



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2026 – 02:26 PM EDT

PDB ID : 13CH / pdb_000013ch
Title : RT XFEL structure of one-flash state of Photosystem II (1F, S2 rich) at 2.02 Angstrom
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Bogacz, I.; Chatterjee, R.; Zhang, M.
Deposited on : 2026-04-28
Resolution : 2.02 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)
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

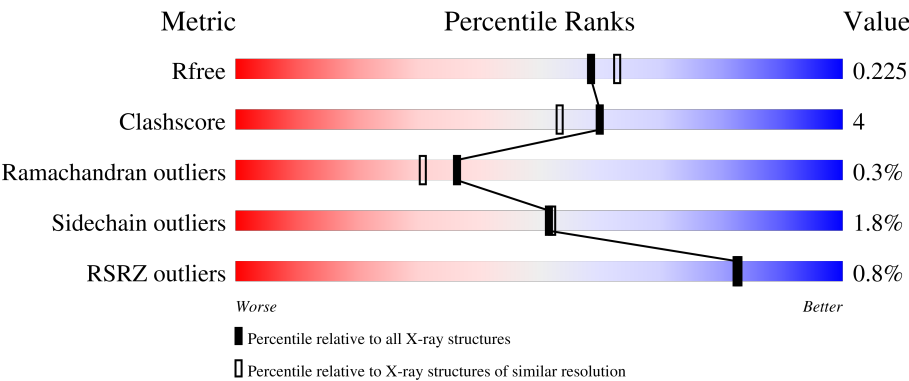
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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.



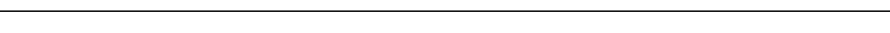
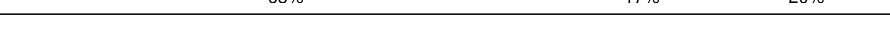
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	% 89%8% .
1	a	344	88%9% ..

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Mol	Chain	Length	Quality of chain
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	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	 66% 5% 28%
16	V	163	 76% 8% 16%
16	v	163	 71% 13% 16%
17	Y	46	 46% 13% 41%
17	y	46	 52% 11% 35%
18	X	41	 88% 5% 7%
18	x	41	 80% 12% 5%
19	Z	62	 79% 21%
19	z	62	 77% 21%
20	R	41	 54% 15% 32%
20	r	41	 41% 22% 32%

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

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

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 104064 atoms, of which 51466 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			4864	1717	2242	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			4851	1714	2232	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	7	0
			7903	2637	3887	670	696	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7826	2614	3842	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6707	2244	3290	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6855	2286	3361	587	608	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5303	1800	2586	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5315	1804	2592	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	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
			1033	335	528	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1007	327	514	80	83			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	conflict	UNP Q8DJ43
h	41	CYS	PHE	conflict	UNP Q8DJ43

- 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			
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
			523	171	267	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

- 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 reaction center protein T.

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

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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 Z.

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

- Molecule 20 is a protein called Photosystem II protein Y.

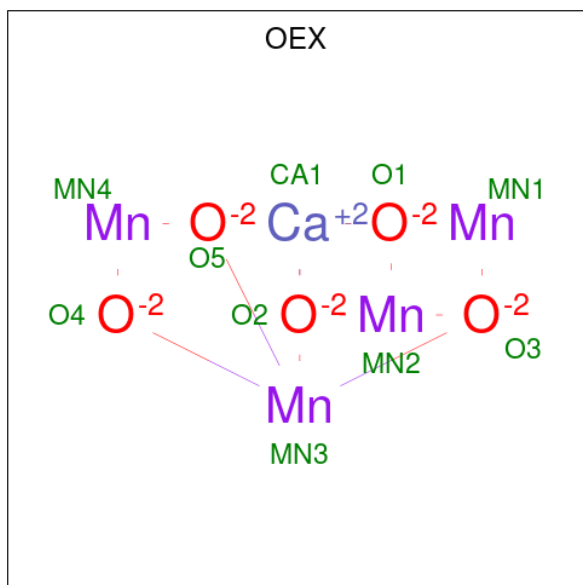
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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

- Molecule 21 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
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

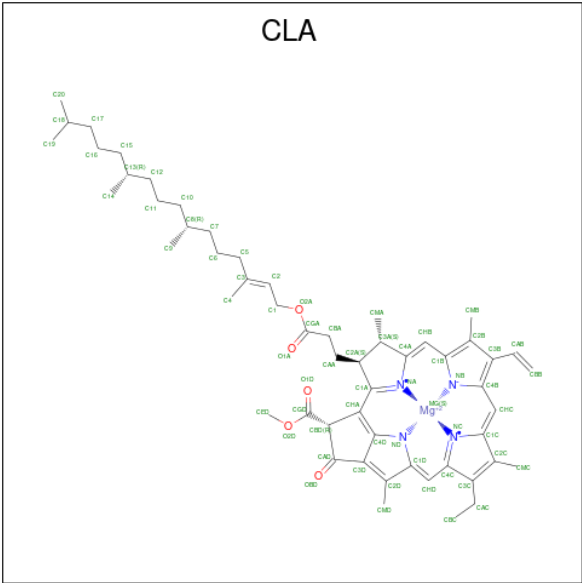
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	a	2	Total	Cl	0	0
			2	2		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	Mg	N	O	0	0
			134	55	69	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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

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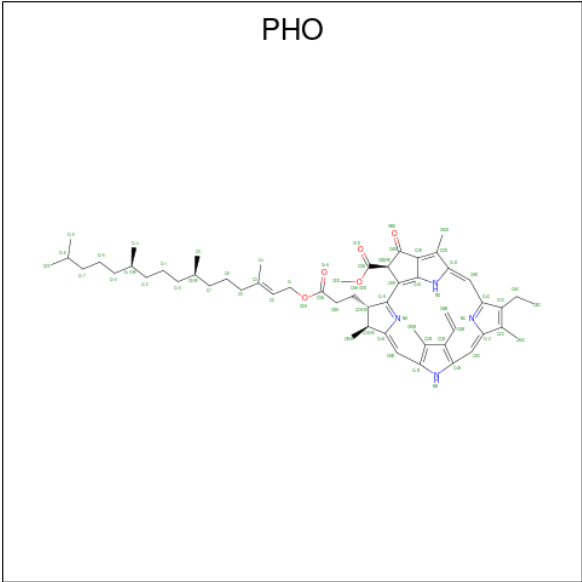
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 134	C 55	H 69	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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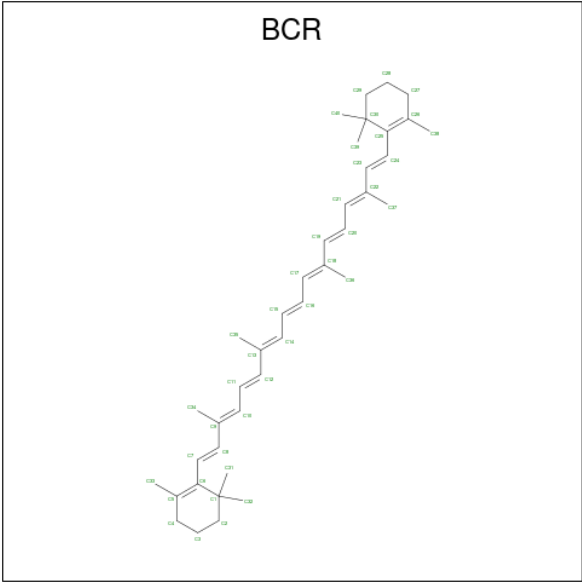
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



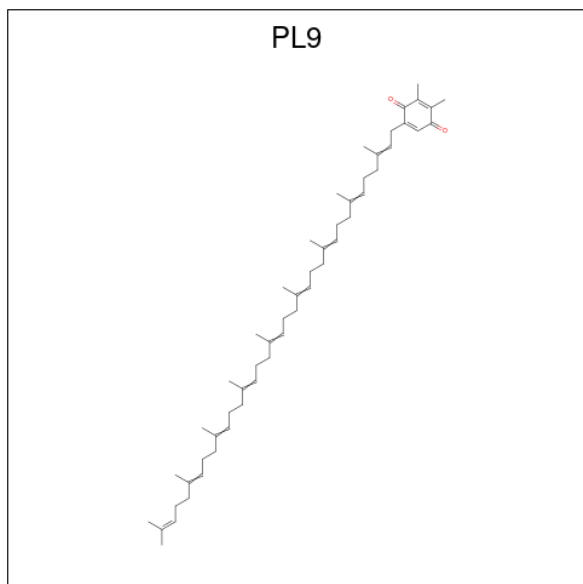
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



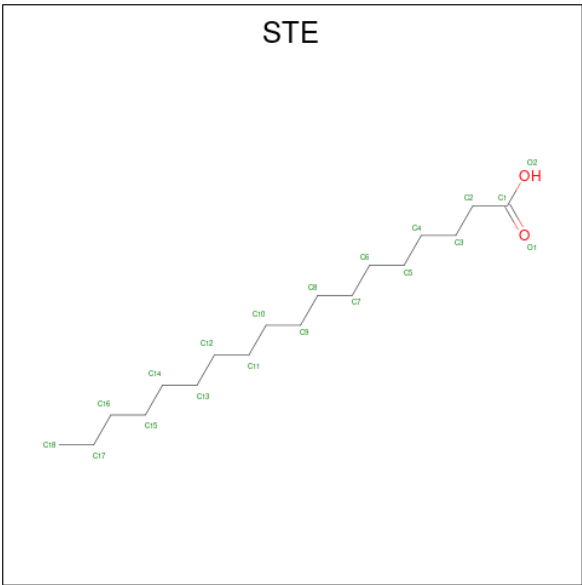
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	T	1	Total	C	H	0	0
			96	40	56		
26	a	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		

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



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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H		0	0
			23	9	14			
28	A	1	Total	C	H		0	0
			50	17	33			
28	A	1	Total	C	H		0	0
			32	11	21			
28	B	1	Total	C	H	O	0	0
			43	15	26	2		
28	B	1	Total	C	H	O	0	0
			46	16	28	2		
28	B	1	Total	C	H	O	0	0
			28	10	16	2		
28	B	1	Total	C	H		0	0
			41	15	26			
28	C	1	Total	C	H	O	0	0
			34	12	20	2		
28	C	1	Total	C	H		0	0
			11	5	6			
28	C	1	Total	C	H		0	0
			17	7	10			
28	C	1	Total	C	H		0	0
			26	10	16			
28	C	1	Total	C	H	O	0	0
			28	10	16	2		
28	C	1	Total	C	H		0	0
			47	16	31			
28	C	1	Total	C	H		0	0
			41	14	27			

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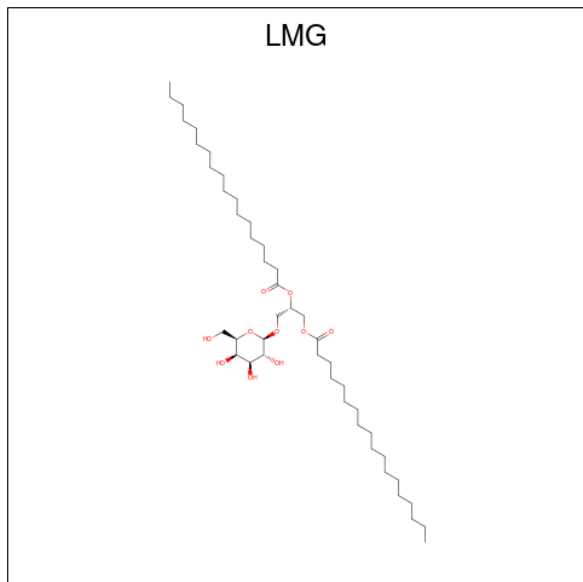
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C H 41 14 27	0	0
28	D	1	Total C H 26 9 17	0	0
28	E	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H 35 12 23	0	0
28	E	1	Total C H O 55 18 35 2	0	0
28	H	1	Total C H 53 18 35	0	0
28	I	1	Total C H O 43 15 26 2	0	0
28	I	1	Total C H O 37 13 22 2	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	M	1	Total C H 44 15 29	0	0
28	X	1	Total C H O 55 18 35 2	0	0
28	Z	1	Total C H 50 17 33	0	0
28	R	1	Total C H O 55 18 35 2	0	0
28	a	1	Total C H O 28 10 16 2	0	0
28	b	1	Total C H 47 16 31	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H O 40 14 24 2	0	0
28	b	1	Total C H 26 10 16	0	0
28	b	1	Total C H 23 8 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b	1	Total C H 32 11 21	0	0
28	c	1	Total C H 35 13 22	0	0
28	c	1	Total C H 53 18 35	0	0
28	d	1	Total C H O 55 18 35 2	0	0
28	d	1	Total C H O 55 18 35 2	0	0
28	d	1	Total C H O 34 12 20 2	0	0
28	e	1	Total C H 26 9 17	0	0
28	e	1	Total C H 26 9 17	0	0
28	e	1	Total C H O 31 11 18 2	0	0
28	f	1	Total C H 23 8 15	0	0
28	h	1	Total C H 29 10 19	0	0
28	i	1	Total C H O 28 10 16 2	0	0
28	i	1	Total C H 14 6 8	0	0
28	j	1	Total C H O 28 10 16 2	0	0
28	j	1	Total C H 47 16 31	0	0
28	l	1	Total C H 53 18 35	0	0
28	m	1	Total C H O 28 10 16 2	0	0
28	t	1	Total C H O 34 12 20 2	0	0
28	t	1	Total C H 26 10 16	0	0
28	x	1	Total C H O 55 18 35 2	0	0
28	z	1	Total C H 23 9 14	0	0

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



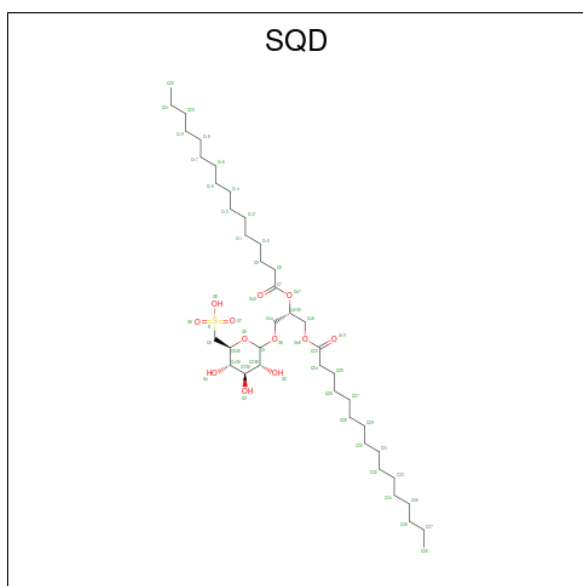
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	B	1	Total	C	H	O	0	0
			105	35	60	10		
29	B	1	Total	C	H	O	0	0
			123	41	72	10		
29	C	1	Total	C	H	O	0	0
			76	26	40	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			120	40	70	10		
29	D	1	Total	C	H	O	0	0
			123	41	72	10		
29	b	1	Total	C	H	O	0	0
			141	45	86	10		
29	c	1	Total	C	H	O	0	0
			71	25	41	5		
29	c	1	Total	C	H	O	0	0
			108	36	62	10		
29	c	1	Total	C	H	O	0	0
			117	38	69	10		
29	c	1	Total	C	H	O	0	0
			117	39	68	10		

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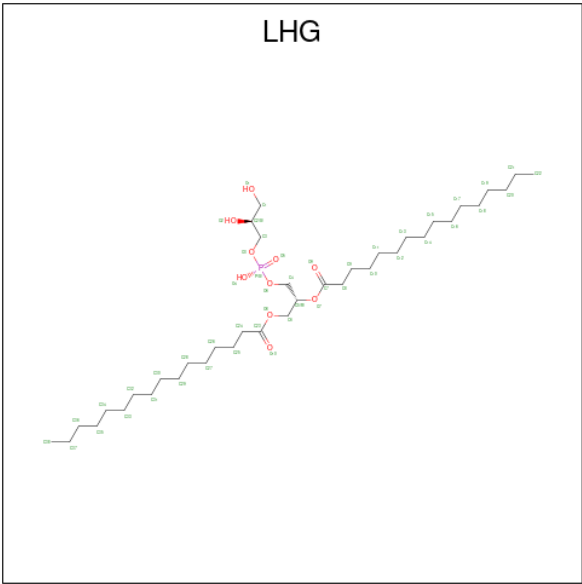
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	d	1	Total	C	H	O	0	0
			102	34	58	10		
29	m	1	Total	C	H	O	0	0
			123	41	72	10		
29	o	1	Total	C	H	O	0	0
			141	45	86	10		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



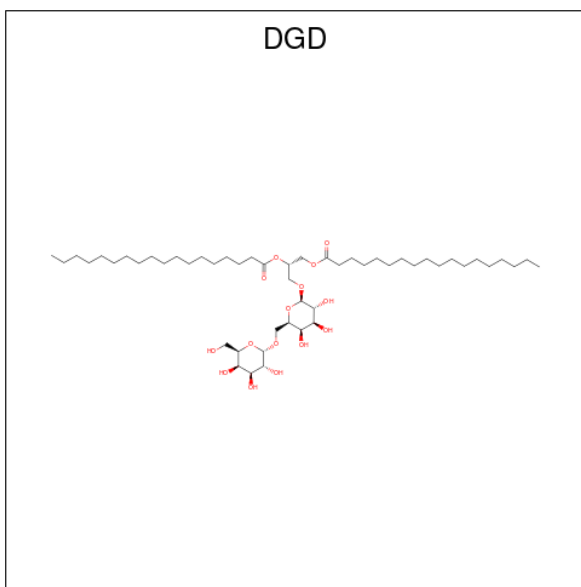
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
30	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
30	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
30	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



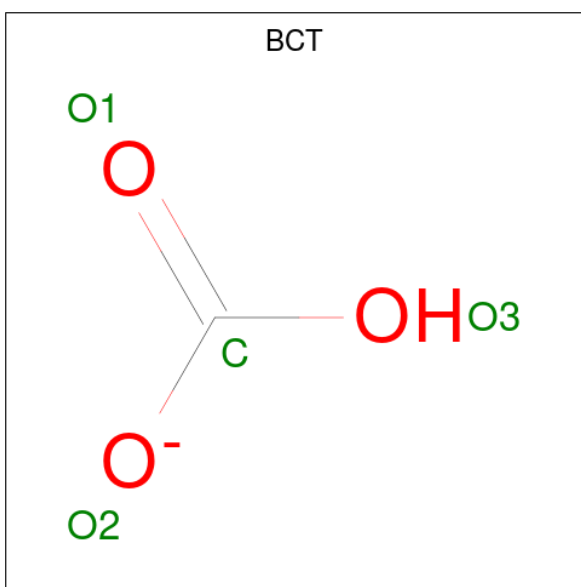
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
31	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



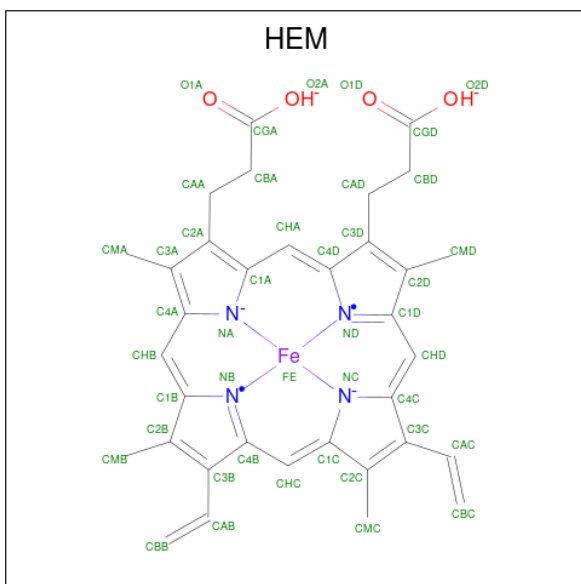
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	H	O	0	0
			162	51	96	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	H	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total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

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



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

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



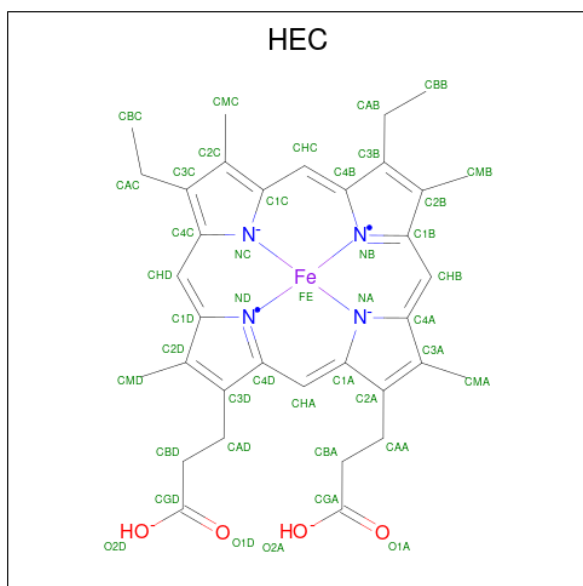
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	31	Total O 31 31	0	0
36	I	6	Total O 6 6	0	0
36	J	14	Total O 14 14	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	7	Total O 7 7	0	0
36	O	109	Total O 109 109	0	0
36	T	12	Total O 12 12	0	0
36	U	43	Total O 43 43	0	0
36	V	72	Total O 72 72	0	0
36	Y	1	Total O 1 1	0	0
36	X	17	Total O 17 17	0	0
36	Z	3	Total O 3 3	0	0
36	R	6	Total O 6 6	0	0
36	a	116	Total O 116 116	0	0
36	b	207	Total O 207 207	0	0
36	c	191	Total O 191 191	0	0
36	d	118	Total O 118 118	0	0
36	e	21	Total O 21 21	0	0
36	f	6	Total O 6 6	0	0
36	h	17	Total O 17 17	0	0

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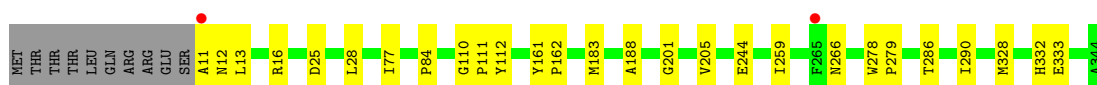
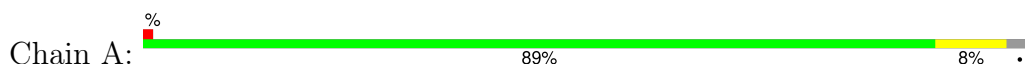
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	i	13	Total 13	O 13	0	0
36	j	7	Total 7	O 7	0	0
36	k	4	Total 4	O 4	0	0
36	l	11	Total 11	O 11	0	0
36	m	6	Total 6	O 6	0	0
36	o	101	Total 101	O 101	0	0
36	t	10	Total 10	O 10	0	0
36	u	74	Total 74	O 74	0	0
36	v	62	Total 62	O 62	0	0
36	y	2	Total 2	O 2	0	0
36	x	15	Total 15	O 15	0	0
36	z	4	Total 4	O 4	0	0
36	r	11	Total 11	O 11	0	0

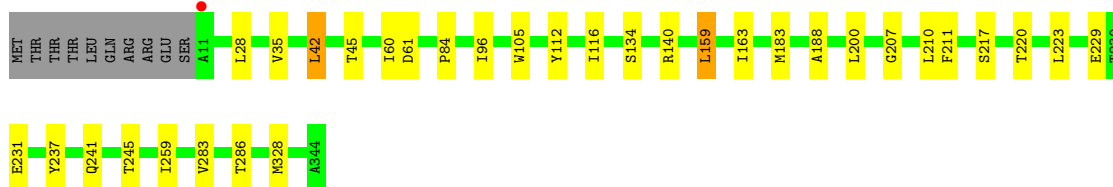
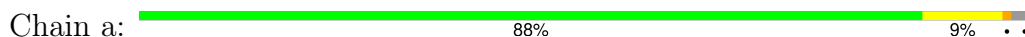
3 Residue-property plots [i](#)

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

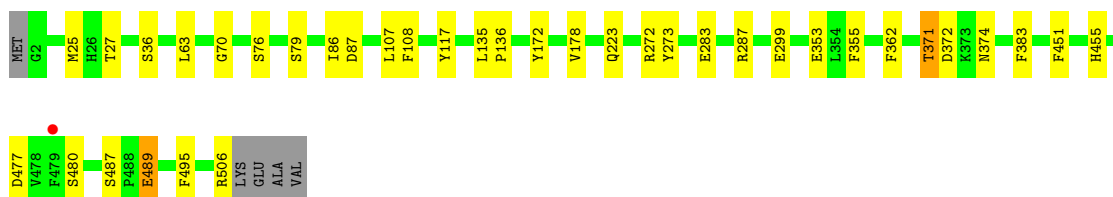
- Molecule 1: Photosystem II protein D1 1



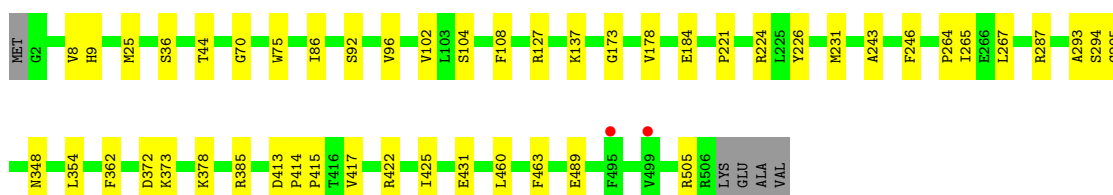
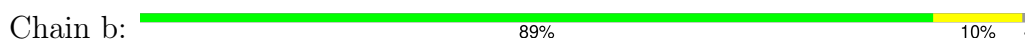
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

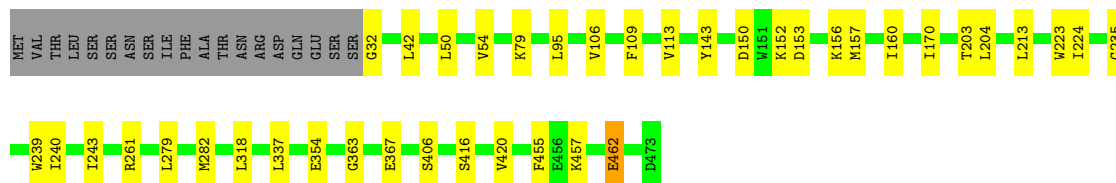


- Molecule 2: Photosystem II CP47 reaction center protein



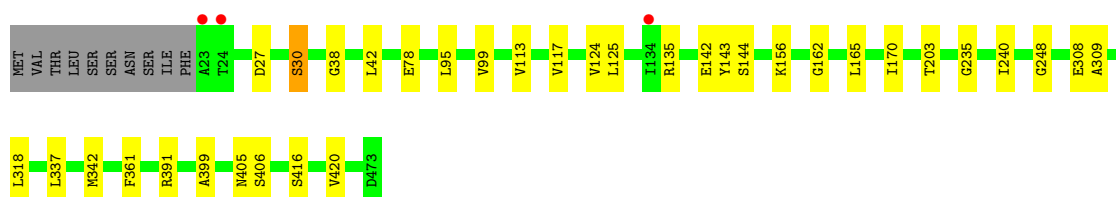
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  90% 7% .



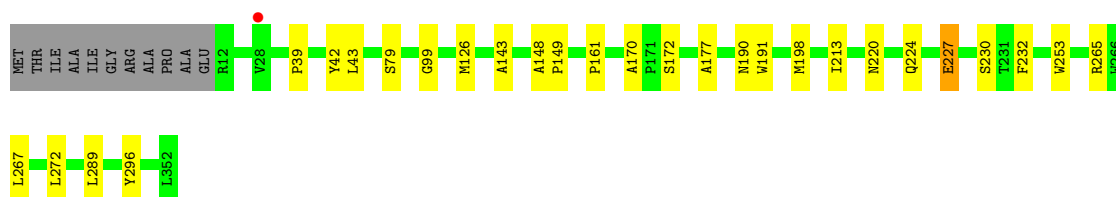
- Molecule 4: Photosystem II D2 protein

Chain D:  90% 7% .



- Molecule 4: Photosystem II D2 protein

Chain d:  89% 8% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  86% 11% .

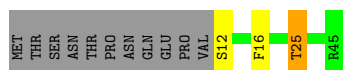


- Molecule 5: Cytochrome b559 subunit alpha

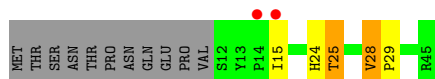
Chain e:  83% 14% .



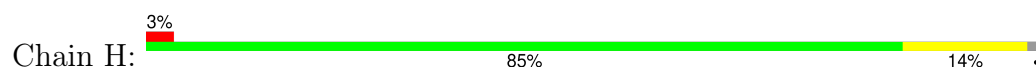
- Molecule 6: Cytochrome b559 subunit beta



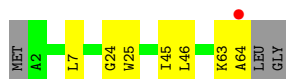
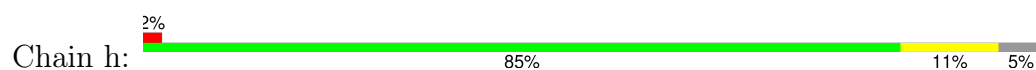
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



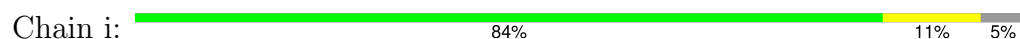
- Molecule 7: Photosystem II reaction center protein H



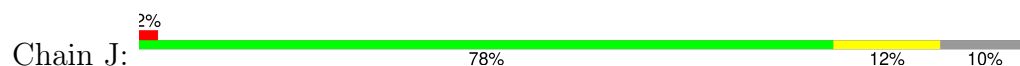
- Molecule 8: Photosystem II reaction center protein I

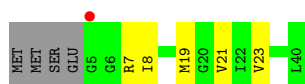


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





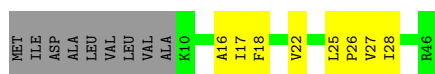
- Molecule 9: Photosystem II reaction center protein J

Chain j: 70% 20% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 63% 17% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 61% 20% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 14%



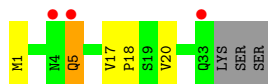
- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11% 3%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 8% 78% 11% 3% 8%

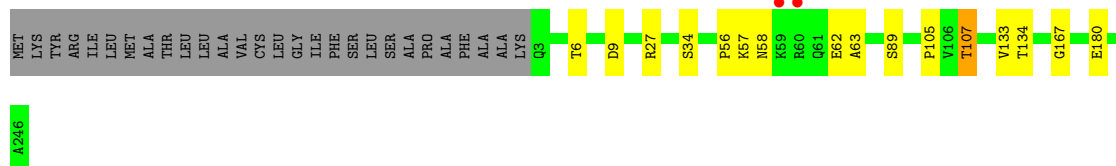
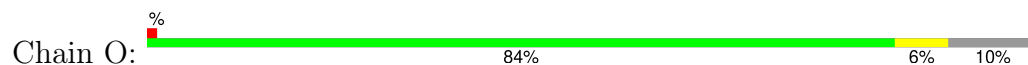


- Molecule 12: Photosystem II reaction center protein M

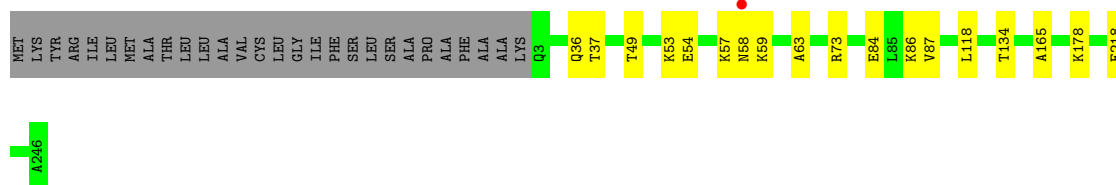
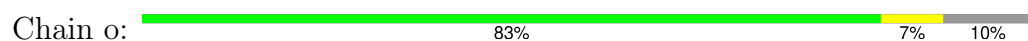
Chain m: 72% 17% 11%



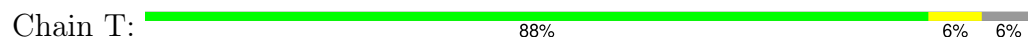
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



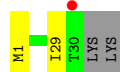
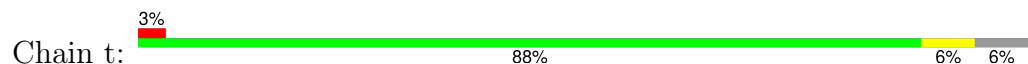
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



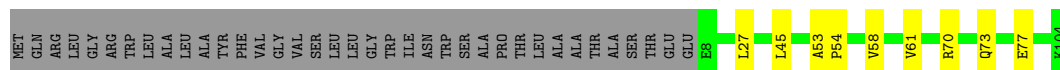
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

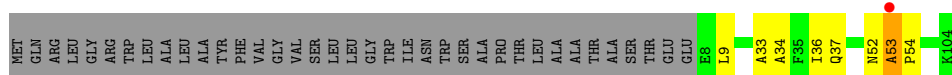


- Molecule 15: Photosystem II 12 kDa extrinsic protein

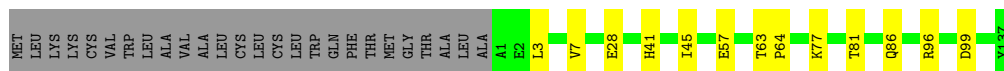


- Molecule 15: Photosystem II 12 kDa extrinsic protein

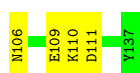




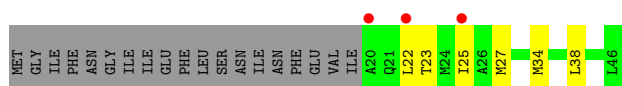
• Molecule 16: Cytochrome c-550



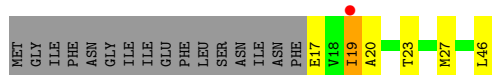
• Molecule 16: Cytochrome c-550



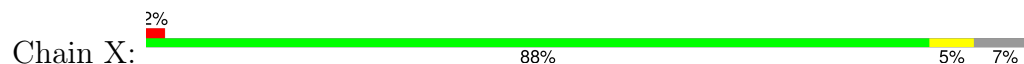
• Molecule 17: Photosystem II reaction center protein Ycf12



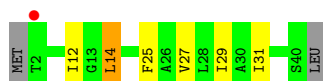
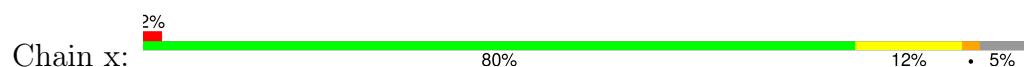
• Molecule 17: Photosystem II reaction center protein Ycf12



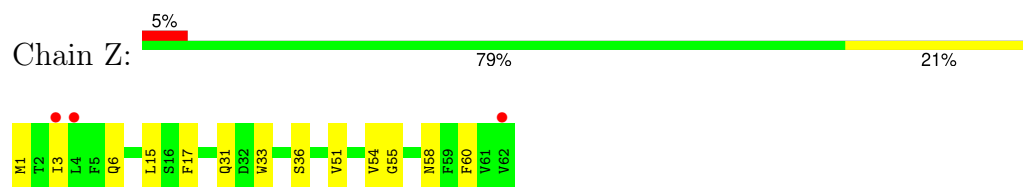
• Molecule 18: Photosystem II reaction center X protein



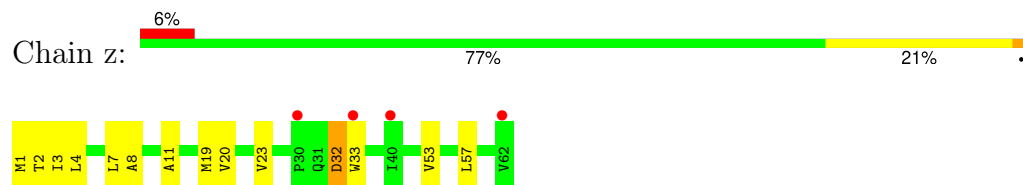
• Molecule 18: Photosystem II reaction center X protein



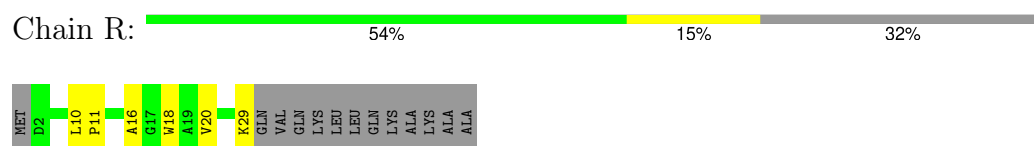
- Molecule 19: Photosystem II reaction center protein Z



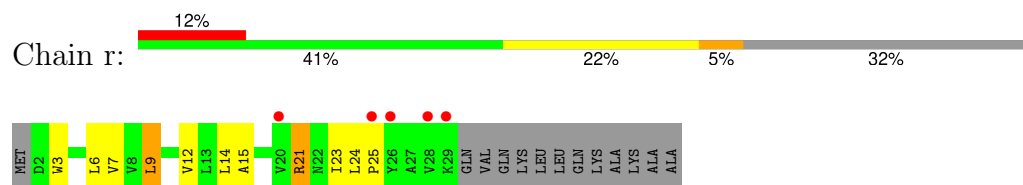
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.54Å 222.87Å 309.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.14 – 2.02 30.14 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.14-2.02) 87.4 (30.14-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.225 0.173 , 0.225	Depositor DCC
R_{free} test set	4689 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	104064	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2707	0.69	0/3692
1	a	0.59	0/2704	0.68	0/3688
2	B	0.55	0/4179	0.64	0/5693
2	b	0.54	0/4127	0.64	0/5623
3	C	0.57	1/3538 (0.0%)	0.65	1/4818 (0.0%)
3	c	0.51	0/3610	0.63	0/4914
4	D	0.59	0/2812	0.65	0/3832
4	d	0.55	0/2821	0.63	0/3844
5	E	0.45	0/688	0.58	0/940
5	e	0.39	0/683	0.53	0/932
6	F	0.41	0/284	0.53	0/387
6	f	0.44	0/284	0.61	0/387
7	H	0.51	0/517	0.62	0/705
7	h	0.42	0/505	0.59	0/689
8	I	0.53	0/293	0.60	0/396
8	i	0.54	0/293	0.58	0/396
9	J	0.49	0/263	0.56	0/356
9	j	0.42	0/263	0.50	0/356
10	K	0.38	0/303	0.51	0/416
10	k	0.40	0/303	0.49	0/416
11	L	0.59	0/311	0.69	0/422
11	l	0.61	0/303	0.64	0/412
12	M	0.56	0/249	0.76	0/341
12	m	0.57	0/244	0.69	0/334
13	O	0.53	0/1904	0.64	0/2585
13	o	0.53	0/1905	0.66	0/2583
14	T	0.53	0/257	0.69	0/349
14	t	0.58	0/255	0.60	0/346
15	U	0.49	0/785	0.60	0/1064
15	u	0.52	0/785	0.68	0/1064
16	V	0.53	0/1085	0.67	0/1473
16	v	0.48	0/1085	0.57	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.36	0/197	0.47	0/264
17	y	0.33	0/219	0.49	0/294
18	X	0.43	0/284	0.58	0/384
18	x	0.38	0/289	0.45	0/391
19	Z	0.34	0/490	0.53	0/669
19	z	0.30	0/488	0.47	0/666
20	R	0.32	0/227	0.48	0/313
20	r	0.26	0/227	0.41	0/313
All	All	0.53	1/42766 (0.0%)	0.63	1/58220 (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
15	u	0	1
16	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	462	GLU	CG-CD	-5.70	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	462	GLU	CA-CB-CG	-6.22	101.67	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
15	u	52	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2242	2519	17	0
1	a	2619	2232	2510	20	0
2	B	4016	3887	3871	23	0
2	b	3984	3842	3842	36	0
3	C	3417	3290	3337	30	3
3	c	3494	3361	3420	22	0
4	D	2717	2586	2621	16	0
4	d	2723	2592	2627	19	0
5	E	666	651	651	8	0
5	e	664	648	648	11	0
6	F	275	282	282	3	0
6	f	275	282	282	4	0
7	H	505	528	528	5	3
7	h	493	514	514	6	0
8	I	296	311	311	4	0
8	i	296	311	311	4	0
9	J	257	268	268	5	0
9	j	257	268	268	7	0
10	K	293	305	305	5	0
10	k	293	305	305	4	0
11	L	304	316	316	4	0
11	l	296	304	304	2	0
12	M	256	267	269	4	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	11	0
13	o	1874	1846	1846	8	0
14	T	258	261	261	2	0
14	t	256	256	256	1	0
15	U	774	773	773	5	0
15	u	774	773	773	5	0
16	V	1064	1070	1073	7	0
16	v	1064	1070	1073	16	0
17	Y	196	217	217	4	0
17	y	218	241	241	5	0
18	X	281	312	312	3	0
18	x	286	316	314	4	0
19	Z	479	516	516	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	477	509	509	8	0
20	R	221	238	238	4	0
20	r	221	238	238	8	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	249	261	264	4	0
24	B	1035	1139	1139	15	0
24	C	839	922	922	17	0
24	D	130	144	144	1	0
24	a	195	213	216	2	0
24	b	1035	1139	1139	20	0
24	c	839	919	919	9	0
24	d	195	216	216	3	0
25	A	64	74	74	0	0
25	D	64	74	74	2	0
25	d	128	148	148	0	0
26	A	40	56	56	2	0
26	B	120	168	168	6	0
26	C	80	112	112	1	0
26	D	40	56	56	5	0
26	H	40	56	56	2	0
26	K	80	112	112	8	0
26	T	40	56	56	5	0
26	a	40	56	56	0	0
26	b	120	168	168	6	0
26	c	80	112	112	6	0
26	d	40	56	56	1	0
26	h	40	56	56	1	0
26	k	80	112	112	3	0
26	t	40	56	56	3	0
27	A	55	80	80	1	0
27	D	55	80	80	1	0
27	a	55	80	80	1	0
27	d	55	80	80	0	0
28	A	37	68	68	1	0
28	B	62	96	96	1	0
28	C	92	153	153	2	0
28	D	9	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	E	44	74	74	1	0
28	H	18	35	35	0	0
28	I	32	48	48	0	0
28	J	12	16	16	0	0
28	M	40	67	67	0	0
28	R	20	35	35	4	0
28	X	20	35	35	1	0
28	Z	17	33	33	0	0
28	a	12	16	16	0	0
28	b	81	142	142	2	0
28	c	31	57	57	1	0
28	d	54	90	90	2	0
28	e	31	52	52	1	0
28	f	8	15	15	0	0
28	h	10	19	19	0	0
28	i	18	24	24	1	0
28	j	28	47	47	0	0
28	l	18	35	35	1	0
28	m	12	16	16	0	0
28	t	24	36	36	2	0
28	x	20	35	35	2	0
28	z	9	14	14	0	0
29	A	48	66	66	0	0
29	B	96	132	132	2	0
29	C	84	106	106	1	0
29	D	101	142	142	1	0
29	b	55	86	86	1	0
29	c	173	240	240	2	0
29	d	44	58	58	1	0
29	m	51	72	72	1	0
29	o	55	86	86	1	0
30	A	95	122	124	1	0
30	B	54	77	78	1	0
30	F	36	45	46	0	0
30	a	108	154	156	3	0
30	b	49	64	65	1	0
30	f	41	48	49	1	0
31	A	49	74	74	2	0
31	D	145	215	214	2	0
31	L	49	74	74	0	0
31	d	137	199	199	8	0
31	e	42	57	57	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	l	49	74	74	0	0
32	A	66	96	96	2	0
32	C	186	246	246	1	0
32	H	62	82	80	0	0
32	c	186	246	243	1	0
32	h	62	82	82	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	F	43	30	30	2	0
34	e	43	30	30	4	0
35	V	43	30	30	0	0
35	v	43	30	30	1	0
36	A	144	0	0	3	0
36	B	221	0	0	4	1
36	C	187	0	0	10	1
36	D	134	0	0	1	0
36	E	29	0	0	0	0
36	F	5	0	0	0	0
36	H	31	0	0	1	0
36	I	6	0	0	0	0
36	J	14	0	0	0	0
36	K	7	0	0	0	0
36	L	11	0	0	0	0
36	M	7	0	0	0	0
36	O	109	0	0	1	0
36	R	6	0	0	0	0
36	T	12	0	0	0	0
36	U	43	0	0	1	0
36	V	72	0	0	1	0
36	X	17	0	0	0	0
36	Y	1	0	0	0	0
36	Z	3	0	0	1	0
36	a	116	0	0	1	0
36	b	207	0	0	8	0
36	c	191	0	0	5	0
36	d	118	0	0	0	0
36	e	21	0	0	1	0
36	f	6	0	0	0	0
36	h	17	0	0	1	0
36	i	13	0	0	2	0
36	j	7	0	0	2	0
36	k	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	11	0	0	0	0
36	m	6	0	0	1	0
36	o	101	0	0	1	0
36	r	11	0	0	1	0
36	t	10	0	0	2	0
36	u	74	0	0	0	0
36	v	62	0	0	2	0
36	x	15	0	0	0	0
36	y	2	0	0	0	0
36	z	4	0	0	0	0
All	All	52598	51466	52195	444	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:ASP:N	36:C:601:HOH:O	1.91	1.04
16:v:6:GLU:OE1	36:v:301:HOH:O	1.80	0.98
13:o:84:GLU:OE2	13:o:86:LYS:NZ	1.96	0.97
24:b:613:CLA:H203	31:d:410:LHG:H223	1.48	0.95
13:O:27:ARG:NH1	36:O:301:HOH:O	2.03	0.92
16:v:77:LYS:NZ	16:v:109:GLU:OE2	2.03	0.91
3:c:27:ASP:OD1	3:c:30:SER:OG	1.89	0.91
1:A:11:ALA:O	1:A:16:ARG:NH2	2.07	0.88
31:e:103:LHG:O4	36:e:201:HOH:O	1.97	0.82
24:B:606:CLA:H141	36:B:917:HOH:O	1.80	0.82
16:v:13:ASN:OD1	16:v:15:GLU:OE1	1.99	0.79
16:v:13:ASN:CG	16:v:15:GLU:OE1	2.26	0.79
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.66	0.78
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.66	0.75
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.68	0.75
5:e:68:ASP:O	5:e:72:ALA:HB2	1.87	0.75
20:r:21:ARG:NH2	36:r:101:HOH:O	2.17	0.75
4:D:332:GLN:NE2	36:D:501:HOH:O	2.19	0.74
2:b:226:TYR:OH	36:b:701:HOH:O	2.03	0.74
15:U:73:GLN:NE2	15:U:77:GLU:OE2	2.19	0.73
13:o:218:GLU:OE2	36:o:401:HOH:O	2.06	0.73
29:c:518:LMG:O9	36:c:601:HOH:O	2.08	0.72
12:m:5:GLN:O	36:m:201:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.73	0.71
8:i:36:ASP:OD1	36:i:201:HOH:O	2.08	0.71
24:b:613:CLA:C20	31:d:410:LHG:H223	2.20	0.70
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.73	0.69
3:C:32:GLY:N	36:C:604:HOH:O	2.24	0.69
1:a:229:GLU:N	1:a:229:GLU:OE1	2.26	0.69
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.75	0.68
7:H:2:ALA:N	36:H:201:HOH:O	2.26	0.68
24:b:613:CLA:H192	31:d:410:LHG:C22	2.24	0.67
4:d:224:GLN:NE2	4:d:227[B]:GLU:OE1	2.27	0.67
15:u:53:ALA:HB1	15:u:54:PRO:CD	2.25	0.67
13:o:57:LYS:O	13:o:59:LYS:N	2.27	0.66
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.79	0.65
3:C:279:LEU:HD12	24:C:509:CLA:HED2	1.80	0.64
2:B:506:ARG:O	36:B:701:HOH:O	2.14	0.64
5:E:25:ILE:HD13	20:R:18:TRP:NE1	2.12	0.64
2:B:283:GLU:OE2	2:B:287[A]:ARG:NE	2.30	0.63
3:C:213:LEU:HG	24:C:506:CLA:H193	1.81	0.63
2:B:371:THR:HG23	2:B:372:ASP:O	1.98	0.63
26:b:618:BCR:H331	26:b:618:BCR:C8	2.29	0.63
1:A:25:ASP:OD1	36:A:701:HOH:O	2.15	0.63
9:j:34:ALA:O	36:j:201:HOH:O	2.15	0.63
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.32	0.62
3:C:170:ILE:HD13	24:C:512:CLA:H112	1.80	0.62
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.79	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.62
1:a:45:THR:HG23	24:d:404:CLA:H201	1.82	0.61
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.00	0.61
2:B:374:ASN:ND2	36:B:704:HOH:O	2.30	0.61
9:J:19:MET:O	9:J:23:VAL:HG23	2.01	0.61
3:c:117:VAL:HG12	29:c:518:LMG:H191	1.81	0.61
24:B:604:CLA:H43	24:B:605:CLA:H2	1.84	0.60
20:R:29:LYS:C	28:R:101:STE:H141	2.27	0.60
20:R:16:ALA:O	20:R:20:VAL:HG23	2.02	0.60
27:A:610:PL9:H361	6:F:25:THR:HG21	1.83	0.59
24:c:509:CLA:H43	24:c:509:CLA:O1A	2.02	0.59
5:e:30:LEU:HD11	34:e:102:HEM:CBB	2.32	0.59
24:B:614:CLA:H151	30:B:623:SQD:H381	1.83	0.59
6:f:24:HIS:O	6:f:28:VAL:HG13	2.03	0.59
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.34	0.59
17:y:17:GLU:HB3	17:y:19:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:23:THR:O	17:y:27:MET:HG3	2.03	0.59
26:K:101:BCR:H331	26:K:101:BCR:C8	2.33	0.59
26:d:407:BCR:H331	26:d:407:BCR:C8	2.33	0.59
3:C:152:LYS:NZ	36:C:603:HOH:O	2.22	0.58
24:c:512:CLA:H142	24:c:513:CLA:H142	1.84	0.58
24:A:608:CLA:H43	24:C:505:CLA:H191	1.84	0.58
36:A:783:HOH:O	13:O:107:THR:HG21	2.04	0.58
26:B:618:BCR:H331	26:B:618:BCR:C8	2.34	0.58
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.38	0.58
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.84	0.58
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.85	0.58
2:B:117:TYR:HA	11:L:1:MET:HE1	1.86	0.57
26:b:619:BCR:H331	26:b:619:BCR:C8	2.34	0.57
6:f:15:ILE:HG21	20:r:23:ILE:HD11	1.86	0.57
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.86	0.56
26:B:619:BCR:H331	26:B:619:BCR:C8	2.35	0.56
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.87	0.56
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.88	0.56
24:B:606:CLA:H191	28:B:622:STE:O1	2.06	0.56
24:b:602:CLA:H92	7:h:46:LEU:HD13	1.88	0.56
9:j:7:ARG:NH2	36:j:202:HOH:O	2.39	0.56
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.88	0.55
10:K:25:LEU:HD22	26:K:102:BCR:H332	1.88	0.55
26:b:618:BCR:H331	26:b:618:BCR:HC8	1.87	0.55
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.36	0.55
24:C:502:CLA:H61	24:C:512:CLA:H42	1.87	0.55
24:b:613:CLA:H192	31:d:410:LHG:H223	1.88	0.55
3:C:156:LYS:NZ	36:C:602:HOH:O	2.21	0.55
4:D:279:LEU:HD22	25:D:402:PHO:HBC3	1.89	0.55
28:d:409:STE:H183	28:d:413:STE:H172	1.88	0.55
1:A:290:ILE:HG13	24:A:605:CLA:HED2	1.89	0.55
4:d:99:GLY:HA3	28:x:101:STE:H41	1.89	0.54
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.90	0.54
26:h:101:BCR:H331	26:h:101:BCR:C8	2.38	0.54
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.88	0.54
24:b:607:CLA:H142	24:b:613:CLA:H171	1.90	0.54
4:d:272:LEU:C	4:d:272:LEU:HD23	2.32	0.54
10:k:10:LYS:N	36:k:204:HOH:O	2.41	0.54
26:T:101:BCR:H382	26:T:101:BCR:H23C	1.90	0.53
30:a:610:SQD:H462	4:d:232:PHE:CE2	2.43	0.53
34:e:102:HEM:HHH	34:e:102:HEM:HBC2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:17:VAL:HB	12:m:18:PRO:HD3	1.90	0.53
3:C:95:LEU:HD21	24:C:501:CLA:OBD	2.09	0.53
24:C:512:CLA:H122	24:C:512:CLA:H91	1.91	0.53
4:D:272:LEU:C	4:D:272:LEU:HD23	2.34	0.53
24:b:602:CLA:H43	7:h:45:ILE:HG22	1.90	0.53
3:C:279:LEU:CD1	24:C:509:CLA:HED2	2.39	0.53
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.90	0.53
10:k:38:VAL:HG23	26:k:101:BCR:H21C	1.91	0.53
31:D:409:LHG:H321	14:T:21:ILE:HD11	1.90	0.52
24:b:614:CLA:H122	24:b:614:CLA:H91	1.92	0.52
3:c:391[B]:ARG:HD3	36:c:663:HOH:O	2.09	0.52
19:z:1:MET:SD	19:z:1:MET:N	2.81	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.92	0.52
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.91	0.52
9:J:8:ILE:HD12	9:J:8:ILE:H	1.74	0.52
13:O:56:PRO:HD3	13:O:63:ALA:HB2	1.92	0.52
17:y:19:ILE:O	17:y:23:THR:HG22	2.09	0.52
1:A:244:GLU:OE1	4:D:264:LYS:NZ	2.43	0.52
26:K:102:BCR:H322	19:Z:17:PHE:CE2	2.45	0.52
24:b:614:CLA:H91	24:b:614:CLA:C12	2.40	0.52
3:c:406:SER:HA	3:c:420:VAL:HG23	1.92	0.52
2:b:422:ARG:O	2:b:425:ILE:HG12	2.10	0.52
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.45	0.52
24:C:513:CLA:H202	28:C:526:STE:C17	2.40	0.51
2:b:287:ARG:HD3	36:b:770:HOH:O	2.08	0.51
2:b:372:ASP:OD2	36:b:703:HOH:O	2.19	0.51
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.91	0.51
26:D:405:BCR:H23C	26:D:405:BCR:H392	1.92	0.51
28:R:101:STE:H91	28:R:101:STE:H32	1.92	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
24:C:513:CLA:H202	28:C:526:STE:H172	1.92	0.51
4:D:13:GLY:O	4:D:17:ILE:HG12	2.11	0.51
2:B:223:GLN:NE2	36:B:711:HOH:O	2.43	0.51
8:i:34:ARG:NH1	36:i:203:HOH:O	2.44	0.51
16:v:99:ASP:N	16:v:99:ASP:OD1	2.42	0.51
13:O:56:PRO:O	13:O:58:ASN:N	2.41	0.50
2:b:184:GLU:OE1	36:b:704:HOH:O	2.19	0.50
29:o:301:LMG:O8	29:o:301:LMG:C10	2.59	0.50
24:C:506:CLA:H143	32:C:521:DGD:CGA	2.41	0.50
2:B:87:ASP:C	2:B:87:ASP:OD1	2.55	0.50
3:C:318:LEU:C	3:C:318:LEU:HD23	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.46	0.50
13:o:57:LYS:HB3	13:o:59:LYS:NZ	2.26	0.50
7:h:63:LYS:O	7:h:64:ALA:HB2	2.12	0.50
2:B:489:GLU:HG2	2:B:495:PHE:CE1	2.47	0.50
19:Z:3:ILE:HA	19:Z:6:GLN:HE21	1.77	0.50
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.27	0.50
13:o:36:GLN:HG3	13:o:37:THR:N	2.27	0.50
4:d:42:TYR:CE1	6:f:25:THR:HG23	2.47	0.49
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.94	0.49
3:C:455:PHE:HD2	8:I:33:LYS:HG3	1.76	0.49
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.27	0.49
1:a:42:LEU:HD13	30:a:611:SQD:H171	1.93	0.49
3:c:391[B]:ARG:NH2	36:c:605:HOH:O	2.45	0.49
26:K:102:BCR:H321	26:K:102:BCR:HC8	1.94	0.49
4:d:267:LEU:C	4:d:267:LEU:HD23	2.36	0.49
3:c:38:GLY:HA3	24:c:511:CLA:HMD2	1.95	0.49
5:e:30:LEU:HD23	20:r:12:VAL:HG12	1.94	0.49
16:v:110:LYS:NZ	16:v:111:ASP:OD1	2.37	0.49
8:I:2:GLU:O	8:I:6:ILE:HG13	2.13	0.49
16:V:99:ASP:OD1	16:V:99:ASP:N	2.46	0.49
24:b:604:CLA:H42	24:b:605:CLA:H2	1.95	0.49
4:D:269:PHE:CD2	31:D:411:LHG:HC12	2.48	0.49
2:B:172:TYR:OH	7:H:63:LYS:HE3	2.13	0.48
26:D:405:BCR:H331	26:D:405:BCR:C8	2.43	0.48
16:V:28:GLU:HG2	36:V:353:HOH:O	2.12	0.48
11:L:20:GLY:O	11:L:24:ILE:HD12	2.13	0.48
12:M:5:GLN:HE21	12:M:5:GLN:CA	2.25	0.48
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.78	0.48
5:e:74:GLN:OE1	5:e:77:GLU:OE1	2.31	0.48
26:D:405:BCR:H402	9:J:21:VAL:CG1	2.44	0.48
13:o:53:LYS:HB2	13:o:53:LYS:HZ3	1.78	0.48
6:F:16:PHE:H	28:R:101:STE:H181	1.79	0.48
24:B:601:CLA:H192	24:B:601:CLA:C15	2.44	0.48
3:C:150:ASP:O	36:C:601:HOH:O	2.20	0.48
15:u:53:ALA:CB	15:u:54:PRO:CD	2.91	0.48
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.96	0.48
31:A:615:LHG:H381	36:A:843:HOH:O	2.13	0.48
3:C:109:PHE:O	3:C:113:VAL:HG23	2.14	0.48
26:T:101:BCR:H311	26:T:101:BCR:C8	2.42	0.48
9:j:18:GLY:O	9:j:21:VAL:HG22	2.13	0.48
24:B:605:CLA:H62	24:B:605:CLA:H41	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:605:CLA:HHC	24:B:605:CLA:HBB1	1.96	0.48
15:U:70:ARG:NH2	36:U:201:HOH:O	2.29	0.48
2:b:221:PRO:HB3	24:b:609:CLA:O1D	2.13	0.48
26:k:101:BCR:H321	26:k:101:BCR:HC8	1.95	0.48
1:a:183:MET:HA	24:a:605:CLA:HMD1	1.95	0.47
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.48	0.47
28:t:102:STE:O1	36:t:201:HOH:O	2.20	0.47
3:C:79:LYS:NZ	36:C:607:HOH:O	2.33	0.47
8:I:7:THR:O	8:I:11:VAL:HG23	2.15	0.47
26:K:102:BCR:H322	19:Z:17:PHE:CZ	2.50	0.47
26:H:101:BCR:H331	26:H:101:BCR:C8	2.43	0.47
18:X:38:GLN:NE2	18:X:38:GLN:HA	2.30	0.47
4:d:39:PRO:O	4:d:43:LEU:HG	2.14	0.47
4:D:131:GLU:O	4:D:135:LEU:HG	2.15	0.47
32:A:617:DGD:HD5	2:b:75:TRP:HB3	1.95	0.47
2:B:506:ARG:HG2	2:B:506:ARG:HH11	1.79	0.47
4:D:150:ILE:O	4:D:154:VAL:HG13	2.15	0.47
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.96	0.47
31:d:410:LHG:H212	12:m:18:PRO:HG3	1.96	0.47
4:D:194:ASN:HA	4:D:295:SER:OG	2.14	0.47
2:b:92:SER:O	2:b:96:VAL:HG23	2.15	0.47
11:l:7:ARG:HH22	28:l:102:STE:H52	1.80	0.47
16:v:41:HIS:HA	16:v:45:ILE:O	2.15	0.47
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.47
26:c:514:BCR:H352	28:c:517:STE:C1	2.45	0.47
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.97	0.46
24:C:512:CLA:H91	24:C:512:CLA:C12	2.45	0.46
26:B:619:BCR:H331	26:B:619:BCR:HC8	1.97	0.46
3:C:150:ASP:C	36:C:601:HOH:O	2.58	0.46
4:D:209:LEU:HD23	4:D:209:LEU:C	2.41	0.46
2:b:137:LYS:HE3	36:h:202:HOH:O	2.14	0.46
2:b:431:GLU:HG2	36:b:706:HOH:O	2.15	0.46
26:c:514:BCR:H24C	26:c:514:BCR:H371	1.81	0.46
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.49	0.46
2:b:489:GLU:OE1	2:b:505:ARG:NH2	2.48	0.46
5:e:23:HIS:HA	5:e:26:THR:OG1	2.16	0.46
26:t:101:BCR:H23C	26:t:101:BCR:H382	1.97	0.46
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.46
2:B:36:SER:OG	26:B:618:BCR:H362	2.15	0.46
24:C:513:CLA:H203	26:K:101:BCR:C17	2.45	0.46
26:D:405:BCR:H20C	26:D:405:BCR:H361	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:245:THR:HB	4:d:265:ARG:HE	1.80	0.46
3:C:50:LEU:O	3:C:54:VAL:HG23	2.15	0.46
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.81	0.46
3:c:337:LEU:HD22	3:c:342:MET:HE3	1.97	0.46
9:j:18:GLY:O	9:j:22:ILE:HD12	2.15	0.46
2:b:373:LYS:HG3	36:b:717:HOH:O	2.15	0.46
7:h:63:LYS:O	7:h:64:ALA:CB	2.64	0.46
5:E:35:TRP:HE1	28:E:103:STE:H141	1.81	0.45
19:Z:55:GLY:HA2	19:Z:58:ASN:CB	2.46	0.45
17:Y:34:MET:O	17:Y:38:LEU:HG	2.16	0.45
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.51	0.45
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.98	0.45
4:d:126:MET:HE3	4:d:143:ALA:O	2.15	0.45
19:z:8:ALA:O	19:z:11:ALA:HB3	2.16	0.45
9:j:19:MET:O	9:j:23:VAL:HG23	2.16	0.45
26:k:102:BCR:H24C	26:k:102:BCR:H371	1.80	0.45
3:C:457:LYS:NZ	36:C:611:HOH:O	2.49	0.45
24:D:404:CLA:H42	7:H:43:LEU:HD11	1.99	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.45
15:U:27:LEU:HD13	15:U:61:VAL:CG1	2.47	0.45
18:X:16:SER:HB3	28:X:101:STE:H112	1.99	0.45
2:b:413:ASP:O	2:b:417:VAL:HG23	2.16	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
13:O:133:VAL:C	13:O:134:THR:HG23	2.42	0.45
19:Z:1:MET:HE3	19:Z:60:PHE:CD2	2.52	0.45
18:x:12:ILE:HD13	28:x:101:STE:H31	1.99	0.45
20:r:9:LEU:O	20:r:12:VAL:HG22	2.17	0.45
2:B:283:GLU:OE2	2:B:287[A]:ARG:NH2	2.50	0.45
2:b:104:SER:OG	30:b:620:SQD:H221	2.17	0.45
17:Y:23:THR:CG2	17:Y:27:MET:HE3	2.47	0.44
1:a:283:VAL:HA	1:a:286:THR:HG22	1.98	0.44
5:E:68:ASP:O	5:E:72:ALA:HB2	2.18	0.44
10:K:25:LEU:HA	10:K:28:ILE:HD12	1.99	0.44
2:B:86:ILE:HG12	2:B:87:ASP:N	2.32	0.44
1:a:210:LEU:C	1:a:210:LEU:HD23	2.43	0.44
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.99	0.44
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.00	0.44
10:k:25:LEU:N	10:k:26:PRO:CD	2.80	0.44
27:D:406:PL9:H412	11:L:29:LEU:HD23	1.99	0.44
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.99	0.44
1:a:217:SER:HA	4:d:272:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:231:MET:HB3	24:b:610:CLA:HBC1	1.99	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.44
24:B:602:CLA:HBB1	24:B:602:CLA:HMB1	1.98	0.44
29:B:620:LMG:O10	29:B:620:LMG:HC72	2.17	0.44
9:J:8:ILE:HD12	9:J:8:ILE:N	2.33	0.44
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.98	0.44
5:e:17:VAL:HB	9:j:7:ARG:HH11	1.82	0.44
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.53	0.44
1:a:207:GLY:O	1:a:211:PHE:CD2	2.70	0.44
1:a:220:THR:HA	1:a:223:LEU:HD13	2.00	0.44
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.81	0.44
5:e:63:ILE:HG23	5:e:64:PRO:HD2	1.99	0.44
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.99	0.44
26:B:619:BCR:H383	26:B:619:BCR:H23C	2.00	0.44
27:a:609:PL9:H251	31:e:103:LHG:H211	2.00	0.44
29:b:623:LMG:O9	29:b:623:LMG:C9	2.65	0.44
8:i:35:LYS:HD2	8:i:35:LYS:N	2.33	0.44
15:u:33:ALA:O	15:u:36:ILE:HG13	2.18	0.44
2:B:135:LEU:N	2:B:136:PRO:CD	2.81	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.44
18:x:27:VAL:HG12	18:x:31:ILE:HD13	1.99	0.44
2:b:44:THR:HG22	28:b:621:STE:H101	2.00	0.43
26:b:618:BCR:H15C	26:b:618:BCR:H351	1.81	0.43
26:c:515:BCR:C8	26:c:515:BCR:H331	2.48	0.43
19:z:4:LEU:HA	19:z:7:LEU:HD12	2.01	0.43
10:K:27:VAL:HG12	10:K:27:VAL:O	2.17	0.43
26:T:101:BCR:H382	26:T:101:BCR:C23	2.48	0.43
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.53	0.43
5:e:17:VAL:HB	9:j:7:ARG:NH1	2.33	0.43
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.06	0.43
3:C:150:ASP:HB3	36:C:601:HOH:O	2.17	0.43
2:b:226:TYR:HA	2:b:231:MET:HG3	1.99	0.43
24:c:501:CLA:H192	24:c:507:CLA:CBB	2.47	0.43
5:e:74:GLN:OE1	5:e:74:GLN:HA	2.17	0.43
26:A:609:BCR:C8	26:A:609:BCR:H331	2.49	0.43
2:B:477:ASP:OD1	2:B:477:ASP:N	2.51	0.43
26:T:101:BCR:HC7	26:T:101:BCR:H331	1.79	0.43
2:b:378:LYS:NZ	36:b:703:HOH:O	2.50	0.43
3:c:95:LEU:HD21	24:c:501:CLA:OBD	2.18	0.43
4:d:198:MET:SD	24:d:404:CLA:HED2	2.58	0.43
32:A:617:DGD:CAB	8:I:1:FME:HCN	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:135:ARG:CD	36:c:637:HOH:O	2.67	0.43
3:c:203:THR:O	3:c:235:GLY:HA3	2.18	0.43
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.43
16:V:77:LYS:O	16:V:96:ARG:HB2	2.18	0.43
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.43
11:l:24:ILE:HD13	12:m:18:PRO:HB2	2.00	0.43
26:K:101:BCR:H20C	26:K:101:BCR:H361	1.85	0.43
15:U:58:VAL:O	15:U:61:VAL:HG22	2.19	0.43
28:i:101:STE:O2	28:i:101:STE:H61	2.19	0.43
16:v:13:ASN:CB	16:v:15:GLU:OE1	2.66	0.43
5:e:53:ASP:O	16:v:1:ALA:N	2.52	0.43
2:b:224:ARG:HG2	7:h:24:GLY:O	2.19	0.43
3:c:142:GLU:N	3:c:142:GLU:OE1	2.52	0.43
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.43
20:r:24:LEU:N	20:r:25:PRO:HD2	2.34	0.43
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.00	0.43
24:c:504:CLA:H141	24:c:508:CLA:H143	2.00	0.43
14:t:29:ILE:HD12	14:t:29:ILE:H	1.83	0.43
17:y:17:GLU:O	17:y:20:ALA:HB3	2.19	0.43
3:C:261:ARG:NE	36:C:605:HOH:O	2.32	0.42
10:K:25:LEU:N	10:K:26:PRO:CD	2.82	0.42
2:b:36:SER:OG	26:b:618:BCR:H362	2.18	0.42
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.42
24:b:604:CLA:HBA2	24:b:612:CLA:H151	2.02	0.42
28:b:627:STE:H171	28:d:413:STE:H52	2.01	0.42
1:A:28:LEU:HD12	30:A:616:SQD:H112	2.01	0.42
24:B:603:CLA:C4D	24:B:605:CLA:H43	2.48	0.42
6:F:16:PHE:H	28:R:101:STE:C18	2.32	0.42
24:C:508:CLA:HBC3	24:C:510:CLA:H71	2.01	0.42
7:H:31:MET:O	7:H:35:MET:HG3	2.19	0.42
2:b:385:ARG:HG2	13:o:165:ALA:O	2.19	0.42
24:b:613:CLA:C18	31:d:410:LHG:H223	2.49	0.42
3:c:156:LYS:NZ	36:c:610:HOH:O	2.51	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.44	0.42
19:z:32:ASP:N	19:z:32:ASP:OD1	2.51	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.42
16:V:81:THR:CG2	16:V:86:GLN:HG2	2.50	0.42
2:b:293:ALA:C	2:b:295:GLY:H	2.27	0.42
16:v:13:ASN:HB2	16:v:15:GLU:OE1	2.19	0.42
20:R:10:LEU:HB3	20:R:11:PRO:HD3	2.01	0.42
1:a:159:LEU:O	1:a:163:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:613:CLA:H203	31:d:410:LHG:C22	2.34	0.42
26:A:609:BCR:H24C	26:A:609:BCR:H371	1.85	0.42
24:B:607:CLA:H193	11:L:27:LEU:HD11	2.02	0.42
24:B:609:CLA:H91	24:B:609:CLA:H112	1.86	0.42
26:C:520:BCR:H15C	26:C:520:BCR:H351	1.95	0.42
26:D:405:BCR:H402	9:J:21:VAL:HG11	2.01	0.42
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.54	0.42
16:v:40:CYS:SG	35:v:201:HEC:HMC1	2.60	0.42
4:D:17:ILE:O	4:D:20:ASP:HB2	2.19	0.42
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	2.01	0.42
19:z:2:THR:O	19:z:3:ILE:C	2.62	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	2.01	0.42
16:V:81:THR:HG23	16:V:86:GLN:HG2	2.01	0.42
19:Z:51:VAL:O	19:Z:54:VAL:O	2.38	0.42
20:r:3:TRP:O	20:r:7:VAL:HG13	2.19	0.42
29:B:620:LMG:O6	29:D:407:LMG:HC3	2.20	0.42
3:C:157:MET:HE2	3:C:160:ILE:HD12	2.01	0.42
25:D:402:PHO:HBC2	25:D:402:PHO:HHD	2.01	0.42
3:c:113:VAL:O	3:c:117:VAL:HG23	2.20	0.42
24:d:406:CLA:H93	18:x:14:LEU:HD22	2.02	0.42
13:o:54:GLU:O	13:o:63:ALA:HB1	2.19	0.42
15:u:34:ALA:O	15:u:37:GLN:HG3	2.19	0.42
24:A:612:CLA:HHC	24:A:612:CLA:HBB1	2.01	0.42
2:b:86:ILE:HD12	2:b:86:ILE:O	2.19	0.42
24:B:606:CLA:H92	26:B:619:BCR:C10	2.50	0.41
24:B:608:CLA:C1A	24:B:608:CLA:CGA	2.98	0.41
5:E:22[A]:ILE:HG23	5:E:23:HIS:HD1	1.85	0.41
26:H:101:BCR:H11C	26:H:101:BCR:H341	1.94	0.41
18:X:38:GLN:HA	18:X:38:GLN:HE21	1.84	0.41
1:A:183:MET:HA	24:A:605:CLA:HMD1	2.02	0.41
2:B:272:ARG:HG3	2:B:273:TYR:N	2.35	0.41
2:b:102:VAL:HA	26:b:618:BCR:C40	2.51	0.41
2:b:414:PRO:N	2:b:415:PRO:CD	2.83	0.41
3:c:405:ASN:HB3	32:c:521:DGD:O1B	2.21	0.41
29:d:414:LMG:C43	28:e:105:STE:C10	2.98	0.41
34:e:102:HEM:HMA1	20:r:23:ILE:HD13	2.00	0.41
19:Z:31:GLN:O	19:Z:33:TRP:N	2.50	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
26:c:515:BCR:H15C	26:c:515:BCR:H351	1.86	0.41
4:d:79:SER:HA	4:d:172:SER:HB3	2.01	0.41
5:e:26:THR:HG22	20:r:15:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:LEU:HD11	29:C:516:LMG:O2	2.20	0.41
3:C:337:LEU:HD23	13:O:105:PRO:CG	2.50	0.41
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.55	0.41
24:b:604:CLA:H41	24:b:604:CLA:H62	1.75	0.41
24:b:613:CLA:C19	31:d:410:LHG:H223	2.49	0.41
16:V:57:GLU:H	16:V:57:GLU:CD	2.29	0.41
30:a:611:SQD:H1	36:a:703:HOH:O	2.20	0.41
24:b:603:CLA:H2	24:b:605:CLA:H91	2.02	0.41
18:x:25:PHE:O	18:x:29:ILE:HG13	2.20	0.41
1:A:84:PRO:HA	1:A:112:TYR:CG	2.56	0.41
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.55	0.41
19:z:19:MET:O	19:z:23:VAL:HG23	2.21	0.41
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.09	0.41
13:O:180:GLU:CD	13:O:180:GLU:H	2.29	0.41
26:c:514:BCR:H15C	26:c:514:BCR:H351	1.90	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.03	0.41
1:A:110:GLY:N	1:A:111:PRO:CD	2.84	0.41
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.03	0.41
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.03	0.41
2:b:231:MET:HE2	24:b:610:CLA:HMC2	2.02	0.41
30:f:101:SQD:O2	30:f:101:SQD:C44	2.68	0.41
28:t:102:STE:C1	36:t:201:HOH:O	2.69	0.41
16:v:80:THR:HA	16:v:86:GLN:O	2.20	0.41
31:A:615:LHG:H241	31:A:615:LHG:H302	2.03	0.41
2:B:299[B]:GLU:H	2:B:299[B]:GLU:CD	2.28	0.41
24:B:601:CLA:H192	24:B:601:CLA:H151	2.02	0.41
2:b:460:LEU:O	2:b:463:PHE:HB3	2.21	0.41
24:b:607:CLA:H142	24:b:613:CLA:C17	2.51	0.41
3:c:143:TYR:HE2	24:c:513:CLA:H2A	1.86	0.41
3:C:239:TRP:O	3:C:243:ILE:HG13	2.21	0.40
24:a:607:CLA:H141	8:i:9:TYR:HD2	1.86	0.40
1:A:11:ALA:O	1:A:16:ARG:CZ	2.66	0.40
1:A:266:ASN:OD1	1:A:266:ASN:C	2.64	0.40
1:A:332:HIS:O	1:A:333:GLU:C	2.64	0.40
13:O:27:ARG:O	13:O:27:ARG:HG2	2.21	0.40
26:c:515:BCR:H11C	26:c:515:BCR:H341	1.96	0.40
26:t:101:BCR:H371	26:t:101:BCR:H24C	1.78	0.40
19:z:53:VAL:O	19:z:57:LEU:HG	2.21	0.40
1:A:13:LEU:HD23	28:A:611:STE:H42	2.03	0.40
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.02	0.40
19:Z:6:GLN:C	36:Z:201:HOH:O	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:86:ILE:HA	36:b:734:HOH:O	2.21	0.40
3:c:135:ARG:NH2	19:z:33:TRP:CD1	2.89	0.40
16:v:90:GLU:HB2	36:v:330:HOH:O	2.21	0.40
3:C:143:TYR:CE2	24:C:513:CLA:HED3	2.56	0.40
3:C:223:TRP:CG	3:C:224:ILE:H	2.40	0.40
3:C:363:GLY:O	3:C:367:GLU:HG2	2.21	0.40
34:F:101:HEM:CMB	34:F:101:HEM:HBB2	2.51	0.40
1:a:60:ILE:HG23	1:a:61:ASP:N	2.37	0.40
10:k:39:TRP:CD1	17:y:46:LEU:HD12	2.57	0.40
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.57	0.40
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.83	0.40

All (4) 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)
3:C:462:GLU:OE1	7:H:3:ARG:NH1[4_557]	1.45	0.75
3:C:462:GLU:OE1	7:H:3:ARG:HH12[4_557]	1.20	0.40
3:C:462:GLU:OE2	7:H:3:ARG:NH2[4_557]	2.12	0.08
36:B:865:HOH:O	36:C:768:HOH:O[1_455]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	31
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	36	31
2	B	510/510 (100%)	503 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	493 (98%)	9 (2%)	2 (0%)	30	22
3	C	441/461 (96%)	432 (98%)	8 (2%)	1 (0%)	43	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	450/461 (98%)	441 (98%)	7 (2%)	2 (0%)	30	22
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	229 (94%)	13 (5%)	1 (0%)	30	22
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	16	8
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	5
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	10
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
All	All	5232/5700 (92%)	5091 (97%)	127 (2%)	14 (0%)	36	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
13	o	58	ASN
15	u	53	ALA
9	J	7	ARG
3	c	416	SER
2	b	127	ARG
2	b	294	SER
10	K	16	ALA
13	O	62	GLU
13	o	73	ARG
3	c	144	SER
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	268 (99%)	2 (1%)	76	77
1	a	269/280 (96%)	262 (97%)	7 (3%)	40	38
2	B	410/407 (101%)	401 (98%)	9 (2%)	45	45
2	b	403/407 (99%)	402 (100%)	1 (0%)	87	88
3	C	345/362 (95%)	342 (99%)	3 (1%)	70	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	353/362 (98%)	346 (98%)	7 (2%)	48	48
4	D	276/283 (98%)	273 (99%)	3 (1%)	65	68
4	d	277/283 (98%)	274 (99%)	3 (1%)	65	68
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	35
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	61
6	F	28/39 (72%)	26 (93%)	2 (7%)	13	7
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	7
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	50
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	31
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	20
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	10
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	26
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	202 (98%)	4 (2%)	50	50
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	41
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	83 (99%)	1 (1%)	63	65
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	65
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	115 (98%)	2 (2%)	53	53
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	17
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	23
19	z	51/52 (98%)	49 (96%)	2 (4%)	28	22
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	18 (82%)	4 (18%)	2	0
All	All	4322/4654 (93%)	4243 (98%)	79 (2%)	51	52

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
2	B	63	LEU
2	B	76	SER
2	B	79	SER
2	B	362	PHE
2	B	371	THR
2	B	480[A]	SER
2	B	480[B]	SER
2	B	487	SER
2	B	489	GLU
3	C	106	VAL
3	C	240	ILE
3	C	354	GLU
4	D	12	ARG
4	D	154	VAL
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	12	SER
6	F	25	THR
7	H	20	LYS
8	I	35	LYS
10	K	22	VAL
12	M	5	GLN
13	O	34	SER
13	O	57	LYS
13	O	89	SER
13	O	107	THR
15	U	45	LEU
16	V	3	LEU
16	V	7	VAL

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Mol	Chain	Res	Type
19	Z	15	LEU
19	Z	36	SER
1	a	28	LEU
1	a	35	VAL
1	a	42	LEU
1	a	134	SER
1	a	159	LEU
1	a	200	LEU
1	a	231	GLU
2	b	362	PHE
3	c	30	SER
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	170	ILE
3	c	240	ILE
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	230	SER
5	e	16	SER
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
9	j	13	VAL
10	k	19	ASP
10	k	27	VAL
10	k	30	VAL
10	k	35	LEU
11	l	21	LEU
11	l	30	LEU
13	o	49	THR
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
13	o	178	LYS
15	u	9	LEU
16	v	18	THR
16	v	52	LEU
17	y	19	ILE
18	x	14	LEU
19	z	20	VAL

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Mol	Chain	Res	Type
19	z	32	ASP
20	r	6	LEU
20	r	9	LEU
20	r	14	LEU
20	r	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	261	GLN
1	A	315	ASN
1	A	338	ASN
2	B	223	GLN
3	C	327	ASN
3	C	418	ASN
4	D	61	HIS
12	M	5	GLN
12	M	32	GLN
13	O	155	ASN
15	U	78	ASN
16	V	106	ASN
18	X	38	GLN
19	Z	6	GLN
19	Z	38	GLN
20	R	22	ASN
1	a	165	GLN
1	a	181	ASN
1	a	234	ASN
1	a	296	ASN
2	b	409	GLN
4	d	350	ASN
7	h	59	ASN
11	l	8	GLN
13	o	58	ASN
13	o	155	ASN
13	o	231	HIS
17	y	45	ASN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	1.07	1 (12%)	8,9,11	1.63	1 (12%)
12	FME	m	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.68	0
12	FME	M	1	12	8,9,10	1.07	1 (12%)	8,9,11	0.68	0
14	FME	T	1	14	8,9,10	0.90	0	8,9,11	1.04	0
8	FME	i	1	8	8,9,10	1.15	0	8,9,11	1.08	0
14	FME	t	1	14	8,9,10	1.15	1 (12%)	8,9,11	1.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.37	1.43	1.46
12	M	1	FME	CA-N	-2.32	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.27	1.43	1.46
12	m	1	FME	CA-N	-2.26	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-3.25	117.82	122.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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
28	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.97	0
28	STE	e	101	-	8,8,19	0.50	0	7,7,19	0.53	0
24	CLA	C	511	3	69,73,73	1.49	11 (15%)	82,113,113	1.36	6 (7%)
24	CLA	b	614	2	69,73,73	1.26	8 (11%)	82,113,113	1.40	12 (14%)
24	CLA	b	608	2	69,73,73	1.18	6 (8%)	82,113,113	1.23	8 (9%)
24	CLA	b	609	2	69,73,73	1.41	10 (14%)	82,113,113	1.42	15 (18%)
28	STE	b	621	-	15,15,19	0.48	0	14,14,19	0.57	0
24	CLA	C	504	36	63,67,73	1.31	7 (11%)	74,105,113	1.42	9 (12%)
28	STE	J	101	-	11,11,19	0.77	0	11,11,19	0.93	0
24	CLA	c	511	3	69,73,73	1.57	7 (10%)	82,113,113	1.54	6 (7%)
24	CLA	d	406	4	69,73,73	1.44	11 (15%)	82,113,113	1.19	8 (9%)
24	CLA	C	507	36	69,73,73	1.27	7 (10%)	82,113,113	1.51	9 (10%)
24	CLA	B	601	36	69,73,73	1.59	10 (14%)	82,113,113	1.51	8 (9%)
29	LMG	C	524	-	48,48,55	0.99	4 (8%)	56,56,63	1.26	3 (5%)
28	STE	e	104	-	8,8,19	0.45	0	7,7,19	0.64	0
26	BCR	b	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.20	5 (8%)
30	SQD	F	102	-	34,36,54	1.47	5 (14%)	42,45,65	2.13	12 (28%)
31	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.20	5 (9%)
24	CLA	A	606	36	69,73,73	1.16	6 (8%)	82,113,113	1.33	9 (10%)
24	CLA	C	501	3	69,73,73	1.35	7 (10%)	82,113,113	1.48	8 (9%)
28	STE	e	105	-	12,12,19	0.74	0	12,12,19	1.25	2 (16%)
28	STE	E	103	-	19,19,19	0.78	0	19,19,19	0.82	0
24	CLA	C	510	3	69,73,73	1.27	11 (15%)	82,113,113	1.24	4 (4%)
28	STE	t	103	-	9,9,19	0.53	0	8,8,19	0.53	0
24	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.38	8 (9%)
24	CLA	B	611	2	69,73,73	1.43	8 (11%)	82,113,113	1.51	12 (14%)
24	CLA	B	616	2	64,68,73	1.64	9 (14%)	76,107,113	1.51	9 (11%)
28	STE	b	622	-	19,19,19	0.58	0	19,19,19	1.13	0
32	DGD	A	617	-	67,67,67	1.21	8 (11%)	81,81,81	1.38	10 (12%)
32	DGD	C	522	-	63,63,67	1.14	6 (9%)	77,77,81	1.38	10 (12%)
32	DGD	h	102	-	63,63,67	1.14	7 (11%)	77,77,81	1.43	11 (14%)
28	STE	d	415	-	13,13,19	0.73	0	13,13,19	0.99	0
29	LMG	c	522	-	46,46,55	1.08	5 (10%)	54,54,63	1.21	4 (7%)
28	STE	B	625	-	11,11,19	0.86	0	11,11,19	1.30	1 (9%)
25	PHO	A	607	-	58,69,69	1.76	11 (18%)	55,99,99	1.71	9 (16%)
28	STE	C	515	-	13,13,19	0.83	0	13,13,19	0.90	0
24	CLA	B	604	2	69,73,73	1.41	7 (10%)	82,113,113	1.80	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	D	411	-	48,48,48	0.90	2 (4%)	51,54,54	1.37	8 (15%)
35	HEC	v	201	16	50,50,50	1.72	5 (10%)	68,82,82	1.35	8 (11%)
25	PHO	D	402	-	58,69,69	1.88	7 (12%)	55,99,99	1.47	8 (14%)
26	BCR	c	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.38	10 (17%)
24	CLA	B	607	36	69,73,73	1.24	6 (8%)	82,113,113	1.44	7 (8%)
24	CLA	C	509	3	69,73,73	1.16	7 (10%)	82,113,113	1.33	9 (10%)
24	CLA	A	605	1	69,73,73	1.22	7 (10%)	82,113,113	1.20	6 (7%)
26	BCR	C	520	-	41,41,41	1.00	2 (4%)	56,56,56	1.21	5 (8%)
24	CLA	C	505	3	69,73,73	1.29	8 (11%)	82,113,113	1.50	6 (7%)
28	STE	t	102	-	13,13,19	0.74	0	13,13,19	1.12	2 (15%)
29	LMG	o	301	-	55,55,55	1.32	6 (10%)	63,63,63	1.55	7 (11%)
24	CLA	c	509	3	69,73,73	1.22	7 (10%)	82,113,113	1.42	6 (7%)
24	CLA	d	404	36	69,73,73	1.50	5 (7%)	82,113,113	1.47	8 (9%)
24	CLA	c	505	3	69,73,73	1.12	6 (8%)	82,113,113	1.35	8 (9%)
28	STE	H	103	-	17,17,19	0.55	0	16,16,19	0.58	0
28	STE	B	622	-	16,16,19	0.71	0	16,16,19	1.16	1 (6%)
26	BCR	h	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.32	11 (19%)
28	STE	b	626	-	7,7,19	0.42	0	6,6,19	0.63	0
28	STE	C	528	-	13,13,19	0.46	0	12,12,19	0.61	0
28	STE	m	102	-	11,11,19	0.79	0	11,11,19	1.06	0
30	SQD	A	616	-	41,43,54	1.76	9 (21%)	51,54,65	1.54	9 (17%)
24	CLA	b	605	2	69,73,73	1.30	10 (14%)	82,113,113	1.51	13 (15%)
29	LMG	m	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.51	10 (16%)
24	CLA	b	607	36	69,73,73	1.11	7 (10%)	82,113,113	1.40	6 (7%)
33	BCT	D	401	22	3,3,3	1.11	0	2,3,3	3.45	1 (50%)
31	LHG	D	410	-	46,46,48	1.18	2 (4%)	49,52,54	1.31	4 (8%)
29	LMG	D	407	-	50,50,55	0.90	2 (4%)	58,58,63	1.19	4 (6%)
28	STE	C	526	-	15,15,19	0.35	0	14,14,19	0.88	0
26	BCR	K	102	-	41,41,41	1.05	3 (7%)	56,56,56	1.21	6 (10%)
24	CLA	a	607	1	69,73,73	1.19	7 (10%)	82,113,113	1.39	11 (13%)
29	LMG	c	523	-	48,48,55	0.97	4 (8%)	56,56,63	1.27	7 (12%)
27	PL9	A	610	-	55,55,55	1.26	5 (9%)	68,69,69	1.54	14 (20%)
24	CLA	b	604	2	69,73,73	1.17	6 (8%)	82,113,113	1.46	8 (9%)
27	PL9	D	406	-	55,55,55	1.19	4 (7%)	68,69,69	1.61	15 (22%)
28	STE	M	103	-	14,14,19	0.40	0	13,13,19	0.83	0
28	STE	M	101	-	14,14,19	0.70	0	14,14,19	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	B	620	-	45,45,55	1.18	3 (6%)	53,53,63	1.29	5 (9%)
24	CLA	b	611	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	11 (13%)
24	CLA	B	612	2	69,73,73	1.17	6 (8%)	82,113,113	1.32	9 (10%)
24	CLA	b	612	2	69,73,73	1.14	8 (11%)	82,113,113	1.40	12 (14%)
26	BCR	t	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	7 (12%)
28	STE	B	624	-	17,17,19	0.66	0	17,17,19	1.00	0
32	DGD	C	521	-	63,63,67	1.08	5 (7%)	77,77,81	1.29	7 (9%)
28	STE	D	412	-	8,8,19	0.48	0	7,7,19	0.58	0
33	BCT	d	401	22	3,3,3	1.04	0	2,3,3	3.11	1 (50%)
24	CLA	d	405	4	69,73,73	1.36	7 (10%)	82,113,113	1.36	8 (9%)
28	STE	j	102	-	15,15,19	0.51	0	14,14,19	0.62	0
24	CLA	c	503	3	69,73,73	1.13	5 (7%)	82,113,113	1.35	8 (9%)
26	BCR	K	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	6 (10%)
28	STE	C	517	-	4,4,19	0.52	0	3,3,19	0.35	0
24	CLA	C	502	3	69,73,73	1.28	7 (10%)	82,113,113	1.44	11 (13%)
24	CLA	A	612	36	69,73,73	1.41	7 (10%)	82,113,113	1.28	8 (9%)
29	LMG	C	516	-	35,35,55	1.51	7 (20%)	43,43,63	1.43	5 (11%)
26	BCR	A	609	-	41,41,41	1.05	3 (7%)	56,56,56	1.29	6 (10%)
28	STE	i	101	-	11,11,19	0.84	0	11,11,19	1.04	1 (9%)
24	CLA	B	608	2	69,73,73	1.23	9 (13%)	82,113,113	1.23	8 (9%)
24	CLA	a	606	36	69,73,73	1.28	9 (13%)	82,113,113	1.40	12 (14%)
31	LHG	L	101	-	48,48,48	1.01	3 (6%)	51,54,54	1.23	4 (7%)
26	BCR	D	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	7 (12%)
28	STE	j	101	-	11,11,19	0.76	0	11,11,19	1.09	1 (9%)
24	CLA	c	512	3	69,73,73	1.29	9 (13%)	82,113,113	1.41	8 (9%)
24	CLA	B	613	2	69,73,73	1.33	10 (14%)	82,113,113	1.26	9 (10%)
26	BCR	T	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.32	8 (14%)
31	LHG	D	409	-	48,48,48	0.99	3 (6%)	51,54,54	1.10	3 (5%)
29	LMG	A	613	-	48,48,55	1.17	8 (16%)	56,56,63	1.41	10 (17%)
32	DGD	C	523	-	63,63,67	0.97	4 (6%)	77,77,81	1.19	6 (7%)
28	STE	C	518	-	6,6,19	0.46	0	5,5,19	0.43	0
28	STE	E	102	-	11,11,19	0.44	0	10,10,19	0.60	0
26	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	7 (12%)
26	BCR	d	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	5 (8%)
31	LHG	A	615	-	48,48,48	1.05	3 (6%)	51,54,54	1.18	3 (5%)
24	CLA	a	605	1	69,73,73	1.35	9 (13%)	82,113,113	1.54	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	616	2	64,68,73	1.21	8 (12%)	76,107,113	1.36	9 (11%)
28	STE	z	101	-	8,8,19	0.45	0	7,7,19	0.54	0
28	STE	M	102	-	9,9,19	0.42	0	8,8,19	0.76	0
25	PHO	d	402	-	58,69,69	2.25	14 (24%)	55,99,99	1.76	8 (14%)
29	LMG	d	414	-	44,44,55	1.11	4 (9%)	52,52,63	1.31	7 (13%)
29	LMG	c	518	-	29,29,55	1.06	2 (6%)	31,31,63	1.06	2 (6%)
30	SQD	B	623	-	52,54,54	1.52	9 (17%)	62,65,65	1.85	14 (22%)
31	LHG	d	411	-	48,48,48	0.83	2 (4%)	51,54,54	1.26	6 (11%)
29	LMG	D	408	-	51,51,55	0.95	3 (5%)	59,59,63	1.42	8 (13%)
28	STE	f	102	-	7,7,19	0.49	0	6,6,19	0.42	0
27	PL9	a	609	-	55,55,55	1.11	6 (10%)	68,69,69	1.60	13 (19%)
26	BCR	C	514	-	41,41,41	1.25	4 (9%)	56,56,56	1.38	6 (10%)
29	LMG	B	621	-	51,51,55	0.99	5 (9%)	59,59,63	1.46	9 (15%)
35	HEC	V	201	16	50,50,50	1.57	4 (8%)	68,82,82	1.27	8 (11%)
24	CLA	c	513	3	69,73,73	1.38	9 (13%)	82,113,113	1.24	9 (10%)
28	STE	I	102	-	14,14,19	0.81	0	14,14,19	1.00	1 (7%)
24	CLA	C	512	3	69,73,73	1.38	8 (11%)	82,113,113	1.60	12 (14%)
30	SQD	a	611	-	52,54,54	1.63	8 (15%)	62,65,65	1.69	9 (14%)
34	HEM	e	102	6,5	50,50,50	1.40	8 (16%)	67,82,82	1.37	7 (10%)
24	CLA	b	610	36	69,73,73	1.24	7 (10%)	82,113,113	1.33	11 (13%)
21	OEX	A	601	3,36,1	0,14,14	-	-	-	-	-
28	STE	x	101	-	19,19,19	0.80	1 (5%)	19,19,19	0.99	1 (5%)
24	CLA	b	602	2	69,73,73	1.17	9 (13%)	82,113,113	1.48	14 (17%)
28	STE	C	519	-	9,9,19	0.43	0	8,8,19	0.58	0
28	STE	Z	101	-	16,16,19	0.50	0	15,15,19	0.52	0
26	BCR	k	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.18	4 (7%)
24	CLA	B	614	2	69,73,73	1.51	7 (10%)	82,113,113	1.41	12 (14%)
26	BCR	H	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	5 (8%)
28	STE	c	516	-	12,12,19	0.43	0	11,11,19	0.69	0
26	BCR	B	618	-	41,41,41	0.99	2 (4%)	56,56,56	1.22	5 (8%)
27	PL9	d	408	-	55,55,55	1.64	5 (9%)	68,69,69	1.76	12 (17%)
28	STE	b	624	-	15,15,19	0.84	1 (6%)	15,15,19	1.11	2 (13%)
28	STE	A	618	-	16,16,19	0.48	0	15,15,19	0.56	0
24	CLA	B	602	2	69,73,73	1.19	8 (11%)	82,113,113	1.14	7 (8%)
24	CLA	c	507	36	69,73,73	1.20	7 (10%)	82,113,113	1.26	10 (12%)
26	BCR	b	617	-	41,41,41	1.10	4 (9%)	56,56,56	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	b	625	-	9,9,19	0.38	0	8,8,19	0.88	0
28	STE	C	527	-	13,13,19	0.39	0	12,12,19	0.75	0
24	CLA	b	613	2	69,73,73	1.36	7 (10%)	82,113,113	1.19	10 (12%)
28	STE	b	627	-	10,10,19	0.52	0	9,9,19	0.51	0
29	LMG	c	524	-	49,49,55	1.07	6 (12%)	57,57,63	1.35	6 (10%)
24	CLA	b	601	36	69,73,73	1.37	9 (13%)	82,113,113	1.43	6 (7%)
28	STE	h	103	-	9,9,19	0.51	0	8,8,19	0.56	0
31	LHG	e	103	-	41,41,48	1.09	4 (9%)	44,47,54	1.28	4 (9%)
26	BCR	B	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	10 (17%)
24	CLA	c	508	3	68,72,73	1.38	10 (14%)	80,111,113	1.33	8 (10%)
24	CLA	c	506	3	69,73,73	1.23	10 (14%)	82,113,113	1.25	12 (14%)
30	SQD	A	614	-	50,52,54	1.62	7 (14%)	60,63,65	2.11	10 (16%)
28	STE	a	612	-	11,11,19	0.84	0	11,11,19	1.00	0
28	STE	X	101	-	19,19,19	0.74	1 (5%)	19,19,19	0.98	0
31	LHG	d	410	-	48,48,48	0.74	1 (2%)	51,54,54	1.35	7 (13%)
24	CLA	B	610	36	69,73,73	1.50	11 (15%)	82,113,113	1.35	9 (10%)
24	CLA	c	510	3	69,73,73	1.15	7 (10%)	82,113,113	1.28	8 (9%)
28	STE	d	413	-	19,19,19	0.65	0	19,19,19	0.77	0
32	DGD	c	521	-	63,63,67	1.00	6 (9%)	77,77,81	1.42	13 (16%)
24	CLA	B	609	2	69,73,73	1.29	6 (8%)	82,113,113	1.34	8 (9%)
26	BCR	a	608	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	7 (12%)
24	CLA	A	608	1	58,62,73	1.37	6 (10%)	68,99,113	1.55	10 (14%)
28	STE	i	102	-	5,5,19	0.45	0	4,4,19	0.42	0
28	STE	A	611	-	8,8,19	0.43	0	7,7,19	0.69	0
24	CLA	b	615	2	69,73,73	1.35	10 (14%)	82,113,113	1.39	10 (12%)
32	DGD	H	102	-	63,63,67	1.15	5 (7%)	77,77,81	1.51	14 (18%)
24	CLA	C	513	3	69,73,73	1.73	8 (11%)	82,113,113	1.43	6 (7%)
25	PHO	d	403	-	58,69,69	2.16	9 (15%)	55,99,99	1.46	7 (12%)
34	HEM	F	101	6,5	50,50,50	1.41	8 (16%)	67,82,82	1.10	3 (4%)
28	STE	c	517	-	17,17,19	0.49	0	16,16,19	0.63	0
28	STE	A	619	-	10,10,19	0.48	0	9,9,19	0.62	0
24	CLA	B	603	2	69,73,73	1.11	7 (10%)	82,113,113	1.49	17 (20%)
24	CLA	B	615	2	69,73,73	1.41	8 (11%)	82,113,113	1.26	8 (9%)
26	BCR	B	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.31	6 (10%)
24	CLA	D	404	4	69,73,73	1.43	11 (15%)	82,113,113	1.26	5 (6%)
29	LMG	b	623	-	55,55,55	1.02	4 (7%)	63,63,63	1.46	7 (11%)
28	STE	I	101	-	16,16,19	0.79	0	16,16,19	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	c	520	-	63,63,67	1.14	10 (15%)	77,77,81	1.35	8 (10%)
28	STE	C	525	-	11,11,19	0.78	0	11,11,19	1.18	1 (9%)
30	SQD	a	610	-	52,54,54	1.43	6 (11%)	62,65,65	2.07	14 (22%)
28	STE	R	101	-	19,19,19	0.74	1 (5%)	19,19,19	1.19	3 (15%)
30	SQD	b	620	-	47,49,54	1.55	7 (14%)	57,60,65	2.04	16 (28%)
24	CLA	c	501	3	69,73,73	1.33	9 (13%)	82,113,113	1.51	7 (8%)
28	STE	B	626	-	14,14,19	0.47	0	13,13,19	0.61	0
24	CLA	b	606	2	69,73,73	1.55	7 (10%)	82,113,113	1.54	9 (10%)
26	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	9 (16%)
28	STE	d	409	-	19,19,19	0.78	0	19,19,19	0.88	1 (5%)
30	SQD	f	101	-	39,41,54	1.70	7 (17%)	49,52,65	1.87	11 (22%)
24	CLA	D	403	4	69,73,73	1.27	8 (11%)	82,113,113	1.39	8 (9%)
24	CLA	b	603	2	69,73,73	1.20	9 (13%)	82,113,113	1.46	11 (13%)
32	DGD	c	519	-	63,63,67	1.27	9 (14%)	77,77,81	1.34	10 (12%)
24	CLA	C	506	3	69,73,73	1.48	10 (14%)	82,113,113	1.24	8 (9%)
26	BCR	k	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.06	3 (5%)
31	LHG	d	412	-	38,38,48	1.15	2 (5%)	41,44,54	1.33	5 (12%)
21	OEX	a	601	3,36,1	0,14,14	-	-	-	-	-
24	CLA	B	606	2	69,73,73	1.41	6 (8%)	82,113,113	1.39	8 (9%)
24	CLA	B	605	2	69,73,73	1.23	5 (7%)	82,113,113	1.34	11 (13%)
28	STE	E	101	-	11,11,19	0.83	0	11,11,19	1.08	1 (9%)
24	CLA	c	502	3	69,73,73	1.24	6 (8%)	82,113,113	1.16	4 (4%)
24	CLA	c	504	36	64,68,73	1.37	9 (14%)	76,107,113	1.37	9 (11%)
24	CLA	C	503	3	69,73,73	1.43	6 (8%)	82,113,113	1.51	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	l	102	-	-	7/15/15/17	-
28	STE	e	101	-	-	2/6/6/17	-
24	CLA	C	511	3	-	2/39/115/115	-
24	CLA	b	614	2	-	12/39/115/115	-
24	CLA	b	608	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	609	2	-	6/39/115/115	-
28	STE	b	621	-	-	7/13/13/17	-
24	CLA	C	504	36	-	7/32/108/115	-
28	STE	J	101	-	-	6/9/9/17	-
24	CLA	c	511	3	-	6/39/115/115	-
24	CLA	d	406	4	-	11/39/115/115	-
24	CLA	C	507	36	-	7/39/115/115	-
24	CLA	B	601	36	-	18/39/115/115	-
29	LMG	C	524	-	-	17/43/63/70	0/1/1/1
28	STE	e	104	-	-	3/6/6/17	-
26	BCR	b	619	-	-	7/29/63/63	0/2/2/2
30	SQD	F	102	-	-	12/28/48/69	0/1/1/1
31	LHG	l	101	-	-	22/53/53/53	-
24	CLA	A	606	36	-	7/39/115/115	-
24	CLA	C	501	3	-	3/39/115/115	-
28	STE	e	105	-	-	5/10/10/17	-
28	STE	E	103	-	-	8/17/17/17	-
24	CLA	C	510	3	-	7/39/115/115	-
28	STE	t	103	-	-	4/7/7/17	-
24	CLA	C	508	3	-	6/39/115/115	-
24	CLA	B	611	2	-	4/39/115/115	-
24	CLA	B	616	2	-	9/33/109/115	-
28	STE	b	622	-	-	7/17/17/17	-
32	DGD	A	617	-	-	24/55/95/95	0/2/2/2
32	DGD	C	522	-	-	17/51/91/95	0/2/2/2
32	DGD	h	102	-	-	16/51/91/95	0/2/2/2
28	STE	d	415	-	-	5/11/11/17	-
29	LMG	c	522	-	-	15/41/61/70	0/1/1/1
28	STE	B	625	-	-	2/9/9/17	-
25	PHO	A	607	-	-	2/37/103/103	0/5/6/6
28	STE	C	515	-	-	4/11/11/17	-
24	CLA	B	604	2	-	8/39/115/115	-
31	LHG	D	411	-	-	16/53/53/53	-
35	HEC	v	201	16	1/1/7/7	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	D	402	-	-	2/37/103/103	0/5/6/6
26	BCR	c	515	-	-	4/29/63/63	0/2/2/2
24	CLA	B	607	36	-	9/39/115/115	-
24	CLA	C	509	3	-	12/39/115/115	-
24	CLA	A	605	1	-	1/39/115/115	-
26	BCR	C	520	-	-	5/29/63/63	0/2/2/2
24	CLA	C	505	3	-	9/39/115/115	-
28	STE	t	102	-	-	5/11/11/17	-
29	LMG	o	301	-	-	26/50/70/70	0/1/1/1
24	CLA	c	509	3	-	10/39/115/115	-
24	CLA	d	404	36	-	0/39/115/115	-
24	CLA	c	505	3	-	11/39/115/115	-
28	STE	H	103	-	-	8/15/15/17	-
28	STE	B	622	-	-	7/14/14/17	-
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
28	STE	b	626	-	-	2/5/5/17	-
28	STE	C	528	-	-	4/11/11/17	-
28	STE	m	102	-	-	2/9/9/17	-
30	SQD	A	616	-	-	14/38/58/69	0/1/1/1
24	CLA	b	605	2	-	5/39/115/115	-
29	LMG	m	101	-	-	18/46/66/70	0/1/1/1
24	CLA	b	607	36	-	14/39/115/115	-
31	LHG	D	410	-	-	15/51/51/53	-
29	LMG	D	407	-	-	21/45/65/70	0/1/1/1
28	STE	C	526	-	-	3/13/13/17	-
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
24	CLA	a	607	1	-	12/39/115/115	-
29	LMG	c	523	-	-	17/43/63/70	0/1/1/1
27	PL9	A	610	-	-	19/53/73/73	0/1/1/1
24	CLA	b	604	2	-	9/39/115/115	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
28	STE	M	103	-	-	8/12/12/17	-
28	STE	M	101	-	-	7/12/12/17	-
29	LMG	B	620	-	-	16/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	611	2	-	7/39/115/115	-
24	CLA	B	612	2	-	8/39/115/115	-
24	CLA	b	612	2	-	3/39/115/115	-
26	BCR	t	101	-	-	4/29/63/63	0/2/2/2
28	STE	B	624	-	-	5/15/15/17	-
32	DGD	C	521	-	-	25/51/91/95	0/2/2/2
28	STE	D	412	-	-	3/6/6/17	-
24	CLA	d	405	4	-	6/39/115/115	-
28	STE	j	102	-	-	6/13/13/17	-
24	CLA	c	503	3	-	9/39/115/115	-
26	BCR	K	101	-	-	5/29/63/63	0/2/2/2
28	STE	C	517	-	-	1/2/2/17	-
24	CLA	C	502	3	-	6/39/115/115	-
24	CLA	A	612	36	-	4/39/115/115	-
29	LMG	C	516	-	-	11/30/50/70	0/1/1/1
26	BCR	A	609	-	-	3/29/63/63	0/2/2/2
28	STE	i	101	-	-	4/9/9/17	-
24	CLA	B	608	2	-	3/39/115/115	-
24	CLA	a	606	36	-	3/39/115/115	-
31	LHG	L	101	-	-	18/53/53/53	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
28	STE	j	101	-	-	5/9/9/17	-
24	CLA	c	512	3	-	17/39/115/115	-
24	CLA	B	613	2	-	13/39/115/115	-
26	BCR	T	101	-	-	3/29/63/63	0/2/2/2
31	LHG	D	409	-	-	21/53/53/53	-
29	LMG	A	613	-	-	17/43/63/70	0/1/1/1
32	DGD	C	523	-	-	15/51/91/95	0/2/2/2
28	STE	C	518	-	-	2/4/4/17	-
28	STE	E	102	-	-	4/9/9/17	-
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
26	BCR	d	407	-	-	8/29/63/63	0/2/2/2
31	LHG	A	615	-	-	26/53/53/53	-
24	CLA	a	605	1	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	616	2	-	6/33/109/115	-
28	STE	z	101	-	-	4/6/6/17	-
28	STE	M	102	-	-	2/7/7/17	-
25	PHO	d	402	-	-	4/37/103/103	0/5/6/6
29	LMG	d	414	-	-	11/39/59/70	0/1/1/1
29	LMG	c	518	-	-	16/31/31/70	-
30	SQD	B	623	-	-	27/49/69/69	0/1/1/1
31	LHG	d	411	-	-	20/53/53/53	-
29	LMG	D	408	-	-	14/46/66/70	0/1/1/1
28	STE	f	102	-	-	3/5/5/17	-
27	PL9	a	609	-	-	20/53/73/73	0/1/1/1
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
29	LMG	B	621	-	-	20/46/66/70	0/1/1/1
24	CLA	c	513	3	-	11/39/115/115	-
28	STE	I	102	-	-	8/12/12/17	-
24	CLA	C	512	3	-	13/39/115/115	-
30	SQD	a	611	-	-	23/49/69/69	0/1/1/1
34	HEM	e	102	6,5	-	5/14/54/54	-
24	CLA	b	610	36	-	6/39/115/115	-
28	STE	x	101	-	-	9/17/17/17	-
24	CLA	b	602	2	-	5/39/115/115	-
28	STE	C	519	-	-	4/7/7/17	-
28	STE	Z	101	-	-	7/14/14/17	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2
24	CLA	B	614	2	-	6/39/115/115	-
26	BCR	H	101	-	-	5/29/63/63	0/2/2/2
28	STE	c	516	-	-	5/10/10/17	-
26	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	PL9	d	408	-	-	10/53/73/73	0/1/1/1
28	STE	b	624	-	-	7/13/13/17	-
28	STE	A	618	-	-	7/14/14/17	-
24	CLA	B	602	2	-	7/39/115/115	-
24	CLA	c	507	36	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	617	-	-	3/29/63/63	0/2/2/2
28	STE	b	625	-	-	2/7/7/17	-
28	STE	C	527	-	-	5/11/11/17	-
24	CLA	b	613	2	-	7/39/115/115	-
28	STE	b	627	-	-	6/8/8/17	-
29	LMG	c	524	-	-	18/44/64/70	0/1/1/1
24	CLA	b	601	36	-	15/39/115/115	-
28	STE	h	103	-	-	4/7/7/17	-
31	LHG	e	103	-	-	21/46/46/53	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
24	CLA	c	508	3	-	8/38/114/115	-
24	CLA	c	506	3	-	12/39/115/115	-
30	SQD	A	614	-	-	19/47/67/69	0/1/1/1
28	STE	a	612	-	-	1/9/9/17	-
28	STE	X	101	-	-	6/17/17/17	-
31	LHG	d	410	-	-	15/53/53/53	-
24	CLA	B	610	36	-	3/39/115/115	-
24	CLA	c	510	3	-	6/39/115/115	-
28	STE	d	413	-	-	8/17/17/17	-
32	DGD	c	521	-	-	18/51/91/95	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-
26	BCR	a	608	-	-	4/29/63/63	0/2/2/2
24	CLA	A	608	1	-	4/26/102/115	-
28	STE	i	102	-	-	1/3/3/17	-
28	STE	A	611	-	-	4/6/6/17	-
24	CLA	b	615	2	-	5/39/115/115	-
32	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	CLA	C	513	3	-	8/39/115/115	-
25	PHO	d	403	-	-	6/37/103/103	0/5/6/6
34	HEM	F	101	6,5	-	3/14/54/54	-
28	STE	c	517	-	-	8/15/15/17	-
28	STE	A	619	-	-	5/8/8/17	-
24	CLA	B	603	2	-	12/39/115/115	-
24	CLA	B	615	2	-	8/39/115/115	-
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	404	4	-	9/39/115/115	-
29	LMG	b	623	-	-	25/50/70/70	0/1/1/1
28	STE	I	101	-	-	6/14/14/17	-
32	DGD	c	520	-	-	19/51/91/95	0/2/2/2
28	STE	C	525	-	-	2/9/9/17	-
30	SQD	a	610	-	-	17/49/69/69	0/1/1/1
28	STE	R	101	-	-	11/17/17/17	-
30	SQD	b	620	-	-	21/44/64/69	0/1/1/1
24	CLA	c	501	3	-	3/39/115/115	-
28	STE	B	626	-	-	8/12/12/17	-
24	CLA	b	606	2	-	6/39/115/115	-
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
28	STE	d	409	-	-	12/17/17/17	-
30	SQD	f	101	-	-	15/36/56/69	0/1/1/1
24	CLA	D	403	4	-	2/39/115/115	-
24	CLA	b	603	2	-	7/39/115/115	-
32	DGD	c	519	-	-	28/51/91/95	0/2/2/2
24	CLA	C	506	3	-	12/39/115/115	-
26	BCR	k	101	-	-	6/29/63/63	0/2/2/2
31	LHG	d	412	-	-	14/43/43/53	-
24	CLA	B	606	2	-	5/39/115/115	-
24	CLA	B	605	2	-	8/39/115/115	-
28	STE	E	101	-	-	5/9/9/17	-
24	CLA	c	502	3	-	4/39/115/115	-
24	CLA	c	504	36	-	4/33/109/115	-
24	CLA	C	503	3	-	6/39/115/115	-

