



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:56 AM UTC

PDB ID : 5MX2 / pdb_00005mx2
Title : Photosystem II depleted of the Mn₄CaO₅ cluster at 2.55 Å resolution
Authors : Zhang, M.; Bommer, M.; Chatterjee, R.; Hussain, R.; Kern, J.; Yano, J.; Dau, H.; Dobbek, H.; Zouni, A.
Deposited on : 2017-01-20
Resolution : 2.20 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)
Xtrriage (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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

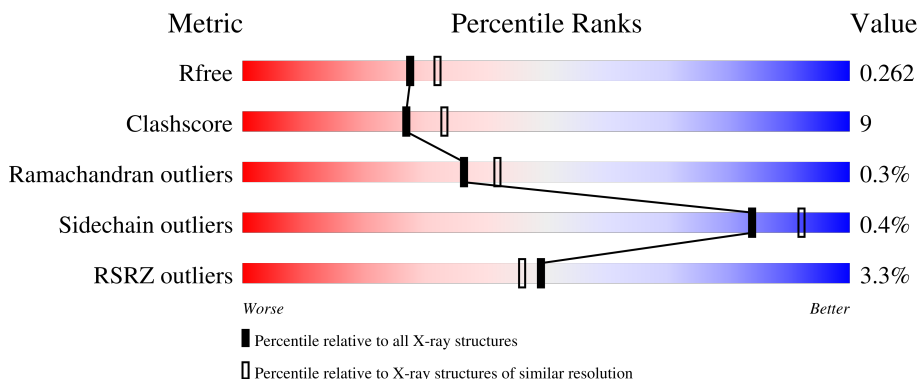
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.








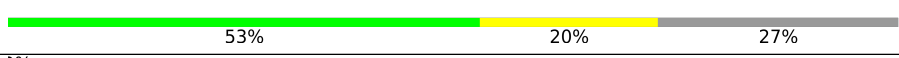

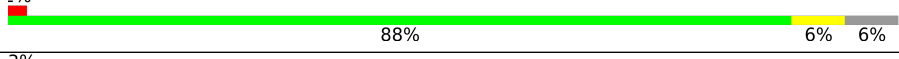
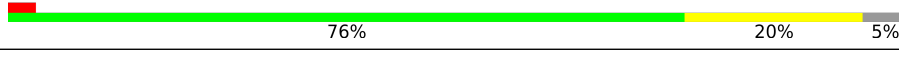
















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	 3% 81% 15% .
1	a	344	 % 76% 20% ..
2	B	510	 2% 82% 17% .
2	b	510	 2% 81% 18% .
3	C	461	 % 84% 13% .




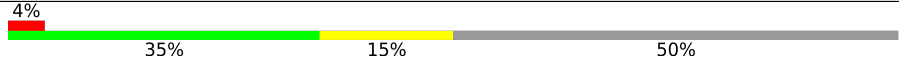
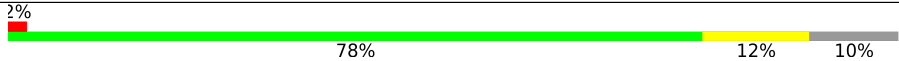
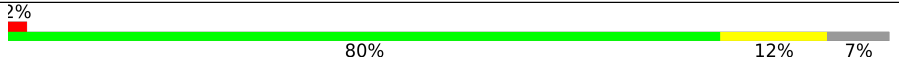
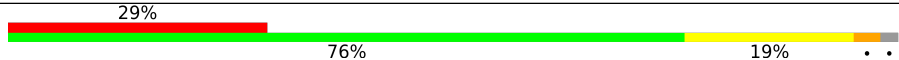
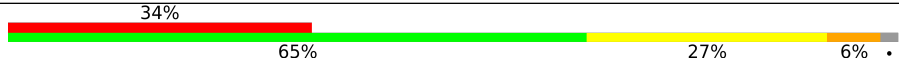
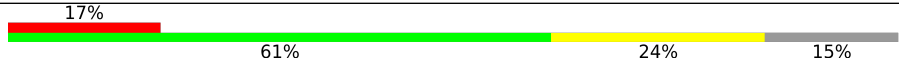
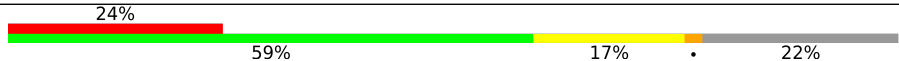
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Mol	Chain	Length	Quality of chain
3	c	461	 80% 17%
4	D	352	 81% 15%
4	d	352	 72% 25%
5	E	84	 71% 25%
5	e	84	 6% 70% 24% 6%
6	F	45	 53% 20% 27%
6	f	45	 2% 56% 16% 27%
7	H	66	 2% 88% 6% 6%
7	h	66	 3% 76% 20% 5%
8	I	38	 74% 13% 13%
8	i	38	 3% 87% 13%
9	J	40	 2% 80% 18%
9	j	40	 2% 68% 15% 18%
10	K	46	 9% 61% 15% 24%
10	k	46	 4% 57% 22% 22%
11	L	37	 81% 16%
11	l	37	 89% 8%
12	M	36	 75% 14% 11%
12	m	36	 75% 14% 11%
13	O	272	 5% 69% 19% 11%
13	o	272	 4% 69% 19% 11%
14	T	32	 66% 22% 12%
14	t	32	 6% 62% 28% 9%
15	U	134	 8% 57% 15% 28%
15	u	134	 63% 9% 28%

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Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	412	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 50407 atoms, of which 0 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
			Total	C	N	O	S			
1	A	333	2617	1714	430	458	15	0	0	0
1	a	333	2617	1714	430	458	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	3980	2611	665	691	13	0	0	0
2	b	503	3958	2599	657	689	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	447	3455	2264	576	602	13	0	0	0
3	c	448	3466	2270	580	603	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	340	2706	1794	440	460	12	0	0	0
4	d	340	2706	1794	440	460	12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			656	428	106	122			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	62	Total	C	N	O	S	0	0	0
			493	330	79	82	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	35	Total	C	N	O	0	0	0
			272	192	37	43			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	36	284	198	41	45	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	L	36	296	197	47	52	0	0	0
11	l	36	296	197	47	52	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	32	249	167	36	45	1	0	0	0
12	m	32	249	167	36	45	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	242	1859	1162	314	379	4	0	0	0
13	o	241	1852	1158	313	377	4	0	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	28	241	170	34	35	2	0	0	0
14	t	29	249	176	35	36	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	96	765	486	128	151	0	0	0
15	u	96	765	486	128	151	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	21	Total	C	N	O	S	0	0	0
			155	102	28	23	2			
17	y	23	Total	C	N	O	S	0	0	0
			171	113	30	25	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0	
			270	182	41	47				
18	x	38	Total	C	N	O	0	0	0	
			281	188	45	48				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			

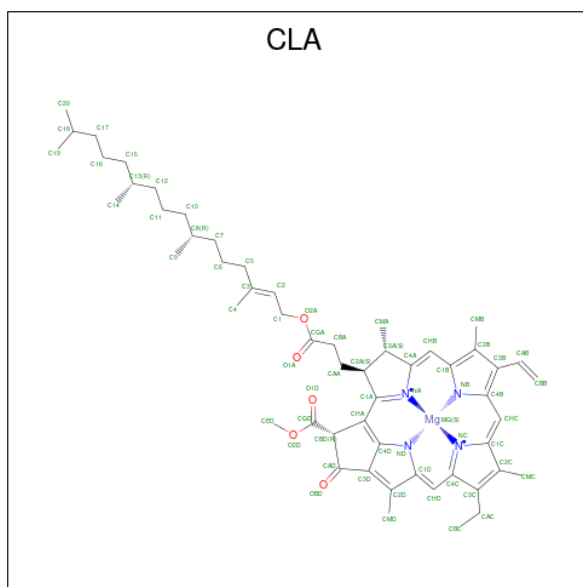
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	35	Total	C	N	O	0	0	0	
			282	191	49	42				
20	r	32	Total	C	N	O	0	0	0	
			257	176	45	36				

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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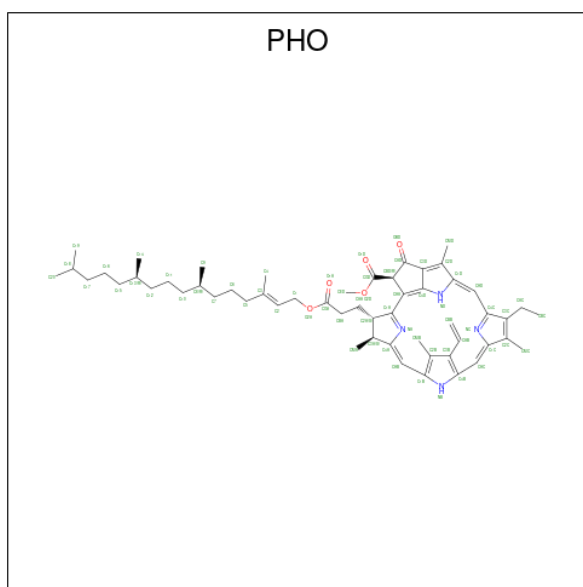
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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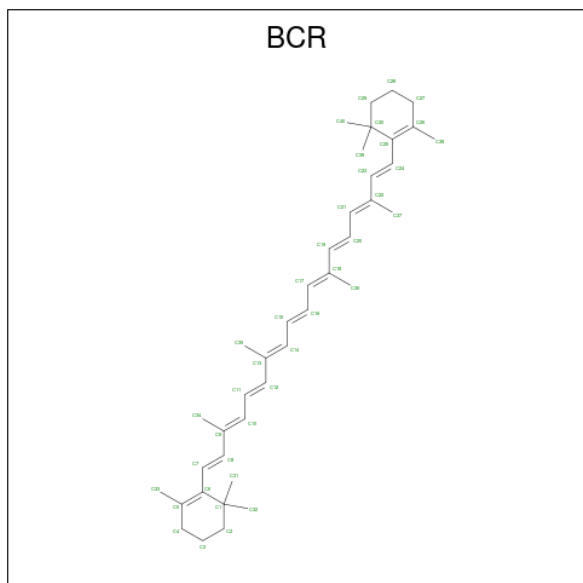
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



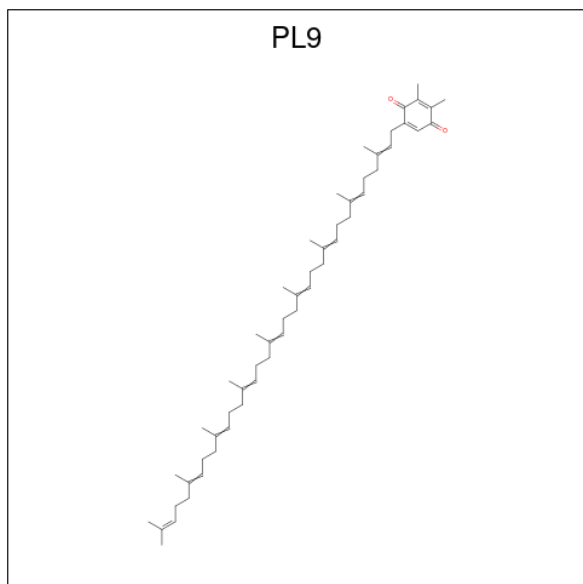
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
23	A	1	64	55	4	5	0	0
23	D	1	64	55	4	5	0	0
23	a	1	64	55	4	5	0	0
23	a	1	64	55	4	5	0	0

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



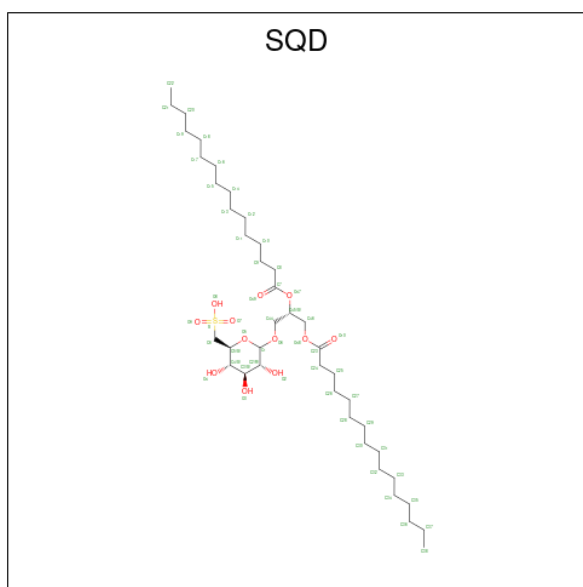
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total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

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



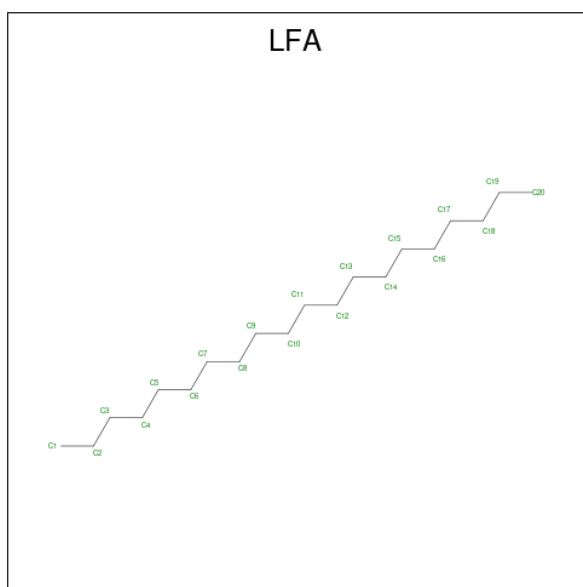
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	A	1	55	53	2	0	0
25	D	1	55	53	2	0	0
25	a	1	55	53	2	0	0
25	d	1	55	53	2	0	0

- Molecule 26 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
			Total	C	O	S		
26	A	1	54	41	12	1	0	0
26	A	1	54	41	12	1	0	0
26	D	1	43	30	12	1	0	0
26	L	1	48	35	12	1	0	0
26	a	1	54	41	12	1	0	0
26	a	1	50	41	9		0	0
26	b	1	54	41	12	1	0	0
26	f	1	43	30	12	1	0	0

- Molecule 27 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 14 14	0	0
27	A	1	Total C 11 11	0	0
27	B	1	Total C 10 10	0	0
27	B	1	Total C 16 16	0	0
27	B	1	Total C 13 13	0	0
27	B	1	Total C 15 15	0	0
27	B	1	Total C 9 9	0	0
27	B	1	Total C 10 10	0	0
27	B	1	Total C 14 14	0	0
27	B	1	Total C 12 12	0	0
27	C	1	Total C 15 15	0	0
27	D	1	Total C 15 15	0	0
27	D	1	Total C 8 8	0	0
27	D	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C 14 14	0	0
27	J	1	Total C 11 11	0	0
27	M	1	Total C 10 10	0	0
27	M	1	Total C 16 16	0	0
27	T	1	Total C 12 12	0	0
27	a	1	Total C 7 7	0	0
27	b	1	Total C 15 15	0	0
27	b	1	Total C 10 10	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 16 16	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 11 11	0	0
27	b	1	Total C 9 9	0	0
27	b	1	Total C 15 15	0	0
27	c	1	Total C 9 9	0	0
27	c	1	Total C 15 15	0	0
27	d	1	Total C 15 15	0	0
27	d	1	Total C 9 9	0	0
27	d	1	Total C 16 16	0	0
27	i	1	Total C 16 16	0	0
27	i	1	Total C 7 7	0	0

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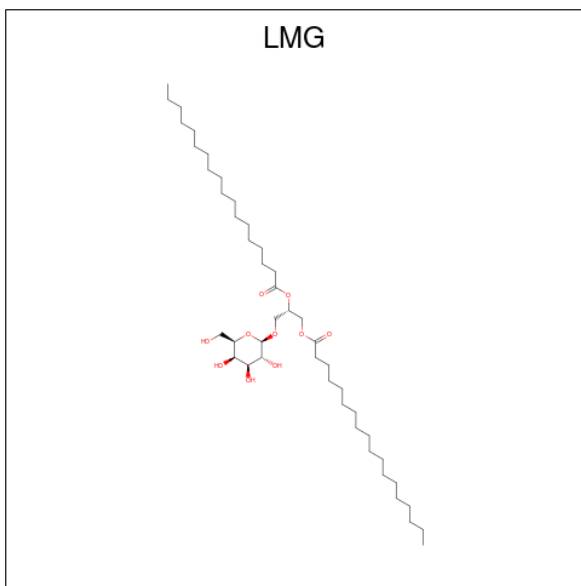
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	j	1	Total C 15 15	0	0
27	m	1	Total C 10 10	0	0
27	m	1	Total C 15 15	0	0
27	t	1	Total C 15 15	0	0

- Molecule 28 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



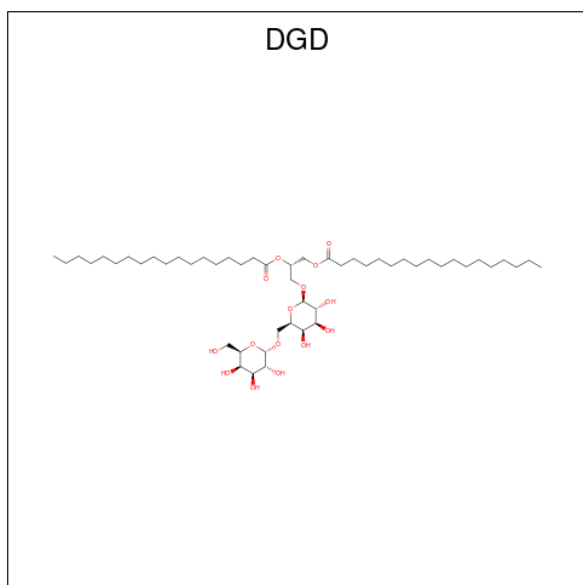
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 36 26 10	0	0
29	C	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	C	1	Total	C	O	0	0
			48	38	10		
29	C	1	Total	C	O	0	0
			44	34	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			39	29	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			41	31	10		
29	f	1	Total	C	O	0	0
			51	41	10		
29	m	1	Total	C	O	0	0
			51	41	10		

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



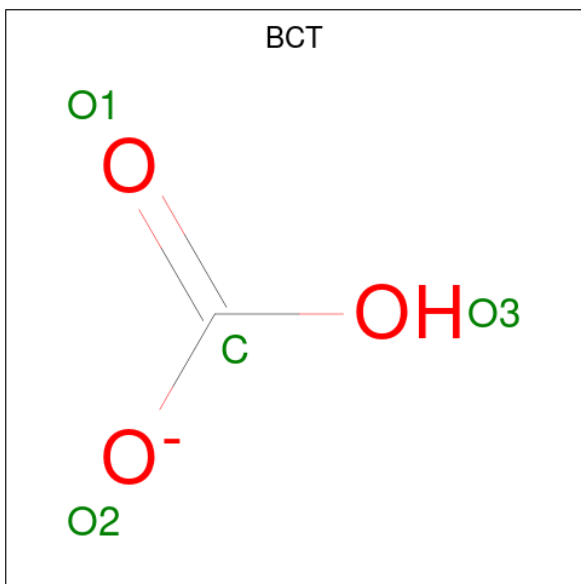
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			62	47	15		
30	C	1	Total	C	O	0	0
			56	41	15		

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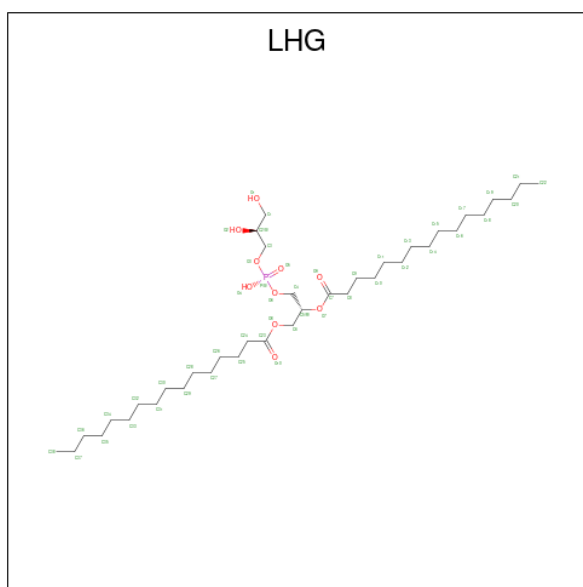
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			62	47	15		
30	H	1	Total	C	O	0	0
			60	45	15		
30	c	1	Total	C	O	0	0
			62	47	15		
30	c	1	Total	C	O	0	0
			55	40	15		
30	c	1	Total	C	O	0	0
			62	47	15		
30	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



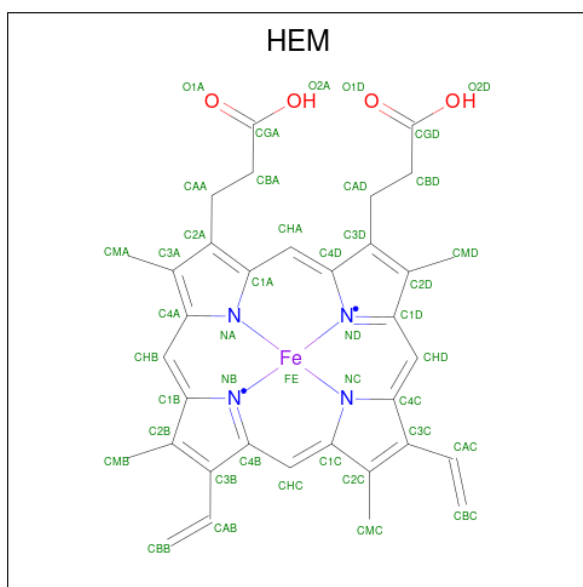
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



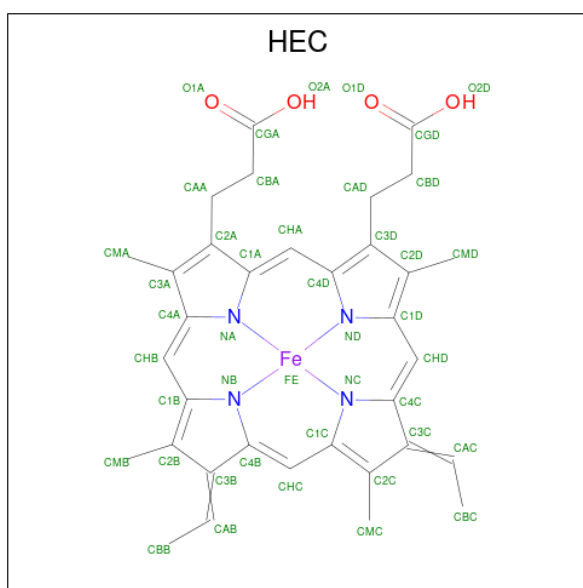
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
32	D	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	E	1	42	31	10	1	0	0
32	L	1	49	38	10	1	0	0
32	b	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	e	1	42	31	10	1	0	0
32	l	1	49	38	10	1	0	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
33	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
34	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	70	Total O 70 70	0	0
35	B	84	Total O 84 84	0	0
35	C	62	Total O 62 62	0	0
35	D	72	Total O 72 72	0	0
35	E	5	Total O 5 5	0	0
35	F	1	Total O 1 1	0	0
35	H	17	Total O 17 17	0	0
35	J	1	Total O 1 1	0	0
35	K	1	Total O 1 1	0	0
35	L	5	Total O 5 5	0	0
35	M	3	Total O 3 3	0	0
35	O	30	Total O 30 30	0	0
35	T	2	Total O 2 2	0	0
35	U	2	Total O 2 2	0	0
35	V	12	Total O 12 12	0	0
35	X	3	Total O 3 3	0	0
35	a	77	Total O 77 77	0	0
35	b	72	Total O 72 72	0	0
35	c	65	Total O 65 65	0	0
35	d	51	Total O 51 51	0	0
35	e	5	Total O 5 5	0	0

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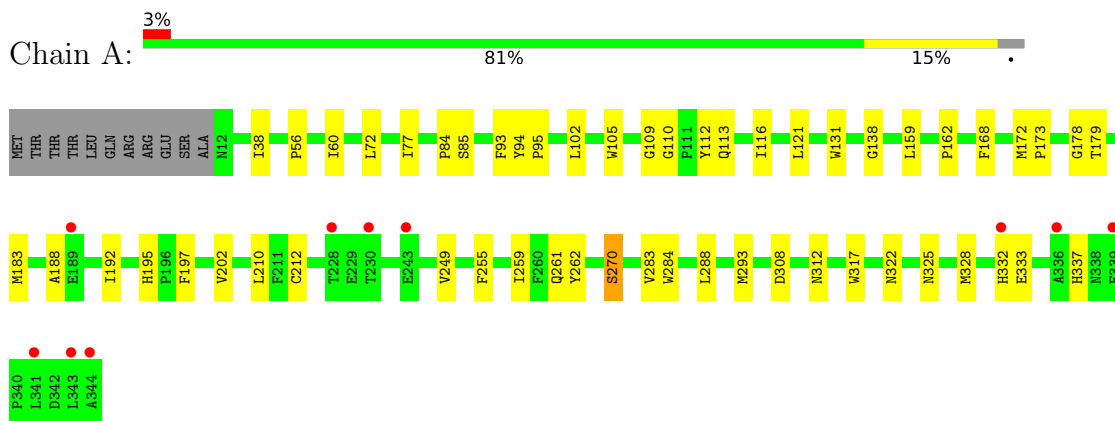
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	f	2	Total O 2 2	0	0
35	h	3	Total O 3 3	0	0
35	l	5	Total O 5 5	0	0
35	m	2	Total O 2 2	0	0
35	o	25	Total O 25 25	0	0
35	t	3	Total O 3 3	0	0
35	u	12	Total O 12 12	0	0
35	v	11	Total O 11 11	0	0

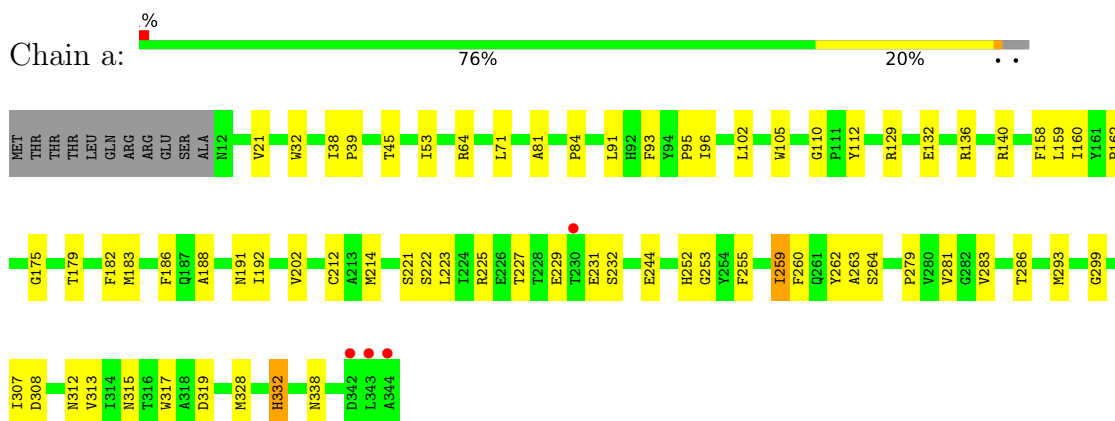
3 Residue-property plots [i](#)

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.

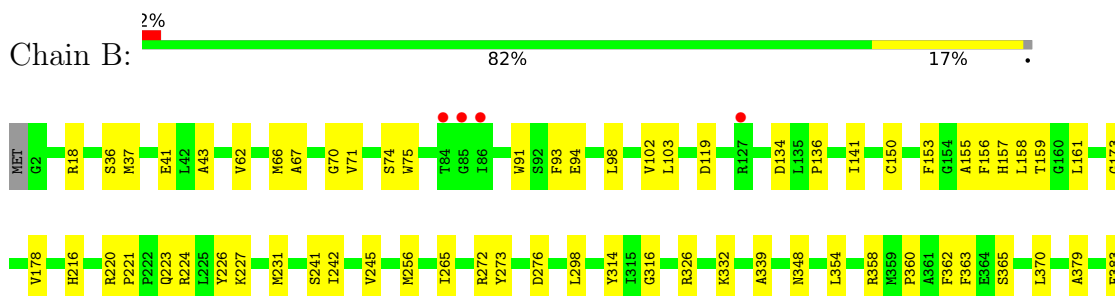
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

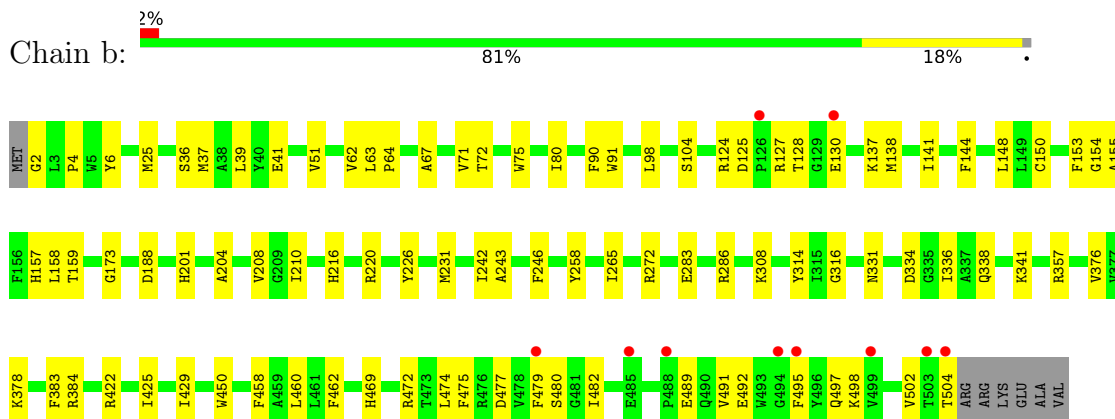


- Molecule 2: Photosystem II CP47 reaction center protein

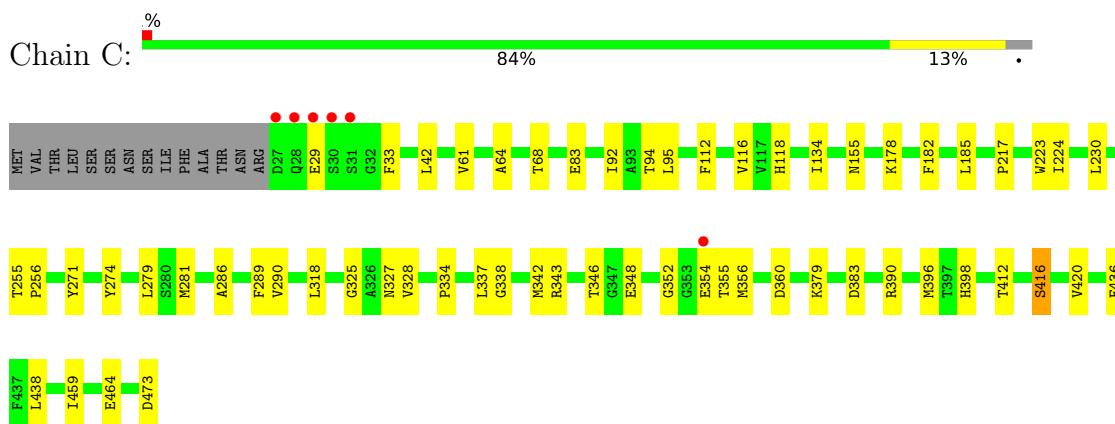




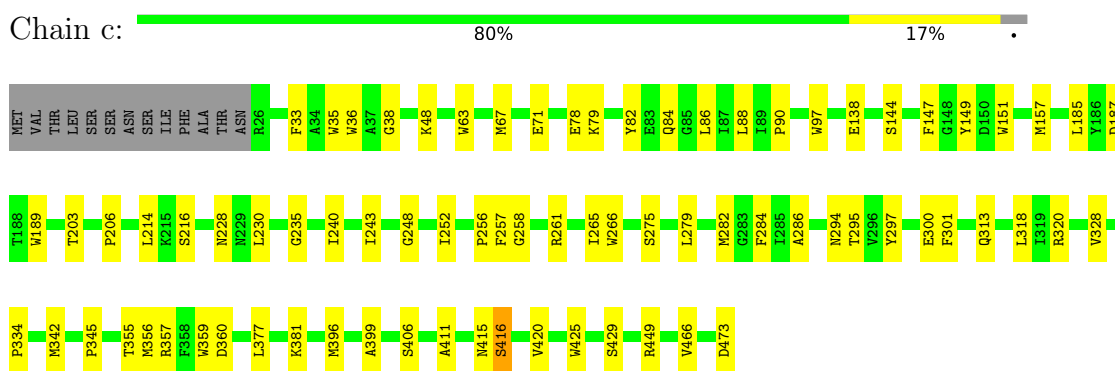
• Molecule 2: Photosystem II CP47 reaction center protein



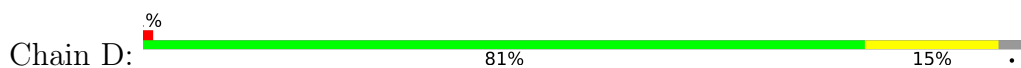
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

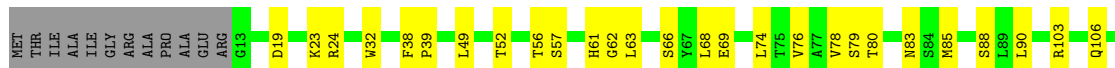


• Molecule 4: Photosystem II D2 protein





● Molecule 4: Photosystem II D2 protein



● Molecule 5: Cytochrome b559 subunit alpha



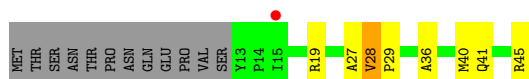
● Molecule 5: Cytochrome b559 subunit alpha



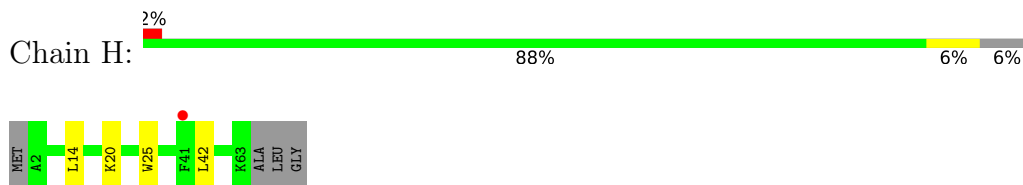
● Molecule 6: Cytochrome b559 subunit beta



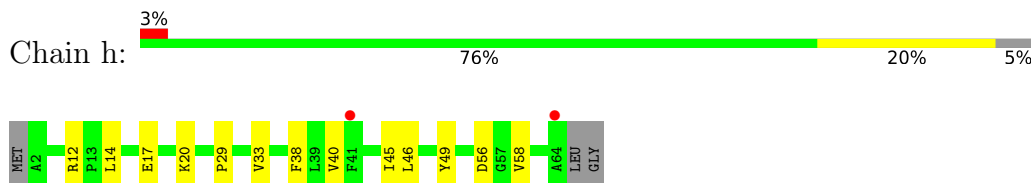
● Molecule 6: Cytochrome b559 subunit beta



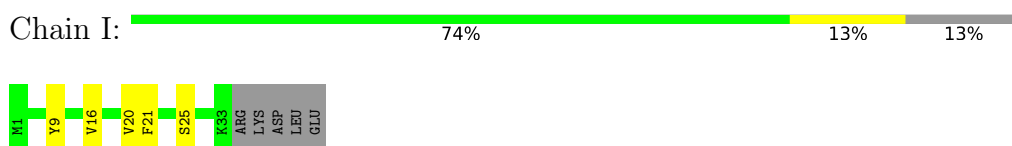
- Molecule 7: Photosystem II reaction center protein H



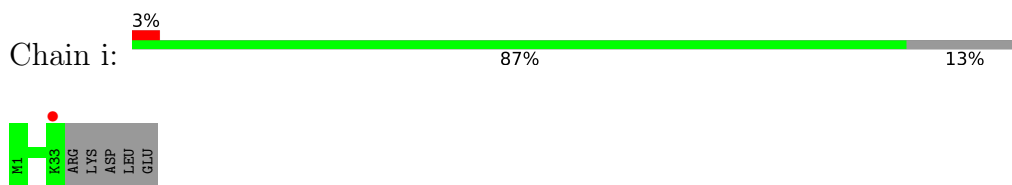
- Molecule 7: Photosystem II reaction center protein H



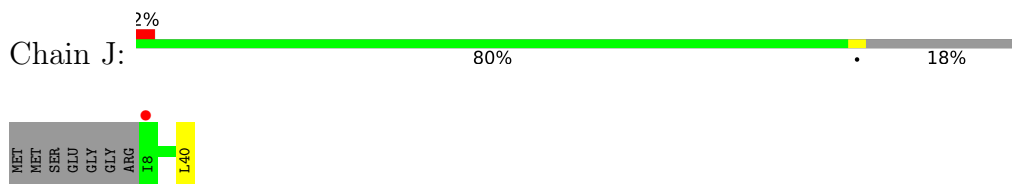
- Molecule 8: Photosystem II reaction center protein I



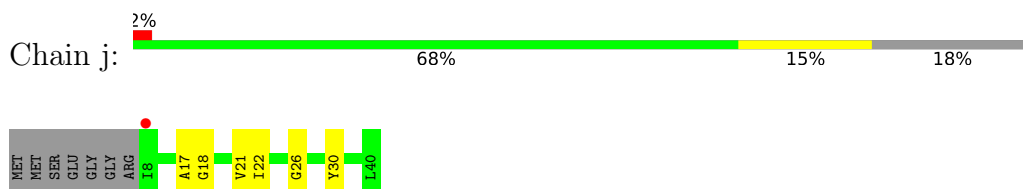
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

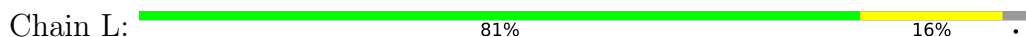




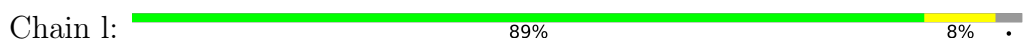
- Molecule 10: Photosystem II reaction center protein K



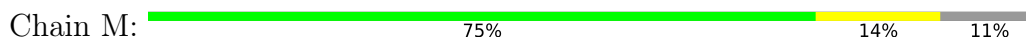
- Molecule 11: Photosystem II reaction center protein L



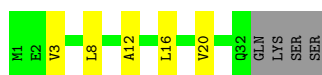
- Molecule 11: Photosystem II reaction center protein L



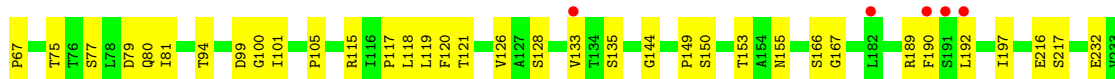
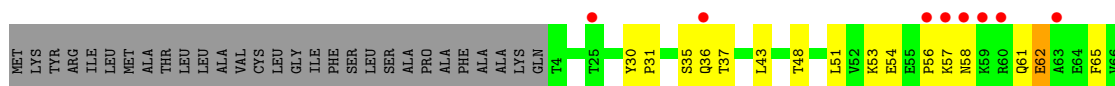
- Molecule 12: Photosystem II reaction center protein M

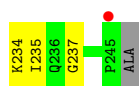


- Molecule 12: Photosystem II reaction center protein M

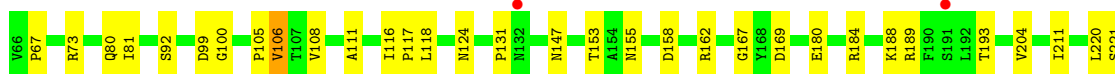


- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 13: Photosystem II manganese-stabilizing polypeptide



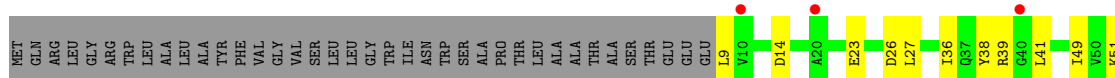
- Molecule 14: Photosystem II reaction center protein T



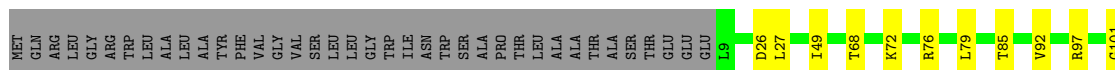
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein

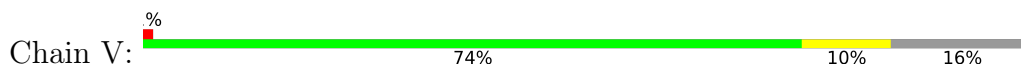


- Molecule 15: Photosystem II 12 kDa extrinsic protein





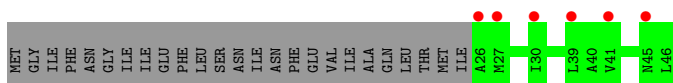
• Molecule 16: Cytochrome c-550



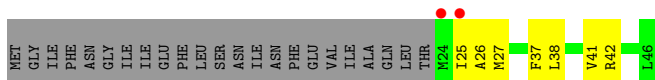
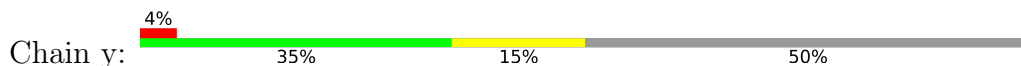
• Molecule 16: Cytochrome c-550



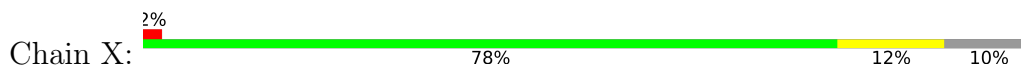
• Molecule 17: Photosystem II reaction center protein Ycf12



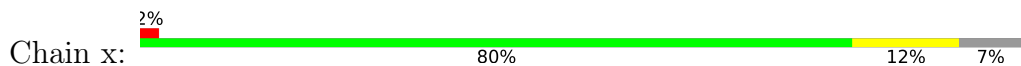
• Molecule 17: Photosystem II reaction center protein Ycf12

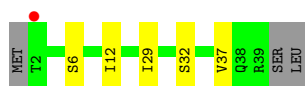


• Molecule 18: Photosystem II reaction center X protein

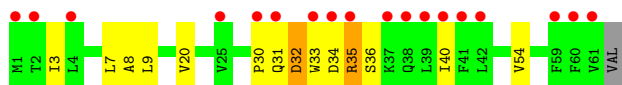
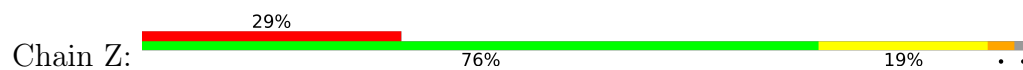


• Molecule 18: Photosystem II reaction center X protein

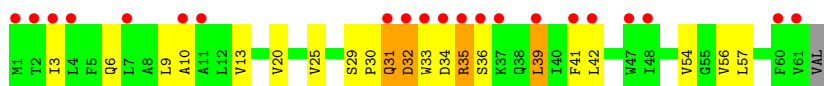




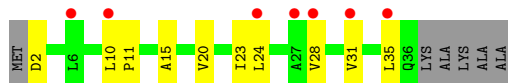
- Molecule 19: Photosystem II reaction center protein Z



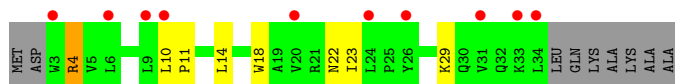
- Molecule 19: Photosystem II reaction center protein Z



- 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	116.33Å 219.62Å 304.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.20 49.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.65-2.20) 92.6 (49.65-2.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.260 0.213 , 0.262	Depositor DCC
R_{free} test set	18229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.673	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50407	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: LMG, CL, LHG, DGD, BCT, BCR, HEC, PHO, FE, PL9, SQD, CLA, HEM, LFA

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	0.50	0/2702	0.51	0/3685
1	a	0.47	0/2702	0.52	0/3685
2	B	0.48	0/4120	0.51	0/5614
2	b	0.46	1/4098 (0.0%)	0.50	0/5586
3	C	0.43	0/3568	0.45	0/4858
3	c	0.44	2/3579 (0.1%)	0.46	0/4872
4	D	0.52	0/2801	0.52	0/3818
4	d	0.47	0/2801	0.51	0/3818
5	E	0.36	0/675	0.43	0/922
5	e	0.49	1/664 (0.2%)	0.47	0/907
6	F	0.36	0/278	0.41	0/379
6	f	0.33	0/278	0.43	0/379
7	H	0.42	0/506	0.48	0/690
7	h	0.37	0/511	0.41	0/697
8	I	0.41	0/273	0.43	0/370
8	i	0.40	0/273	0.41	0/370
9	J	0.37	0/244	0.39	0/332
9	j	0.29	0/244	0.32	0/332
10	K	0.32	0/282	0.42	0/391
10	k	0.34	0/294	0.50	0/405
11	L	0.49	0/303	0.48	0/412
11	l	0.47	0/303	0.48	0/412
12	M	0.47	0/252	0.49	0/344
12	m	0.41	0/252	0.41	0/344
13	O	0.38	0/1890	0.45	0/2564
13	o	0.41	0/1883	0.47	0/2554
14	T	0.50	0/250	0.43	0/338
14	t	0.44	0/258	0.42	0/349
15	U	0.24	0/776	0.37	0/1052
15	u	0.37	0/776	0.45	0/1052
16	V	0.38	0/1085	0.40	0/1473
16	v	0.37	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.22	0/156	0.38	0/207
17	y	0.27	0/172	0.37	0/228
18	X	0.37	0/273	0.33	0/370
18	x	0.25	0/284	0.33	0/384
19	Z	0.27	0/482	0.46	0/659
19	z	0.34	0/482	0.60	1/659 (0.2%)
20	R	0.25	0/288	0.37	0/395
20	r	0.28	0/263	0.57	0/361
All	All	0.44	4/42406 (0.0%)	0.48	1/57740 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
19	z	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	-8.62	1.13	1.33
2	b	2	GLY	C-N	-6.22	1.20	1.33
3	c	399	ALA	C-N	-6.04	1.19	1.33
3	c	78	GLU	C-N	-5.73	1.21	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
19	z	39	LEU	CA-CB-CG	5.72	136.31	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	81	ALA	Peptide
19	z	35	ARG	Peptide

