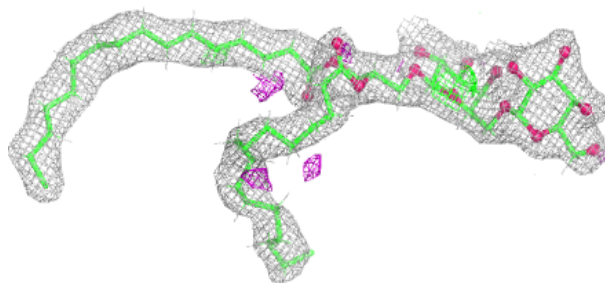
**Electron density around STE d 411:**

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



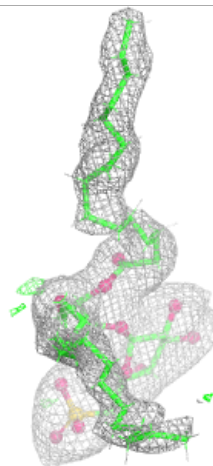
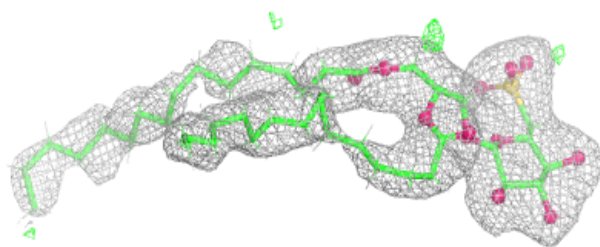
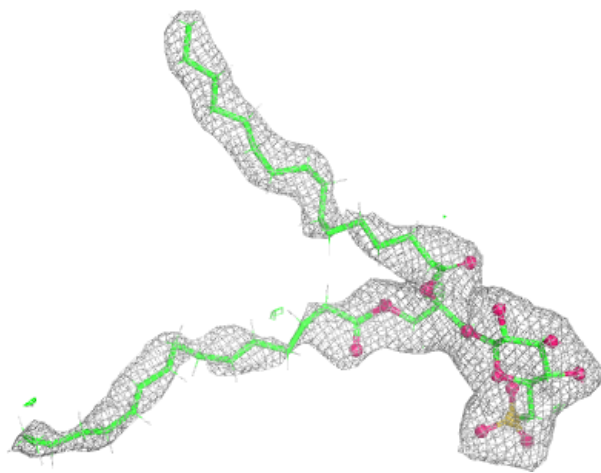
Electron density around DGD h 101:

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



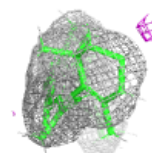
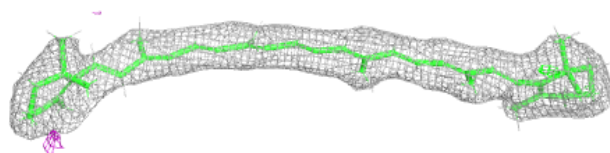
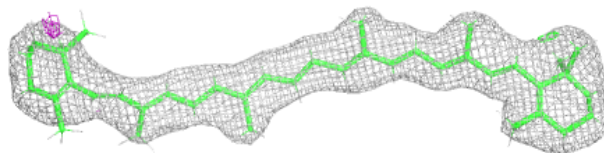
Electron density around SQD a 411:

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

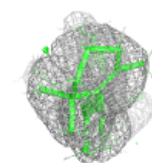
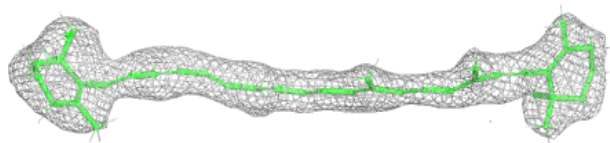


Electron density around BCR d 405:

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

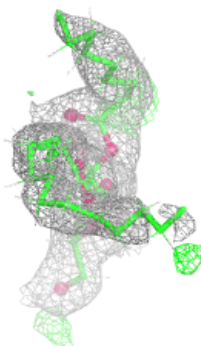
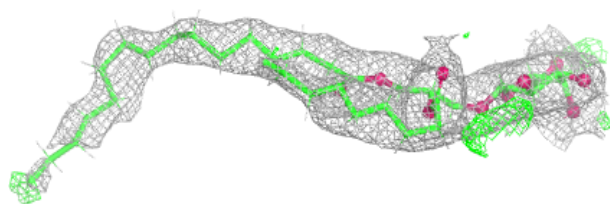
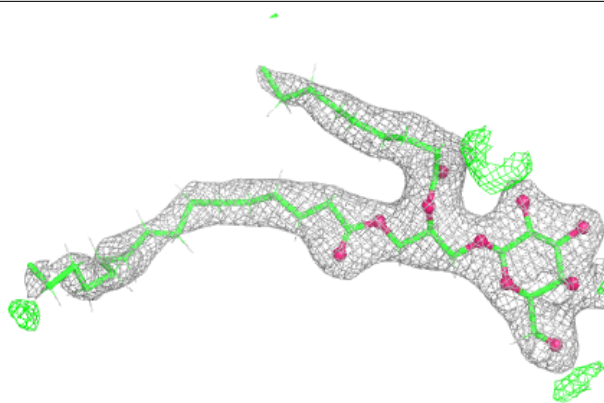
**Electron density around BCR k 101:**

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

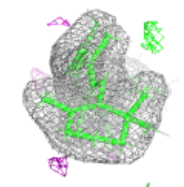
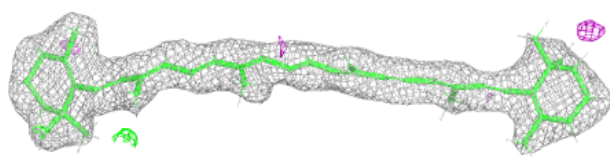
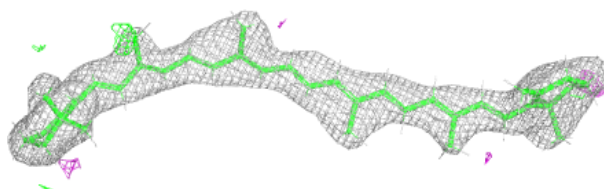


Electron density around LMG d 410:

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

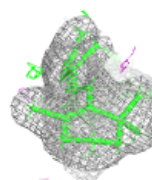
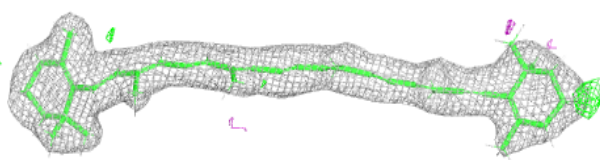
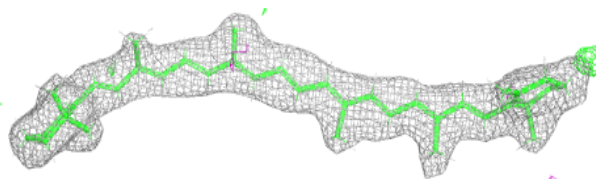
**Electron density around BCR x 101:**

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

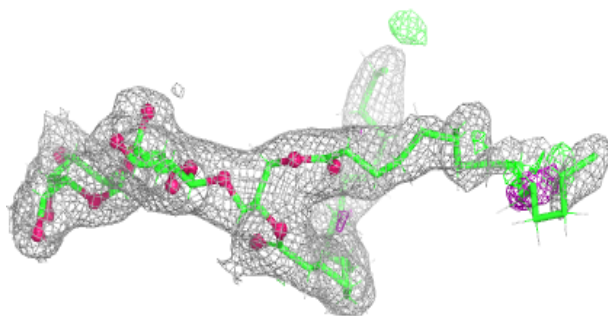
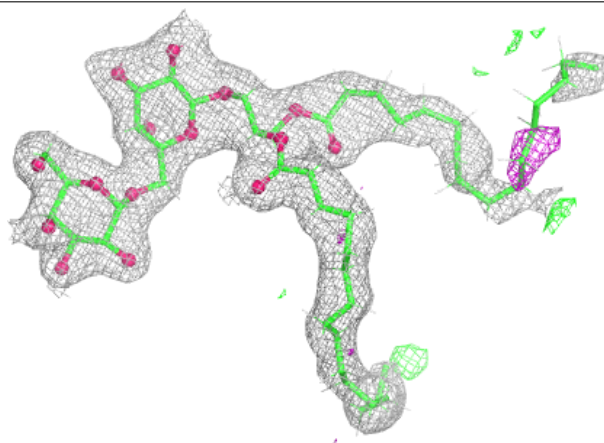


Electron density around BCR H 101:

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

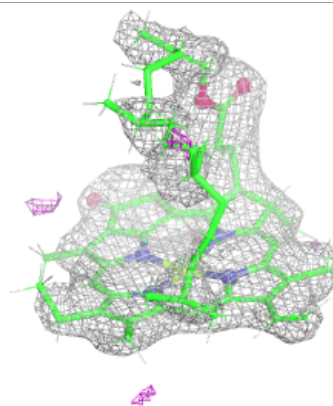
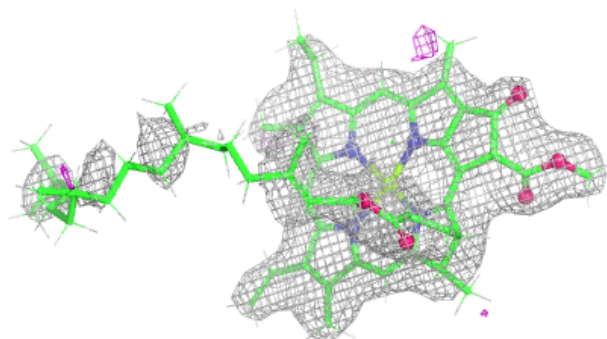
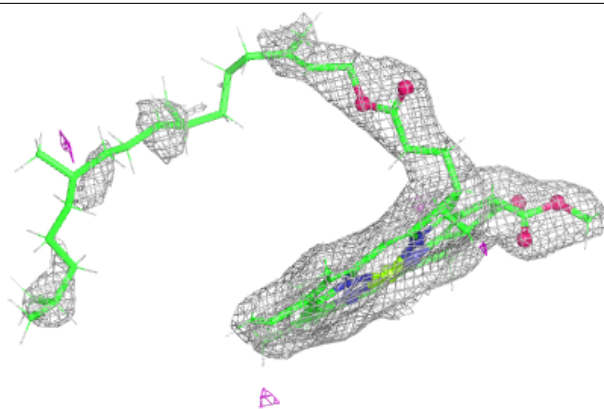
**Electron density around DGD C 516:**

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

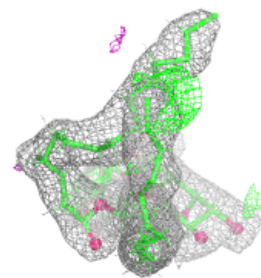
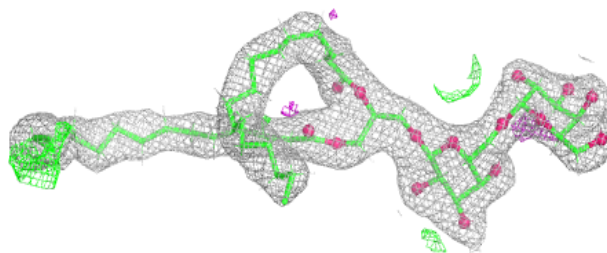
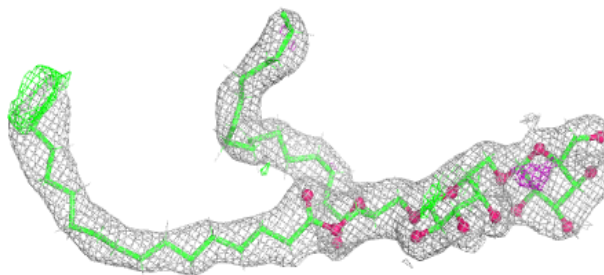


Electron density around CLA c 513:

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

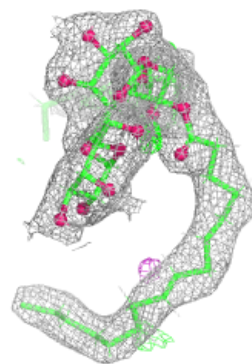
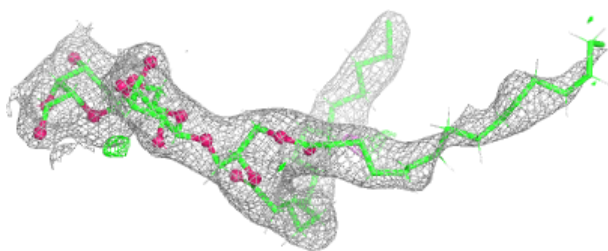
**Electron density around DGD H 102:**

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

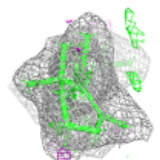
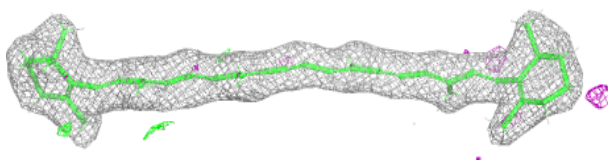
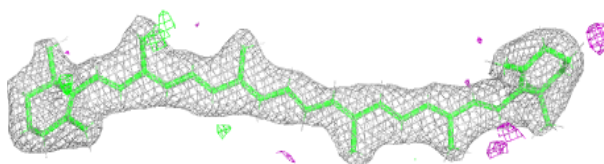


Electron density around DGD c 517:

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

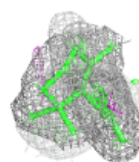
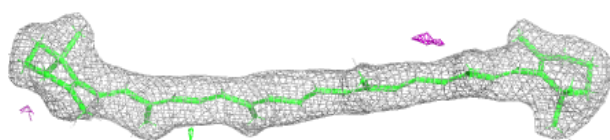
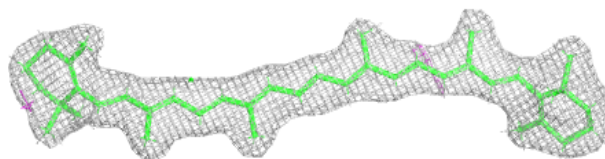
**Electron density around BCR B 618:**

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

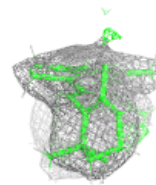
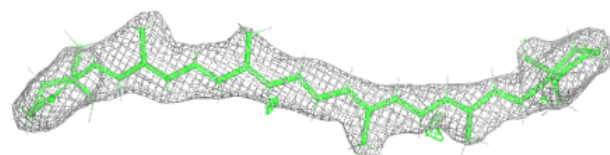
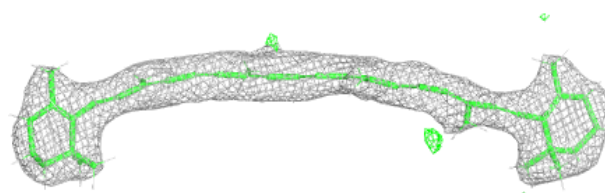


Electron density around BCR B 619:

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

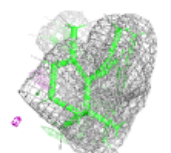
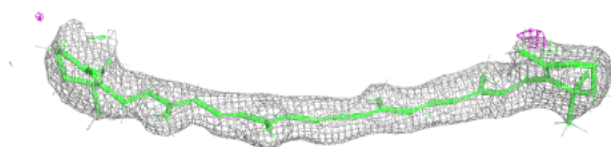
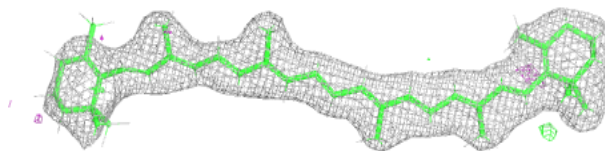
**Electron density around BCR k 102:**

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



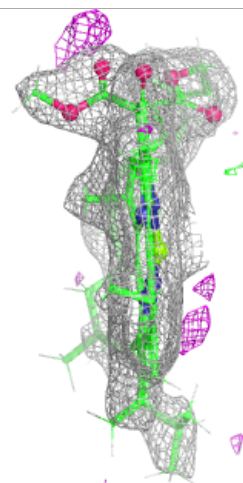
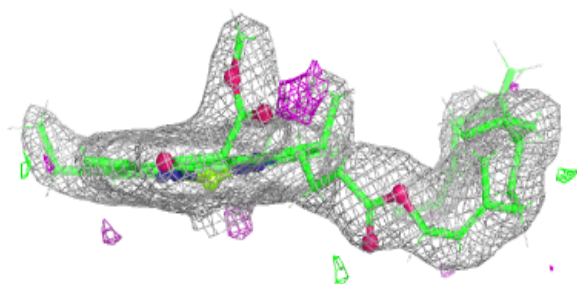
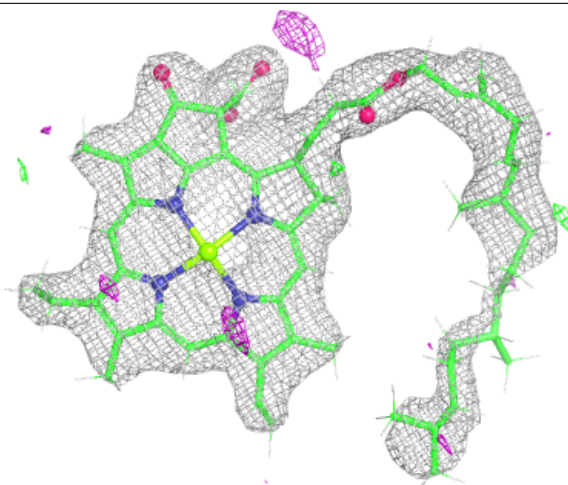
Electron density around BCR D 404:

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



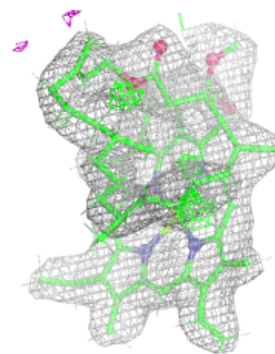
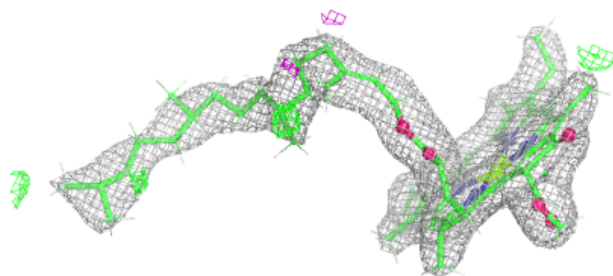
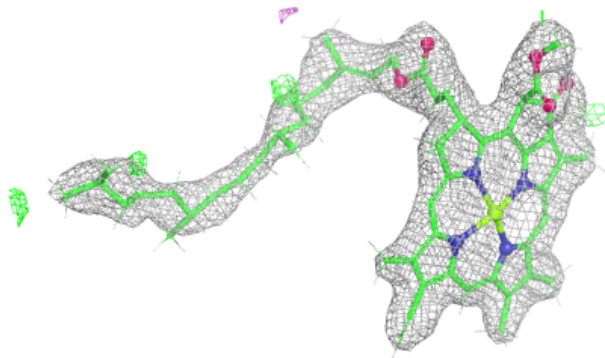
Electron density around CLA C 512:

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



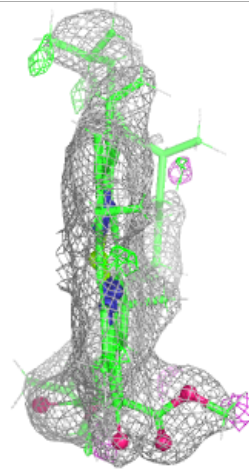
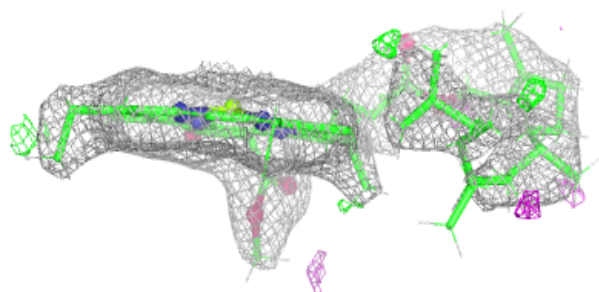
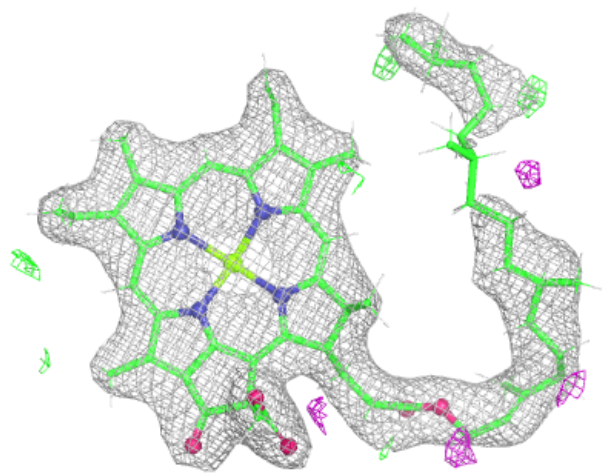
Electron density around CLA c 511:

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



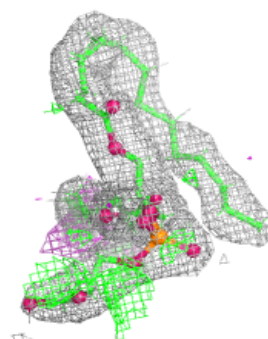
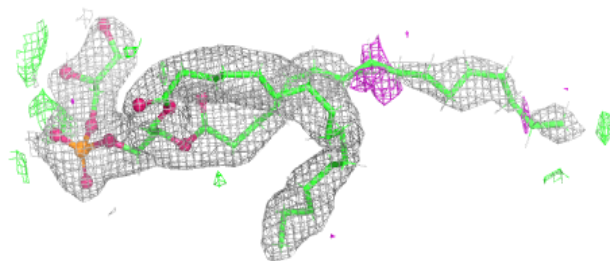
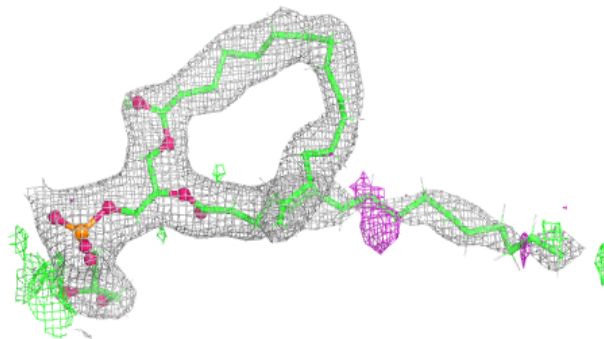
Electron density around CLA c 512:

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

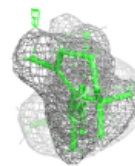
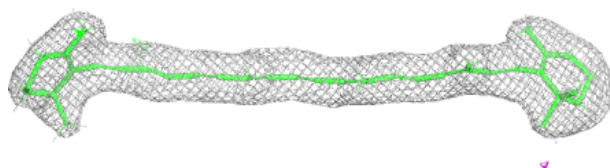
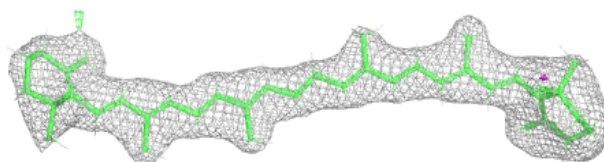


Electron density around LHG d 407:

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

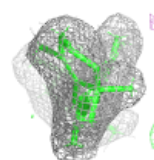
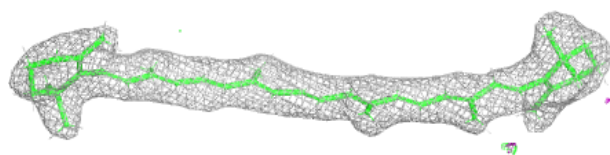
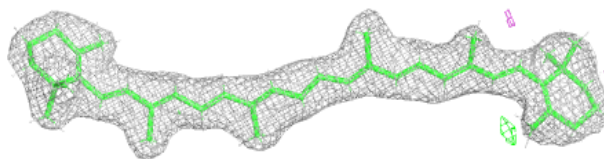
**Electron density around BCR b 618:**