All (901) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C1B-C2B	10.35	1.50	1.39
25	d	403	PHO	C1B-C2B	10.06	1.50	1.39
25	D	402	PHO	C1B-C2B	8.74	1.49	1.39
24	C	513	CLA	MG-ND	8.44	2.22	2.05
24	c	511	CLA	MG-NA	8.20	2.25	2.06
25	d	402	PHO	C3B-C4B	8.17	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	408	PL9	C6-C1	-8.04	1.35	1.48
25	d	403	PHO	C3B-C4B	7.87	1.49	1.41
24	B	601	CLA	MG-NA	7.80	2.24	2.06
24	d	404	CLA	MG-NA	7.79	2.24	2.06
25	D	402	PHO	C3B-C4B	7.64	1.49	1.41
24	B	606	CLA	MG-NA	7.62	2.24	2.06
24	C	503	CLA	MG-NA	7.42	2.23	2.06
24	b	606	CLA	MG-NA	7.36	2.23	2.06
24	B	610	CLA	MG-ND	-7.29	1.91	2.05
35	v	201	HEC	C3D-C2D	7.26	1.52	1.36
24	C	506	CLA	MG-NA	7.03	2.23	2.06
35	V	201	HEC	C3D-C2D	6.66	1.51	1.36
24	d	405	CLA	MG-NA	6.62	2.22	2.06
24	B	614	CLA	MG-ND	-6.56	1.92	2.05
25	A	607	PHO	C1B-C2B	6.49	1.46	1.39
24	B	616	CLA	MG-NA	6.46	2.21	2.06
24	b	609	CLA	MG-NA	6.39	2.21	2.06
24	C	512	CLA	MG-NB	6.34	2.18	2.05
24	B	611	CLA	MG-NA	6.08	2.20	2.06
24	C	511	CLA	MG-NA	6.00	2.20	2.06
24	b	613	CLA	MG-ND	-5.84	1.94	2.05
25	A	607	PHO	C3B-C4B	5.75	1.47	1.41
24	D	404	CLA	MG-NB	-5.62	1.94	2.05
24	A	612	CLA	MG-NB	5.61	2.16	2.05
24	A	608	CLA	MG-ND	-5.58	1.94	2.05
35	v	201	HEC	FE-NA	5.56	2.13	1.95
24	B	609	CLA	MG-NA	5.33	2.18	2.06
24	C	513	CLA	MG-NB	-5.24	1.95	2.05
24	C	501	CLA	MG-NA	5.11	2.18	2.06
24	b	610	CLA	MG-NB	-5.03	1.95	2.05
24	C	507	CLA	MG-NA	5.02	2.18	2.06
30	f	101	SQD	O48-C23	5.02	1.48	1.33
24	B	604	CLA	MG-NA	5.01	2.18	2.06
24	B	616	CLA	MG-NB	-5.00	1.95	2.05
29	o	301	LMG	C4-C5	4.98	1.63	1.53
31	D	410	LHG	P-O6	4.94	1.78	1.59
30	A	616	SQD	O48-C23	4.93	1.47	1.33
24	b	606	CLA	MG-NC	4.84	2.17	2.06
24	B	615	CLA	MG-NC	4.78	2.17	2.06
24	B	604	CLA	MG-NC	4.73	2.17	2.06
25	d	403	PHO	C1D-C2D	4.73	1.44	1.39
24	C	508	CLA	MG-ND	4.72	2.15	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	614	SQD	O48-C23	4.72	1.47	1.33
24	C	501	CLA	C1D-ND	4.66	1.44	1.37
30	a	611	SQD	O48-C23	4.66	1.46	1.33
24	B	614	CLA	MG-NA	4.60	2.17	2.06
24	C	502	CLA	MG-NA	4.55	2.17	2.06
26	h	101	BCR	C30-C25	-4.55	1.48	1.53
30	B	623	SQD	O48-C23	4.51	1.46	1.33
24	C	504	CLA	MG-NA	4.50	2.17	2.06
24	b	601	CLA	MG-NA	4.49	2.16	2.06
24	c	513	CLA	MG-NA	4.48	2.16	2.06
24	B	613	CLA	MG-NA	4.47	2.16	2.06
30	F	102	SQD	O48-C23	4.45	1.46	1.33
29	B	620	LMG	C4-C5	4.44	1.62	1.53
24	c	508	CLA	MG-NB	4.44	2.14	2.05
26	c	515	BCR	C1-C6	-4.42	1.48	1.53
24	a	605	CLA	MG-NC	4.40	2.16	2.06
24	d	406	CLA	MG-NB	-4.36	1.97	2.05
24	D	404	CLA	C1D-ND	4.36	1.43	1.37
24	c	512	CLA	MG-NB	4.33	2.14	2.05
27	d	408	PL9	C3-C4	-4.33	1.42	1.49
24	A	606	CLA	MG-NA	4.33	2.16	2.06
24	c	504	CLA	MG-ND	-4.31	1.97	2.05
24	C	513	CLA	MG-NC	4.28	2.16	2.06
24	a	605	CLA	MG-NB	4.28	2.14	2.05
24	d	406	CLA	MG-ND	-4.25	1.97	2.05
24	B	614	CLA	C1D-ND	4.20	1.43	1.37
26	b	618	BCR	C30-C25	-4.15	1.48	1.53
25	d	402	PHO	C1D-C2D	4.10	1.44	1.39
24	C	511	CLA	C1D-ND	4.10	1.43	1.37
34	e	102	HEM	FE-NA	4.10	2.08	1.95
29	C	516	LMG	O1-C1	4.08	1.47	1.40
24	c	502	CLA	MG-NA	4.07	2.15	2.06
24	D	404	CLA	MG-ND	-4.06	1.97	2.05
24	A	605	CLA	C1D-ND	4.01	1.43	1.37
26	C	514	BCR	C1-C6	-3.98	1.48	1.53
24	B	601	CLA	C4B-NB	3.97	1.43	1.37
24	B	616	CLA	C1D-ND	3.97	1.43	1.37
24	b	616	CLA	MG-NA	3.97	2.15	2.06
30	a	611	SQD	O47-C7	3.95	1.45	1.34
24	B	601	CLA	C1D-ND	3.95	1.43	1.37
32	c	519	DGD	C4D-C3D	3.94	1.62	1.52
24	B	616	CLA	MG-ND	3.93	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	605	CLA	MG-NA	3.93	2.15	2.06
24	B	604	CLA	C1D-ND	3.92	1.43	1.37
30	b	620	SQD	O48-C23	3.92	1.44	1.33
24	D	403	CLA	MG-NB	3.90	2.13	2.05
24	B	614	CLA	C4B-NB	3.90	1.43	1.37
24	b	611	CLA	MG-NA	3.90	2.15	2.06
24	c	513	CLA	MG-ND	-3.89	1.98	2.05
26	B	619	BCR	C30-C25	-3.87	1.48	1.53
24	A	608	CLA	C4B-NB	3.87	1.42	1.37
24	a	607	CLA	MG-NC	-3.86	1.97	2.06
24	b	601	CLA	C1D-ND	3.85	1.42	1.37
24	B	610	CLA	MG-NA	3.84	2.15	2.06
24	b	614	CLA	MG-NC	3.83	2.15	2.06
24	c	506	CLA	MG-NC	3.83	2.15	2.06
24	c	509	CLA	MG-ND	-3.82	1.98	2.05
24	B	607	CLA	C1D-ND	3.80	1.42	1.37
24	C	513	CLA	MG-NA	3.79	2.15	2.06
24	b	614	CLA	C1D-ND	3.78	1.42	1.37
24	C	506	CLA	MG-NB	3.78	2.13	2.05
34	F	101	HEM	FE-NC	3.76	2.07	1.95
24	A	612	CLA	C4B-NB	3.76	1.42	1.37
24	b	610	CLA	C1D-ND	3.75	1.42	1.37
29	o	301	LMG	C4-C3	3.74	1.62	1.52
24	B	608	CLA	C1D-ND	3.74	1.42	1.37
24	B	610	CLA	C1D-ND	3.73	1.42	1.37
24	c	504	CLA	C4B-NB	3.73	1.42	1.37
24	c	501	CLA	MG-NA	3.72	2.15	2.06
26	H	101	BCR	C30-C25	-3.71	1.49	1.53
24	b	604	CLA	C4B-NB	3.71	1.42	1.37
24	b	605	CLA	MG-ND	3.71	2.13	2.05
26	K	102	BCR	C30-C25	-3.69	1.49	1.53
30	A	614	SQD	O47-C45	-3.68	1.37	1.46
29	C	516	LMG	C7-C8	3.68	1.62	1.50
24	c	501	CLA	C1D-ND	3.68	1.42	1.37
35	V	201	HEC	FE-ND	3.67	2.06	1.94
24	C	512	CLA	MG-NA	3.67	2.15	2.06
30	a	611	SQD	O5-C1	3.66	1.51	1.41
31	A	615	LHG	P-O6	3.66	1.73	1.59
24	b	611	CLA	MG-ND	3.65	2.13	2.05
24	C	504	CLA	MG-NB	3.65	2.13	2.05
25	A	607	PHO	C4D-ND	-3.64	1.33	1.38
24	B	612	CLA	MG-NB	3.63	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	610	SQD	O48-C23	3.63	1.43	1.33
24	C	505	CLA	MG-NA	3.63	2.14	2.06
24	b	601	CLA	C4B-NB	3.63	1.42	1.37
24	B	615	CLA	C4B-NB	3.63	1.42	1.37
35	V	201	HEC	FE-NB	3.62	2.06	1.94
29	c	518	LMG	C7-C8	3.61	1.59	1.51
24	a	606	CLA	C4B-NB	3.61	1.42	1.37
24	C	505	CLA	CHC-C1C	3.60	1.45	1.38
24	B	605	CLA	C1B-C2B	3.60	1.51	1.43
24	C	502	CLA	C4B-NB	3.59	1.42	1.37
24	c	511	CLA	C4B-NB	3.59	1.42	1.37
27	D	406	PL9	C6-C1	-3.57	1.42	1.48
26	B	619	BCR	C1-C6	-3.57	1.49	1.53
24	b	613	CLA	C1D-ND	3.57	1.42	1.37
24	d	406	CLA	C4B-NB	3.57	1.42	1.37
24	A	612	CLA	C1D-ND	3.57	1.42	1.37
24	C	505	CLA	MG-NC	3.56	2.14	2.06
24	c	508	CLA	C1D-ND	3.56	1.42	1.37
24	c	501	CLA	C4B-NB	3.56	1.42	1.37
24	C	510	CLA	C1D-ND	3.55	1.42	1.37
26	b	617	BCR	C1-C6	-3.55	1.49	1.53
24	B	611	CLA	MG-ND	3.55	2.12	2.05
30	A	616	SQD	C24-C23	3.55	1.61	1.50
30	f	101	SQD	O47-C7	3.54	1.44	1.34
29	m	101	LMG	C4-C3	3.53	1.61	1.52
30	f	101	SQD	O47-C45	-3.53	1.38	1.46
31	d	412	LHG	C24-C23	3.52	1.60	1.50
24	b	604	CLA	C1D-ND	3.50	1.42	1.37
24	c	501	CLA	MG-ND	-3.49	1.98	2.05
26	K	101	BCR	C1-C6	-3.49	1.49	1.53
24	B	615	CLA	C1D-ND	3.49	1.42	1.37
32	H	102	DGD	O5D-C1E	3.49	1.46	1.40
24	b	615	CLA	MG-NC	3.47	2.14	2.06
24	C	501	CLA	C4B-NB	3.46	1.42	1.37
26	C	514	BCR	C30-C25	-3.46	1.49	1.53
30	A	616	SQD	O5-C1	3.45	1.50	1.41
24	c	508	CLA	CHC-C1C	3.45	1.45	1.38
27	d	408	PL9	C53-C6	-3.44	1.43	1.50
30	a	610	SQD	O47-C45	-3.44	1.38	1.46
30	b	620	SQD	O5-C1	3.43	1.50	1.41
24	c	503	CLA	MG-NC	3.43	2.14	2.06
31	d	412	LHG	P-O6	3.42	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	406	CLA	C1D-ND	3.42	1.42	1.37
24	C	508	CLA	C3B-C4B	3.41	1.52	1.42
24	c	507	CLA	C1D-ND	3.41	1.42	1.37
26	B	617	BCR	C1-C6	-3.41	1.49	1.53
30	A	616	SQD	O47-C45	-3.40	1.38	1.46
31	L	101	LHG	O7-C5	-3.39	1.38	1.46
24	a	606	CLA	MG-NB	3.39	2.12	2.05
24	b	609	CLA	C1D-ND	3.39	1.42	1.37
24	C	510	CLA	MG-NB	3.39	2.12	2.05
24	c	508	CLA	MG-NA	3.38	2.14	2.06
24	C	511	CLA	C4B-NB	3.38	1.42	1.37
24	B	605	CLA	C4B-NB	3.38	1.42	1.37
24	a	606	CLA	MG-NA	3.37	2.14	2.06
24	c	513	CLA	MG-NB	3.36	2.12	2.05
25	A	607	PHO	C1A-C2A	3.36	1.55	1.51
25	d	403	PHO	C4D-CHA	3.35	1.44	1.39
24	b	605	CLA	MG-NB	-3.35	1.99	2.05
24	c	505	CLA	MG-NC	3.34	2.14	2.06
24	c	504	CLA	MG-NC	3.34	2.14	2.06
24	B	605	CLA	C3B-C4B	3.33	1.52	1.42
26	c	514	BCR	C1-C6	-3.33	1.49	1.53
26	B	618	BCR	C30-C25	-3.32	1.49	1.53
26	D	405	BCR	C1-C6	-3.32	1.49	1.53
24	b	605	CLA	MG-NA	3.32	2.14	2.06
26	c	514	BCR	C30-C25	-3.31	1.49	1.53
24	B	611	CLA	C1B-C2B	3.31	1.50	1.43
30	B	623	SQD	O47-C45	-3.31	1.38	1.46
30	b	620	SQD	O47-C7	3.31	1.43	1.34
24	b	606	CLA	C1B-C2B	3.30	1.50	1.43
30	A	614	SQD	C24-C23	3.30	1.60	1.50
24	b	606	CLA	C1D-ND	3.29	1.42	1.37
27	D	406	PL9	C52-C5	-3.29	1.44	1.50
32	A	617	DGD	C3E-C2E	3.29	1.60	1.52
26	A	609	BCR	C1-C6	-3.29	1.49	1.53
32	C	523	DGD	C4D-C5D	3.28	1.60	1.53
24	A	612	CLA	C3B-C4B	3.28	1.52	1.42
24	A	605	CLA	C1B-C2B	3.26	1.50	1.43
24	c	512	CLA	C1D-ND	3.26	1.42	1.37
26	k	102	BCR	C1-C6	-3.25	1.49	1.53
25	d	402	PHO	CMB-C2B	-3.25	1.45	1.51
24	c	506	CLA	C1D-ND	3.25	1.42	1.37
24	b	602	CLA	MG-NC	3.25	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1D-ND	3.25	1.42	1.37
24	b	607	CLA	MG-ND	-3.24	1.99	2.05
29	C	516	LMG	C4-C5	3.24	1.59	1.53
32	h	102	DGD	C4D-C3D	3.24	1.60	1.52
30	A	616	SQD	O47-C7	3.24	1.43	1.34
24	B	613	CLA	C4B-NB	3.23	1.42	1.37
29	o	301	LMG	C3-C2	3.23	1.60	1.52
24	b	615	CLA	C1D-ND	3.23	1.42	1.37
24	c	509	CLA	C1D-ND	3.23	1.42	1.37
24	b	608	CLA	CHC-C1C	3.22	1.44	1.38
26	k	101	BCR	C30-C25	-3.22	1.49	1.53
24	A	606	CLA	C1D-ND	3.21	1.42	1.37
24	b	608	CLA	C1D-ND	3.20	1.42	1.37
24	C	509	CLA	C1D-ND	3.20	1.42	1.37
24	d	405	CLA	C1B-C2B	3.20	1.50	1.43
24	C	507	CLA	C1B-C2B	3.18	1.50	1.43
30	b	620	SQD	C24-C23	3.18	1.59	1.50
26	K	102	BCR	C1-C6	-3.18	1.49	1.53
24	a	606	CLA	CHC-C1C	3.17	1.44	1.38
24	b	601	CLA	C1B-C2B	3.17	1.50	1.43
24	a	605	CLA	C1D-ND	3.17	1.42	1.37
24	B	602	CLA	MG-NC	-3.17	1.98	2.06
24	c	511	CLA	CHC-C1C	3.16	1.44	1.38
24	B	609	CLA	C1B-C2B	3.16	1.50	1.43
24	c	503	CLA	C1D-ND	3.16	1.42	1.37
24	D	403	CLA	MG-NA	3.15	2.13	2.06
24	c	510	CLA	C1D-ND	3.15	1.42	1.37
25	d	402	PHO	CMD-C2D	-3.14	1.45	1.51
24	c	510	CLA	MG-NA	3.14	2.13	2.06
24	a	607	CLA	C1D-ND	3.14	1.42	1.37
26	c	515	BCR	C30-C25	-3.14	1.49	1.53
24	B	607	CLA	MG-NC	3.13	2.13	2.06
24	b	612	CLA	C1D-ND	3.13	1.42	1.37
24	c	512	CLA	C1B-C2B	3.13	1.50	1.43
24	D	403	CLA	C1D-ND	3.12	1.42	1.37
24	b	615	CLA	MG-NA	3.12	2.13	2.06
24	c	513	CLA	C1D-ND	3.12	1.42	1.37
35	V	201	HEC	CMB-C2B	3.11	1.57	1.50
24	B	605	CLA	C1D-ND	3.11	1.41	1.37
24	C	511	CLA	MG-NB	-3.10	1.99	2.05
24	c	509	CLA	C1B-C2B	3.10	1.50	1.43
24	c	511	CLA	C1B-C2B	3.10	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C1C	3.09	1.44	1.38
29	C	524	LMG	O7-C8	-3.08	1.39	1.46
31	l	101	LHG	O7-C5	-3.08	1.39	1.46
24	d	406	CLA	CMD-C2D	-3.07	1.44	1.50
30	F	102	SQD	C24-C23	3.07	1.59	1.50
31	D	409	LHG	O8-C6	-3.07	1.38	1.45
24	B	609	CLA	C1D-ND	3.06	1.41	1.37
24	C	505	CLA	C1B-C2B	3.06	1.50	1.43
24	B	609	CLA	CMD-C2D	-3.06	1.44	1.50
24	C	509	CLA	MG-NA	3.05	2.13	2.06
25	d	403	PHO	CAC-C3C	-3.05	1.46	1.51
24	C	511	CLA	C1B-C2B	3.05	1.50	1.43
24	C	507	CLA	C4B-NB	3.05	1.41	1.37
31	D	409	LHG	O7-C5	-3.05	1.39	1.46
26	t	101	BCR	C1-C6	-3.04	1.49	1.53
30	F	102	SQD	O5-C1	3.04	1.49	1.41
30	a	611	SQD	C24-C23	3.03	1.59	1.50
24	B	608	CLA	MG-NA	3.03	2.13	2.06
31	e	103	LHG	O8-C23	3.03	1.42	1.33
26	d	407	BCR	C1-C6	-3.03	1.49	1.53
24	B	616	CLA	C4B-NB	3.03	1.41	1.37
24	C	512	CLA	C1D-ND	3.03	1.41	1.37
31	A	615	LHG	O7-C5	-3.02	1.39	1.46
24	b	603	CLA	MG-NA	3.02	2.13	2.06
24	B	606	CLA	CMD-C2D	-3.02	1.44	1.50
24	b	614	CLA	CHC-C1C	3.02	1.44	1.38
24	C	513	CLA	C1D-ND	3.01	1.41	1.37
24	b	603	CLA	CMB-C2B	-3.01	1.44	1.50
24	c	502	CLA	MG-NC	-3.01	1.99	2.06
24	b	608	CLA	C3B-C4B	3.01	1.51	1.42
24	b	615	CLA	C4B-NB	3.01	1.41	1.37
24	B	615	CLA	MG-NB	3.00	2.11	2.05
32	A	617	DGD	C4D-C5D	3.00	1.59	1.53
26	K	101	BCR	C30-C25	-2.99	1.50	1.53
30	a	610	SQD	O47-C7	2.99	1.42	1.34
29	c	524	LMG	C4-C5	2.99	1.59	1.53
27	A	610	PL9	C7-C3	-2.98	1.47	1.51
25	d	402	PHO	C3D-C4D	2.98	1.45	1.41
24	B	608	CLA	CMD-C2D	-2.98	1.44	1.50
24	d	404	CLA	C1B-C2B	2.97	1.50	1.43
32	C	522	DGD	C4D-C3D	2.97	1.60	1.52
32	H	102	DGD	O2D-C2D	-2.97	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	612	CLA	C1B-C2B	2.97	1.50	1.43
32	c	519	DGD	C1D-C2D	2.96	1.61	1.52
25	D	402	PHO	C4D-ND	-2.96	1.34	1.38
24	C	509	CLA	CMD-C2D	-2.96	1.44	1.50
24	b	609	CLA	C4B-NB	2.96	1.41	1.37
24	b	611	CLA	MG-NB	-2.95	1.99	2.05
24	b	603	CLA	CMC-C2C	-2.95	1.44	1.50
24	b	606	CLA	C4B-NB	2.95	1.41	1.37
24	b	609	CLA	MG-NB	2.95	2.11	2.05
29	B	620	LMG	C7-C8	2.95	1.60	1.50
26	D	405	BCR	C30-C25	-2.95	1.50	1.53
29	B	620	LMG	C4-C3	2.95	1.60	1.52
26	B	617	BCR	C30-C25	-2.95	1.50	1.53
30	a	611	SQD	O47-C45	-2.95	1.39	1.46
30	b	620	SQD	O47-C45	-2.94	1.39	1.46
27	A	610	PL9	C3-C4	-2.94	1.45	1.49
32	c	519	DGD	O2G-C2G	-2.94	1.39	1.46
32	C	521	DGD	C4E-C3E	2.94	1.60	1.52
24	B	603	CLA	C1D-ND	2.94	1.41	1.37
24	B	612	CLA	C1B-C2B	2.94	1.50	1.43
24	B	607	CLA	MG-NA	2.94	2.13	2.06
29	A	613	LMG	C1-C2	2.94	1.61	1.52
24	B	602	CLA	C1D-ND	2.94	1.41	1.37
24	C	508	CLA	C1B-C2B	2.93	1.50	1.43
24	a	606	CLA	C1D-ND	2.93	1.41	1.37
24	b	605	CLA	C1B-C2B	2.93	1.50	1.43
30	B	623	SQD	O47-C7	2.93	1.42	1.34
30	A	614	SQD	O47-C7	2.92	1.42	1.34
25	d	402	PHO	C4D-CHA	2.92	1.43	1.39
24	C	511	CLA	C3B-C4B	2.92	1.51	1.42
26	k	102	BCR	C30-C25	-2.92	1.50	1.53
29	d	414	LMG	O1-C7	-2.92	1.38	1.43
24	B	616	CLA	C1B-C2B	2.92	1.50	1.43
24	b	615	CLA	MG-NB	2.91	2.11	2.05
24	C	502	CLA	C1D-ND	2.91	1.41	1.37
24	B	602	CLA	C1B-C2B	2.91	1.50	1.43
24	C	506	CLA	MG-NC	-2.91	1.99	2.06
24	B	615	CLA	CHC-C1C	2.90	1.44	1.38
24	C	506	CLA	C1D-ND	2.90	1.41	1.37
26	a	608	BCR	C38-C26	-2.90	1.46	1.50
26	b	619	BCR	C1-C6	-2.89	1.50	1.53
24	A	612	CLA	CHC-C1C	2.89	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	MG-NC	-2.89	1.99	2.06
24	d	405	CLA	C4B-NB	2.89	1.41	1.37
29	D	407	LMG	C4-C5	2.89	1.59	1.53
24	B	602	CLA	MG-NA	2.88	2.13	2.06
32	c	519	DGD	O2E-C2E	-2.88	1.35	1.43
29	c	524	LMG	O1-C7	-2.88	1.38	1.43
24	c	502	CLA	C1D-ND	2.88	1.41	1.37
30	A	614	SQD	O5-C1	2.88	1.49	1.41
29	c	522	LMG	C4-C3	2.88	1.59	1.52
24	b	602	CLA	C1B-C2B	2.87	1.49	1.43
24	B	613	CLA	C1B-C2B	2.87	1.49	1.43
24	C	503	CLA	C4B-NB	2.87	1.41	1.37
24	b	606	CLA	CHC-C1C	2.87	1.44	1.38
24	C	502	CLA	C1B-C2B	2.87	1.49	1.43
24	C	510	CLA	C1B-C2B	2.87	1.49	1.43
24	a	607	CLA	MG-ND	-2.87	2.00	2.05
30	f	101	SQD	O5-C1	2.86	1.49	1.41
24	d	404	CLA	C1D-ND	2.86	1.41	1.37
29	B	621	LMG	C9-C8	2.86	1.59	1.50
24	A	608	CLA	C1D-ND	2.86	1.41	1.37
24	B	606	CLA	C1B-C2B	2.86	1.49	1.43
31	e	103	LHG	P-O6	2.85	1.70	1.59
32	c	519	DGD	C3G-C2G	2.84	1.59	1.50
26	t	101	BCR	C30-C25	-2.84	1.50	1.53
27	A	610	PL9	C41-C39	2.84	1.57	1.51
32	A	617	DGD	C1E-C2E	2.84	1.60	1.52
24	b	612	CLA	MG-ND	-2.84	2.00	2.05
24	B	613	CLA	CHC-C1C	2.83	1.44	1.38
31	e	103	LHG	C24-C23	2.83	1.58	1.50
24	c	507	CLA	MG-ND	2.83	2.11	2.05
24	b	605	CLA	MG-NC	-2.82	1.99	2.06
29	o	301	LMG	C9-C8	2.82	1.59	1.50
24	b	613	CLA	MG-NB	-2.82	2.00	2.05
24	B	614	CLA	C1B-C2B	2.82	1.49	1.43
24	b	613	CLA	C4B-NB	2.81	1.41	1.37
24	c	508	CLA	C3B-C4B	2.81	1.50	1.42
24	C	501	CLA	C1B-C2B	2.81	1.49	1.43
24	d	405	CLA	CMD-C2D	-2.80	1.45	1.50
24	b	616	CLA	C1D-ND	2.80	1.41	1.37
24	b	611	CLA	C1B-C2B	2.80	1.49	1.43
24	b	602	CLA	C4B-NB	2.79	1.41	1.37
24	b	615	CLA	C3B-C4B	2.79	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	414	LMG	O7-C8	-2.78	1.40	1.46
29	c	522	LMG	O1-C1	2.78	1.44	1.40
24	c	511	CLA	C3B-C4B	2.78	1.50	1.42
24	B	612	CLA	C3B-C4B	2.77	1.50	1.42
24	a	607	CLA	C1B-C2B	2.77	1.49	1.43
25	A	607	PHO	C3D-C4D	2.77	1.45	1.41
30	f	101	SQD	C24-C23	2.76	1.58	1.50
34	F	101	HEM	FE-NB	2.75	2.03	1.94
32	A	617	DGD	O1G-C1G	-2.75	1.39	1.45
32	A	617	DGD	C4D-C3D	2.75	1.59	1.52
24	c	507	CLA	C1B-C2B	2.74	1.49	1.43
24	B	601	CLA	MG-NB	-2.74	2.00	2.05
29	d	414	LMG	O6-C5	-2.74	1.37	1.44
35	v	201	HEC	FE-ND	2.74	2.03	1.94
25	d	403	PHO	CMD-C2D	-2.74	1.46	1.51
26	C	520	BCR	C30-C25	-2.74	1.50	1.53
34	e	102	HEM	CAC-C3C	2.73	1.54	1.47
34	F	101	HEM	CAC-C3C	2.73	1.54	1.47
30	B	623	SQD	O5-C1	2.73	1.48	1.41
24	d	405	CLA	C3B-C4B	2.73	1.50	1.42
24	B	607	CLA	CMB-C2B	-2.73	1.45	1.50
24	c	513	CLA	C1B-C2B	2.73	1.49	1.43
30	a	610	SQD	O5-C1	2.72	1.48	1.41
25	d	403	PHO	CMC-C2C	-2.72	1.46	1.50
29	C	524	LMG	C7-C8	2.72	1.59	1.50
24	c	504	CLA	CMC-C2C	-2.72	1.45	1.50
24	c	510	CLA	C4B-NB	2.72	1.41	1.37
24	B	611	CLA	CHC-C1C	2.71	1.43	1.38
25	d	402	PHO	CMC-C2C	-2.70	1.46	1.50
24	A	606	CLA	C4B-NB	2.70	1.41	1.37
24	B	615	CLA	C1B-C2B	2.69	1.49	1.43
24	C	503	CLA	C1B-C2B	2.69	1.49	1.43
24	d	405	CLA	CHC-C1C	2.69	1.43	1.38
26	B	617	BCR	C33-C5	-2.69	1.46	1.50
24	a	605	CLA	C1B-C2B	2.69	1.49	1.43
24	c	506	CLA	CHC-C1C	2.69	1.43	1.38
31	D	411	LHG	O7-C5	-2.69	1.40	1.46
26	b	617	BCR	C30-C25	-2.68	1.50	1.53
24	B	613	CLA	C1D-ND	2.68	1.41	1.37
24	c	511	CLA	MG-NC	2.68	2.12	2.06
24	c	501	CLA	CHC-C1C	2.68	1.43	1.38
29	D	408	LMG	C7-C8	2.68	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C1B-C2B	2.67	1.49	1.43
24	B	606	CLA	C1D-ND	2.67	1.41	1.37
24	d	406	CLA	C1B-C2B	2.67	1.49	1.43
26	d	407	BCR	C30-C25	-2.67	1.50	1.53
24	b	607	CLA	C1B-NB	-2.67	1.34	1.37
24	b	608	CLA	CMD-C2D	-2.67	1.45	1.50
34	F	101	HEM	FE-NA	2.67	2.04	1.95
29	A	613	LMG	O1-C1	2.66	1.44	1.40
31	D	409	LHG	P-O3	2.65	1.69	1.59
30	f	101	SQD	O9-S	2.65	1.52	1.45
24	b	602	CLA	CMD-C2D	-2.65	1.45	1.50
32	A	617	DGD	C3G-C2G	2.65	1.59	1.50
24	B	612	CLA	C1D-ND	2.65	1.41	1.37
30	a	611	SQD	O7-S	2.65	1.52	1.45
32	c	520	DGD	C4D-C3D	2.65	1.59	1.52
24	C	510	CLA	C3B-C4B	2.65	1.50	1.42
24	c	512	CLA	C4B-NB	2.64	1.41	1.37
24	D	403	CLA	CMD-C2D	-2.64	1.45	1.50
24	C	513	CLA	C1B-C2B	2.64	1.49	1.43
24	B	613	CLA	CMB-C2B	-2.63	1.45	1.50
24	c	508	CLA	C1B-C2B	2.63	1.49	1.43
24	C	506	CLA	C4B-NB	2.63	1.41	1.37
29	c	523	LMG	O1-C1	2.62	1.44	1.40
26	A	609	BCR	C30-C25	-2.62	1.50	1.53
25	D	402	PHO	CMD-C2D	-2.62	1.46	1.51
31	D	410	LHG	C3-C2	2.62	1.59	1.51
29	o	301	LMG	C7-C8	2.62	1.59	1.50
29	c	522	LMG	C7-C8	2.61	1.59	1.50
24	c	509	CLA	C4B-NB	2.61	1.41	1.37
24	b	614	CLA	MG-NB	2.61	2.11	2.05
24	b	613	CLA	C1B-C2B	2.61	1.49	1.43
24	b	610	CLA	C4B-NB	2.61	1.41	1.37
25	d	402	PHO	CBD-CGD	-2.61	1.49	1.52
24	c	502	CLA	CMD-C2D	-2.61	1.45	1.50
24	B	604	CLA	C3B-C4B	2.61	1.50	1.42
24	B	603	CLA	MG-NA	2.61	2.12	2.06
29	b	623	LMG	C9-C8	2.60	1.58	1.50
24	B	602	CLA	C4B-NB	2.60	1.41	1.37
24	b	605	CLA	C1D-ND	2.60	1.41	1.37
32	c	521	DGD	C4D-C5D	2.59	1.58	1.53
26	T	101	BCR	C1-C6	-2.59	1.50	1.53
24	c	502	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	408	PL9	C26-C24	-2.59	1.46	1.51
26	k	101	BCR	C1-C6	-2.59	1.50	1.53
29	A	613	LMG	C7-C8	2.59	1.58	1.50
24	B	607	CLA	C1B-C2B	2.58	1.49	1.43
24	b	602	CLA	C1D-ND	2.57	1.41	1.37
24	B	604	CLA	C1B-C2B	2.57	1.49	1.43
24	b	603	CLA	C1B-NB	-2.57	1.34	1.37
24	b	604	CLA	C1B-C2B	2.57	1.49	1.43
29	c	524	LMG	O7-C8	-2.57	1.40	1.46
27	d	408	PL9	C52-C5	-2.56	1.45	1.50
24	b	615	CLA	CHC-C1C	2.56	1.43	1.38
24	B	603	CLA	C1B-C2B	2.56	1.49	1.43
24	c	513	CLA	CMB-C2B	-2.56	1.45	1.50
24	b	605	CLA	C4B-NB	2.55	1.41	1.37
24	d	405	CLA	C1D-ND	2.55	1.41	1.37
24	b	616	CLA	C1B-C2B	2.55	1.49	1.43
29	C	516	LMG	C4-C3	2.55	1.58	1.52
24	b	615	CLA	C1B-C2B	2.54	1.49	1.43
24	C	501	CLA	C3D-C4D	2.54	1.49	1.44
24	c	512	CLA	CHC-C1C	2.54	1.43	1.38
24	b	614	CLA	C1B-NB	-2.54	1.34	1.37
24	c	505	CLA	CMB-C2B	-2.54	1.45	1.50
24	c	508	CLA	MG-NC	2.53	2.12	2.06
34	F	101	HEM	CMD-C2D	2.53	1.56	1.50
32	c	519	DGD	O3G-C3G	-2.53	1.39	1.43
24	C	503	CLA	C1D-ND	2.53	1.41	1.37
24	a	607	CLA	MG-NA	2.53	2.12	2.06
32	C	522	DGD	C1G-C2G	2.53	1.58	1.50
31	A	615	LHG	O8-C23	2.53	1.40	1.33
24	A	605	CLA	C4B-NB	2.52	1.41	1.37
30	A	614	SQD	O9-S	2.52	1.52	1.45
24	c	509	CLA	C3B-C4B	2.52	1.50	1.42
24	c	513	CLA	C3B-C4B	2.51	1.50	1.42
24	c	501	CLA	CMC-C2C	-2.51	1.45	1.50
24	a	606	CLA	CMD-C2D	-2.51	1.45	1.50
24	c	508	CLA	C4B-NB	2.51	1.41	1.37
24	C	510	CLA	CMB-C2B	-2.51	1.45	1.50
24	b	609	CLA	C3B-C4B	2.50	1.50	1.42
24	c	504	CLA	CHC-C1C	2.50	1.43	1.38
24	B	601	CLA	C1B-C2B	2.50	1.49	1.43
29	A	613	LMG	O1-C7	-2.50	1.39	1.43
26	c	515	BCR	C33-C5	-2.50	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	CHC-C1C	2.50	1.43	1.38
24	C	505	CLA	MG-ND	2.50	2.10	2.05
32	c	520	DGD	O2E-C2E	-2.49	1.36	1.43
24	B	610	CLA	C1B-C2B	2.49	1.49	1.43
24	a	605	CLA	CHC-C1C	2.49	1.43	1.38
35	v	201	HEC	CMD-C2D	2.49	1.55	1.50
24	B	608	CLA	C1B-C2B	2.49	1.49	1.43
32	c	519	DGD	O3E-C3E	-2.49	1.36	1.43
31	d	410	LHG	C24-C23	2.48	1.57	1.50
29	D	408	LMG	C4-C5	2.48	1.58	1.53
24	b	601	CLA	CMC-C2C	-2.48	1.45	1.50
24	C	505	CLA	C4B-NB	2.48	1.41	1.37
24	B	608	CLA	MG-ND	-2.48	2.00	2.05
30	A	616	SQD	O9-S	2.48	1.52	1.45
24	D	404	CLA	CMD-C2D	-2.48	1.45	1.50
24	C	509	CLA	MG-ND	-2.47	2.00	2.05
29	C	516	LMG	O8-C28	2.47	1.40	1.33
32	H	102	DGD	C4E-C5E	2.47	1.58	1.53
24	c	508	CLA	C3C-C2C	2.47	1.42	1.36
24	c	501	CLA	C1B-NB	-2.47	1.34	1.37
24	c	505	CLA	C1B-C2B	2.47	1.48	1.43
24	C	507	CLA	CHC-C1C	2.47	1.43	1.38
24	b	601	CLA	C3B-C4B	2.46	1.49	1.42
24	B	611	CLA	C1D-ND	2.46	1.41	1.37
25	d	402	PHO	C4D-ND	-2.46	1.34	1.38
27	a	609	PL9	C47-C48	2.46	1.57	1.50
24	A	612	CLA	MG-NA	2.46	2.12	2.06
32	C	521	DGD	O1G-C1A	2.46	1.40	1.33
24	c	510	CLA	C1B-C2B	2.46	1.48	1.43
32	c	521	DGD	O2G-C1B	2.45	1.41	1.34
32	h	102	DGD	C4E-C5E	2.44	1.58	1.53
24	c	505	CLA	C3B-C4B	2.44	1.49	1.42
25	A	607	PHO	C3D-CAD	-2.44	1.43	1.47
32	A	617	DGD	O3G-C1D	2.44	1.44	1.40
32	C	522	DGD	C1E-C2E	2.44	1.59	1.52
25	A	607	PHO	CMC-C2C	-2.44	1.46	1.50
24	C	511	CLA	CHC-C1C	2.44	1.43	1.38
24	C	508	CLA	MG-NA	2.43	2.12	2.06
24	d	406	CLA	CMC-C2C	-2.43	1.45	1.50
30	B	623	SQD	C24-C23	2.43	1.57	1.50
24	c	511	CLA	C1D-ND	2.43	1.41	1.37
24	b	609	CLA	CMD-C2D	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3B-C4B	2.43	1.49	1.42
24	C	509	CLA	C3B-C4B	2.42	1.49	1.42
24	B	610	CLA	CHC-C1C	2.42	1.43	1.38
24	b	609	CLA	CHC-C1C	2.42	1.43	1.38
24	b	616	CLA	C4B-NB	2.42	1.41	1.37
24	C	506	CLA	C3B-C4B	2.41	1.49	1.42
27	a	609	PL9	C46-C44	2.41	1.56	1.51
24	C	512	CLA	CHC-C1C	2.41	1.43	1.38
32	c	521	DGD	O5D-C1E	2.41	1.44	1.40
24	b	603	CLA	C1D-ND	2.41	1.41	1.37
24	c	510	CLA	CMB-C2B	-2.41	1.45	1.50
24	D	403	CLA	MG-NC	2.41	2.12	2.06
32	C	523	DGD	O3G-C3G	-2.40	1.39	1.43
24	c	507	CLA	CMB-C2B	-2.40	1.45	1.50
32	h	102	DGD	C1E-C2E	2.40	1.59	1.52
30	f	101	SQD	O7-S	2.39	1.51	1.45
29	D	408	LMG	O6-C5	-2.39	1.38	1.44
29	C	516	LMG	C9-C8	2.39	1.58	1.50
24	C	510	CLA	CHC-C1C	2.39	1.43	1.38
29	C	516	LMG	C3-C2	2.39	1.58	1.52
26	A	609	BCR	C33-C5	-2.39	1.47	1.50
24	B	610	CLA	C4B-NB	2.39	1.41	1.37
30	a	610	SQD	C24-C23	2.39	1.57	1.50
29	b	623	LMG	C4-C5	2.39	1.58	1.53
24	B	612	CLA	CMC-C2C	-2.38	1.45	1.50
24	B	613	CLA	CMD-C2D	-2.38	1.45	1.50
24	C	512	CLA	C3B-C4B	2.38	1.49	1.42
31	D	411	LHG	C24-C23	2.38	1.57	1.50
32	c	521	DGD	C6D-C5D	2.38	1.58	1.51
24	C	511	CLA	CMB-C2B	-2.37	1.45	1.50
29	B	621	LMG	O4-C4	-2.37	1.37	1.43
24	A	608	CLA	C1B-C2B	2.37	1.48	1.43
24	A	605	CLA	C3B-C4B	2.36	1.49	1.42
25	d	403	PHO	CMB-C2B	-2.36	1.46	1.51
24	C	508	CLA	CHC-C1C	2.36	1.43	1.38
24	C	506	CLA	MG-ND	-2.36	2.01	2.05
24	D	404	CLA	CHC-C4B	-2.36	1.34	1.39
25	D	402	PHO	CMC-C2C	-2.35	1.46	1.50
34	e	102	HEM	C3B-C2B	-2.35	1.32	1.37
24	b	615	CLA	CMB-C2B	-2.35	1.45	1.50
24	c	512	CLA	C3B-C4B	2.35	1.49	1.42
24	b	602	CLA	C1A-CHA	-2.35	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	618	BCR	C1-C6	-2.35	1.50	1.53
24	B	610	CLA	C3B-C4B	2.35	1.49	1.42
24	B	603	CLA	C3B-C4B	2.35	1.49	1.42
30	B	623	SQD	O5-C5	2.35	1.50	1.44
34	e	102	HEM	CAB-C3B	2.34	1.53	1.47
24	b	611	CLA	CMD-C2D	-2.34	1.46	1.50
24	B	608	CLA	C4B-NB	2.34	1.40	1.37
24	c	505	CLA	CHC-C1C	2.34	1.43	1.38
25	A	607	PHO	C1D-ND	2.34	1.42	1.38
24	b	611	CLA	C1D-C2D	2.33	1.50	1.45
29	m	101	LMG	C4-C5	2.33	1.58	1.53
32	C	521	DGD	C3G-C2G	2.33	1.58	1.50
24	B	609	CLA	C3B-C4B	2.33	1.49	1.42
30	F	102	SQD	O9-S	2.33	1.51	1.45
24	C	504	CLA	C3B-C4B	2.33	1.49	1.42
24	c	508	CLA	CMC-C2C	-2.33	1.46	1.50
24	c	506	CLA	C3B-C4B	2.32	1.49	1.42
24	B	603	CLA	C1B-NB	-2.32	1.34	1.37
24	c	505	CLA	C4B-NB	2.32	1.40	1.37
24	C	512	CLA	CMB-C2B	-2.32	1.46	1.50
29	b	623	LMG	C4-C3	2.32	1.58	1.52
27	a	609	PL9	C46-C47	2.32	1.61	1.53
24	c	503	CLA	C1B-C2B	2.32	1.48	1.43
34	F	101	HEM	CMA-C3A	2.31	1.55	1.50
30	A	616	SQD	O7-S	2.31	1.51	1.45
32	c	521	DGD	O1G-C1A	2.31	1.40	1.33
24	b	612	CLA	CMC-C2C	-2.31	1.46	1.50
24	c	507	CLA	CMC-C2C	-2.31	1.46	1.50
24	C	513	CLA	C4B-NB	2.31	1.40	1.37
24	b	609	CLA	O2D-CGD	2.31	1.38	1.33
27	A	610	PL9	C41-C42	2.31	1.61	1.53
29	c	523	LMG	C4-C3	2.30	1.58	1.52
24	a	607	CLA	C4B-NB	2.30	1.40	1.37
24	c	503	CLA	CMC-C2C	-2.30	1.46	1.50
26	T	101	BCR	C27-C26	-2.30	1.46	1.51
24	b	612	CLA	C3B-C4B	2.30	1.49	1.42
24	d	404	CLA	CMB-C2B	-2.30	1.46	1.50
24	b	606	CLA	C3B-C4B	2.30	1.49	1.42
24	c	503	CLA	C4B-NB	2.30	1.40	1.37
32	c	521	DGD	O3D-C3D	-2.29	1.37	1.43
24	B	602	CLA	C3B-C4B	2.29	1.49	1.42
24	a	606	CLA	MG-NC	2.29	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C4C-C3C	2.29	1.48	1.45
26	B	618	BCR	C1-C6	-2.29	1.50	1.53
24	C	506	CLA	C1B-C2B	2.29	1.48	1.43
24	b	614	CLA	C3B-C4B	2.29	1.49	1.42
24	a	605	CLA	C3D-C4D	2.28	1.49	1.44
30	a	611	SQD	O9-S	2.28	1.51	1.45
24	b	605	CLA	C3B-C4B	2.28	1.49	1.42
24	b	601	CLA	CHC-C1C	2.28	1.43	1.38
24	d	406	CLA	CHC-C1C	2.27	1.43	1.38
24	b	610	CLA	C3D-C4D	2.27	1.49	1.44
30	a	611	SQD	O5-C5	2.27	1.49	1.44
24	b	609	CLA	C1B-C2B	2.27	1.48	1.43
31	L	101	LHG	C24-C23	2.27	1.57	1.50
29	A	613	LMG	C3-C2	2.27	1.58	1.52
24	b	612	CLA	C4B-NB	2.27	1.40	1.37
24	B	612	CLA	CHC-C1C	2.27	1.43	1.38
25	D	402	PHO	CMB-C2B	-2.27	1.47	1.51
30	a	610	SQD	O7-S	2.26	1.51	1.45
24	b	615	CLA	CMD-C2D	-2.26	1.46	1.50
24	c	509	CLA	CMD-C2D	-2.26	1.46	1.50
24	D	403	CLA	CAA-C2A	-2.26	1.50	1.54
24	b	607	CLA	C1B-C2B	2.26	1.48	1.43
31	d	411	LHG	C1-C2	-2.26	1.43	1.51
34	e	102	HEM	CMC-C2C	2.26	1.55	1.50
24	B	601	CLA	CMB-C2B	-2.26	1.46	1.50
24	D	404	CLA	MG-NC	2.25	2.11	2.06
24	C	509	CLA	C1B-C2B	2.25	1.48	1.43
24	c	507	CLA	C1B-NB	-2.25	1.34	1.37
24	b	616	CLA	CMC-C2C	-2.25	1.46	1.50
27	D	406	PL9	C7-C3	-2.25	1.48	1.51
24	a	606	CLA	C1B-C2B	2.25	1.48	1.43
34	F	101	HEM	CAB-C3B	2.25	1.53	1.47
29	d	414	LMG	C7-C8	2.25	1.57	1.50
26	T	101	BCR	C30-C25	-2.24	1.50	1.53
24	b	610	CLA	C1B-C2B	2.24	1.48	1.43
24	c	512	CLA	MG-NC	2.24	2.11	2.06
24	B	611	CLA	MG-NB	2.24	2.10	2.05
26	a	608	BCR	C1-C6	-2.24	1.50	1.53
24	B	608	CLA	C1B-NB	-2.24	1.34	1.37
30	B	623	SQD	C8-C7	2.24	1.57	1.50
32	C	523	DGD	O6E-C1E	2.24	1.47	1.41
27	a	609	PL9	C6-C1	-2.24	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	610	PL9	C25-C24	-2.24	1.45	1.50
32	H	102	DGD	C4D-C5D	2.23	1.57	1.53
24	D	404	CLA	C3D-C4D	2.23	1.49	1.44
24	c	501	CLA	C1B-C2B	2.23	1.48	1.43
32	c	520	DGD	C1E-C2E	2.23	1.59	1.52
29	c	524	LMG	O6-C5	-2.23	1.38	1.44
25	A	607	PHO	C1C-NC	-2.23	1.30	1.37
24	C	508	CLA	C1D-ND	2.23	1.40	1.37
24	B	604	CLA	CMC-C2C	-2.23	1.46	1.50
24	b	613	CLA	MG-NA	2.23	2.11	2.06
29	c	523	LMG	O7-C8	-2.23	1.41	1.46
24	d	404	CLA	MG-ND	2.23	2.10	2.05
24	C	505	CLA	C3B-C4B	2.22	1.49	1.42
24	C	509	CLA	C3D-C4D	2.22	1.49	1.44
26	b	619	BCR	C30-C25	-2.22	1.50	1.53
31	d	411	LHG	C4-C5	2.22	1.57	1.50
24	C	503	CLA	C3B-C4B	2.22	1.49	1.42
24	c	504	CLA	CMD-C2D	-2.21	1.46	1.50
24	C	507	CLA	C3B-C4B	2.21	1.49	1.42
24	A	608	CLA	MG-NC	2.21	2.11	2.06
24	b	608	CLA	C1B-C2B	2.21	1.48	1.43
24	a	605	CLA	C3B-C4B	2.21	1.49	1.42
29	b	623	LMG	O8-C28	2.21	1.39	1.33
24	C	504	CLA	C1B-C2B	2.21	1.48	1.43
26	C	514	BCR	C33-C5	-2.21	1.47	1.50
24	A	606	CLA	C3B-C4B	2.21	1.49	1.42
24	c	504	CLA	C1B-C2B	2.21	1.48	1.43
24	b	603	CLA	CMD-C2D	-2.21	1.46	1.50
24	a	605	CLA	MG-ND	2.21	2.10	2.05
25	A	607	PHO	C4D-CHA	2.21	1.42	1.39
32	h	102	DGD	O3G-C3G	-2.21	1.39	1.43
32	c	520	DGD	C6D-C5D	2.21	1.58	1.51
24	B	613	CLA	C3B-C4B	2.20	1.49	1.42
24	B	601	CLA	C3B-C4B	2.20	1.49	1.42
24	b	607	CLA	C4B-NB	2.20	1.40	1.37
24	C	501	CLA	C3B-C4B	2.20	1.49	1.42
24	b	602	CLA	CMB-C2B	-2.20	1.46	1.50
24	B	610	CLA	CMB-C2B	-2.20	1.46	1.50
32	c	520	DGD	C4E-C5E	2.20	1.57	1.53
24	d	406	CLA	C3B-C4B	2.20	1.49	1.42
34	e	102	HEM	FE-NB	2.20	2.01	1.94
24	B	602	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	520	DGD	O5D-C1E	2.20	1.43	1.40
24	b	608	CLA	C4B-NB	2.20	1.40	1.37
24	b	610	CLA	C3B-C4B	2.19	1.49	1.42
24	b	616	CLA	CMD-C2D	-2.19	1.46	1.50
24	b	604	CLA	MG-NA	2.19	2.11	2.06
24	b	604	CLA	CMD-C2D	-2.19	1.46	1.50
24	b	602	CLA	C3B-C4B	2.19	1.49	1.42
29	A	613	LMG	C14-C13	2.19	1.62	1.51
24	c	512	CLA	MG-NA	2.19	2.11	2.06
34	F	101	HEM	C2A-C3A	-2.19	1.33	1.38
24	B	615	CLA	CMB-C2B	-2.19	1.46	1.50
28	x	101	STE	C2-C1	2.19	1.55	1.50
29	o	301	LMG	C1-C2	2.19	1.58	1.52
24	c	506	CLA	O2D-CGD	2.18	1.38	1.33
29	C	524	LMG	C1-C2	2.18	1.58	1.52
24	A	606	CLA	C1B-C2B	2.18	1.48	1.43
25	d	402	PHO	C3D-CAD	-2.18	1.43	1.47
24	b	611	CLA	C3B-C4B	2.18	1.49	1.42
24	b	609	CLA	C3D-C4D	2.18	1.49	1.44
30	b	620	SQD	O9-S	2.18	1.51	1.45
24	D	404	CLA	CMC-C2C	-2.18	1.46	1.50
24	B	608	CLA	C3D-C4D	2.18	1.49	1.44
24	C	510	CLA	O2A-CGA	2.18	1.39	1.33
24	B	614	CLA	CHC-C1C	2.17	1.42	1.38
24	C	503	CLA	C1D-C2D	2.17	1.49	1.45
32	C	521	DGD	C2A-C1A	-2.17	1.44	1.50
24	B	616	CLA	CMC-C2C	-2.17	1.46	1.50
32	c	520	DGD	C6E-C5E	2.17	1.59	1.51
24	C	506	CLA	CHC-C1C	2.17	1.42	1.38
24	a	605	CLA	C1D-C2D	2.17	1.49	1.45
32	c	520	DGD	C4D-C5D	2.17	1.57	1.53
24	B	606	CLA	C3B-C4B	2.16	1.49	1.42
24	b	601	CLA	O2A-CGA	2.16	1.39	1.33
24	A	608	CLA	C1D-C2D	2.16	1.49	1.45
32	H	102	DGD	C1G-C2G	2.16	1.57	1.50
25	D	402	PHO	C4D-CHA	2.16	1.42	1.39
35	v	201	HEC	CMA-C3A	2.16	1.55	1.50
24	b	612	CLA	MG-NA	2.16	2.11	2.06
24	C	510	CLA	CMD-C2D	-2.16	1.46	1.50
24	B	611	CLA	C3B-C4B	2.16	1.49	1.42
24	b	610	CLA	CMB-C2B	-2.15	1.46	1.50
24	b	614	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	407	LMG	C7-C8	2.15	1.57	1.50
24	c	502	CLA	CHC-C4B	-2.15	1.34	1.39
24	c	510	CLA	CHC-C1C	2.15	1.42	1.38
32	C	523	DGD	O1G-C1G	-2.15	1.40	1.45
25	d	403	PHO	C3D-CAD	-2.14	1.43	1.47
32	h	102	DGD	C3G-C2G	2.14	1.57	1.50
27	a	609	PL9	C36-C34	2.14	1.55	1.51
24	A	605	CLA	CMC-C2C	-2.14	1.46	1.50
24	C	512	CLA	C1B-C2B	2.14	1.48	1.43
24	C	512	CLA	CMD-C2D	-2.14	1.46	1.50
24	a	607	CLA	C3B-C4B	2.14	1.49	1.42
24	c	501	CLA	CMD-C2D	-2.14	1.46	1.50
25	d	402	PHO	C3B-C2B	-2.14	1.37	1.40
24	b	614	CLA	C4B-NB	2.13	1.40	1.37
26	C	520	BCR	C33-C5	-2.13	1.47	1.50
24	B	603	CLA	CMB-C2B	-2.13	1.46	1.50
24	c	504	CLA	C3B-C4B	2.13	1.49	1.42
26	b	617	BCR	C33-C5	-2.13	1.47	1.50
24	C	501	CLA	CHC-C1C	2.13	1.42	1.38
32	C	522	DGD	C6E-C5E	2.13	1.59	1.51
24	B	611	CLA	CMB-C2B	-2.13	1.46	1.50
32	C	522	DGD	O3D-C3D	-2.13	1.37	1.43
24	C	504	CLA	O2D-CGD	2.12	1.38	1.33
32	c	520	DGD	O5D-C6D	2.12	1.47	1.43
24	b	605	CLA	C3D-C4D	2.12	1.49	1.44
24	c	513	CLA	MG-NC	-2.12	2.01	2.06
24	D	404	CLA	C1B-C2B	2.12	1.48	1.43
24	d	406	CLA	MG-NA	2.12	2.11	2.06
24	c	506	CLA	C1B-C2B	2.12	1.48	1.43
24	B	607	CLA	C3B-C4B	2.12	1.48	1.42
29	m	101	LMG	C1-C2	2.11	1.58	1.52
24	b	607	CLA	CMD-C2D	-2.11	1.46	1.50
24	b	603	CLA	C1B-C2B	2.11	1.48	1.43
24	C	511	CLA	MG-NC	2.11	2.11	2.06
29	A	613	LMG	C16-C15	2.11	1.62	1.51
32	C	522	DGD	O5D-C6D	-2.11	1.40	1.43
24	B	601	CLA	CMC-C2C	-2.11	1.46	1.50
24	C	508	CLA	MG-NB	2.11	2.10	2.05
26	K	102	BCR	C33-C5	-2.11	1.47	1.50
24	C	510	CLA	C3D-C4D	2.11	1.48	1.44
24	b	605	CLA	C1D-C2D	2.10	1.49	1.45
24	a	606	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CMC-C2C	-2.10	1.46	1.50
34	e	102	HEM	C2A-C3A	-2.10	1.33	1.38
29	C	524	LMG	C4-C3	2.10	1.57	1.52
29	B	621	LMG	C4-C3	2.10	1.57	1.52
24	b	612	CLA	C1B-C2B	2.10	1.48	1.43
24	B	609	CLA	O2D-CGD	2.10	1.38	1.33
24	B	606	CLA	CHC-C1C	2.10	1.42	1.38
29	c	522	LMG	C4-C5	2.10	1.57	1.53
27	a	609	PL9	C40-C39	-2.10	1.45	1.50
24	B	616	CLA	CMB-C2B	-2.10	1.46	1.50
24	b	607	CLA	C1D-ND	2.10	1.40	1.37
29	c	518	LMG	C9-C8	2.10	1.57	1.50
30	A	616	SQD	C46-C45	2.10	1.57	1.50
31	L	101	LHG	O6-C4	-2.10	1.36	1.44
32	c	519	DGD	C1G-C2G	2.10	1.57	1.50
25	A	607	PHO	O2D-CGD	2.10	1.38	1.33
24	B	613	CLA	C3D-C4D	2.09	1.48	1.44
24	c	506	CLA	C4B-NB	2.09	1.40	1.37
24	b	612	CLA	CHC-C1C	2.09	1.42	1.38
29	B	621	LMG	C4-C5	2.09	1.57	1.53
24	c	506	CLA	C1B-NB	-2.09	1.35	1.37
29	c	523	LMG	C9-C8	2.09	1.57	1.50
24	B	610	CLA	C3D-C4D	2.09	1.48	1.44
32	c	520	DGD	O2G-C2G	-2.09	1.41	1.46
24	C	508	CLA	C3C-C2C	2.09	1.41	1.36
26	T	101	BCR	C4-C5	-2.08	1.47	1.51
30	A	616	SQD	O5-C5	2.08	1.49	1.44
32	h	102	DGD	O2D-C2D	-2.08	1.37	1.43
24	c	509	CLA	C3C-C2C	2.08	1.41	1.36
24	B	603	CLA	C4B-NB	2.08	1.40	1.37
24	B	601	CLA	C3D-C4D	2.08	1.48	1.44
29	c	524	LMG	C1-C2	2.08	1.58	1.52
29	A	613	LMG	C4-C3	2.08	1.57	1.52
34	e	102	HEM	CMB-C2B	2.08	1.55	1.50
24	b	602	CLA	MG-ND	-2.08	2.01	2.05
24	B	614	CLA	CMC-C2C	-2.08	1.46	1.50
24	C	504	CLA	C1D-ND	2.08	1.40	1.37
24	c	512	CLA	C3D-C4D	2.08	1.48	1.44
24	c	510	CLA	C3B-C4B	2.08	1.48	1.42
24	B	616	CLA	CHC-C4B	-2.08	1.34	1.39
30	A	614	SQD	C8-C7	2.08	1.56	1.50
25	d	402	PHO	O2D-CGD	2.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	BCR	C36-C18	-2.07	1.46	1.50
32	c	519	DGD	O5D-C1E	2.07	1.43	1.40
24	b	603	CLA	O2D-CGD	2.07	1.38	1.33
24	B	608	CLA	CHC-C1C	2.07	1.42	1.38
24	C	511	CLA	CMC-C2C	-2.07	1.46	1.50
24	b	616	CLA	MG-ND	-2.07	2.01	2.05
30	B	623	SQD	O9-S	2.06	1.50	1.45
24	B	602	CLA	MG-NB	2.06	2.09	2.05
31	e	103	LHG	C6-C5	2.06	1.57	1.50
26	b	617	BCR	C4-C5	-2.06	1.47	1.51
24	D	404	CLA	MG-NA	2.06	2.11	2.06
25	d	402	PHO	C4C-NC	2.06	1.44	1.37
24	C	506	CLA	CMC-C2C	-2.06	1.46	1.50
24	c	504	CLA	CMB-C2B	-2.06	1.46	1.50
29	B	621	LMG	C1-C2	2.06	1.58	1.52
30	b	620	SQD	O5-C5	2.05	1.49	1.44
29	c	524	LMG	C3-C2	2.05	1.57	1.52
24	b	613	CLA	CMD-C2D	-2.05	1.46	1.50
28	b	624	STE	C2-C1	2.05	1.55	1.50
28	X	101	STE	C2-C1	2.05	1.55	1.50
24	c	513	CLA	C4B-NB	2.05	1.40	1.37
24	c	507	CLA	C3D-C4D	2.04	1.48	1.44
32	C	521	DGD	C4D-C3D	2.04	1.57	1.52
24	B	604	CLA	CHC-C1C	2.04	1.42	1.38
24	d	406	CLA	C1A-CHA	-2.04	1.34	1.43
24	B	613	CLA	C4D-CHA	2.04	1.45	1.38
24	C	510	CLA	MG-NC	2.04	2.11	2.06
24	A	606	CLA	CMC-C2C	-2.03	1.46	1.50
24	C	508	CLA	C4C-C3C	2.03	1.48	1.45
28	R	101	STE	C2-C1	2.03	1.55	1.50
24	B	615	CLA	MG-NA	2.03	2.11	2.06
24	b	604	CLA	CMC-C2C	-2.03	1.46	1.50
24	b	616	CLA	CMB-C2B	-2.02	1.46	1.50
24	c	506	CLA	CHC-C4B	-2.02	1.34	1.39
24	b	601	CLA	CMD-C2D	-2.02	1.46	1.50
24	C	511	CLA	C4D-CHA	2.02	1.45	1.38
27	D	406	PL9	C50-C49	2.02	1.55	1.50
29	c	522	LMG	C6-C5	2.02	1.58	1.51
24	C	502	CLA	C4D-CHA	2.01	1.45	1.38
24	D	403	CLA	C1B-NB	-2.01	1.35	1.37
24	D	404	CLA	CMB-C2B	-2.01	1.46	1.50
24	C	507	CLA	C3D-C4D	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C4B-NB	2.01	1.40	1.37
24	b	603	CLA	C4B-NB	2.01	1.40	1.37
30	B	623	SQD	O7-S	2.01	1.50	1.45
32	h	102	DGD	C6D-C5D	2.01	1.57	1.51
24	B	610	CLA	CMC-C2C	-2.01	1.46	1.50
24	B	610	CLA	MG-NC	-2.01	2.01	2.06
26	k	102	BCR	C33-C5	-2.01	1.47	1.50
24	A	605	CLA	C1D-C2D	2.01	1.49	1.45
32	A	617	DGD	O5D-C1E	2.01	1.43	1.40
24	B	601	CLA	C3C-C2C	2.00	1.41	1.36
24	c	506	CLA	CMD-C2D	-2.00	1.46	1.50
30	F	102	SQD	O7-S	2.00	1.50	1.45
24	C	513	CLA	C3B-C4B	2.00	1.48	1.42

All (1229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C4A-NA-C1A	12.69	112.47	106.68
24	C	507	CLA	C4A-NA-C1A	9.48	111.00	106.68
24	c	511	CLA	C4A-NA-C1A	9.46	110.99	106.68
24	B	601	CLA	C4A-NA-C1A	9.07	110.82	106.68
24	C	505	CLA	C4A-NA-C1A	8.37	110.50	106.68
24	C	513	CLA	C4A-NA-C1A	8.28	110.46	106.68
24	b	606	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	C	511	CLA	C4A-NA-C1A	8.13	110.39	106.68
24	b	601	CLA	C4A-NA-C1A	8.06	110.36	106.68
24	d	404	CLA	C4A-NA-C1A	7.92	110.29	106.68
24	B	616	CLA	C4A-NA-C1A	7.88	110.27	106.68
25	A	607	PHO	C4D-CHA-CBD	-7.86	104.69	108.45
25	d	402	PHO	C4D-CHA-CBD	-7.79	104.72	108.45
30	b	620	SQD	O6-C1-C2	7.66	119.90	108.27
30	A	614	SQD	O6-C1-C2	7.61	119.84	108.27
24	c	509	CLA	C4A-NA-C1A	7.49	110.10	106.68
30	a	610	SQD	O6-C1-C2	7.45	119.58	108.27
24	B	607	CLA	C4A-NA-C1A	7.30	110.01	106.68
24	C	512	CLA	C4A-NA-C1A	7.14	109.94	106.68
24	B	606	CLA	C4A-NA-C1A	7.12	109.93	106.68
24	b	607	CLA	C4A-NA-C1A	7.09	109.91	106.68
24	b	604	CLA	C4A-NA-C1A	6.89	109.82	106.68
24	a	605	CLA	C4A-NA-C1A	6.86	109.81	106.68
24	C	503	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	b	614	CLA	C4A-NA-C1A	6.73	109.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	610	SQD	C1-O5-C5	-6.63	100.77	113.72
24	B	609	CLA	C4A-NA-C1A	6.62	109.70	106.68
24	C	510	CLA	C4A-NA-C1A	6.60	109.69	106.68
24	D	403	CLA	C4A-NA-C1A	6.55	109.67	106.68
30	B	623	SQD	C1-O5-C5	-6.36	101.30	113.72
27	a	609	PL9	C7-C3-C4	6.32	122.12	116.91
27	d	408	PL9	C7-C3-C4	6.32	122.12	116.91
24	c	501	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	B	615	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	B	614	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	c	512	CLA	C4A-NA-C1A	6.17	109.49	106.68
24	C	501	CLA	C4A-NA-C1A	6.13	109.48	106.68
24	C	508	CLA	C4A-NA-C1A	6.07	109.45	106.68
30	F	102	SQD	C1-O5-C5	-6.02	101.96	113.72
24	b	615	CLA	C4A-NA-C1A	5.92	109.38	106.68
24	C	502	CLA	C4A-NA-C1A	5.91	109.38	106.68
24	d	405	CLA	C4A-NA-C1A	5.90	109.37	106.68
30	A	614	SQD	O7-S-C6	5.85	115.49	106.76
24	c	504	CLA	C4A-NA-C1A	5.85	109.35	106.68
30	a	611	SQD	O7-S-C6	5.84	115.48	106.76
24	b	616	CLA	C4A-NA-C1A	5.83	109.34	106.68
29	o	301	LMG	C1-C2-C3	-5.72	97.97	110.01
24	A	608	CLA	C4A-NA-C1A	5.72	109.29	106.68
24	c	501	CLA	O2D-CGD-O1D	-5.71	112.73	123.85
24	A	612	CLA	C4A-NA-C1A	5.63	109.25	106.68
30	A	614	SQD	C1-O5-C5	-5.62	102.75	113.72
24	C	509	CLA	C4A-NA-C1A	5.61	109.24	106.68
24	c	513	CLA	C4A-NA-C1A	5.56	109.22	106.68
30	f	101	SQD	O6-C1-C2	5.56	116.72	108.27
24	C	501	CLA	O2D-CGD-O1D	-5.50	113.14	123.85
24	B	611	CLA	C4A-NA-C1A	5.48	109.18	106.68
24	a	606	CLA	C4A-NA-C1A	5.35	109.12	106.68
24	c	508	CLA	C4A-NA-C1A	5.32	109.10	106.68
30	A	614	SQD	O9-S-O7	-5.27	96.69	113.82
24	c	510	CLA	C4A-NA-C1A	5.18	109.04	106.68
24	c	505	CLA	C4A-NA-C1A	5.18	109.04	106.68
24	b	603	CLA	O2D-CGD-O1D	-5.11	113.91	123.85
24	b	602	CLA	O2D-CGD-O1D	-5.07	113.97	123.85
24	C	506	CLA	C4A-NA-C1A	5.06	108.99	106.68
24	D	404	CLA	C4A-NA-C1A	5.03	108.98	106.68
30	F	102	SQD	O6-C1-C2	5.01	115.89	108.27
24	B	603	CLA	C4A-NA-C1A	4.90	108.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	606	CLA	C4A-NA-C1A	4.89	108.91	106.68
24	b	606	CLA	O2D-CGD-O1D	-4.88	114.34	123.85
24	b	603	CLA	O2D-CGD-CBD	4.87	119.75	111.23
30	F	102	SQD	O9-S-C6	4.84	113.99	106.76
30	a	611	SQD	O47-C7-C8	4.82	121.91	111.48
32	c	521	DGD	C3D-C4D-C5D	-4.82	101.49	110.23
24	a	605	CLA	C3B-C4B-NB	-4.80	106.25	110.53
30	a	610	SQD	O9-S-C6	4.78	113.89	106.76
33	D	401	BCT	O2-C-O1	4.72	131.75	119.68
24	B	610	CLA	O2D-CGD-O1D	-4.66	114.77	123.85
24	b	615	CLA	C3B-C4B-NB	-4.64	106.38	110.53
35	V	201	HEC	C1D-ND-C4D	4.64	110.70	105.21
24	C	508	CLA	O2D-CGD-O1D	-4.64	114.82	123.85
24	C	504	CLA	C4A-NA-C1A	4.63	108.79	106.68
30	f	101	SQD	O9-S-O7	-4.62	98.81	113.82
27	a	609	PL9	C7-C3-C2	-4.58	117.99	123.39
24	C	501	CLA	O2D-CGD-CBD	4.55	119.19	111.23
32	H	102	DGD	O3G-C3G-C2G	-4.55	99.76	110.82
24	C	506	CLA	C3B-C4B-NB	-4.51	106.51	110.53
24	C	503	CLA	C7-C6-C5	-4.50	101.26	113.26
25	d	403	PHO	O1D-CGD-CBD	4.49	131.54	124.72
27	D	406	PL9	C7-C3-C4	4.49	120.61	116.91
31	d	411	LHG	O4-P-O5	4.48	133.29	112.44
30	F	102	SQD	O8-S-C6	4.45	114.56	105.97
27	d	408	PL9	C37-C38-C39	-4.43	117.49	127.62
24	B	614	CLA	O2D-CGD-O1D	-4.42	115.25	123.85
24	b	605	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
24	B	611	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
24	b	610	CLA	O2D-CGD-O1D	-4.34	115.40	123.85
30	B	623	SQD	O47-C7-C8	4.33	120.85	111.48
31	D	410	LHG	O4-P-O5	4.32	132.53	112.44
24	c	509	CLA	O2A-CGA-O1A	-4.30	112.87	123.63
30	A	614	SQD	C1-C2-C3	-4.29	100.98	110.01
30	f	101	SQD	C1-O5-C5	-4.29	105.35	113.72
27	A	610	PL9	C40-C39-C41	4.28	122.66	115.23
25	d	403	PHO	C2B-C1B-NB	-4.27	106.34	109.43
24	a	607	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
24	b	609	CLA	C3B-C4B-NB	-4.25	106.73	110.53
30	a	611	SQD	O9-S-O7	-4.23	100.05	113.82
24	b	602	CLA	C4A-NA-C1A	4.23	108.61	106.68
24	c	512	CLA	C1-C2-C3	-4.22	119.29	126.20
31	e	103	LHG	O4-P-O5	4.21	132.03	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	601	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
29	b	623	LMG	C1-O6-C5	-4.20	105.53	113.72
24	b	605	CLA	C4-C3-C5	4.19	122.50	115.23
31	L	101	LHG	O4-P-O5	4.18	131.90	112.44
24	b	608	CLA	C3B-C4B-NB	-4.18	106.80	110.53
24	c	502	CLA	C4A-NA-C1A	4.17	108.58	106.68
24	C	512	CLA	O2D-CGD-O1D	-4.17	115.74	123.85
24	c	501	CLA	O2D-CGD-CBD	4.15	118.48	111.23
30	A	614	SQD	O47-C7-C8	4.14	120.44	111.48
24	b	609	CLA	C4A-NA-C1A	4.14	108.57	106.68
32	C	522	DGD	O3G-C3G-C2G	-4.14	100.76	110.82
25	d	402	PHO	C2B-C1B-NB	-4.13	106.44	109.43
24	a	607	CLA	C4A-NA-C1A	4.12	108.56	106.68
26	b	617	BCR	C2-C1-C6	4.12	116.42	110.44
24	c	511	CLA	C3B-C4B-NB	-4.11	106.86	110.53
29	b	623	LMG	O1-C1-C2	-4.10	102.04	108.27
33	d	401	BCT	O2-C-O1	4.10	130.17	119.68
30	A	614	SQD	O5-C1-C2	-4.09	101.97	110.37
29	o	301	LMG	O1-C1-C2	4.08	114.47	108.27
24	c	505	CLA	C3B-C4B-NB	-4.05	106.91	110.53
24	C	504	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
31	d	410	LHG	O4-P-O5	4.03	131.20	112.44
32	h	102	DGD	C3D-C4D-C5D	-4.03	102.92	110.23
24	c	503	CLA	C4A-NA-C1A	4.03	108.52	106.68
26	B	619	BCR	C2-C1-C6	4.03	116.29	110.44
26	D	405	BCR	C2-C1-C6	4.03	116.29	110.44
25	A	607	PHO	CMB-C2B-C3B	4.03	132.73	124.68
25	d	402	PHO	CBC-CAC-C3C	-4.03	107.11	112.87
24	C	512	CLA	C3B-C4B-NB	-4.03	106.94	110.53
30	f	101	SQD	O5-C1-C2	-4.02	102.11	110.37
24	B	610	CLA	O2D-CGD-CBD	4.01	118.25	111.23
24	A	605	CLA	C4A-NA-C1A	4.01	108.51	106.68
27	d	408	PL9	C22-C23-C24	-3.99	118.49	127.62
31	d	412	LHG	O4-P-O5	3.98	130.97	112.44
24	B	612	CLA	C4A-NA-C1A	3.97	108.49	106.68
31	l	101	LHG	O4-P-O5	3.97	130.90	112.44
24	a	607	CLA	C4-C3-C5	3.96	122.11	115.23
29	c	524	LMG	O6-C1-O1	-3.95	100.70	110.04
31	A	615	LHG	O4-P-O5	3.95	130.81	112.44
24	b	602	CLA	O2D-CGD-CBD	3.94	118.12	111.23
30	B	623	SQD	C3-C4-C5	3.93	117.37	110.23
27	d	408	PL9	C42-C43-C44	-3.93	118.63	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C42-C43-C44	-3.93	118.63	127.62
27	A	610	PL9	C22-C23-C24	-3.92	118.65	127.62
30	b	620	SQD	O5-C1-C2	-3.92	102.31	110.37
32	C	521	DGD	O3G-C3G-C2G	-3.92	101.29	110.82
24	a	607	CLA	O2D-CGD-CBD	3.91	118.07	111.23
24	B	613	CLA	C1-C2-C3	-3.91	119.79	126.20
25	D	402	PHO	O1D-CGD-CBD	3.90	130.64	124.72
30	f	101	SQD	O9-S-C6	3.90	112.57	106.76
24	b	607	CLA	C3B-C4B-NB	-3.87	107.07	110.53
30	B	623	SQD	O48-C23-C24	3.87	123.63	111.83
29	o	301	LMG	O6-C1-C2	-3.86	102.43	110.37
32	A	617	DGD	C4E-C3E-C2E	-3.86	104.05	110.83
24	C	512	CLA	CMB-C2B-C1B	-3.86	119.54	125.42
24	b	611	CLA	C4A-NA-C1A	3.86	108.44	106.68
30	a	610	SQD	C1-C2-C3	-3.84	101.93	110.01
30	A	616	SQD	O7-S-C6	3.83	112.48	106.76
24	B	605	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
24	b	602	CLA	CHB-C4A-NA	3.82	129.91	124.40
27	d	408	PL9	C7-C3-C2	-3.82	118.89	123.39
24	b	611	CLA	O2D-CGD-O1D	-3.81	116.42	123.85
25	D	402	PHO	O2D-CGD-O1D	-3.81	116.43	123.85
24	B	611	CLA	O2D-CGD-CBD	3.81	117.89	111.23
24	a	606	CLA	O2D-CGD-CBD	3.81	117.89	111.23
24	b	610	CLA	C4A-NA-C1A	3.80	108.41	106.68
24	B	601	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
25	d	403	PHO	C4D-CHA-CBD	-3.76	106.65	108.45
31	D	411	LHG	O4-P-O5	3.76	129.91	112.44
24	A	612	CLA	C3B-C4B-NB	-3.74	107.19	110.53
29	m	101	LMG	O7-C10-O9	-3.74	114.97	123.70
24	B	612	CLA	C3B-C4B-NB	-3.73	107.20	110.53
24	d	404	CLA	O2D-CGD-CBD	3.72	117.73	111.23
31	d	412	LHG	O8-C23-O10	-3.72	114.32	123.63
24	C	502	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
25	D	402	PHO	C2B-C1B-NB	-3.69	106.77	109.43
30	b	620	SQD	O47-C7-C8	3.69	119.45	111.48
31	D	410	LHG	O8-C23-O10	-3.67	114.44	123.63
24	b	612	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
24	B	605	CLA	C3B-C4B-NB	-3.66	107.26	110.53
31	D	411	LHG	O8-C23-C24	3.65	122.96	111.83
34	e	102	HEM	CBA-CAA-C2A	-3.65	102.45	112.53
34	e	102	HEM	CBD-CAD-C3D	-3.64	102.46	112.53
35	v	201	HEC	C1D-ND-C4D	3.62	109.50	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
30	b	620	SQD	C1-C2-C3	-3.62	102.40	110.01
24	b	605	CLA	C4A-NA-C1A	3.61	108.33	106.68
31	d	412	LHG	O8-C23-C24	3.60	122.83	111.83
26	B	617	BCR	C2-C1-C6	3.60	115.67	110.44
24	c	507	CLA	C4A-NA-C1A	3.60	108.32	106.68
35	v	201	HEC	CHA-C4D-ND	3.56	128.26	124.42
24	C	503	CLA	C3B-C4B-NB	-3.56	107.35	110.53
24	C	508	CLA	C3B-C4B-NB	-3.54	107.37	110.53
24	B	616	CLA	CHC-C4B-NB	3.52	129.33	124.05
30	b	620	SQD	O7-S-C6	3.52	112.01	106.76
24	B	605	CLA	O1D-CGD-CBD	3.52	131.46	124.52
24	c	508	CLA	C3B-C4B-NB	-3.52	107.39	110.53
24	c	508	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
30	b	620	SQD	C1-O5-C5	-3.52	106.85	113.72
24	C	505	CLA	C3B-C4B-NB	-3.52	107.39	110.53
24	B	603	CLA	C1D-ND-C4D	3.51	108.78	106.31
26	b	618	BCR	C37-C22-C21	-3.50	117.14	122.82
31	D	409	LHG	O4-P-O5	3.50	128.73	112.44
24	c	503	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
24	c	506	CLA	C2D-C1D-ND	-3.49	106.67	110.13
26	b	619	BCR	C27-C26-C25	3.49	127.42	122.70
24	a	605	CLA	O1D-CGD-CBD	3.49	131.40	124.52
24	c	504	CLA	C3B-C4B-NB	-3.49	107.42	110.53
24	C	513	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
24	c	512	CLA	C3B-C4B-NB	-3.47	107.43	110.53
24	c	503	CLA	C3B-C4B-NB	-3.46	107.44	110.53
24	B	613	CLA	C3B-C4B-NB	-3.45	107.45	110.53
30	A	616	SQD	O6-C1-C2	3.45	113.51	108.27
26	b	618	BCR	C2-C1-C6	3.44	115.44	110.44
29	C	516	LMG	O6-C5-C4	3.44	115.90	109.70
30	A	616	SQD	O47-C7-C8	3.44	118.92	111.48
24	b	604	CLA	CHB-C4A-NA	3.44	129.36	124.40
24	C	504	CLA	CMB-C2B-C3B	3.43	134.62	126.55
26	C	514	BCR	C27-C26-C25	3.43	127.33	122.70
30	B	623	SQD	C25-C24-C23	-3.42	101.16	113.69
24	b	611	CLA	O2D-CGD-CBD	3.42	117.20	111.23
27	A	610	PL9	O1-C4-C3	-3.41	117.13	120.73
24	C	509	CLA	C1-C2-C3	-3.41	120.61	126.20
24	D	403	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	A	608	CLA	O2D-CGD-CBD	3.41	117.19	111.23
24	b	614	CLA	C3B-C4B-NB	-3.41	107.49	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	PHO	C1-C2-C3	-3.40	120.62	126.20
32	c	520	DGD	C3G-O3G-C1D	3.40	121.09	113.80
24	A	612	CLA	O2D-CGD-CBD	3.39	117.16	111.23
24	D	404	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
24	A	608	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
24	c	512	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
24	c	512	CLA	CHB-C4A-NA	3.38	129.28	124.40
24	B	603	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	D	402	PHO	C4D-CHA-CBD	-3.38	106.84	108.45
24	B	604	CLA	C6-C5-C3	-3.37	105.25	113.47
24	B	606	CLA	C3B-C4B-NB	-3.37	107.52	110.53
24	B	603	CLA	C4-C3-C5	3.37	121.08	115.23
24	B	612	CLA	C11-C12-C13	-3.36	104.79	115.97
26	H	101	BCR	C38-C26-C25	-3.36	120.82	124.48
32	c	521	DGD	O3G-C3G-C2G	-3.35	102.67	110.82
30	a	610	SQD	O47-C7-C8	3.35	118.72	111.48
24	C	511	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
24	B	602	CLA	CHB-C4A-NA	3.34	129.22	124.40
24	c	509	CLA	CHB-C4A-NA	3.34	129.22	124.40
24	B	601	CLA	O2D-CGD-CBD	3.34	117.06	111.23
24	c	504	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
26	c	514	BCR	C2-C1-C6	3.33	115.28	110.44
24	b	612	CLA	CAC-C3C-C4C	3.33	129.12	124.79
24	C	510	CLA	C3B-C4B-NB	-3.33	107.56	110.53
24	C	512	CLA	C1-C2-C3	-3.32	120.75	126.20
24	B	610	CLA	CHB-C4A-NA	3.32	129.20	124.40
24	b	605	CLA	CHD-C1D-ND	-3.32	120.13	124.80
24	b	601	CLA	C3B-C4B-NB	-3.32	107.57	110.53
24	A	606	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
24	C	501	CLA	C3B-C4B-NB	-3.31	107.57	110.53
24	c	507	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
30	b	620	SQD	C3-C4-C5	3.31	116.23	110.23
29	B	620	LMG	O6-C5-C4	3.31	115.66	109.70
24	b	604	CLA	C3B-C4B-NB	-3.30	107.58	110.53
27	A	610	PL9	C30-C29-C28	-3.29	115.17	123.63
24	C	502	CLA	C3B-C4B-NB	-3.29	107.59	110.53
26	A	609	BCR	C27-C26-C25	3.29	127.15	122.70
26	c	515	BCR	C35-C13-C14	-3.29	117.49	122.82
30	b	620	SQD	O9-S-O7	-3.28	103.15	113.82
32	A	617	DGD	O5D-C1E-C2E	3.28	113.25	108.27
24	b	612	CLA	CHB-C4A-NA	3.28	129.13	124.40
26	K	101	BCR	C2-C1-C6	3.27	115.19	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	611	SQD	C3-C4-C5	3.27	116.16	110.23
24	B	602	CLA	O2D-CGD-CBD	3.27	116.94	111.23
24	B	604	CLA	CHB-C4A-NA	3.26	129.11	124.40
24	B	613	CLA	C4A-NA-C1A	3.26	108.17	106.68
24	d	404	CLA	C3B-C4B-NB	-3.26	107.62	110.53
26	b	617	BCR	C29-C30-C25	3.25	115.16	110.44
24	b	611	CLA	C2D-C1D-ND	-3.24	106.92	110.13
24	C	502	CLA	CAA-C2A-C3A	-3.24	104.24	113.00
30	a	610	SQD	O9-S-O7	-3.24	103.29	113.82
26	A	609	BCR	C2-C1-C6	3.24	115.14	110.44
24	c	505	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
24	b	603	CLA	CHD-C1D-ND	-3.22	120.27	124.80
24	a	606	CLA	CHB-C4A-NA	3.21	129.03	124.40
24	B	604	CLA	C3B-C4B-NB	-3.21	107.67	110.53
24	c	501	CLA	CMB-C2B-C1B	-3.20	120.54	125.42
26	B	619	BCR	C29-C30-C25	3.19	115.08	110.44
26	T	101	BCR	C27-C26-C25	3.19	127.01	122.70
24	b	614	CLA	CHD-C1D-ND	-3.19	120.31	124.80
32	c	519	DGD	C3D-C4D-C5D	-3.19	104.46	110.23
32	H	102	DGD	O6E-C5E-C4E	3.18	115.44	109.70
24	D	404	CLA	O1D-CGD-CBD	3.18	130.80	124.52
24	C	513	CLA	O2D-CGD-CBD	3.18	116.79	111.23
29	B	620	LMG	C1-C2-C3	-3.18	103.33	110.01
32	c	519	DGD	O3E-C3E-C2E	-3.17	102.89	110.38
24	b	616	CLA	C3B-C4B-NB	-3.17	107.70	110.53
29	D	408	LMG	O1-C1-C2	-3.17	103.46	108.27
27	D	406	PL9	C37-C38-C39	-3.16	120.38	127.62
26	A	609	BCR	C39-C30-C25	3.16	115.20	110.24
24	C	509	CLA	C3B-C4B-NB	-3.16	107.71	110.53
30	a	610	SQD	C3-C4-C5	3.15	115.95	110.23
30	A	616	SQD	O9-S-O7	-3.15	103.57	113.82
24	a	606	CLA	C3B-C4B-NB	-3.15	107.72	110.53
26	C	514	BCR	C36-C18-C17	-3.15	117.71	122.82
34	F	101	HEM	CBD-CAD-C3D	-3.15	103.83	112.53
26	c	515	BCR	C27-C26-C25	3.15	126.95	122.70
24	C	512	CLA	CHB-C4A-NA	3.14	128.93	124.40
31	d	410	LHG	O8-C23-C24	3.13	121.39	111.83
30	a	610	SQD	O8-S-C6	3.13	112.02	105.97
24	b	604	CLA	O2A-CGA-O1A	-3.12	115.81	123.63
26	h	101	BCR	C27-C26-C25	3.12	126.92	122.70
26	a	608	BCR	C29-C30-C25	3.12	114.97	110.44
32	C	522	DGD	O2D-C2D-C1D	-3.11	102.67	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	611	SQD	O48-C23-C24	3.11	121.31	111.83
29	B	621	LMG	O7-C10-O9	-3.11	116.44	123.70
29	A	613	LMG	O1-C1-C2	3.11	112.99	108.27
27	A	610	PL9	C7-C3-C4	3.11	119.47	116.91
24	b	601	CLA	O1D-CGD-CBD	3.10	130.64	124.52
24	b	605	CLA	C1-O2A-CGA	-3.10	109.14	116.65
24	b	612	CLA	C1-C2-C3	-3.10	121.11	126.20
24	b	616	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
24	d	406	CLA	C3B-C4B-NB	-3.09	107.77	110.53
24	b	606	CLA	O2D-CGD-CBD	3.09	116.63	111.23
27	d	408	PL9	C40-C39-C41	3.08	120.57	115.23
24	C	509	CLA	CED-O2D-CGD	3.08	122.89	115.92
24	C	507	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
30	F	102	SQD	C1-C2-C3	-3.07	103.55	110.01
24	B	608	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	B	602	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	b	605	CLA	C1-C2-C3	-3.06	121.19	126.20
24	B	608	CLA	C4A-NA-C1A	3.06	108.07	106.68
24	d	405	CLA	C3B-C4B-NB	-3.05	107.81	110.53
26	c	514	BCR	C27-C26-C25	3.04	126.82	122.70
30	F	102	SQD	O48-C23-C24	3.04	121.11	111.83
29	B	621	LMG	O1-C7-C8	-3.04	103.42	110.82
26	a	608	BCR	C27-C26-C25	3.04	126.81	122.70
26	c	515	BCR	C15-C16-C17	-3.04	117.30	123.52
24	D	403	CLA	C3B-C4B-NB	-3.03	107.82	110.53
29	b	623	LMG	C8-O7-C10	3.03	125.04	117.80
32	h	102	DGD	O3G-C3G-C2G	-3.02	103.46	110.82
29	C	516	LMG	C7-O1-C1	3.02	120.28	113.80
29	b	623	LMG	O2-C2-C1	-3.02	102.88	110.08
26	k	102	BCR	C27-C26-C25	3.02	126.79	122.70
29	D	408	LMG	O8-C28-O10	-3.02	116.08	123.63
26	T	101	BCR	C7-C8-C9	-3.02	121.77	126.23
32	h	102	DGD	O6E-C5E-C4E	3.02	115.14	109.70
30	A	616	SQD	O48-C23-C24	3.02	121.03	111.83
26	B	617	BCR	C33-C5-C6	-3.01	121.19	124.48
26	C	520	BCR	C29-C30-C25	3.01	114.81	110.44
31	d	411	LHG	O8-C23-C24	3.01	121.01	111.83
29	C	516	LMG	O2-C2-C1	-3.01	102.91	110.08
24	b	608	CLA	C4A-NA-C1A	3.00	108.05	106.68
30	f	101	SQD	O7-S-C6	2.99	111.23	106.76
30	B	623	SQD	O5-C5-C4	2.99	115.09	109.70
31	L	101	LHG	C11-C10-C9	-2.99	99.27	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	605	CLA	CHB-C4A-NA	2.99	128.71	124.40
24	B	606	CLA	CGD-CBD-CAD	-2.98	101.21	110.85
24	c	513	CLA	CHB-C4A-NA	2.97	128.69	124.40
24	b	611	CLA	C1D-ND-C4D	2.97	108.40	106.31
24	b	609	CLA	O1D-CGD-CBD	2.97	130.37	124.52
29	C	524	LMG	O7-C10-O9	-2.97	116.77	123.70
25	d	403	PHO	O2D-CGD-O1D	-2.96	118.08	123.85
24	C	507	CLA	CHB-C4A-NA	2.96	128.68	124.40
24	B	611	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	C	503	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	b	601	CLA	CHB-C4A-NA	2.96	128.67	124.40
24	c	504	CLA	CHB-C4A-NA	2.96	128.67	124.40
26	B	617	BCR	C29-C30-C25	2.96	114.74	110.44
24	b	610	CLA	CAA-CBA-CGA	-2.96	104.81	113.21
24	b	611	CLA	CHD-C1D-C2D	2.95	131.62	125.49
26	b	618	BCR	C15-C14-C13	-2.95	123.14	127.28
24	b	612	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
29	B	620	LMG	O8-C28-O10	-2.95	116.26	123.63
31	D	410	LHG	O8-C23-C24	2.94	120.81	111.83
24	c	510	CLA	CHB-C4A-NA	2.94	128.65	124.40
26	C	514	BCR	C2-C1-C6	2.94	114.71	110.44
26	H	101	BCR	C27-C26-C25	2.93	126.67	122.70
27	A	610	PL9	O2-C1-C2	-2.93	115.16	121.83
24	a	605	CLA	CHB-C4A-NA	2.93	128.63	124.40
24	B	605	CLA	C4A-NA-C1A	2.93	108.02	106.68
30	b	620	SQD	O2-C2-C1	2.93	117.06	110.08
26	K	102	BCR	C27-C26-C25	2.92	126.65	122.70
24	b	613	CLA	C1-C2-C3	-2.92	121.41	126.20
31	d	410	LHG	O8-C23-O10	-2.92	116.32	123.63
24	D	403	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
24	C	503	CLA	C6-C5-C3	2.92	120.57	113.47
24	B	607	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
32	c	520	DGD	O3G-C3G-C2G	-2.91	103.74	110.82
26	t	101	BCR	C7-C8-C9	-2.91	121.93	126.23
32	C	522	DGD	C6D-O5D-C1E	2.91	120.03	113.80
24	B	616	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	B	614	CLA	CHB-C4A-NA	2.91	128.59	124.40
32	c	519	DGD	CDB-CCB-CBB	-2.90	99.69	114.37
24	C	512	CLA	CMB-C2B-C3B	2.90	133.36	126.55
30	A	614	SQD	O9-S-C6	2.90	111.08	106.76
34	e	102	HEM	CHB-C1B-NB	2.90	127.95	124.37
29	m	101	LMG	C9-C8-C7	-2.89	105.04	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	C6-C5-C3	2.89	120.51	113.47
24	B	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
27	a	609	PL9	C27-C28-C29	-2.89	121.01	127.62
32	C	521	DGD	CDB-CCB-CBB	-2.89	99.76	114.37
24	b	610	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	c	503	CLA	C11-C12-C13	-2.88	106.38	115.97
24	B	613	CLA	CED-O2D-CGD	2.88	122.46	115.92
28	R	101	STE	C3-C2-C1	-2.88	106.98	114.51
32	C	523	DGD	O3D-C3D-C4D	-2.88	103.58	110.38
32	H	102	DGD	CDB-CCB-CBB	-2.88	99.82	114.37
29	A	613	LMG	O6-C1-O1	-2.87	103.26	110.04
31	d	410	LHG	C11-C10-C9	-2.87	99.87	114.37
24	C	512	CLA	O2D-CGD-CBD	2.87	116.24	111.23
30	F	102	SQD	O8-S-O9	-2.86	104.23	111.40
32	H	102	DGD	O5E-C6E-C5E	-2.86	101.58	111.33
24	B	609	CLA	C3B-C4B-NB	-2.86	107.97	110.53
26	H	101	BCR	C24-C23-C22	-2.86	122.00	126.23
24	b	612	CLA	CMB-C2B-C3B	2.86	133.28	126.55
26	C	514	BCR	C33-C5-C6	-2.86	121.36	124.48
24	b	614	CLA	CMD-C2D-C1D	2.86	129.76	124.73
30	B	623	SQD	O6-C1-C2	2.86	112.61	108.27
24	d	405	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
24	c	506	CLA	C1D-ND-C4D	2.85	108.31	106.31
27	A	610	PL9	O2-C1-C6	2.85	125.02	120.48
24	b	615	CLA	C11-C12-C13	-2.85	106.49	115.97
24	A	605	CLA	CAC-C3C-C4C	2.85	128.50	124.79
29	B	621	LMG	O1-C1-C2	-2.85	103.94	108.27
29	C	524	LMG	O1-C7-C8	-2.85	103.89	110.82
24	B	614	CLA	C4-C3-C5	2.84	120.17	115.23
26	B	618	BCR	C29-C30-C25	2.84	114.57	110.44
25	d	402	PHO	CMB-C2B-C3B	2.84	130.35	124.68
24	C	508	CLA	CHD-C1D-ND	-2.84	120.81	124.80
29	m	101	LMG	O7-C10-C11	2.84	117.62	111.48
27	a	609	PL9	C35-C34-C36	2.84	120.15	115.23
24	b	603	CLA	CHC-C4B-NB	2.83	128.30	124.05
24	B	615	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	B	601	CLA	C1-O2A-CGA	2.83	123.51	116.65
24	B	610	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
24	b	610	CLA	C1D-ND-C4D	-2.83	104.33	106.31
24	a	606	CLA	C2D-C1D-ND	-2.83	107.33	110.13
26	H	101	BCR	C2-C1-C6	2.82	114.54	110.44
26	K	101	BCR	C15-C14-C13	-2.82	123.32	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	617	DGD	O5E-C6E-C5E	-2.82	101.73	111.33
24	b	604	CLA	C6-C7-C8	-2.82	106.59	115.97
32	H	102	DGD	C1E-O6E-C5E	2.82	119.22	113.72
29	b	623	LMG	O8-C28-O10	-2.82	116.58	123.63
24	c	507	CLA	CHB-C4A-NA	2.81	128.46	124.40
26	k	101	BCR	C38-C26-C25	-2.81	121.42	124.48
24	A	606	CLA	CAC-C3C-C4C	2.81	128.44	124.79
35	V	201	HEC	C1D-C2D-C3D	-2.81	104.03	106.98
32	h	102	DGD	C6D-C5D-C4D	2.81	117.96	112.07
24	b	612	CLA	C11-C12-C13	-2.81	106.64	115.97
24	A	606	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
24	A	612	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	c	506	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
24	b	610	CLA	O1D-CGD-CBD	2.80	130.04	124.52
29	o	301	LMG	C1-O6-C5	-2.80	108.26	113.72
29	c	523	LMG	O6-C1-O1	-2.80	103.44	110.04
35	v	201	HEC	CHB-C1B-NB	2.80	127.43	124.42
24	B	603	CLA	C5-C3-C2	-2.79	114.90	121.17
24	c	504	CLA	O2D-CGD-CBD	2.79	116.10	111.23
30	A	616	SQD	O5-C5-C4	2.78	114.71	109.70
24	b	613	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
24	B	602	CLA	C3B-C4B-NB	-2.77	108.05	110.53
24	c	506	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	D	402	PHO	C3B-C4B-NB	-2.77	105.66	107.46
24	b	605	CLA	C3B-C4B-NB	-2.77	108.06	110.53
24	C	501	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
30	a	610	SQD	C25-C24-C23	-2.77	103.56	113.69
24	C	509	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
24	a	606	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
29	B	620	LMG	O6-C1-O1	-2.75	103.54	110.04
24	D	403	CLA	O2D-CGD-CBD	2.75	116.04	111.23
26	b	618	BCR	C35-C13-C14	-2.75	118.36	122.82
31	D	411	LHG	C11-C10-C9	-2.75	100.47	114.37
29	c	522	LMG	O6-C1-O1	-2.75	103.55	110.04
27	D	406	PL9	C7-C3-C2	-2.74	120.16	123.39
24	A	605	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
26	a	608	BCR	C7-C8-C9	-2.74	122.18	126.23
24	b	603	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
24	C	513	CLA	C3B-C4B-NB	-2.74	108.09	110.53
24	a	606	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
32	C	521	DGD	O1G-C1A-C2A	-2.74	103.49	111.83
32	H	102	DGD	O2G-C1B-O1B	-2.74	117.31	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CHB-C4A-NA	2.73	128.35	124.40
24	b	614	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
27	a	609	PL9	O2-C1-C6	2.73	124.82	120.48
32	A	617	DGD	C1D-C2D-C3D	-2.73	104.27	110.01
24	B	612	CLA	CMB-C2B-C3B	2.73	132.96	126.55
26	b	619	BCR	C2-C1-C6	2.73	114.40	110.44
26	b	617	BCR	C27-C26-C25	2.73	126.39	122.70
26	K	101	BCR	C35-C13-C14	-2.72	118.40	122.82
29	m	101	LMG	O3-C3-C2	-2.72	103.96	110.38
24	C	512	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
30	F	102	SQD	C3-C4-C5	2.72	115.16	110.23
24	c	507	CLA	CHD-C1D-ND	-2.71	120.99	124.80
32	H	102	DGD	C1D-O6D-C5D	-2.71	108.43	113.72
24	b	609	CLA	CHC-C4B-NB	2.70	128.10	124.05
24	B	610	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	C	520	BCR	C2-C1-C6	2.70	114.36	110.44
24	B	607	CLA	CHB-C4A-NA	2.69	128.29	124.40
24	c	503	CLA	O1D-CGD-CBD	2.69	129.82	124.52
32	A	617	DGD	CDB-CCB-CBB	-2.68	100.80	114.37
29	o	301	LMG	C9-C8-C7	-2.68	105.53	111.78
26	a	608	BCR	C33-C5-C6	-2.68	121.56	124.48
27	a	609	PL9	O2-C1-C2	-2.68	115.72	121.83
24	b	615	CLA	CHB-C1B-NB	2.68	128.07	124.05
26	K	101	BCR	C33-C5-C6	-2.68	121.56	124.48
32	c	521	DGD	O2D-C2D-C3D	-2.68	104.05	110.38
32	c	521	DGD	O6D-C1D-O3G	-2.68	103.71	110.04
24	c	502	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
32	c	520	DGD	O6D-C1D-O3G	-2.68	103.71	110.04
24	C	506	CLA	CHB-C4A-NA	2.68	128.27	124.40
24	B	610	CLA	CHA-C1A-NA	-2.68	120.33	126.39
24	b	612	CLA	O1D-CGD-CBD	2.68	129.80	124.52
24	c	508	CLA	CHB-C4A-NA	2.68	128.26	124.40
24	C	513	CLA	CHD-C1D-ND	-2.67	121.04	124.80
24	C	507	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
24	c	505	CLA	C6-C7-C8	-2.67	107.10	115.97
27	D	406	PL9	C20-C19-C21	2.67	119.85	115.23
24	c	513	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
28	B	622	STE	O2-C1-C2	2.66	122.42	114.00
29	B	621	LMG	C6-C5-C4	-2.66	106.48	113.02
26	B	619	BCR	C3-C4-C5	-2.65	109.32	114.06
24	C	511	CLA	CHB-C4A-NA	2.65	128.23	124.40
31	l	101	LHG	C11-C10-C9	-2.65	100.95	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C12-C13-C14	-2.65	121.56	127.62
28	B	625	STE	O2-C1-C2	2.65	122.37	114.00
24	d	404	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	C	504	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	B	601	CLA	C3B-C4B-NB	-2.65	108.17	110.53
24	C	502	CLA	O1D-CGD-CBD	2.65	129.74	124.52
32	H	102	DGD	O2D-C2D-C1D	-2.64	103.78	110.08
24	C	505	CLA	CAC-C3C-C4C	2.64	128.23	124.79
24	b	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	d	407	BCR	C2-C1-C6	2.64	114.27	110.44
24	a	606	CLA	C1D-ND-C4D	2.64	108.16	106.31
26	h	101	BCR	C2-C1-C6	2.63	114.26	110.44
32	c	521	DGD	CDB-CCB-CBB	-2.63	101.08	114.37
25	A	607	PHO	CMA-C3A-C4A	-2.63	108.95	114.61
24	c	513	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
32	h	102	DGD	C4E-C3E-C2E	-2.62	106.23	110.83
24	A	608	CLA	C2C-C1C-NC	2.62	112.73	109.98
24	c	503	CLA	C7-C6-C5	-2.62	106.28	113.26
24	d	406	CLA	CHA-C1A-NA	-2.62	120.46	126.39
27	D	406	PL9	C22-C23-C24	-2.62	121.63	127.62
30	a	610	SQD	O48-C23-C24	2.62	119.81	111.83
24	C	508	CLA	O1D-CGD-CBD	2.62	129.68	124.52
34	F	101	HEM	CHC-C4B-NB	2.61	127.23	124.42
24	C	504	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	D	402	PHO	CMB-C2B-C3B	2.61	129.90	124.68
25	d	402	PHO	O2A-CGA-O1A	-2.61	117.10	123.63
29	c	524	LMG	O7-C10-O9	-2.61	117.61	123.70
29	c	523	LMG	O2-C2-C1	-2.61	103.86	110.08
24	b	609	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	b	620	SQD	O8-S-C6	2.60	110.99	105.97
28	x	101	STE	O2-C1-C2	2.60	122.22	114.00
24	b	616	CLA	CAA-CBA-CGA	-2.60	105.83	113.21
24	B	609	CLA	C1-C2-C3	-2.60	121.94	126.20
32	H	102	DGD	O6D-C1D-O3G	-2.60	103.91	110.04
24	B	605	CLA	C1-O2A-CGA	-2.60	110.37	116.65
32	A	617	DGD	C3E-C4E-C5E	-2.59	105.53	110.23
31	l	101	LHG	C27-C26-C25	-2.59	101.27	114.37
26	a	608	BCR	C30-C25-C26	-2.59	119.10	122.64
32	c	519	DGD	O3G-C3G-C2G	-2.59	104.52	110.82
27	a	609	PL9	C40-C39-C41	2.59	119.72	115.23
27	d	408	PL9	C40-C39-C38	-2.59	116.99	123.63
24	b	602	CLA	C3B-C4B-NB	-2.58	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CMB-C2B-C1B	-2.58	121.48	125.42
25	A	607	PHO	C5-C3-C2	2.58	126.96	121.17
31	d	410	LHG	O8-C6-C5	-2.58	100.96	108.40
32	C	522	DGD	O6D-C1D-O3G	-2.58	103.95	110.04
24	C	511	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
32	C	521	DGD	O5D-C6D-C5D	-2.58	103.61	109.42
27	A	610	PL9	C7-C3-C2	-2.58	120.35	123.39
29	c	522	LMG	O3-C3-C2	-2.58	104.30	110.38
29	m	101	LMG	O8-C28-O10	-2.58	117.18	123.63
24	c	507	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	c	515	BCR	C2-C1-C6	2.58	114.18	110.44
29	d	414	LMG	C3-C4-C5	-2.58	105.56	110.23
24	A	608	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
30	B	623	SQD	O9-S-C6	2.57	110.60	106.76
30	f	101	SQD	O47-C7-C8	2.57	120.39	110.93
24	B	616	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
24	b	615	CLA	C6-C5-C3	-2.57	107.20	113.47
24	B	611	CLA	CHD-C4C-NC	2.57	128.22	124.23
30	a	610	SQD	C44-O6-C1	-2.57	108.29	113.80
29	A	613	LMG	C38-C37-C36	-2.57	101.39	114.37
29	D	407	LMG	O6-C1-O1	-2.57	103.98	110.04
24	c	502	CLA	C1-C2-C3	-2.57	121.99	126.20
26	D	405	BCR	C38-C26-C25	-2.57	121.68	124.48
31	D	411	LHG	O3-P-O5	-2.57	98.76	108.94
24	b	608	CLA	O2D-CGD-CBD	2.57	115.72	111.23
31	D	411	LHG	O8-C23-O10	-2.56	117.21	123.63
24	b	602	CLA	C1-C2-C3	-2.56	122.00	126.20
26	d	407	BCR	C38-C26-C25	-2.56	121.69	124.48
29	d	414	LMG	O2-C2-C1	-2.56	103.97	110.08
30	F	102	SQD	O9-S-O7	-2.56	105.49	113.82
24	a	605	CLA	C2A-C1A-CHA	2.56	128.31	123.87
24	b	612	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	A	608	CLA	CMC-C2C-C1C	2.56	129.03	125.03
26	c	515	BCR	C33-C5-C6	-2.56	121.69	124.48
35	V	201	HEC	CHB-C4A-NA	2.56	127.24	124.45
24	B	603	CLA	C16-C15-C13	-2.55	107.48	115.97
24	B	611	CLA	CHB-C4A-NA	2.55	128.09	124.40
29	m	101	LMG	C40-C39-C38	-2.55	101.47	114.37
24	B	608	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	t	101	BCR	C2-C1-C6	2.55	114.14	110.44
32	C	523	DGD	CBB-CAB-C9B	-2.55	101.48	114.37
27	d	408	PL9	C7-C8-C9	-2.55	122.44	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	610	SQD	O5-C1-C2	-2.55	105.14	110.37
24	B	608	CLA	CHA-C1A-NA	-2.55	120.62	126.39
24	C	502	CLA	C4D-CHA-C1A	2.55	124.28	121.24
32	c	520	DGD	CBB-CAB-C9B	-2.55	101.50	114.37
24	b	606	CLA	CHB-C1B-NB	2.54	127.87	124.05
24	C	504	CLA	CED-O2D-CGD	2.54	121.69	115.92
24	b	610	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	A	606	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	C	507	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	B	610	CLA	C4A-NA-C1A	2.53	107.83	106.68
26	K	102	BCR	C33-C5-C6	-2.53	121.72	124.48
32	C	522	DGD	O5D-C6D-C5D	-2.53	103.72	109.42
24	B	615	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	H	102	DGD	C3D-C4D-C5D	-2.53	105.65	110.23
31	A	615	LHG	O8-C23-C24	2.53	119.54	111.83
29	c	524	LMG	C32-C31-C30	-2.53	101.60	114.37
24	C	509	CLA	CHB-C4A-NA	2.53	128.04	124.40
25	D	402	PHO	C1A-C2A-C3A	-2.52	100.44	102.84
24	B	614	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	B	604	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	B	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	c	506	CLA	CMB-C2B-C3B	2.52	132.47	126.55
24	a	606	CLA	C4-C3-C5	2.52	119.60	115.23
35	v	201	HEC	C1D-C2D-C3D	-2.52	104.33	106.98
24	B	608	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
26	T	101	BCR	C3-C4-C5	-2.51	109.57	114.06
24	d	405	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	b	603	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	A	617	DGD	C3G-C2G-C1G	-2.51	105.93	111.78
24	C	511	CLA	O2D-CGD-CBD	2.51	115.62	111.23
24	a	607	CLA	CHB-C4A-NA	2.51	128.02	124.40
27	a	609	PL9	C37-C38-C39	-2.51	121.88	127.62
24	b	604	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
24	C	508	CLA	CHB-C4A-NA	2.51	128.02	124.40
31	D	410	LHG	C11-C10-C9	-2.51	101.69	114.37
24	c	511	CLA	O2D-CGD-CBD	2.51	115.61	111.23
29	D	407	LMG	O6-C5-C4	2.50	114.21	109.70
24	A	612	CLA	CHB-C4A-NA	2.50	128.01	124.40
31	l	101	LHG	C18-C17-C16	-2.50	101.72	114.37
25	A	607	PHO	C2B-C1B-NB	-2.50	107.62	109.43
26	c	514	BCR	C3-C4-C5	-2.50	109.60	114.06
31	e	103	LHG	C11-C10-C9	-2.50	101.74	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	PHO	C1-C2-C3	-2.49	122.11	126.20
31	d	412	LHG	C26-C25-C24	2.49	122.28	113.13
31	A	615	LHG	C11-C10-C9	-2.49	101.79	114.37
29	B	620	LMG	O3-C3-C2	-2.49	104.51	110.38
24	B	605	CLA	CHD-C1D-ND	-2.49	121.30	124.80
26	d	407	BCR	C33-C5-C6	-2.49	121.77	124.48
24	B	614	CLA	O2D-CGD-CBD	2.48	115.57	111.23
30	a	611	SQD	O5-C1-C2	2.48	115.47	110.37
24	B	616	CLA	C3B-C4B-NB	-2.48	108.31	110.53
26	K	101	BCR	C27-C26-C25	2.48	126.06	122.70
25	A	607	PHO	O2D-CGD-CBD	2.48	113.67	110.95
26	a	608	BCR	C35-C13-C14	-2.48	118.80	122.82
28	C	525	STE	O2-C1-C2	2.48	121.83	114.00
29	A	613	LMG	C36-C35-C34	-2.48	101.85	114.37
32	c	519	DGD	O6D-C1D-O3G	-2.48	104.19	110.04
24	b	605	CLA	CHB-C1B-NB	2.48	127.76	124.05
29	m	101	LMG	C6-C5-C4	-2.47	106.95	113.02
24	b	613	CLA	CHA-C1A-NA	-2.47	120.80	126.39
24	C	503	CLA	O2A-C1-C2	-2.47	98.60	108.11
24	B	603	CLA	CHB-C4A-NA	2.47	127.96	124.40
27	a	609	PL9	C22-C23-C24	-2.47	121.97	127.62
24	B	611	CLA	C1D-ND-C4D	2.47	108.04	106.31
30	F	102	SQD	O5-C1-C2	-2.47	105.30	110.37
24	B	606	CLA	O2A-CGA-O1A	-2.46	117.46	123.63
26	b	618	BCR	C29-C30-C25	2.46	114.02	110.44
32	C	523	DGD	O3G-C3G-C2G	-2.46	104.82	110.82
29	A	613	LMG	O7-C10-C11	2.46	116.81	111.48
30	F	102	SQD	O48-C23-O10	-2.46	117.47	123.63
29	o	301	LMG	C38-C37-C36	-2.46	101.94	114.37
28	R	101	STE	O2-C1-C2	2.46	121.77	114.00
24	c	512	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
31	D	411	LHG	C20-C19-C18	-2.46	101.95	114.37
26	C	514	BCR	C32-C1-C6	-2.45	106.39	110.24
24	A	608	CLA	CHC-C4B-NB	2.45	127.73	124.05
24	a	605	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
26	K	102	BCR	C30-C25-C26	-2.45	119.28	122.64
24	C	506	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
24	B	605	CLA	C4D-C3D-CAD	-2.45	105.44	108.11
32	c	521	DGD	O6E-C5E-C4E	2.45	114.11	109.70
24	c	511	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	c	510	CLA	O1D-CGD-CBD	2.45	129.35	124.52
24	d	405	CLA	CHA-C4D-ND	2.45	137.60	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	BCR	C27-C26-C25	2.45	126.01	122.70
30	a	611	SQD	C17-C16-C15	-2.45	102.00	114.37
29	c	523	LMG	O1-C1-C2	-2.45	104.56	108.27
27	D	406	PL9	C36-C34-C33	-2.45	115.67	121.17
28	e	105	STE	C3-C2-C1	-2.45	108.12	114.51
24	C	501	CLA	CHB-C1B-NB	2.45	127.72	124.05
32	c	520	DGD	O3G-C1D-C2D	-2.44	104.56	108.27
26	K	102	BCR	C39-C30-C25	-2.44	106.42	110.24
30	B	623	SQD	O9-S-O7	-2.44	105.89	113.82
24	b	605	CLA	O1D-CGD-CBD	2.44	129.33	124.52
35	V	201	HEC	CBD-CAD-C3D	-2.44	105.80	112.53
26	B	617	BCR	C11-C10-C9	-2.43	123.86	127.28
26	T	101	BCR	C2-C1-C6	2.43	113.97	110.44
29	D	408	LMG	C3-C4-C5	-2.43	105.82	110.23
29	B	621	LMG	C9-C8-C7	-2.43	106.12	111.78
29	C	516	LMG	C6-C5-C4	-2.43	107.06	113.02
26	b	618	BCR	C30-C25-C26	-2.43	119.32	122.64
24	b	612	CLA	C4A-NA-C1A	2.43	107.79	106.68
24	B	606	CLA	CHC-C4B-NB	2.43	127.69	124.05
29	c	522	LMG	C40-C39-C38	-2.43	102.11	114.37
24	c	507	CLA	CMB-C2B-C3B	2.43	132.25	126.55
24	C	502	CLA	CHD-C1D-ND	-2.42	121.39	124.80
26	B	617	BCR	C27-C26-C25	2.42	125.98	122.70
26	t	101	BCR	C35-C13-C14	-2.42	118.89	122.82
26	B	617	BCR	C3-C4-C5	-2.42	109.74	114.06
24	b	602	CLA	C2D-C1D-ND	-2.42	107.73	110.13
24	b	616	CLA	C1-C2-C3	-2.42	122.23	126.20
24	b	612	CLA	C9-C8-C10	-2.42	102.66	111.27
27	D	406	PL9	C40-C39-C41	2.42	119.42	115.23
26	B	618	BCR	C35-C13-C14	-2.42	118.90	122.82
24	c	505	CLA	CHB-C4A-NA	2.41	127.89	124.40
26	k	101	BCR	C33-C5-C6	-2.41	121.85	124.48
24	B	616	CLA	CAC-C3C-C4C	2.41	127.93	124.79
29	d	414	LMG	O1-C7-C8	-2.41	104.95	110.82
24	b	614	CLA	C1-C2-C3	-2.41	122.24	126.20
30	f	101	SQD	C1-C2-C3	-2.41	104.93	110.01
25	A	607	PHO	C1-C2-C3	-2.41	122.25	126.20
24	a	607	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
25	d	402	PHO	OBD-CAD-CBD	-2.41	122.29	125.82
24	c	505	CLA	C11-C10-C8	-2.41	107.96	115.97
29	c	523	LMG	O3-C3-C2	-2.41	104.70	110.38
24	b	608	CLA	O2A-CGA-O1A	-2.41	117.61	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	406	CLA	C1-C2-C3	-2.40	122.26	126.20
24	B	609	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
24	b	616	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	C	506	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
32	H	102	DGD	C1D-C2D-C3D	-2.40	104.95	110.01
24	C	508	CLA	O2D-CGD-CBD	2.40	115.43	111.23
26	a	608	BCR	C11-C10-C9	-2.40	123.91	127.28
24	b	609	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
26	b	617	BCR	C11-C10-C9	-2.40	123.91	127.28
24	C	502	CLA	CHA-C1A-NA	-2.40	120.95	126.39
28	E	101	STE	O2-C1-C2	2.40	121.58	114.00
31	e	103	LHG	O8-C23-C24	2.40	119.15	111.83
24	C	512	CLA	C6-C5-C3	-2.40	107.62	113.47
24	b	608	CLA	C2D-C1D-ND	-2.40	107.75	110.13
26	K	102	BCR	C8-C7-C6	-2.40	120.59	127.00
32	c	521	DGD	C6D-C5D-C4D	2.40	117.09	112.07
24	b	609	CLA	CBC-CAC-C3C	-2.39	105.93	112.42
28	t	102	STE	O2-C1-O1	-2.39	117.18	123.33
27	d	408	PL9	C36-C34-C33	-2.39	115.80	121.17
24	b	615	CLA	CHA-C4D-ND	2.39	137.48	132.55
24	b	611	CLA	CHD-C1D-ND	-2.39	121.44	124.80
30	f	101	SQD	C25-C24-C23	-2.39	104.94	113.69
26	B	619	BCR	C30-C25-C26	-2.39	119.37	122.64
29	c	523	LMG	C6-C5-C4	-2.39	107.16	113.02
31	e	103	LHG	C20-C19-C18	-2.39	102.31	114.37
30	B	623	SQD	O47-C7-O49	-2.39	118.13	123.70
31	d	411	LHG	O7-C7-C8	-2.38	106.32	111.48
27	a	609	PL9	C42-C43-C44	-2.38	122.17	127.62
26	b	619	BCR	C30-C25-C26	-2.38	119.38	122.64
26	b	618	BCR	C27-C26-C25	2.38	125.92	122.70
30	A	616	SQD	C9-C8-C7	-2.38	104.96	113.69
24	B	603	CLA	CHC-C4B-NB	2.38	127.62	124.05
24	B	603	CLA	C2D-C1D-ND	-2.38	107.77	110.13
28	b	624	STE	O2-C1-O1	-2.38	117.21	123.33
27	D	406	PL9	C27-C28-C29	-2.38	122.17	127.62
24	C	503	CLA	CHD-C1D-ND	-2.38	121.45	124.80
32	c	519	DGD	CBB-CAB-C9B	-2.38	102.34	114.37
24	c	508	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
24	b	603	CLA	OBD-CAD-C3D	2.38	133.98	128.42
26	k	101	BCR	C27-C26-C25	2.38	125.92	122.70
29	C	524	LMG	O6-C1-O1	-2.37	104.43	110.04
26	D	405	BCR	C24-C23-C22	-2.37	122.72	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	623	SQD	O8-S-C6	2.37	110.55	105.97
24	C	506	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
35	V	201	HEC	CAD-CBD-CGD	-2.37	107.38	113.67
24	d	405	CLA	C2D-C1D-ND	-2.37	107.78	110.13
24	B	606	CLA	C1-C2-C3	-2.37	122.32	126.20
26	b	617	BCR	C33-C5-C6	-2.37	121.90	124.48
29	C	516	LMG	O6-C1-C2	-2.36	105.51	110.37
25	A	607	PHO	C3B-C4B-NB	-2.36	105.92	107.46
24	b	614	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
24	c	505	CLA	O2D-CGD-CBD	2.36	115.35	111.23
24	A	608	CLA	CHB-C1B-NB	2.36	127.58	124.05
29	m	101	LMG	O1-C7-C8	-2.36	105.09	110.82
24	B	614	CLA	O1D-CGD-CBD	2.36	129.16	124.52
32	c	521	DGD	O1G-C1A-O1A	-2.35	117.74	123.63
24	C	504	CLA	C4-C3-C5	2.35	119.31	115.23
29	A	613	LMG	C1-O6-C5	-2.35	109.13	113.72
30	B	623	SQD	C1-C2-C3	-2.35	105.06	110.01
32	C	521	DGD	O6D-C1D-O3G	-2.35	104.49	110.04
24	C	508	CLA	CHD-C1D-C2D	2.35	130.38	125.49
24	B	607	CLA	CHB-C1B-NB	2.35	127.57	124.05
24	b	605	CLA	O2D-CGD-CBD	2.35	115.33	111.23
24	C	502	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
29	D	408	LMG	C38-C37-C36	-2.34	102.52	114.37
24	D	404	CLA	CHC-C4B-NB	2.34	127.56	124.05
24	b	608	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	c	506	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	c	506	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	c	509	CLA	C1-O2A-CGA	-2.34	110.99	116.65
31	l	101	LHG	C20-C19-C18	-2.34	102.55	114.37
24	c	509	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	B	614	CLA	CBC-CAC-C3C	-2.34	106.09	112.42
24	b	615	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
24	b	610	CLA	CHD-C1D-ND	-2.34	121.52	124.80
24	b	604	CLA	CMA-C3A-C4A	2.33	118.04	111.77
24	C	505	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
30	b	620	SQD	O48-C23-C24	2.33	118.94	111.83
24	B	613	CLA	CHA-C1A-NA	-2.33	121.11	126.39
26	B	617	BCR	C15-C16-C17	-2.33	118.75	123.52
26	B	619	BCR	C27-C26-C25	2.33	125.85	122.70
24	B	603	CLA	C2A-C1A-CHA	2.33	127.91	123.87
30	b	620	SQD	O9-S-C6	2.32	110.23	106.76
24	c	509	CLA	O2A-CGA-CBA	2.32	118.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	620	SQD	O48-C23-O10	-2.32	117.82	123.63
24	c	511	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
32	c	520	DGD	O5D-C6D-C5D	-2.32	104.19	109.42
24	c	510	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	t	101	BCR	C1-C6-C5	-2.32	119.46	122.64
26	C	520	BCR	C27-C26-C25	2.32	125.83	122.70
24	C	510	CLA	CHB-C4A-NA	2.31	127.74	124.40
24	B	605	CLA	C7-C6-C5	-2.31	107.10	113.26
24	B	603	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
24	d	404	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
27	D	406	PL9	C50-C49-C48	-2.31	115.72	122.66
30	b	620	SQD	C46-O48-C23	-2.31	108.67	117.12
24	b	609	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
27	D	406	PL9	C8-C7-C3	2.31	118.00	112.03
24	b	612	CLA	C16-C15-C13	-2.31	108.30	115.97
24	b	614	CLA	CHB-C4A-NA	2.31	127.73	124.40
26	c	515	BCR	C7-C8-C9	-2.30	122.83	126.23
32	C	521	DGD	C3D-C4D-C5D	-2.30	106.06	110.23
24	b	605	CLA	CHD-C1D-C2D	2.30	130.28	125.49
32	c	519	DGD	C3B-C2B-C1B	-2.30	105.26	113.69
24	b	606	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	c	507	CLA	C4-C3-C5	2.30	119.22	115.23
31	D	411	LHG	C15-C14-C13	-2.30	102.75	114.37
24	c	506	CLA	CHD-C1D-C2D	2.30	130.26	125.49
24	B	611	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	B	608	CLA	CMB-C2B-C3B	2.29	131.95	126.55
32	h	102	DGD	O6D-C1D-O3G	-2.29	104.62	110.04
24	B	603	CLA	C6-C7-C8	-2.29	108.34	115.97
32	c	520	DGD	CDB-CCB-CBB	-2.29	102.78	114.37
24	C	501	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
30	f	101	SQD	O48-C23-C24	2.29	118.82	111.83
26	h	101	BCR	C35-C13-C14	-2.29	119.11	122.82
27	A	610	PL9	C37-C38-C39	-2.29	122.38	127.62
24	b	602	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
26	C	520	BCR	C15-C16-C17	-2.29	118.84	123.52
24	A	608	CLA	CHD-C1D-ND	-2.29	121.58	124.80
26	T	101	BCR	C40-C30-C25	2.29	113.83	110.24
26	B	617	BCR	C8-C7-C6	-2.28	120.89	127.00
32	h	102	DGD	C1E-O6E-C5E	2.28	118.18	113.72
32	c	519	DGD	O3G-C1D-C2D	-2.28	104.81	108.27
24	A	605	CLA	C4-C3-C5	2.28	119.19	115.23
24	b	602	CLA	CMA-C3A-C4A	-2.28	105.64	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CHB-C4A-NA	2.28	127.69	124.40
31	D	411	LHG	O7-C7-C8	-2.28	106.55	111.48
24	B	609	CLA	C2D-C1D-ND	-2.28	107.87	110.13
27	A	610	PL9	C20-C19-C21	2.28	119.18	115.23
24	B	609	CLA	C7-C6-C5	-2.28	107.19	113.26
32	A	617	DGD	O5D-C6D-C5D	-2.28	104.29	109.42
30	A	614	SQD	O47-C7-O49	-2.28	118.38	123.70
24	B	613	CLA	CHB-C1B-NB	2.28	127.46	124.05
24	a	607	CLA	CMB-C2B-C1B	-2.27	121.95	125.42
24	b	613	CLA	CMB-C2B-C3B	2.27	131.90	126.55
26	k	102	BCR	C2-C1-C6	2.27	113.74	110.44
24	B	605	CLA	C11-C10-C8	-2.27	108.41	115.97
29	D	408	LMG	O3-C3-C2	-2.27	105.02	110.38
24	b	610	CLA	C1-C2-C3	-2.27	122.47	126.20
32	C	521	DGD	CBB-CAB-C9B	-2.27	102.89	114.37
27	a	609	PL9	C31-C29-C28	2.27	126.26	121.17
26	K	102	BCR	C40-C30-C25	2.27	113.80	110.24
24	c	507	CLA	CHD-C4C-NC	2.27	127.75	124.23
24	b	613	CLA	C16-C15-C13	-2.27	108.42	115.97
29	m	101	LMG	O6-C1-O1	-2.27	104.68	110.04
24	B	603	CLA	CHD-C4C-NC	2.27	127.75	124.23
24	b	603	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
24	b	614	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
24	B	612	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
24	c	506	CLA	CHA-C1A-NA	-2.26	121.26	126.39
24	b	613	CLA	CED-O2D-CGD	2.26	121.05	115.92
27	A	610	PL9	C7-C8-C9	-2.26	122.93	126.83
24	C	502	CLA	C2A-C1A-CHA	2.26	127.79	123.87
24	b	606	CLA	CHA-C1A-NA	-2.26	121.27	126.39
34	F	101	HEM	CBA-CAA-C2A	-2.26	106.28	112.53
32	c	521	DGD	C1D-C2D-C3D	-2.26	105.26	110.01
24	B	601	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
24	B	614	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
24	A	606	CLA	CMB-C2B-C3B	2.26	131.86	126.55
28	j	101	STE	O2-C1-C2	2.25	121.12	114.00
24	b	609	CLA	CHA-C1A-NA	-2.25	121.29	126.39
26	K	101	BCR	C15-C16-C17	-2.25	118.91	123.52
30	A	616	SQD	C10-C9-C8	-2.25	104.87	113.13
24	c	501	CLA	CHB-C1B-NB	2.25	127.42	124.05
24	c	510	CLA	C3B-C4B-NB	-2.24	108.53	110.53
29	c	522	LMG	O2-C2-C1	-2.24	104.73	110.08
24	B	609	CLA	CHB-C4A-NA	2.24	127.64	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C15-C14-C13	-2.24	124.13	127.28
24	a	605	CLA	O2D-CGD-CBD	-2.24	107.31	111.23
32	C	523	DGD	O3E-C3E-C2E	-2.24	105.10	110.38
35	V	201	HEC	CHD-C4C-NC	2.24	127.92	123.86
26	h	101	BCR	C35-C13-C12	2.23	121.50	118.09
29	d	414	LMG	C38-C37-C36	-2.23	103.08	114.37
24	b	611	CLA	C7-C6-C5	-2.23	107.31	113.26
24	b	613	CLA	CHB-C1B-NB	2.23	127.40	124.05
24	a	606	CLA	O1A-CGA-CBA	2.23	132.50	123.78
26	B	618	BCR	C39-C30-C25	-2.23	106.75	110.24
24	C	502	CLA	CHD-C4C-NC	2.23	127.69	124.23
26	h	101	BCR	C34-C9-C8	-2.23	114.68	118.09
32	c	521	DGD	C3G-C2G-C1G	-2.23	106.59	111.78
26	b	618	BCR	C3-C4-C5	-2.23	110.08	114.06
30	a	611	SQD	O49-C7-C8	-2.23	115.08	123.78
26	c	515	BCR	C1-C6-C5	-2.23	119.59	122.64
24	B	616	CLA	C4D-CHA-C1A	2.22	123.90	121.24
27	d	408	PL9	C8-C7-C3	2.22	117.78	112.03
24	C	503	CLA	O1D-CGD-CBD	2.22	128.90	124.52
24	B	613	CLA	C2B-C1B-NB	-2.22	108.02	110.33
32	H	102	DGD	C7B-C6B-C5B	-2.22	103.14	114.37
24	B	616	CLA	O2D-CGD-CBD	2.22	115.11	111.23
26	d	407	BCR	C7-C8-C9	-2.22	122.95	126.23
24	d	406	CLA	CMB-C2B-C3B	2.22	131.77	126.55
32	C	522	DGD	O3G-C1D-C2D	-2.22	104.91	108.27
24	C	507	CLA	CHC-C4B-NB	2.22	127.37	124.05
29	B	621	LMG	O3-C3-C2	-2.22	105.15	110.38
26	B	617	BCR	C24-C23-C22	-2.22	122.96	126.23
24	B	605	CLA	CHD-C1D-C2D	2.21	130.09	125.49
27	A	610	PL9	C12-C13-C14	-2.21	122.56	127.62
32	H	102	DGD	O5D-C1E-C2E	2.21	111.64	108.27
24	a	605	CLA	C1D-ND-C4D	2.21	107.86	106.31
31	L	101	LHG	C18-C17-C16	-2.21	103.19	114.37
24	b	602	CLA	CHA-C4D-ND	2.21	137.11	132.55
29	c	523	LMG	O7-C10-O9	-2.21	118.54	123.70
24	c	510	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	b	602	CLA	CMB-C2B-C3B	2.21	131.74	126.55
24	c	513	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	B	617	BCR	C34-C9-C10	-2.20	119.24	122.82
24	b	603	CLA	CMA-C3A-C4A	2.20	117.70	111.77
24	B	608	CLA	C11-C12-C13	-2.20	108.64	115.97
31	D	409	LHG	C18-C17-C16	-2.20	103.24	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C40-C39-C38	-2.20	117.97	123.63
26	c	515	BCR	C35-C13-C12	2.20	121.45	118.09
24	C	505	CLA	C1D-ND-C4D	2.20	107.86	106.31
24	C	504	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
32	c	521	DGD	C5B-C4B-C3B	-2.20	103.26	114.37
26	k	102	BCR	C40-C30-C25	2.20	113.69	110.24
27	a	609	PL9	C45-C44-C43	-2.20	117.99	123.63
24	d	406	CLA	C11-C10-C8	-2.20	108.67	115.97
24	A	612	CLA	CHD-C1D-ND	-2.20	121.71	124.80
26	b	618	BCR	C15-C16-C17	-2.19	119.03	123.52
32	h	102	DGD	O5E-C6E-C5E	-2.19	103.86	111.33
24	B	615	CLA	CAC-C3C-C4C	2.19	127.64	124.79
24	B	603	CLA	CHD-C4C-C3C	-2.19	121.58	124.77
29	o	301	LMG	O6-C5-C4	2.19	113.65	109.70
26	c	515	BCR	C30-C25-C26	-2.19	119.64	122.64
27	A	610	PL9	C40-C39-C38	-2.19	118.00	123.63
30	a	611	SQD	C1-C2-C3	2.19	114.62	110.01
24	a	607	CLA	C2C-C1C-NC	2.19	112.28	109.98
24	B	601	CLA	C2A-C1A-CHA	2.19	127.67	123.87
24	C	506	CLA	O1D-CGD-CBD	2.19	128.83	124.52
26	H	101	BCR	C1-C6-C5	-2.19	119.65	122.64
28	i	101	STE	O2-C1-C2	2.19	120.91	114.00
24	C	506	CLA	CMB-C2B-C3B	2.19	131.69	126.55
24	c	508	CLA	C1D-ND-C4D	2.18	107.84	106.31
32	A	617	DGD	CFB-CEB-CDB	-2.18	103.33	114.37
29	c	518	LMG	C8-O7-C10	2.18	123.02	117.80
24	b	608	CLA	CHB-C1B-NB	2.18	127.32	124.05
24	c	507	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
26	t	101	BCR	C27-C26-C25	2.18	125.65	122.70
32	H	102	DGD	CBB-CAB-C9B	-2.18	103.34	114.37
24	B	614	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	a	606	CLA	CED-O2D-CGD	-2.18	110.97	115.92
29	B	621	LMG	C8-O7-C10	2.18	123.01	117.80
30	B	623	SQD	C44-O6-C1	-2.18	109.13	113.80
26	C	520	BCR	C3-C4-C5	-2.18	110.18	114.06
24	b	602	CLA	C16-C15-C13	-2.17	108.74	115.97
24	C	505	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
24	a	607	CLA	C1-C2-C3	-2.17	122.64	126.20
28	d	409	STE	O2-C1-C2	2.17	120.87	114.00
29	D	408	LMG	C40-C39-C38	-2.17	103.40	114.37
26	c	514	BCR	C15-C16-C17	-2.17	119.08	123.52
24	A	608	CLA	C3B-C4B-NB	-2.17	108.59	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C41-C39-C38	-2.17	116.30	121.17
24	c	506	CLA	C1-O2A-CGA	2.17	121.89	116.65
25	d	402	PHO	C14-C13-C12	-2.17	103.55	111.27
24	b	615	CLA	CED-O2D-CGD	2.17	120.83	115.92
34	e	102	HEM	CAB-C3B-C2B	-2.17	121.39	128.43
24	A	612	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
27	d	408	PL9	C27-C28-C29	-2.16	122.68	127.62
26	t	101	BCR	C3-C4-C5	-2.16	110.20	114.06
24	B	607	CLA	CMA-C3A-C4A	2.16	117.58	111.77
32	C	523	DGD	O6D-C1D-O3G	-2.16	104.94	110.04
31	L	101	LHG	C5-O7-C7	-2.16	112.63	117.80
24	a	605	CLA	C4D-CHA-C1A	2.16	123.82	121.24
24	B	603	CLA	CHD-C1D-C2D	2.16	129.97	125.49
29	A	613	LMG	C40-C39-C38	-2.15	103.47	114.37
35	V	201	HEC	CAC-C3C-C4C	-2.15	121.95	124.91
29	A	613	LMG	C1-C2-C3	-2.15	105.48	110.01
29	b	623	LMG	O6-C5-C6	2.15	111.77	106.44
27	D	406	PL9	C30-C29-C31	-2.15	111.49	115.23
24	b	615	CLA	CHC-C1C-NC	2.15	127.55	124.31
29	b	623	LMG	C3-C4-C5	-2.15	106.33	110.23
29	d	414	LMG	O1-C1-C2	-2.15	105.01	108.27
24	A	606	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	c	502	CLA	CHB-C4A-NA	2.15	127.50	124.40
24	B	604	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	B	612	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
28	e	105	STE	O2-C1-C2	2.15	120.78	114.00
24	b	607	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
24	B	611	CLA	C1-C2-C3	-2.15	122.68	126.20
30	F	102	SQD	O2-C2-C3	2.15	115.44	110.38
24	b	602	CLA	C6-C7-C8	-2.15	108.83	115.97
24	d	404	CLA	C2A-C1A-CHA	2.15	127.59	123.87
24	b	606	CLA	O1D-CGD-CBD	2.14	128.74	124.52
24	d	406	CLA	CHA-C4D-ND	2.14	136.96	132.55
29	D	408	LMG	O2-C2-C1	-2.14	104.98	110.08
32	c	519	DGD	C7B-C6B-C5B	-2.14	103.56	114.37
24	c	501	CLA	O1D-CGD-CBD	2.14	128.73	124.52
24	b	605	CLA	O1A-CGA-CBA	2.14	132.13	123.78
30	A	614	SQD	C3-C4-C5	2.13	114.10	110.23
24	b	609	CLA	CMB-C2B-C3B	2.13	131.57	126.55
24	C	509	CLA	O1D-CGD-CBD	2.13	128.73	124.52
31	d	411	LHG	C20-C19-C18	-2.13	103.58	114.37
26	b	619	BCR	C38-C26-C25	-2.13	122.16	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	O1D-CGD-CBD	2.13	128.72	124.52
26	A	609	BCR	C7-C8-C9	-2.13	123.08	126.23
24	C	501	CLA	CHB-C4A-NA	2.13	127.47	124.40
26	c	514	BCR	C8-C7-C6	-2.13	121.31	127.00
26	C	514	BCR	C15-C16-C17	-2.13	119.16	123.52
26	t	101	BCR	C15-C16-C17	-2.13	119.16	123.52
24	B	611	CLA	C9-C8-C10	-2.13	103.68	111.27
24	c	511	CLA	O1A-CGA-CBA	2.13	132.11	123.78
32	h	102	DGD	CBB-CAB-C9B	-2.13	103.61	114.37
24	C	512	CLA	CHC-C1C-NC	2.13	127.52	124.31
24	c	506	CLA	CHA-C4D-ND	2.13	136.94	132.55
32	C	523	DGD	CDB-CCB-CBB	-2.13	103.62	114.37
34	e	102	HEM	CAC-C3C-C4C	2.13	129.90	124.82
24	d	405	CLA	C1-C2-C3	-2.13	122.71	126.20
24	B	611	CLA	CHD-C1D-C2D	2.12	129.91	125.49
24	b	613	CLA	O1D-CGD-CBD	2.12	128.71	124.52
35	V	201	HEC	CAC-C3C-C2C	2.12	130.25	126.89
29	B	621	LMG	C1-O6-C5	-2.12	109.58	113.72
24	b	616	CLA	CHC-C4B-NB	2.12	127.23	124.05
24	b	614	CLA	CHD-C1D-C2D	2.12	129.90	125.49
24	c	513	CLA	CMB-C2B-C3B	2.12	131.53	126.55
24	c	513	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	c	504	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	A	606	CLA	C3B-C4B-NB	-2.11	108.64	110.53
24	C	507	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	A	610	PL9	C36-C34-C33	-2.11	116.43	121.17
24	D	404	CLA	C2C-C1C-NC	2.11	112.20	109.98
30	b	620	SQD	O4-C4-C3	-2.11	105.41	110.38
24	d	406	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	B	615	CLA	C16-C15-C13	-2.11	108.96	115.97
25	A	607	PHO	C2D-C1D-ND	2.11	110.95	109.43
30	f	101	SQD	O5-C5-C4	2.11	113.50	109.70
24	b	609	CLA	C6-C5-C3	2.11	118.60	113.47
35	v	201	HEC	CBA-CAA-C2A	-2.10	106.71	112.53
29	D	407	LMG	O1-C7-C8	-2.10	105.70	110.82
24	b	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	b	613	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
28	R	101	STE	O2-C1-O1	-2.10	117.93	123.33
24	B	614	CLA	CAC-C3C-C4C	2.10	127.52	124.79
30	A	616	SQD	O48-C23-O10	-2.10	118.37	123.63
26	b	617	BCR	C32-C1-C6	-2.10	106.95	110.24
24	B	602	CLA	O2A-CGA-O1A	-2.10	118.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C16-C15-C14	-2.10	119.22	123.52
24	c	508	CLA	O2D-CGD-CBD	2.10	114.90	111.23
31	d	410	LHG	C20-C19-C18	-2.10	103.76	114.37
24	b	616	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
24	b	610	CLA	C3D-C4D-ND	2.10	113.39	109.99
24	C	503	CLA	CHB-C1B-NB	2.10	127.19	124.05
32	C	522	DGD	C1D-C2D-C3D	-2.09	105.60	110.01
24	b	609	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
32	c	521	DGD	C8B-C7B-C6B	-2.09	103.78	114.37
27	a	609	PL9	C46-C44-C43	2.09	125.87	121.17
26	T	101	BCR	C30-C25-C26	-2.09	119.78	122.64
26	D	405	BCR	C15-C16-C17	-2.09	119.24	123.52
32	h	102	DGD	C1D-C2D-C3D	-2.09	105.61	110.01
26	h	101	BCR	C11-C10-C9	-2.09	124.35	127.28
31	d	410	LHG	C15-C14-C13	-2.09	103.80	114.37
26	A	609	BCR	C15-C16-C17	-2.09	119.24	123.52
24	c	504	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
24	B	603	CLA	CHA-C1A-NA	-2.09	121.66	126.39
24	c	512	CLA	C11-C10-C8	-2.09	109.02	115.97
24	c	507	CLA	CHB-C1B-NB	2.09	127.18	124.05
26	h	101	BCR	C7-C8-C9	-2.09	123.15	126.23
24	b	614	CLA	CHA-C4D-ND	2.09	136.85	132.55
29	A	613	LMG	O5-C6-C5	-2.09	104.23	111.33
24	B	601	CLA	CHA-C4D-ND	2.09	136.85	132.55
26	d	407	BCR	C28-C27-C26	-2.08	110.34	114.06
24	B	615	CLA	CHC-C4B-NB	2.08	127.17	124.05
24	C	511	CLA	C3B-C4B-NB	-2.08	108.67	110.53
28	b	624	STE	O2-C1-C2	2.08	120.58	114.00
24	b	607	CLA	CHC-C4B-NB	2.08	127.17	124.05
24	C	509	CLA	CHA-C1A-NA	-2.08	121.68	126.39
24	c	508	CLA	CHD-C1D-ND	-2.08	121.87	124.80
26	D	405	BCR	C28-C27-C26	-2.08	110.34	114.06
24	b	607	CLA	CHB-C4A-NA	2.08	127.40	124.40
31	D	409	LHG	C11-C10-C9	-2.08	103.86	114.37
24	D	403	CLA	C4-C3-C5	2.08	118.84	115.23
24	b	604	CLA	C1-C2-C3	-2.08	122.79	126.20
24	b	603	CLA	CMB-C2B-C3B	2.08	131.44	126.55
24	c	513	CLA	C3B-C4B-NB	-2.08	108.68	110.53
24	c	512	CLA	O1D-CGD-CBD	2.08	128.61	124.52
24	A	612	CLA	C1D-ND-C4D	2.08	107.77	106.31
24	B	610	CLA	CMD-C2D-C3D	2.08	132.45	127.69
30	a	610	SQD	C9-C8-C7	-2.08	106.09	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	CHD-C1D-C2D	2.07	129.80	125.49
24	B	606	CLA	O2D-CGD-CBD	2.07	114.86	111.23
24	C	512	CLA	C2A-C3A-C4A	2.07	105.22	101.87
24	b	608	CLA	CMB-C2B-C3B	2.07	131.43	126.55
24	B	614	CLA	C2A-C1A-CHA	2.07	127.47	123.87
29	c	523	LMG	O1-C7-C8	-2.07	105.78	110.82
34	e	102	HEM	O2D-CGD-CBD	2.07	120.55	114.00
24	c	504	CLA	CMC-C2C-C1C	2.07	128.27	125.03
24	B	607	CLA	CHC-C4B-NB	2.07	127.16	124.05
29	A	613	LMG	O6-C1-C2	-2.07	106.11	110.37
24	B	613	CLA	C11-C10-C8	-2.07	109.08	115.97
24	B	615	CLA	C7-C6-C5	-2.07	107.74	113.26
26	T	101	BCR	C38-C26-C27	-2.07	109.18	113.60
30	b	620	SQD	O5-C5-C4	2.07	113.43	109.70
24	b	610	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	B	610	CLA	C2A-C1A-CHA	2.07	127.46	123.87
28	I	102	STE	O2-C1-C2	2.07	120.53	114.00
24	B	611	CLA	C6-C7-C8	-2.07	109.09	115.97
24	C	504	CLA	CHD-C4C-C3C	-2.06	121.76	124.77
32	A	617	DGD	O6E-C1E-O5D	-2.06	105.17	110.04
24	b	606	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
32	c	520	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
25	D	402	PHO	C1-C2-C3	-2.06	122.82	126.20
24	b	609	CLA	C1D-ND-C4D	2.06	107.76	106.31
29	B	621	LMG	C38-C37-C36	-2.06	103.96	114.37
24	b	611	CLA	C20-C18-C19	-2.06	101.34	110.53
24	b	609	CLA	C2D-C1D-ND	-2.06	108.09	110.13
32	C	522	DGD	CBB-CAB-C9B	-2.06	103.96	114.37
24	c	503	CLA	C4-C3-C5	2.06	118.80	115.23
26	h	101	BCR	C39-C30-C25	-2.06	107.02	110.24
32	C	522	DGD	O2G-C1B-O1B	-2.06	118.90	123.70
24	B	615	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
24	b	614	CLA	CMB-C2B-C3B	2.05	131.38	126.55
24	a	607	CLA	C5-C3-C2	-2.05	116.56	121.17
24	a	606	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	c	505	CLA	CHD-C1D-ND	-2.05	121.91	124.80
30	B	623	SQD	C9-C8-C7	-2.05	106.17	113.69
24	C	510	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
26	h	101	BCR	C8-C9-C10	2.05	122.23	119.01
26	B	619	BCR	C1-C6-C5	-2.05	119.83	122.64
24	b	605	CLA	CHD-C4C-NC	2.05	127.41	124.23
26	A	609	BCR	C38-C26-C25	-2.05	122.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4D-CHA-C1A	2.05	123.69	121.24
24	c	504	CLA	CHD-C4C-NC	2.05	127.41	124.23
26	c	514	BCR	C24-C23-C22	-2.05	123.21	126.23
32	h	102	DGD	CAB-C9B-C8B	-2.05	104.03	114.37
31	d	411	LHG	O8-C6-C5	-2.04	102.50	108.40
26	B	618	BCR	C15-C16-C17	-2.04	119.33	123.52
32	c	521	DGD	O5E-C6E-C5E	-2.04	104.37	111.33
24	a	607	CLA	C3D-C4D-ND	2.04	113.31	109.99
26	h	101	BCR	C30-C25-C26	-2.04	119.84	122.64
24	b	616	CLA	CAC-C3C-C4C	2.04	127.45	124.79
24	B	607	CLA	C2C-C1C-NC	2.04	112.13	109.98
29	c	524	LMG	C38-C37-C36	-2.04	104.05	114.37
24	b	611	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
29	d	414	LMG	O7-C10-O9	-2.04	118.94	123.70
30	a	610	SQD	C46-O48-C23	-2.04	109.67	117.12
26	D	405	BCR	C7-C8-C9	-2.04	123.22	126.23
26	T	101	BCR	C1-C6-C5	-2.04	119.85	122.64
24	A	606	CLA	CHC-C1C-NC	2.04	127.38	124.31
29	m	101	LMG	C37-C36-C35	-2.04	104.08	114.37
27	d	408	PL9	C50-C49-C48	-2.04	116.55	122.66
32	C	522	DGD	C3D-C4D-C5D	-2.04	106.54	110.23
35	v	201	HEC	CAB-C3B-C4B	2.03	127.44	124.79
24	b	609	CLA	C3C-C4C-NC	-2.03	107.83	110.43
24	b	601	CLA	C2A-C3A-C4A	2.03	105.15	101.87
26	k	102	BCR	C24-C23-C22	-2.03	123.23	126.23
24	b	606	CLA	C2A-C1A-CHA	2.03	127.39	123.87
24	C	513	CLA	CHD-C1D-C2D	2.03	129.71	125.49
24	B	606	CLA	CHD-C4C-C3C	-2.03	121.82	124.77
24	c	510	CLA	C1-C2-C3	-2.03	122.87	126.20
29	c	524	LMG	O5-C6-C5	-2.03	104.43	111.33
35	v	201	HEC	C1B-C2B-C3B	2.03	109.11	106.98
29	d	414	LMG	O6-C1-O1	-2.03	105.25	110.04
31	d	411	LHG	C18-C17-C16	-2.03	104.13	114.37
26	B	618	BCR	C40-C30-C25	2.03	113.42	110.24
24	C	503	CLA	CHC-C4B-NB	2.02	127.09	124.05
24	d	406	CLA	CAC-C3C-C4C	2.02	127.42	124.79
29	D	407	LMG	C1-C2-C3	-2.02	105.75	110.01
24	D	403	CLA	C2B-C1B-NB	-2.02	108.23	110.33
34	e	102	HEM	C3B-C2B-C1B	2.02	107.93	106.41
24	B	602	CLA	C6-C5-C3	-2.02	108.55	113.47
24	B	616	CLA	C1D-ND-C4D	2.02	107.73	106.31
24	b	607	CLA	O2A-CGA-O1A	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	t	102	STE	O2-C1-C2	2.02	120.38	114.00
26	b	619	BCR	C33-C5-C6	-2.02	122.28	124.48
28	I	101	STE	O2-C1-C2	2.02	120.37	114.00
24	c	501	CLA	C3B-C4B-NB	-2.02	108.73	110.53
24	d	404	CLA	C2B-C1B-NB	-2.02	108.23	110.33
29	D	408	LMG	C17-C16-C15	-2.02	104.18	114.37
25	d	403	PHO	CAA-CBA-CGA	-2.01	107.49	113.21
26	c	515	BCR	C4-C5-C6	2.01	125.43	122.70
24	B	612	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	b	602	CLA	C11-C10-C8	-2.01	109.27	115.97
24	c	503	CLA	C5-C3-C2	-2.01	116.65	121.17
24	C	507	CLA	CHA-C4D-ND	2.01	136.70	132.55
24	B	603	CLA	CHB-C1B-NB	2.01	127.07	124.05
24	C	509	CLA	CHA-C4D-ND	2.01	136.70	132.55
24	B	605	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	B	613	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	C	507	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	c	513	CLA	CHD-C1D-C2D	2.01	129.66	125.49
24	A	605	CLA	CHC-C4B-NB	2.01	127.06	124.05
29	c	524	LMG	O1-C7-C8	-2.01	105.94	110.82
24	B	602	CLA	C1-C2-C3	-2.01	122.91	126.20
31	d	412	LHG	C29-C28-C27	-2.01	104.23	114.37
29	c	518	LMG	O7-C10-O9	-2.01	119.02	123.70
24	B	609	CLA	CHA-C1A-NA	-2.00	121.85	126.39
35	v	201	HEC	CHD-C1D-ND	2.00	126.84	124.37
25	d	403	PHO	CMB-C2B-C3B	2.00	128.68	124.68
24	b	615	CLA	CHB-C4A-NA	2.00	127.29	124.40
32	c	519	DGD	O6E-C5E-C4E	2.00	113.31	109.70