5.2 Too-close contacts [i](#)

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	2617	0	2514	43	0
1	a	2617	0	2514	57	0
2	B	3980	0	3841	65	0
2	b	3958	0	3815	80	0
3	C	3455	0	3376	46	0
3	c	3466	0	3389	71	0
4	D	2706	0	2608	45	0
4	d	2706	0	2608	75	0
5	E	656	0	638	21	0
5	e	645	0	628	22	0
6	F	269	0	277	10	0
6	f	269	0	277	8	0
7	H	493	0	513	4	0
7	h	498	0	518	13	0
8	I	266	0	282	4	0
8	i	266	0	282	0	0
9	J	238	0	249	1	0
9	j	238	0	249	6	0
10	K	272	0	279	5	0
10	k	284	0	292	8	0
11	L	296	0	304	6	0
11	l	296	0	304	2	0
12	M	249	0	268	5	0
12	m	249	0	268	5	0
13	O	1859	0	1833	37	0
13	o	1852	0	1826	39	0
14	T	241	0	244	4	0
14	t	249	0	255	11	0
15	U	765	0	767	13	0
15	u	765	0	767	7	0
16	V	1064	0	1073	13	0
16	v	1064	0	1073	18	0
17	Y	155	0	175	0	0
17	y	171	0	195	4	0
18	X	270	0	299	4	0
18	x	281	0	312	3	0
19	Z	471	0	507	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	471	0	507	17	0
20	R	282	0	313	7	0
20	r	257	0	290	9	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	260	0	288	9	0
22	B	975	0	1080	35	0
22	C	845	0	936	41	0
22	D	130	0	144	6	0
22	H	65	0	72	1	0
22	a	195	0	216	12	0
22	b	1040	0	1152	39	0
22	c	845	0	936	52	0
22	d	195	0	216	7	0
23	A	64	0	74	1	0
23	D	64	0	74	2	0
23	a	128	0	148	5	0
24	A	40	0	56	1	0
24	B	120	0	168	9	0
24	C	80	0	112	5	0
24	D	40	0	56	4	0
24	H	40	0	56	4	0
24	K	80	0	112	5	0
24	T	40	0	56	1	0
24	a	40	0	56	1	0
24	b	120	0	168	6	0
24	c	120	0	168	12	0
24	d	40	0	56	3	0
24	h	40	0	56	6	0
24	k	40	0	56	4	0
24	t	40	0	56	8	0
25	A	55	0	80	6	0
25	D	55	0	80	6	0
25	a	55	0	80	4	0
25	d	55	0	80	3	0
26	A	108	0	156	4	0
26	D	43	0	53	1	0
26	L	48	0	63	4	0
26	a	104	0	153	5	0
26	b	54	0	78	8	0
26	f	43	0	53	2	0
27	A	25	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	99	0	187	9	0
27	C	15	0	29	0	0
27	D	33	0	57	2	0
27	I	14	0	24	0	0
27	J	11	0	18	0	0
27	M	26	0	47	4	0
27	T	12	0	23	0	0
27	a	7	0	10	0	0
27	b	100	0	183	6	0
27	c	24	0	43	3	0
27	d	40	0	77	2	0
27	i	23	0	41	0	0
27	j	15	0	29	4	0
27	m	25	0	45	1	0
27	t	15	0	29	3	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	B	87	0	114	2	0
29	C	143	0	196	9	0
29	D	51	0	72	1	0
29	b	39	0	48	2	0
29	c	143	0	196	14	0
29	f	51	0	72	2	0
29	m	51	0	72	3	0
30	C	180	0	234	7	0
30	H	60	0	78	3	0
30	c	179	0	232	16	0
30	h	62	0	82	7	0
31	D	4	0	0	0	0
31	a	4	0	0	0	0
32	D	147	0	222	19	0
32	E	42	0	57	4	0
32	L	49	0	74	6	0
32	b	49	0	74	2	0
32	d	98	0	148	20	0
32	e	42	0	57	2	0
32	l	49	0	74	1	0
33	E	43	0	30	9	0
33	e	43	0	30	7	0
34	V	43	0	30	2	0
34	v	43	0	30	1	0
35	A	70	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	84	0	0	3	0
35	C	62	0	0	2	0
35	D	72	0	0	2	0
35	E	5	0	0	0	0
35	F	1	0	0	0	0
35	H	17	0	0	1	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	5	0	0	1	0
35	M	3	0	0	0	0
35	O	30	0	0	2	0
35	T	2	0	0	0	0
35	U	2	0	0	0	0
35	V	12	0	0	0	0
35	X	3	0	0	0	0
35	a	77	0	0	5	0
35	b	72	0	0	0	0
35	c	65	0	0	6	0
35	d	51	0	0	2	0
35	e	5	0	0	1	0
35	f	2	0	0	0	0
35	h	3	0	0	0	0
35	l	5	0	0	0	0
35	m	2	0	0	0	0
35	o	25	0	0	4	0
35	t	3	0	0	0	0
35	u	12	0	0	1	0
35	v	11	0	0	3	0
All	All	50407	0	51279	931	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (931) 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)
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.43	0.99
3:c:189:TRP:HE1	3:c:295:THR:HG22	1.36	0.89
2:b:357:ARG:NH2	4:d:337:GLU:O	2.07	0.88
32:D:409:LHG:H352	32:D:409:LHG:H151	1.53	0.88
11:L:7:ARG:NH2	26:L:101:SQD:O8	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:128:THR:HG22	2:b:130:GLU:H	1.40	0.85
4:d:192:THR:HG23	22:d:402:CLA:HBC2	1.60	0.84
15:U:39:ARG:NH2	16:V:60:ALA:O	2.10	0.83
19:z:33:TRP:HA	19:z:36:SER:HB2	1.63	0.80
32:b:628:LHG:O4	4:d:141:TYR:OH	1.99	0.80
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.48	0.79
2:B:91:TRP:HE1	27:B:622:LFA:H32	1.48	0.79
19:Z:31:GLN:O	19:Z:33:TRP:N	2.16	0.78
19:Z:34:ASP:OD1	19:Z:35:ARG:N	2.16	0.78
2:b:124:ARG:O	7:h:12:ARG:NH2	2.17	0.77
13:o:189:ARG:NH2	35:o:303:HOH:O	2.17	0.76
2:B:155:ALA:O	2:B:159:THR:OG1	2.04	0.76
13:O:99:ASP:OD2	13:O:100:GLY:N	2.19	0.76
4:D:144:ILE:O	4:D:147:SER:OG	2.03	0.75
5:E:13:ILE:HG21	33:E:102:HEM:HAD1	1.68	0.75
4:d:103:ARG:HH21	5:e:77:GLU:HG2	1.50	0.74
22:c:504:CLA:H172	22:c:511:CLA:HBB2	1.69	0.74
2:b:155:ALA:O	2:b:159:THR:OG1	2.03	0.73
4:d:79:SER:HA	4:d:172:SER:HB3	1.69	0.73
3:C:217:PRO:HD3	29:C:501:LMG:H332	1.69	0.73
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.52	0.73
1:a:286:THR:OG1	22:a:404:CLA:O1D	2.06	0.72
29:B:619:LMG:HC5	27:t:101:LFA:H141	1.70	0.72
5:e:60:GLN:NE2	5:e:62:SER:O	2.23	0.72
3:c:411:ALA:O	35:c:601:HOH:O	2.07	0.72
5:e:26:THR:HB	33:e:102:HEM:HAB	1.70	0.72
3:C:343:ARG:NH1	13:O:77:SER:O	2.22	0.72
2:B:119:ASP:OD1	35:B:701:HOH:O	2.08	0.71
3:c:228:ASN:HA	3:c:295:THR:HG21	1.73	0.71
3:c:313:GLN:HA	3:c:396:MET:HE3	1.72	0.71
1:A:85:SER:HA	1:A:109:GLY:HA3	1.72	0.71
32:D:407:LHG:H222	12:M:18:PRO:HD3	1.72	0.71
26:a:410:SQD:H251	32:d:407:LHG:H131	1.73	0.71
1:a:315:ASN:ND2	4:d:332:GLN:OE1	2.25	0.70
2:B:156:PHE:HD1	2:B:161:LEU:HD22	1.57	0.70
22:c:511:CLA:H201	10:k:30:VAL:HG22	1.72	0.70
32:d:407:LHG:H382	32:d:407:LHG:H112	1.74	0.70
13:O:94:THR:HG1	13:O:128:SER:HG	1.37	0.70
19:z:56:VAL:HG23	19:z:57:LEU:HD23	1.74	0.69
3:c:240:ILE:HG13	22:c:502:CLA:HAB	1.74	0.69
22:C:504:CLA:H172	22:C:511:CLA:HBB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:BCR:H383	26:L:101:SQD:H111	1.72	0.69
32:D:407:LHG:H351	32:D:407:LHG:H121	1.73	0.69
2:b:39:LEU:HD22	27:b:623:LFA:H92	1.74	0.68
2:b:91:TRP:HE1	27:b:625:LFA:H62	1.57	0.68
10:k:13:GLU:HG3	10:k:14:ALA:N	2.07	0.68
22:c:505:CLA:H191	32:d:407:LHG:H341	1.74	0.68
3:c:318:LEU:HD21	3:c:328:VAL:HG21	1.76	0.68
19:Z:32:ASP:O	19:Z:36:SER:OG	2.10	0.68
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.29	0.68
33:E:102:HEM:HAC	6:F:27:ALA:HB1	1.75	0.68
27:A:413:LFA:H101	2:b:75:TRP:HB3	1.75	0.67
20:r:4:ARG:HH21	20:r:4:ARG:HG3	1.59	0.67
2:B:496:TYR:HB3	2:B:504:THR:HG23	1.77	0.67
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.77	0.67
22:C:502:CLA:HBB1	22:C:502:CLA:H71	1.75	0.67
13:o:111:ALA:O	35:o:301:HOH:O	2.11	0.67
25:a:409:PL9:H502	4:d:39:PRO:HG3	1.75	0.67
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.76	0.67
1:a:299:GLY:O	35:a:501:HOH:O	2.12	0.66
29:c:501:LMG:H242	22:c:506:CLA:H92	1.78	0.66
16:v:83:ASP:OD2	35:v:302:HOH:O	2.12	0.66
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.76	0.66
19:z:34:ASP:OD1	19:z:35:ARG:N	2.25	0.66
4:D:56:THR:HB	5:E:49:THR:HG23	1.76	0.66
5:E:60:GLN:NE2	5:E:62:SER:O	2.29	0.66
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.31	0.66
13:O:75:THR:OG1	35:O:301:HOH:O	2.08	0.66
1:a:332:HIS:NE2	35:a:509:HOH:O	2.29	0.65
3:c:359:TRP:O	35:c:602:HOH:O	2.14	0.65
1:A:308:ASP:OD1	1:A:312:ASN:N	2.29	0.65
13:o:59:LYS:HB3	13:o:61:GLN:OE1	1.97	0.65
4:D:186:GLN:NE2	4:D:322:ASN:OD1	2.24	0.65
32:L:102:LHG:H271	12:M:22:LEU:HD21	1.78	0.65
11:L:2:GLU:O	35:L:201:HOH:O	2.13	0.65
13:o:155:ASN:O	35:o:302:HOH:O	2.14	0.65
14:t:4:ILE:HD13	24:t:102:BCR:H391	1.79	0.65
4:D:344:GLU:OE1	35:D:502:HOH:O	2.14	0.65
26:A:409:SQD:H251	32:D:409:LHG:H131	1.79	0.64
3:c:377:LEU:H	13:o:80:GLN:HE22	1.46	0.64
25:A:408:PL9:H502	4:D:39:PRO:HG3	1.79	0.64
19:Z:31:GLN:C	19:Z:33:TRP:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:THR:HB	33:E:102:HEM:HAB	1.79	0.64
32:E:101:LHG:H132	6:F:23:VAL:HG12	1.79	0.64
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.80	0.64
5:E:67:THR:HB	5:E:75:GLN:HE22	1.64	0.63
1:a:253:GLY:HA3	2:b:491:VAL:HG13	1.80	0.63
2:B:348:ASN:HB3	2:B:354:LEU:HD11	1.80	0.63
3:C:281:MET:HG3	29:C:501:LMG:H412	1.81	0.63
22:C:505:CLA:H201	32:D:409:LHG:H342	1.79	0.63
1:a:231:GLU:O	35:a:503:HOH:O	2.14	0.63
26:a:410:SQD:H272	32:d:407:LHG:H141	1.80	0.63
4:d:56:THR:OG1	4:d:57:SER:N	2.32	0.63
22:C:502:CLA:C3D	22:C:504:CLA:H2	2.29	0.63
22:b:604:CLA:H101	22:b:611:CLA:H18	1.80	0.63
22:c:502:CLA:C3D	22:c:504:CLA:H2	2.28	0.63
2:B:74:SER:OG	2:B:94:GLU:OE2	2.16	0.63
24:c:523:BCR:H363	10:k:31:LEU:HD22	1.79	0.63
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.81	0.63
3:c:279:LEU:HD23	3:c:282:MET:HE3	1.81	0.62
5:e:8:ARG:HD3	5:e:13:ILE:HG12	1.80	0.62
2:b:489:GLU:HA	2:b:492:GLU:HB2	1.81	0.62
32:D:409:LHG:H132	32:D:409:LHG:H372	1.80	0.62
22:b:606:CLA:H43	22:b:607:CLA:H2	1.82	0.62
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.80	0.62
22:c:509:CLA:H92	32:d:407:LHG:H371	1.82	0.62
19:z:36:SER:HA	19:z:39:LEU:CD1	2.29	0.62
32:D:409:LHG:H112	32:D:409:LHG:H382	1.81	0.62
22:b:605:CLA:H193	22:b:611:CLA:H111	1.80	0.62
5:E:7:GLU:N	5:E:7:GLU:OE1	2.30	0.62
18:X:3:ILE:HA	18:X:7:LEU:HD23	1.81	0.62
24:t:102:BCR:HC8	24:t:102:BCR:H311	1.82	0.62
4:D:236:ASN:ND2	4:D:238:THR:OG1	2.32	0.61
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.13	0.61
5:e:25:ILE:HD12	20:r:18:TRP:CD1	2.35	0.61
1:a:338:ASN:N	21:a:403:CL:CL	2.56	0.61
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.82	0.61
22:a:404:CLA:H201	32:d:406:LHG:H321	1.82	0.61
15:u:27:LEU:HD22	15:u:49:ILE:HG21	1.81	0.61
26:b:601:SQD:H121	22:b:616:CLA:H52	1.81	0.61
3:C:223:TRP:CD1	29:C:501:LMG:H331	2.35	0.61
2:b:497:GLN:HB2	2:b:504:THR:OG1	1.99	0.61
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.81	0.61
22:A:403:CLA:H201	32:D:408:LHG:H332	1.82	0.61
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.81	0.60
13:o:61:GLN:OE1	13:o:61:GLN:N	2.31	0.60
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.83	0.60
4:d:199:MET:HG2	25:d:405:PL9:H312	1.84	0.60
33:e:102:HEM:CGD	6:f:19:ARG:HH21	2.14	0.60
17:y:37:PHE:O	17:y:41:VAL:HG23	2.01	0.60
1:A:121:LEU:HD11	22:C:506:CLA:H171	1.82	0.60
2:B:276:ASP:OD1	35:B:702:HOH:O	2.16	0.60
13:o:23:ASP:HB2	13:o:25:THR:HG22	1.83	0.60
4:d:186:GLN:HB2	22:d:402:CLA:HBC1	1.82	0.60
25:A:408:PL9:H261	32:E:101:LHG:H223	1.82	0.60
3:C:29:GLU:CD	3:C:29:GLU:H	2.09	0.60
2:b:141:ILE:HD11	7:h:14:LEU:HD22	1.83	0.60
22:C:511:CLA:H43	32:D:409:LHG:H383	1.84	0.60
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	1.84	0.59
25:D:406:PL9:H311	32:L:102:LHG:H201	1.83	0.59
4:d:66:SER:OG	4:d:69:GLU:OE2	2.20	0.59
3:c:67:MET:HE2	10:k:26:PRO:HB3	1.85	0.59
1:a:140:ARG:HH22	32:d:407:LHG:HC42	1.68	0.59
5:E:58:GLN:NE2	16:V:2:GLU:O	2.29	0.59
2:b:383:PHE:N	4:d:344:GLU:O	2.35	0.59
12:M:24:ILE:HD13	27:M:102:LFA:H111	1.85	0.59
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.85	0.59
3:C:396:MET:HE3	16:V:48:THR:HG22	1.85	0.59
3:C:155:ASN:HD22	3:C:255:THR:HG22	1.67	0.58
16:v:38:ALA:O	16:v:42:VAL:HG13	2.03	0.58
2:B:62:VAL:HB	22:B:604:CLA:HED3	1.86	0.58
13:O:36:GLN:OE1	13:O:37:THR:N	2.36	0.58
2:b:475:PHE:HB2	2:b:479:PHE:HE2	1.68	0.58
13:o:59:LYS:CB	13:o:61:GLN:OE1	2.52	0.58
19:z:34:ASP:CG	19:z:35:ARG:H	2.11	0.58
22:b:616:CLA:H161	29:m:103:LMG:H422	1.85	0.58
2:B:256:MET:HG3	2:B:448:ARG:HG3	1.84	0.58
3:C:95:LEU:HD13	22:C:503:CLA:H142	1.86	0.58
4:d:312:GLU:OE1	4:d:317:LYS:NZ	2.36	0.58
1:A:283:VAL:HG21	23:D:402:PHO:HBC3	1.86	0.58
2:B:67:ALA:HA	2:B:71:VAL:O	2.02	0.58
3:c:256:PRO:HA	22:c:507:CLA:HED2	1.85	0.58
22:C:502:CLA:H203	22:C:508:CLA:H13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:LYS:NZ	2:B:438:ASN:O	2.30	0.58
4:D:56:THR:OG1	4:D:57:SER:N	2.36	0.58
24:C:516:BCR:HC41	8:I:20:VAL:HG13	1.85	0.58
3:c:473:ASP:OXT	14:t:28:ARG:NH1	2.36	0.58
22:c:508:CLA:H142	24:c:515:BCR:H362	1.86	0.57
4:D:24:ARG:HH11	18:X:37:VAL:HG12	1.68	0.57
25:a:409:PL9:H453	26:f:102:SQD:H261	1.86	0.57
6:f:41:GLN:OE1	29:f:101:LMG:O4	2.16	0.57
27:B:623:LFA:H22	1:a:102:LEU:HD12	1.85	0.57
4:D:126:MET:HE3	4:D:143:ALA:O	2.05	0.57
13:O:153:THR:HA	13:O:190:PHE:HE2	1.69	0.57
3:c:429:SER:HB3	30:c:517:DGD:HBT2	1.85	0.57
4:d:83:ASN:OD1	4:d:166:SER:OG	2.20	0.57
5:E:26:THR:HB	33:E:102:HEM:CAB	2.35	0.57
22:b:607:CLA:H8	22:b:614:CLA:H191	1.87	0.56
29:c:519:LMG:H301	29:c:519:LMG:H181	1.87	0.56
12:m:12:ALA:HA	27:t:101:LFA:H13	1.88	0.56
32:D:409:LHG:H361	32:D:409:LHG:H121	1.85	0.56
16:v:86:GLN:NE2	35:v:304:HOH:O	2.38	0.56
29:C:522:LMG:O2	29:C:522:LMG:HC71	2.05	0.56
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.88	0.56
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.88	0.56
1:a:160:ILE:HD11	30:c:516:DGD:HBE1	1.88	0.55
15:u:76:ARG:HA	15:u:79:LEU:HG	1.88	0.55
2:b:231:MET:HE2	22:b:612:CLA:HMC1	1.88	0.55
3:c:360:ASP:O	30:c:516:DGD:O2E	2.17	0.55
4:d:68:LEU:HD13	6:f:40:MET:HE2	1.88	0.55
12:m:8:LEU:HD11	27:t:101:LFA:H52	1.88	0.55
2:B:37:MET:O	2:B:41:GLU:HG3	2.06	0.55
15:u:26:ASP:OD2	15:u:85:THR:OG1	2.21	0.55
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.42	0.55
3:c:82:TYR:O	35:c:603:HOH:O	2.18	0.55
13:o:169:ASP:OD1	13:o:169:ASP:N	2.40	0.55
1:a:140:ARG:NH2	32:d:407:LHG:HC42	2.22	0.55
22:a:404:CLA:H51	23:a:406:PHO:C3B	2.36	0.55
22:b:604:CLA:H42	30:h:102:DGD:HB51	1.89	0.55
1:A:325:ASN:HA	1:A:328:MET:HE3	1.89	0.55
5:E:13:ILE:HG21	33:E:102:HEM:CAD	2.36	0.55
2:b:472:ARG:HA	2:b:479:PHE:CE2	2.41	0.55
3:c:334:PRO:HA	13:o:153:THR:OG1	2.07	0.55
22:c:503:CLA:HBB2	22:c:511:CLA:H151	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.89	0.55
2:B:216:HIS:CE1	22:B:608:CLA:NA	2.75	0.55
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.89	0.55
20:r:4:ARG:HH21	20:r:4:ARG:CG	2.19	0.55
13:o:106:VAL:HG13	13:o:118:LEU:HG	1.89	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.55
1:a:283:VAL:HA	1:a:286:THR:HG22	1.88	0.55
22:a:405:CLA:H172	14:t:10:PHE:HE1	1.72	0.55
4:D:79:SER:HA	4:D:172:SER:HB3	1.89	0.54
32:D:408:LHG:H322	14:T:21:ILE:HD11	1.88	0.54
19:z:33:TRP:HA	19:z:36:SER:CB	2.34	0.54
16:v:87:GLU:OE2	16:v:96:ARG:NH1	2.38	0.54
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.42	0.54
3:c:248:GLY:O	3:c:252:ILE:HG13	2.07	0.54
22:c:512:CLA:H171	19:z:20:VAL:HA	1.89	0.54
3:C:473:ASP:OD2	35:C:601:HOH:O	2.18	0.54
27:M:101:LFA:H82	26:b:601:SQD:H252	1.90	0.54
19:z:3:ILE:O	19:z:6:GLN:HG2	2.08	0.54
2:B:98:LEU:HD12	27:B:626:LFA:H22	1.89	0.54
13:o:28:GLY:O	35:o:304:HOH:O	2.18	0.54
1:a:263:ALA:HA	32:e:101:LHG:H272	1.88	0.54
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.89	0.54
4:D:302:GLU:OE1	4:D:315:TYR:OH	2.11	0.54
13:O:197:ILE:HG13	13:O:217:SER:HB3	1.90	0.54
3:c:286:ALA:HB2	22:c:503:CLA:HMD1	1.89	0.54
33:E:102:HEM:CAC	6:F:27:ALA:HB1	2.37	0.54
2:b:98:LEU:HD13	27:b:626:LFA:H101	1.90	0.54
3:C:64:ALA:O	3:C:68:THR:OG1	2.25	0.54
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.43	0.54
16:V:28:GLU:OE1	16:V:31:ARG:NH2	2.33	0.54
3:c:406:SER:HA	3:c:420:VAL:HG23	1.89	0.54
7:h:38:PHE:HD2	24:h:101:BCR:H311	1.73	0.54
13:o:124:ASN:HD22	13:o:147:ASN:HB2	1.73	0.54
15:U:92:VAL:HG12	15:U:97:ARG:HD2	1.89	0.53
4:d:24:ARG:HE	18:x:37:VAL:HG22	1.73	0.53
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.17	0.53
3:c:415:ASN:O	3:c:416:SER:OG	2.20	0.53
20:R:2:ASP:OD1	20:R:2:ASP:N	2.40	0.53
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.56	0.53
4:D:103:ARG:NH2	5:E:77:GLU:HG2	2.19	0.53
2:B:385:ARG:NH2	15:U:14:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:26:VAL:HG21	32:L:102:LHG:H192	1.90	0.53
4:d:350:ASN:O	4:d:352:LEU:N	2.35	0.53
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.91	0.53
1:A:332:HIS:NE2	35:A:508:HOH:O	2.33	0.53
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	1.89	0.53
22:B:603:CLA:H93	22:B:604:CLA:HAB	1.91	0.53
1:a:227:THR:HB	1:a:231:GLU:HG3	1.90	0.53
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.90	0.53
4:D:87:HIS:ND1	30:H:103:DGD:O2D	2.33	0.53
3:c:67:MET:HE1	22:c:505:CLA:CHD	2.39	0.53
13:O:35:SER:O	13:O:35:SER:OG	2.27	0.52
1:a:132:GLU:O	1:a:136:ARG:HG2	2.10	0.52
2:b:475:PHE:HB2	2:b:479:PHE:CE2	2.43	0.52
2:B:339:ALA:HB2	13:o:58:ASN:HD21	1.74	0.52
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.44	0.52
30:c:517:DGD:O5E	29:c:519:LMG:O3	2.14	0.52
2:B:141:ILE:HD11	7:H:14:LEU:HD22	1.92	0.52
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.43	0.52
3:C:438:LEU:HD11	22:C:506:CLA:HBB1	1.90	0.52
1:a:229:GLU:CD	1:a:229:GLU:H	2.16	0.52
23:a:414:PHO:HBC3	4:d:279:LEU:HD22	1.91	0.52
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.91	0.52
20:r:18:TRP:O	20:r:22:ASN:ND2	2.36	0.52
2:B:216:HIS:HE1	22:B:608:CLA:C1A	2.22	0.52
13:O:149:PRO:HA	13:O:192:LEU:HD12	1.92	0.52
22:a:407:CLA:H193	22:c:506:CLA:H13	1.92	0.52
2:b:283:GLU:OE2	2:b:286:ARG:NH2	2.43	0.52
3:c:466:VAL:HG13	4:d:251:ARG:HD2	1.90	0.52
3:C:223:TRP:CG	3:C:224:ILE:H	2.28	0.52
16:V:93:PRO:HG3	16:V:101:PHE:CD1	2.45	0.52
1:a:45:THR:HG21	26:a:412:SQD:H221	1.90	0.52
17:y:38:LEU:O	17:y:42:ARG:HD2	2.09	0.52
32:D:408:LHG:HC62	11:L:15:THR:HG23	1.91	0.52
18:X:2:THR:OG1	18:X:3:ILE:N	2.43	0.52
27:B:624:LFA:H62	27:D:413:LFA:H31	1.90	0.52
2:b:458:PHE:HB3	22:b:606:CLA:HBC2	1.92	0.52
10:K:17:ILE:HD12	10:K:17:ILE:H	1.75	0.51
2:b:128:THR:HG21	2:b:130:GLU:HG2	1.92	0.51
3:c:206:PRO:HD3	29:c:522:LMG:HC91	1.91	0.51
3:c:216:SER:HB2	29:c:501:LMG:HC71	1.92	0.51
3:c:279:LEU:HD12	22:c:510:CLA:HED2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:519:LMG:H141	29:c:519:LMG:H292	1.92	0.51
1:A:202:VAL:HG11	22:A:404:CLA:C3D	2.41	0.51
25:D:406:PL9:H401	32:D:408:LHG:H211	1.92	0.51
4:d:103:ARG:NH2	5:e:77:GLU:HG2	2.23	0.51
10:K:40:GLN:HA	10:K:43:VAL:HG22	1.92	0.51
26:b:601:SQD:H81	24:b:619:BCR:H383	1.92	0.51
13:o:99:ASP:OD1	13:o:100:GLY:N	2.34	0.51
26:L:101:SQD:H292	27:m:101:LFA:H142	1.93	0.51
4:d:56:THR:HG22	35:e:201:HOH:O	2.10	0.51
25:A:408:PL9:H261	32:E:101:LHG:H191	1.93	0.51
29:c:501:LMG:H381	30:c:516:DGD:HB41	1.92	0.51
22:c:502:CLA:C4D	22:c:504:CLA:H2	2.41	0.51
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.37	0.51
27:M:101:LFA:H102	26:b:601:SQD:H261	1.92	0.51
2:b:62:VAL:HB	22:b:607:CLA:HED3	1.93	0.51
4:d:291:LEU:HD21	30:h:102:DGD:HBN1	1.93	0.51
32:d:406:LHG:HC62	11:l:15:THR:HG23	1.93	0.51
2:b:216:HIS:HE1	22:b:611:CLA:C1A	2.24	0.51
3:c:147:PHE:CD2	22:c:514:CLA:H3A	2.46	0.51
2:b:201:HIS:HB2	22:b:604:CLA:CHB	2.41	0.51
3:c:265:ILE:HG13	3:c:449:ARG:HD3	1.92	0.51
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.45	0.51
9:j:17:ALA:O	9:j:21:VAL:HG23	2.10	0.51
20:R:28:VAL:HA	20:R:31:VAL:HG12	1.93	0.51
22:C:514:CLA:HBB1	22:C:514:CLA:HMB1	1.93	0.51
3:c:33:PHE:HE2	22:c:509:CLA:HED1	1.75	0.51
3:c:149:TYR:CZ	22:c:510:CLA:H191	2.45	0.51
22:c:505:CLA:H72	30:c:517:DGD:HBF1	1.93	0.51
19:z:31:GLN:O	19:z:33:TRP:N	2.44	0.50
3:C:325:GLY:O	15:U:51:LYS:NZ	2.45	0.50
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.93	0.50
22:B:606:CLA:C4B	29:B:619:LMG:H142	2.42	0.50
2:b:25:MET:HE3	24:b:619:BCR:H23C	1.94	0.50
5:e:9:PRO:O	5:e:13:ILE:HG13	2.11	0.50
19:z:32:ASP:O	19:z:36:SER:OG	2.26	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.47	0.50
22:c:512:CLA:H202	24:k:101:BCR:H17C	1.93	0.50
4:d:141:TYR:HA	4:d:144:ILE:HD12	1.93	0.50
1:A:56:PRO:HB2	13:O:115:ARG:NH2	2.26	0.50
1:A:138:GLY:O	35:A:501:HOH:O	2.20	0.50
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:64:ARG:NH1	13:o:105:PRO:O	2.45	0.50
3:c:300:GLU:OE2	35:c:604:HOH:O	2.19	0.50
5:e:60:GLN:HG2	5:e:62:SER:H	1.76	0.50
22:B:607:CLA:HHC	22:B:607:CLA:HBB1	1.93	0.50
2:b:37:MET:O	2:b:41:GLU:HG3	2.11	0.50
2:b:242:ILE:HG23	2:b:462:PHE:CD2	2.40	0.50
2:b:331:ASN:ND2	2:b:336:ILE:HG12	2.27	0.50
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.93	0.50
32:D:407:LHG:H351	32:D:407:LHG:H101	1.93	0.50
16:V:92:HIS:CD2	34:V:201:HEC:ND	2.79	0.50
22:c:505:CLA:H51	30:c:518:DGD:HB72	1.93	0.50
22:d:401:CLA:HMB1	22:d:401:CLA:HBB1	1.93	0.50
2:B:98:LEU:O	2:B:102:VAL:HG23	2.12	0.50
3:C:134:ILE:HG21	22:C:512:CLA:H43	1.92	0.50
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.47	0.50
22:C:514:CLA:H61	24:C:515:BCR:H281	1.93	0.49
13:O:53:LYS:NZ	13:O:232:GLU:OE1	2.39	0.49
2:b:314:TYR:CZ	2:b:316:GLY:HA3	2.46	0.49
1:a:183:MET:HB3	22:a:404:CLA:HBC2	1.94	0.49
22:B:604:CLA:H8	22:B:611:CLA:H191	1.93	0.49
22:B:607:CLA:H162	22:D:404:CLA:H3A	1.94	0.49
2:B:156:PHE:CD1	2:B:161:LEU:HD22	2.43	0.49
22:B:601:CLA:H101	22:B:608:CLA:H18	1.94	0.49
8:I:21:PHE:O	8:I:25:SER:OG	2.26	0.49
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.93	0.49
4:d:352:LEU:O	16:v:134:LYS:NZ	2.37	0.49
27:d:410:LFA:H22	18:x:12:ILE:HD13	1.95	0.49
2:B:36:SER:OG	24:B:617:BCR:H362	2.13	0.49
2:B:157:HIS:HE1	22:B:605:CLA:NA	2.10	0.49
24:H:102:BCR:H331	24:H:102:BCR:C8	2.42	0.49
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.48	0.49
33:E:102:HEM:HBA2	20:R:23:ILE:HD13	1.95	0.49
15:U:76:ARG:HA	15:U:79:LEU:HG	1.94	0.49
3:c:97:TRP:CE2	27:c:521:LFA:H52	2.48	0.49
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.48	0.49
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.47	0.49
22:C:509:CLA:H92	32:D:409:LHG:H371	1.93	0.49
3:c:33:PHE:CE2	22:c:509:CLA:HED1	2.47	0.49
22:c:505:CLA:H151	22:c:509:CLA:H143	1.93	0.49
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.47	0.49
1:A:261:GLN:HB3	2:B:493:TRP:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:522:LMG:H121	29:C:522:LMG:O10	2.12	0.49
4:D:24:ARG:HB2	4:D:26:ARG:NH2	2.27	0.49
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.94	0.49
22:c:511:CLA:H43	32:d:407:LHG:H383	1.94	0.49
1:A:284:TRP:O	1:A:288:LEU:HG	2.13	0.48
14:T:20:ALA:O	14:T:24:ARG:HB3	2.12	0.48
2:b:104:SER:OG	26:b:601:SQD:H223	2.12	0.48
2:b:272:ARG:NH1	4:d:164:GLN:HA	2.27	0.48
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.48
22:C:512:CLA:H143	19:Z:20:VAL:HG13	1.95	0.48
4:D:274:VAL:HG22	25:D:406:PL9:H222	1.96	0.48
22:d:403:CLA:H193	7:h:40:VAL:HG11	1.95	0.48
30:C:519:DGD:HBN2	32:D:409:LHG:H211	1.95	0.48
22:c:514:CLA:C4B	24:c:524:BCR:H383	2.43	0.48
2:B:472:ARG:O	2:B:476:ARG:HB2	2.13	0.48
2:b:188:ASP:OD1	7:h:58:VAL:HA	2.12	0.48
3:c:88:LEU:HB3	22:c:504:CLA:HED3	1.95	0.48
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.95	0.48
29:C:520:LMG:H192	10:K:27:VAL:HG11	1.95	0.48
11:L:26:VAL:HG11	32:L:102:LHG:H212	1.95	0.48
3:c:35:TRP:CZ2	27:c:520:LFA:H112	2.48	0.48
32:d:407:LHG:H372	32:d:407:LHG:H142	1.96	0.48
2:B:221:PRO:HA	22:B:608:CLA:HED3	1.96	0.48
3:C:338:GLY:N	35:C:605:HOH:O	2.42	0.48
1:a:307:ILE:HD13	1:a:313:VAL:HA	1.96	0.48
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.96	0.48
22:a:407:CLA:H143	22:c:506:CLA:H193	1.95	0.48
4:d:154:VAL:HG21	30:h:102:DGD:HAF1	1.95	0.48
6:f:36:ALA:O	6:f:40:MET:HG3	2.14	0.48
22:B:606:CLA:H203	32:D:407:LHG:H142	1.95	0.48
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.96	0.48
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.94	0.48
1:A:72:LEU:HD11	27:b:623:LFA:H82	1.95	0.48
13:O:36:GLN:O	35:O:302:HOH:O	2.20	0.48
1:a:223:LEU:HD13	4:d:265:ARG:HD3	1.96	0.48
1:a:225:ARG:HD3	2:b:480:SER:HB2	1.94	0.48
1:A:173:PRO:HB2	1:A:178:GLY:HA3	1.95	0.48
22:C:502:CLA:C2D	22:C:504:CLA:H2	2.44	0.48
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.48	0.48
33:e:102:HEM:C3C	6:f:27:ALA:HB1	2.49	0.48
22:A:412:CLA:H2	23:D:402:PHO:C2B	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.48	0.47
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.96	0.47
13:o:117:PRO:O	13:o:221:SER:HB2	2.14	0.47
26:D:412:SQD:H242	6:F:21:VAL:HG21	1.96	0.47
12:M:20:VAL:HG11	12:m:20:VAL:HB	1.95	0.47
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.96	0.47
2:B:422:ARG:O	2:B:425:ILE:HG12	2.15	0.47
24:B:617:BCR:H381	24:t:102:BCR:H341	1.96	0.47
5:e:26:THR:HB	33:e:102:HEM:CAB	2.42	0.47
29:c:519:LMG:H151	17:y:25:ILE:HD11	1.96	0.47
7:h:49:TYR:CD2	30:h:102:DGD:HB31	2.49	0.47
5:E:10:PHE:CE1	33:E:102:HEM:HBD2	2.48	0.47
13:O:155:ASN:ND2	15:U:100:ASN:O	2.45	0.47
3:c:63:TRP:HE1	3:c:67:MET:HE3	1.79	0.47
4:d:319:LEU:O	4:d:323:GLU:HG3	2.15	0.47
13:o:53:LYS:HB2	13:o:65:PHE:CE2	2.49	0.47
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.49	0.47
22:a:407:CLA:H43	22:c:506:CLA:H191	1.97	0.47
24:h:101:BCR:C8	24:h:101:BCR:H331	2.45	0.47
10:k:43:VAL:O	10:k:46:ARG:HG3	2.14	0.47
16:v:92:HIS:CD2	34:v:201:HEC:ND	2.82	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.47
22:B:604:CLA:HBB1	22:B:605:CLA:H51	1.97	0.47
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.50	0.47
24:D:405:BCR:H363	6:F:33:PHE:HB3	1.97	0.47
5:E:36:LEU:HA	5:E:39:SER:OG	2.15	0.47
25:a:409:PL9:H28	25:a:409:PL9:H322	1.69	0.47
2:b:220:ARG:NH2	7:h:17:GLU:O	2.48	0.47
22:c:504:CLA:HAB	27:c:521:LFA:H141	1.97	0.47
30:c:518:DGD:HB22	30:c:518:DGD:HB52	1.64	0.47
4:d:49:LEU:HD13	24:d:404:BCR:C15	2.45	0.47
4:d:61:HIS:CD2	4:d:79:SER:HB3	2.50	0.47
19:z:35:ARG:O	19:z:39:LEU:HD12	2.15	0.47
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.96	0.47
1:A:172:MET:SD	1:A:179:THR:HG23	2.55	0.47
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.80	0.47
4:D:85:MET:HA	5:E:69:ARG:HG3	1.96	0.47
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.50	0.47
3:C:318:LEU:HD21	3:C:328:VAL:HG21	1.97	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.47
3:c:257:PHE:O	3:c:261:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:404:BCR:H15C	24:d:404:BCR:H351	1.70	0.47
33:e:102:HEM:CAC	6:f:27:ALA:HB1	2.44	0.47
12:m:12:ALA:O	12:m:16:LEU:HG	2.15	0.47
3:c:313:GLN:HA	3:c:396:MET:CE	2.42	0.47
16:v:55:ARG:NH2	16:v:132:GLY:HA2	2.30	0.47
3:C:420:VAL:N	30:C:518:DGD:O3E	2.32	0.46
24:H:102:BCR:H24C	24:H:102:BCR:H371	1.75	0.46
19:Z:36:SER:O	19:Z:40:ILE:HG13	2.15	0.46
2:b:460:LEU:HG	4:d:280:TRP:CZ3	2.50	0.46
3:c:275:SER:HB3	22:c:510:CLA:HED3	1.97	0.46
5:e:18:ARG:NH1	33:e:102:HEM:O2A	2.42	0.46
22:C:512:CLA:H171	19:Z:20:VAL:HA	1.96	0.46
23:a:414:PHO:HBC1	4:d:275:PRO:HB2	1.97	0.46
4:d:274:VAL:HG22	25:d:405:PL9:H222	1.96	0.46
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.97	0.46
2:b:258:TYR:CE2	30:h:102:DGD:HG12	2.50	0.46
2:b:469:HIS:CE1	22:b:613:CLA:NA	2.83	0.46
5:e:73:LYS:O	5:e:77:GLU:HG3	2.15	0.46
22:B:603:CLA:H43	22:B:604:CLA:H2	1.97	0.46
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.96	0.46
16:V:36:ALA:HB3	34:V:201:HEC:HBB1	1.97	0.46
1:a:202:VAL:HG11	22:d:401:CLA:C3D	2.46	0.46
22:b:609:CLA:H42	29:m:103:LMG:H311	1.97	0.46
22:c:507:CLA:H13	22:c:507:CLA:H192	1.97	0.46
13:O:79:ASP:OD1	13:O:80:GLN:N	2.42	0.46
1:a:21:VAL:HG11	1:a:32:TRP:CE3	2.49	0.46
29:c:501:LMG:H211	30:c:516:DGD:HA72	1.97	0.46
4:d:143:ALA:N	35:d:502:HOH:O	2.28	0.46
13:o:51:LEU:HD23	13:o:67:PRO:HA	1.97	0.46
4:d:56:THR:HG21	5:e:50:PRO:HD3	1.97	0.46
5:e:13:ILE:HG21	33:e:102:HEM:HAD1	1.98	0.46
16:v:57:GLU:O	16:v:61:LEU:HD12	2.15	0.46
25:A:408:PL9:H151	25:A:408:PL9:H171	1.54	0.46
2:b:286:ARG:HG2	2:b:286:ARG:HH11	1.79	0.46
22:b:615:CLA:H51	32:b:628:LHG:H361	1.98	0.46
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.97	0.46
32:d:406:LHG:H291	14:t:17:PHE:CE1	2.51	0.46
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.97	0.46
22:C:511:CLA:HMB1	22:C:511:CLA:HBB1	1.98	0.46
26:f:102:SQD:H362	26:f:102:SQD:H332	1.49	0.46
13:o:158:ASP:OD2	13:o:162:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:41:HIS:HA	16:v:45:ILE:O	2.15	0.46
22:B:602:CLA:C4D	22:B:604:CLA:H43	2.46	0.46
13:O:61:GLN:HG2	13:O:62:GLU:N	2.31	0.46
1:a:262:TYR:CD2	32:e:101:LHG:HC5	2.51	0.46
22:b:607:CLA:H62	22:b:607:CLA:H41	1.73	0.46
22:b:616:CLA:H62	22:b:616:CLA:H41	1.55	0.46
22:c:514:CLA:H61	24:c:524:BCR:H271	1.98	0.46
32:d:407:LHG:H121	32:d:407:LHG:H361	1.98	0.46
19:z:25:VAL:O	19:z:29:SER:OG	2.20	0.46
3:C:342:MET:SD	3:C:356:MET:HE2	2.56	0.45
22:C:506:CLA:H141	8:I:16:VAL:HG22	1.97	0.45
13:O:51:LEU:HD23	13:O:67:PRO:HA	1.97	0.45
1:a:244:GLU:HG2	4:d:242:GLU:HA	1.98	0.45
1:a:308:ASP:OD1	1:a:312:ASN:N	2.48	0.45
2:b:138:MET:HE3	22:b:617:CLA:CHD	2.46	0.45
22:b:605:CLA:H62	22:b:605:CLA:H41	1.84	0.45
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.96	0.45
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.81	0.45
3:c:151:TRP:HA	3:c:157:MET:HE3	1.97	0.45
20:r:10:LEU:HB3	20:r:11:PRO:HD3	1.98	0.45
1:A:322:ASN:OD1	3:C:412:THR:HA	2.16	0.45
22:B:604:CLA:H8	22:B:611:CLA:C19	2.46	0.45
3:C:390:ARG:HD3	16:V:90:GLU:O	2.17	0.45
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.97	0.45
24:a:408:BCR:H15C	24:a:408:BCR:H351	1.81	0.45
2:b:314:TYR:OH	2:b:334:ASP:OD2	2.28	0.45
22:c:511:CLA:HBB1	22:c:511:CLA:HMB1	1.98	0.45
17:y:26:ALA:HB3	17:y:27:MET:HE2	1.98	0.45
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.98	0.45
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.45
2:b:75:TRP:CH2	27:b:622:LFA:H41	2.52	0.45
22:c:505:CLA:H43	30:c:518:DGD:HB51	1.99	0.45
22:B:613:CLA:H92	22:B:613:CLA:H61	1.80	0.45
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.32	0.45
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.99	0.45
15:U:27:LEU:HD22	15:U:49:ILE:HG21	1.98	0.45
9:j:30:TYR:HA	27:j:101:LFA:H62	1.98	0.45
22:C:508:CLA:HAA2	22:C:508:CLA:HBD	1.99	0.45
15:U:70:ARG:O	15:U:74:ILE:HG13	2.17	0.45
2:b:4:PRO:HB3	2:b:6:TYR:CE1	2.52	0.45
3:c:294:ASN:HA	3:c:297:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:32:TRP:CD2	27:d:409:LFA:H32	2.51	0.45
19:z:10:ALA:O	19:z:13:VAL:HG22	2.17	0.45
1:A:270:SER:OG	26:A:409:SQD:O49	2.22	0.45
22:C:503:CLA:H61	22:C:513:CLA:H42	1.99	0.45
1:a:21:VAL:HG11	1:a:32:TRP:CZ3	2.52	0.45
1:a:221:SER:O	4:d:138:VAL:HB	2.16	0.45
1:a:223:LEU:HD22	4:d:265:ARG:HG2	1.98	0.45
1:a:232:SER:OG	32:l:101:LHG:O5	2.13	0.45
26:b:601:SQD:H181	26:b:601:SQD:H212	1.81	0.45
4:d:126:MET:HE3	4:d:143:ALA:O	2.16	0.45
32:d:406:LHG:H331	14:t:21:ILE:HD11	1.98	0.45
5:e:60:GLN:HE21	5:e:62:SER:HB2	1.81	0.45
22:B:607:CLA:HBB2	4:D:123:ILE:HG12	1.99	0.45
13:O:216:GLU:OE1	13:O:234:LYS:HD3	2.17	0.45
2:b:383:PHE:CE1	13:o:167:GLY:HA2	2.51	0.45
4:d:223:PHE:CZ	4:d:245:SER:HB2	2.51	0.45
7:h:49:TYR:CE2	30:h:102:DGD:HB31	2.51	0.45
13:o:92:SER:HB3	13:o:131:PRO:HA	1.98	0.45
13:o:188:LYS:HD2	13:o:225:MET:HE3	1.99	0.45
16:v:93:PRO:HG3	16:v:101:PHE:CD1	2.51	0.45
22:A:406:CLA:H203	22:C:507:CLA:H101	1.99	0.45
9:J:40:LEU:OXT	16:V:30:LYS:NZ	2.43	0.45
10:K:25:LEU:HD21	24:K:101:BCR:HC41	1.99	0.45
29:D:410:LMG:H161	29:D:410:LMG:H192	1.68	0.45
3:c:71:GLU:OE1	3:c:86:LEU:HB3	2.18	0.45
3:c:275:SER:OG	22:c:510:CLA:OBD	2.26	0.45
13:o:26:ALA:C	13:o:27:ARG:HD2	2.41	0.45
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.32	0.44
4:D:162:LEU:HD13	30:H:103:DGD:HBT2	1.97	0.44
24:D:405:BCR:H15C	24:D:405:BCR:H351	1.83	0.44
2:b:125:ASP:OD1	2:b:127:ARG:HB3	2.17	0.44
2:b:376:VAL:O	2:b:378:LYS:HG2	2.16	0.44
3:c:189:TRP:HE1	3:c:295:THR:CG2	2.19	0.44
3:c:284:PHE:HB3	30:c:516:DGD:HB62	1.98	0.44
20:r:10:LEU:O	20:r:14:LEU:HD12	2.18	0.44
1:A:131:TRP:CH2	22:C:506:CLA:HAA2	2.52	0.44
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.99	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.79	0.44
4:D:146:PHE:C	4:D:149:PRO:HD2	2.42	0.44
1:a:308:ASP:O	6:f:45:ARG:NH1	2.51	0.44
30:h:102:DGD:O4E	30:h:102:DGD:O5E	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:56:THR:OG1	35:v:301:HOH:O	2.11	0.44
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.52	0.44
3:C:94:THR:HG22	22:C:502:CLA:HED1	2.00	0.44
3:C:436:PHE:CZ	22:C:505:CLA:H172	2.53	0.44
22:C:509:CLA:HBC3	22:C:511:CLA:H71	1.99	0.44
24:C:515:BCR:H15C	24:C:515:BCR:H351	1.84	0.44
2:b:489:GLU:HB3	2:b:495:PHE:CD2	2.53	0.44
3:c:63:TRP:NE1	3:c:67:MET:HE3	2.32	0.44
3:c:345:PRO:HB3	13:o:73:ARG:HD3	2.00	0.44
22:c:506:CLA:HBC2	24:c:515:BCR:H341	1.99	0.44
30:c:517:DGD:HA42	27:j:101:LFA:H142	1.97	0.44
4:d:336:HIS:CD2	4:d:337:GLU:HG2	2.52	0.44
22:A:406:CLA:H203	22:A:406:CLA:H152	2.00	0.44
2:B:504:THR:O	2:B:504:THR:OG1	2.35	0.44
22:B:607:CLA:CBB	4:D:123:ILE:HG12	2.48	0.44
24:B:617:BCR:H20C	24:B:617:BCR:H361	1.81	0.44
13:O:48:THR:HG23	13:O:237:GLY:HA2	1.99	0.44
1:a:182:PHE:O	1:a:186:PHE:HB2	2.18	0.44
2:b:216:HIS:HE1	22:b:611:CLA:CHA	2.31	0.44
2:b:220:ARG:HG3	7:h:20:LYS:HD2	1.98	0.44
3:c:38:GLY:HA3	22:c:512:CLA:HMD2	1.99	0.44
3:C:42:LEU:HD21	22:C:512:CLA:H2A	2.00	0.44
24:H:102:BCR:H331	24:H:102:BCR:HC8	1.99	0.44
27:M:102:LFA:H152	27:M:102:LFA:H121	1.82	0.44
19:Z:3:ILE:O	19:Z:7:LEU:HG	2.17	0.44
2:b:498:LYS:HB3	2:b:504:THR:HG21	1.99	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.98	0.44
22:b:603:CLA:HBB2	24:h:101:BCR:H351	2.00	0.44
3:c:258:GLY:HA2	3:c:261:ARG:NH1	2.33	0.44
3:c:261:ARG:HA	3:c:266:TRP:CZ2	2.53	0.44
22:c:502:CLA:H172	22:c:508:CLA:HMB2	1.99	0.44
24:c:515:BCR:H20C	24:c:515:BCR:H361	1.84	0.44
2:B:75:TRP:HB3	27:B:623:LFA:H51	1.99	0.44
2:B:370:LEU:HB2	2:B:379:ALA:HB3	1.99	0.44
24:B:616:BCR:H24C	24:B:616:BCR:H371	1.81	0.44
24:B:617:BCR:H382	24:t:102:BCR:H11C	1.99	0.44
22:C:502:CLA:CGA	22:C:502:CLA:H3A	2.48	0.44
22:D:404:CLA:H41	22:D:404:CLA:H62	1.81	0.44
1:a:175:GLY:O	1:a:179:THR:OG1	2.22	0.44
2:b:450:TRP:CZ3	4:d:293:LEU:HD21	2.52	0.44
22:b:603:CLA:HMA3	29:b:624:LMG:H291	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:74:LEU:HD22	4:d:175:VAL:HG11	1.99	0.44
22:d:403:CLA:H91	22:d:403:CLA:H112	1.63	0.44
5:e:8:ARG:HB3	5:e:13:ILE:HD11	2.00	0.44
5:e:74:GLN:O	5:e:78:THR:HG22	2.18	0.44
26:A:411:SQD:H222	22:A:412:CLA:H191	1.99	0.44
2:B:43:ALA:HA	27:B:627:LFA:H61	1.99	0.44
13:O:120:PHE:HD1	13:O:235:ILE:HD13	1.83	0.44
1:a:53:ILE:HG12	1:a:71:LEU:HD12	2.00	0.44
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.00	0.44
10:k:21:LEU:O	10:k:25:LEU:HG	2.17	0.44
3:C:33:PHE:CE1	22:C:509:CLA:HED1	2.53	0.44
3:C:256:PRO:HA	22:C:507:CLA:HED2	1.99	0.44
25:D:406:PL9:H322	32:L:102:LHG:H222	2.00	0.44
22:c:509:CLA:H42	32:d:407:LHG:H381	1.99	0.44
24:h:101:BCR:H341	24:h:101:BCR:H11C	1.67	0.44
9:j:26:GLY:HA2	27:j:101:LFA:H121	2.00	0.44
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.53	0.43
2:B:358:ARG:O	2:B:360:PRO:HD3	2.18	0.43
4:D:103:ARG:HD3	4:D:106:GLN:NE2	2.33	0.43
22:b:606:CLA:HMD3	22:b:614:CLA:H192	1.99	0.43
9:j:18:GLY:O	9:j:22:ILE:HG13	2.18	0.43
13:o:234:LYS:HB2	13:o:234:LYS:HE2	1.72	0.43
1:A:262:TYR:HE2	4:D:27:PHE:HE1	1.65	0.43
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.53	0.43
24:c:523:BCR:H371	9:j:18:GLY:HA3	1.99	0.43
4:d:351:ALA:HA	15:u:101:GLY:O	2.18	0.43
2:B:220:ARG:HD2	2:B:220:ARG:HA	1.77	0.43
5:E:26:THR:HG22	20:R:15:ALA:HB1	1.99	0.43
13:O:150:SER:HB3	13:O:190:PHE:CZ	2.53	0.43
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.00	0.43
1:a:319:ASP:OD1	35:a:505:HOH:O	2.21	0.43
22:a:405:CLA:C1B	23:a:406:PHO:H192	2.49	0.43
19:z:31:GLN:C	19:z:33:TRP:N	2.76	0.43
19:z:41:PHE:HD2	19:z:42:LEU:HG	1.83	0.43
2:B:363:PHE:HB3	2:B:365:SER:O	2.19	0.43
33:E:102:HEM:CGD	6:F:19:ARG:HH21	2.31	0.43
24:K:102:BCR:H15C	24:K:102:BCR:H351	1.71	0.43
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.90	0.43
24:T:101:BCR:H351	24:T:101:BCR:H15C	1.81	0.43
1:a:281:VAL:HB	26:a:410:SQD:H171	2.00	0.43
2:b:67:ALA:HA	2:b:71:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.00	0.43
1:A:337:HIS:CD2	4:D:352:LEU:HD11	2.53	0.43
24:B:616:BCR:H341	24:B:616:BCR:H11C	1.74	0.43
24:B:618:BCR:H15C	24:B:618:BCR:H351	1.77	0.43
16:V:122:GLU:HG3	16:V:126:LEU:HD12	2.01	0.43
32:d:406:LHG:H142	32:d:406:LHG:H171	1.90	0.43
24:H:102:BCR:H11C	24:H:102:BCR:H341	1.73	0.43
1:a:91:LEU:HD23	1:a:91:LEU:HA	1.85	0.43
1:a:252:HIS:HD2	1:a:264:SER:OG	2.01	0.43
2:b:36:SER:OG	24:b:620:BCR:H362	2.19	0.43
4:d:52:THR:HB	4:d:76:VAL:HB	2.00	0.43
14:t:11:ALA:HB3	24:t:102:BCR:H363	2.01	0.43
2:B:134:ASP:OD1	2:B:136:PRO:HD2	2.19	0.43
2:B:383:PHE:O	13:O:166:SER:HA	2.17	0.43
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.06	0.43
22:C:504:CLA:H101	22:C:504:CLA:H62	1.72	0.43
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.78	0.43
18:X:15:LEU:HD23	18:X:15:LEU:HA	1.71	0.43
2:b:157:HIS:HE1	22:b:608:CLA:NA	2.15	0.43
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.53	0.43
24:b:620:BCR:H15C	24:b:620:BCR:H351	1.80	0.43
3:c:36:TRP:CD1	3:c:36:TRP:H	2.37	0.43
3:c:67:MET:CE	10:k:26:PRO:HB3	2.48	0.43
32:d:407:LHG:H242	32:d:407:LHG:H272	1.41	0.43
22:C:510:CLA:HAA2	22:C:510:CLA:HBD	2.01	0.43
4:D:68:LEU:HD13	6:F:40:MET:HE2	2.01	0.43
22:D:404:CLA:ND	27:D:414:LFA:H112	2.34	0.43
5:E:65:LEU:HD12	5:E:66:VAL:H	1.83	0.43
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.54	0.43
22:b:603:CLA:CED	29:b:624:LMG:HC61	2.49	0.43
22:b:604:CLA:H91	22:b:604:CLA:H111	1.78	0.43
29:c:519:LMG:H242	9:j:22:ILE:HD13	2.01	0.43
10:k:39:TRP:O	10:k:43:VAL:HG22	2.19	0.43
1:A:94:TYR:H	1:A:113:GLN:HE22	1.67	0.43
1:A:322:ASN:OD1	35:A:502:HOH:O	2.22	0.43
22:B:615:CLA:HAA2	22:B:615:CLA:HBD	2.00	0.43
3:C:360:ASP:O	30:C:517:DGD:O2E	2.29	0.43
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.84	0.43
2:b:482:ILE:HG22	4:d:138:VAL:HA	2.01	0.43
3:c:67:MET:O	3:c:71:GLU:HG3	2.19	0.43
22:c:505:CLA:H193	22:c:511:CLA:H72	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:18:LYS:HD3	13:o:46:GLN:NE2	2.33	0.43
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	2.01	0.42
25:a:409:PL9:H402	4:d:38:PHE:CG	2.53	0.42
2:b:137:LYS:HD2	7:h:14:LEU:O	2.17	0.42
4:d:103:ARG:HD3	4:d:106:GLN:OE1	2.19	0.42
22:H:101:CLA:C1B	22:H:101:CLA:H143	2.49	0.42
30:H:103:DGD:HB51	30:H:103:DGD:HB21	1.78	0.42
10:K:18:PHE:O	10:K:21:LEU:N	2.52	0.42
13:O:189:ARG:HD2	15:U:9:LEU:HD22	2.01	0.42
3:c:187:ASP:HB2	3:c:230:LEU:HD12	2.01	0.42
22:c:507:CLA:H72	24:c:515:BCR:H10C	2.01	0.42
30:c:517:DGD:HB92	30:c:517:DGD:HBW2	1.80	0.42
4:d:88:SER:HB2	5:e:69:ARG:NH2	2.34	0.42
4:d:259:ILE:HD13	32:d:406:LHG:H281	2.01	0.42
4:d:284:ILE:HD13	29:m:103:LMG:H241	2.01	0.42
22:B:615:CLA:H141	22:B:615:CLA:H161	1.78	0.42
3:C:334:PRO:HA	13:O:153:THR:OG1	2.19	0.42
26:L:101:SQD:H161	26:L:101:SQD:H131	1.84	0.42
13:O:31:PRO:HA	13:O:135:SER:OG	2.19	0.42
2:b:90:PHE:CZ	22:b:608:CLA:H151	2.53	0.42
22:b:617:CLA:H101	22:b:617:CLA:H13	1.92	0.42
24:b:620:BCR:H24C	24:b:620:BCR:H371	1.83	0.42
24:d:404:BCR:H372	29:f:101:LMG:H301	2.00	0.42
5:e:23:HIS:HA	5:e:26:THR:OG1	2.19	0.42
16:v:64:PRO:HD2	16:v:66:ARG:NH2	2.34	0.42
1:A:112:TYR:O	1:A:116:ILE:HG12	2.19	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.01	0.42
22:B:611:CLA:H122	22:B:611:CLA:H8	1.81	0.42
5:E:10:PHE:O	5:E:14:ILE:HG12	2.19	0.42
24:K:101:BCR:H11C	24:K:101:BCR:H341	1.89	0.42
3:c:216:SER:HA	29:c:501:LMG:H292	2.02	0.42
24:t:102:BCR:H15C	24:t:102:BCR:H351	1.74	0.42
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.42
4:D:282:SER:OG	22:D:403:CLA:HED3	2.19	0.42
24:K:102:BCR:H20C	24:K:102:BCR:H361	1.82	0.42
2:b:384:ARG:CZ	4:d:348:ARG:HD3	2.49	0.42
22:c:505:CLA:HHC	22:c:505:CLA:HAB	1.84	0.42
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.07	0.42
24:A:407:BCR:H15C	24:A:407:BCR:H351	1.88	0.42
2:B:326:ARG:O	2:B:444:ARG:HG2	2.20	0.42
3:C:112:PHE:O	3:C:116:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:HB2	2:b:338:GLN:O	2.20	0.42
19:Z:7:LEU:HD12	19:Z:8:ALA:N	2.34	0.42
22:a:405:CLA:H172	14:t:10:PHE:CE1	2.54	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
3:c:243:ILE:HG12	29:c:522:LMG:H201	2.02	0.42
22:c:503:CLA:HBD	22:c:503:CLA:HAA1	2.00	0.42
32:d:407:LHG:H352	32:d:407:LHG:H151	2.01	0.42
20:R:20:VAL:O	20:R:24:LEU:HB2	2.19	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.02	0.42
22:A:406:CLA:H11	8:I:9:TYR:CZ	2.55	0.42
22:B:609:CLA:HHC	22:B:609:CLA:HBB1	2.01	0.42
27:B:620:LFA:C10	26:a:412:SQD:H381	2.49	0.42
3:C:271:TYR:HA	3:C:274:TYR:CD2	2.55	0.42
3:C:327:ASN:HB3	13:O:99:ASP:OD1	2.20	0.42
29:C:520:LMG:H191	29:C:520:LMG:H331	2.01	0.42
7:H:20:LYS:HA	35:H:216:HOH:O	2.19	0.42
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.55	0.42
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.54	0.42
2:b:148:LEU:HD23	2:b:148:LEU:HA	1.93	0.42
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.34	0.42
3:c:342:MET:SD	3:c:356:MET:HE2	2.58	0.42
25:d:405:PL9:H33	11:l:26:VAL:CG1	2.49	0.42
3:C:92:ILE:HD11	22:C:504:CLA:HED2	2.02	0.42
13:O:133:VAL:O	13:O:133:VAL:HG23	2.20	0.42
2:b:477:ASP:CG	4:d:134:ARG:HH22	2.28	0.42
1:A:38:ILE:HG12	26:A:411:SQD:H142	2.01	0.42
2:B:476:ARG:O	2:B:476:ARG:HG2	2.19	0.42
22:C:508:CLA:H142	24:C:516:BCR:H16C	2.02	0.42
24:D:405:BCR:H11C	24:D:405:BCR:H341	1.91	0.42
13:O:54:GLU:O	13:O:56:PRO:HD3	2.20	0.42
22:c:507:CLA:HMC2	22:c:508:CLA:H101	2.02	0.42
24:k:101:BCR:H24C	24:k:101:BCR:H371	1.65	0.42
13:o:153:THR:HB	35:u:205:HOH:O	2.20	0.42
22:B:615:CLA:H52	22:B:615:CLA:H11	1.89	0.42
3:C:279:LEU:HD12	22:C:510:CLA:HED2	2.02	0.42
24:c:524:BCR:H24C	24:c:524:BCR:H371	1.89	0.42
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.55	0.42
1:A:159:LEU:C	1:A:162:PRO:HD2	2.45	0.41
22:A:406:CLA:HMA2	29:C:501:LMG:H131	2.02	0.41
3:C:379:LYS:HA	3:C:383:ASP:OD2	2.21	0.41
25:D:406:PL9:H371	25:D:406:PL9:H351	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:126:VAL:O	13:O:144:GLY:HA3	2.20	0.41
3:c:90:PRO:HB3	3:c:301:PHE:HB3	2.01	0.41
29:c:519:LMG:H141	29:c:519:LMG:H171	1.77	0.41
18:x:29:ILE:O	18:x:32:SER:OG	2.20	0.41
20:r:29:LYS:HD3	20:r:29:LYS:HA	1.80	0.41
1:A:179:THR:O	1:A:183:MET:HG3	2.20	0.41
2:B:486:LEU:HD11	2:B:490:GLN:CD	2.45	0.41
22:B:612:CLA:HBB1	22:B:612:CLA:HMB1	2.02	0.41
24:B:617:BCR:H371	24:B:617:BCR:H24C	1.82	0.41
24:C:516:BCR:H24C	24:C:516:BCR:H371	1.79	0.41
16:V:32:LEU:HD13	16:V:111:ASP:HB3	2.02	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.35	0.41
2:b:460:LEU:HG	4:d:280:TRP:HZ3	1.85	0.41
3:c:377:LEU:H	13:o:80:GLN:NE2	2.17	0.41
4:d:80:THR:HG22	4:d:111:TRP:NE1	2.35	0.41
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.74	0.41
1:A:255:PHE:CZ	25:A:408:PL9:H13	2.56	0.41
21:A:402:CL:CL	3:C:354:GLU:HG2	2.58	0.41
3:C:286:ALA:HB2	22:C:503:CLA:HMD1	2.01	0.41
22:C:502:CLA:CHB	22:C:502:CLA:H2	2.50	0.41
4:D:103:ARG:HE	5:E:77:GLU:CG	2.32	0.41
32:E:101:LHG:H223	32:E:101:LHG:H191	1.92	0.41
2:b:474:LEU:HD23	2:b:474:LEU:HA	1.88	0.41
22:b:605:CLA:C4D	22:b:607:CLA:H43	2.50	0.41
5:e:25:ILE:HD12	20:r:18:TRP:CG	2.54	0.41
22:a:405:CLA:HED2	4:d:198:MET:SD	2.59	0.41
30:c:516:DGD:HG11	35:c:613:HOH:O	2.20	0.41
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.55	0.41
13:o:184:ARG:NH2	13:o:229:GLU:OE1	2.54	0.41
19:z:31:GLN:C	19:z:33:TRP:H	2.28	0.41
2:B:241:SER:O	2:B:245:VAL:HG23	2.20	0.41
29:C:501:LMG:C25	22:C:506:CLA:HBB2	2.50	0.41
1:a:159:LEU:C	1:a:162:PRO:HD2	2.45	0.41
1:a:332:HIS:O	1:a:332:HIS:ND1	2.54	0.41
2:b:204:ALA:O	2:b:208:VAL:HG23	2.20	0.41
2:b:384:ARG:HH11	15:u:102:LEU:HG	1.84	0.41
22:c:502:CLA:H143	22:c:502:CLA:H161	1.95	0.41
22:c:513:CLA:C1B	24:c:524:BCR:H401	2.50	0.41
30:c:517:DGD:HBF2	30:c:517:DGD:HBE1	1.90	0.41
4:d:90:LEU:HA	4:d:90:LEU:HD23	1.66	0.41
4:d:142:ASN:HB3	35:d:502:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:518:DGD:HBE2	30:C:518:DGD:HBF1	1.83	0.41
5:E:5:THR:HG23	5:E:7:GLU:OE1	2.21	0.41
15:U:36:ILE:CD1	16:V:51:SER:HB3	2.49	0.41
2:b:341:LYS:HD2	2:b:429:ILE:HG22	2.02	0.41
22:b:603:CLA:HHD	24:h:101:BCR:H383	2.03	0.41
3:c:214:LEU:O	29:c:501:LMG:H291	2.20	0.41
22:c:508:CLA:HAA2	22:c:508:CLA:HBD	2.02	0.41
24:c:524:BCR:H15C	24:c:524:BCR:H351	1.77	0.41
7:h:29:PRO:O	7:h:33:VAL:HG23	2.20	0.41
24:k:101:BCR:H15C	24:k:101:BCR:H351	1.83	0.41
20:r:23:ILE:HD12	20:r:23:ILE:HA	1.90	0.41
2:B:153:PHE:CE2	2:B:158:LEU:HD11	2.56	0.41
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.01	0.41
3:C:223:TRP:CE3	30:C:517:DGD:HB21	2.56	0.41
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.55	0.41
22:b:616:CLA:H93	22:b:616:CLA:H111	1.81	0.41
3:c:48:LYS:NZ	3:c:138:GLU:HB3	2.36	0.41
4:d:19:ASP:O	4:d:23:LYS:HG2	2.21	0.41
4:d:85:MET:CE	4:d:90:LEU:HD21	2.51	0.41
2:B:18:ARG:NH1	35:B:703:HOH:O	2.20	0.41
22:C:506:CLA:CHC	22:C:506:CLA:H51	2.51	0.41
22:b:617:CLA:HBC3	22:b:618:CLA:HBC1	2.02	0.41
22:c:514:CLA:HMB3	22:c:514:CLA:HBB1	2.03	0.41
32:d:407:LHG:H321	32:d:407:LHG:H291	1.75	0.41
5:e:36:LEU:HA	5:e:39:SER:HG	1.86	0.41
15:u:68:THR:O	15:u:72:LYS:HG3	2.21	0.41
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.84	0.41
2:B:66:MET:HE3	2:B:93:PHE:HD1	1.86	0.41
2:B:98:LEU:HD12	27:B:626:LFA:C2	2.50	0.41
2:B:223:GLN:O	2:B:227:LYS:HG2	2.21	0.41
2:B:386:ALA:HB3	15:U:102:LEU:HD22	2.03	0.41
22:B:610:CLA:H112	22:B:610:CLA:H72	1.78	0.41
27:B:628:LFA:H81	14:t:4:ILE:HD11	2.03	0.41
22:C:503:CLA:H102	22:C:504:CLA:CHB	2.51	0.41
4:D:322:ASN:O	4:D:326:ARG:HG3	2.20	0.41
32:L:102:LHG:H102	32:L:102:LHG:H241	2.03	0.41
13:O:119:LEU:O	13:O:121:THR:HG22	2.20	0.41
14:T:25:GLU:HA	14:T:26:PRO:HD3	1.92	0.41
2:b:153:PHE:CE2	2:b:158:LEU:HD11	2.56	0.41
2:b:216:HIS:CE1	22:b:611:CLA:C1A	3.04	0.41
22:b:604:CLA:H111	22:b:604:CLA:H152	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:608:CLA:HAA1	22:b:608:CLA:HBD	2.03	0.41
3:c:357:ARG:O	35:c:605:HOH:O	2.22	0.41
24:c:524:BCR:H11C	24:c:524:BCR:H341	1.88	0.41
5:e:60:GLN:HG2	5:e:61:ARG:N	2.36	0.41
27:j:101:LFA:H13	27:j:101:LFA:H42	1.87	0.41
14:t:8:PHE:HD1	24:t:102:BCR:H372	1.85	0.41
14:t:15:ALA:HA	24:t:102:BCR:H12C	2.02	0.41
16:v:32:LEU:HB3	16:v:115:ILE:HD11	2.03	0.41
1:A:210:LEU:HD12	23:A:405:PHO:NB	2.35	0.41
22:C:509:CLA:H92	32:D:409:LHG:C37	2.51	0.41
4:D:23:LYS:HD3	4:D:135:LEU:HD21	2.03	0.41
4:D:307:GLU:HG3	35:D:554:HOH:O	2.21	0.41
32:D:407:LHG:H121	32:D:407:LHG:H332	2.03	0.41
5:E:23:HIS:HA	5:E:26:THR:OG1	2.20	0.41
1:a:158:PHE:O	1:a:162:PRO:HG2	2.21	0.41
23:a:414:PHO:H61	22:d:402:CLA:H111	2.03	0.41
22:b:614:CLA:H122	22:b:614:CLA:H8	1.84	0.41
4:d:62:GLY:O	4:d:63:LEU:HD23	2.21	0.41
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.02	0.40
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.92	0.40
2:b:150:CYS:HB2	22:b:605:CLA:CMC	2.51	0.40
2:b:422:ARG:O	2:b:425:ILE:HG12	2.21	0.40
3:c:279:LEU:CD1	22:c:510:CLA:HED2	2.51	0.40
3:c:318:LEU:HD23	3:c:318:LEU:O	2.20	0.40
3:c:425:TRP:HE3	30:c:517:DGD:HBT1	1.86	0.40
22:c:512:CLA:C3B	24:k:101:BCR:H393	2.51	0.40
5:e:7:GLU:OE1	5:e:7:GLU:N	2.46	0.40
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.86	0.40
22:B:605:CLA:HAA1	22:B:605:CLA:HBD	2.04	0.40
3:C:337:LEU:HD23	13:O:105:PRO:HG2	2.04	0.40
22:C:502:CLA:HAA1	22:C:502:CLA:HBD	2.03	0.40
11:L:14:ARG:HG2	11:L:18:TYR:CE2	2.56	0.40
19:Z:31:GLN:HA	19:Z:33:TRP:CE3	2.57	0.40
22:a:405:CLA:O1A	22:a:405:CLA:H43	2.21	0.40
26:b:601:SQD:H383	26:b:601:SQD:H351	1.80	0.40
3:c:228:ASN:OD1	3:c:228:ASN:N	2.53	0.40
3:c:320:ARG:HD2	16:v:49:ASN:OD1	2.21	0.40
13:o:54:GLU:O	13:o:56:PRO:HD3	2.21	0.40
22:B:612:CLA:HAA2	22:B:612:CLA:HBD	2.04	0.40
22:B:613:CLA:HMD1	12:M:21:PHE:HE1	1.86	0.40
4:D:49:LEU:HD13	24:D:405:BCR:C15	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:115:ARG:O	13:O:117:PRO:HD3	2.21	0.40
1:a:129:ARG:NH1	35:a:517:HOH:O	2.49	0.40
22:b:608:CLA:H161	22:b:608:CLA:H122	1.98	0.40
22:c:504:CLA:H203	22:c:511:CLA:HAB	2.03	0.40
13:o:108:VAL:HG23	13:o:116:ILE:HB	2.03	0.40
13:o:180:GLU:H	13:o:180:GLU:CD	2.30	0.40
1:A:183:MET:HA	22:A:403:CLA:HMD2	2.03	0.40
22:B:602:CLA:H3A	22:B:602:CLA:O1A	2.21	0.40
22:B:607:CLA:H8	22:B:608:CLA:H13	2.04	0.40
3:C:217:PRO:HB2	30:C:517:DGD:HA32	2.03	0.40
3:C:223:TRP:HE3	30:C:517:DGD:HB21	1.86	0.40
25:A:408:PL9:HC8	25:A:408:PL9:HC2	1.77	0.40
2:B:150:CYS:HB2	22:B:602:CLA:CMC	2.52	0.40
2:B:272:ARG:HG3	2:B:273:TYR:N	2.37	0.40
22:B:602:CLA:C3D	22:B:604:CLA:H43	2.52	0.40
3:C:352:GLY:O	3:C:355:THR:HG22	2.21	0.40
25:D:406:PL9:H471	25:D:406:PL9:H43	1.65	0.40
2:b:39:LEU:HD13	27:b:623:LFA:H112	2.03	0.40
2:b:502:VAL:C	2:b:504:THR:H	2.29	0.40
26:b:601:SQD:H301	26:b:601:SQD:H332	1.75	0.40
22:b:616:CLA:H8	24:b:619:BCR:H362	2.04	0.40
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.57	0.40
7:h:38:PHE:CD2	24:h:101:BCR:HC7	2.57	0.40
7:h:45:ILE:HG13	7:h:46:LEU:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	36	42
2	B	503/510 (99%)	478 (95%)	25 (5%)	0	100	100
2	b	501/510 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	445/461 (96%)	433 (97%)	11 (2%)	1 (0%)	43	51
3	c	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	43	51
4	D	338/352 (96%)	327 (97%)	11 (3%)	0	100	100
4	d	338/352 (96%)	321 (95%)	17 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	60/66 (91%)	56 (93%)	4 (7%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	31/38 (82%)	30 (97%)	1 (3%)	0	100	100
8	i	31/38 (82%)	31 (100%)	0	0	100	100
9	J	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
9	j	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
10	K	33/46 (72%)	32 (97%)	1 (3%)	0	100	100
10	k	34/46 (74%)	33 (97%)	1 (3%)	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	30/36 (83%)	30 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	222 (92%)	15 (6%)	3 (1%)	9	8
13	o	239/272 (88%)	223 (93%)	14 (6%)	2 (1%)	16	16
14	T	26/32 (81%)	26 (100%)	0	0	100	100
14	t	27/32 (84%)	25 (93%)	2 (7%)	0	100	100
15	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
15	u	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	19
16	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	19/46 (41%)	18 (95%)	1 (5%)	0	100	100
17	y	21/46 (46%)	21 (100%)	0	0	100	100
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	59/62 (95%)	54 (92%)	2 (3%)	3 (5%)	1	0
19	z	59/62 (95%)	53 (90%)	3 (5%)	3 (5%)	1	0
20	R	33/41 (80%)	32 (97%)	0	1 (3%)	3	1
20	r	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5173/5700 (91%)	4951 (96%)	205 (4%)	17 (0%)	36	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	32	ASP
19	Z	35	ARG
3	c	416	SER
19	z	30	PRO
19	z	32	ASP
3	C	416	SER
19	Z	30	PRO
19	z	31	GLN
13	O	62	GLU
13	o	62	GLU
13	o	57	LYS
20	R	35	LEU
1	a	259	ILE
13	O	101	ILE
16	V	45	ILE
1	A	259	ILE