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

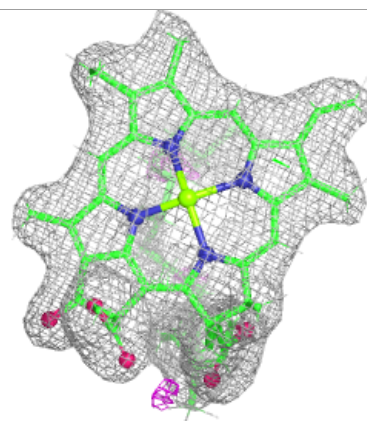
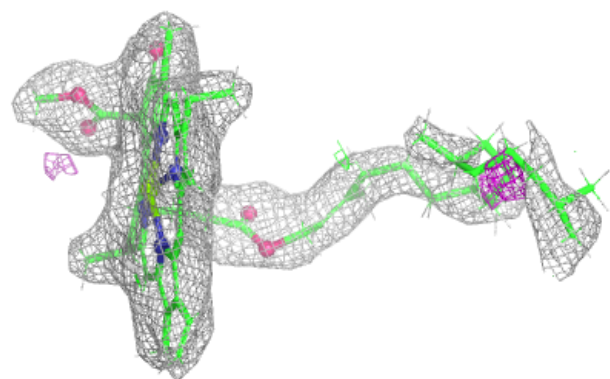
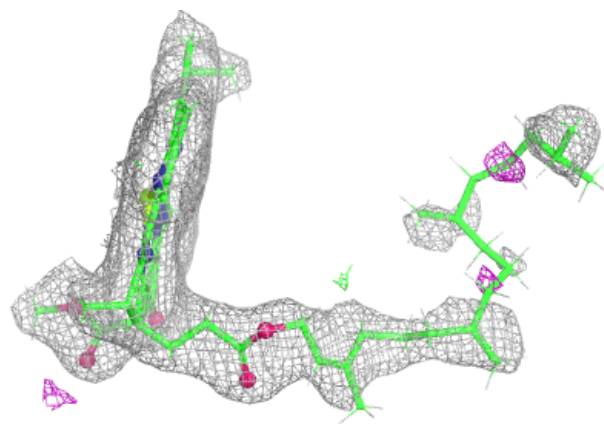


Electron density around BCR b 619:

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

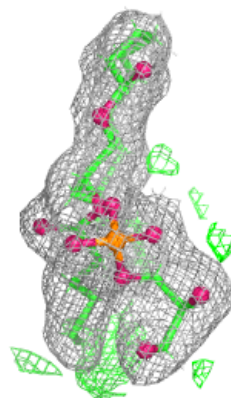
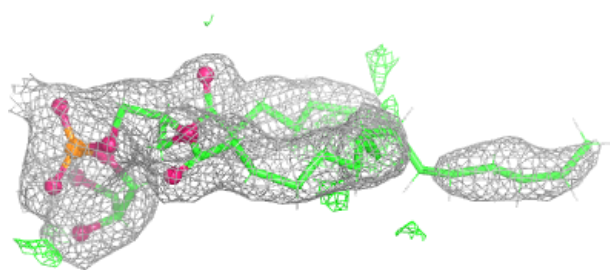
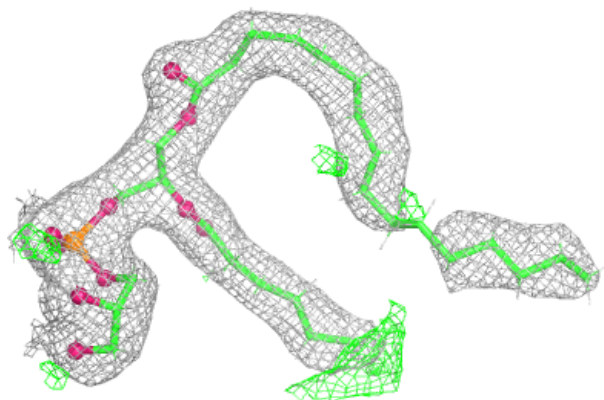
**Electron density around CLA c 506:**

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

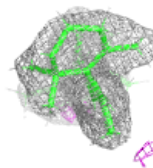
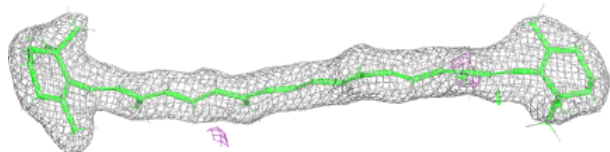
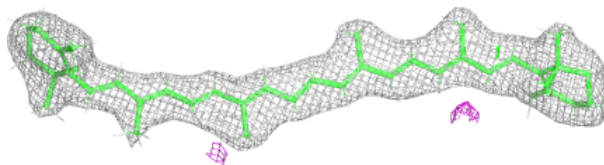


Electron density around LHG d 409:

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

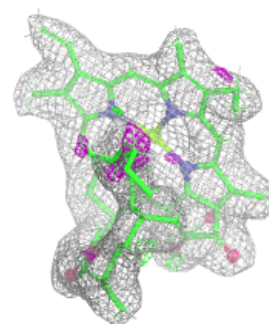
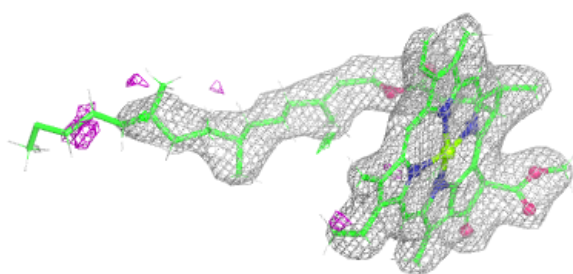
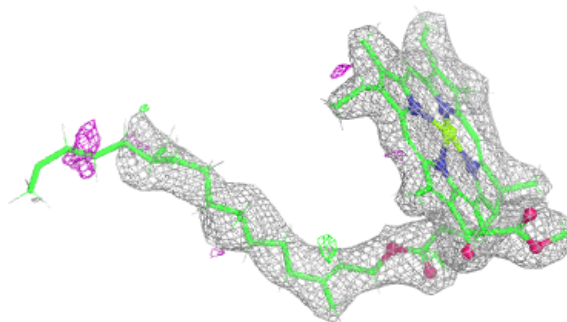
**Electron density around BCR C 514:**

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

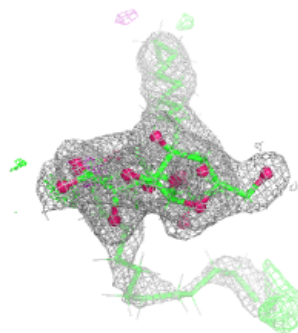
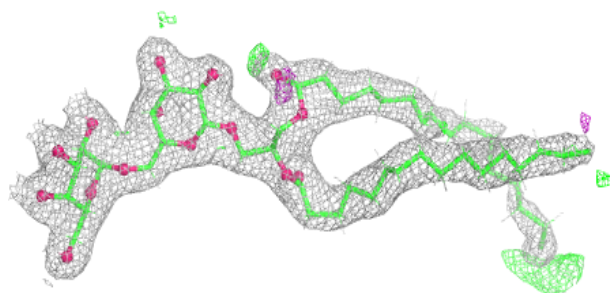
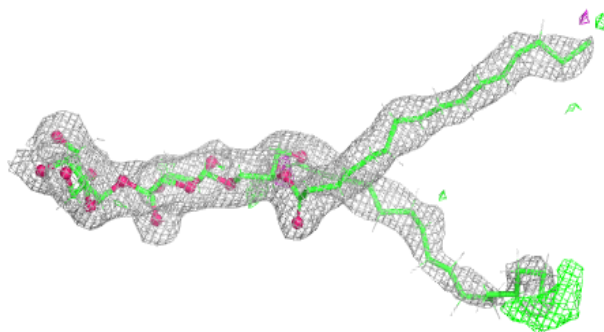


Electron density around CLA c 508:

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

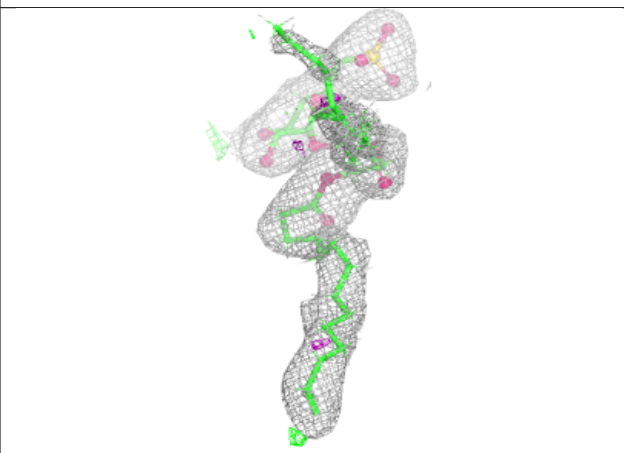
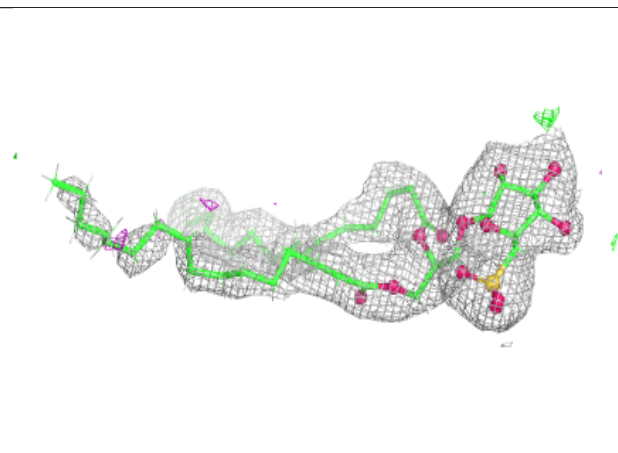
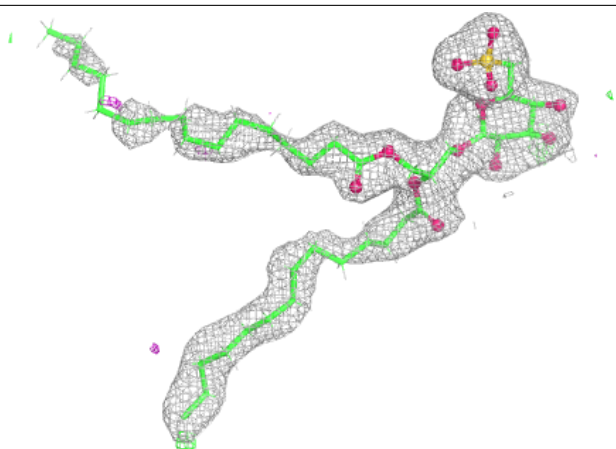
**Electron density around DGD C 515:**

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

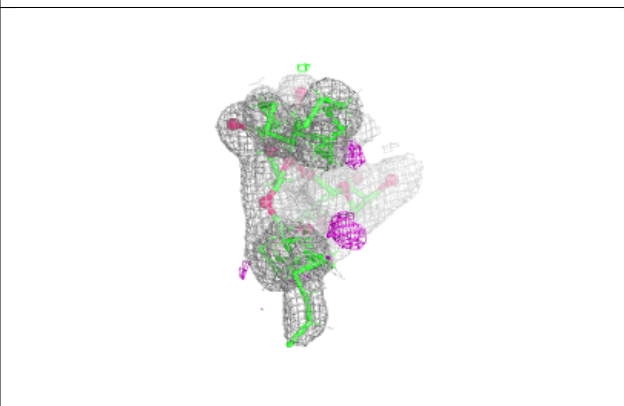
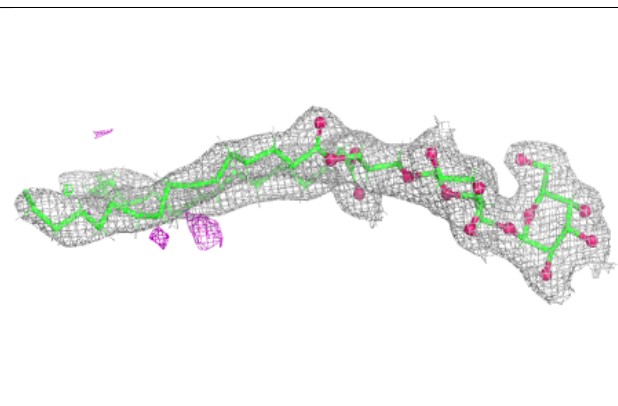
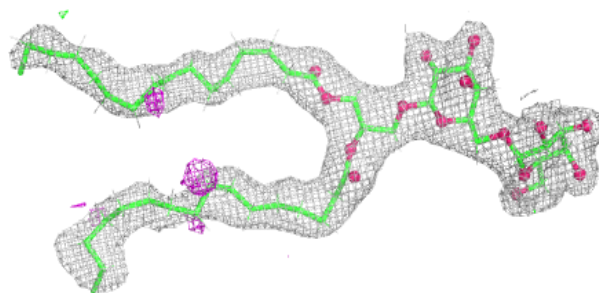


Electron density around SQD A 413:

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

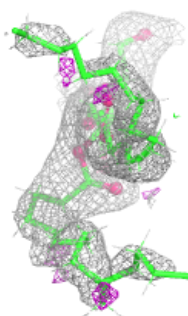
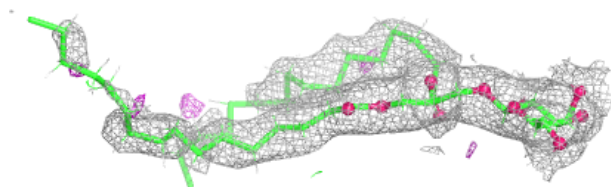
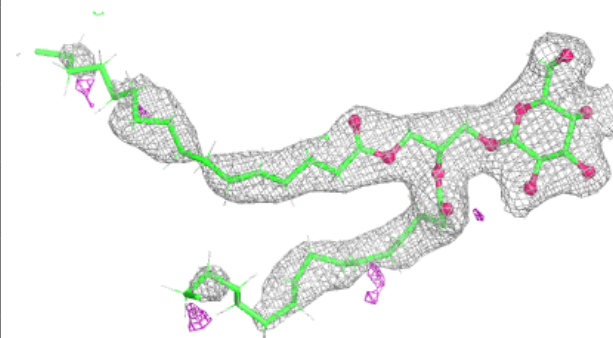
**Electron density around DGD C 517:**

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

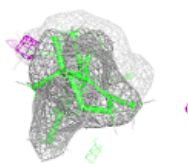
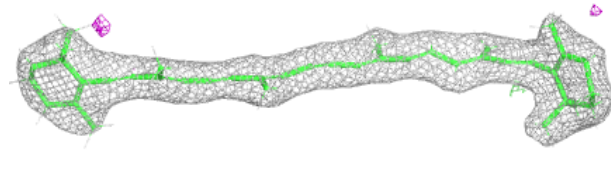
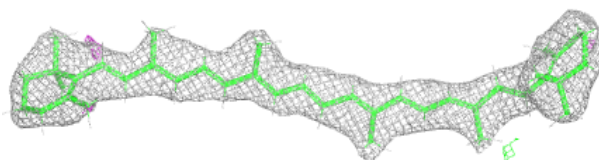


Electron density around LMG D 406:

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

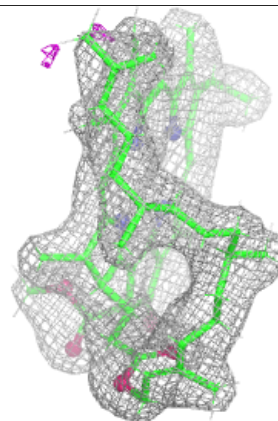
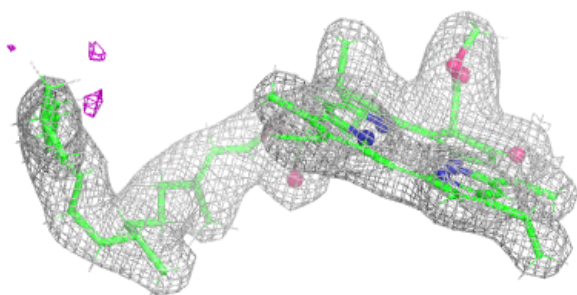
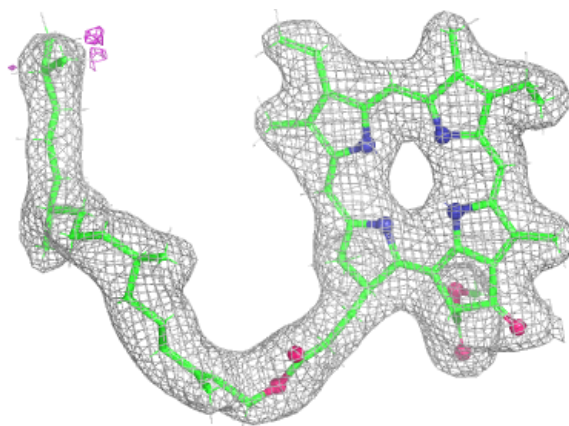
**Electron density around BCR c 515:**

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

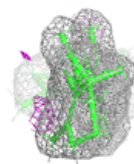
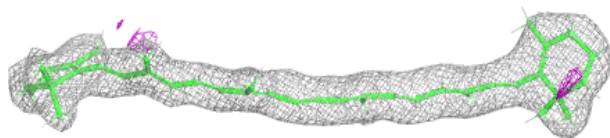
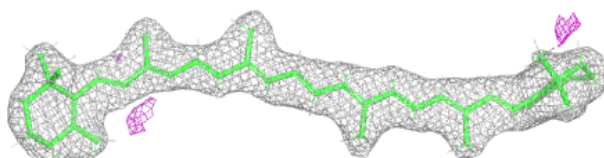


Electron density around PHO d 402:

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

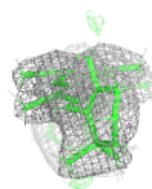
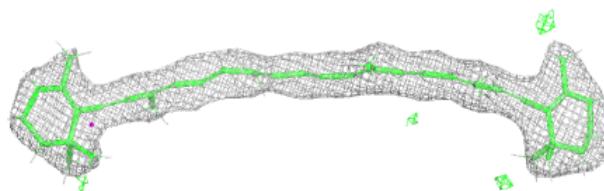
**Electron density around BCR B 617:**

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

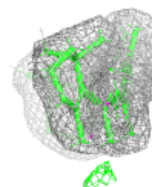
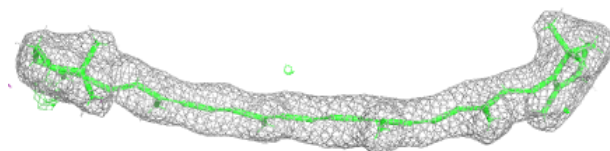
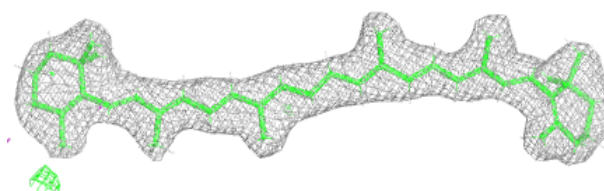


Electron density around BCR K 102:

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

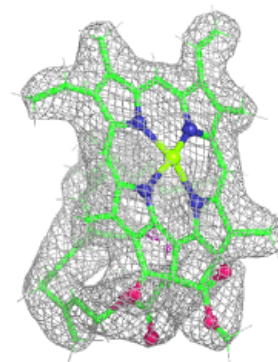
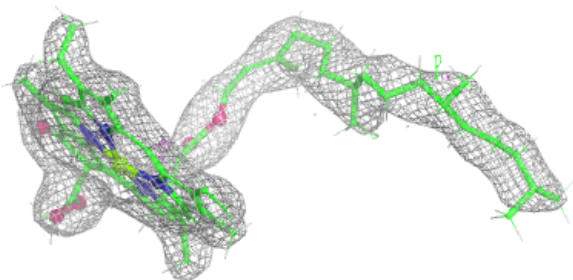
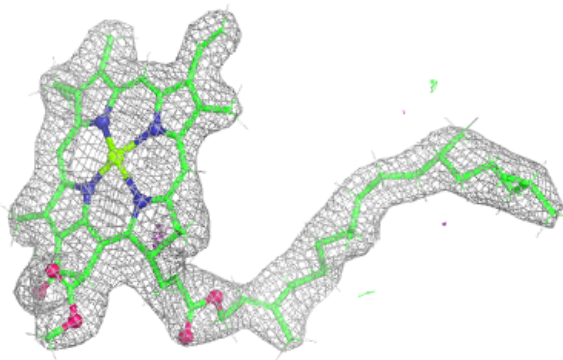
**Electron density around BCR T 101:**

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

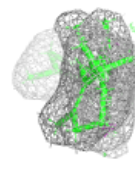
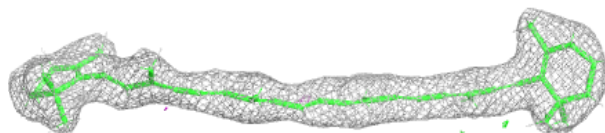
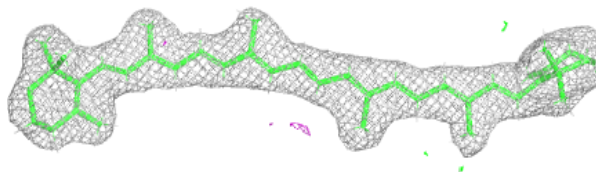


Electron density around CLA C 511:

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

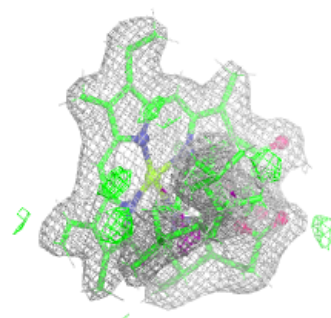
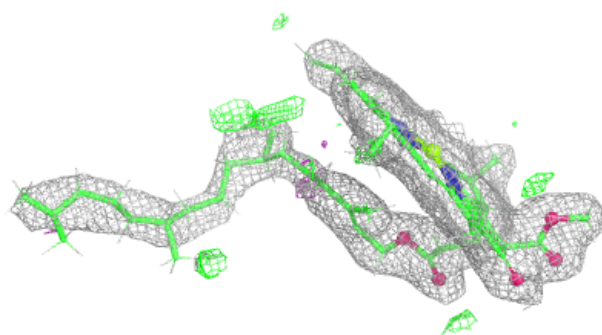
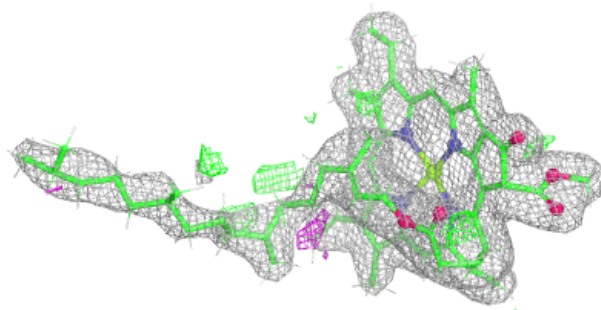
**Electron density around BCR b 617:**

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

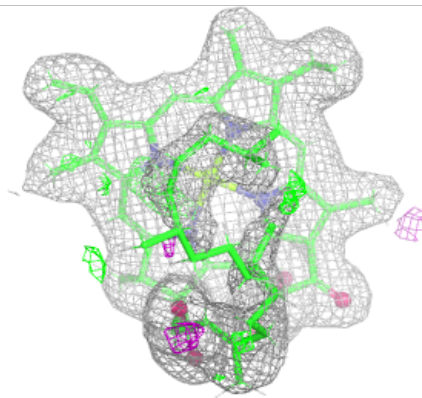
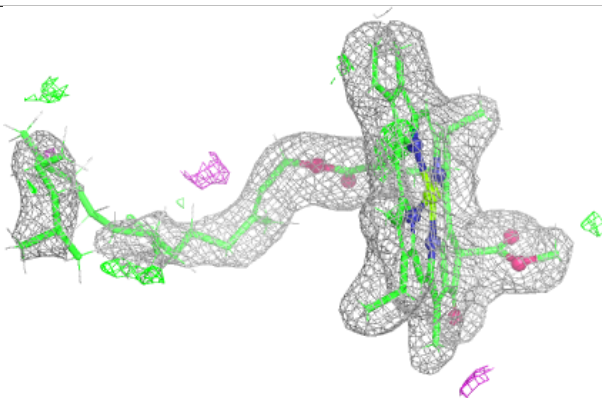
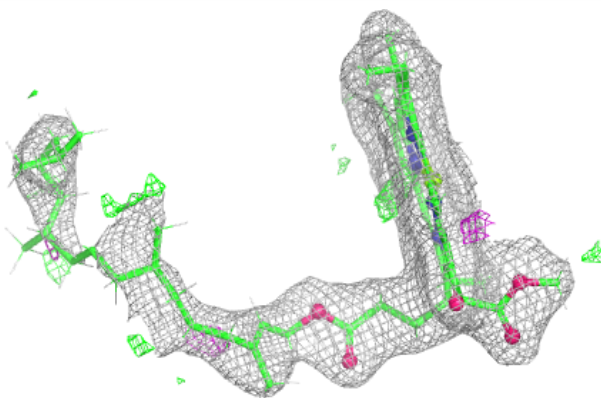