All (2) chirality outliers are listed below:

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

All (1762) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	C4B-C3B-CAB-CBB
24	C	512	CLA	C11-C10-C8-C9
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
26	A	609	BCR	C20-C21-C22-C37
26	B	619	BCR	C11-C12-C13-C35
26	C	514	BCR	C21-C22-C23-C24
26	D	405	BCR	C21-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C26
26	H	101	BCR	C16-C17-C18-C36
26	K	101	BCR	C16-C17-C18-C36
26	K	102	BCR	C1-C6-C7-C8
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C21-C22-C23-C24
26	K	102	BCR	C37-C22-C23-C24
26	b	619	BCR	C11-C10-C9-C34
26	h	101	BCR	C20-C21-C22-C37
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C21-C22-C23-C24
27	A	610	PL9	C27-C28-C29-C30
27	A	610	PL9	C27-C28-C29-C31
27	A	610	PL9	C30-C29-C31-C32
27	A	610	PL9	C42-C43-C44-C45
27	D	406	PL9	C32-C33-C34-C36
27	a	609	PL9	C12-C13-C14-C15
27	a	609	PL9	C22-C23-C24-C25
27	a	609	PL9	C35-C34-C36-C37
27	a	609	PL9	C47-C48-C49-C50
27	d	408	PL9	C32-C33-C34-C36
27	d	408	PL9	C38-C39-C41-C42
29	A	613	LMG	O9-C10-O7-C8
29	C	516	LMG	C2-C1-O1-C7
29	C	524	LMG	C11-C10-O7-C8
29	b	623	LMG	O6-C1-O1-C7
29	b	623	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
29	c	518	LMG	O1-C7-C8-C9
29	c	518	LMG	O1-C7-C8-O7
29	c	518	LMG	O10-C28-O8-C9
29	c	524	LMG	O6-C1-O1-C7
30	A	616	SQD	O6-C44-C45-O47
30	B	623	SQD	C2-C1-O6-C44
30	B	623	SQD	O5-C1-O6-C44
30	B	623	SQD	O6-C44-C45-O47
30	B	623	SQD	O49-C7-O47-C45
30	B	623	SQD	C8-C7-O47-C45
30	F	102	SQD	C2-C1-O6-C44
30	F	102	SQD	O5-C1-O6-C44
30	a	611	SQD	O6-C44-C45-O47
30	a	611	SQD	O5-C5-C6-S
30	a	611	SQD	C5-C6-S-O7
30	a	611	SQD	C5-C6-S-O8
30	a	611	SQD	C5-C6-S-O9
30	b	620	SQD	C8-C7-O47-C45
30	f	101	SQD	O5-C1-O6-C44
31	A	615	LHG	C3-O3-P-O5
31	D	409	LHG	C3-O3-P-O4
31	D	409	LHG	C3-O3-P-O6
31	D	409	LHG	C4-O6-P-O4
31	D	411	LHG	C3-O3-P-O4
31	D	411	LHG	C3-O3-P-O6
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O4
31	d	411	LHG	O1-C1-C2-C3
31	d	411	LHG	C1-C2-C3-O3
31	d	411	LHG	C4-O6-P-O3
31	d	411	LHG	C4-O6-P-O4
31	e	103	LHG	O1-C1-C2-C3
31	e	103	LHG	C3-O3-P-O4
31	e	103	LHG	C3-O3-P-O6
31	l	101	LHG	C4-O6-P-O5
24	B	601	CLA	O1A-CGA-O2A-C1
29	B	621	LMG	O10-C28-O8-C9
30	F	102	SQD	O10-C23-O48-C46
30	f	101	SQD	O10-C23-O48-C46
27	A	610	PL9	C47-C48-C49-C50
27	A	610	PL9	C47-C48-C49-C51
27	a	609	PL9	C47-C48-C49-C51

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CBA-CGA-O2A-C1
30	F	102	SQD	C24-C23-O48-C46
29	B	620	LMG	O10-C28-O8-C9
29	o	301	LMG	O10-C28-O8-C9
29	D	407	LMG	O9-C10-O7-C8
32	A	617	DGD	O1B-C1B-O2G-C2G
24	B	616	CLA	CBA-CGA-O2A-C1
29	B	621	LMG	C29-C28-O8-C9
29	o	301	LMG	C29-C28-O8-C9
30	f	101	SQD	C24-C23-O48-C46
24	C	501	CLA	CBD-CGD-O2D-CED
29	A	613	LMG	C11-C10-O7-C8
24	B	603	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	B	603	CLA	C2-C3-C5-C6
24	b	604	CLA	C2-C3-C5-C6
27	A	610	PL9	C33-C34-C36-C37
27	a	609	PL9	C33-C34-C36-C37
24	c	511	CLA	CBD-CGD-O2D-CED
24	B	601	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C3-C5-C6-C7
24	b	614	CLA	C3-C5-C6-C7
29	A	613	LMG	C29-C28-O8-C9
29	c	518	LMG	C29-C28-O8-C9
30	b	620	SQD	C24-C23-O48-C46
27	d	408	PL9	C32-C33-C34-C35
27	d	408	PL9	C42-C43-C44-C45
27	A	610	PL9	C32-C33-C34-C36
27	a	609	PL9	C22-C23-C24-C26
29	A	613	LMG	O10-C28-O8-C9
29	C	516	LMG	O10-C28-O8-C9
30	b	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O49-C7-O47-C45
24	A	608	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	B	616	CLA	CBD-CGD-O2D-CED
25	d	403	PHO	CBD-CGD-O2D-CED
31	D	409	LHG	O2-C2-C3-O3
31	D	411	LHG	O2-C2-C3-O3
31	d	410	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	d	411	LHG	O2-C2-C3-O3
29	b	623	LMG	O6-C5-C6-O5
32	A	617	DGD	O6E-C5E-C6E-O5E
24	B	616	CLA	O1A-CGA-O2A-C1
29	D	407	LMG	C11-C10-O7-C8
29	C	524	LMG	O6-C5-C6-O5
24	C	509	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	CBD-CGD-O2D-CED
29	C	524	LMG	C4-C5-C6-O5
29	B	620	LMG	C29-C28-O8-C9
24	B	605	CLA	C4-C3-C5-C6
24	a	607	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	a	607	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	c	507	CLA	C2-C3-C5-C6
27	A	610	PL9	C28-C29-C31-C32
29	b	623	LMG	O10-C28-O8-C9
27	A	610	PL9	C39-C41-C42-C43
27	a	609	PL9	C24-C26-C27-C28
27	a	609	PL9	C44-C46-C47-C48
24	b	601	CLA	CBD-CGD-O2D-CED
32	A	617	DGD	C4E-C5E-C6E-O5E
35	v	201	HEC	C2C-C3C-CAC-CBC
29	D	407	LMG	O6-C1-O1-C7
32	A	617	DGD	O6D-C1D-O3G-C3G
30	F	102	SQD	C44-C45-C46-O48
24	B	601	CLA	CBD-CGD-O2D-CED
24	c	501	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	CBD-CGD-O2D-CED
29	D	408	LMG	C10-C11-C12-C13
29	A	613	LMG	O6-C5-C6-O5
35	V	201	HEC	C2C-C3C-CAC-CBC
27	D	406	PL9	C22-C23-C24-C25
29	c	524	LMG	O9-C10-O7-C8
31	A	615	LHG	C1-C2-C3-O3
31	D	411	LHG	C1-C2-C3-O3
31	d	410	LHG	C1-C2-C3-O3
24	c	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	C	516	LMG	C29-C28-O8-C9
31	A	615	LHG	C27-C28-C29-C30
24	B	614	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
27	A	610	PL9	C35-C34-C36-C37
24	B	614	CLA	C2-C3-C5-C6
24	B	611	CLA	C11-C12-C13-C14
24	B	613	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	C	513	CLA	C11-C12-C13-C14
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C10-C8-C9
24	b	613	CLA	C11-C12-C13-C14
24	c	509	CLA	C11-C12-C13-C14
24	c	512	CLA	C6-C7-C8-C9
24	d	406	CLA	C6-C7-C8-C9
25	A	607	PHO	C14-C13-C15-C16
29	b	623	LMG	C2-C1-O1-C7
29	c	524	LMG	C2-C1-O1-C7
28	d	413	STE	C7-C8-C9-C10
28	x	101	STE	C1-C2-C3-C4
29	d	414	LMG	C10-C11-C12-C13
29	o	301	LMG	O6-C5-C6-O5
29	A	613	LMG	C4-C5-C6-O5
26	B	618	BCR	C37-C22-C23-C24
26	T	101	BCR	C36-C18-C19-C20
26	b	618	BCR	C37-C22-C23-C24
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
26	d	407	BCR	C21-C22-C23-C24
24	B	606	CLA	C2A-CAA-CBA-CGA
29	c	518	LMG	C28-C29-C30-C31
24	C	501	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	O6-C5-C6-O5
27	D	406	PL9	C37-C38-C39-C40
24	d	405	CLA	C3-C5-C6-C7
31	d	410	LHG	C7-C8-C9-C10
24	c	512	CLA	O1A-CGA-O2A-C1
35	V	201	HEC	C2B-C3B-CAB-CBB
24	B	601	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	b	613	CLA	C11-C10-C8-C7
29	m	101	LMG	C29-C28-O8-C9
24	C	505	CLA	C13-C15-C16-C17
28	R	101	STE	C1-C2-C3-C4
29	o	301	LMG	C28-C29-C30-C31
32	H	102	DGD	O6E-C5E-C6E-O5E
27	A	610	PL9	C24-C26-C27-C28
27	a	609	PL9	C34-C36-C37-C38
24	c	513	CLA	C3-C5-C6-C7
28	C	525	STE	C2-C3-C4-C5
29	b	623	LMG	C4-C5-C6-O5
28	M	101	STE	C1-C2-C3-C4
28	b	622	STE	C1-C2-C3-C4
29	D	407	LMG	C28-C29-C30-C31
29	c	523	LMG	C28-C29-C30-C31
29	d	414	LMG	C28-C29-C30-C31
30	F	102	SQD	C23-C24-C25-C26
32	c	521	DGD	C1A-C2A-C3A-C4A
24	C	508	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	C5-C6-C7-C8
24	b	613	CLA	C13-C15-C16-C17
24	b	606	CLA	C2A-CAA-CBA-CGA
26	K	101	BCR	C10-C11-C12-C13
24	B	606	CLA	C8-C10-C11-C12
24	B	611	CLA	C8-C10-C11-C12
24	a	607	CLA	C5-C6-C7-C8
24	b	607	CLA	C5-C6-C7-C8
28	E	101	STE	C1-C2-C3-C4
30	A	614	SQD	C23-C24-C25-C26
30	a	610	SQD	C7-C8-C9-C10
31	l	101	LHG	C23-C24-C25-C26
24	b	601	CLA	C3-C5-C6-C7
28	B	626	STE	C5-C6-C7-C8
24	B	601	CLA	C5-C6-C7-C8
24	B	603	CLA	C5-C6-C7-C8
24	B	606	CLA	C13-C15-C16-C17
24	B	608	CLA	C15-C16-C17-C18
24	C	509	CLA	C10-C11-C12-C13
24	c	503	CLA	C8-C10-C11-C12
24	c	507	CLA	C5-C6-C7-C8
31	e	103	LHG	O2-C2-C3-O3
30	B	623	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	O10-C23-O8-C6
28	J	101	STE	C1-C2-C3-C4
28	i	101	STE	C1-C2-C3-C4
31	A	615	LHG	C23-C24-C25-C26
24	B	613	CLA	C8-C10-C11-C12
24	b	601	CLA	C5-C6-C7-C8
31	e	103	LHG	O10-C23-O8-C6
24	A	612	CLA	C15-C16-C17-C18
24	C	506	CLA	C15-C16-C17-C18
24	C	507	CLA	C13-C15-C16-C17
24	b	601	CLA	C10-C11-C12-C13
29	C	524	LMG	C29-C28-O8-C9
24	C	509	CLA	C13-C15-C16-C17
30	A	616	SQD	C12-C13-C14-C15
24	c	506	CLA	O1A-CGA-O2A-C1
31	e	103	LHG	C1-C2-C3-O3
24	c	506	CLA	CBA-CGA-O2A-C1
30	B	623	SQD	C24-C23-O48-C46
24	B	607	CLA	C8-C10-C11-C12
24	B	614	CLA	C15-C16-C17-C18
24	C	513	CLA	C8-C10-C11-C12
24	b	607	CLA	C8-C10-C11-C12
24	c	508	CLA	C8-C10-C11-C12
24	c	512	CLA	C8-C10-C11-C12
24	B	616	CLA	O1D-CGD-O2D-CED
24	c	511	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	C10-C11-C12-C13
24	B	616	CLA	C5-C6-C7-C8
24	C	508	CLA	C10-C11-C12-C13
24	a	607	CLA	C13-C15-C16-C17
24	b	608	CLA	C13-C15-C16-C17
24	c	508	CLA	C10-C11-C12-C13
35	v	201	HEC	C4C-C3C-CAC-CBC
24	B	607	CLA	C5-C6-C7-C8
24	C	503	CLA	C5-C6-C7-C8
24	b	606	CLA	C15-C16-C17-C18
24	c	507	CLA	C8-C10-C11-C12
29	b	623	LMG	C29-C28-O8-C9
24	B	602	CLA	C13-C15-C16-C17
24	C	510	CLA	C8-C10-C11-C12
30	f	101	SQD	C8-C7-O47-C45
24	D	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	d	403	PHO	O1D-CGD-O2D-CED
30	f	101	SQD	O49-C7-O47-C45
29	D	407	LMG	C2-C1-O1-C7
32	C	522	DGD	C2E-C1E-O5D-C6D
32	c	520	DGD	C2E-C1E-O5D-C6D
24	B	604	CLA	C10-C11-C12-C13
26	A	609	BCR	C35-C13-C14-C15
26	B	617	BCR	C11-C10-C9-C34
26	B	618	BCR	C35-C13-C14-C15
26	C	514	BCR	C16-C17-C18-C36
26	C	520	BCR	C11-C10-C9-C34
26	D	405	BCR	C20-C21-C22-C37
26	K	101	BCR	C35-C13-C14-C15
26	K	102	BCR	C35-C13-C14-C15
26	K	102	BCR	C16-C17-C18-C36
26	a	608	BCR	C35-C13-C14-C15
26	a	608	BCR	C20-C21-C22-C37
26	b	618	BCR	C35-C13-C14-C15
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C16-C17-C18-C36
26	c	514	BCR	C20-C21-C22-C37
26	c	515	BCR	C20-C21-C22-C37
26	d	407	BCR	C35-C13-C14-C15
26	d	407	BCR	C16-C17-C18-C36
26	h	101	BCR	C11-C10-C9-C34
26	h	101	BCR	C35-C13-C14-C15
26	k	101	BCR	C35-C13-C14-C15
26	k	102	BCR	C20-C21-C22-C37
26	c	515	BCR	C11-C12-C13-C35
26	d	407	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C17-C18-C19-C20
24	C	505	CLA	C10-C11-C12-C13
31	D	410	LHG	O1-C1-C2-C3
31	e	103	LHG	C23-C24-C25-C26
30	b	620	SQD	C46-C45-O47-C7
24	b	609	CLA	C16-C17-C18-C19
24	c	503	CLA	C16-C17-C18-C20
24	c	509	CLA	C16-C17-C18-C20
24	C	509	CLA	O1D-CGD-O2D-CED
24	c	512	CLA	O1D-CGD-O2D-CED
24	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	C10-C11-C12-C13
26	K	101	BCR	C16-C17-C18-C19
26	h	101	BCR	C11-C10-C9-C8
32	C	522	DGD	O6E-C1E-O5D-C6D
24	b	607	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C8-C10-C11-C12
24	C	506	CLA	CBD-CGD-O2D-CED
29	B	621	LMG	C28-C29-C30-C31
32	c	519	DGD	O6D-C5D-C6D-O5D
24	B	601	CLA	C2-C1-O2A-CGA
24	c	506	CLA	C2-C1-O2A-CGA
24	C	513	CLA	C16-C17-C18-C19
24	b	609	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
35	V	201	HEC	C4C-C3C-CAC-CBC
24	A	605	CLA	C15-C16-C17-C18
28	B	626	STE	C2-C3-C4-C5
28	B	626	STE	C4-C5-C6-C7
28	b	621	STE	C6-C7-C8-C9
29	B	621	LMG	C33-C34-C35-C36
30	A	614	SQD	C30-C31-C32-C33
30	b	620	SQD	C17-C18-C19-C20
32	C	521	DGD	C3A-C4A-C5A-C6A
32	c	520	DGD	C5A-C6A-C7A-C8A
32	h	102	DGD	C2B-C3B-C4B-C5B
28	C	527	STE	C13-C14-C15-C16
28	b	621	STE	C9-C10-C11-C12
28	j	102	STE	C6-C7-C8-C9
29	C	524	LMG	C11-C12-C13-C14
29	D	408	LMG	C20-C21-C22-C23
29	D	408	LMG	C35-C36-C37-C38
29	m	101	LMG	C16-C17-C18-C19
29	o	301	LMG	C31-C32-C33-C34
31	D	410	LHG	C15-C16-C17-C18
31	D	411	LHG	C16-C17-C18-C19
31	d	411	LHG	C17-C18-C19-C20
32	h	102	DGD	C8A-C9A-CAA-CBA
29	m	101	LMG	C10-C11-C12-C13
24	c	503	CLA	C15-C16-C17-C18
28	E	103	STE	C9-C10-C11-C12
28	c	516	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C12-C13-C14-C15
29	b	623	LMG	C22-C23-C24-C25
29	o	301	LMG	C14-C15-C16-C17
30	A	614	SQD	C15-C16-C17-C18
30	A	614	SQD	C28-C29-C30-C31
31	l	101	LHG	C11-C12-C13-C14
32	C	522	DGD	C4A-C5A-C6A-C7A
32	C	522	DGD	C6A-C7A-C8A-C9A
32	C	523	DGD	C6A-C7A-C8A-C9A
24	C	511	CLA	CBA-CGA-O2A-C1
28	C	519	STE	C7-C8-C9-C10
28	Z	101	STE	C10-C11-C12-C13
28	d	413	STE	C12-C13-C14-C15
28	e	105	STE	C5-C6-C7-C8
28	f	102	STE	C13-C14-C15-C16
28	j	101	STE	C4-C5-C6-C7
29	C	524	LMG	C37-C38-C39-C40
29	c	524	LMG	C15-C16-C17-C18
30	A	616	SQD	C10-C11-C12-C13
31	A	615	LHG	C10-C11-C12-C13
31	L	101	LHG	C28-C29-C30-C31
31	l	101	LHG	C17-C18-C19-C20
32	A	617	DGD	C8B-C9B-CAB-CBB
32	c	519	DGD	C4A-C5A-C6A-C7A
32	c	519	DGD	C7B-C8B-C9B-CAB
29	C	524	LMG	O9-C10-O7-C8
31	e	103	LHG	O1-C1-C2-O2
28	C	526	STE	C7-C8-C9-C10
28	J	101	STE	C6-C7-C8-C9
31	D	411	LHG	C28-C29-C30-C31
31	d	412	LHG	C29-C30-C31-C32
32	A	617	DGD	C6B-C7B-C8B-C9B
24	c	504	CLA	C5-C6-C7-C8
24	b	610	CLA	C4B-C3B-CAB-CBB
29	c	522	LMG	C28-C29-C30-C31
28	I	101	STE	C2-C3-C4-C5
30	A	616	SQD	C9-C10-C11-C12
31	A	615	LHG	C15-C16-C17-C18
24	C	513	CLA	C16-C17-C18-C20
24	B	601	CLA	O1D-CGD-O2D-CED
29	B	621	LMG	C17-C18-C19-C20
30	a	610	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	D	409	LHG	C18-C19-C20-C21
31	d	412	LHG	C28-C29-C30-C31
28	R	101	STE	C9-C10-C11-C12
28	d	409	STE	C5-C6-C7-C8
29	D	407	LMG	C16-C17-C18-C19
31	d	411	LHG	C12-C13-C14-C15
24	c	508	CLA	C11-C12-C13-C15
28	C	528	STE	C12-C13-C14-C15
28	E	101	STE	C3-C4-C5-C6
28	t	103	STE	C3-C4-C5-C6
29	b	623	LMG	C29-C30-C31-C32
30	A	614	SQD	C12-C13-C14-C15
31	d	411	LHG	C30-C31-C32-C33
31	A	615	LHG	O2-C2-C3-O3
30	f	101	SQD	C23-C24-C25-C26
24	B	605	CLA	C13-C15-C16-C17
24	c	512	CLA	C13-C15-C16-C17
28	B	626	STE	C7-C8-C9-C10
28	Z	101	STE	C14-C15-C16-C17
28	d	409	STE	C6-C7-C8-C9
28	h	103	STE	C12-C13-C14-C15
29	B	621	LMG	C35-C36-C37-C38
29	D	407	LMG	C30-C31-C32-C33
29	b	623	LMG	C15-C16-C17-C18
24	B	601	CLA	C3A-C2A-CAA-CBA
28	t	102	STE	C7-C8-C9-C10
31	d	412	LHG	C33-C34-C35-C36
32	C	523	DGD	C6B-C7B-C8B-C9B
32	c	521	DGD	C5A-C6A-C7A-C8A
32	C	523	DGD	C8A-C9A-CAA-CBA
24	b	615	CLA	C5-C6-C7-C8
29	c	524	LMG	C28-C29-C30-C31
30	B	623	SQD	O10-C23-O48-C46
28	A	618	STE	C10-C11-C12-C13
28	d	409	STE	C14-C15-C16-C17
30	B	623	SQD	C27-C28-C29-C30
28	A	618	STE	C13-C14-C15-C16
28	M	101	STE	C5-C6-C7-C8
30	B	623	SQD	C32-C33-C34-C35
31	d	410	LHG	C10-C11-C12-C13
31	D	409	LHG	C1-C2-C3-O3
28	B	624	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	R	101	STE	C11-C10-C9-C8
28	d	413	STE	C2-C3-C4-C5
29	D	407	LMG	C36-C37-C38-C39
30	A	614	SQD	C27-C28-C29-C30
30	F	102	SQD	C34-C35-C36-C37
32	A	617	DGD	C5B-C6B-C7B-C8B
24	C	512	CLA	C3-C5-C6-C7
28	d	413	STE	C1-C2-C3-C4
32	c	520	DGD	C1B-C2B-C3B-C4B
28	A	619	STE	C14-C15-C16-C17
28	B	626	STE	C9-C10-C11-C12
28	C	526	STE	C4-C5-C6-C7
28	b	622	STE	C4-C5-C6-C7
28	b	622	STE	C12-C13-C14-C15
29	B	620	LMG	C34-C35-C36-C37
29	c	522	LMG	C39-C40-C41-C42
29	d	414	LMG	C37-C38-C39-C40
30	A	614	SQD	C9-C10-C11-C12
30	a	611	SQD	C33-C34-C35-C36
30	f	101	SQD	C29-C30-C31-C32
31	d	410	LHG	C28-C29-C30-C31
31	e	103	LHG	C24-C25-C26-C27
32	c	521	DGD	C7A-C8A-C9A-CAA
32	c	521	DGD	C5B-C6B-C7B-C8B
28	A	611	STE	C3-C4-C5-C6
29	B	621	LMG	C18-C19-C20-C21
29	D	408	LMG	C39-C40-C41-C42
29	b	623	LMG	C23-C24-C25-C26
30	F	102	SQD	C30-C31-C32-C33
32	c	519	DGD	C7A-C8A-C9A-CAA
28	H	103	STE	C4-C5-C6-C7
28	Z	101	STE	C6-C7-C8-C9
28	i	101	STE	C2-C3-C4-C5
31	D	410	LHG	C13-C14-C15-C16
28	d	409	STE	C12-C13-C14-C15
28	d	413	STE	C11-C12-C13-C14
29	A	613	LMG	C16-C17-C18-C19
29	c	522	LMG	C14-C15-C16-C17
29	m	101	LMG	C17-C18-C19-C20
29	o	301	LMG	C34-C35-C36-C37
30	B	623	SQD	C17-C18-C19-C20
31	d	412	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	C9A-CAA-CBA-CCA
24	a	607	CLA	C16-C17-C18-C20
29	D	407	LMG	C10-C11-C12-C13
26	B	617	BCR	C1-C6-C7-C8
26	D	405	BCR	C23-C24-C25-C30
28	C	518	STE	C4-C5-C6-C7
28	e	101	STE	C11-C12-C13-C14
30	f	101	SQD	C28-C29-C30-C31
31	L	101	LHG	C17-C18-C19-C20
32	c	519	DGD	C5A-C6A-C7A-C8A
29	C	516	LMG	C11-C10-O7-C8
24	c	509	CLA	C10-C11-C12-C13
28	M	103	STE	C11-C10-C9-C8
29	A	613	LMG	C13-C14-C15-C16
29	B	620	LMG	C32-C33-C34-C35
30	a	611	SQD	C27-C28-C29-C30
28	c	517	STE	C12-C13-C14-C15
28	i	101	STE	C5-C6-C7-C8
29	c	523	LMG	C38-C39-C40-C41
29	d	414	LMG	C33-C34-C35-C36
32	C	521	DGD	C2A-C3A-C4A-C5A
31	d	412	LHG	C23-C24-C25-C26
30	A	614	SQD	C29-C30-C31-C32
30	F	102	SQD	C27-C28-C29-C30
30	a	611	SQD	C14-C15-C16-C17
31	l	101	LHG	C32-C33-C34-C35
32	c	520	DGD	C6A-C7A-C8A-C9A
24	C	511	CLA	O1A-CGA-O2A-C1
28	A	618	STE	C6-C7-C8-C9
28	M	103	STE	C13-C14-C15-C16
28	Z	101	STE	C11-C12-C13-C14
29	D	407	LMG	C31-C32-C33-C34
30	A	616	SQD	C14-C15-C16-C17
30	a	611	SQD	C11-C10-C9-C8
32	A	617	DGD	C2A-C3A-C4A-C5A
32	C	523	DGD	C7B-C8B-C9B-CAB
32	c	521	DGD	C4B-C5B-C6B-C7B
29	b	623	LMG	O9-C10-O7-C8
24	c	509	CLA	C4-C3-C5-C6
27	d	408	PL9	C45-C44-C46-C47
24	b	601	CLA	O1D-CGD-O2D-CED
29	D	407	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	C12-C13-C14-C15
32	C	521	DGD	C8A-C9A-CAA-CBA
32	h	102	DGD	C5B-C6B-C7B-C8B
27	a	609	PL9	C32-C33-C34-C36
26	T	101	BCR	C18-C19-C20-C21
26	b	619	BCR	C10-C11-C12-C13
31	D	410	LHG	C25-C26-C27-C28
31	D	410	LHG	C27-C28-C29-C30
32	A	617	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	C3B-C4B-C5B-C6B
32	c	519	DGD	C5B-C6B-C7B-C8B
32	c	521	DGD	CCB-CDB-CEB-CFB
29	c	523	LMG	C29-C28-O8-C9
29	o	301	LMG	C23-C24-C25-C26
32	c	519	DGD	C6A-C7A-C8A-C9A
28	M	103	STE	C9-C10-C11-C12
29	A	613	LMG	C30-C31-C32-C33
29	b	623	LMG	C38-C39-C40-C41
30	B	623	SQD	C11-C12-C13-C14
31	d	412	LHG	C31-C32-C33-C34
26	b	617	BCR	C6-C7-C8-C9
32	c	520	DGD	O6E-C1E-O5D-C6D
28	C	528	STE	C10-C11-C12-C13
31	e	103	LHG	C15-C16-C17-C18
28	B	622	STE	C9-C10-C11-C12
29	B	620	LMG	C33-C34-C35-C36
29	d	414	LMG	C34-C35-C36-C37
29	o	301	LMG	C20-C21-C22-C23
30	F	102	SQD	C24-C25-C26-C27
32	H	102	DGD	C7A-C8A-C9A-CAA
28	M	101	STE	C4-C5-C6-C7
28	d	409	STE	C4-C5-C6-C7
29	c	522	LMG	C13-C14-C15-C16
28	B	622	STE	C7-C8-C9-C10
29	m	101	LMG	C32-C33-C34-C35
30	a	611	SQD	C34-C35-C36-C37
30	b	620	SQD	C10-C11-C12-C13
31	e	103	LHG	C17-C18-C19-C20
24	b	607	CLA	C16-C17-C18-C20
29	c	522	LMG	C11-C10-O7-C8
32	A	617	DGD	C2B-C1B-O2G-C2G
24	B	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	B	624	STE	C4-C5-C6-C7
28	C	515	STE	C11-C10-C9-C8
28	a	612	STE	C2-C3-C4-C5
29	c	523	LMG	C35-C36-C37-C38
32	C	523	DGD	C5B-C6B-C7B-C8B
26	B	619	BCR	C7-C8-C9-C34
26	C	520	BCR	C37-C22-C23-C24
30	a	611	SQD	C29-C30-C31-C32
32	c	521	DGD	C4A-C5A-C6A-C7A
32	C	522	DGD	C5D-C6D-O5D-C1E
28	R	101	STE	C13-C14-C15-C16
29	D	408	LMG	C33-C34-C35-C36
24	B	615	CLA	C16-C17-C18-C20
24	a	607	CLA	C16-C17-C18-C19
24	b	611	CLA	C16-C17-C18-C19
29	c	524	LMG	C38-C39-C40-C41
27	a	609	PL9	C45-C44-C46-C47
28	d	409	STE	C1-C2-C3-C4
28	d	409	STE	C7-C8-C9-C10
28	m	102	STE	C2-C3-C4-C5
31	D	409	LHG	C11-C10-C9-C8
31	d	412	LHG	C25-C26-C27-C28
32	H	102	DGD	CCA-CDA-CEA-CFA
24	c	506	CLA	C8-C10-C11-C12
28	R	101	STE	C6-C7-C8-C9
28	J	101	STE	C5-C6-C7-C8
30	A	614	SQD	C32-C33-C34-C35
32	c	521	DGD	C3A-C4A-C5A-C6A
28	A	618	STE	C4-C5-C6-C7
28	m	102	STE	C4-C5-C6-C7
29	D	407	LMG	C34-C35-C36-C37
29	c	523	LMG	C31-C32-C33-C34
30	a	611	SQD	C9-C10-C11-C12
29	c	523	LMG	C10-C11-C12-C13
28	D	412	STE	C12-C13-C14-C15
30	A	614	SQD	C25-C26-C27-C28
29	c	523	LMG	O9-C10-O7-C8
28	E	101	STE	C4-C5-C6-C7
28	M	103	STE	C14-C15-C16-C17
30	b	620	SQD	C29-C30-C31-C32
32	H	102	DGD	C9B-CAB-CBB-CCB
24	d	406	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	F	101	HEM	C4C-C3C-CAC-CBC
24	B	615	CLA	C16-C17-C18-C19
24	b	607	CLA	C16-C17-C18-C19
24	c	503	CLA	C16-C17-C18-C19
28	b	626	STE	C14-C15-C16-C17
28	d	409	STE	C3-C4-C5-C6
29	c	518	LMG	C32-C33-C34-C35
31	d	410	LHG	C14-C15-C16-C17
31	D	411	LHG	C23-C24-C25-C26
32	c	519	DGD	C1B-C2B-C3B-C4B
24	C	505	CLA	C15-C16-C17-C18
24	C	507	CLA	C10-C11-C12-C13
24	C	513	CLA	C13-C15-C16-C17
28	I	102	STE	C5-C6-C7-C8
29	C	516	LMG	C14-C15-C16-C17
32	C	521	DGD	C4B-C5B-C6B-C7B
29	D	407	LMG	O6-C5-C6-O5
29	D	408	LMG	O6-C5-C6-O5
29	c	523	LMG	O7-C8-C9-O8
30	a	610	SQD	O47-C45-C46-O48
29	C	524	LMG	O10-C28-O8-C9
28	b	627	STE	C12-C13-C14-C15
28	d	409	STE	C13-C14-C15-C16
29	C	516	LMG	C11-C12-C13-C14
31	D	409	LHG	C12-C13-C14-C15
31	e	103	LHG	C11-C10-C9-C8
32	A	617	DGD	CAA-CBA-CCA-CDA
32	c	519	DGD	C6B-C7B-C8B-C9B
28	Z	101	STE	C9-C10-C11-C12
28	h	103	STE	C11-C12-C13-C14
31	D	409	LHG	C30-C31-C32-C33
28	C	519	STE	C6-C7-C8-C9
28	c	517	STE	C11-C10-C9-C8
29	C	524	LMG	C32-C33-C34-C35
30	a	610	SQD	C16-C17-C18-C19
29	d	414	LMG	O6-C5-C6-O5
24	b	607	CLA	C10-C11-C12-C13
28	X	101	STE	C3-C4-C5-C6
29	c	518	LMG	C30-C31-C32-C33
29	o	301	LMG	C38-C39-C40-C41
31	d	410	LHG	C32-C33-C34-C35
32	C	522	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
24	A	608	CLA	C4-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
28	B	624	STE	C11-C10-C9-C8
28	b	622	STE	C3-C4-C5-C6
28	d	413	STE	C9-C10-C11-C12
32	A	617	DGD	CCA-CDA-CEA-CFA
24	c	503	CLA	CBD-CGD-O2D-CED
28	l	102	STE	C6-C7-C8-C9
28	b	624	STE	C9-C10-C11-C12
31	A	615	LHG	C24-C25-C26-C27
24	C	510	CLA	C13-C15-C16-C17
31	l	101	LHG	C7-C8-C9-C10
29	D	407	LMG	C32-C33-C34-C35
32	H	102	DGD	C6B-C7B-C8B-C9B
28	I	102	STE	C2-C3-C4-C5
28	e	101	STE	C13-C14-C15-C16
32	c	519	DGD	O6E-C5E-C6E-O5E
29	c	523	LMG	C41-C42-C43-C44
32	c	520	DGD	CAB-CBB-CCB-CDB
24	C	503	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
24	B	614	CLA	C8-C10-C11-C12
28	b	622	STE	C9-C10-C11-C12
29	c	524	LMG	C18-C19-C20-C21
32	C	521	DGD	O6E-C5E-C6E-O5E
29	c	522	LMG	O9-C10-O7-C8
32	h	102	DGD	CAB-CBB-CCB-CDB
24	B	604	CLA	C11-C10-C8-C7
24	B	607	CLA	C11-C10-C8-C7
24	B	615	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C15
24	b	606	CLA	C6-C7-C8-C10
24	b	611	CLA	C11-C12-C13-C15
24	b	612	CLA	C12-C13-C15-C16
24	b	613	CLA	C11-C12-C13-C15
24	c	505	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C12-C13-C15
24	c	512	CLA	C6-C7-C8-C10
24	d	405	CLA	C6-C7-C8-C10
24	d	406	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	C	506	CLA	O1D-CGD-O2D-CED
24	c	513	CLA	CBA-CGA-O2A-C1
24	B	603	CLA	C15-C16-C17-C18
32	C	523	DGD	C4B-C5B-C6B-C7B
32	h	102	DGD	CCB-CDB-CEB-CFB
27	D	406	PL9	C43-C44-C46-C47
27	D	406	PL9	C47-C48-C49-C50
28	M	103	STE	C11-C12-C13-C14
32	c	519	DGD	C9A-CAA-CBA-CCA
29	c	523	LMG	O6-C5-C6-O5
29	b	623	LMG	C16-C17-C18-C19
30	b	620	SQD	C28-C29-C30-C31
32	h	102	DGD	C3B-C4B-C5B-C6B
24	B	612	CLA	C10-C11-C12-C13
29	c	524	LMG	C11-C10-O7-C8
29	o	301	LMG	C11-C10-O7-C8
24	B	601	CLA	C11-C12-C13-C14
24	B	604	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C14-C13-C15-C16
24	a	607	CLA	C14-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C9
24	b	612	CLA	C14-C13-C15-C16
24	c	505	CLA	C6-C7-C8-C9
24	c	505	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	c	513	CLA	C14-C13-C15-C16
28	x	101	STE	C3-C4-C5-C6
28	B	625	STE	C2-C3-C4-C5
28	H	103	STE	C7-C8-C9-C10
28	H	103	STE	C11-C10-C9-C8
31	D	411	LHG	C27-C28-C29-C30
32	h	102	DGD	C6A-C7A-C8A-C9A
24	C	512	CLA	C13-C15-C16-C17
27	a	609	PL9	C32-C33-C34-C35
29	B	620	LMG	O6-C5-C6-O5
24	c	501	CLA	O1D-CGD-O2D-CED
29	o	301	LMG	C4-C5-C6-O5
28	E	103	STE	C1-C2-C3-C4
29	b	623	LMG	C10-C11-C12-C13
29	D	407	LMG	O1-C7-C8-C9
29	b	623	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c	523	LMG	C7-C8-C9-O8
31	e	103	LHG	C4-C5-C6-O8
32	A	617	DGD	C1G-C2G-C3G-O3G
28	H	103	STE	C10-C11-C12-C13
28	d	415	STE	C5-C6-C7-C8
28	t	102	STE	C2-C3-C4-C5
29	D	408	LMG	C30-C31-C32-C33
30	b	620	SQD	C16-C17-C18-C19
31	d	412	LHG	C30-C31-C32-C33
29	m	101	LMG	C34-C35-C36-C37
24	C	506	CLA	C10-C11-C12-C13
28	C	527	STE	C14-C15-C16-C17
28	e	105	STE	C3-C4-C5-C6
29	c	524	LMG	C37-C38-C39-C40
32	H	102	DGD	C3B-C4B-C5B-C6B
32	c	519	DGD	C8A-C9A-CAA-CBA
24	c	502	CLA	C16-C17-C18-C20
28	J	101	STE	C2-C3-C4-C5
28	e	105	STE	C7-C8-C9-C10
30	a	610	SQD	C27-C28-C29-C30
31	A	615	LHG	C28-C29-C30-C31
32	c	521	DGD	C8A-C9A-CAA-CBA
30	B	623	SQD	C45-C46-O48-C23
32	c	519	DGD	C4D-C5D-C6D-O5D
28	d	413	STE	C5-C6-C7-C8
30	A	614	SQD	C13-C14-C15-C16
31	D	411	LHG	C25-C26-C27-C28
26	k	102	BCR	C16-C17-C18-C36
28	I	102	STE	C9-C10-C11-C12
28	x	101	STE	C4-C5-C6-C7
31	D	410	LHG	C32-C33-C34-C35
24	C	510	CLA	C4-C3-C5-C6
24	b	614	CLA	C5-C6-C7-C8
24	c	506	CLA	C13-C15-C16-C17
28	B	624	STE	C1-C2-C3-C4
28	M	101	STE	C6-C7-C8-C9
29	m	101	LMG	C37-C38-C39-C40
29	o	301	LMG	C18-C19-C20-C21
24	b	603	CLA	C8-C10-C11-C12
29	c	522	LMG	C36-C37-C38-C39
29	C	524	LMG	C14-C15-C16-C17
30	a	610	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	c	524	LMG	C32-C33-C34-C35
31	A	615	LHG	C24-C23-O8-C6
30	a	611	SQD	C10-C11-C12-C13
32	C	523	DGD	C4A-C5A-C6A-C7A
32	C	523	DGD	O6D-C5D-C6D-O5D
26	c	514	BCR	C10-C11-C12-C13
24	C	506	CLA	C13-C15-C16-C17
28	b	621	STE	C7-C8-C9-C10
28	j	102	STE	C5-C6-C7-C8
28	x	101	STE	C5-C6-C7-C8
29	A	613	LMG	C35-C36-C37-C38
29	c	523	LMG	C36-C37-C38-C39
30	A	616	SQD	C11-C10-C9-C8
30	a	610	SQD	C13-C14-C15-C16
28	X	101	STE	C7-C8-C9-C10
29	C	524	LMG	C16-C17-C18-C19
29	c	518	LMG	C16-C17-C18-C19
29	m	101	LMG	C13-C14-C15-C16
26	C	520	BCR	C11-C10-C9-C8
26	b	619	BCR	C11-C10-C9-C8
26	h	101	BCR	C20-C21-C22-C23
31	D	411	LHG	C24-C25-C26-C27
28	x	101	STE	C7-C8-C9-C10
31	D	411	LHG	C29-C30-C31-C32
32	c	519	DGD	C4B-C5B-C6B-C7B
29	D	408	LMG	C19-C20-C21-C22
31	D	409	LHG	C15-C16-C17-C18
32	C	522	DGD	CAB-CBB-CCB-CDB
27	A	610	PL9	C15-C14-C16-C17
24	C	510	CLA	C2-C3-C5-C6
24	b	611	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
28	t	103	STE	C7-C8-C9-C10
28	b	625	STE	C4-C5-C6-C7
28	z	101	STE	C4-C5-C6-C7
30	a	611	SQD	C25-C26-C27-C28
32	c	519	DGD	CAA-CBA-CCA-CDA
29	c	523	LMG	C16-C17-C18-C19
29	d	414	LMG	C30-C31-C32-C33
32	C	521	DGD	C5B-C6B-C7B-C8B
32	C	523	DGD	CCB-CDB-CEB-CFB
32	c	520	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
24	A	608	CLA	C6-C7-C8-C9
28	h	103	STE	C9-C10-C11-C12
31	d	412	LHG	C9-C10-C11-C12
32	c	521	DGD	CDA-CEA-CFA-CGA
29	B	621	LMG	C30-C31-C32-C33
29	c	524	LMG	C11-C12-C13-C14
31	L	101	LHG	C30-C31-C32-C33
32	C	522	DGD	CCA-CDA-CEA-CFA
32	A	617	DGD	O2G-C2G-C3G-O3G
28	C	519	STE	C9-C10-C11-C12
29	B	620	LMG	C29-C30-C31-C32
31	l	101	LHG	C33-C34-C35-C36
29	m	101	LMG	C22-C23-C24-C25
31	L	101	LHG	C19-C20-C21-C22
30	a	610	SQD	C32-C33-C34-C35
30	b	620	SQD	C18-C19-C20-C21
32	h	102	DGD	CBA-CCA-CDA-CEA
28	D	412	STE	C15-C16-C17-C18
28	c	516	STE	C10-C11-C12-C13
28	c	516	STE	C5-C6-C7-C8
24	b	610	CLA	C4C-C3C-CAC-CBC
32	C	523	DGD	C9A-CAA-CBA-CCA
28	D	412	STE	C10-C11-C12-C13
32	C	521	DGD	C9A-CAA-CBA-CCA
28	M	103	STE	C4-C5-C6-C7
28	b	627	STE	C15-C16-C17-C18
24	C	510	CLA	C15-C16-C17-C18
28	b	627	STE	C13-C14-C15-C16
30	A	614	SQD	C24-C25-C26-C27
32	C	521	DGD	C5A-C6A-C7A-C8A
27	d	408	PL9	C47-C48-C49-C51
28	j	102	STE	C15-C16-C17-C18
30	a	610	SQD	C8-C7-O47-C45
28	b	626	STE	C15-C16-C17-C18
28	c	517	STE	C15-C16-C17-C18
29	B	620	LMG	C17-C18-C19-C20
31	L	101	LHG	C18-C19-C20-C21
29	D	408	LMG	C18-C19-C20-C21
30	b	620	SQD	C7-C8-C9-C10
29	b	623	LMG	C17-C18-C19-C20
28	b	625	STE	C7-C8-C9-C10
24	C	509	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	505	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
27	D	406	PL9	C28-C29-C31-C32
28	b	621	STE	C11-C10-C9-C8
28	x	101	STE	C10-C11-C12-C13
24	b	602	CLA	C13-C15-C16-C17
31	d	411	LHG	C19-C20-C21-C22
28	x	101	STE	C11-C10-C9-C8
32	H	102	DGD	C5A-C6A-C7A-C8A
30	F	102	SQD	C45-C44-O6-C1
31	D	409	LHG	O1-C1-C2-O2
31	d	411	LHG	O1-C1-C2-O2
24	B	607	CLA	C11-C10-C8-C9
24	B	612	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C14
24	C	512	CLA	C11-C12-C13-C14
24	a	606	CLA	C11-C10-C8-C9
24	b	601	CLA	C11-C10-C8-C9
24	b	611	CLA	C11-C12-C13-C14
24	b	613	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	d	405	CLA	C6-C7-C8-C9
24	d	406	CLA	C11-C12-C13-C14
28	R	101	STE	C4-C5-C6-C7
29	c	524	LMG	C35-C36-C37-C38
31	l	101	LHG	C11-C10-C9-C8
32	C	521	DGD	CCA-CDA-CEA-CFA
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
28	R	101	STE	C10-C11-C12-C13
30	B	623	SQD	C9-C10-C11-C12
31	A	615	LHG	C29-C30-C31-C32
31	L	101	LHG	C26-C27-C28-C29
28	E	102	STE	C11-C10-C9-C8
24	b	613	CLA	C15-C16-C17-C18
24	b	616	CLA	C5-C6-C7-C8
29	c	518	LMG	C14-C15-C16-C17
30	f	101	SQD	C2-C1-O6-C44
28	E	102	STE	C11-C12-C13-C14
28	j	101	STE	C5-C6-C7-C8
30	B	623	SQD	C13-C14-C15-C16
31	d	410	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	e	103	LHG	C11-C12-C13-C14
32	C	521	DGD	C3B-C4B-C5B-C6B
31	l	101	LHG	O6-C4-C5-C6
29	B	621	LMG	C19-C20-C21-C22
29	c	522	LMG	C29-C30-C31-C32
24	B	604	CLA	C11-C12-C13-C15
24	B	604	CLA	C12-C13-C15-C16
24	B	611	CLA	C11-C12-C13-C15
24	B	612	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C10-C8-C7
24	a	606	CLA	C11-C10-C8-C7
24	b	601	CLA	C6-C7-C8-C10
24	b	603	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C12-C13-C15
24	c	505	CLA	C6-C7-C8-C10
24	c	506	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
24	C	508	CLA	C15-C16-C17-C18
28	C	528	STE	C5-C6-C7-C8
32	C	522	DGD	CDB-CEB-CFB-CGB
32	c	521	DGD	CAB-CBB-CCB-CDB
32	C	521	DGD	C1B-C2B-C3B-C4B
28	e	104	STE	C10-C11-C12-C13
31	A	615	LHG	C19-C20-C21-C22
32	c	520	DGD	CDA-CEA-CFA-CGA
30	B	623	SQD	C18-C19-C20-C21
30	b	620	SQD	C25-C26-C27-C28
24	B	604	CLA	C13-C15-C16-C17
24	D	404	CLA	C16-C17-C18-C20
31	D	410	LHG	C17-C18-C19-C20
31	l	101	LHG	C35-C36-C37-C38
32	C	523	DGD	CDA-CEA-CFA-CGA
32	C	523	DGD	C5A-C6A-C7A-C8A
30	a	610	SQD	C9-C10-C11-C12
28	C	519	STE	C3-C4-C5-C6
24	c	510	CLA	C4-C3-C5-C6
27	D	406	PL9	C45-C44-C46-C47
24	B	609	CLA	C13-C15-C16-C17
31	A	615	LHG	C35-C36-C37-C38
32	c	520	DGD	CBB-CCB-CDB-CEB
24	c	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	e	103	LHG	C24-C23-O8-C6
26	k	102	BCR	C9-C10-C11-C12
24	C	509	CLA	C16-C17-C18-C20
24	B	601	CLA	C13-C15-C16-C17
32	A	617	DGD	CDA-CEA-CFA-CGA
32	H	102	DGD	CAB-CBB-CCB-CDB
32	c	520	DGD	CBA-CCA-CDA-CEA
24	c	503	CLA	C5-C6-C7-C8
24	C	504	CLA	CBD-CGD-O2D-CED
28	I	101	STE	C5-C6-C7-C8
29	b	623	LMG	C36-C37-C38-C39
29	d	414	LMG	C39-C40-C41-C42
29	m	101	LMG	C30-C31-C32-C33
35	V	201	HEC	C4B-C3B-CAB-CBB
28	b	624	STE	C2-C3-C4-C5
32	c	520	DGD	CCA-CDA-CEA-CFA
29	B	621	LMG	C7-C8-C9-O8
29	C	516	LMG	C7-C8-C9-O8
30	a	610	SQD	C44-C45-C46-O48
31	A	615	LHG	C4-C5-C6-O8
32	A	617	DGD	O1G-C1G-C2G-C3G
28	C	528	STE	C7-C8-C9-C10
28	I	102	STE	C4-C5-C6-C7
29	c	523	LMG	C17-C18-C19-C20
24	d	405	CLA	C16-C17-C18-C20
24	C	512	CLA	C10-C11-C12-C13
28	E	103	STE	C10-C11-C12-C13
31	D	409	LHG	C29-C30-C31-C32
31	L	101	LHG	C11-C10-C9-C8
24	b	611	CLA	C4-C3-C5-C6
27	a	609	PL9	C20-C19-C21-C22
29	m	101	LMG	C28-C29-C30-C31
27	A	610	PL9	C13-C14-C16-C17
30	b	620	SQD	C14-C15-C16-C17
32	C	522	DGD	CBB-CCB-CDB-CEB
28	f	102	STE	C12-C13-C14-C15
24	B	613	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C19
29	c	518	LMG	O9-C10-O7-C8
28	E	102	STE	C7-C8-C9-C10
28	j	102	STE	C3-C4-C5-C6
26	H	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	d	411	LHG	C28-C29-C30-C31
32	H	102	DGD	CBB-CCB-CDB-CEB
32	C	521	DGD	O1G-C1A-C2A-C3A
28	X	101	STE	C4-C5-C6-C7
28	X	101	STE	C11-C10-C9-C8
32	A	617	DGD	C4B-C5B-C6B-C7B
28	b	627	STE	C10-C11-C12-C13
32	h	102	DGD	C9B-CAB-CBB-CCB
24	C	509	CLA	C8-C10-C11-C12
31	A	615	LHG	C11-C12-C13-C14
29	C	516	LMG	C17-C18-C19-C20
28	b	627	STE	C9-C10-C11-C12
31	D	409	LHG	C25-C26-C27-C28
31	l	101	LHG	C29-C30-C31-C32
24	d	405	CLA	C16-C17-C18-C19
24	C	507	CLA	C5-C6-C7-C8
29	B	621	LMG	O7-C8-C9-O8
29	o	301	LMG	O7-C8-C9-O8
32	A	617	DGD	O1G-C1G-C2G-O2G
28	M	102	STE	C3-C4-C5-C6
31	A	615	LHG	C30-C31-C32-C33
31	d	412	LHG	C32-C33-C34-C35
29	c	522	LMG	C4-C5-C6-O5
27	a	609	PL9	C4-C3-C7-C8
31	D	409	LHG	C32-C33-C34-C35
24	b	609	CLA	C4-C3-C5-C6
30	b	620	SQD	C11-C12-C13-C14
32	A	617	DGD	C8A-C9A-CAA-CBA
24	C	505	CLA	C2-C3-C5-C6
24	c	510	CLA	C2-C3-C5-C6
27	a	609	PL9	C43-C44-C46-C47
28	c	516	STE	C6-C7-C8-C9
29	B	621	LMG	C31-C32-C33-C34
29	c	523	LMG	C14-C15-C16-C17
24	c	503	CLA	O1D-CGD-O2D-CED
28	A	619	STE	C10-C11-C12-C13
30	b	620	SQD	C11-C10-C9-C8
32	h	102	DGD	C7B-C8B-C9B-CAB
24	B	604	CLA	C11-C10-C8-C9
24	B	604	CLA	C14-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C14
24	b	605	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C12-C13-C14
35	v	201	HEC	C2B-C3B-CAB-CBB
26	d	407	BCR	C22-C23-C24-C25
30	F	102	SQD	C33-C34-C35-C36
24	d	406	CLA	C3-C5-C6-C7
28	c	517	STE	C4-C5-C6-C7
29	c	518	LMG	C17-C18-C19-C20
31	D	409	LHG	C34-C35-C36-C37
28	B	624	STE	C2-C3-C4-C5
29	D	408	LMG	C17-C18-C19-C20
32	H	102	DGD	C8A-C9A-CAA-CBA
28	C	527	STE	C5-C6-C7-C8
30	A	614	SQD	C26-C27-C28-C29
28	E	101	STE	C7-C8-C9-C10
29	o	301	LMG	C30-C31-C32-C33
31	D	410	LHG	O1-C1-C2-O2
24	c	509	CLA	CAA-CBA-CGA-O2A
24	B	610	CLA	C16-C17-C18-C19
24	D	404	CLA	C16-C17-C18-C19
24	c	509	CLA	C16-C17-C18-C19
28	I	101	STE	C7-C8-C9-C10
31	d	410	LHG	C16-C17-C18-C19
26	H	101	BCR	C20-C21-C22-C37
26	c	514	BCR	C16-C17-C18-C36
26	k	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C11-C10-C9-C34
28	E	102	STE	C9-C10-C11-C12
32	C	521	DGD	CDA-CEA-CFA-CGA
32	c	520	DGD	CCB-CDB-CEB-CFB
24	c	502	CLA	C16-C17-C18-C19
24	d	406	CLA	C16-C17-C18-C19
30	b	620	SQD	C30-C31-C32-C33
30	f	101	SQD	C33-C34-C35-C36
24	c	513	CLA	C13-C15-C16-C17
26	B	617	BCR	C7-C8-C9-C34
28	l	102	STE	C4-C5-C6-C7
24	A	606	CLA	C12-C13-C15-C16
24	B	613	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	b	602	CLA	C6-C7-C8-C10
24	b	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	C11-C12-C13-C15
24	b	614	CLA	C12-C13-C15-C16
24	d	406	CLA	C12-C13-C15-C16
28	j	101	STE	C1-C2-C3-C4
28	C	527	STE	C11-C10-C9-C8
32	c	519	DGD	C2B-C3B-C4B-C5B
24	B	602	CLA	C8-C10-C11-C12
24	B	616	CLA	C8-C10-C11-C12
26	c	514	BCR	C11-C12-C13-C14
26	c	514	BCR	C17-C18-C19-C20
24	b	607	CLA	CBA-CGA-O2A-C1
28	j	102	STE	C11-C10-C9-C8
29	o	301	LMG	C8-C7-O1-C1
32	c	520	DGD	C2G-C3G-O3G-C1D
32	c	520	DGD	C5D-C6D-O5D-C1E
24	B	613	CLA	C13-C15-C16-C17
30	a	610	SQD	O49-C7-O47-C45
28	C	525	STE	C3-C4-C5-C6
24	C	506	CLA	C4-C3-C5-C6
32	H	102	DGD	O1A-C1A-O1G-C1G
28	M	102	STE	C1-C2-C3-C4
28	z	101	STE	C1-C2-C3-C4
24	c	508	CLA	C15-C16-C17-C18
32	H	102	DGD	C4B-C5B-C6B-C7B
29	D	407	LMG	C39-C40-C41-C42
24	b	615	CLA	C13-C15-C16-C17
30	B	623	SQD	C46-C45-O47-C7
24	b	611	CLA	C16-C17-C18-C20
24	c	505	CLA	C16-C17-C18-C20
29	C	524	LMG	C30-C31-C32-C33
24	a	606	CLA	C15-C16-C17-C18
26	d	407	BCR	C16-C17-C18-C19
31	l	101	LHG	O6-C4-C5-O7
28	M	101	STE	C2-C3-C4-C5
29	c	522	LMG	C38-C39-C40-C41
29	o	301	LMG	O6-C1-O1-C7
32	C	522	DGD	O6D-C1D-O3G-C3G
31	D	411	LHG	C18-C19-C20-C21
29	B	620	LMG	C7-C8-C9-O8
30	A	616	SQD	O6-C44-C45-C46
30	B	623	SQD	O6-C44-C45-C46
30	a	611	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
34	e	102	HEM	C4B-C3B-CAB-CBB
24	b	616	CLA	C11-C12-C13-C14
28	J	101	STE	C7-C8-C9-C10
28	A	618	STE	C14-C15-C16-C17
24	c	512	CLA	C10-C11-C12-C13
32	A	617	DGD	C5A-C6A-C7A-C8A
29	B	620	LMG	O7-C8-C9-O8
29	C	516	LMG	O1-C7-C8-O7
29	C	516	LMG	O7-C8-C9-O8
29	D	407	LMG	O1-C7-C8-O7
29	b	623	LMG	O1-C7-C8-O7
30	A	614	SQD	O6-C44-C45-O47
31	A	615	LHG	O7-C5-C6-O8
32	c	519	DGD	O1G-C1G-C2G-O2G
24	B	607	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	a	605	CLA	C2C-C3C-CAC-CBC
29	m	101	LMG	C12-C13-C14-C15
29	m	101	LMG	C19-C20-C21-C22
29	o	301	LMG	C17-C18-C19-C20
24	b	607	CLA	O1A-CGA-O2A-C1
28	B	626	STE	C3-C4-C5-C6
29	d	414	LMG	C35-C36-C37-C38
30	A	614	SQD	C16-C17-C18-C19
29	A	613	LMG	C39-C40-C41-C42
32	c	521	DGD	C2A-C3A-C4A-C5A
29	B	620	LMG	C28-C29-C30-C31
24	D	404	CLA	O1D-CGD-O2D-CED
28	C	527	STE	C7-C8-C9-C10
29	b	623	LMG	C13-C14-C15-C16
29	c	524	LMG	C36-C37-C38-C39
30	A	614	SQD	C31-C32-C33-C34
24	C	504	CLA	O1D-CGD-O2D-CED
30	B	623	SQD	C24-C25-C26-C27
24	C	502	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C19
24	b	603	CLA	C13-C15-C16-C17
31	D	410	LHG	C2-C3-O3-P
29	B	621	LMG	C34-C35-C36-C37
29	d	414	LMG	C15-C16-C17-C18
30	a	610	SQD	C14-C15-C16-C17
24	A	606	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	Z	101	STE	C11-C10-C9-C8
29	o	301	LMG	C16-C17-C18-C19
29	o	301	LMG	C32-C33-C34-C35
28	b	621	STE	C3-C4-C5-C6
28	I	101	STE	C3-C4-C5-C6
32	c	520	DGD	C5B-C6B-C7B-C8B
24	B	613	CLA	C16-C17-C18-C19
31	D	410	LHG	O9-C7-O7-C5
24	C	508	CLA	O1D-CGD-O2D-CED
26	c	515	BCR	C37-C22-C23-C24
28	d	415	STE	C3-C4-C5-C6
24	b	601	CLA	C4B-C3B-CAB-CBB
31	A	615	LHG	C9-C10-C11-C12
28	j	101	STE	C7-C8-C9-C10
30	a	611	SQD	C18-C19-C20-C21
32	H	102	DGD	CDA-CEA-CFA-CGA
29	D	408	LMG	C38-C39-C40-C41
24	b	610	CLA	C2C-C3C-CAC-CBC
29	b	623	LMG	C19-C20-C21-C22
32	c	519	DGD	O1B-C1B-O2G-C2G
28	t	102	STE	C11-C10-C9-C8
31	l	101	LHG	C15-C16-C17-C18
24	B	601	CLA	C11-C10-C8-C7
24	B	616	CLA	C11-C10-C8-C7
24	C	505	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C12-C13-C15
24	C	509	CLA	C12-C13-C15-C16
24	a	607	CLA	C12-C13-C15-C16
24	b	601	CLA	C12-C13-C15-C16
24	b	604	CLA	C12-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C10
24	b	614	CLA	C11-C10-C8-C7
25	d	402	PHO	C6-C7-C8-C10
28	b	621	STE	C11-C12-C13-C14
32	C	521	DGD	C9B-CAB-CBB-CCB
24	c	511	CLA	C16-C17-C18-C20
28	t	103	STE	C5-C6-C7-C8
29	C	524	LMG	C12-C13-C14-C15
31	A	615	LHG	C32-C33-C34-C35
32	C	521	DGD	C4A-C5A-C6A-C7A
24	D	403	CLA	C2C-C3C-CAC-CBC
28	H	103	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	d	412	LHG	C2-C3-O3-P
24	B	610	CLA	C16-C17-C18-C20
24	b	602	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
29	m	101	LMG	C14-C15-C16-C17
30	f	101	SQD	C27-C28-C29-C30
32	c	520	DGD	C3B-C4B-C5B-C6B
28	C	517	STE	C3-C4-C5-C6
31	D	411	LHG	O9-C7-O7-C5
28	A	618	STE	C2-C3-C4-C5
28	C	515	STE	C3-C4-C5-C6
30	b	620	SQD	C9-C10-C11-C12
32	C	523	DGD	CCA-CDA-CEA-CFA
24	C	513	CLA	C11-C10-C8-C9
24	b	614	CLA	C14-C13-C15-C16
24	d	406	CLA	C14-C13-C15-C16
32	C	521	DGD	O1A-C1A-O1G-C1G
30	a	611	SQD	C32-C33-C34-C35
29	c	524	LMG	C14-C15-C16-C17
31	D	410	LHG	C31-C32-C33-C34
26	d	407	BCR	C13-C14-C15-C16
32	c	520	DGD	C7B-C8B-C9B-CAB
29	o	301	LMG	C33-C34-C35-C36
28	t	103	STE	C2-C3-C4-C5
31	e	103	LHG	C19-C20-C21-C22
31	D	409	LHG	C10-C11-C12-C13
24	c	507	CLA	C13-C15-C16-C17
31	d	411	LHG	C29-C30-C31-C32
29	C	516	LMG	O1-C7-C8-C9
29	o	301	LMG	C7-C8-C9-O8
30	A	614	SQD	O6-C44-C45-C46
32	C	521	DGD	O1G-C1G-C2G-C3G
24	A	608	CLA	C2-C3-C5-C6
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	B	607	CLA	C16-C17-C18-C19
31	A	615	LHG	C33-C34-C35-C36
28	M	103	STE	C15-C16-C17-C18
29	b	623	LMG	C35-C36-C37-C38
29	c	518	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	C	524	LMG	C18-C19-C20-C21
29	c	524	LMG	C31-C32-C33-C34
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
25	d	403	PHO	CHA-CBD-CGD-O1D
25	d	403	PHO	CHA-CBD-CGD-O2D
31	A	615	LHG	C3-O3-P-O4
31	A	615	LHG	C3-O3-P-O6
31	D	411	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	d	411	LHG	C3-O3-P-O5
31	d	411	LHG	C4-O6-P-O5
24	c	508	CLA	O1A-CGA-O2A-C1
28	B	622	STE	C5-C6-C7-C8
28	E	103	STE	C5-C6-C7-C8
25	D	402	PHO	C2C-C3C-CAC-CBC
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	512	CLA	C2B-C3B-CAB-CBB
26	H	101	BCR	C23-C24-C25-C26
28	l	102	STE	C10-C11-C12-C13
24	C	506	CLA	C2-C3-C5-C6
31	A	615	LHG	C34-C35-C36-C37
31	d	410	LHG	C27-C28-C29-C30
24	A	606	CLA	C15-C16-C17-C18
24	a	605	CLA	C15-C16-C17-C18
29	A	613	LMG	C12-C13-C14-C15
32	h	102	DGD	C9A-CAA-CBA-CCA
28	d	409	STE	C11-C12-C13-C14
29	c	524	LMG	C29-C30-C31-C32
29	B	621	LMG	C40-C41-C42-C43
30	f	101	SQD	C32-C33-C34-C35
30	B	623	SQD	C19-C20-C21-C22
28	i	101	STE	C6-C7-C8-C9
28	j	101	STE	C2-C3-C4-C5
31	d	411	LHG	C23-C24-C25-C26
29	A	613	LMG	C15-C16-C17-C18
27	A	610	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C8-C10-C11-C12
29	D	407	LMG	C7-C8-O7-C10
29	o	301	LMG	C7-C8-O7-C10
30	b	620	SQD	C13-C14-C15-C16
24	B	607	CLA	C10-C11-C12-C13
24	b	609	CLA	C2-C3-C5-C6
24	B	603	CLA	C16-C17-C18-C20
24	d	406	CLA	C16-C17-C18-C20
28	A	611	STE	C1-C2-C3-C4
24	A	606	CLA	C14-C13-C15-C16
24	B	601	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	C	508	CLA	C11-C12-C13-C14
24	b	601	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C12-C13-C14
32	c	521	DGD	C8B-C9B-CAB-CBB
24	B	603	CLA	C6-C7-C8-C10
24	B	606	CLA	C6-C7-C8-C10
24	B	613	CLA	C6-C7-C8-C10
26	A	609	BCR	C11-C10-C9-C8
26	D	405	BCR	C11-C10-C9-C8
26	t	101	BCR	C12-C13-C14-C15
31	e	103	LHG	O6-C4-C5-O7
28	H	103	STE	C2-C3-C4-C5
29	B	621	LMG	C21-C22-C23-C24
29	D	407	LMG	C37-C38-C39-C40
30	B	623	SQD	C28-C29-C30-C31
32	c	519	DGD	O1G-C1A-C2A-C3A
30	B	623	SQD	C35-C36-C37-C38
29	B	621	LMG	C15-C16-C17-C18
32	C	521	DGD	CBB-CCB-CDB-CEB
30	A	616	SQD	C2-C1-O6-C44
24	c	510	CLA	C10-C11-C12-C13
27	a	609	PL9	C21-C22-C23-C24
31	l	101	LHG	C24-C25-C26-C27
32	h	102	DGD	C4A-C5A-C6A-C7A
30	a	610	SQD	O6-C44-C45-O47
31	e	103	LHG	O7-C5-C6-O8
32	C	521	DGD	O1G-C1G-C2G-O2G
32	H	102	DGD	O2G-C1B-C2B-C3B
32	h	102	DGD	C3A-C4A-C5A-C6A
24	A	606	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C16-C17-C18-C19
31	l	101	LHG	C8-C7-O7-C5
31	d	410	LHG	C33-C34-C35-C36
28	c	517	STE	C10-C11-C12-C13
25	d	403	PHO	C2C-C3C-CAC-CBC
24	c	505	CLA	C16-C17-C18-C19
28	E	103	STE	C11-C10-C9-C8
28	M	103	STE	C5-C6-C7-C8
32	C	522	DGD	C9A-CAA-CBA-CCA
26	K	101	BCR	C7-C8-C9-C34
26	a	608	BCR	C7-C8-C9-C34
28	I	102	STE	C6-C7-C8-C9
32	h	102	DGD	C6B-C7B-C8B-C9B
24	c	508	CLA	CBA-CGA-O2A-C1
32	A	617	DGD	C4A-C5A-C6A-C7A
31	D	409	LHG	C13-C14-C15-C16
30	A	616	SQD	O5-C1-O6-C44
24	a	605	CLA	C4C-C3C-CAC-CBC
28	c	517	STE	C3-C4-C5-C6
24	B	613	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C6-C7-C8-C9
24	C	505	CLA	C6-C7-C8-C9
24	C	509	CLA	C14-C13-C15-C16
24	b	604	CLA	C14-C13-C15-C16
24	c	508	CLA	C11-C12-C13-C14
28	X	101	STE	C10-C11-C12-C13
32	H	102	DGD	CDB-CEB-CFB-CGB
24	B	603	CLA	C16-C17-C18-C19
29	B	621	LMG	C39-C40-C41-C42
24	B	601	CLA	C4-C3-C5-C6
28	e	104	STE	C13-C14-C15-C16
27	d	408	PL9	C43-C44-C46-C47
32	c	521	DGD	O6D-C5D-C6D-O5D
32	c	521	DGD	CAA-CBA-CCA-CDA
29	m	101	LMG	O10-C28-O8-C9
28	l	102	STE	C1-C2-C3-C4
32	C	522	DGD	C3A-C4A-C5A-C6A
24	C	502	CLA	C16-C17-C18-C19
28	A	611	STE	C2-C3-C4-C5
29	B	621	LMG	C37-C38-C39-C40
32	A	617	DGD	C7B-C8B-C9B-CAB
32	C	521	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
28	b	624	STE	C11-C10-C9-C8
24	a	607	CLA	C11-C10-C8-C7
24	b	609	CLA	C11-C12-C13-C15
24	c	504	CLA	C8-C10-C11-C12
24	a	607	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	C38-C39-C40-C41
24	B	605	CLA	C16-C17-C18-C19
32	H	102	DGD	C8B-C9B-CAB-CBB
31	D	409	LHG	C33-C34-C35-C36
35	v	201	HEC	CAD-CBD-CGD-O1D
26	a	608	BCR	C16-C17-C18-C36
26	c	515	BCR	C16-C17-C18-C36
24	B	607	CLA	C15-C16-C17-C18
30	A	614	SQD	C7-C8-C9-C10
24	d	405	CLA	C2-C1-O2A-CGA
24	c	509	CLA	C13-C15-C16-C17
28	d	413	STE	C10-C11-C12-C13
28	e	104	STE	C14-C15-C16-C17
29	D	408	LMG	C14-C15-C16-C17
31	d	412	LHG	C24-C25-C26-C27
24	B	605	CLA	C16-C17-C18-C20
32	c	519	DGD	O1G-C1G-C2G-C3G
28	A	619	STE	C11-C12-C13-C14
32	C	523	DGD	CAA-CBA-CCA-CDA
24	B	602	CLA	C11-C12-C13-C14
24	B	613	CLA	C6-C7-C8-C9
24	b	614	CLA	C6-C7-C8-C9
31	A	615	LHG	C16-C17-C18-C19
32	h	102	DGD	C1A-C2A-C3A-C4A
32	C	522	DGD	C2B-C3B-C4B-C5B
32	C	521	DGD	CDB-CEB-CFB-CGB
29	A	613	LMG	C9-C8-O7-C10
28	I	101	STE	O1-C1-C2-C3
28	t	102	STE	O1-C1-C2-C3
30	f	101	SQD	C34-C35-C36-C37
24	c	512	CLA	C4-C3-C5-C6
29	c	522	LMG	C17-C18-C19-C20
28	e	105	STE	C4-C5-C6-C7
28	b	622	STE	C6-C7-C8-C9
28	C	518	STE	C2-C3-C4-C5
28	M	101	STE	O1-C1-C2-C3
24	B	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	C	515	STE	C5-C6-C7-C8
24	b	601	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
26	H	101	BCR	C20-C21-C22-C23
34	e	102	HEM	CAD-CBD-CGD-O1D
29	C	524	LMG	C17-C18-C19-C20
29	D	407	LMG	C29-C30-C31-C32
24	B	601	CLA	C2B-C3B-CAB-CBB
24	b	610	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	B	618	BCR	C23-C24-C25-C26
26	B	618	BCR	C23-C24-C25-C30
26	C	520	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C30
32	c	519	DGD	C2B-C1B-O2G-C2G
34	F	101	HEM	CAD-CBD-CGD-O1D
31	D	410	LHG	O10-C23-O8-C6
32	c	519	DGD	O1A-C1A-O1G-C1G
29	b	623	LMG	C11-C12-C13-C14
32	H	102	DGD	C3A-C4A-C5A-C6A
27	a	609	PL9	C25-C24-C26-C27
31	D	410	LHG	C34-C35-C36-C37
31	d	410	LHG	C11-C10-C9-C8
35	v	201	HEC	CAD-CBD-CGD-O2D
28	b	624	STE	C11-C12-C13-C14
24	B	602	CLA	C11-C12-C13-C15
24	C	512	CLA	C12-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C10
24	b	606	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	503	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C12-C13-C15
24	d	406	CLA	C6-C7-C8-C10
24	c	501	CLA	C2A-CAA-CBA-CGA
28	H	103	STE	C12-C13-C14-C15
31	l	101	LHG	C12-C13-C14-C15
28	l	102	STE	C5-C6-C7-C8
29	A	613	LMG	C18-C19-C20-C21
30	a	611	SQD	C30-C31-C32-C33
31	D	409	LHG	C11-C12-C13-C14
28	R	101	STE	C12-C13-C14-C15
28	h	103	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C27-C28-C29-C30
24	B	601	CLA	C2-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
28	t	102	STE	O2-C1-C2-C3
24	b	616	CLA	C11-C12-C13-C15
30	B	623	SQD	C31-C32-C33-C34
31	D	409	LHG	C16-C17-C18-C19
28	B	622	STE	O2-C1-C2-C3
24	C	503	CLA	C8-C10-C11-C12
30	a	611	SQD	C28-C29-C30-C31
29	c	518	LMG	C12-C13-C14-C15
31	l	101	LHG	C10-C11-C12-C13
30	B	623	SQD	C23-C24-C25-C26
28	d	415	STE	C7-C8-C9-C10
24	c	505	CLA	C15-C16-C17-C18
27	a	609	PL9	C15-C14-C16-C17
30	b	620	SQD	C24-C25-C26-C27
30	f	101	SQD	C26-C27-C28-C29
31	l	101	LHG	O10-C23-O8-C6
24	C	513	CLA	C5-C6-C7-C8
32	C	523	DGD	CAB-CBB-CCB-CDB
34	e	102	HEM	CAD-CBD-CGD-O2D
29	c	523	LMG	C15-C16-C17-C18
31	d	411	LHG	C9-C10-C11-C12
31	e	103	LHG	C7-C8-C9-C10
28	B	626	STE	C10-C11-C12-C13
31	d	410	LHG	C12-C13-C14-C15
31	L	101	LHG	C35-C36-C37-C38
30	a	610	SQD	O6-C44-C45-C46
28	b	624	STE	O2-C1-C2-C3
24	C	501	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
32	A	617	DGD	CBA-CCA-CDA-CEA
32	c	519	DGD	CBA-CCA-CDA-CEA
28	M	101	STE	O2-C1-C2-C3
24	B	611	CLA	C15-C16-C17-C18
32	C	521	DGD	O6D-C5D-C6D-O5D
35	V	201	HEC	CAD-CBD-CGD-O2D
35	v	201	HEC	C4B-C3B-CAB-CBB
32	h	102	DGD	O2G-C1B-C2B-C3B
31	e	103	LHG	C13-C14-C15-C16
28	A	618	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	C	522	DGD	C2A-C3A-C4A-C5A
24	D	404	CLA	O1A-CGA-O2A-C1
28	B	622	STE	O1-C1-C2-C3
28	I	101	STE	O2-C1-C2-C3
24	b	610	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C19
25	D	402	PHO	CHA-CBD-CGD-O1D
25	d	402	PHO	CHA-CBD-CGD-O1D
26	d	407	BCR	C11-C10-C9-C34
34	F	101	HEM	CAD-CBD-CGD-O2D
31	e	103	LHG	O6-C4-C5-C6
28	d	415	STE	C4-C5-C6-C7
29	c	523	LMG	C11-C10-O7-C8
28	R	101	STE	C5-C6-C7-C8
28	z	101	STE	C3-C4-C5-C6
29	b	623	LMG	C37-C38-C39-C40
29	B	620	LMG	C35-C36-C37-C38
32	c	521	DGD	C7B-C8B-C9B-CAB
28	f	102	STE	C14-C15-C16-C17
24	b	605	CLA	C11-C12-C13-C14
24	b	606	CLA	C11-C12-C13-C14
24	c	511	CLA	C6-C7-C8-C9
29	c	518	LMG	C33-C34-C35-C36
30	A	616	SQD	C45-C44-O6-C1
32	C	522	DGD	C2G-C3G-O3G-C1D
24	b	614	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	C2-C1-O2A-CGA
24	c	506	CLA	C16-C17-C18-C20
28	e	105	STE	C6-C7-C8-C9
28	x	101	STE	O2-C1-C2-C3
28	B	622	STE	C11-C10-C9-C8
31	d	412	LHG	O1-C1-C2-C3
28	b	624	STE	O1-C1-C2-C3
31	D	409	LHG	C17-C18-C19-C20
25	d	402	PHO	O2A-C1-C2-C3
26	K	102	BCR	C18-C19-C20-C21
28	X	101	STE	C11-C12-C13-C14
28	I	102	STE	C11-C10-C9-C8
31	l	101	LHG	C31-C32-C33-C34
24	C	505	CLA	C8-C10-C11-C12
28	x	101	STE	O1-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	Z	101	STE	C7-C8-C9-C10
28	H	103	STE	C9-C10-C11-C12
24	c	505	CLA	C10-C11-C12-C13
28	R	101	STE	C14-C15-C16-C17
27	A	610	PL9	C19-C21-C22-C23
28	B	622	STE	C2-C3-C4-C5
28	b	624	STE	C3-C4-C5-C6
28	E	103	STE	C6-C7-C8-C9
29	c	524	LMG	C40-C41-C42-C43
28	b	627	STE	C14-C15-C16-C17
28	R	101	STE	C7-C8-C9-C10
29	c	524	LMG	C19-C20-C21-C22
31	d	410	LHG	C34-C35-C36-C37
24	d	406	CLA	C4-C3-C5-C6
27	D	406	PL9	C20-C19-C21-C22
30	b	620	SQD	C27-C28-C29-C30
32	c	520	DGD	C8B-C9B-CAB-CBB
29	d	414	LMG	O7-C10-C11-C12
29	A	613	LMG	O1-C7-C8-O7
28	c	516	STE	C3-C4-C5-C6
24	c	509	CLA	C8-C10-C11-C12
24	B	613	CLA	C14-C13-C15-C16
24	a	607	CLA	C6-C7-C8-C9
24	b	602	CLA	C6-C7-C8-C9
24	b	611	CLA	C14-C13-C15-C16
24	c	503	CLA	C11-C10-C8-C9
25	d	402	PHO	C6-C7-C8-C9
24	a	605	CLA	C16-C17-C18-C19
28	d	415	STE	C11-C10-C9-C8
30	a	611	SQD	C12-C13-C14-C15
29	D	408	LMG	O7-C10-C11-C12
26	b	619	BCR	C11-C12-C13-C14
29	c	522	LMG	O7-C10-C11-C12
24	A	612	CLA	C11-C12-C13-C15
24	B	603	CLA	C11-C10-C8-C7
24	B	615	CLA	C11-C10-C8-C7
24	D	404	CLA	C12-C13-C15-C16
24	b	605	CLA	C11-C12-C13-C15
24	c	511	CLA	C6-C7-C8-C10
24	c	512	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C10-C8-C7
24	b	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	o	301	LMG	C15-C16-C17-C18
24	B	602	CLA	C2B-C3B-CAB-CBB
24	B	603	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	b	601	CLA	C2B-C3B-CAB-CBB
26	C	520	BCR	C23-C24-C25-C26
26	K	102	BCR	C23-C24-C25-C30
26	b	617	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
31	d	411	LHG	O9-C7-O7-C5
28	E	103	STE	C11-C12-C13-C14
24	C	506	CLA	C2-C1-O2A-CGA
31	l	101	LHG	C26-C27-C28-C29
28	E	101	STE	C6-C7-C8-C9
32	c	519	DGD	O6E-C1E-O5D-C6D
24	B	605	CLA	C5-C6-C7-C8
31	D	411	LHG	C11-C10-C9-C8
29	o	301	LMG	O7-C10-C11-C12
32	c	519	DGD	O2G-C1B-C2B-C3B
27	a	609	PL9	C18-C19-C21-C22
27	d	408	PL9	C28-C29-C31-C32
24	b	609	CLA	O1D-CGD-O2D-CED
30	a	611	SQD	C8-C7-O47-C45
29	D	408	LMG	O10-C28-O8-C9
30	B	623	SQD	C25-C26-C27-C28
31	d	411	LHG	C11-C12-C13-C14
24	A	606	CLA	C8-C10-C11-C12
24	c	506	CLA	C15-C16-C17-C18
32	C	522	DGD	CDA-CEA-CFA-CGA
24	a	607	CLA	CBA-CGA-O2A-C1
27	A	610	PL9	C42-C43-C44-C46
32	c	521	DGD	C9B-CAB-CBB-CCB
28	c	517	STE	C6-C7-C8-C9
32	H	102	DGD	C4E-C5E-C6E-O5E
28	d	409	STE	O1-C1-C2-C3
34	e	102	HEM	CAA-CBA-CGA-O2A
31	d	410	LHG	C35-C36-C37-C38
24	A	612	CLA	C11-C12-C13-C14
24	B	603	CLA	C11-C10-C8-C9
24	C	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	b	601	CLA	C14-C13-C15-C16
24	b	614	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C10-C8-C9
24	B	612	CLA	CAA-CBA-CGA-O2A
29	C	524	LMG	O1-C7-C8-C9
32	c	519	DGD	C1G-C2G-C3G-O3G
31	d	411	LHG	C34-C35-C36-C37
24	B	601	CLA	C4B-C3B-CAB-CBB
24	B	602	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	c	510	CLA	CAA-CBA-CGA-O2A
34	e	102	HEM	CAA-CBA-CGA-O1A
30	a	611	SQD	O49-C7-O47-C45
29	B	620	LMG	C8-C9-O8-C28
28	B	626	STE	C6-C7-C8-C9
31	D	410	LHG	C10-C11-C12-C13
30	a	611	SQD	C2-C1-O6-C44
31	L	101	LHG	O10-C23-O8-C6
31	L	101	LHG	C14-C15-C16-C17
30	A	614	SQD	C17-C18-C19-C20
28	b	622	STE	C14-C15-C16-C17
28	d	409	STE	O2-C1-C2-C3
24	B	612	CLA	C8-C10-C11-C12
27	D	406	PL9	C15-C14-C16-C17
24	D	403	CLA	C2-C1-O2A-CGA
24	B	608	CLA	C11-C12-C13-C15
24	B	613	CLA	C11-C12-C13-C15
24	C	510	CLA	C11-C10-C8-C7
24	b	604	CLA	C11-C10-C8-C7
30	f	101	SQD	C25-C26-C27-C28
28	I	102	STE	O1-C1-C2-C3
28	I	102	STE	O2-C1-C2-C3
24	A	612	CLA	C16-C17-C18-C19
24	a	605	CLA	C16-C17-C18-C20
29	o	301	LMG	C9-C8-O7-C10
29	m	101	LMG	C36-C37-C38-C39
24	b	603	CLA	C2A-CAA-CBA-CGA
31	d	411	LHG	C35-C36-C37-C38
29	D	407	LMG	C14-C15-C16-C17
27	A	610	PL9	C21-C22-C23-C24
31	L	101	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	C3A-C2A-CAA-CBA
24	C	512	CLA	C3A-C2A-CAA-CBA
25	d	403	PHO	C3A-C2A-CAA-CBA
30	A	616	SQD	O48-C23-C24-C25
32	C	521	DGD	O2G-C1B-C2B-C3B
28	C	526	STE	C12-C13-C14-C15
24	c	509	CLA	CAA-CBA-CGA-O1A
24	D	404	CLA	CBA-CGA-O2A-C1
28	J	101	STE	C4-C5-C6-C7
24	B	610	CLA	C8-C10-C11-C12
30	a	610	SQD	C31-C32-C33-C34
24	b	613	CLA	CAA-CBA-CGA-O2A
28	A	611	STE	C4-C5-C6-C7
27	d	408	PL9	C36-C37-C38-C39
24	b	602	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	C2A-CAA-CBA-CGA
24	C	503	CLA	C6-C7-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	D	404	CLA	C6-C7-C8-C9
24	b	612	CLA	C11-C10-C8-C9
24	c	505	CLA	C11-C12-C13-C14
28	E	103	STE	C2-C3-C4-C5
32	c	519	DGD	O1B-C1B-C2B-C3B
28	z	101	STE	C5-C6-C7-C8
24	C	506	CLA	C5-C6-C7-C8
27	A	610	PL9	C40-C39-C41-C42
27	d	408	PL9	C15-C14-C16-C17
30	A	616	SQD	O5-C5-C6-S
29	B	621	LMG	C22-C23-C24-C25
32	c	520	DGD	O1B-C1B-C2B-C3B
32	c	521	DGD	O1A-C1A-C2A-C3A
32	C	521	DGD	CBA-CCA-CDA-CEA
28	b	621	STE	C10-C11-C12-C13
30	B	623	SQD	C10-C11-C12-C13
28	i	102	STE	C9-C10-C11-C12
29	B	620	LMG	O7-C10-C11-C12
31	L	101	LHG	O7-C7-C8-C9
24	B	612	CLA	CAA-CBA-CGA-O1A
24	c	510	CLA	CAA-CBA-CGA-O1A
29	c	518	LMG	O9-C10-C11-C12
31	D	410	LHG	O10-C23-C24-C25
28	j	102	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	l	102	STE	C2-C3-C4-C5
29	B	621	LMG	C8-C7-O1-C1
29	m	101	LMG	C8-C7-O1-C1
30	a	610	SQD	C45-C44-O6-C1
32	C	521	DGD	C5D-C6D-O5D-C1E
29	m	101	LMG	C38-C39-C40-C41
29	C	524	LMG	C40-C41-C42-C43
30	A	616	SQD	O47-C7-C8-C9
29	c	522	LMG	O1-C7-C8-C9
31	L	101	LHG	C33-C34-C35-C36
29	c	522	LMG	O9-C10-C11-C12
30	A	616	SQD	O10-C23-C24-C25
24	b	601	CLA	C13-C15-C16-C17
28	A	619	STE	C15-C16-C17-C18
31	d	412	LHG	O10-C23-C24-C25
24	B	608	CLA	C16-C17-C18-C19
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	612	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
25	A	607	PHO	CAD-CBD-CGD-O2D
31	l	101	LHG	C16-C17-C18-C19
30	B	623	SQD	O48-C23-C24-C25
31	D	411	LHG	C32-C33-C34-C35
24	B	613	CLA	C5-C6-C7-C8
28	l	102	STE	C7-C8-C9-C10
24	b	601	CLA	CAA-CBA-CGA-O2A
24	A	606	CLA	C16-C17-C18-C19
24	B	603	CLA	C2A-CAA-CBA-CGA
29	B	620	LMG	O9-C10-C11-C12
24	c	505	CLA	C13-C15-C16-C17
29	c	518	LMG	O8-C28-C29-C30
28	A	619	STE	C13-C14-C15-C16
28	B	625	STE	O2-C1-C2-C3
28	C	515	STE	O2-C1-C2-C3
31	L	101	LHG	O9-C7-C8-C9
28	c	517	STE	C11-C12-C13-C14

There are no ring outliers.

110 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	l	102	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	511	CLA	1	0
24	b	614	CLA	2	0
24	b	609	CLA	1	0
28	b	621	STE	1	0
24	c	511	CLA	2	0
24	d	406	CLA	1	0
24	B	601	CLA	2	0
26	b	619	BCR	1	0
24	C	501	CLA	1	0
28	e	105	STE	1	0
28	E	103	STE	1	0
24	C	510	CLA	1	0
24	C	508	CLA	1	0
32	A	617	DGD	2	0
24	B	604	CLA	1	0
31	D	411	LHG	1	0
35	v	201	HEC	1	0
25	D	402	PHO	2	0
26	c	515	BCR	3	0
24	B	607	CLA	1	0
24	C	509	CLA	3	0
24	A	605	CLA	2	0
26	C	520	BCR	1	0
24	C	505	CLA	1	0
28	t	102	STE	2	0
29	o	301	LMG	1	0
24	c	509	CLA	1	0
24	d	404	CLA	2	0
28	B	622	STE	1	0
26	h	101	BCR	1	0
30	A	616	SQD	1	0
24	b	605	CLA	2	0
29	m	101	LMG	1	0
24	b	607	CLA	2	0
29	D	407	LMG	1	0
28	C	526	STE	2	0
26	K	102	BCR	4	0
24	a	607	CLA	1	0
27	A	610	PL9	1	0
24	b	604	CLA	3	0
27	D	406	PL9	1	0
29	B	620	LMG	2	0

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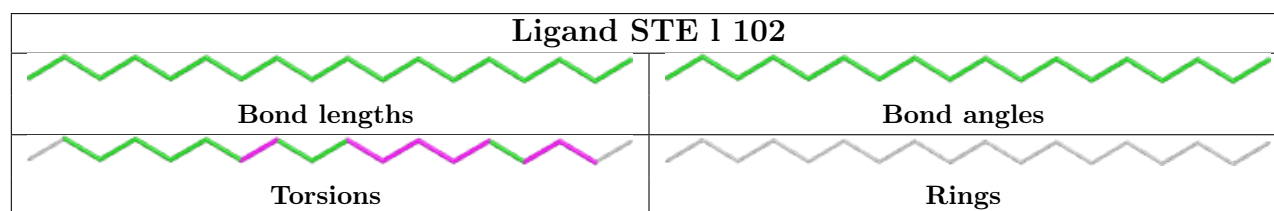
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	612	CLA	1	0
26	t	101	BCR	3	0
32	C	521	DGD	1	0
26	K	101	BCR	4	0
24	C	502	CLA	1	0
24	A	612	CLA	1	0
29	C	516	LMG	1	0
26	A	609	BCR	2	0
28	i	101	STE	1	0
24	B	608	CLA	1	0
26	D	405	BCR	5	0
24	c	512	CLA	1	0
24	B	613	CLA	1	0
26	T	101	BCR	5	0
31	D	409	LHG	1	0
26	c	514	BCR	3	0
26	d	407	BCR	1	0
31	A	615	LHG	2	0
24	a	605	CLA	1	0
29	d	414	LMG	1	0
29	c	518	LMG	2	0
30	B	623	SQD	1	0
27	a	609	PL9	1	0
24	c	513	CLA	2	0
24	C	512	CLA	4	0
30	a	611	SQD	2	0
34	e	102	HEM	4	0
24	b	610	CLA	2	0
28	x	101	STE	2	0
24	b	602	CLA	2	0
26	k	102	BCR	1	0
24	B	614	CLA	1	0
26	H	101	BCR	2	0
26	B	618	BCR	2	0
24	B	602	CLA	1	0
24	c	507	CLA	2	0
24	b	613	CLA	9	0
28	b	627	STE	1	0
31	e	103	LHG	2	0
24	c	508	CLA	1	0
28	X	101	STE	1	0
31	d	410	LHG	8	0

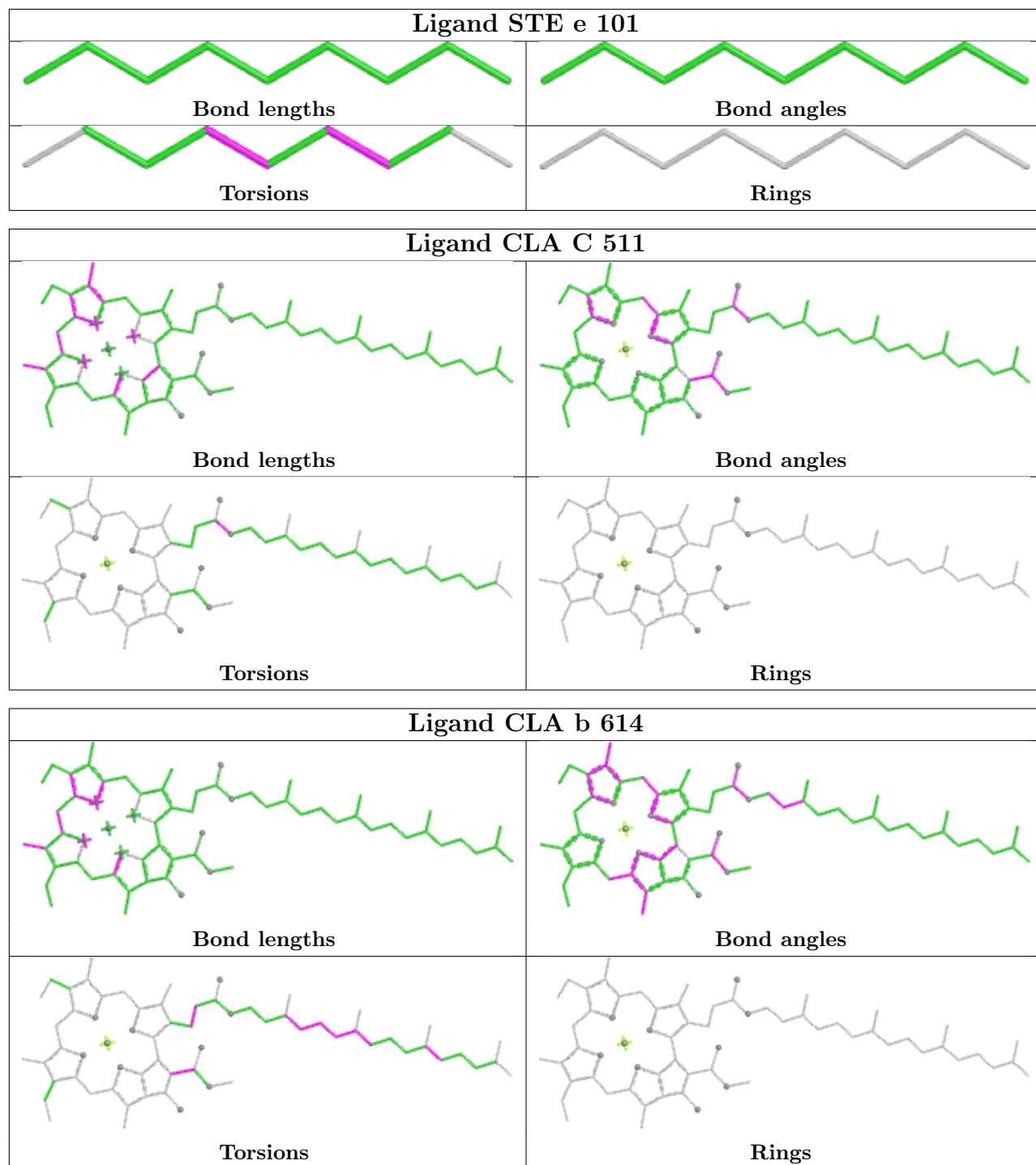
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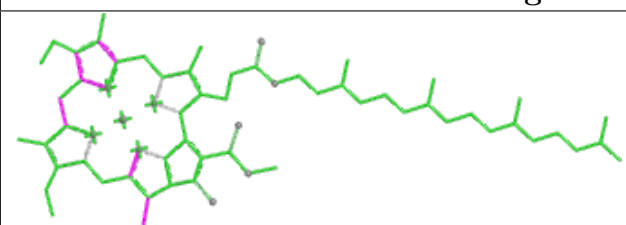
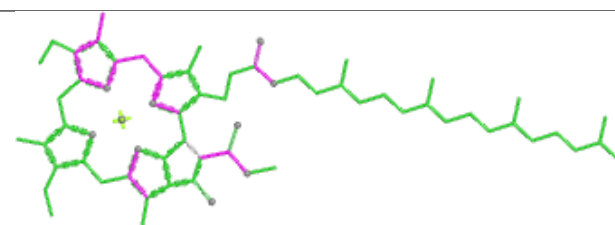
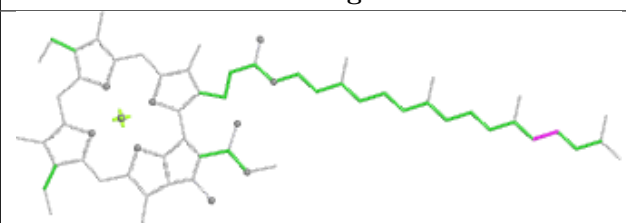
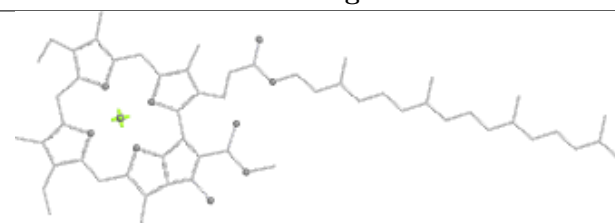
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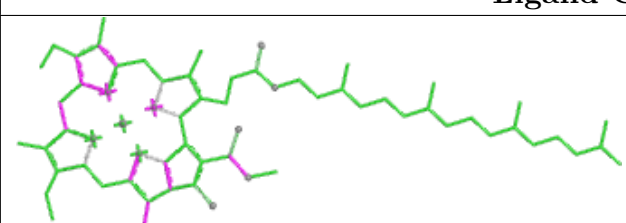
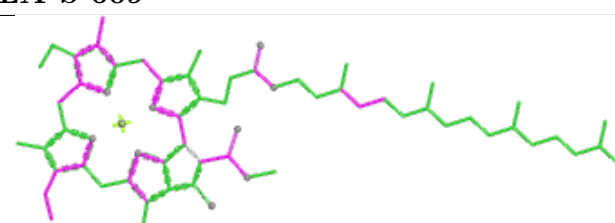
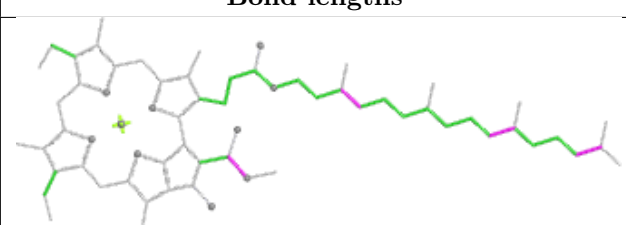
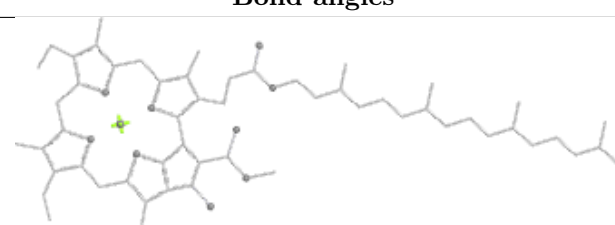
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	413	STE	2	0
32	c	521	DGD	1	0
24	B	609	CLA	1	0
24	A	608	CLA	1	0
28	A	611	STE	1	0
24	C	513	CLA	4	0
34	F	101	HEM	2	0
28	c	517	STE	1	0
24	B	603	CLA	1	0
26	B	619	BCR	4	0
24	D	404	CLA	1	0
29	b	623	LMG	1	0
30	a	610	SQD	1	0
28	R	101	STE	4	0
30	b	620	SQD	1	0
24	c	501	CLA	3	0
26	b	618	BCR	5	0
28	d	409	STE	1	0
30	f	101	SQD	1	0
24	b	603	CLA	1	0
24	C	506	CLA	2	0
26	k	101	BCR	2	0
24	B	606	CLA	3	0
24	B	605	CLA	4	0
24	c	504	CLA	1	0

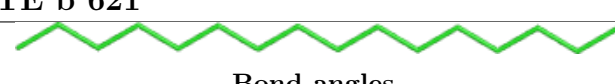
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



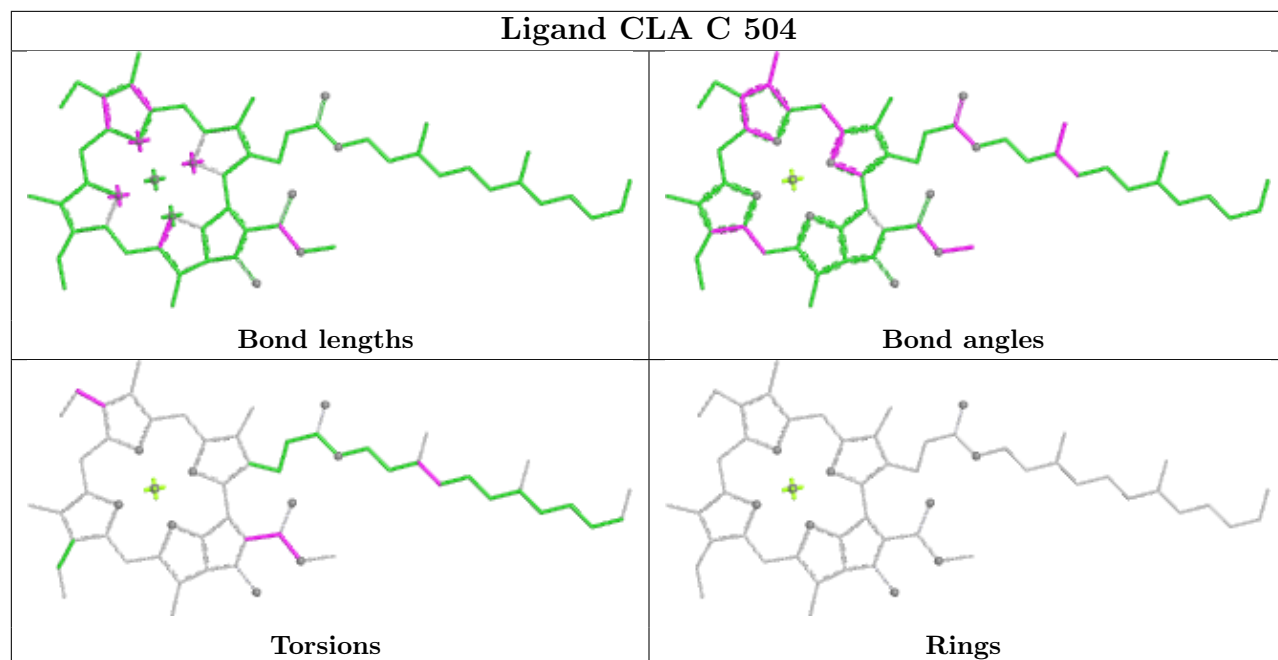


Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

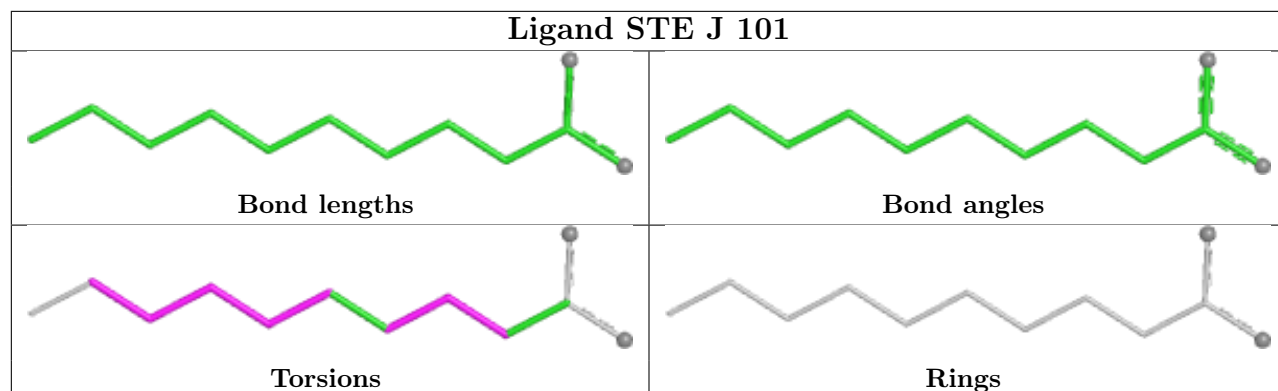
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

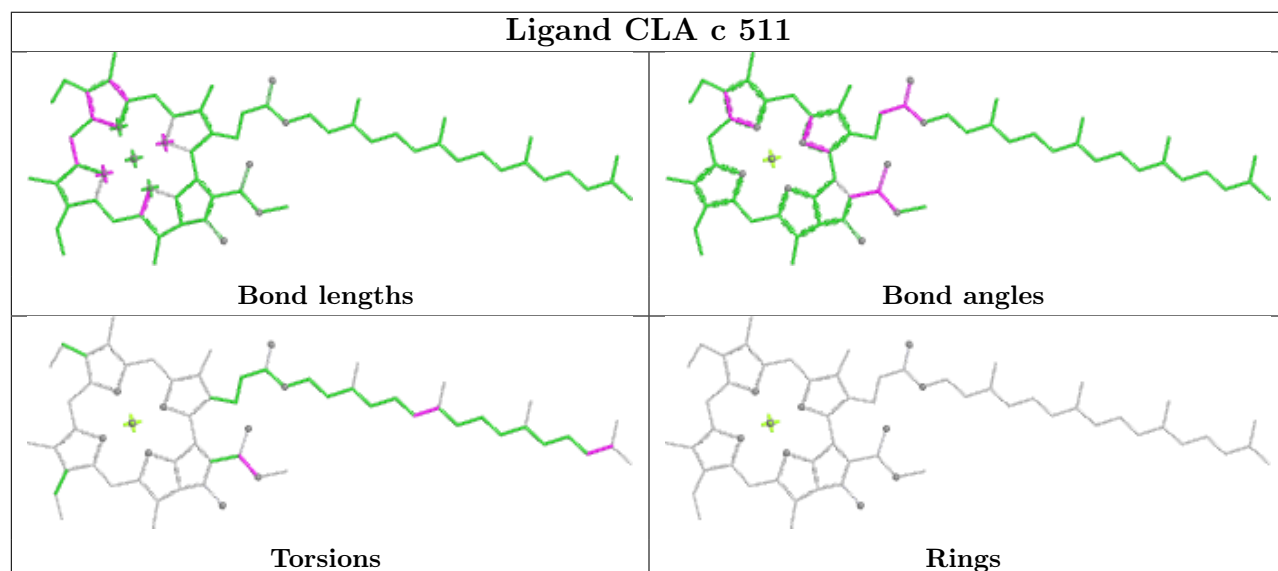
Ligand CLA C 504



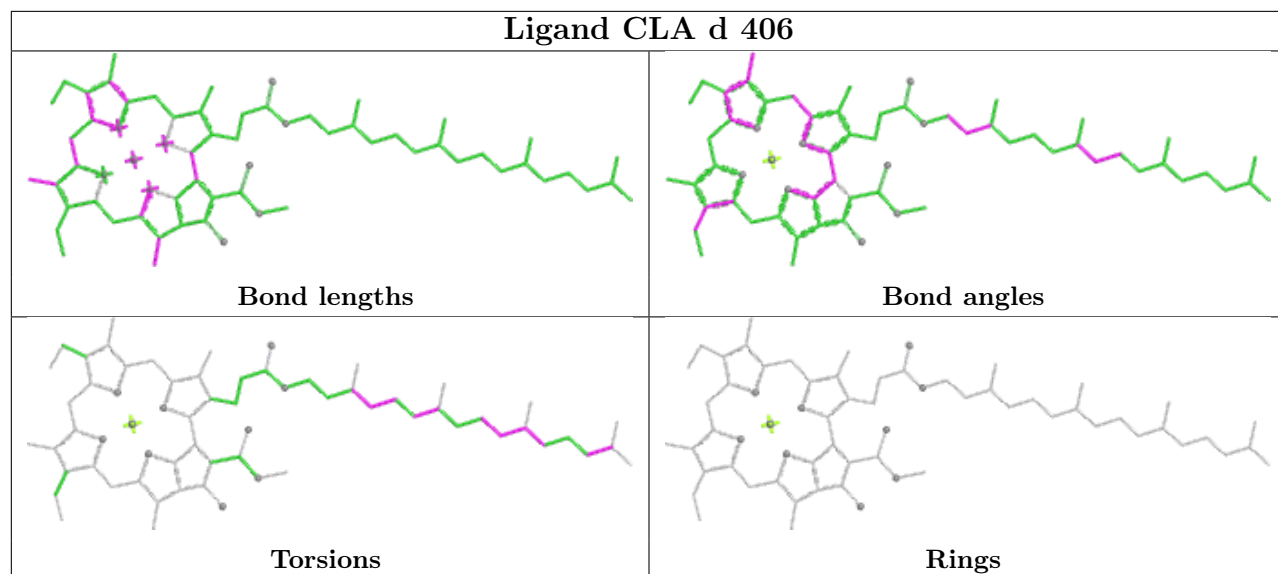
Ligand STE J 101



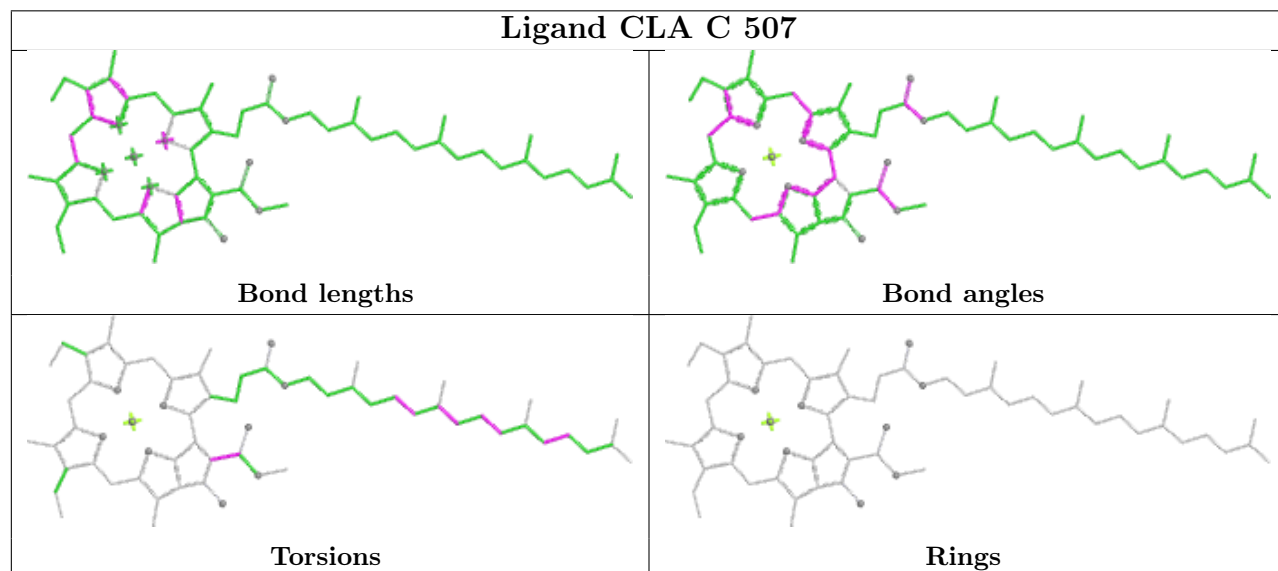
Ligand CLA c 511



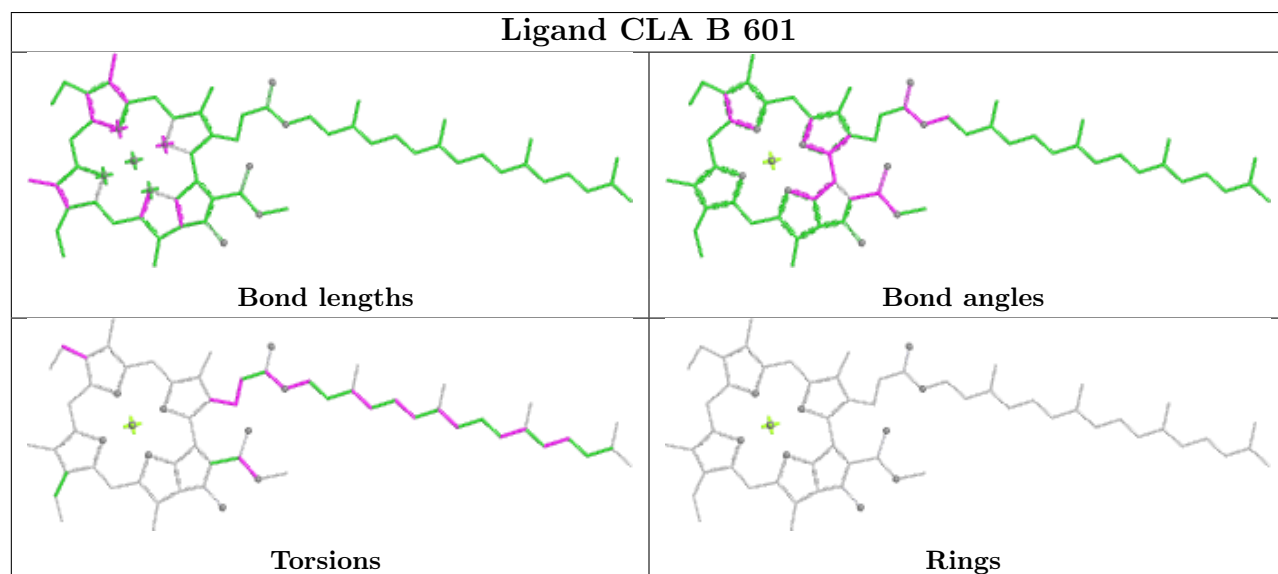
Ligand CLA d 406

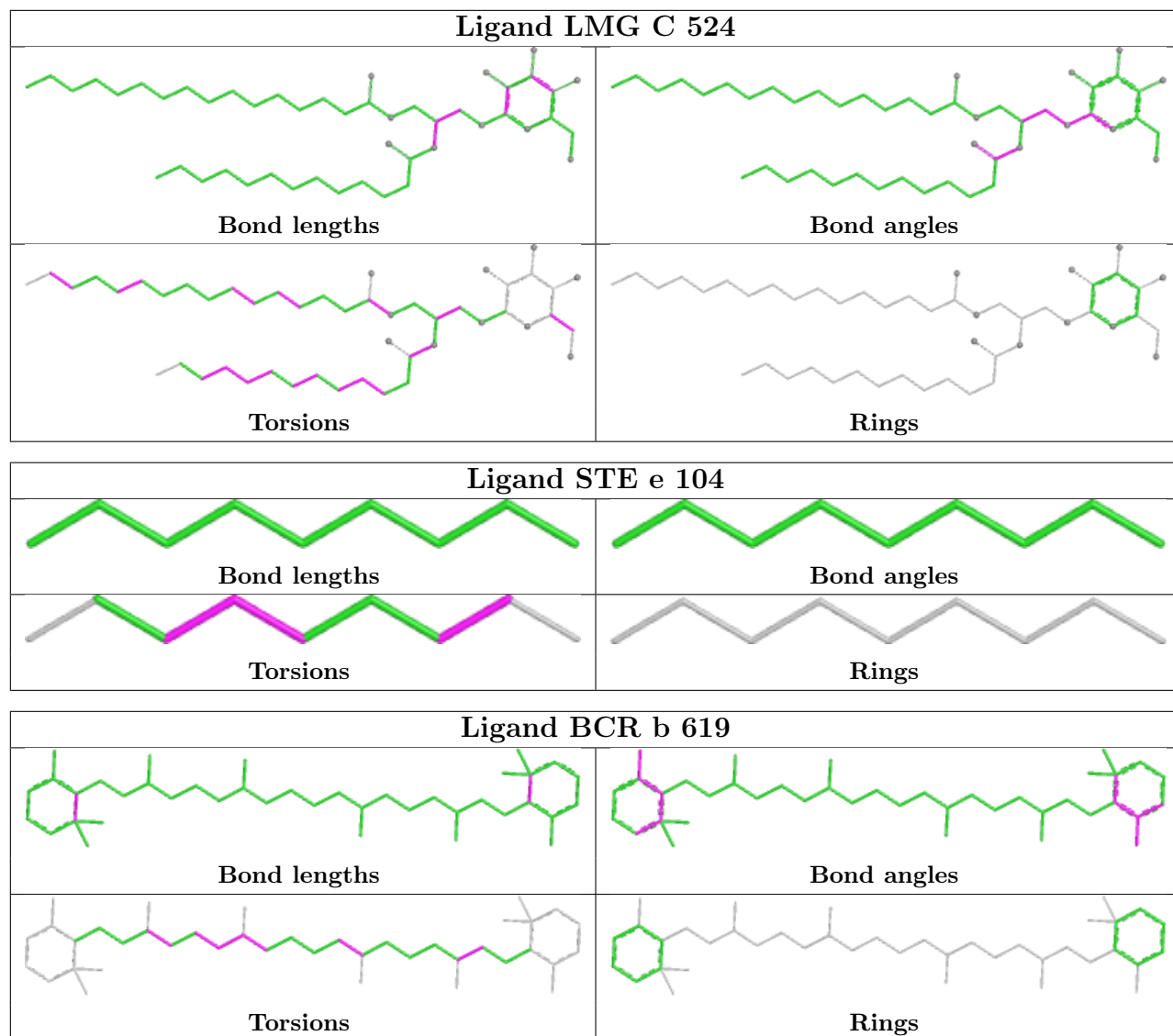


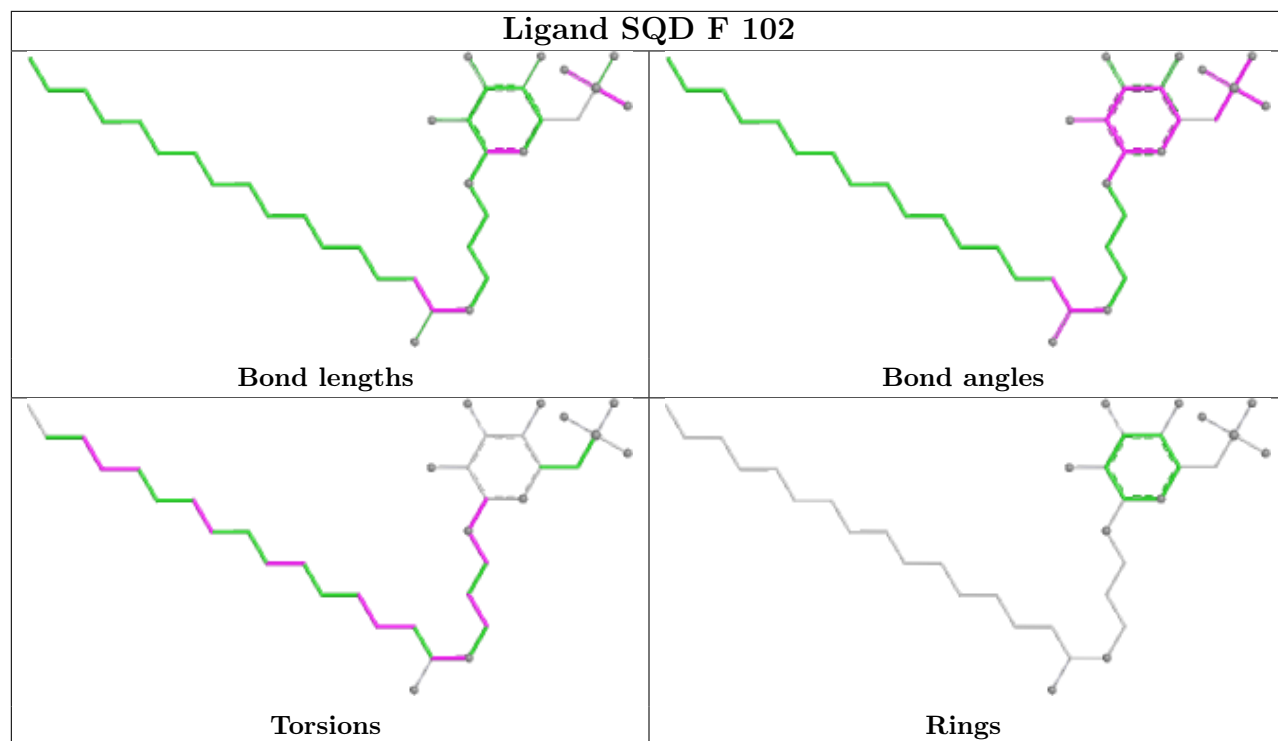
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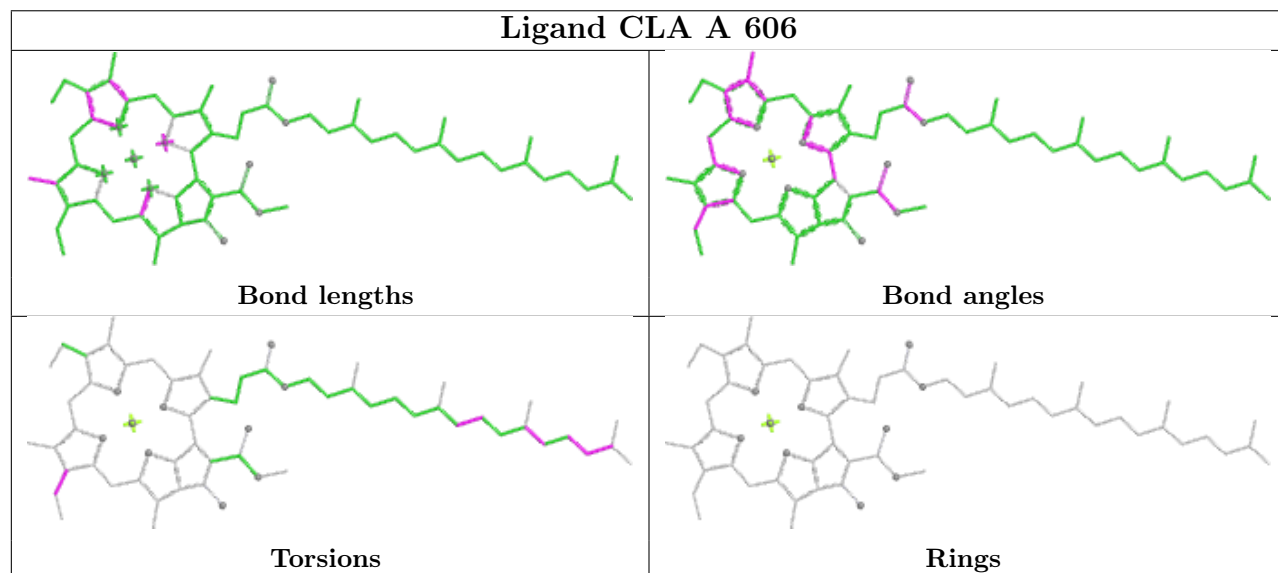
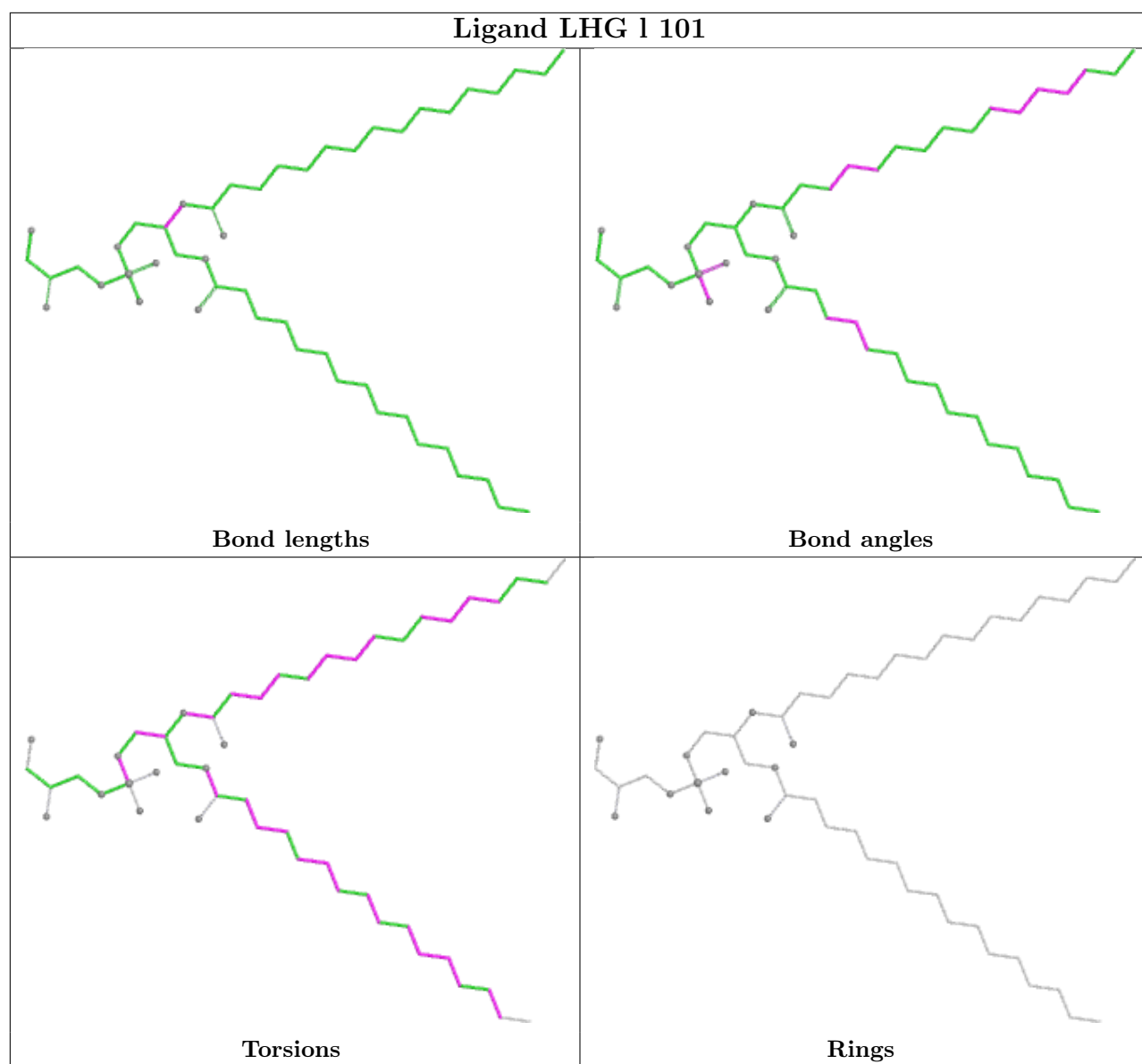