5.3.2 Protein sidechains [i](#)

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%)	269 (100%)	1 (0%)	84	92
1	a	270/280 (96%)	268 (99%)	2 (1%)	76	87
2	B	403/407 (99%)	402 (100%)	1 (0%)	87	94
2	b	401/407 (98%)	401 (100%)	0	100	100
3	C	349/362 (96%)	346 (99%)	3 (1%)	70	84
3	c	350/362 (97%)	348 (99%)	2 (1%)	78	89
4	D	275/283 (97%)	275 (100%)	0	100	100
4	d	275/283 (97%)	275 (100%)	0	100	100
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	75
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	26 (96%)	1 (4%)	30	41
7	H	53/55 (96%)	53 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	66
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	30/35 (86%)	30 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	28/37 (76%)	28 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	51
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	205 (100%)	1 (0%)	81	90
13	o	205/228 (90%)	204 (100%)	1 (0%)	81	90
14	T	25/29 (86%)	24 (96%)	1 (4%)	28	38
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	63	78
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	15/37 (40%)	15 (100%)	0	100	100
17	y	17/37 (46%)	17 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	47
19	Z	51/52 (98%)	51 (100%)	0	100	100
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	30/33 (91%)	30 (100%)	0	100	100
20	r	27/33 (82%)	26 (96%)	1 (4%)	30	41
All	All	4297/4660 (92%)	4278 (100%)	19 (0%)	84	92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	SER
2	B	362	PHE
3	C	289	PHE
3	C	290	VAL
3	C	416	SER
5	E	4	THR
13	O	118	LEU
14	T	2	GLU
15	U	23	GLU
1	a	222	SER
1	a	332	HIS
3	c	144	SER
3	c	355	THR
6	f	28	VAL
7	h	56	ASP
11	l	10	VAL
13	o	106	VAL
18	x	6	SER
20	r	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	113	GLN

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Mol	Chain	Res	Type
2	B	497	GLN
3	C	155	ASN
3	C	311	GLN
3	C	322	GLN
3	C	327	ASN
4	D	106	GLN
4	D	186	GLN
4	D	236	ASN
4	D	322	ASN
4	D	332	GLN
4	D	336	HIS
10	K	40	GLN
15	U	71	GLN
15	U	73	GLN
16	V	118	HIS
1	a	252	HIS
1	a	315	ASN
2	b	53	ASN
2	b	282	GLN
2	b	331	ASN
2	b	374	ASN
3	c	201	ASN
3	c	327	ASN
3	c	332	GLN
3	c	418	ASN
4	d	61	HIS
4	d	186	GLN
4	d	224	GLN
4	d	250	ASN
4	d	332	GLN
5	e	82	GLN
6	f	44	GLN
10	k	40	GLN
11	l	37	ASN
12	m	4	ASN
12	m	32	GLN
13	o	36	GLN
13	o	58	ASN
13	o	80	GLN
13	o	88	ASN
13	o	124	ASN
13	o	236	GLN

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Mol	Chain	Res	Type
16	v	86	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	614	-	69,73,73	1.36	9 (13%)	82,113,113	1.33	10 (12%)
22	CLA	b	610	-	69,73,73	1.52	8 (11%)	82,113,113	1.33	7 (8%)
22	CLA	C	514	-	69,73,73	1.66	9 (13%)	82,113,113	1.17	9 (10%)
30	DGD	C	519	-	63,63,67	0.83	3 (4%)	77,77,81	1.10	7 (9%)
22	CLA	D	404	-	69,73,73	1.86	12 (17%)	82,113,113	1.19	9 (10%)
22	CLA	C	507	-	69,73,73	1.82	12 (17%)	82,113,113	1.36	10 (12%)
22	CLA	C	512	3	69,73,73	1.56	9 (13%)	82,113,113	1.22	8 (9%)
27	LFA	D	413	-	7,7,19	0.13	0	6,6,18	0.33	0
22	CLA	A	403	-	69,73,73	1.55	9 (13%)	82,113,113	1.43	8 (9%)
27	LFA	M	101	-	9,9,19	0.18	0	8,8,18	0.64	0
22	CLA	C	505	35	69,73,73	1.74	10 (14%)	82,113,113	1.18	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	610	-	69,73,73	1.55	9 (13%)	82,113,113	1.38	11 (13%)
27	LFA	D	411	-	14,14,19	0.10	0	13,13,18	0.25	0
27	LFA	B	623	-	12,12,19	0.07	0	11,11,18	0.23	0
22	CLA	b	613	-	69,73,73	1.50	9 (13%)	82,113,113	1.31	9 (10%)
29	LMG	C	520	-	48,48,55	0.94	2 (4%)	56,56,63	1.16	5 (8%)
26	SQD	a	410	-	52,54,54	1.05	3 (5%)	62,65,65	1.34	11 (17%)
29	LMG	b	624	-	39,39,55	1.12	3 (7%)	47,47,63	1.12	6 (12%)
22	CLA	c	504	-	69,73,73	1.60	9 (13%)	82,113,113	1.17	8 (9%)
24	BCR	H	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	B	615	-	69,73,73	1.70	9 (13%)	82,113,113	1.43	10 (12%)
27	LFA	b	630	-	14,14,19	0.09	0	13,13,18	0.37	0
31	BCT	D	401	28	3,3,3	0.86	0	2,3,3	0.72	0
34	HEC	V	201	16	46,50,50	1.78	6 (13%)	58,82,82	1.05	4 (6%)
27	LFA	i	102	-	6,6,19	0.11	0	5,5,18	0.16	0
22	CLA	a	405	35	69,73,73	1.48	8 (11%)	82,113,113	1.24	9 (10%)
24	BCR	b	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	14 (25%)
27	LFA	J	101	-	10,10,19	0.12	0	9,9,18	0.36	0
27	LFA	b	625	-	15,15,19	0.09	0	14,14,18	0.38	0
29	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	6 (10%)
22	CLA	B	605	-	69,73,73	1.50	8 (11%)	82,113,113	1.31	7 (8%)
22	CLA	C	504	-	69,73,73	1.47	7 (10%)	82,113,113	1.10	9 (10%)
22	CLA	B	603	-	69,73,73	1.55	7 (10%)	82,113,113	1.28	9 (10%)
22	CLA	A	412	35	69,73,73	1.54	10 (14%)	82,113,113	1.21	9 (10%)
22	CLA	a	404	-	69,73,73	1.53	7 (10%)	82,113,113	1.28	7 (8%)
22	CLA	c	507	-	69,73,73	1.67	8 (11%)	82,113,113	1.38	10 (12%)
22	CLA	b	604	-	69,73,73	1.60	10 (14%)	82,113,113	1.31	10 (12%)
22	CLA	b	617	-	69,73,73	1.51	9 (13%)	82,113,113	1.24	9 (10%)
24	BCR	c	523	-	41,41,41	0.86	1 (2%)	56,56,56	1.86	13 (23%)
26	SQD	b	601	-	52,54,54	1.06	3 (5%)	62,65,65	1.52	13 (20%)
27	LFA	d	408	-	14,14,19	0.12	0	13,13,18	0.42	0
22	CLA	b	603	35	69,73,73	1.59	7 (10%)	82,113,113	1.14	10 (12%)
22	CLA	c	506	-	69,73,73	1.57	9 (13%)	82,113,113	1.11	8 (9%)
22	CLA	B	607	-	69,73,73	1.55	9 (13%)	82,113,113	1.19	7 (8%)
22	CLA	c	505	35	69,73,73	1.66	9 (13%)	82,113,113	1.15	8 (9%)
22	CLA	c	512	3	69,73,73	1.57	9 (13%)	82,113,113	1.23	9 (10%)
22	CLA	B	602	-	69,73,73	1.59	9 (13%)	82,113,113	1.29	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LFA	a	411	-	6,6,19	0.10	0	5,5,18	0.22	0
27	LFA	j	101	-	14,14,19	0.11	0	13,13,18	0.43	0
23	PHO	a	414	-	58,69,69	1.36	7 (12%)	55,99,99	1.72	4 (7%)
32	LHG	D	408	-	48,48,48	0.88	3 (6%)	51,54,54	1.19	4 (7%)
27	LFA	i	101	-	15,15,19	0.12	0	14,14,18	0.38	0
23	PHO	a	406	-	58,69,69	1.15	6 (10%)	55,99,99	1.66	4 (7%)
27	LFA	m	102	-	14,14,19	0.13	0	13,13,18	0.40	0
22	CLA	A	406	-	69,73,73	2.01	14 (20%)	82,113,113	1.17	9 (10%)
31	BCT	a	413	28	3,3,3	0.87	0	2,3,3	0.23	0
23	PHO	D	402	-	58,69,69	1.23	7 (12%)	55,99,99	1.76	6 (10%)
26	SQD	L	101	-	46,48,54	1.15	3 (6%)	56,59,65	3.33	10 (17%)
29	LMG	m	103	-	51,51,55	0.84	3 (5%)	59,59,63	1.38	8 (13%)
24	BCR	a	408	-	41,41,41	0.88	1 (2%)	56,56,56	1.44	11 (19%)
24	BCR	c	524	-	41,41,41	0.78	1 (2%)	56,56,56	1.74	14 (25%)
33	HEM	E	102	6,5	50,50,50	1.42	9 (18%)	67,82,82	1.15	5 (7%)
26	SQD	a	412	-	50,50,54	0.89	2 (4%)	58,58,65	1.18	6 (10%)
23	PHO	A	405	-	58,69,69	1.25	8 (13%)	55,99,99	1.68	4 (7%)
22	CLA	c	510	-	69,73,73	1.70	10 (14%)	82,113,113	1.21	12 (14%)
22	CLA	d	402	-	69,73,73	1.51	9 (13%)	82,113,113	1.09	4 (4%)
27	LFA	M	102	-	15,15,19	0.21	0	14,14,18	0.65	0
22	CLA	B	611	-	69,73,73	1.72	8 (11%)	82,113,113	1.18	7 (8%)
29	LMG	B	619	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	2 (3%)
29	LMG	D	410	-	51,51,55	0.96	2 (3%)	59,59,63	0.94	2 (3%)
24	BCR	d	404	-	41,41,41	0.93	2 (4%)	56,56,56	2.21	16 (28%)
27	LFA	B	627	-	13,13,19	0.12	0	12,12,18	0.51	0
24	BCR	c	515	-	41,41,41	0.87	2 (4%)	56,56,56	1.40	7 (12%)
26	SQD	D	412	-	41,43,54	1.18	3 (7%)	51,54,65	1.74	10 (19%)
24	BCR	B	617	-	41,41,41	0.85	2 (4%)	56,56,56	1.62	13 (23%)
24	BCR	k	101	-	41,41,41	0.86	1 (2%)	56,56,56	1.84	12 (21%)
22	CLA	b	611	-	69,73,73	1.72	12 (17%)	82,113,113	1.25	8 (9%)
29	LMG	c	501	-	51,51,55	0.87	3 (5%)	59,59,63	1.25	5 (8%)
22	CLA	b	615	-	69,73,73	1.90	11 (15%)	82,113,113	1.25	8 (9%)
27	LFA	B	626	-	9,9,19	0.11	0	8,8,18	0.45	0
27	LFA	B	625	-	8,8,19	0.11	0	7,7,18	0.31	0
27	LFA	b	623	-	11,11,19	0.09	0	10,10,18	0.39	0
24	BCR	K	101	-	41,41,41	0.81	2 (4%)	56,56,56	1.66	11 (19%)
27	LFA	A	410	-	13,13,19	0.09	0	12,12,18	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LFA	b	626	-	11,11,19	0.09	0	10,10,18	0.30	0
30	DGD	h	102	-	63,63,67	0.82	2 (3%)	77,77,81	1.01	3 (3%)
27	LFA	d	409	-	8,8,19	0.11	0	7,7,18	0.26	0
22	CLA	C	503	-	69,73,73	1.59	8 (11%)	82,113,113	1.13	9 (10%)
22	CLA	b	614	-	69,73,73	1.83	11 (15%)	82,113,113	1.29	10 (12%)
32	LHG	b	628	-	48,48,48	0.90	3 (6%)	51,54,54	1.13	5 (9%)
22	CLA	C	510	-	69,73,73	1.80	10 (14%)	82,113,113	1.18	9 (10%)
27	LFA	C	521	-	14,14,19	0.08	0	13,13,18	0.33	0
22	CLA	C	513	-	69,73,73	1.66	9 (13%)	82,113,113	1.18	10 (12%)
22	CLA	B	612	-	69,73,73	1.60	9 (13%)	82,113,113	1.22	7 (8%)
29	LMG	B	621	-	36,36,55	1.06	2 (5%)	44,44,63	1.23	5 (11%)
30	DGD	c	516	-	63,63,67	0.84	3 (4%)	77,77,81	1.14	6 (7%)
22	CLA	H	101	35	69,73,73	1.64	10 (14%)	82,113,113	1.13	7 (8%)
22	CLA	C	511	-	69,73,73	1.56	7 (10%)	82,113,113	1.25	11 (13%)
22	CLA	c	503	-	69,73,73	1.70	9 (13%)	82,113,113	1.23	10 (12%)
29	LMG	C	522	-	44,44,55	1.06	3 (6%)	52,52,63	1.60	9 (17%)
22	CLA	C	509	-	69,73,73	1.58	8 (11%)	82,113,113	1.16	9 (10%)
27	LFA	I	101	-	13,13,19	0.09	0	12,12,18	0.36	0
29	LMG	C	501	-	51,51,55	0.89	2 (3%)	59,59,63	1.10	3 (5%)
32	LHG	e	101	-	41,41,48	0.98	2 (4%)	44,47,54	1.07	3 (6%)
22	CLA	B	606	35	69,73,73	1.83	10 (14%)	82,113,113	1.22	10 (12%)
32	LHG	D	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.03	2 (3%)
22	CLA	b	618	-	69,73,73	1.71	11 (15%)	82,113,113	1.26	8 (9%)
27	LFA	B	628	-	11,11,19	0.10	0	10,10,18	0.37	0
33	HEM	e	102	6,5	50,50,50	1.39	7 (14%)	67,82,82	1.01	3 (4%)
22	CLA	c	514	-	69,73,73	1.78	10 (14%)	82,113,113	1.21	10 (12%)
24	BCR	K	102	-	41,41,41	0.84	1 (2%)	56,56,56	1.92	12 (21%)
22	CLA	c	509	-	69,73,73	1.61	9 (13%)	82,113,113	1.26	8 (9%)
32	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.20	4 (7%)
25	PL9	A	408	-	55,55,55	0.64	2 (3%)	68,69,69	2.00	22 (32%)
22	CLA	b	606	-	69,73,73	1.62	10 (14%)	82,113,113	1.38	11 (13%)
24	BCR	B	616	-	41,41,41	0.84	1 (2%)	56,56,56	1.70	11 (19%)
27	LFA	b	627	-	10,10,19	0.09	0	9,9,18	0.35	0
22	CLA	B	613	-	69,73,73	1.55	10 (14%)	82,113,113	1.30	5 (6%)
26	SQD	f	102	-	41,43,54	1.19	4 (9%)	51,54,65	1.63	10 (19%)
24	BCR	B	618	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	H	103	-	61,61,67	0.84	2 (3%)	75,75,81	1.20	5 (6%)
22	CLA	c	508	35	69,73,73	1.73	10 (14%)	82,113,113	1.29	8 (9%)
22	CLA	C	502	-	69,73,73	1.72	11 (15%)	82,113,113	1.37	12 (14%)
32	LHG	L	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.12	3 (5%)
27	LFA	d	410	-	15,15,19	0.08	0	14,14,18	0.36	0
22	CLA	C	508	35	69,73,73	1.78	9 (13%)	82,113,113	1.21	10 (12%)
22	CLA	a	407	-	69,73,73	1.86	10 (14%)	82,113,113	1.19	10 (12%)
22	CLA	b	609	35	69,73,73	1.84	11 (15%)	82,113,113	1.31	10 (12%)
29	LMG	c	522	-	41,41,55	1.04	2 (4%)	49,49,63	1.61	11 (22%)
22	CLA	c	502	-	69,73,73	1.73	9 (13%)	82,113,113	1.27	9 (10%)
27	LFA	B	620	-	9,9,19	0.18	0	8,8,18	0.43	0
27	LFA	T	102	-	11,11,19	0.13	0	10,10,18	0.42	0
24	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.52	9 (16%)
30	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.23	7 (9%)
27	LFA	B	624	-	14,14,19	0.09	0	13,13,18	0.31	0
32	LHG	d	406	-	48,48,48	0.93	4 (8%)	51,54,54	1.17	5 (9%)
27	LFA	b	629	-	8,8,19	0.11	0	7,7,18	0.32	0
27	LFA	t	101	-	14,14,19	0.14	0	13,13,18	0.52	0
32	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
22	CLA	B	609	35	69,73,73	1.85	11 (15%)	82,113,113	1.31	10 (12%)
22	CLA	B	608	-	69,73,73	1.60	8 (11%)	82,113,113	1.22	10 (12%)
22	CLA	c	511	-	69,73,73	1.65	9 (13%)	82,113,113	1.27	7 (8%)
24	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.80	17 (30%)
27	LFA	c	520	-	8,8,19	0.11	0	7,7,18	0.37	0
30	DGD	c	517	-	56,56,67	0.89	2 (3%)	70,70,81	1.10	4 (5%)
22	CLA	b	607	-	69,73,73	1.48	10 (14%)	82,113,113	1.24	8 (9%)
27	LFA	B	622	-	15,15,19	0.11	0	14,14,18	0.32	0
22	CLA	D	403	-	69,73,73	1.62	8 (11%)	82,113,113	1.37	7 (8%)
27	LFA	b	602	-	14,14,19	0.12	0	13,13,18	0.43	0
22	CLA	b	608	-	69,73,73	1.65	11 (15%)	82,113,113	1.29	8 (9%)
22	CLA	c	513	-	69,73,73	1.61	9 (13%)	82,113,113	1.19	8 (9%)
24	BCR	A	407	-	41,41,41	0.82	0	56,56,56	1.57	11 (19%)
30	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	2 (2%)
24	BCR	D	405	-	41,41,41	0.93	2 (4%)	56,56,56	1.90	13 (23%)
22	CLA	B	601	-	69,73,73	1.58	8 (11%)	82,113,113	1.33	7 (8%)
24	BCR	T	101	-	41,41,41	0.90	2 (4%)	56,56,56	2.03	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	d	407	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	3 (5%)
27	LFA	D	414	-	9,9,19	0.19	0	8,8,18	0.51	0
24	BCR	t	102	-	41,41,41	0.86	1 (2%)	56,56,56	1.94	14 (25%)
26	SQD	A	409	-	52,54,54	1.05	3 (5%)	62,65,65	1.63	11 (17%)
25	PL9	a	409	-	55,55,55	0.61	2 (3%)	68,69,69	1.79	18 (26%)
34	HEC	v	201	16	46,50,50	1.80	6 (13%)	58,82,82	1.09	4 (6%)
22	CLA	A	404	35	69,73,73	1.52	8 (11%)	82,113,113	1.21	9 (10%)
22	CLA	B	604	-	69,73,73	1.45	8 (11%)	82,113,113	1.28	8 (9%)
22	CLA	C	506	-	69,73,73	1.64	9 (13%)	82,113,113	1.19	8 (9%)
22	CLA	b	616	-	69,73,73	1.51	8 (11%)	82,113,113	1.14	6 (7%)
24	BCR	b	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.80	13 (23%)
25	PL9	d	405	-	55,55,55	0.66	3 (5%)	68,69,69	1.74	15 (22%)
27	LFA	A	413	-	10,10,19	0.08	0	9,9,18	0.43	0
22	CLA	d	403	-	69,73,73	1.88	11 (15%)	82,113,113	1.18	9 (10%)
24	BCR	h	101	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
26	SQD	A	411	-	52,54,54	1.07	3 (5%)	62,65,65	1.31	8 (12%)
27	LFA	c	521	-	14,14,19	0.09	0	13,13,18	0.34	0
22	CLA	b	612	35	69,73,73	1.84	11 (15%)	82,113,113	1.44	7 (8%)
25	PL9	D	406	-	55,55,55	0.72	3 (5%)	68,69,69	1.62	15 (22%)
24	BCR	C	516	-	41,41,41	0.94	2 (4%)	56,56,56	1.76	10 (17%)
22	CLA	d	401	35	69,73,73	1.62	9 (13%)	82,113,113	1.19	11 (13%)
30	DGD	C	518	-	57,57,67	0.86	2 (3%)	71,71,81	1.27	9 (12%)
22	CLA	b	605	-	69,73,73	1.71	10 (14%)	82,113,113	1.25	6 (7%)
27	LFA	m	101	-	9,9,19	0.13	0	8,8,18	0.44	0
32	LHG	l	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.23	5 (9%)
29	LMG	f	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	5 (8%)
27	LFA	b	622	-	9,9,19	0.13	0	8,8,18	0.33	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
22	CLA	B	614	-	1/1/15/20	10/39/115/115	-
22	CLA	b	610	-	1/1/15/20	3/39/115/115	-
22	CLA	C	514	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	C	519	-	-	6/51/91/95	0/2/2/2
22	CLA	D	404	-	1/1/15/20	5/39/115/115	-
22	CLA	C	507	-	1/1/15/20	4/39/115/115	-
22	CLA	C	512	3	1/1/15/20	1/39/115/115	-
27	LFA	D	413	-	-	2/5/5/17	-
22	CLA	A	403	-	1/1/15/20	1/39/115/115	-
27	LFA	M	101	-	-	2/7/7/17	-
22	CLA	C	505	35	1/1/15/20	5/39/115/115	-
22	CLA	B	610	-	1/1/15/20	3/39/115/115	-
27	LFA	D	411	-	-	5/12/12/17	-
27	LFA	B	623	-	-	6/10/10/17	-
22	CLA	b	613	-	1/1/15/20	7/39/115/115	-
29	LMG	C	520	-	-	10/43/63/70	0/1/1/1
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
29	LMG	b	624	-	-	13/34/54/70	0/1/1/1
22	CLA	c	504	-	1/1/15/20	4/39/115/115	-
24	BCR	H	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/15/20	7/39/115/115	-
27	LFA	b	630	-	-	6/12/12/17	-
34	HEC	V	201	16	-	5/14/54/54	-
27	LFA	i	102	-	-	2/4/4/17	-
22	CLA	a	405	35	1/1/15/20	5/39/115/115	-
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
27	LFA	J	101	-	-	1/8/8/17	-
27	LFA	b	625	-	-	6/13/13/17	-
29	LMG	c	519	-	-	10/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	5/39/115/115	-
22	CLA	C	504	-	1/1/15/20	5/39/115/115	-
22	CLA	B	603	-	1/1/15/20	1/39/115/115	-
22	CLA	A	412	35	1/1/15/20	0/39/115/115	-
22	CLA	a	404	-	1/1/15/20	2/39/115/115	-
22	CLA	c	507	-	1/1/15/20	5/39/115/115	-
22	CLA	b	604	-	1/1/15/20	5/39/115/115	-
22	CLA	b	617	-	1/1/15/20	3/39/115/115	-
24	BCR	c	523	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	b	601	-	-	11/49/69/69	0/1/1/1
27	LFA	d	408	-	-	5/12/12/17	-
22	CLA	b	603	35	1/1/15/20	8/39/115/115	-
22	CLA	c	506	-	1/1/15/20	7/39/115/115	-
22	CLA	B	607	-	1/1/15/20	2/39/115/115	-
22	CLA	c	505	35	1/1/15/20	4/39/115/115	-
22	CLA	c	512	3	1/1/15/20	0/39/115/115	-
22	CLA	B	602	-	1/1/15/20	4/39/115/115	-
27	LFA	a	411	-	-	1/4/4/17	-
27	LFA	j	101	-	-	3/12/12/17	-
23	PHO	a	414	-	-	0/37/103/103	0/5/6/6
32	LHG	D	408	-	-	10/53/53/53	-
27	LFA	i	101	-	-	6/13/13/17	-
23	PHO	a	406	-	-	3/37/103/103	0/5/6/6
27	LFA	m	102	-	-	4/12/12/17	-
22	CLA	A	406	-	1/1/15/20	2/39/115/115	-
23	PHO	D	402	-	-	4/37/103/103	0/5/6/6
26	SQD	L	101	-	-	18/43/63/69	0/1/1/1
29	LMG	m	103	-	-	17/46/66/70	0/1/1/1
24	BCR	a	408	-	-	2/29/63/63	0/2/2/2
24	BCR	c	524	-	-	2/29/63/63	0/2/2/2
33	HEM	E	102	6,5	-	6/14/54/54	-
26	SQD	a	412	-	-	15/44/64/69	0/1/1/1
23	PHO	A	405	-	-	0/37/103/103	0/5/6/6
22	CLA	c	510	-	1/1/15/20	3/39/115/115	-
22	CLA	d	402	-	1/1/15/20	3/39/115/115	-
27	LFA	M	102	-	-	5/13/13/17	-
22	CLA	B	611	-	1/1/15/20	3/39/115/115	-
29	LMG	B	619	-	-	15/46/66/70	0/1/1/1
29	LMG	D	410	-	-	5/46/66/70	0/1/1/1
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
27	LFA	B	627	-	-	8/11/11/17	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
26	SQD	D	412	-	-	6/38/58/69	0/1/1/1
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	k	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/15/20	6/39/115/115	-
29	LMG	c	501	-	-	17/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/15/20	4/39/115/115	-
27	LFA	B	626	-	-	4/7/7/17	-
27	LFA	B	625	-	-	0/6/6/17	-
27	LFA	b	623	-	-	0/9/9/17	-
24	BCR	K	101	-	-	4/29/63/63	0/2/2/2
27	LFA	A	410	-	-	6/11/11/17	-
27	LFA	b	626	-	-	6/9/9/17	-
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
27	LFA	d	409	-	-	2/6/6/17	-
22	CLA	C	503	-	1/1/15/20	4/39/115/115	-
22	CLA	b	614	-	1/1/15/20	3/39/115/115	-
32	LHG	b	628	-	-	12/53/53/53	-
22	CLA	C	510	-	1/1/15/20	6/39/115/115	-
27	LFA	C	521	-	-	5/12/12/17	-
22	CLA	C	513	-	1/1/15/20	2/39/115/115	-
22	CLA	B	612	-	1/1/15/20	2/39/115/115	-
29	LMG	B	621	-	-	8/31/51/70	0/1/1/1
30	DGD	c	516	-	-	13/51/91/95	0/2/2/2
22	CLA	H	101	35	1/1/15/20	9/39/115/115	-
22	CLA	C	511	-	1/1/15/20	1/39/115/115	-
22	CLA	c	503	-	1/1/15/20	2/39/115/115	-
29	LMG	C	522	-	-	16/39/59/70	0/1/1/1
22	CLA	C	509	-	1/1/15/20	2/39/115/115	-
27	LFA	I	101	-	-	6/11/11/17	-
29	LMG	C	501	-	-	15/46/66/70	0/1/1/1
32	LHG	e	101	-	-	13/46/46/53	-
22	CLA	B	606	35	1/1/15/20	6/39/115/115	-
32	LHG	D	409	-	-	17/53/53/53	-
22	CLA	b	618	-	1/1/15/20	4/39/115/115	-
27	LFA	B	628	-	-	2/9/9/17	-
33	HEM	e	102	6,5	-	7/14/54/54	-
22	CLA	c	514	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/15/20	3/39/115/115	-
32	LHG	D	407	-	-	15/53/53/53	-
25	PL9	A	408	-	-	8/53/73/73	0/1/1/1
22	CLA	b	606	-	1/1/15/20	6/39/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
27	LFA	b	627	-	-	3/8/8/17	-
22	CLA	B	613	-	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	17/38/58/69	0/1/1/1
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
30	DGD	H	103	-	-	12/49/89/95	0/2/2/2
22	CLA	c	508	35	1/1/15/20	4/39/115/115	-
22	CLA	C	502	-	1/1/15/20	1/39/115/115	-
32	LHG	L	102	-	-	15/53/53/53	-
27	LFA	d	410	-	-	5/13/13/17	-
22	CLA	C	508	35	1/1/15/20	2/39/115/115	-
22	CLA	a	407	-	1/1/15/20	4/39/115/115	-
22	CLA	b	609	35	1/1/15/20	5/39/115/115	-
29	LMG	c	522	-	-	10/36/56/70	0/1/1/1
22	CLA	c	502	-	1/1/15/20	4/39/115/115	-
27	LFA	B	620	-	-	5/7/7/17	-
27	LFA	T	102	-	-	2/9/9/17	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
27	LFA	B	624	-	-	8/12/12/17	-
32	LHG	d	406	-	-	16/53/53/53	-
27	LFA	b	629	-	-	0/6/6/17	-
27	LFA	t	101	-	-	3/12/12/17	-
32	LHG	E	101	-	-	20/46/46/53	-
22	CLA	B	609	35	1/1/15/20	3/39/115/115	-
22	CLA	B	608	-	1/1/15/20	6/39/115/115	-
22	CLA	c	511	-	1/1/15/20	3/39/115/115	-
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	LFA	c	520	-	-	0/6/6/17	-
30	DGD	c	517	-	-	14/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	607	-	1/1/15/20	8/39/115/115	-
27	LFA	B	622	-	-	2/13/13/17	-
22	CLA	D	403	-	1/1/15/20	3/39/115/115	-
27	LFA	b	602	-	-	5/12/12/17	-
22	CLA	b	608	-	1/1/15/20	4/39/115/115	-
22	CLA	c	513	-	1/1/15/20	2/39/115/115	-
24	BCR	A	407	-	-	3/29/63/63	0/2/2/2
30	DGD	c	518	-	-	18/51/91/95	0/2/2/2
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	4/39/115/115	-
24	BCR	T	101	-	-	8/29/63/63	0/2/2/2
32	LHG	d	407	-	-	25/53/53/53	-
27	LFA	D	414	-	-	0/7/7/17	-
24	BCR	t	102	-	-	6/29/63/63	0/2/2/2
26	SQD	A	409	-	-	11/49/69/69	0/1/1/1
25	PL9	a	409	-	-	15/53/73/73	0/1/1/1
34	HEC	v	201	16	-	5/14/54/54	-
22	CLA	A	404	35	1/1/15/20	2/39/115/115	-
22	CLA	B	604	-	1/1/15/20	11/39/115/115	-
22	CLA	C	506	-	1/1/15/20	6/39/115/115	-
22	CLA	b	616	-	1/1/15/20	11/39/115/115	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	PL9	d	405	-	-	11/53/73/73	0/1/1/1
27	LFA	A	413	-	-	5/8/8/17	-
22	CLA	d	403	-	1/1/15/20	8/39/115/115	-
24	BCR	h	101	-	-	3/29/63/63	0/2/2/2
26	SQD	A	411	-	-	22/49/69/69	0/1/1/1
27	LFA	c	521	-	-	4/12/12/17	-
22	CLA	b	612	35	1/1/15/20	7/39/115/115	-
25	PL9	D	406	-	-	13/53/73/73	0/1/1/1
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
22	CLA	d	401	35	1/1/15/20	3/39/115/115	-
30	DGD	C	518	-	-	14/45/85/95	0/2/2/2
22	CLA	b	605	-	1/1/15/20	5/39/115/115	-
27	LFA	m	101	-	-	1/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	l	101	-	-	20/53/53/53	-
29	LMG	f	101	-	-	8/46/66/70	0/1/1/1
27	LFA	b	622	-	-	3/7/7/17	-