Electron density around CLA C 505:

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

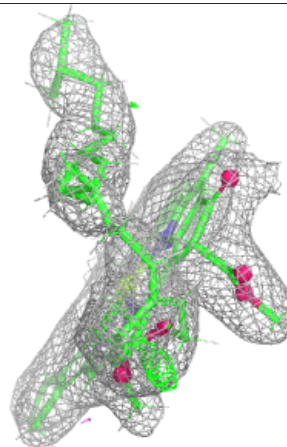
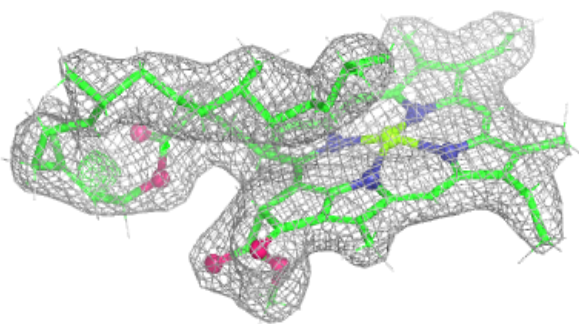
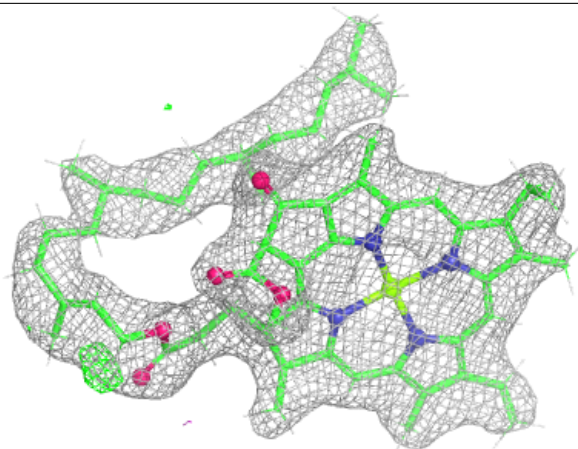
**Electron density around CLA C 506:**

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



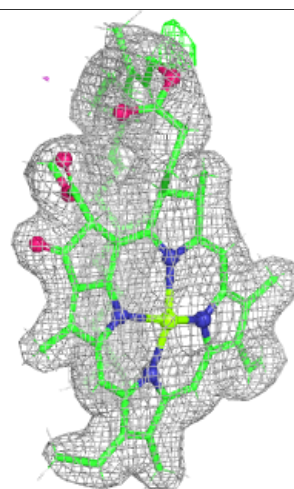
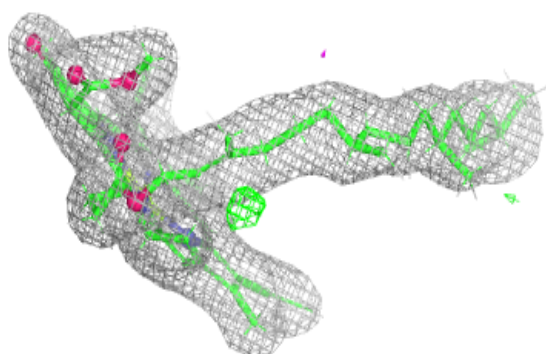
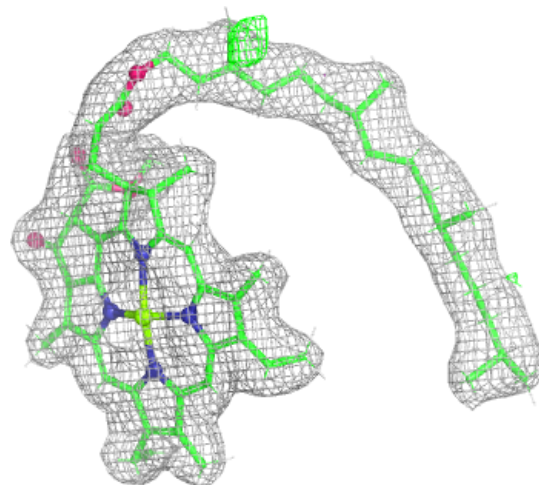
Electron density around CLA c 509:

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



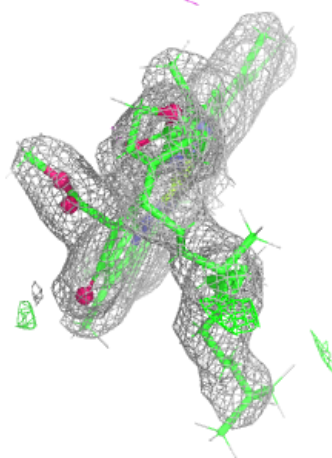
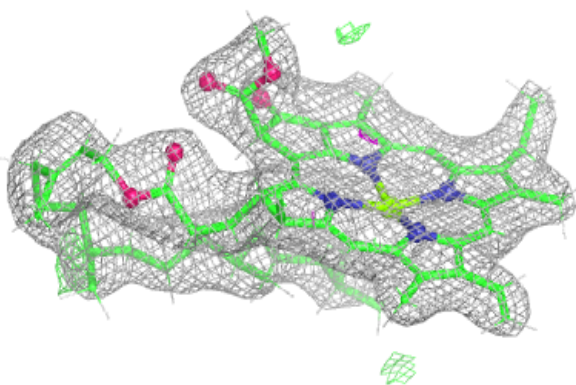
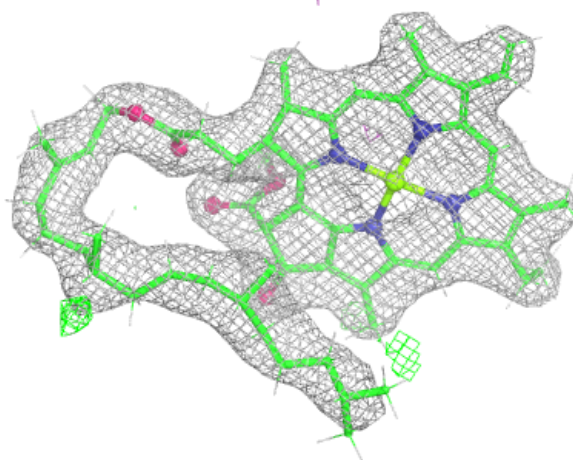
Electron density around CLA C 507:

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



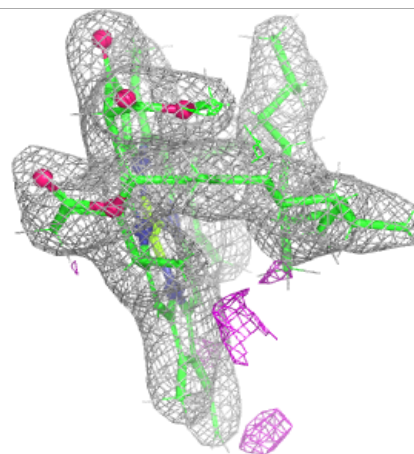
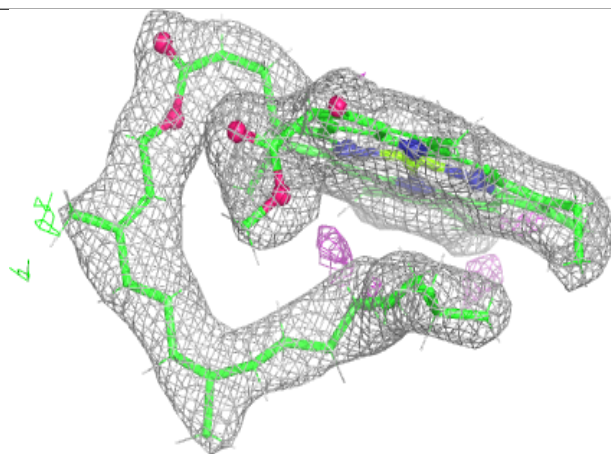
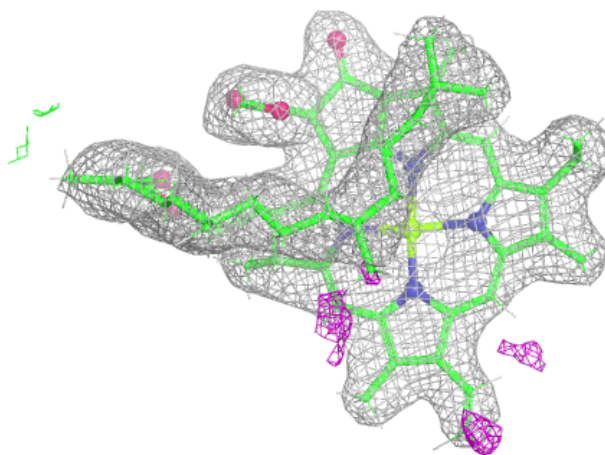
Electron density around CLA C 509:

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



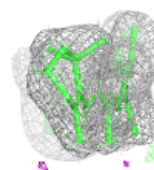
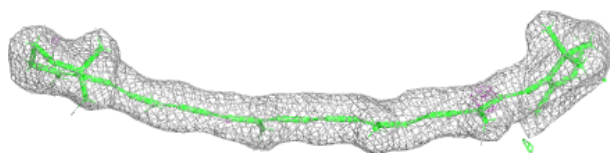
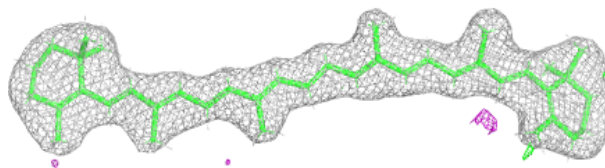
Electron density around CLA C 510:

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

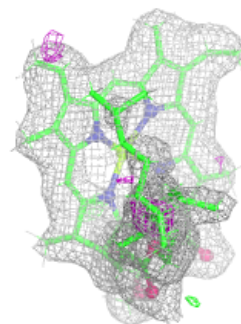
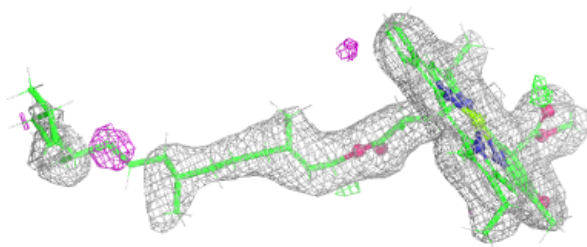
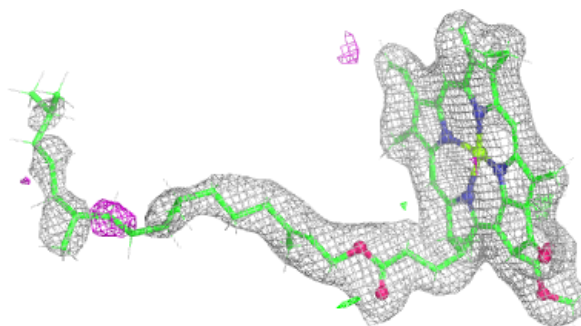


Electron density around BCR t 101:

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

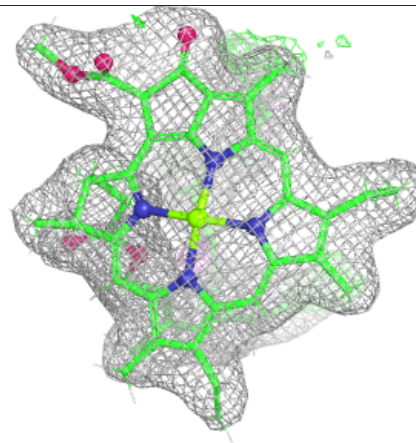
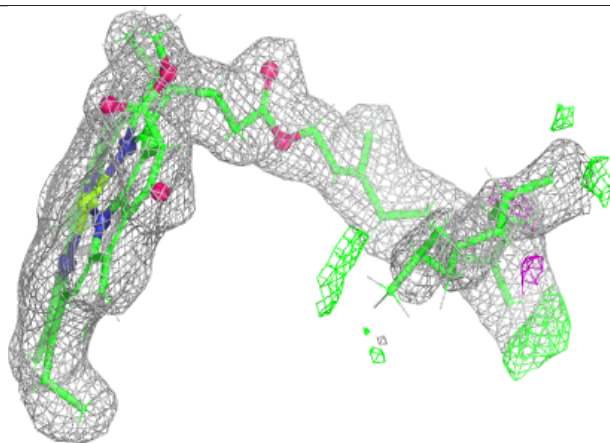
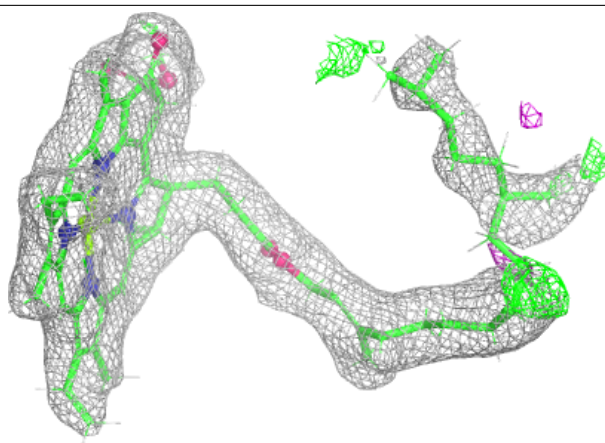
**Electron density around CLA d 404:**

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

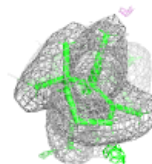
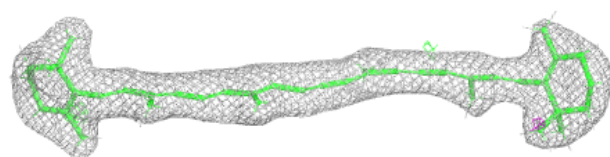
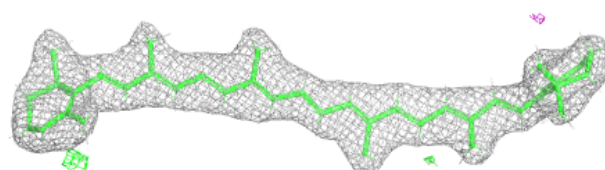


Electron density around CLA B 606:

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

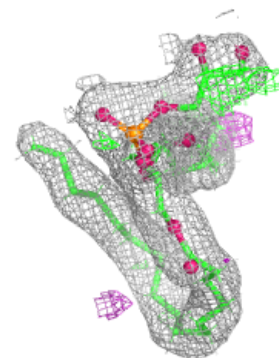
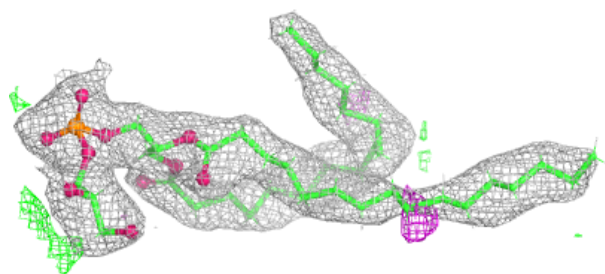
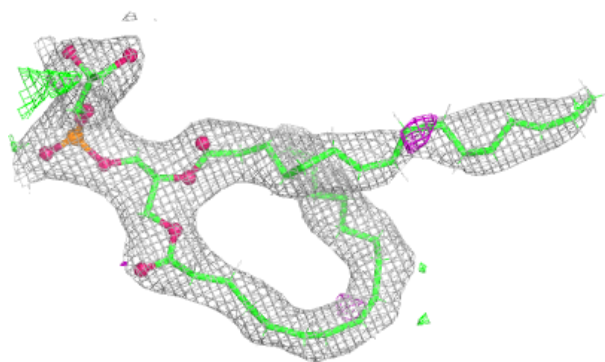
**Electron density around BCR A 406:**

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

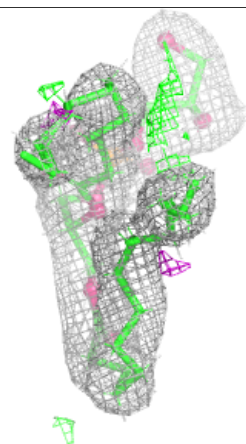
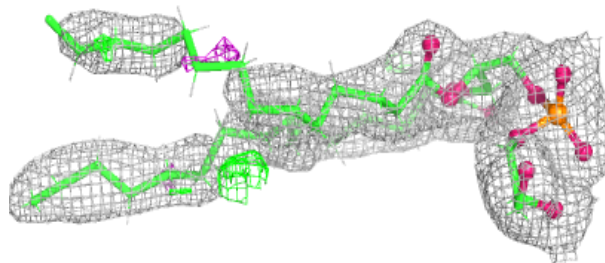
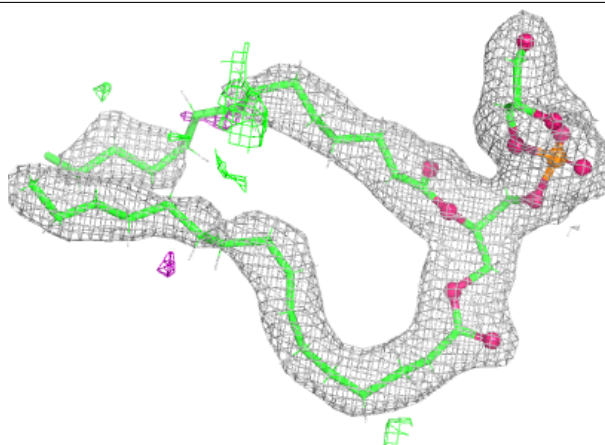


Electron density around LHG B 622:

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

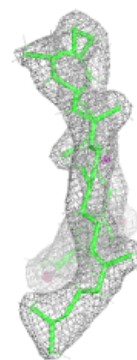
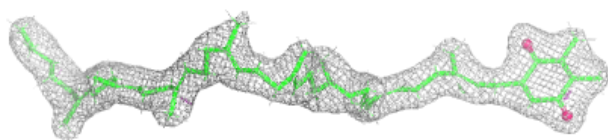
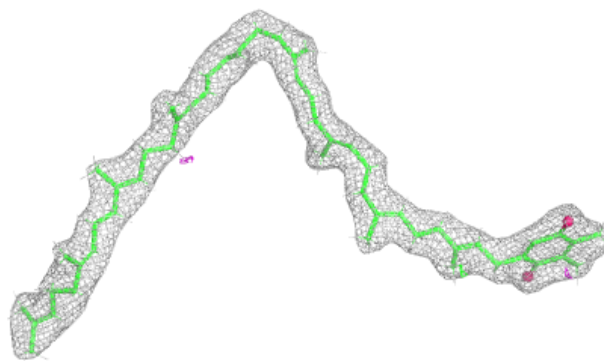
**Electron density around LHG D 409:**

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

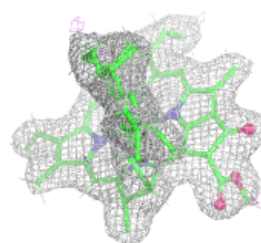
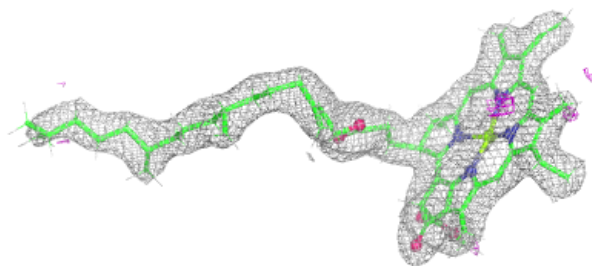
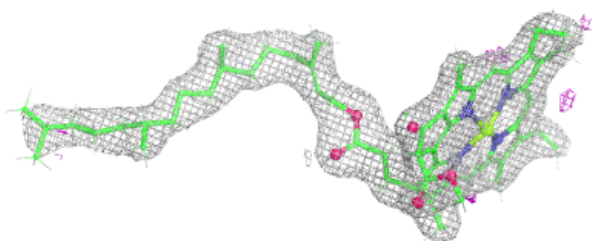


Electron density around PL9 D 405:

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

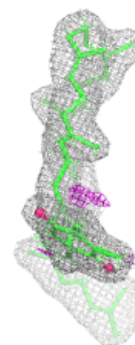
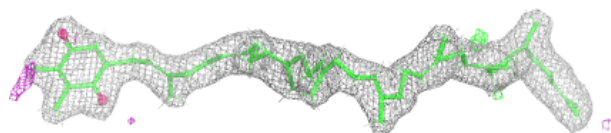
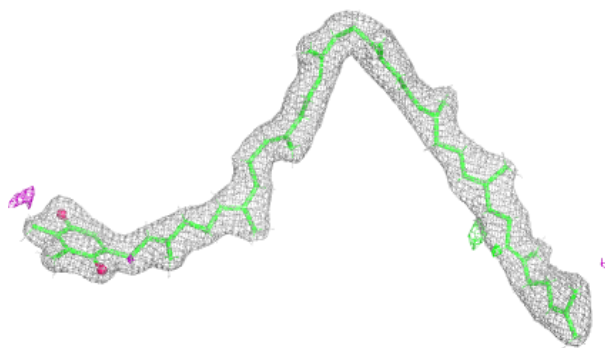
**Electron density around CLA C 502:**

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



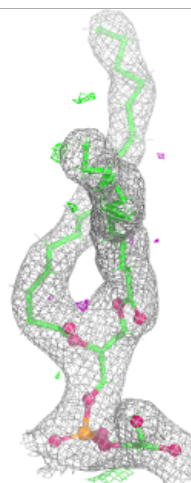
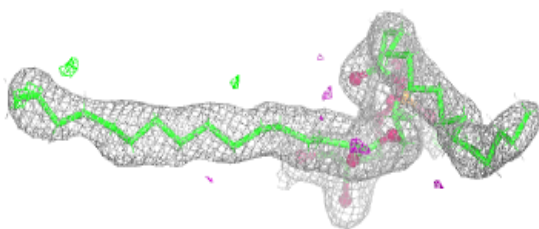
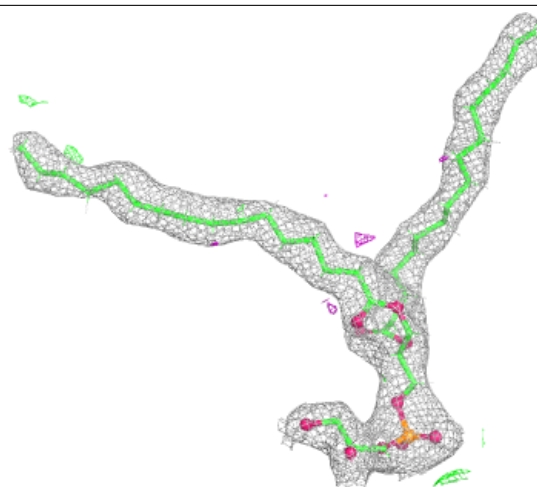
Electron density around PL9 d 406:

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



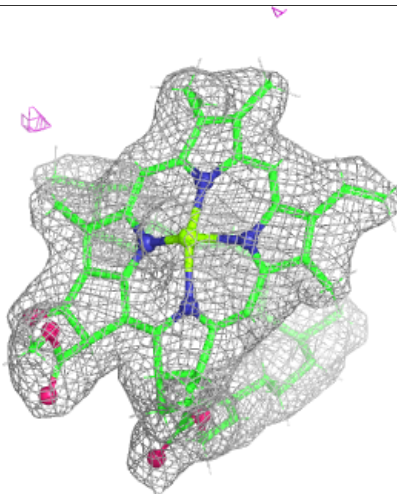
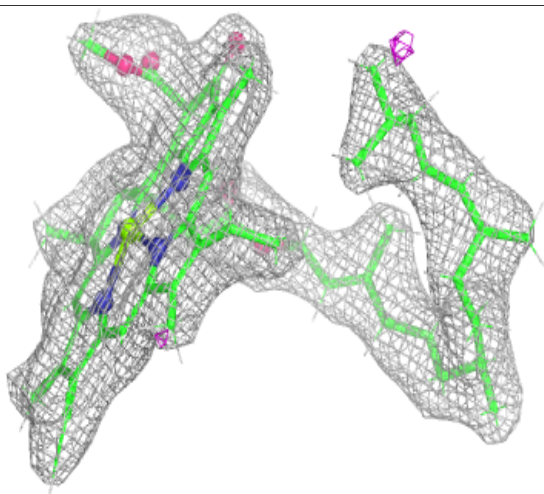
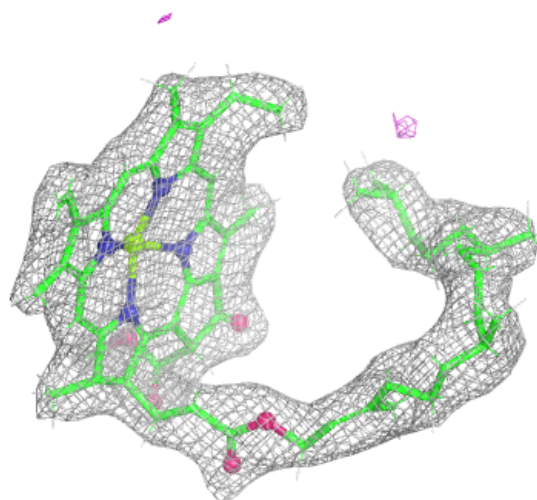
Electron density around LHG 1 101:

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



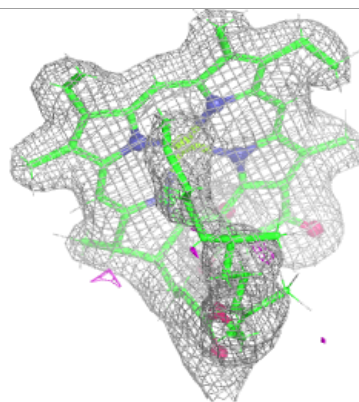
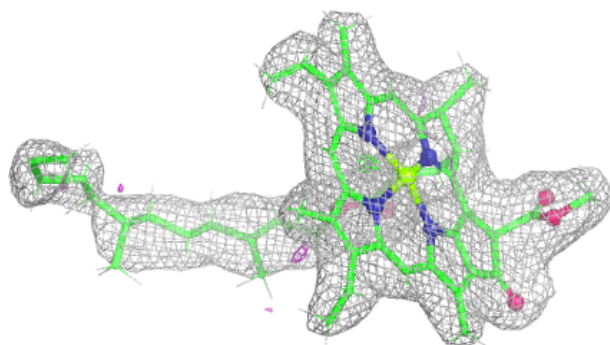
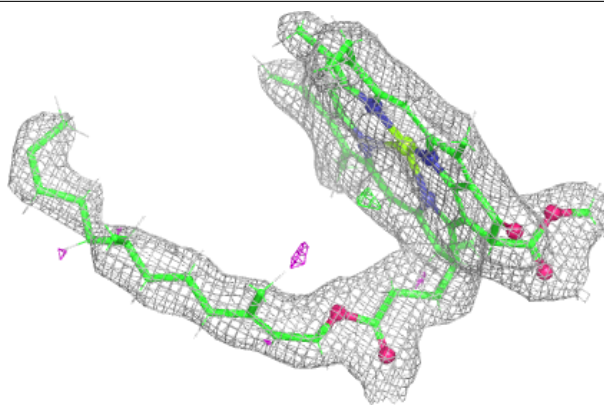
Electron density around CLA C 503:

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

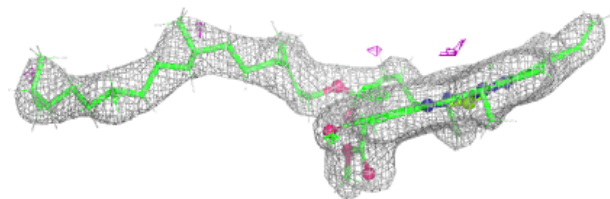
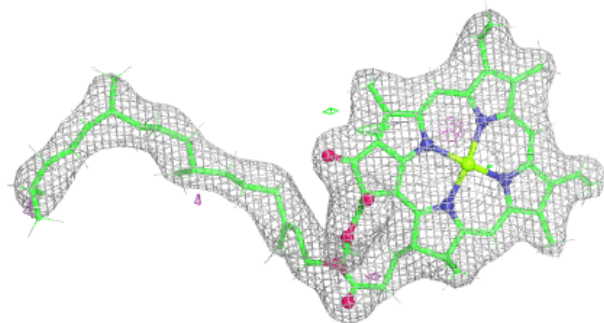


Electron density around CLA C 504:

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

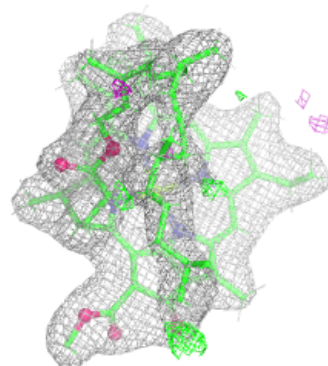
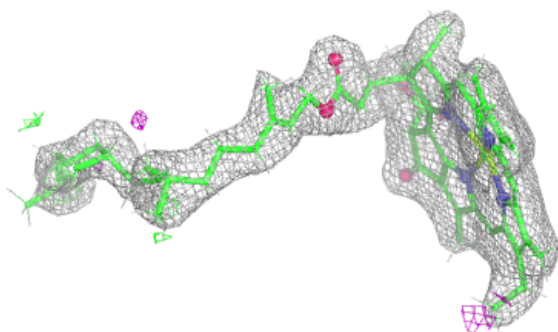
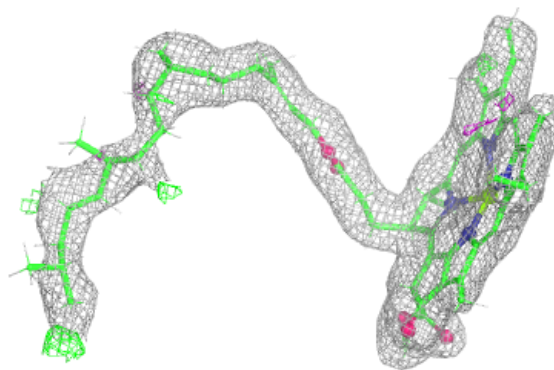
**Electron density around CLA b 602:**

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

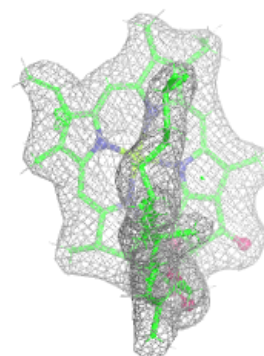
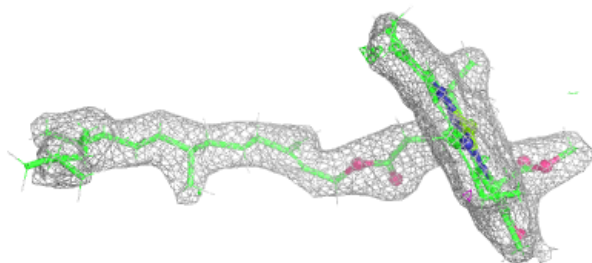
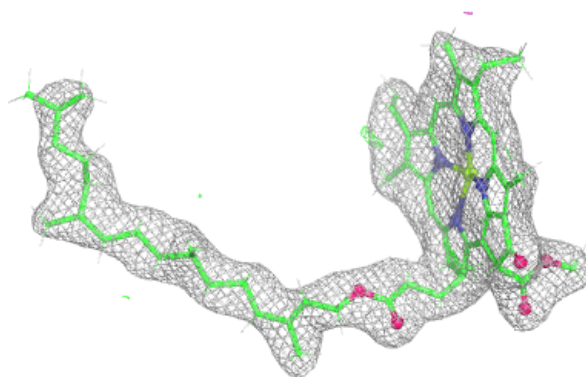


Electron density around CLA b 606:

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

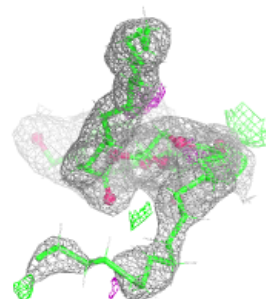
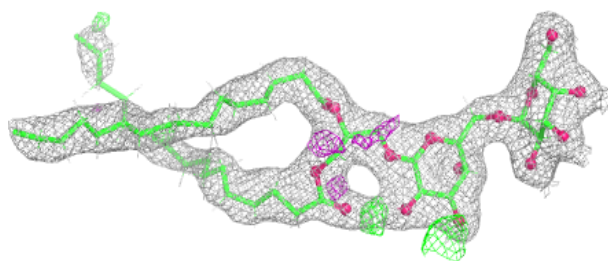
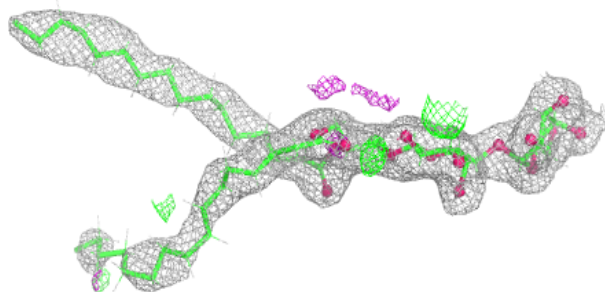
**Electron density around CLA b 609:**

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

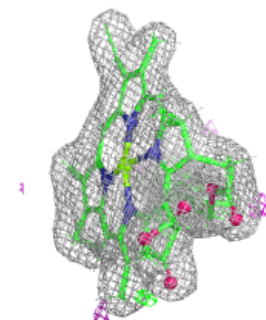
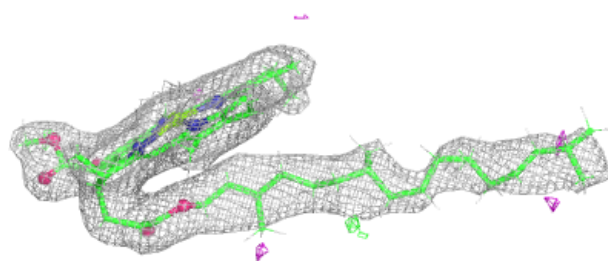
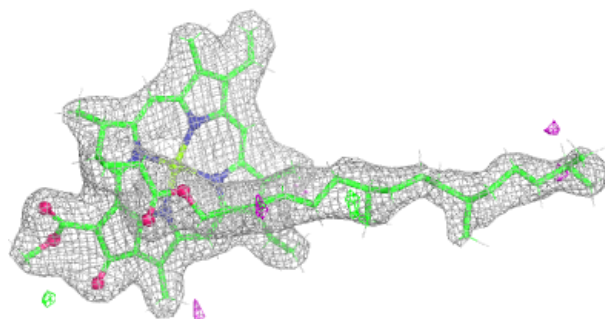


Electron density around DGD c 516:

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

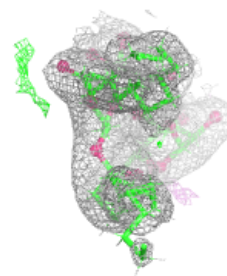
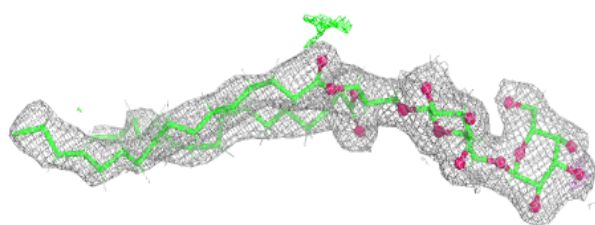
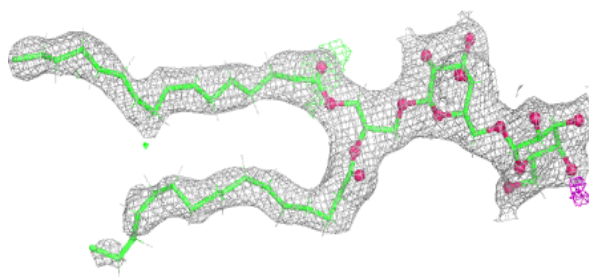
**Electron density around CLA b 614:**

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



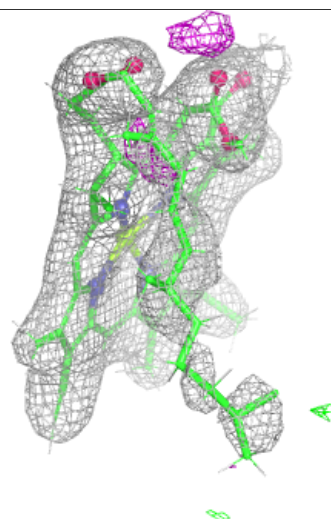
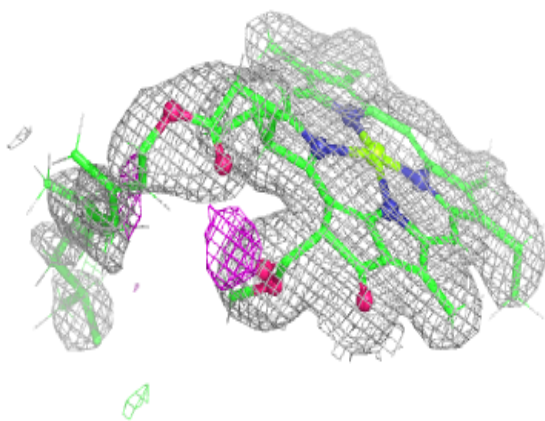
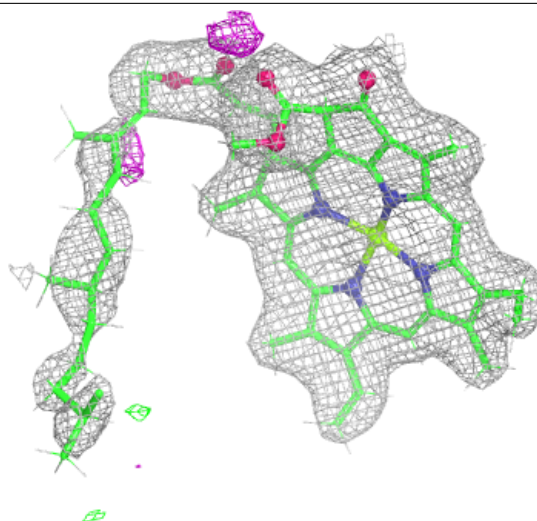
Electron density around DGD c 518:

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



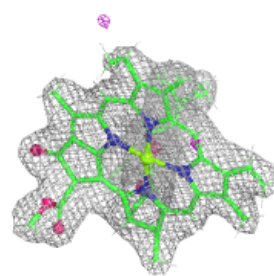
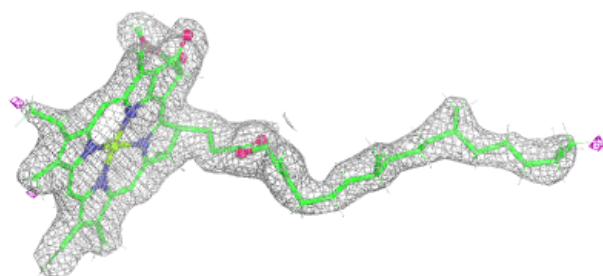
Electron density around CLA b 616:

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



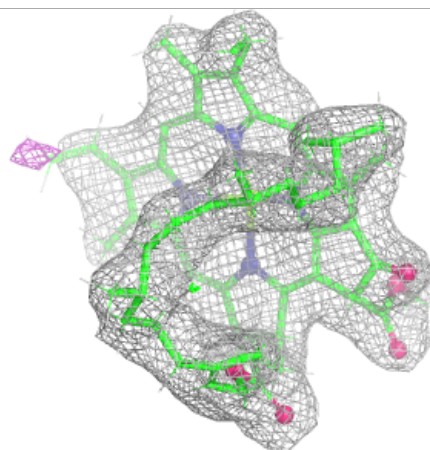
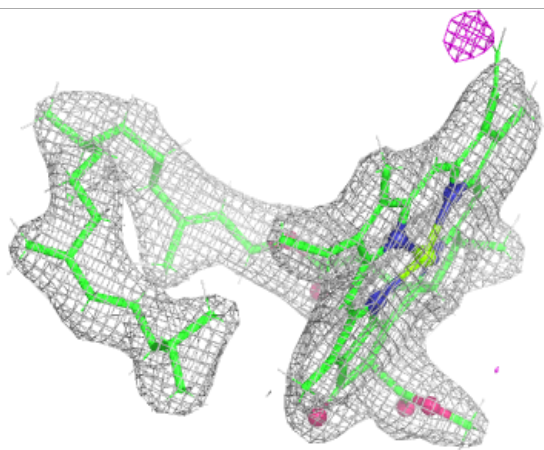
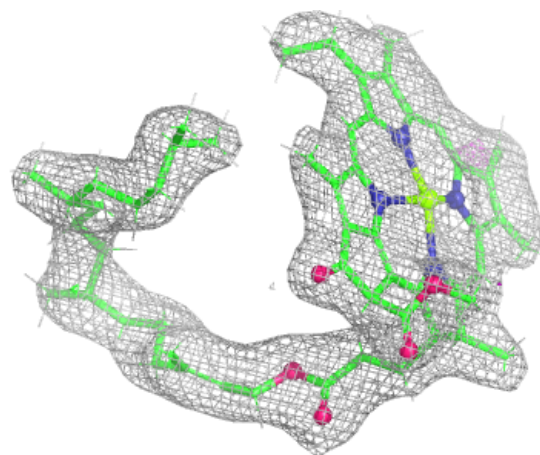
Electron density around CLA c 502:

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

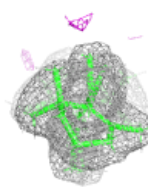
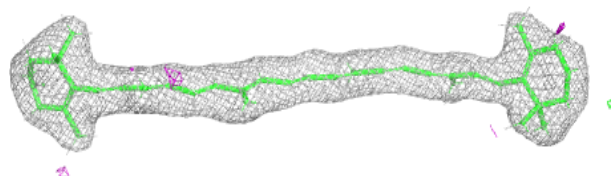
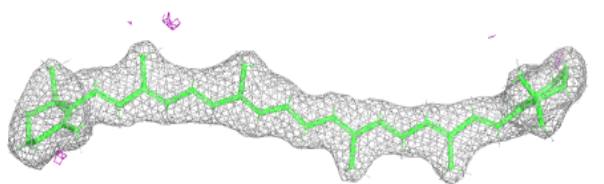


Electron density around CLA c 503:

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

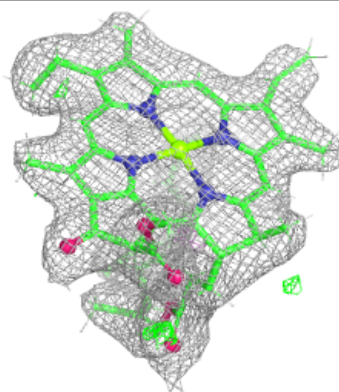
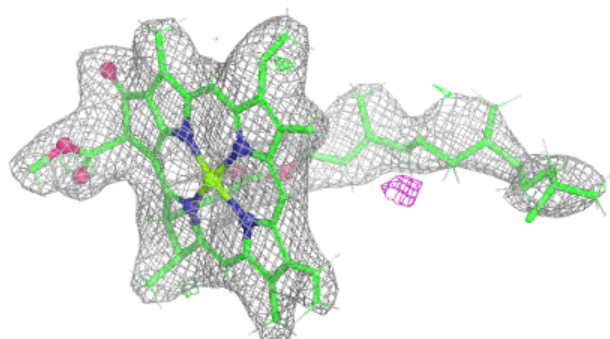
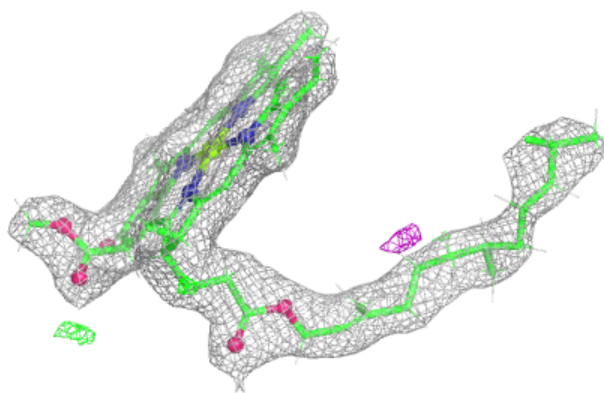
**Electron density around BCR a 405:**

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

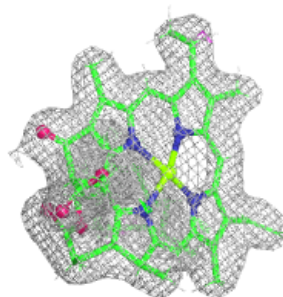
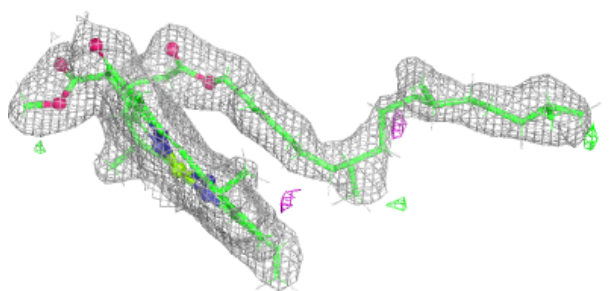
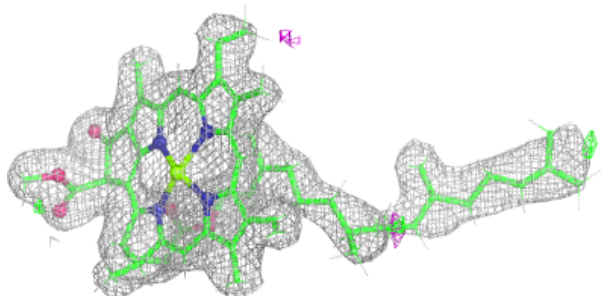


Electron density around CLA c 504:

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

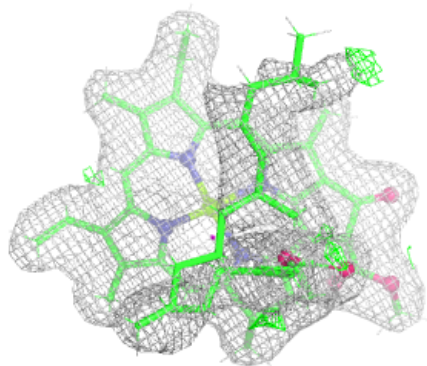
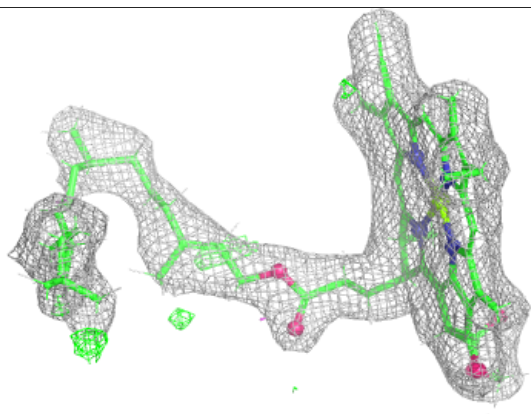
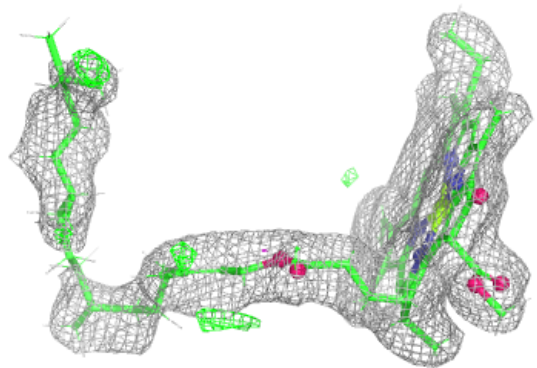
**Electron density around CLA c 505:**