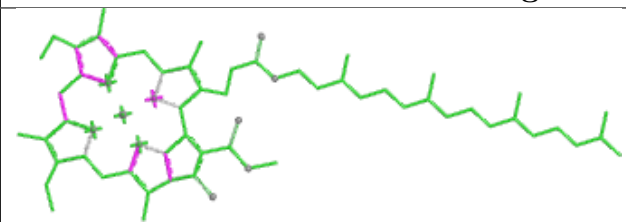
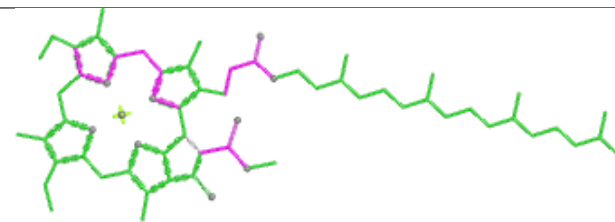
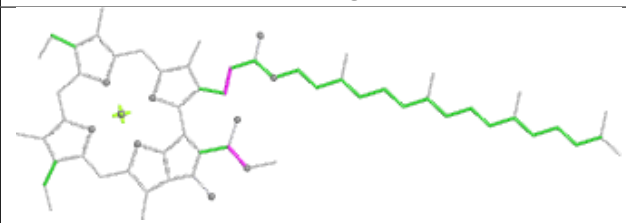
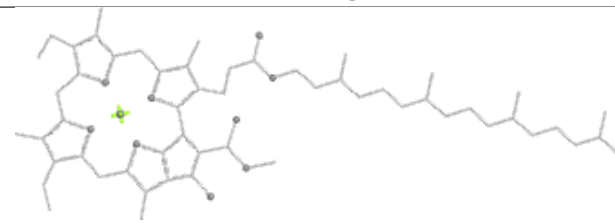
Ligand CLA B 601

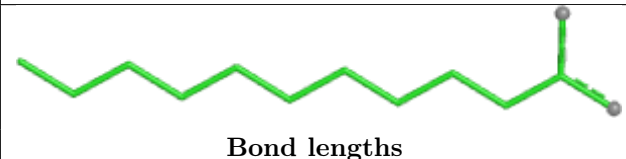
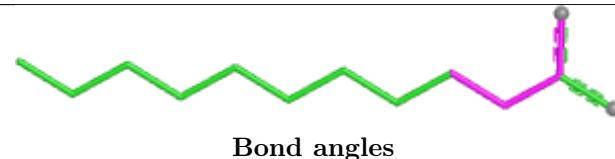
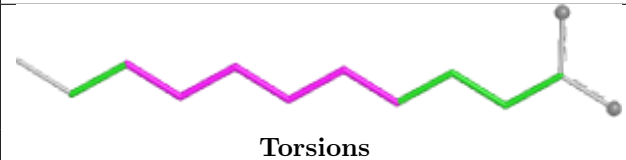
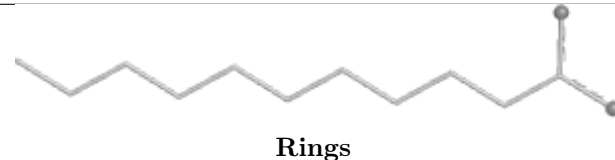


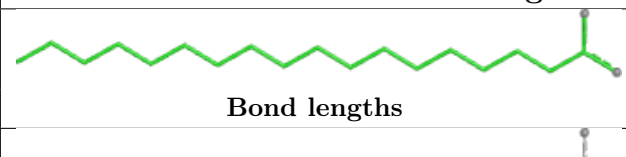
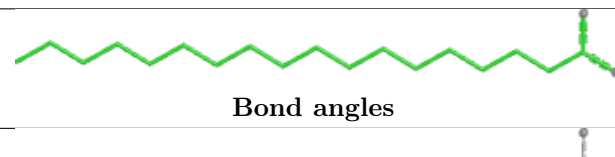




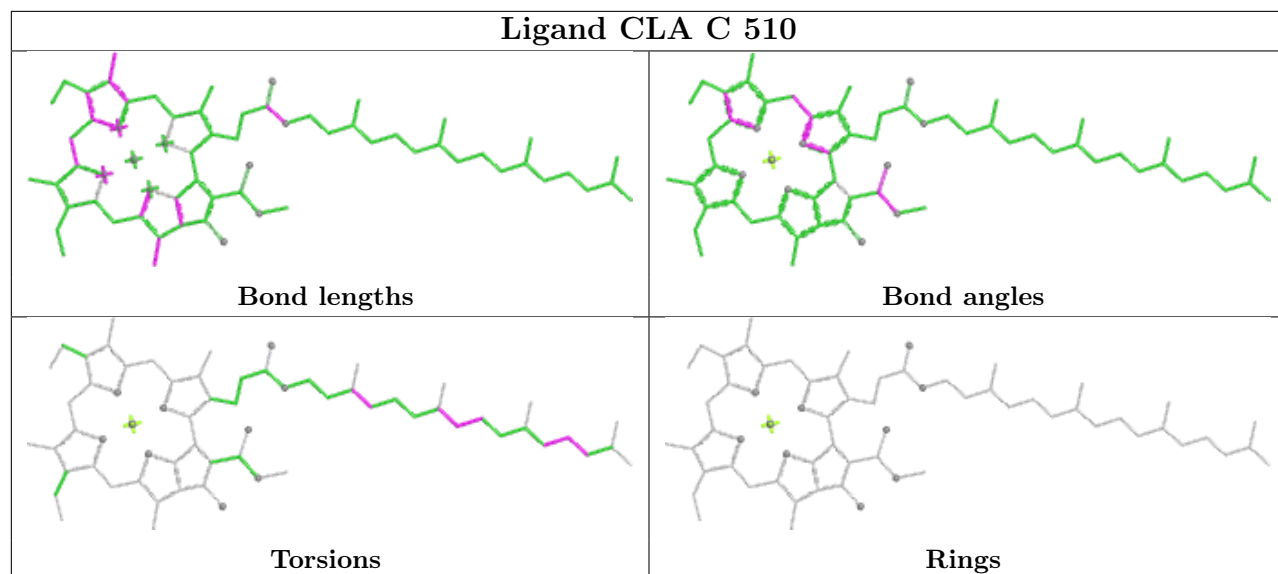


Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

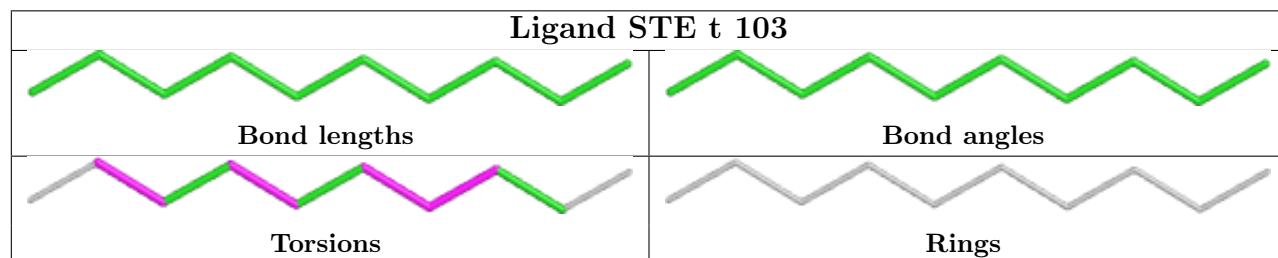
Ligand STE e 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

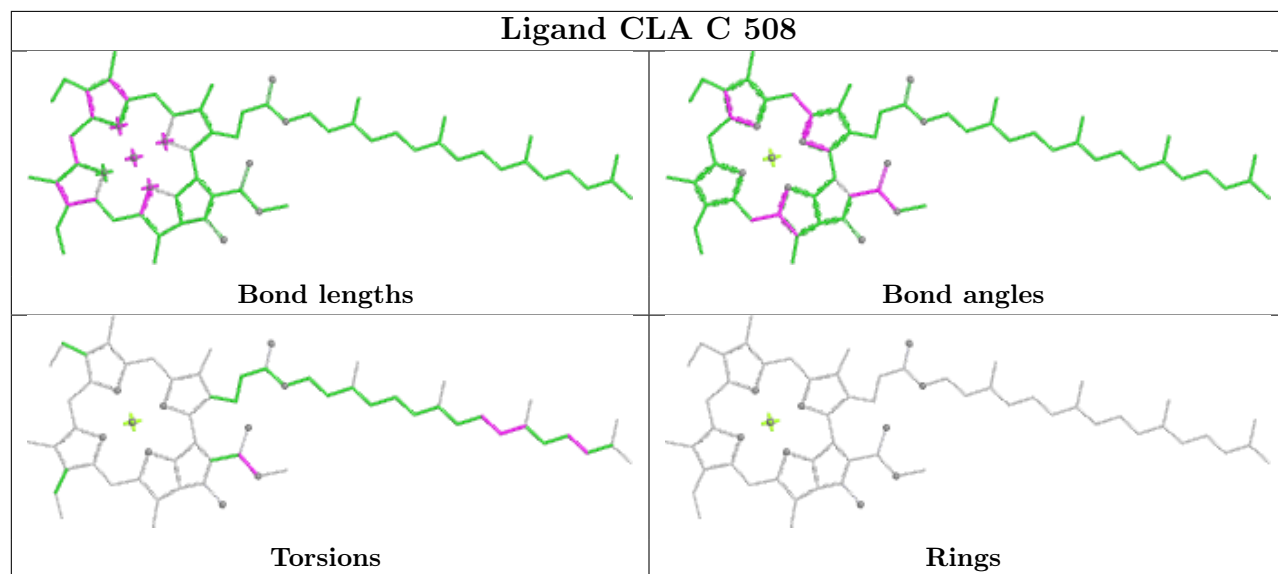
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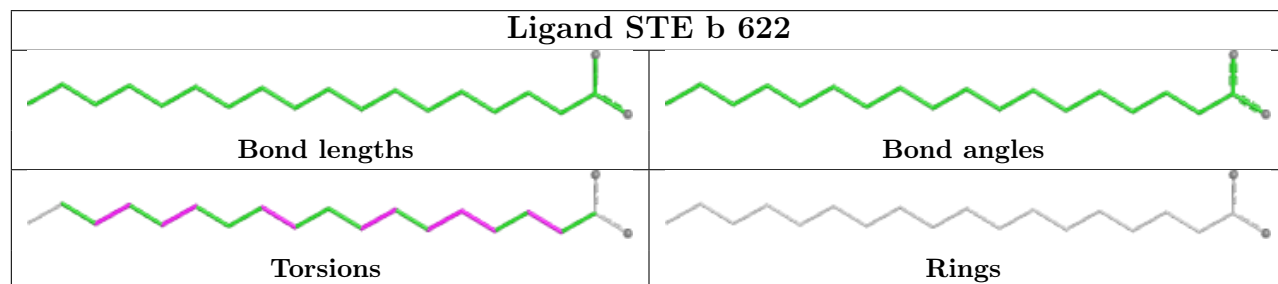
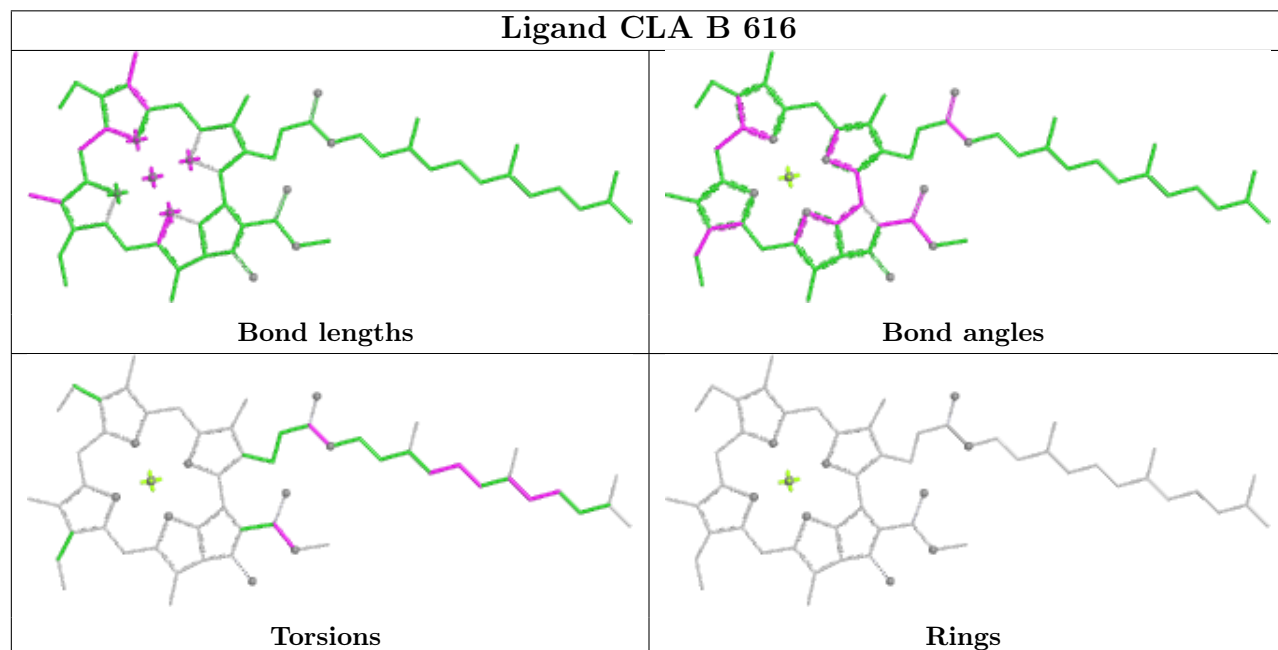
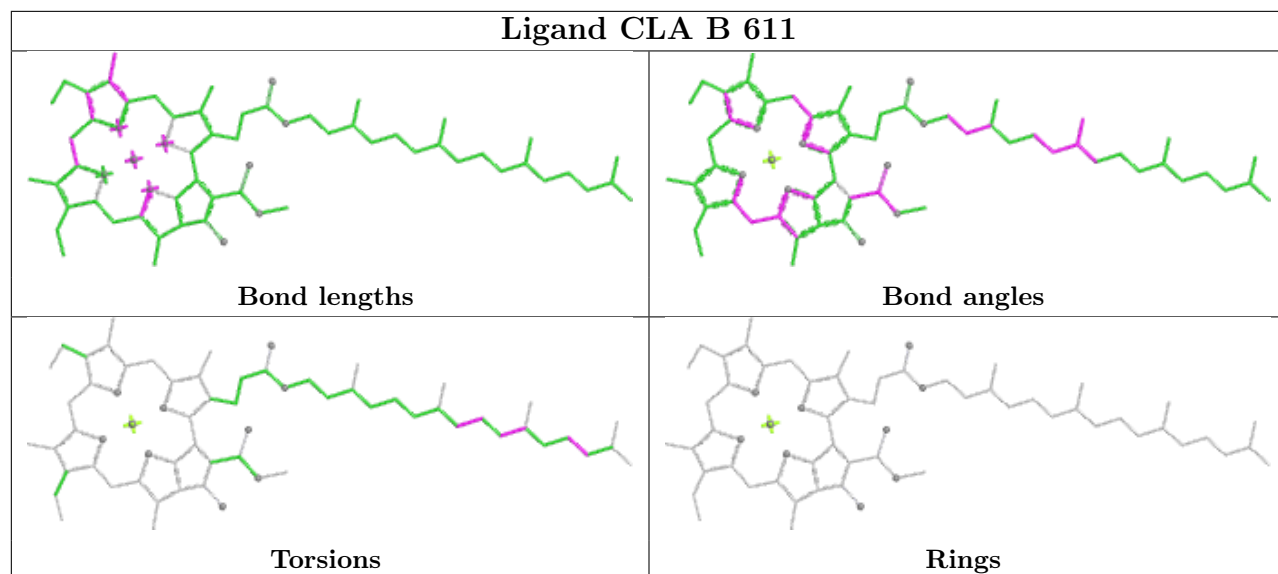


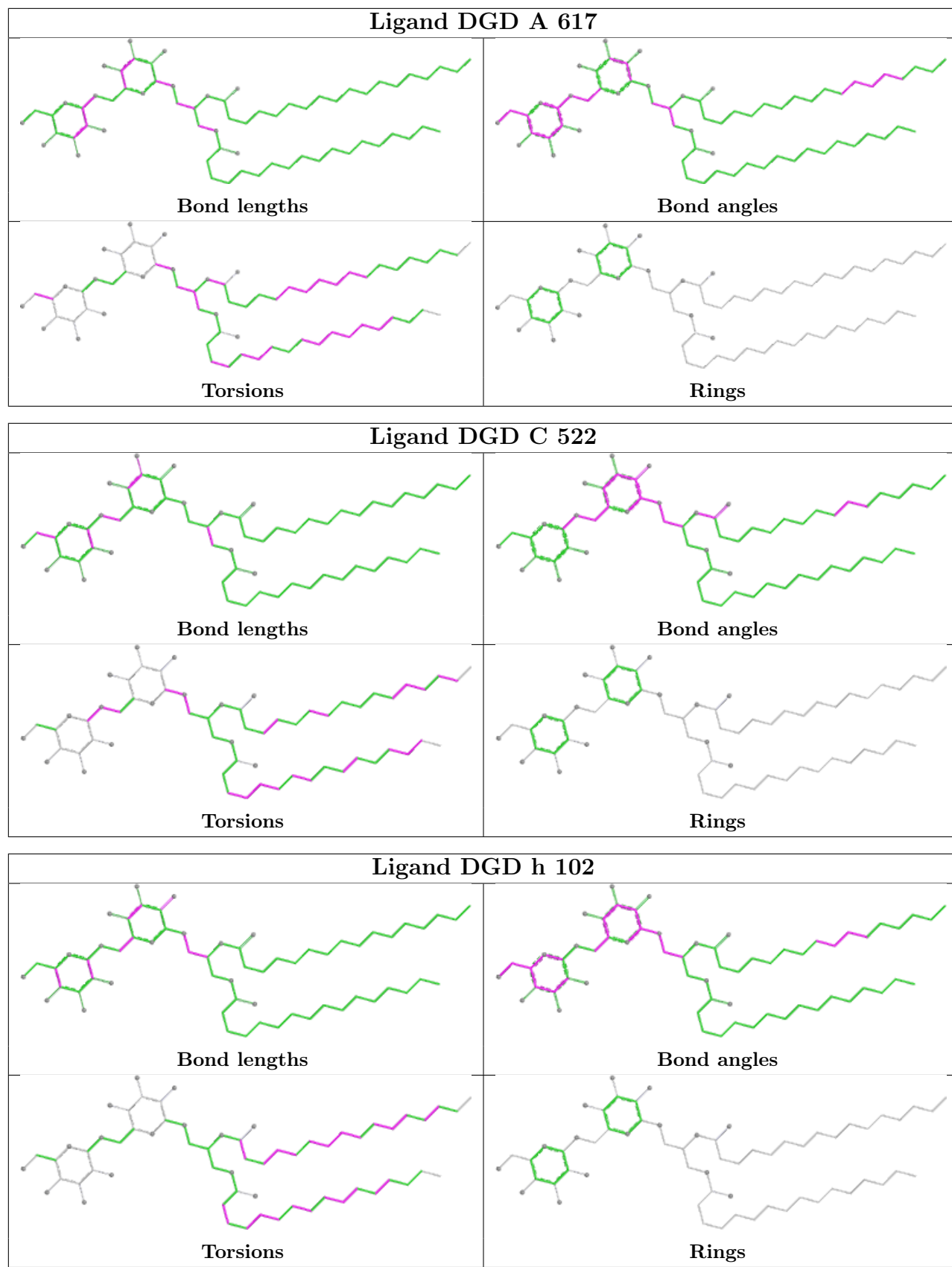
Ligand STE t 103

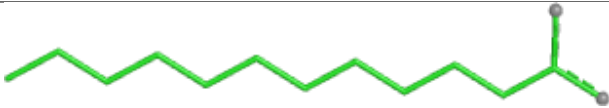
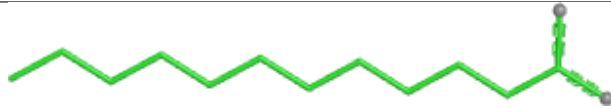
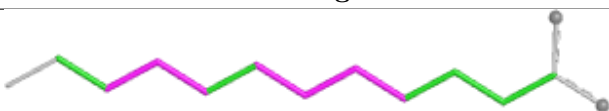
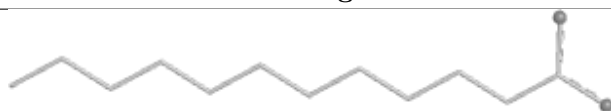


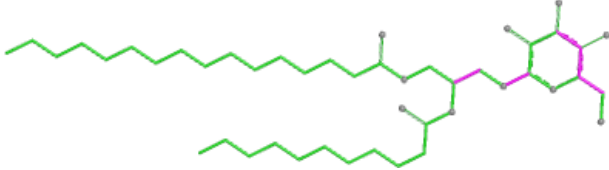
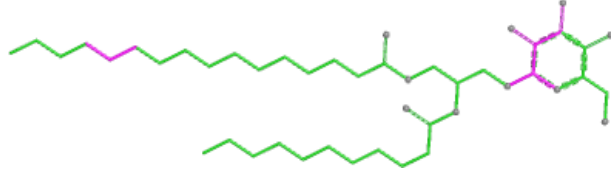
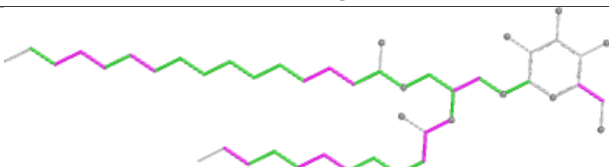
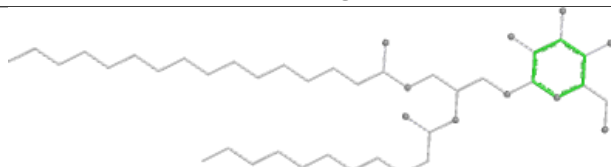
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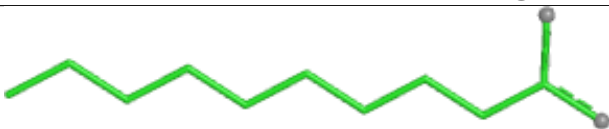
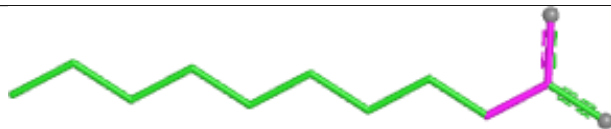
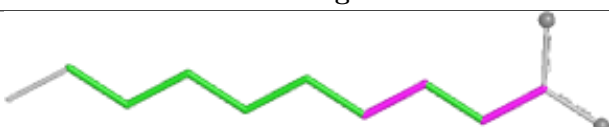
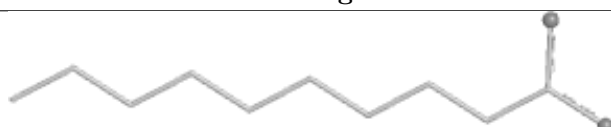


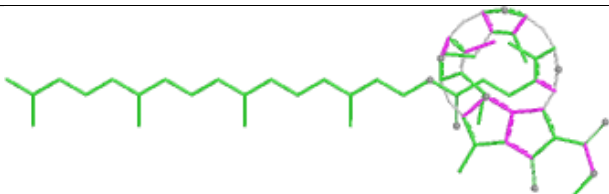
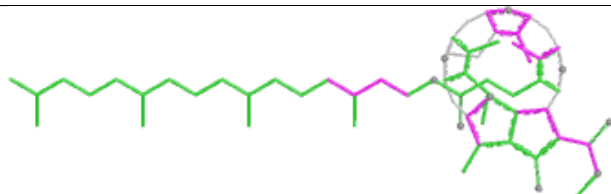
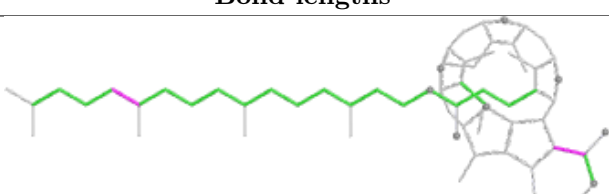
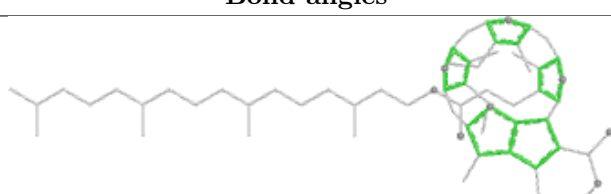


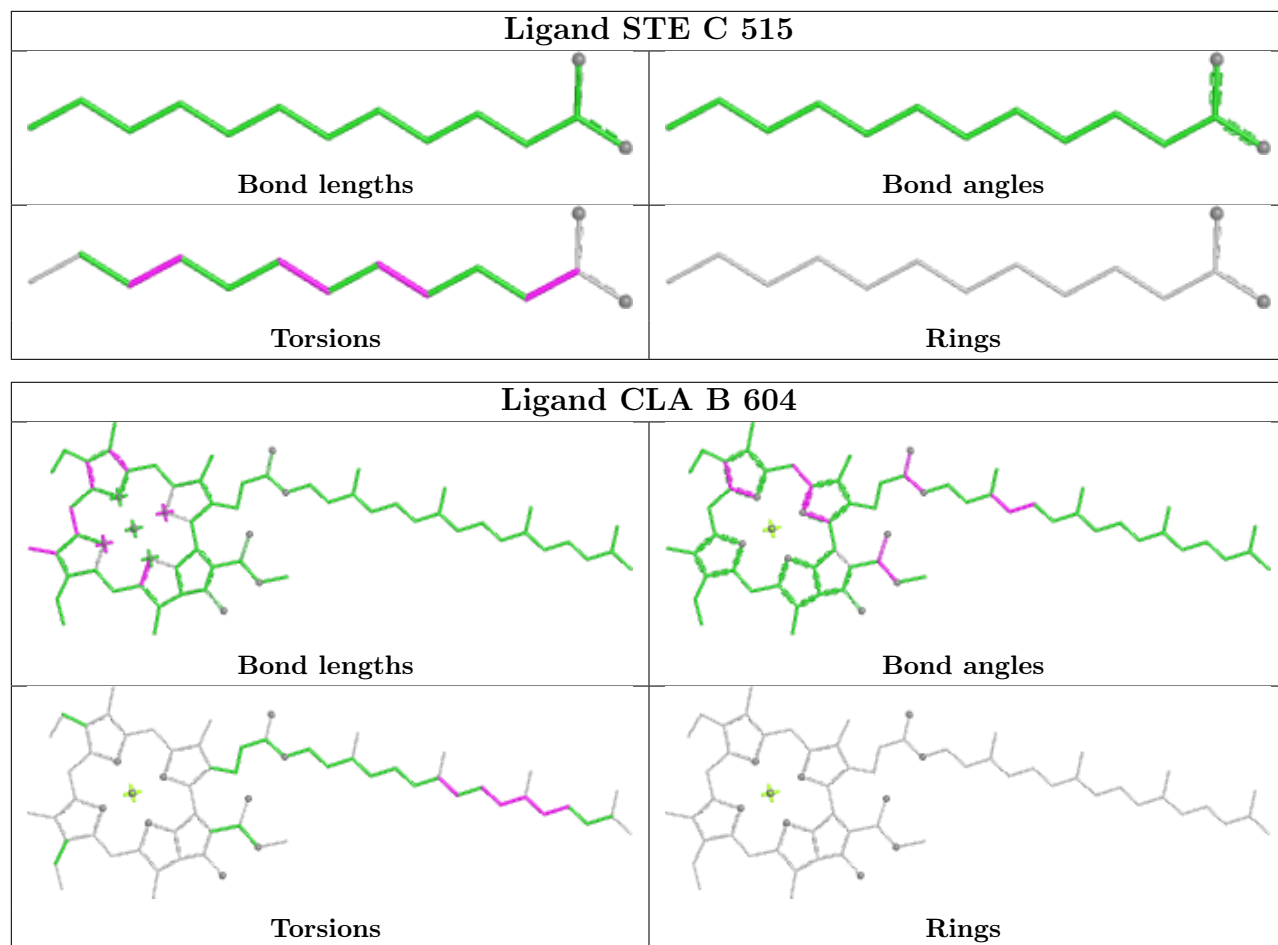


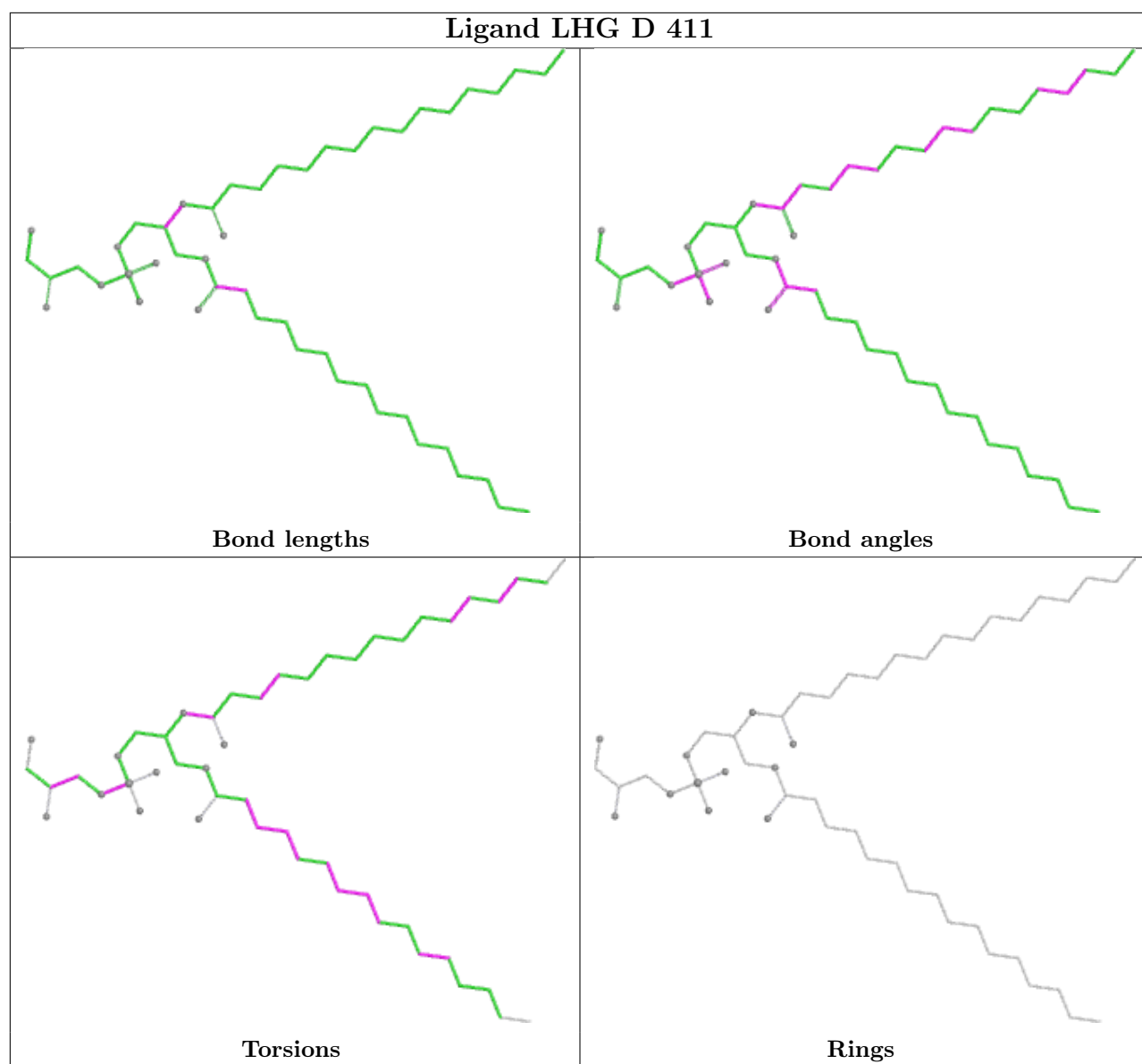
Ligand STE d 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

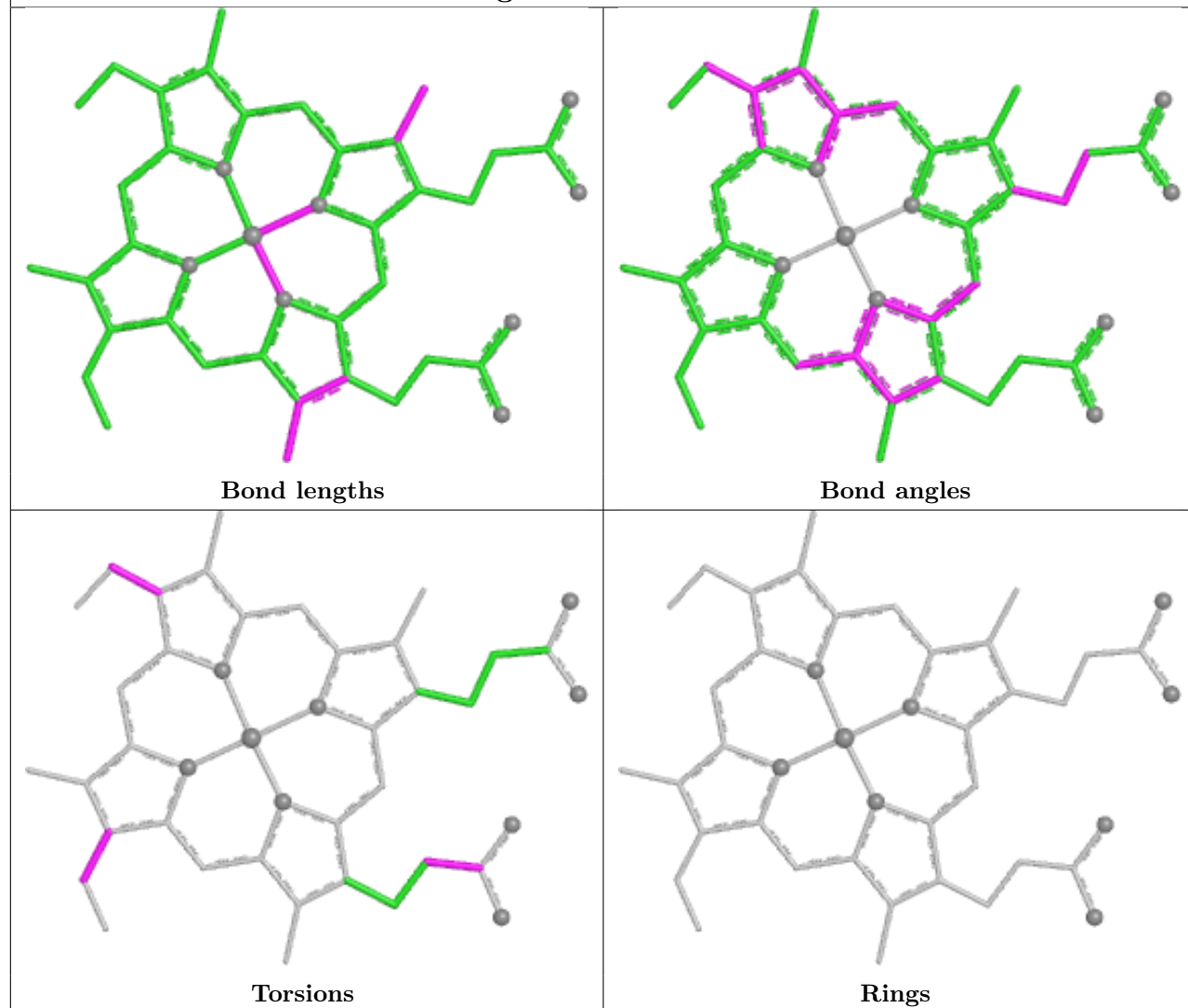
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

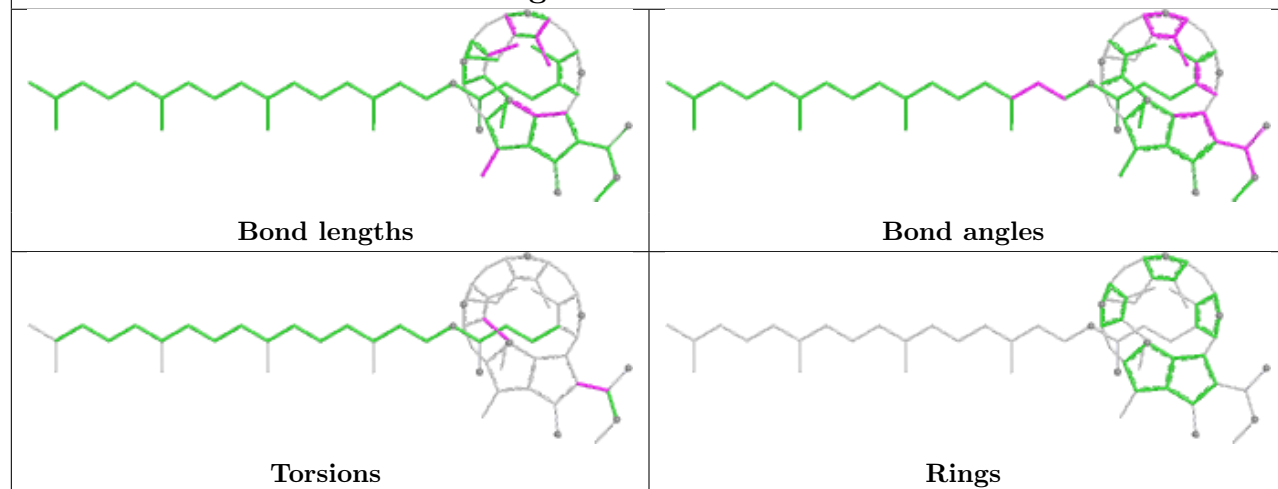




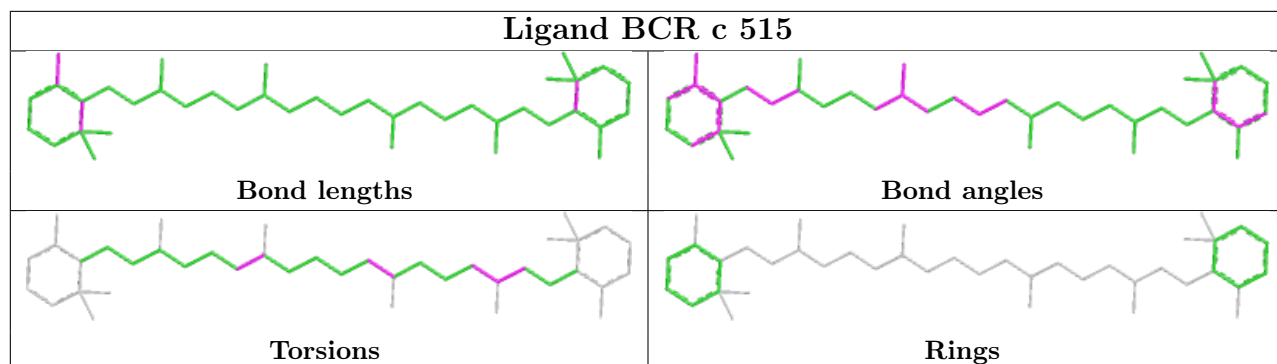
Ligand HEC v 201



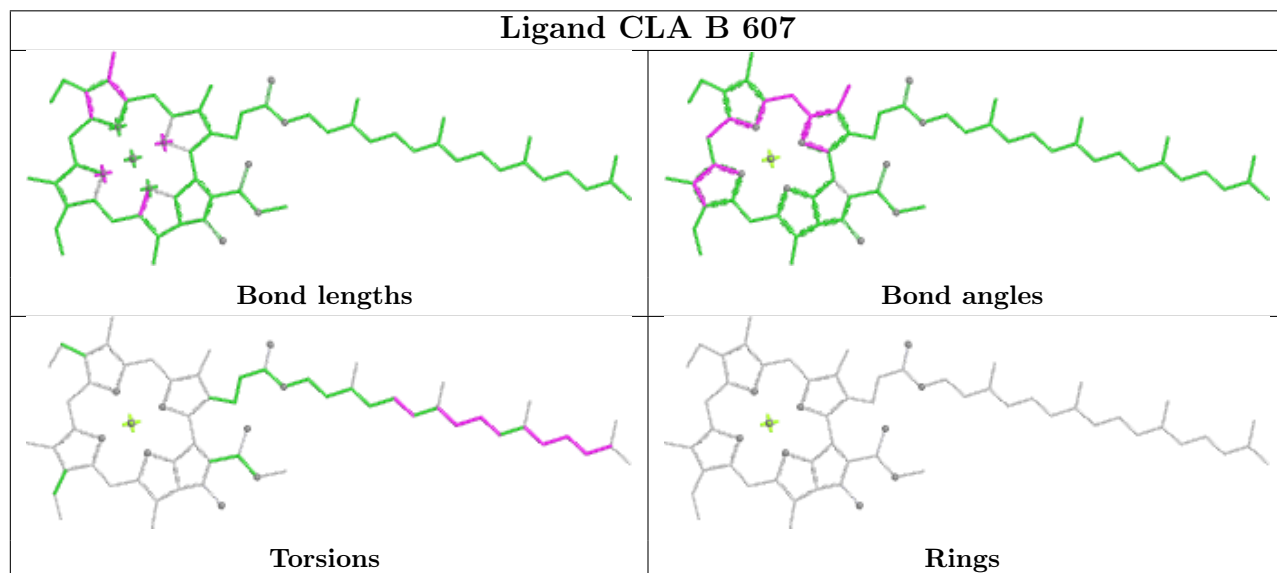
Ligand PHO D 402



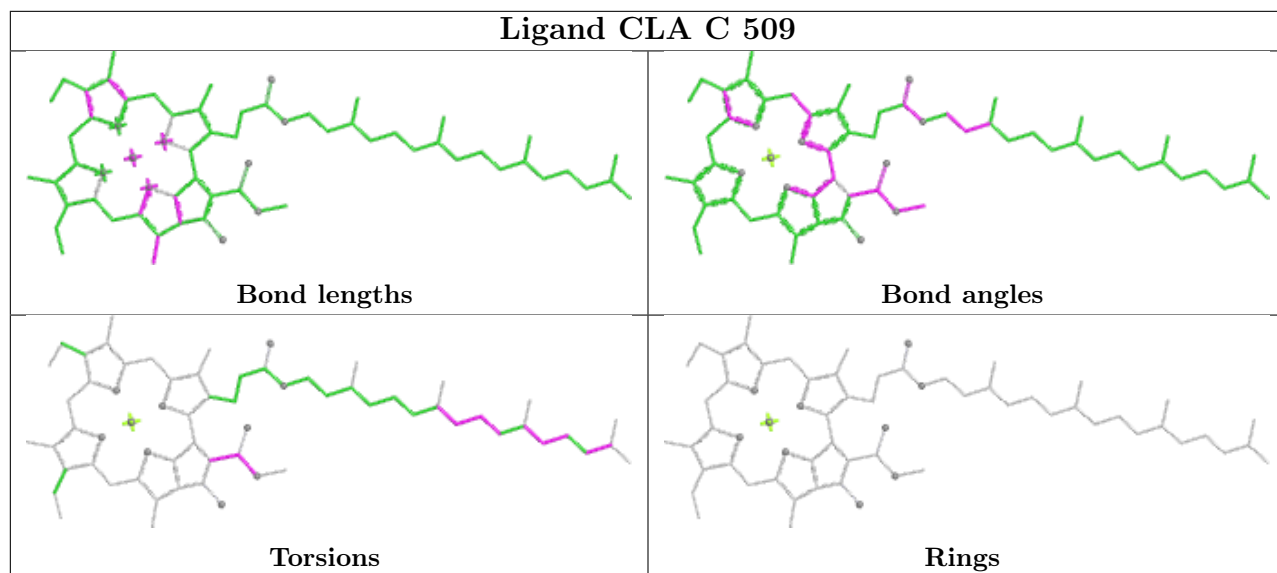
Ligand BCR c 515

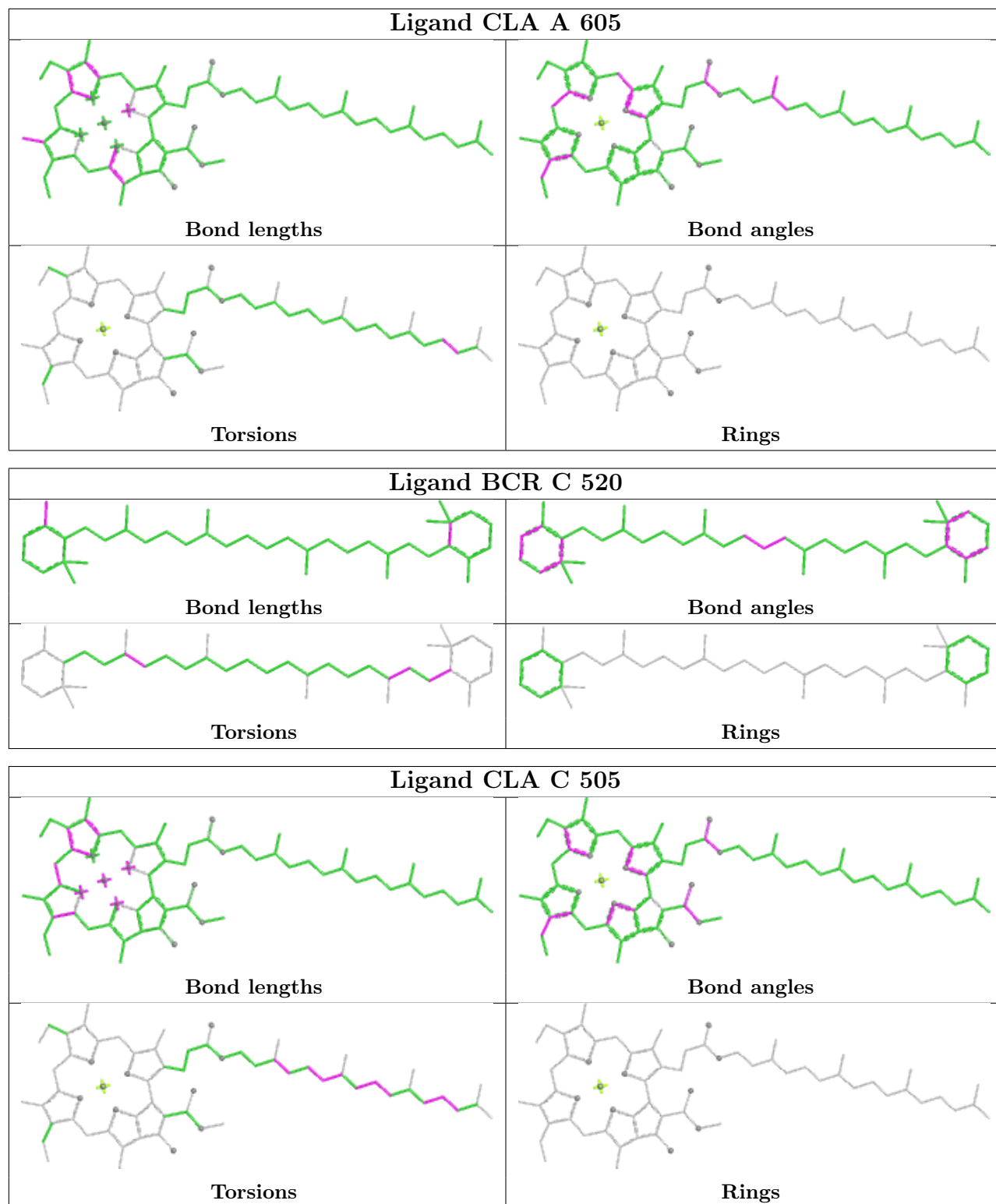


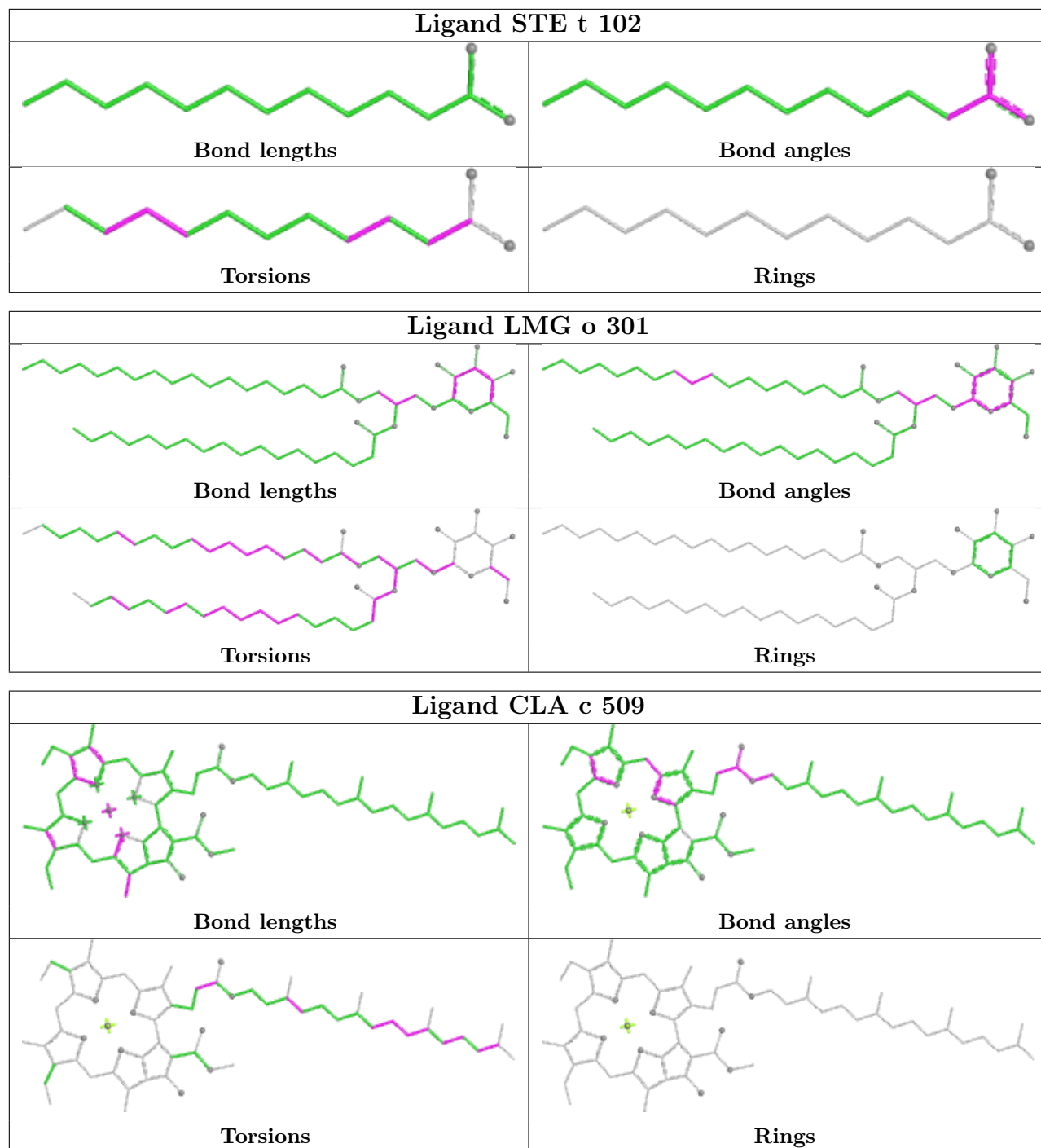
Ligand CLA B 607

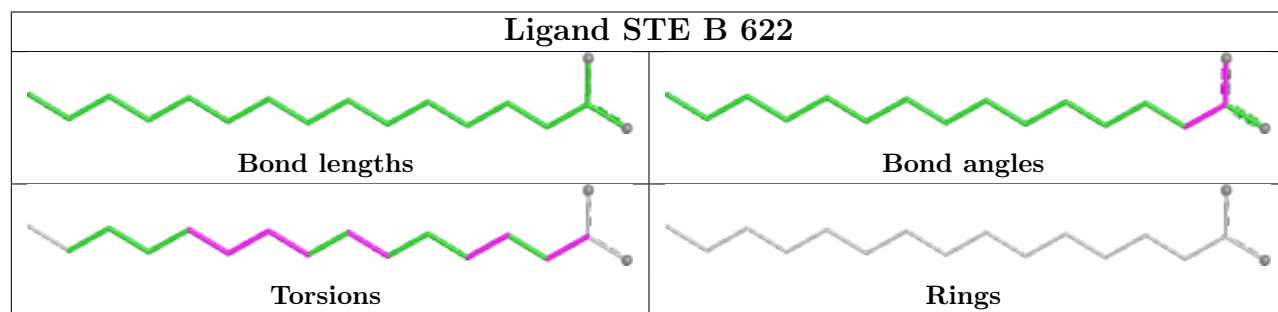
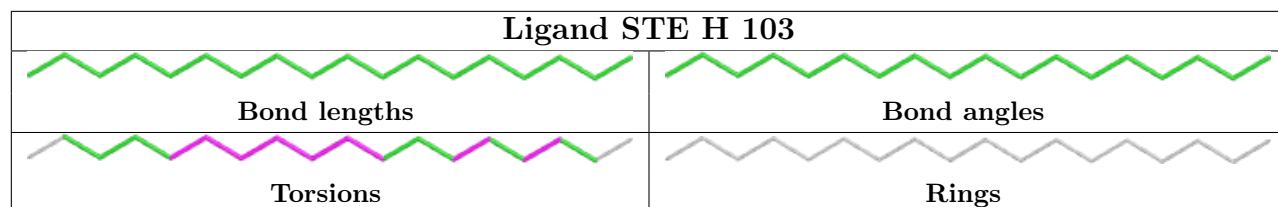
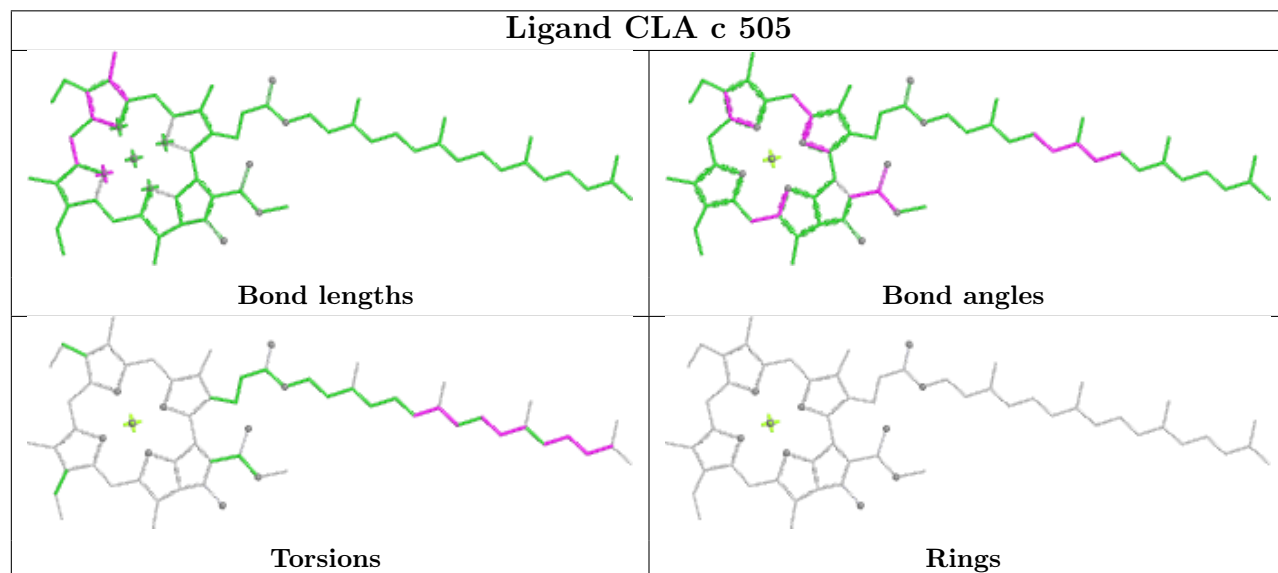
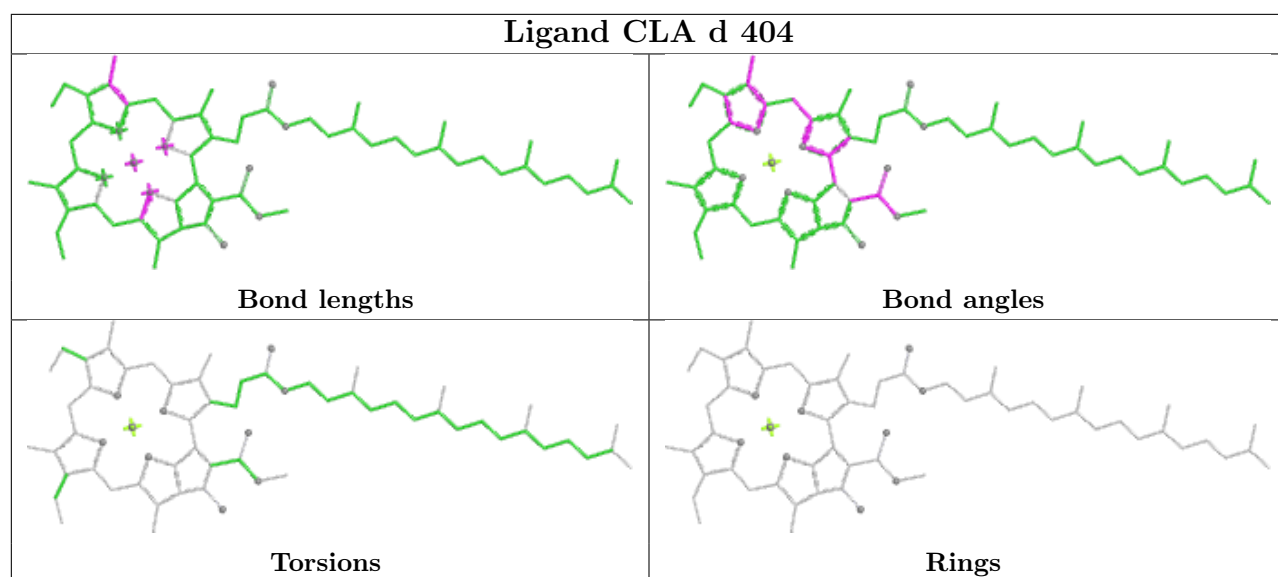


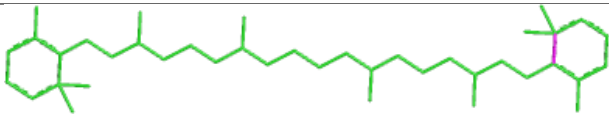
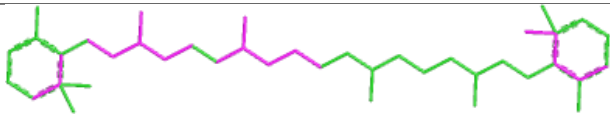
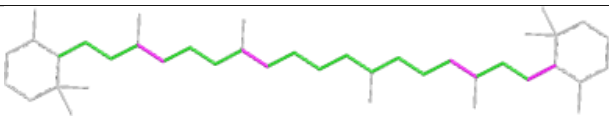
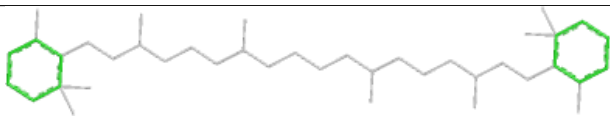
Ligand CLA C 509

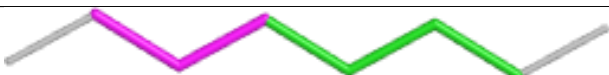


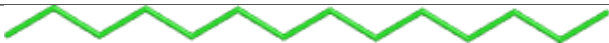
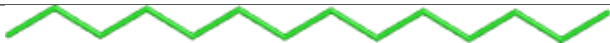


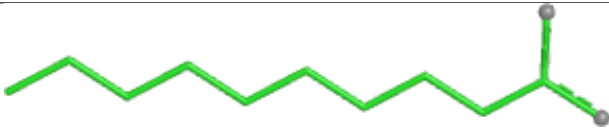
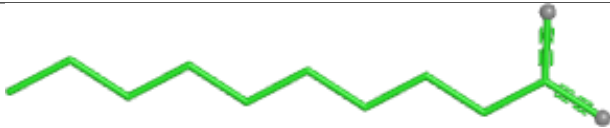
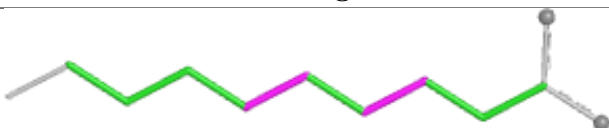
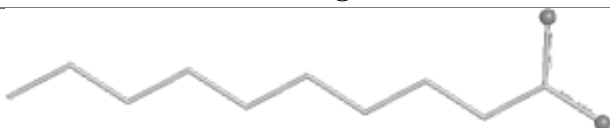




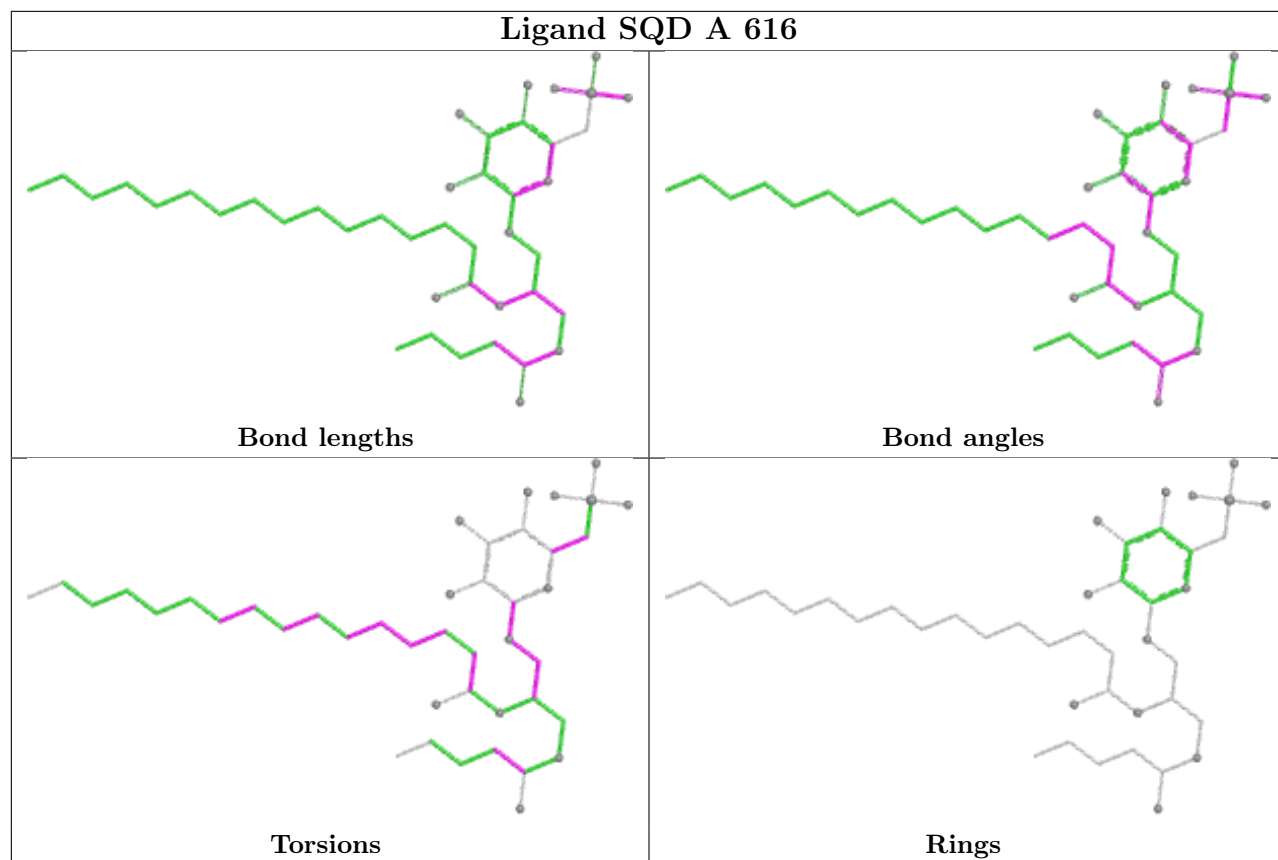
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

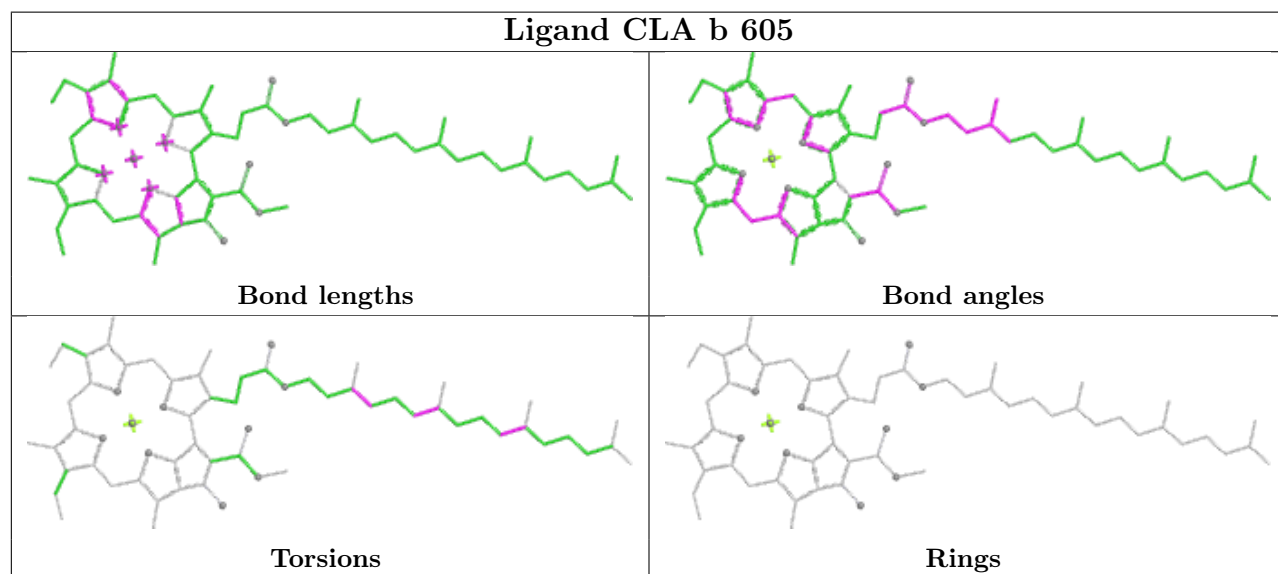
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Bond lengths	Bond angles
	
Torsions	Rings

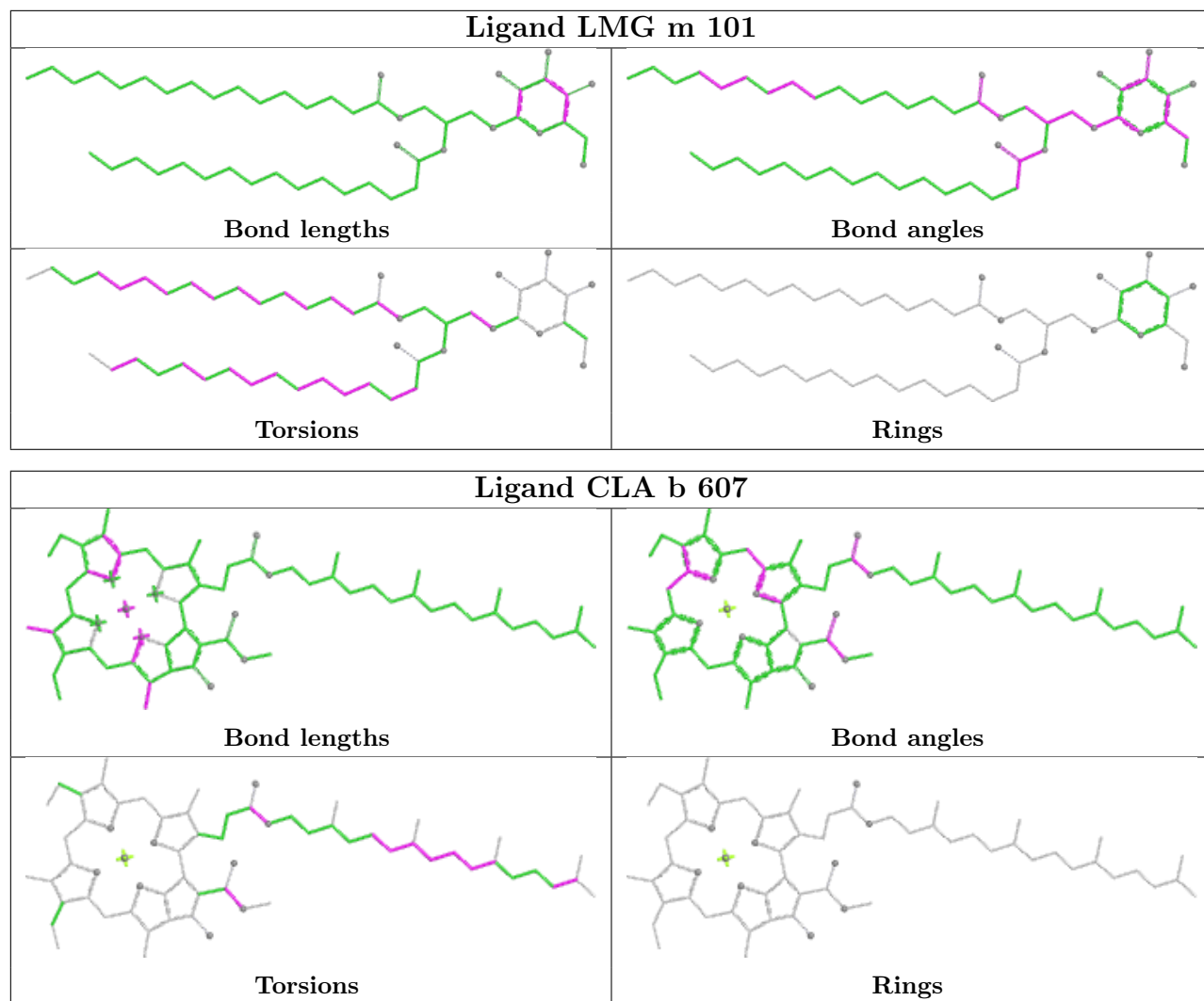
Ligand STE m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

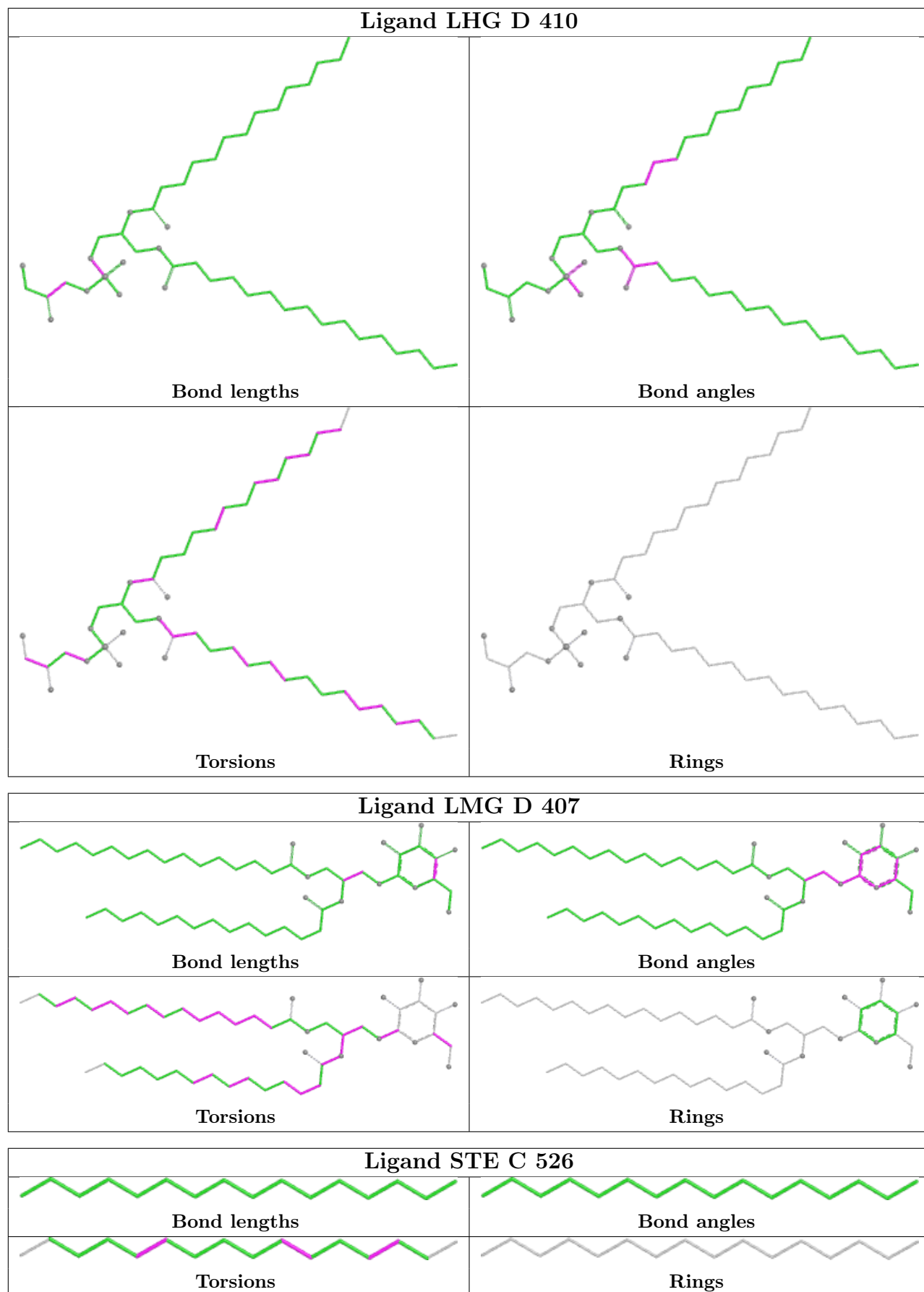
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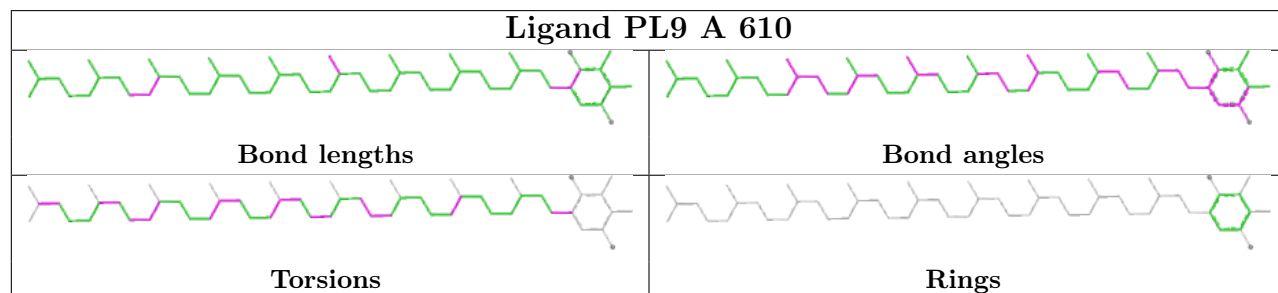
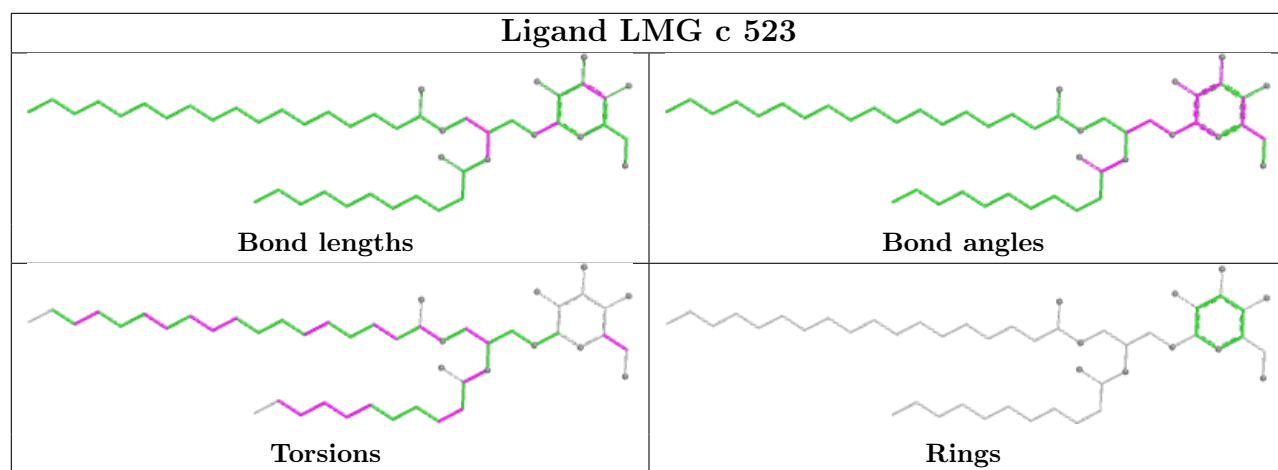
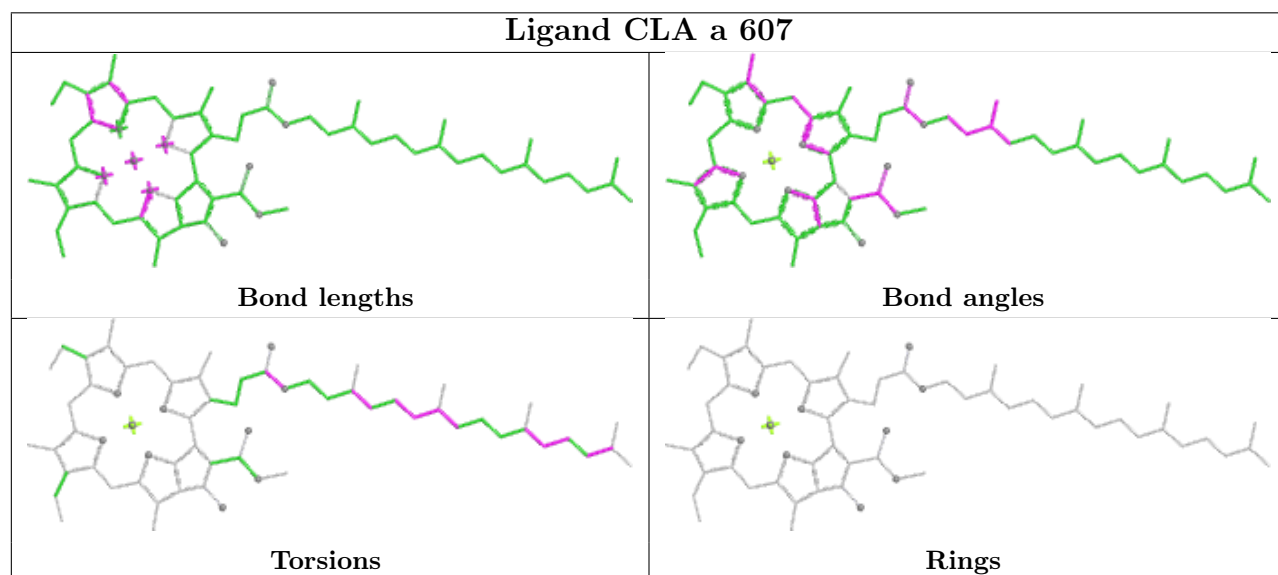
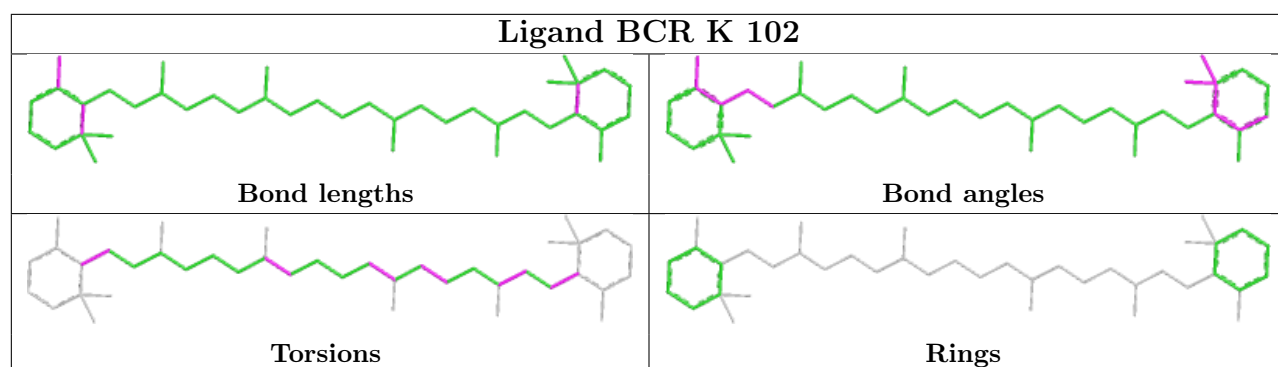


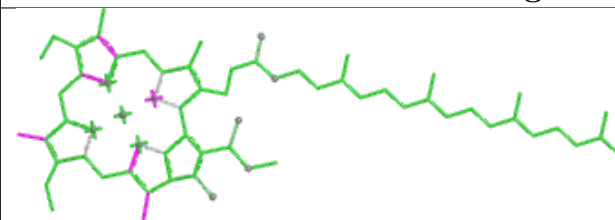
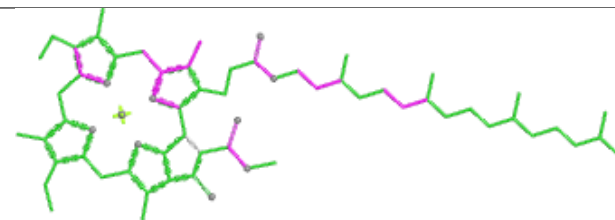
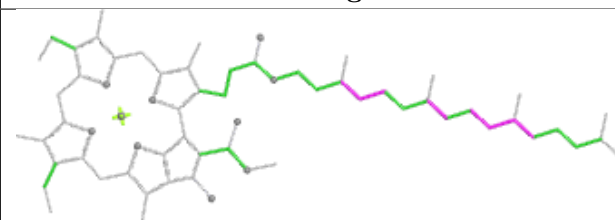
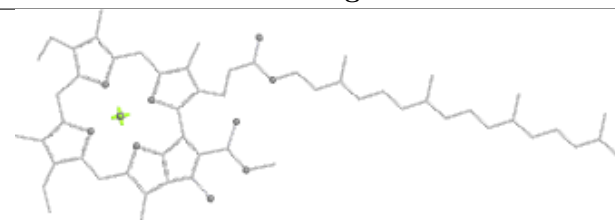
Ligand CLA b 605

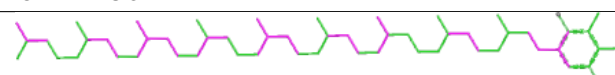
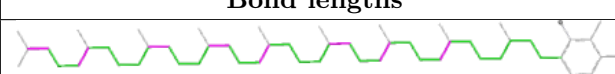
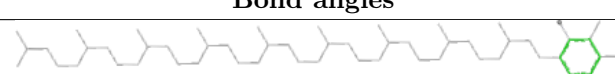






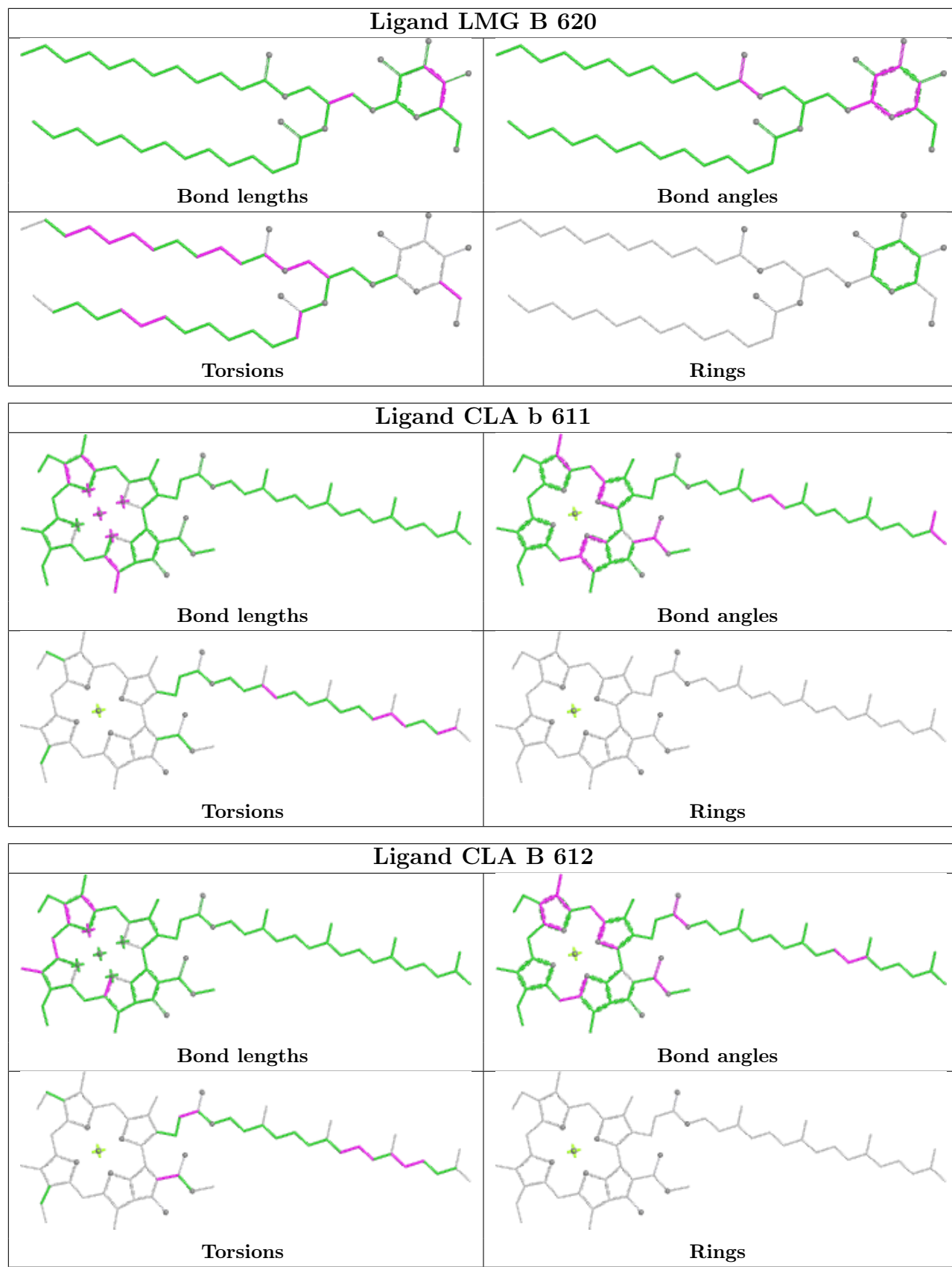


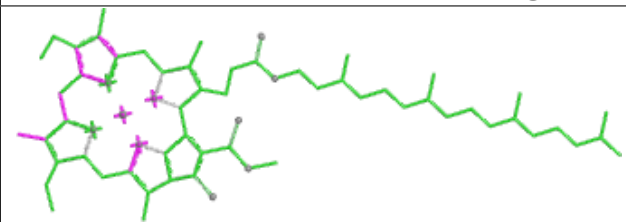
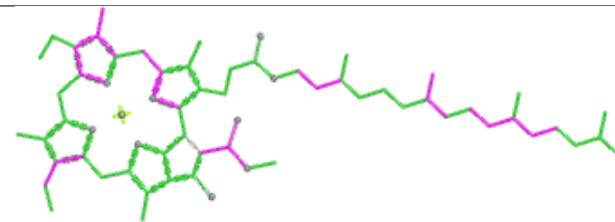
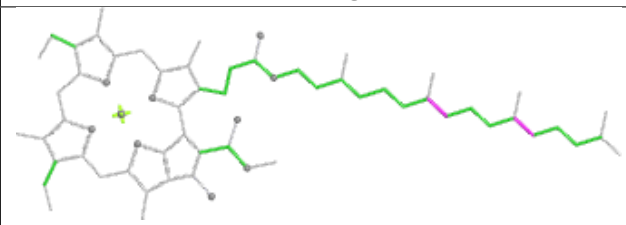
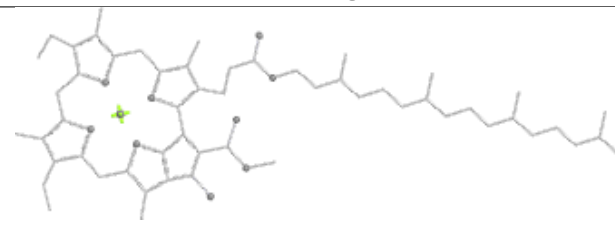
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

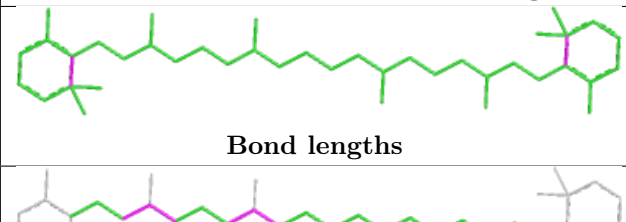
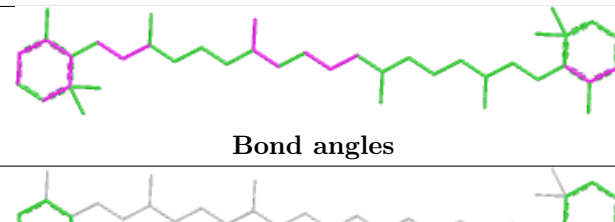
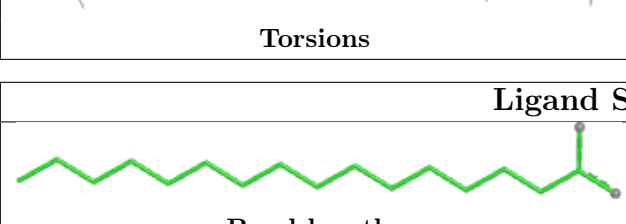
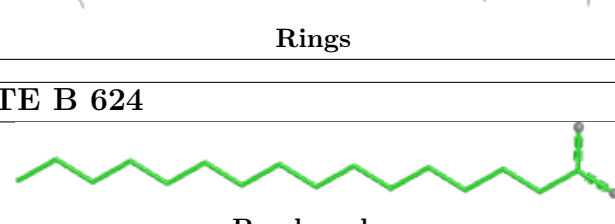
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

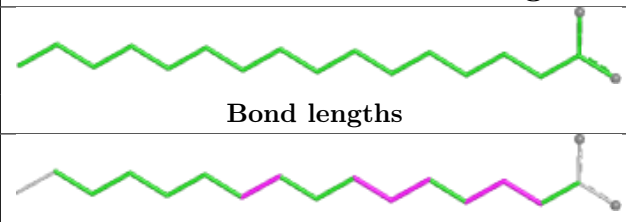
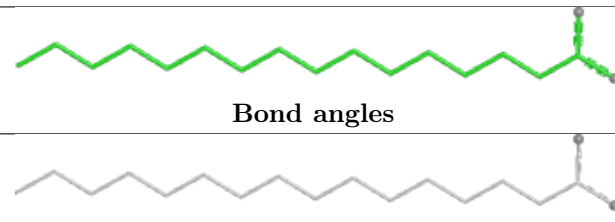
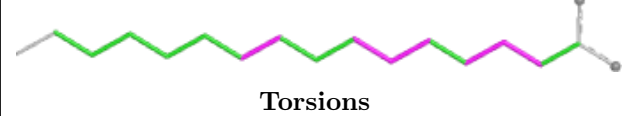
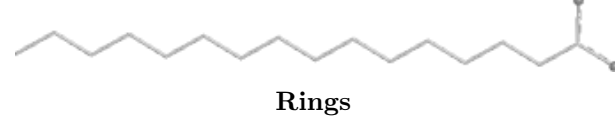
Ligand STE M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

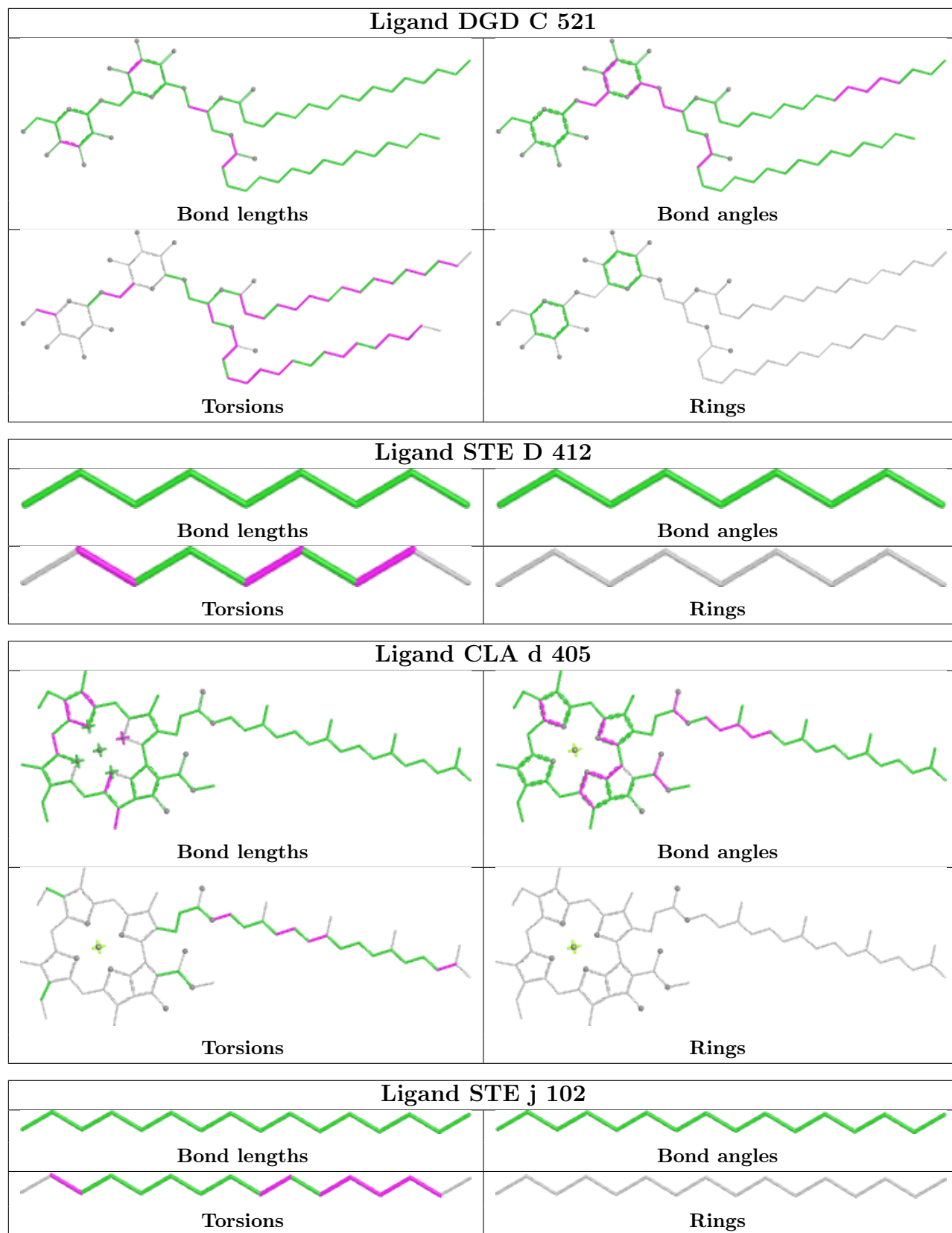
Ligand STE M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

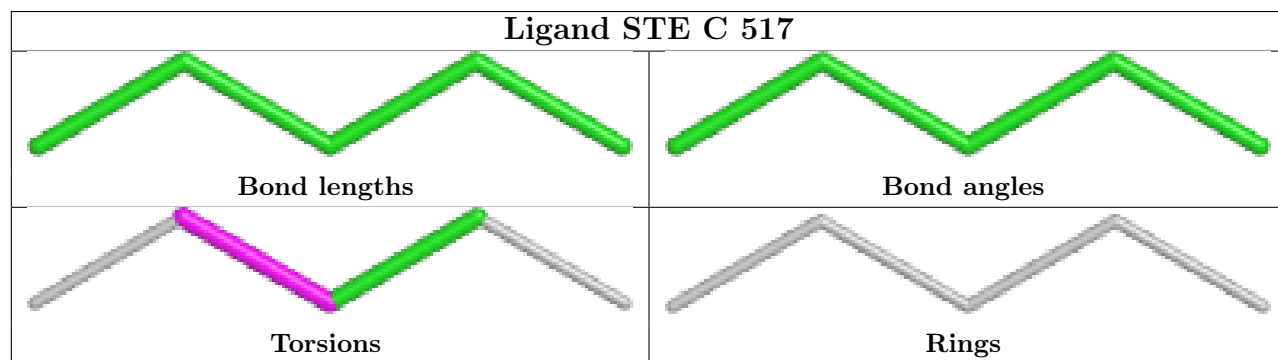
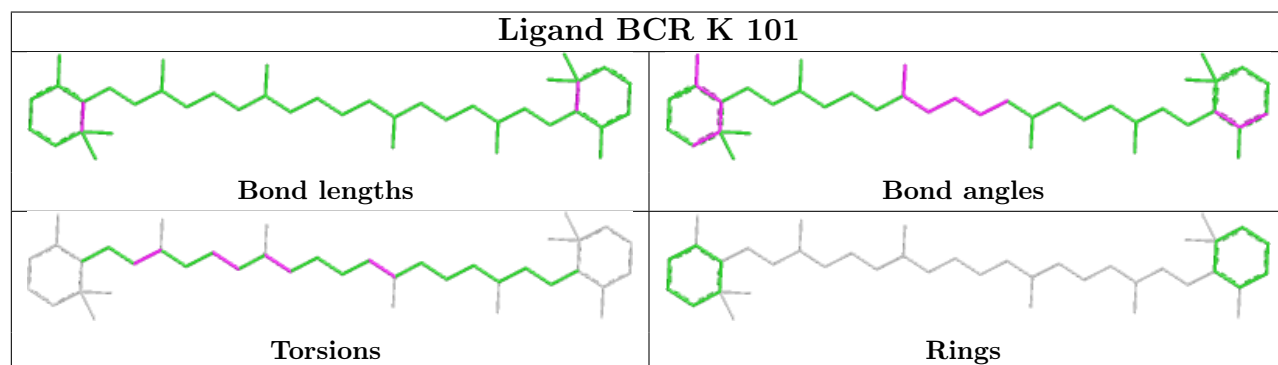
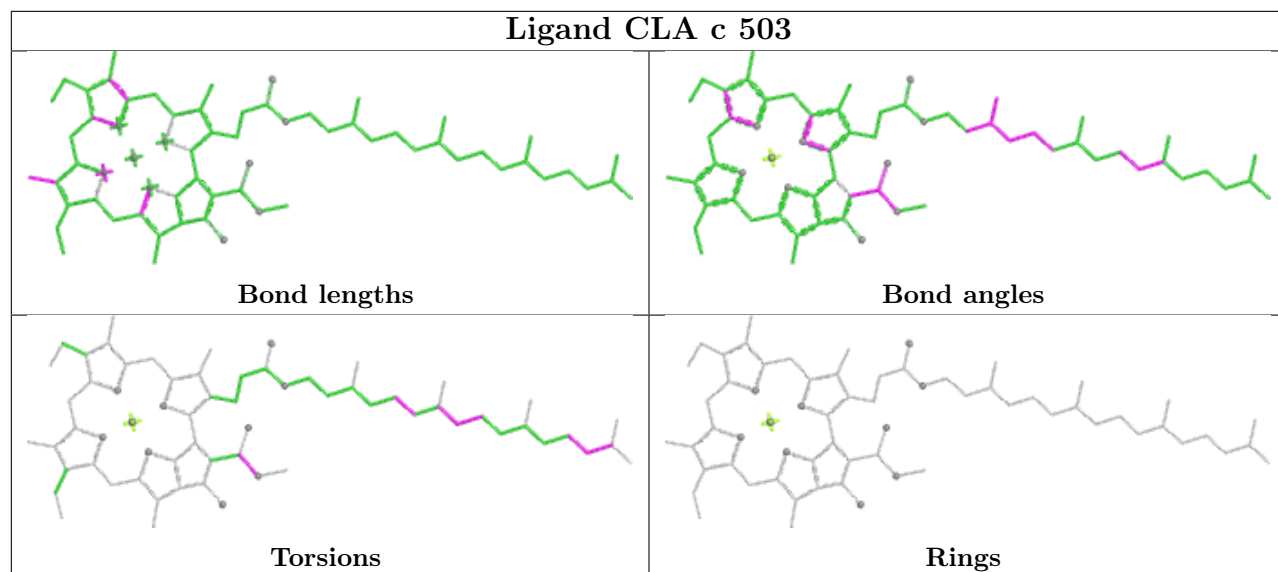


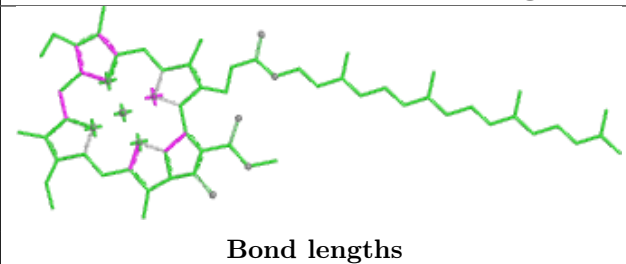
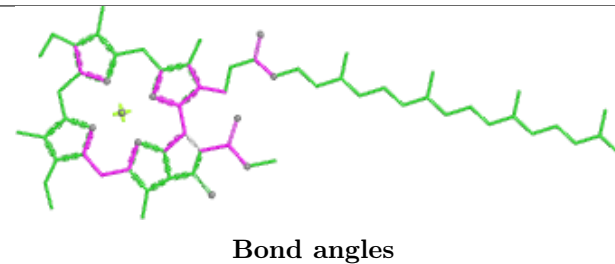
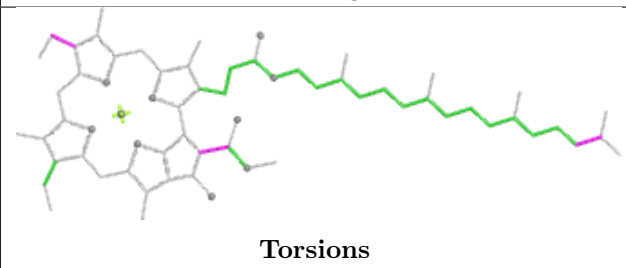
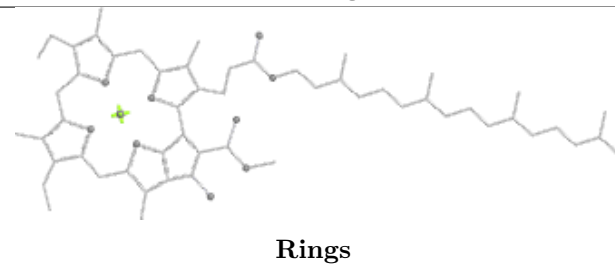
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

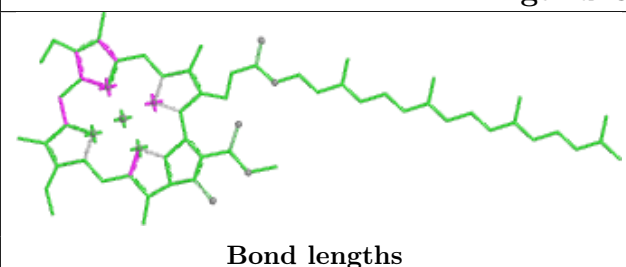
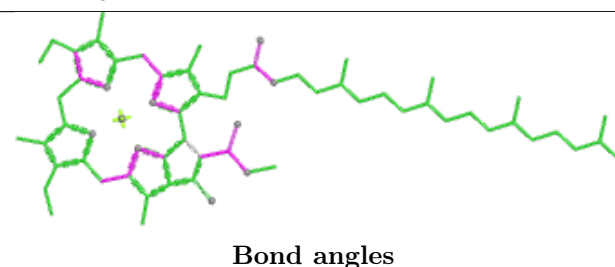
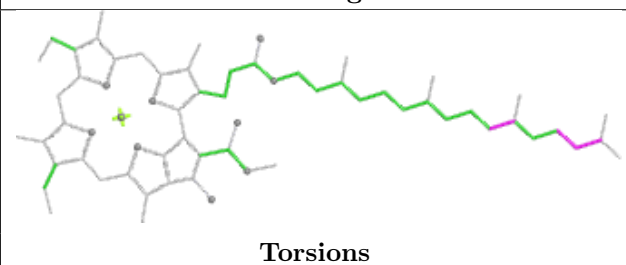
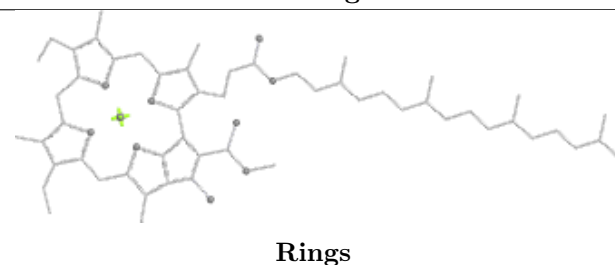
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

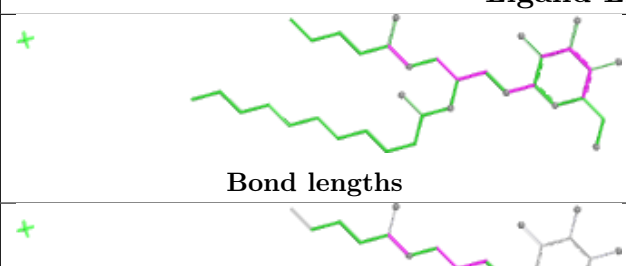
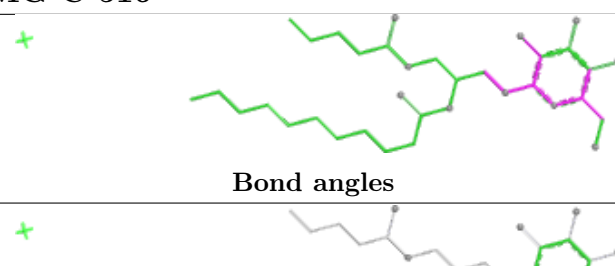
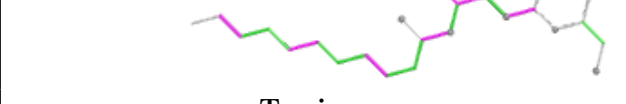
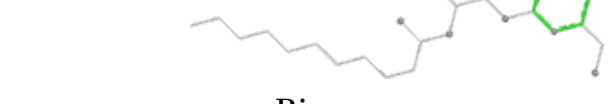
Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

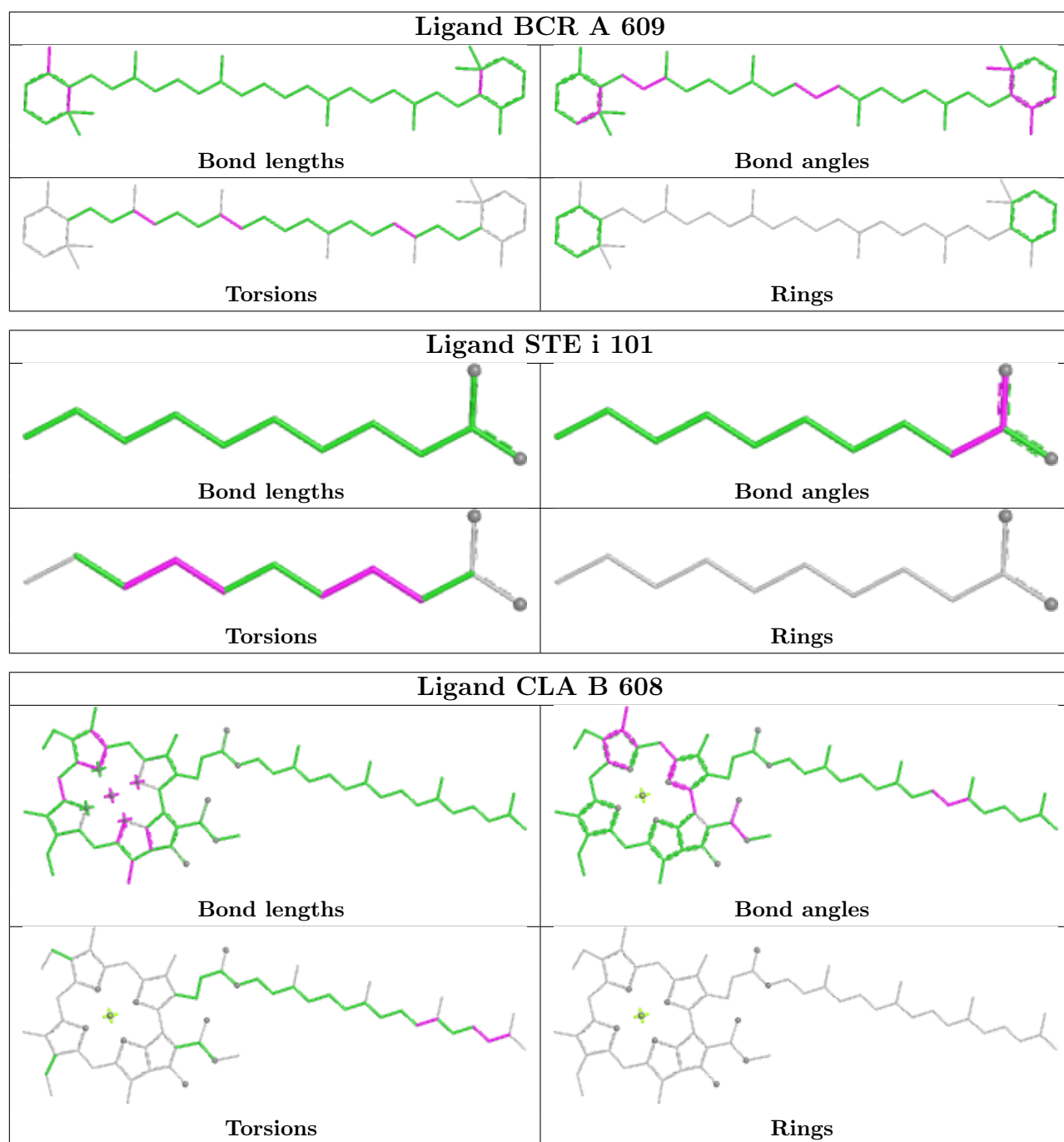


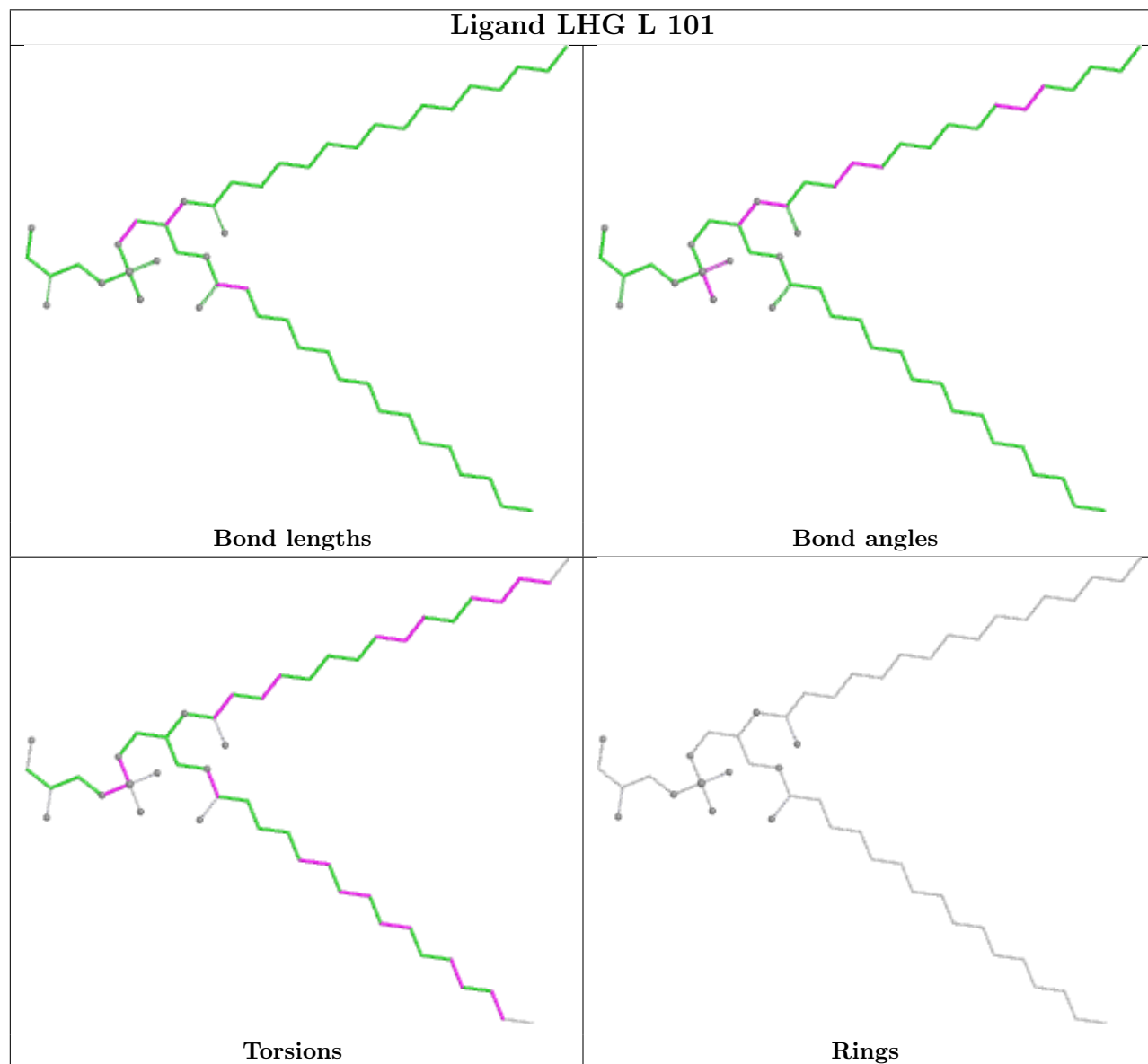
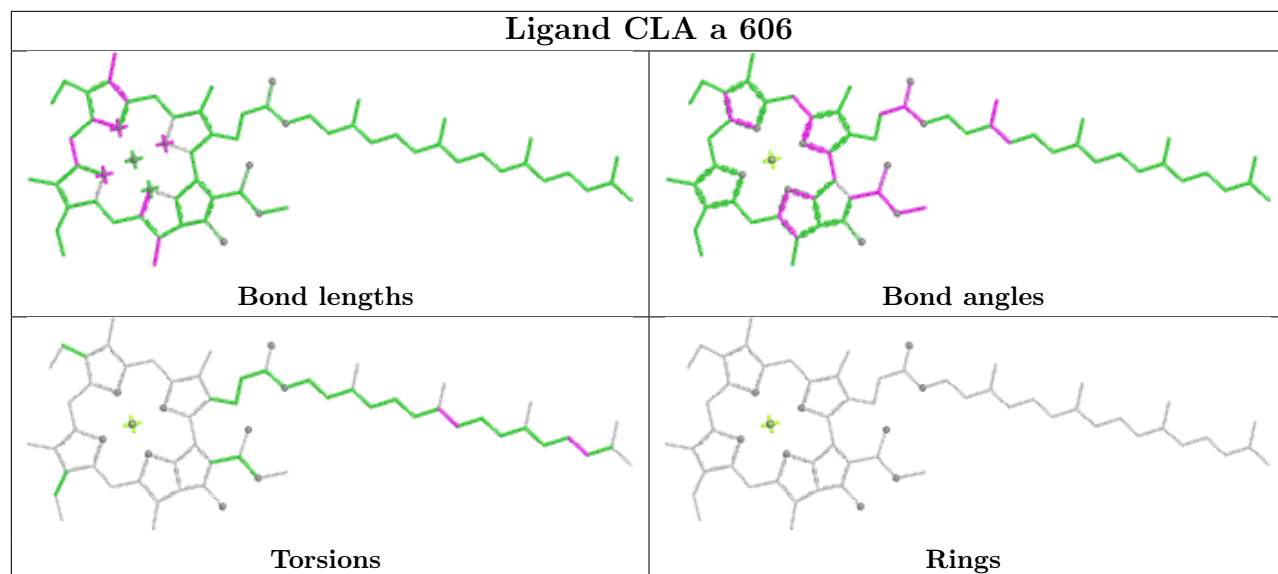


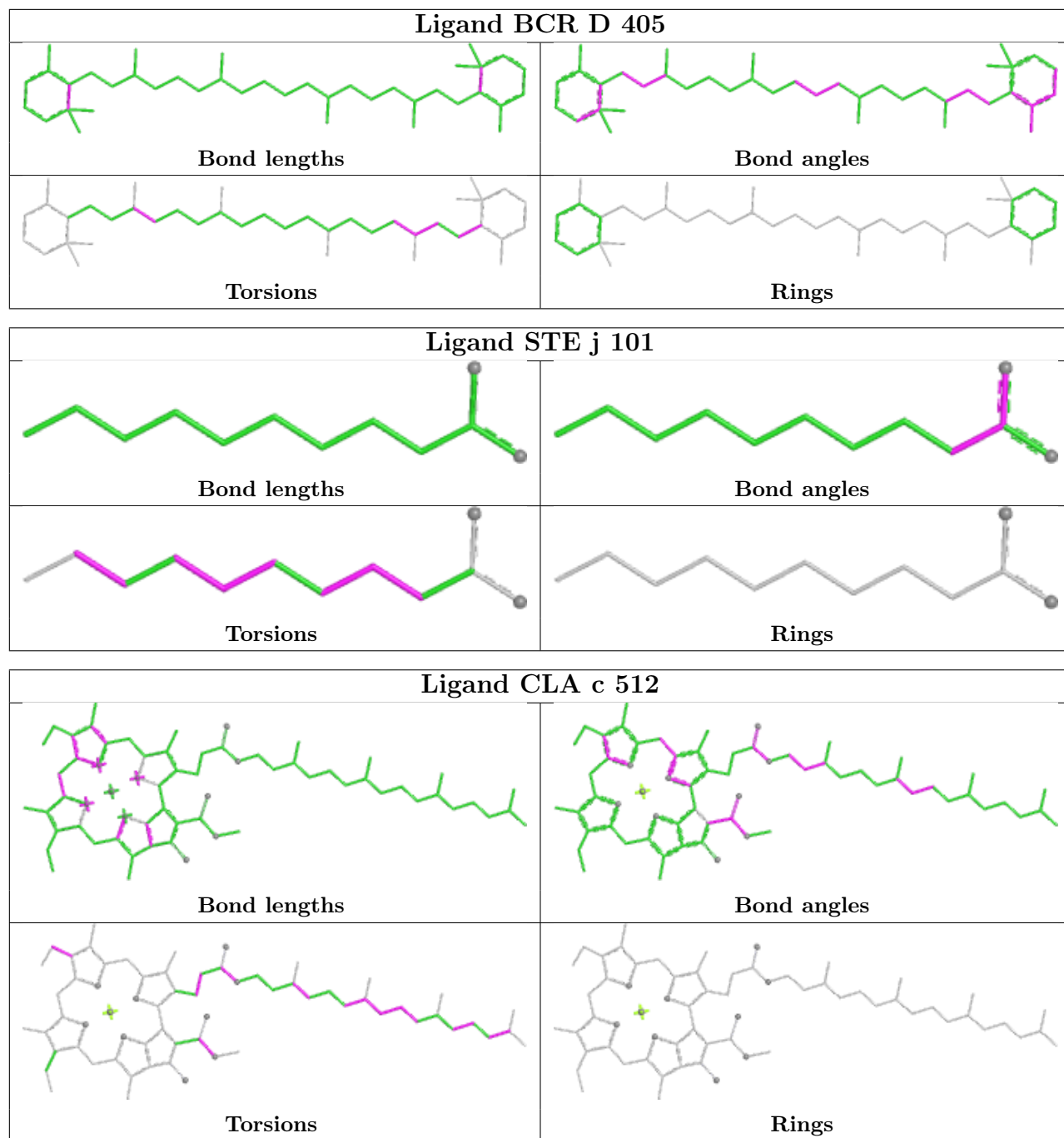
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