All (843) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	MG-ND	-8.30	1.89	2.05
22	A	406	CLA	MG-NB	-8.25	1.89	2.05
22	D	404	CLA	MG-NB	-8.11	1.89	2.05
22	d	403	CLA	MG-NB	-8.10	1.89	2.05
22	c	508	CLA	MG-NB	-8.07	1.89	2.05
22	b	615	CLA	MG-NB	-8.05	1.89	2.05
22	C	507	CLA	MG-ND	-8.05	1.89	2.05
22	a	407	CLA	MG-ND	-8.04	1.89	2.05
22	d	403	CLA	MG-ND	-8.02	1.89	2.05
22	b	614	CLA	MG-ND	-7.81	1.90	2.05
22	B	606	CLA	MG-ND	-7.79	1.90	2.05
22	C	510	CLA	MG-ND	-7.75	1.90	2.05
22	c	514	CLA	MG-NB	-7.74	1.90	2.05
22	C	505	CLA	MG-NB	-7.59	1.90	2.05
22	c	510	CLA	MG-ND	-7.51	1.90	2.05
22	B	609	CLA	MG-ND	-7.51	1.90	2.05
22	C	510	CLA	MG-NB	-7.50	1.90	2.05
22	a	407	CLA	MG-NB	-7.47	1.91	2.05
22	B	611	CLA	MG-NB	-7.46	1.91	2.05
22	D	404	CLA	MG-ND	-7.40	1.91	2.05
22	b	612	CLA	MG-NB	-7.37	1.91	2.05
22	B	610	CLA	MG-NB	-7.35	1.91	2.05
22	C	505	CLA	MG-ND	-7.34	1.91	2.05
22	C	502	CLA	MG-ND	-7.30	1.91	2.05
22	c	502	CLA	MG-ND	-7.29	1.91	2.05
22	A	406	CLA	MG-ND	-7.29	1.91	2.05
22	b	611	CLA	MG-NB	-7.28	1.91	2.05
22	c	503	CLA	MG-ND	-7.26	1.91	2.05
22	c	502	CLA	MG-NB	-7.25	1.91	2.05
22	C	508	CLA	MG-ND	-7.23	1.91	2.05
22	C	502	CLA	MG-NB	-7.23	1.91	2.05
22	C	514	CLA	MG-NB	-7.20	1.91	2.05
22	c	507	CLA	MG-ND	-7.17	1.91	2.05
22	b	611	CLA	MG-ND	-7.16	1.91	2.05
22	c	514	CLA	MG-ND	-7.14	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	MG-NB	-7.12	1.91	2.05
22	B	615	CLA	MG-NB	-7.08	1.91	2.05
22	A	404	CLA	MG-ND	-7.06	1.91	2.05
22	b	605	CLA	MG-NB	-7.04	1.91	2.05
22	H	101	CLA	MG-NB	-7.03	1.91	2.05
22	C	514	CLA	MG-ND	-7.00	1.91	2.05
22	b	609	CLA	MG-NB	-7.00	1.91	2.05
22	c	503	CLA	MG-NB	-6.98	1.91	2.05
22	c	505	CLA	MG-NB	-6.97	1.92	2.05
22	b	605	CLA	MG-ND	-6.93	1.92	2.05
22	c	511	CLA	MG-NB	-6.88	1.92	2.05
22	B	603	CLA	MG-NB	-6.86	1.92	2.05
22	B	608	CLA	MG-ND	-6.85	1.92	2.05
22	b	604	CLA	MG-NB	-6.82	1.92	2.05
22	b	606	CLA	MG-NB	-6.71	1.92	2.05
22	c	505	CLA	MG-ND	-6.70	1.92	2.05
22	C	509	CLA	MG-NB	-6.70	1.92	2.05
22	c	512	CLA	MG-NB	-6.68	1.92	2.05
22	b	618	CLA	MG-ND	-6.67	1.92	2.05
22	b	616	CLA	MG-NB	-6.65	1.92	2.05
22	C	508	CLA	MG-NB	-6.60	1.92	2.05
22	c	509	CLA	MG-NB	-6.60	1.92	2.05
22	C	507	CLA	MG-NB	-6.59	1.92	2.05
22	b	608	CLA	MG-NB	-6.58	1.92	2.05
22	H	101	CLA	MG-ND	-6.57	1.92	2.05
22	C	512	CLA	MG-NB	-6.57	1.92	2.05
22	B	611	CLA	MG-ND	-6.57	1.92	2.05
22	d	401	CLA	MG-ND	-6.54	1.92	2.05
22	c	510	CLA	MG-NB	-6.53	1.92	2.05
22	b	603	CLA	MG-ND	-6.53	1.92	2.05
22	b	618	CLA	MG-NB	-6.53	1.92	2.05
22	c	507	CLA	MG-NB	-6.52	1.92	2.05
22	b	608	CLA	MG-ND	-6.52	1.92	2.05
22	B	609	CLA	MG-NB	-6.51	1.92	2.05
22	C	513	CLA	MG-NB	-6.47	1.93	2.05
22	D	403	CLA	MG-NB	-6.45	1.93	2.05
22	b	613	CLA	MG-NB	-6.43	1.93	2.05
22	a	405	CLA	MG-ND	-6.42	1.93	2.05
22	c	506	CLA	MG-NB	-6.41	1.93	2.05
22	b	612	CLA	MG-ND	-6.41	1.93	2.05
22	B	606	CLA	MG-NB	-6.40	1.93	2.05
22	C	511	CLA	MG-NB	-6.38	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	MG-ND	-6.38	1.93	2.05
22	b	603	CLA	MG-NB	-6.37	1.93	2.05
22	C	503	CLA	MG-NB	-6.37	1.93	2.05
22	d	401	CLA	MG-NB	-6.35	1.93	2.05
22	C	513	CLA	MG-ND	-6.35	1.93	2.05
22	B	608	CLA	MG-NB	-6.34	1.93	2.05
22	c	513	CLA	MG-ND	-6.27	1.93	2.05
22	c	508	CLA	MG-ND	-6.27	1.93	2.05
22	c	512	CLA	MG-ND	-6.24	1.93	2.05
22	c	513	CLA	MG-NB	-6.23	1.93	2.05
22	b	615	CLA	MG-ND	-6.22	1.93	2.05
22	C	503	CLA	MG-ND	-6.22	1.93	2.05
22	B	612	CLA	MG-NB	-6.22	1.93	2.05
23	a	414	PHO	C3A-C2A	-6.21	1.49	1.54
22	C	512	CLA	MG-ND	-6.20	1.93	2.05
22	c	511	CLA	MG-ND	-6.18	1.93	2.05
22	C	511	CLA	MG-ND	-6.12	1.93	2.05
22	B	602	CLA	MG-ND	-6.10	1.93	2.05
22	d	402	CLA	MG-ND	-6.10	1.93	2.05
22	a	404	CLA	MG-ND	-6.09	1.93	2.05
22	c	504	CLA	MG-NB	-6.09	1.93	2.05
22	B	602	CLA	MG-NB	-6.08	1.93	2.05
22	B	601	CLA	MG-NB	-6.07	1.93	2.05
22	B	604	CLA	C4B-NB	6.04	1.45	1.37
22	B	612	CLA	MG-ND	-6.00	1.93	2.05
22	C	504	CLA	MG-ND	-6.00	1.93	2.05
22	A	403	CLA	MG-NB	-5.99	1.93	2.05
22	b	606	CLA	MG-ND	-5.98	1.93	2.05
22	B	615	CLA	MG-ND	-5.96	1.94	2.05
22	C	506	CLA	MG-ND	-5.92	1.94	2.05
22	b	604	CLA	MG-ND	-5.90	1.94	2.05
22	a	404	CLA	MG-NB	-5.88	1.94	2.05
22	A	412	CLA	MG-NB	-5.84	1.94	2.05
22	C	509	CLA	MG-ND	-5.82	1.94	2.05
22	c	504	CLA	MG-ND	-5.78	1.94	2.05
22	C	506	CLA	MG-NB	-5.75	1.94	2.05
22	B	613	CLA	C4B-NB	5.75	1.45	1.37
22	B	601	CLA	C4B-NB	5.70	1.45	1.37
22	c	504	CLA	C4B-NB	5.69	1.45	1.37
22	b	610	CLA	MG-NB	-5.67	1.94	2.05
22	B	606	CLA	MG-NC	-5.63	1.92	2.06
22	b	607	CLA	C4B-NB	5.62	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	MG-ND	-5.62	1.94	2.05
22	C	504	CLA	C4B-NB	5.57	1.45	1.37
22	A	404	CLA	MG-NB	-5.52	1.94	2.05
22	B	613	CLA	MG-ND	-5.49	1.94	2.05
34	V	201	HEC	CBC-CAC	-5.48	1.29	1.49
22	B	601	CLA	MG-ND	-5.48	1.94	2.05
22	b	603	CLA	C4B-NB	5.47	1.45	1.37
34	V	201	HEC	CBB-CAB	-5.47	1.29	1.49
22	A	412	CLA	MG-ND	-5.44	1.95	2.05
34	v	201	HEC	CBC-CAC	-5.43	1.29	1.49
22	b	617	CLA	MG-NB	-5.43	1.95	2.05
34	v	201	HEC	CBB-CAB	-5.43	1.29	1.49
22	c	509	CLA	MG-ND	-5.39	1.95	2.05
22	c	507	CLA	C4B-NB	5.38	1.44	1.37
22	b	618	CLA	MG-NC	-5.34	1.93	2.06
22	b	609	CLA	MG-NC	-5.33	1.93	2.06
22	B	603	CLA	MG-ND	-5.33	1.95	2.05
22	B	608	CLA	C4B-NB	5.30	1.44	1.37
22	a	407	CLA	MG-NC	-5.30	1.93	2.06
22	C	507	CLA	MG-NC	-5.29	1.93	2.06
22	B	613	CLA	MG-NB	-5.28	1.95	2.05
22	B	605	CLA	MG-NB	-5.28	1.95	2.05
22	D	403	CLA	MG-ND	-5.21	1.95	2.05
22	b	610	CLA	MG-ND	-5.21	1.95	2.05
22	b	616	CLA	C4B-NB	5.20	1.44	1.37
22	C	506	CLA	C4B-NB	5.19	1.44	1.37
22	C	508	CLA	MG-NC	-5.19	1.94	2.06
22	A	406	CLA	MG-NC	-5.18	1.94	2.06
22	b	617	CLA	MG-ND	-5.17	1.95	2.05
22	A	403	CLA	MG-ND	-5.14	1.95	2.05
22	B	607	CLA	MG-NB	-5.13	1.95	2.05
22	b	612	CLA	MG-NC	-5.09	1.94	2.06
22	b	615	CLA	MG-NC	-5.09	1.94	2.06
22	B	615	CLA	MG-NC	-5.05	1.94	2.06
22	A	406	CLA	MG-NA	-5.04	1.94	2.06
22	D	404	CLA	MG-NC	-5.04	1.94	2.06
22	H	101	CLA	C4B-NB	5.02	1.44	1.37
22	C	513	CLA	C4B-NB	5.00	1.44	1.37
22	B	602	CLA	C4B-NB	5.00	1.44	1.37
22	b	616	CLA	MG-ND	-4.99	1.95	2.05
22	D	403	CLA	MG-NC	-4.98	1.94	2.06
22	b	613	CLA	MG-NC	-4.94	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	MG-NC	-4.93	1.94	2.06
23	a	406	PHO	C1B-C2B	4.93	1.45	1.39
23	A	405	PHO	C3A-C2A	-4.91	1.50	1.54
22	b	617	CLA	MG-NC	-4.89	1.94	2.06
22	B	607	CLA	MG-NC	-4.89	1.94	2.06
22	B	607	CLA	C4B-NB	4.89	1.44	1.37
22	c	503	CLA	MG-NC	-4.85	1.94	2.06
22	d	402	CLA	MG-NB	-4.85	1.96	2.05
22	c	505	CLA	MG-NC	-4.82	1.94	2.06
22	C	511	CLA	C4B-NB	4.81	1.44	1.37
22	B	604	CLA	MG-NC	-4.79	1.94	2.06
22	C	503	CLA	MG-NC	-4.79	1.94	2.06
22	b	611	CLA	C4B-NB	4.79	1.44	1.37
22	B	603	CLA	C4B-NB	4.78	1.44	1.37
22	B	609	CLA	C4B-NB	4.77	1.44	1.37
22	c	509	CLA	MG-NC	-4.77	1.94	2.06
22	c	506	CLA	C4B-NB	4.74	1.44	1.37
22	B	604	CLA	MG-ND	-4.73	1.96	2.05
22	b	612	CLA	C3A-C2A	-4.72	1.41	1.54
22	b	606	CLA	C4B-NB	4.70	1.44	1.37
22	d	403	CLA	MG-NC	-4.70	1.95	2.06
22	b	614	CLA	MG-NA	-4.70	1.95	2.06
22	A	412	CLA	MG-NC	-4.67	1.95	2.06
22	B	609	CLA	C3A-C2A	-4.67	1.41	1.54
22	b	604	CLA	MG-NC	-4.67	1.95	2.06
23	a	414	PHO	C1B-C2B	4.65	1.44	1.39
22	B	614	CLA	MG-ND	-4.65	1.96	2.05
22	B	611	CLA	MG-NA	-4.64	1.95	2.06
22	D	403	CLA	C4B-NB	4.63	1.43	1.37
26	L	101	SQD	O8-S	4.62	1.64	1.47
22	B	601	CLA	MG-NC	-4.62	1.95	2.06
22	c	513	CLA	MG-NC	-4.62	1.95	2.06
22	C	512	CLA	C4B-NB	4.61	1.43	1.37
23	D	402	PHO	C1B-C2B	4.61	1.44	1.39
22	c	502	CLA	MG-NC	-4.61	1.95	2.06
23	D	402	PHO	C3B-C2B	-4.59	1.34	1.40
22	a	405	CLA	MG-NB	-4.59	1.96	2.05
22	b	607	CLA	MG-ND	-4.58	1.96	2.05
22	c	502	CLA	C4B-NB	4.57	1.43	1.37
22	b	615	CLA	C4B-NB	4.57	1.43	1.37
22	C	513	CLA	MG-NC	-4.55	1.95	2.06
22	B	614	CLA	C4B-NB	4.55	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	MG-NC	-4.53	1.95	2.06
22	b	614	CLA	MG-NC	-4.53	1.95	2.06
22	c	514	CLA	MG-NC	-4.53	1.95	2.06
29	b	624	LMG	O8-C28	4.53	1.46	1.33
22	b	605	CLA	MG-NC	-4.52	1.95	2.06
22	C	502	CLA	MG-NC	-4.51	1.95	2.06
34	v	201	HEC	CAB-C3B	4.49	1.49	1.35
22	B	609	CLA	MG-NC	-4.47	1.95	2.06
22	C	504	CLA	MG-NB	-4.45	1.97	2.05
22	d	402	CLA	MG-NA	-4.45	1.95	2.06
22	c	508	CLA	C4B-NB	4.45	1.43	1.37
22	B	615	CLA	C4B-NB	4.44	1.43	1.37
22	B	610	CLA	MG-NC	-4.42	1.95	2.06
22	B	613	CLA	MG-NC	-4.42	1.95	2.06
22	C	509	CLA	MG-NC	-4.42	1.95	2.06
22	c	509	CLA	C4B-NB	4.40	1.43	1.37
34	V	201	HEC	CAB-C3B	4.39	1.49	1.35
22	b	608	CLA	MG-NC	-4.38	1.95	2.06
26	A	411	SQD	O8-S	4.38	1.63	1.47
22	d	403	CLA	MG-NA	-4.38	1.95	2.06
22	A	404	CLA	C4B-NB	4.37	1.43	1.37
32	L	102	LHG	O8-C23	4.36	1.46	1.33
22	b	607	CLA	MG-NC	-4.35	1.95	2.06
22	c	511	CLA	C4B-NB	4.34	1.43	1.37
22	B	614	CLA	MG-NC	-4.34	1.96	2.06
22	C	509	CLA	C4B-NB	4.33	1.43	1.37
22	a	404	CLA	MG-NC	-4.33	1.96	2.06
22	c	506	CLA	MG-NC	-4.32	1.96	2.06
22	C	510	CLA	MG-NC	-4.31	1.96	2.06
22	B	605	CLA	C4B-NB	4.29	1.43	1.37
29	D	410	LMG	O8-C28	4.28	1.45	1.33
22	c	514	CLA	MG-NA	-4.28	1.96	2.06
22	d	402	CLA	MG-NC	-4.27	1.96	2.06
26	D	412	SQD	O47-C7	4.27	1.46	1.34
22	b	607	CLA	MG-NB	-4.27	1.97	2.05
29	C	522	LMG	O7-C10	4.26	1.46	1.34
22	C	514	CLA	MG-NC	-4.26	1.96	2.06
34	v	201	HEC	CAC-C3C	4.25	1.48	1.35
29	C	520	LMG	O8-C28	4.25	1.45	1.33
22	C	507	CLA	C4B-NB	4.25	1.43	1.37
22	c	511	CLA	MG-NC	-4.25	1.96	2.06
22	c	508	CLA	MG-NC	-4.24	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	410	LMG	O7-C10	4.24	1.46	1.34
22	b	610	CLA	MG-NC	-4.23	1.96	2.06
22	B	611	CLA	C4B-NB	4.23	1.43	1.37
22	B	610	CLA	MG-ND	-4.23	1.97	2.05
32	E	101	LHG	O8-C23	4.23	1.45	1.33
22	A	403	CLA	C4B-NB	4.23	1.43	1.37
26	b	601	SQD	O8-S	4.22	1.63	1.47
22	c	513	CLA	C4B-NB	4.22	1.43	1.37
29	c	522	LMG	O7-C10	4.20	1.46	1.34
23	A	405	PHO	C1B-C2B	4.20	1.44	1.39
22	d	401	CLA	MG-NC	-4.19	1.96	2.06
22	b	617	CLA	C4B-NB	4.17	1.43	1.37
22	b	615	CLA	C3A-C2A	-4.17	1.43	1.54
22	B	612	CLA	MG-NC	-4.17	1.96	2.06
29	B	619	LMG	O7-C10	4.17	1.46	1.34
29	c	519	LMG	O8-C28	4.17	1.45	1.33
22	C	505	CLA	MG-NC	-4.16	1.96	2.06
22	b	605	CLA	C4B-NB	4.15	1.43	1.37
22	A	412	CLA	MG-NA	-4.15	1.96	2.06
22	b	608	CLA	C4B-NB	4.14	1.43	1.37
22	b	613	CLA	MG-ND	-4.13	1.97	2.05
22	C	511	CLA	MG-NC	-4.12	1.96	2.06
22	c	504	CLA	MG-NC	-4.10	1.96	2.06
22	B	602	CLA	MG-NC	-4.10	1.96	2.06
26	a	410	SQD	O8-S	4.09	1.62	1.47
22	c	512	CLA	C4B-NB	4.09	1.43	1.37
22	C	514	CLA	C4B-NB	4.09	1.43	1.37
22	B	612	CLA	C3A-C2A	-4.08	1.43	1.54
29	C	501	LMG	O8-C28	4.07	1.45	1.33
26	a	410	SQD	O48-C23	4.07	1.45	1.33
30	H	103	DGD	O1G-C1A	4.06	1.45	1.33
32	E	101	LHG	O7-C7	4.05	1.45	1.34
22	A	403	CLA	MG-NC	-4.05	1.96	2.06
22	b	611	CLA	MG-NC	-4.05	1.96	2.06
26	f	102	SQD	O48-C23	4.05	1.45	1.33
22	c	510	CLA	MG-NA	-4.04	1.96	2.06
29	f	101	LMG	O8-C28	4.04	1.45	1.33
22	c	514	CLA	C4B-NB	4.03	1.43	1.37
22	a	407	CLA	MG-NA	-4.03	1.96	2.06
30	c	518	DGD	O2G-C1B	4.03	1.45	1.34
22	B	605	CLA	MG-NC	-4.03	1.96	2.06
22	c	510	CLA	MG-NC	-4.03	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C4B-NB	4.02	1.43	1.37
22	D	403	CLA	C3A-C2A	-4.02	1.43	1.54
22	c	507	CLA	MG-NC	-4.02	1.96	2.06
22	a	405	CLA	MG-NC	-4.02	1.96	2.06
26	A	409	SQD	O8-S	4.02	1.62	1.47
22	C	510	CLA	MG-NA	-4.01	1.96	2.06
26	f	102	SQD	O8-S	4.01	1.62	1.47
29	c	522	LMG	O8-C28	4.00	1.45	1.33
34	V	201	HEC	CAC-C3C	3.99	1.47	1.35
29	B	619	LMG	O8-C28	3.99	1.45	1.33
30	c	516	DGD	O1G-C1A	3.99	1.45	1.33
30	c	517	DGD	O1G-C1A	3.98	1.45	1.33
32	e	101	LHG	O8-C23	3.98	1.44	1.33
29	b	624	LMG	O7-C10	3.98	1.45	1.34
26	L	101	SQD	O47-C7	3.96	1.45	1.34
32	d	406	LHG	O7-C7	3.95	1.45	1.34
22	C	503	CLA	C4B-NB	3.95	1.43	1.37
22	C	508	CLA	C3A-C2A	-3.95	1.43	1.54
22	C	512	CLA	MG-NC	-3.94	1.96	2.06
22	b	616	CLA	MG-NC	-3.94	1.96	2.06
32	e	101	LHG	O7-C7	3.94	1.45	1.34
22	b	613	CLA	C4B-NB	3.94	1.43	1.37
22	B	614	CLA	MG-NB	-3.93	1.98	2.05
22	B	603	CLA	MG-NC	-3.93	1.96	2.06
22	C	508	CLA	MG-NA	-3.93	1.96	2.06
22	c	510	CLA	C4B-NB	3.92	1.43	1.37
22	A	403	CLA	C3A-C2A	-3.92	1.43	1.54
22	B	607	CLA	MG-ND	-3.92	1.98	2.05
29	C	522	LMG	O8-C28	3.91	1.44	1.33
29	c	501	LMG	O8-C28	3.91	1.44	1.33
26	a	412	SQD	O47-C7	3.90	1.45	1.34
22	A	403	CLA	MG-NA	-3.89	1.97	2.06
26	D	412	SQD	O8-S	3.88	1.61	1.47
26	L	101	SQD	O48-C23	3.87	1.44	1.33
29	B	621	LMG	O7-C10	3.86	1.45	1.34
30	h	102	DGD	O1G-C1A	3.86	1.44	1.33
30	C	518	DGD	O1G-C1A	3.85	1.44	1.33
26	A	409	SQD	O48-C23	3.85	1.44	1.33
22	C	505	CLA	C4B-NB	3.84	1.42	1.37
30	c	518	DGD	O1G-C1A	3.84	1.44	1.33
29	C	520	LMG	O7-C10	3.84	1.45	1.34
26	D	412	SQD	O48-C23	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	411	SQD	O48-C23	3.81	1.44	1.33
32	b	628	LHG	O8-C23	3.81	1.44	1.33
26	b	601	SQD	O48-C23	3.81	1.44	1.33
22	c	503	CLA	C4B-NB	3.80	1.42	1.37
29	c	519	LMG	O7-C10	3.80	1.45	1.34
22	b	612	CLA	MG-NA	-3.80	1.97	2.06
22	c	511	CLA	C3A-C2A	-3.80	1.44	1.54
22	H	101	CLA	MG-NC	-3.80	1.97	2.06
30	C	518	DGD	O2G-C1B	3.79	1.45	1.34
29	C	501	LMG	O7-C10	3.78	1.45	1.34
30	C	517	DGD	O1G-C1A	3.78	1.44	1.33
29	B	621	LMG	O8-C28	3.77	1.44	1.33
33	e	102	HEM	FE-ND	3.77	2.06	1.94
26	a	412	SQD	O48-C23	3.77	1.44	1.33
22	b	610	CLA	C4B-NB	3.76	1.42	1.37
22	B	609	CLA	MG-NA	-3.76	1.97	2.06
26	A	411	SQD	O47-C7	3.75	1.44	1.34
26	f	102	SQD	O47-C7	3.74	1.44	1.34
26	b	601	SQD	O47-C7	3.74	1.44	1.34
22	a	405	CLA	C4B-NB	3.74	1.42	1.37
30	c	517	DGD	O2G-C1B	3.74	1.44	1.34
26	A	409	SQD	O47-C7	3.74	1.44	1.34
32	d	407	LHG	O7-C7	3.73	1.44	1.34
22	c	513	CLA	MG-NA	-3.73	1.97	2.06
22	b	610	CLA	MG-NA	-3.72	1.97	2.06
22	B	607	CLA	MG-NA	-3.72	1.97	2.06
29	f	101	LMG	O7-C10	3.70	1.44	1.34
22	B	612	CLA	C4B-NB	3.70	1.42	1.37
26	a	410	SQD	O47-C7	3.70	1.44	1.34
22	b	610	CLA	C3A-C2A	-3.70	1.44	1.54
22	C	503	CLA	MG-NA	-3.69	1.97	2.06
29	m	103	LMG	O8-C28	3.67	1.44	1.33
22	C	510	CLA	C4B-NB	3.67	1.42	1.37
22	C	508	CLA	C4B-NB	3.66	1.42	1.37
22	c	509	CLA	MG-NA	-3.65	1.97	2.06
22	b	604	CLA	C4B-NB	3.65	1.42	1.37
22	a	404	CLA	C3A-C2A	-3.65	1.44	1.54
22	C	504	CLA	MG-NC	-3.64	1.97	2.06
22	B	608	CLA	MG-NC	-3.60	1.97	2.06
22	C	513	CLA	MG-NA	-3.59	1.97	2.06
30	C	519	DGD	O1G-C1A	3.58	1.43	1.33
22	d	401	CLA	MG-NA	-3.58	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	MG-NA	-3.57	1.97	2.06
30	h	102	DGD	O2G-C1B	3.57	1.44	1.34
22	B	606	CLA	MG-NA	-3.57	1.97	2.06
30	C	519	DGD	O2G-C1B	3.57	1.44	1.34
22	d	401	CLA	C4B-NB	3.56	1.42	1.37
22	C	505	CLA	MG-NA	-3.55	1.97	2.06
32	D	409	LHG	O8-C23	3.55	1.43	1.33
32	D	407	LHG	O8-C23	3.54	1.43	1.33
29	c	501	LMG	O7-C10	3.54	1.44	1.34
30	C	517	DGD	O2G-C1B	3.53	1.44	1.34
32	L	102	LHG	O7-C7	3.53	1.44	1.34
22	b	615	CLA	C1D-C2D	-3.53	1.38	1.45
22	c	512	CLA	MG-NC	-3.52	1.97	2.06
22	C	514	CLA	MG-NA	-3.52	1.97	2.06
30	H	103	DGD	O2G-C1B	3.52	1.44	1.34
22	D	404	CLA	C4B-NB	3.52	1.42	1.37
22	D	404	CLA	MG-NA	-3.50	1.98	2.06
32	l	101	LHG	O8-C23	3.49	1.43	1.33
32	d	407	LHG	O8-C23	3.49	1.43	1.33
22	C	506	CLA	MG-NA	-3.49	1.98	2.06
22	c	505	CLA	MG-NA	-3.48	1.98	2.06
32	D	408	LHG	O8-C23	3.46	1.43	1.33
22	b	603	CLA	MG-NC	-3.45	1.98	2.06
22	B	610	CLA	MG-NA	-3.45	1.98	2.06
22	A	406	CLA	C3A-C2A	-3.41	1.45	1.54
23	a	414	PHO	C3B-C4B	3.40	1.45	1.41
22	B	610	CLA	C4B-NB	3.39	1.42	1.37
22	b	618	CLA	MG-NA	-3.38	1.98	2.06
32	l	101	LHG	O7-C7	3.38	1.43	1.34
23	a	406	PHO	C3B-C2B	-3.38	1.35	1.40
22	a	405	CLA	C3A-C2A	-3.38	1.45	1.54
22	b	617	CLA	MG-NA	-3.38	1.98	2.06
22	B	615	CLA	C3A-C2A	-3.37	1.45	1.54
32	D	409	LHG	O7-C7	3.36	1.43	1.34
22	B	611	CLA	MG-NC	-3.36	1.98	2.06
22	C	502	CLA	C3A-C2A	-3.34	1.45	1.54
22	B	601	CLA	MG-NA	-3.34	1.98	2.06
22	C	510	CLA	C1D-C2D	-3.33	1.38	1.45
32	b	628	LHG	O7-C7	3.32	1.43	1.34
22	b	615	CLA	MG-NA	-3.32	1.98	2.06
32	D	407	LHG	O7-C7	3.32	1.43	1.34
29	m	103	LMG	O7-C10	3.31	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C4B-NB	3.30	1.42	1.37
22	a	404	CLA	MG-NA	-3.30	1.98	2.06
24	C	516	BCR	C1-C6	-3.28	1.49	1.53
22	b	604	CLA	MG-NA	-3.25	1.98	2.06
22	A	406	CLA	C1D-C2D	-3.24	1.38	1.45
22	C	509	CLA	MG-NA	-3.24	1.98	2.06
22	c	503	CLA	MG-NA	-3.23	1.98	2.06
22	C	508	CLA	C1D-C2D	-3.22	1.39	1.45
22	c	511	CLA	MG-NA	-3.22	1.98	2.06
22	C	511	CLA	MG-NA	-3.22	1.98	2.06
22	B	612	CLA	C1D-C2D	-3.20	1.39	1.45
22	a	404	CLA	C4B-NB	3.18	1.42	1.37
22	D	404	CLA	C1D-C2D	-3.17	1.39	1.45
22	b	614	CLA	C3A-C2A	-3.17	1.45	1.54
22	B	609	CLA	C1D-C2D	-3.16	1.39	1.45
23	A	405	PHO	C3D-C4D	-3.16	1.36	1.41
23	D	402	PHO	C3A-C2A	-3.16	1.52	1.54
22	d	403	CLA	C1D-C2D	-3.15	1.39	1.45
22	b	609	CLA	C1D-C2D	-3.15	1.39	1.45
22	b	607	CLA	MG-NA	-3.14	1.98	2.06
22	B	606	CLA	C1D-C2D	-3.13	1.39	1.45
22	D	403	CLA	MG-NA	-3.12	1.98	2.06
23	A	405	PHO	C3B-C2B	-3.11	1.36	1.40
22	c	508	CLA	MG-NA	-3.10	1.98	2.06
22	c	508	CLA	C3A-C2A	-3.10	1.46	1.54
22	a	407	CLA	C1D-C2D	-3.09	1.39	1.45
22	B	607	CLA	C3D-C4D	-3.09	1.37	1.44
22	b	613	CLA	MG-NA	-3.08	1.98	2.06
22	B	606	CLA	CHD-C4C	-3.07	1.32	1.39
33	E	102	HEM	FE-ND	3.06	2.04	1.94
22	B	604	CLA	MG-NB	-3.06	1.99	2.05
22	c	512	CLA	MG-NA	-3.05	1.99	2.06
22	b	607	CLA	C3A-C2A	-3.05	1.46	1.54
22	C	513	CLA	C1D-C2D	-3.04	1.39	1.45
23	a	406	PHO	C3B-C4B	3.03	1.44	1.41
30	c	516	DGD	O2G-C1B	3.03	1.42	1.34
22	d	402	CLA	C4B-NB	3.03	1.41	1.37
22	c	505	CLA	C4B-NB	3.02	1.41	1.37
22	c	506	CLA	MG-NA	-3.02	1.99	2.06
32	D	408	LHG	O7-C7	3.02	1.42	1.34
22	A	404	CLA	C3D-C4D	-3.01	1.37	1.44
22	a	407	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	C1D-C2D	-3.01	1.39	1.45
23	D	402	PHO	C3B-C4B	3.01	1.44	1.41
22	B	604	CLA	C3D-C4D	-2.99	1.37	1.44
22	b	606	CLA	C3A-C2A	-2.99	1.46	1.54
22	b	605	CLA	C1D-C2D	-2.98	1.39	1.45
22	b	618	CLA	C4B-NB	2.98	1.41	1.37
22	A	406	CLA	CHD-C4C	-2.97	1.32	1.39
22	b	603	CLA	MG-NA	-2.97	1.99	2.06
22	C	506	CLA	C1D-C2D	-2.96	1.39	1.45
22	c	504	CLA	C1D-C2D	-2.95	1.39	1.45
33	e	102	HEM	FE-NA	2.94	2.04	1.95
32	d	406	LHG	O8-C23	2.94	1.41	1.33
22	B	602	CLA	C1D-C2D	-2.94	1.39	1.45
22	B	606	CLA	C3B-C2B	-2.94	1.31	1.41
22	C	505	CLA	C1D-C2D	-2.94	1.39	1.45
22	B	615	CLA	C1D-C2D	-2.93	1.39	1.45
22	b	612	CLA	C1D-C2D	-2.93	1.39	1.45
22	C	505	CLA	C3A-C2A	-2.92	1.46	1.54
22	d	402	CLA	C1D-C2D	-2.92	1.39	1.45
22	C	507	CLA	C1D-C2D	-2.91	1.39	1.45
33	e	102	HEM	C3D-C2D	2.90	1.43	1.36
24	K	102	BCR	C30-C25	-2.89	1.50	1.53
22	B	611	CLA	C3D-C4D	-2.89	1.37	1.44
24	B	618	BCR	C1-C6	-2.88	1.50	1.53
22	b	604	CLA	C1D-C2D	-2.88	1.39	1.45
22	C	504	CLA	C1D-C2D	-2.88	1.39	1.45
22	c	503	CLA	C1D-C2D	-2.88	1.39	1.45
22	b	611	CLA	MG-NA	-2.88	1.99	2.06
22	b	608	CLA	MG-NA	-2.88	1.99	2.06
22	b	618	CLA	C1D-C2D	-2.88	1.39	1.45
22	C	509	CLA	C1D-C2D	-2.88	1.39	1.45
33	E	102	HEM	FE-NB	2.87	2.03	1.94
23	A	405	PHO	C3B-C4B	2.87	1.44	1.41
22	H	101	CLA	MG-NA	-2.87	1.99	2.06
22	b	617	CLA	C1D-C2D	-2.87	1.39	1.45
22	b	608	CLA	C1D-C2D	-2.87	1.39	1.45
22	B	608	CLA	C1D-C2D	-2.86	1.39	1.45
32	D	407	LHG	O7-C5	-2.85	1.39	1.46
22	b	609	CLA	MG-NA	-2.84	1.99	2.06
22	b	614	CLA	C1D-C2D	-2.84	1.39	1.45
22	b	618	CLA	C3A-C2A	-2.84	1.46	1.54
22	C	503	CLA	C1D-C2D	-2.84	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C1D-C2D	-2.84	1.39	1.45
22	c	514	CLA	C1D-C2D	-2.84	1.39	1.45
34	V	201	HEC	O2D-CGD	-2.84	1.21	1.30
22	c	510	CLA	C3A-C2A	-2.83	1.46	1.54
22	b	615	CLA	C4C-C3C	-2.82	1.40	1.45
22	c	506	CLA	C1D-C2D	-2.82	1.39	1.45
33	e	102	HEM	FE-NB	2.82	2.03	1.94
22	B	615	CLA	MG-NA	-2.82	1.99	2.06
22	c	502	CLA	C3A-C2A	-2.82	1.46	1.54
22	C	504	CLA	MG-NA	-2.82	1.99	2.06
24	k	101	BCR	C1-C6	-2.82	1.50	1.53
23	a	414	PHO	C3B-C2B	-2.81	1.36	1.40
22	c	508	CLA	C1D-C2D	-2.80	1.39	1.45
22	c	504	CLA	MG-NA	-2.80	1.99	2.06
22	C	502	CLA	C1D-C2D	-2.80	1.39	1.45
34	v	201	HEC	C3C-C2C	-2.79	1.31	1.41
24	c	523	BCR	C1-C6	-2.79	1.50	1.53
22	d	401	CLA	C4C-C3C	2.79	1.49	1.45
22	C	506	CLA	C3D-C4D	-2.78	1.37	1.44
22	C	514	CLA	C1D-C2D	-2.78	1.39	1.45
22	b	609	CLA	CHD-C4C	-2.77	1.32	1.39
22	C	512	CLA	C1D-C2D	-2.76	1.39	1.45
22	d	401	CLA	C3D-C4D	-2.76	1.38	1.44
22	c	511	CLA	C1D-C2D	-2.76	1.39	1.45
22	b	606	CLA	C1D-C2D	-2.76	1.39	1.45
22	a	405	CLA	MG-NA	-2.76	1.99	2.06
22	b	611	CLA	C1D-C2D	-2.75	1.39	1.45
22	A	406	CLA	C3B-C2B	-2.75	1.31	1.41
22	c	502	CLA	C1D-C2D	-2.75	1.39	1.45
22	C	512	CLA	MG-NA	-2.75	1.99	2.06
22	b	614	CLA	CHC-C1C	-2.74	1.33	1.38
22	b	609	CLA	C4B-NB	2.74	1.41	1.37
34	V	201	HEC	C3C-C2C	-2.74	1.31	1.41
34	v	201	HEC	O2D-CGD	-2.74	1.21	1.30
22	B	602	CLA	C3D-C4D	-2.74	1.38	1.44
22	b	613	CLA	C3D-C4D	-2.74	1.38	1.44
22	H	101	CLA	C1D-C2D	-2.73	1.39	1.45
29	C	522	LMG	O1-C1	2.73	1.44	1.40
22	b	612	CLA	C3D-C4D	-2.73	1.38	1.44
22	b	610	CLA	C3D-C4D	-2.73	1.38	1.44
22	d	403	CLA	C4B-NB	2.73	1.41	1.37
22	c	509	CLA	C1D-C2D	-2.73	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	C3D-C4D	-2.72	1.38	1.44
24	t	102	BCR	C30-C25	-2.72	1.50	1.53
24	B	617	BCR	C1-C6	-2.72	1.50	1.53
22	B	608	CLA	C3D-C4D	-2.72	1.38	1.44
22	B	610	CLA	C3D-C4D	-2.71	1.38	1.44
32	D	408	LHG	O7-C5	-2.71	1.40	1.46
22	B	606	CLA	C3D-C4D	-2.71	1.38	1.44
22	c	509	CLA	C3D-C4D	-2.71	1.38	1.44
22	B	613	CLA	C1D-C2D	-2.71	1.40	1.45
22	C	507	CLA	C3A-C2A	-2.71	1.47	1.54
22	b	618	CLA	CHD-C4C	-2.70	1.33	1.39
22	B	604	CLA	C1D-C2D	-2.70	1.40	1.45
23	a	414	PHO	C3D-C4D	-2.70	1.37	1.41
33	E	102	HEM	FE-NA	2.70	2.04	1.95
22	B	607	CLA	C3B-C2B	-2.70	1.32	1.41
22	C	510	CLA	C3A-C2A	-2.70	1.47	1.54
22	b	607	CLA	C1D-C2D	-2.70	1.40	1.45
22	c	510	CLA	C1D-C2D	-2.69	1.40	1.45
22	A	404	CLA	C3A-C2A	-2.69	1.47	1.54
24	c	515	BCR	C1-C6	-2.69	1.50	1.53
22	b	605	CLA	C3A-C2A	-2.69	1.47	1.54
22	B	614	CLA	C3D-C4D	-2.69	1.38	1.44
22	b	616	CLA	C1D-C2D	-2.68	1.40	1.45
22	c	510	CLA	C3D-C4D	-2.68	1.38	1.44
22	c	513	CLA	C1D-C2D	-2.68	1.40	1.45
22	d	402	CLA	C3D-C4D	-2.68	1.38	1.44
24	T	101	BCR	C30-C25	-2.67	1.50	1.53
22	C	508	CLA	C3D-C4D	-2.67	1.38	1.44
22	d	403	CLA	C3D-C4D	-2.66	1.38	1.44
22	B	609	CLA	CBC-CAC	-2.66	1.40	1.51
22	b	617	CLA	C3D-C4D	-2.66	1.38	1.44
22	C	513	CLA	C3A-C2A	-2.66	1.47	1.54
22	c	513	CLA	C3A-C2A	-2.66	1.47	1.54
22	c	502	CLA	C3D-C4D	-2.65	1.38	1.44
22	d	401	CLA	C1D-C2D	-2.65	1.40	1.45
23	a	406	PHO	C3D-C4D	-2.65	1.37	1.41
22	D	404	CLA	C3D-C4D	-2.65	1.38	1.44
22	A	406	CLA	C3D-C4D	-2.65	1.38	1.44
22	B	609	CLA	C3D-C4D	-2.64	1.38	1.44
22	b	614	CLA	C3D-C4D	-2.64	1.38	1.44
22	a	407	CLA	C3A-C2A	-2.64	1.47	1.54
22	D	404	CLA	CAB-C3B	-2.64	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	C3D-C4D	-2.64	1.38	1.44
33	E	102	HEM	C3D-C2D	2.63	1.42	1.36
22	b	605	CLA	C3D-C4D	-2.63	1.38	1.44
22	B	614	CLA	C1D-C2D	-2.62	1.40	1.45
22	C	508	CLA	CHD-C4C	-2.62	1.33	1.39
22	B	607	CLA	C1D-C2D	-2.61	1.40	1.45
22	B	601	CLA	C3D-C4D	-2.61	1.38	1.44
22	c	507	CLA	C1D-C2D	-2.61	1.40	1.45
22	b	605	CLA	MG-NA	-2.61	2.00	2.06
22	B	611	CLA	C1D-C2D	-2.61	1.40	1.45
22	A	406	CLA	C1C-NC	-2.61	1.33	1.37
33	e	102	HEM	O2D-CGD	-2.60	1.22	1.30
22	c	512	CLA	C1D-C2D	-2.60	1.40	1.45
32	d	406	LHG	O8-C6	-2.60	1.39	1.45
22	C	506	CLA	C3B-C2B	-2.60	1.32	1.41
22	b	603	CLA	C1D-C2D	-2.59	1.40	1.45
22	A	412	CLA	C3D-C4D	-2.59	1.38	1.44
22	C	510	CLA	CHC-C1C	-2.59	1.33	1.38
22	a	407	CLA	CHD-C4C	-2.58	1.33	1.39
30	c	516	DGD	O2G-C2G	-2.57	1.40	1.46
22	b	610	CLA	C1D-C2D	-2.57	1.40	1.45
22	C	511	CLA	C1D-C2D	-2.57	1.40	1.45
22	b	613	CLA	C1D-C2D	-2.57	1.40	1.45
22	C	507	CLA	C3D-C4D	-2.57	1.38	1.44
22	c	509	CLA	C3A-C2A	-2.56	1.47	1.54
22	b	615	CLA	C3D-C4D	-2.56	1.38	1.44
32	b	628	LHG	O7-C5	-2.56	1.40	1.46
22	B	615	CLA	C3D-C4D	-2.56	1.38	1.44
22	b	604	CLA	C3D-C4D	-2.56	1.38	1.44
22	b	605	CLA	CHD-C4C	-2.56	1.33	1.39
22	d	403	CLA	CHD-C4C	-2.56	1.33	1.39
22	a	405	CLA	C3D-C4D	-2.55	1.38	1.44
22	d	403	CLA	CHC-C1C	-2.55	1.33	1.38
33	E	102	HEM	O2D-CGD	-2.55	1.22	1.30
22	D	403	CLA	C1D-C2D	-2.53	1.40	1.45
22	A	404	CLA	MG-NC	-2.53	2.00	2.06
22	b	607	CLA	C3B-C2B	-2.53	1.32	1.41
22	b	609	CLA	C4C-C3C	-2.53	1.40	1.45
22	c	504	CLA	C3D-C4D	-2.52	1.38	1.44
22	c	507	CLA	C3D-C4D	-2.52	1.38	1.44
22	d	402	CLA	C3B-C2B	-2.51	1.32	1.41
22	C	511	CLA	C3D-C4D	-2.51	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	C3D-C4D	-2.51	1.38	1.44
22	b	607	CLA	C3D-C4D	-2.50	1.38	1.44
24	a	408	BCR	C30-C25	-2.50	1.50	1.53
22	b	606	CLA	C3D-C4D	-2.50	1.38	1.44
22	A	404	CLA	C1D-C2D	-2.49	1.40	1.45
22	a	407	CLA	C3D-C4D	-2.49	1.38	1.44
22	b	612	CLA	C3B-C2B	-2.49	1.32	1.41
22	C	507	CLA	MG-NA	-2.48	2.00	2.06
22	C	510	CLA	C3D-C4D	-2.48	1.38	1.44
24	B	616	BCR	C1-C6	-2.48	1.50	1.53
22	b	611	CLA	C3D-C4D	-2.48	1.38	1.44
22	c	505	CLA	C3D-C4D	-2.48	1.38	1.44
22	c	502	CLA	MG-NA	-2.47	2.00	2.06
24	d	404	BCR	C30-C25	-2.47	1.50	1.53
22	B	603	CLA	C3D-C4D	-2.47	1.38	1.44
22	C	514	CLA	C3D-C4D	-2.47	1.38	1.44
22	b	618	CLA	CHC-C1C	-2.47	1.33	1.38
22	B	602	CLA	C3A-C2A	-2.47	1.47	1.54
22	B	601	CLA	C1D-C2D	-2.46	1.40	1.45
25	A	408	PL9	C6-C5	2.46	1.47	1.35
24	b	621	BCR	C1-C6	-2.46	1.50	1.53
22	b	611	CLA	C3A-C2A	-2.46	1.47	1.54
30	C	519	DGD	O2G-C2G	-2.46	1.40	1.46
22	a	407	CLA	CHC-C1C	-2.46	1.33	1.38
22	B	610	CLA	C1D-C2D	-2.46	1.40	1.45
22	D	403	CLA	C3D-C4D	-2.46	1.38	1.44
22	C	504	CLA	C3D-C4D	-2.46	1.38	1.44
22	c	503	CLA	C3D-C4D	-2.45	1.38	1.44
22	c	507	CLA	MG-NA	-2.45	2.00	2.06
22	b	608	CLA	CHD-C4C	-2.44	1.33	1.39
22	c	511	CLA	C3D-C4D	-2.44	1.38	1.44
25	D	406	PL9	C3-C4	-2.44	1.45	1.49
22	C	513	CLA	C3D-C4D	-2.44	1.38	1.44
22	C	507	CLA	C1B-NB	-2.44	1.34	1.37
22	c	512	CLA	C3A-C2A	-2.43	1.47	1.54
22	B	606	CLA	C4C-C3C	-2.43	1.40	1.45
22	B	602	CLA	CHD-C4C	-2.43	1.33	1.39
25	D	406	PL9	C6-C5	2.43	1.47	1.35
22	C	502	CLA	C3D-C4D	-2.43	1.38	1.44
22	c	513	CLA	C3D-C4D	-2.43	1.38	1.44
22	b	618	CLA	C3D-C4D	-2.43	1.38	1.44
22	c	514	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	412	CLA	C3A-C2A	-2.41	1.47	1.54
22	B	612	CLA	MG-NA	-2.41	2.00	2.06
22	b	614	CLA	C1C-NC	-2.41	1.34	1.37
32	D	409	LHG	O7-C5	-2.41	1.40	1.46
22	b	608	CLA	C3A-C2A	-2.40	1.48	1.54
22	a	405	CLA	C1D-C2D	-2.40	1.40	1.45
22	c	506	CLA	CHD-C4C	-2.40	1.33	1.39
22	A	412	CLA	C1D-C2D	-2.39	1.40	1.45
22	c	514	CLA	CHD-C4C	-2.39	1.33	1.39
22	c	502	CLA	CHD-C4C	-2.39	1.33	1.39
22	C	513	CLA	CHD-C4C	-2.39	1.33	1.39
22	c	508	CLA	C3D-C4D	-2.38	1.38	1.44
22	B	613	CLA	MG-NA	-2.38	2.00	2.06
22	B	614	CLA	C3A-C2A	-2.37	1.48	1.54
22	B	614	CLA	C3B-C2B	-2.37	1.33	1.41
25	a	409	PL9	C6-C5	2.37	1.46	1.35
22	B	602	CLA	MG-NA	-2.37	2.00	2.06
22	C	509	CLA	C3D-C4D	-2.36	1.38	1.44
22	A	406	CLA	CHC-C1C	-2.36	1.33	1.38
22	B	601	CLA	C3A-C2A	-2.36	1.48	1.54
22	C	502	CLA	CHD-C4C	-2.35	1.33	1.39
22	a	404	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	516	BCR	C30-C25	-2.35	1.50	1.53
22	B	610	CLA	C3A-C2A	-2.35	1.48	1.54
24	D	405	BCR	C30-C25	-2.34	1.50	1.53
23	D	402	PHO	C3D-C2D	2.34	1.43	1.39
22	B	605	CLA	C3B-C2B	-2.34	1.33	1.41
22	C	505	CLA	CHD-C4C	-2.34	1.33	1.39
22	B	613	CLA	C3B-C2B	-2.34	1.33	1.41
22	b	615	CLA	CHD-C4C	-2.34	1.33	1.39
22	C	505	CLA	C3D-C4D	-2.33	1.38	1.44
32	l	101	LHG	O7-C5	-2.33	1.41	1.46
22	c	503	CLA	CHD-C4C	-2.32	1.33	1.39
22	B	609	CLA	C3B-C2B	-2.32	1.33	1.41
22	B	613	CLA	C3D-C4D	-2.31	1.39	1.44
33	E	102	HEM	FE-NC	2.30	2.02	1.95
22	A	412	CLA	C4C-C3C	2.30	1.48	1.45
25	d	405	PL9	C6-C5	2.30	1.46	1.35
22	H	101	CLA	C3D-C4D	-2.30	1.39	1.44
22	B	612	CLA	C3D-C4D	-2.29	1.39	1.44
22	D	404	CLA	CHD-C4C	-2.29	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	514	CLA	CHC-C1C	-2.29	1.33	1.38
22	C	512	CLA	C3D-C4D	-2.29	1.39	1.44
33	E	102	HEM	C3C-C2C	-2.29	1.32	1.37
22	c	512	CLA	C3D-C4D	-2.29	1.39	1.44
24	D	405	BCR	C1-C6	-2.28	1.50	1.53
22	b	613	CLA	C3B-C2B	-2.28	1.33	1.41
22	c	503	CLA	C3A-C2A	-2.28	1.48	1.54
22	b	611	CLA	CHD-C4C	-2.27	1.34	1.39
22	B	614	CLA	MG-NA	-2.27	2.00	2.06
33	E	102	HEM	C4D-ND	-2.27	1.36	1.40
22	c	505	CLA	CHD-C4C	-2.27	1.34	1.39
22	b	616	CLA	C3D-C4D	-2.26	1.39	1.44
22	C	506	CLA	CHD-C4C	-2.26	1.34	1.39
29	b	624	LMG	O1-C1	2.26	1.44	1.40
22	b	614	CLA	C4B-NB	2.26	1.40	1.37
22	c	514	CLA	C3A-C2A	-2.26	1.48	1.54
23	D	402	PHO	CHA-CBD	2.26	1.54	1.51
22	C	512	CLA	CHC-C1C	-2.26	1.34	1.38
22	C	507	CLA	C3B-C2B	-2.26	1.33	1.41
22	B	605	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	406	CLA	CAB-C3B	-2.25	1.41	1.47
22	b	608	CLA	C3B-C2B	-2.25	1.33	1.41
24	B	617	BCR	C30-C25	-2.24	1.50	1.53
22	C	510	CLA	CHD-C4C	-2.24	1.34	1.39
22	A	412	CLA	C4B-NB	2.24	1.40	1.37
25	A	408	PL9	C2-C1	-2.24	1.38	1.44
30	c	518	DGD	O2G-C2G	-2.24	1.41	1.46
22	b	618	CLA	C3B-C2B	-2.23	1.33	1.41
22	b	609	CLA	C3A-C2A	-2.23	1.48	1.54
22	B	605	CLA	CHD-C4C	-2.23	1.34	1.39
22	D	404	CLA	CHC-C1C	-2.23	1.34	1.38
22	B	613	CLA	C3A-C2A	-2.23	1.48	1.54
22	d	403	CLA	CAB-C3B	-2.23	1.41	1.47
22	B	604	CLA	C3B-C2B	-2.23	1.33	1.41
25	d	405	PL9	C2-C1	-2.22	1.38	1.44
22	b	616	CLA	MG-NA	-2.22	2.01	2.06
22	b	614	CLA	CHD-C4C	-2.22	1.34	1.39
22	D	404	CLA	C3B-C2B	-2.22	1.33	1.41
24	C	515	BCR	C30-C25	-2.22	1.50	1.53
22	b	604	CLA	C1C-NC	-2.21	1.34	1.37
24	c	515	BCR	C30-C25	-2.21	1.51	1.53
32	d	406	LHG	O7-C5	-2.20	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C3A-C2A	-2.20	1.48	1.54
22	b	608	CLA	C3D-C4D	-2.20	1.39	1.44
23	a	406	PHO	CHA-CBD	2.20	1.54	1.51
32	d	407	LHG	O7-C5	-2.20	1.41	1.46
22	C	502	CLA	C3B-C2B	-2.19	1.33	1.41
22	A	403	CLA	C1D-C2D	-2.19	1.41	1.45
22	B	610	CLA	CHC-C1C	-2.19	1.34	1.38
22	B	608	CLA	CHD-C4C	-2.18	1.34	1.39
22	A	406	CLA	CHD-C1D	-2.18	1.34	1.38
22	d	401	CLA	CHC-C1C	-2.18	1.34	1.38
22	C	502	CLA	MG-NA	-2.18	2.01	2.06
22	H	101	CLA	C3B-C2B	-2.18	1.33	1.41
25	D	406	PL9	C2-C1	-2.18	1.39	1.44
22	c	510	CLA	CHC-C1C	-2.18	1.34	1.38
23	D	402	PHO	C3D-C4D	-2.18	1.38	1.41
24	b	619	BCR	C1-C6	-2.18	1.51	1.53
25	d	405	PL9	C3-C4	-2.17	1.46	1.49
22	b	603	CLA	C3D-C4D	-2.17	1.39	1.44
22	c	506	CLA	C3D-C4D	-2.17	1.39	1.44
22	A	404	CLA	MG-NA	-2.17	2.01	2.06
22	C	507	CLA	CHC-C1C	-2.17	1.34	1.38
22	C	514	CLA	CHD-C4C	-2.17	1.34	1.39
33	e	102	HEM	FE-NC	2.16	2.02	1.95
33	e	102	HEM	C3C-C2C	-2.16	1.32	1.37
24	K	101	BCR	C30-C25	-2.16	1.51	1.53
22	H	101	CLA	C3A-C2A	-2.16	1.48	1.54
23	a	406	PHO	C3D-C2D	2.15	1.43	1.39
22	B	612	CLA	CHD-C4C	-2.15	1.34	1.39
22	c	506	CLA	C3B-C2B	-2.15	1.33	1.41
24	K	101	BCR	C1-C6	-2.14	1.51	1.53
22	C	507	CLA	CHD-C4C	-2.14	1.34	1.39
23	a	414	PHO	CHA-CBD	2.14	1.54	1.51
22	b	604	CLA	C3A-C2A	-2.13	1.48	1.54
22	B	607	CLA	CHD-C4C	-2.13	1.34	1.39
22	c	509	CLA	CHD-C4C	-2.13	1.34	1.39
23	A	405	PHO	C3D-CAD	-2.13	1.43	1.47
25	a	409	PL9	C2-C1	-2.12	1.39	1.44
22	B	615	CLA	CHD-C4C	-2.12	1.34	1.39
22	C	514	CLA	CHC-C1C	-2.12	1.34	1.38
22	D	404	CLA	C3A-C2A	-2.12	1.48	1.54
22	b	611	CLA	CHC-C1C	-2.11	1.34	1.38
22	c	510	CLA	CHD-C4C	-2.11	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	CHD-C4C	-2.11	1.34	1.39
22	C	509	CLA	CHD-C4C	-2.11	1.34	1.39
22	c	508	CLA	CHD-C4C	-2.10	1.34	1.39
22	b	616	CLA	C3B-C2B	-2.10	1.34	1.41
22	c	505	CLA	CHC-C1C	-2.10	1.34	1.38
22	B	613	CLA	CHD-C4C	-2.10	1.34	1.39
24	d	404	BCR	C1-C6	-2.10	1.51	1.53
22	c	504	CLA	C3A-C2A	-2.10	1.48	1.54
22	b	613	CLA	CHC-C1C	-2.09	1.34	1.38
22	b	612	CLA	CHD-C4C	-2.09	1.34	1.39
22	B	608	CLA	CHC-C1C	-2.09	1.34	1.38
26	f	102	SQD	O47-C45	-2.09	1.41	1.46
29	c	501	LMG	O7-C8	-2.08	1.41	1.46
29	m	103	LMG	O7-C8	-2.08	1.41	1.46
22	B	603	CLA	CHC-C1C	-2.08	1.34	1.38
22	b	617	CLA	CHD-C4C	-2.08	1.34	1.39
22	C	512	CLA	CHD-C4C	-2.08	1.34	1.39
22	b	611	CLA	C3B-C2B	-2.07	1.34	1.41
24	T	101	BCR	C1-C6	-2.07	1.51	1.53
22	b	612	CLA	CHC-C1C	-2.07	1.34	1.38
22	C	503	CLA	CHD-C4C	-2.07	1.34	1.39
22	c	508	CLA	CHC-C1C	-2.07	1.34	1.38
22	b	608	CLA	CHC-C1C	-2.07	1.34	1.38
22	b	607	CLA	CAB-C3B	-2.07	1.41	1.47
22	d	402	CLA	C3A-C2A	-2.06	1.48	1.54
22	b	609	CLA	C3B-C2B	-2.06	1.34	1.41
22	A	406	CLA	C1B-NB	-2.06	1.35	1.37
22	b	606	CLA	CHD-C4C	-2.05	1.34	1.39
33	E	102	HEM	C1B-NB	-2.05	1.36	1.40
22	b	617	CLA	C3B-C2B	-2.04	1.34	1.41
22	C	502	CLA	CHC-C1C	-2.04	1.34	1.38
22	b	606	CLA	C3B-C2B	-2.04	1.34	1.41
22	c	504	CLA	CHD-C4C	-2.04	1.34	1.39
22	d	403	CLA	C3B-C2B	-2.04	1.34	1.41
22	b	606	CLA	CHC-C1C	-2.03	1.34	1.38
22	b	615	CLA	CHD-C1D	-2.03	1.34	1.38
22	c	511	CLA	CHD-C4C	-2.03	1.34	1.39
22	H	101	CLA	CHD-C4C	-2.03	1.34	1.39
22	b	604	CLA	CHD-C4C	-2.03	1.34	1.39
22	B	606	CLA	CAB-C3B	-2.03	1.42	1.47
23	a	414	PHO	C3D-C2D	2.02	1.43	1.39
22	B	611	CLA	C3B-C2B	-2.02	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	PHO	CHA-CBD	2.02	1.54	1.51
22	b	605	CLA	C3B-C2B	-2.02	1.34	1.41
22	c	512	CLA	C1D-ND	2.02	1.40	1.37
24	c	524	BCR	C30-C25	-2.02	1.51	1.53
22	b	611	CLA	CAB-C3B	-2.02	1.42	1.47
22	B	609	CLA	CHC-C1C	-2.01	1.34	1.38
22	A	412	CLA	CHC-C1C	-2.01	1.34	1.38
22	C	505	CLA	CHC-C1C	-2.01	1.34	1.38
23	A	405	PHO	C3D-C2D	2.00	1.43	1.39
22	A	403	CLA	C1C-NC	-2.00	1.34	1.37