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



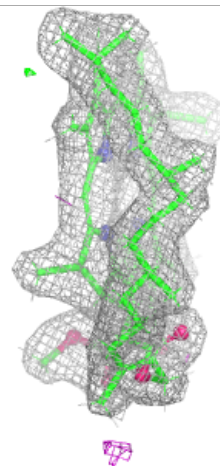
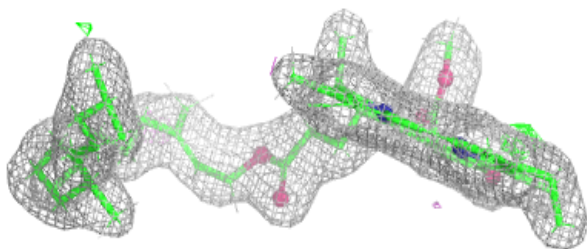
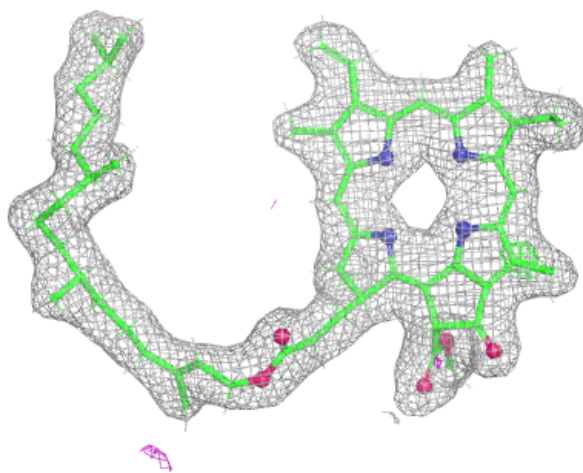
Electron density around CLA a 404:

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



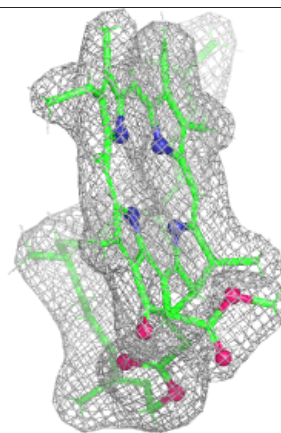
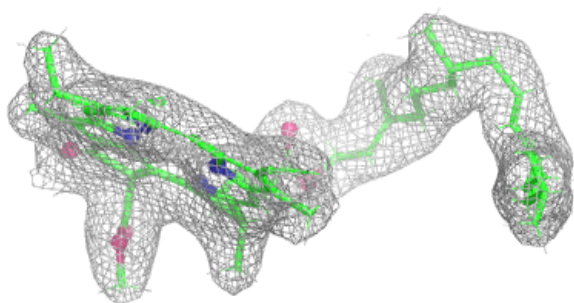
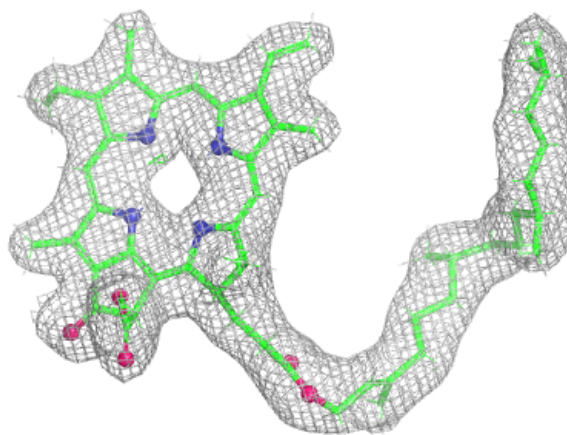
Electron density around PHO A 404:

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



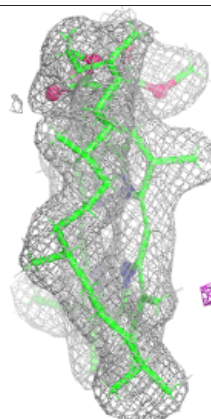
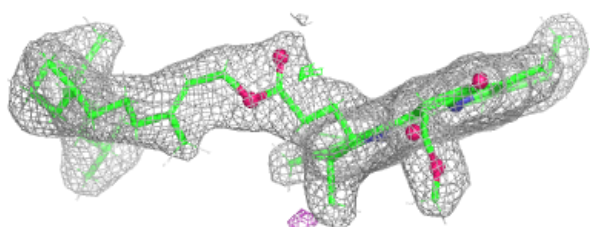
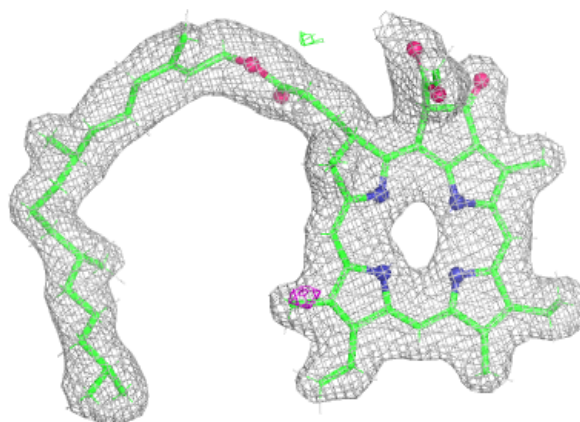
Electron density around PHO D 401:

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

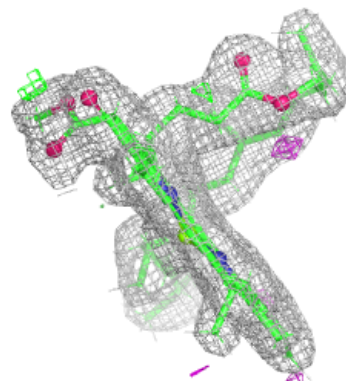
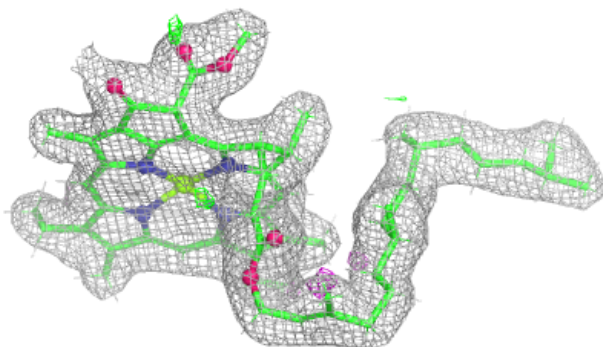
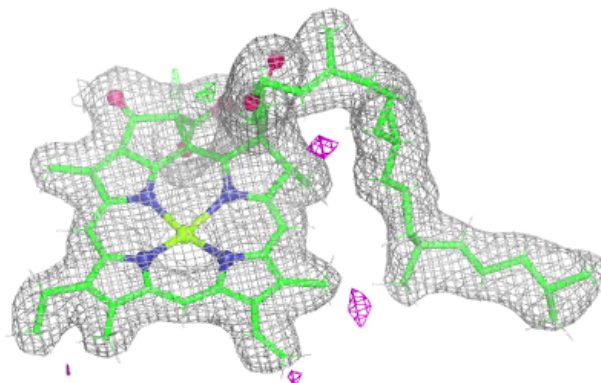


Electron density around PHO d 401:

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

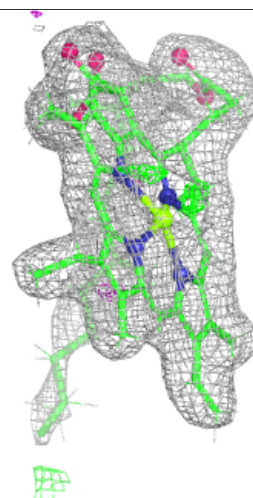
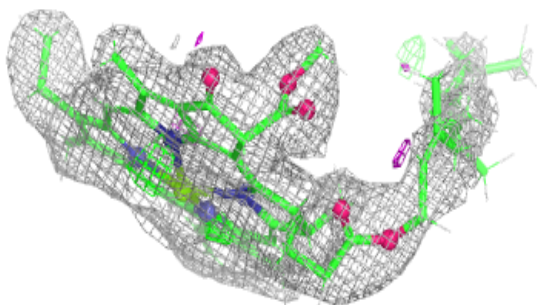
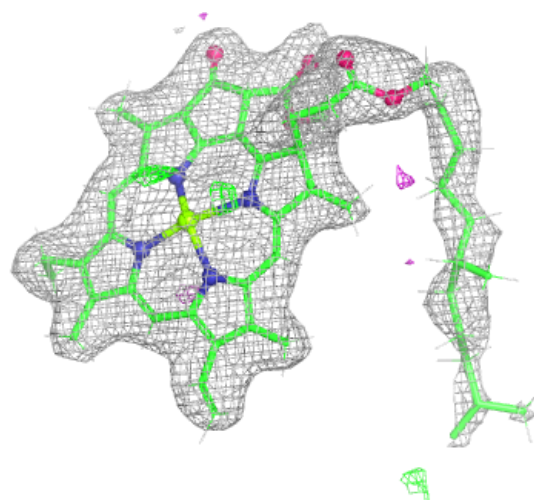
**Electron density around CLA a 410:**

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



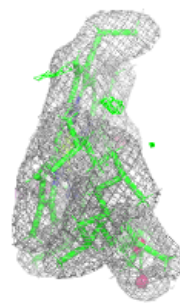
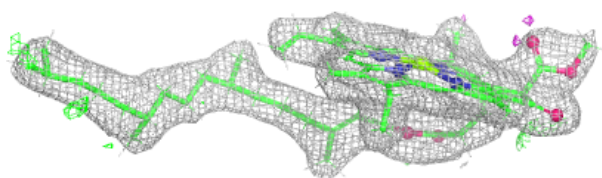
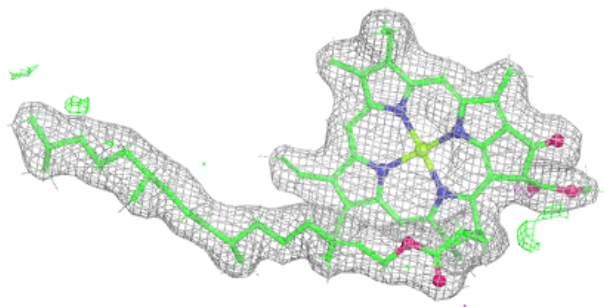
Electron density around CLA B 616:

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

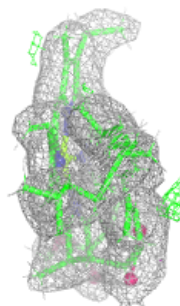
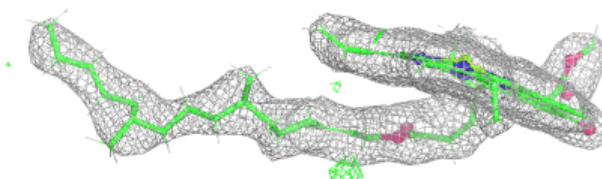
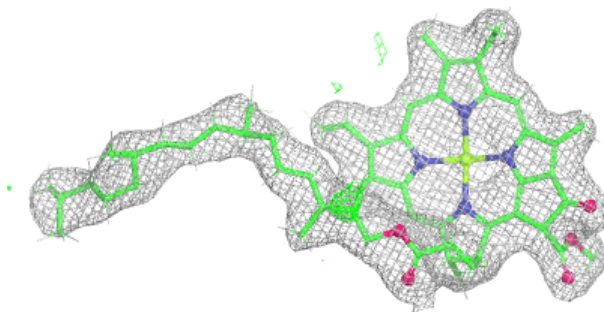


Electron density around CLA C 501:

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

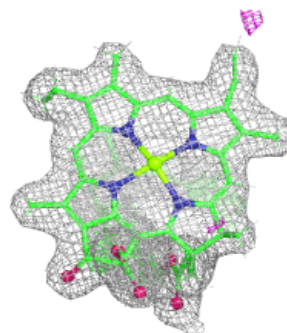
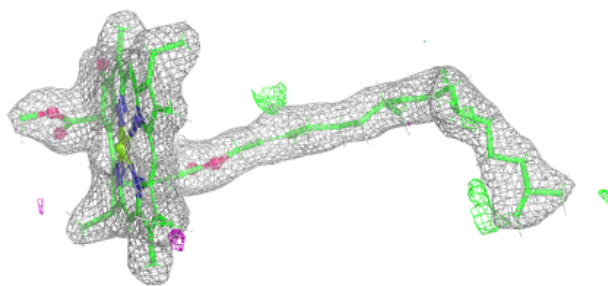
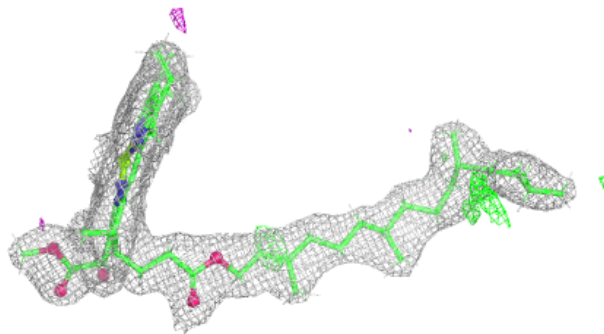
**Electron density around CLA b 603:**

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

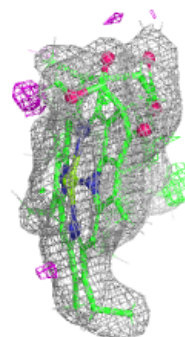
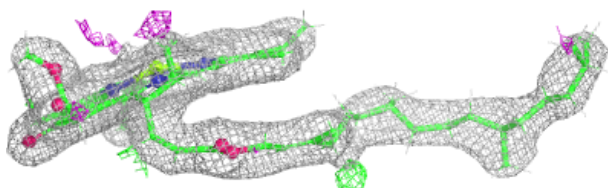
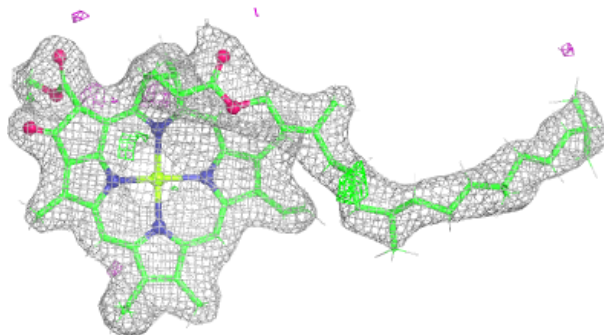


Electron density around CLA b 605:

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

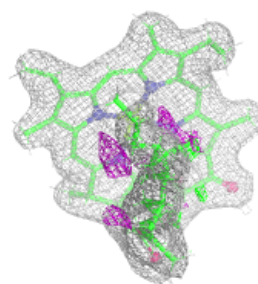
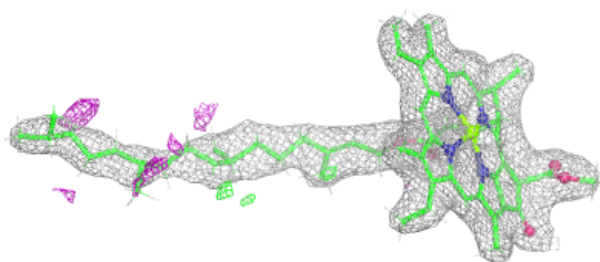
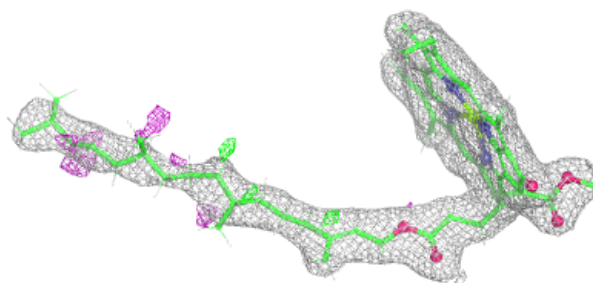
**Electron density around CLA B 603:**

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

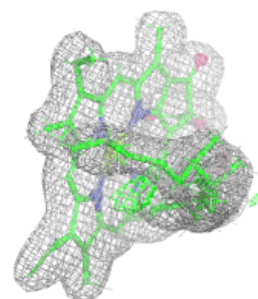
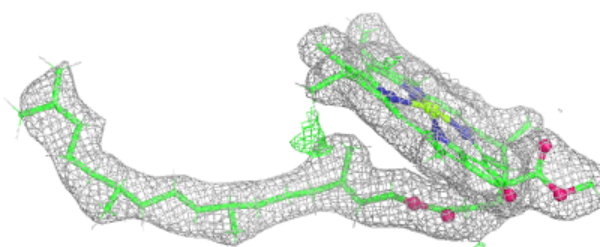
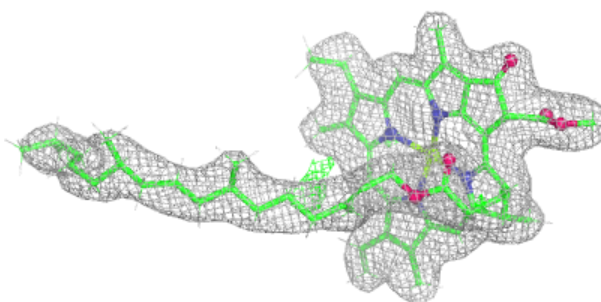


Electron density around CLA b 607:

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

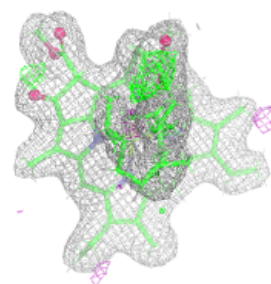
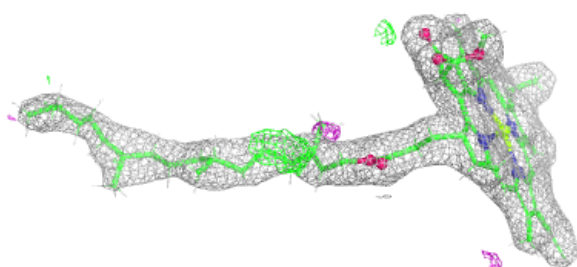
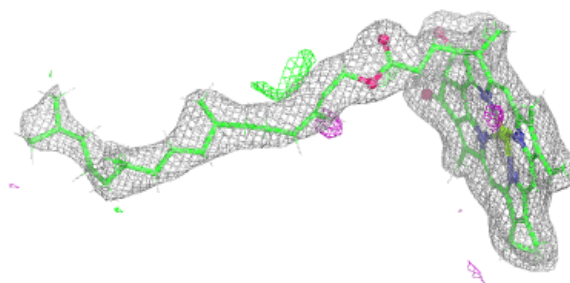
**Electron density around CLA b 608:**

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

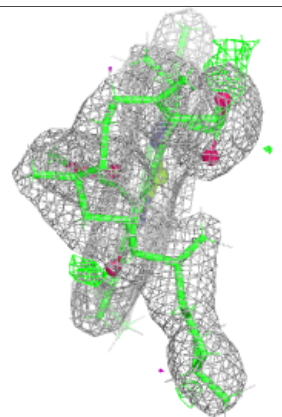
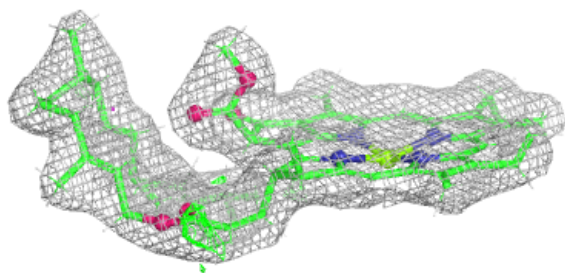
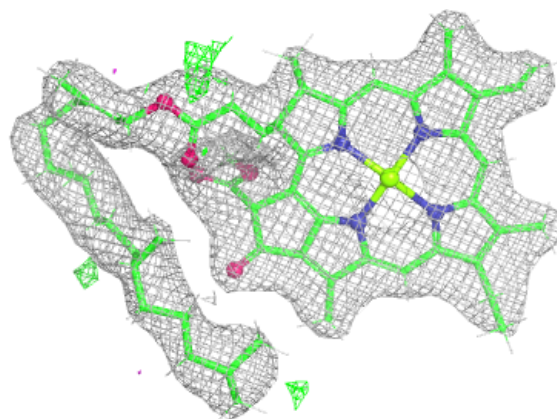


Electron density around CLA B 604:

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

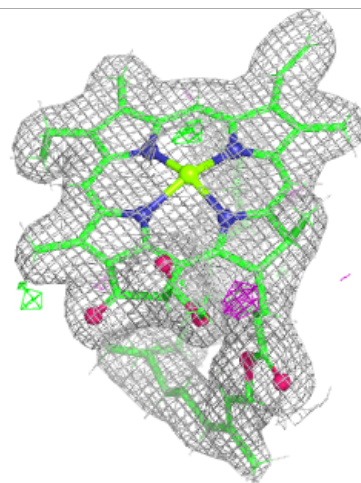
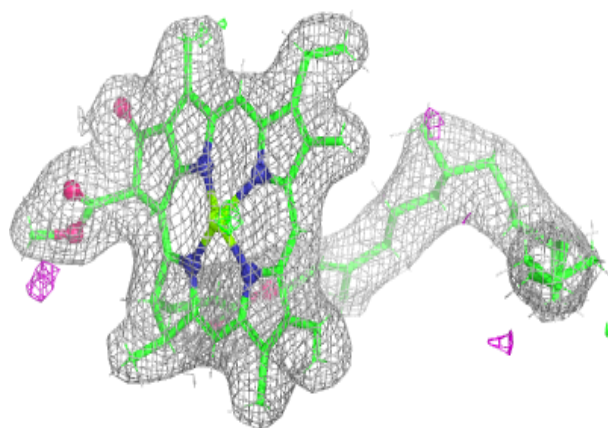
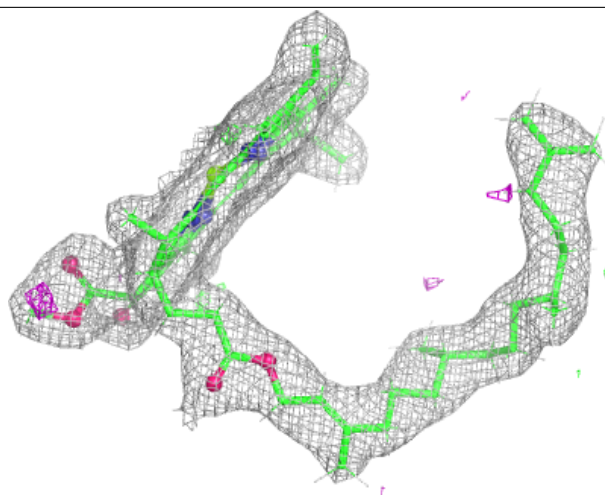
**Electron density around CLA b 610:**

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



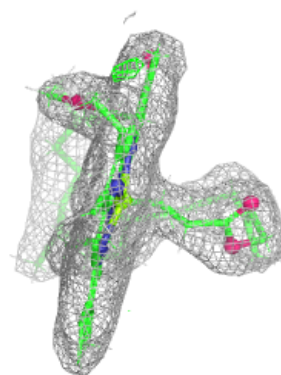
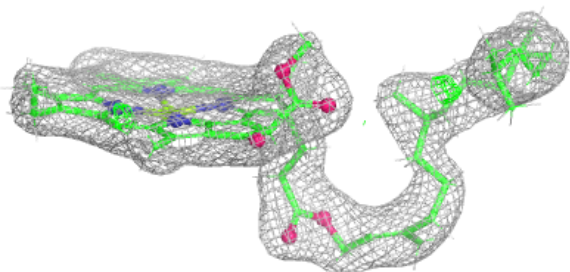
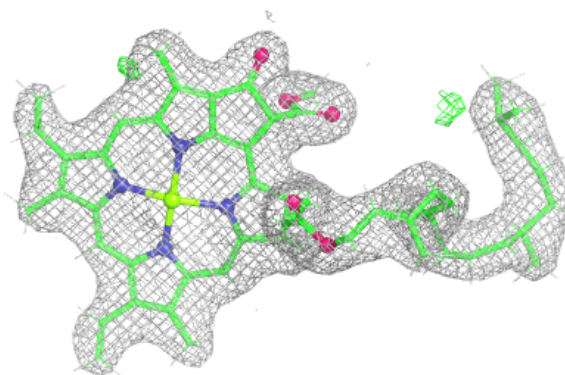
Electron density around CLA b 611:

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

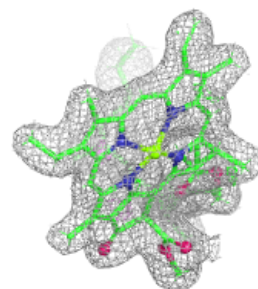
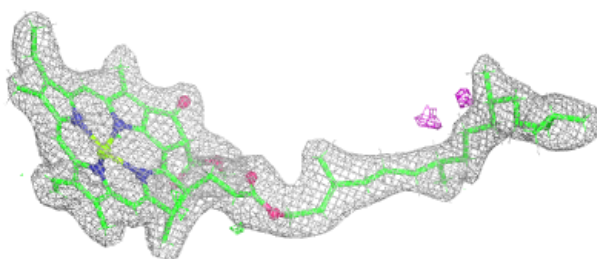
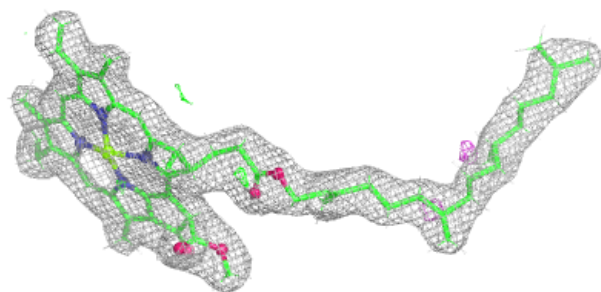


Electron density around CLA b 612:

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

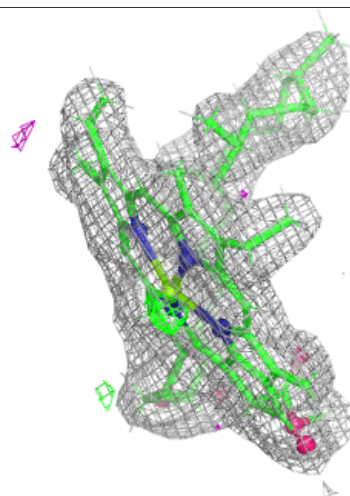
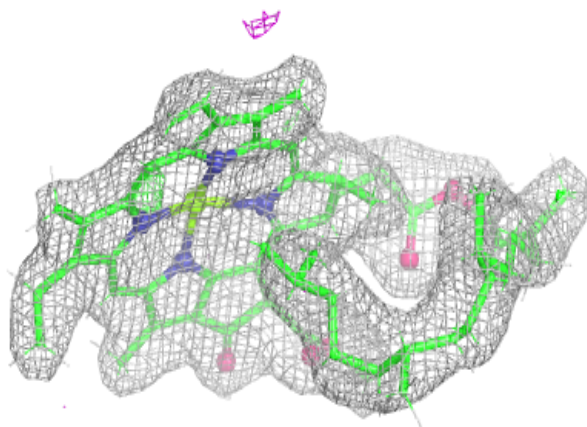
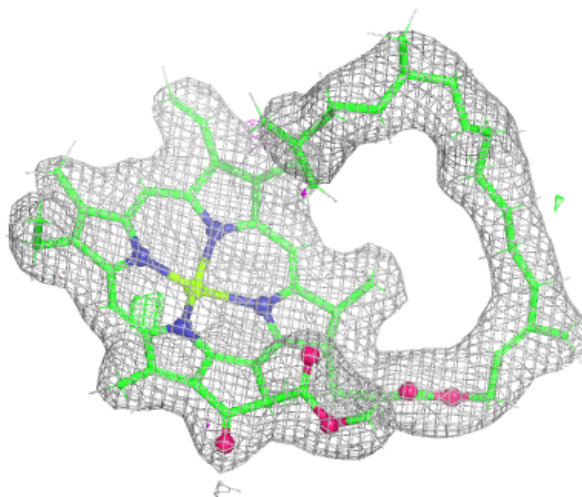
**Electron density around CLA A 402:**

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



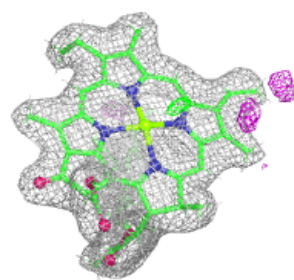
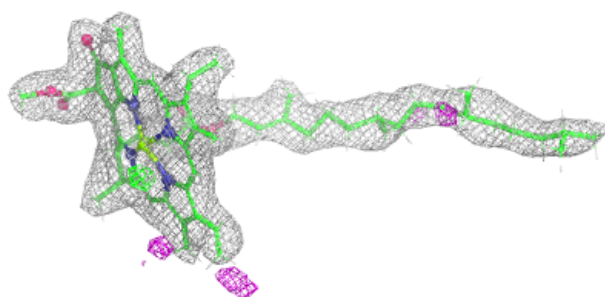
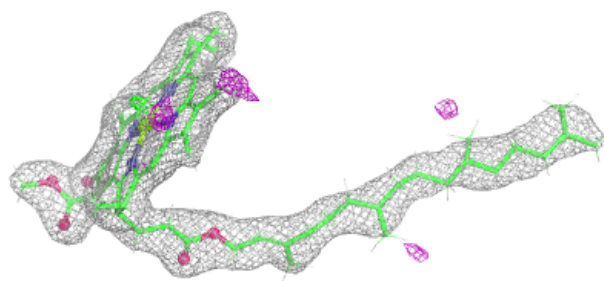
Electron density around CLA b 615:

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

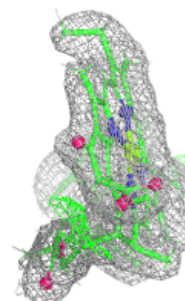
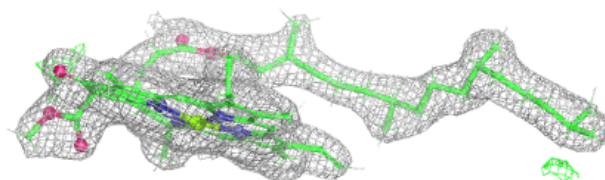
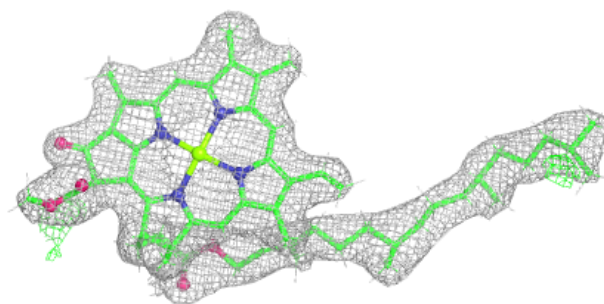


Electron density around CLA B 607:

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

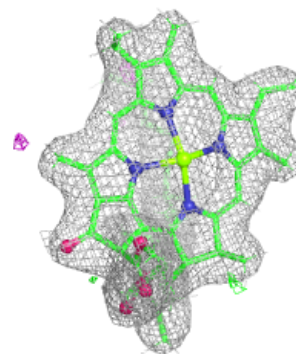
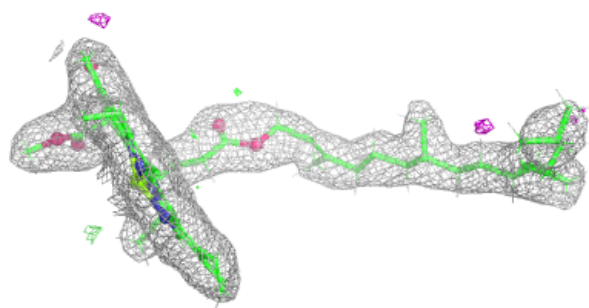
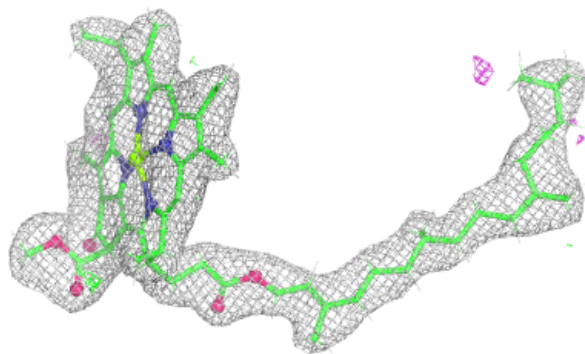
**Electron density around CLA c 501:**

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



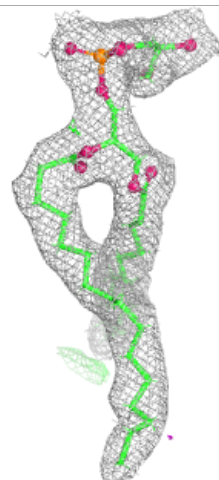
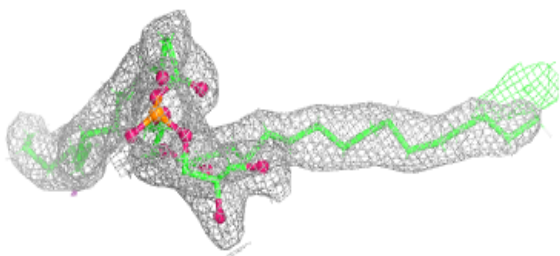
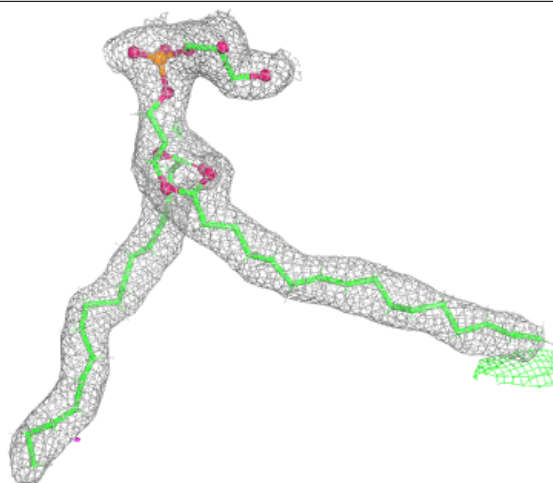
Electron density around CLA B 609:

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



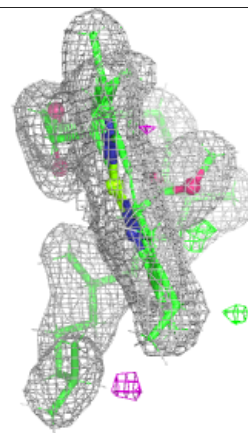
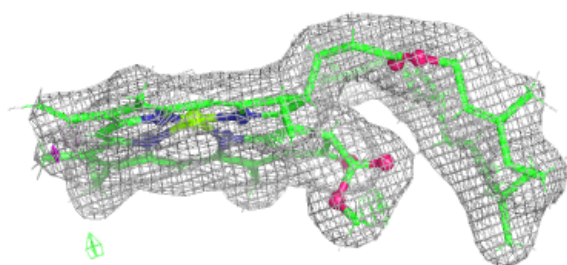
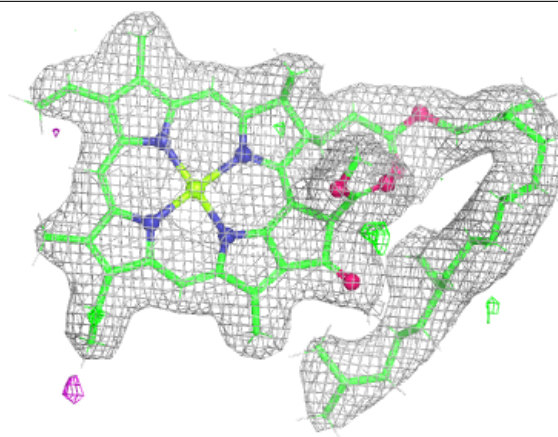
Electron density around LHG B 621:

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



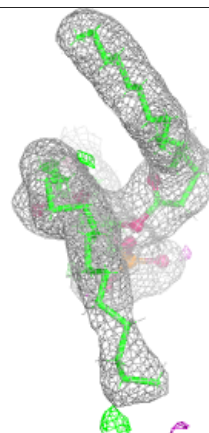
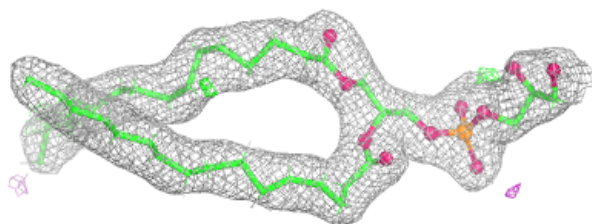
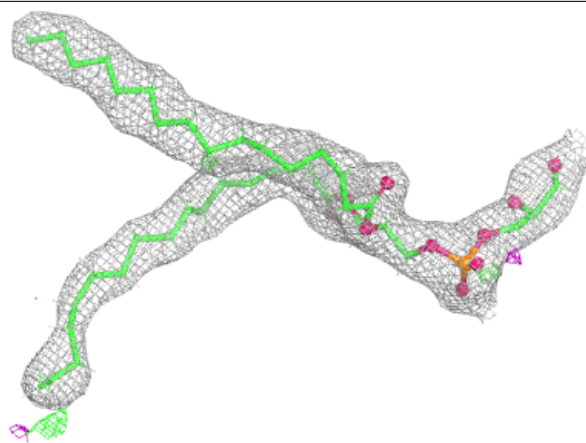
Electron density around CLA B 610:

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



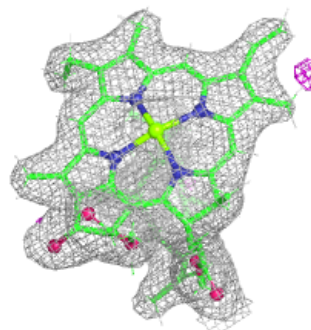
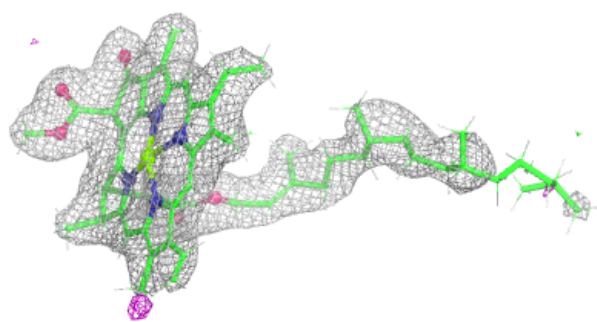
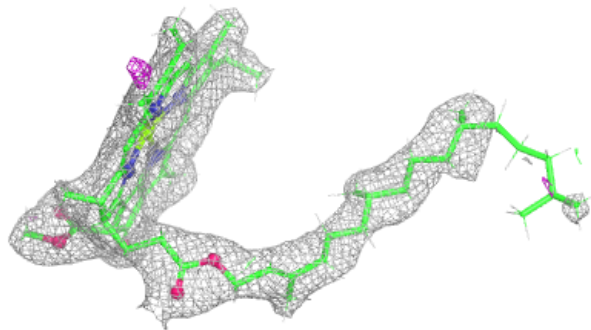
Electron density around LHG D 408:

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



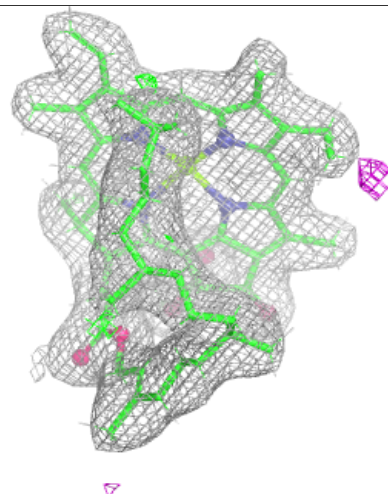
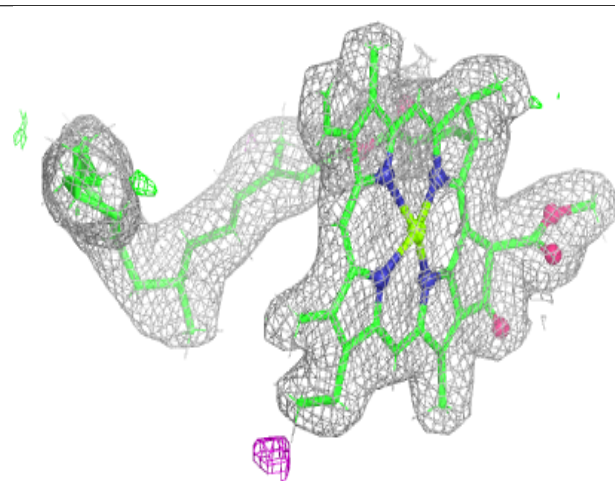
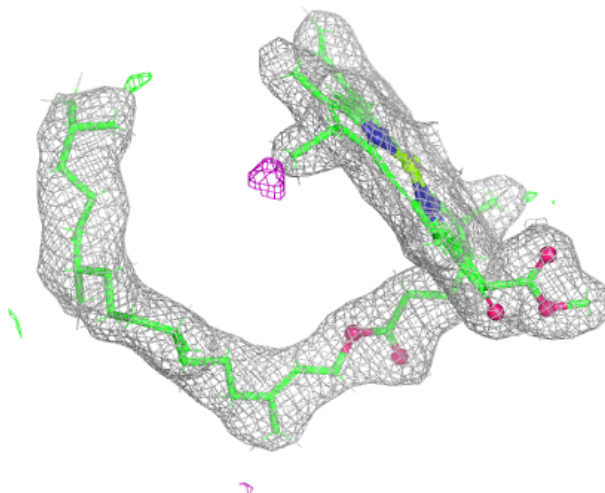
Electron density around CLA C 508:

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



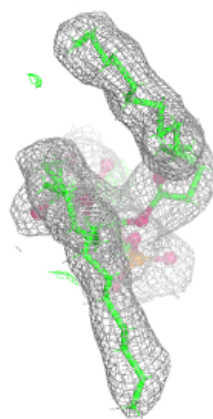
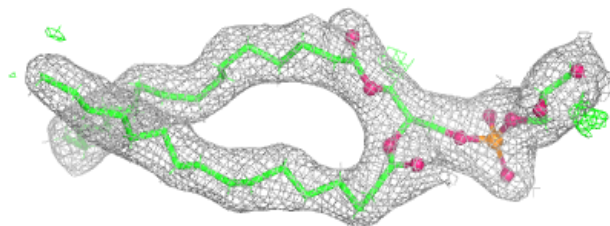
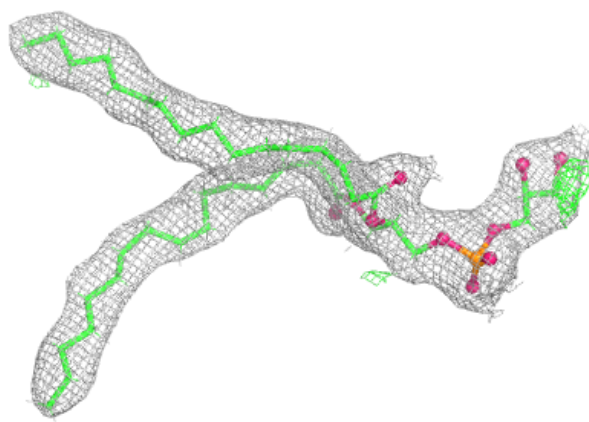
Electron density around CLA B 611:

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



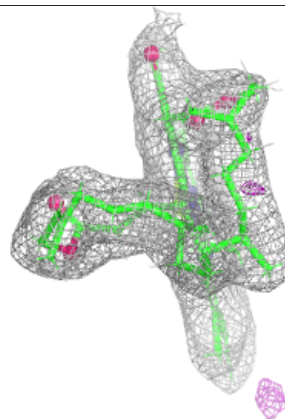
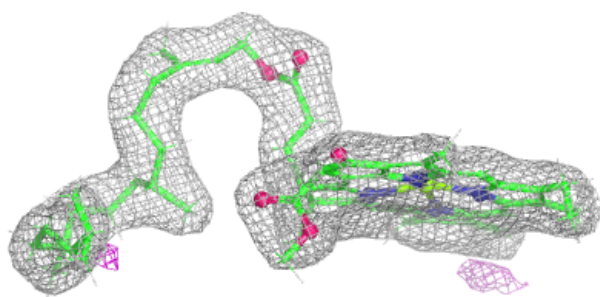
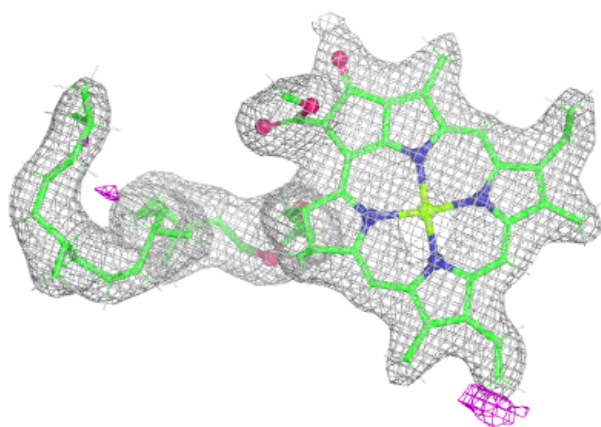
Electron density around LHG d 408:

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



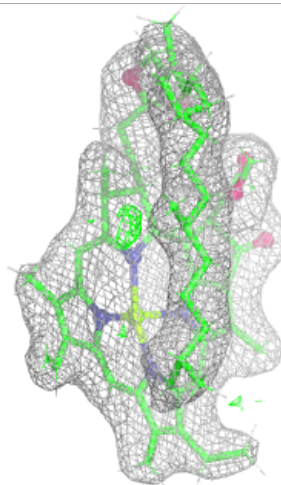
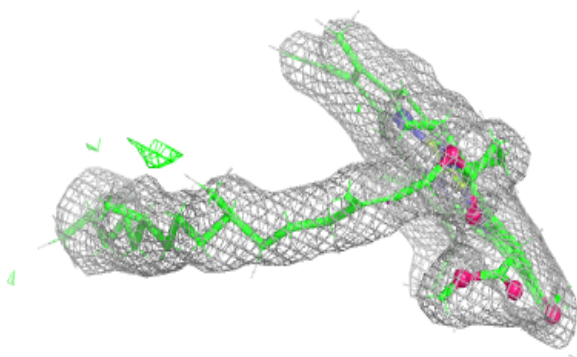
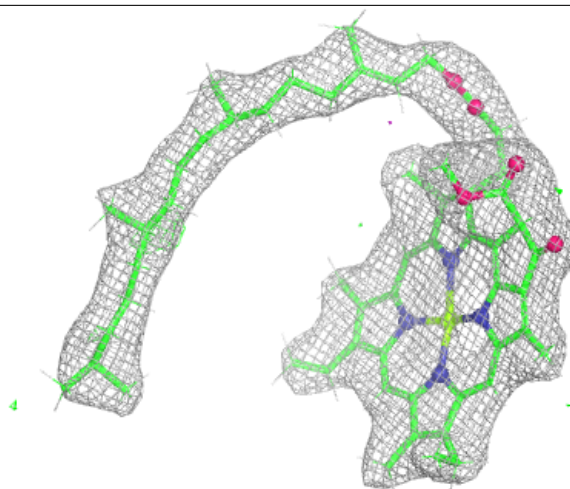
Electron density around CLA B 612:

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



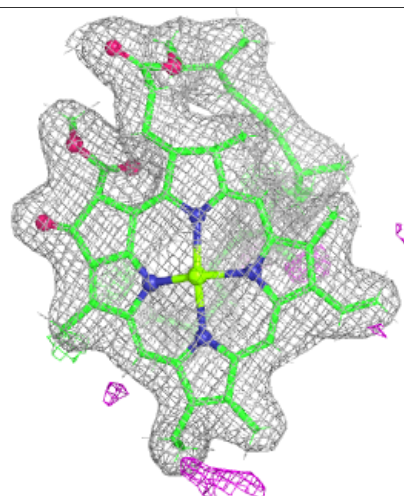
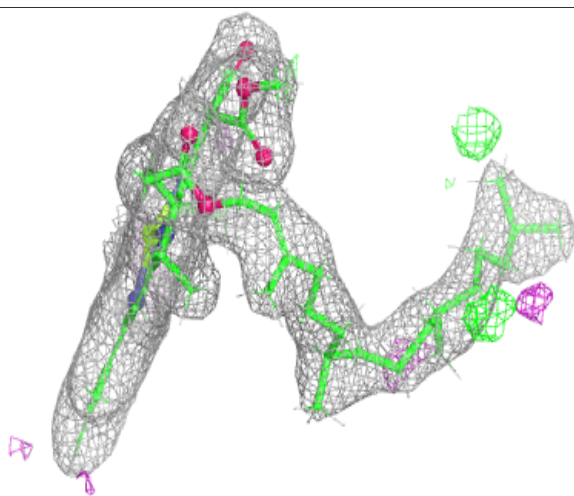
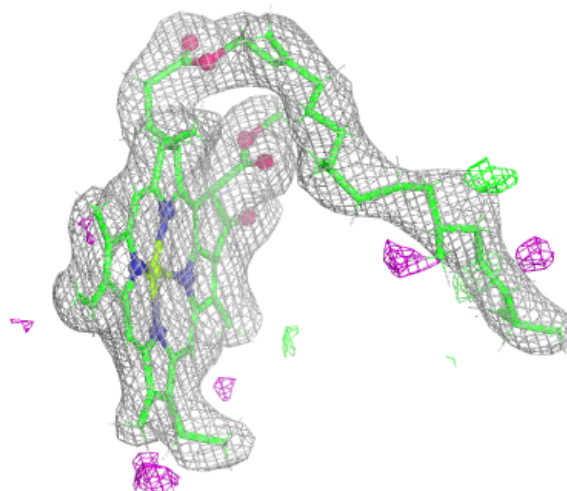
Electron density around CLA c 507:

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



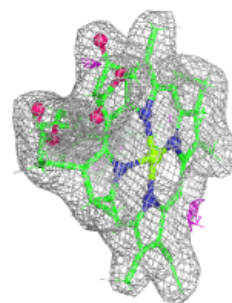
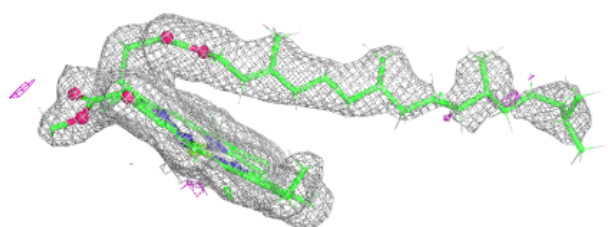
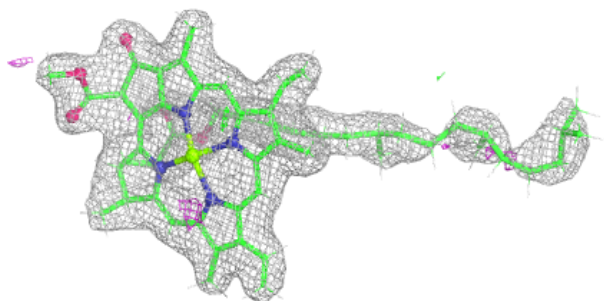
Electron density around CLA B 613:

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



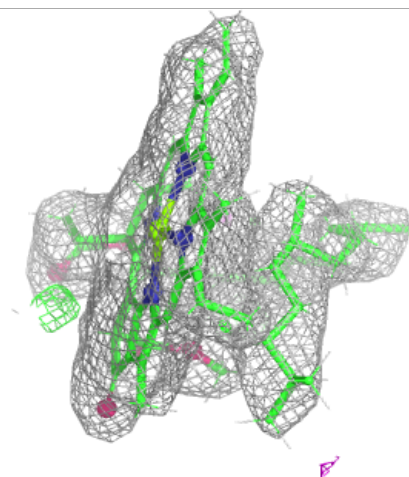
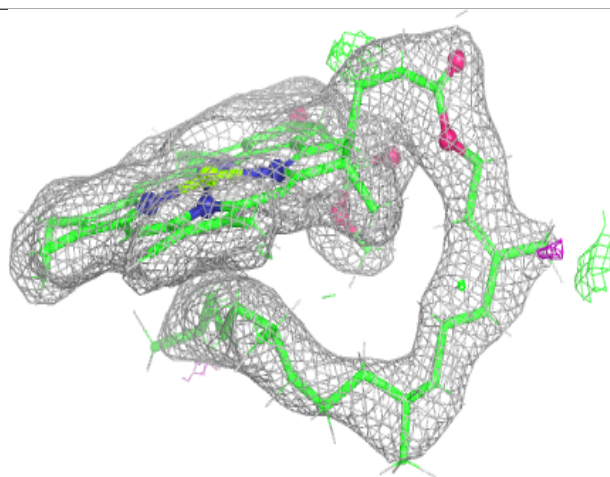
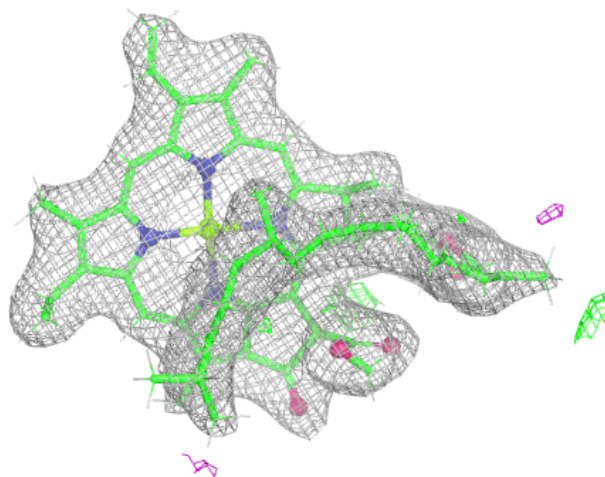
Electron density around CLA B 614:

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



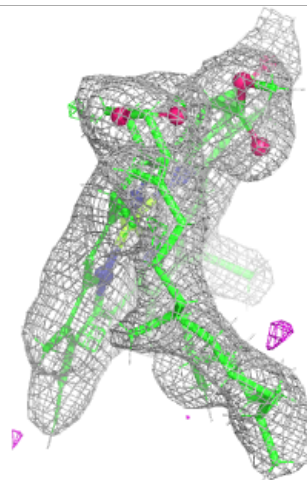
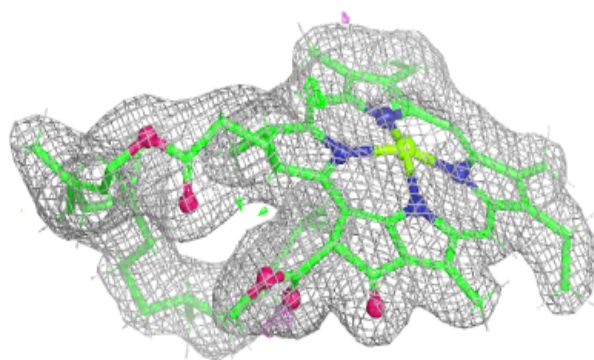
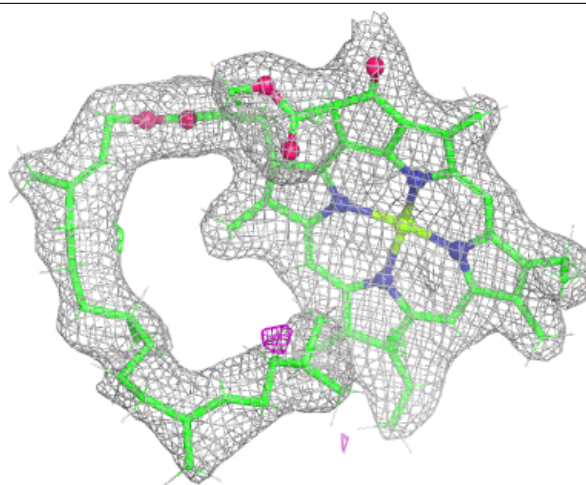
Electron density around CLA c 510:

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



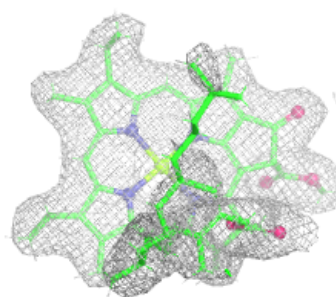
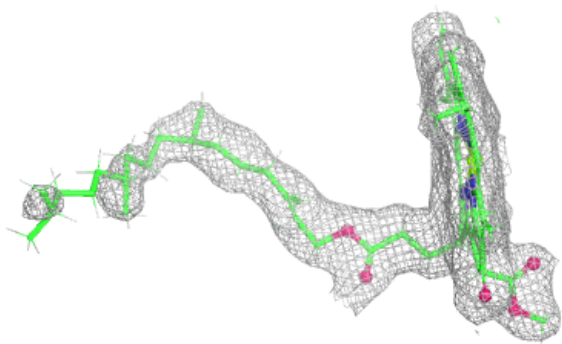
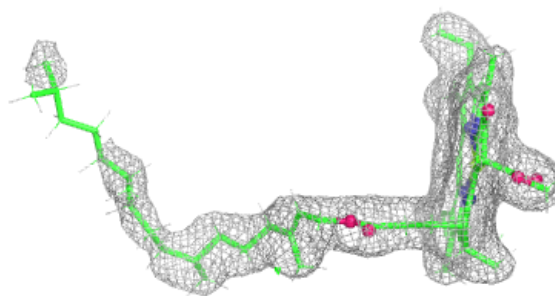
Electron density around CLA B 615:

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

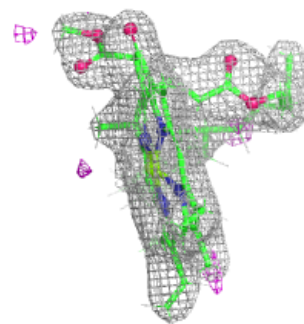
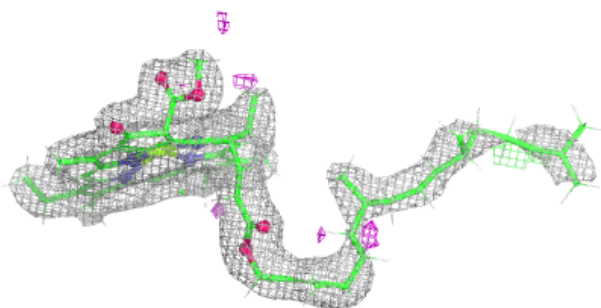
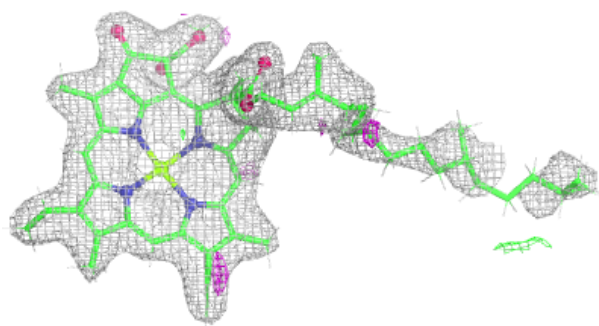


Electron density around CLA D 403:

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

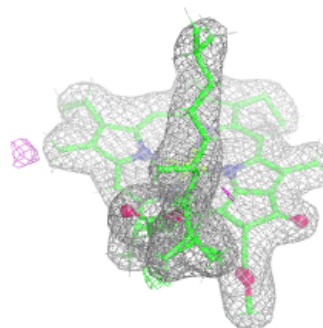
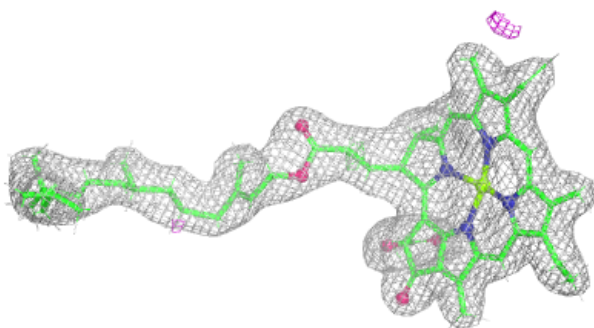
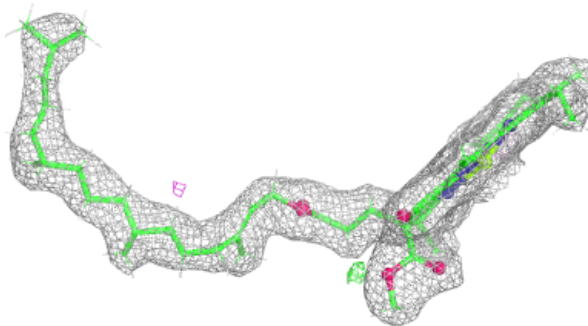
**Electron density around CLA a 403:**

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



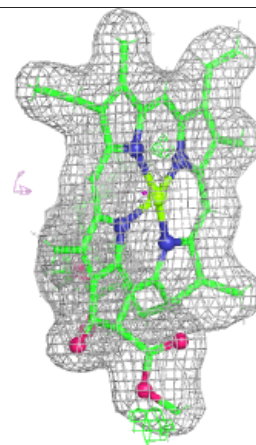
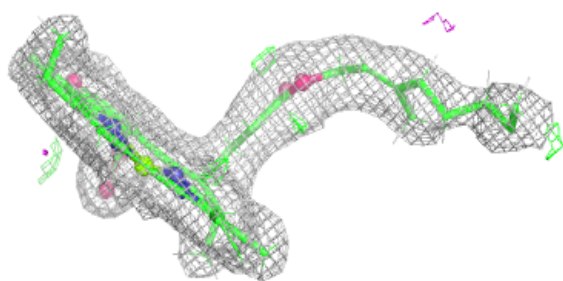
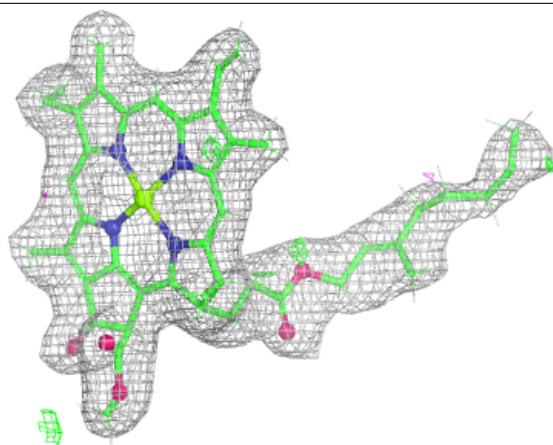
Electron density around CLA d 403:

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



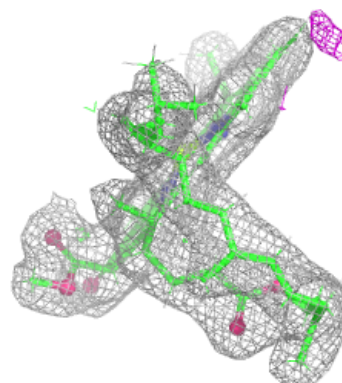
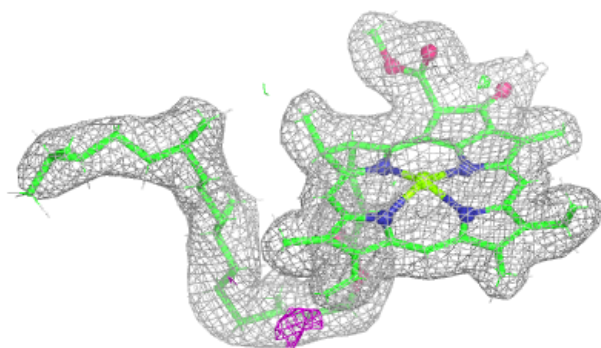
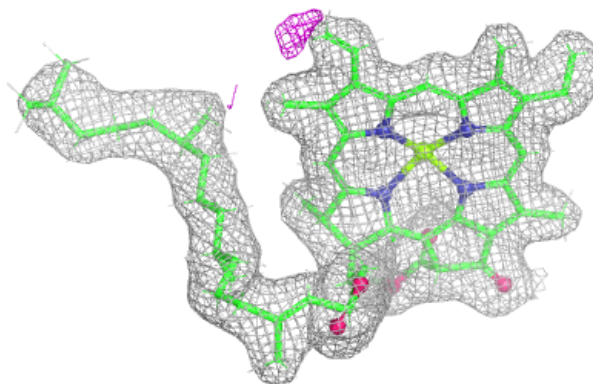
Electron density around CLA A 405:

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

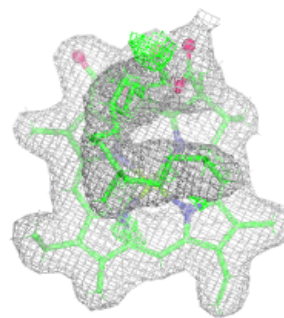
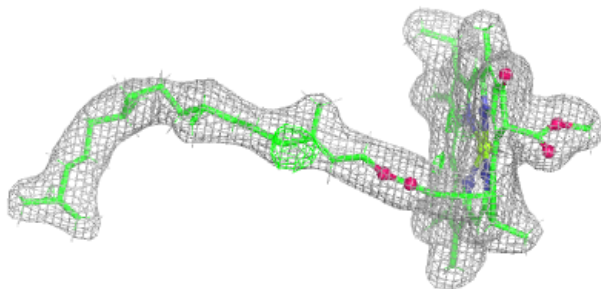
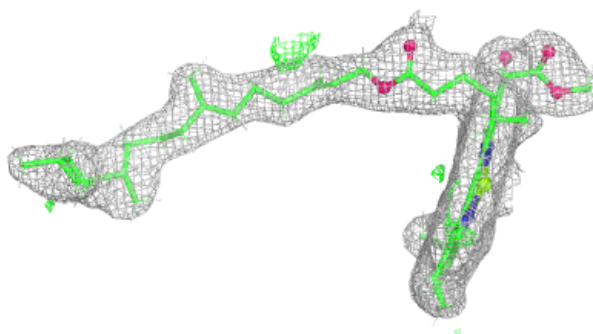


Electron density around CLA A 411:

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

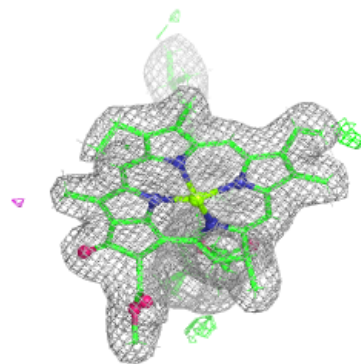
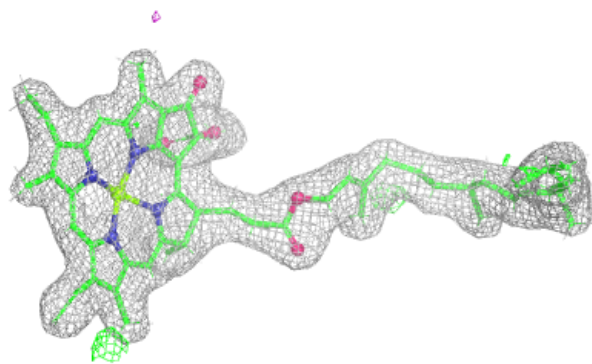
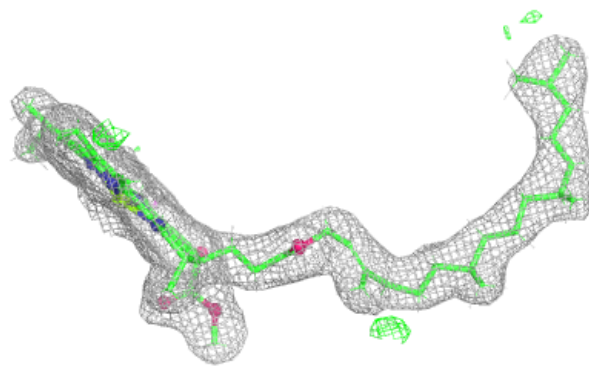
**Electron density around CLA B 605:**

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



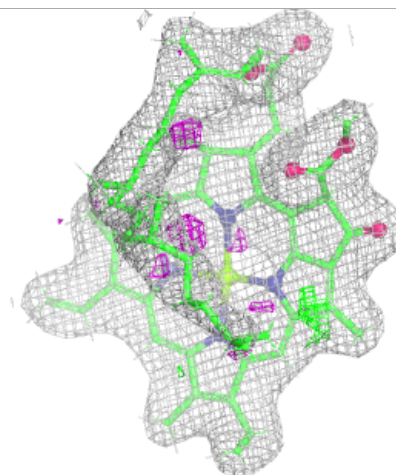
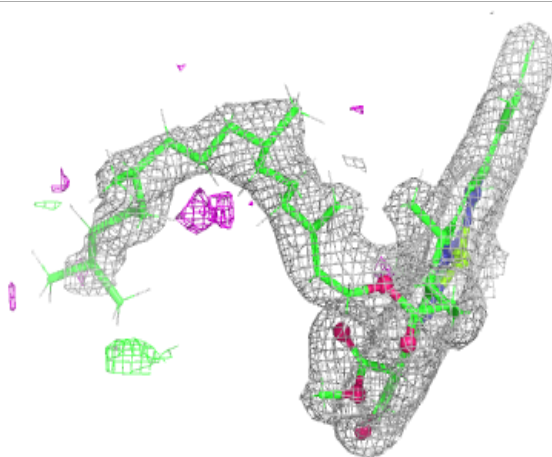
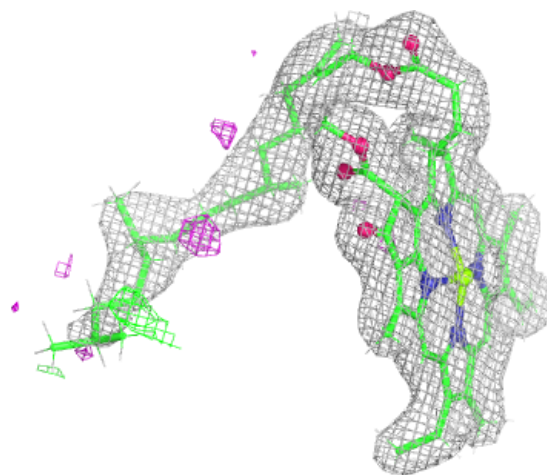
Electron density around CLA D 402:

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



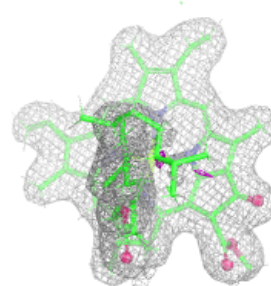
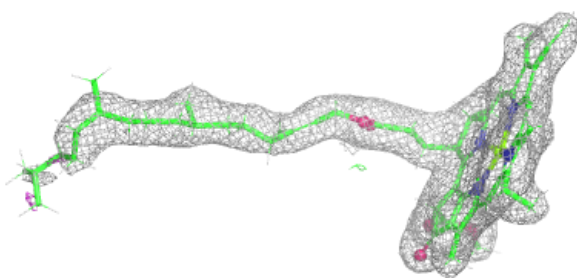
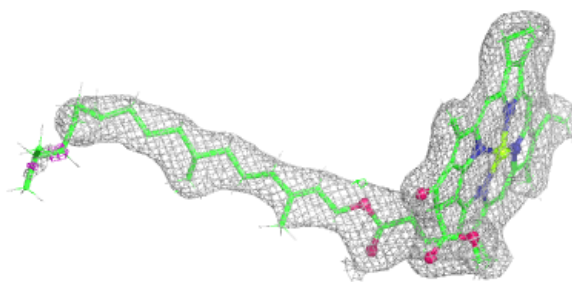
Electron density around CLA b 613:

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

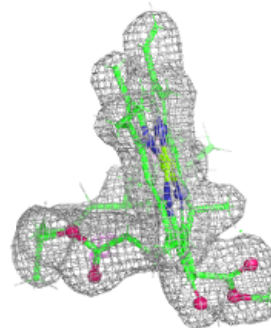
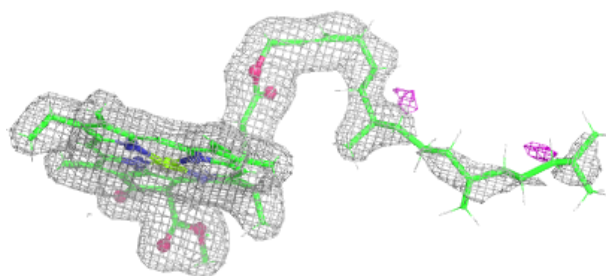
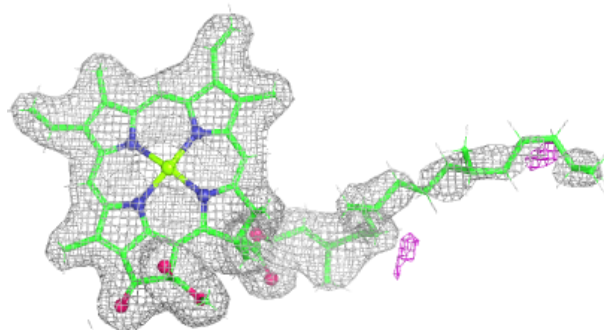