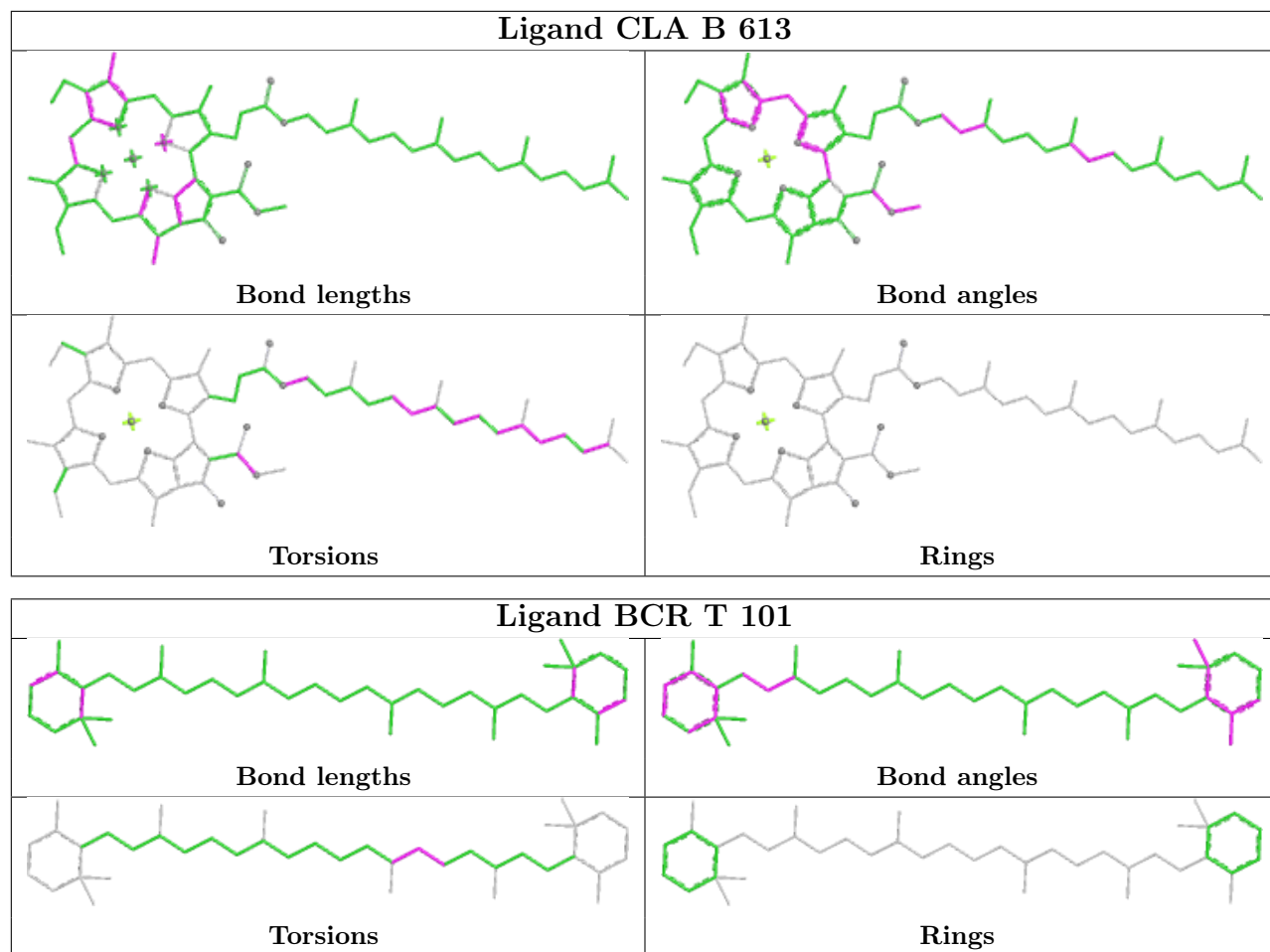
Ligand CLA A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

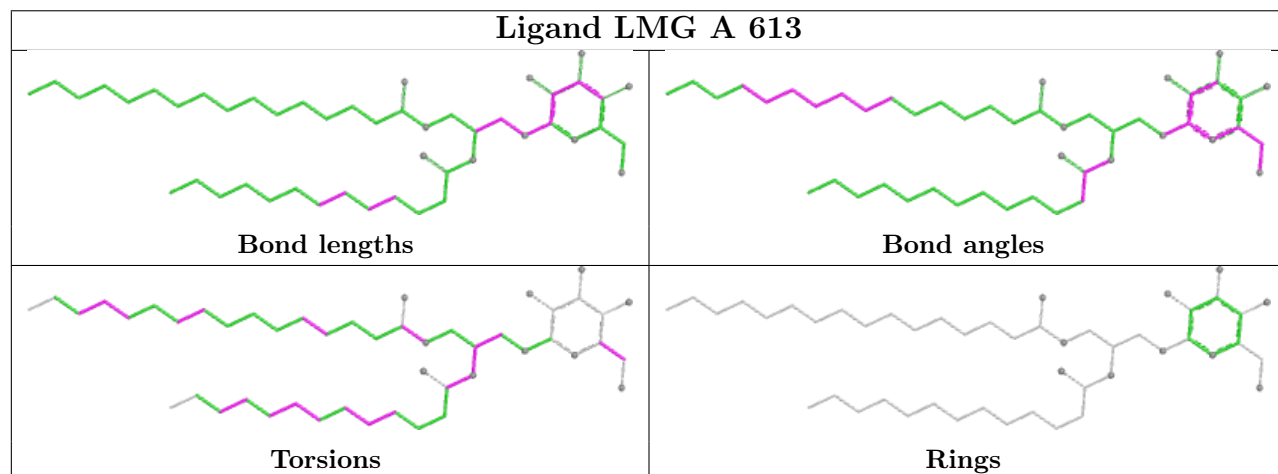
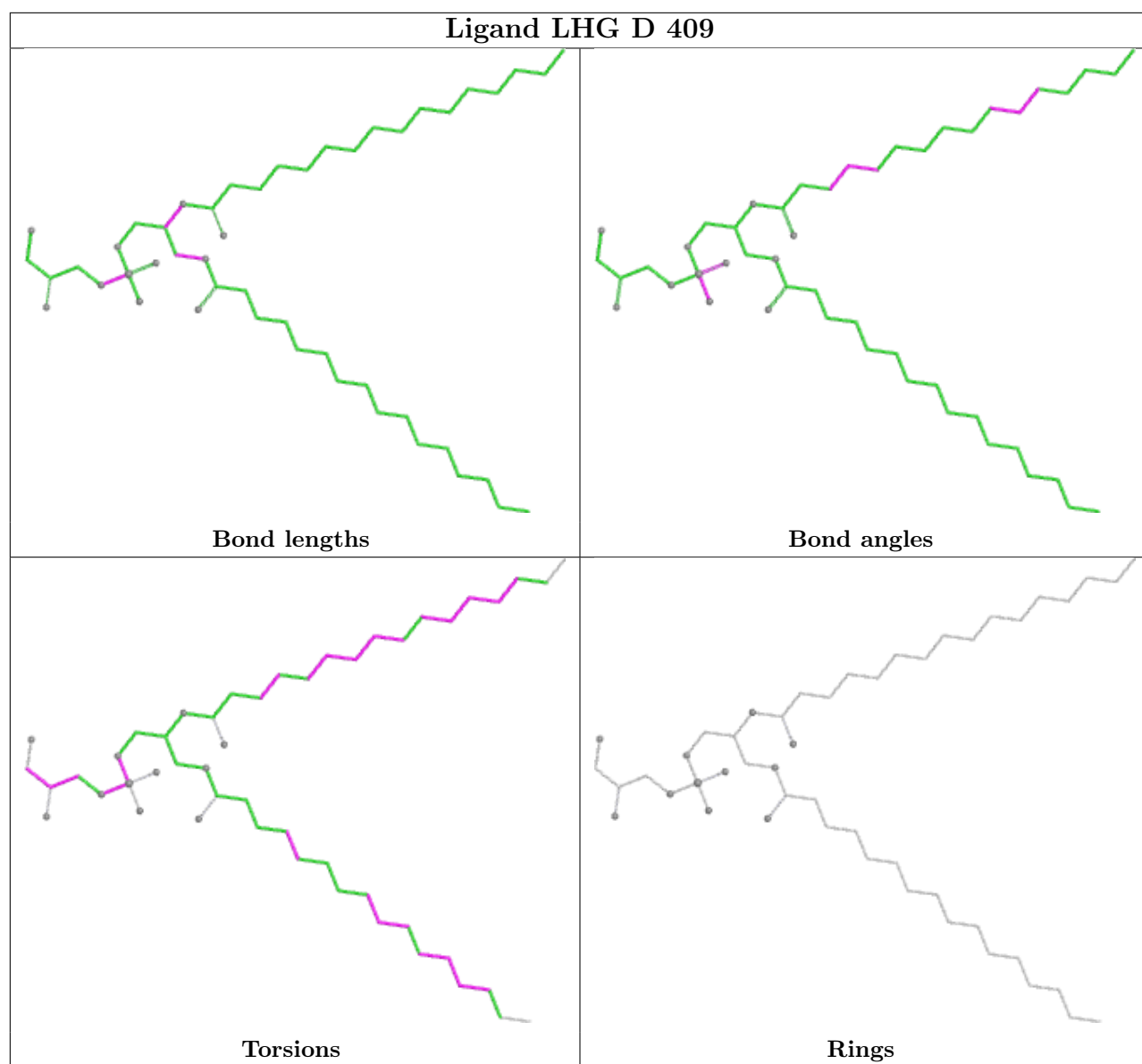
Ligand LMG C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

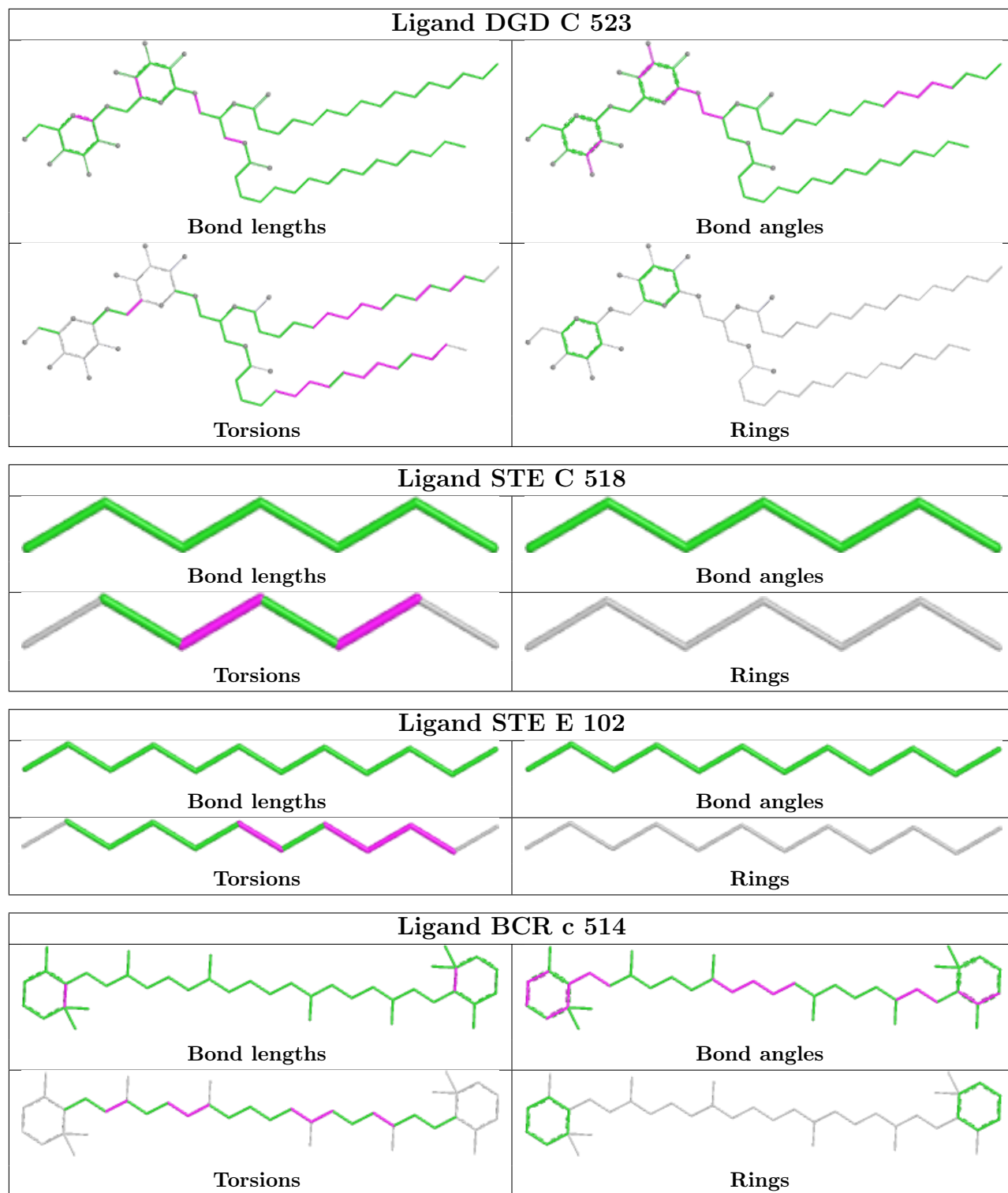


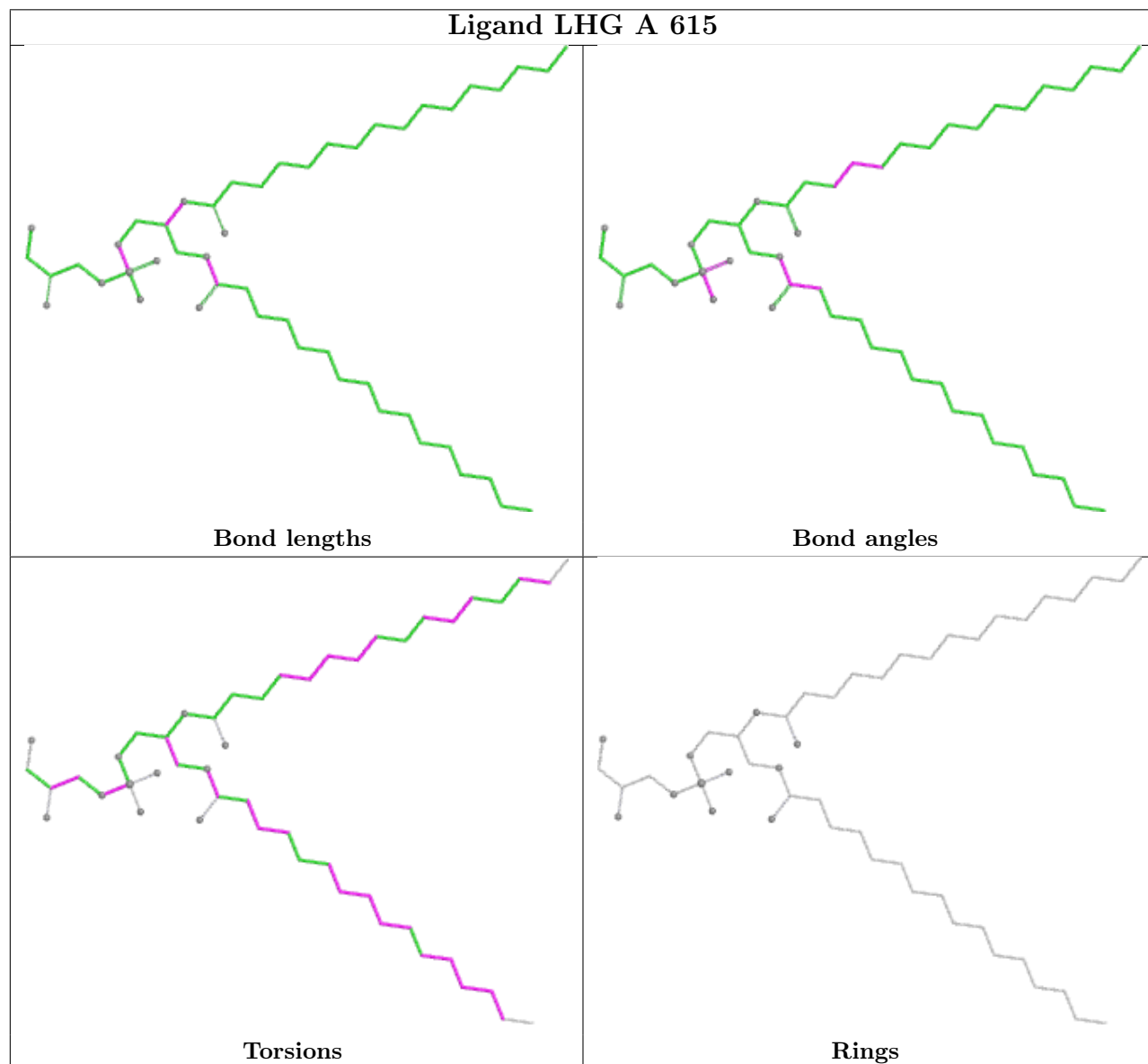
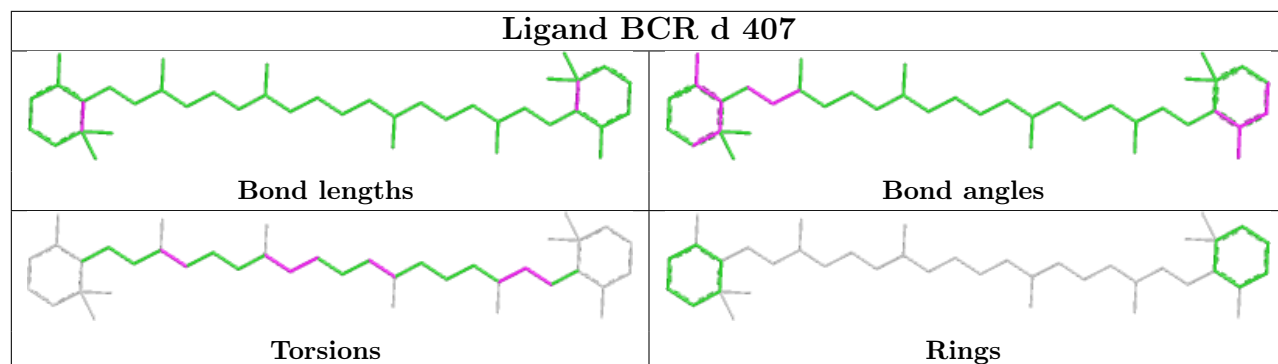


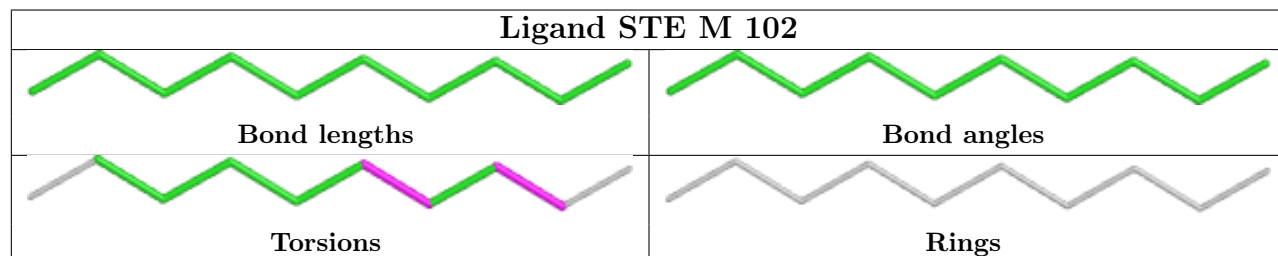
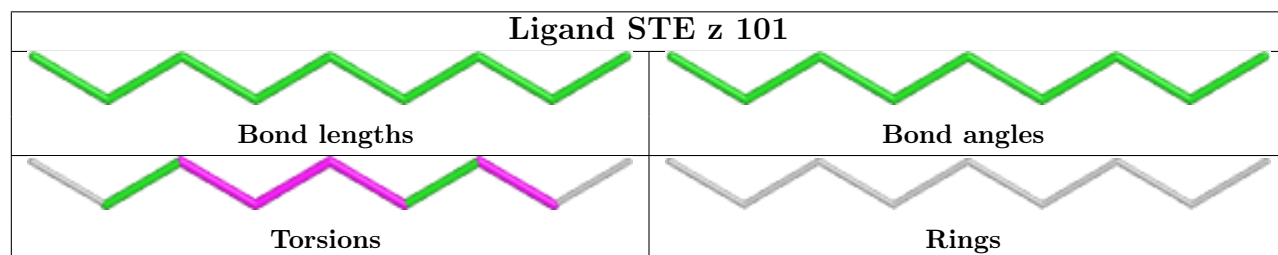
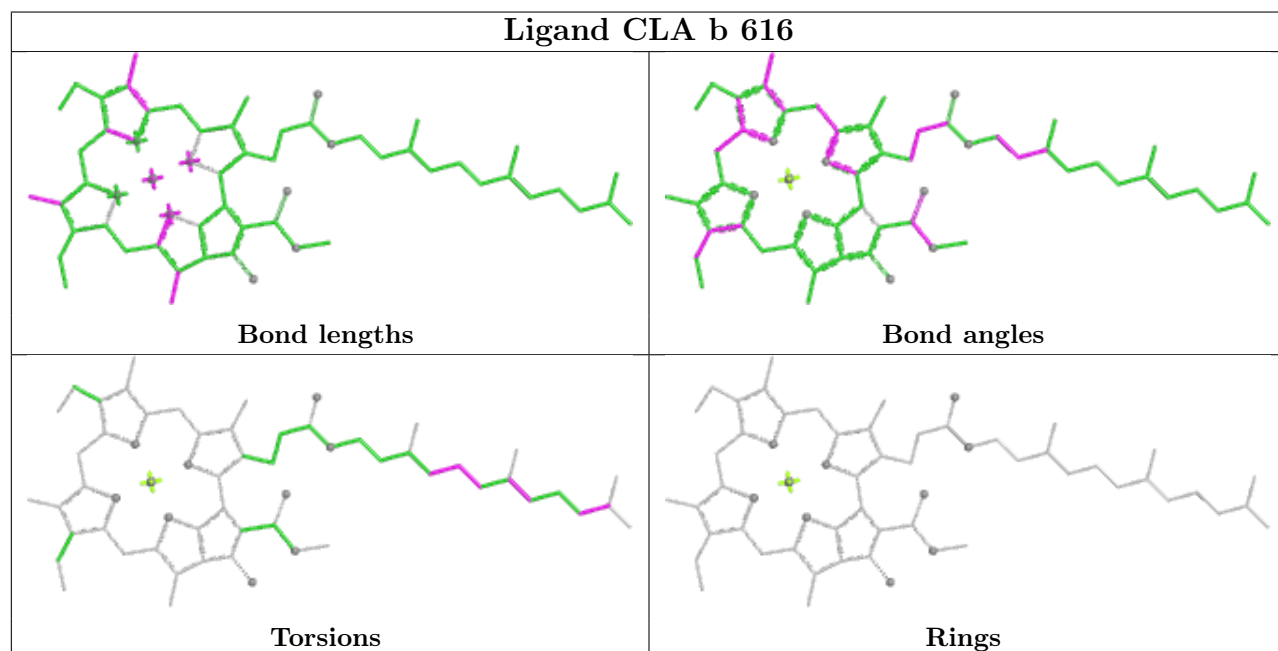
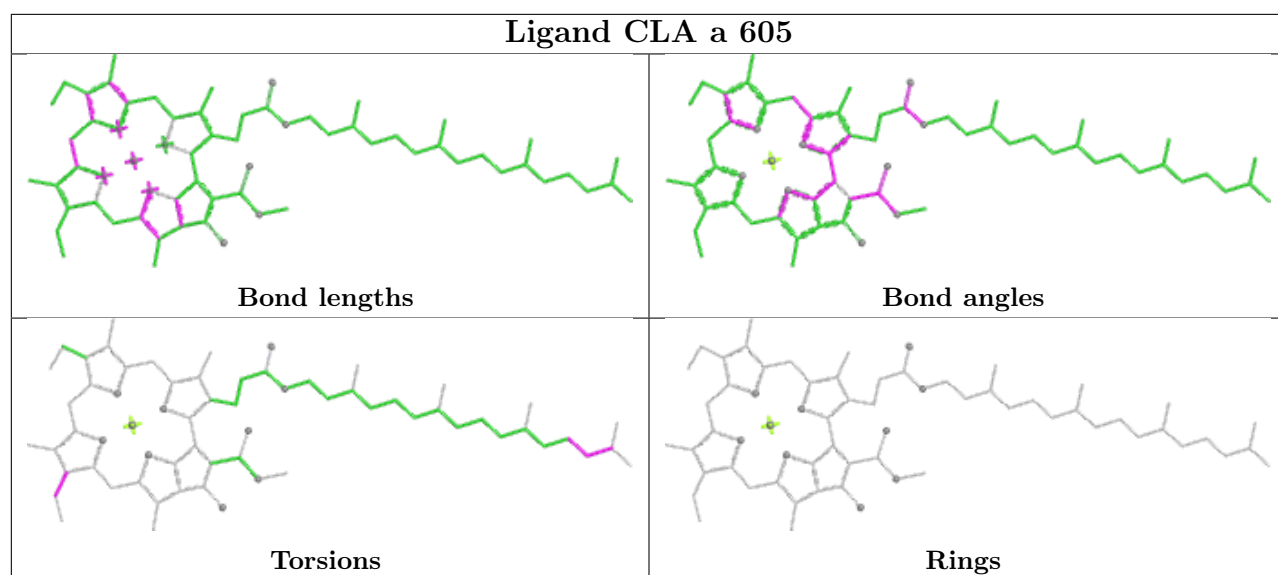




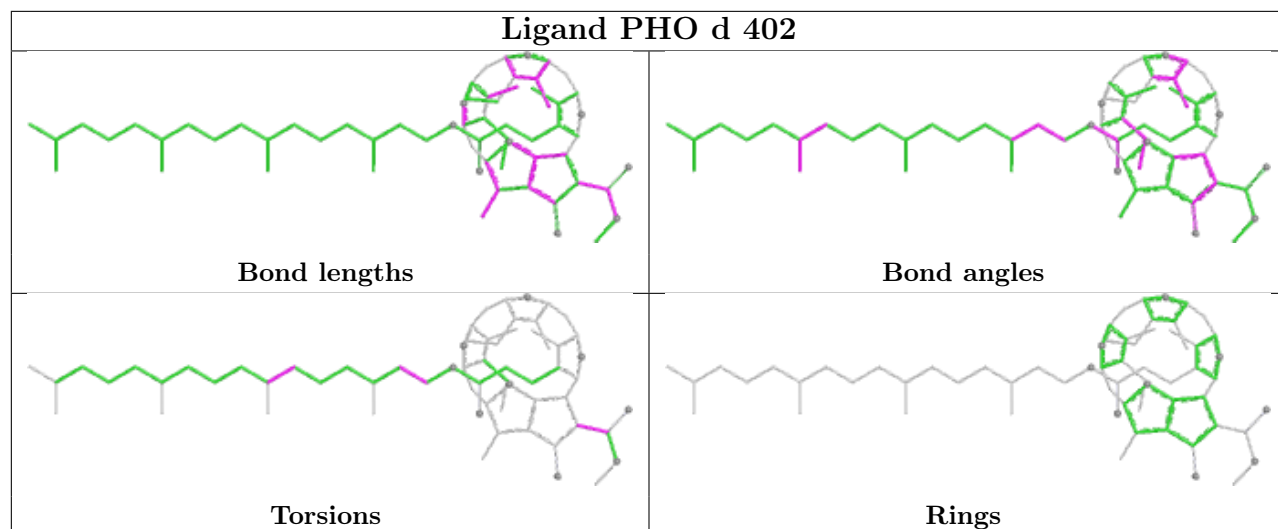




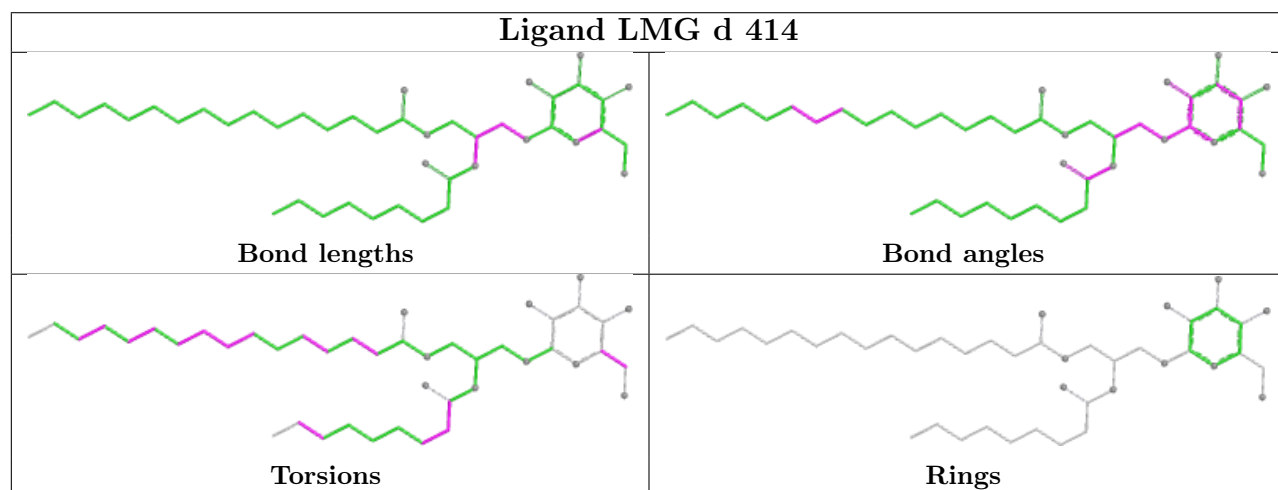




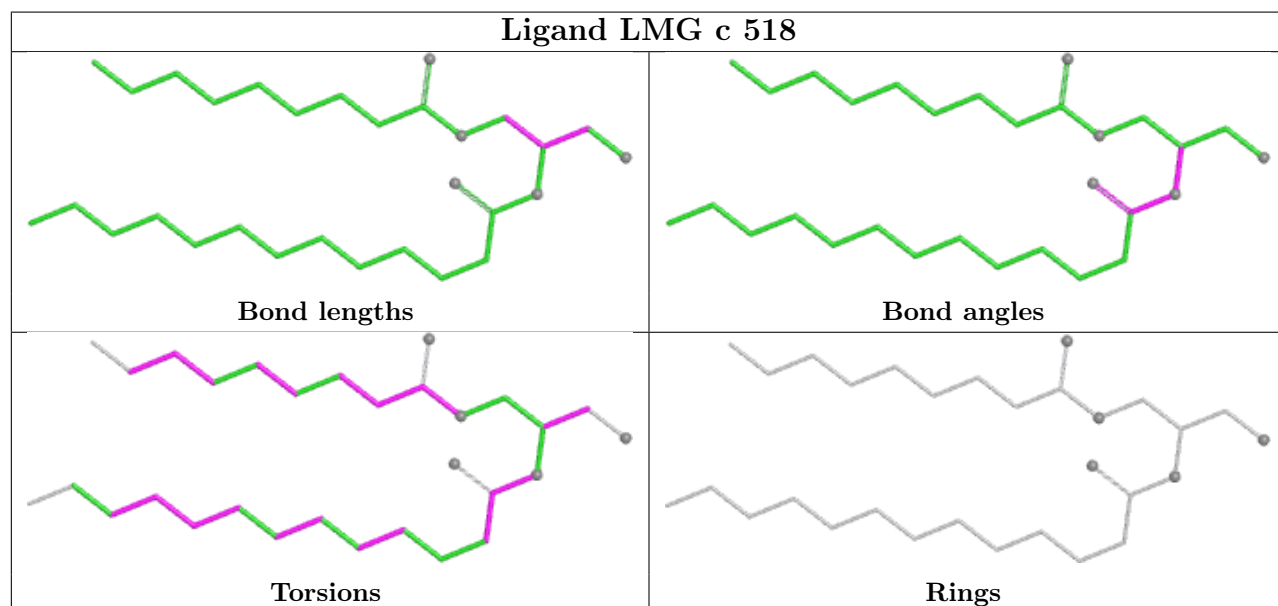
Ligand PHO d 402

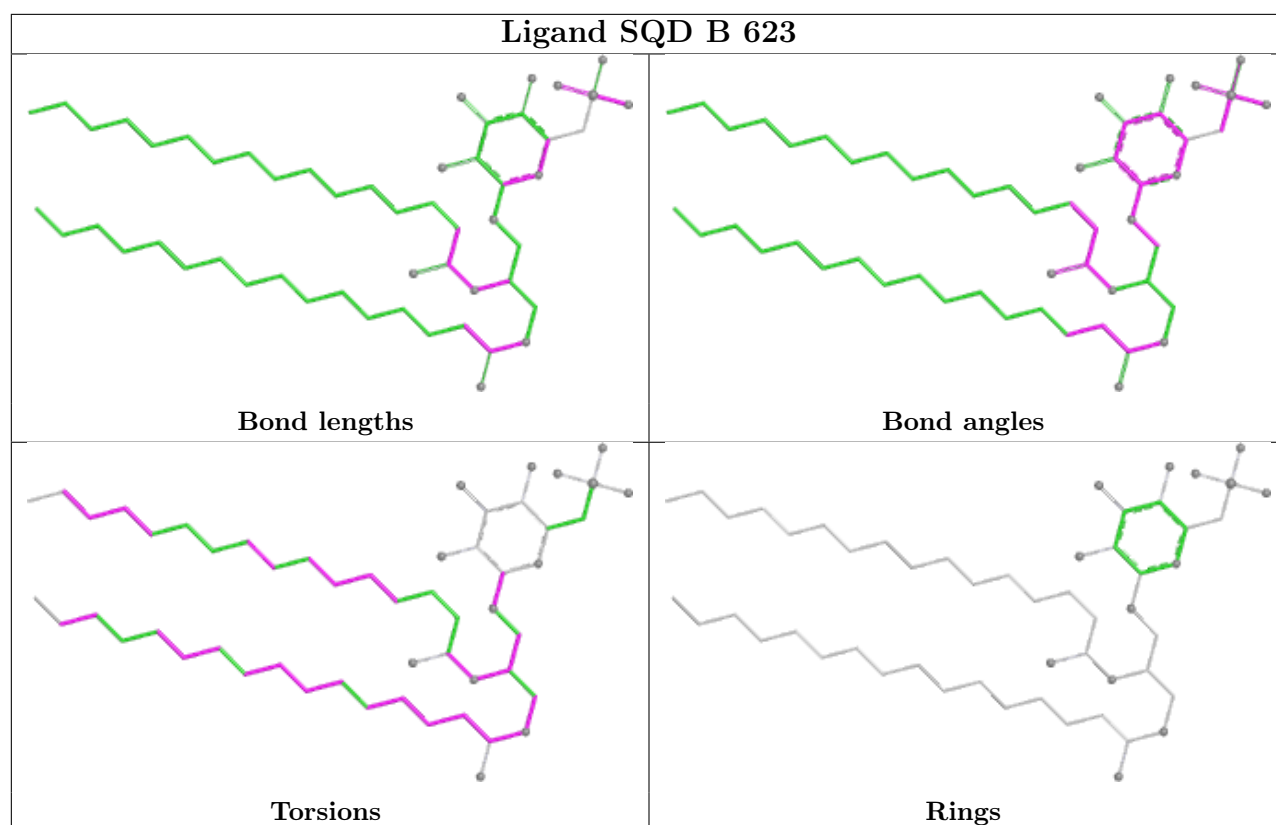


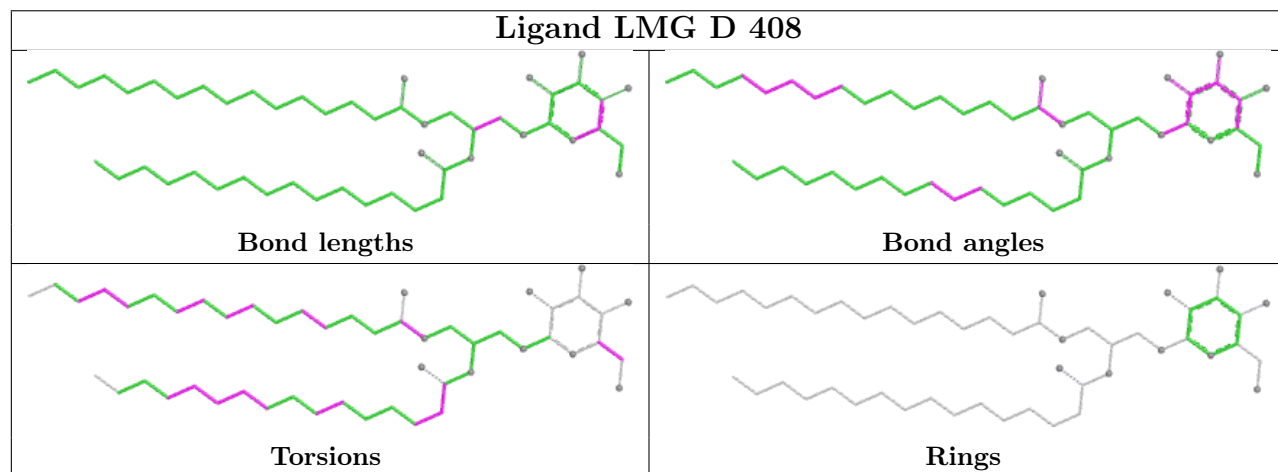
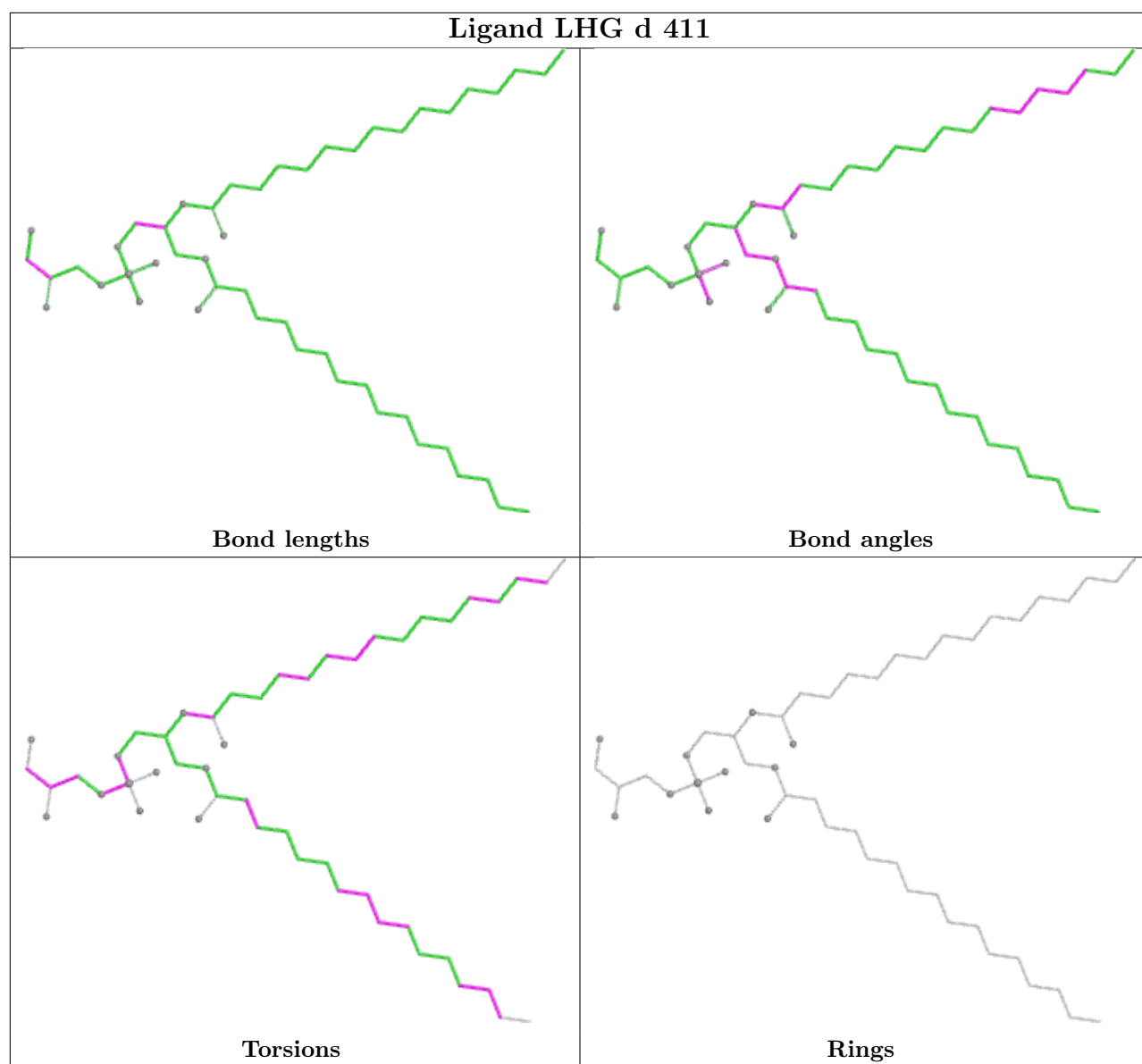
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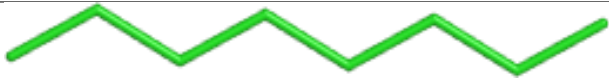
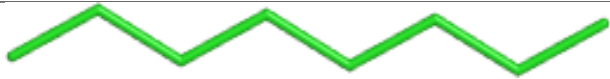


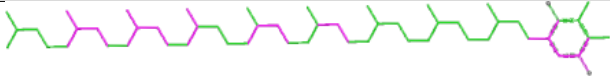
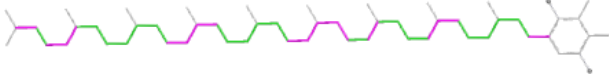
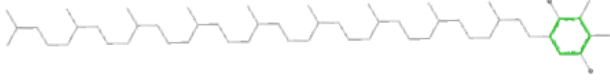
Ligand LMG c 518

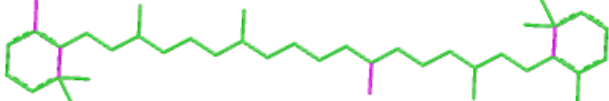
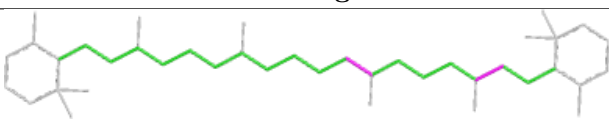
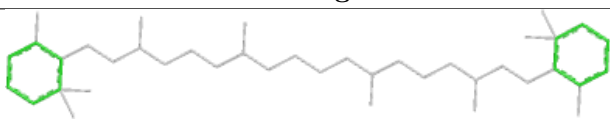


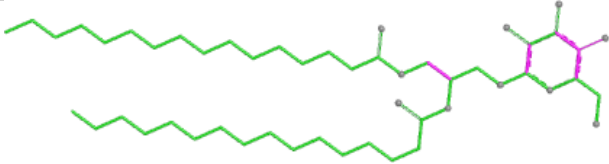
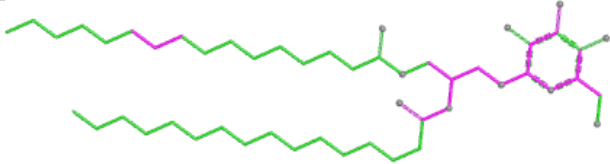
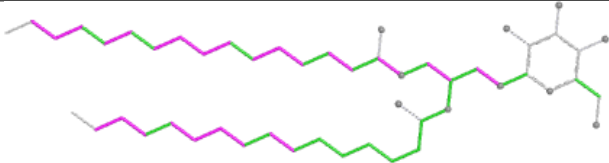
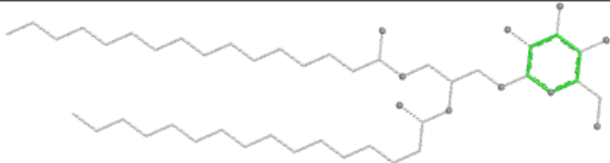




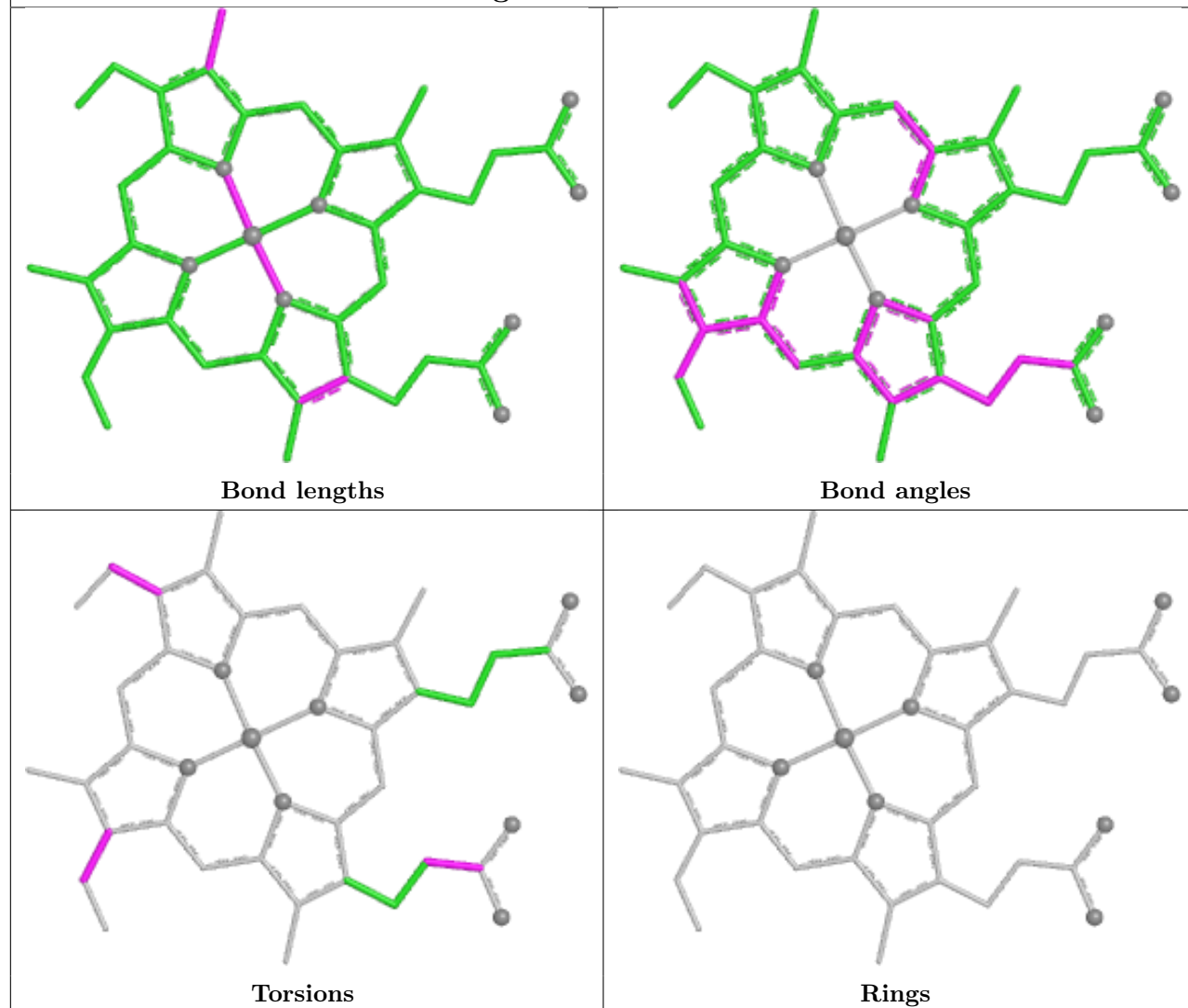
Ligand STE f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 a 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

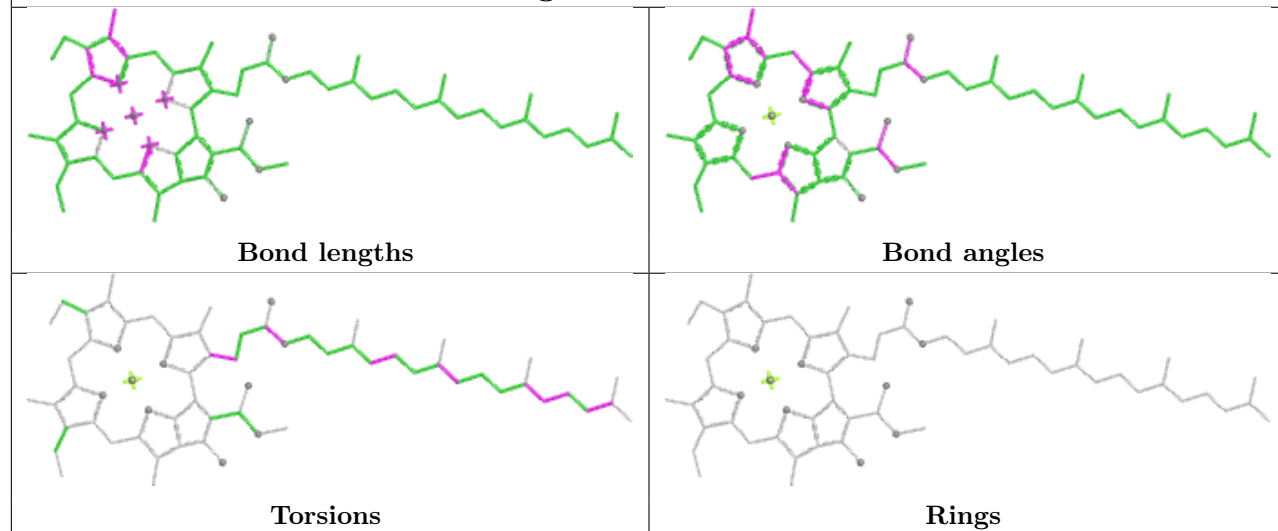
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

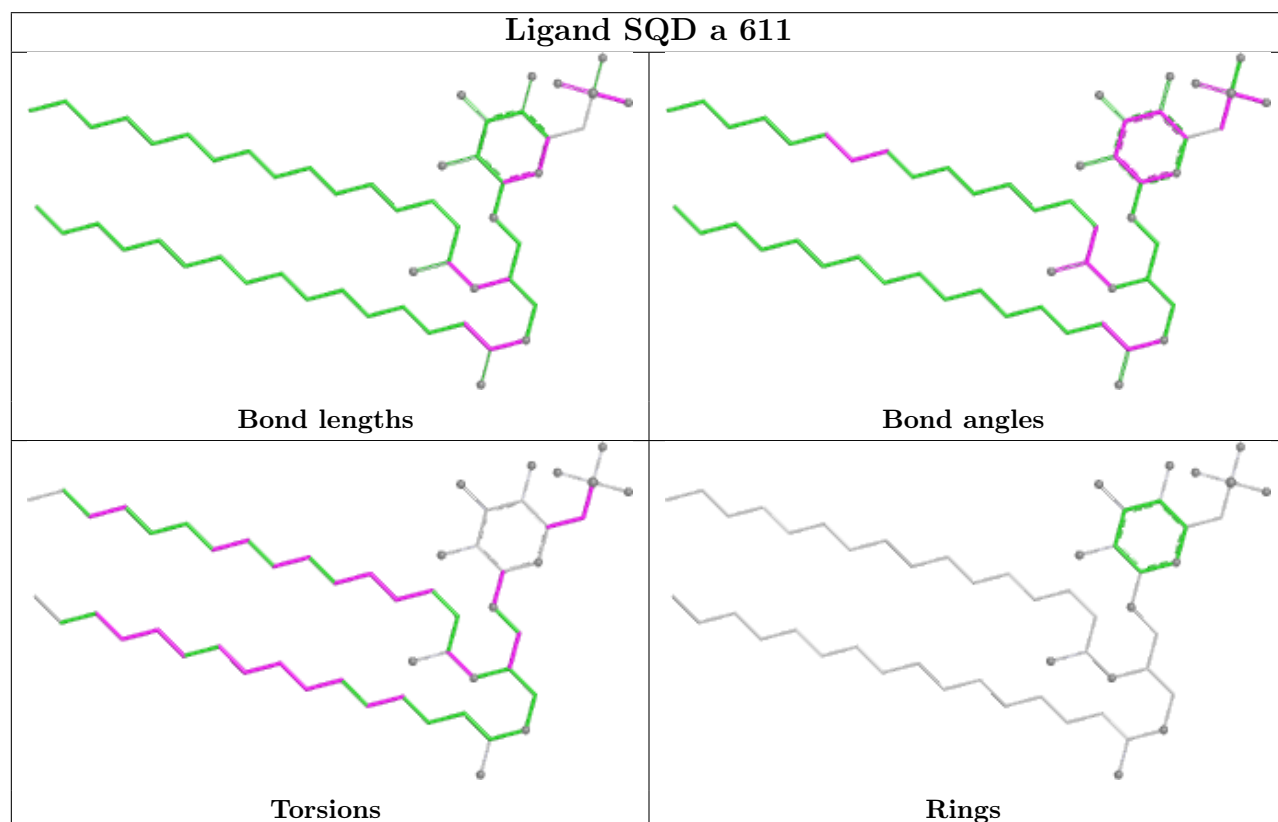
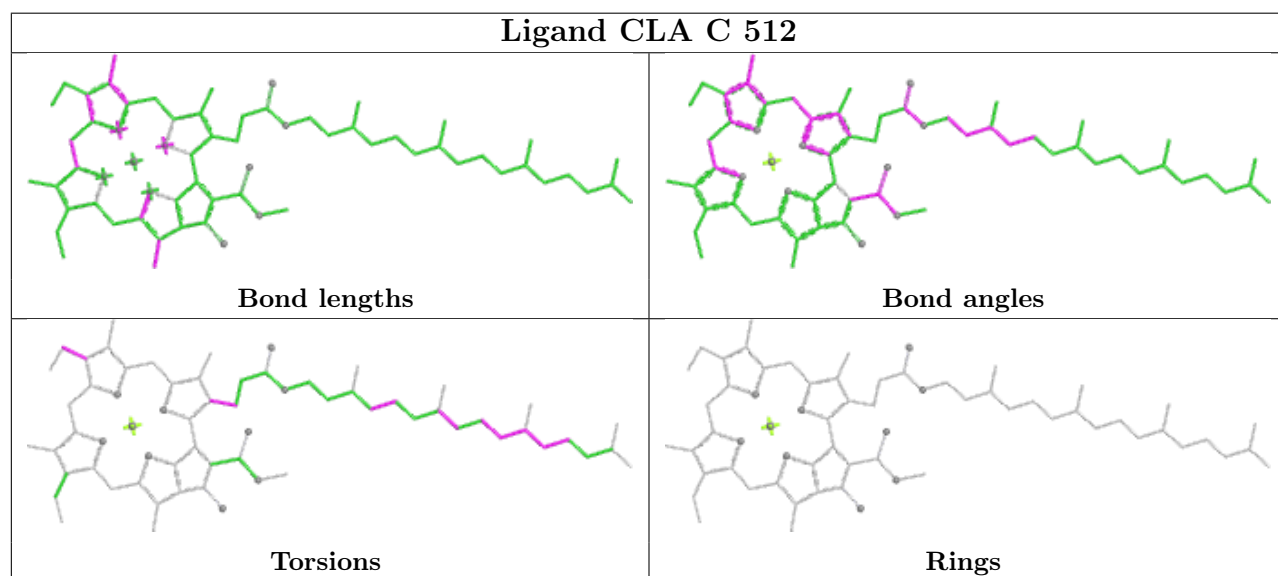
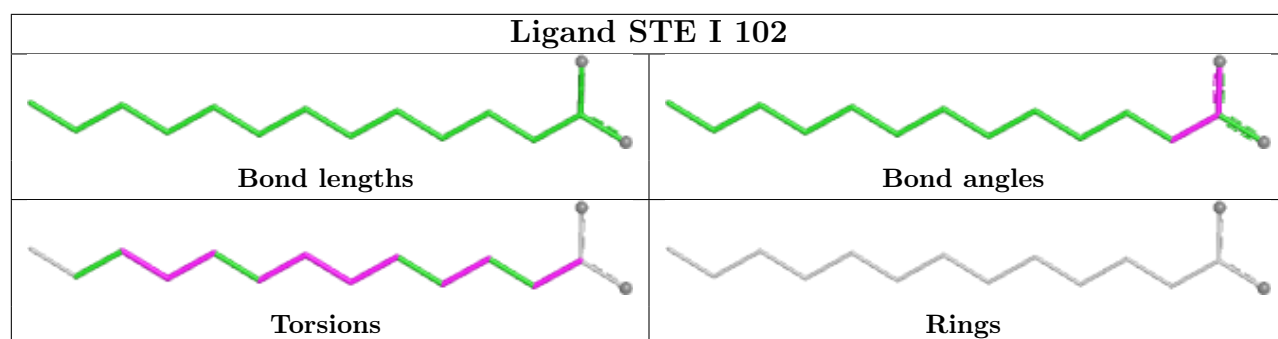
Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC V 201

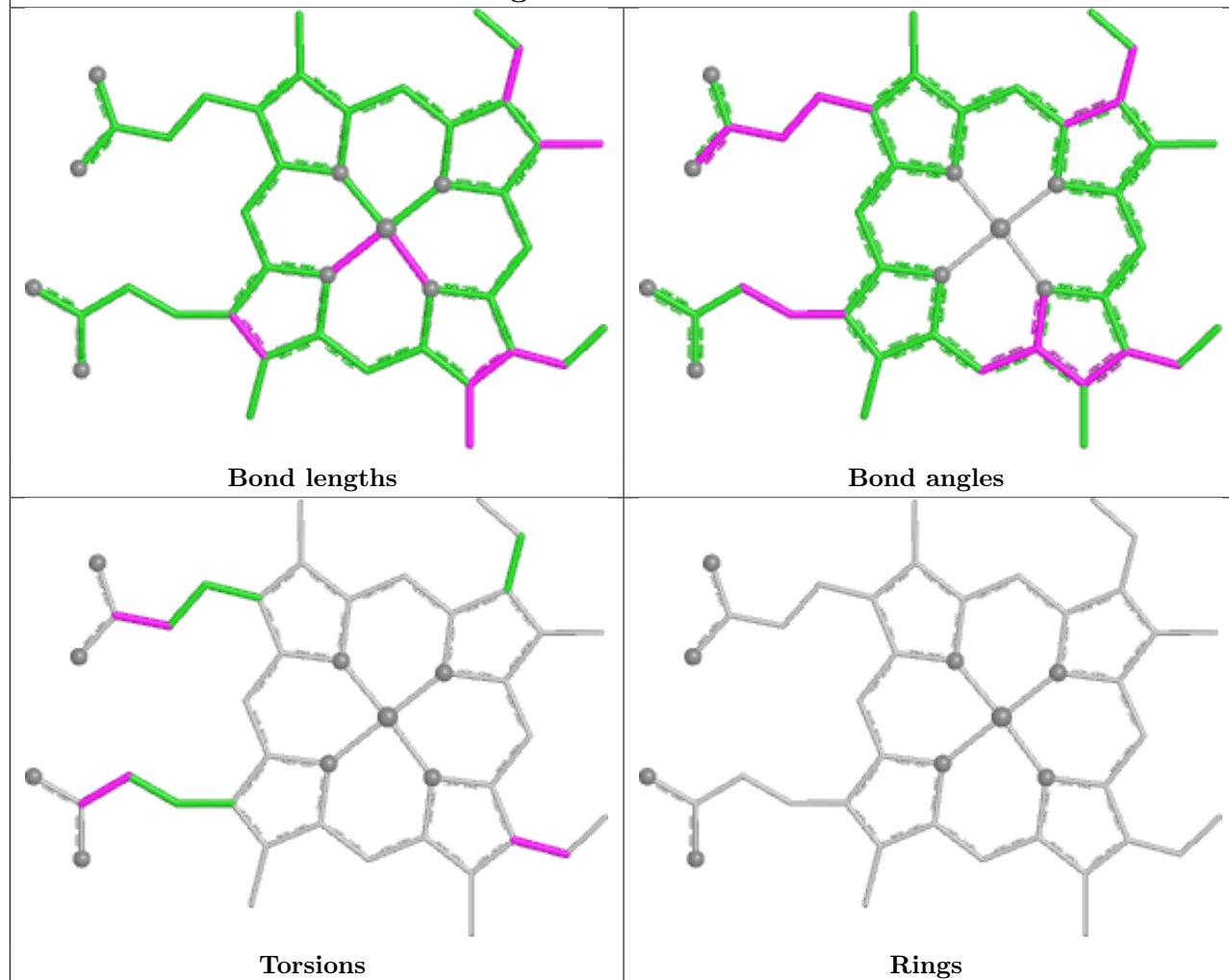


Ligand CLA c 513

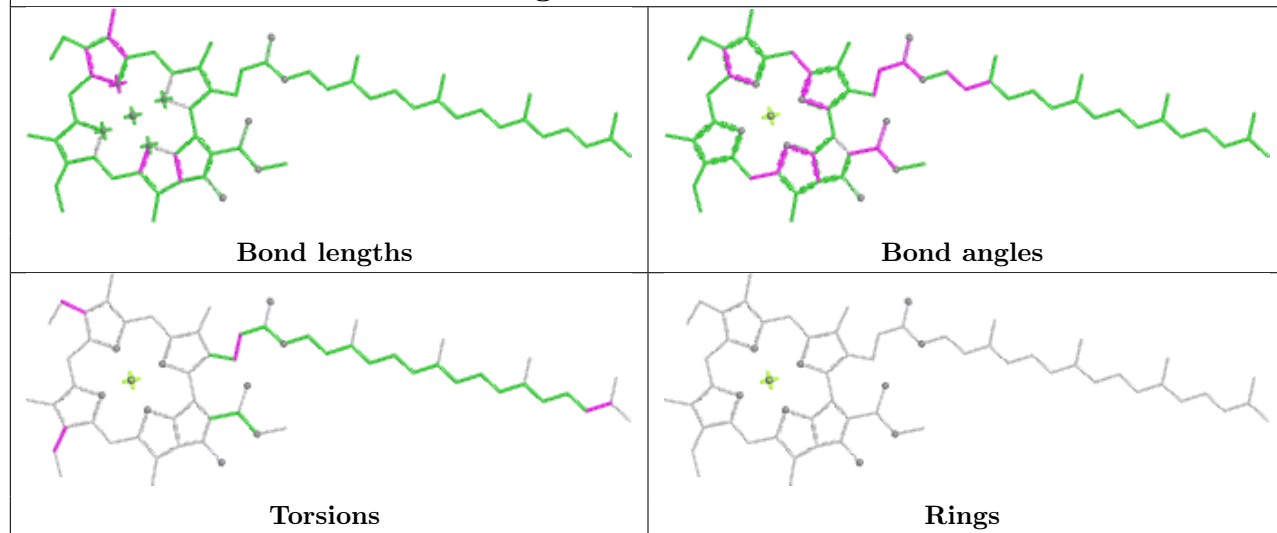


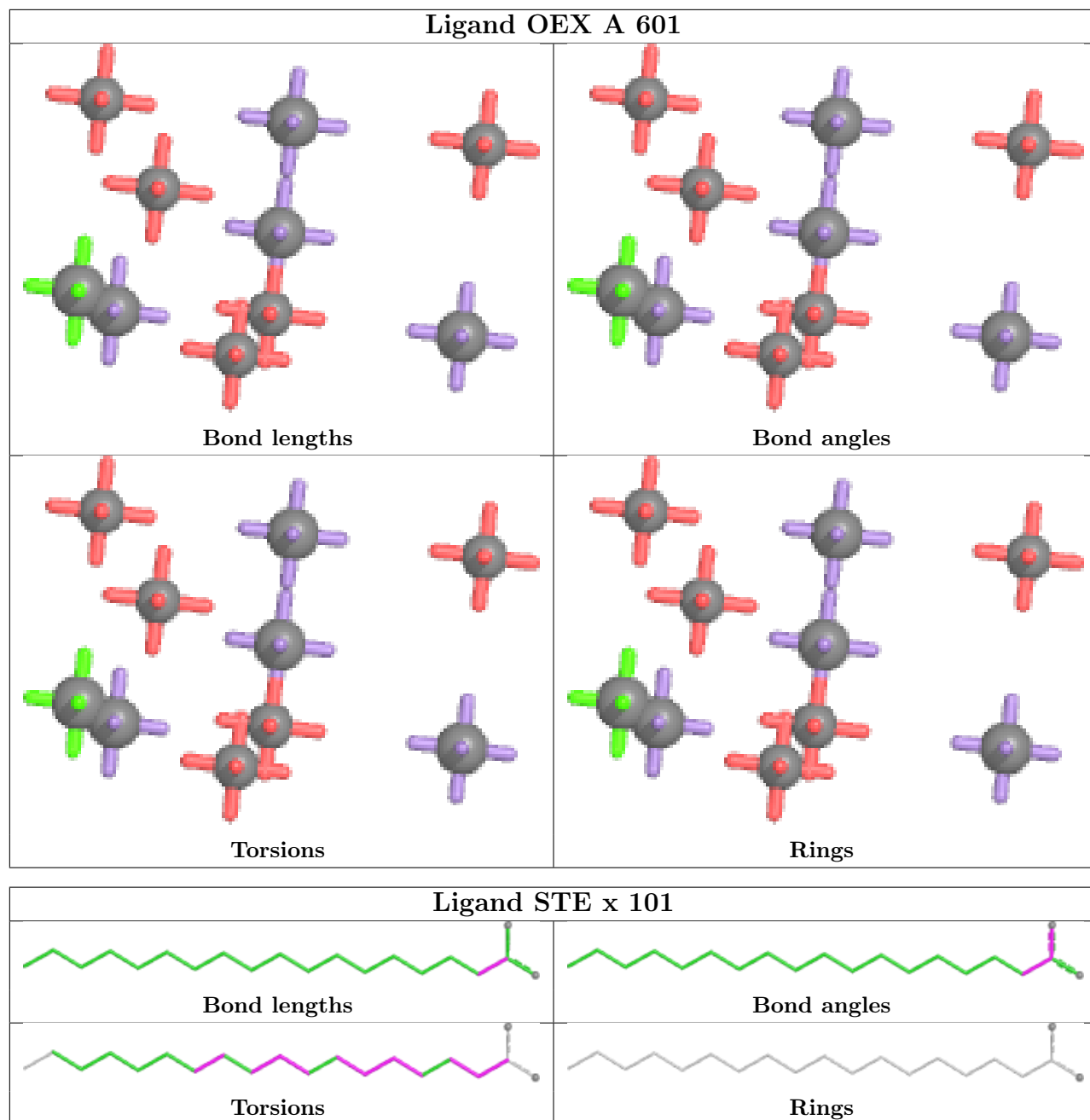


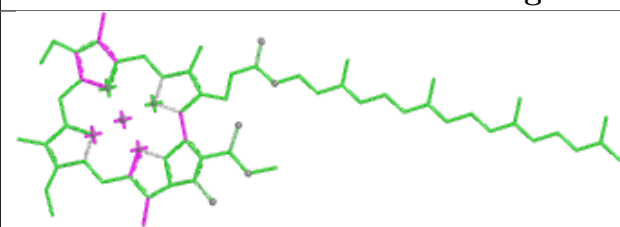
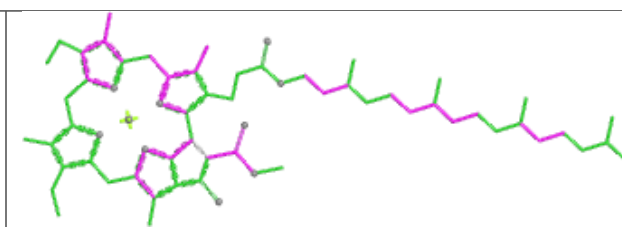
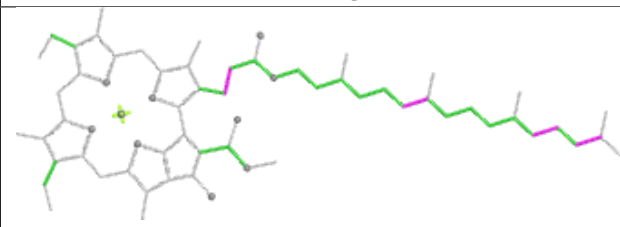
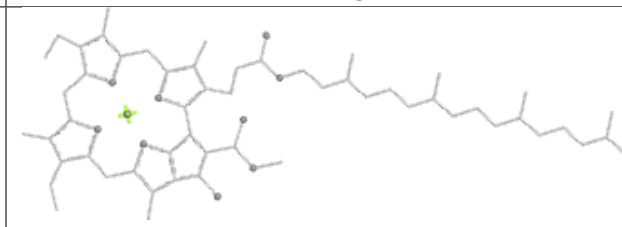
Ligand HEM e 102



Ligand CLA b 610

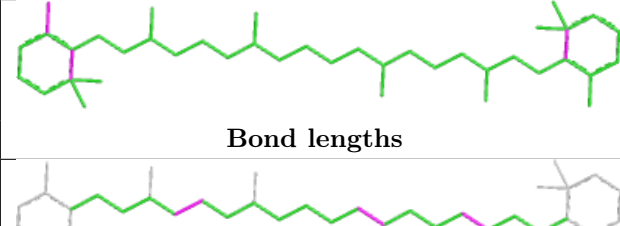
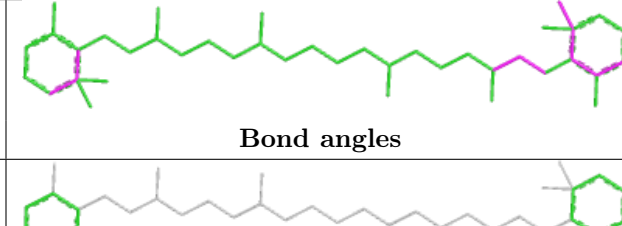
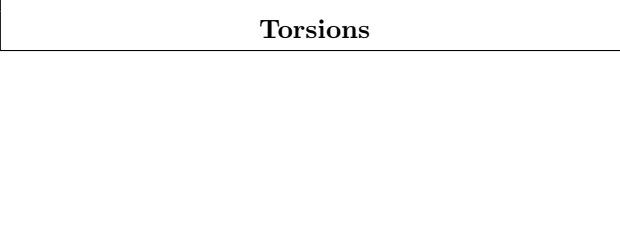
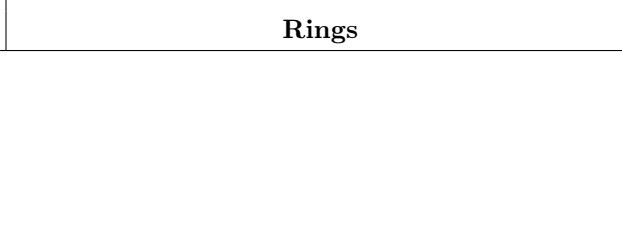


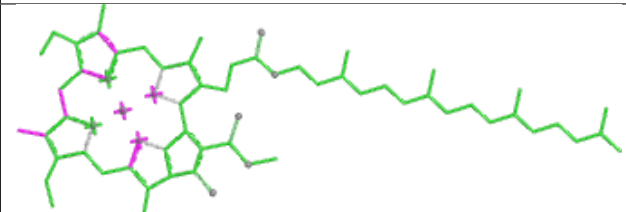
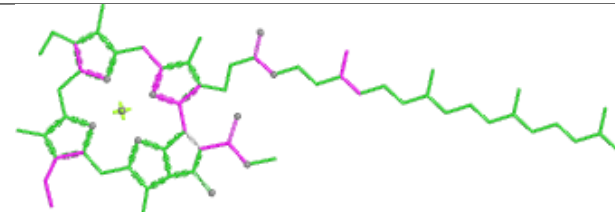
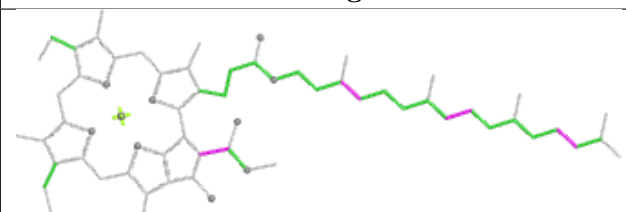
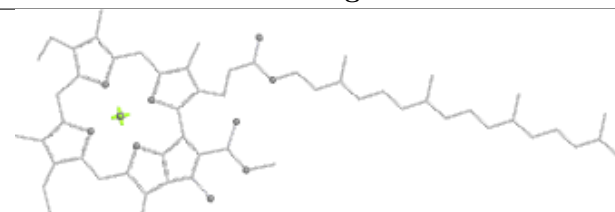


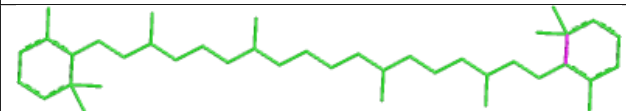
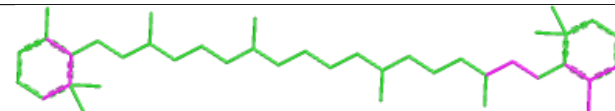
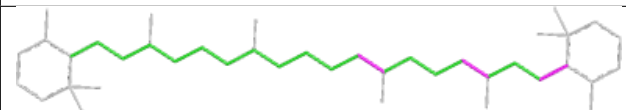
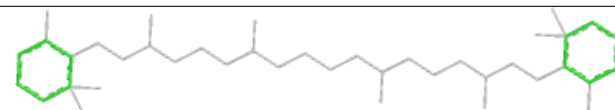
Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

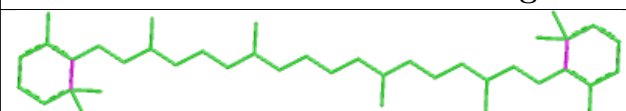
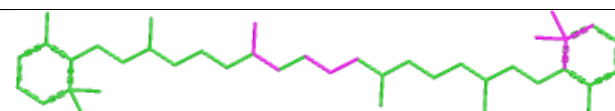
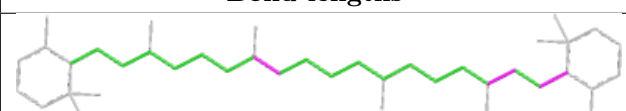
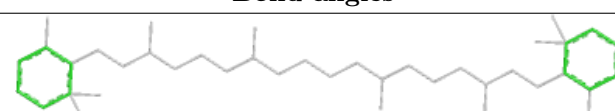
Ligand STE Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

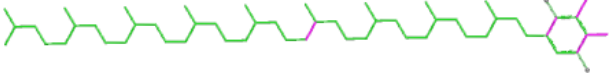
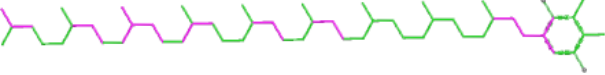
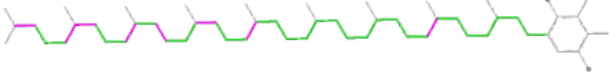
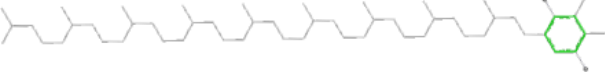
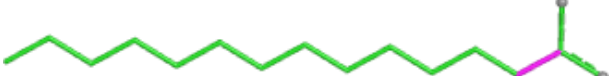
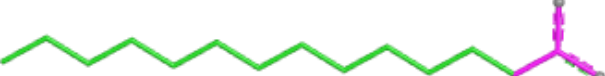
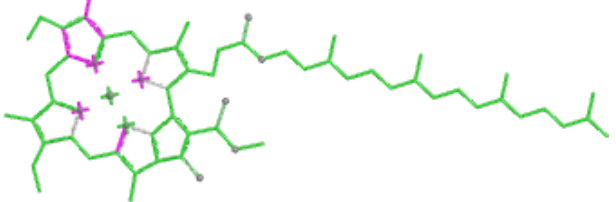
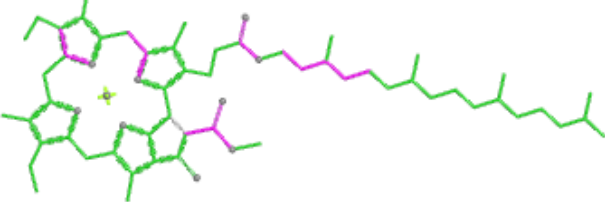
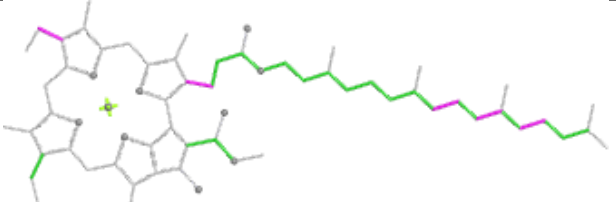
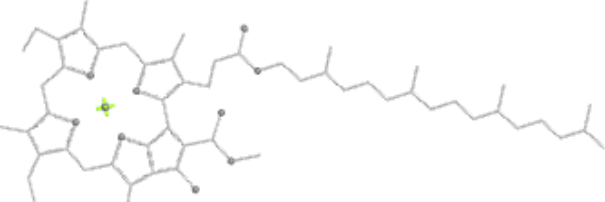
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

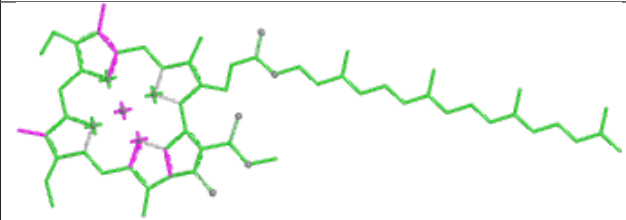
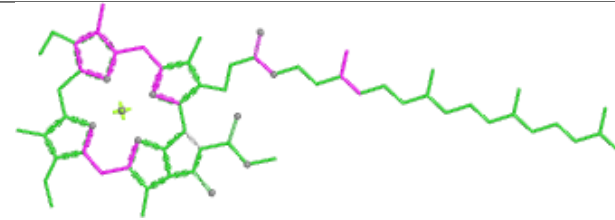
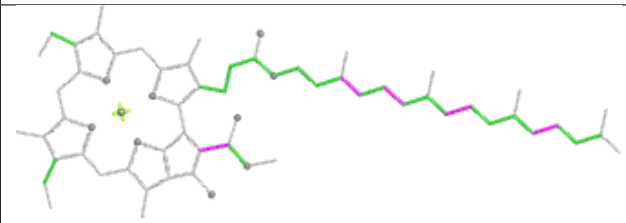
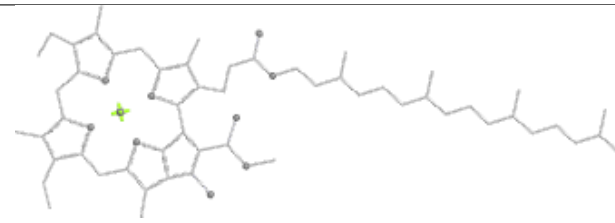
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

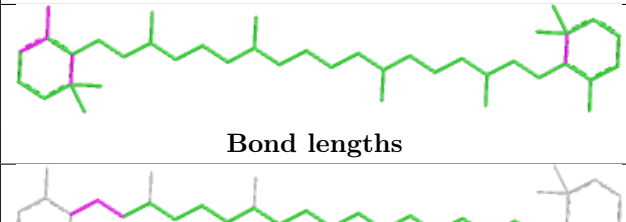
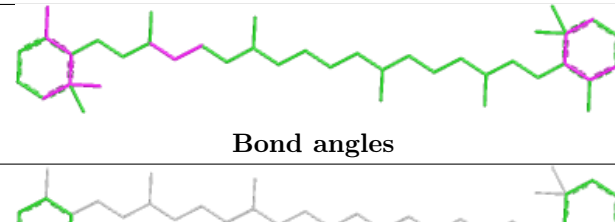
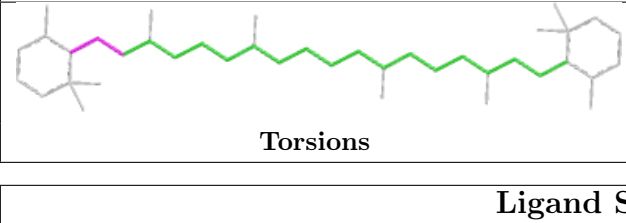
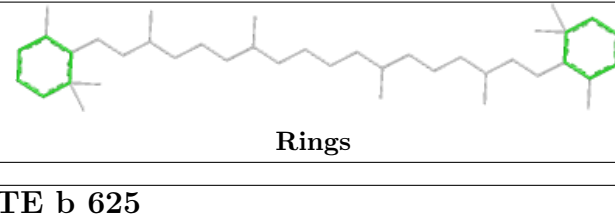
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

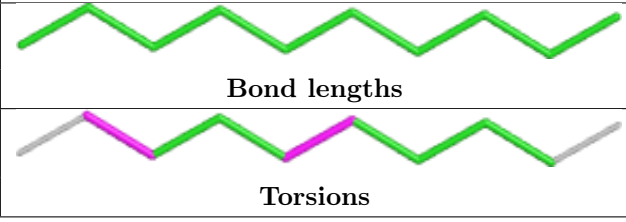
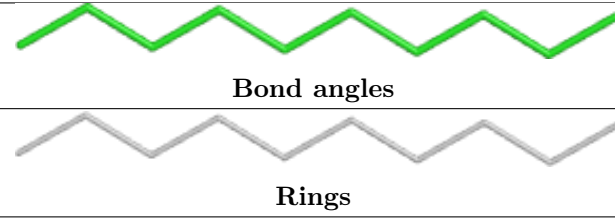
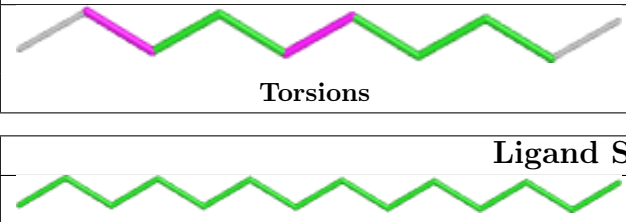
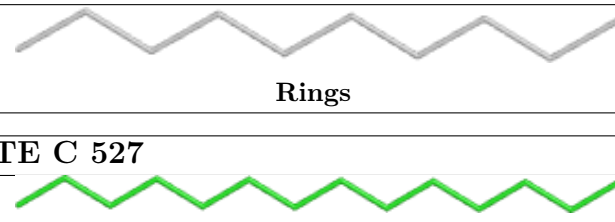
Ligand STE c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

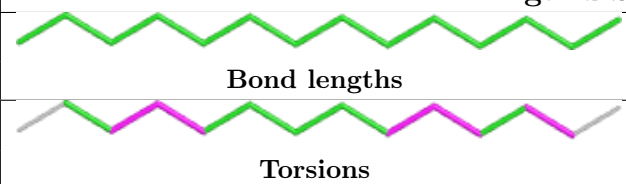
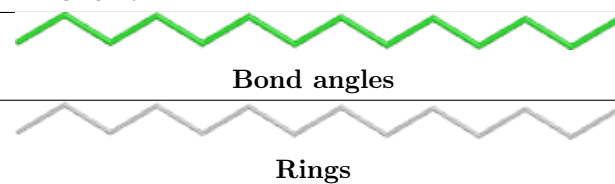
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

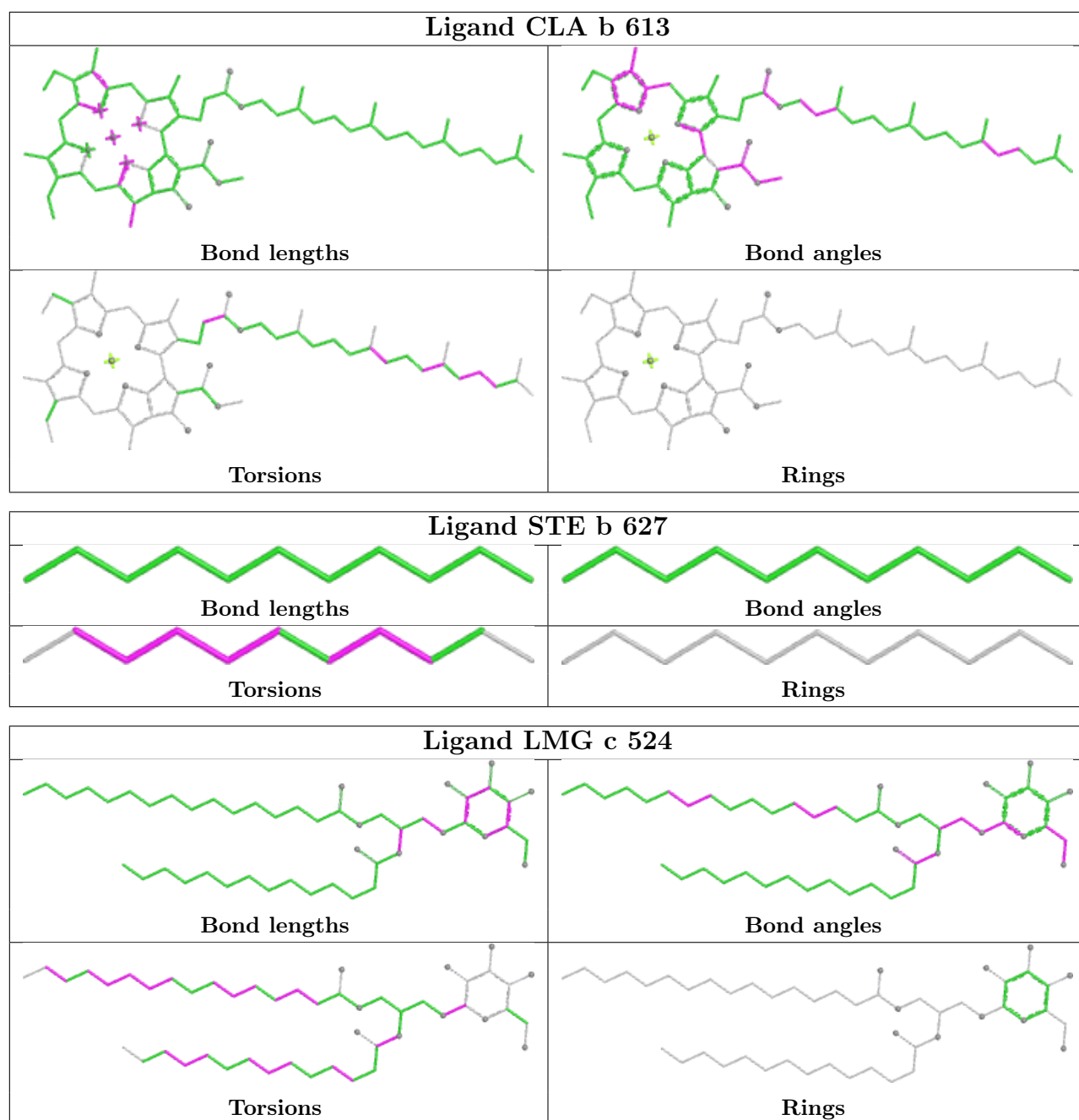
Ligand PL9 d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE A 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

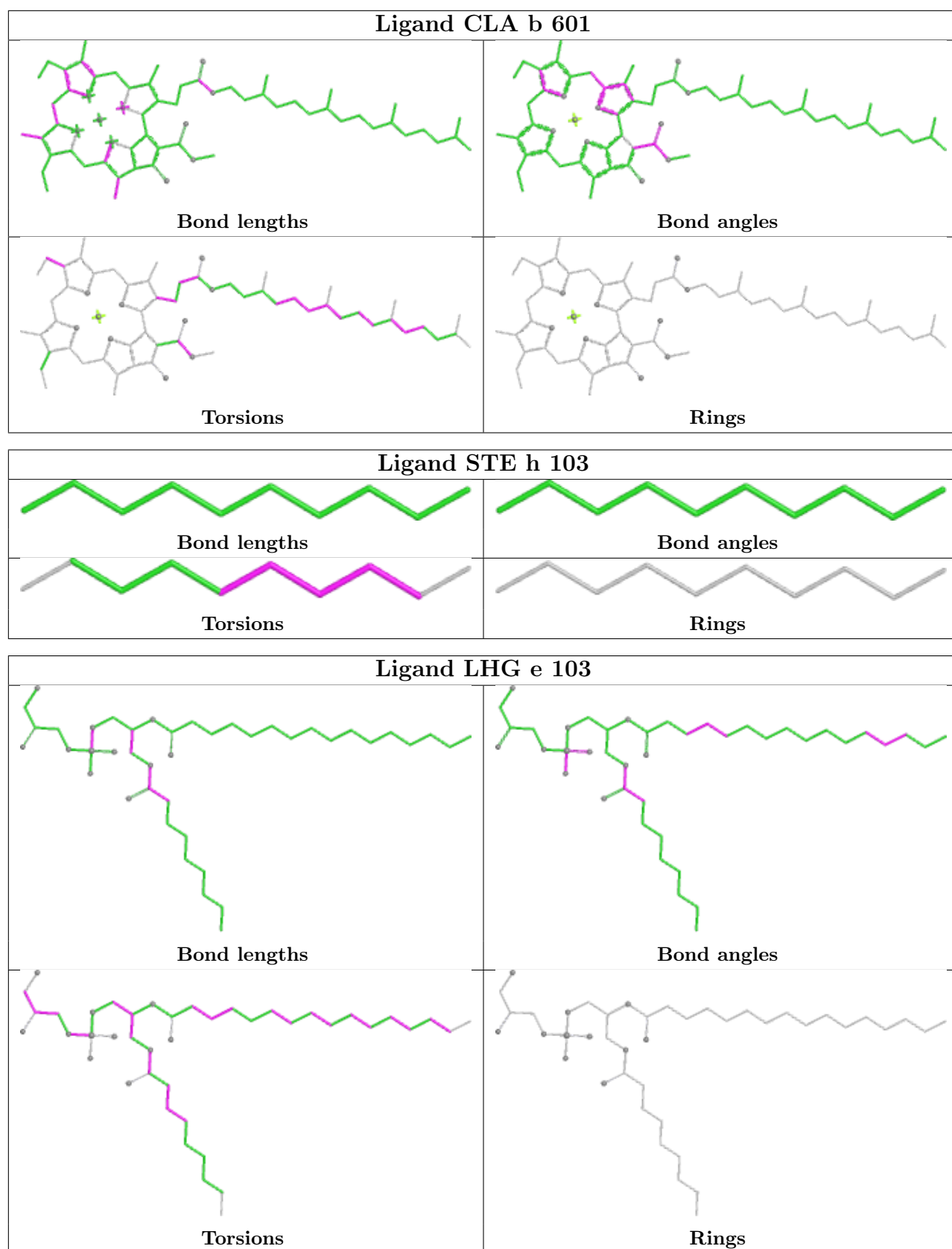
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

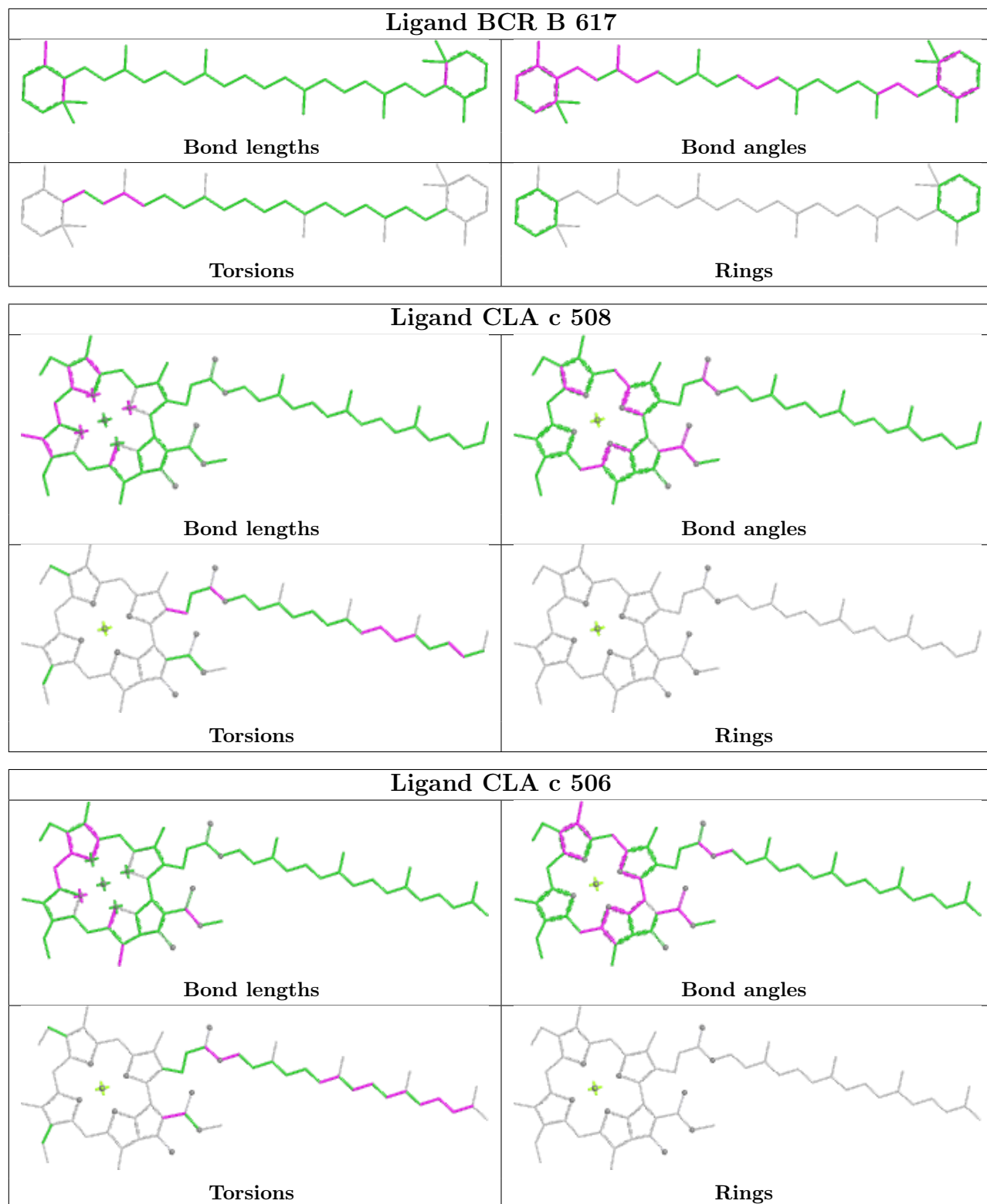
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

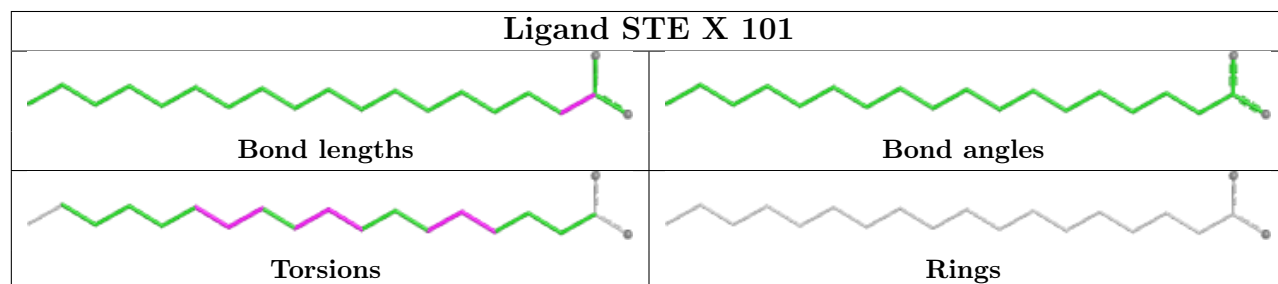
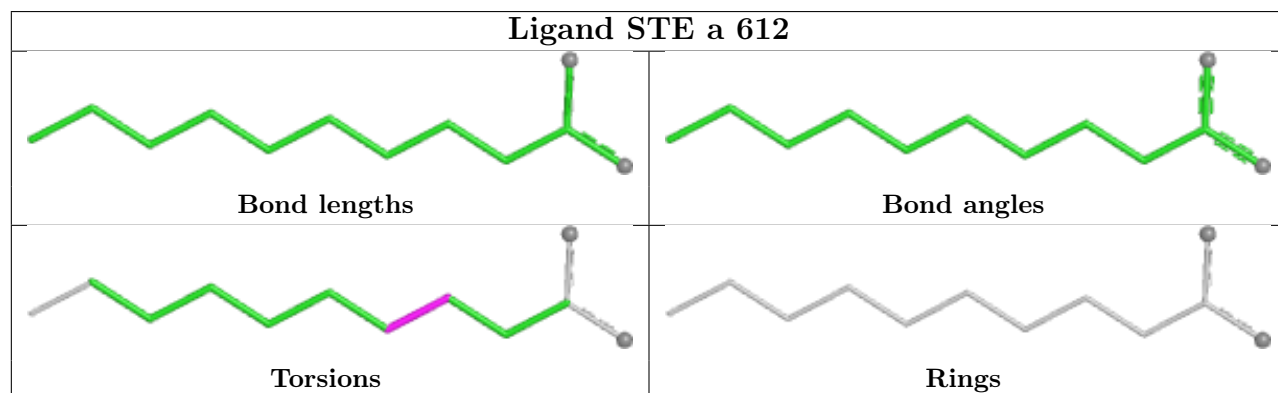
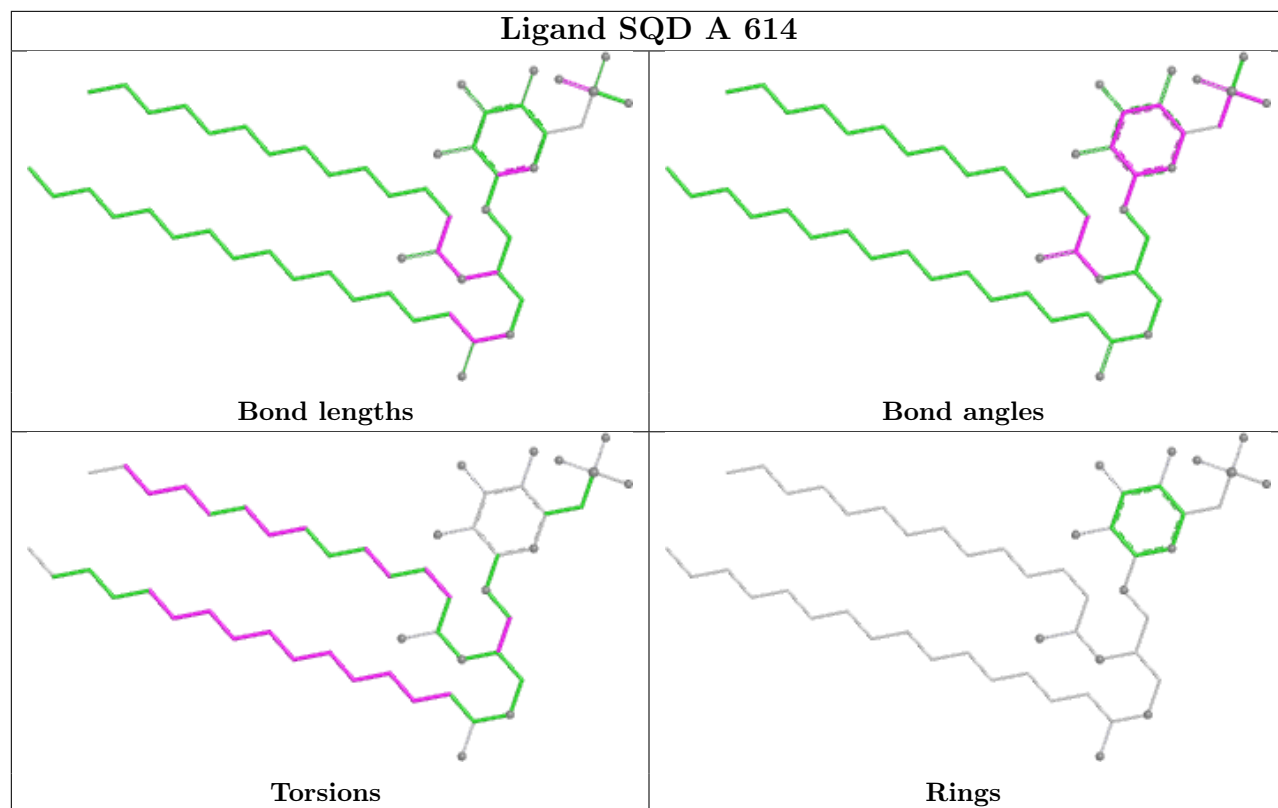
Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

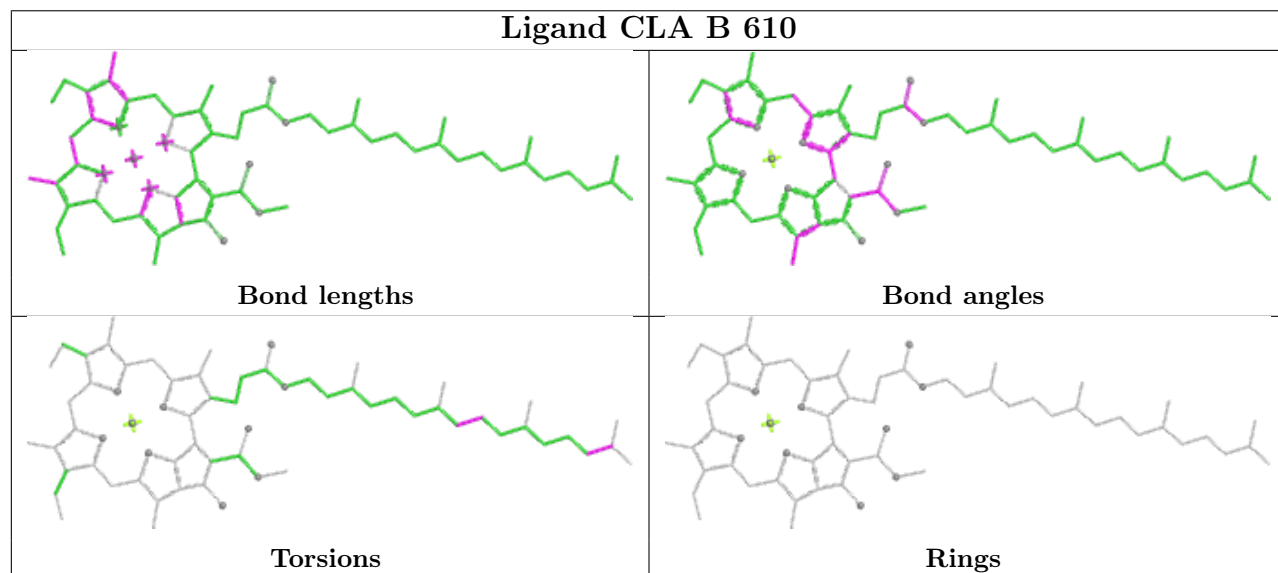
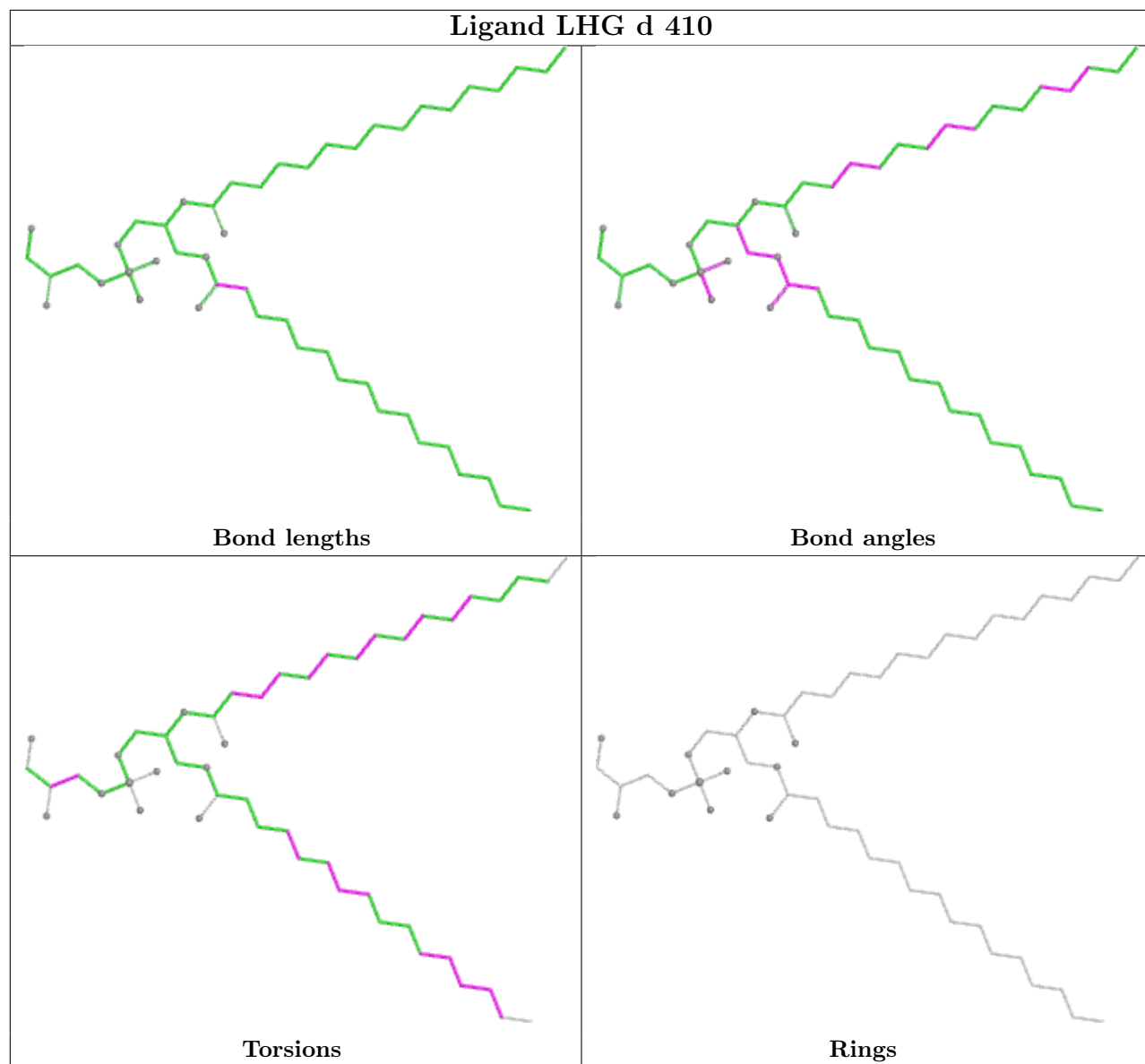
Ligand STE C 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

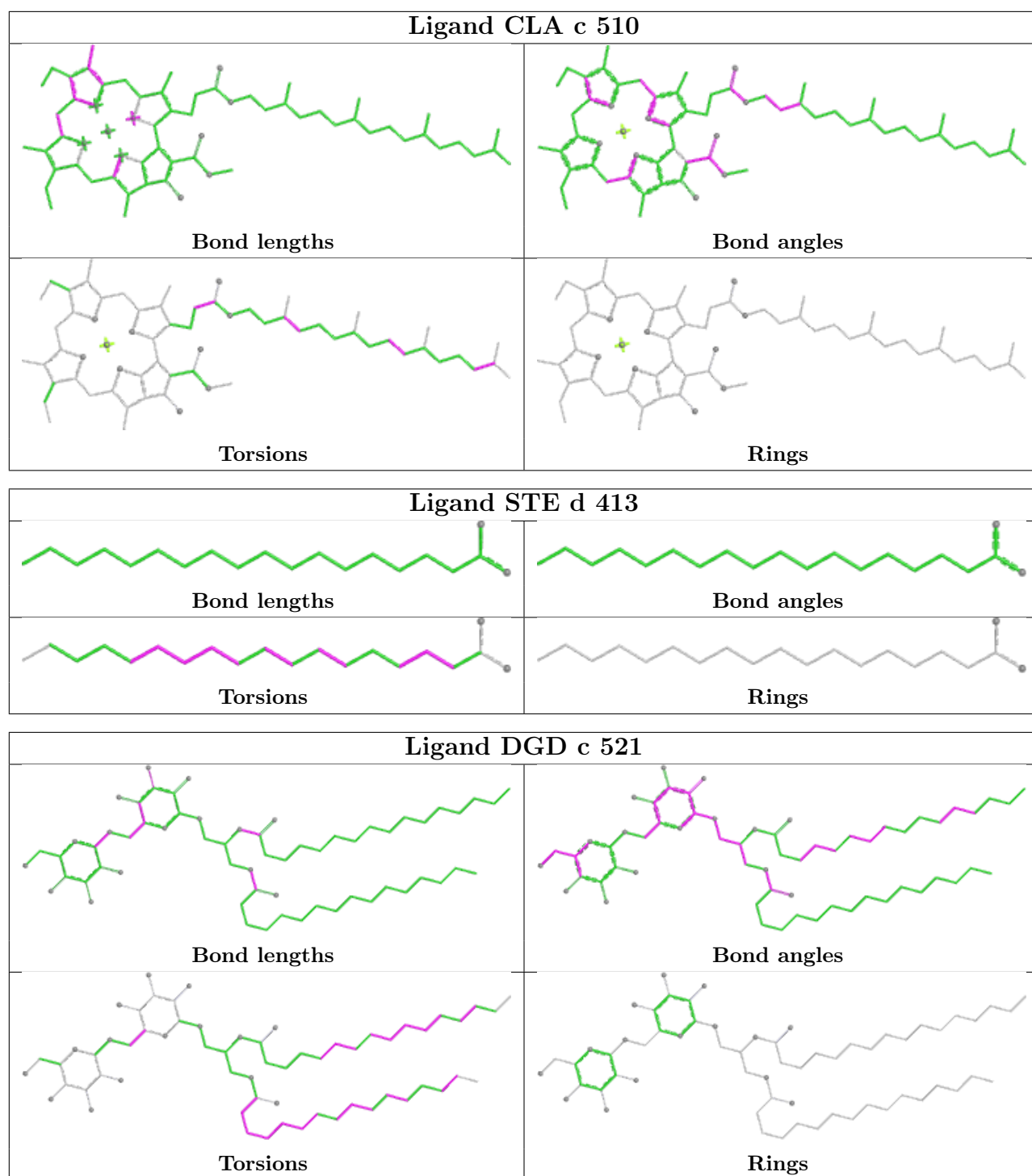




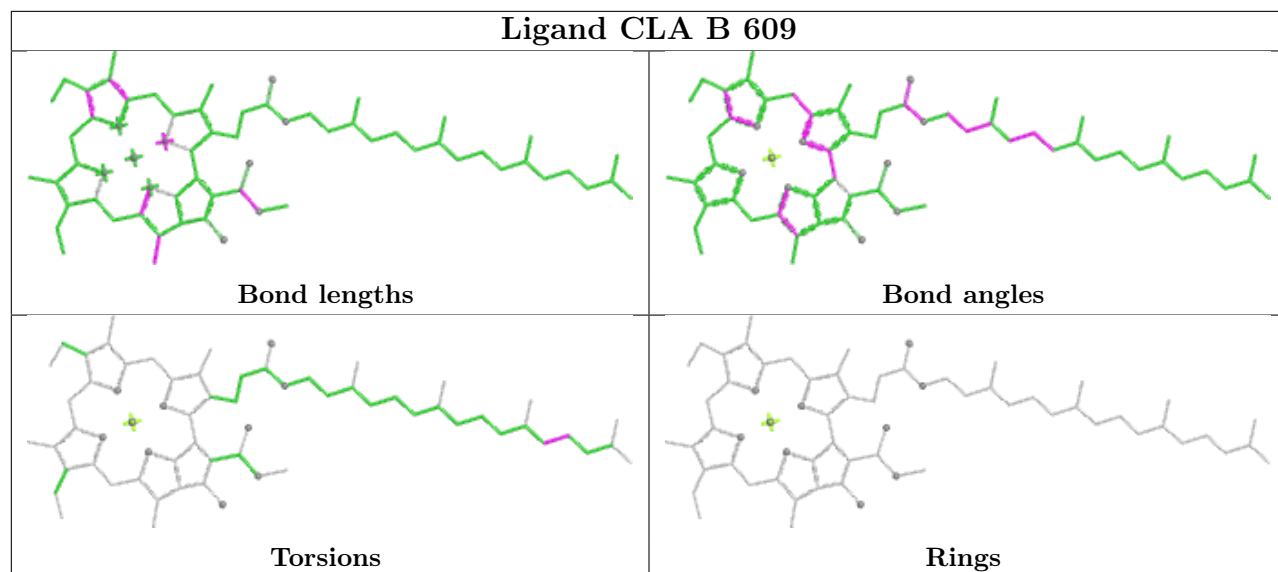




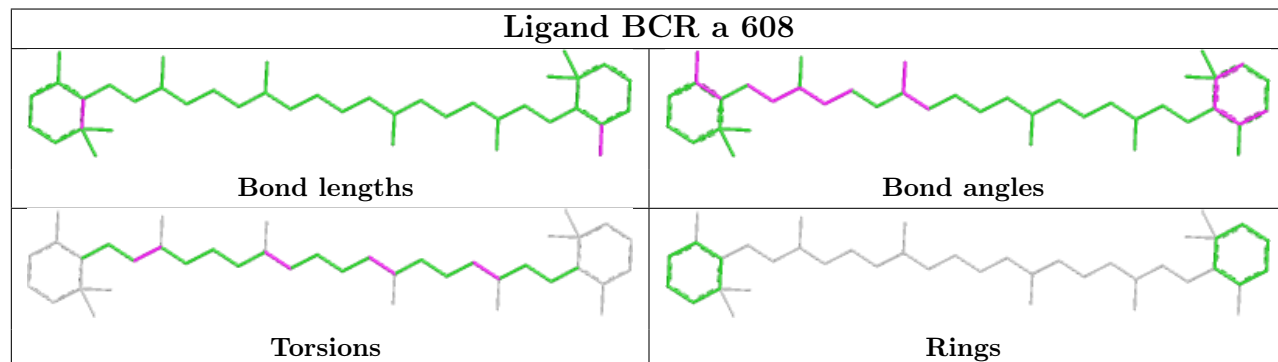




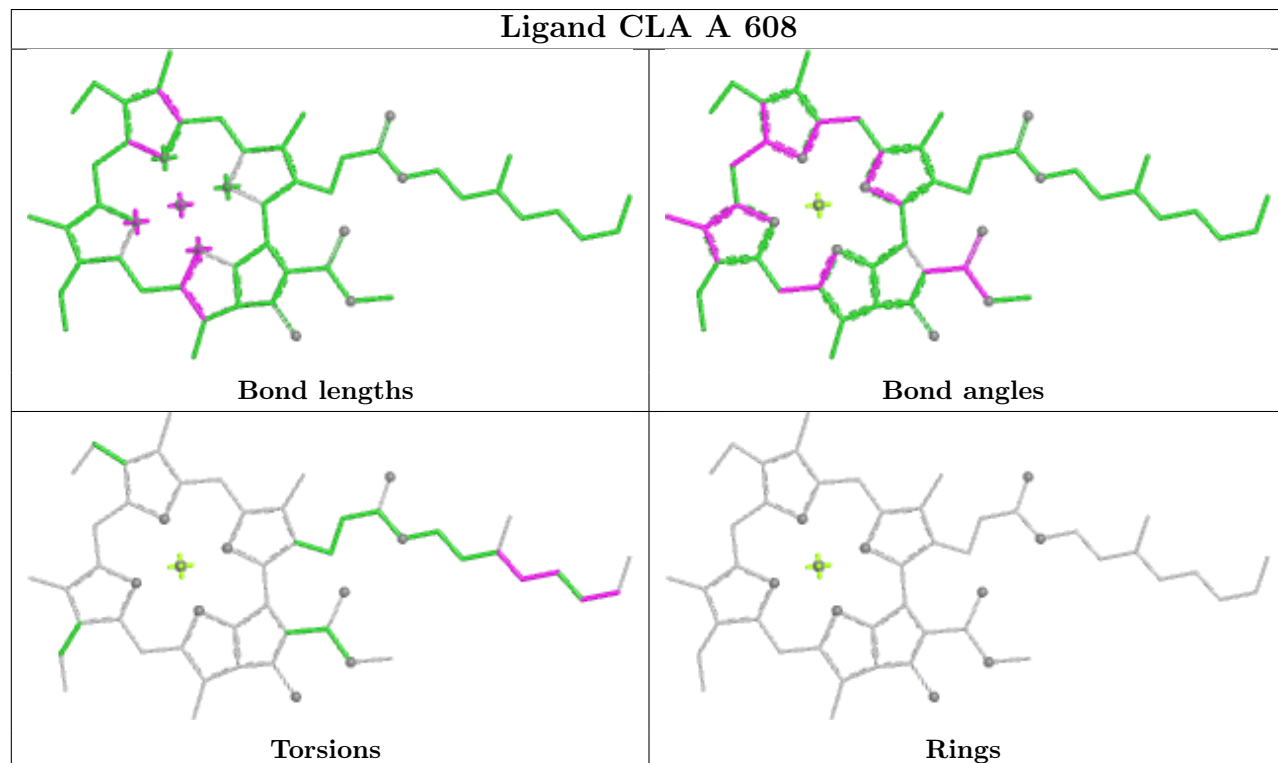
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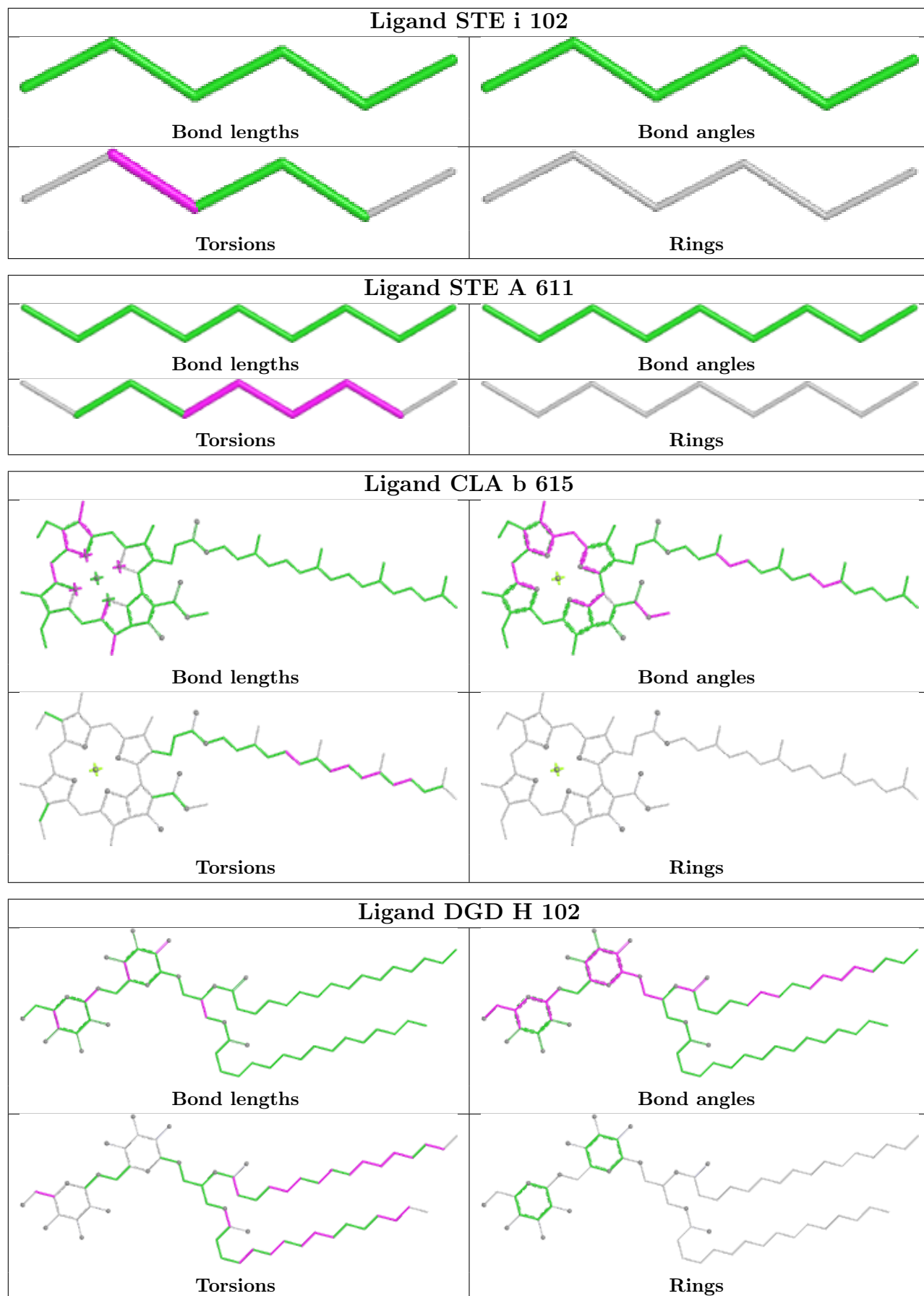


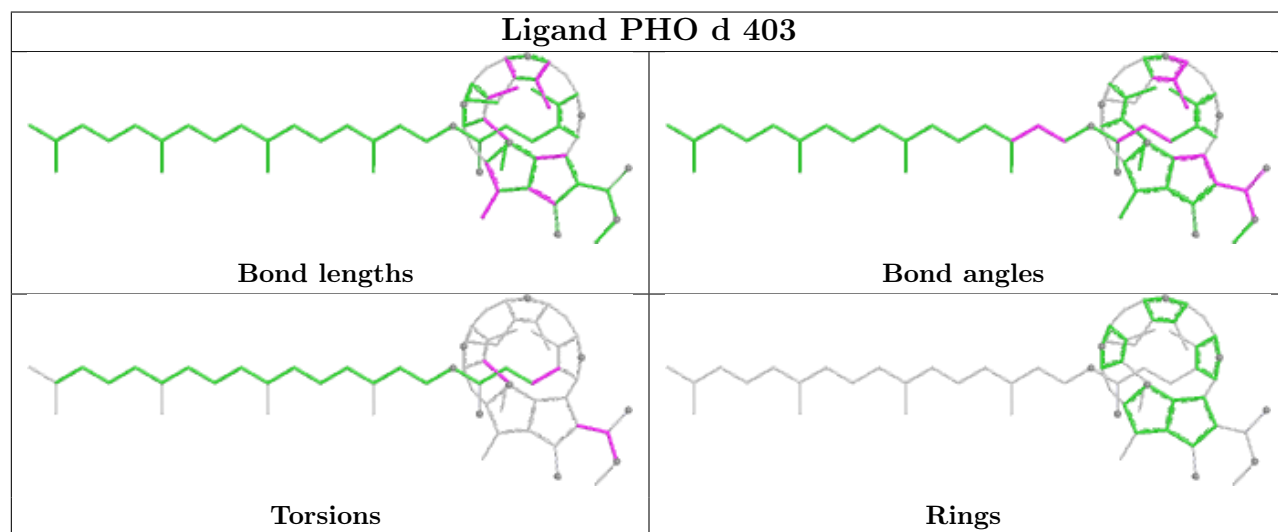
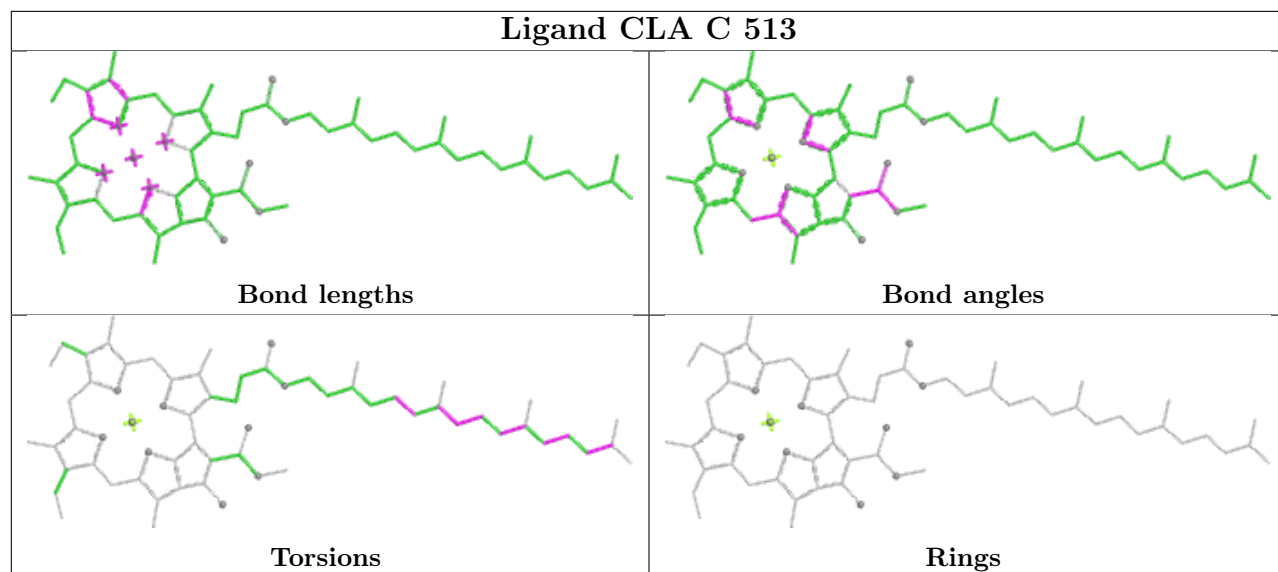
Ligand BCR a 608