All (1216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O9-S-C6	-14.76	84.72	106.76
26	L	101	SQD	O8-S-O9	-10.70	84.64	111.40
23	D	402	PHO	C4D-CHA-CBD	-10.32	103.51	108.45
26	L	101	SQD	O9-S-O7	-10.30	80.32	113.82
23	a	414	PHO	C4D-CHA-CBD	-10.08	103.62	108.45
23	a	406	PHO	C4D-CHA-CBD	-9.60	103.85	108.45
23	A	405	PHO	C4D-CHA-CBD	-9.34	103.98	108.45
26	L	101	SQD	O7-S-C6	8.72	119.78	106.76
22	A	403	CLA	C4A-NA-C1A	-8.52	102.79	106.68
22	B	615	CLA	C4A-NA-C1A	-8.10	102.98	106.68
22	b	610	CLA	C4A-NA-C1A	-8.09	102.99	106.68
22	C	507	CLA	C4A-NA-C1A	-8.02	103.02	106.68
22	b	612	CLA	C4A-NA-C1A	-7.94	103.06	106.68
22	b	606	CLA	C4A-NA-C1A	-7.72	103.16	106.68
22	C	502	CLA	C4A-NA-C1A	-7.69	103.17	106.68
22	c	507	CLA	C4A-NA-C1A	-7.32	103.34	106.68
22	D	403	CLA	C4A-NA-C1A	-7.24	103.38	106.68
22	b	611	CLA	C4A-NA-C1A	-7.07	103.45	106.68
22	B	613	CLA	C4A-NA-C1A	-7.01	103.48	106.68
22	c	502	CLA	C4A-NA-C1A	-6.97	103.50	106.68
22	a	404	CLA	C4A-NA-C1A	-6.86	103.55	106.68
22	b	605	CLA	C4A-NA-C1A	-6.86	103.55	106.68
22	B	609	CLA	C4A-NA-C1A	-6.83	103.56	106.68
22	b	608	CLA	C4A-NA-C1A	-6.73	103.61	106.68
22	b	609	CLA	C4A-NA-C1A	-6.73	103.61	106.68
22	c	511	CLA	C4A-NA-C1A	-6.73	103.61	106.68
22	a	405	CLA	C4A-NA-C1A	-6.65	103.65	106.68
22	B	614	CLA	C4A-NA-C1A	-6.58	103.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C4A-NA-C1A	-6.50	103.71	106.68
22	b	604	CLA	C4A-NA-C1A	-6.48	103.72	106.68
22	C	508	CLA	C4A-NA-C1A	-6.47	103.72	106.68
22	c	509	CLA	C4A-NA-C1A	-6.47	103.73	106.68
22	A	404	CLA	C4A-NA-C1A	-6.41	103.75	106.68
22	b	615	CLA	C4A-NA-C1A	-6.40	103.76	106.68
22	B	601	CLA	C4A-NA-C1A	-6.39	103.76	106.68
22	B	602	CLA	C4A-NA-C1A	-6.39	103.77	106.68
22	B	612	CLA	C4A-NA-C1A	-6.37	103.77	106.68
22	c	503	CLA	C4A-NA-C1A	-6.27	103.82	106.68
22	c	508	CLA	C4A-NA-C1A	-6.24	103.83	106.68
25	A	408	PL9	C7-C8-C9	-6.21	116.14	126.83
22	B	604	CLA	C4A-NA-C1A	-6.14	103.88	106.68
22	C	505	CLA	C4A-NA-C1A	-6.06	103.91	106.68
24	d	404	BCR	C28-C27-C26	-6.03	103.30	114.06
22	b	618	CLA	C4A-NA-C1A	-6.03	103.93	106.68
22	b	607	CLA	C4A-NA-C1A	-5.98	103.95	106.68
22	B	603	CLA	C4A-NA-C1A	-5.97	103.96	106.68
22	C	506	CLA	C4A-NA-C1A	-5.91	103.98	106.68
24	T	101	BCR	C20-C21-C22	-5.88	119.03	127.28
24	h	101	BCR	C11-C10-C9	-5.88	119.03	127.28
22	b	617	CLA	C4A-NA-C1A	-5.87	104.00	106.68
24	K	102	BCR	C7-C8-C9	-5.85	117.58	126.23
22	B	605	CLA	C4A-NA-C1A	-5.84	104.01	106.68
24	H	102	BCR	C7-C8-C9	-5.84	117.60	126.23
24	D	405	BCR	C24-C23-C22	-5.80	117.66	126.23
22	b	614	CLA	C4A-NA-C1A	-5.79	104.04	106.68
29	m	103	LMG	O7-C10-C11	5.78	123.99	111.48
24	T	101	BCR	C33-C5-C6	-5.78	118.18	124.48
22	B	607	CLA	C4A-NA-C1A	-5.74	104.06	106.68
22	b	613	CLA	C4A-NA-C1A	-5.71	104.07	106.68
25	a	409	PL9	C7-C8-C9	-5.70	117.00	126.83
22	B	608	CLA	C4A-NA-C1A	-5.70	104.08	106.68
24	d	404	BCR	C24-C23-C22	-5.63	117.91	126.23
24	K	101	BCR	C33-C5-C6	-5.62	118.35	124.48
22	c	504	CLA	C4A-NA-C1A	-5.58	104.13	106.68
24	H	102	BCR	C11-C10-C9	-5.56	119.48	127.28
24	T	101	BCR	C24-C23-C22	-5.56	118.01	126.23
22	c	512	CLA	C4A-NA-C1A	-5.50	104.17	106.68
24	c	523	BCR	C28-C27-C26	-5.50	104.25	114.06
22	b	616	CLA	C4A-NA-C1A	-5.50	104.17	106.68
24	h	101	BCR	C7-C8-C9	-5.47	118.14	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C4A-NA-C1A	-5.42	104.21	106.68
22	c	510	CLA	C4A-NA-C1A	-5.39	104.22	106.68
24	C	516	BCR	C7-C8-C9	-5.38	118.28	126.23
29	C	522	LMG	O1-C1-C2	5.37	116.44	108.27
24	c	523	BCR	C33-C5-C6	-5.37	118.62	124.48
24	d	404	BCR	C15-C14-C13	-5.35	119.78	127.28
22	D	404	CLA	C4A-NA-C1A	-5.34	104.24	106.68
29	c	522	LMG	O7-C10-C11	5.30	122.94	111.48
22	A	406	CLA	C4A-NA-C1A	-5.28	104.27	106.68
24	k	101	BCR	C24-C23-C22	-5.26	118.46	126.23
24	B	618	BCR	C7-C8-C9	-5.19	118.56	126.23
25	d	405	PL9	C7-C8-C9	-5.17	117.92	126.83
22	C	513	CLA	C4A-NA-C1A	-5.17	104.32	106.68
22	B	606	CLA	C4A-NA-C1A	-5.16	104.33	106.68
22	d	401	CLA	C4A-NA-C1A	-5.12	104.34	106.68
24	B	617	BCR	C28-C27-C26	-5.09	104.99	114.06
22	C	514	CLA	C4A-NA-C1A	-5.08	104.36	106.68
22	c	505	CLA	C4A-NA-C1A	-5.04	104.38	106.68
22	A	412	CLA	C4A-NA-C1A	-5.01	104.39	106.68
24	K	102	BCR	C15-C14-C13	-5.01	120.26	127.28
24	t	102	BCR	C33-C5-C6	-5.00	119.03	124.48
30	C	517	DGD	O2G-C1B-C2B	4.99	122.27	111.48
26	L	101	SQD	O8-S-C6	4.98	115.60	105.97
22	C	504	CLA	C4A-NA-C1A	-4.98	104.41	106.68
22	C	510	CLA	C4A-NA-C1A	-4.96	104.42	106.68
22	c	513	CLA	C4A-NA-C1A	-4.94	104.42	106.68
26	f	102	SQD	C45-O47-C7	-4.93	106.00	117.80
22	a	407	CLA	C4A-NA-C1A	-4.92	104.43	106.68
24	D	405	BCR	C38-C26-C25	-4.92	119.12	124.48
26	A	409	SQD	O6-C1-C2	4.92	115.74	108.27
26	D	412	SQD	O6-C1-C2	4.88	115.68	108.27
24	c	515	BCR	C33-C5-C6	-4.85	119.19	124.48
24	t	102	BCR	C24-C23-C22	-4.80	119.13	126.23
29	c	501	LMG	C8-O7-C10	-4.79	106.33	117.80
24	c	524	BCR	C28-C27-C26	-4.77	105.55	114.06
22	c	514	CLA	C4A-NA-C1A	-4.77	104.50	106.68
24	d	404	BCR	C33-C5-C6	-4.77	119.28	124.48
22	d	402	CLA	C4A-NA-C1A	-4.76	104.51	106.68
22	b	603	CLA	C4A-NA-C1A	-4.72	104.52	106.68
30	H	103	DGD	O2G-C1B-C2B	4.71	121.68	111.48
22	C	512	CLA	C4A-NA-C1A	-4.69	104.54	106.68
29	C	522	LMG	O6-C5-C6	4.62	117.89	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	619	LMG	O7-C10-C11	4.60	121.44	111.48
22	b	612	CLA	C1-C2-C3	-4.59	118.67	126.20
22	C	511	CLA	C4A-NA-C1A	-4.59	104.59	106.68
22	d	403	CLA	C4A-NA-C1A	-4.54	104.61	106.68
24	C	516	BCR	C24-C23-C22	-4.54	119.52	126.23
24	B	618	BCR	C15-C14-C13	-4.52	120.94	127.28
29	B	621	LMG	O7-C10-C11	4.50	121.22	111.48
22	c	507	CLA	C1-C2-C3	-4.49	118.83	126.20
29	C	522	LMG	O7-C10-C11	4.49	121.19	111.48
22	B	605	CLA	C1-C2-C3	-4.47	118.87	126.20
22	c	506	CLA	C4A-NA-C1A	-4.46	104.64	106.68
32	d	406	LHG	O7-C7-C8	4.46	121.12	111.48
22	B	611	CLA	C4A-NA-C1A	-4.45	104.65	106.68
24	b	619	BCR	C29-C30-C25	4.45	116.90	110.44
22	H	101	CLA	C4A-NA-C1A	-4.42	104.66	106.68
24	D	405	BCR	C7-C8-C9	-4.40	119.72	126.23
26	D	412	SQD	O9-S-C6	4.39	113.32	106.76
24	B	618	BCR	C1-C6-C5	-4.39	116.64	122.64
29	c	519	LMG	O7-C10-C11	4.39	120.97	111.48
23	a	406	PHO	C2B-C1B-NB	-4.38	106.26	109.43
23	D	402	PHO	C2B-C1B-NB	-4.37	106.27	109.43
26	A	409	SQD	C1-O5-C5	-4.36	105.21	113.72
22	b	613	CLA	C1-C2-C3	-4.36	119.06	126.20
25	d	405	PL9	C37-C38-C39	-4.33	117.72	127.62
24	c	524	BCR	C16-C17-C18	-4.31	121.23	127.28
26	b	601	SQD	O6-C1-C2	4.30	114.80	108.27
29	C	520	LMG	O7-C10-C11	4.29	120.76	111.48
29	f	101	LMG	O7-C10-C11	4.29	120.76	111.48
22	c	508	CLA	C4D-C3D-CAD	4.27	112.74	108.11
24	C	516	BCR	C33-C5-C6	-4.26	119.84	124.48
23	A	405	PHO	C1-C2-C3	-4.25	119.23	126.20
32	d	407	LHG	C6-C5-C4	-4.24	101.90	111.78
24	C	515	BCR	C7-C8-C9	-4.24	119.96	126.23
24	b	621	BCR	C15-C14-C13	-4.23	121.34	127.28
26	A	409	SQD	O47-C7-C8	4.21	120.59	111.48
22	B	606	CLA	C4D-C3D-CAD	4.19	112.66	108.11
23	A	405	PHO	C2B-C1B-NB	-4.19	106.40	109.43
24	t	102	BCR	C7-C8-C9	-4.19	120.04	126.23
26	D	412	SQD	C44-O6-C1	-4.15	104.89	113.80
24	k	101	BCR	C7-C8-C9	-4.13	120.13	126.23
25	A	408	PL9	C37-C38-C39	-4.10	118.23	127.62
24	k	101	BCR	C20-C21-C22	-4.10	121.53	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	414	PHO	C2B-C1B-NB	-4.09	106.47	109.43
34	v	201	HEC	CBD-CAD-C3D	-4.09	101.23	112.53
26	b	601	SQD	O47-C7-C8	4.08	120.31	111.48
26	A	409	SQD	O5-C1-C2	-4.08	101.99	110.37
22	A	403	CLA	C1D-ND-C4D	-4.07	103.46	106.31
24	t	102	BCR	C3-C4-C5	-4.06	106.81	114.06
26	D	412	SQD	C1-C2-C3	-4.04	101.52	110.01
24	b	621	BCR	C7-C8-C9	-4.03	120.27	126.23
24	c	524	BCR	C15-C14-C13	-4.03	121.63	127.28
24	d	404	BCR	C16-C17-C18	-4.03	121.63	127.28
32	D	407	LHG	O8-C23-C24	4.02	124.10	111.83
26	D	412	SQD	O47-C7-C8	4.02	120.17	111.48
24	b	619	BCR	C33-C5-C6	-3.99	120.13	124.48
32	E	101	LHG	O7-C7-C8	3.98	120.09	111.48
24	A	407	BCR	C29-C30-C25	3.98	116.22	110.44
25	d	405	PL9	C27-C28-C29	-3.97	118.53	127.62
26	A	411	SQD	O47-C7-C8	3.97	120.07	111.48
24	c	523	BCR	C16-C17-C18	-3.96	121.72	127.28
25	a	409	PL9	C32-C33-C34	-3.95	118.58	127.62
24	B	618	BCR	C28-C27-C26	-3.93	107.05	114.06
22	b	614	CLA	C1-C2-C3	-3.89	119.82	126.20
24	K	102	BCR	C38-C26-C25	-3.89	120.24	124.48
25	A	408	PL9	C22-C23-C24	-3.88	118.73	127.62
22	C	503	CLA	C4A-NA-C1A	-3.88	104.91	106.68
24	b	621	BCR	C28-C27-C26	-3.86	107.17	114.06
29	c	522	LMG	O8-C28-C29	3.83	123.52	111.83
32	D	409	LHG	O7-C7-C8	3.82	119.74	111.48
24	b	621	BCR	C16-C17-C18	-3.81	121.93	127.28
24	k	101	BCR	C33-C5-C6	-3.81	120.33	124.48
24	K	102	BCR	C24-C23-C22	-3.80	120.62	126.23
29	b	624	LMG	O7-C10-C11	3.80	119.69	111.48
24	t	102	BCR	C15-C14-C13	-3.79	121.97	127.28
29	C	501	LMG	O7-C10-C11	3.76	119.62	111.48
26	f	102	SQD	O47-C7-C8	3.76	119.61	111.48
32	b	628	LHG	O7-C7-C8	3.75	119.60	111.48
29	c	501	LMG	O7-C10-C11	3.75	119.60	111.48
26	f	102	SQD	C44-O6-C1	-3.75	105.75	113.80
24	H	102	BCR	C24-C23-C22	-3.74	120.71	126.23
29	c	522	LMG	C8-O7-C10	-3.73	108.86	117.80
32	D	408	LHG	O7-C7-C8	3.73	119.55	111.48
23	a	414	PHO	C1-C2-C3	-3.73	120.09	126.20
22	B	605	CLA	C1D-ND-C4D	-3.72	103.70	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C4D-C3D-CAD	3.70	112.12	108.11
32	l	101	LHG	O7-C7-C8	3.69	119.47	111.48
22	D	403	CLA	C4D-C3D-CAD	3.68	112.11	108.11
24	K	102	BCR	C20-C21-C22	-3.67	122.13	127.28
24	B	616	BCR	C15-C14-C13	-3.67	122.14	127.28
22	b	608	CLA	C1D-ND-C4D	-3.66	103.74	106.31
24	b	620	BCR	C15-C14-C13	-3.66	122.15	127.28
22	C	510	CLA	C1-C2-C3	-3.66	120.20	126.20
24	B	616	BCR	C33-C5-C6	-3.65	120.50	124.48
22	D	403	CLA	C1D-ND-C4D	-3.64	103.76	106.31
30	c	516	DGD	O2G-C1B-C2B	3.63	119.34	111.48
22	C	506	CLA	C1-C2-C3	-3.63	120.25	126.20
24	b	619	BCR	C7-C8-C9	-3.63	120.86	126.23
24	t	102	BCR	C16-C17-C18	-3.63	122.19	127.28
26	L	101	SQD	O8-S-O7	3.62	120.45	111.40
24	B	618	BCR	C29-C30-C25	3.61	115.69	110.44
30	C	518	DGD	O2G-C1B-C2B	3.61	119.29	111.48
22	B	604	CLA	CHD-C1D-ND	-3.60	119.73	124.80
25	A	408	PL9	C53-C6-C1	3.60	122.64	115.28
24	b	621	BCR	C33-C5-C6	-3.59	120.56	124.48
22	B	610	CLA	C1-C2-C3	-3.58	120.33	126.20
24	b	621	BCR	C29-C30-C25	3.57	115.62	110.44
22	B	605	CLA	C4D-C3D-CAD	3.57	111.98	108.11
30	c	517	DGD	O2G-C1B-C2B	3.57	119.20	111.48
24	B	617	BCR	C24-C23-C22	-3.56	120.97	126.23
26	a	410	SQD	O47-C7-C8	3.56	119.17	111.48
25	D	406	PL9	C25-C24-C26	3.55	121.39	115.23
32	L	102	LHG	O7-C7-C8	3.55	119.16	111.48
24	b	621	BCR	C1-C6-C5	-3.54	117.80	122.64
22	B	603	CLA	C4D-C3D-CAD	3.54	111.95	108.11
24	C	515	BCR	C11-C10-C9	-3.54	122.32	127.28
24	k	101	BCR	C16-C17-C18	-3.54	122.32	127.28
22	a	404	CLA	C4D-C3D-CAD	3.53	111.94	108.11
26	f	102	SQD	O9-S-C6	3.53	112.03	106.76
25	A	408	PL9	C17-C18-C19	-3.53	119.56	127.62
24	K	102	BCR	C33-C5-C6	-3.52	120.64	124.48
24	b	620	BCR	C33-C5-C6	-3.52	120.65	124.48
22	b	618	CLA	C4D-C3D-CAD	3.52	111.92	108.11
22	H	101	CLA	C4D-C3D-CAD	3.51	111.92	108.11
32	e	101	LHG	O7-C7-C8	3.51	119.07	111.48
22	C	511	CLA	C1-C2-C3	-3.51	120.45	126.20
24	B	616	BCR	C11-C10-C9	-3.50	122.37	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C1D-ND-C4D	-3.49	103.86	106.31
24	b	619	BCR	C28-C27-C26	-3.49	107.84	114.06
24	D	405	BCR	C33-C5-C6	-3.48	120.69	124.48
24	H	102	BCR	C29-C30-C25	3.47	115.49	110.44
22	C	512	CLA	C1D-ND-C4D	-3.47	103.88	106.31
22	b	618	CLA	C1D-ND-C4D	-3.46	103.88	106.31
24	H	102	BCR	C16-C17-C18	-3.46	122.43	127.28
25	D	406	PL9	C20-C19-C21	3.46	121.23	115.23
22	b	609	CLA	C4D-C3D-CAD	3.46	111.86	108.11
22	d	401	CLA	C2C-C1C-NC	3.46	113.61	109.98
24	t	102	BCR	C20-C21-C22	-3.46	122.43	127.28
24	C	515	BCR	C38-C26-C25	-3.45	120.72	124.48
25	D	406	PL9	C45-C44-C46	3.44	121.19	115.23
26	b	601	SQD	C1-O5-C5	-3.44	107.01	113.72
24	D	405	BCR	C15-C14-C13	-3.44	122.46	127.28
24	B	616	BCR	C16-C17-C18	-3.43	122.47	127.28
32	d	407	LHG	O7-C7-C8	3.43	118.89	111.48
24	k	101	BCR	C38-C26-C25	-3.42	120.75	124.48
22	c	509	CLA	C4D-C3D-CAD	3.41	111.81	108.11
22	c	512	CLA	C4D-C3D-CAD	3.41	111.81	108.11
25	a	409	PL9	C17-C18-C19	-3.41	119.82	127.62
24	b	619	BCR	C11-C10-C9	-3.41	122.50	127.28
26	A	409	SQD	C1-C2-C3	-3.41	102.84	110.01
22	D	403	CLA	CHD-C1D-ND	-3.40	120.02	124.80
22	c	502	CLA	C4D-C3D-CAD	3.40	111.79	108.11
26	A	409	SQD	C45-O47-C7	-3.39	109.69	117.80
29	c	519	LMG	C8-O7-C10	-3.39	109.69	117.80
22	C	507	CLA	C1-C2-C3	-3.38	120.65	126.20
22	B	614	CLA	C4D-C3D-CAD	3.38	111.78	108.11
22	B	601	CLA	C1D-ND-C4D	-3.38	103.94	106.31
22	C	514	CLA	C4D-C3D-CAD	3.38	111.78	108.11
29	C	520	LMG	O8-C28-C29	3.38	122.14	111.83
26	f	102	SQD	O6-C1-C2	3.38	113.40	108.27
25	D	406	PL9	C17-C18-C19	-3.37	119.91	127.62
24	d	404	BCR	C27-C26-C25	-3.37	118.15	122.70
24	B	616	BCR	C24-C23-C22	-3.37	121.25	126.23
22	d	403	CLA	C2C-C1C-NC	3.37	113.52	109.98
24	d	404	BCR	C38-C26-C27	3.36	120.77	113.60
22	b	603	CLA	C4D-C3D-CAD	3.36	111.76	108.11
26	A	411	SQD	C45-O47-C7	-3.36	109.75	117.80
25	D	406	PL9	C12-C13-C14	-3.36	119.93	127.62
24	b	620	BCR	C28-C27-C26	-3.36	108.07	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m	103	LMG	C8-O7-C10	-3.36	109.76	117.80
26	b	601	SQD	C3-C4-C5	3.36	116.32	110.23
25	a	409	PL9	C22-C23-C24	-3.35	119.94	127.62
29	c	522	LMG	O6-C5-C6	3.35	114.75	106.44
24	C	516	BCR	C21-C20-C19	-3.34	113.51	123.20
24	c	515	BCR	C7-C8-C9	-3.34	121.29	126.23
22	C	513	CLA	C1D-ND-C4D	-3.33	103.98	106.31
25	A	408	PL9	C32-C33-C34	-3.33	120.00	127.62
22	C	508	CLA	C4D-C3D-CAD	3.33	111.72	108.11
22	C	511	CLA	C4D-C3D-CAD	3.33	111.72	108.11
32	l	101	LHG	O8-C23-C24	3.32	121.96	111.83
29	c	519	LMG	O8-C28-C29	3.31	121.94	111.83
30	C	517	DGD	O1G-C1A-C2A	3.31	121.94	111.83
26	A	411	SQD	O48-C23-C24	3.30	121.91	111.83
22	H	101	CLA	C1D-ND-C4D	-3.30	104.00	106.31
25	A	408	PL9	C30-C29-C31	3.30	120.96	115.23
22	b	606	CLA	C4D-C3D-CAD	3.30	111.69	108.11
25	D	406	PL9	C37-C38-C39	-3.30	120.08	127.62
22	b	612	CLA	C4D-C3D-CAD	3.30	111.69	108.11
24	B	618	BCR	C16-C17-C18	-3.30	122.66	127.28
22	B	611	CLA	C4D-C3D-CAD	3.29	111.68	108.11
29	m	103	LMG	O7-C10-O9	-3.29	116.01	123.70
22	c	513	CLA	C1D-ND-C4D	-3.28	104.01	106.31
22	B	601	CLA	CHD-C1D-ND	-3.28	120.19	124.80
22	B	609	CLA	C4D-C3D-CAD	3.28	111.66	108.11
24	T	101	BCR	C15-C14-C13	-3.26	122.70	127.28
25	d	405	PL9	C17-C18-C19	-3.26	120.16	127.62
22	B	610	CLA	CHD-C1D-ND	-3.26	120.21	124.80
22	b	610	CLA	C1-C2-C3	-3.26	120.86	126.20
22	c	511	CLA	C1D-ND-C4D	-3.26	104.03	106.31
22	a	404	CLA	C1D-ND-C4D	-3.25	104.03	106.31
22	d	403	CLA	C4D-C3D-CAD	3.25	111.64	108.11
22	a	404	CLA	CHD-C1D-ND	-3.25	120.23	124.80
25	a	409	PL9	C12-C13-C14	-3.24	120.21	127.62
22	b	607	CLA	CHD-C1D-ND	-3.24	120.24	124.80
22	b	604	CLA	C4D-C3D-CAD	3.23	111.62	108.11
22	c	514	CLA	C4D-C3D-CAD	3.23	111.62	108.11
26	L	101	SQD	O47-C7-C8	3.22	118.45	111.48
24	K	101	BCR	C38-C26-C25	-3.22	120.97	124.48
24	B	617	BCR	C33-C5-C6	-3.22	120.97	124.48
22	D	403	CLA	C1-C2-C3	-3.22	120.92	126.20
22	C	512	CLA	C1-C2-C3	-3.22	120.92	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C15-C14-C13	-3.21	122.78	127.28
22	B	613	CLA	CHD-C1D-ND	-3.21	120.29	124.80
24	K	102	BCR	C10-C11-C12	-3.20	113.92	123.20
24	H	102	BCR	C28-C27-C26	-3.20	108.34	114.06
24	B	618	BCR	C4-C5-C6	-3.19	118.39	122.70
24	K	101	BCR	C24-C23-C22	-3.19	121.51	126.23
22	D	404	CLA	C4D-C3D-CAD	3.19	111.57	108.11
24	c	523	BCR	C29-C30-C25	3.19	115.07	110.44
30	H	103	DGD	O1G-C1A-C2A	3.19	121.56	111.83
22	d	402	CLA	C4D-C3D-CAD	3.18	111.56	108.11
24	d	404	BCR	C38-C26-C25	-3.18	121.02	124.48
24	B	617	BCR	C15-C14-C13	-3.18	122.83	127.28
22	b	609	CLA	C1-C2-C3	-3.17	121.00	126.20
22	B	602	CLA	C4D-C3D-CAD	3.17	111.55	108.11
24	h	101	BCR	C16-C17-C18	-3.17	122.83	127.28
22	B	611	CLA	C1-C2-C3	-3.17	121.01	126.20
22	b	613	CLA	CHD-C1D-ND	-3.16	120.35	124.80
22	b	617	CLA	C1-C2-C3	-3.16	121.02	126.20
22	B	613	CLA	C1D-ND-C4D	-3.16	104.09	106.31
24	d	404	BCR	C7-C8-C9	-3.16	121.56	126.23
22	C	509	CLA	C1-C2-C3	-3.16	121.03	126.20
22	B	601	CLA	C4D-C3D-CAD	3.15	111.53	108.11
22	b	616	CLA	C1D-ND-C4D	-3.15	104.10	106.31
30	h	102	DGD	O1G-C1A-C2A	3.15	121.43	111.83
24	C	515	BCR	C20-C21-C22	-3.14	122.87	127.28
24	C	516	BCR	C15-C14-C13	-3.14	122.87	127.28
25	a	409	PL9	C45-C44-C46	3.14	120.68	115.23
22	B	614	CLA	CHD-C1D-ND	-3.14	120.39	124.80
34	V	201	HEC	CBD-CAD-C3D	-3.14	103.86	112.53
26	a	412	SQD	O48-C23-C24	3.14	121.39	111.83
32	D	407	LHG	O8-C23-O10	-3.13	115.79	123.63
32	l	101	LHG	C6-C5-C4	-3.13	104.49	111.78
30	c	516	DGD	C2G-O2G-C1B	-3.13	110.31	117.80
29	D	410	LMG	O7-C10-C11	3.12	118.24	111.48
25	d	405	PL9	C42-C43-C44	-3.12	120.48	127.62
26	a	410	SQD	O6-C1-C2	3.12	113.01	108.27
32	b	628	LHG	O8-C23-C24	3.12	121.34	111.83
24	a	408	BCR	C15-C14-C13	-3.12	122.91	127.28
25	d	405	PL9	C12-C13-C14	-3.12	120.49	127.62
25	a	409	PL9	C37-C38-C39	-3.11	120.49	127.62
24	h	101	BCR	C15-C14-C13	-3.11	122.91	127.28
25	d	405	PL9	C53-C6-C1	3.11	121.65	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	C4D-C3D-CAD	3.11	111.49	108.11
22	B	615	CLA	C1D-ND-C4D	-3.10	104.13	106.31
23	a	406	PHO	C2D-C1D-ND	-3.10	107.19	109.43
33	E	102	HEM	CBA-CAA-C2A	-3.10	103.97	112.53
26	a	412	SQD	O47-C7-C8	3.10	118.18	111.48
22	b	617	CLA	CHD-C1D-ND	-3.10	120.45	124.80
24	A	407	BCR	C7-C8-C9	-3.09	121.66	126.23
30	h	102	DGD	O2G-C1B-C2B	3.09	118.17	111.48
22	B	601	CLA	C1-C2-C3	-3.09	121.13	126.20
25	A	408	PL9	C12-C13-C14	-3.08	120.57	127.62
22	b	608	CLA	C1-C2-C3	-3.08	121.15	126.20
22	c	513	CLA	C4D-C3D-CAD	3.08	111.45	108.11
22	c	512	CLA	C1D-ND-C4D	-3.08	104.15	106.31
22	c	506	CLA	C4D-C3D-CAD	3.08	111.45	108.11
30	H	103	DGD	C1D-O6D-C5D	-3.07	107.72	113.72
32	D	407	LHG	O7-C7-C8	3.07	118.13	111.48
30	C	519	DGD	O2G-C1B-C2B	3.07	118.13	111.48
22	b	610	CLA	CHD-C1D-ND	-3.07	120.48	124.80
22	c	504	CLA	C4D-C3D-CAD	3.07	111.44	108.11
23	a	414	PHO	C2D-C1D-ND	-3.07	107.21	109.43
22	b	603	CLA	C1D-ND-C4D	-3.06	104.16	106.31
25	a	409	PL9	C53-C6-C1	3.06	121.54	115.28
22	B	607	CLA	CHD-C1D-ND	-3.06	120.50	124.80
26	A	409	SQD	C44-O6-C1	-3.06	107.25	113.80
25	d	405	PL9	C40-C39-C41	3.06	120.53	115.23
22	b	607	CLA	C1D-ND-C4D	-3.05	104.17	106.31
22	B	608	CLA	CHA-C1A-NA	-3.05	119.49	126.39
22	b	608	CLA	C4D-C3D-CAD	3.04	111.41	108.11
24	c	523	BCR	C27-C26-C25	-3.04	118.59	122.70
22	b	613	CLA	C2C-C1C-NC	3.04	113.18	109.98
32	E	101	LHG	O8-C23-C24	3.04	121.11	111.83
24	C	516	BCR	C15-C16-C17	-3.04	117.30	123.52
22	a	407	CLA	C2C-C1C-NC	3.04	113.17	109.98
22	B	608	CLA	C2C-C1C-NC	3.03	113.17	109.98
29	C	520	LMG	C8-O7-C10	-3.03	110.54	117.80
30	c	518	DGD	O2G-C1B-C2B	3.03	118.04	111.48
24	k	101	BCR	C10-C11-C12	-3.03	114.42	123.20
22	A	412	CLA	C2C-C1C-NC	3.03	113.16	109.98
22	c	507	CLA	C4D-C3D-CAD	3.02	111.39	108.11
22	C	503	CLA	C4D-C3D-CAD	3.02	111.39	108.11
22	c	503	CLA	C1-C2-C3	-3.02	121.25	126.20
30	c	517	DGD	O1G-C1A-C2A	3.01	121.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	PHO	C2D-C1D-ND	-3.01	107.25	109.43
22	c	514	CLA	C1D-ND-C4D	-3.01	104.20	106.31
22	C	502	CLA	C1D-ND-C4D	-3.00	104.20	106.31
22	B	613	CLA	C4D-C3D-CAD	3.00	111.36	108.11
24	c	524	BCR	C29-C30-C25	2.99	114.79	110.44
24	K	102	BCR	C39-C30-C25	-2.99	105.55	110.24
22	c	507	CLA	C1D-ND-C4D	-2.99	104.21	106.31
24	c	523	BCR	C21-C20-C19	-2.98	114.55	123.20
24	C	515	BCR	C15-C14-C13	-2.98	123.10	127.28
30	C	518	DGD	O1G-C1A-C2A	2.98	120.91	111.83
22	C	502	CLA	C4D-C3D-CAD	2.98	111.34	108.11
22	b	616	CLA	CHD-C1D-ND	-2.97	120.62	124.80
22	b	604	CLA	C1D-ND-C4D	-2.97	104.23	106.31
25	D	406	PL9	C27-C28-C29	-2.97	120.83	127.62
23	D	402	PHO	C2D-C1D-ND	-2.97	107.29	109.43
22	b	605	CLA	C1D-ND-C4D	-2.97	104.23	106.31
24	C	515	BCR	C24-C23-C22	-2.97	121.85	126.23
22	b	617	CLA	C1D-ND-C4D	-2.96	104.23	106.31
22	c	508	CLA	C1D-ND-C4D	-2.96	104.23	106.31
29	m	103	LMG	O8-C28-C29	2.95	120.83	111.83
30	C	518	DGD	O1G-C1A-O1A	-2.95	116.25	123.63
24	C	515	BCR	C33-C5-C6	-2.95	121.27	124.48
30	c	516	DGD	C4E-C3E-C2E	-2.95	105.66	110.83
26	a	410	SQD	O9-S-C6	2.95	111.16	106.76
32	b	628	LHG	C5-O7-C7	-2.94	110.75	117.80
22	B	610	CLA	C2C-C1C-NC	2.94	113.07	109.98
22	C	511	CLA	C1D-ND-C4D	-2.94	104.25	106.31
22	C	504	CLA	C4D-C3D-CAD	2.94	111.29	108.11
22	B	613	CLA	C1-C2-C3	-2.94	121.39	126.20
22	d	401	CLA	C1-C2-C3	-2.93	121.39	126.20
24	c	524	BCR	C11-C10-C9	-2.93	123.17	127.28
30	C	518	DGD	C6D-C5D-C4D	2.92	118.20	112.07
25	A	408	PL9	C27-C28-C29	-2.92	120.93	127.62
25	A	408	PL9	C15-C14-C16	2.92	120.30	115.23
24	c	523	BCR	C15-C14-C13	-2.92	123.18	127.28
22	c	511	CLA	C1-C2-C3	-2.92	121.41	126.20
22	A	403	CLA	CHD-C1D-ND	-2.92	120.69	124.80
25	D	406	PL9	C7-C8-C9	-2.92	121.80	126.83
22	C	512	CLA	C2C-C1C-NC	2.92	113.04	109.98
33	E	102	HEM	O2D-CGD-CBD	2.91	123.20	114.00
24	d	404	BCR	C29-C30-C25	2.91	114.67	110.44
24	t	102	BCR	C33-C5-C4	2.91	119.80	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C20-C19-C18	-2.91	118.39	126.36
22	a	407	CLA	C1D-ND-C4D	-2.91	104.27	106.31
24	t	102	BCR	C39-C30-C25	-2.91	105.69	110.24
22	B	602	CLA	C1D-ND-C4D	-2.90	104.27	106.31
24	K	101	BCR	C23-C24-C25	-2.90	119.25	127.00
22	C	503	CLA	C1D-ND-C4D	-2.90	104.28	106.31
26	A	411	SQD	O7-S-C6	2.90	111.08	106.76
24	b	620	BCR	C24-C23-C22	-2.90	121.95	126.23
22	B	608	CLA	C4D-C3D-CAD	2.89	111.24	108.11
22	C	504	CLA	C1D-ND-C4D	-2.88	104.29	106.31
32	D	408	LHG	O8-C23-C24	2.88	120.63	111.83
22	D	404	CLA	CHD-C1D-ND	-2.88	120.75	124.80
22	a	407	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
30	C	519	DGD	O3G-C3G-C2G	-2.87	103.83	110.82
22	A	403	CLA	C4D-C3D-CAD	2.87	111.22	108.11
30	C	519	DGD	O1G-C1A-C2A	2.87	120.58	111.83
29	f	101	LMG	C8-O7-C10	-2.87	110.93	117.80
22	A	412	CLA	CHD-C1D-ND	-2.87	120.77	124.80
26	D	412	SQD	O48-C23-C24	2.87	120.57	111.83
22	c	508	CLA	C1-C2-C3	-2.86	121.50	126.20
24	K	102	BCR	C16-C17-C18	-2.86	123.27	127.28
22	c	504	CLA	C1D-ND-C4D	-2.86	104.31	106.31
22	b	616	CLA	C1-C2-C3	-2.86	121.52	126.20
32	d	406	LHG	O8-C23-C24	2.86	120.54	111.83
22	A	406	CLA	C2C-C1C-NC	2.85	112.98	109.98
22	C	505	CLA	C4D-C3D-CAD	2.85	111.20	108.11
24	C	515	BCR	C16-C17-C18	-2.85	123.28	127.28
22	B	604	CLA	C4D-C3D-CAD	2.85	111.20	108.11
24	B	616	BCR	C34-C9-C10	-2.85	118.20	122.82
22	c	506	CLA	C1D-ND-C4D	-2.84	104.32	106.31
22	d	401	CLA	CHD-C1D-ND	-2.84	120.80	124.80
22	b	605	CLA	C4D-C3D-CAD	2.84	111.19	108.11
22	C	510	CLA	C4D-C3D-CAD	2.84	111.19	108.11
24	B	616	BCR	C28-C27-C26	-2.84	109.00	114.06
24	B	618	BCR	C10-C11-C12	-2.83	115.00	123.20
22	c	505	CLA	C1D-ND-C4D	-2.83	104.33	106.31
22	a	405	CLA	CHD-C1D-ND	-2.83	120.82	124.80
22	d	401	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	C	516	BCR	C11-C10-C9	-2.82	123.32	127.28
30	C	517	DGD	C2G-O2G-C1B	-2.82	111.06	117.80
22	a	407	CLA	C4D-C3D-CAD	2.81	111.16	108.11
26	b	601	SQD	O7-S-C6	2.81	110.96	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	C4D-C3D-CAD	2.81	111.16	108.11
24	k	101	BCR	C15-C16-C17	-2.81	117.78	123.52
22	b	614	CLA	C1D-ND-C4D	-2.80	104.34	106.31
22	d	403	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
29	C	522	LMG	O2-C2-C3	-2.80	103.78	110.38
22	c	508	CLA	CHD-C1D-ND	-2.80	120.87	124.80
22	b	604	CLA	C1-C2-C3	-2.79	121.63	126.20
24	d	404	BCR	C30-C25-C26	-2.78	118.83	122.64
22	c	503	CLA	C1D-ND-C4D	-2.78	104.36	106.31
22	C	509	CLA	C1D-ND-C4D	-2.78	104.36	106.31
22	B	614	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
22	B	603	CLA	C2C-C1C-NC	2.77	112.90	109.98
22	c	509	CLA	CHD-C1D-ND	-2.77	120.90	124.80
22	B	615	CLA	C1-C2-C3	-2.77	121.66	126.20
24	A	407	BCR	C16-C17-C18	-2.77	123.40	127.28
22	c	505	CLA	C1-C2-C3	-2.76	121.67	126.20
24	D	405	BCR	C21-C20-C19	-2.76	115.19	123.20
24	h	101	BCR	C34-C9-C10	-2.76	118.34	122.82
22	D	404	CLA	C2C-C1C-NC	2.76	112.88	109.98
22	c	502	CLA	CHD-C1D-ND	-2.76	120.92	124.80
22	c	510	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	k	101	BCR	C21-C20-C19	-2.75	115.22	123.20
22	A	412	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
22	b	612	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	C	509	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	A	406	CLA	C1-C2-C3	-2.75	121.69	126.20
22	C	503	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	b	613	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
22	c	507	CLA	CHD-C1D-ND	-2.74	120.94	124.80
22	c	511	CLA	C4D-C3D-CAD	2.74	111.08	108.11
24	T	101	BCR	C33-C5-C4	2.74	119.44	113.60
22	b	612	CLA	C1D-ND-C4D	-2.74	104.39	106.31
24	D	405	BCR	C30-C25-C26	-2.74	118.89	122.64
22	C	514	CLA	C1D-ND-C4D	-2.74	104.39	106.31
30	C	518	DGD	O3G-C1D-C2D	2.74	112.43	108.27
22	b	609	CLA	C1D-CHD-C4C	-2.74	120.21	126.02
25	A	408	PL9	C20-C19-C21	2.73	119.97	115.23
24	A	407	BCR	C33-C5-C6	-2.73	121.50	124.48
24	a	408	BCR	C40-C30-C25	-2.73	105.96	110.24
26	a	412	SQD	C45-O47-C7	-2.73	111.27	117.80
22	c	504	CLA	CHD-C1D-ND	-2.72	120.97	124.80
22	a	405	CLA	C1D-ND-C4D	-2.72	104.40	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	523	BCR	C8-C7-C6	-2.72	119.72	127.00
22	B	614	CLA	CHC-C1C-NC	2.72	128.41	124.31
24	B	617	BCR	C7-C8-C9	-2.72	122.21	126.23
29	c	522	LMG	O8-C28-O10	-2.72	116.82	123.63
29	c	522	LMG	O7-C10-O9	-2.72	117.35	123.70
22	B	611	CLA	CHD-C1D-ND	-2.72	120.98	124.80
24	b	620	BCR	C7-C8-C9	-2.72	122.21	126.23
22	c	514	CLA	CGD-CBD-CAD	-2.71	102.06	110.85
22	d	403	CLA	C1D-CHD-C4C	-2.71	120.25	126.02
22	b	607	CLA	C4D-C3D-CAD	2.71	111.05	108.11
22	D	404	CLA	C1D-ND-C4D	-2.71	104.41	106.31
24	D	405	BCR	C16-C17-C18	-2.71	123.48	127.28
22	b	614	CLA	C2C-C1C-NC	2.71	112.83	109.98
26	b	601	SQD	C45-O47-C7	-2.71	111.32	117.80
22	b	617	CLA	C4D-C3D-CAD	2.71	111.05	108.11
24	B	617	BCR	C39-C30-C25	-2.71	106.00	110.24
30	C	518	DGD	O5D-C1E-C2E	2.70	112.38	108.27
24	B	618	BCR	C33-C5-C4	2.70	119.34	113.60
22	B	610	CLA	CHC-C1C-C2C	-2.70	119.29	126.95
29	C	501	LMG	O8-C28-C29	2.70	120.05	111.83
22	B	606	CLA	C1D-CHD-C4C	-2.70	120.29	126.02
22	b	606	CLA	CHD-C1D-ND	-2.69	121.01	124.80
26	A	409	SQD	O48-C23-C24	2.69	120.05	111.83
24	C	516	BCR	C10-C11-C12	-2.69	115.40	123.20
24	t	102	BCR	C1-C6-C7	2.69	122.95	115.65
22	B	602	CLA	C4D-CHA-C1A	-2.69	118.03	121.24
22	B	602	CLA	C1-C2-C3	-2.69	121.79	126.20
24	a	408	BCR	C3-C4-C5	-2.69	109.26	114.06
25	A	408	PL9	C45-C44-C46	2.69	119.89	115.23
23	a	406	PHO	C1-C2-C3	-2.69	121.79	126.20
24	B	617	BCR	C29-C30-C25	2.69	114.34	110.44
24	b	620	BCR	C38-C26-C25	-2.69	121.55	124.48
30	c	518	DGD	O1G-C1A-C2A	2.69	120.02	111.83
22	C	502	CLA	CHD-C1D-ND	-2.68	121.03	124.80
29	c	501	LMG	C7-O1-C1	-2.68	108.04	113.80
34	v	201	HEC	O2D-CGD-CBD	2.68	122.48	114.00
22	b	613	CLA	C4D-C3D-CAD	2.68	111.02	108.11
22	C	510	CLA	C2C-C1C-NC	2.68	112.80	109.98
22	A	404	CLA	CHD-C1D-ND	-2.68	121.03	124.80
22	C	514	CLA	C2C-C1C-NC	2.68	112.80	109.98
24	A	407	BCR	C38-C26-C25	-2.68	121.56	124.48
26	a	410	SQD	C1-C2-C3	-2.68	104.38	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	CHD-C1D-ND	-2.67	121.04	124.80
32	D	409	LHG	O8-C23-C24	2.67	119.98	111.83
32	d	406	LHG	O8-C23-O10	-2.67	116.95	123.63
24	B	617	BCR	C38-C26-C25	-2.67	121.57	124.48
22	B	615	CLA	CHD-C1D-ND	-2.66	121.05	124.80
22	B	615	CLA	C1D-CHD-C4C	-2.66	120.36	126.02
22	A	406	CLA	C1D-ND-C4D	-2.66	104.45	106.31
22	C	507	CLA	C2C-C1C-NC	2.66	112.77	109.98
29	c	522	LMG	O1-C7-C8	2.66	117.28	110.82
22	C	512	CLA	CHD-C1D-ND	-2.65	121.07	124.80
24	B	616	BCR	C29-C30-C25	2.65	114.29	110.44
22	B	606	CLA	C1-C2-C3	-2.65	121.85	126.20
22	c	513	CLA	CHD-C1D-ND	-2.65	121.07	124.80
22	b	618	CLA	CHD-C1D-ND	-2.65	121.08	124.80
24	T	101	BCR	C11-C10-C9	-2.64	123.58	127.28
24	K	101	BCR	C15-C14-C13	-2.63	123.59	127.28
25	a	409	PL9	C35-C34-C36	2.63	119.80	115.23
24	c	524	BCR	C7-C8-C9	-2.63	122.34	126.23
32	L	102	LHG	C6-C5-C4	-2.63	105.66	111.78
29	f	101	LMG	O8-C28-C29	2.63	119.85	111.83
25	a	409	PL9	C10-C9-C11	2.63	119.79	115.23
22	b	614	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	c	509	CLA	C1D-ND-C4D	-2.63	104.47	106.31
25	a	409	PL9	C40-C39-C41	2.63	119.79	115.23
24	C	515	BCR	C35-C13-C12	2.63	122.10	118.09
22	B	608	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
22	B	615	CLA	C4D-C3D-CAD	2.62	110.95	108.11
25	d	405	PL9	C35-C34-C36	2.62	119.78	115.23
22	C	514	CLA	C1-C2-C3	-2.62	121.91	126.20
26	a	412	SQD	C9-C8-C7	-2.62	104.11	113.69
22	d	402	CLA	CHD-C1D-ND	-2.61	121.12	124.80
24	b	621	BCR	C33-C5-C4	2.61	119.17	113.60
22	B	612	CLA	C1D-ND-C4D	-2.61	104.48	106.31
24	C	515	BCR	C21-C20-C19	-2.61	115.65	123.20
24	B	618	BCR	C3-C4-C5	-2.61	109.41	114.06
22	B	603	CLA	CHA-C1A-NA	-2.61	120.49	126.39
22	b	606	CLA	CHA-C4D-ND	2.60	137.92	132.55
22	C	511	CLA	CHD-C1D-ND	-2.60	121.14	124.80
22	b	606	CLA	CHA-C1A-NA	-2.60	120.50	126.39
22	B	612	CLA	C4D-C3D-CAD	2.60	110.93	108.11
22	c	514	CLA	CHD-C1D-ND	-2.60	121.14	124.80
22	A	406	CLA	C4D-C3D-CAD	2.60	110.93	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C4D-C3D-CAD	2.60	110.93	108.11
24	b	621	BCR	C39-C30-C25	-2.59	106.18	110.24