Electron density around CLA b 604:

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

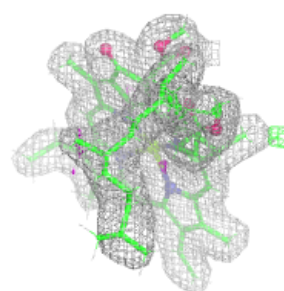
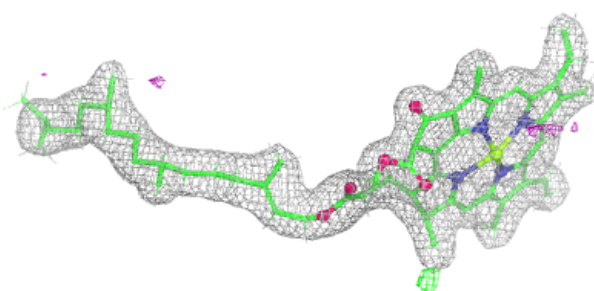
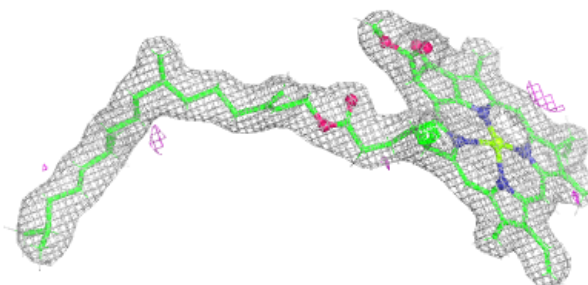
**Electron density around CLA A 403:**

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

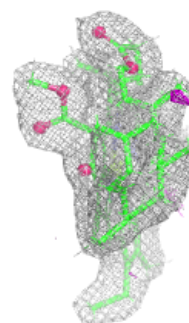
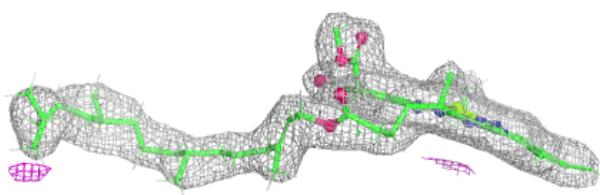
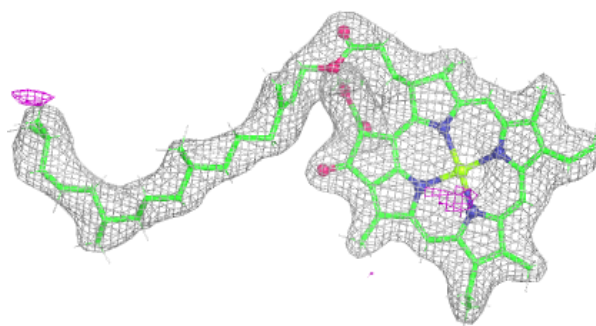


Electron density around CLA a 402:

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

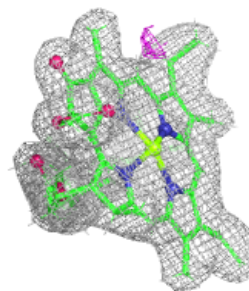
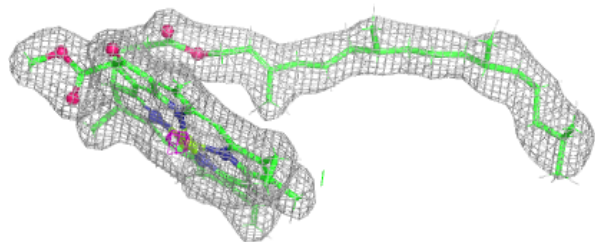
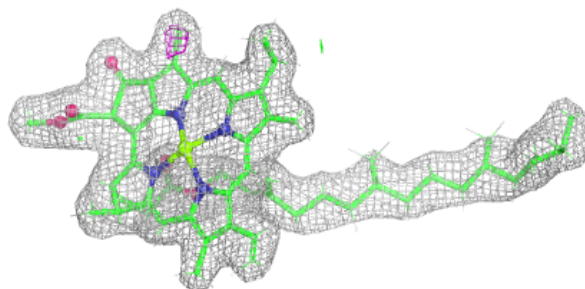
**Electron density around CLA B 602:**

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



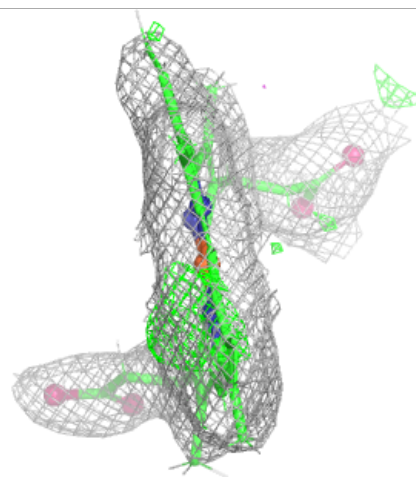
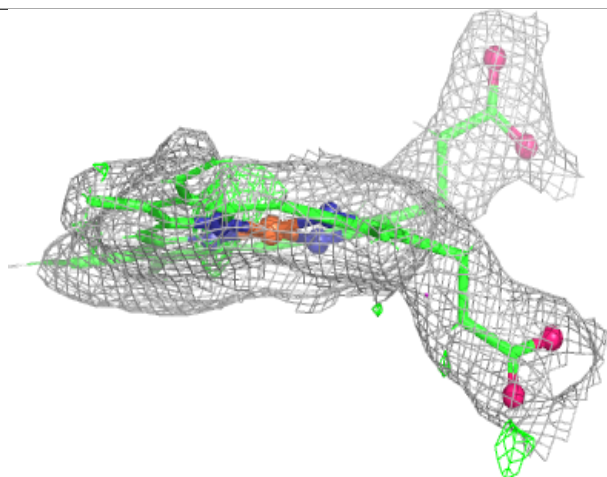
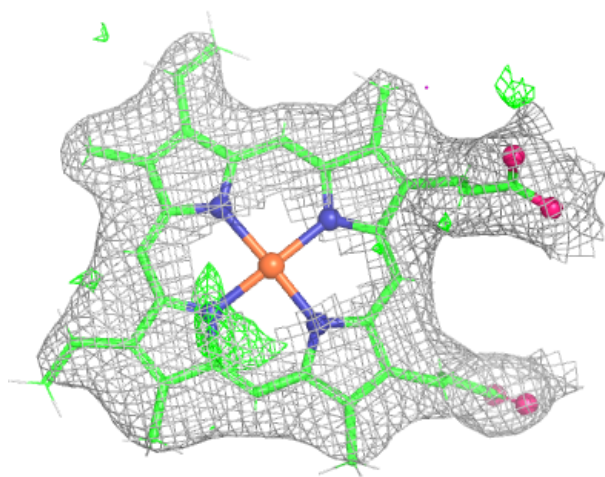
Electron density around CLA B 608:

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



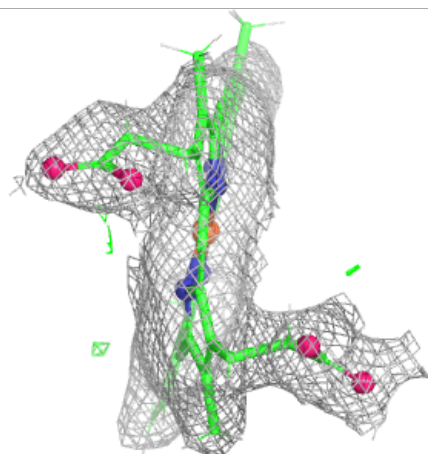
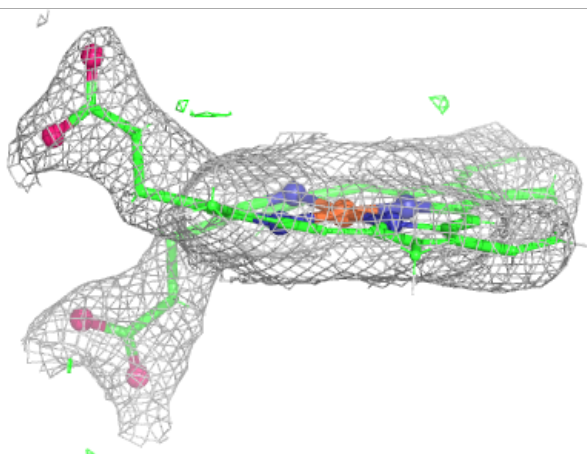
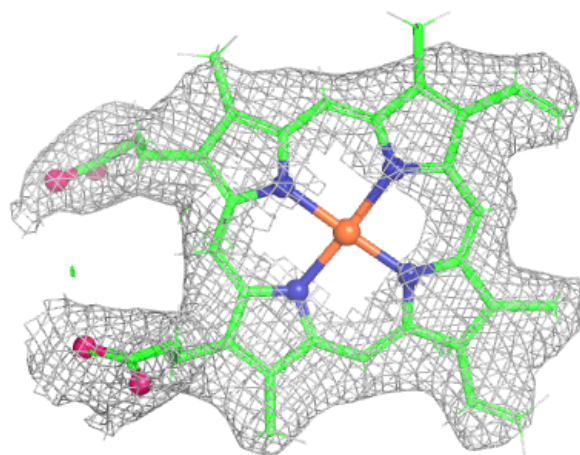
Electron density around HEM F 101:

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



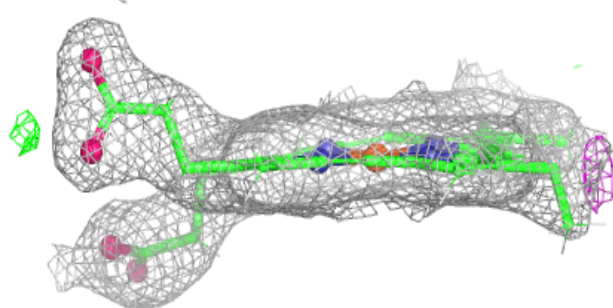
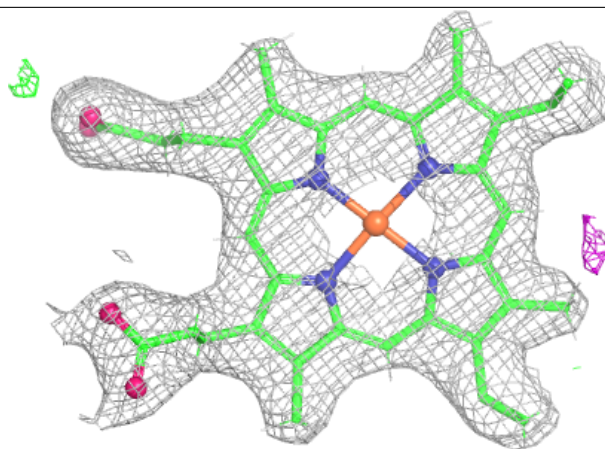
Electron density around HEM e 101:

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



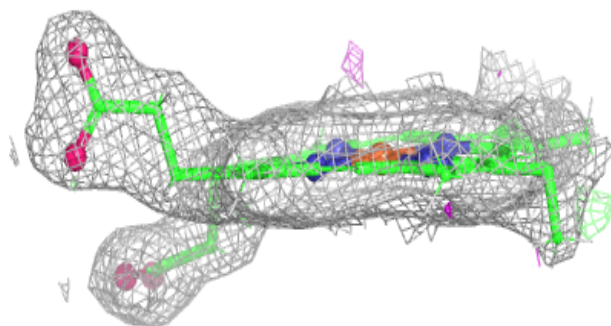
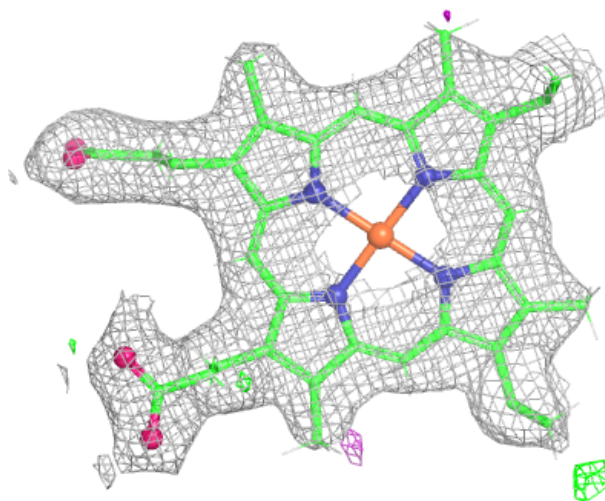
Electron density around HEC V 201:

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



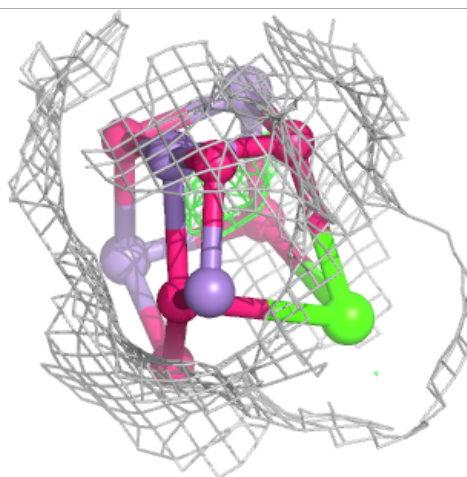
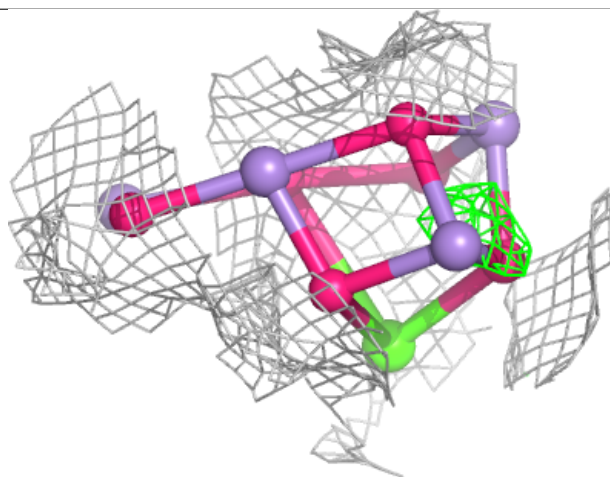
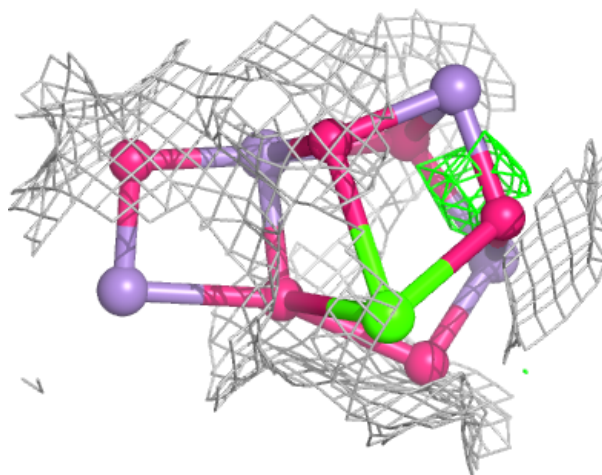
Electron density around HEC v 201:

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



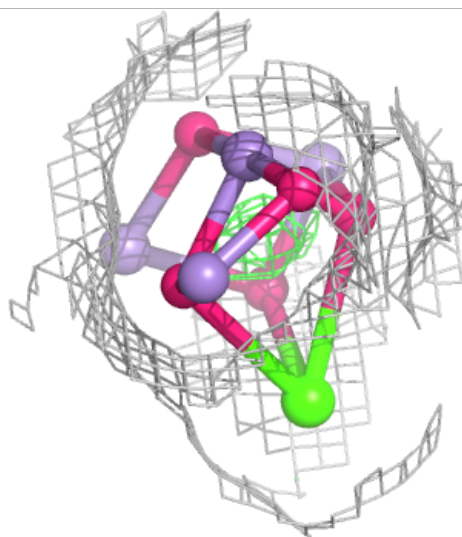
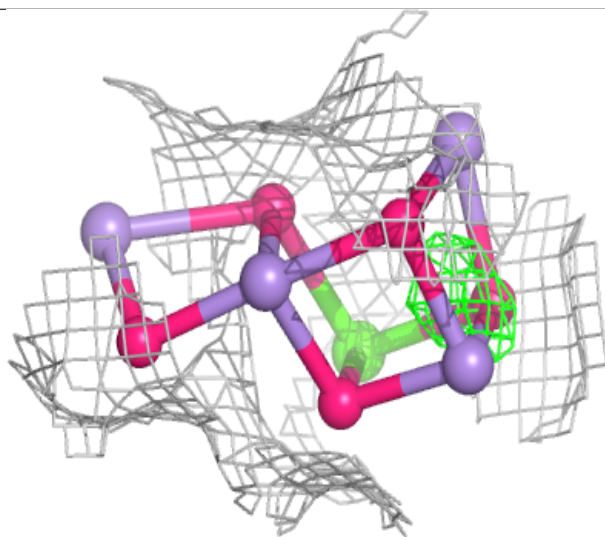
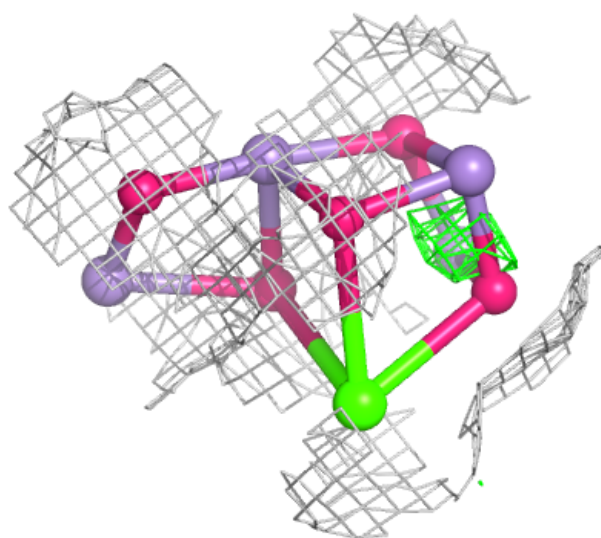
Electron density around OEY A 417 (B):

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



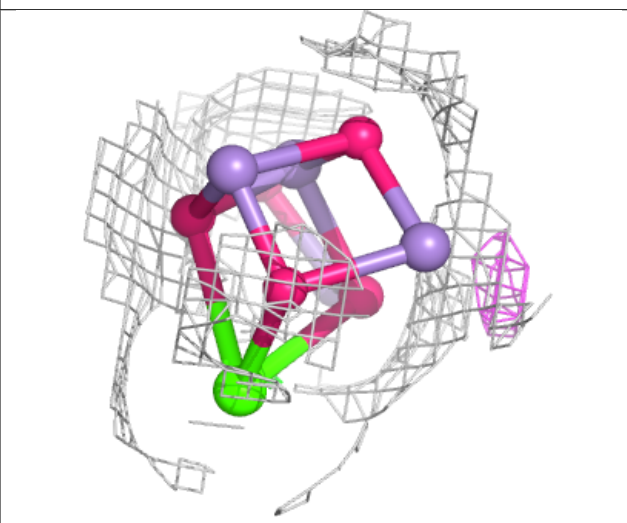
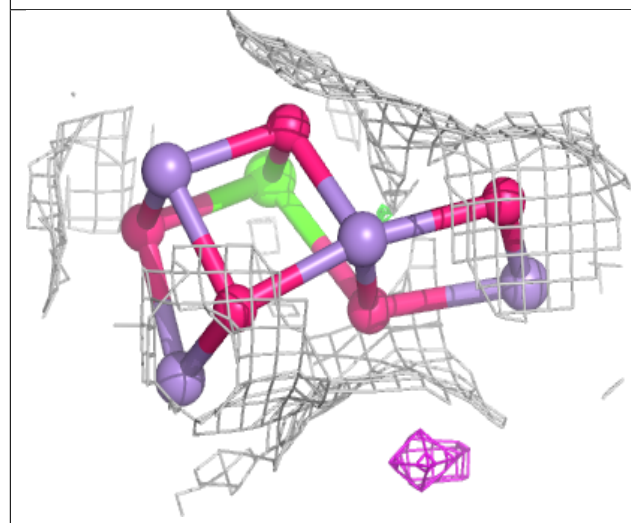
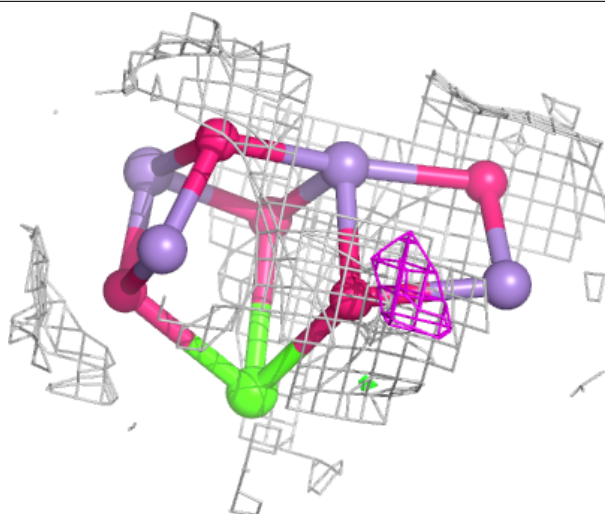
Electron density around OEX A 418 (A):

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



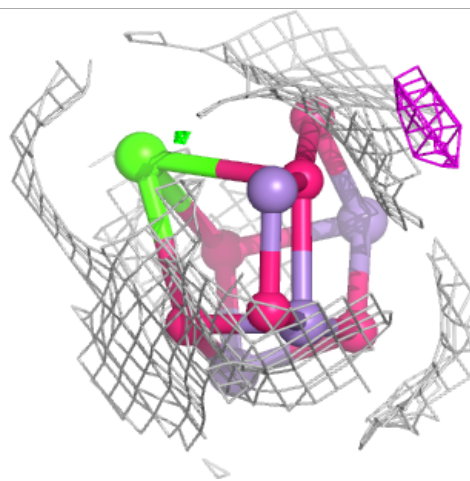
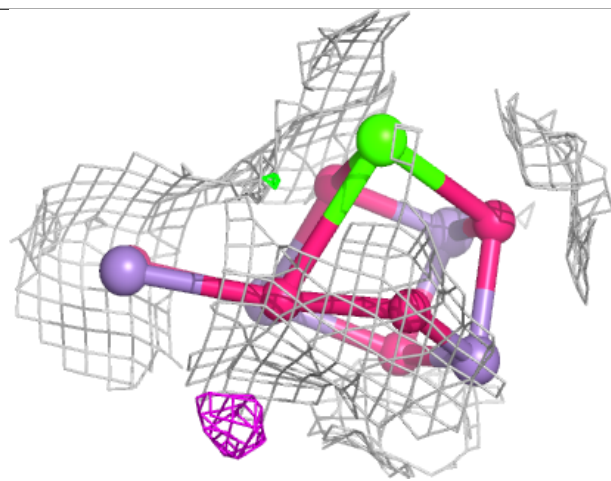
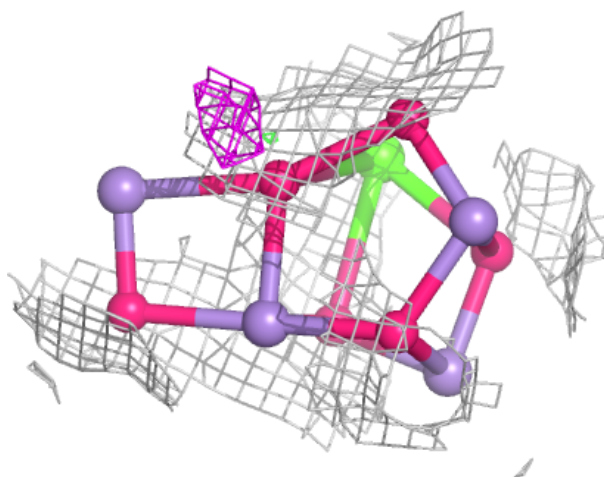
Electron density around OEX a 417 (A):

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



Electron density around OEY a 418 (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.