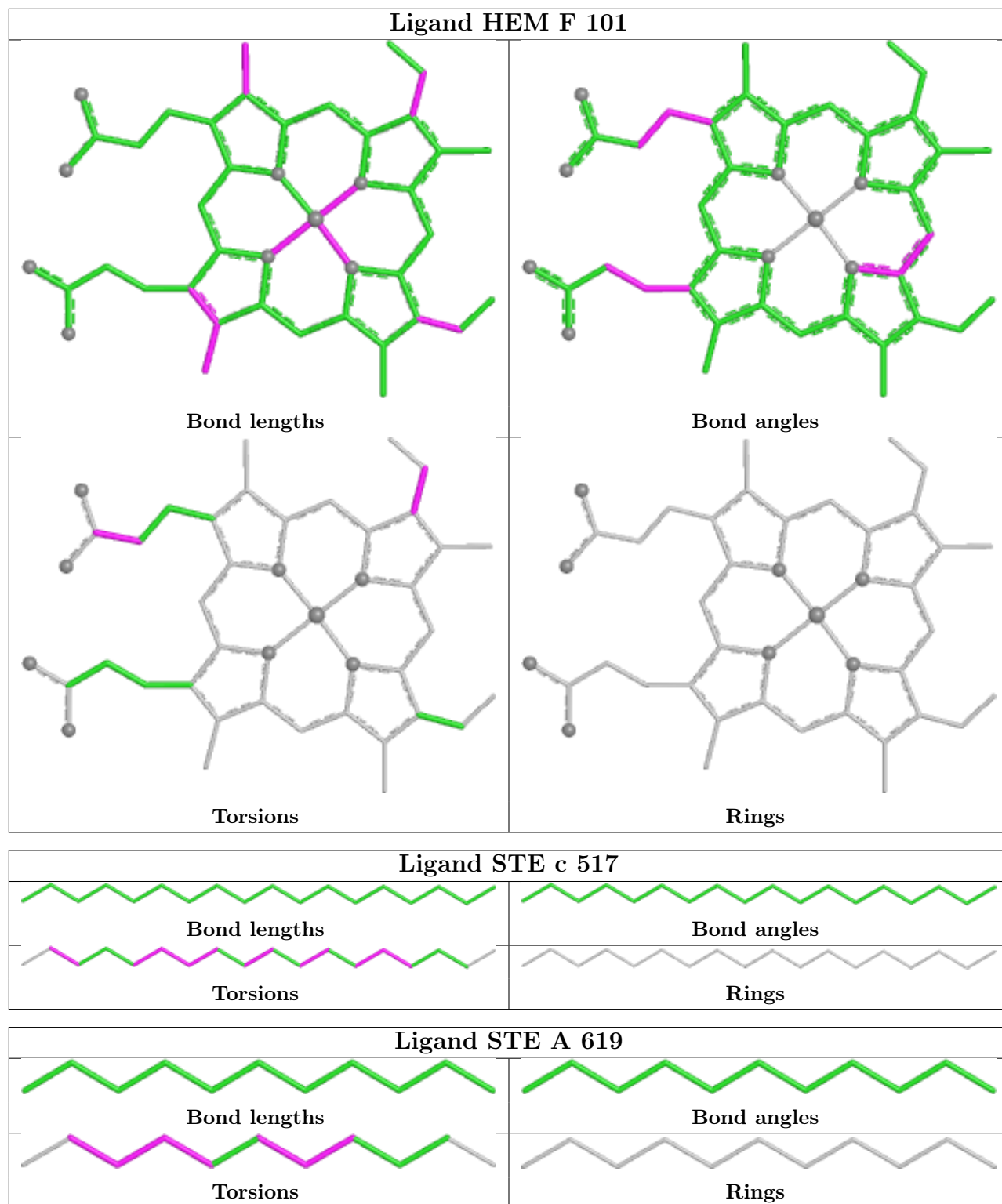


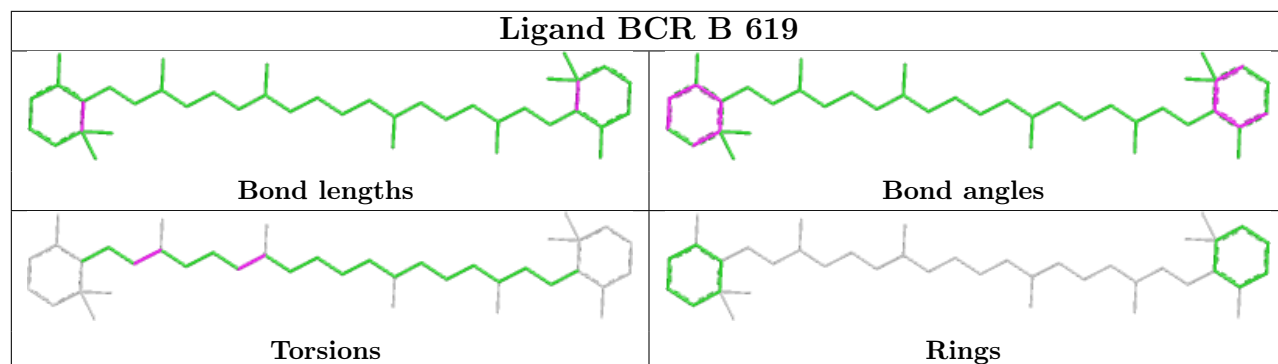
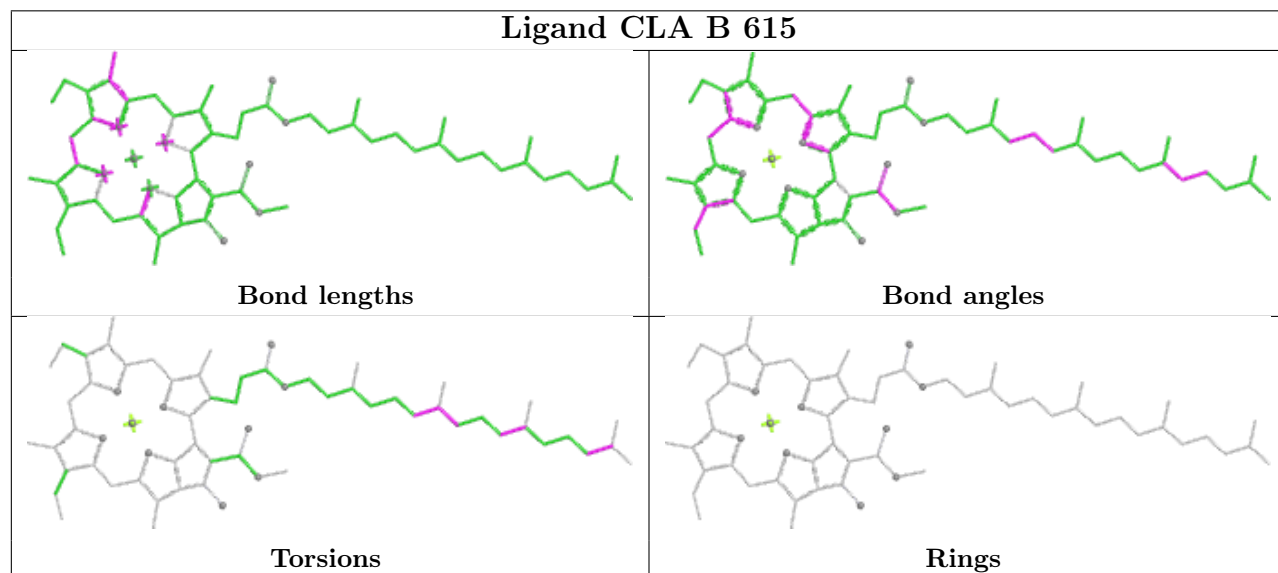
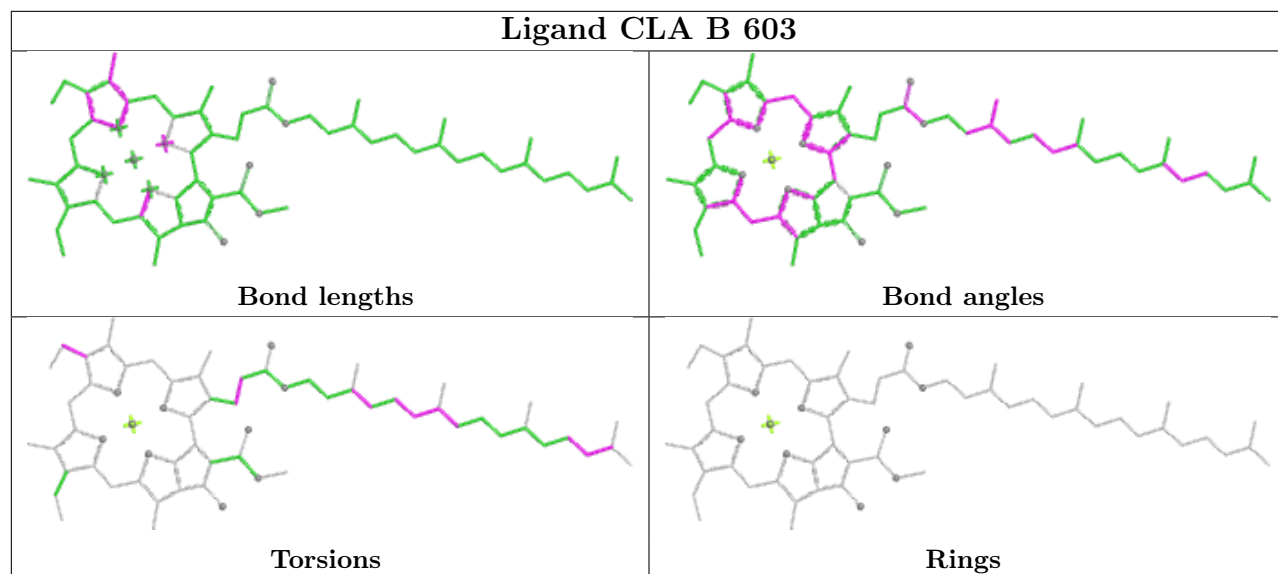
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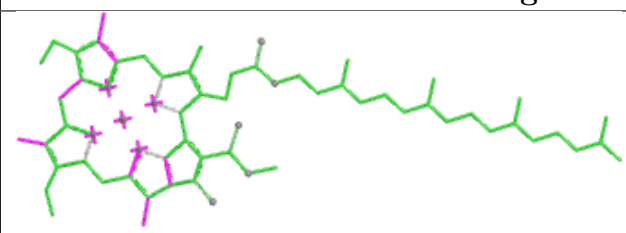
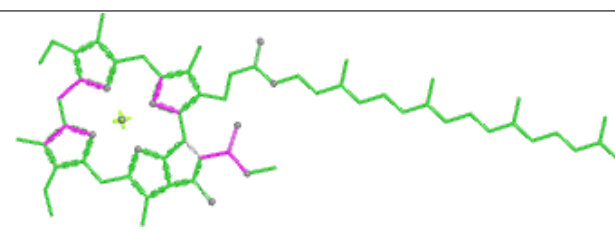
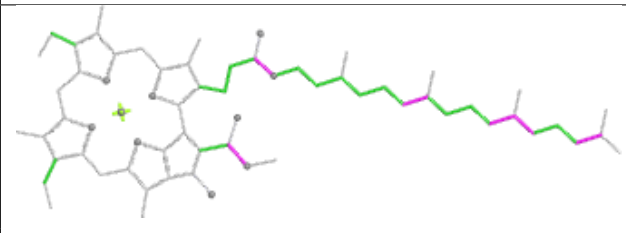
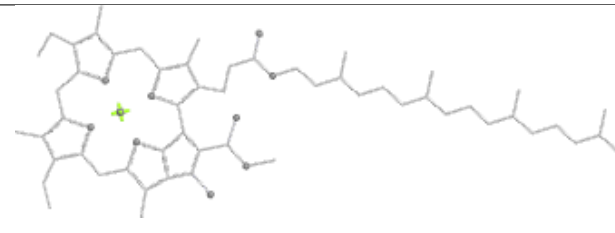


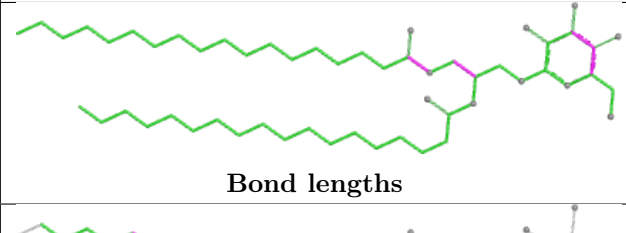
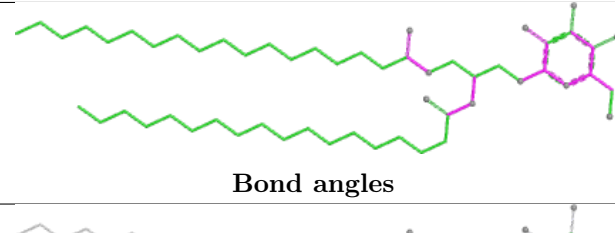
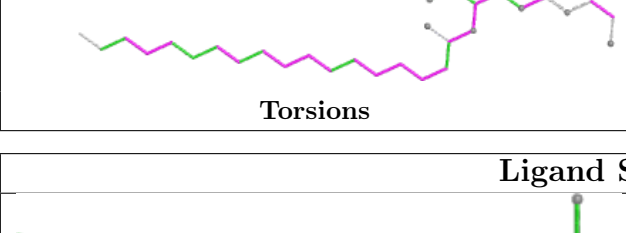
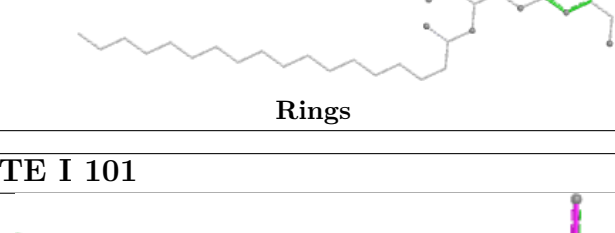


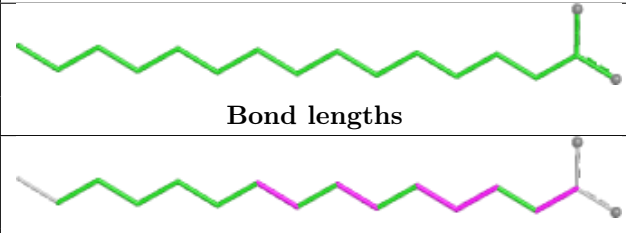
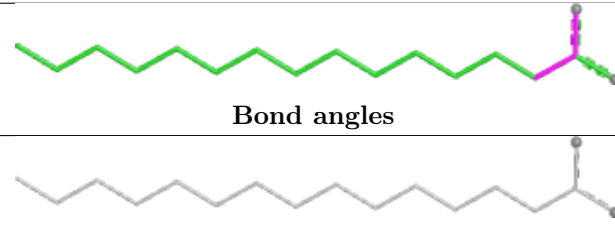
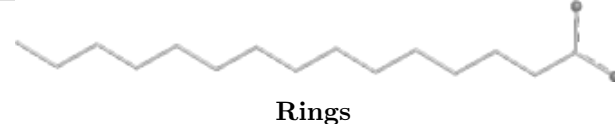


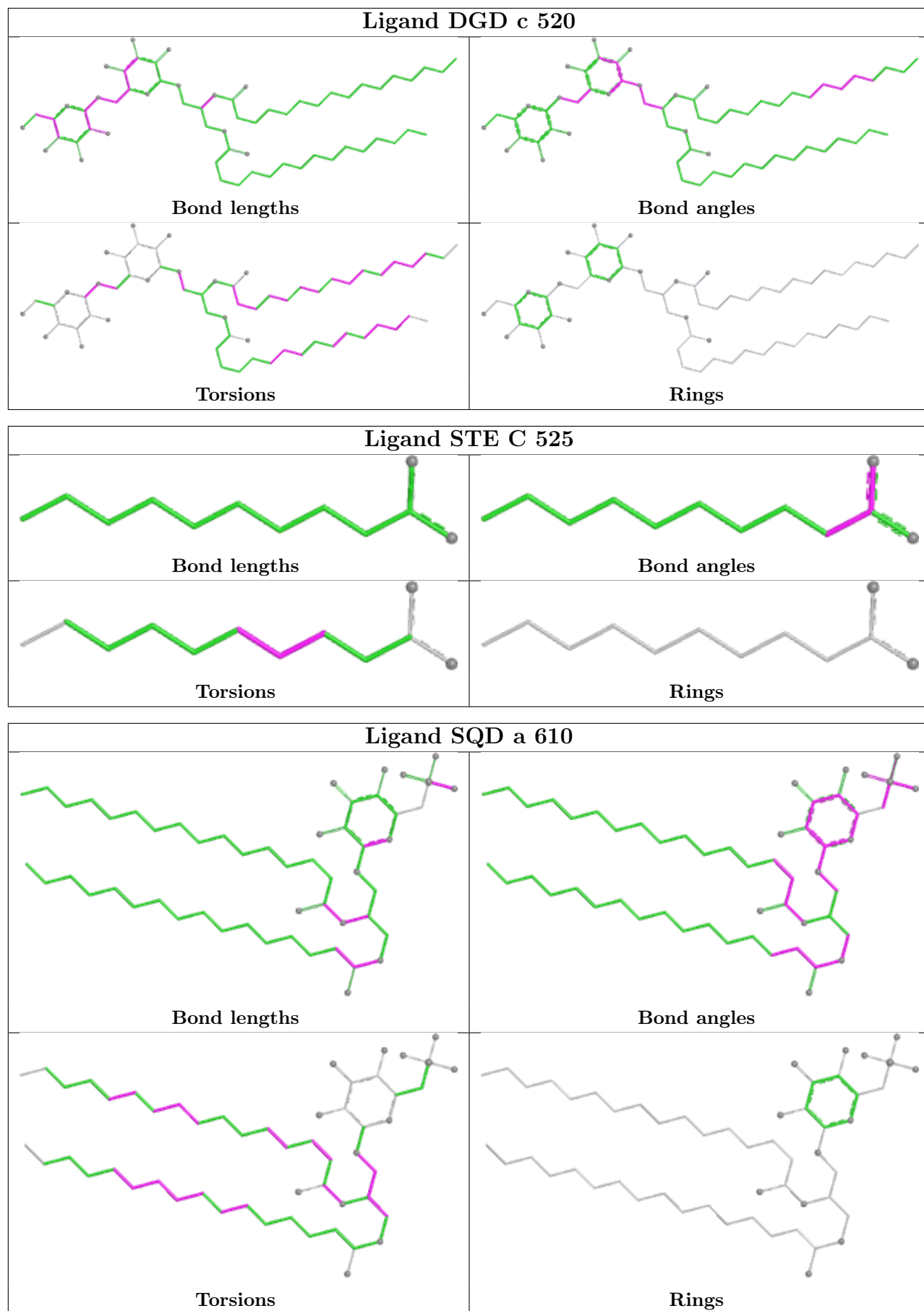


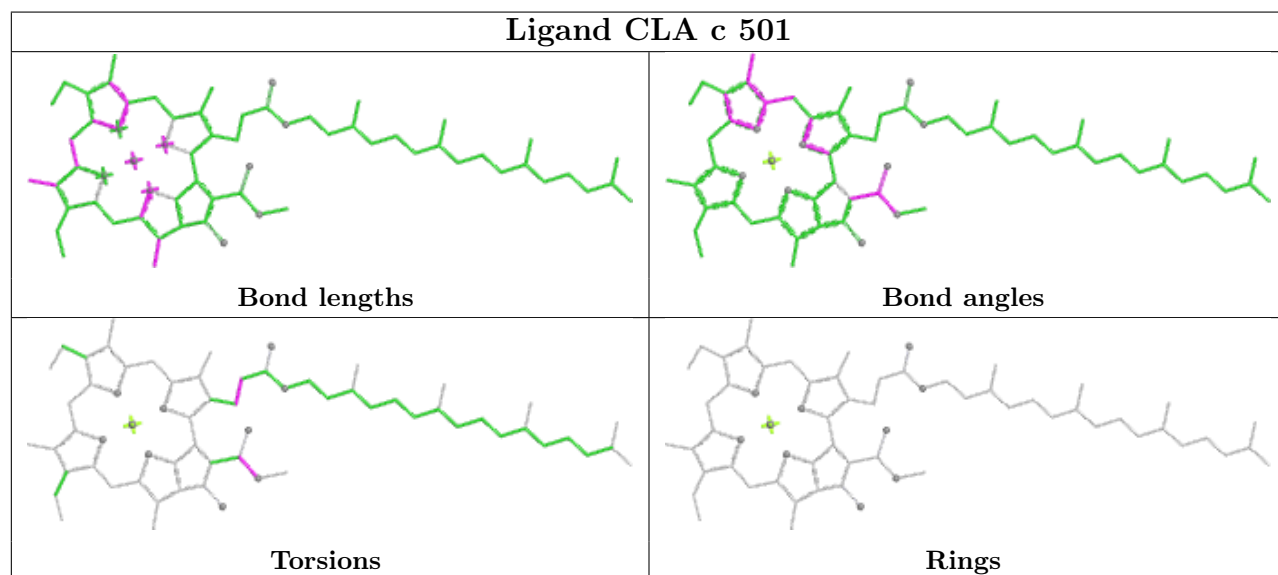
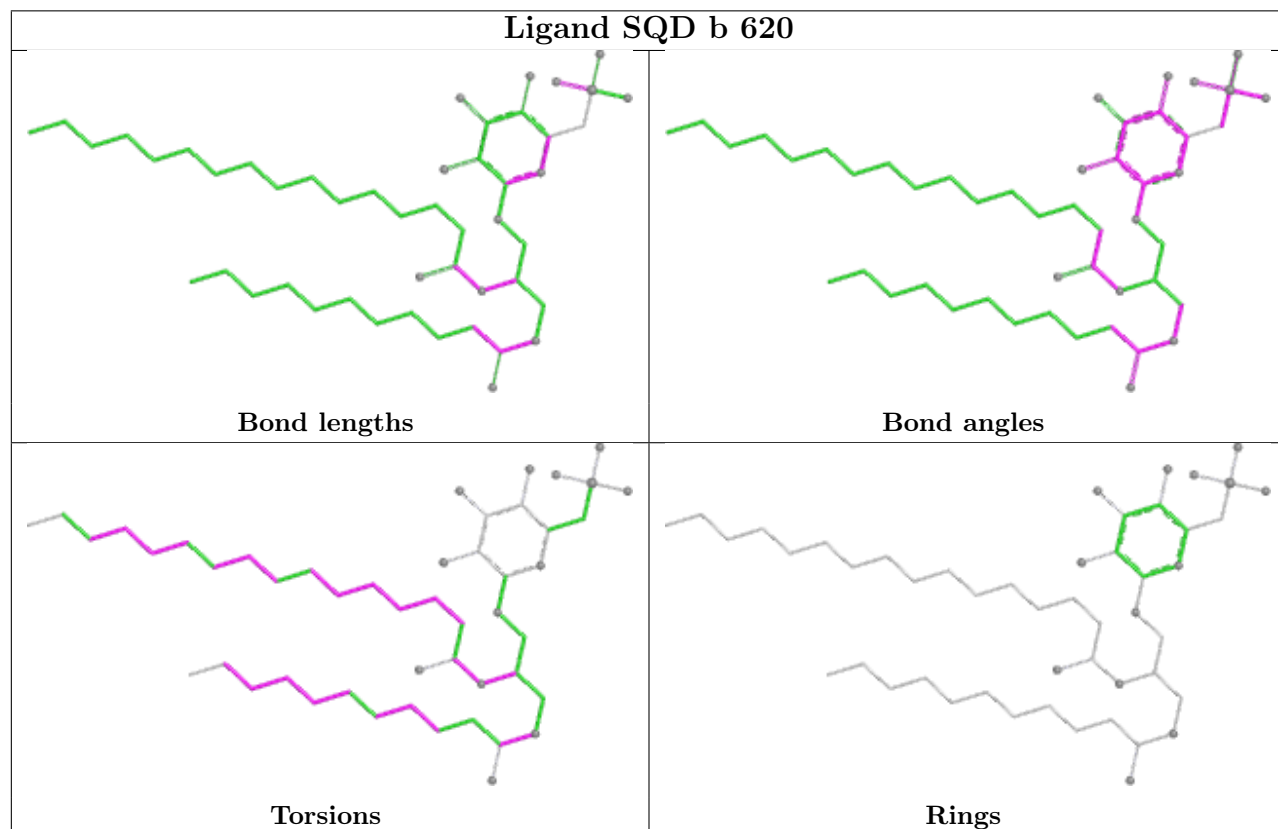
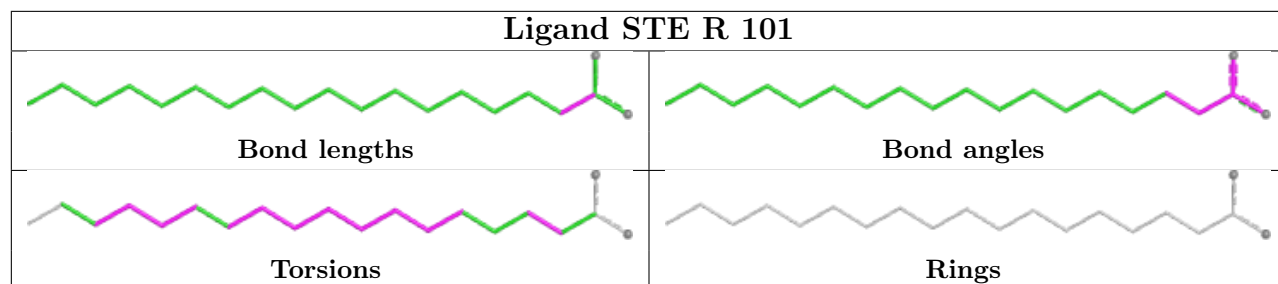


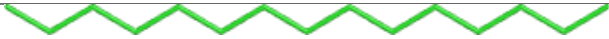
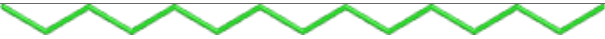
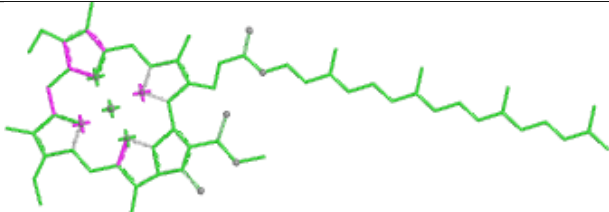
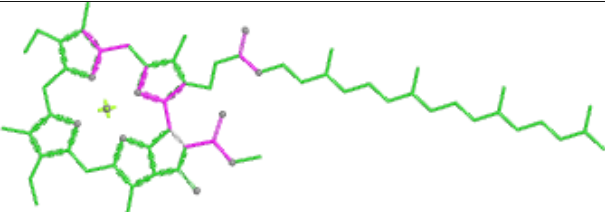
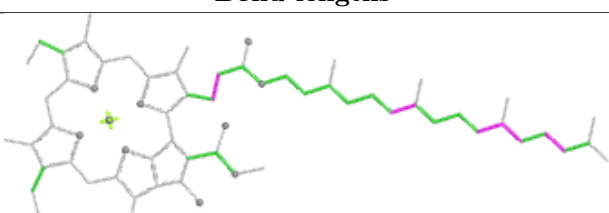
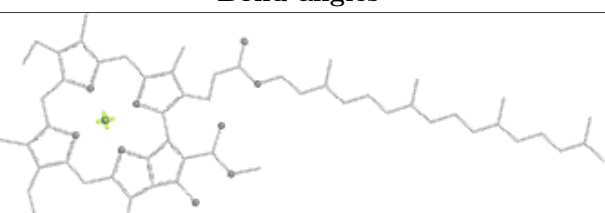
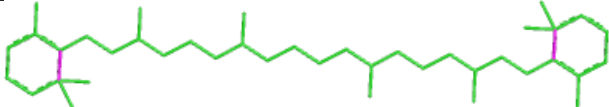
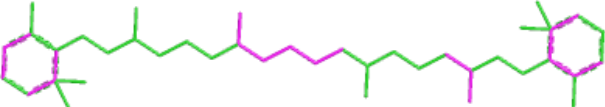
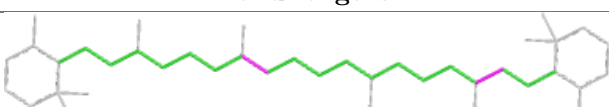
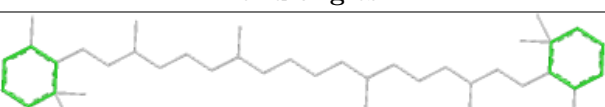
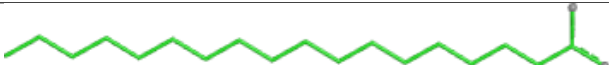
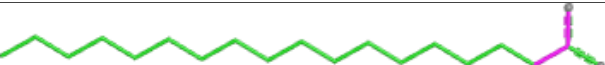
Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

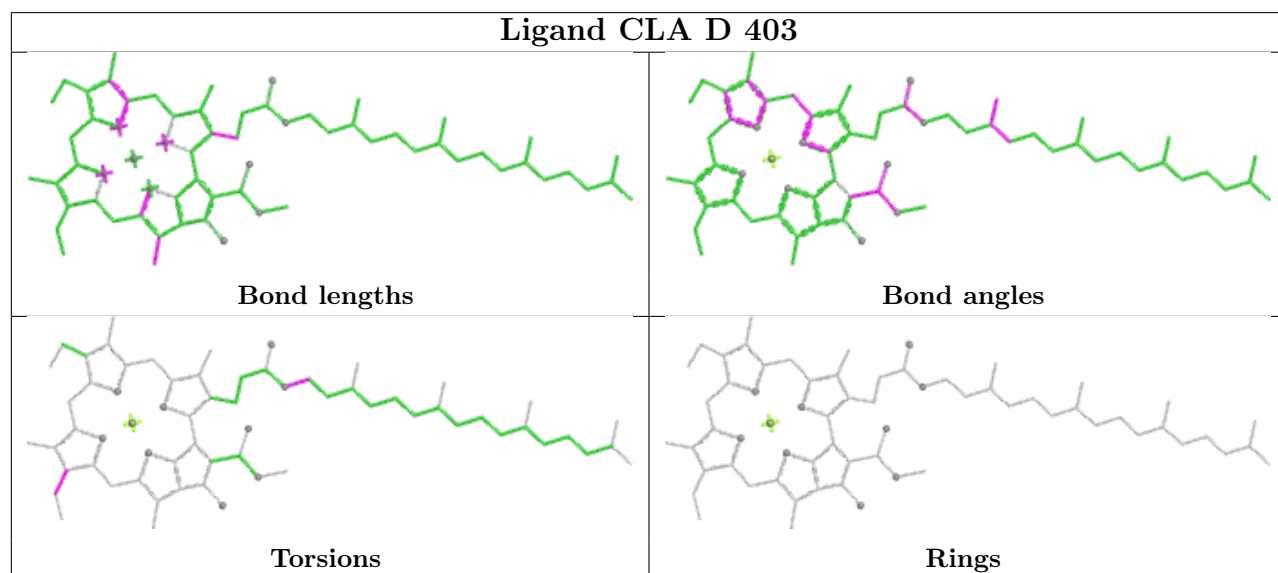
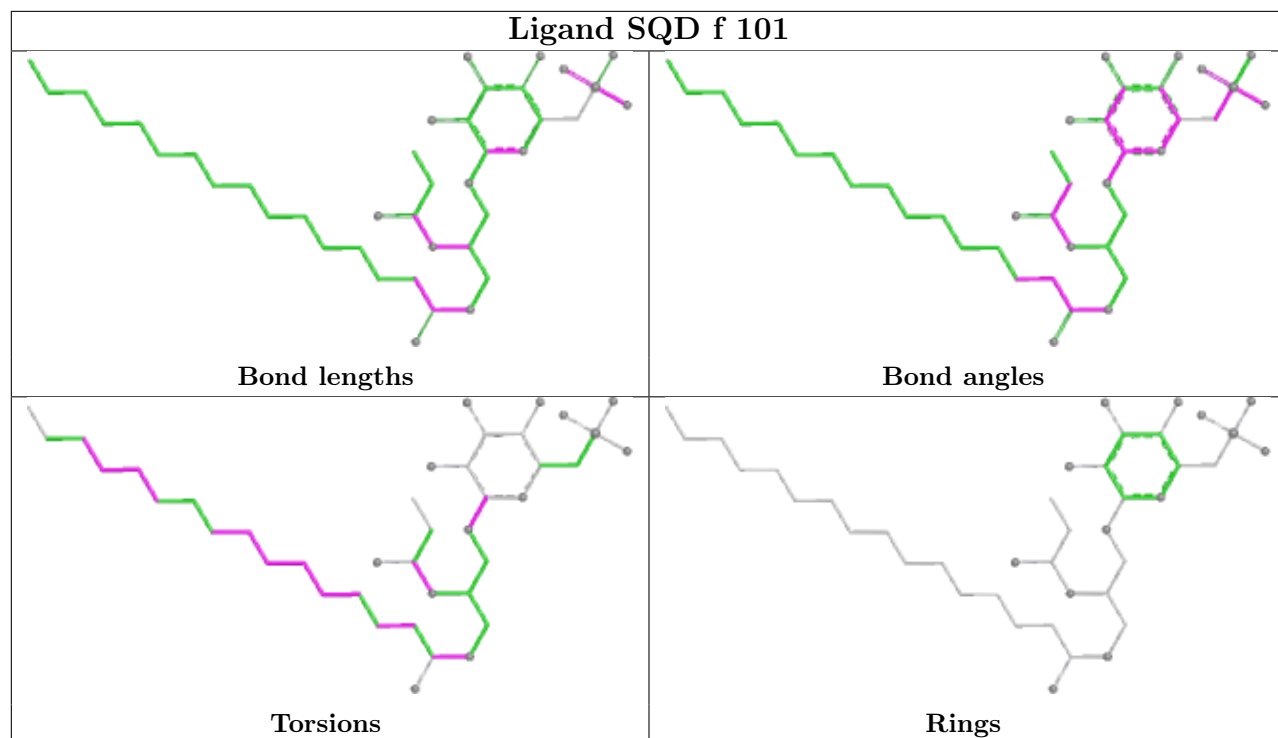
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

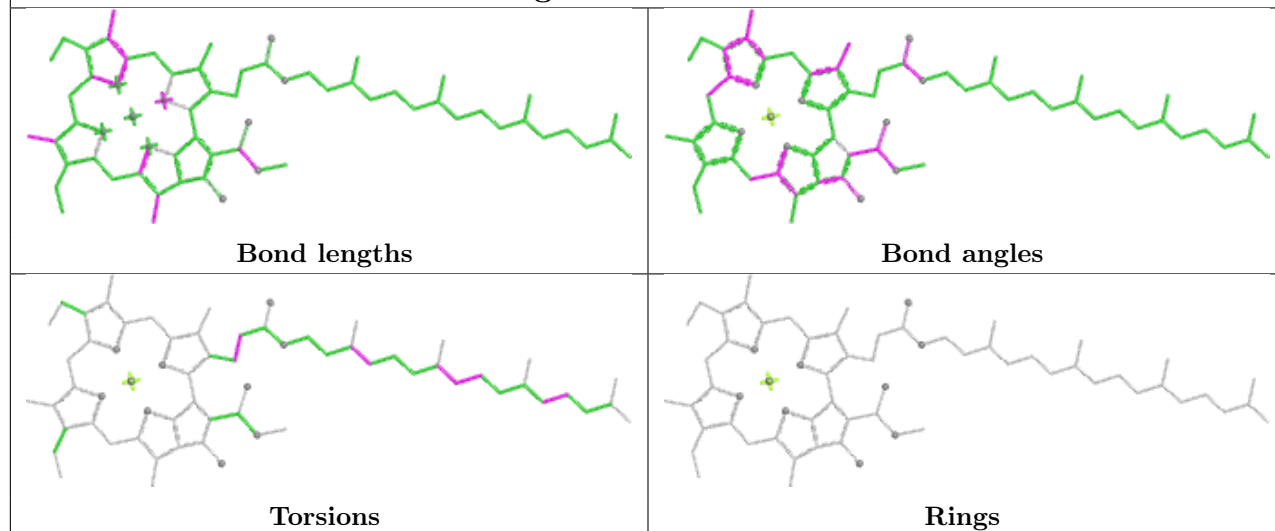




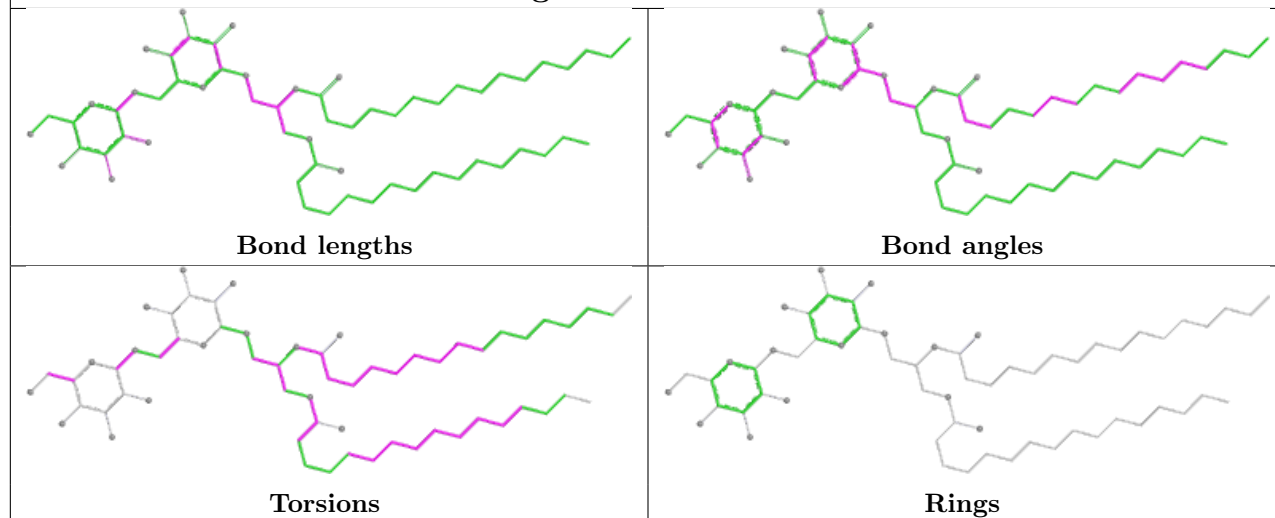
Ligand STE B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings



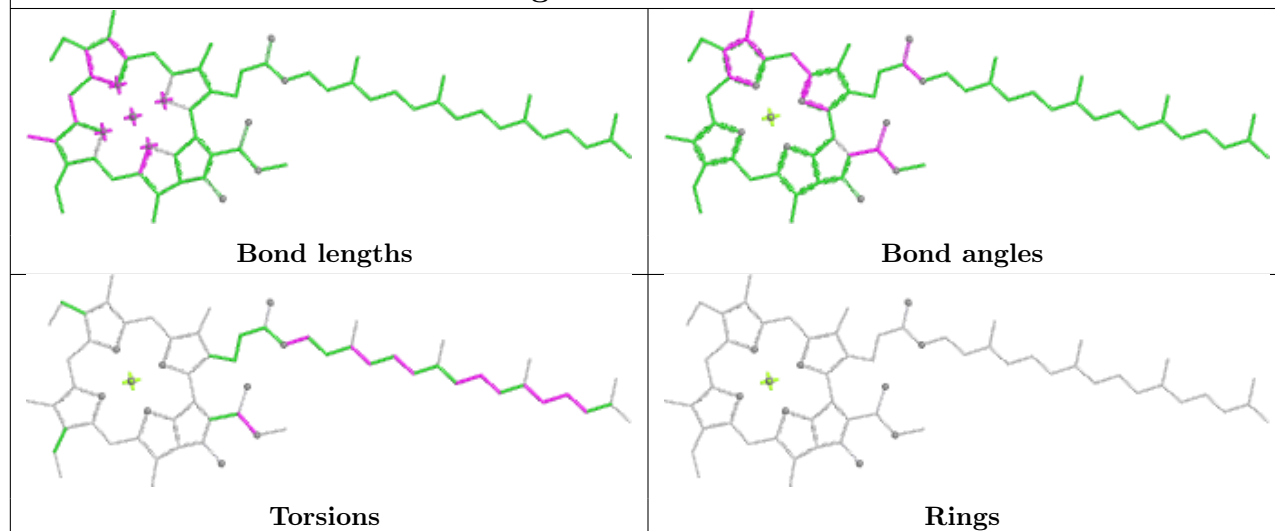
Ligand CLA b 603



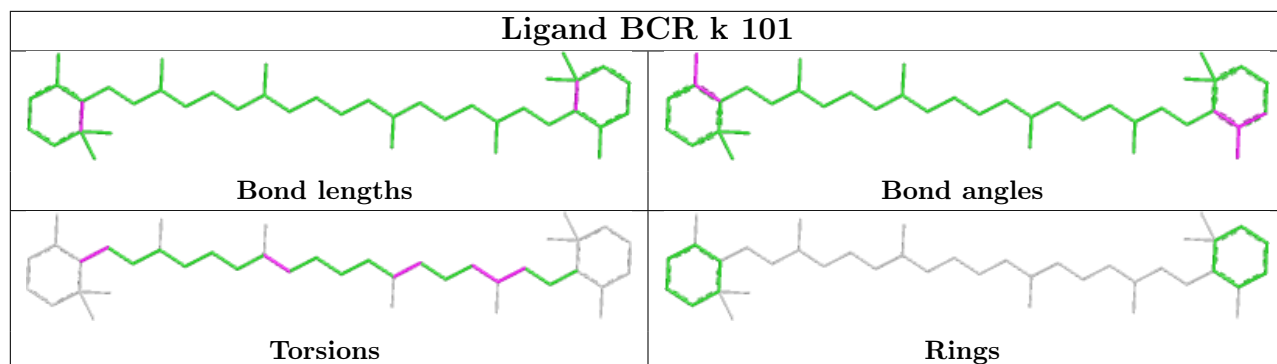
Ligand DGD c 519



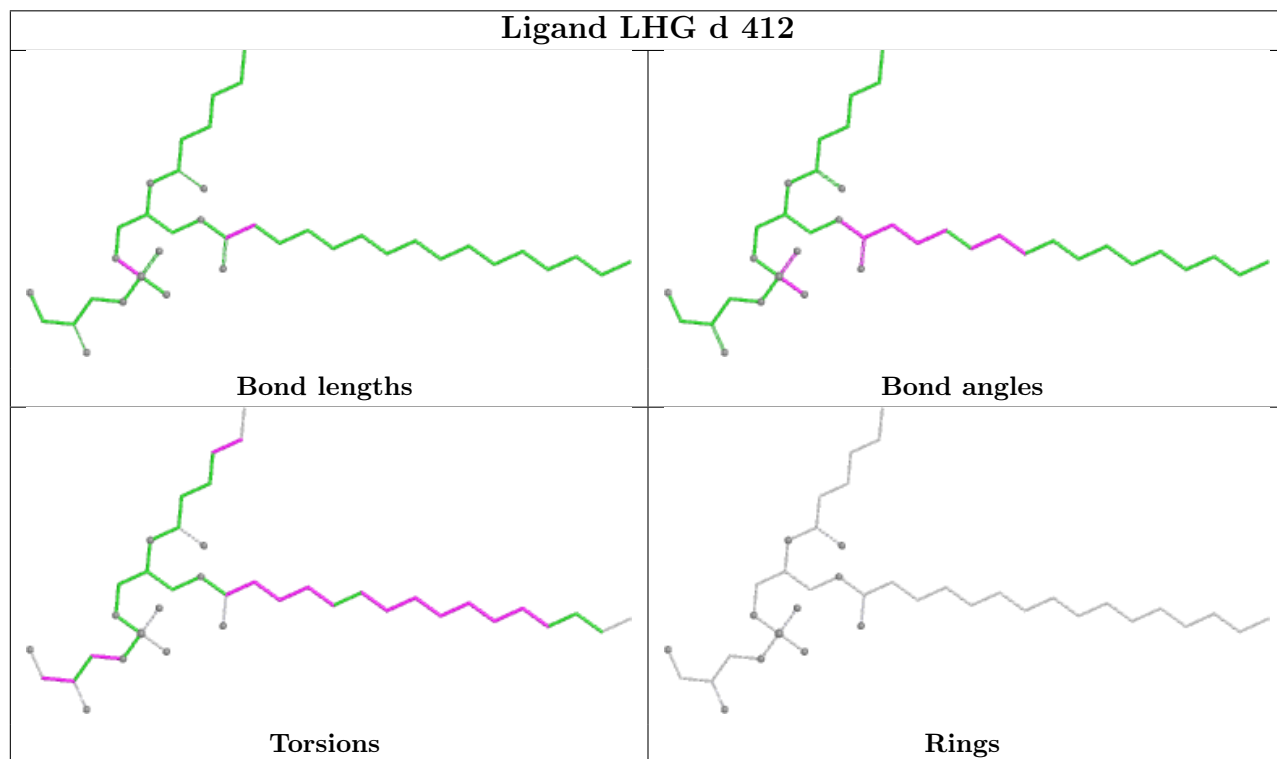
Ligand CLA C 506

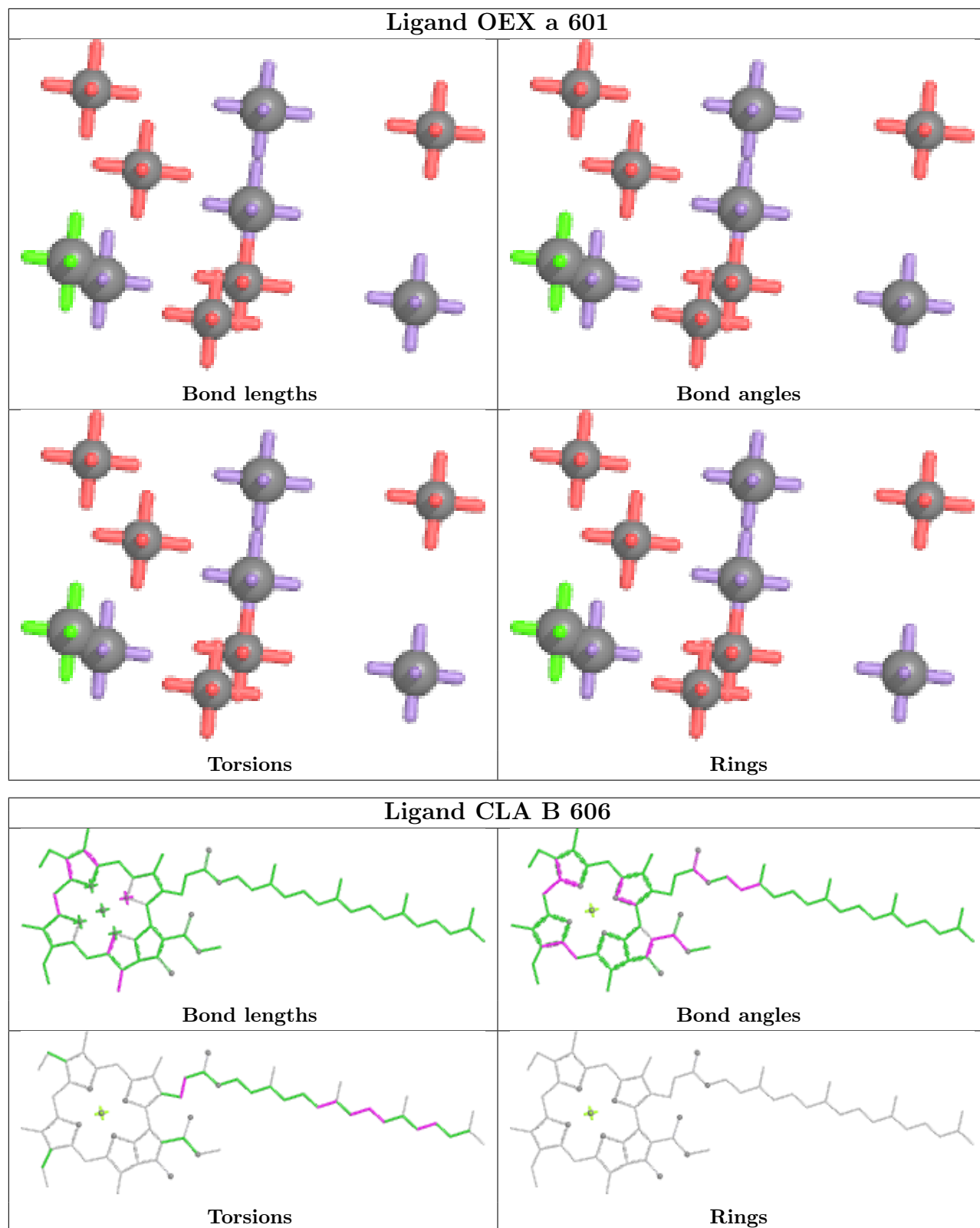


Ligand BCR k 101

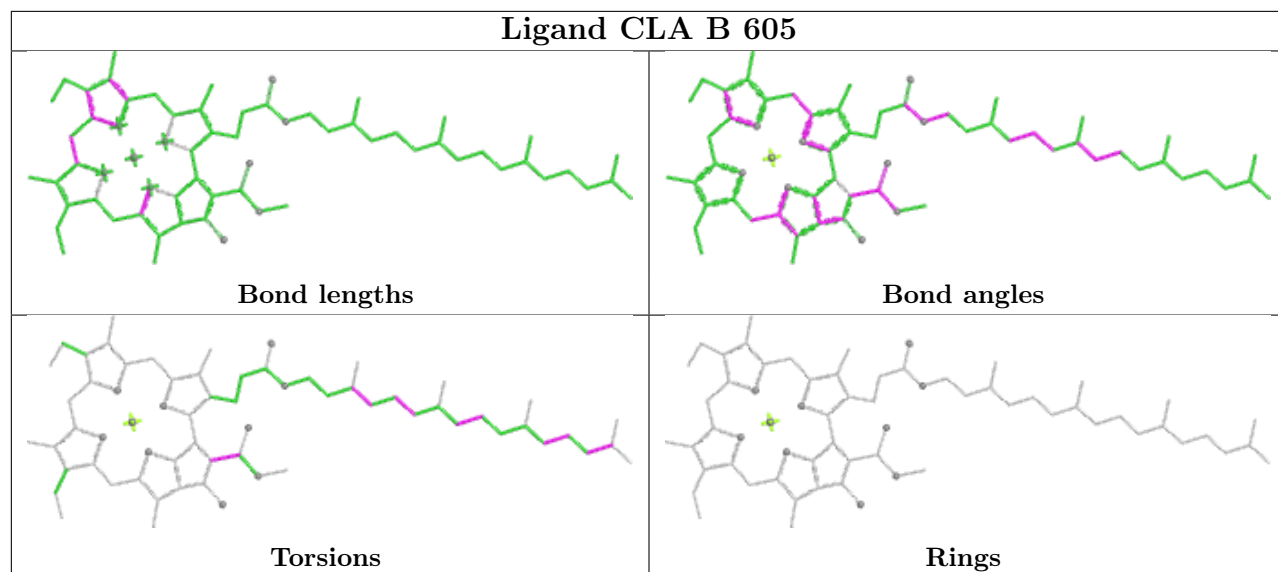


Ligand LHG d 412

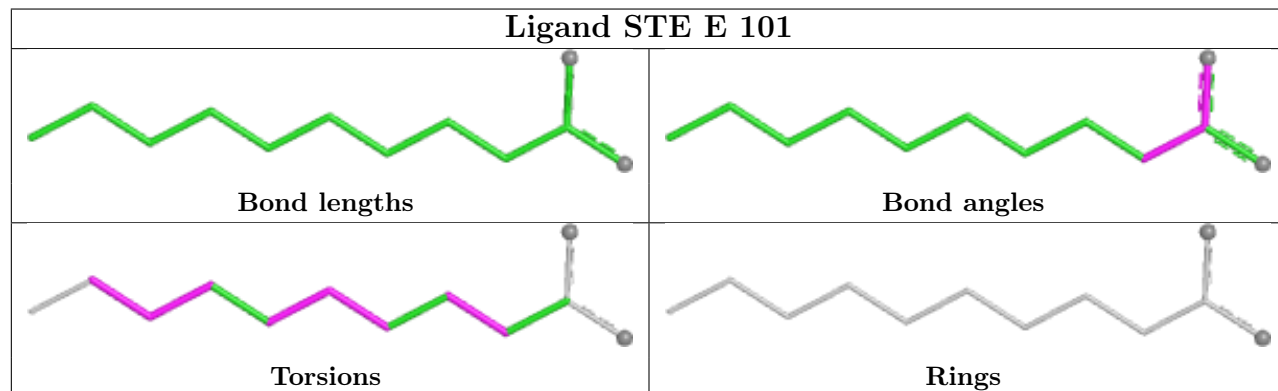




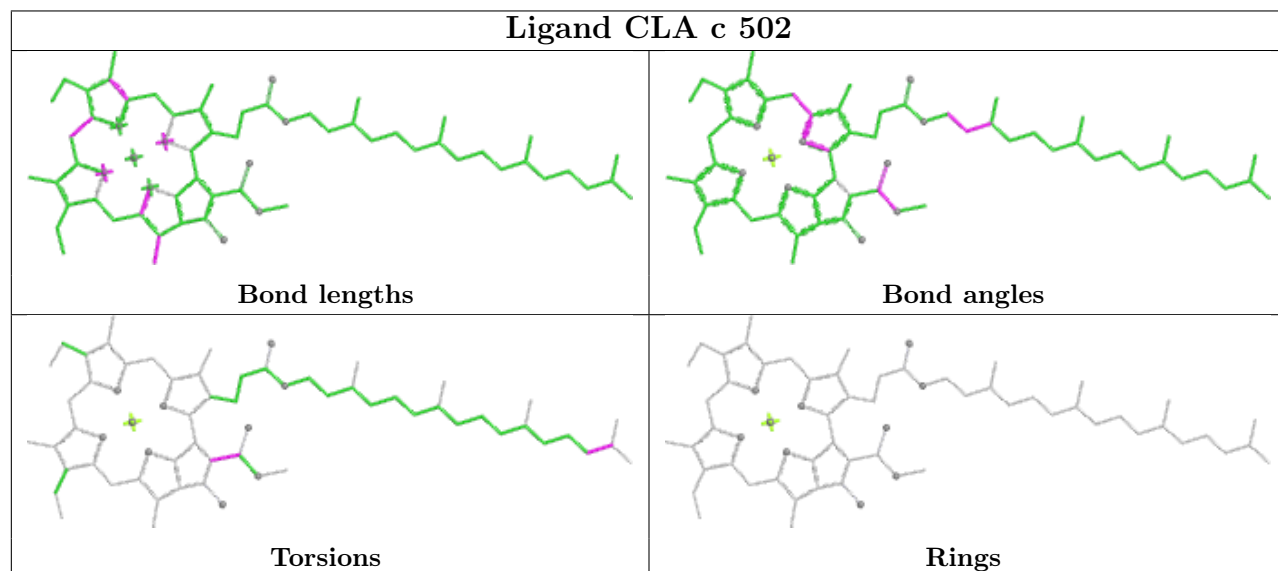
Ligand CLA B 605

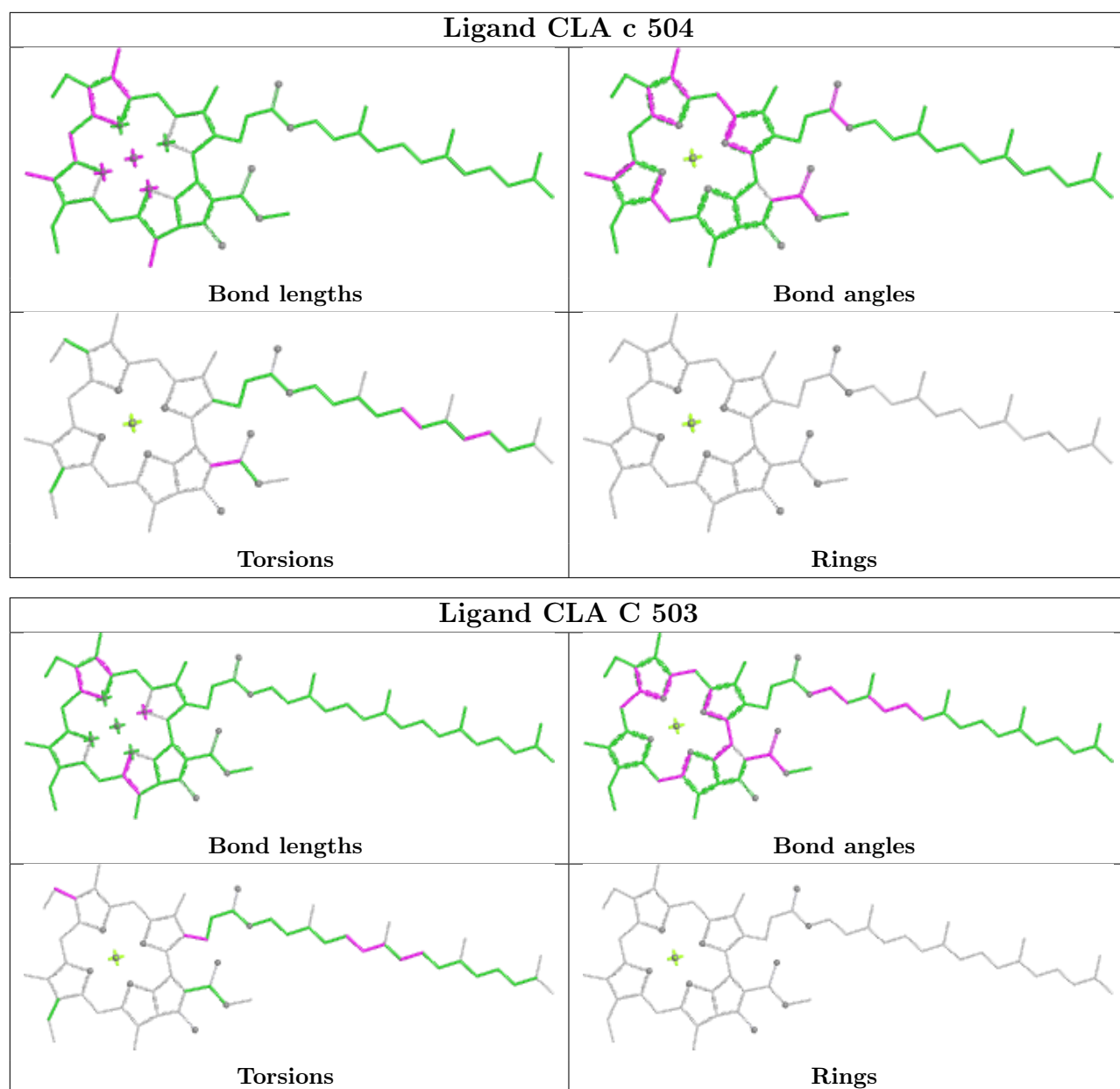


Ligand STE E 101



Ligand CLA c 502





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%)	-0.67	2 (0%) 85 86	23, 30, 52, 81	0
1	a	334/344 (97%)	-0.57	1 (0%) 90 90	22, 32, 63, 77	0
2	B	505/510 (99%)	-0.56	1 (0%) 91 91	18, 35, 68, 96	5 (0%)
2	b	505/510 (99%)	-0.41	2 (0%) 88 89	26, 38, 74, 110	1 (0%)
3	C	442/461 (95%)	-0.53	0 100 100	25, 39, 58, 84	0
3	c	451/461 (97%)	-0.39	3 (0%) 84 84	23, 42, 69, 102	1 (0%)
4	D	341/352 (96%)	-0.69	0 100 100	23, 33, 51, 82	0
4	d	341/352 (96%)	-0.55	1 (0%) 90 90	25, 36, 62, 87	1 (0%)
5	E	82/84 (97%)	0.07	1 (1%) 76 76	31, 54, 73, 87	1 (1%)
5	e	82/84 (97%)	0.25	0 100 100	41, 63, 83, 92	0
6	F	34/45 (75%)	-0.20	0 100 100	39, 46, 64, 84	0
6	f	34/45 (75%)	0.13	2 (5%) 28 27	42, 53, 82, 96	0
7	H	65/66 (98%)	-0.32	2 (3%) 51 51	36, 45, 61, 81	0
7	h	63/66 (95%)	-0.00	1 (1%) 70 70	44, 54, 67, 76	0
8	I	35/38 (92%)	-0.35	0 100 100	32, 42, 76, 81	0
8	i	35/38 (92%)	-0.41	0 100 100	32, 43, 78, 91	0
9	J	36/40 (90%)	0.04	1 (2%) 55 54	39, 54, 80, 99	0
9	j	36/40 (90%)	0.16	0 100 100	39, 60, 91, 97	0
10	K	37/46 (80%)	-0.12	0 100 100	44, 57, 74, 83	0
10	k	37/46 (80%)	0.08	0 100 100	47, 60, 76, 85	0
11	L	37/37 (100%)	-0.69	0 100 100	26, 31, 66, 73	0
11	l	36/37 (97%)	-0.58	0 100 100	27, 33, 70, 82	0
12	M	32/36 (88%)	-0.39	3 (9%) 14 13	28, 36, 66, 80	0
12	m	31/36 (86%)	-0.54	0 100 100	29, 37, 51, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.33	2 (0%) 82 83	26, 44, 86, 128	1 (0%)
13	o	244/272 (89%)	-0.38	1 (0%) 88 89	25, 43, 82, 125	0
14	T	29/32 (90%)	-0.70	0 100 100	27, 34, 65, 78	0
14	t	29/32 (90%)	-0.56	1 (3%) 48 47	28, 35, 80, 90	0
15	U	97/134 (72%)	-0.36	0 100 100	31, 45, 71, 94	0
15	u	97/134 (72%)	-0.38	1 (1%) 79 80	32, 43, 58, 89	0
16	V	137/163 (84%)	-0.49	0 100 100	29, 42, 60, 76	0
16	v	137/163 (84%)	-0.15	0 100 100	35, 49, 74, 90	0
17	Y	27/46 (58%)	0.91	3 (11%) 10 9	56, 79, 105, 108	0
17	y	30/46 (65%)	0.67	1 (3%) 49 48	63, 77, 106, 118	0
18	X	38/41 (92%)	0.01	1 (2%) 57 57	43, 55, 78, 88	0
18	x	39/41 (95%)	0.13	1 (2%) 57 57	50, 65, 85, 94	0
19	Z	62/62 (100%)	0.53	3 (4%) 35 35	58, 72, 109, 126	0
19	z	62/62 (100%)	0.69	4 (6%) 25 24	58, 78, 116, 134	0
20	R	28/41 (68%)	0.60	0 100 100	63, 71, 89, 99	0
20	r	28/41 (68%)	1.07	5 (17%) 3 3	75, 89, 106, 113	0
All	All	5293/5700 (92%)	-0.38	43 (0%) 82 83	18, 40, 77, 134	10 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	3.8
13	o	58	ASN	3.3
12	M	4	ASN	3.2
7	h	64	ALA	2.9
17	Y	20	ALA	2.9
19	Z	62	VAL	2.9
17	Y	25	ILE	2.9
3	c	24	THR	2.9
9	J	5	GLY	2.9
17	Y	22	LEU	2.8
1	a	11	ALA	2.7
3	c	23	ALA	2.7
14	t	30	THR	2.6
15	u	53	ALA	2.6
2	b	495	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
19	Z	4	LEU	2.5
2	b	499	VAL	2.4
1	A	11	ALA	2.4
20	r	26	TYR	2.4
6	f	15	ILE	2.4
20	r	29	LYS	2.4
7	H	66	GLY	2.4
5	E	79	PHE	2.4
20	r	20	VAL	2.4
18	x	2	THR	2.4
19	z	30	PRO	2.3
7	H	65	LEU	2.3
17	y	19	ILE	2.2
3	c	134	ILE	2.1
19	Z	3	ILE	2.1
13	O	60	ARG	2.1
1	A	265	PHE	2.1
2	B	479[A]	PHE	2.1
6	f	14	PRO	2.1
19	z	40	ILE	2.1
12	M	33	GLN	2.0
18	X	2	THR	2.0
13	O	59	LYS	2.0
4	d	28	VAL	2.0
19	z	62	VAL	2.0
20	r	28	VAL	2.0
12	M	5	GLN	2.0
20	r	25	PRO	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
8	FME	I	1	10/11	0.95	0.09	36,52,65,65	0
12	FME	M	1	10/11	0.95	0.09	39,47,67,72	0
8	FME	i	1	10/11	0.95	0.08	34,47,61,65	0
14	FME	T	1	10/11	0.96	0.08	29,45,68,69	0
14	FME	t	1	10/11	0.96	0.07	29,42,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	m	1	10/11	0.98	0.06	29,45,70,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	C	528	14/20	0.65	0.20	51,82,107,107	0
28	STE	i	101	12/20	0.65	0.17	50,90,107,109	0
28	STE	C	518	7/20	0.66	0.15	47,69,81,81	0
28	STE	j	102	16/20	0.67	0.21	61,82,104,110	0
28	STE	A	619	11/20	0.68	0.18	47,85,112,119	0
28	STE	H	103	18/20	0.68	0.19	49,74,87,88	0
28	STE	E	102	12/20	0.69	0.18	53,83,111,112	0
28	STE	c	517	18/20	0.70	0.18	61,85,105,107	0
28	STE	C	517	5/20	0.71	0.21	47,62,75,75	0
28	STE	I	101	17/20	0.72	0.18	51,76,88,89	0
28	STE	C	519	10/20	0.73	0.15	54,91,107,109	0
28	STE	i	102	6/20	0.74	0.23	45,75,84,84	0
28	STE	e	101	9/20	0.76	0.20	54,75,90,91	0
31	LHG	e	103	42/49	0.76	0.15	61,89,112,130	0
28	STE	e	104	9/20	0.77	0.17	50,69,86,87	0
28	STE	c	516	13/20	0.77	0.14	51,78,88,91	0
28	STE	A	618	17/20	0.77	0.13	48,73,85,88	0
28	STE	d	415	14/20	0.77	0.14	53,74,90,100	0
28	STE	R	101	20/20	0.77	0.15	48,67,81,83	0
29	LMG	D	407	50/55	0.78	0.16	36,71,126,141	0
31	LHG	A	615	49/49	0.78	0.15	50,84,118,128	0
28	STE	B	626	15/20	0.78	0.20	44,64,87,91	0
29	LMG	c	518	30/55	0.79	0.14	45,75,101,108	0
28	STE	b	627	11/20	0.79	0.19	56,73,84,88	0
28	STE	f	102	8/20	0.79	0.20	48,76,81,83	0
28	STE	t	103	10/20	0.80	0.13	46,64,69,77	0
28	STE	C	527	14/20	0.80	0.15	55,80,117,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	A	611	9/20	0.80	0.18	49,71,90,97	0
28	STE	a	612	12/20	0.80	0.14	40,71,77,83	0
28	STE	e	105	13/20	0.80	0.16	71,88,103,104	0
28	STE	h	103	10/20	0.81	0.16	52,75,93,100	0
28	STE	E	101	12/20	0.81	0.14	53,76,89,94	0
29	LMG	b	623	55/55	0.81	0.16	47,73,92,108	0
27	PL9	A	610	55/55	0.82	0.14	39,65,93,97	0
28	STE	z	101	9/20	0.82	0.17	49,74,83,87	0
29	LMG	c	523	48/55	0.82	0.14	53,80,107,118	0
29	LMG	B	620	45/55	0.82	0.14	37,62,110,132	0
28	STE	b	624	16/20	0.82	0.16	49,69,94,101	0
28	STE	b	621	16/20	0.83	0.18	41,55,108,110	0
27	PL9	a	609	55/55	0.83	0.14	41,67,89,96	0
28	STE	b	625	10/20	0.83	0.15	45,60,68,72	0
28	STE	E	103	20/20	0.83	0.13	43,69,84,85	0
29	LMG	o	301	55/55	0.84	0.13	33,62,84,87	0
28	STE	B	625	12/20	0.84	0.13	46,65,77,81	0
28	STE	C	515	14/20	0.84	0.13	53,67,80,81	0
28	STE	M	103	15/20	0.85	0.17	47,62,95,101	0
28	STE	j	101	12/20	0.85	0.12	44,59,73,73	0
28	STE	d	409	20/20	0.85	0.13	39,63,81,82	0
28	STE	d	413	20/20	0.85	0.13	50,72,91,94	0
28	STE	Z	101	17/20	0.85	0.15	48,72,97,99	0
28	STE	C	526	16/20	0.85	0.12	47,60,69,70	0
29	LMG	C	516	36/55	0.85	0.12	40,63,87,99	0
32	DGD	A	617	66/66	0.85	0.12	47,69,90,98	0
30	SQD	a	611	54/54	0.86	0.12	38,64,101,120	0
29	LMG	C	524	48/55	0.86	0.12	48,74,95,104	0
28	STE	I	102	15/20	0.86	0.13	43,59,73,73	0
28	STE	J	101	12/20	0.86	0.12	52,67,75,79	0
29	LMG	A	613	48/55	0.87	0.10	37,58,72,87	0
28	STE	m	102	12/20	0.87	0.14	45,59,79,92	0
28	STE	B	624	18/20	0.87	0.11	48,60,73,74	0
29	LMG	c	522	46/55	0.87	0.12	43,72,90,98	0
28	STE	C	525	12/20	0.87	0.14	37,53,67,68	0
28	STE	x	101	20/20	0.88	0.12	37,57,75,89	0
28	STE	D	412	9/20	0.88	0.12	49,66,75,81	0
28	STE	b	622	20/20	0.88	0.10	41,59,86,91	0
24	CLA	b	601	65/65	0.88	0.11	44,68,97,113	0
28	STE	M	102	10/20	0.89	0.13	41,59,67,77	0
30	SQD	B	623	54/54	0.89	0.10	38,61,90,97	0
28	STE	B	622	17/20	0.90	0.11	33,54,75,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	A	616	43/54	0.90	0.09	42,61,106,119	0
26	BCR	k	101	40/40	0.90	0.10	45,62,74,82	0
28	STE	M	101	15/20	0.90	0.11	35,51,66,73	0
30	SQD	f	101	41/54	0.90	0.11	51,78,95,100	0
28	STE	b	626	8/20	0.90	0.11	44,60,80,80	0
29	LMG	c	524	49/55	0.90	0.10	35,59,95,115	0
29	LMG	m	101	51/55	0.90	0.09	36,53,67,80	0
26	BCR	K	101	40/40	0.91	0.10	41,58,69,73	0
28	STE	t	102	14/20	0.91	0.09	43,56,64,69	0
28	STE	l	102	18/20	0.91	0.12	34,53,94,94	0
26	BCR	h	101	40/40	0.92	0.09	34,56,80,80	0
29	LMG	B	621	51/55	0.92	0.09	27,51,77,86	0
30	SQD	F	102	36/54	0.92	0.11	42,74,90,102	0
30	SQD	a	610	54/54	0.92	0.10	40,66,93,99	0
24	CLA	B	601	65/65	0.92	0.09	33,61,94,95	0
30	SQD	b	620	49/54	0.92	0.09	41,59,87,98	0
24	CLA	c	513	65/65	0.92	0.10	44,70,95,103	0
24	CLA	C	513	65/65	0.92	0.10	44,65,92,99	0
26	BCR	K	102	40/40	0.92	0.09	40,54,75,77	0
30	SQD	A	614	52/54	0.92	0.09	32,61,90,97	0
32	DGD	H	102	62/66	0.92	0.09	34,50,62,69	0
26	BCR	H	101	40/40	0.93	0.07	32,51,65,69	0
28	STE	X	101	20/20	0.93	0.09	37,51,71,77	0
24	CLA	c	512	65/65	0.93	0.09	37,59,89,98	0
26	BCR	k	102	40/40	0.93	0.10	40,57,69,80	0
26	BCR	D	405	40/40	0.93	0.09	30,46,96,107	0
26	BCR	c	514	40/40	0.93	0.09	46,61,74,79	0
32	DGD	C	522	62/66	0.93	0.09	32,52,103,122	0
26	BCR	d	407	40/40	0.93	0.09	33,54,93,98	0
32	DGD	c	520	62/66	0.93	0.09	32,52,92,101	0
32	DGD	h	102	62/66	0.93	0.09	35,53,68,75	0
29	LMG	D	408	51/55	0.94	0.09	26,58,88,96	0
26	BCR	B	619	40/40	0.94	0.07	24,40,61,68	0
26	BCR	c	515	40/40	0.94	0.08	30,45,67,74	0
26	BCR	C	520	40/40	0.94	0.09	38,53,69,69	0
24	CLA	c	511	65/65	0.94	0.08	39,53,68,81	0
24	CLA	C	512	65/65	0.94	0.09	39,54,98,102	0
31	LHG	d	410	49/49	0.94	0.09	34,54,78,86	0
29	LMG	d	414	44/55	0.94	0.09	33,55,93,100	0
24	CLA	c	509	65/65	0.94	0.09	33,47,67,74	0
26	BCR	B	618	40/40	0.94	0.06	23,40,52,57	0
26	BCR	b	617	40/40	0.94	0.07	27,41,52,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	b	618	40/40	0.94	0.06	25,40,61,65	0
26	BCR	b	619	40/40	0.94	0.07	30,46,65,70	0
26	BCR	t	101	40/40	0.95	0.06	29,41,60,64	0
24	CLA	c	504	60/65	0.95	0.07	26,45,83,85	0
24	CLA	c	506	65/65	0.95	0.09	26,49,102,105	0
24	CLA	c	508	64/65	0.95	0.08	29,45,96,112	0
24	CLA	C	511	65/65	0.95	0.07	32,49,68,74	0
26	BCR	T	101	40/40	0.95	0.06	26,39,57,62	0
24	CLA	B	606	65/65	0.95	0.07	21,36,71,79	0
24	CLA	C	503	65/65	0.95	0.07	30,43,53,56	0
24	CLA	C	510	65/65	0.95	0.07	29,45,62,70	0
31	LHG	d	412	39/49	0.95	0.09	31,48,72,82	0
26	BCR	A	609	40/40	0.95	0.06	24,35,46,48	0
31	LHG	l	101	49/49	0.95	0.07	32,46,58,62	0
26	BCR	B	617	40/40	0.95	0.07	25,39,54,58	0
24	CLA	b	609	65/65	0.95	0.07	28,45,65,79	0
32	DGD	C	523	62/66	0.95	0.08	28,50,79,94	0
24	CLA	b	612	65/65	0.95	0.07	22,33,47,55	0
26	BCR	C	514	40/40	0.95	0.07	27,41,55,57	0
24	CLA	c	503	65/65	0.95	0.07	30,44,57,60	0
24	CLA	C	501	65/65	0.96	0.06	24,36,51,61	0
24	CLA	c	510	65/65	0.96	0.07	29,48,68,80	0
24	CLA	B	609	65/65	0.96	0.07	26,38,62,65	0
24	CLA	a	606	65/65	0.96	0.08	23,41,97,103	0
24	CLA	C	504	59/65	0.96	0.07	29,43,89,94	0
24	CLA	d	406	65/65	0.96	0.08	23,50,91,105	0
25	PHO	d	403	64/64	0.96	0.06	26,37,48,58	0
27	PL9	D	406	55/55	0.96	0.06	22,34,47,51	0
24	CLA	b	602	65/65	0.96	0.08	27,45,70,74	0
27	PL9	d	408	55/55	0.96	0.06	23,35,47,47	0
24	CLA	b	606	65/65	0.96	0.07	24,39,74,84	0
24	CLA	b	608	65/65	0.96	0.07	23,43,72,76	0
24	CLA	C	505	65/65	0.96	0.08	24,40,66,71	0
24	CLA	b	610	65/65	0.96	0.07	23,39,52,58	0
24	CLA	C	506	65/65	0.96	0.09	27,43,93,99	0
31	LHG	D	410	47/49	0.96	0.08	27,50,84,101	0
31	LHG	D	411	49/49	0.96	0.08	29,47,73,83	0
24	CLA	b	614	65/65	0.96	0.07	23,39,78,93	0
31	LHG	d	411	49/49	0.96	0.07	23,44,53,64	0
24	CLA	b	615	65/65	0.96	0.07	25,41,61,73	0
24	CLA	b	616	60/65	0.96	0.08	25,44,86,93	0
24	CLA	c	502	65/65	0.96	0.06	27,43,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	508	65/65	0.96	0.07	28,43,116,126	0
32	DGD	C	521	62/66	0.96	0.08	22,41,85,94	0
26	BCR	a	608	40/40	0.96	0.06	20,33,48,50	0
24	CLA	C	509	65/65	0.96	0.08	24,46,66,74	0
24	CLA	c	505	65/65	0.96	0.07	25,42,67,73	0
32	DGD	c	519	62/66	0.96	0.08	20,42,75,88	0
24	CLA	B	612	65/65	0.96	0.06	19,34,46,53	0
32	DGD	c	521	62/66	0.96	0.08	29,55,80,94	0
24	CLA	B	615	65/65	0.96	0.07	22,39,66,75	0
33	BCT	D	401	4/4	0.96	0.08	28,30,33,40	0
33	BCT	d	401	4/4	0.96	0.08	28,30,46,55	0
24	CLA	a	607	65/65	0.97	0.08	19,33,83,91	0
24	CLA	d	404	65/65	0.97	0.06	20,30,49,52	0
24	CLA	d	405	65/65	0.97	0.06	20,34,62,69	0
24	CLA	B	614	65/65	0.97	0.07	18,37,84,90	0
25	PHO	A	607	64/64	0.97	0.05	18,29,40,43	0
25	PHO	D	402	64/64	0.97	0.05	21,33,43,47	0
25	PHO	d	402	64/64	0.97	0.05	22,31,40,41	0
24	CLA	A	605	65/65	0.97	0.05	17,29,51,60	0
24	CLA	b	603	65/65	0.97	0.06	20,36,73,82	0
24	CLA	b	605	65/65	0.97	0.05	20,35,49,58	0
24	CLA	B	616	60/65	0.97	0.08	20,39,87,102	0
24	CLA	b	607	65/65	0.97	0.06	19,36,70,81	0
24	CLA	B	602	65/65	0.97	0.06	22,37,68,73	0
24	CLA	C	502	65/65	0.97	0.06	26,39,60,72	0
24	CLA	B	603	65/65	0.97	0.06	18,34,67,74	0
31	LHG	D	409	49/49	0.97	0.06	22,40,57,66	0
24	CLA	b	611	65/65	0.97	0.05	22,35,55,61	0
24	CLA	B	604	65/65	0.97	0.07	20,33,74,87	0
31	LHG	L	101	49/49	0.97	0.06	28,43,62,68	0
24	CLA	b	613	65/65	0.97	0.06	20,35,73,90	0
24	CLA	B	605	65/65	0.97	0.06	19,31,49,55	0
24	CLA	A	606	65/65	0.97	0.08	20,36,101,115	0
24	CLA	C	507	65/65	0.97	0.06	24,41,58,61	0
24	CLA	c	501	65/65	0.97	0.06	27,41,56,58	0
24	CLA	B	607	65/65	0.97	0.06	17,31,58,71	0
24	CLA	B	608	65/65	0.97	0.05	20,36,59,69	0
24	CLA	A	608	54/65	0.97	0.06	18,34,58,68	0
24	CLA	B	610	65/65	0.97	0.06	22,33,45,50	0
24	CLA	B	611	65/65	0.97	0.05	21,30,48,58	0
24	CLA	c	507	65/65	0.97	0.07	25,46,61,66	0
24	CLA	A	612	65/65	0.97	0.06	21,29,55,56	0

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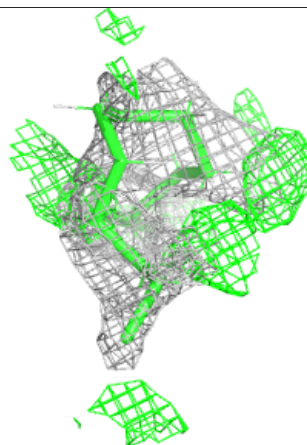
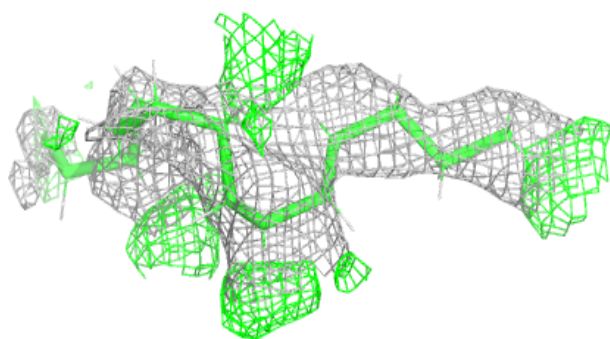
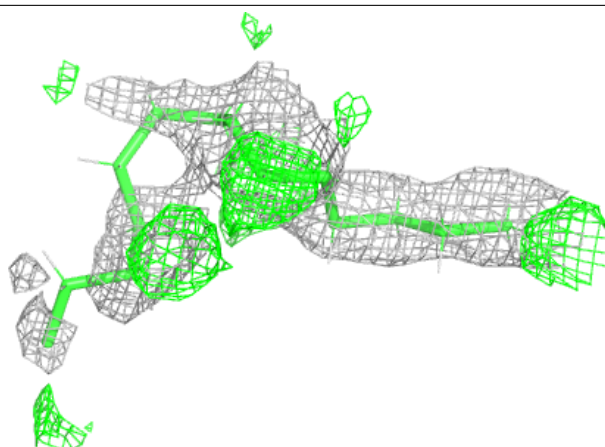
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	D	403	65/65	0.97	0.05	19,31,57,63	0
24	CLA	D	404	65/65	0.97	0.08	21,43,112,127	0
24	CLA	a	605	65/65	0.97	0.05	18,29,49,57	0
24	CLA	B	613	65/65	0.97	0.06	19,32,70,77	0
34	HEM	e	102	43/43	0.97	0.09	45,57,80,83	0
34	HEM	F	101	43/43	0.98	0.08	33,48,65,69	0
24	CLA	b	604	65/65	0.98	0.06	21,34,86,99	0
35	HEC	v	201	43/43	0.98	0.06	30,37,47,52	0
23	CL	A	604	1/1	0.99	0.04	28,28,28,28	0
21	OEX	A	601	10/10	0.99	0.03	26,27,30,30	0
22	FE2	a	602	1/1	0.99	0.02	31,31,31,31	0
35	HEC	V	201	43/43	0.99	0.06	22,32,45,47	0
23	CL	A	603	1/1	0.99	0.03	26,26,26,26	0
22	FE2	A	602	1/1	1.00	0.01	26,26,26,26	0
21	OEX	a	601	10/10	1.00	0.02	23,26,29,31	0
23	CL	a	603	1/1	1.00	0.03	28,28,28,28	0
23	CL	a	604	1/1	1.00	0.04	28,28,28,28	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.

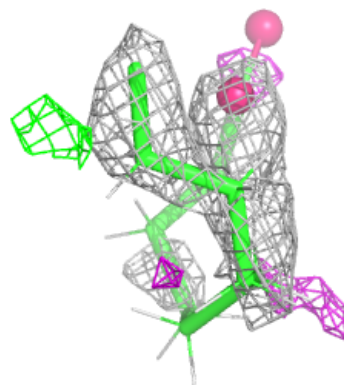
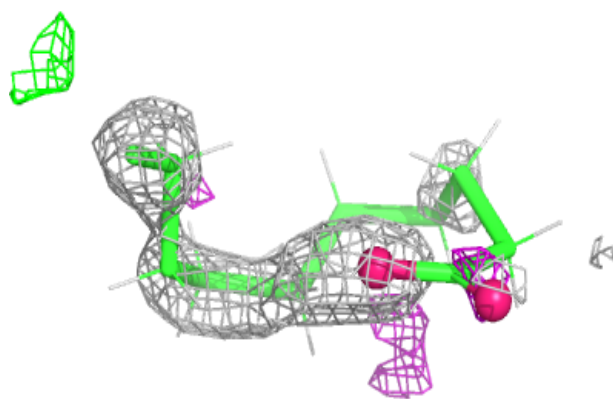
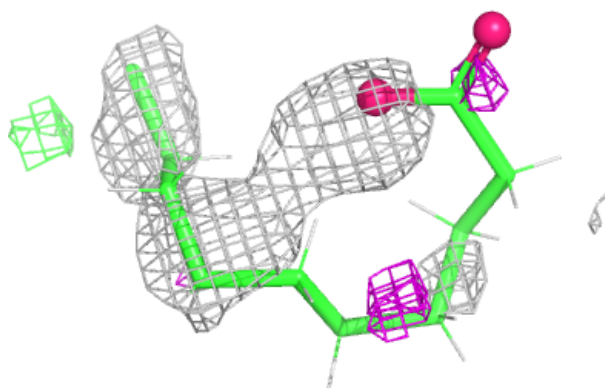
Electron density around STE C 528:

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



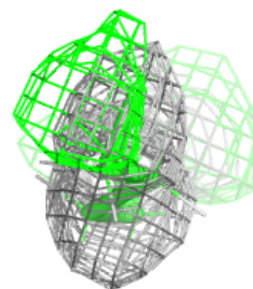
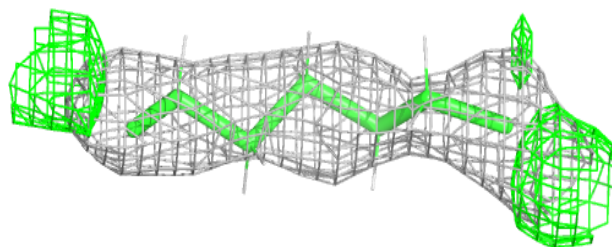
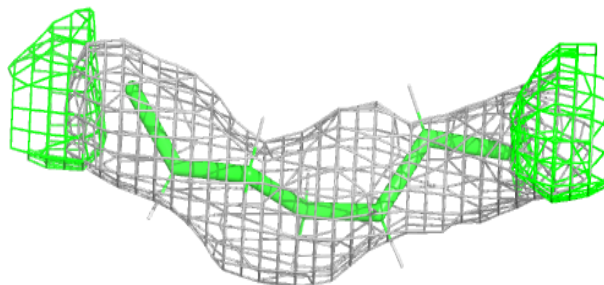
Electron density around STE i 101:

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

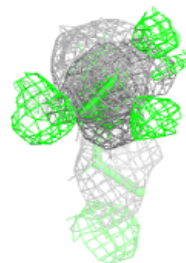
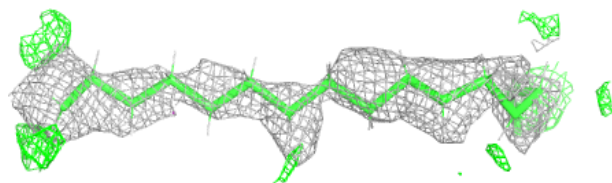
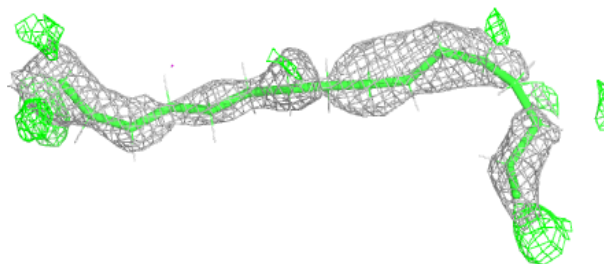


Electron density around STE C 518:

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

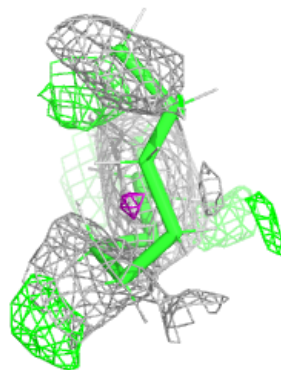
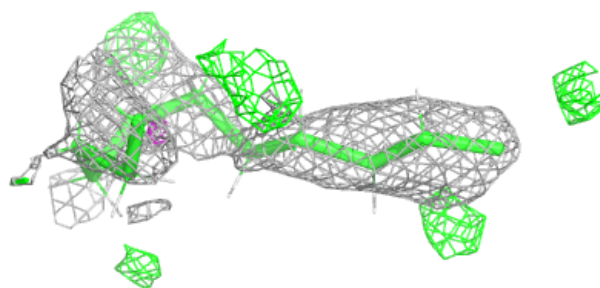
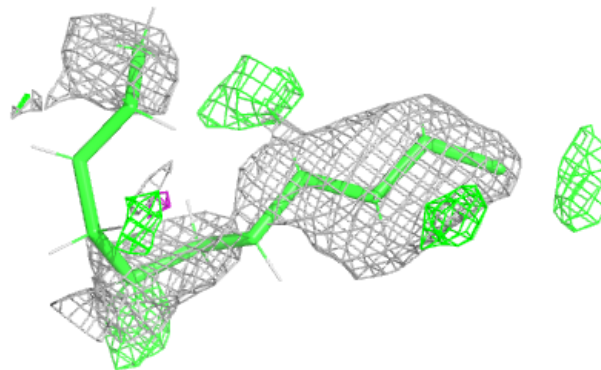
**Electron density around STE j 102:**

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

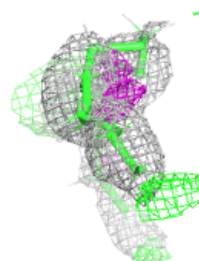
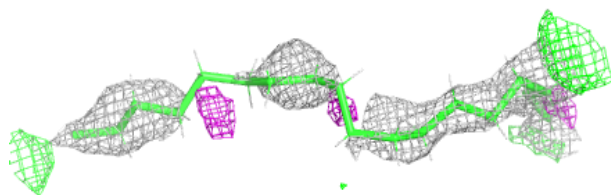
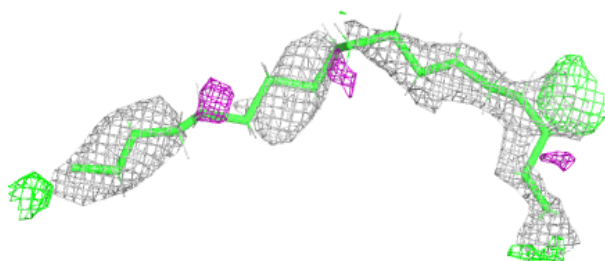


Electron density around STE A 619:

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

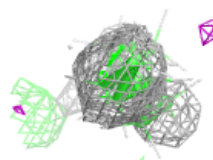
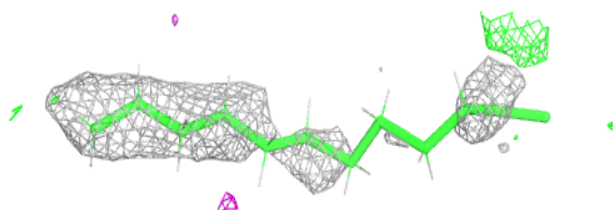
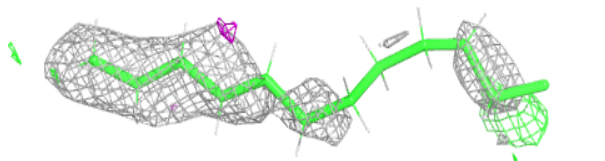
**Electron density around STE H 103:**

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

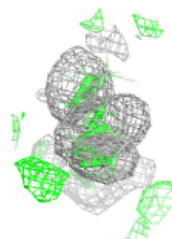
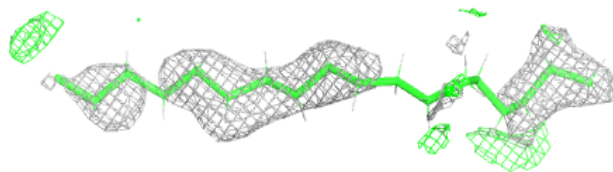
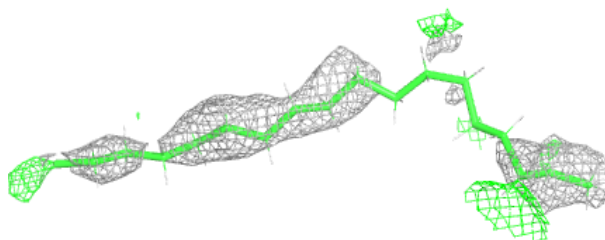


Electron density around STE E 102:

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

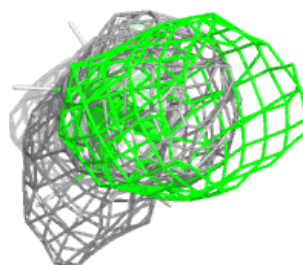
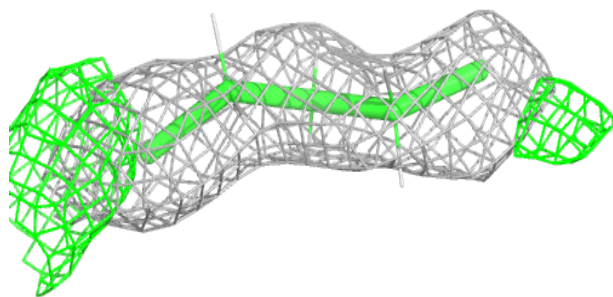
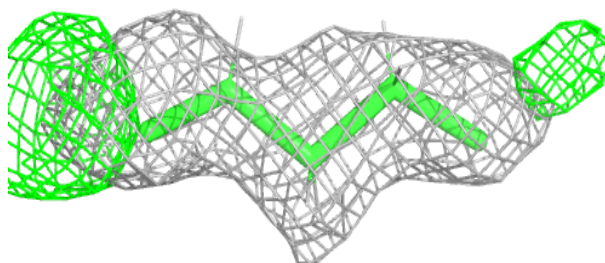
**Electron density around STE c 517:**

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

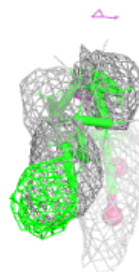
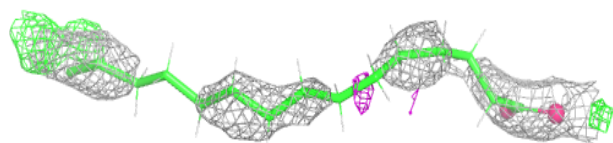
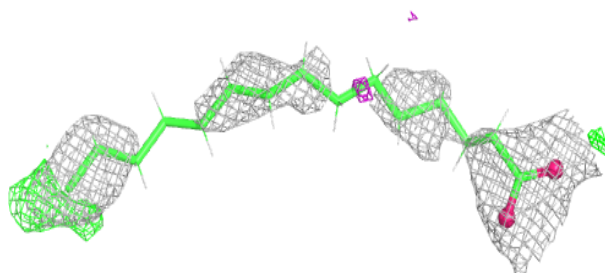


Electron density around STE C 517:

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

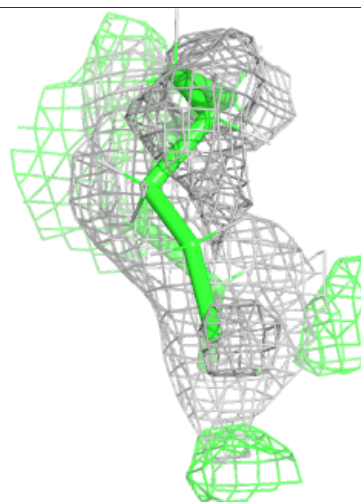
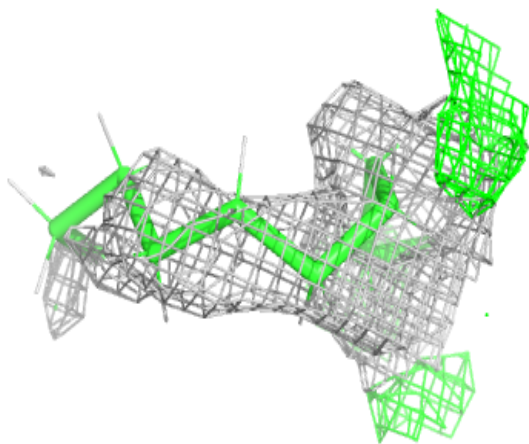
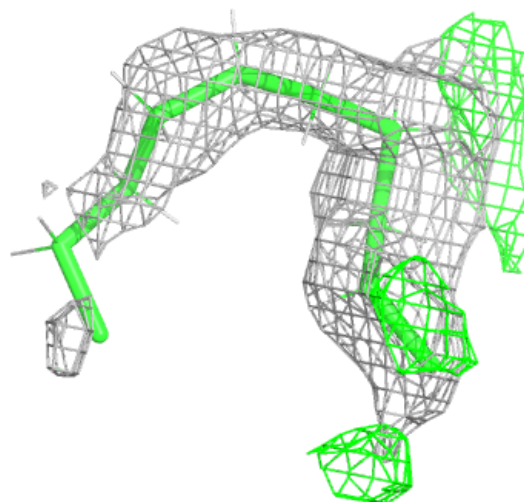
**Electron density around STE I 101:**

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



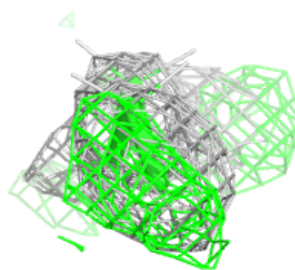
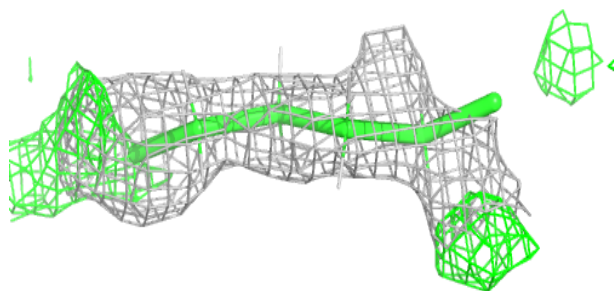
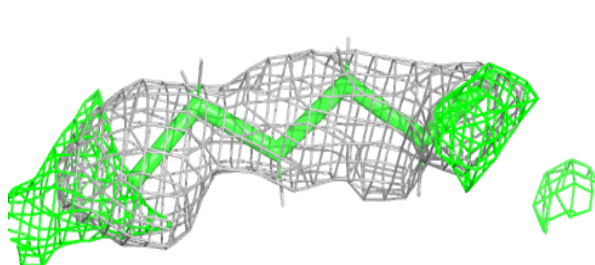
Electron density around STE C 519:

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and green (positive)

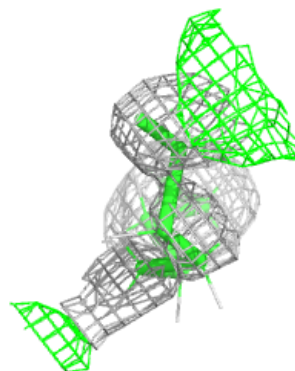
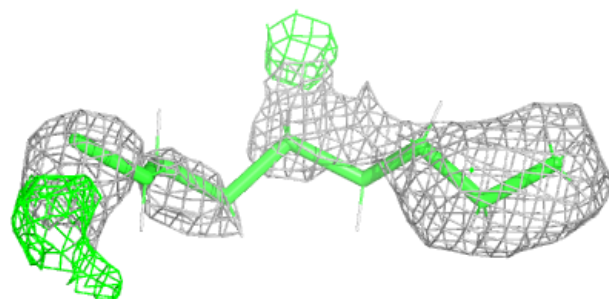
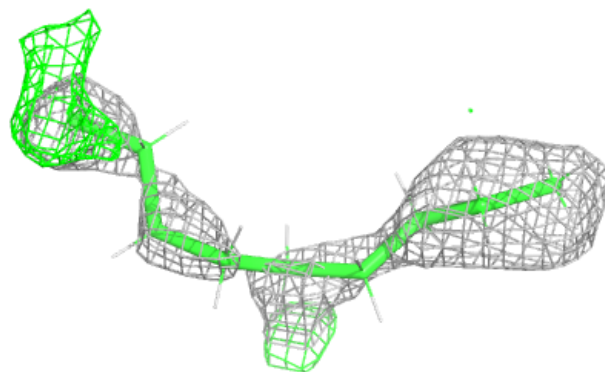


Electron density around STE i 102:

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and green (positive)

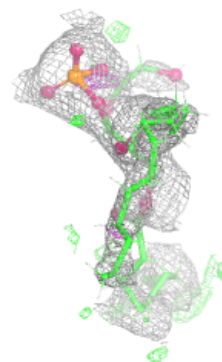
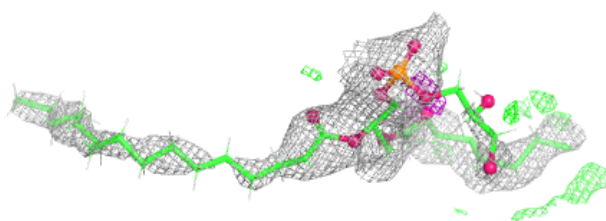
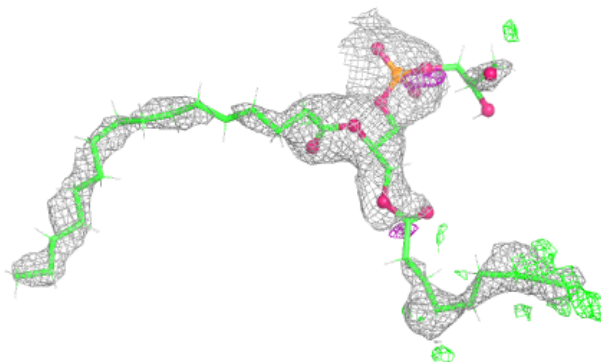
**Electron density around STE e 101:**

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and green (positive)

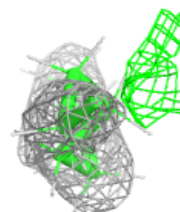
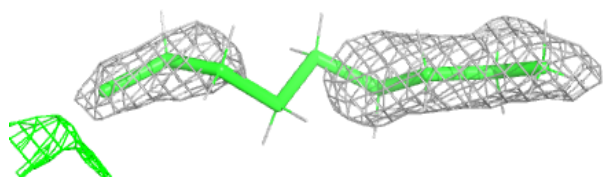
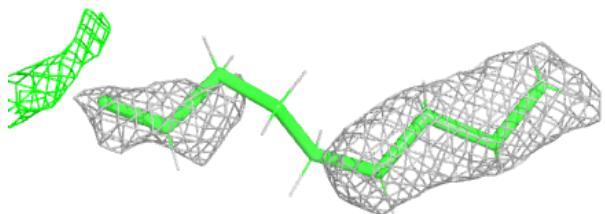


Electron density around LHG e 103:

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

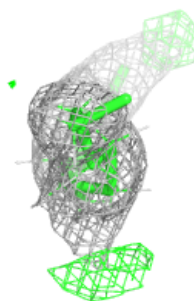
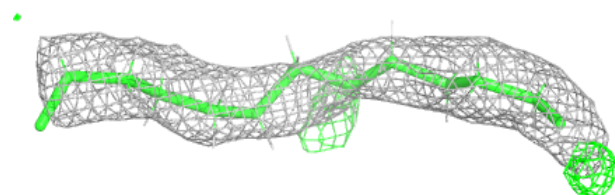
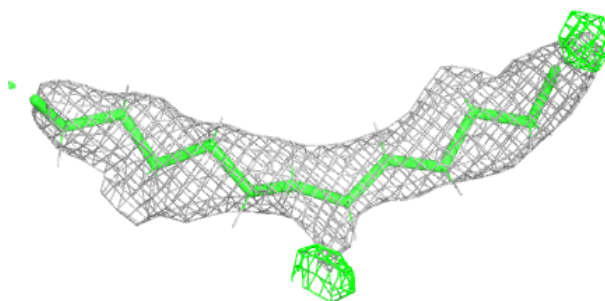
**Electron density around STE e 104:**

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

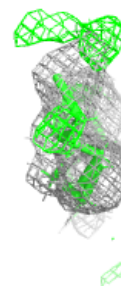
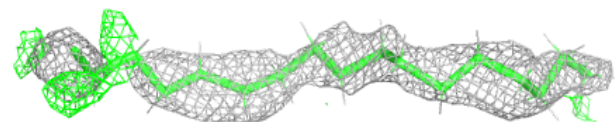
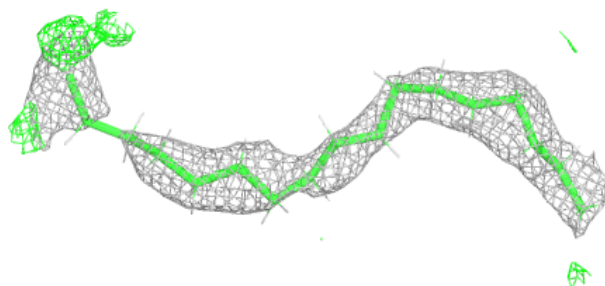


Electron density around STE c 516:

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

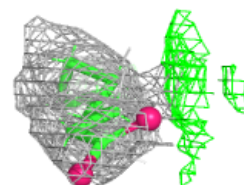
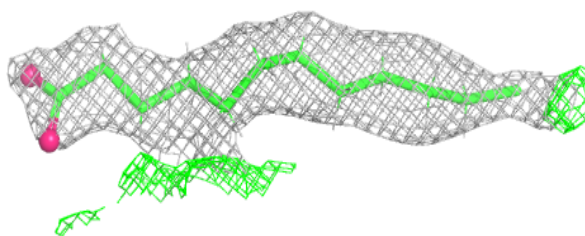
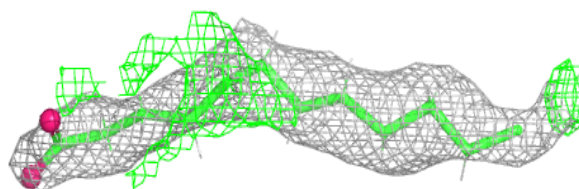
**Electron density around STE A 618:**

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

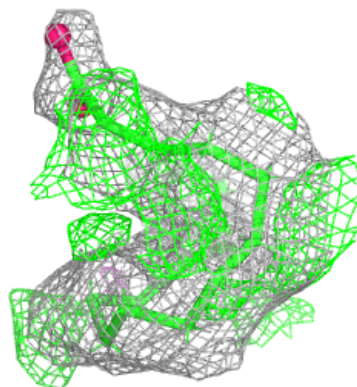
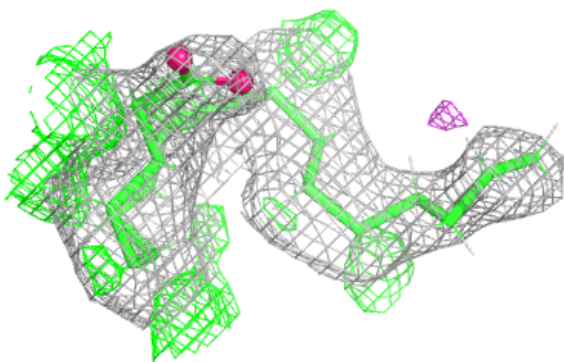
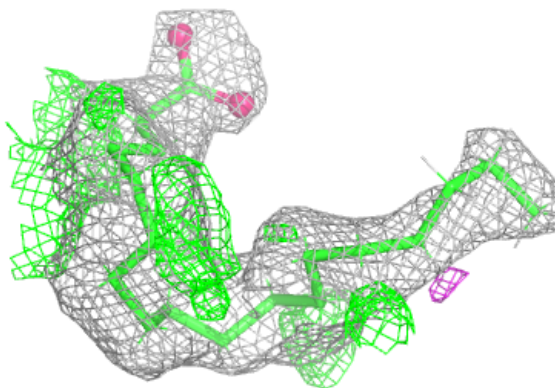


Electron density around STE d 415:

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

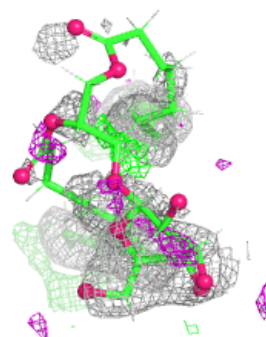
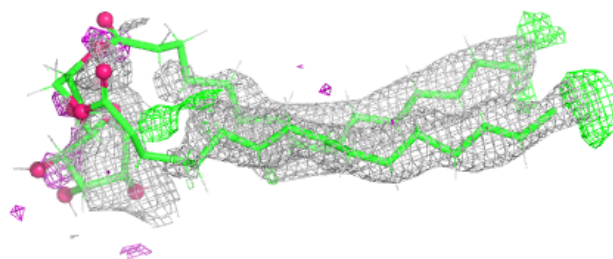
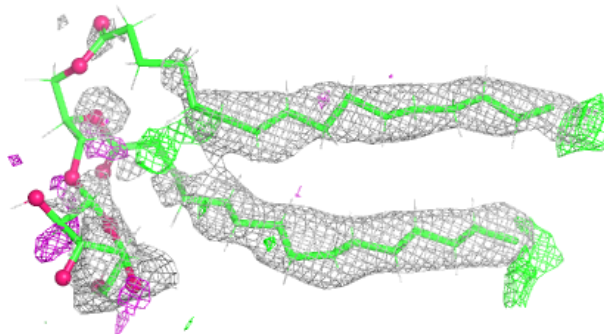
**Electron density around STE R 101:**

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

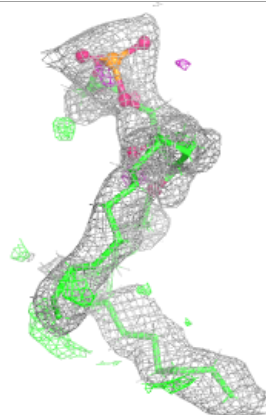
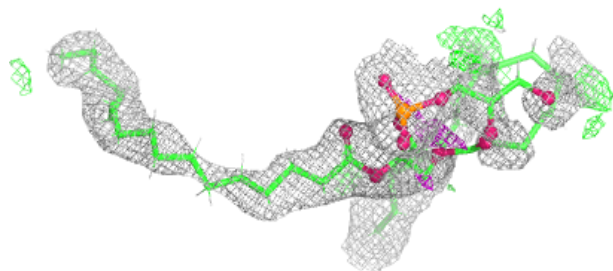
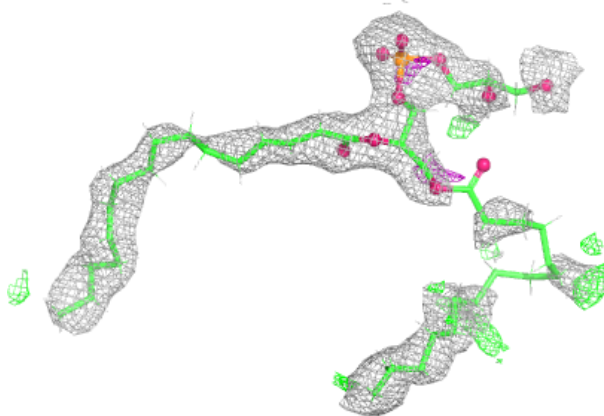


Electron density around LMG D 407:

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

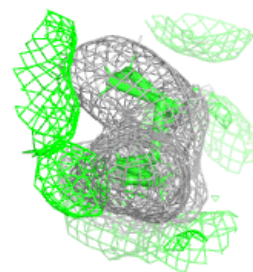
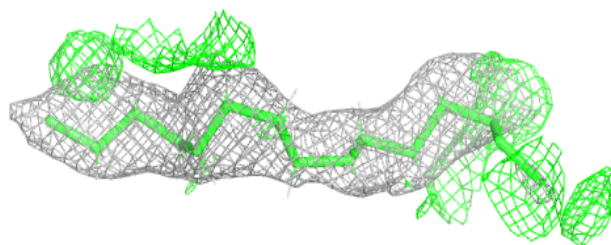
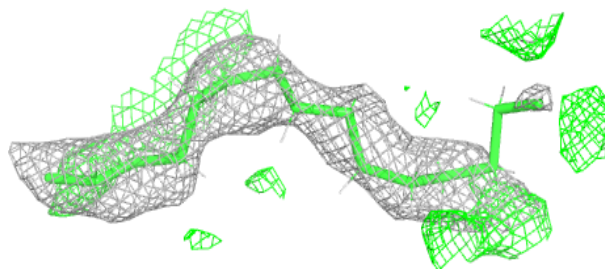
**Electron density around LHG A 615:**

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

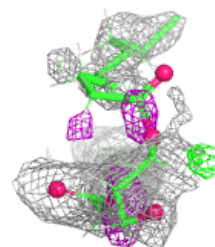
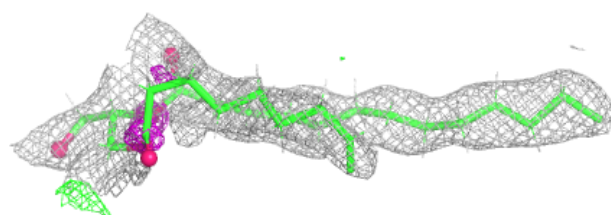
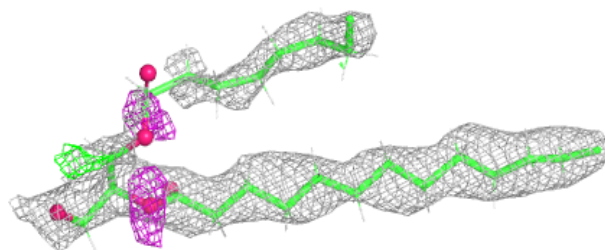


Electron density around STE B 626:

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

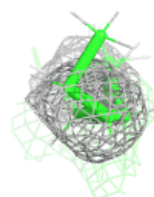
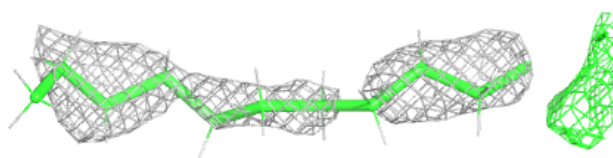
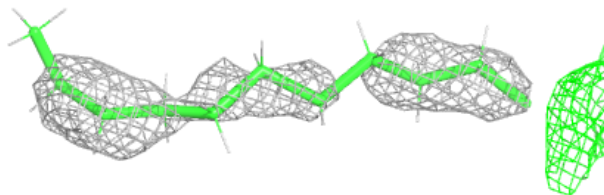
**Electron density around LMG c 518:**

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

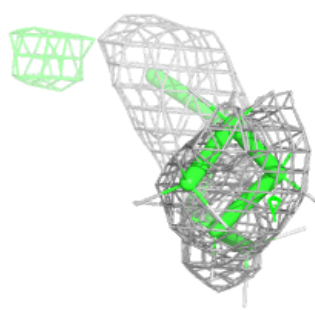
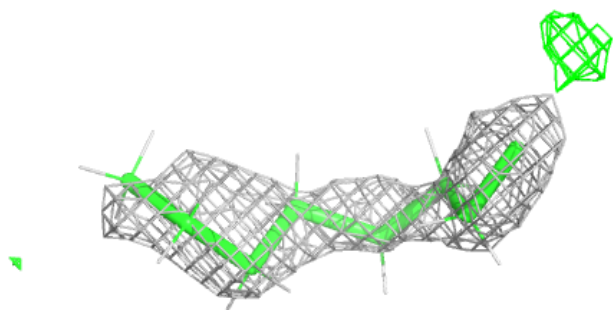
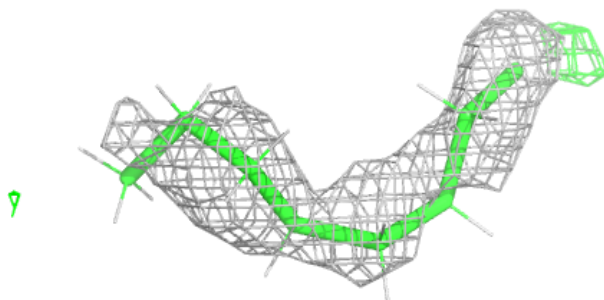


Electron density around STE b 627:

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

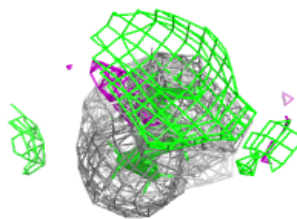
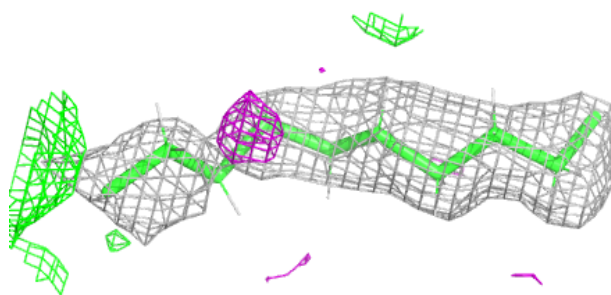
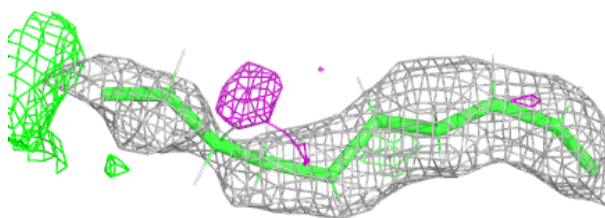
**Electron density around STE f 102:**

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

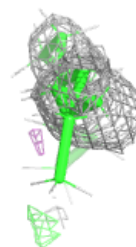
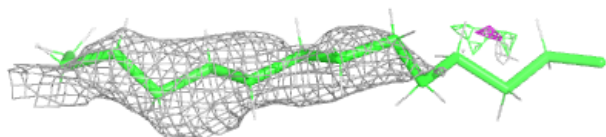
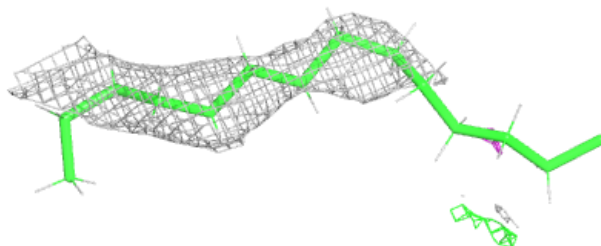


Electron density around STE t 103:

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

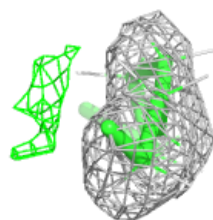
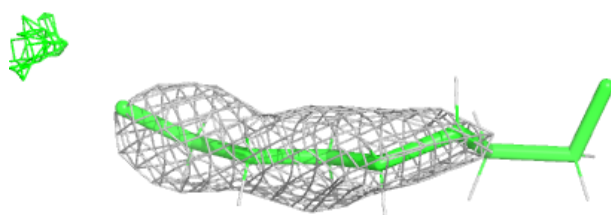
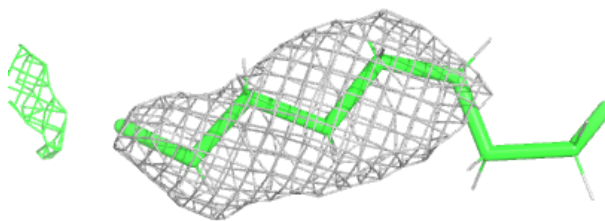
**Electron density around STE C 527:**

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

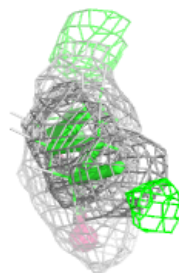
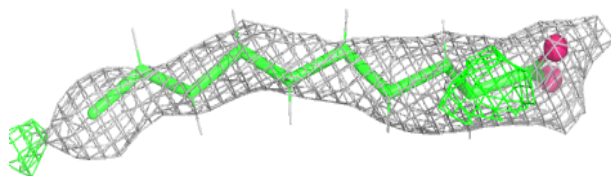
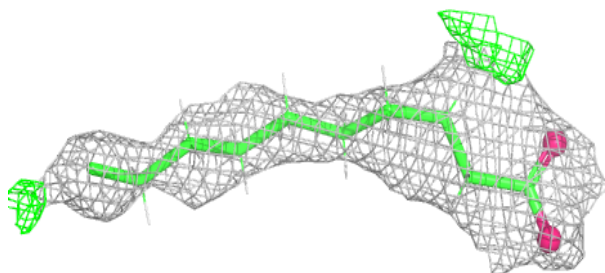


Electron density around STE A 611:

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

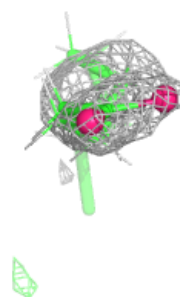
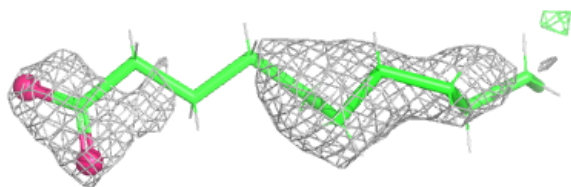
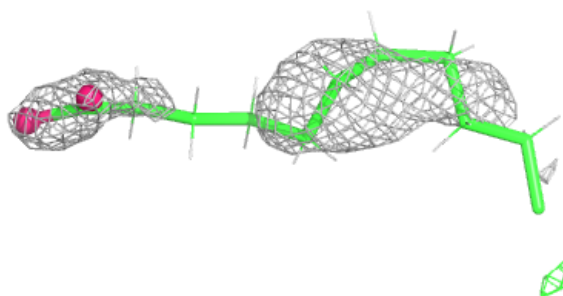
**Electron density around STE a 612:**

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

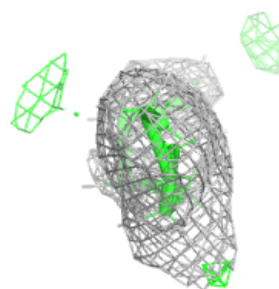
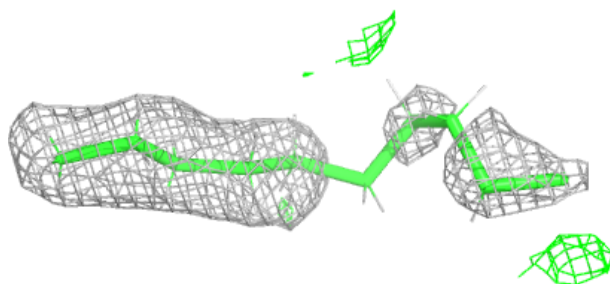
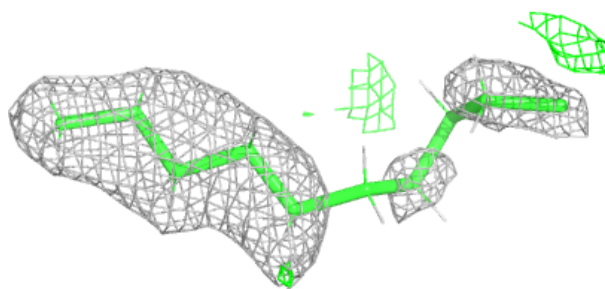


Electron density around STE e 105:

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

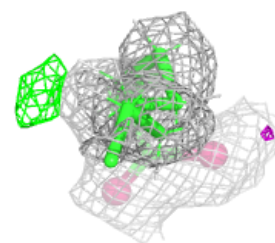
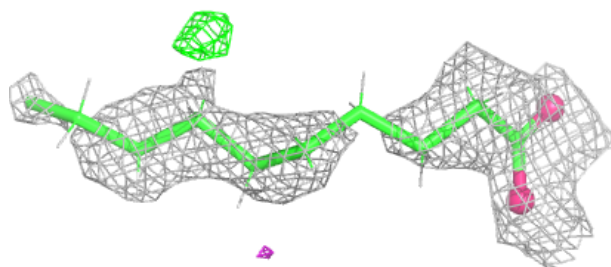
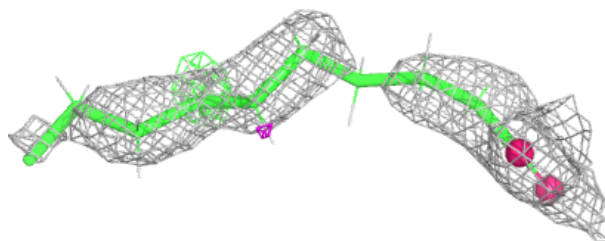
**Electron density around STE h 103:**

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

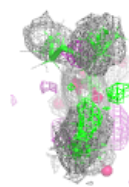
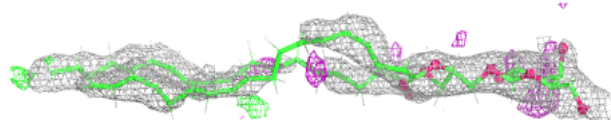
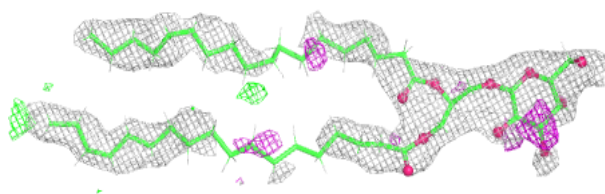


Electron density around STE E 101:

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

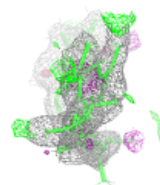
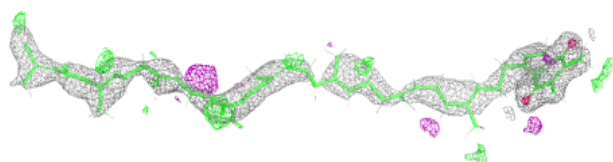
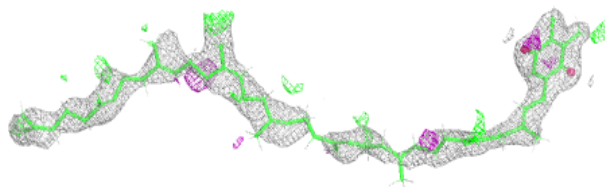
**Electron density around LMG b 623:**

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

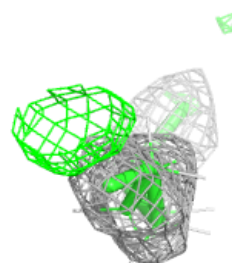
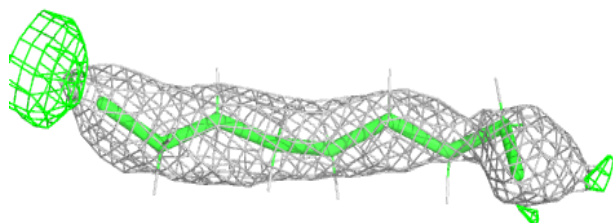
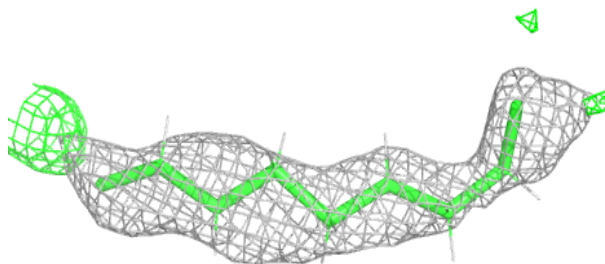