22	c	512	CLA	C1-C2-C3	-2.59	121.95	126.20
22	A	404	CLA	C4D-C3D-CAD	2.59	110.92	108.11
22	b	604	CLA	C4D-CHA-C1A	-2.59	118.16	121.24
22	B	612	CLA	CHD-C1D-ND	-2.59	121.16	124.80
24	K	101	BCR	C16-C17-C18	-2.59	123.65	127.28
24	H	102	BCR	C31-C1-C6	-2.58	106.19	110.24
22	b	607	CLA	C1-C2-C3	-2.58	121.97	126.20
26	D	412	SQD	C45-O47-C7	-2.58	111.62	117.80
29	c	519	LMG	O8-C28-O10	-2.58	117.18	123.63
24	a	408	BCR	C7-C8-C9	-2.58	122.42	126.23
22	C	502	CLA	C2C-C1C-NC	2.58	112.69	109.98
22	c	512	CLA	C2C-C1C-NC	2.58	112.69	109.98
22	b	617	CLA	CHC-C1C-NC	2.57	128.19	124.31
22	C	514	CLA	CHD-C1D-ND	-2.57	121.19	124.80
24	h	101	BCR	C31-C1-C6	-2.57	106.22	110.24
24	k	101	BCR	C11-C10-C9	-2.56	123.69	127.28
30	C	517	DGD	C4D-C3D-C2D	-2.56	106.33	110.83
22	C	512	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
24	d	404	BCR	C10-C11-C12	-2.56	115.78	123.20
23	D	402	PHO	C1A-C2A-C3A	-2.56	100.40	102.84
22	b	615	CLA	C1D-ND-C4D	-2.56	104.52	106.31
24	H	102	BCR	C16-C15-C14	-2.56	118.29	123.52
22	B	603	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
22	b	611	CLA	C1D-ND-C4D	-2.55	104.52	106.31
22	c	502	CLA	C1D-ND-C4D	-2.55	104.52	106.31
29	b	624	LMG	O8-C28-C29	2.55	119.61	111.83
33	E	102	HEM	C3B-C2B-C1B	2.55	108.33	106.41
25	d	405	PL9	C15-C14-C16	2.55	119.65	115.23
26	a	410	SQD	O7-S-C6	2.55	110.56	106.76
22	c	504	CLA	C2C-C1C-NC	2.54	112.66	109.98
24	K	102	BCR	C15-C16-C17	-2.54	118.31	123.52
25	A	408	PL9	C37-C36-C34	-2.54	104.76	113.19
30	H	103	DGD	O2G-C1B-O1B	-2.54	117.76	123.70
22	C	505	CLA	C2C-C1C-NC	2.54	112.65	109.98
22	A	412	CLA	C4D-C3D-CAD	2.54	110.86	108.11
29	C	501	LMG	C8-O7-C10	-2.54	111.72	117.80
22	B	605	CLA	CHD-C1D-ND	-2.54	121.23	124.80
22	C	509	CLA	C2C-C1C-NC	2.53	112.64	109.98
22	C	513	CLA	C4D-C3D-CAD	2.53	110.85	108.11
22	B	615	CLA	CHC-C1C-NC	2.53	128.12	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C1D-ND-C4D	-2.53	104.54	106.31
22	d	402	CLA	C1D-ND-C4D	-2.53	104.54	106.31
22	b	611	CLA	C4D-C3D-CAD	2.52	110.85	108.11
24	t	102	BCR	C7-C6-C5	-2.52	115.74	121.56
22	b	614	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
22	b	618	CLA	C1D-CHD-C4C	-2.52	120.66	126.02
22	B	604	CLA	C1D-ND-C4D	-2.52	104.54	106.31
24	K	101	BCR	C10-C11-C12	-2.52	115.89	123.20
22	C	510	CLA	C1D-CHD-C4C	-2.52	120.66	126.02
22	B	610	CLA	C1D-ND-C4D	-2.52	104.54	106.31
22	b	614	CLA	C4D-C3D-CAD	2.52	110.84	108.11
22	c	510	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
25	A	408	PL9	C42-C43-C44	-2.52	121.86	127.62
22	c	505	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	C	511	CLA	CHC-C1C-C2C	-2.51	119.80	126.95
24	c	515	BCR	C15-C16-C17	-2.51	118.38	123.52
22	c	512	CLA	CHD-C1D-ND	-2.51	121.27	124.80
24	A	407	BCR	C2-C1-C6	2.50	114.07	110.44
26	b	601	SQD	O48-C23-C24	2.50	119.45	111.83
29	B	621	LMG	O8-C28-C29	2.50	119.45	111.83
22	b	604	CLA	CHA-C4D-ND	2.50	137.70	132.55
24	c	524	BCR	C27-C26-C25	-2.49	119.33	122.70
22	c	514	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
22	c	503	CLA	CHD-C1D-ND	-2.49	121.29	124.80
22	H	101	CLA	CHD-C1D-ND	-2.49	121.29	124.80
22	C	505	CLA	C1D-CHD-C4C	-2.49	120.72	126.02
26	A	411	SQD	O48-C23-O10	-2.49	117.40	123.63
24	b	620	BCR	C29-C30-C25	2.49	114.06	110.44
24	A	407	BCR	C28-C27-C26	-2.49	109.62	114.06
34	V	201	HEC	O2D-CGD-CBD	2.49	121.87	114.00
26	f	102	SQD	C1-C2-C3	-2.49	104.78	110.01
22	C	514	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
22	b	607	CLA	CHC-C1C-NC	2.48	128.05	124.31
22	b	611	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	b	605	CLA	CMA-C3A-C4A	2.48	118.44	111.77
24	K	101	BCR	C11-C10-C9	-2.48	123.80	127.28
24	K	101	BCR	C8-C7-C6	-2.48	120.38	127.00
30	C	519	DGD	O5E-C6E-C5E	-2.47	102.92	111.33
24	D	405	BCR	C38-C26-C27	2.47	118.86	113.60
26	D	412	SQD	O48-C23-O10	-2.47	117.45	123.63
25	A	408	PL9	C25-C24-C26	2.47	119.52	115.23
22	C	503	CLA	C1-C2-C3	-2.47	122.15	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	407	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	c	511	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	B	611	CLA	C2C-C1C-NC	2.47	112.57	109.98
22	C	507	CLA	CHA-C1A-NA	-2.46	120.81	126.39
22	b	608	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	B	606	CLA	CHC-C1C-NC	2.46	128.02	124.31
32	d	406	LHG	O8-C6-C5	-2.46	101.30	108.40
24	d	404	BCR	C2-C3-C4	-2.46	105.87	111.28
25	d	405	PL9	C45-C44-C46	2.46	119.50	115.23
29	c	519	LMG	O7-C10-O9	-2.46	117.95	123.70
25	A	408	PL9	C2-C1-C6	2.46	121.92	119.00
24	a	408	BCR	C38-C26-C25	-2.46	121.80	124.48
22	C	508	CLA	C1D-CHD-C4C	-2.46	120.79	126.02
24	K	102	BCR	C2-C1-C6	2.46	114.01	110.44
22	a	407	CLA	CHC-C1C-NC	2.46	128.01	124.31
22	b	617	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
30	C	517	DGD	O1G-C1A-O1A	-2.45	117.49	123.63
22	B	601	CLA	CHC-C1C-NC	2.45	128.01	124.31
25	D	406	PL9	C15-C14-C16	2.45	119.49	115.23
22	C	506	CLA	C4D-C3D-CAD	2.45	110.77	108.11
22	C	509	CLA	C4D-C3D-CAD	2.45	110.77	108.11
22	A	404	CLA	CHA-C1A-NA	-2.45	120.84	126.39
29	B	621	LMG	O7-C10-O9	-2.45	117.99	123.70
22	c	510	CLA	CHD-C1D-ND	-2.44	121.36	124.80
22	C	510	CLA	C1D-ND-C4D	-2.44	104.60	106.31
24	h	101	BCR	C8-C9-C10	2.44	122.85	119.01
22	c	514	CLA	C2C-C1C-NC	2.44	112.54	109.98
32	l	101	LHG	O8-C23-O10	-2.44	117.53	123.63
22	C	507	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
26	a	410	SQD	C45-O47-C7	-2.44	111.96	117.80
24	T	101	BCR	C32-C1-C6	-2.44	106.42	110.24
25	D	406	PL9	C53-C6-C1	2.44	120.27	115.28
26	A	409	SQD	O9-S-C6	2.43	110.39	106.76
24	b	619	BCR	C34-C9-C10	-2.43	118.87	122.82
24	H	102	BCR	C2-C1-C6	2.43	113.97	110.44
22	B	615	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
22	c	513	CLA	C2C-C1C-NC	2.43	112.53	109.98
29	C	522	LMG	O8-C28-C29	2.43	119.23	111.83
24	c	523	BCR	C16-C15-C14	-2.43	118.55	123.52
26	f	102	SQD	O48-C23-C24	2.42	119.22	111.83
24	a	408	BCR	C2-C1-C6	2.42	113.96	110.44
22	B	607	CLA	C4D-C3D-CAD	2.42	110.73	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	BCR	C24-C23-C22	-2.42	122.66	126.23
26	D	412	SQD	C1-O5-C5	-2.42	109.00	113.72
22	B	604	CLA	C1-C2-C3	-2.42	122.23	126.20
22	B	604	CLA	CHC-C1C-NC	2.42	127.95	124.31
29	B	619	LMG	O8-C28-C29	2.42	119.21	111.83
22	c	514	CLA	C1-C2-C3	-2.42	122.24	126.20
22	b	615	CLA	C4D-C3D-CAD	2.42	110.73	108.11
22	B	603	CLA	CHA-C4D-ND	2.41	137.53	132.55
22	b	606	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
24	c	523	BCR	C38-C26-C27	2.41	118.74	113.60
26	a	410	SQD	O48-C23-C24	2.41	119.19	111.83
26	a	412	SQD	O48-C23-O10	-2.41	117.60	123.63
24	c	524	BCR	C23-C24-C25	-2.40	120.57	127.00
29	b	624	LMG	C1-C2-C3	2.40	115.06	110.01
30	C	517	DGD	O2G-C1B-O1B	-2.40	118.09	123.70
29	c	522	LMG	C6-C5-C4	-2.40	107.13	113.02
22	b	611	CLA	CHA-C1A-NA	-2.40	120.96	126.39
24	T	101	BCR	C3-C4-C5	-2.40	109.78	114.06
22	b	615	CLA	C1D-CHD-C4C	-2.40	120.92	126.02
22	C	511	CLA	C2C-C1C-NC	2.40	112.50	109.98
22	B	602	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	b	611	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
22	b	618	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
22	b	618	CLA	CHC-C1C-NC	2.39	127.92	124.31
32	E	101	LHG	O8-C23-O10	-2.39	117.64	123.63
22	c	507	CLA	CHA-C1A-NA	-2.39	120.97	126.39
22	d	403	CLA	C1D-ND-C4D	-2.39	104.63	106.31
24	A	407	BCR	C3-C4-C5	-2.39	109.80	114.06
22	c	506	CLA	C1-C2-C3	-2.39	122.29	126.20
22	A	404	CLA	CHA-C4D-ND	2.39	137.47	132.55
22	c	506	CLA	CHD-C1D-ND	-2.39	121.44	124.80
22	A	406	CLA	CHC-C1C-C2C	-2.39	120.17	126.95
22	c	513	CLA	CHC-C1C-C2C	-2.39	120.17	126.95
25	D	406	PL9	C35-C34-C36	2.39	119.37	115.23
22	C	511	CLA	C3D-C2D-C1D	2.38	109.08	105.83
32	d	407	LHG	O8-C23-C24	2.38	119.10	111.83
22	D	404	CLA	CHC-C1C-C2C	-2.38	120.17	126.95
32	D	408	LHG	O8-C23-O10	-2.38	117.67	123.63
22	C	513	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
24	C	515	BCR	C3-C4-C5	-2.38	109.81	114.06
24	B	618	BCR	C21-C20-C19	-2.38	116.30	123.20
22	C	503	CLA	C1D-CHD-C4C	-2.38	120.96	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	BCR	C36-C18-C19	2.38	121.72	118.09
24	B	617	BCR	C32-C1-C6	-2.38	106.51	110.24
22	b	613	CLA	C1D-ND-C4D	-2.38	104.64	106.31
32	e	101	LHG	O8-C23-C24	2.38	119.08	111.83
22	B	606	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
22	B	602	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
26	L	101	SQD	O6-C44-C45	-2.38	105.04	110.82
26	A	411	SQD	C3-C4-C5	2.38	114.54	110.23
22	c	504	CLA	CHC-C1C-C2C	-2.38	120.20	126.95
24	h	101	BCR	C38-C26-C25	-2.37	121.89	124.48
22	C	506	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	C	513	CLA	C1D-CHD-C4C	-2.37	120.98	126.02
26	L	101	SQD	O48-C23-C24	2.37	119.06	111.83
32	e	101	LHG	C5-O7-C7	-2.37	112.13	117.80
22	A	406	CLA	C1D-CHD-C4C	-2.37	120.99	126.02
22	B	602	CLA	C2C-C1C-NC	2.37	112.47	109.98
22	B	606	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	b	619	BCR	C37-C22-C21	-2.36	118.98	122.82
29	C	522	LMG	O1-C7-C8	2.36	116.56	110.82
24	C	516	BCR	C29-C30-C25	2.36	113.87	110.44
22	C	504	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
22	b	611	CLA	C2C-C1C-NC	2.35	112.45	109.98
30	C	518	DGD	C3G-O3G-C1D	-2.35	108.75	113.80
22	b	609	CLA	CHA-C1A-NA	-2.35	121.06	126.39
24	B	616	BCR	C21-C20-C19	-2.35	116.39	123.20
29	C	520	LMG	O7-C10-O9	-2.35	118.21	123.70
30	H	103	DGD	C2G-O2G-C1B	-2.35	112.17	117.80
22	c	502	CLA	CHA-C1A-NA	-2.35	121.07	126.39
22	b	607	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
22	b	610	CLA	C4D-C3D-CAD	2.35	110.65	108.11
24	A	407	BCR	C36-C18-C17	-2.34	119.02	122.82
22	B	608	CLA	CHD-C1D-ND	-2.34	121.50	124.80
24	c	515	BCR	C29-C30-C25	2.34	113.84	110.44
22	C	502	CLA	C1-C2-C3	-2.34	122.36	126.20
25	d	405	PL9	C30-C29-C31	2.34	119.29	115.23
22	C	505	CLA	C1-C2-C3	-2.34	122.36	126.20
22	B	602	CLA	CMA-C3A-C4A	2.34	118.06	111.77
22	C	508	CLA	CHA-C4D-ND	2.34	137.38	132.55
26	A	411	SQD	O8-S-C6	2.34	110.49	105.97
24	H	102	BCR	C20-C21-C22	-2.34	124.00	127.28
22	c	509	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
33	E	102	HEM	C4D-ND-C1D	2.33	107.97	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	CHA-C1A-NA	-2.33	121.11	126.39
22	c	512	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
25	A	408	PL9	C22-C21-C19	-2.33	105.46	113.19
22	B	606	CLA	CAA-CBA-CGA	2.33	119.83	113.21
24	h	101	BCR	C2-C1-C6	2.33	113.83	110.44
24	b	621	BCR	C3-C4-C5	-2.33	109.90	114.06
24	t	102	BCR	C2-C1-C6	2.33	113.83	110.44
24	b	619	BCR	C36-C18-C19	2.33	121.65	118.09
22	b	605	CLA	CHD-C1D-ND	-2.33	121.53	124.80
24	h	101	BCR	C33-C5-C6	-2.33	121.94	124.48
24	D	405	BCR	C3-C4-C5	-2.33	109.91	114.06
24	C	515	BCR	C16-C15-C14	-2.33	118.76	123.52
22	C	510	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
22	B	614	CLA	C2C-C1C-NC	2.32	112.42	109.98
24	K	101	BCR	C21-C20-C19	-2.32	116.47	123.20
22	d	401	CLA	CHA-C1A-NA	-2.32	121.13	126.39
23	D	402	PHO	CMA-C3A-C4A	-2.32	109.61	114.61
22	a	407	CLA	C1D-CHD-C4C	-2.32	121.10	126.02
24	H	102	BCR	C15-C14-C13	-2.32	124.03	127.28
30	C	519	DGD	O1G-C1A-O1A	-2.31	117.84	123.63
25	D	406	PL9	C10-C9-C11	2.31	119.24	115.23
22	C	507	CLA	C4D-C3D-CAD	2.31	110.62	108.11
22	B	607	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
29	c	522	LMG	C7-O1-C1	-2.31	108.85	113.80
22	b	604	CLA	C1D-CHD-C4C	-2.31	121.12	126.02
25	A	408	PL9	C35-C34-C36	2.31	119.23	115.23
22	B	609	CLA	CHA-C1A-NA	-2.31	121.17	126.39
33	E	102	HEM	O2A-CGA-CBA	2.30	121.27	114.00
22	B	609	CLA	C1D-CHD-C4C	-2.30	121.13	126.02
24	T	101	BCR	C27-C26-C25	-2.30	119.60	122.70
22	C	503	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
22	c	510	CLA	C1D-ND-C4D	-2.30	104.70	106.31
26	f	102	SQD	O47-C7-O49	-2.30	118.34	123.70
22	c	505	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
22	c	505	CLA	C1D-CHD-C4C	-2.29	121.15	126.02
22	a	405	CLA	C1-C2-C3	-2.29	122.45	126.20
22	B	609	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
24	K	102	BCR	C21-C20-C19	-2.29	116.57	123.20
30	h	102	DGD	O1G-C1A-O1A	-2.29	117.91	123.63
22	d	403	CLA	CHA-C1A-NA	-2.29	121.21	126.39
25	a	409	PL9	C15-C14-C16	2.28	119.19	115.23
25	d	405	PL9	C2-C1-C6	2.28	121.71	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	C2C-C1C-NC	2.28	112.38	109.98
22	b	604	CLA	C2C-C1C-NC	2.28	112.38	109.98
24	D	405	BCR	C35-C13-C14	-2.28	119.12	122.82
24	d	404	BCR	C39-C30-C25	-2.28	106.67	110.24
22	B	601	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
25	a	409	PL9	C27-C28-C29	-2.28	122.41	127.62
22	A	403	CLA	CHC-C1C-C2C	-2.28	120.48	126.95
29	C	522	LMG	C1-O6-C5	-2.28	109.28	113.72
22	B	615	CLA	C3D-C2D-C1D	2.27	108.93	105.83
22	b	614	CLA	C2A-C3A-C4A	2.27	105.54	101.87
30	c	516	DGD	O2G-C1B-O1B	-2.27	118.39	123.70
22	b	616	CLA	C4D-C3D-CAD	2.27	110.57	108.11
22	C	505	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	a	408	BCR	C10-C11-C12	-2.27	116.62	123.20
22	b	615	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	c	514	CLA	C1D-CHD-C4C	-2.27	121.20	126.02
24	T	101	BCR	C30-C25-C26	-2.27	119.54	122.64
25	A	408	PL9	C7-C3-C2	-2.27	120.72	123.39
34	V	201	HEC	CAD-CBD-CGD	2.27	119.68	113.67
22	d	401	CLA	CHA-C4D-ND	2.27	137.22	132.55
22	b	603	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
26	a	412	SQD	O6-C1-C2	2.27	111.71	108.27
22	A	404	CLA	C2C-C1C-NC	2.27	112.36	109.98
22	A	412	CLA	C1-C2-C3	-2.26	122.49	126.20
22	C	511	CLA	C1D-CHD-C4C	-2.26	121.21	126.02
22	C	504	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	b	619	BCR	C30-C25-C26	-2.26	119.54	122.64
24	D	405	BCR	C30-C25-C24	2.26	121.79	115.65
22	C	505	CLA	C1D-ND-C4D	-2.26	104.72	106.31
22	c	508	CLA	CHA-C1A-NA	-2.26	121.27	126.39
22	a	407	CLA	C1-C2-C3	-2.26	122.49	126.20
22	C	514	CLA	C1D-CHD-C4C	-2.26	121.22	126.02
22	a	404	CLA	C2C-C1C-NC	2.26	112.35	109.98
22	A	412	CLA	CHC-C1C-NC	2.26	127.71	124.31
22	a	405	CLA	C4D-C3D-CAD	2.26	110.56	108.11
22	b	614	CLA	C1D-CHD-C4C	-2.26	121.22	126.02
25	A	408	PL9	C10-C9-C11	2.26	119.14	115.23
22	B	612	CLA	C2C-C1C-NC	2.26	112.35	109.98
29	c	522	LMG	C1-O6-C5	-2.25	109.32	113.72
22	B	611	CLA	CHA-C4D-ND	2.25	137.19	132.55
29	c	501	LMG	O8-C28-C29	2.25	118.70	111.83
22	B	606	CLA	CHA-C1A-NA	-2.25	121.30	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	O3G-C1D-C2D	2.25	111.69	108.27
22	B	604	CLA	CHD-C1D-C2D	2.25	130.16	125.49
22	B	604	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
22	B	612	CLA	CHA-C1A-NA	-2.25	121.30	126.39
22	C	511	CLA	CHC-C1C-NC	2.25	127.69	124.31
29	m	103	LMG	O1-C7-C8	-2.25	105.36	110.82
32	b	628	LHG	O8-C23-O10	-2.24	118.02	123.63
24	T	101	BCR	C37-C22-C21	-2.24	119.18	122.82
24	T	101	BCR	C1-C6-C7	2.24	121.73	115.65
22	c	504	CLA	CHA-C1A-NA	-2.24	121.31	126.39
22	c	509	CLA	C2C-C1C-NC	2.24	112.34	109.98
22	A	412	CLA	C1D-ND-C4D	-2.24	104.74	106.31
24	B	617	BCR	C21-C20-C19	-2.24	116.70	123.20
24	C	515	BCR	C2-C1-C6	2.24	113.69	110.44
22	C	510	CLA	CHA-C4D-ND	2.24	137.17	132.55
22	b	608	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
22	b	604	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
30	C	519	DGD	C2G-O2G-C1B	-2.24	112.44	117.80
32	D	408	LHG	O7-C7-O9	-2.24	118.47	123.70
24	k	101	BCR	C8-C7-C6	-2.24	121.02	127.00
22	b	603	CLA	C1D-CHD-C4C	-2.24	121.27	126.02
22	c	503	CLA	C2C-C1C-NC	2.24	112.33	109.98
22	C	506	CLA	CHA-C1A-NA	-2.23	121.33	126.39
22	B	609	CLA	C3D-C2D-C1D	2.23	108.88	105.83
22	c	511	CLA	C1D-CHD-C4C	-2.23	121.27	126.02
22	c	502	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
24	C	515	BCR	C37-C22-C23	2.23	121.50	118.09
24	c	523	BCR	C23-C24-C25	-2.23	121.04	127.00
24	B	616	BCR	C7-C8-C9	-2.23	122.94	126.23
24	t	102	BCR	C35-C13-C14	-2.23	119.21	122.82
26	A	409	SQD	O8-S-C6	2.22	110.27	105.97
22	C	508	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
32	b	628	LHG	O7-C7-O9	-2.22	118.51	123.70
24	a	408	BCR	C37-C22-C21	-2.22	119.22	122.82
22	b	609	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
22	b	609	CLA	CHD-C1D-ND	-2.22	121.68	124.80
33	e	102	HEM	O2D-CGD-CBD	2.22	121.01	114.00
26	a	410	SQD	O48-C23-O10	-2.22	118.08	123.63
29	m	103	LMG	C4-C3-C2	-2.22	106.94	110.83
22	C	511	CLA	CHA-C4D-ND	2.22	137.12	132.55
29	D	410	LMG	O8-C28-C29	2.22	118.59	111.83
26	b	601	SQD	O47-C7-O49	-2.22	118.53	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	518	DGD	C1D-O6D-C5D	-2.22	109.39	113.72
24	C	516	BCR	C36-C18-C19	2.21	121.47	118.09
22	b	603	CLA	C2C-C1C-NC	2.21	112.31	109.98
22	A	404	CLA	C3D-C2D-C1D	2.21	108.85	105.83
24	A	407	BCR	C15-C14-C13	-2.21	124.18	127.28
24	c	515	BCR	C23-C24-C25	-2.21	121.09	127.00
29	m	103	LMG	O8-C28-O10	-2.21	118.10	123.63
22	B	608	CLA	C1D-ND-C4D	-2.21	104.76	106.31
22	b	609	CLA	C1-O2A-CGA	2.21	122.00	116.65
22	a	404	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
22	c	513	CLA	C4D-CHA-C1A	-2.21	118.61	121.24
26	A	409	SQD	O47-C7-O49	-2.21	118.54	123.70
22	c	510	CLA	CHA-C4D-ND	2.21	137.10	132.55
25	d	405	PL9	C25-C24-C26	2.21	119.06	115.23
24	b	620	BCR	C21-C20-C19	-2.21	116.81	123.20
22	B	602	CLA	CHA-C4D-ND	2.21	137.10	132.55
24	T	101	BCR	C28-C27-C26	-2.20	110.12	114.06
24	c	524	BCR	C33-C5-C6	-2.20	122.08	124.48
24	c	515	BCR	C15-C14-C13	-2.20	124.19	127.28
22	C	507	CLA	CHD-C1D-ND	-2.20	121.70	124.80
22	D	404	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	a	408	BCR	C29-C30-C25	2.20	113.63	110.44
29	b	624	LMG	C9-O8-C28	2.20	125.15	117.12
25	a	409	PL9	C10-C9-C8	-2.20	117.99	123.63
22	B	614	CLA	CHA-C1A-NA	-2.19	121.42	126.39
22	c	503	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
22	D	404	CLA	C1D-CHD-C4C	-2.19	121.36	126.02
34	V	201	HEC	CMD-C2D-C1D	2.19	128.76	125.42
22	a	405	CLA	C3D-C2D-C1D	2.19	108.82	105.83
22	B	612	CLA	CAA-CBA-CGA	2.19	119.43	113.21
22	A	403	CLA	C2C-C1C-NC	2.19	112.28	109.98
29	f	101	LMG	O7-C10-O9	-2.19	118.58	123.70
25	D	406	PL9	C22-C23-C24	-2.19	122.61	127.62
22	C	503	CLA	CHC-C1C-NC	2.19	127.61	124.31
22	d	401	CLA	C4D-C3D-CAD	2.19	110.48	108.11
22	C	507	CLA	CHA-C4D-ND	2.19	137.06	132.55
22	b	613	CLA	C3D-C2D-C1D	2.19	108.82	105.83
25	a	409	PL9	C30-C29-C31	2.19	119.03	115.23
22	C	509	CLA	CHA-C1A-NA	-2.18	121.45	126.39
22	A	406	CLA	CHD-C1D-ND	-2.18	121.73	124.80
22	C	508	CLA	C1D-ND-C4D	-2.18	104.78	106.31
22	b	604	CLA	CHD-C1D-ND	-2.18	121.73	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	601	SQD	O5-C1-C2	-2.18	105.89	110.37
22	C	505	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
25	A	408	PL9	C40-C39-C41	2.18	119.01	115.23
24	H	102	BCR	C34-C9-C10	-2.18	119.29	122.82
22	C	509	CLA	C1D-CHD-C4C	-2.18	121.40	126.02
29	c	522	LMG	O6-C1-O1	2.17	115.18	110.04
22	b	613	CLA	CHC-C1C-NC	2.17	127.58	124.31
22	C	508	CLA	CHC-C1C-NC	2.17	127.58	124.31
30	C	519	DGD	C3G-C2G-C1G	-2.17	106.72	111.78
24	d	404	BCR	C36-C18-C17	-2.17	119.30	122.82
24	b	619	BCR	C39-C30-C25	-2.17	106.84	110.24
24	B	616	BCR	C34-C9-C8	2.17	121.40	118.09
22	b	618	CLA	C1-C2-C3	-2.16	122.65	126.20
22	C	507	CLA	C1D-CHD-C4C	-2.16	121.42	126.02
22	C	514	CLA	CHA-C1A-NA	-2.16	121.49	126.39
22	a	407	CLA	CHA-C1A-NA	-2.16	121.49	126.39
22	b	617	CLA	CHA-C4D-ND	2.16	137.00	132.55
22	b	610	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
22	B	609	CLA	CHA-C4D-ND	2.16	137.00	132.55
22	c	503	CLA	C4D-C3D-CAD	2.16	110.45	108.11
26	a	410	SQD	C1-O5-C5	-2.16	109.51	113.72
25	D	406	PL9	C32-C33-C34	-2.15	122.69	127.62
26	a	410	SQD	O5-C1-C2	-2.15	105.95	110.37
22	c	512	CLA	CHA-C1A-NA	-2.15	121.52	126.39
30	c	517	DGD	O1G-C1A-O1A	-2.15	118.25	123.63
22	H	101	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
22	C	509	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
22	C	502	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
22	b	612	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
24	c	523	BCR	C10-C11-C12	-2.14	116.99	123.20
24	c	523	BCR	C34-C9-C8	2.14	121.36	118.09
24	c	524	BCR	C24-C23-C22	-2.14	123.07	126.23
22	b	603	CLA	CHD-C1D-ND	-2.13	121.80	124.80
24	B	618	BCR	C11-C10-C9	-2.13	124.29	127.28
22	A	412	CLA	C1D-CHD-C4C	-2.13	121.48	126.02
26	f	102	SQD	C3-C4-C5	2.13	114.10	110.23
22	C	513	CLA	C4D-CHA-C1A	-2.13	118.70	121.24
32	l	101	LHG	C25-C24-C23	-2.13	105.88	113.69
22	B	611	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
30	C	518	DGD	C2G-O2G-C1B	-2.13	112.69	117.80
22	b	609	CLA	CHA-C4D-ND	2.13	136.95	132.55
22	B	607	CLA	C2C-C1C-NC	2.13	112.22	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	C4-C3-C2	-2.13	107.09	110.83
22	c	503	CLA	C1D-CHD-C4C	-2.13	121.49	126.02
29	m	103	LMG	C9-C8-C7	-2.13	106.82	111.78
24	B	617	BCR	C8-C7-C6	-2.13	121.31	127.00
29	b	624	LMG	O6-C5-C6	2.13	111.71	106.44
26	A	411	SQD	C4-C3-C2	2.13	114.56	110.83
22	c	506	CLA	CHA-C1A-NA	-2.13	121.58	126.39
22	C	504	CLA	C2C-C1C-NC	2.13	112.22	109.98
22	c	514	CLA	CHC-C1C-NC	2.13	127.51	124.31
22	b	611	CLA	C1-C2-C3	-2.13	122.71	126.20
24	a	408	BCR	C37-C22-C23	2.13	121.33	118.09
22	B	603	CLA	C1D-ND-C4D	-2.13	104.82	106.31
22	A	404	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
32	D	407	LHG	O3-P-O5	-2.12	100.51	108.94
26	b	601	SQD	O9-S-C6	2.12	109.93	106.76
22	B	607	CLA	C3D-C2D-C1D	2.12	108.73	105.83
22	b	606	CLA	CHC-C1C-NC	2.12	127.51	124.31
22	c	502	CLA	C1D-CHD-C4C	-2.12	121.51	126.02
24	h	101	BCR	C20-C21-C22	-2.12	124.30	127.28
22	B	608	CLA	C1-C2-C3	-2.12	122.72	126.20
22	C	502	CLA	CHA-C1A-NA	-2.12	121.59	126.39
24	C	515	BCR	C28-C27-C26	-2.12	110.28	114.06
22	c	507	CLA	C3D-C2D-C1D	2.12	108.72	105.83
22	c	511	CLA	C3D-C2D-C1D	2.12	108.72	105.83
22	c	510	CLA	C1D-CHD-C4C	-2.12	121.52	126.02
22	c	507	CLA	CHA-C4D-ND	2.11	136.91	132.55
22	d	403	CLA	CHA-C4D-ND	2.11	136.91	132.55
24	c	524	BCR	C38-C26-C27	2.11	118.10	113.60
22	C	506	CLA	CHC-C1C-NC	2.11	127.49	124.31
24	d	404	BCR	C3-C4-C5	-2.11	110.29	114.06
29	b	624	LMG	C6-C5-C4	-2.11	107.84	113.02
22	C	508	CLA	CHD-C1D-ND	-2.11	121.83	124.80
22	c	508	CLA	CHA-C4D-ND	2.11	136.90	132.55
22	b	609	CLA	CHC-C1C-NC	2.11	127.48	124.31
22	c	503	CLA	CHA-C1A-NA	-2.11	121.62	126.39
34	v	201	HEC	CAD-CBD-CGD	2.11	119.25	113.67
25	a	409	PL9	C51-C49-C50	2.11	119.44	114.59
22	d	401	CLA	CHD-C1D-C2D	2.11	129.87	125.49
22	C	508	CLA	C1-C2-C3	-2.11	122.75	126.20
22	b	610	CLA	C2C-C1C-NC	2.11	112.19	109.98
25	d	405	PL9	C10-C9-C11	2.10	118.88	115.23
22	c	505	CLA	CHC-C1C-NC	2.10	127.48	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	621	LMG	C8-O7-C10	-2.10	112.77	117.80
24	K	101	BCR	C16-C15-C14	-2.10	119.22	123.52
25	a	409	PL9	C37-C36-C34	-2.10	106.23	113.19
22	C	508	CLA	CHA-C1A-NA	-2.10	121.64	126.39
22	d	403	CLA	CHC-C1C-NC	2.10	127.47	124.31
22	a	405	CLA	C4D-CHA-C1A	-2.10	118.74	121.24
34	v	201	HEC	CHD-C4C-C3C	2.10	128.74	125.21
22	C	513	CLA	CHD-C1D-ND	-2.10	121.85	124.80
22	c	506	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
24	c	524	BCR	C15-C16-C17	-2.10	119.23	123.52
22	c	506	CLA	C2C-C1C-NC	2.10	112.18	109.98
22	D	404	CLA	C1-C2-C3	-2.10	122.76	126.20
22	B	610	CLA	CHC-C1C-NC	2.09	127.47	124.31
22	c	513	CLA	C3A-C2A-C1A	2.09	104.47	101.34
33	e	102	HEM	C1B-NB-C4B	2.09	107.68	105.21
26	b	601	SQD	O48-C23-O10	-2.09	118.40	123.63
22	C	504	CLA	CHC-C1C-NC	2.09	127.46	124.31
24	B	618	BCR	C33-C5-C6	-2.09	122.21	124.48
22	C	502	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
30	c	516	DGD	O1G-C1A-C2A	2.08	118.19	111.83
22	d	401	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
24	b	621	BCR	C27-C26-C25	-2.08	119.89	122.70
22	b	605	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
22	b	606	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
24	b	620	BCR	C8-C7-C6	-2.08	121.44	127.00
22	C	513	CLA	C3A-C2A-C1A	2.08	104.45	101.34
22	d	401	CLA	CHC-C1C-NC	2.08	127.44	124.31
22	b	603	CLA	CHA-C4D-ND	2.08	136.83	132.55
24	b	619	BCR	C38-C26-C25	-2.07	122.22	124.48
24	B	618	BCR	C16-C15-C14	-2.07	119.28	123.52
22	B	608	CLA	CHA-C4D-ND	2.07	136.83	132.55
26	D	412	SQD	O5-C1-C2	-2.07	106.11	110.37
24	B	617	BCR	C38-C26-C27	2.07	118.01	113.60
22	C	507	CLA	C3D-C2D-C1D	2.07	108.66	105.83
22	A	406	CLA	CHA-C1A-NA	-2.07	121.70	126.39
22	b	615	CLA	C1-C2-C3	-2.07	122.81	126.20
22	a	405	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
26	f	102	SQD	O8-S-C6	2.07	109.96	105.97
24	b	621	BCR	C37-C22-C23	2.07	121.25	118.09
22	B	614	CLA	C2A-C3A-C4A	2.07	105.21	101.87
22	c	512	CLA	C2A-C3A-C4A	2.07	105.21	101.87
22	B	609	CLA	CHD-C1D-ND	-2.07	121.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	C2C-C1C-NC	2.07	112.15	109.98
24	B	618	BCR	C37-C22-C23	2.06	121.24	118.09
24	h	101	BCR	C28-C27-C26	-2.06	110.38	114.06
22	b	606	CLA	C2C-C1C-NC	2.06	112.15	109.98
22	b	612	CLA	C1D-CHD-C4C	-2.06	121.64	126.02
29	f	101	LMG	O8-C28-O10	-2.06	118.47	123.63
22	C	502	CLA	C3D-C2D-C1D	2.06	108.64	105.83
33	e	102	HEM	C3B-C2B-C1B	2.06	107.96	106.41
24	h	101	BCR	C24-C23-C22	-2.06	123.19	126.23
26	b	601	SQD	C1-C2-C3	-2.06	105.68	110.01
24	t	102	BCR	C36-C18-C17	-2.06	119.48	122.82
22	H	101	CLA	C2C-C1C-NC	2.06	112.14	109.98
22	B	605	CLA	CHA-C4D-ND	2.06	136.79	132.55
29	C	520	LMG	O8-C28-O10	-2.06	118.49	123.63
29	C	522	LMG	C3-C4-C5	-2.06	106.50	110.23
22	C	506	CLA	CHC-C1C-C2C	-2.06	121.11	126.95
22	a	405	CLA	CHA-C1A-NA	-2.06	121.74	126.39
22	C	502	CLA	CMA-C3A-C4A	2.05	117.29	111.77
25	a	409	PL9	C47-C48-C49	-2.05	120.80	127.64
22	c	509	CLA	C1D-CHD-C4C	-2.05	121.66	126.02
22	C	512	CLA	CHA-C1A-NA	-2.05	121.75	126.39
22	A	404	CLA	CHD-C1D-C2D	2.05	129.75	125.49
22	c	504	CLA	C1D-CHD-C4C	-2.05	121.67	126.02
22	b	608	CLA	CHA-C1A-NA	-2.05	121.75	126.39
24	D	405	BCR	C1-C6-C7	2.05	121.20	115.65
22	B	609	CLA	CHC-C1C-NC	2.05	127.39	124.31
24	c	524	BCR	C21-C20-C19	-2.05	117.27	123.20
23	D	402	PHO	C1-C2-C3	-2.05	122.85	126.20
22	b	603	CLA	CHA-C1A-NA	-2.04	121.76	126.39
22	B	606	CLA	CHD-C1D-ND	-2.04	121.93	124.80
22	c	503	CLA	C3D-C2D-C1D	2.04	108.62	105.83
22	c	502	CLA	CHA-C4D-ND	2.04	136.76	132.55
22	b	615	CLA	CHA-C1A-NA	-2.04	121.77	126.39
22	B	610	CLA	C1D-CHD-C4C	-2.04	121.69	126.02
26	a	410	SQD	C44-O6-C1	-2.04	109.42	113.80
24	a	408	BCR	C21-C20-C19	-2.04	117.29	123.20
24	b	619	BCR	C1-C6-C7	2.04	121.17	115.65
22	H	101	CLA	C1D-CHD-C4C	-2.04	121.69	126.02
22	b	603	CLA	C3D-C2D-C1D	2.04	108.61	105.83
29	c	519	LMG	C4-C3-C2	-2.04	107.26	110.83
24	C	515	BCR	C23-C24-C25	-2.04	121.56	127.00
22	B	615	CLA	CHA-C4D-ND	2.03	136.75	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C2-C3-C4	-2.03	106.80	111.28
25	A	408	PL9	O2-C1-C2	-2.03	117.20	121.83
22	b	615	CLA	C3A-C2A-C1A	2.03	104.38	101.34
22	B	610	CLA	CHD-C1D-C2D	2.03	129.71	125.49
22	C	503	CLA	CHA-C1A-NA	-2.03	121.79	126.39
22	B	614	CLA	C1D-CHD-C4C	-2.03	121.70	126.02
26	b	601	SQD	O5-C5-C4	2.03	113.36	109.70
22	B	610	CLA	C3D-C2D-C1D	2.03	108.60	105.83
22	c	507	CLA	C2C-C1C-NC	2.03	112.11	109.98
29	B	621	LMG	O8-C28-O10	-2.03	118.55	123.63
22	b	614	CLA	CHC-C1C-NC	2.03	127.37	124.31
22	C	504	CLA	C1D-CHD-C4C	-2.03	121.71	126.02
22	b	617	CLA	C1D-CHD-C4C	-2.03	121.72	126.02
24	b	621	BCR	C11-C10-C9	-2.02	124.44	127.28
30	c	516	DGD	O6D-C5D-C6D	2.02	110.71	106.69
22	b	607	CLA	CHA-C1A-NA	-2.02	121.81	126.39
22	c	508	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
22	D	403	CLA	C1D-CHD-C4C	-2.02	121.72	126.02
22	B	608	CLA	C3D-C2D-C1D	2.02	108.59	105.83
22	C	513	CLA	CHC-C1C-NC	2.02	127.35	124.31
22	C	505	CLA	CMA-C3A-C4A	2.02	117.20	111.77
22	C	502	CLA	CHA-C4D-ND	2.02	136.71	132.55
22	c	510	CLA	CHA-C1A-NA	-2.02	121.82	126.39
30	C	517	DGD	C4E-C3E-C2E	-2.02	107.29	110.83
22	B	607	CLA	CHA-C1A-NA	-2.02	121.82	126.39
22	B	603	CLA	C1D-CHD-C4C	-2.02	121.73	126.02
22	c	509	CLA	CHC-C1C-NC	2.02	127.35	124.31
22	D	403	CLA	C3A-C2A-C1A	2.01	104.36	101.34
22	C	506	CLA	C3D-C2D-C1D	2.01	108.58	105.83
22	c	507	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
22	B	605	CLA	C4D-CHA-C1A	-2.01	118.84	121.24
29	c	501	LMG	O7-C10-O9	-2.01	119.00	123.70
22	B	609	CLA	C2C-C1C-NC	2.01	112.09	109.98
24	B	617	BCR	C15-C16-C17	-2.01	119.40	123.52
22	A	403	CLA	C3D-C2D-C1D	2.01	108.58	105.83
24	c	524	BCR	C36-C18-C17	-2.01	119.56	122.82
22	b	610	CLA	CHA-C1A-NA	-2.01	121.84	126.39
22	a	404	CLA	C3D-C2D-C1D	2.01	108.57	105.83
22	b	606	CLA	C2A-C3A-C4A	2.01	105.11	101.87
25	D	406	PL9	C51-C49-C50	2.01	119.21	114.59
22	b	608	CLA	C2C-C1C-NC	2.01	112.09	109.98
22	c	502	CLA	CHC-C1C-NC	2.01	127.33	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
32	d	406	LHG	O7-C7-O9	-2.01	119.02	123.70
29	C	522	LMG	O8-C28-O10	-2.01	118.61	123.63
22	c	510	CLA	CHC-C1C-NC	2.01	127.33	124.31
24	c	515	BCR	C21-C20-C19	-2.00	117.39	123.20
24	H	102	BCR	C3-C4-C5	-2.00	110.48	114.06
22	c	510	CLA	C1-C2-C3	-2.00	122.92	126.20
24	b	619	BCR	C24-C23-C22	-2.00	123.27	126.23
22	C	510	CLA	CHD-C1D-ND	-2.00	121.98	124.80
24	C	515	BCR	C34-C9-C10	-2.00	119.57	122.82
22	A	403	CLA	C1D-CHD-C4C	-2.00	121.77	126.02
32	L	102	LHG	O8-C23-C24	2.00	117.94	111.83

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	406	CLA	ND
22	A	412	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	514	CLA	ND
22	D	403	CLA	ND
22	D	404	CLA	ND
22	H	101	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	407	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	b	618	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND
22	d	401	CLA	ND

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Mol	Chain	Res	Type	Atom
22	d	402	CLA	ND
22	d	403	CLA	ND

All (1105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	613	CLA	C4B-C3B-CAB-CBB
22	B	613	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	C2B-C3B-CAB-CBB
22	B	614	CLA	C4B-C3B-CAB-CBB
22	C	506	CLA	C4B-C3B-CAB-CBB
22	H	101	CLA	CAD-CBD-CGD-O1D
22	H	101	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	C2B-C3B-CAB-CBB
22	b	603	CLA	C4B-C3B-CAB-CBB
22	b	603	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	C2B-C3B-CAB-CBB
22	b	607	CLA	C4B-C3B-CAB-CBB
22	b	613	CLA	C2B-C3B-CAB-CBB
22	b	613	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	CAD-CBD-CGD-O1D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	C2B-C3B-CAB-CBB
22	c	502	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
24	D	405	BCR	C7-C8-C9-C10
24	D	405	BCR	C21-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	K	102	BCR	C7-C8-C9-C10
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	T	101	BCR	C17-C18-C19-C20
24	T	101	BCR	C36-C18-C19-C20
24	T	101	BCR	C21-C22-C23-C24
24	T	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	b	621	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C34
24	d	404	BCR	C21-C22-C23-C24
24	h	101	BCR	C7-C8-C9-C10
24	h	101	BCR	C7-C8-C9-C34
26	A	411	SQD	O6-C44-C45-O47
26	A	411	SQD	O5-C5-C6-S
26	A	411	SQD	C5-C6-S-O7
26	A	411	SQD	C5-C6-S-O8
26	A	411	SQD	C5-C6-S-O9
26	L	101	SQD	C46-C45-O47-C7
26	L	101	SQD	C5-C6-S-O7
26	L	101	SQD	C5-C6-S-O8
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	C8-C7-O47-C45
29	C	522	LMG	O6-C1-O1-C7
29	b	624	LMG	C11-C10-O7-C8
32	D	408	LHG	C4-O6-P-O3
32	D	408	LHG	C4-O6-P-O4
32	D	409	LHG	C4-O6-P-O4
32	E	101	LHG	C3-O3-P-O4
32	E	101	LHG	C3-O3-P-O6
32	E	101	LHG	C4-O6-P-O4
32	L	102	LHG	C3-O3-P-O4
32	L	102	LHG	C3-O3-P-O6
32	L	102	LHG	C4-O6-P-O3
32	L	102	LHG	C4-O6-P-O4
32	L	102	LHG	C4-O6-P-O5
32	b	628	LHG	C3-O3-P-O4
32	b	628	LHG	C3-O3-P-O6
32	d	406	LHG	C3-O3-P-O4
32	d	406	LHG	C3-O3-P-O6
32	d	406	LHG	C4-O6-P-O3
32	d	406	LHG	C4-O6-P-O4
32	d	407	LHG	C3-O3-P-O5
32	d	407	LHG	C4-O6-P-O5
32	e	101	LHG	C3-O3-P-O4
32	e	101	LHG	C3-O3-P-O5
32	e	101	LHG	C3-O3-P-O6
32	l	101	LHG	C3-O3-P-O4
32	l	101	LHG	C3-O3-P-O6
32	l	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
32	l	101	LHG	C4-O6-P-O4
32	l	101	LHG	C4-O6-P-O5
33	E	102	HEM	C2B-C3B-CAB-CBB
33	E	102	HEM	C3D-CAD-CBD-CGD
33	e	102	HEM	C2B-C3B-CAB-CBB
33	e	102	HEM	C4B-C3B-CAB-CBB
33	e	102	HEM	C2C-C3C-CAC-CBC
34	V	201	HEC	C2B-C3B-CAB-CBB
34	V	201	HEC	C4B-C3B-CAB-CBB
34	v	201	HEC	C2B-C3B-CAB-CBB
34	v	201	HEC	C4B-C3B-CAB-CBB
26	L	101	SQD	O49-C7-O47-C45
26	f	102	SQD	O49-C7-O47-C45
29	b	624	LMG	O9-C10-O7-C8
22	B	613	CLA	C3-C5-C6-C7
22	b	616	CLA	C3-C5-C6-C7
22	b	605	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
25	A	408	PL9	C15-C14-C16-C17
25	a	409	PL9	C45-C44-C46-C47
22	b	605	CLA	C2-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
25	A	408	PL9	C13-C14-C16-C17
22	d	403	CLA	C3-C5-C6-C7
32	E	101	LHG	O2-C2-C3-O3
26	L	101	SQD	C24-C23-O48-C46
26	L	101	SQD	C8-C7-O47-C45
22	a	407	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
25	A	408	PL9	C9-C11-C12-C13
25	A	408	PL9	C14-C16-C17-C18
25	a	409	PL9	C19-C21-C22-C23
26	L	101	SQD	O10-C23-O48-C46
30	c	516	DGD	O6E-C5E-C6E-O5E
32	E	101	LHG	C1-C2-C3-O3
29	C	522	LMG	C29-C28-O8-C9
30	C	518	DGD	O6E-C5E-C6E-O5E
27	D	413	LFA	C3-C4-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	a	407	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	604	CLA	C4-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
25	a	409	PL9	C43-C44-C46-C47
22	B	604	CLA	C14-C13-C15-C16
22	B	608	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	H	101	CLA	C11-C10-C8-C9
22	b	612	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C10-C8-C9
32	D	409	LHG	C24-C25-C26-C27
30	c	517	DGD	O6E-C5E-C6E-O5E
29	c	522	LMG	C2-C1-O1-C7
30	c	517	DGD	C9B-CAB-CBB-CCB
30	C	518	DGD	C4E-C5E-C6E-O5E
30	c	517	DGD	C4E-C5E-C6E-O5E
24	D	405	BCR	C7-C8-C9-C34
24	K	102	BCR	C7-C8-C9-C34
24	T	101	BCR	C7-C8-C9-C34
24	d	404	BCR	C37-C22-C23-C24
24	t	102	BCR	C7-C8-C9-C34
24	t	102	BCR	C37-C22-C23-C24
24	T	101	BCR	C7-C8-C9-C10
24	t	102	BCR	C21-C22-C23-C24
29	b	624	LMG	C10-C11-C12-C13
29	c	501	LMG	C11-C12-C13-C14
22	B	615	CLA	C13-C15-C16-C17
30	c	516	DGD	C6A-C7A-C8A-C9A
30	h	102	DGD	C4B-C5B-C6B-C7B
22	H	101	CLA	C10-C11-C12-C13
26	f	102	SQD	C33-C34-C35-C36
22	D	403	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	b	607	CLA	C15-C16-C17-C18
25	a	409	PL9	C34-C36-C37-C38
22	C	504	CLA	C5-C6-C7-C8
26	A	409	SQD	C7-C8-C9-C10
29	B	619	LMG	C10-C11-C12-C13
29	c	522	LMG	C28-C29-C30-C31
29	C	522	LMG	O10-C28-O8-C9
22	B	601	CLA	C15-C16-C17-C18
22	a	404	CLA	C15-C16-C17-C18
22	d	403	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C2A-CAA-CBA-CGA
29	B	621	LMG	C10-C11-C12-C13
29	c	519	LMG	C10-C11-C12-C13
30	c	516	DGD	C1B-C2B-C3B-C4B
30	c	518	DGD	O6D-C1D-O3G-C3G
32	d	407	LHG	C24-C25-C26-C27
22	B	613	CLA	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
30	C	517	DGD	O6E-C5E-C6E-O5E
26	L	101	SQD	C23-C24-C25-C26
22	B	606	CLA	C3-C5-C6-C7
29	C	501	LMG	C28-C29-C30-C31
30	C	518	DGD	C1A-C2A-C3A-C4A
22	b	605	CLA	C5-C6-C7-C8
26	b	601	SQD	C7-C8-C9-C10
22	c	507	CLA	C13-C15-C16-C17
22	b	608	CLA	C2A-CAA-CBA-CGA
22	b	604	CLA	C13-C15-C16-C17
27	M	102	LFA	C12-C13-C14-C15
22	b	610	CLA	C13-C15-C16-C17
30	c	518	DGD	C2D-C1D-O3G-C3G
22	B	601	CLA	C13-C15-C16-C17
24	H	102	BCR	C7-C8-C9-C34
24	c	524	BCR	C7-C8-C9-C34
24	d	404	BCR	C7-C8-C9-C34
24	k	101	BCR	C11-C12-C13-C35
24	H	102	BCR	C7-C8-C9-C10
22	b	612	CLA	C2A-CAA-CBA-CGA
22	b	603	CLA	C8-C10-C11-C12
32	D	409	LHG	O1-C1-C2-C3
32	d	407	LHG	O1-C1-C2-C3
29	c	522	LMG	O6-C1-O1-C7
29	B	619	LMG	C32-C33-C34-C35
30	C	519	DGD	C2A-C1A-O1G-C1G
22	b	604	CLA	C8-C10-C11-C12
30	c	517	DGD	C3B-C4B-C5B-C6B
27	B	623	LFA	C5-C6-C7-C8
27	b	630	LFA	C9-C10-C11-C12
29	c	501	LMG	C18-C19-C20-C21
26	a	412	SQD	C15-C16-C17-C18
27	B	627	LFA	C9-C10-C11-C12
27	C	521	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	C	501	LMG	C15-C16-C17-C18
27	b	602	LFA	C11-C10-C9-C8
27	i	101	LFA	C10-C11-C12-C13
29	C	501	LMG	C18-C19-C20-C21
29	C	520	LMG	C31-C32-C33-C34
32	d	407	LHG	C31-C32-C33-C34
27	D	411	LFA	C3-C4-C5-C6
27	d	408	LFA	C2-C3-C4-C5
27	t	101	LFA	C5-C6-C7-C8
29	c	501	LMG	C36-C37-C38-C39
32	d	407	LHG	C16-C17-C18-C19
26	A	409	SQD	C10-C11-C12-C13
26	A	411	SQD	C34-C35-C36-C37
27	C	521	LFA	C7-C8-C9-C10
32	b	628	LHG	C15-C16-C17-C18
22	H	101	CLA	C4B-C3B-CAB-CBB
22	a	405	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
26	a	410	SQD	C33-C34-C35-C36
30	h	102	DGD	C3B-C4B-C5B-C6B
22	b	616	CLA	C8-C10-C11-C12
32	D	408	LHG	C14-C15-C16-C17
32	d	406	LHG	C11-C10-C9-C8
32	l	101	LHG	C13-C14-C15-C16
27	B	624	LFA	C6-C7-C8-C9
26	L	101	SQD	C7-C8-C9-C10
22	A	403	CLA	C15-C16-C17-C18
26	a	410	SQD	C14-C15-C16-C17
26	f	102	SQD	C29-C30-C31-C32
26	f	102	SQD	C31-C32-C33-C34
29	C	520	LMG	C35-C36-C37-C38
32	L	102	LHG	C13-C14-C15-C16
27	j	101	LFA	C3-C4-C5-C6
29	D	410	LMG	C20-C21-C22-C23
32	d	407	LHG	C32-C33-C34-C35
29	m	103	LMG	C32-C33-C34-C35
26	A	411	SQD	C7-C8-C9-C10
26	L	101	SQD	C16-C17-C18-C19
32	D	408	LHG	C11-C10-C9-C8
27	B	623	LFA	C3-C4-C5-C6
29	m	103	LMG	C18-C19-C20-C21
27	B	627	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	C	501	LMG	C36-C37-C38-C39
29	m	103	LMG	C31-C32-C33-C34
30	c	517	DGD	C1A-C2A-C3A-C4A
32	D	407	LHG	C7-C8-C9-C10
26	b	601	SQD	C10-C11-C12-C13
29	b	624	LMG	C29-C30-C31-C32
32	d	407	LHG	C30-C31-C32-C33
32	e	101	LHG	C12-C13-C14-C15
30	c	516	DGD	C4E-C5E-C6E-O5E
27	d	409	LFA	C5-C6-C7-C8
29	B	619	LMG	C19-C20-C21-C22
30	H	103	DGD	C3B-C4B-C5B-C6B
32	D	407	LHG	C18-C19-C20-C21
32	e	101	LHG	C27-C28-C29-C30
32	l	101	LHG	C18-C19-C20-C21
29	C	522	LMG	C32-C33-C34-C35
29	c	501	LMG	C39-C40-C41-C42
32	D	407	LHG	C34-C35-C36-C37
30	C	519	DGD	O1A-C1A-O1G-C1G
22	B	613	CLA	C2B-C3B-CAB-CBB
22	C	506	CLA	C2B-C3B-CAB-CBB
22	H	101	CLA	C2B-C3B-CAB-CBB
24	B	616	BCR	C1-C6-C7-C8
24	B	616	BCR	C5-C6-C7-C8
24	K	101	BCR	C1-C6-C7-C8
24	K	101	BCR	C5-C6-C7-C8
24	b	619	BCR	C1-C6-C7-C8
24	c	523	BCR	C1-C6-C7-C8
24	c	523	BCR	C5-C6-C7-C8
24	t	102	BCR	C1-C6-C7-C8
24	t	102	BCR	C5-C6-C7-C8
29	D	410	LMG	C14-C15-C16-C17
32	e	101	LHG	C14-C15-C16-C17
26	a	412	SQD	C8-C7-O47-C45
22	C	504	CLA	C15-C16-C17-C18
26	a	412	SQD	C28-C29-C30-C31
29	B	619	LMG	C38-C39-C40-C41
33	E	102	HEM	C2A-CAA-CBA-CGA
22	B	605	CLA	C2A-CAA-CBA-CGA
29	m	103	LMG	C10-C11-C12-C13
26	b	601	SQD	C16-C17-C18-C19
27	B	627	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	D	408	LHG	C16-C17-C18-C19
27	D	411	LFA	C11-C10-C9-C8
32	D	409	LHG	C12-C13-C14-C15
25	D	406	PL9	C30-C29-C31-C32
26	A	411	SQD	C31-C32-C33-C34
32	L	102	LHG	C16-C17-C18-C19
29	C	520	LMG	C39-C40-C41-C42
32	L	102	LHG	C27-C28-C29-C30
22	C	510	CLA	C14-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C14
27	C	521	LFA	C5-C6-C7-C8
26	a	410	SQD	C27-C28-C29-C30
30	c	517	DGD	O6E-C1E-O5D-C6D
27	B	626	LFA	C5-C6-C7-C8
27	b	625	LFA	C7-C8-C9-C10
26	a	410	SQD	C26-C27-C28-C29
27	a	411	LFA	C6-C7-C8-C9
27	c	521	LFA	C4-C5-C6-C7
30	h	102	DGD	CDB-CEB-CFB-CGB
27	D	413	LFA	C5-C6-C7-C8
26	b	601	SQD	C8-C7-O47-C45
29	c	501	LMG	C11-C10-O7-C8
22	b	616	CLA	C13-C15-C16-C17
26	L	101	SQD	C27-C28-C29-C30
26	b	601	SQD	C28-C29-C30-C31
24	b	621	BCR	C37-C22-C23-C24
29	m	103	LMG	C15-C16-C17-C18
24	t	102	BCR	C7-C8-C9-C10
27	b	602	LFA	C2-C3-C4-C5
32	l	101	LHG	C28-C29-C30-C31
30	C	517	DGD	C8A-C9A-CAA-CBA
22	c	506	CLA	C4-C3-C5-C6
25	D	406	PL9	C15-C14-C16-C17
25	D	406	PL9	C40-C39-C41-C42
25	a	409	PL9	C30-C29-C31-C32
25	d	405	PL9	C45-C44-C46-C47
29	C	522	LMG	O6-C5-C6-O5
33	E	102	HEM	C2C-C3C-CAC-CBC
32	d	407	LHG	C25-C26-C27-C28
22	b	613	CLA	C15-C16-C17-C18
29	c	522	LMG	O6-C5-C6-O5
29	C	501	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	b	628	LHG	C25-C26-C27-C28
25	D	406	PL9	C39-C41-C42-C43
33	E	102	HEM	C4B-C3B-CAB-CBB
33	E	102	HEM	C4C-C3C-CAC-CBC
33	e	102	HEM	C4C-C3C-CAC-CBC
26	A	411	SQD	C27-C28-C29-C30
27	b	602	LFA	C11-C12-C13-C14
29	b	624	LMG	C14-C15-C16-C17
29	c	519	LMG	C17-C18-C19-C20
27	B	623	LFA	C4-C5-C6-C7
26	a	410	SQD	C7-C8-C9-C10
27	C	521	LFA	C2-C3-C4-C5
30	h	102	DGD	C2B-C3B-C4B-C5B
26	A	411	SQD	O47-C45-C46-O48
26	a	410	SQD	O6-C44-C45-O47
29	C	522	LMG	O7-C8-C9-O8
32	d	407	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
26	L	101	SQD	C12-C13-C14-C15
32	E	101	LHG	C9-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
27	B	628	LFA	C9-C10-C11-C12
27	D	411	LFA	C7-C8-C9-C10
27	B	622	LFA	C3-C4-C5-C6
29	B	621	LMG	C29-C30-C31-C32
32	D	408	LHG	C30-C31-C32-C33
22	D	404	CLA	C16-C17-C18-C20
22	b	604	CLA	C5-C6-C7-C8
30	H	103	DGD	C6A-C7A-C8A-C9A
25	d	405	PL9	C15-C14-C16-C17
22	b	606	CLA	C3-C5-C6-C7
25	d	405	PL9	C13-C14-C16-C17
25	d	405	PL9	C43-C44-C46-C47
29	c	501	LMG	O9-C10-O7-C8
29	c	519	LMG	C13-C14-C15-C16
27	B	620	LFA	C5-C6-C7-C8
27	c	521	LFA	C6-C7-C8-C9
26	a	410	SQD	C16-C17-C18-C19
26	f	102	SQD	C27-C28-C29-C30
27	A	413	LFA	C9-C10-C11-C12
26	b	601	SQD	O49-C7-O47-C45
27	I	101	LFA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	d	408	LFA	C4-C5-C6-C7
32	e	101	LHG	C17-C18-C19-C20
22	B	602	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	b	608	CLA	C6-C7-C8-C10
22	d	403	CLA	C6-C7-C8-C10
26	f	102	SQD	C32-C33-C34-C35
27	b	630	LFA	C10-C11-C12-C13
26	A	411	SQD	C13-C14-C15-C16
22	C	507	CLA	C10-C11-C12-C13
30	c	518	DGD	C1B-C2B-C3B-C4B
32	d	407	LHG	C27-C28-C29-C30
22	B	608	CLA	C4-C3-C5-C6
22	b	618	CLA	C2-C3-C5-C6
22	c	506	CLA	C2-C3-C5-C6
25	a	409	PL9	C12-C11-C9-C8
25	a	409	PL9	C28-C29-C31-C32
27	I	101	LFA	C3-C4-C5-C6
32	b	628	LHG	C13-C14-C15-C16
22	B	614	CLA	C14-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C9
27	B	624	LFA	C5-C6-C7-C8
27	b	626	LFA	C6-C7-C8-C9
32	E	101	LHG	C17-C18-C19-C20
29	B	621	LMG	O6-C5-C6-O5
30	c	518	DGD	C2A-C1A-O1G-C1G
30	C	518	DGD	CAB-CBB-CCB-CDB
29	D	410	LMG	O6-C5-C6-O5
29	b	624	LMG	C11-C12-C13-C14
30	c	516	DGD	CAB-CBB-CCB-CDB
26	D	412	SQD	C2-C1-O6-C44
29	C	522	LMG	C2-C1-O1-C7
30	c	517	DGD	C2E-C1E-O5D-C6D
26	A	409	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
32	d	407	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
22	B	603	CLA	C3-C5-C6-C7
26	A	411	SQD	C25-C26-C27-C28
26	L	101	SQD	C26-C27-C28-C29
27	b	626	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	519	DGD	CBA-CCA-CDA-CEA
32	d	407	LHG	C24-C23-O8-C6
29	f	101	LMG	O6-C5-C6-O5
26	b	601	SQD	C26-C27-C28-C29
27	B	623	LFA	C11-C10-C9-C8
27	b	625	LFA	C10-C11-C12-C13
29	m	103	LMG	C35-C36-C37-C38
22	b	611	CLA	C4-C3-C5-C6
22	b	618	CLA	C4-C3-C5-C6
25	D	406	PL9	C45-C44-C46-C47
22	B	608	CLA	C2-C3-C5-C6
22	b	611	CLA	C2-C3-C5-C6
25	D	406	PL9	C13-C14-C16-C17
25	D	406	PL9	C28-C29-C31-C32
25	D	406	PL9	C38-C39-C41-C42
25	D	406	PL9	C43-C44-C46-C47
27	i	102	LFA	C6-C7-C8-C9
26	b	601	SQD	C32-C33-C34-C35
27	B	624	LFA	C2-C3-C4-C5
29	b	624	LMG	O6-C5-C6-O5
30	C	518	DGD	O6D-C5D-C6D-O5D
22	B	604	CLA	C13-C15-C16-C17
27	b	602	LFA	C3-C4-C5-C6
29	B	619	LMG	C20-C21-C22-C23
26	A	411	SQD	C15-C16-C17-C18
29	c	519	LMG	C38-C39-C40-C41
27	t	101	LFA	C12-C13-C14-C15
32	D	407	LHG	C9-C10-C11-C12
22	c	513	CLA	O2A-C1-C2-C3
26	A	409	SQD	C17-C18-C19-C20
27	m	102	LFA	C5-C6-C7-C8
29	B	619	LMG	C31-C32-C33-C34
29	c	519	LMG	C14-C15-C16-C17
30	C	517	DGD	C4B-C5B-C6B-C7B
32	l	101	LHG	C32-C33-C34-C35
27	b	622	LFA	C2-C3-C4-C5
27	b	627	LFA	C11-C10-C9-C8
29	c	501	LMG	C32-C33-C34-C35
29	m	103	LMG	C39-C40-C41-C42
25	D	406	PL9	C35-C34-C36-C37
25	a	409	PL9	C25-C24-C26-C27
22	d	401	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	M	101	LFA	C7-C8-C9-C10
29	c	501	LMG	C21-C22-C23-C24
26	A	409	SQD	O6-C44-C45-O47
26	a	410	SQD	C24-C25-C26-C27
27	B	627	LFA	C6-C7-C8-C9
32	l	101	LHG	C14-C15-C16-C17
22	C	511	CLA	C8-C10-C11-C12
27	B	624	LFA	C1-C2-C3-C4
29	B	621	LMG	C34-C35-C36-C37
25	a	409	PL9	C24-C26-C27-C28
29	c	522	LMG	C19-C20-C21-C22
27	b	625	LFA	C1-C2-C3-C4
26	A	409	SQD	C11-C12-C13-C14
32	D	407	LHG	C23-C24-C25-C26
22	c	504	CLA	C15-C16-C17-C18
29	m	103	LMG	C36-C37-C38-C39
29	c	501	LMG	C28-C29-C30-C31
29	c	501	LMG	C31-C32-C33-C34
27	I	101	LFA	C6-C7-C8-C9
26	a	412	SQD	O49-C7-O47-C45
32	D	409	LHG	O1-C1-C2-O2
32	d	407	LHG	O1-C1-C2-O2
22	b	611	CLA	C6-C7-C8-C9
22	d	403	CLA	C6-C7-C8-C9
27	B	627	LFA	C2-C3-C4-C5
27	M	102	LFA	C6-C7-C8-C9
30	H	103	DGD	C4B-C5B-C6B-C7B
30	c	517	DGD	C2A-C3A-C4A-C5A
32	d	406	LHG	C25-C26-C27-C28
22	b	612	CLA	C13-C15-C16-C17
22	c	507	CLA	C15-C16-C17-C18
22	b	608	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	C4B-C3B-CAB-CBB
22	d	402	CLA	C4B-C3B-CAB-CBB
26	A	411	SQD	C14-C15-C16-C17
27	b	630	LFA	C2-C3-C4-C5
27	M	102	LFA	C2-C3-C4-C5
30	C	518	DGD	CDB-CEB-CFB-CGB
22	D	404	CLA	C16-C17-C18-C19
30	C	518	DGD	C5B-C6B-C7B-C8B
26	a	412	SQD	C9-C10-C11-C12
22	B	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
22	b	603	CLA	C10-C11-C12-C13
30	c	516	DGD	CAA-CBA-CCA-CDA
30	h	102	DGD	C1B-C2B-C3B-C4B
26	L	101	SQD	C29-C30-C31-C32
27	d	410	LFA	C4-C5-C6-C7
27	i	101	LFA	C3-C4-C5-C6
25	a	409	PL9	C12-C11-C9-C10
22	c	511	CLA	C8-C10-C11-C12
26	a	410	SQD	C25-C26-C27-C28
27	d	410	LFA	C11-C10-C9-C8
29	c	501	LMG	C33-C34-C35-C36
30	c	518	DGD	O1A-C1A-O1G-C1G
32	d	407	LHG	O10-C23-O8-C6
30	c	516	DGD	C2A-C1A-O1G-C1G
27	b	625	LFA	C12-C13-C14-C15
26	A	411	SQD	O6-C44-C45-C46
26	A	411	SQD	C44-C45-C46-O48
26	L	101	SQD	C44-C45-C46-O48
26	a	410	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
29	C	501	LMG	C7-C8-C9-O8
29	C	522	LMG	C7-C8-C9-O8
27	I	101	LFA	C9-C10-C11-C12
22	B	601	CLA	C16-C17-C18-C20
29	C	520	LMG	C30-C31-C32-C33
27	D	411	LFA	C9-C10-C11-C12
25	A	408	PL9	C12-C11-C9-C10
26	a	412	SQD	C12-C13-C14-C15
27	A	410	LFA	C7-C8-C9-C10
29	c	522	LMG	C13-C14-C15-C16
32	D	409	LHG	C29-C30-C31-C32
32	D	407	LHG	C17-C18-C19-C20
29	f	101	LMG	C10-C11-C12-C13
22	B	615	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
30	h	102	DGD	C4E-C5E-C6E-O5E
24	D	405	BCR	C1-C6-C7-C8
24	b	619	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	621	BCR	C5-C6-C7-C8
30	h	102	DGD	C5B-C6B-C7B-C8B
22	b	615	CLA	C13-C15-C16-C17
22	B	601	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C20
22	c	507	CLA	C5-C6-C7-C8
22	d	403	CLA	C10-C11-C12-C13
29	b	624	LMG	O1-C7-C8-O7
30	c	518	DGD	O1G-C1G-C2G-O2G
25	D	406	PL9	C4-C3-C7-C8
25	d	405	PL9	C4-C3-C7-C8
30	C	519	DGD	CCB-CDB-CEB-CFB
26	D	412	SQD	C31-C32-C33-C34
29	f	101	LMG	C15-C16-C17-C18
32	b	628	LHG	C16-C17-C18-C19
26	A	411	SQD	C18-C19-C20-C21
27	m	102	LFA	C4-C5-C6-C7
32	E	101	LHG	C11-C10-C9-C8
29	B	619	LMG	C28-C29-C30-C31
27	m	102	LFA	C6-C7-C8-C9
32	D	409	LHG	C28-C29-C30-C31
22	B	606	CLA	C14-C13-C15-C16
22	D	403	CLA	C14-C13-C15-C16
22	c	508	CLA	C14-C13-C15-C16
29	C	520	LMG	C12-C13-C14-C15
27	A	410	LFA	C2-C3-C4-C5
32	D	407	LHG	C28-C29-C30-C31
32	L	102	LHG	C32-C33-C34-C35
30	C	518	DGD	C5A-C6A-C7A-C8A
30	c	518	DGD	CCB-CDB-CEB-CFB
27	B	620	LFA	C7-C8-C9-C10
29	c	501	LMG	C40-C41-C42-C43
30	H	103	DGD	CBB-CCB-CDB-CEB
32	d	406	LHG	C23-C24-C25-C26
32	d	406	LHG	O2-C2-C3-O3
26	a	412	SQD	O47-C7-C8-C9
30	h	102	DGD	O2G-C1B-C2B-C3B
29	m	103	LMG	C34-C35-C36-C37
27	i	101	LFA	C1-C2-C3-C4
30	C	517	DGD	C7B-C8B-C9B-CAB
32	L	102	LHG	C33-C34-C35-C36
32	l	101	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	d	408	LFA	C1-C2-C3-C4
26	L	101	SQD	C25-C26-C27-C28
27	B	624	LFA	C7-C8-C9-C10
27	m	101	LFA	C7-C8-C9-C10
30	H	103	DGD	CAB-CBB-CCB-CDB
22	H	101	CLA	C8-C10-C11-C12
22	C	505	CLA	C13-C15-C16-C17
22	B	604	CLA	C12-C13-C15-C16
22	C	509	CLA	C12-C13-C15-C16
22	a	407	CLA	C11-C10-C8-C7
22	b	606	CLA	C6-C7-C8-C10
30	C	519	DGD	C6B-C7B-C8B-C9B
32	E	101	LHG	C18-C19-C20-C21
32	E	101	LHG	C28-C29-C30-C31
29	b	624	LMG	C34-C35-C36-C37
22	a	405	CLA	C15-C16-C17-C18
27	J	101	LFA	C5-C6-C7-C8
24	d	404	BCR	C7-C8-C9-C10
32	D	409	LHG	C30-C31-C32-C33
30	c	517	DGD	C5D-C6D-O5D-C1E
29	c	522	LMG	C18-C19-C20-C21
29	m	103	LMG	C11-C10-O7-C8
25	A	408	PL9	C12-C11-C9-C8
26	a	412	SQD	C17-C18-C19-C20
27	B	627	LFA	C7-C8-C9-C10
27	C	521	LFA	C1-C2-C3-C4
32	e	101	LHG	C28-C29-C30-C31
32	D	407	LHG	C32-C33-C34-C35
29	C	501	LMG	C35-C36-C37-C38
29	m	103	LMG	C11-C12-C13-C14
29	f	101	LMG	C30-C31-C32-C33
32	l	101	LHG	O6-C4-C5-O7
30	C	517	DGD	C2A-C3A-C4A-C5A
26	D	412	SQD	O5-C1-O6-C44
30	C	518	DGD	O6E-C1E-O5D-C6D
26	D	412	SQD	C44-C45-C46-O48
29	C	501	LMG	O1-C7-C8-C9
22	b	609	CLA	C16-C17-C18-C20
26	f	102	SQD	C35-C36-C37-C38
32	D	407	LHG	C19-C20-C21-C22
30	C	517	DGD	C4D-C5D-C6D-O5D
22	B	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	H	103	DGD	C6B-C7B-C8B-C9B
32	d	406	LHG	C16-C17-C18-C19
22	b	607	CLA	C10-C11-C12-C13
27	c	521	LFA	C3-C4-C5-C6
27	T	102	LFA	C9-C10-C11-C12
22	H	101	CLA	C3-C5-C6-C7
29	B	619	LMG	C17-C18-C19-C20
29	B	619	LMG	C37-C38-C39-C40
30	c	516	DGD	C2A-C3A-C4A-C5A
26	L	101	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
30	H	103	DGD	O1G-C1G-C2G-O2G
30	h	102	DGD	O1G-C1G-C2G-O2G
22	B	605	CLA	C11-C10-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	a	407	CLA	C11-C10-C8-C9
29	C	501	LMG	C16-C17-C18-C19
29	c	519	LMG	C18-C19-C20-C21
27	i	101	LFA	C7-C8-C9-C10
30	c	516	DGD	O1A-C1A-O1G-C1G
27	B	620	LFA	C1-C2-C3-C4
32	L	102	LHG	C14-C15-C16-C17
32	E	101	LHG	C25-C26-C27-C28
29	b	624	LMG	C31-C32-C33-C34
32	E	101	LHG	C24-C25-C26-C27
32	l	101	LHG	C26-C27-C28-C29
22	c	505	CLA	C13-C15-C16-C17
29	c	501	LMG	C35-C36-C37-C38
22	C	507	CLA	C3-C5-C6-C7
27	I	101	LFA	C7-C8-C9-C10
22	B	611	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C19
26	A	409	SQD	C13-C14-C15-C16
24	B	618	BCR	C7-C8-C9-C34
24	k	101	BCR	C7-C8-C9-C34
29	C	501	LMG	C22-C23-C24-C25
30	H	103	DGD	C5B-C6B-C7B-C8B
22	b	612	CLA	C4B-C3B-CAB-CBB
29	C	522	LMG	C28-C29-C30-C31
26	b	601	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	D	406	PL9	C33-C34-C36-C37
24	c	524	BCR	C7-C8-C9-C10
24	k	101	BCR	C7-C8-C9-C10
27	b	630	LFA	C6-C7-C8-C9
27	b	622	LFA	C7-C8-C9-C10
30	c	516	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C2B-C1B-O2G-C2G
29	m	103	LMG	O9-C10-O7-C8
29	c	519	LMG	C12-C13-C14-C15
27	b	627	LFA	C10-C11-C12-C13
22	H	101	CLA	C11-C10-C8-C7
32	b	628	LHG	C24-C25-C26-C27
22	B	610	CLA	C16-C17-C18-C19
22	d	401	CLA	C16-C17-C18-C19
23	a	406	PHO	C16-C17-C18-C19
27	b	630	LFA	C1-C2-C3-C4
27	i	101	LFA	C12-C13-C14-C15
27	B	627	LFA	C11-C12-C13-C14
32	d	407	LHG	C9-C10-C11-C12
32	l	101	LHG	C15-C16-C17-C18
27	B	623	LFA	C9-C10-C11-C12
32	l	101	LHG	C11-C12-C13-C14
34	V	201	HEC	C4C-C3C-CAC-CBC
27	A	410	LFA	C11-C10-C9-C8
32	e	101	LHG	C19-C20-C21-C22
33	e	102	HEM	C3D-CAD-CBD-CGD
26	L	101	SQD	C24-C25-C26-C27
22	B	602	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
22	b	618	CLA	C11-C10-C8-C9
30	H	103	DGD	C2B-C3B-C4B-C5B
27	B	626	LFA	C7-C8-C9-C10
27	m	102	LFA	C2-C3-C4-C5
26	D	412	SQD	O47-C45-C46-O48
29	C	501	LMG	O1-C7-C8-O7
29	C	501	LMG	O7-C8-C9-O8
29	C	522	LMG	O1-C7-C8-O7
29	C	501	LMG	C13-C14-C15-C16
29	b	624	LMG	O1-C7-C8-C9
30	c	518	DGD	O1G-C1G-C2G-C3G
30	h	102	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C25-C26-C27-C28
29	c	522	LMG	C14-C15-C16-C17
30	c	517	DGD	C6B-C7B-C8B-C9B
27	b	626	LFA	C7-C8-C9-C10
32	d	407	LHG	C12-C13-C14-C15
26	f	102	SQD	C11-C10-C9-C8
22	B	606	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
26	A	411	SQD	C33-C34-C35-C36
30	C	518	DGD	C9B-CAB-CBB-CCB
27	A	413	LFA	C6-C7-C8-C9
32	D	407	LHG	C30-C31-C32-C33
29	c	522	LMG	C29-C28-O8-C9
27	B	624	LFA	C10-C11-C12-C13
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
24	k	101	BCR	C19-C20-C21-C22
32	D	408	LHG	C4-O6-P-O5
32	D	409	LHG	C4-O6-P-O3
32	D	409	LHG	C4-O6-P-O5
32	E	101	LHG	C4-O6-P-O3
32	E	101	LHG	C4-O6-P-O5
32	L	102	LHG	C3-O3-P-O5
32	d	406	LHG	C4-O6-P-O5
32	d	407	LHG	C4-O6-P-O3
32	d	407	LHG	C4-O6-P-O4
32	l	101	LHG	C3-O3-P-O5
29	C	522	LMG	C20-C21-C22-C23
22	B	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C13-C15-C16-C17
22	a	405	CLA	C2B-C3B-CAB-CBB
22	b	608	CLA	C2B-C3B-CAB-CBB
22	b	612	CLA	C2B-C3B-CAB-CBB
22	c	504	CLA	C2B-C3B-CAB-CBB
22	c	506	CLA	C2B-C3B-CAB-CBB
24	b	621	BCR	C1-C6-C7-C8
26	a	412	SQD	C29-C30-C31-C32
32	d	406	LHG	C34-C35-C36-C37
29	C	522	LMG	C10-C11-C12-C13
24	K	101	BCR	C37-C22-C23-C24
32	D	409	LHG	C2-C3-O3-P
29	c	501	LMG	C29-C30-C31-C32
26	a	412	SQD	C18-C19-C20-C21
25	a	409	PL9	C4-C3-C7-C8
26	A	411	SQD	O10-C23-O48-C46
27	T	102	LFA	C6-C7-C8-C9
22	c	504	CLA	C10-C11-C12-C13
27	A	413	LFA	C7-C8-C9-C10
30	C	517	DGD	O6D-C5D-C6D-O5D
30	H	103	DGD	O2G-C1B-C2B-C3B
22	B	606	CLA	C13-C15-C16-C17
32	e	101	LHG	C15-C16-C17-C18
27	B	626	LFA	C2-C3-C4-C5
27	M	102	LFA	C7-C8-C9-C10
27	M	102	LFA	C11-C12-C13-C14
32	l	101	LHG	O6-C4-C5-C6
26	A	409	SQD	C30-C31-C32-C33
27	b	622	LFA	C4-C5-C6-C7
22	B	604	CLA	C11-C10-C8-C9
27	b	626	LFA	C11-C12-C13-C14
22	B	602	CLA	C6-C7-C8-C10
32	d	406	LHG	C30-C31-C32-C33
22	a	405	CLA	C16-C17-C18-C20
26	A	411	SQD	C24-C23-O48-C46
30	C	518	DGD	C2E-C1E-O5D-C6D
32	l	101	LHG	C16-C17-C18-C19
27	d	410	LFA	C3-C4-C5-C6
29	b	624	LMG	C29-C28-O8-C9
23	D	402	PHO	C16-C17-C18-C19
30	c	518	DGD	C9B-CAB-CBB-CCB
26	A	409	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	d	409	LFA	C4-C5-C6-C7
29	b	624	LMG	O10-C28-O8-C9
27	B	620	LFA	C6-C7-C8-C9
29	B	619	LMG	C13-C14-C15-C16
29	f	101	LMG	C39-C40-C41-C42
29	B	621	LMG	C31-C32-C33-C34
29	C	501	LMG	C11-C12-C13-C14
29	C	520	LMG	C10-C11-C12-C13
25	a	409	PL9	C35-C34-C36-C37
22	C	510	CLA	C16-C17-C18-C20
32	d	407	LHG	C34-C35-C36-C37
22	B	607	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
24	K	101	BCR	C21-C22-C23-C24
24	b	621	BCR	C21-C22-C23-C24
29	C	522	LMG	C8-C7-O1-C1
32	D	407	LHG	C31-C32-C33-C34
32	D	409	LHG	C11-C12-C13-C14
29	c	501	LMG	C17-C18-C19-C20
22	c	514	CLA	C16-C17-C18-C20
22	B	608	CLA	C11-C10-C8-C9
22	b	606	CLA	C6-C7-C8-C9
32	D	407	LHG	C15-C16-C17-C18
32	D	409	LHG	C24-C23-O8-C6
32	d	406	LHG	C24-C23-O8-C6
22	A	404	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	C4B-C3B-CAB-CBB
27	b	627	LFA	C5-C6-C7-C8
32	b	628	LHG	C27-C28-C29-C30
26	a	412	SQD	C19-C20-C21-C22
26	f	102	SQD	O10-C23-O48-C46
27	M	101	LFA	C6-C7-C8-C9
25	d	405	PL9	C30-C29-C31-C32
25	d	405	PL9	C40-C39-C41-C42
22	C	506	CLA	C2-C3-C5-C6
25	a	409	PL9	C33-C34-C36-C37
27	I	101	LFA	C5-C6-C7-C8
27	B	623	LFA	C2-C3-C4-C5
29	c	519	LMG	C19-C20-C21-C22
22	b	614	CLA	C12-C13-C15-C16
26	a	412	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	d	407	LHG	C29-C30-C31-C32
32	E	101	LHG	C14-C15-C16-C17
26	f	102	SQD	C24-C23-O48-C46
29	c	519	LMG	C29-C30-C31-C32
30	c	516	DGD	C4D-C5D-C6D-O5D
32	E	101	LHG	O7-C5-C6-O8
22	D	404	CLA	C3A-C2A-CAA-CBA
29	f	101	LMG	C14-C15-C16-C17
32	d	406	LHG	C28-C29-C30-C31
27	A	410	LFA	C10-C11-C12-C13
27	b	626	LFA	C9-C10-C11-C12
32	E	101	LHG	C27-C28-C29-C30
30	C	517	DGD	C5A-C6A-C7A-C8A
22	B	604	CLA	C10-C11-C12-C13
29	D	410	LMG	C10-C11-C12-C13
25	d	405	PL9	C24-C26-C27-C28
25	d	405	PL9	C39-C41-C42-C43
30	H	103	DGD	O1G-C1G-C2G-C3G
27	j	101	LFA	C5-C6-C7-C8
32	d	407	LHG	C15-C16-C17-C18
29	c	522	LMG	O10-C28-O8-C9
22	B	613	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	611	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C10-C8-C9
23	D	402	PHO	C14-C13-C15-C16
29	B	619	LMG	C33-C34-C35-C36
30	C	519	DGD	CDB-CEB-CFB-CGB
27	b	630	LFA	C11-C10-C9-C8
27	b	625	LFA	C9-C10-C11-C12
29	m	103	LMG	C37-C38-C39-C40
32	D	408	LHG	C26-C27-C28-C29
25	a	409	PL9	C23-C24-C26-C27
27	b	626	LFA	C4-C5-C6-C7
34	v	201	HEC	CAD-CBD-CGD-O1D
30	h	102	DGD	O1B-C1B-C2B-C3B
22	A	404	CLA	C2B-C3B-CAB-CBB
22	C	502	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	d	402	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	A	407	BCR	C23-C24-C25-C30
24	D	405	BCR	C5-C6-C7-C8
24	a	408	BCR	C1-C6-C7-C8
27	B	628	LFA	C10-C11-C12-C13
26	f	102	SQD	C24-C25-C26-C27
22	a	405	CLA	C16-C17-C18-C19
22	C	505	CLA	C4-C3-C5-C6
32	d	407	LHG	C35-C36-C37-C38
22	B	613	CLA	C2-C3-C5-C6
25	d	405	PL9	C28-C29-C31-C32
25	d	405	PL9	C38-C39-C41-C42
32	L	102	LHG	C11-C10-C9-C8
34	v	201	HEC	CAD-CBD-CGD-O2D
30	h	102	DGD	O6E-C5E-C6E-O5E
22	B	613	CLA	C11-C12-C13-C15
22	C	504	CLA	C6-C7-C8-C10
27	t	101	LFA	C4-C5-C6-C7
22	B	614	CLA	C16-C17-C18-C19
22	B	607	CLA	C15-C16-C17-C18
30	c	517	DGD	O1G-C1G-C2G-O2G
32	D	409	LHG	C9-C10-C11-C12
27	B	624	LFA	C11-C10-C9-C8
32	L	102	LHG	C26-C27-C28-C29
32	d	406	LHG	C26-C27-C28-C29
27	A	410	LFA	C4-C5-C6-C7
33	e	102	HEM	CAA-CBA-CGA-O2A
22	b	609	CLA	C16-C17-C18-C19
27	d	410	LFA	C7-C8-C9-C10
30	C	517	DGD	CDA-CEA-CFA-CGA
27	i	101	LFA	C2-C3-C4-C5
22	B	614	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
32	l	101	LHG	C27-C28-C29-C30
27	A	413	LFA	C10-C11-C12-C13
22	B	605	CLA	C8-C10-C11-C12
27	c	521	LFA	C12-C13-C14-C15
32	D	409	LHG	O10-C23-O8-C6
32	D	409	LHG	C25-C26-C27-C28
22	D	404	CLA	C4-C3-C5-C6
22	b	617	CLA	C4-C3-C5-C6
30	C	517	DGD	C8B-C9B-CAB-CBB
32	d	406	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	O6D-C5D-C6D-O5D
22	b	603	CLA	CAA-CBA-CGA-O2A
30	h	102	DGD	C5A-C6A-C7A-C8A
30	c	518	DGD	C1G-C2G-C3G-O3G
22	C	504	CLA	C10-C11-C12-C13
27	B	626	LFA	C3-C4-C5-C6
29	m	103	LMG	C30-C31-C32-C33
27	B	622	LFA	C4-C5-C6-C7
32	b	628	LHG	O6-C4-C5-O7
22	B	614	CLA	C4-C3-C5-C6
22	C	506	CLA	C4-C3-C5-C6
27	A	410	LFA	C3-C4-C5-C6
26	D	412	SQD	O48-C23-C24-C25
27	d	410	LFA	C6-C7-C8-C9
30	h	102	DGD	C2A-C3A-C4A-C5A
26	a	410	SQD	C9-C10-C11-C12
29	C	522	LMG	C14-C15-C16-C17
29	C	522	LMG	C29-C30-C31-C32
34	V	201	HEC	CAD-CBD-CGD-O2D
29	B	619	LMG	C12-C13-C14-C15
26	a	410	SQD	C18-C19-C20-C21
22	A	406	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
27	b	625	LFA	C13-C14-C15-C16
33	e	102	HEM	CAA-CBA-CGA-O1A
26	b	601	SQD	C29-C30-C31-C32
30	c	518	DGD	C7B-C8B-C9B-CAB
27	B	620	LFA	C2-C3-C4-C5
27	D	411	LFA	C11-C12-C13-C14
30	C	518	DGD	C4D-C5D-C6D-O5D
26	A	411	SQD	C26-C27-C28-C29
27	B	627	LFA	C10-C11-C12-C13
22	B	608	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C7
27	B	624	LFA	C9-C10-C11-C12
34	V	201	HEC	CAD-CBD-CGD-O1D
22	C	507	CLA	C16-C17-C18-C19
27	d	408	LFA	C3-C4-C5-C6
22	b	613	CLA	C14-C13-C15-C16
22	b	617	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
29	D	410	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C2-C1-O2A-CGA
30	C	517	DGD	CAB-CBB-CCB-CDB
27	A	413	LFA	C4-C5-C6-C7
26	a	410	SQD	O47-C7-C8-C9
32	b	628	LHG	C14-C15-C16-C17
29	f	101	LMG	C29-C30-C31-C32
30	c	517	DGD	CAB-CBB-CCB-CDB
22	B	604	CLA	C15-C16-C17-C18
23	a	406	PHO	C15-C16-C17-C18
29	C	520	LMG	C17-C18-C19-C20
30	h	102	DGD	O1B-C1B-O2G-C2G
22	B	615	CLA	C3-C5-C6-C7
30	c	518	DGD	C7A-C8A-C9A-CAA
22	b	614	CLA	CAA-CBA-CGA-O2A
22	b	607	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
22	B	614	CLA	C16-C17-C18-C20
30	c	518	DGD	O6D-C5D-C6D-O5D
30	c	516	DGD	C1A-C2A-C3A-C4A
32	L	102	LHG	C18-C19-C20-C21
32	E	101	LHG	O8-C23-C24-C25
22	B	608	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15
22	b	605	CLA	C6-C7-C8-C10
22	b	609	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C10-C8-C7
22	c	509	CLA	C12-C13-C15-C16
22	B	605	CLA	C2B-C3B-CAB-CBB
22	b	616	CLA	C2B-C3B-CAB-CBB
22	d	401	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C5-C6-C7-C8
24	H	102	BCR	C1-C6-C7-C8
24	a	408	BCR	C5-C6-C7-C8
24	b	621	BCR	C23-C24-C25-C26
24	b	621	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C30
22	b	610	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
32	d	407	LHG	C2-C3-O3-P
27	j	101	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	A	411	SQD	C16-C17-C18-C19
26	a	412	SQD	C26-C27-C28-C29
29	B	621	LMG	O7-C10-C11-C12
27	d	408	LFA	C5-C6-C7-C8
22	B	602	CLA	C13-C15-C16-C17
32	D	407	LHG	C33-C34-C35-C36
30	c	518	DGD	C2B-C3B-C4B-C5B
25	A	408	PL9	C4-C3-C7-C8
29	c	519	LMG	C20-C21-C22-C23
30	c	517	DGD	CDB-CEB-CFB-CGB
30	c	517	DGD	O6D-C5D-C6D-O5D
29	m	103	LMG	O8-C28-C29-C30
26	a	412	SQD	C33-C34-C35-C36
22	C	505	CLA	C2-C3-C5-C6
32	l	101	LHG	C30-C31-C32-C33
22	B	604	CLA	C6-C7-C8-C9
22	d	402	CLA	C11-C12-C13-C14
30	C	517	DGD	O2G-C1B-C2B-C3B
30	h	102	DGD	C1G-C2G-C3G-O3G
22	A	406	CLA	C16-C17-C18-C20
29	m	103	LMG	C16-C17-C18-C19
30	C	518	DGD	C7B-C8B-C9B-CAB
22	D	404	CLA	C1A-C2A-CAA-CBA
30	C	517	DGD	C3A-C4A-C5A-C6A
27	b	602	LFA	C1-C2-C3-C4
22	b	603	CLA	C4-C3-C5-C6
29	C	501	LMG	O6-C1-O1-C7
32	D	409	LHG	C33-C34-C35-C36
32	D	407	LHG	O7-C5-C6-O8
24	B	618	BCR	C7-C8-C9-C10
24	k	101	BCR	C11-C12-C13-C14
32	d	407	LHG	C14-C15-C16-C17
22	b	611	CLA	C16-C17-C18-C20
26	b	601	SQD	C33-C34-C35-C36
32	e	101	LHG	C13-C14-C15-C16
30	H	103	DGD	C4E-C5E-C6E-O5E
32	D	407	LHG	C26-C27-C28-C29
22	C	514	CLA	C8-C10-C11-C12
22	b	616	CLA	C2-C1-O2A-CGA
22	b	612	CLA	C11-C12-C13-C15
22	b	616	CLA	C12-C13-C15-C16
22	b	617	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C29-C28-O8-C9
29	B	619	LMG	C30-C31-C32-C33
29	B	619	LMG	O8-C28-C29-C30
22	B	611	CLA	C10-C11-C12-C13
30	h	102	DGD	C8A-C9A-CAA-CBA
32	b	628	LHG	C26-C27-C28-C29
22	C	504	CLA	C8-C10-C11-C12
22	C	510	CLA	C16-C17-C18-C19
22	b	610	CLA	C16-C17-C18-C19
22	b	612	CLA	C16-C17-C18-C20
25	A	408	PL9	C26-C27-C28-C29
25	D	406	PL9	C11-C12-C13-C14
22	C	509	CLA	C13-C15-C16-C17
23	D	402	PHO	C3A-C2A-CAA-CBA
34	v	201	HEC	C4C-C3C-CAC-CBC
29	B	621	LMG	O9-C10-C11-C12
22	d	403	CLA	C13-C15-C16-C17
22	C	507	CLA	C16-C17-C18-C20
22	C	513	CLA	CAA-CBA-CGA-O2A
26	a	412	SQD	O49-C7-C8-C9
32	b	628	LHG	C24-C23-O8-C6
29	c	501	LMG	C10-C11-C12-C13
22	c	510	CLA	C5-C6-C7-C8
26	a	410	SQD	C11-C12-C13-C14
22	c	505	CLA	C15-C16-C17-C18
32	D	408	LHG	C32-C33-C34-C35
22	b	614	CLA	CAA-CBA-CGA-O1A
32	E	101	LHG	O10-C23-C24-C25
30	c	518	DGD	C8B-C9B-CAB-CBB
30	C	517	DGD	C5D-C6D-O5D-C1E
29	C	520	LMG	O10-C28-O8-C9
30	c	518	DGD	O2G-C2G-C3G-O3G
30	c	518	DGD	CAA-CBA-CCA-CDA
32	E	101	LHG	C12-C13-C14-C15
29	f	101	LMG	C20-C21-C22-C23
29	B	619	LMG	O10-C28-C29-C30
22	c	511	CLA	CAA-CBA-CGA-O2A
26	A	409	SQD	O47-C7-C8-C9
29	C	522	LMG	C17-C18-C19-C20
32	D	408	LHG	O10-C23-O8-C6
25	a	409	PL9	C29-C31-C32-C33
29	B	621	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	C1A-C2A-C3A-C4A
22	b	606	CLA	C13-C15-C16-C17
29	m	103	LMG	O10-C28-C29-C30
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	a	404	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
23	D	402	PHO	CAD-CBD-CGD-O2D
23	a	406	PHO	CAD-CBD-CGD-O2D
30	C	518	DGD	C6B-C7B-C8B-C9B
22	C	512	CLA	C16-C17-C18-C20
22	c	506	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
22	C	513	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
26	A	409	SQD	O49-C7-C8-C9
29	c	501	LMG	C13-C14-C15-C16
27	i	102	LFA	C11-C10-C9-C8

There are no ring outliers.