Electron density around PL9 A 610:

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

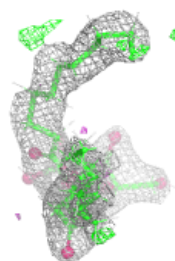
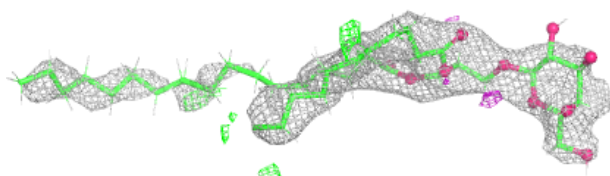
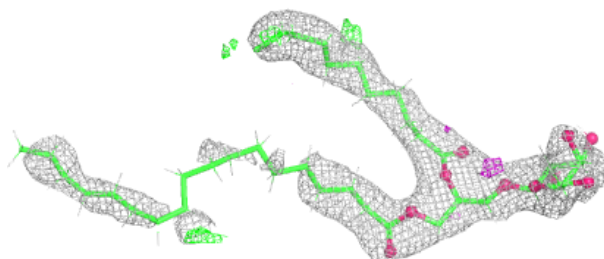
**Electron density around STE z 101:**

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

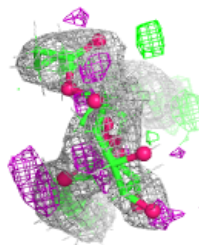
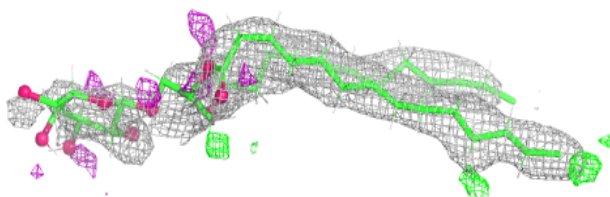
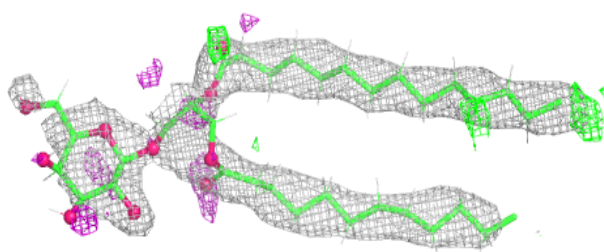


Electron density around LMG c 523:

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

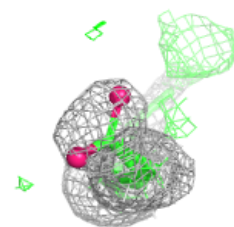
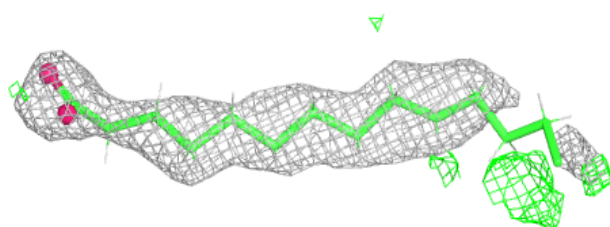
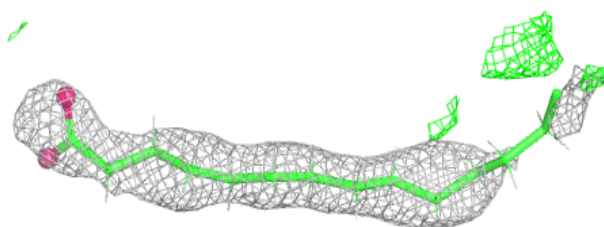
**Electron density around LMG B 620:**

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

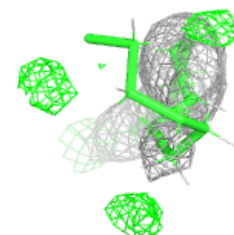
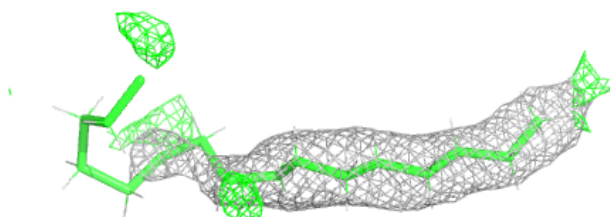
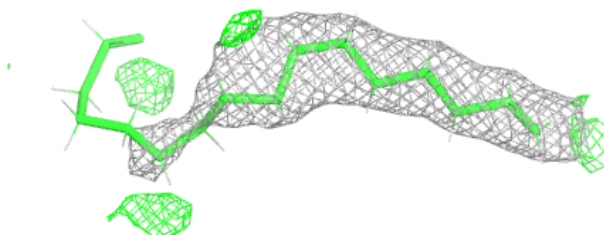


Electron density around STE b 624:

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

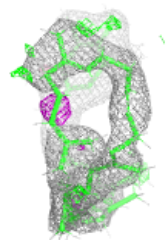
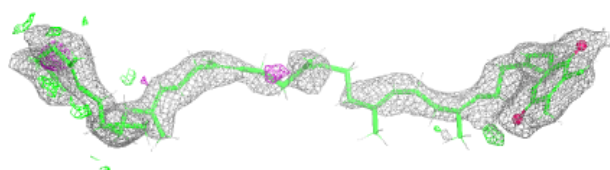
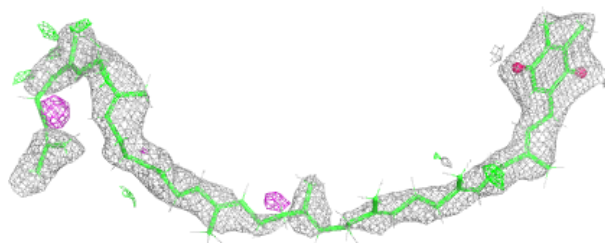
**Electron density around STE b 621:**

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

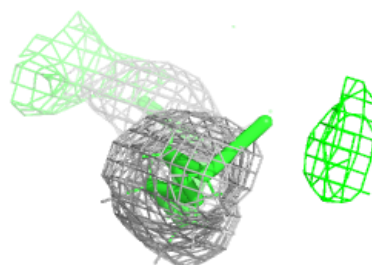
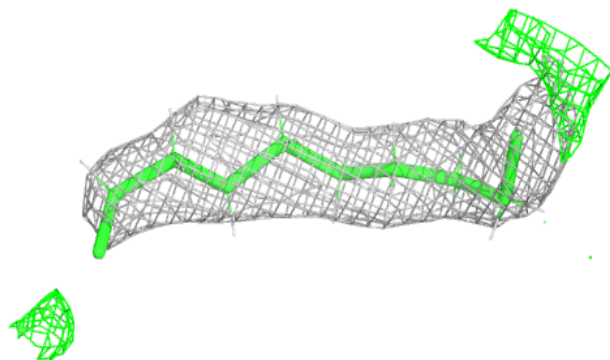
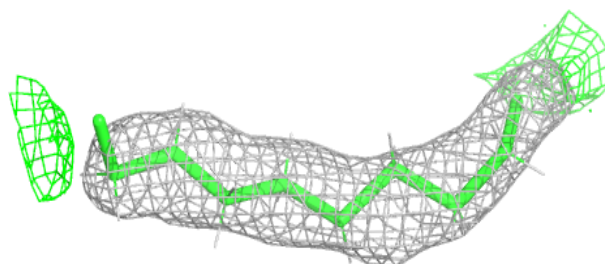


Electron density around PL9 a 609:

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

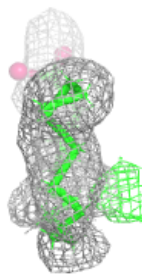
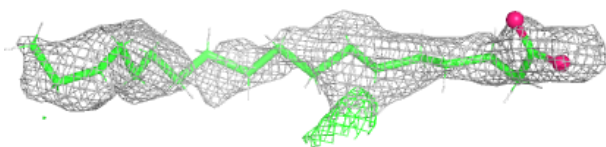
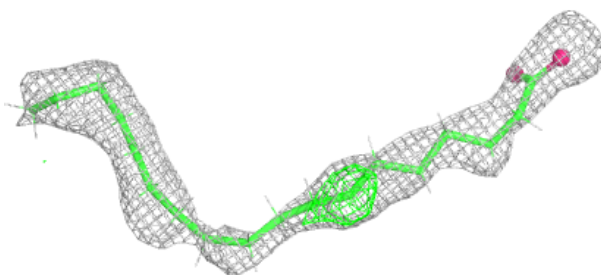
**Electron density around STE b 625:**

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

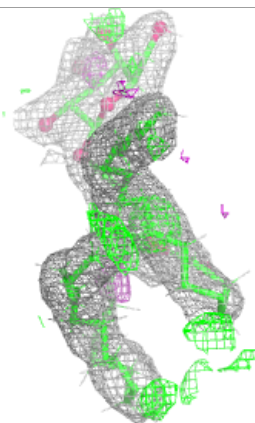
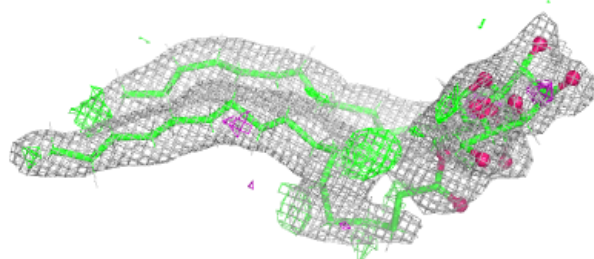
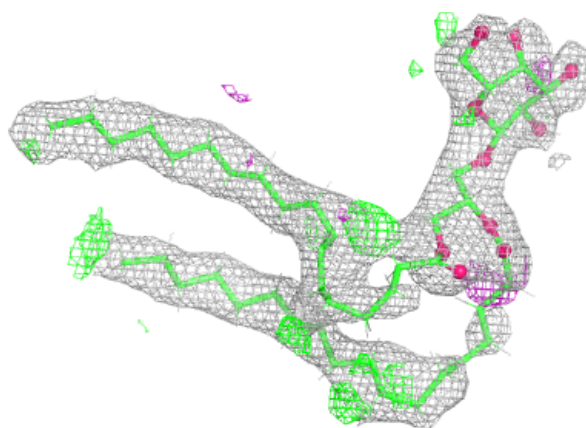


Electron density around STE E 103:

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

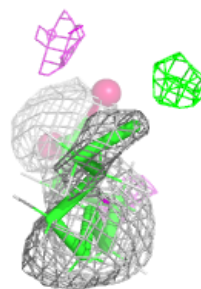
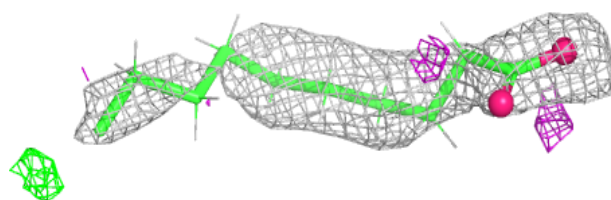
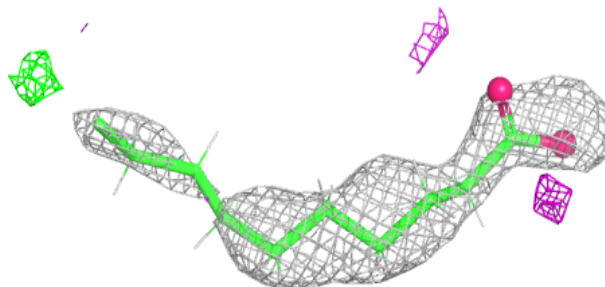
**Electron density around LMG o 301:**

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

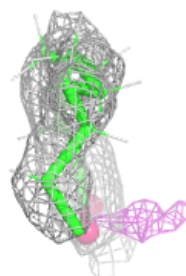
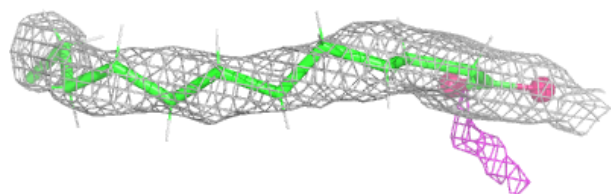
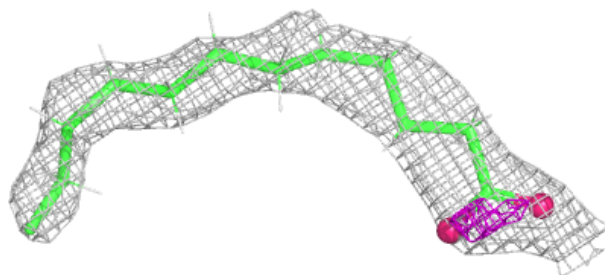


Electron density around STE B 625:

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

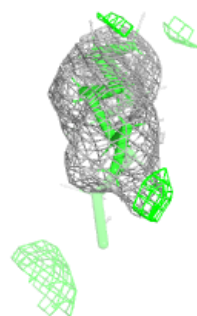
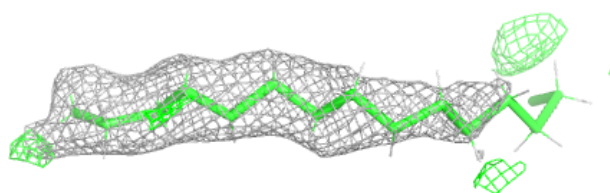
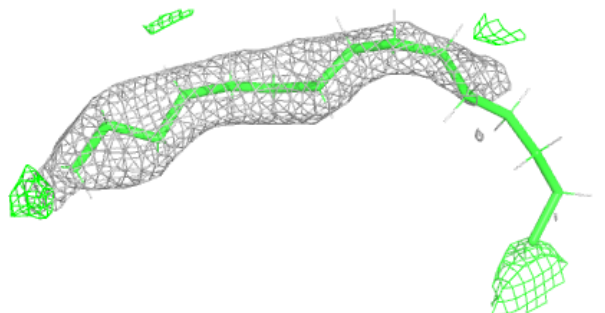
**Electron density around STE C 515:**

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

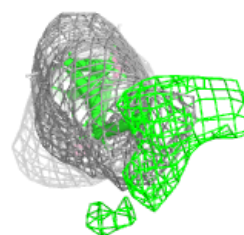
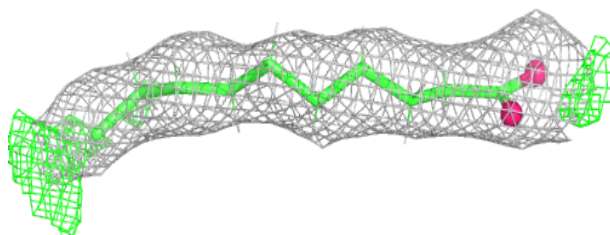
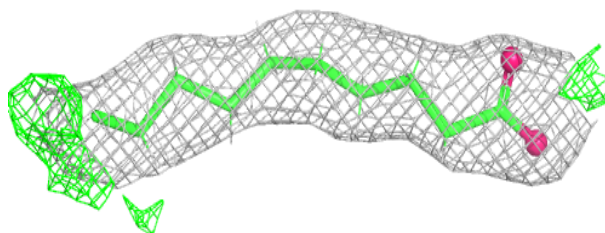


Electron density around STE M 103:

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

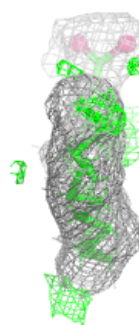
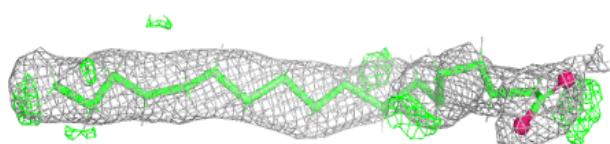
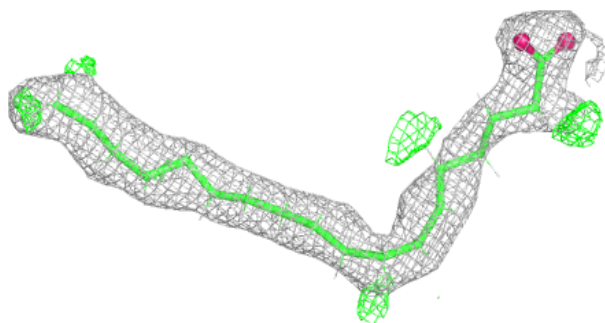
**Electron density around STE j 101:**

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

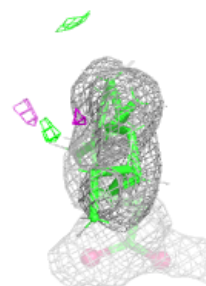
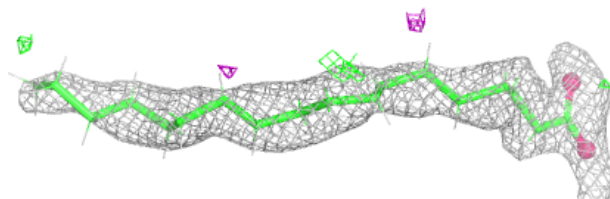
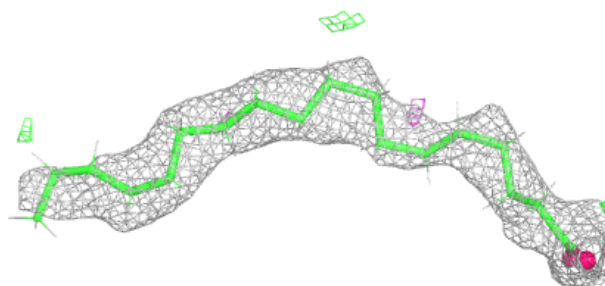


Electron density around STE d 409:

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

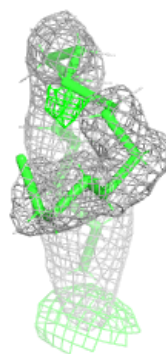
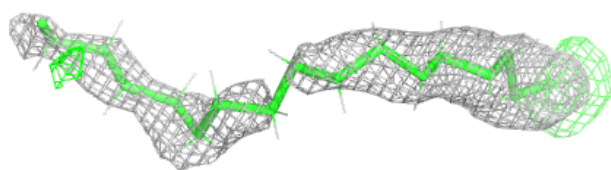
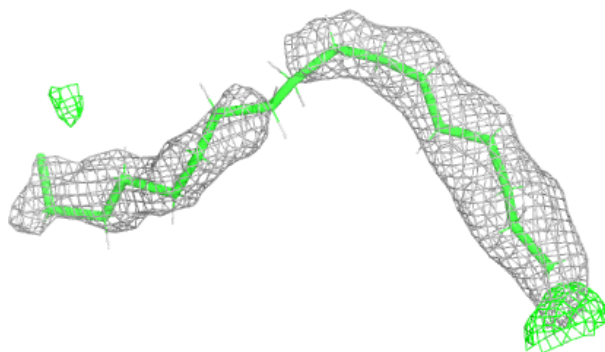
**Electron density around STE d 413:**

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

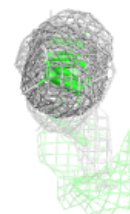
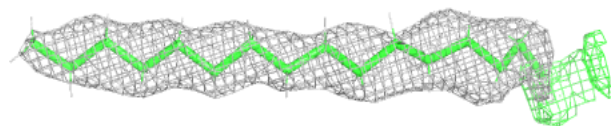
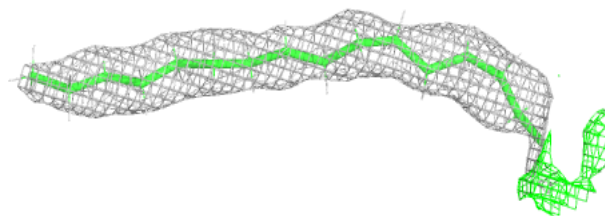


Electron density around STE Z 101:

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

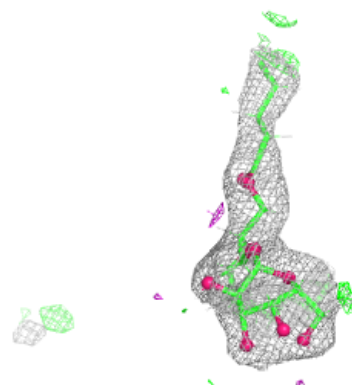
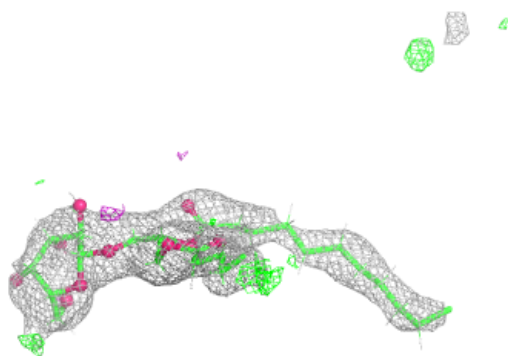
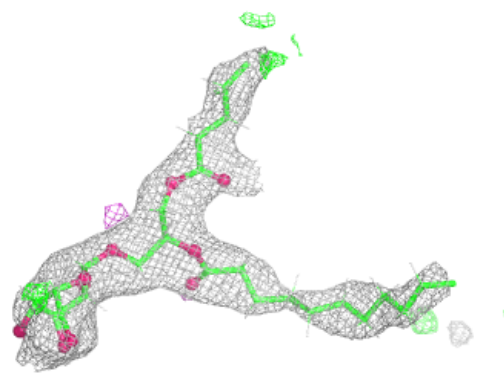
**Electron density around STE C 526:**

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

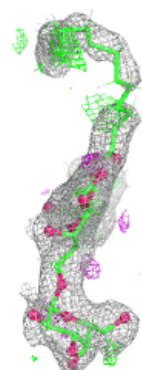
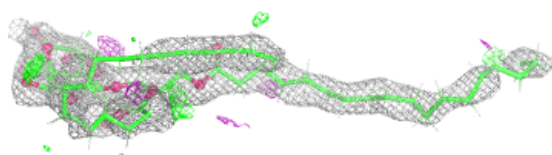
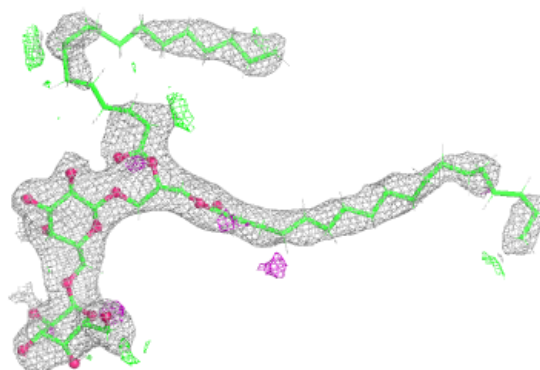


Electron density around LMG C 516:

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

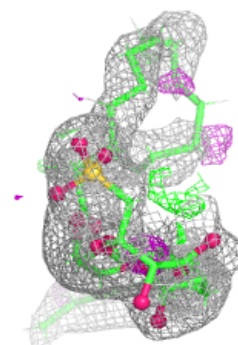
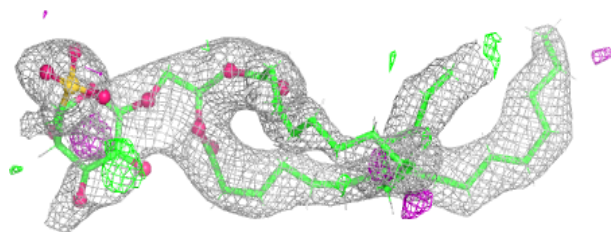
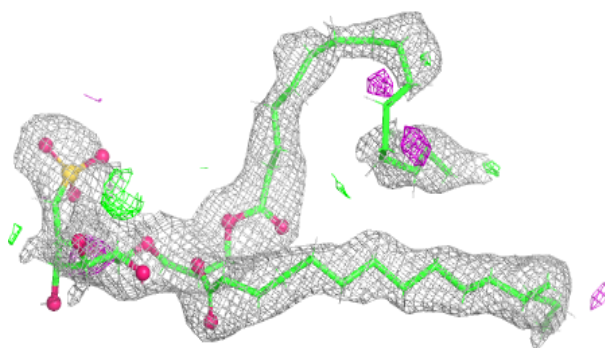
**Electron density around DGD A 617:**

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



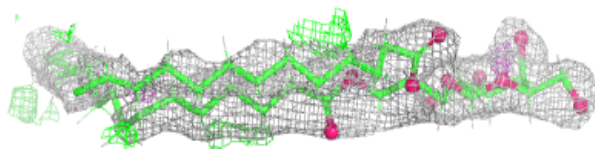
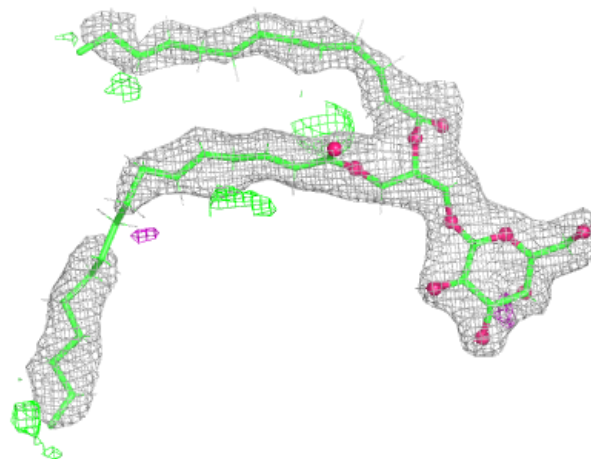
Electron density around SQD a 611:

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



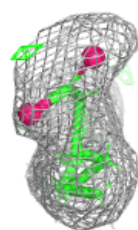
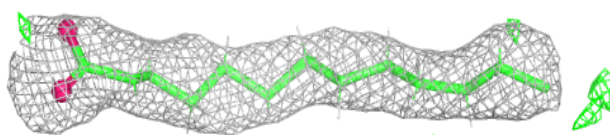
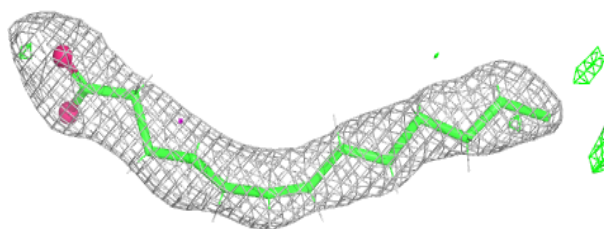
Electron density around LMG C 524:

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

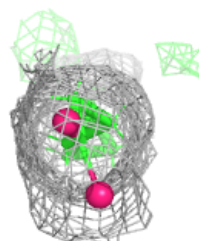
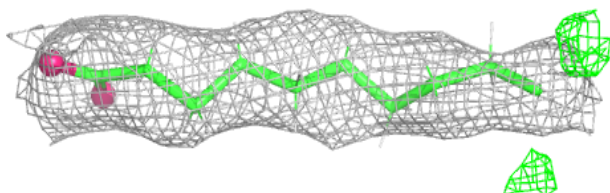
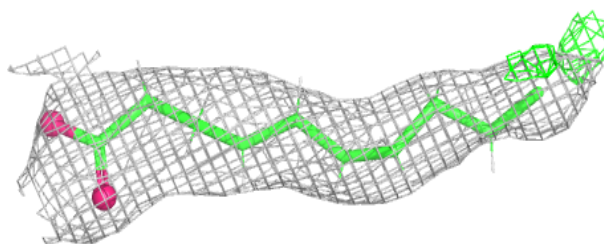


Electron density around STE I 102:

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

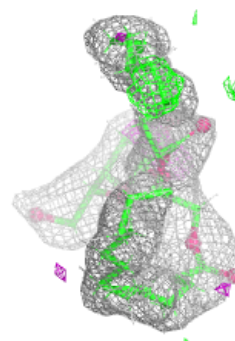
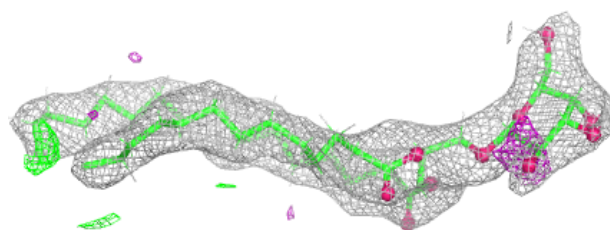
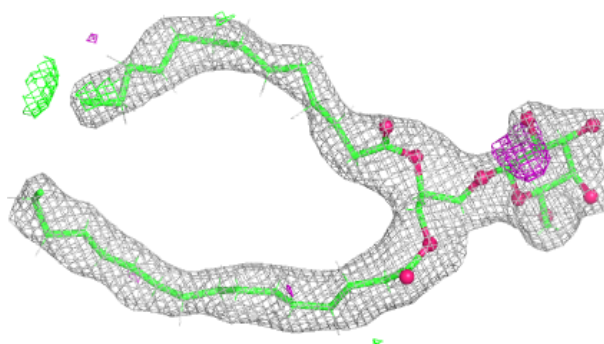
**Electron density around STE J 101:**

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

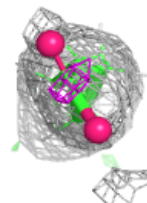
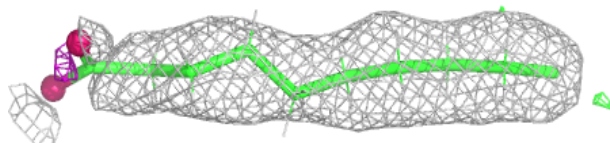
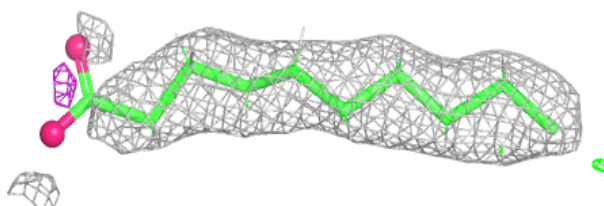


Electron density around LMG A 613:

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

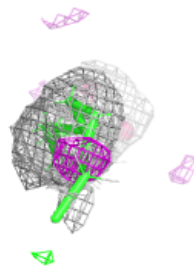
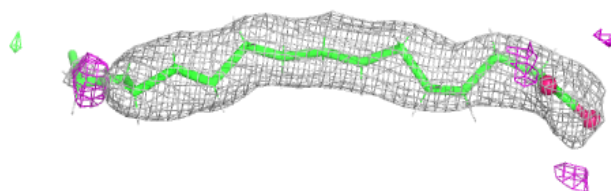
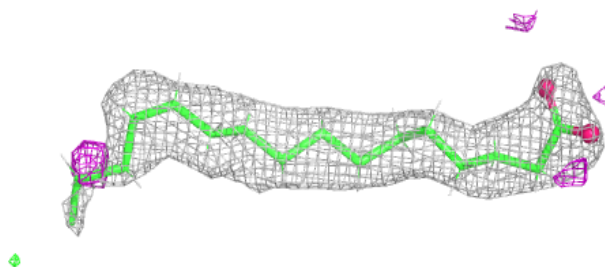
**Electron density around STE m 102:**

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



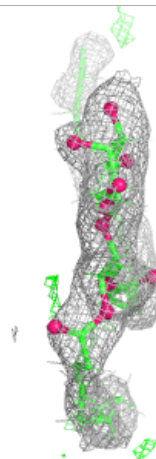
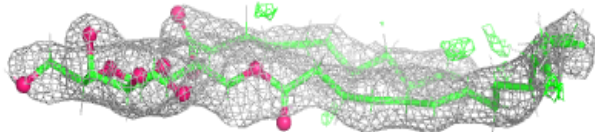
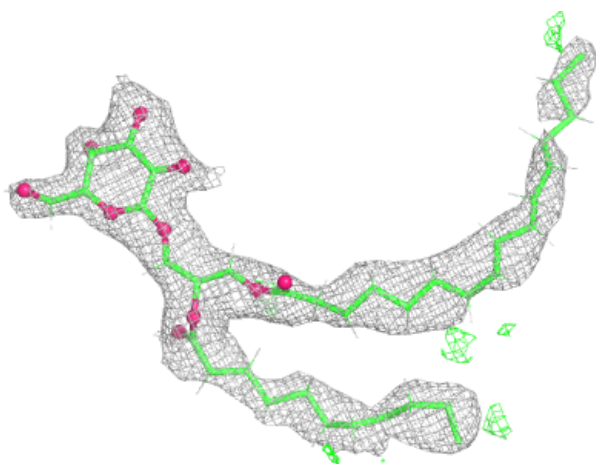
Electron density around STE B 624:

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



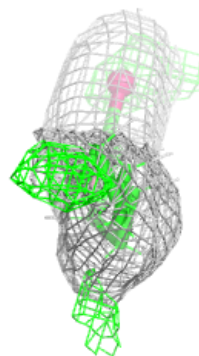
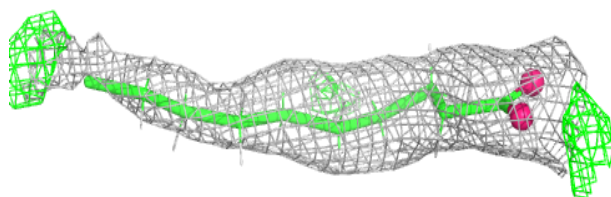
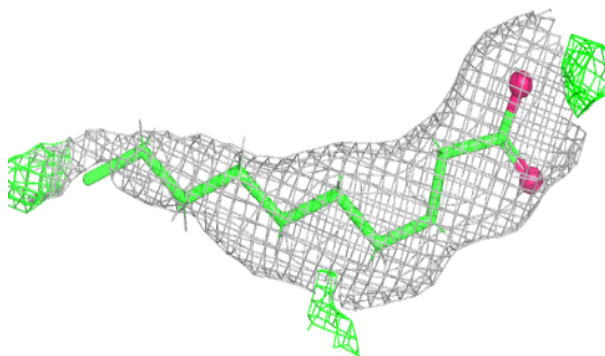
Electron density around LMG c 522:

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

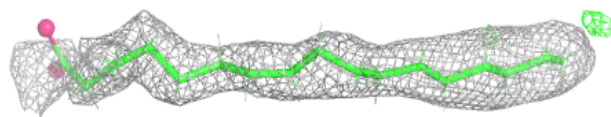
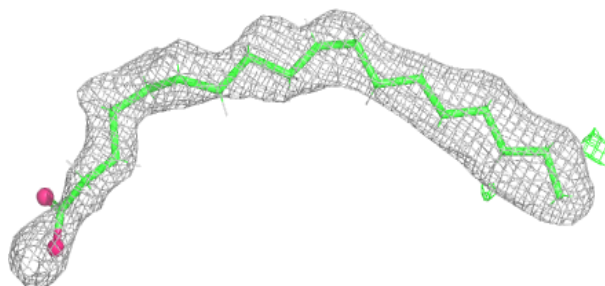


Electron density around STE C 525:

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

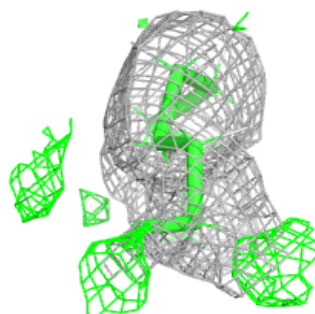
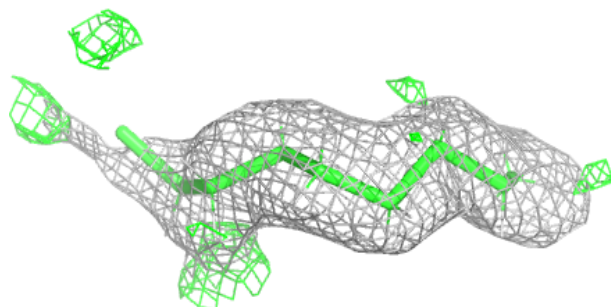
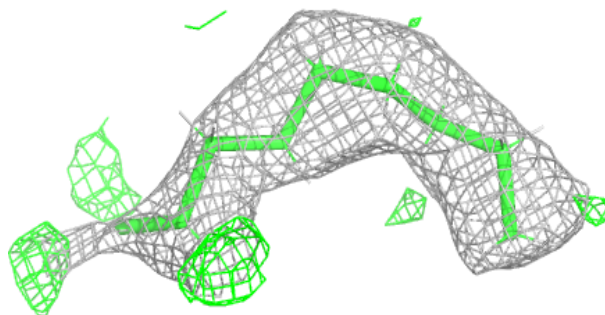
**Electron density around STE x 101:**

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

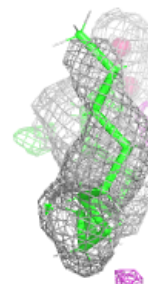
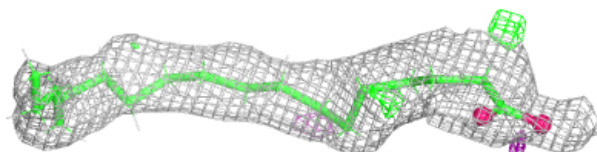
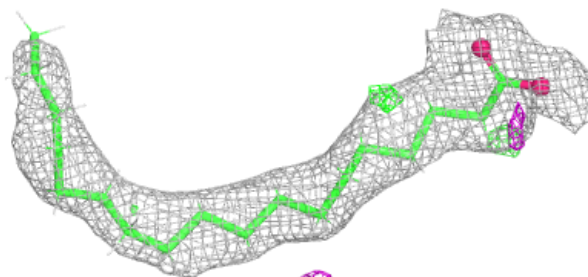


Electron density around STE D 412:

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

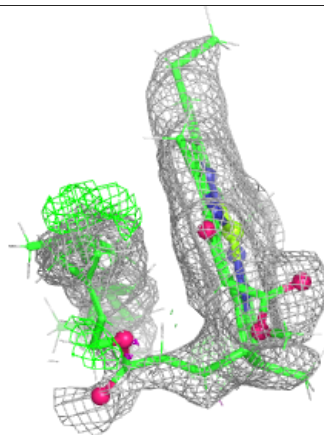
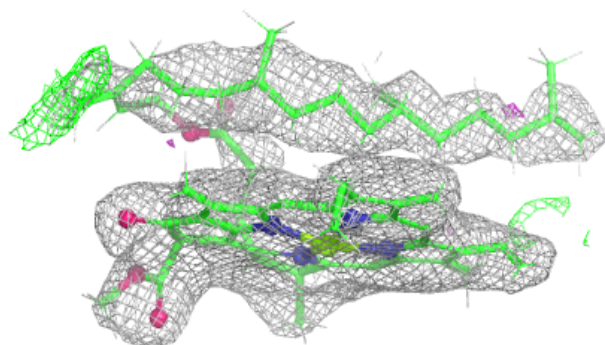
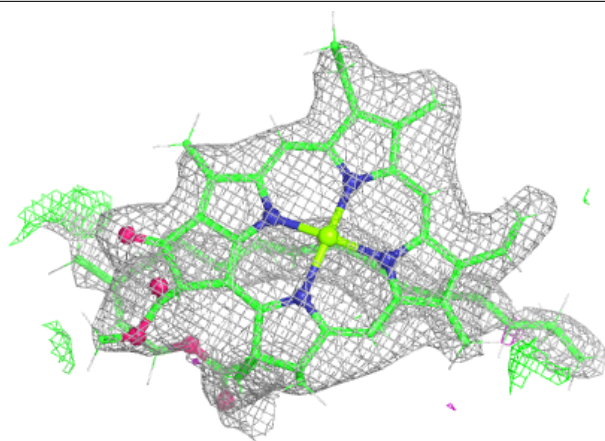
**Electron density around STE b 622:**

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

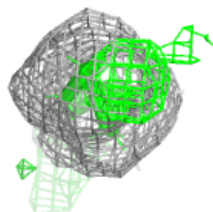
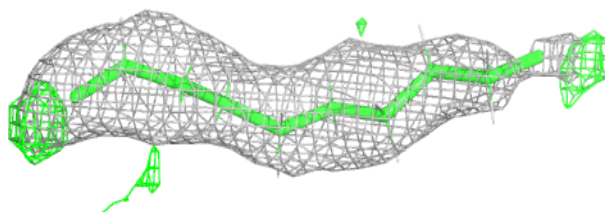
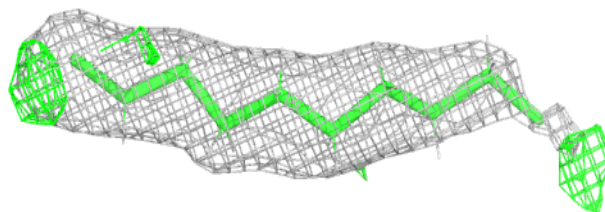


Electron density around CLA b 601:

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

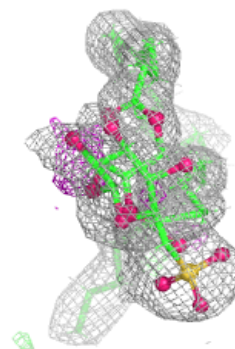
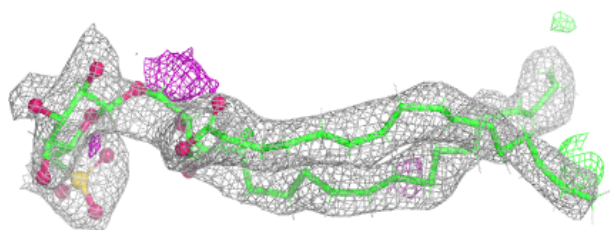
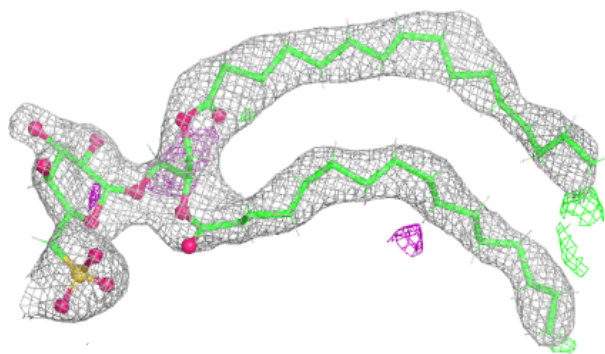
**Electron density around STE M 102:**

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

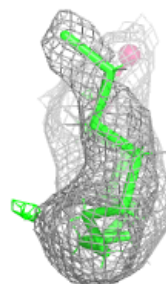
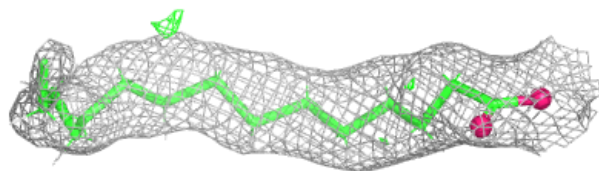
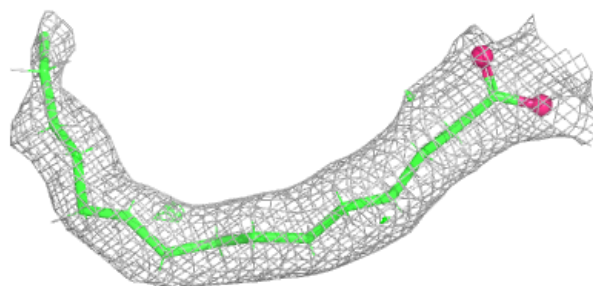


Electron density around SQD B 623:

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

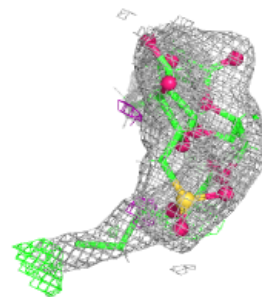
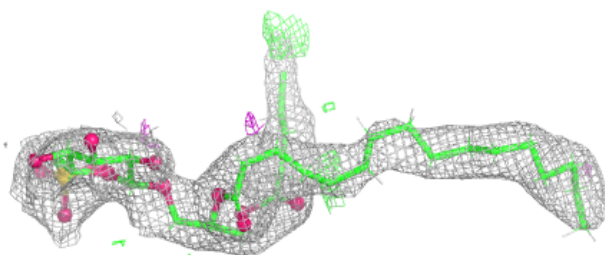
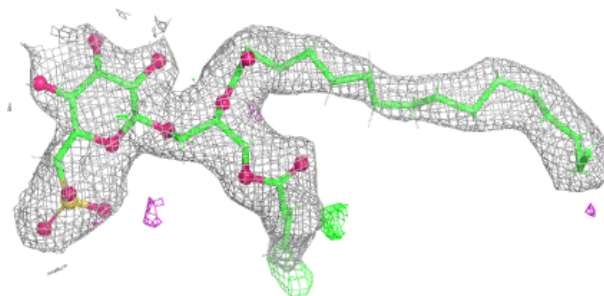
**Electron density around STE B 622:**

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

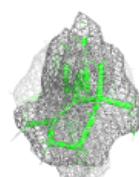
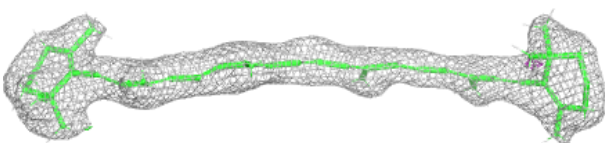
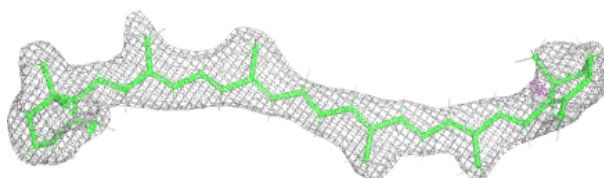


Electron density around SQD A 616:

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

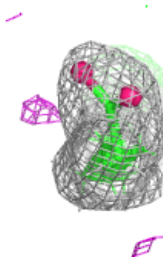
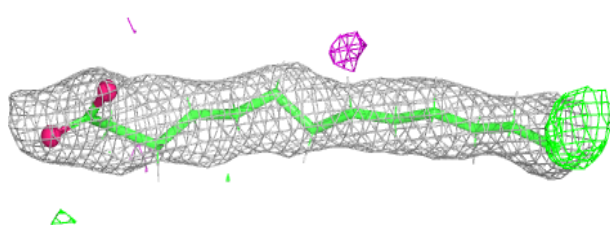
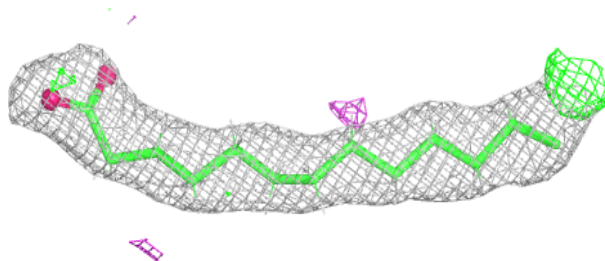
**Electron density around BCR k 101:**

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

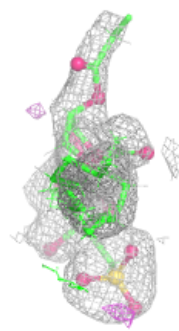
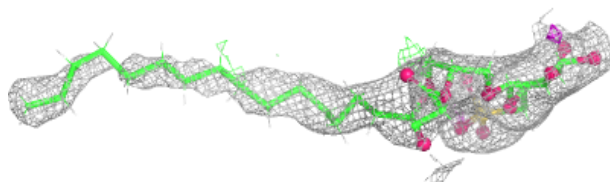
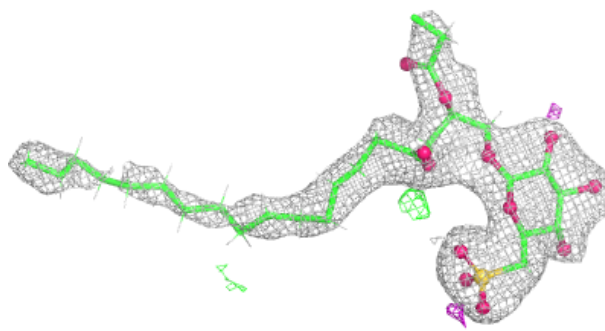


Electron density around STE M 101:

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

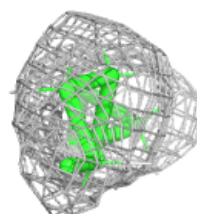
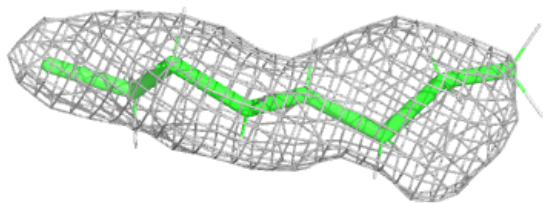
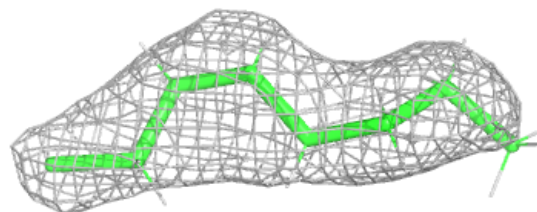
**Electron density around SQD f 101:**

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

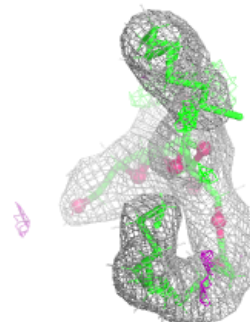
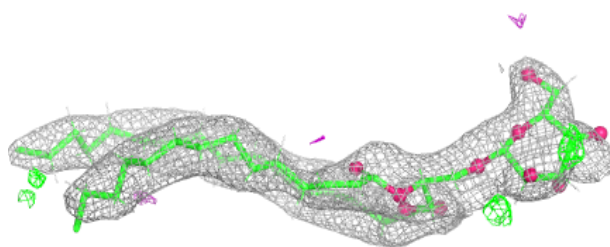
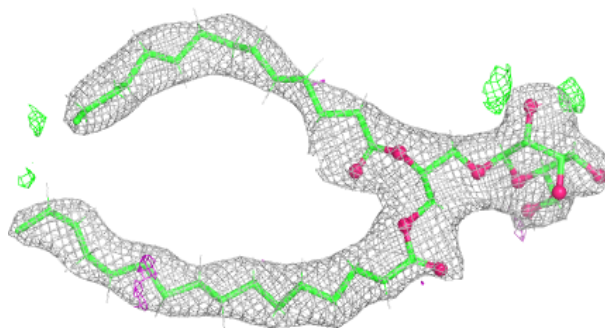


Electron density around STE b 626:

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

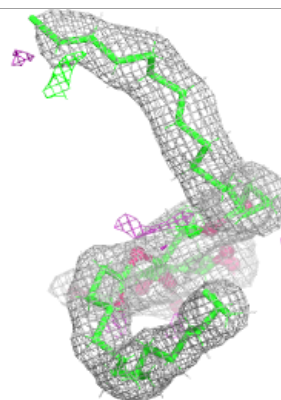
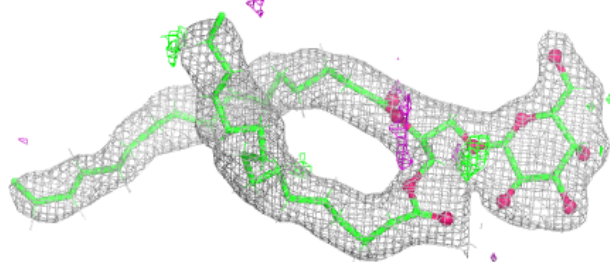
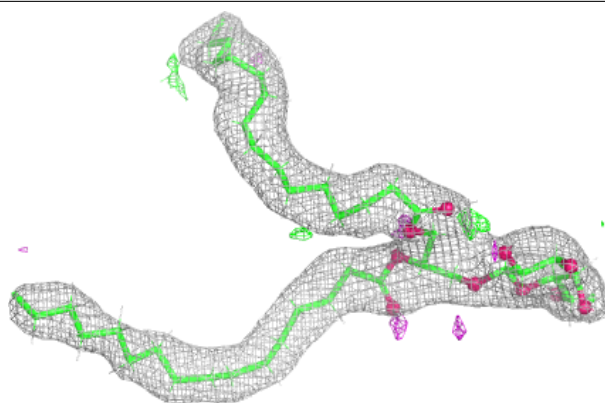
**Electron density around LMG c 524:**

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

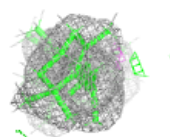
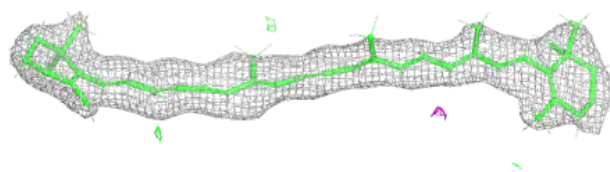
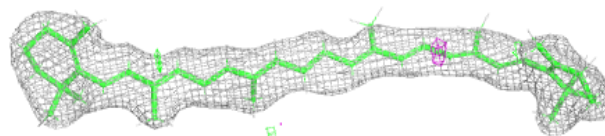


Electron density around LMG m 101:

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

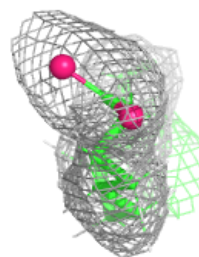
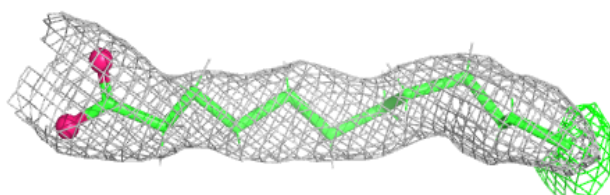
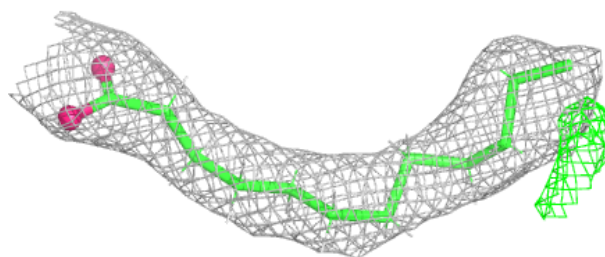
**Electron density around BCR K 101:**

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

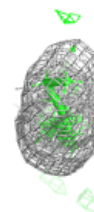
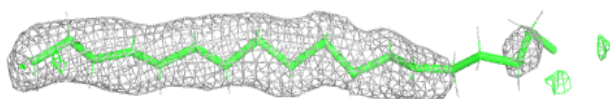
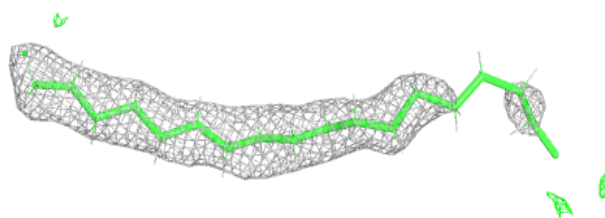


Electron density around STE t 102:

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

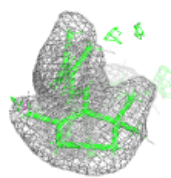
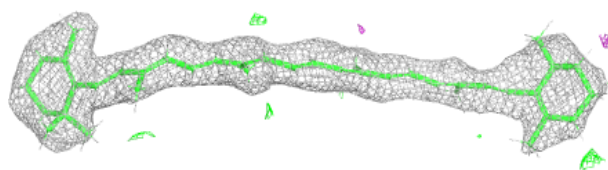
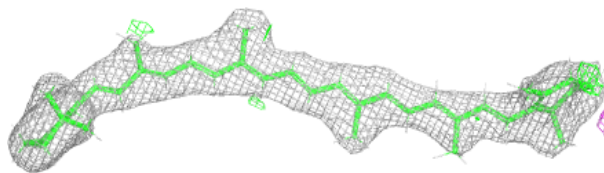
**Electron density around STE l 102:**

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

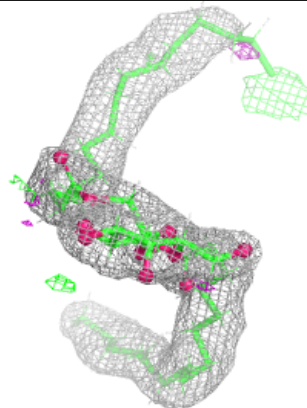
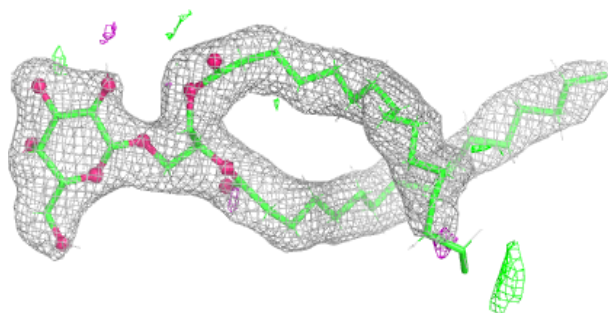
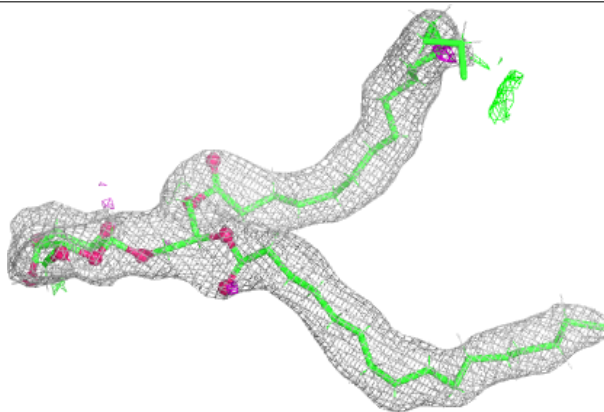


Electron density around BCR h 101:

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

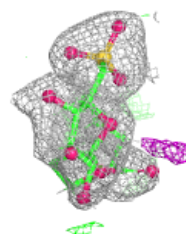
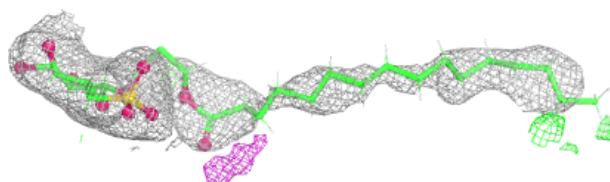
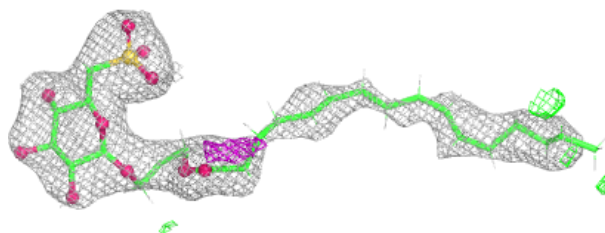
**Electron density around LMG B 621:**

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



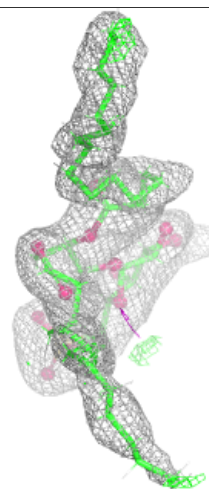
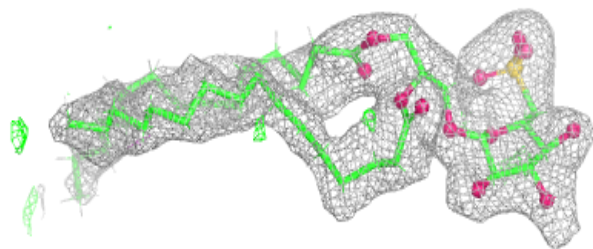
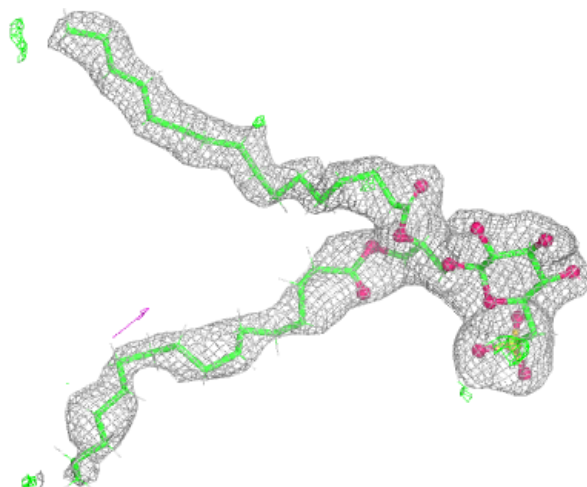
Electron density around SQD F 102:

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



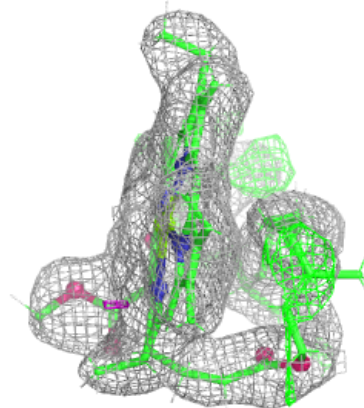
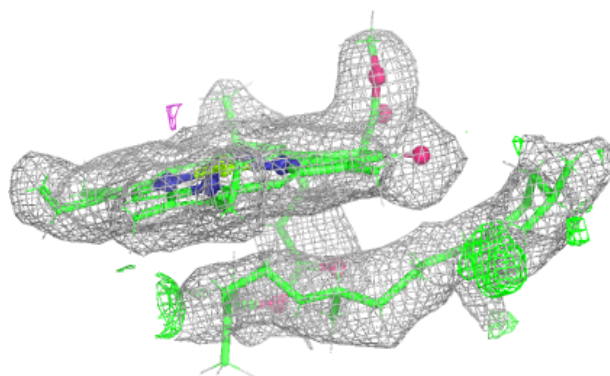
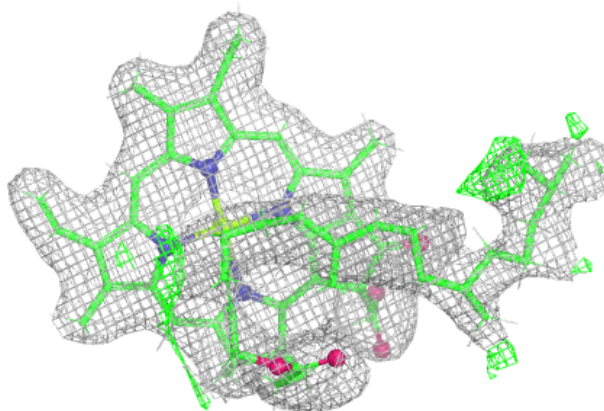
Electron density around SQD a 610:

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

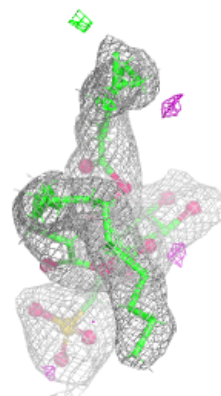
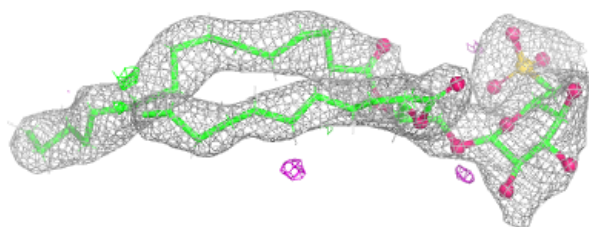
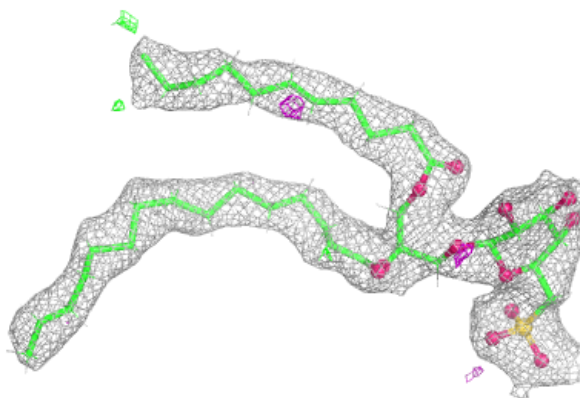


Electron density around CLA B 601:

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

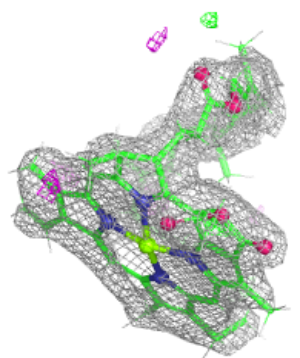
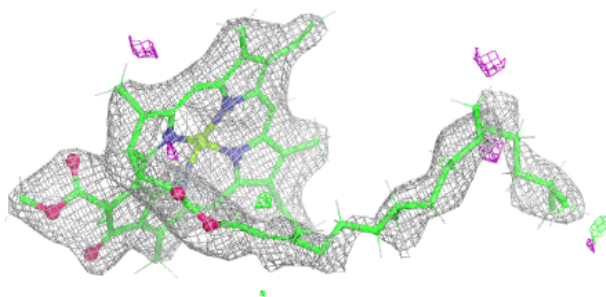
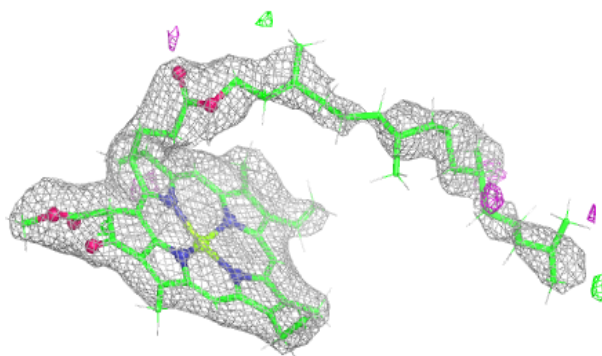
**Electron density around SQD b 620:**

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

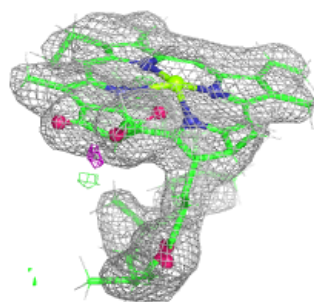
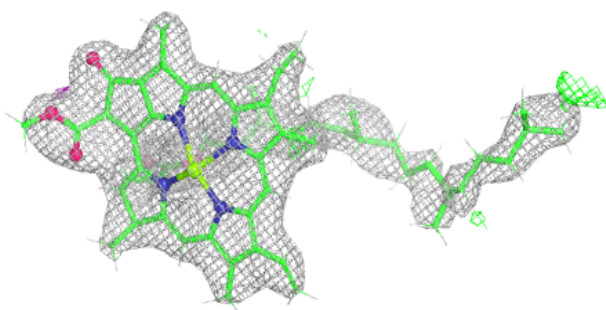
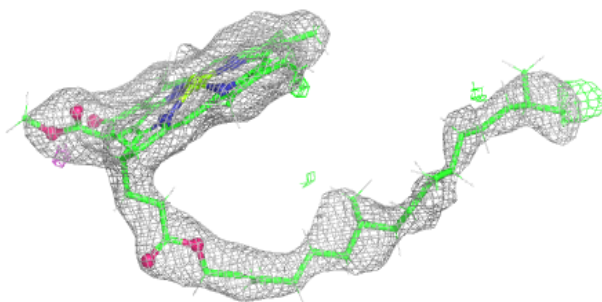


Electron density around CLA c 513:

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

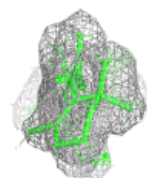
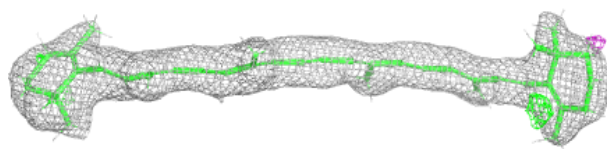
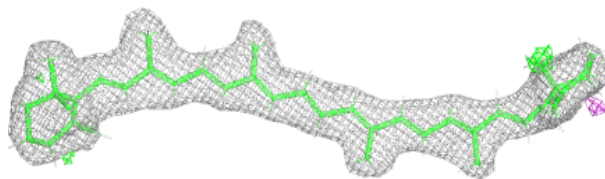
**Electron density around CLA C 513:**

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



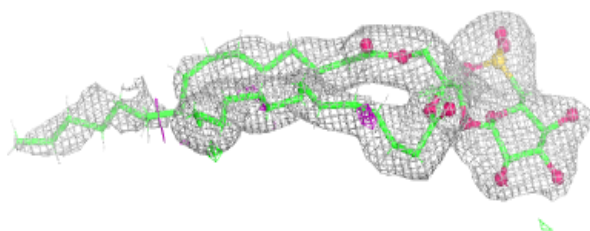
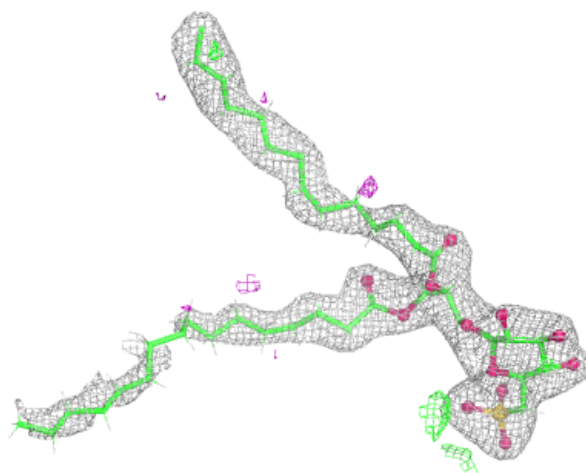
Electron density around BCR K 102:

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



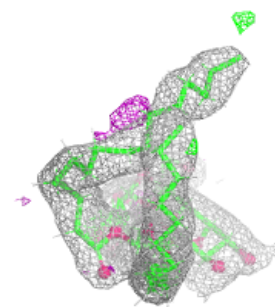
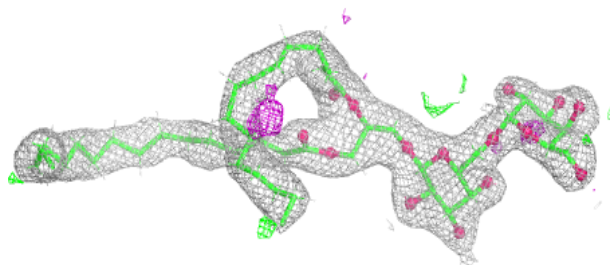
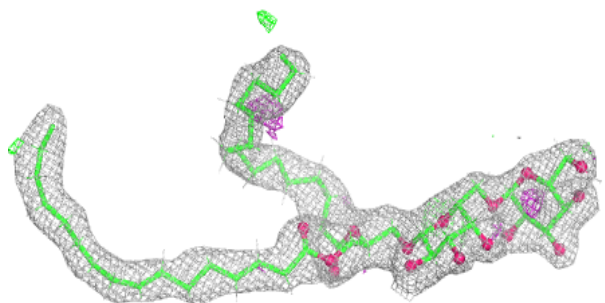
Electron density around SQD A 614:

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

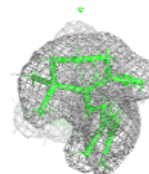
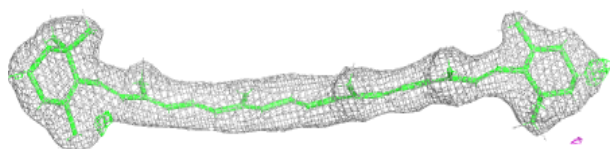
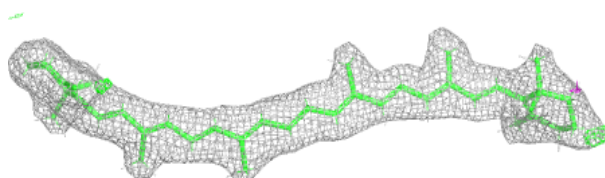


Electron density around DGD H 102:

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

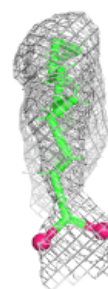
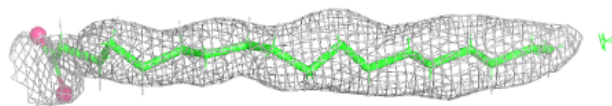
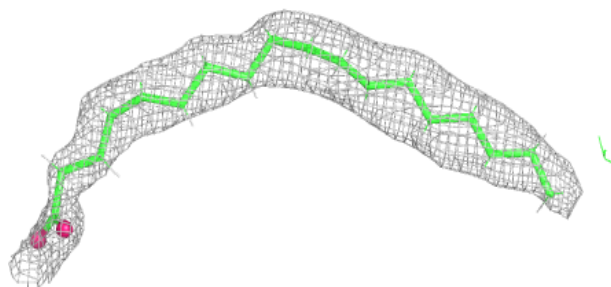
**Electron density around BCR H 101:**

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



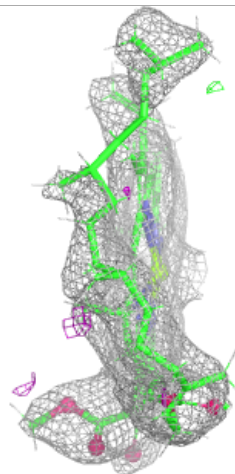
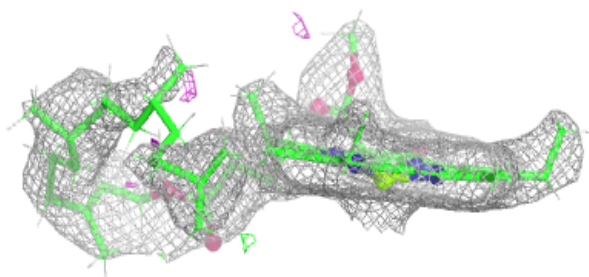
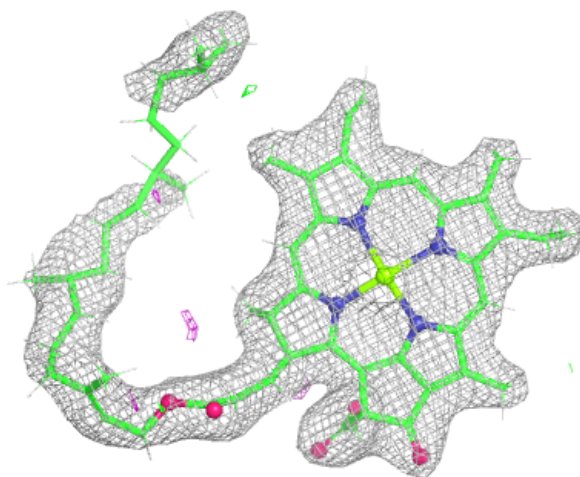
Electron density around STE X 101:

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



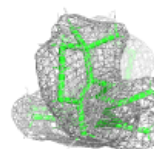
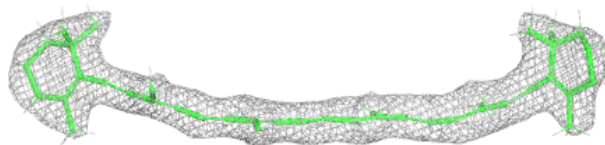
Electron density around CLA c 512:

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

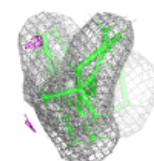
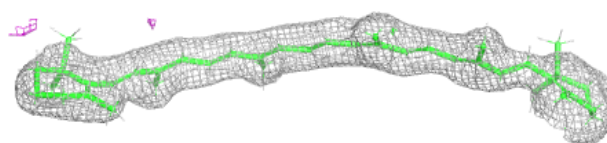


Electron density around BCR k 102:

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

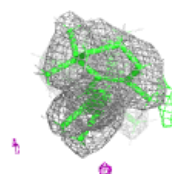
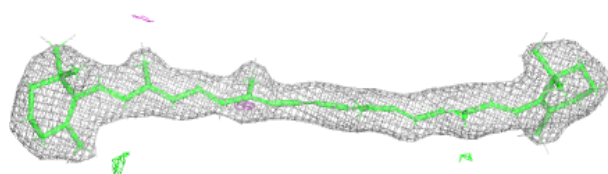
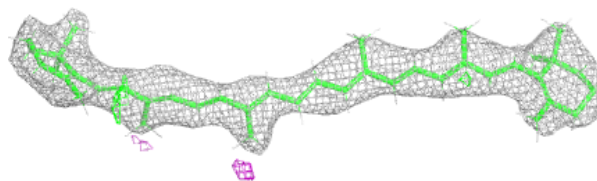
**Electron density around BCR D 405:**

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

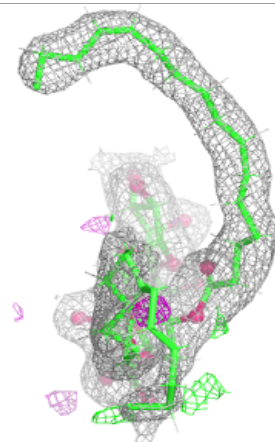
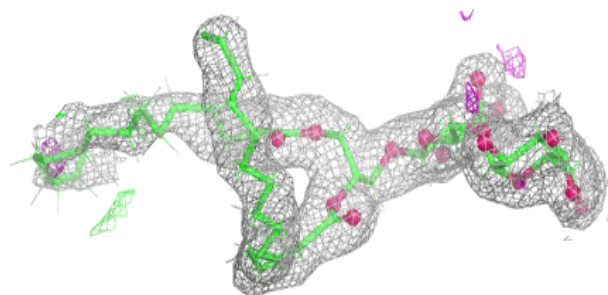
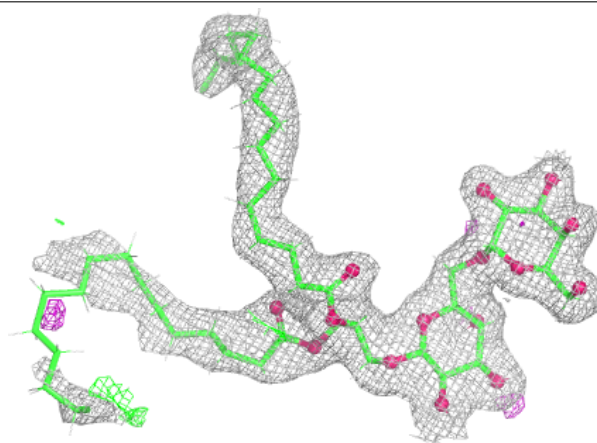


Electron density around BCR c 514:

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

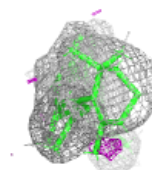
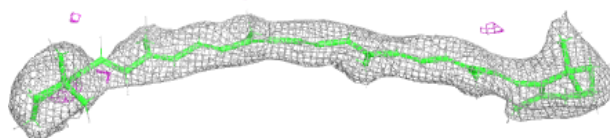
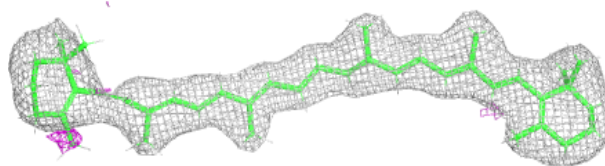
**Electron density around DGD C 522:**

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

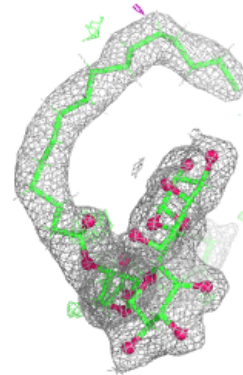
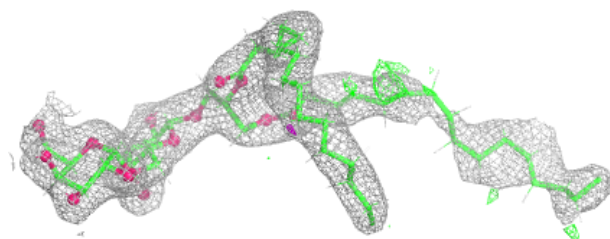
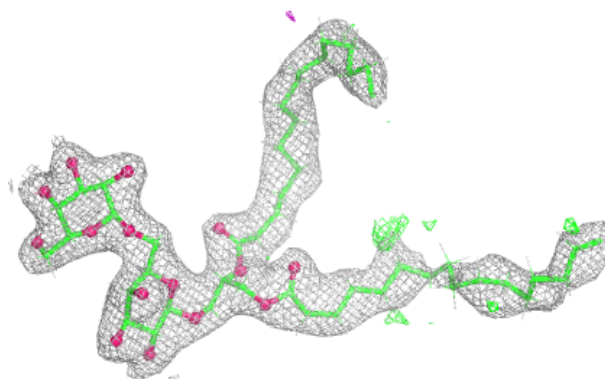


Electron density around BCR d 407:

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

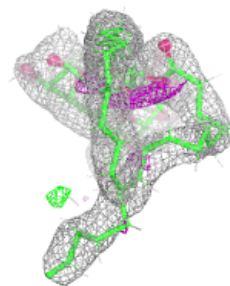
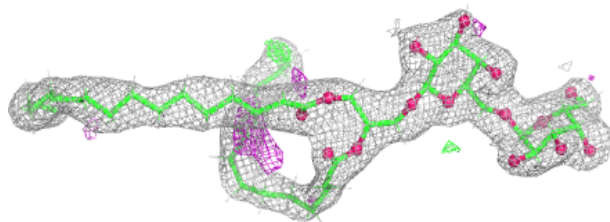
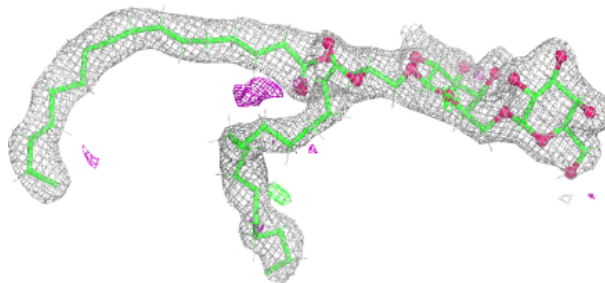
**Electron density around DGD c 520:**

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

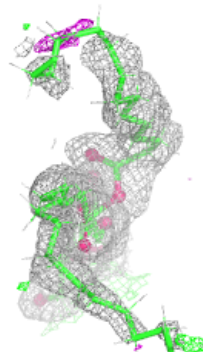
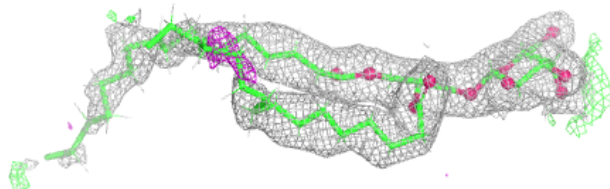
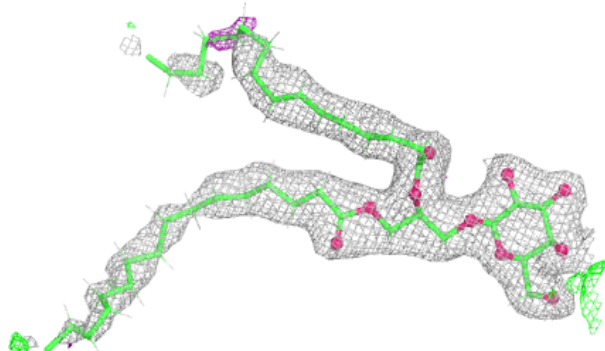


Electron density around DGD h 102:

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

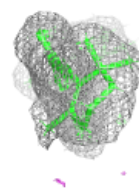
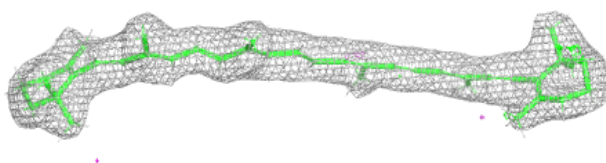
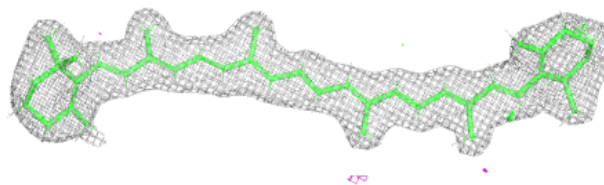
**Electron density around LMG D 408:**

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

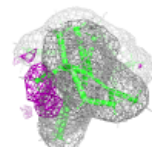
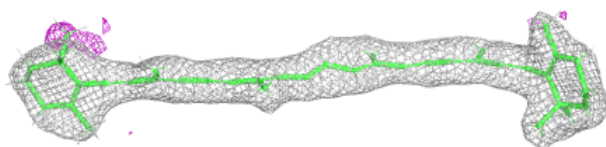
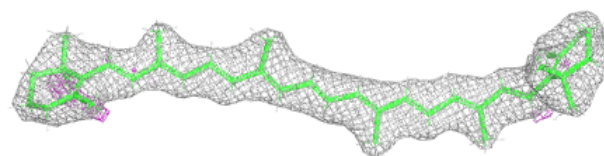


Electron density around BCR B 619:

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

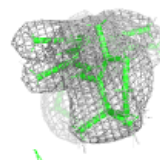
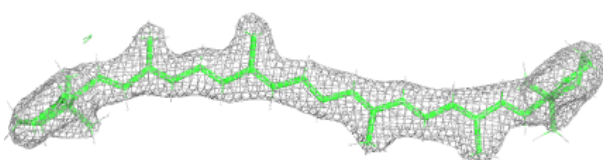
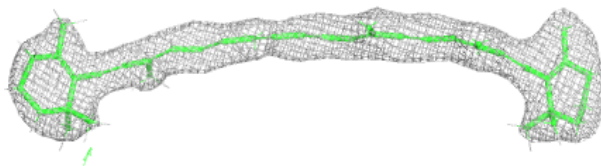
**Electron density around BCR c 515:**

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

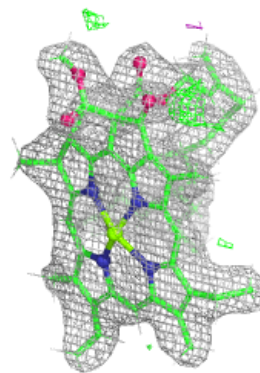
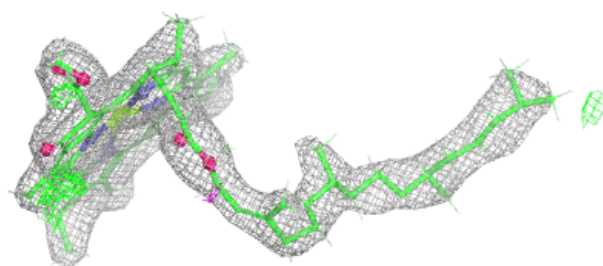
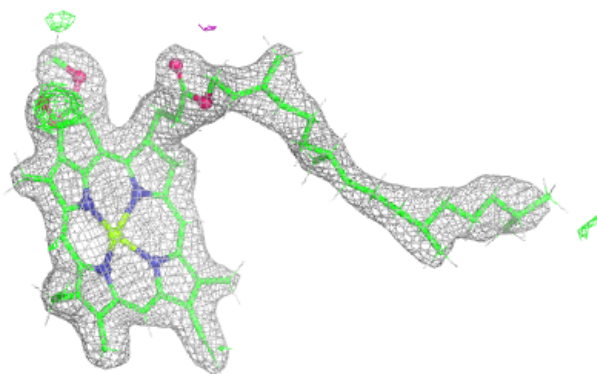


Electron density around BCR C 520:

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

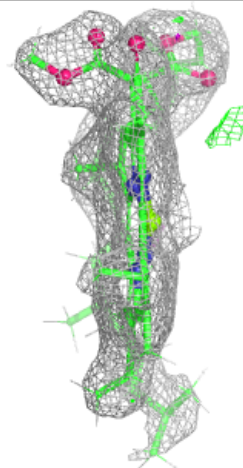
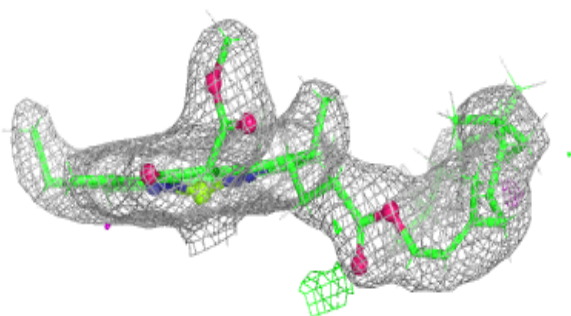
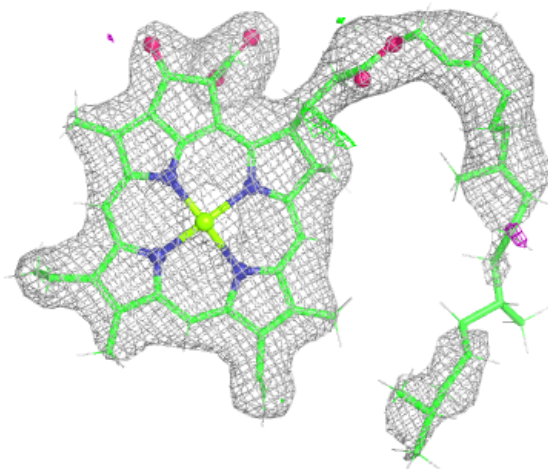
**Electron density around CLA c 511:**

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



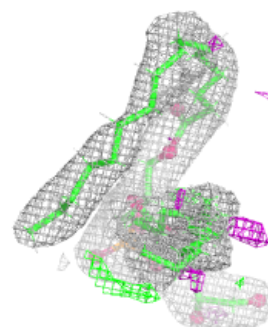
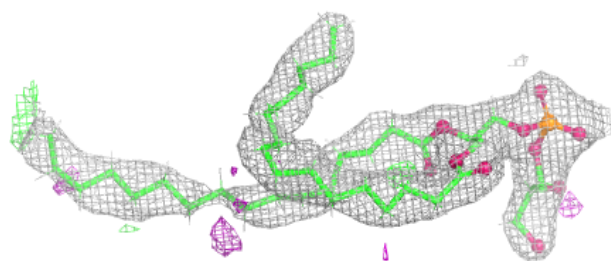
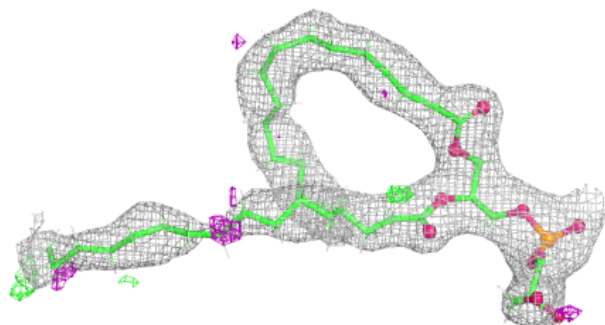
Electron density around CLA C 512:

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

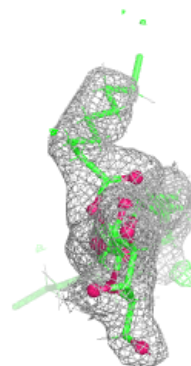
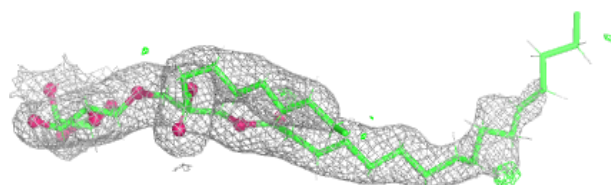
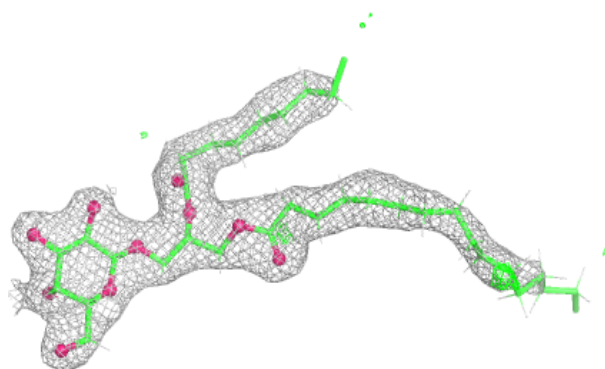


Electron density around LHG d 410:

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

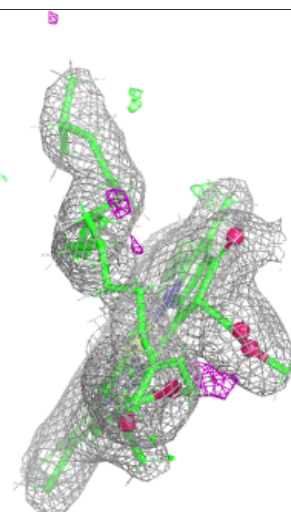
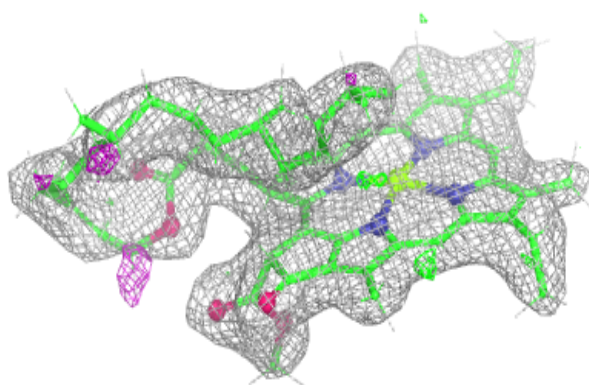
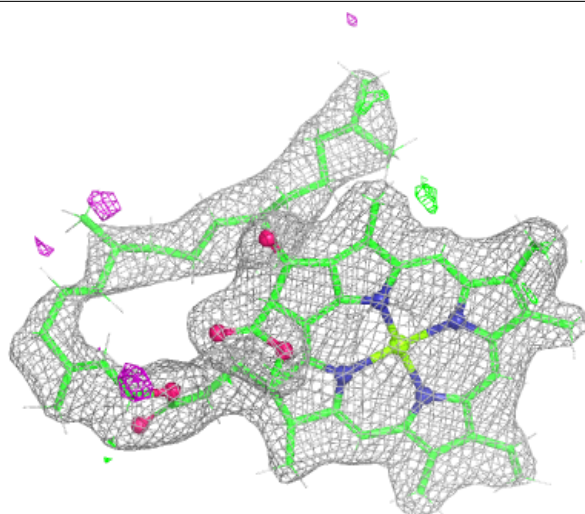
**Electron density around LMG d 414:**

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



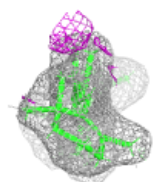
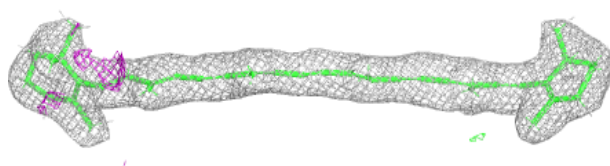
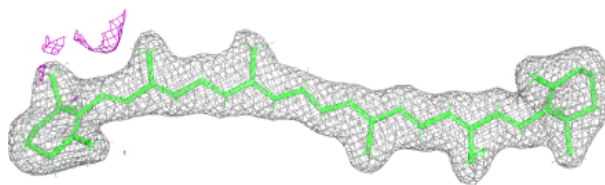
Electron density around CLA c 509:

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

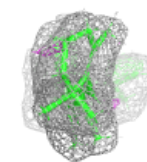
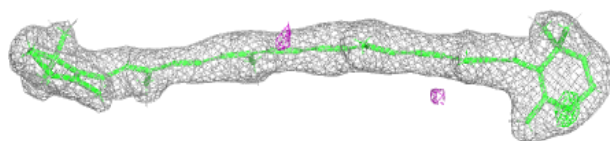
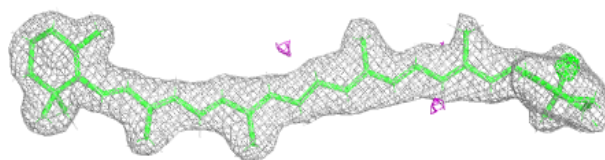


Electron density around BCR B 618:

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

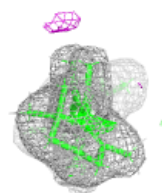
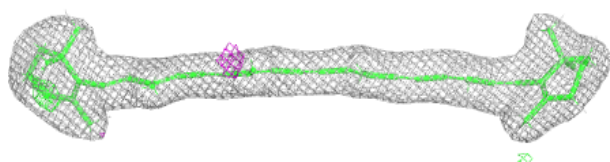
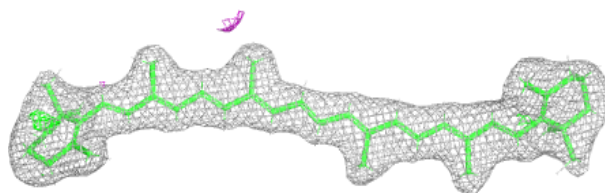
**Electron density around BCR b 617:**

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

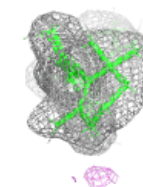
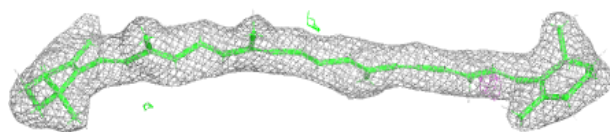
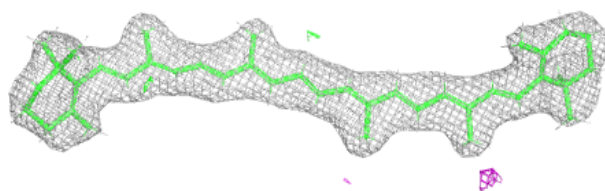


Electron density around BCR b 618:

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

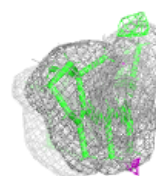
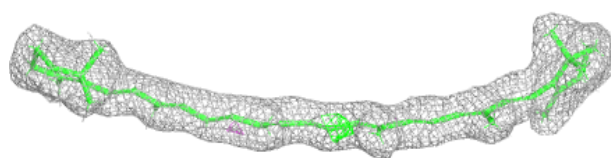
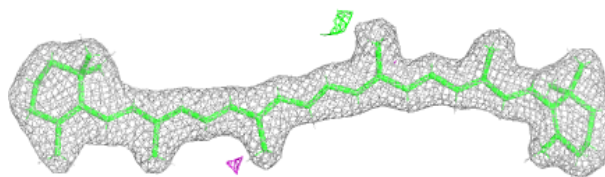
**Electron density around BCR b 619:**

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

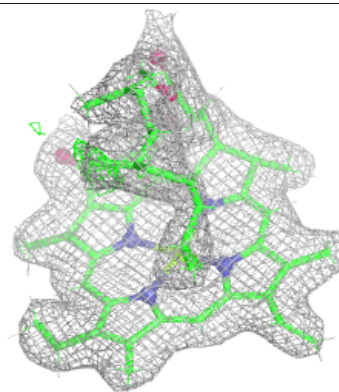
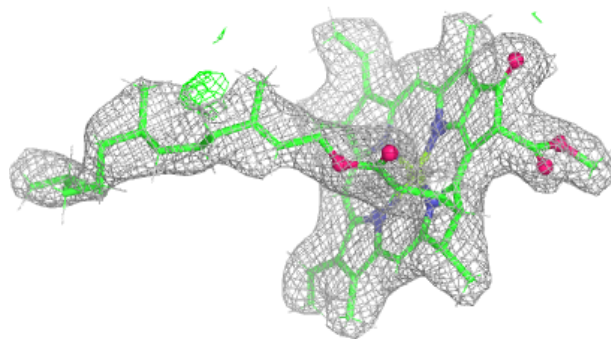
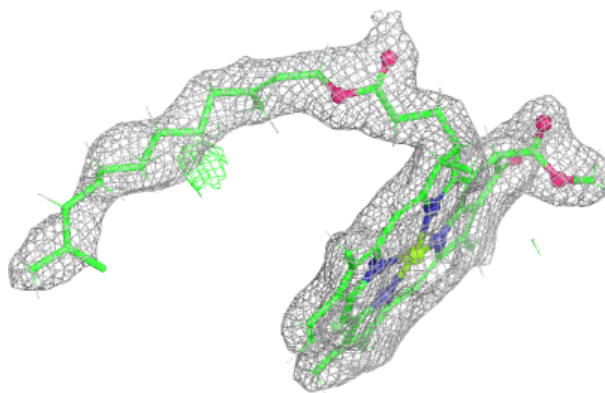


Electron density around BCR t 101:

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

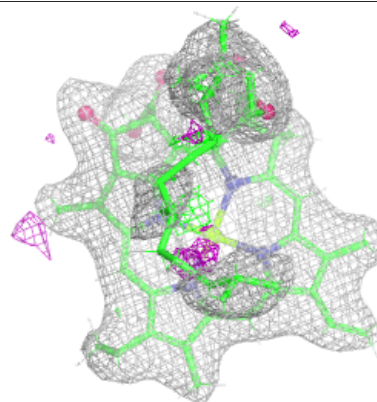
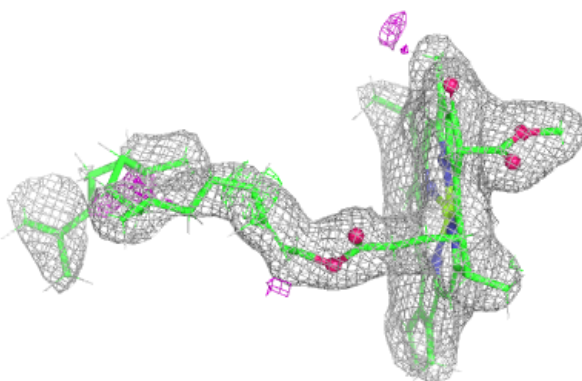
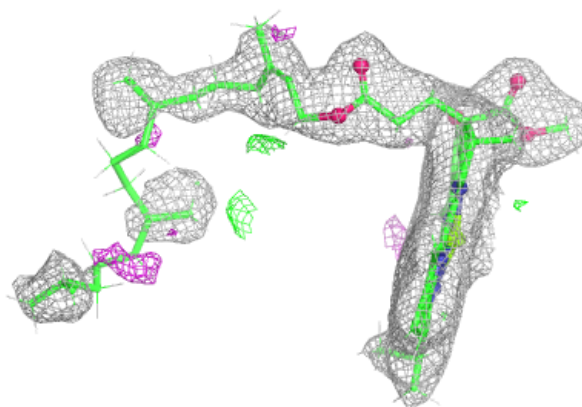
**Electron density around CLA c 504:**

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

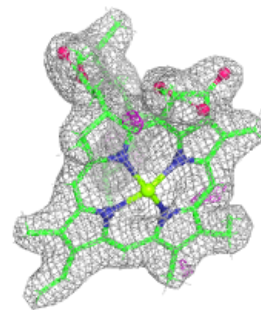
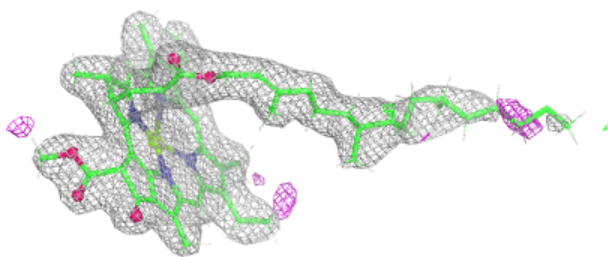
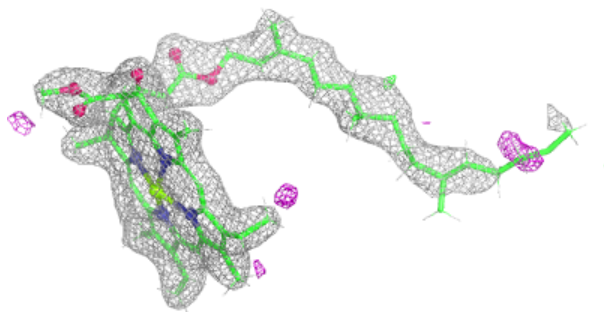


Electron density around CLA c 506:

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

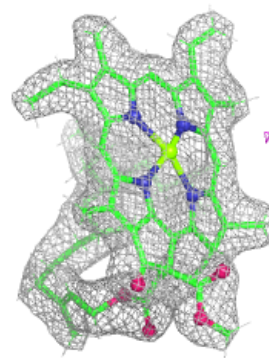
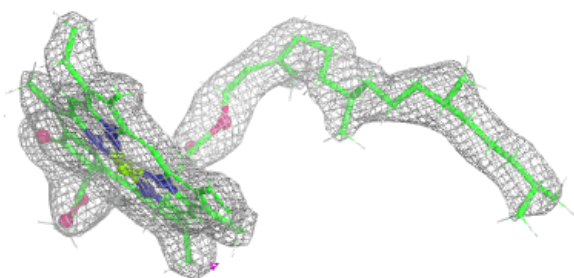
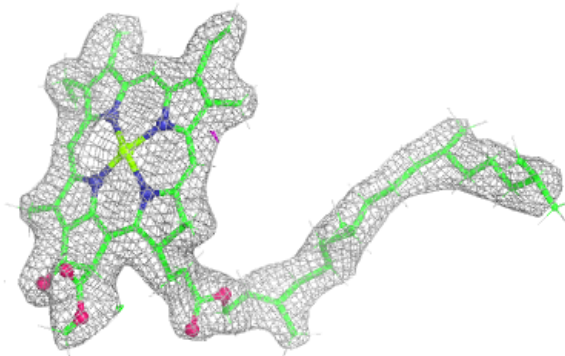
**Electron density around CLA c 508:**

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

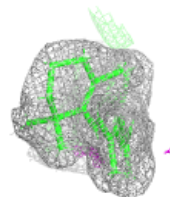
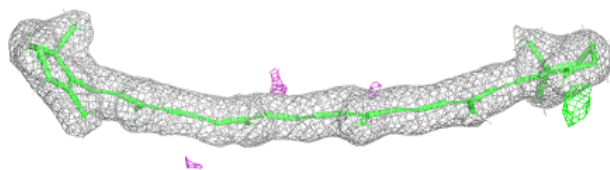
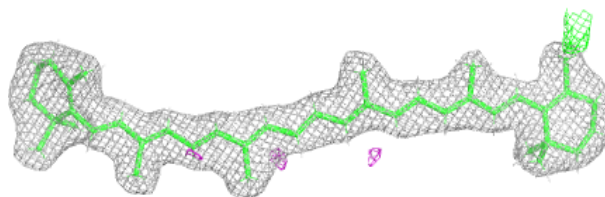


Electron density around CLA C 511:

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

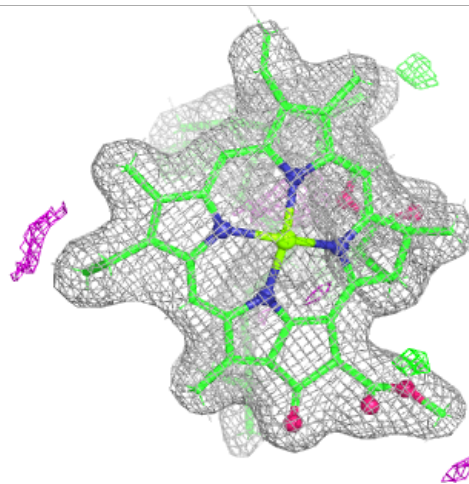
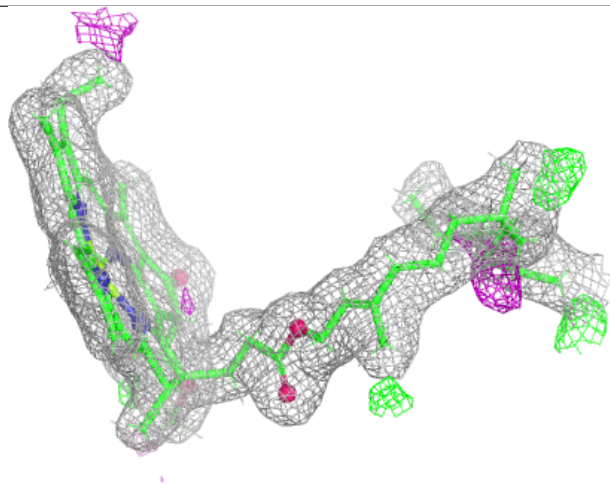
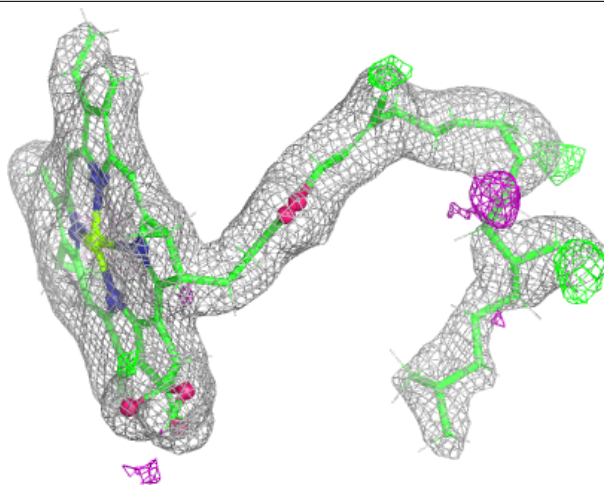
**Electron density around BCR T 101:**

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



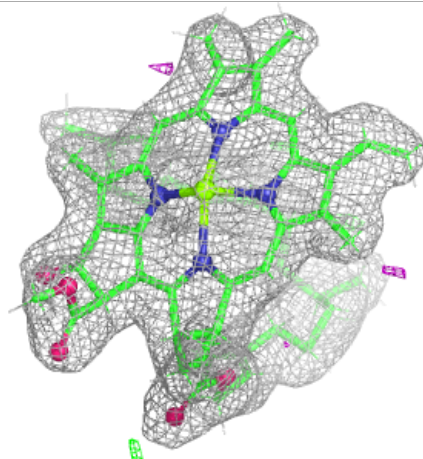
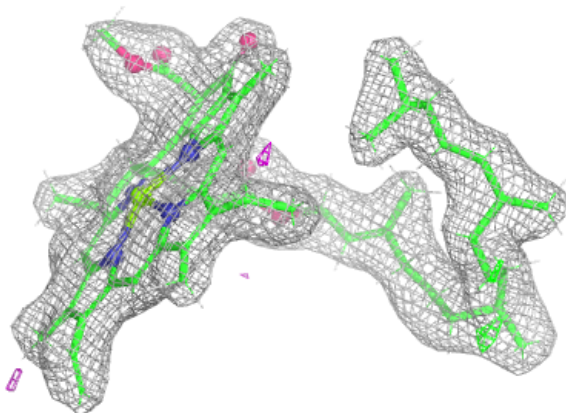
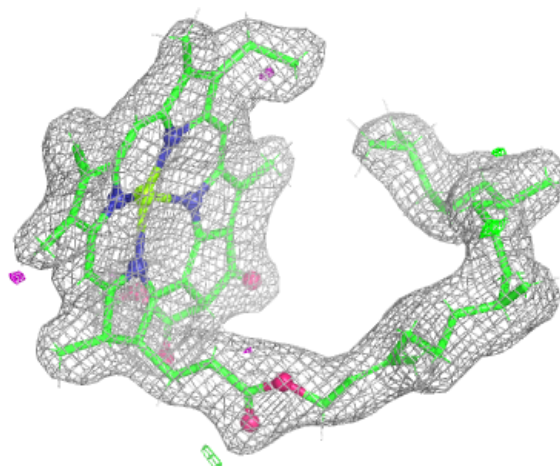
Electron density around CLA B 606:

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



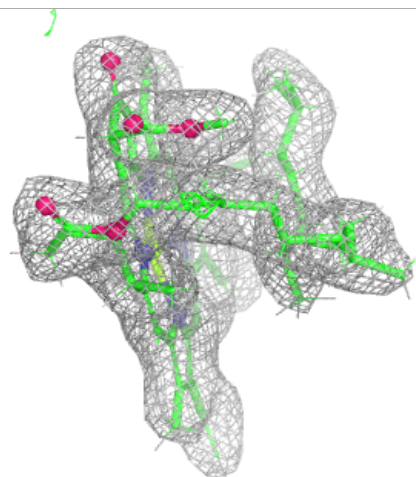
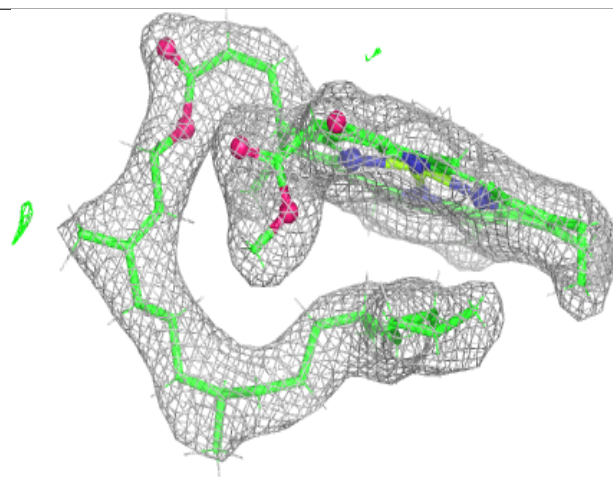
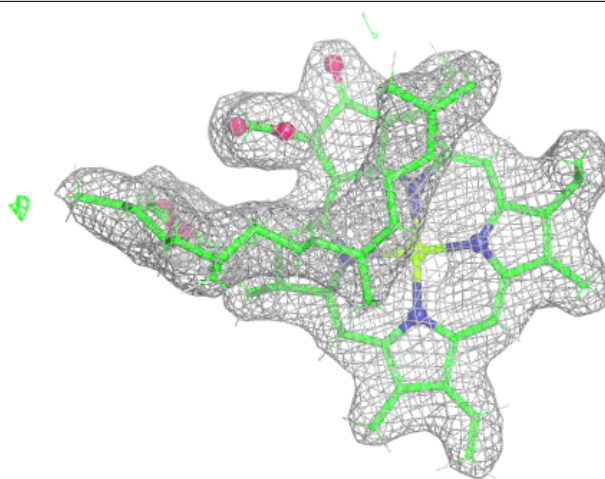
Electron density around CLA C 503:

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



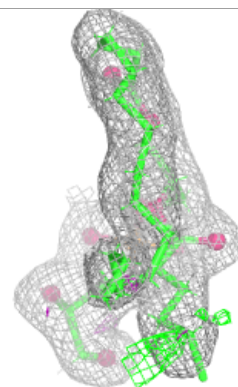
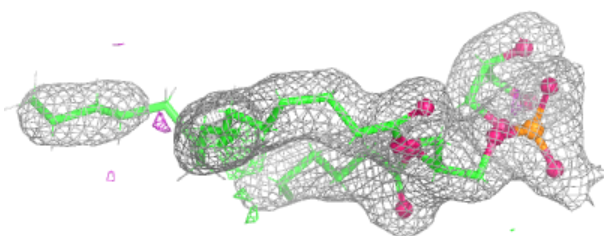
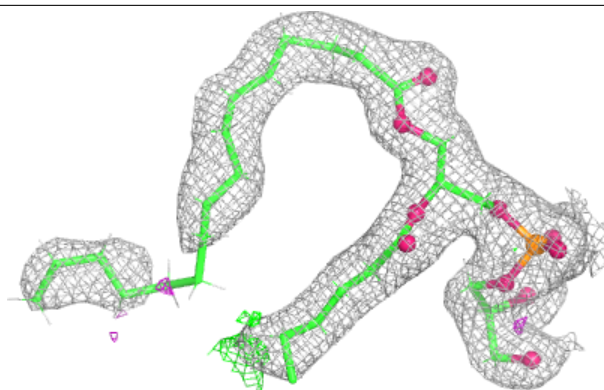
Electron density around CLA C 510:

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

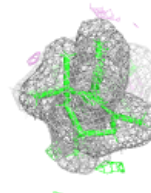
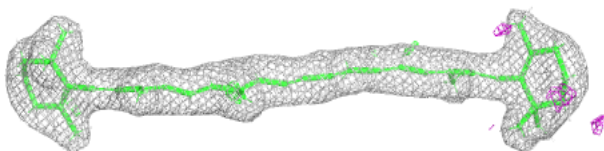
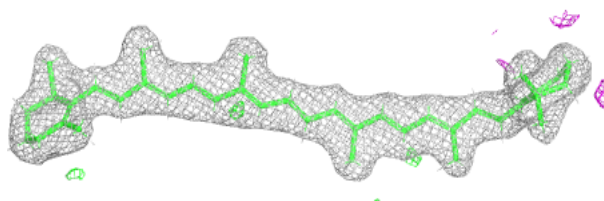


Electron density around LHG d 412:

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

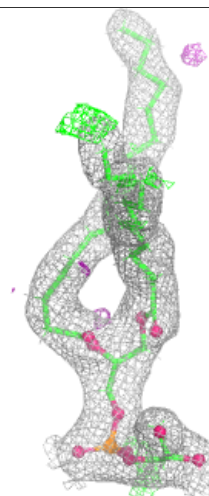
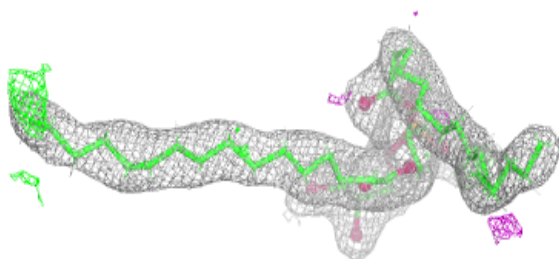
**Electron density around BCR A 609:**

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



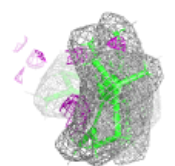
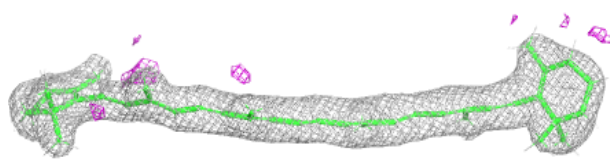
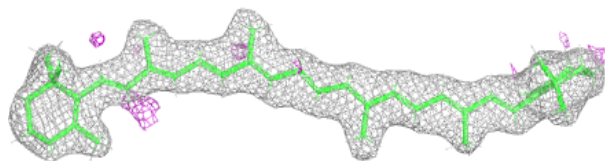
Electron density around LHG 1 101:

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

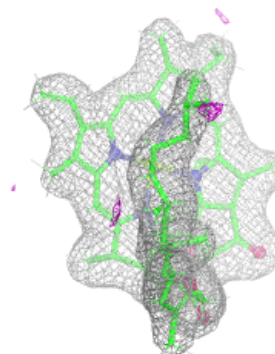
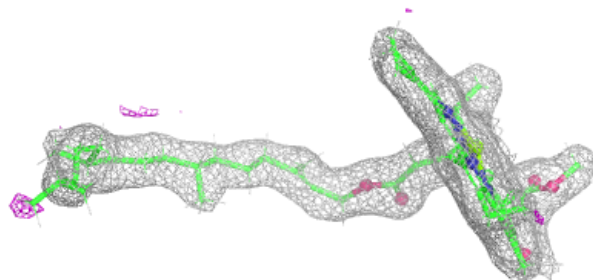
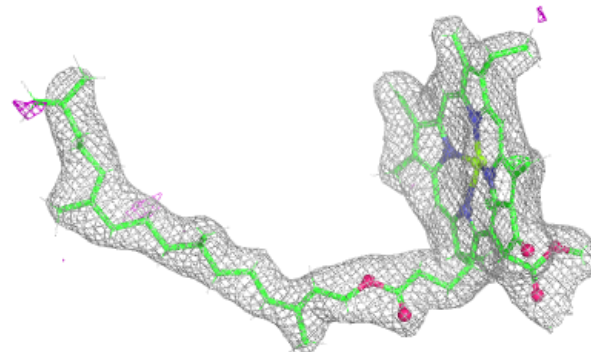


Electron density around BCR B 617:

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

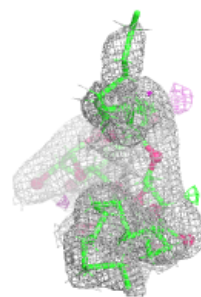
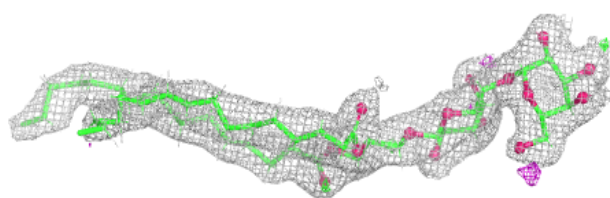
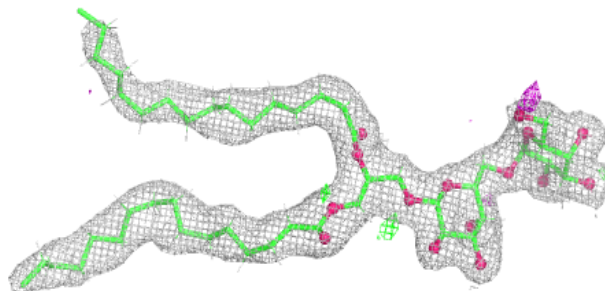
**Electron density around CLA b 609:**

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

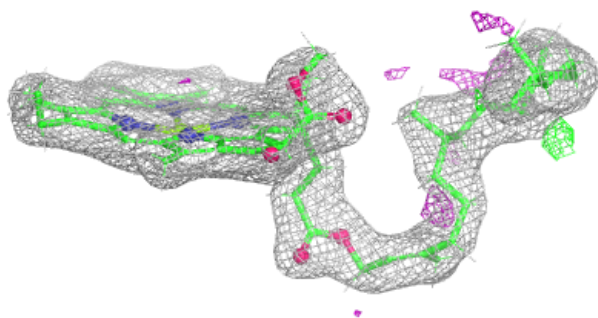
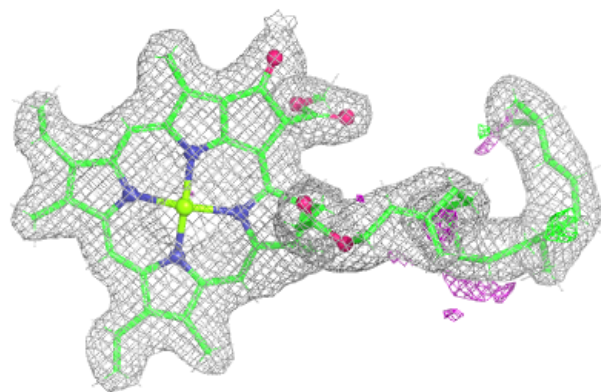


Electron density around DGD C 523:

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

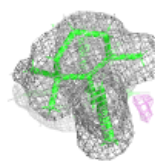
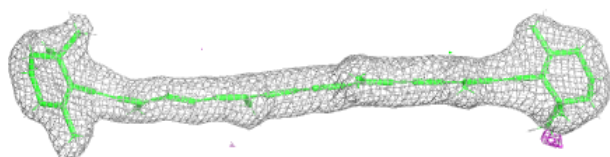
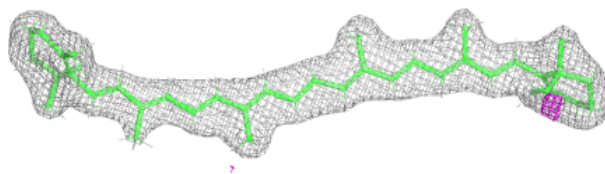
**Electron density around CLA b 612:**

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



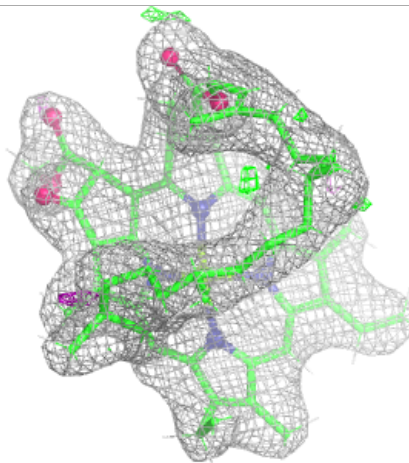
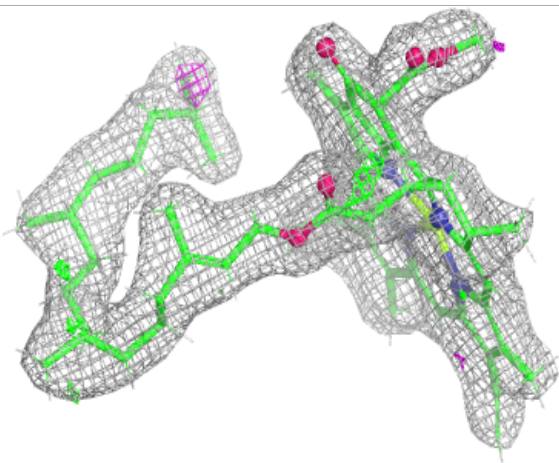
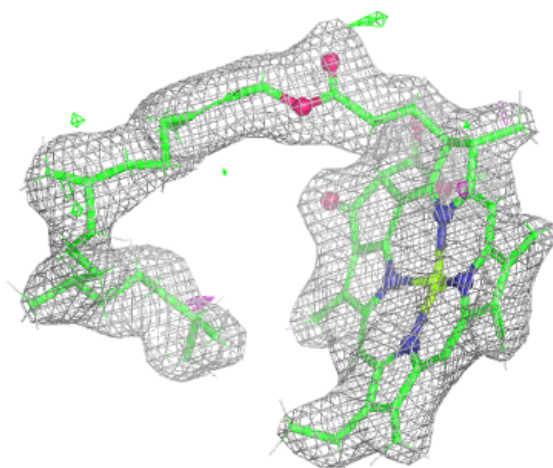
Electron density around BCR C 514:

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



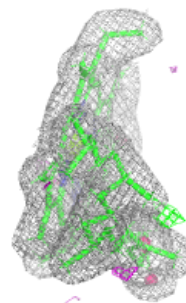
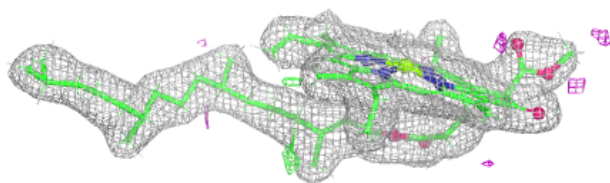
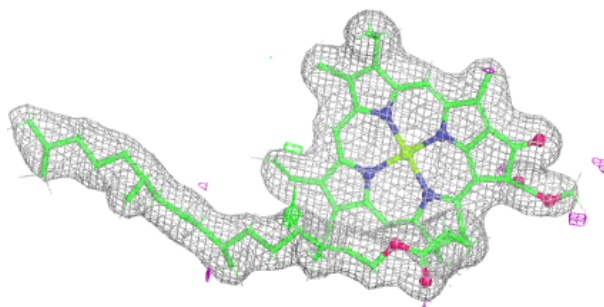
Electron density around CLA c 503:

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



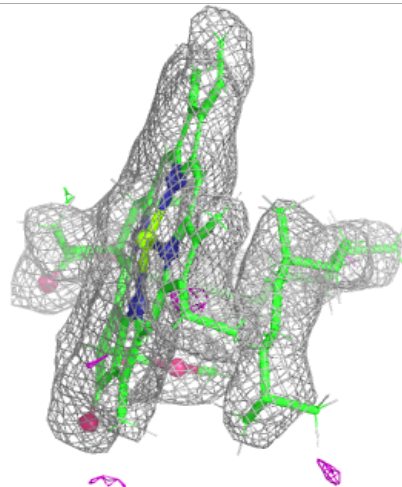
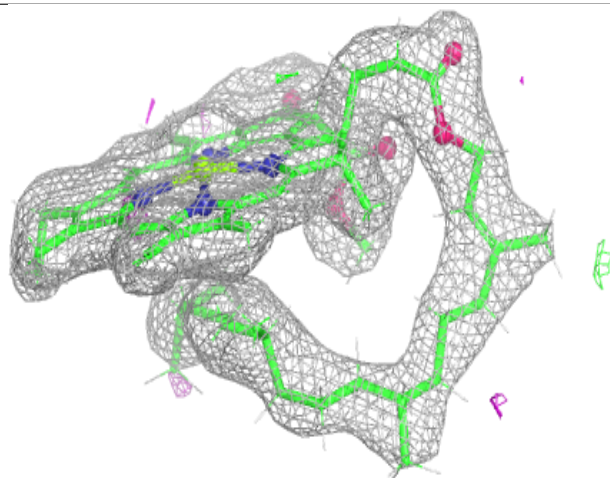
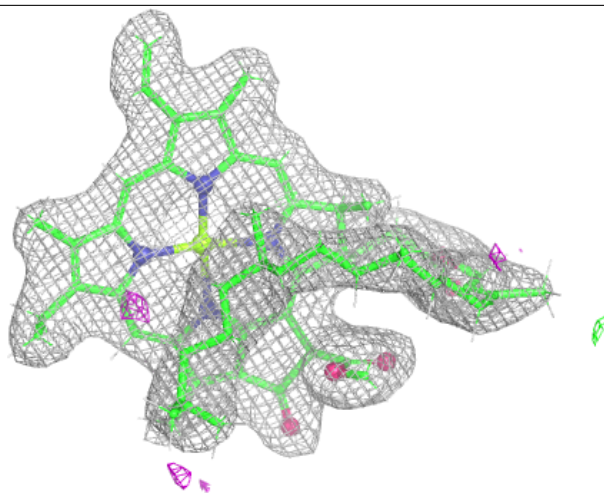
Electron density around CLA C 501:

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



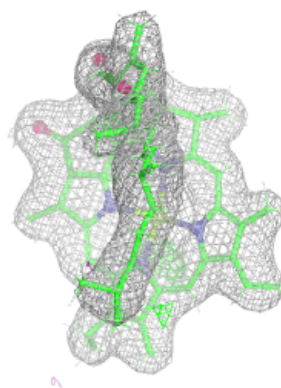
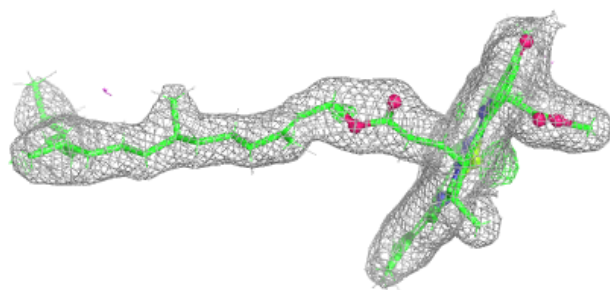
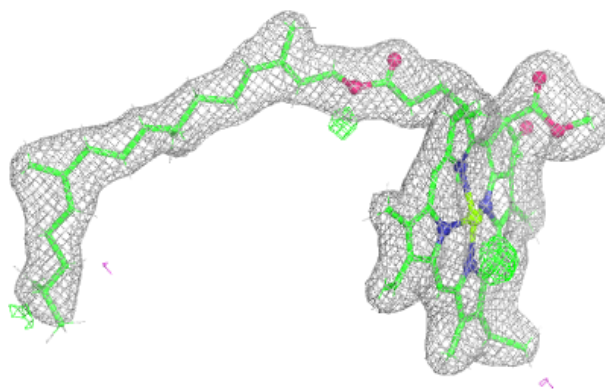
Electron density around CLA c 510:

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

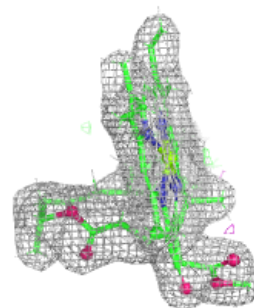
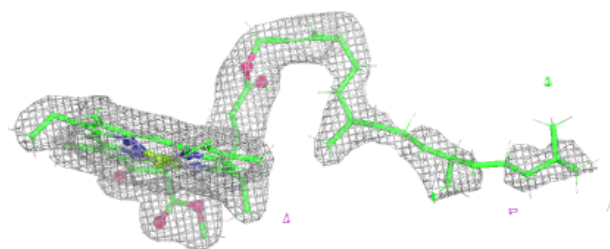
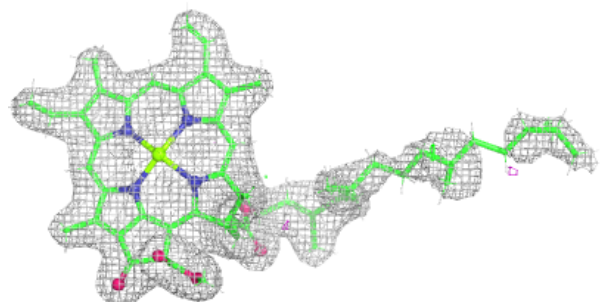


Electron density around CLA B 609:

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

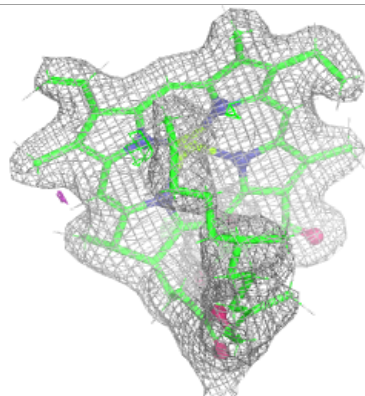
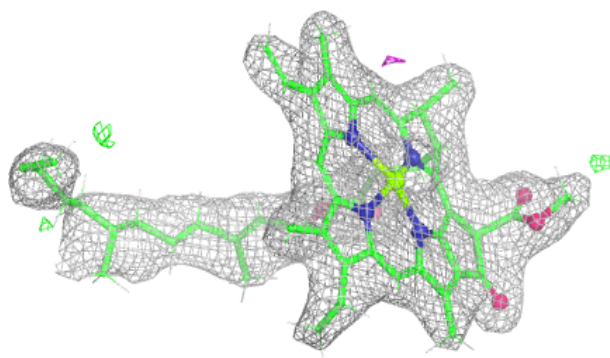
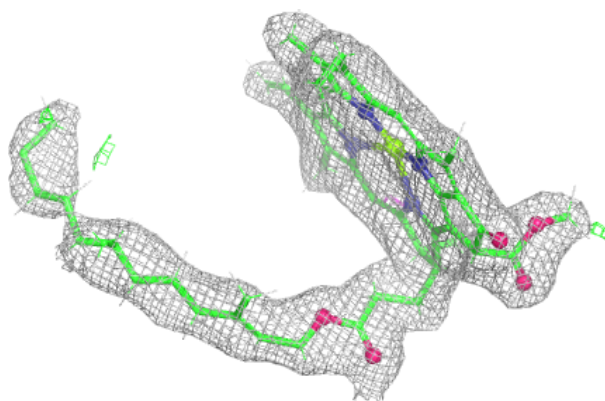
**Electron density around CLA a 606:**

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

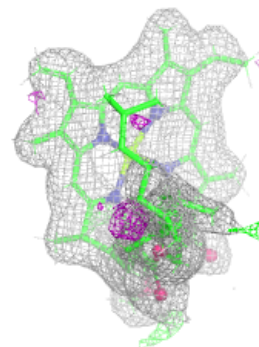
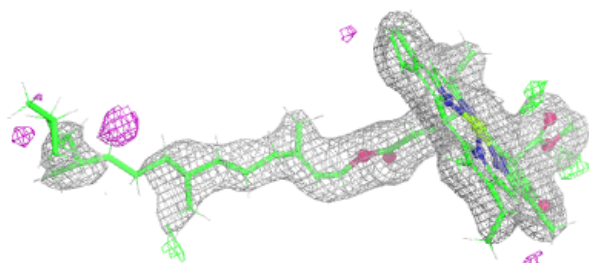
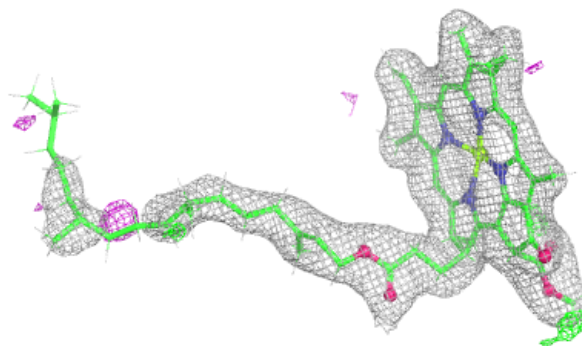


Electron density around CLA C 504:

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

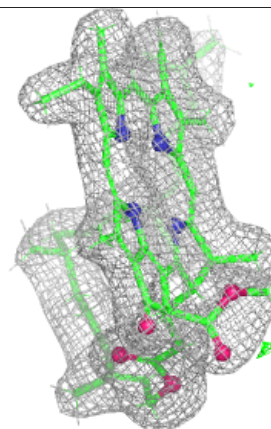
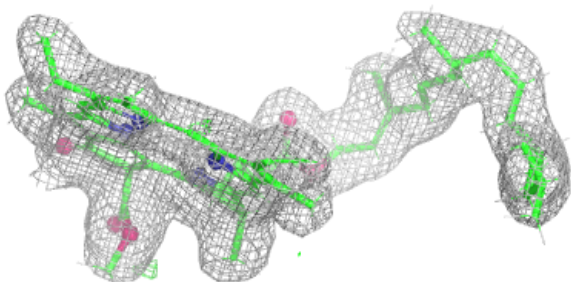
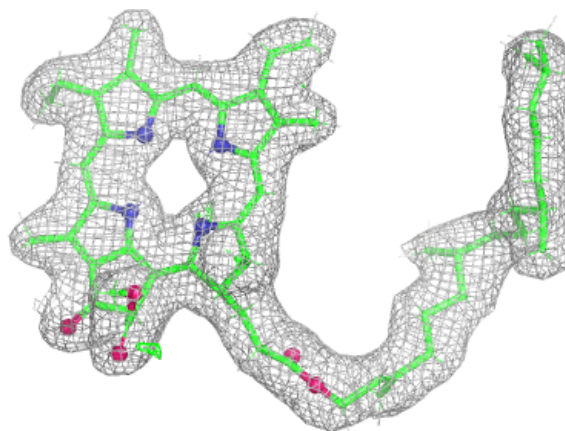
**Electron density around CLA d 406:**

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

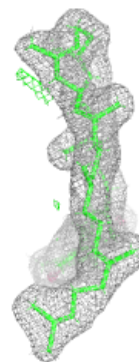
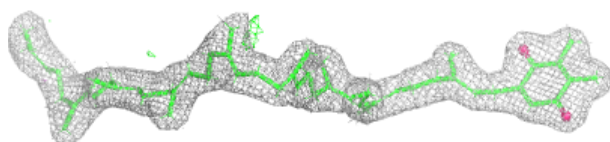
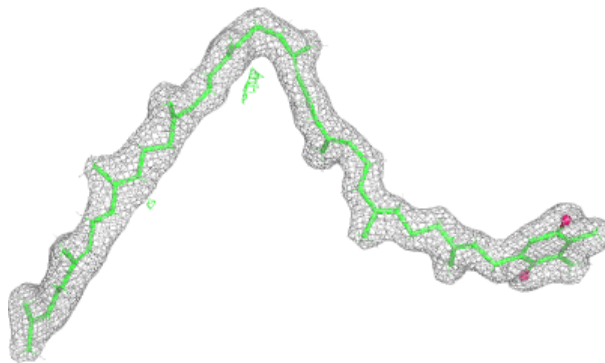


Electron density around PHO d 403:

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

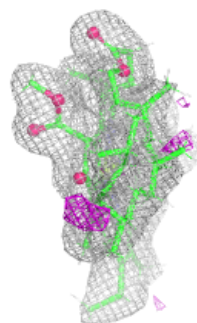
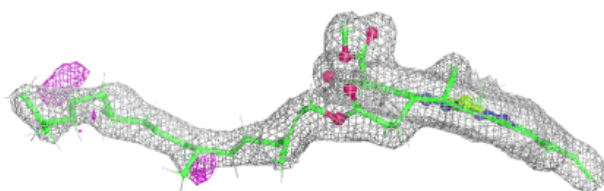
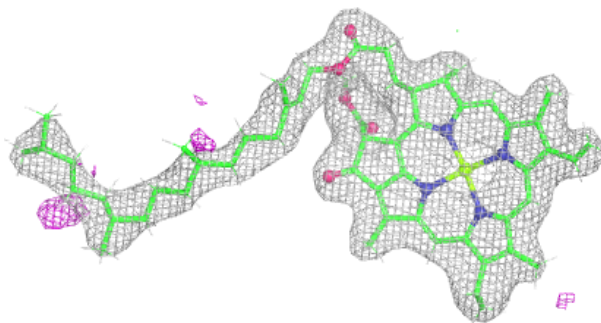
**Electron density around PL9 D 406:**

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

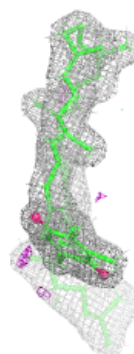
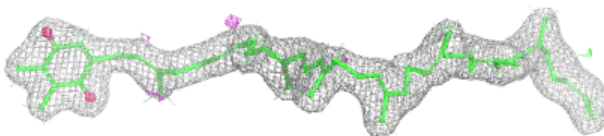
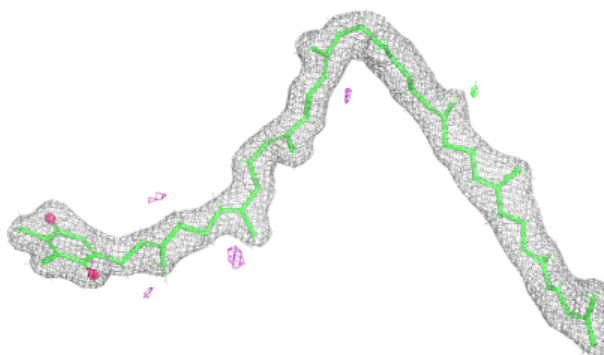


Electron density around CLA b 602:

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

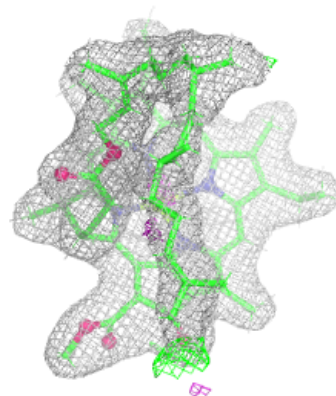
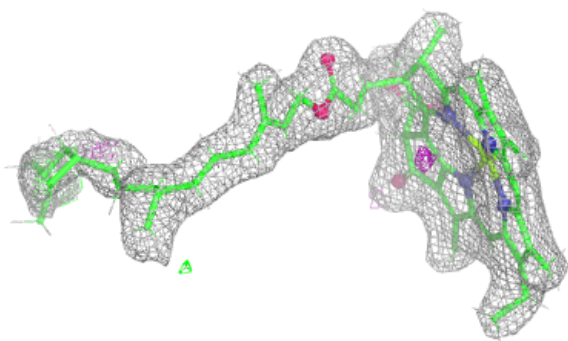
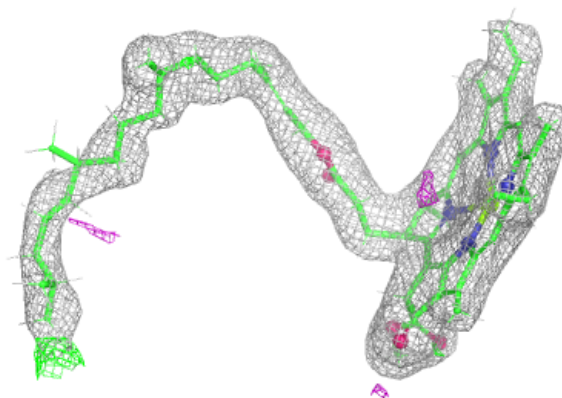
**Electron density around PL9 d 408:**

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

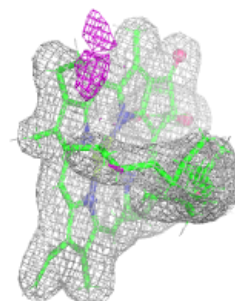
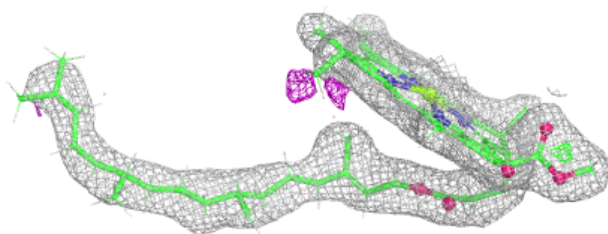
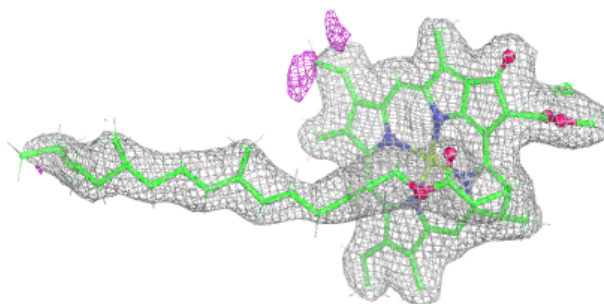


Electron density around CLA b 606:

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

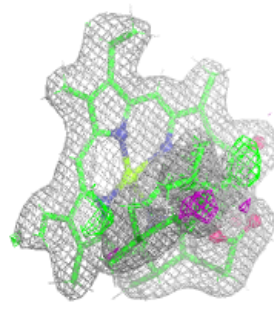
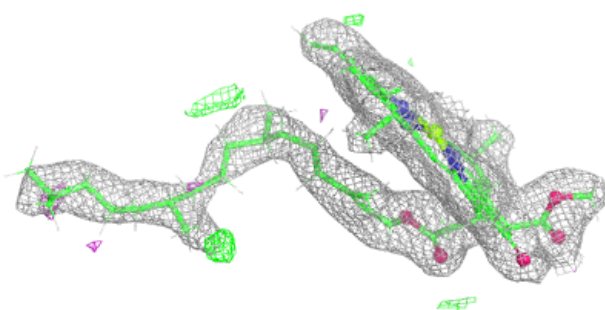
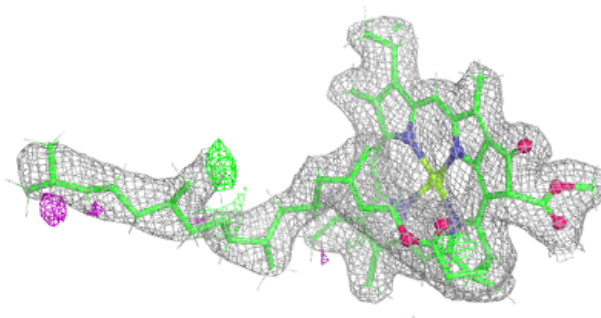
**Electron density around CLA b 608:**

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

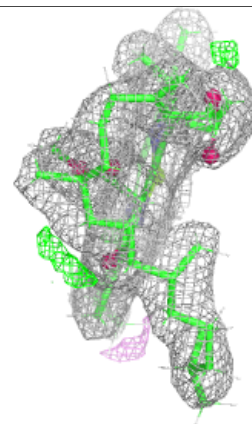
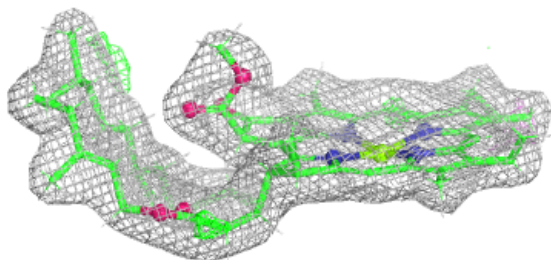
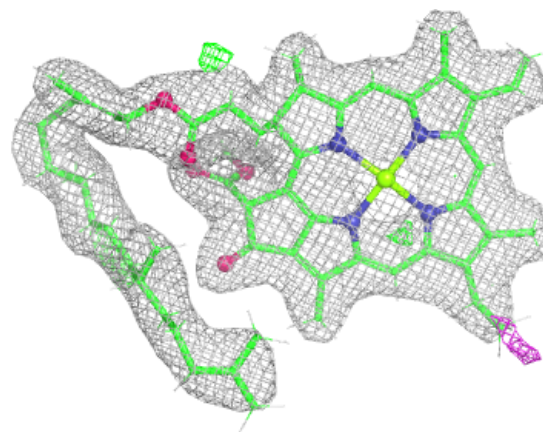


Electron density around CLA C 505:

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

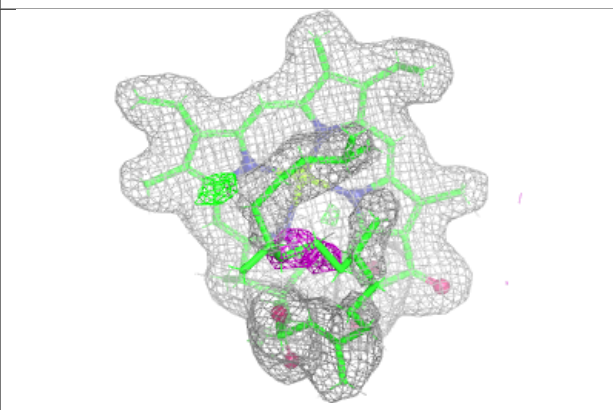
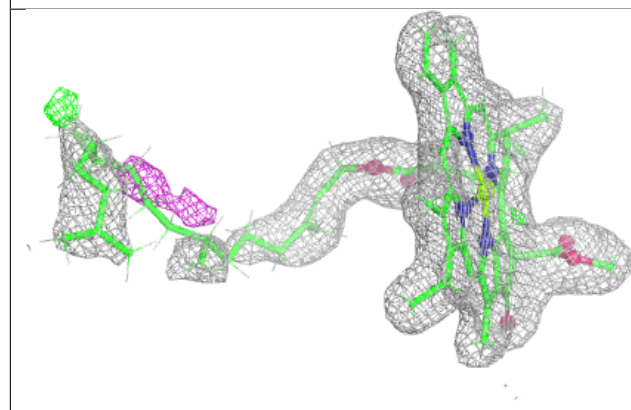
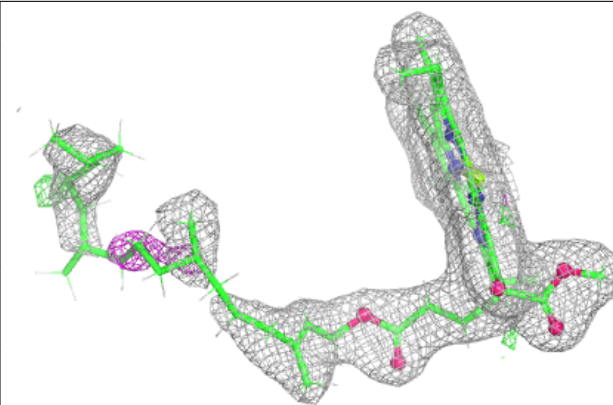
**Electron density around CLA b 610:**

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

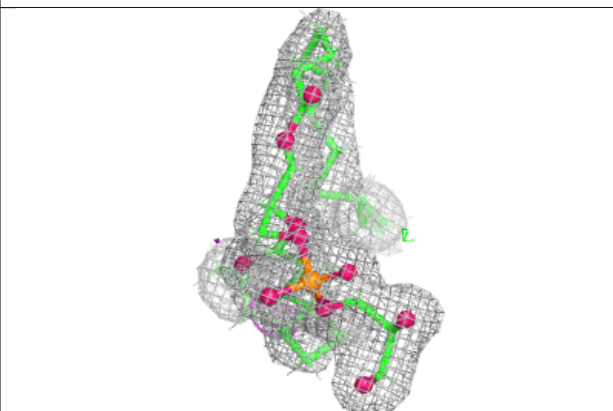
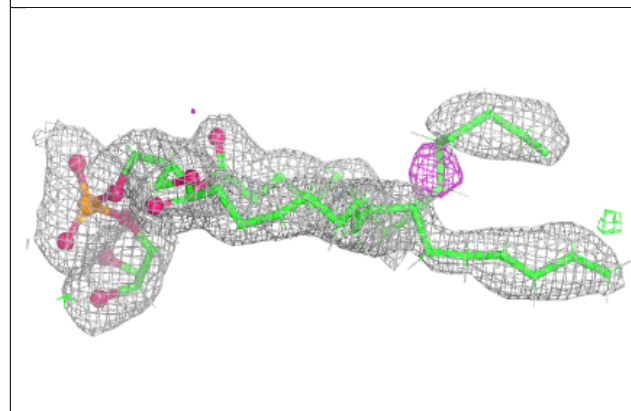
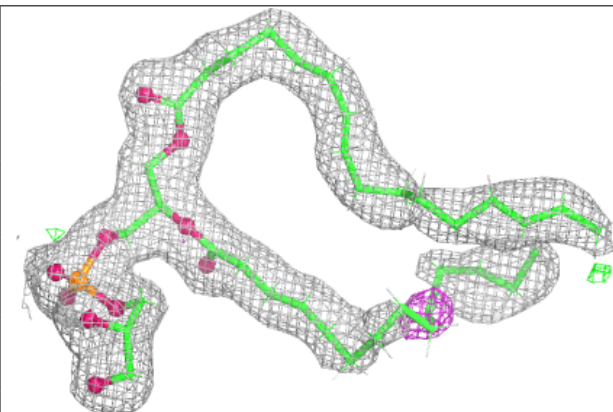


Electron density around CLA C 506:

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

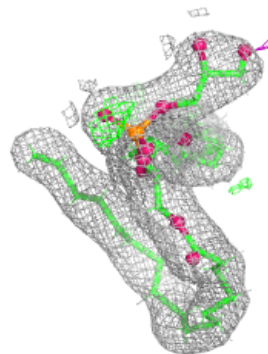
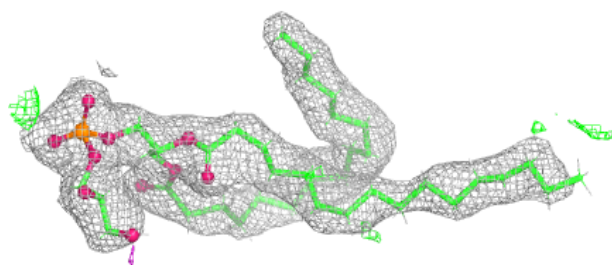
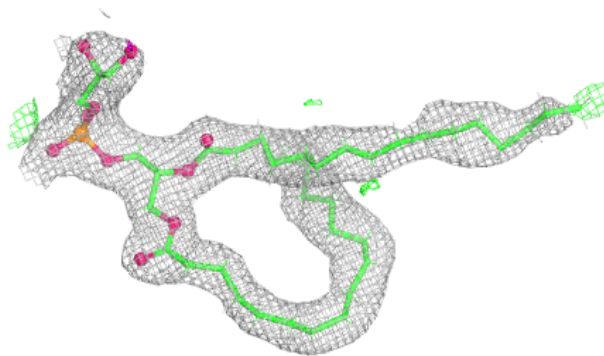
**Electron density around LHG D 410:**

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

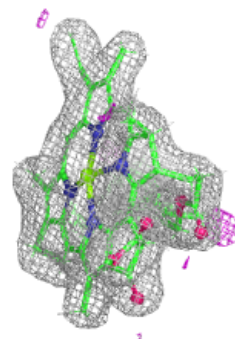
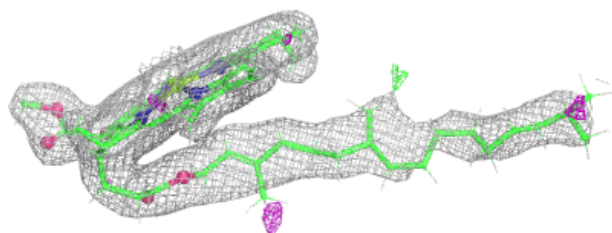
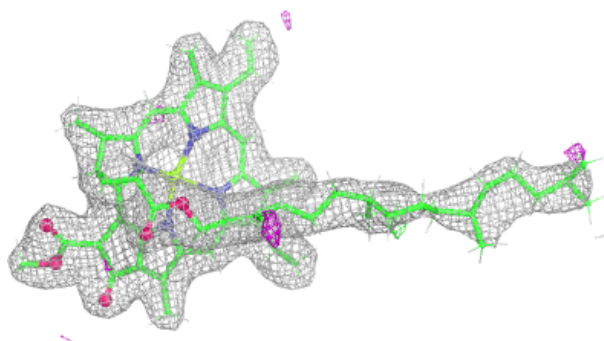


Electron density around LHG D 411:

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

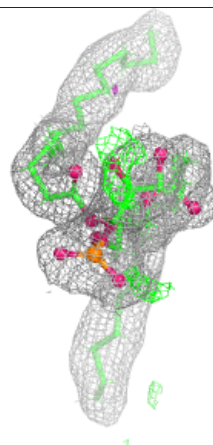
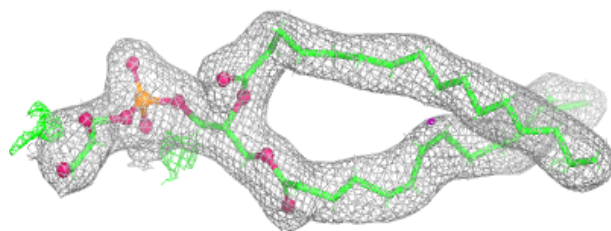
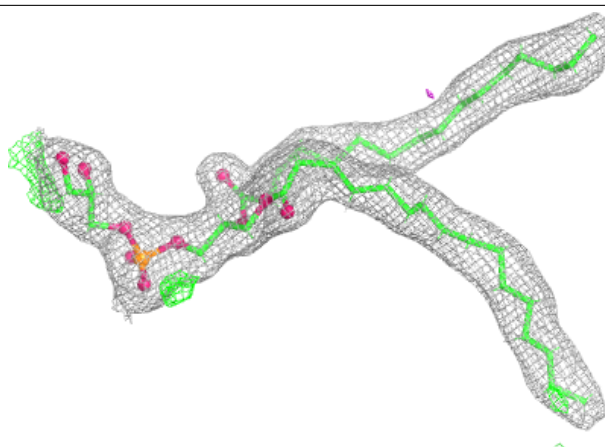
**Electron density around CLA b 614:**

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



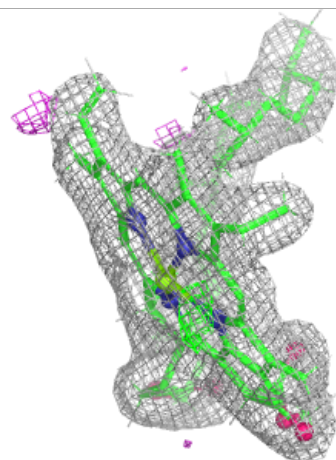
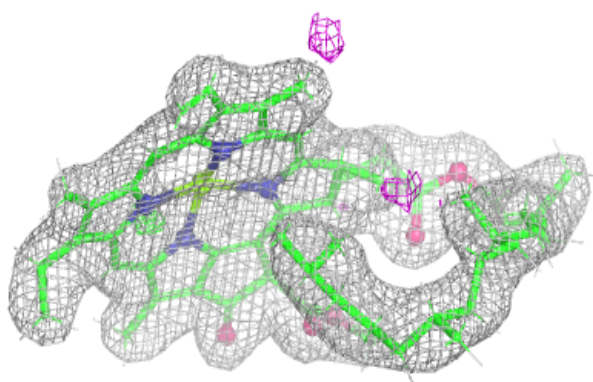
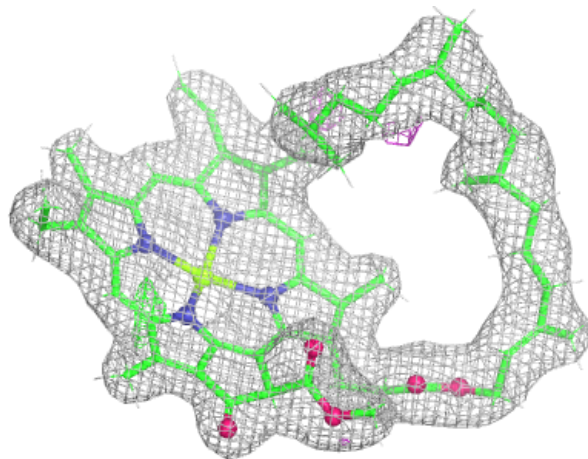
Electron density around LHG d 411:

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



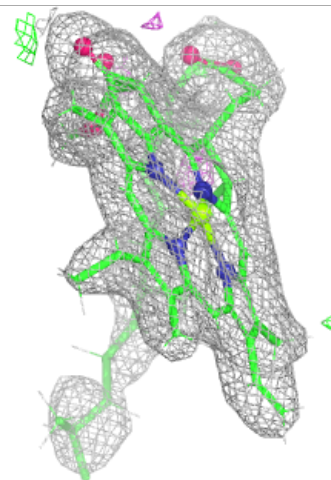
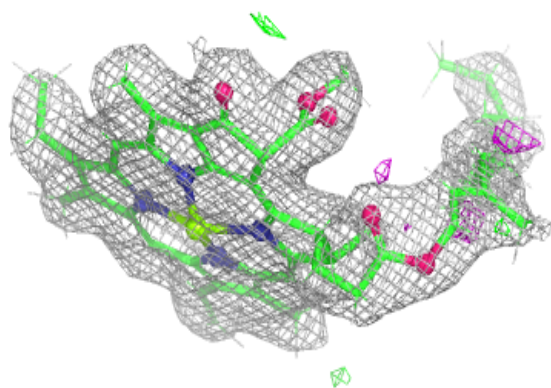
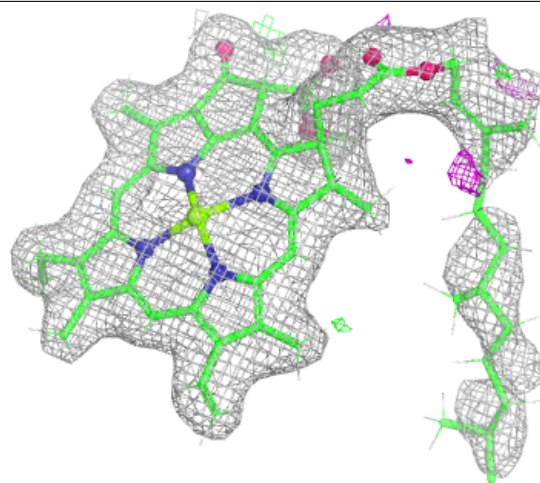
Electron density around CLA b 615:

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



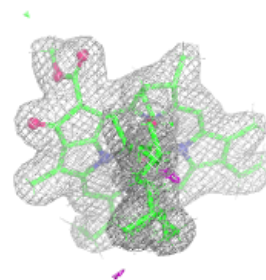
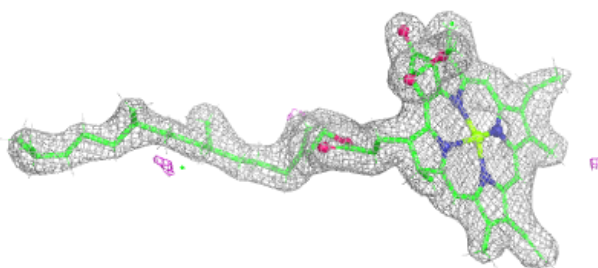
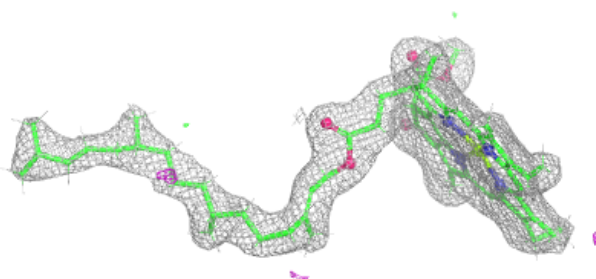
Electron density around CLA b 616:

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

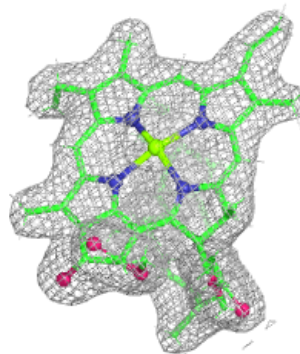
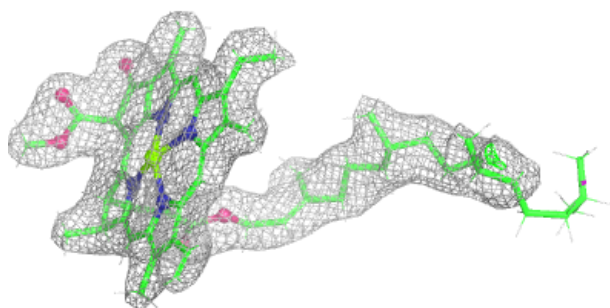
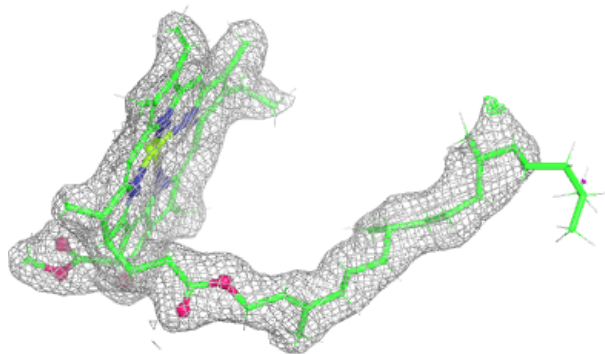


Electron density around CLA c 502:

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

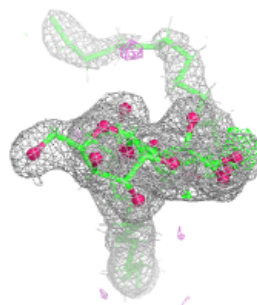
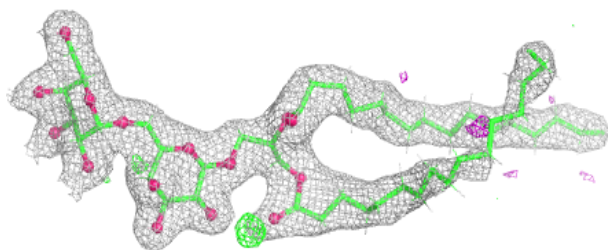
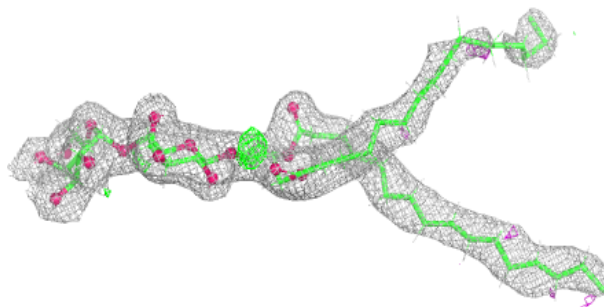
**Electron density around CLA C 508:**

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

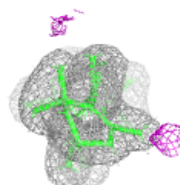
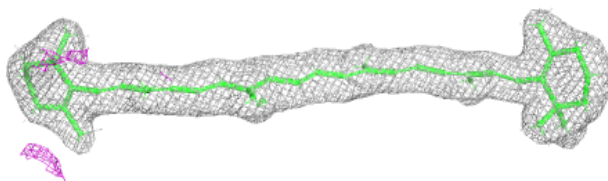
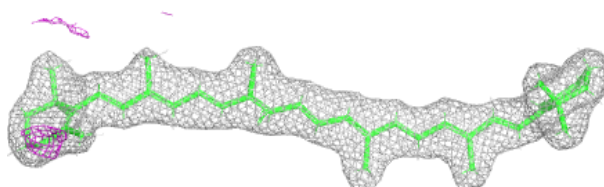


Electron density around DGD C 521:

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

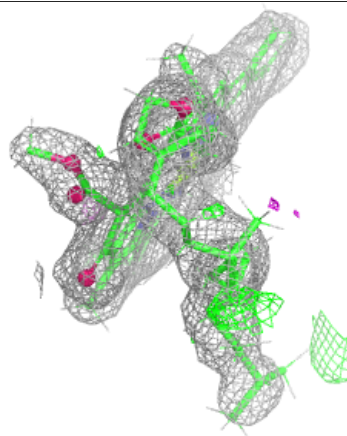
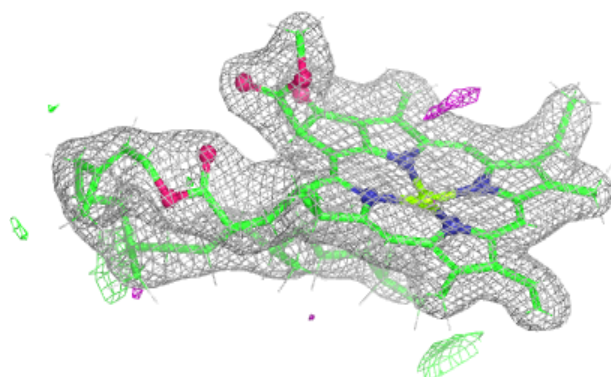
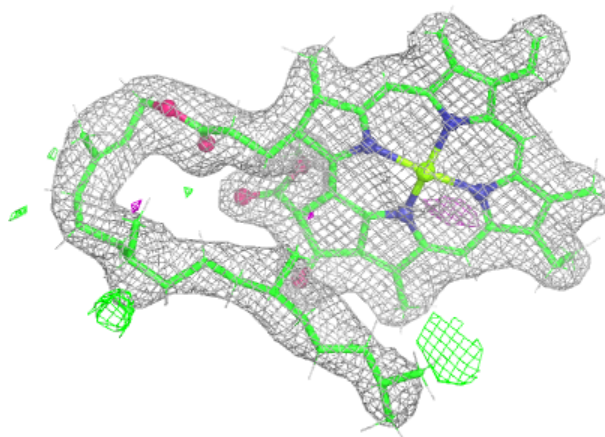
**Electron density around BCR a 608:**

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

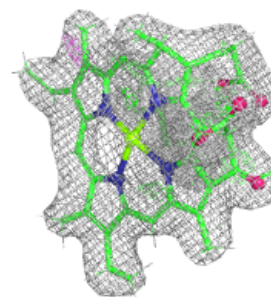
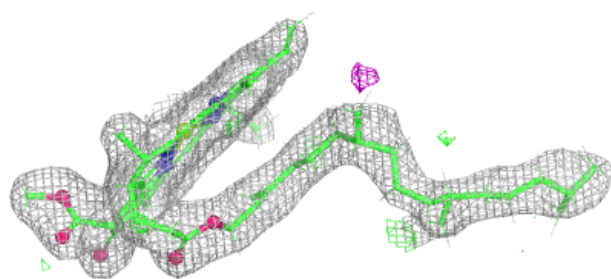
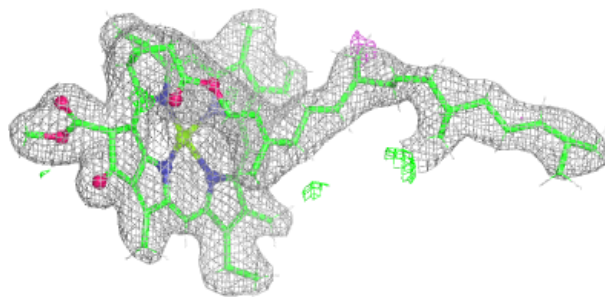


Electron density around CLA C 509:

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

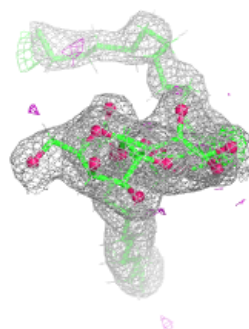
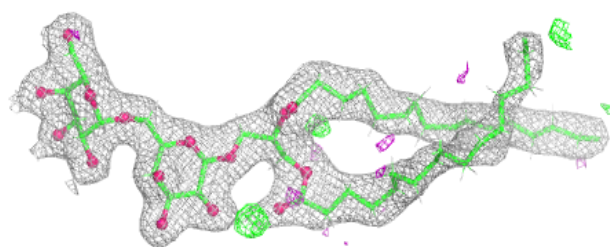
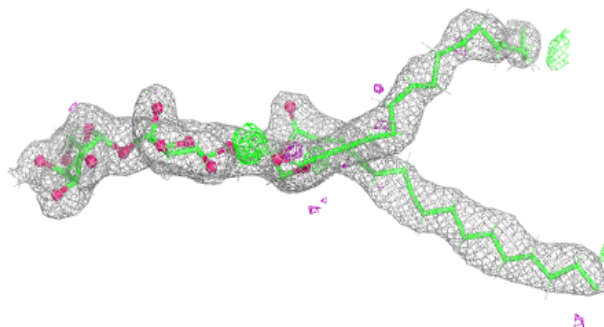
**Electron density around CLA c 505:**

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

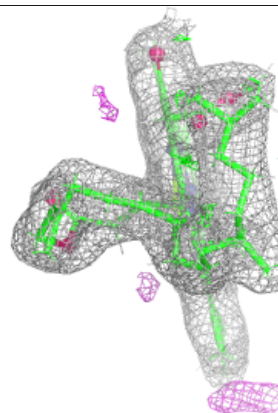
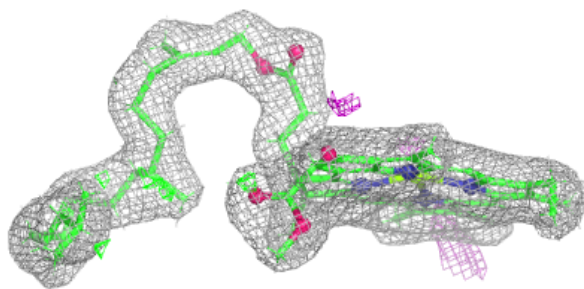
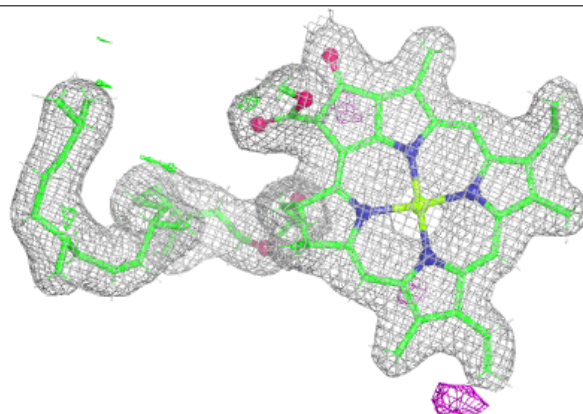


Electron density around DGD c 519:

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

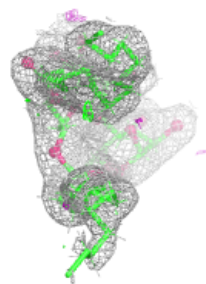
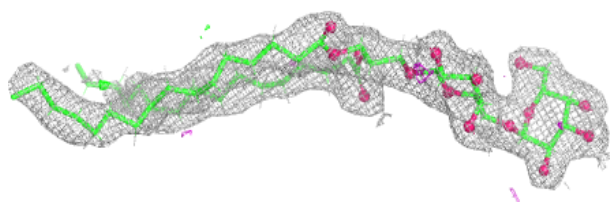
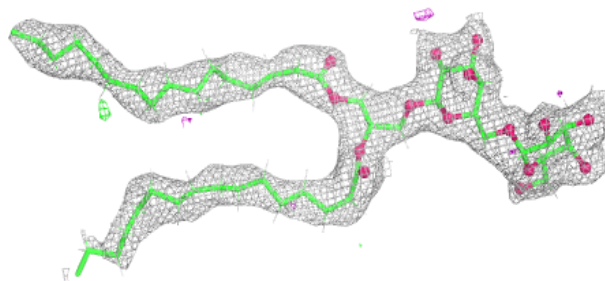
**Electron density around CLA B 612:**

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



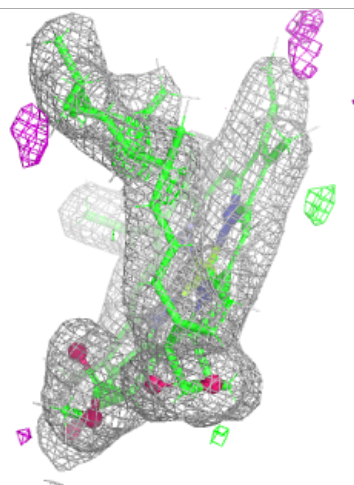
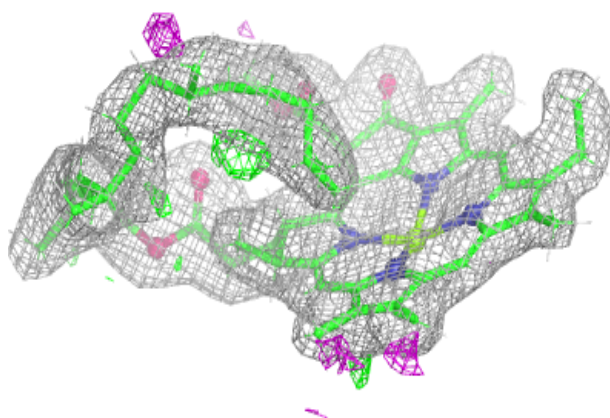
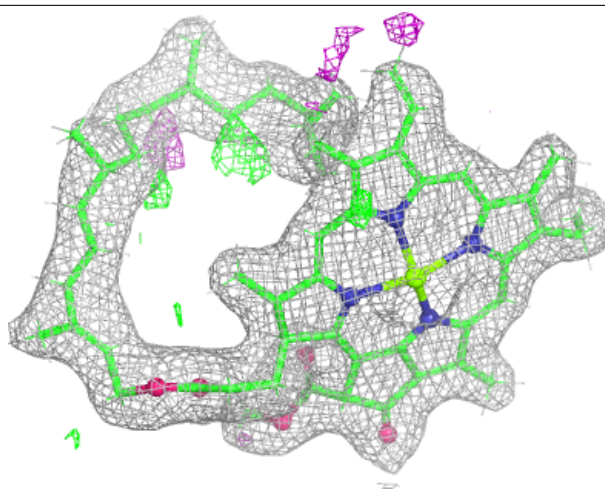
Electron density around DGD c 521:

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



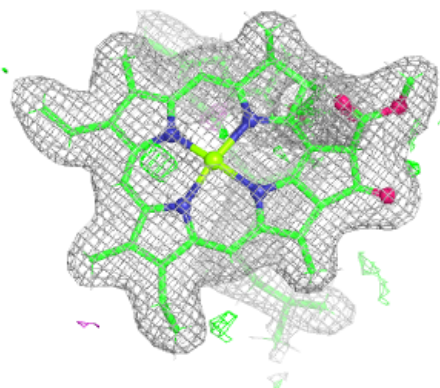
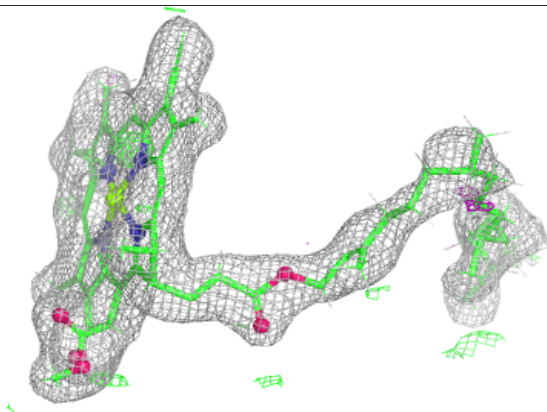
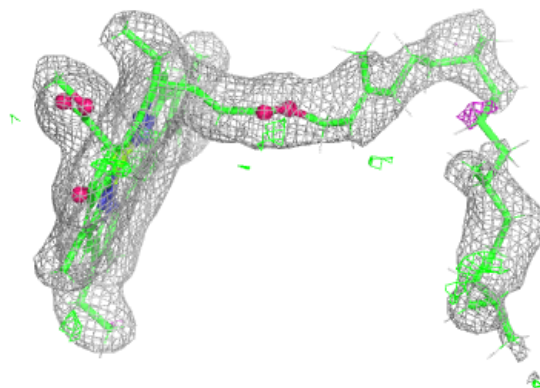
Electron density around CLA B 615:

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

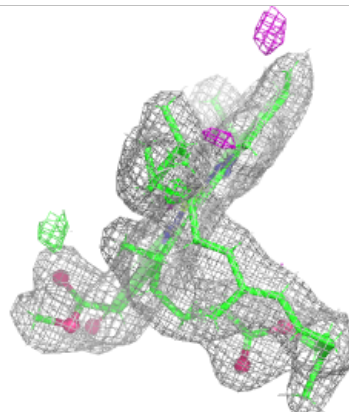
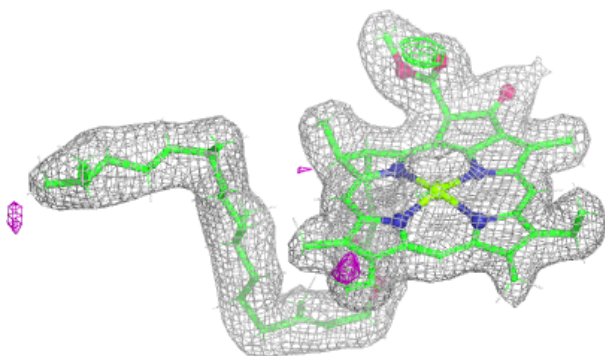
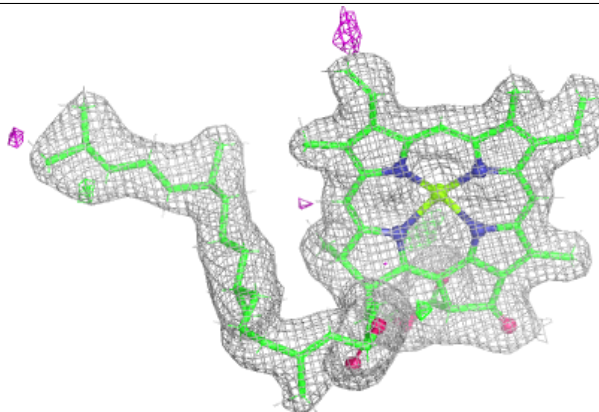


Electron density around CLA a 607:

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

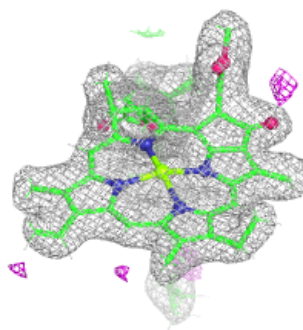
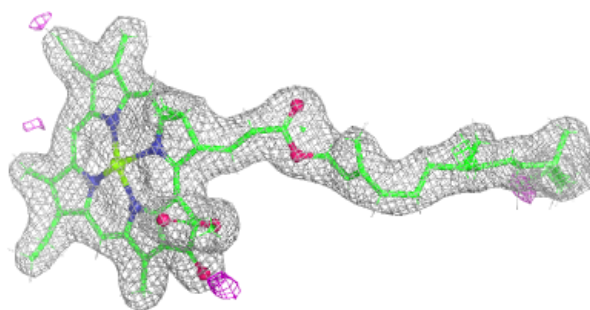
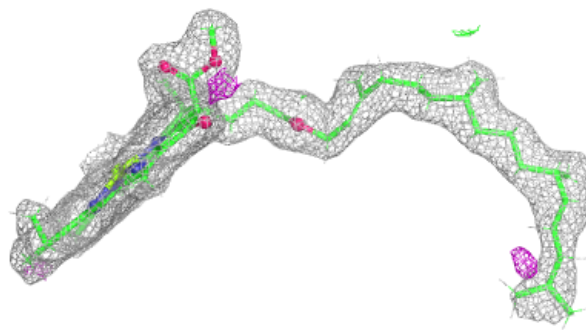
**Electron density around CLA d 404:**

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

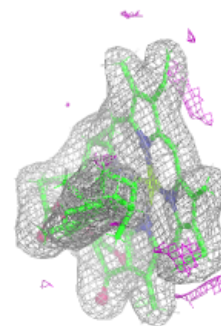
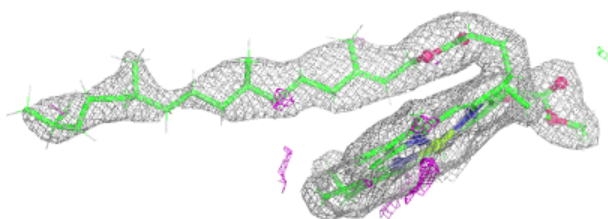
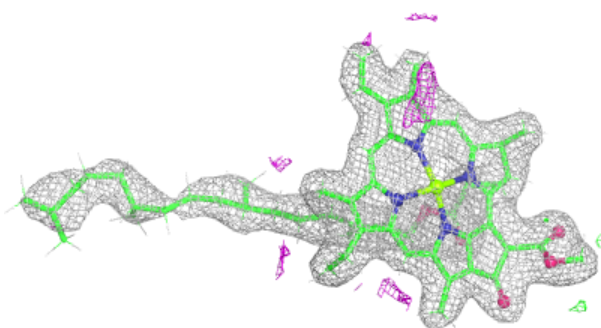


Electron density around CLA d 405:

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

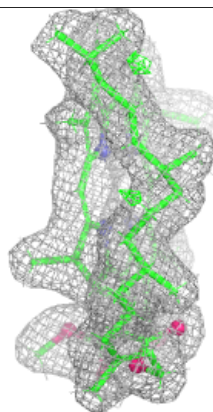
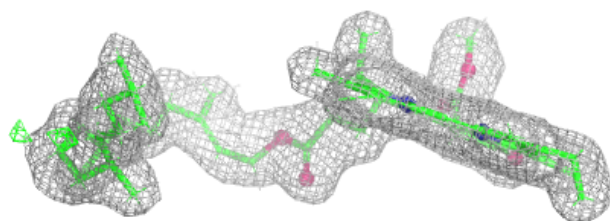
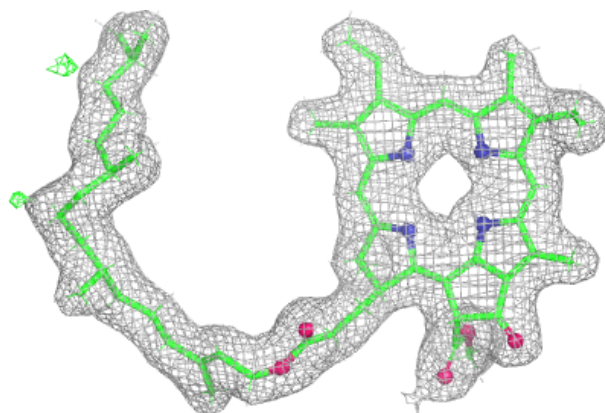
**Electron density around CLA B 614:**

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



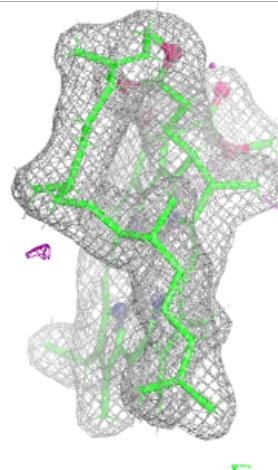
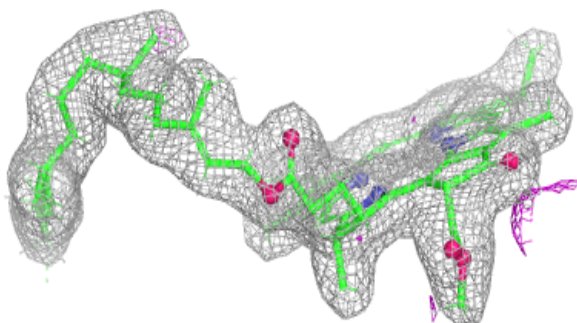
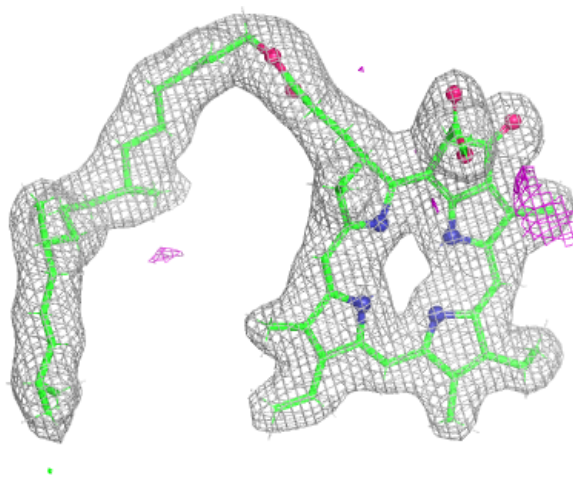
Electron density around PHO A 607:

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



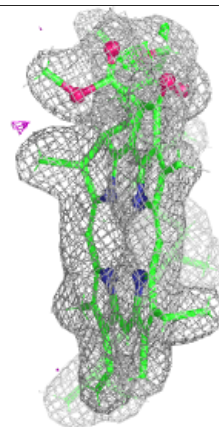
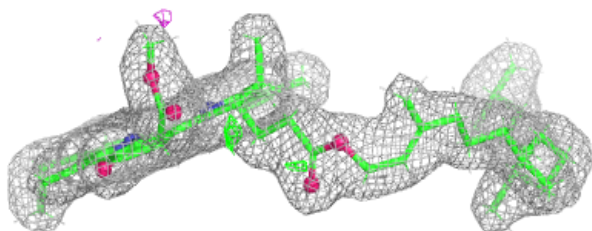
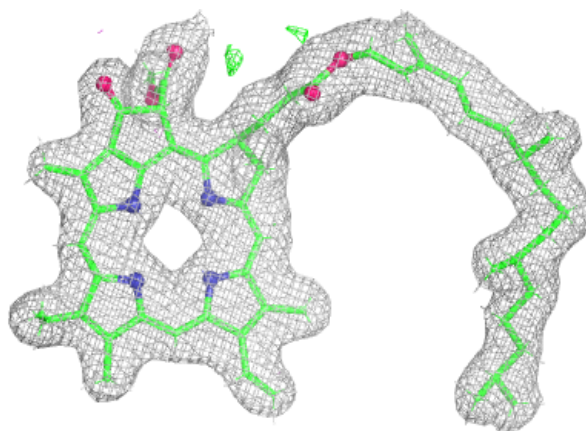
Electron density around PHO D 402:

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

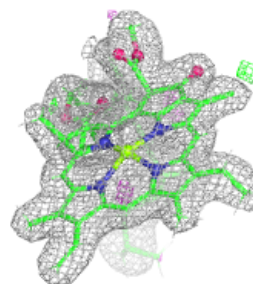
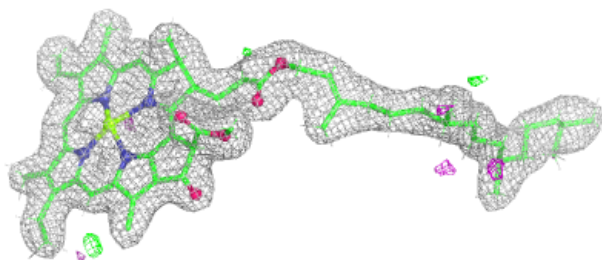
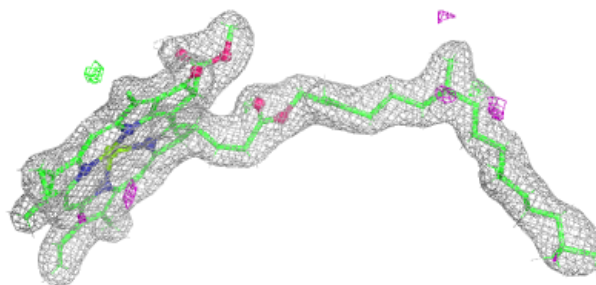


Electron density around PHO d 402:

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

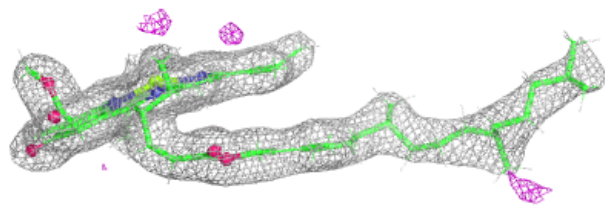
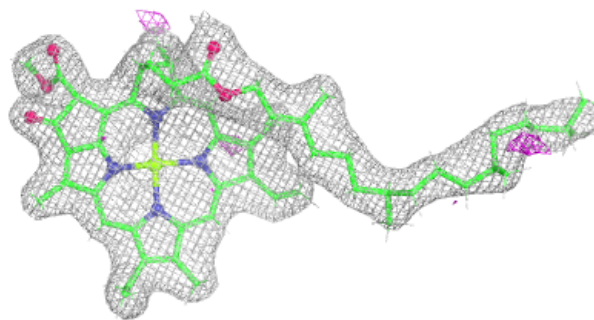
**Electron density around CLA A 605:**

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

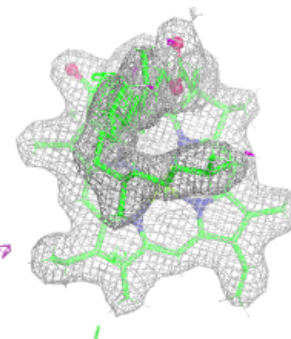
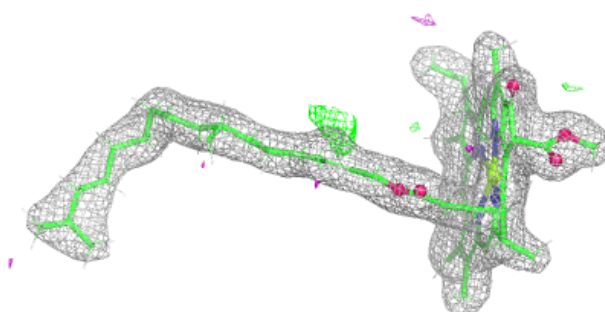
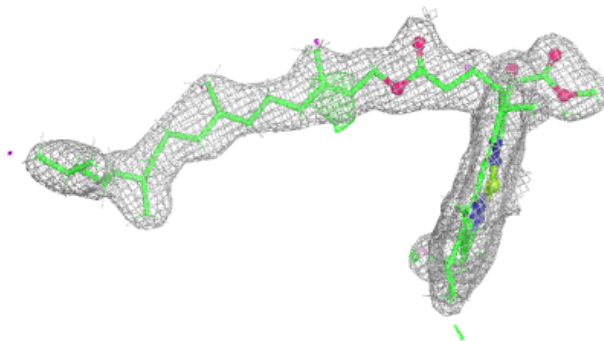


Electron density around CLA b 603:

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

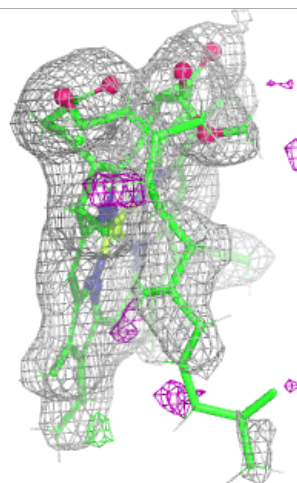
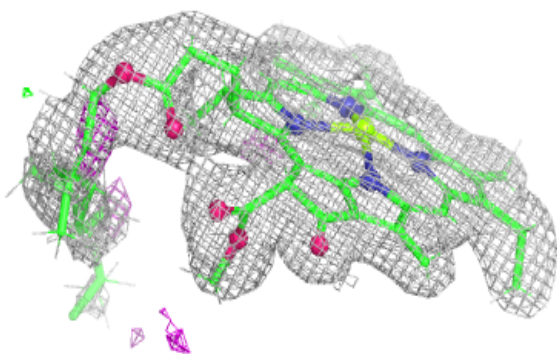
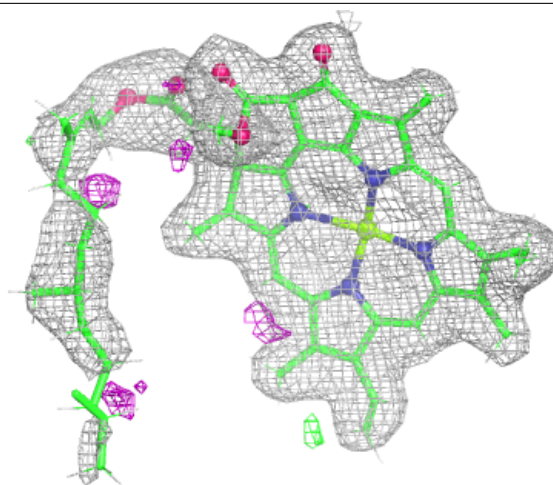
**Electron density around CLA b 605:**

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



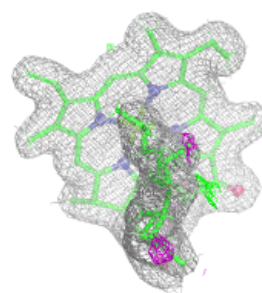
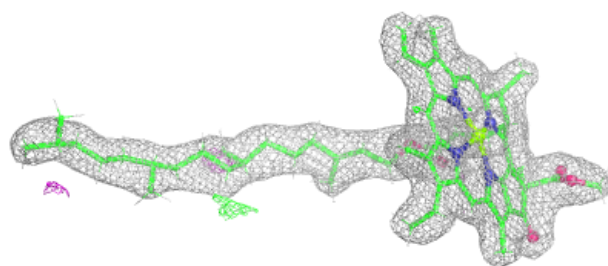
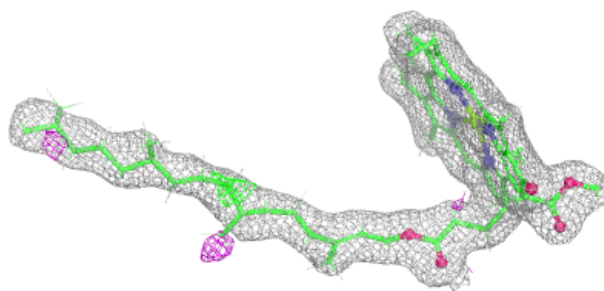
Electron density around CLA B 616:

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

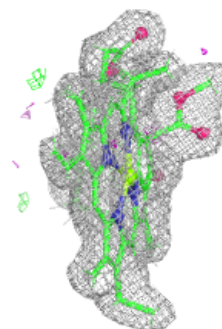
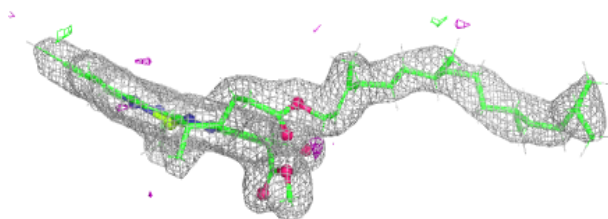
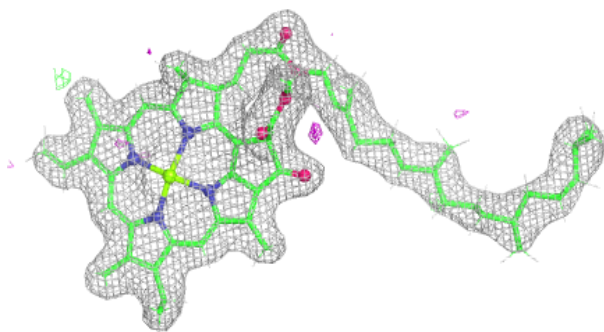


Electron density around CLA b 607:

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

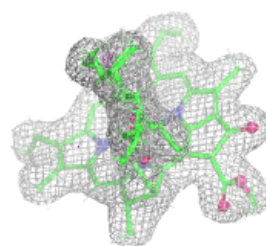
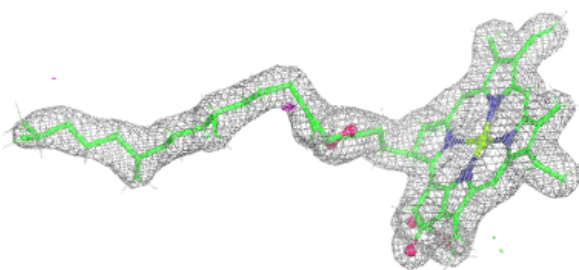
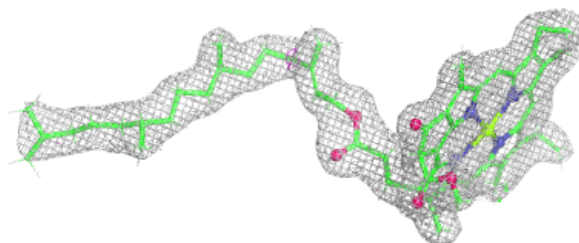
**Electron density around CLA B 602:**

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

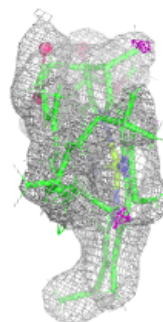
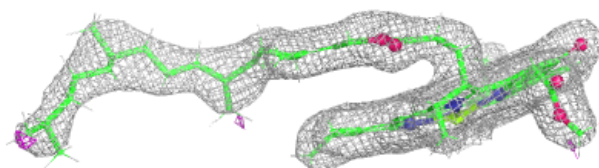
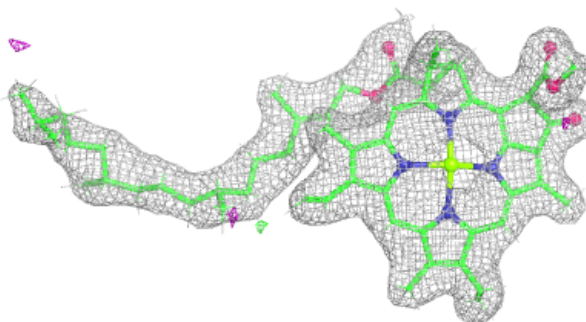


Electron density around CLA C 502:

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

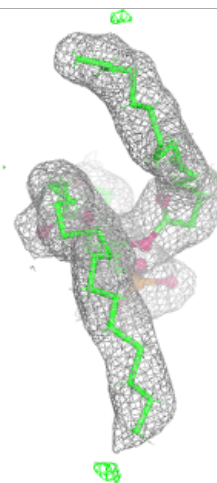
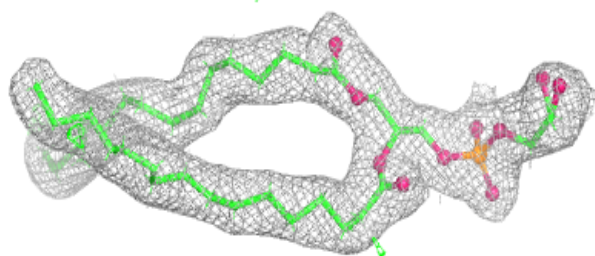
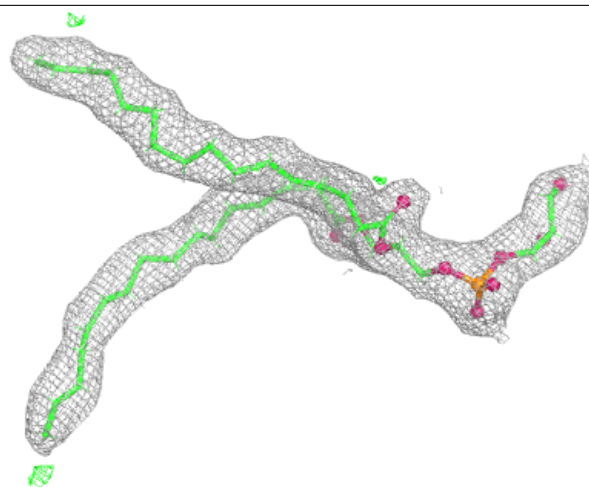
**Electron density around CLA B 603:**

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



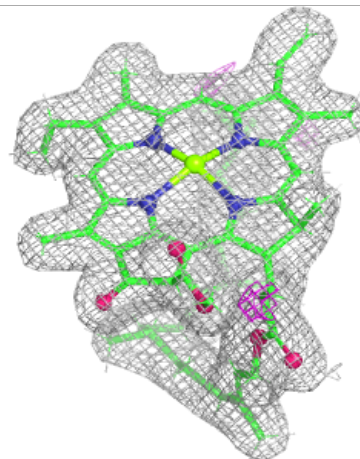
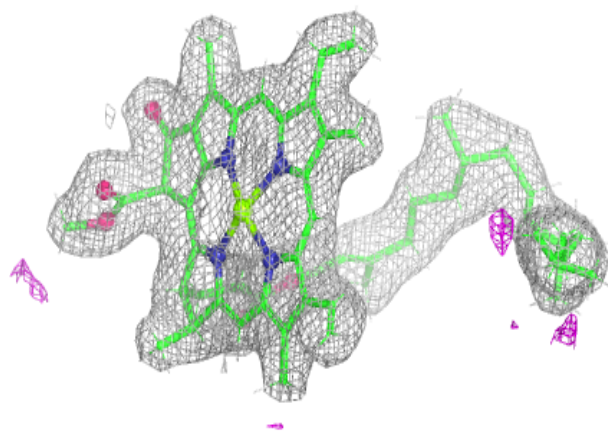
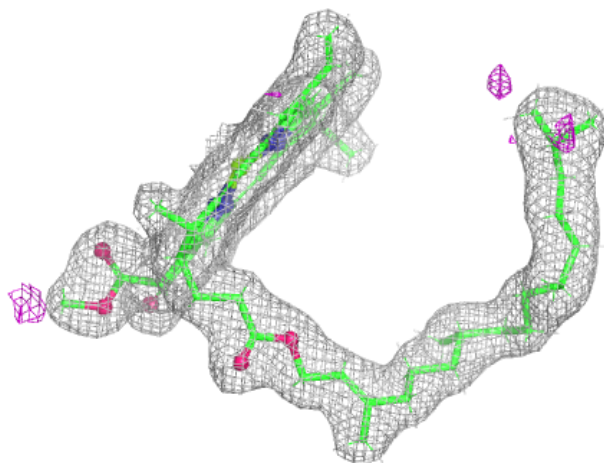
Electron density around LHG D 409:

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



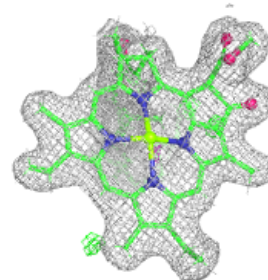
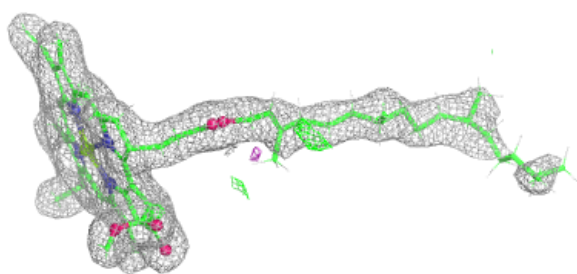
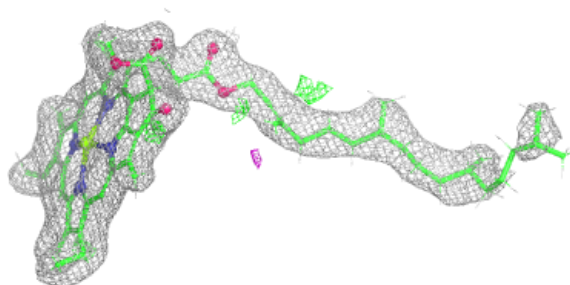
Electron density around CLA b 611:

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



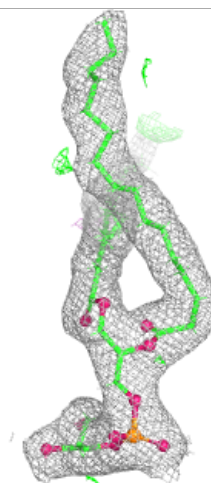
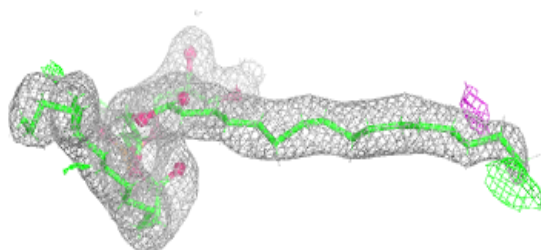
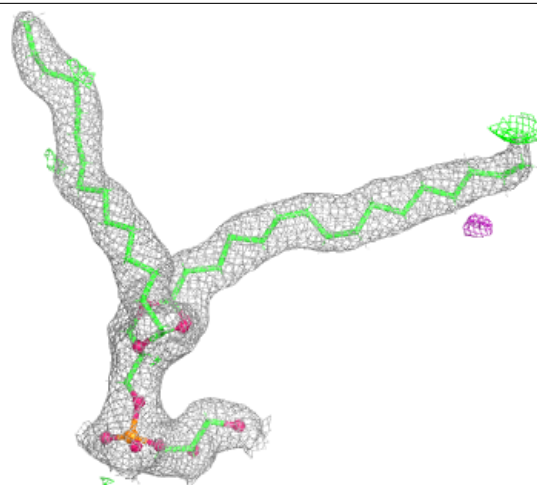
Electron density around CLA B 604:

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



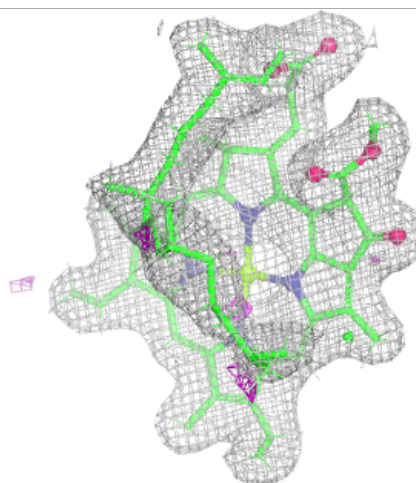
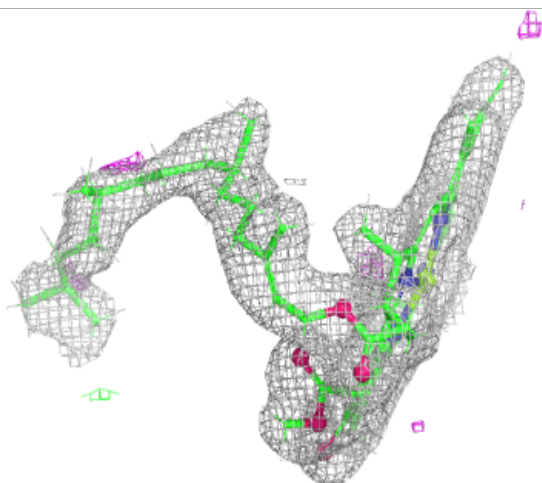
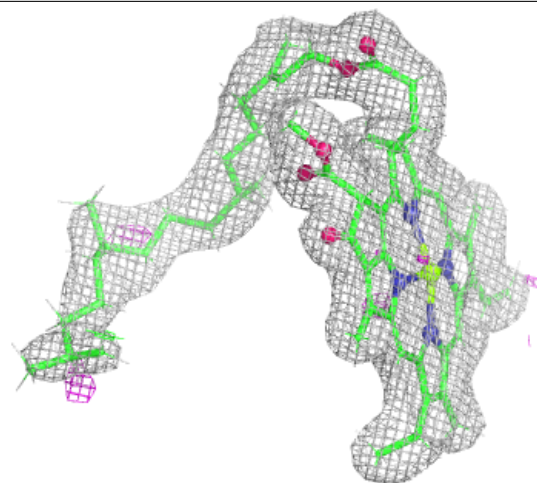
Electron density around LHG L 101:

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



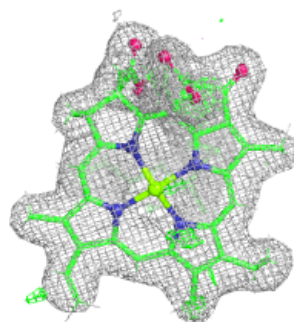
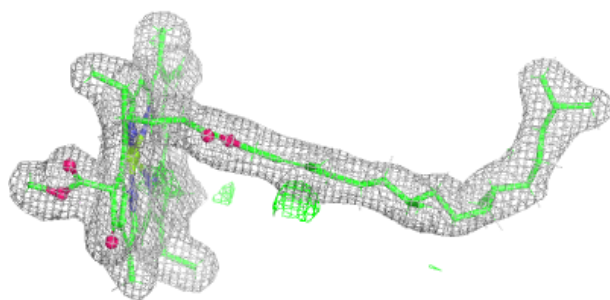
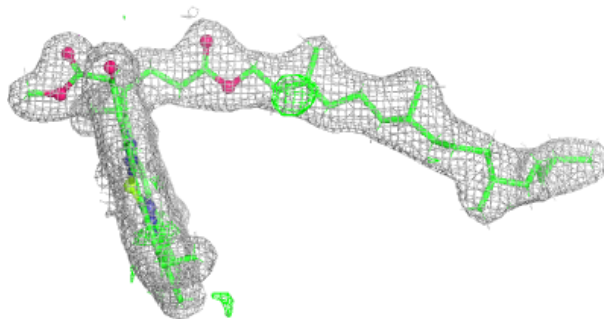
Electron density around CLA b 613:

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

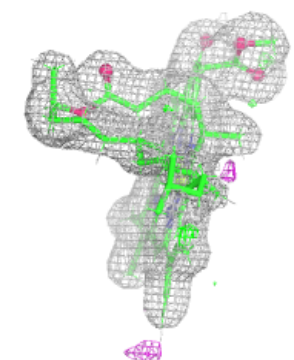
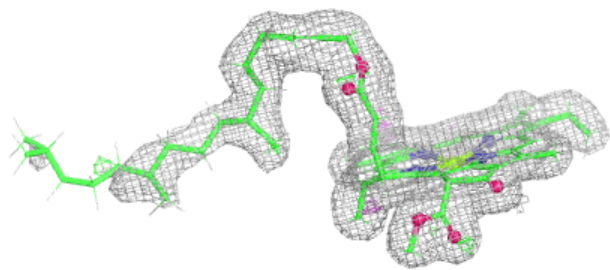
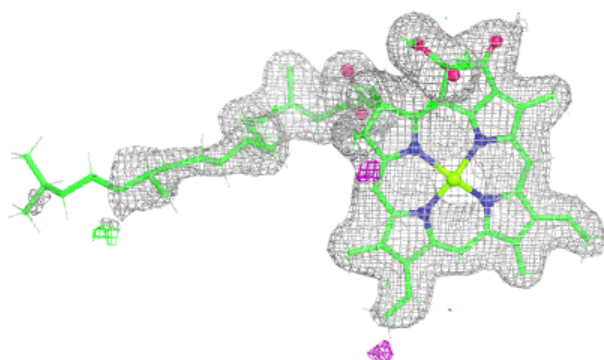


Electron density around CLA B 605:

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

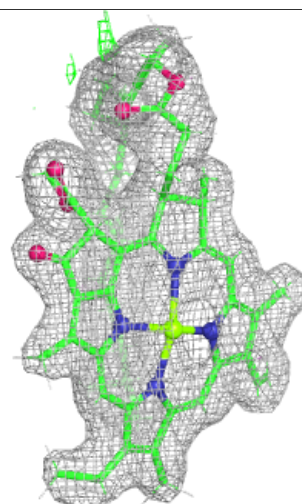
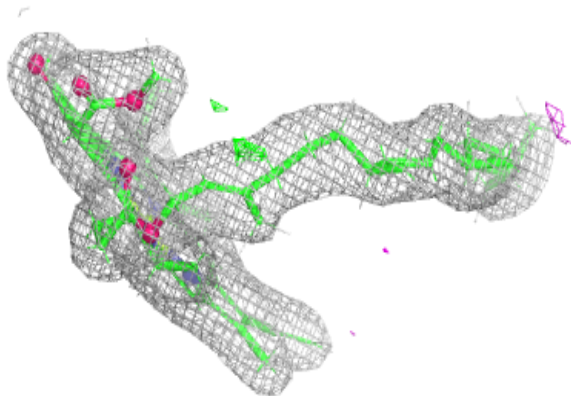
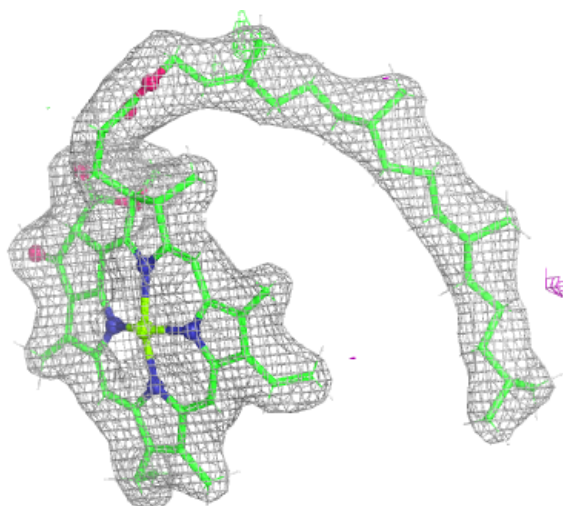
**Electron density around CLA A 606:**

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



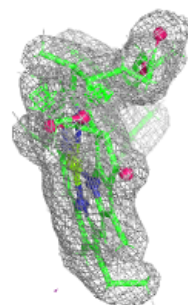
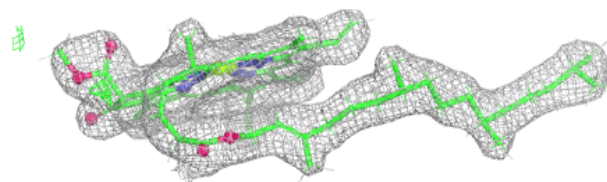
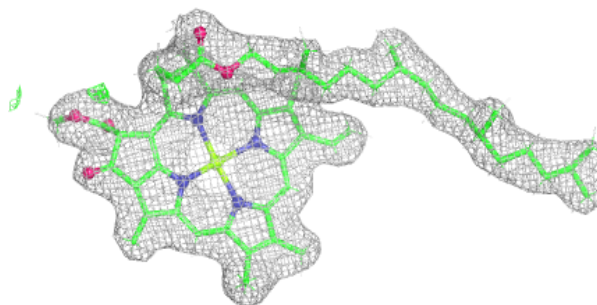
Electron density around CLA C 507:

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

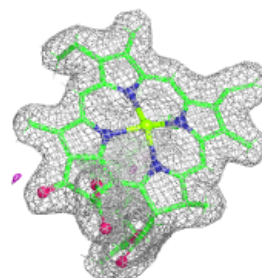
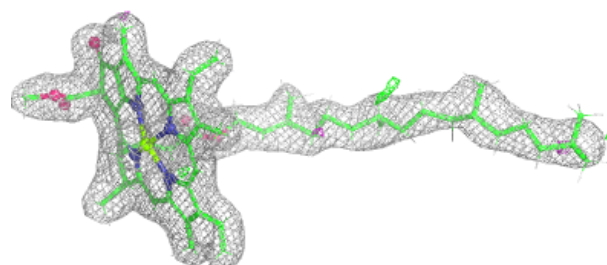
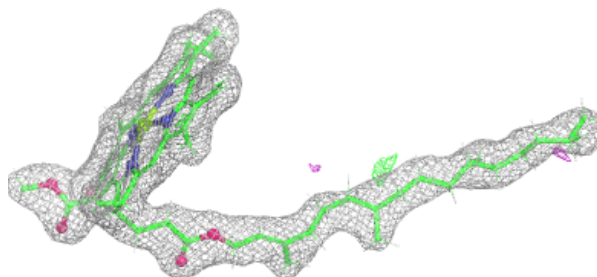


Electron density around CLA c 501:

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

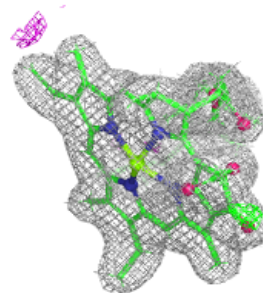
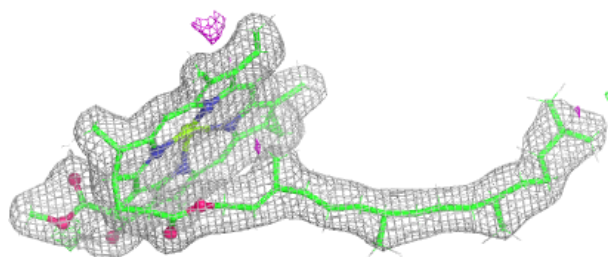
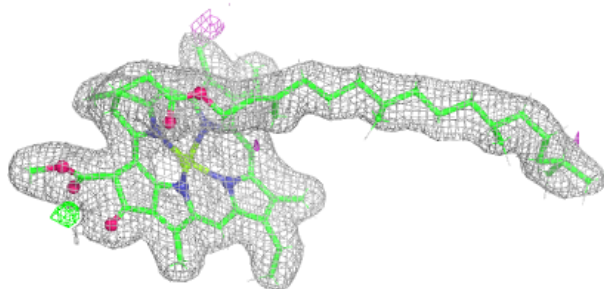
**Electron density around CLA B 607:**

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

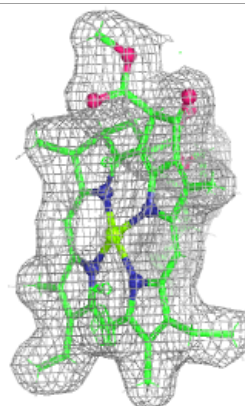
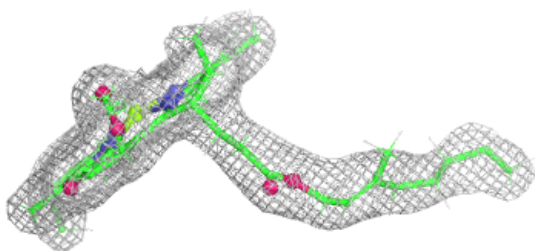
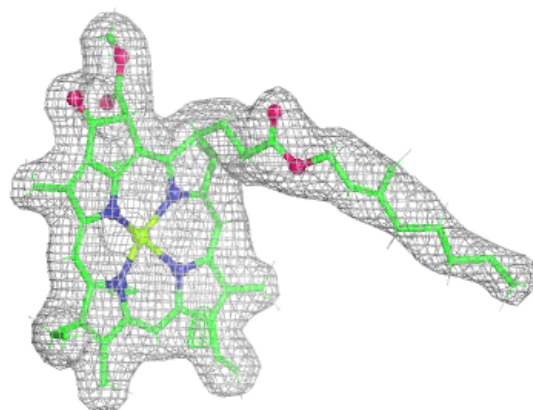


Electron density around CLA B 608:

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

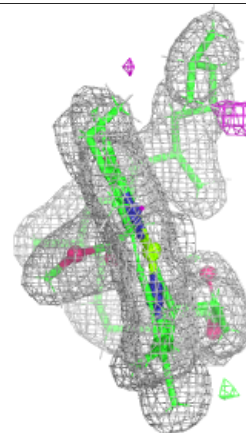
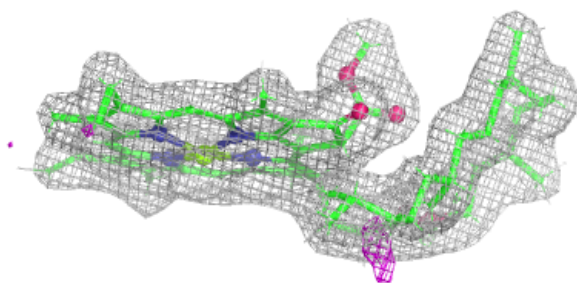
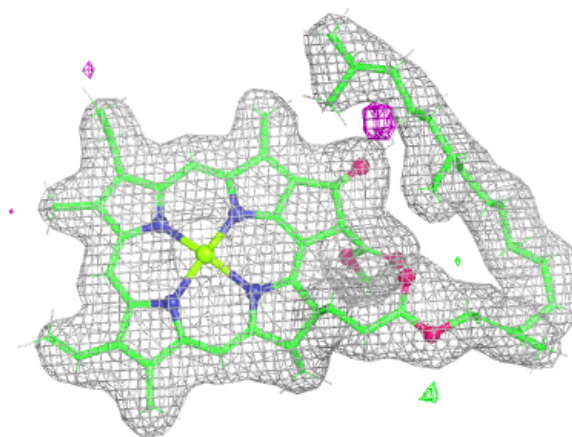
**Electron density around CLA A 608:**

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



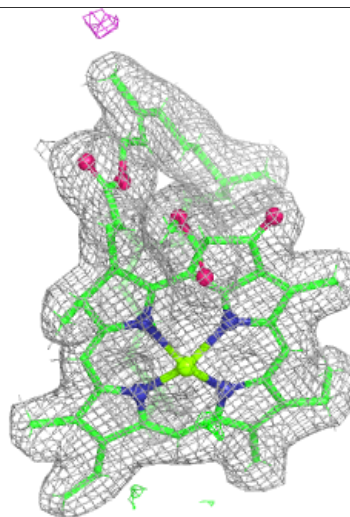
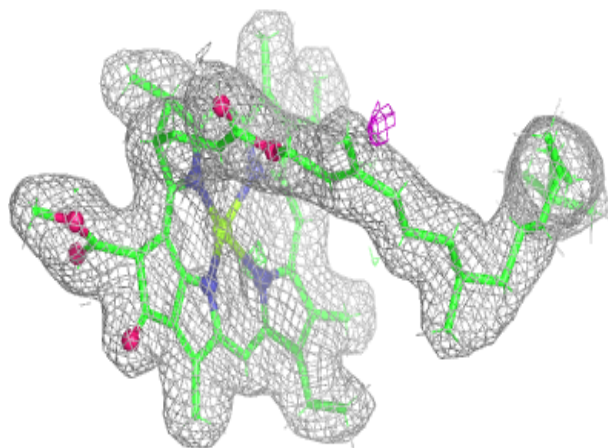
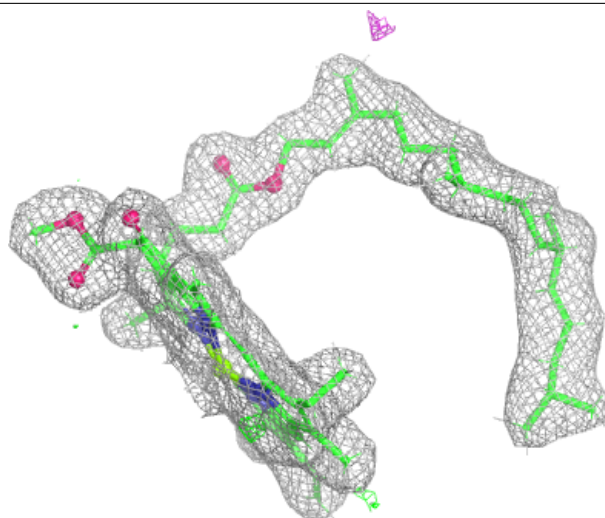
Electron density around CLA B 610:

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



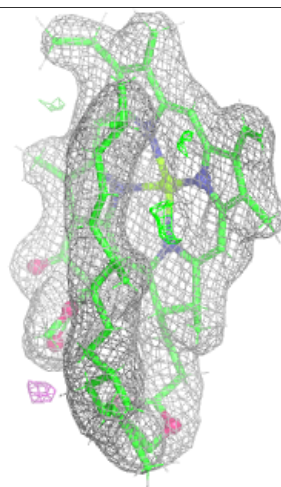
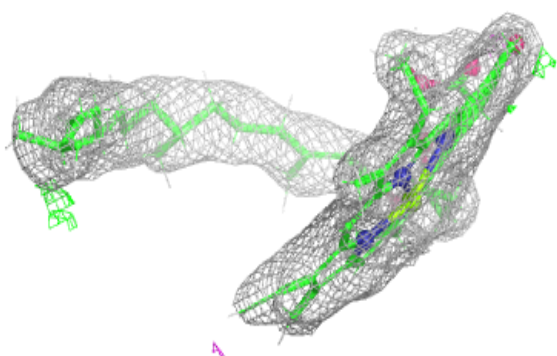
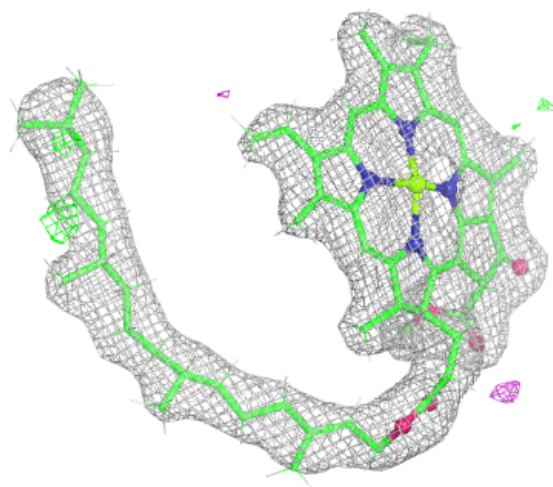
Electron density around CLA B 611:

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



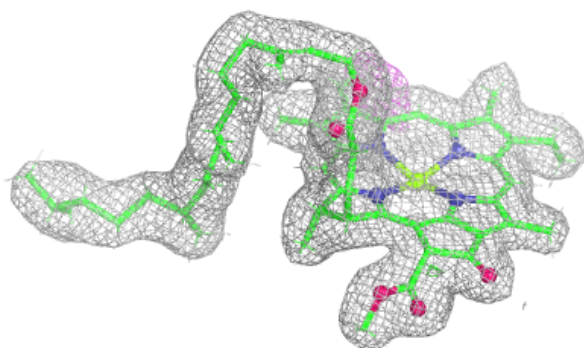
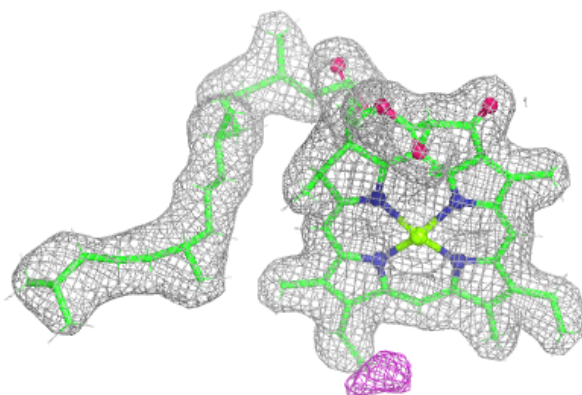
Electron density around CLA c 507:

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

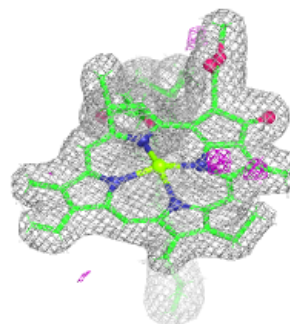
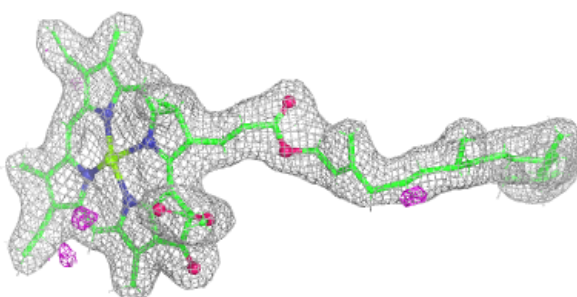
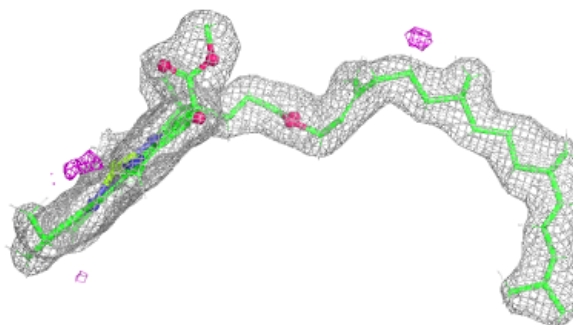


Electron density around CLA A 612:

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

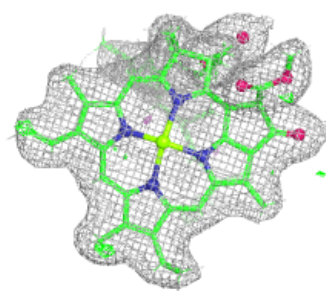
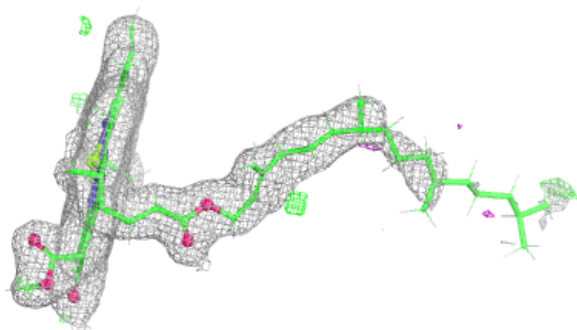
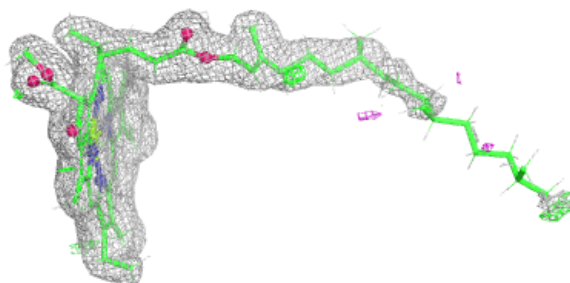
**Electron density around CLA D 403:**

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

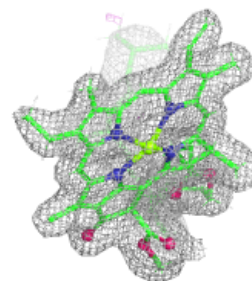
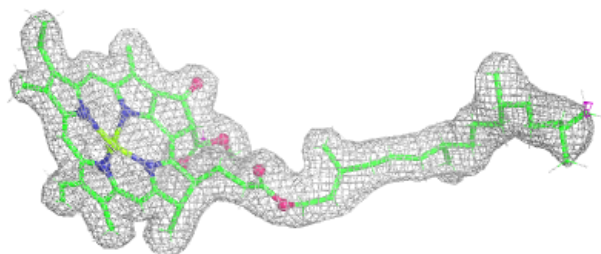
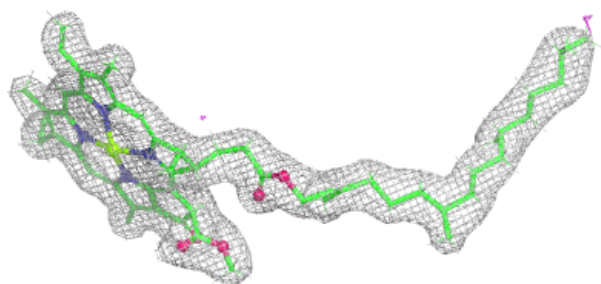


Electron density around CLA D 404:

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

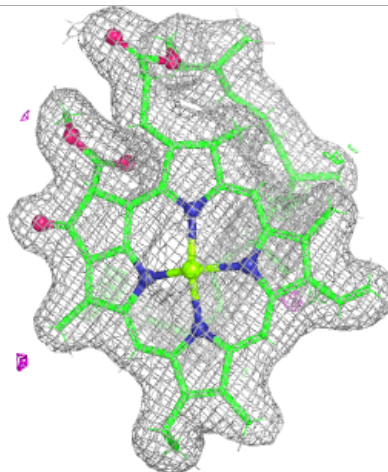
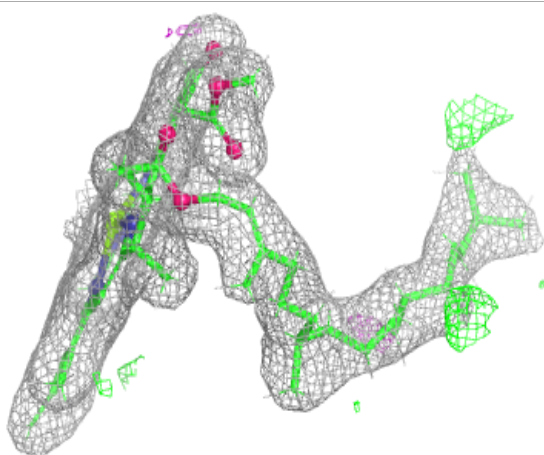
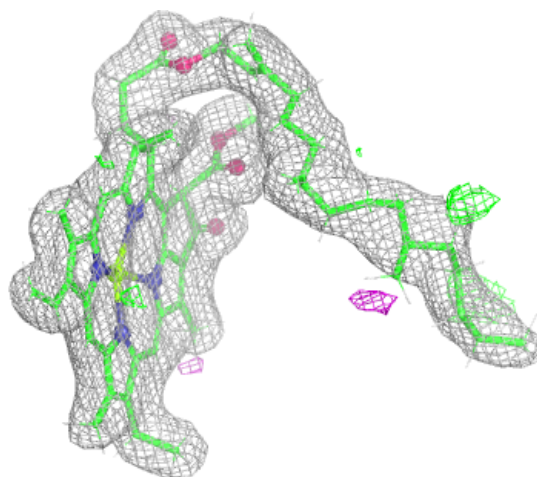
**Electron density around CLA a 605:**

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



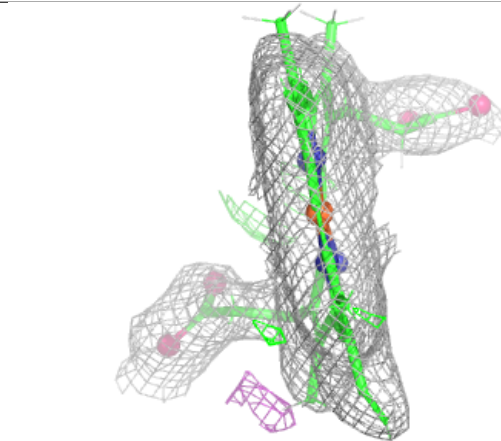
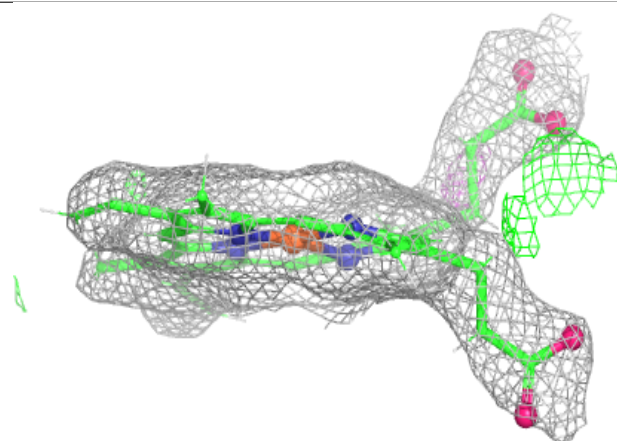
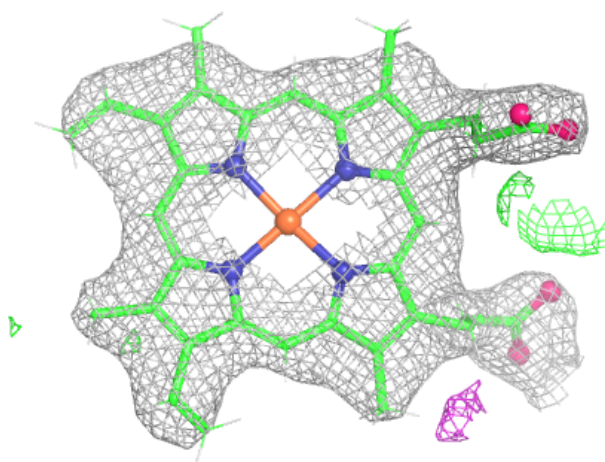
Electron density around CLA B 613:

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



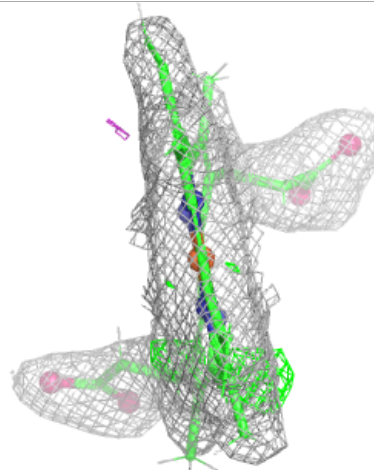
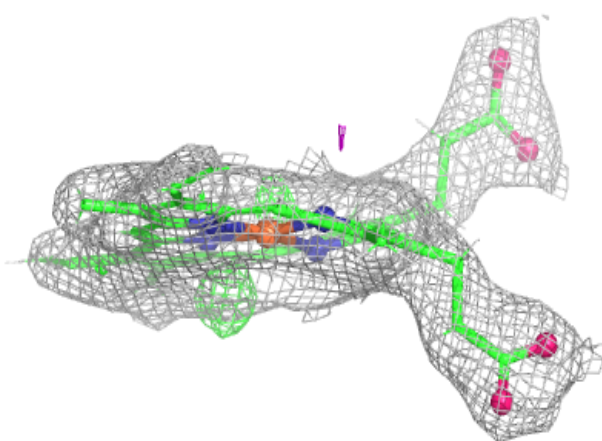
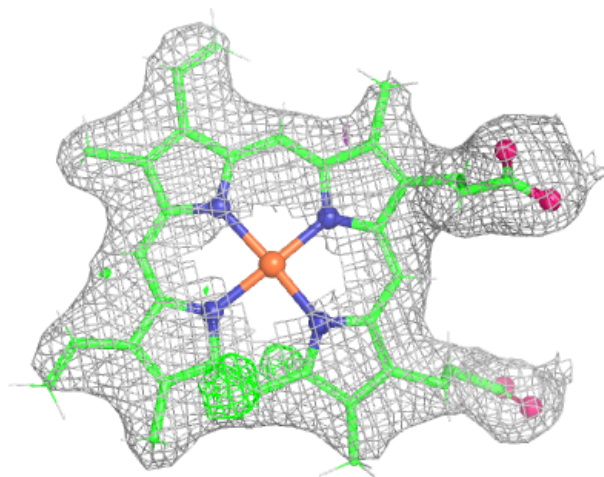
Electron density around HEM e 102:

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



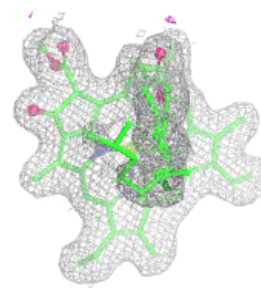
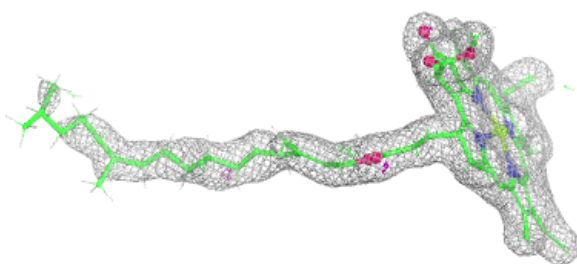
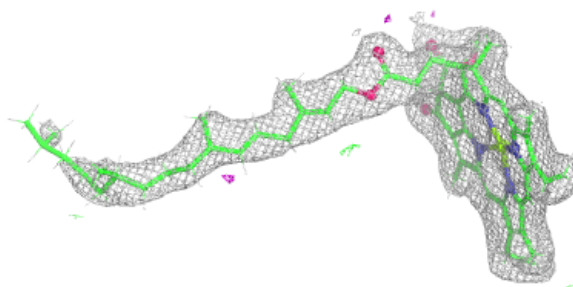
Electron density around HEM F 101:

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



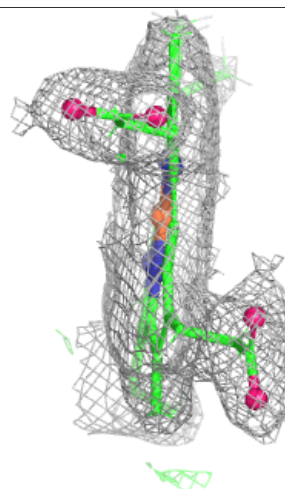
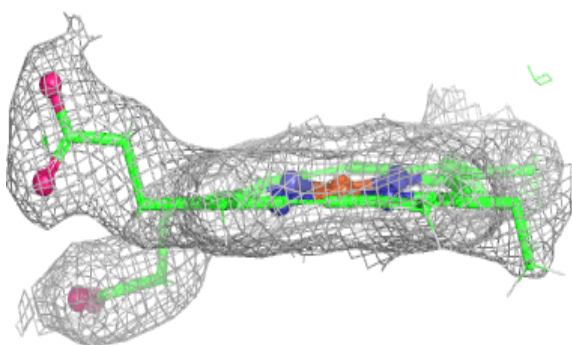
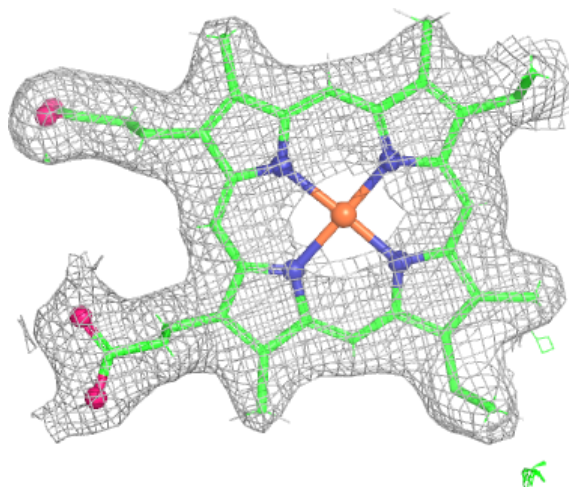
Electron density around CLA b 604:

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



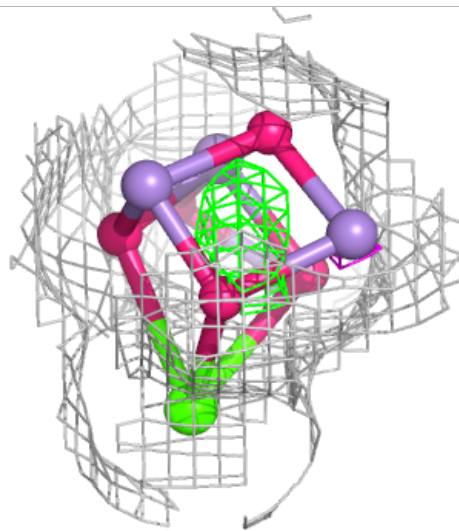
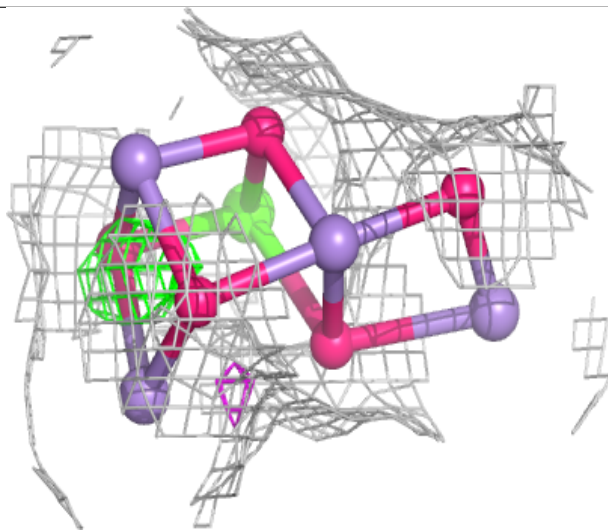
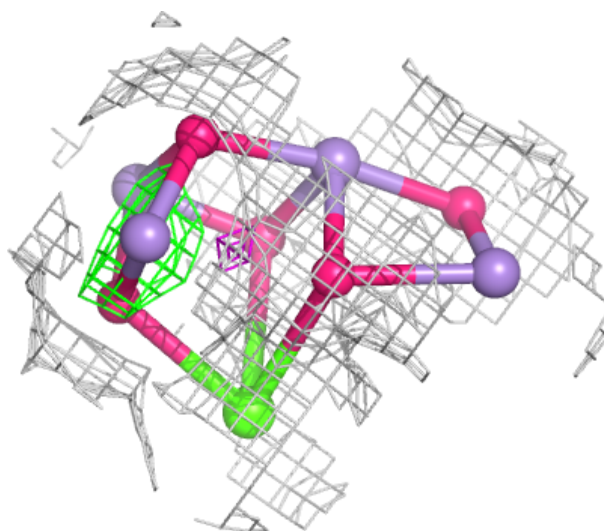
Electron density around HEC v 201:

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



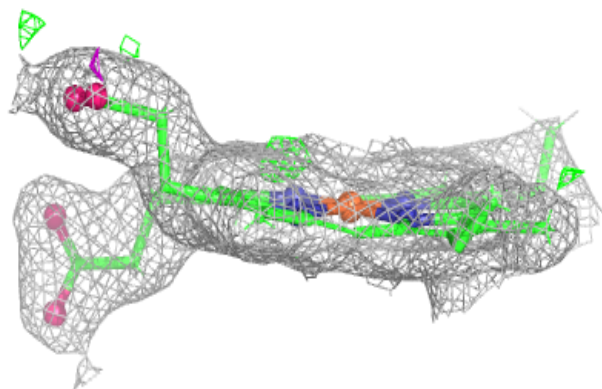
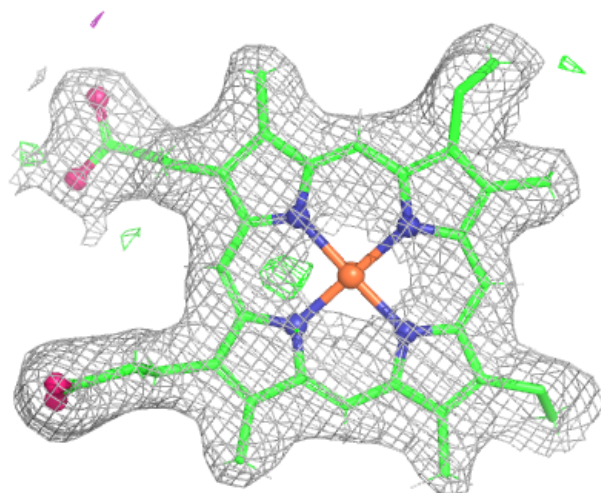
Electron density around OEX A 601:

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



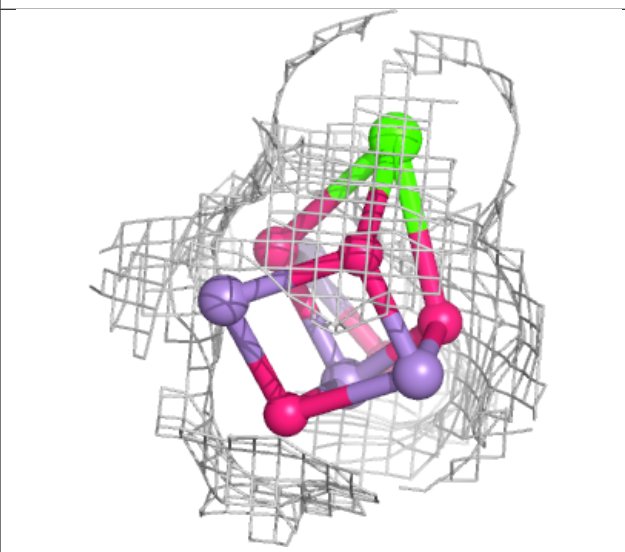
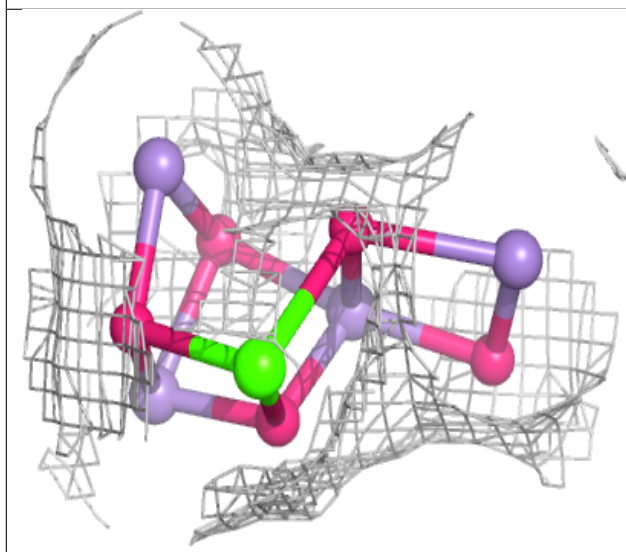
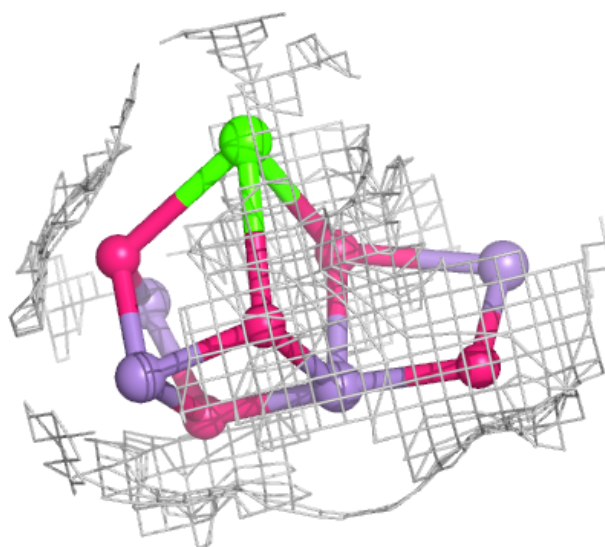
Electron density around HEC V 201:

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



Electron density around OEX a 601:

$2mF_o-DF_c$ (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.