161 monomers are involved in 421 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	514	CLA	2	0
30	C	519	DGD	1	0
22	D	404	CLA	3	0
22	C	507	CLA	2	0
22	C	512	CLA	4	0
27	D	413	LFA	1	0
22	A	403	CLA	2	0
27	M	101	LFA	2	0
22	C	505	CLA	2	0
22	B	610	CLA	1	0
27	B	623	LFA	2	0
22	b	613	CLA	1	0
29	C	520	LMG	2	0
26	a	410	SQD	3	0
29	b	624	LMG	2	0
22	c	504	CLA	6	0
24	H	102	BCR	4	0
22	B	615	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	V	201	HEC	2	0
22	a	405	CLA	5	0
27	b	625	LFA	1	0
29	c	519	LMG	6	0
22	B	605	CLA	3	0
22	C	504	CLA	6	0
22	B	603	CLA	3	0
22	A	412	CLA	2	0
22	a	404	CLA	4	0
22	c	507	CLA	4	0
22	b	604	CLA	5	0
22	b	617	CLA	3	0
24	c	523	BCR	2	0
26	b	601	SQD	8	0
22	b	603	CLA	4	0
22	c	506	CLA	5	0
22	B	607	CLA	5	0
22	c	505	CLA	8	0
22	c	512	CLA	4	0
22	B	602	CLA	4	0
27	j	101	LFA	4	0
23	a	414	PHO	3	0
32	D	408	LHG	4	0
23	a	406	PHO	2	0
22	A	406	CLA	4	0
23	D	402	PHO	2	0
26	L	101	SQD	4	0
29	m	103	LMG	3	0
24	a	408	BCR	1	0
24	c	524	BCR	6	0
33	E	102	HEM	9	0
26	a	412	SQD	2	0
23	A	405	PHO	1	0
22	c	510	CLA	5	0
22	d	402	CLA	3	0
27	M	102	LFA	2	0
22	B	611	CLA	3	0
29	B	619	LMG	2	0
29	D	410	LMG	1	0
24	d	404	BCR	3	0
27	B	627	LFA	1	0
24	c	515	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	412	SQD	1	0
24	B	617	BCR	5	0
24	k	101	BCR	4	0
22	b	611	CLA	5	0
29	c	501	LMG	6	0
22	b	615	CLA	1	0
27	B	626	LFA	2	0
27	b	623	LFA	3	0
24	K	101	BCR	2	0
27	b	626	LFA	1	0
30	h	102	DGD	7	0
27	d	409	LFA	1	0
22	C	503	CLA	4	0
22	b	614	CLA	3	0
32	b	628	LHG	2	0
22	C	510	CLA	2	0
22	C	513	CLA	1	0
22	B	612	CLA	2	0
30	c	516	DGD	6	0
22	H	101	CLA	1	0
22	C	511	CLA	4	0
22	c	503	CLA	3	0
29	C	522	LMG	2	0
22	C	509	CLA	4	0
29	C	501	LMG	5	0
32	e	101	LHG	2	0
22	B	606	CLA	2	0
32	D	409	LHG	10	0
22	b	618	CLA	1	0
27	B	628	LFA	1	0
33	e	102	HEM	7	0
22	c	514	CLA	4	0
24	K	102	BCR	3	0
22	c	509	CLA	5	0
32	D	407	LHG	5	0
25	A	408	PL9	6	0
22	b	606	CLA	3	0
24	B	616	BCR	3	0
22	B	613	CLA	2	0
26	f	102	SQD	2	0
24	B	618	BCR	1	0
30	H	103	DGD	3	0

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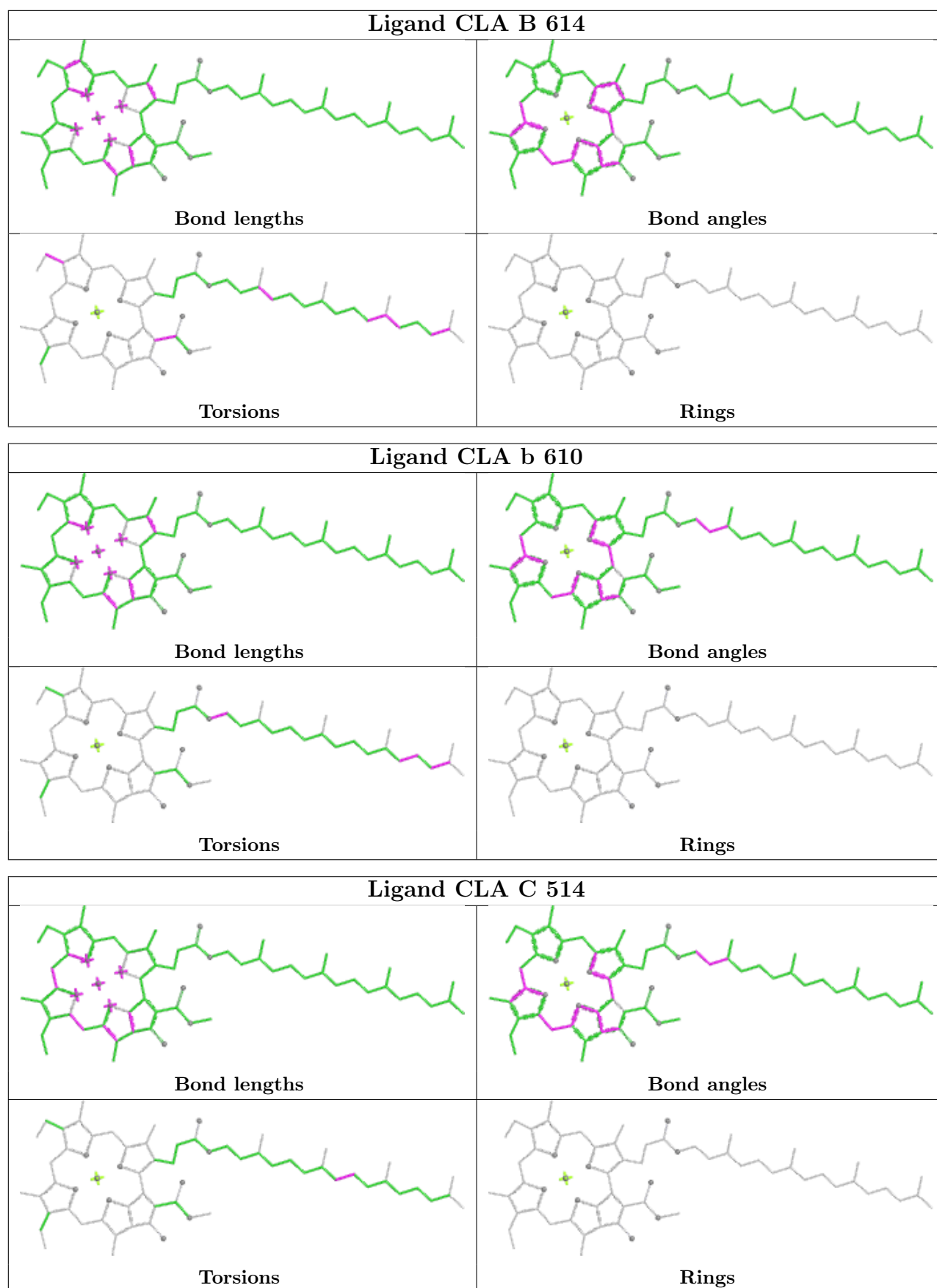
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	508	CLA	4	0
22	C	502	CLA	8	0
32	L	102	LHG	6	0
27	d	410	LFA	1	0
22	C	508	CLA	3	0
22	a	407	CLA	3	0
22	b	609	CLA	1	0
29	c	522	LMG	2	0
22	c	502	CLA	5	0
27	B	620	LFA	1	0
24	b	620	BCR	3	0
30	C	517	DGD	4	0
27	B	624	LFA	1	0
32	d	406	LHG	6	0
27	t	101	LFA	3	0
32	E	101	LHG	4	0
22	B	609	CLA	1	0
22	B	608	CLA	5	0
22	c	511	CLA	7	0
24	C	515	BCR	2	0
27	c	520	LFA	1	0
30	c	517	DGD	7	0
22	b	607	CLA	5	0
27	B	622	LFA	1	0
22	D	403	CLA	3	0
22	b	608	CLA	4	0
22	c	513	CLA	1	0
24	A	407	BCR	1	0
30	c	518	DGD	3	0
24	D	405	BCR	4	0
22	B	601	CLA	1	0
24	T	101	BCR	1	0
32	d	407	LHG	14	0
27	D	414	LFA	1	0
24	t	102	BCR	8	0
26	A	409	SQD	2	0
25	a	409	PL9	4	0
34	v	201	HEC	1	0
22	A	404	CLA	1	0
22	B	604	CLA	9	0
22	C	506	CLA	6	0
22	b	616	CLA	5	0

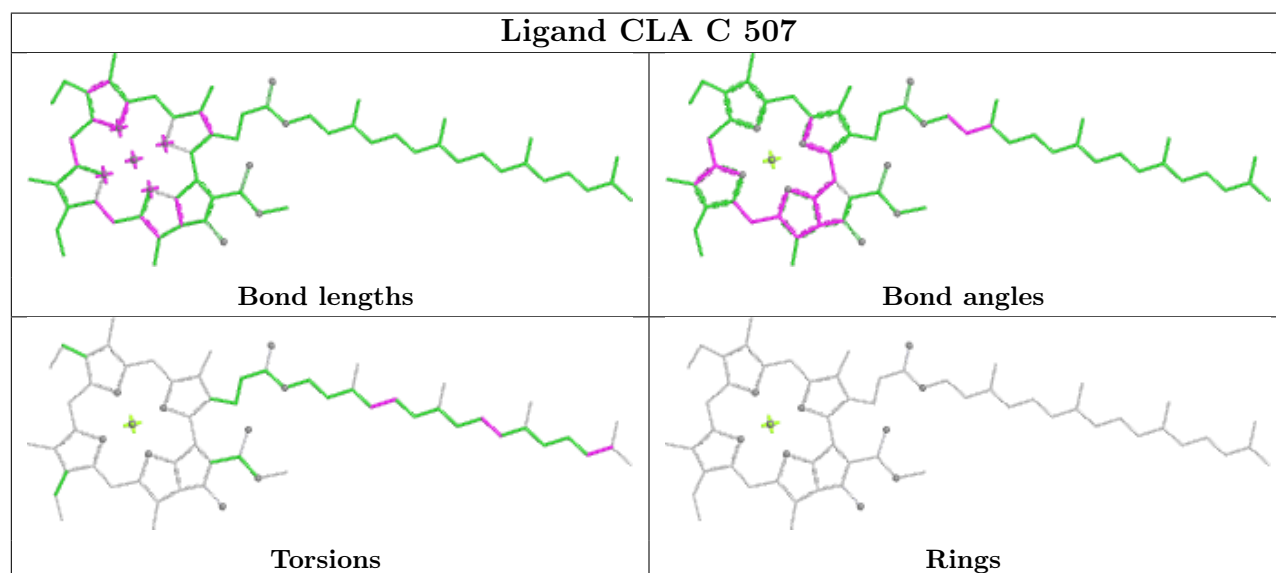
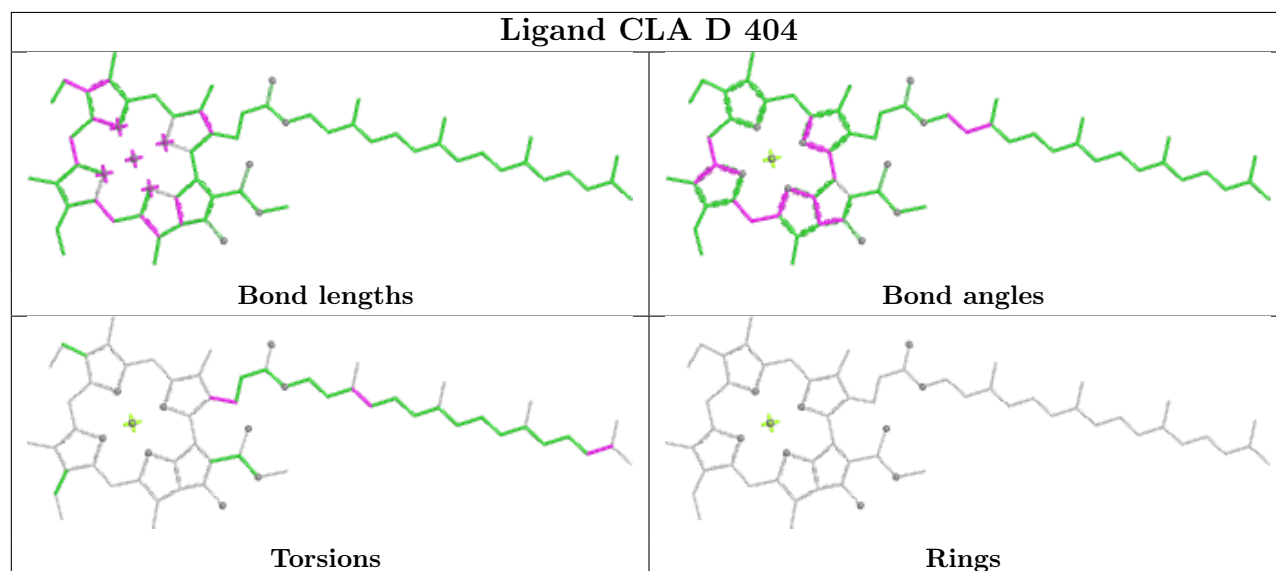
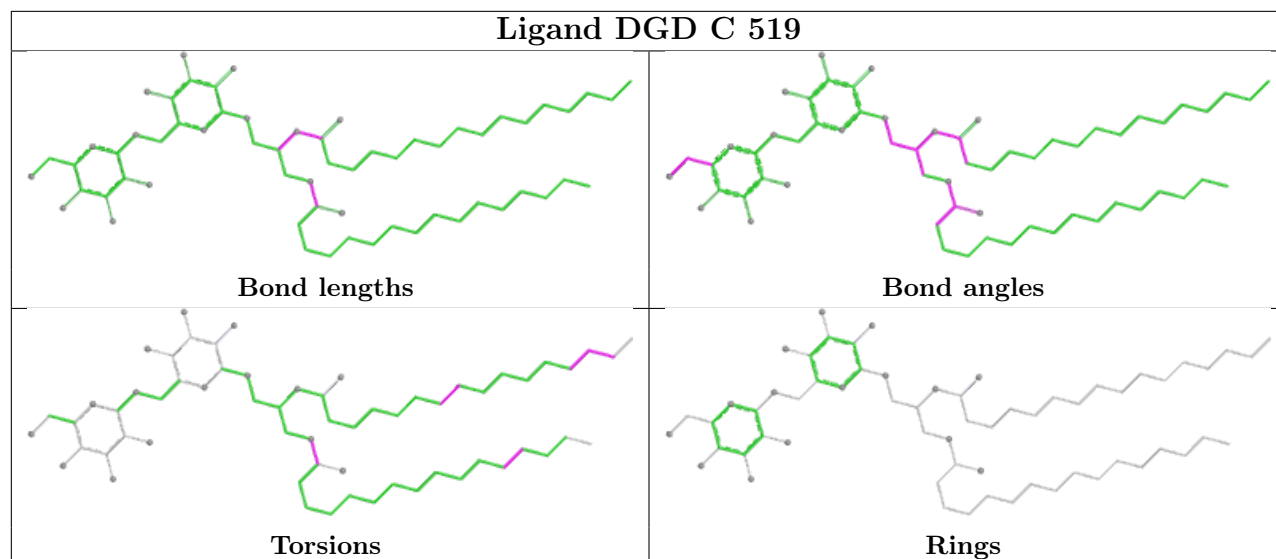
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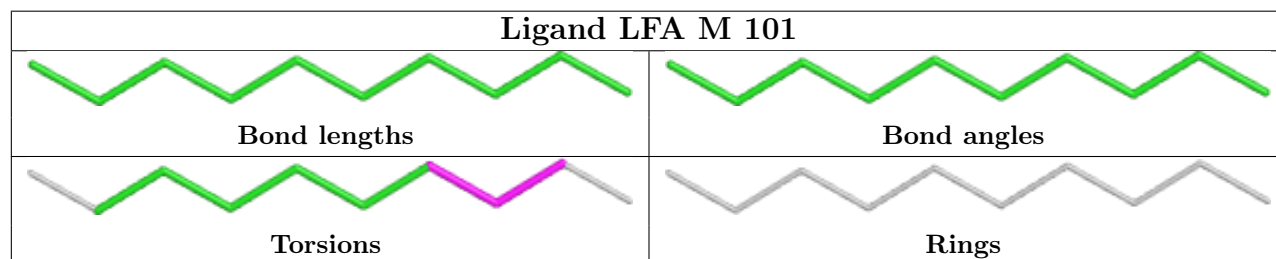
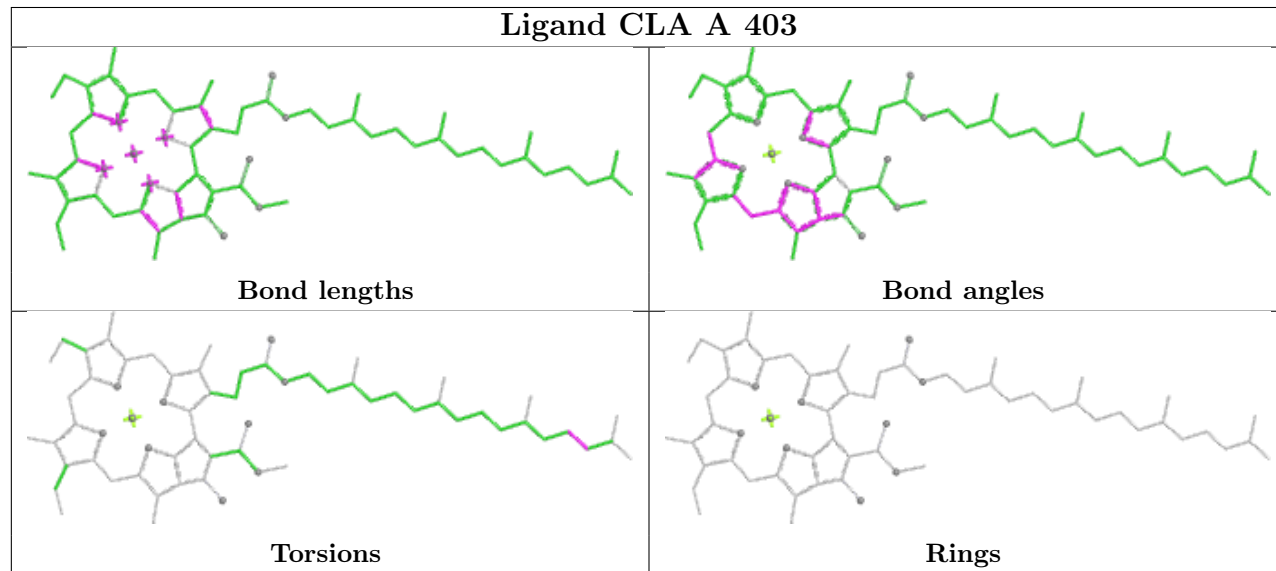
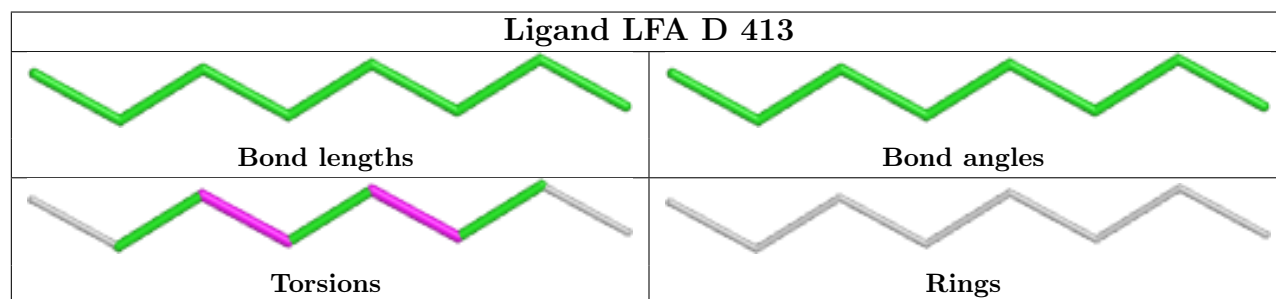
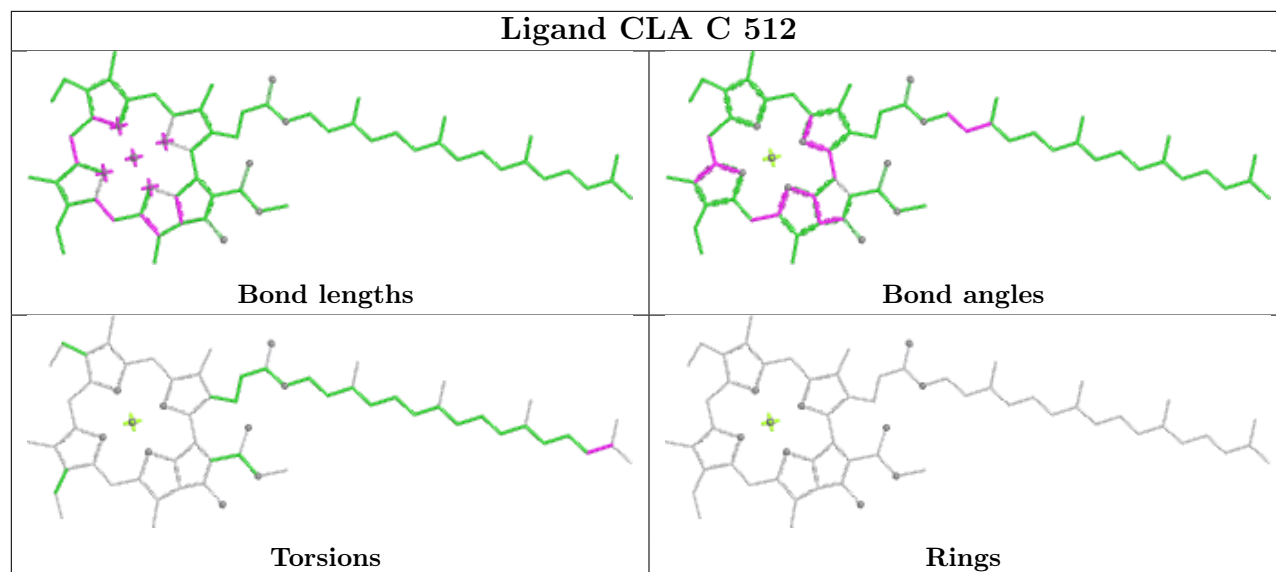
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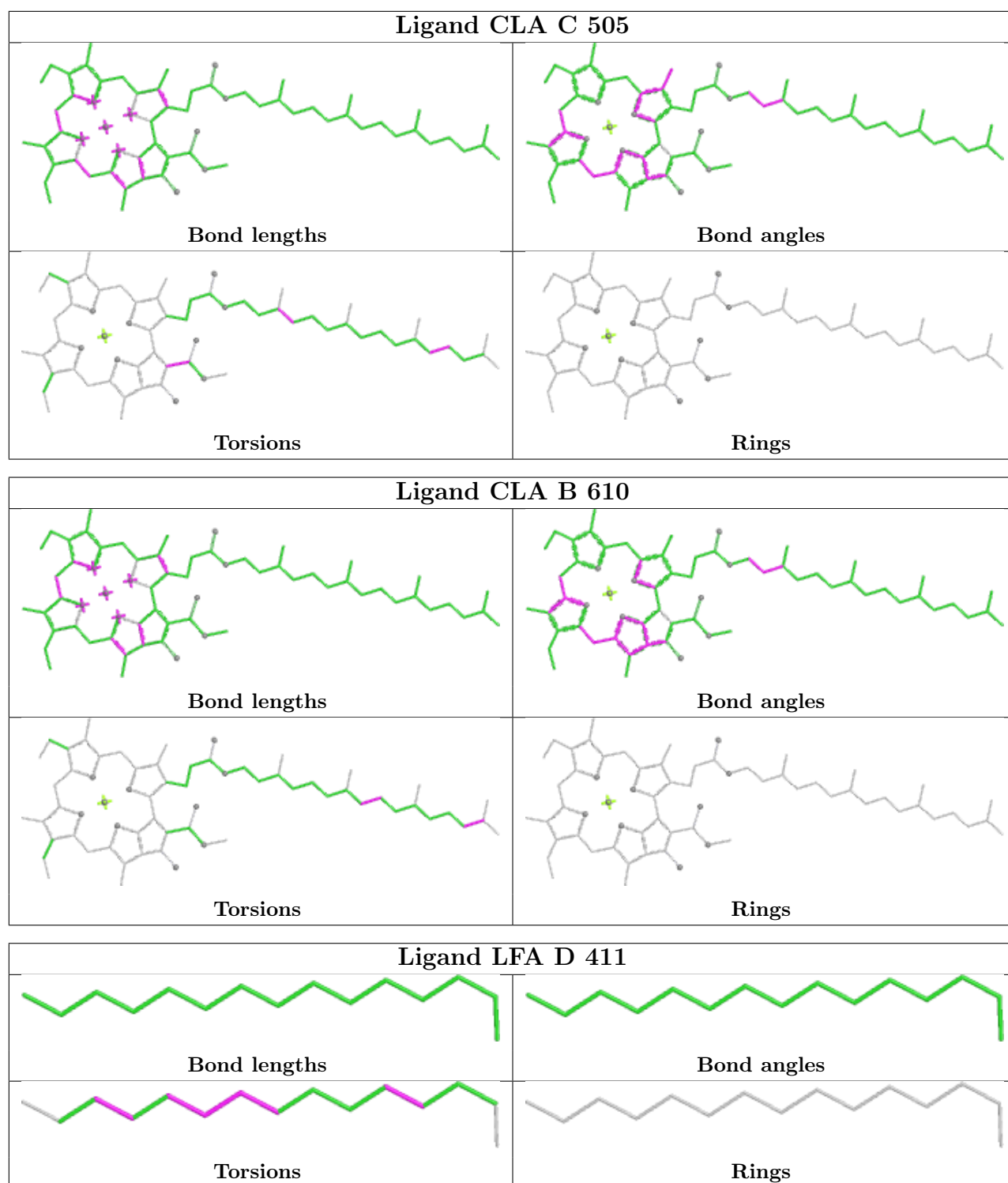
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	619	BCR	3	0
25	d	405	PL9	3	0
27	A	413	LFA	1	0
22	d	403	CLA	2	0
24	h	101	BCR	6	0
26	A	411	SQD	2	0
27	c	521	LFA	2	0
22	b	612	CLA	1	0
25	D	406	PL9	6	0
24	C	516	BCR	3	0
22	d	401	CLA	2	0
30	C	518	DGD	2	0
22	b	605	CLA	4	0
27	m	101	LFA	1	0
32	l	101	LHG	1	0
29	f	101	LMG	2	0
27	b	622	LFA	1	0

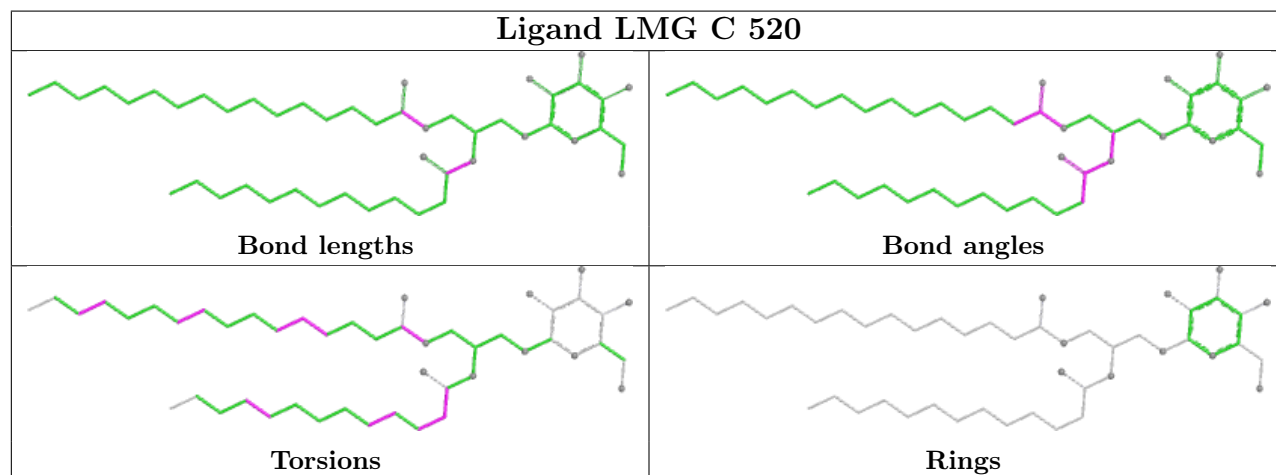
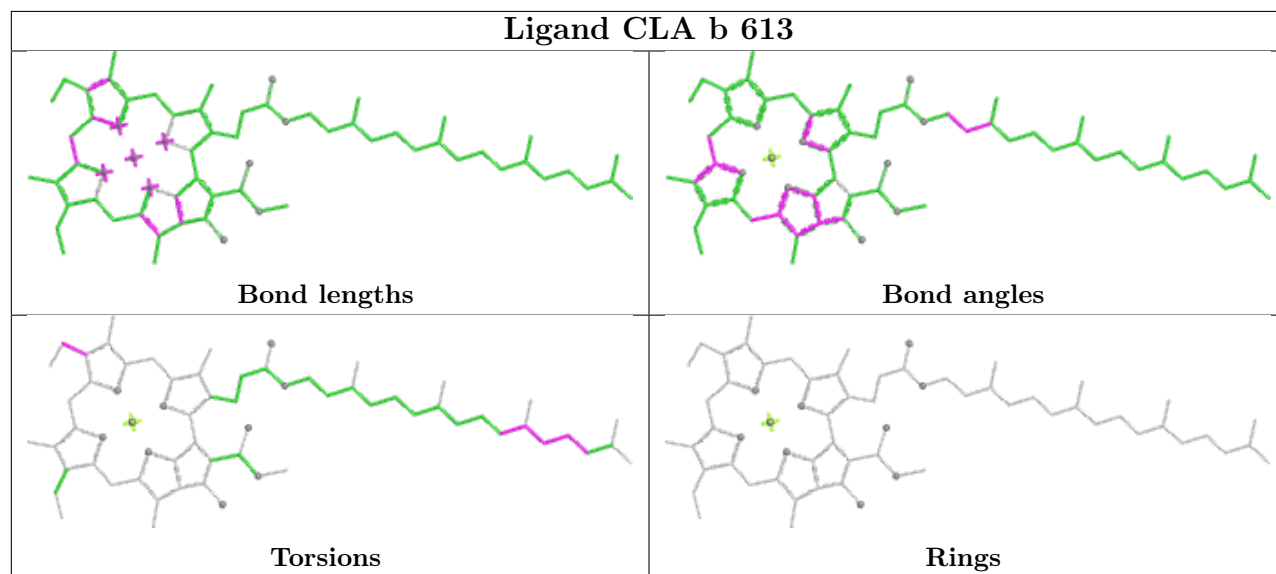
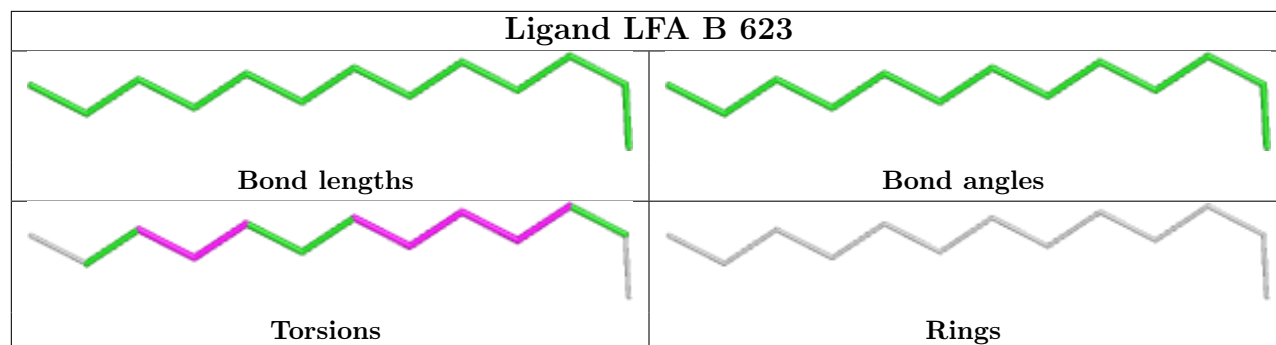
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

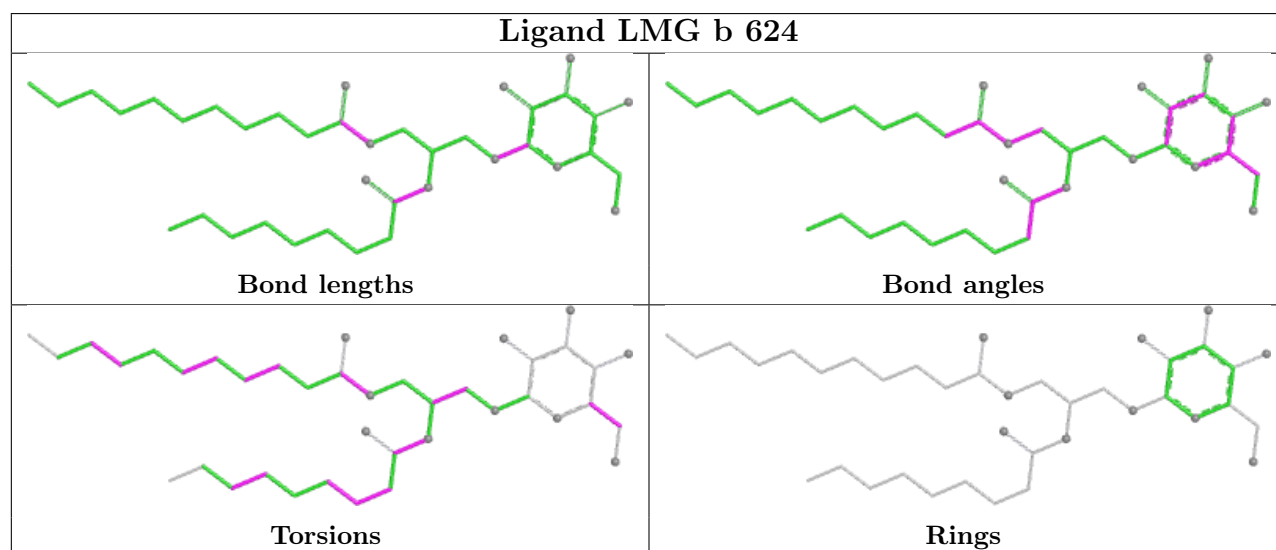
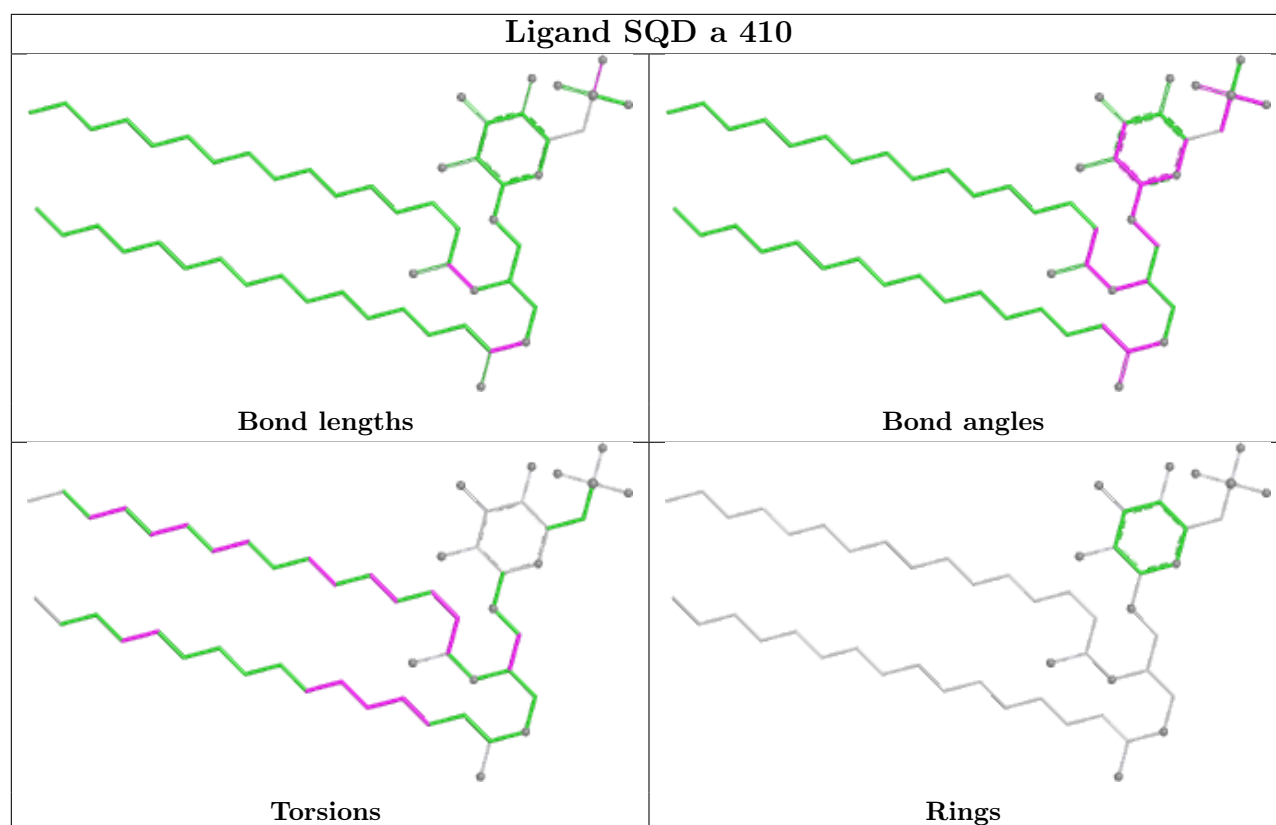


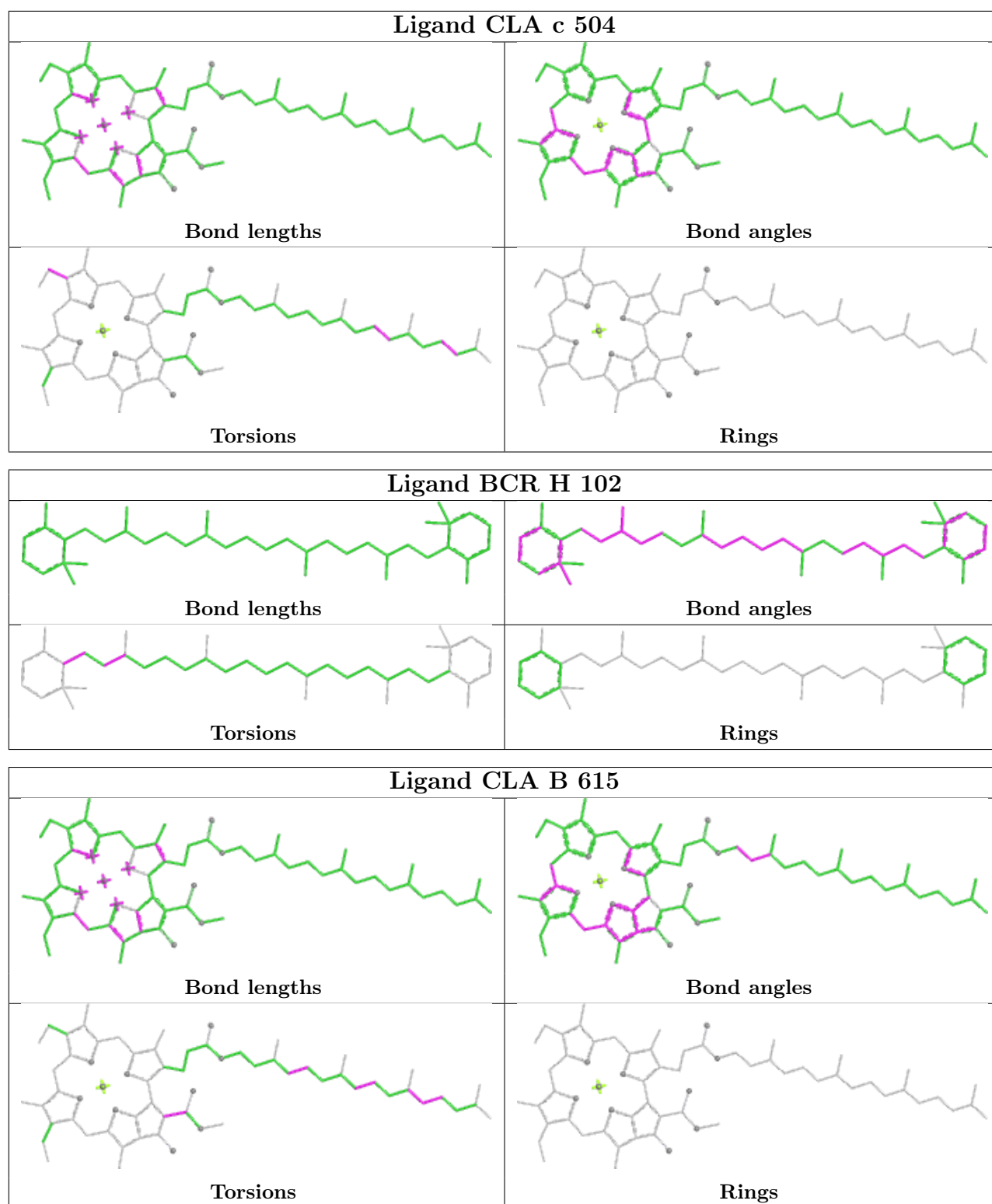


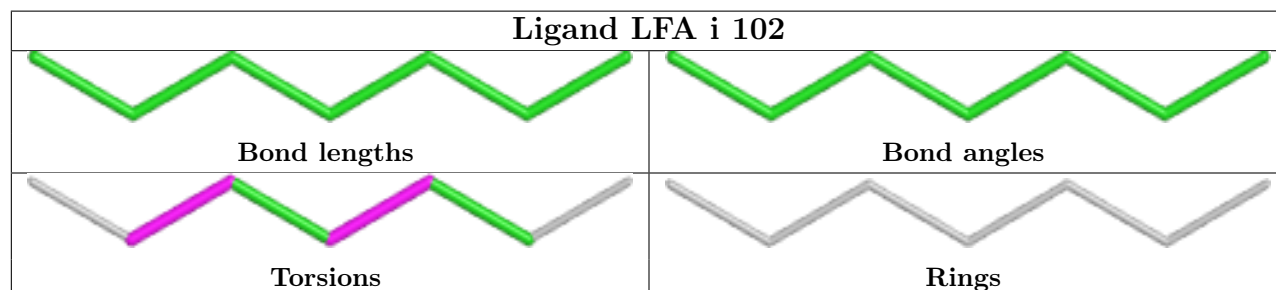
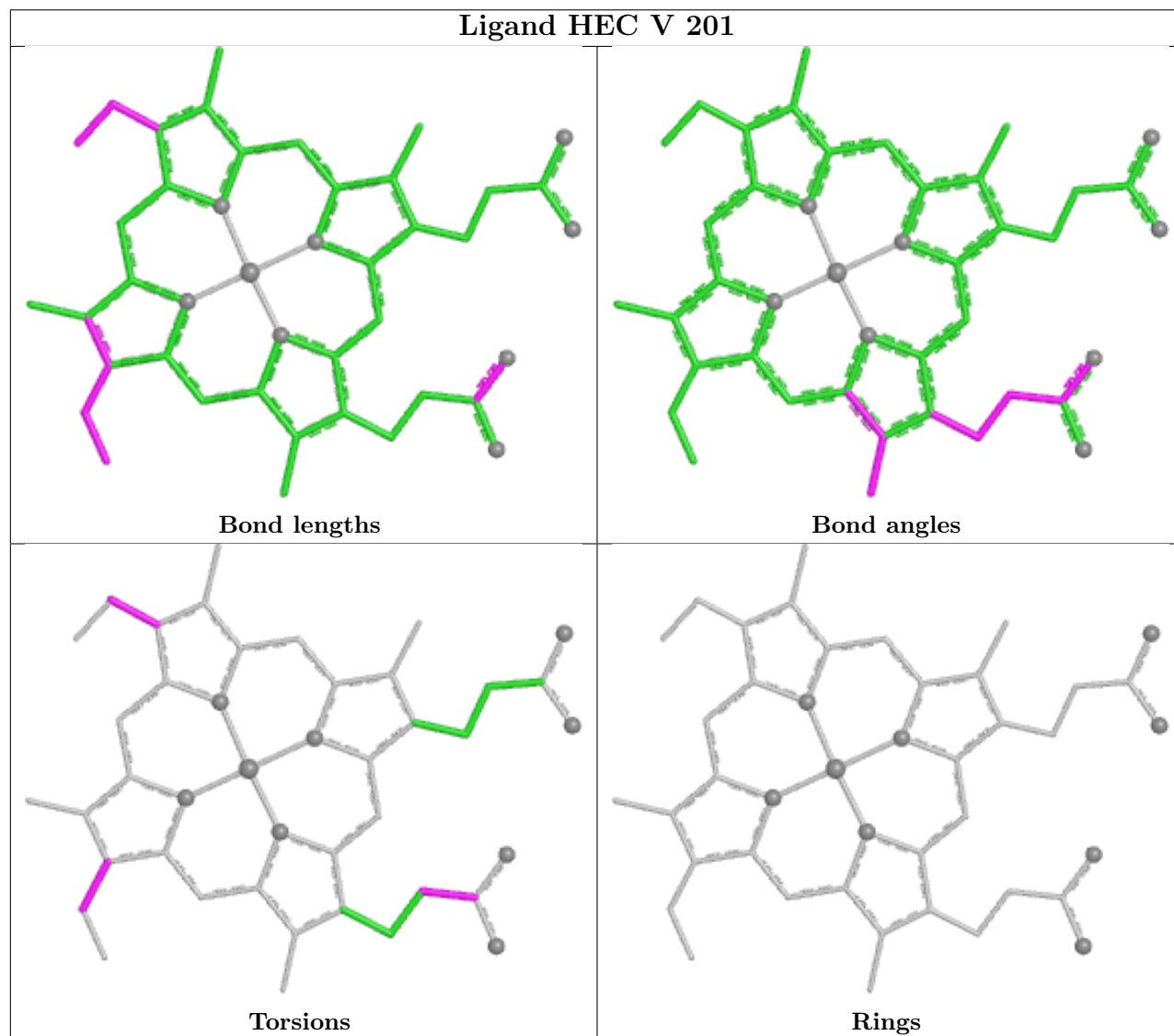
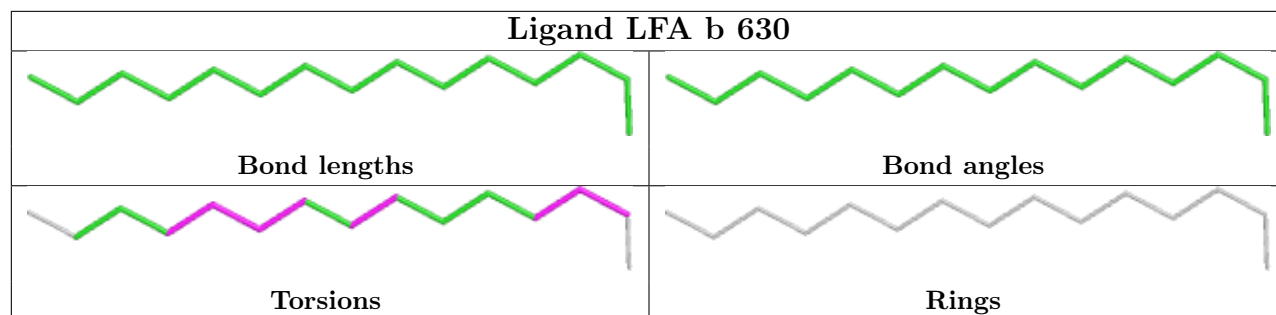


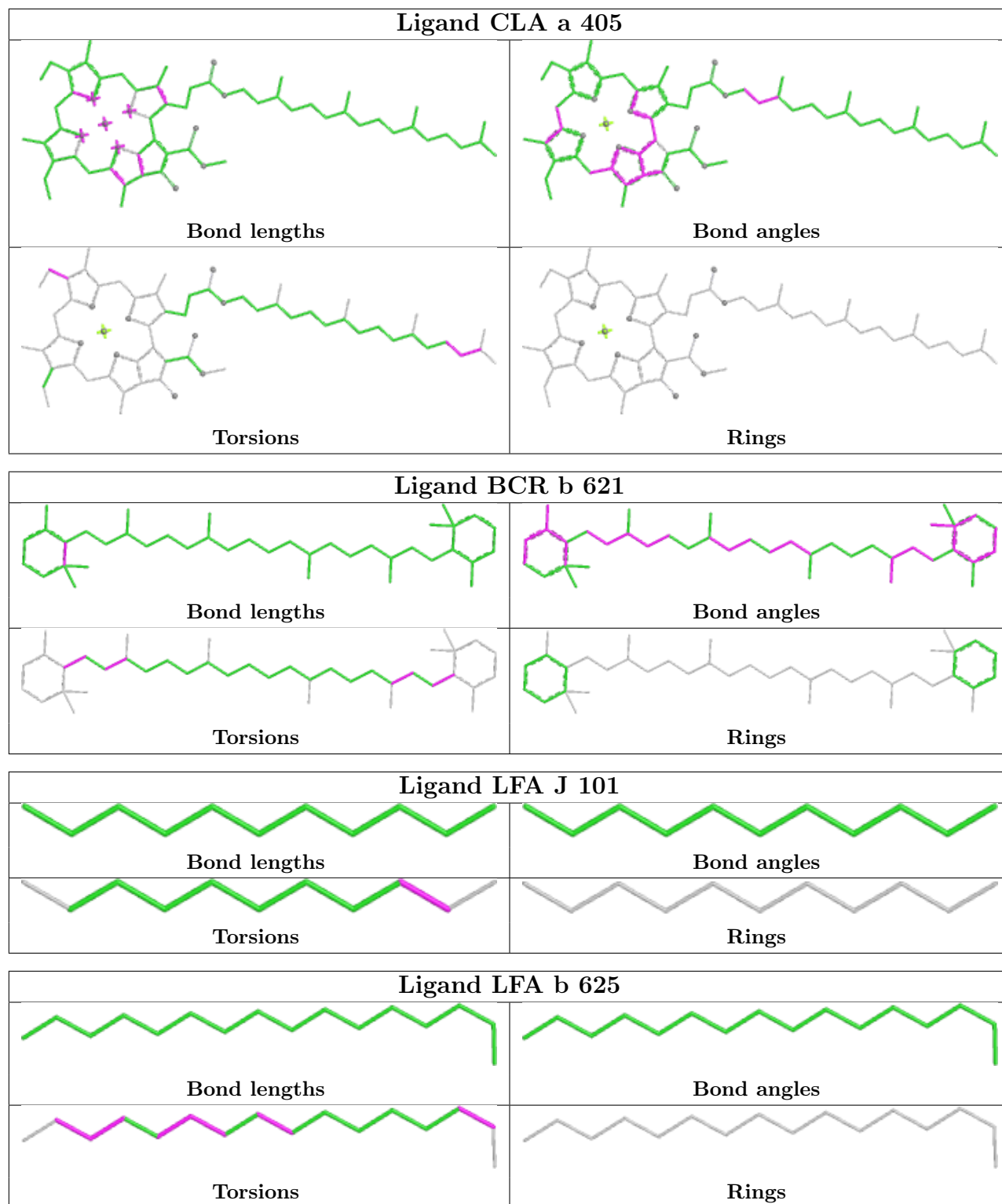


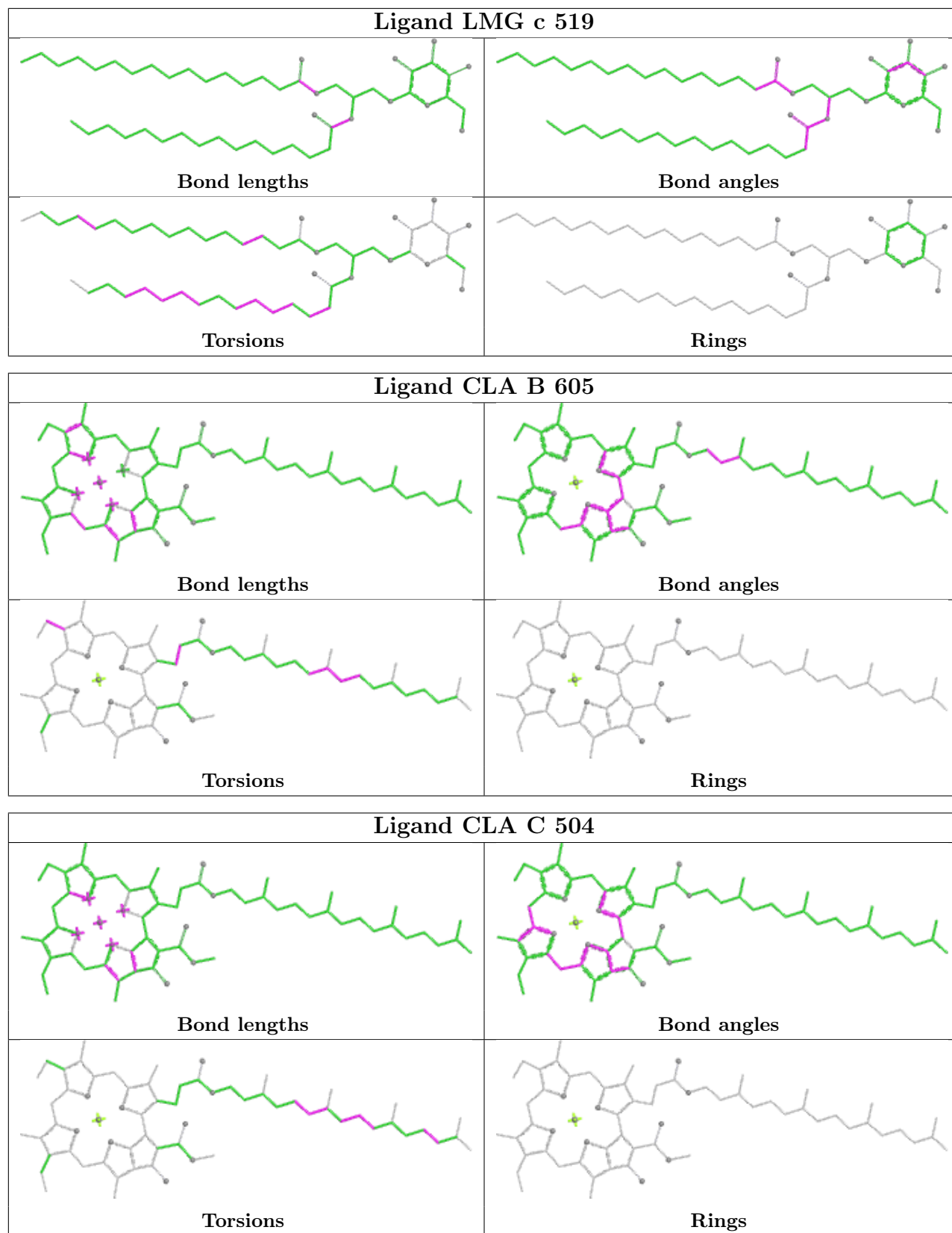


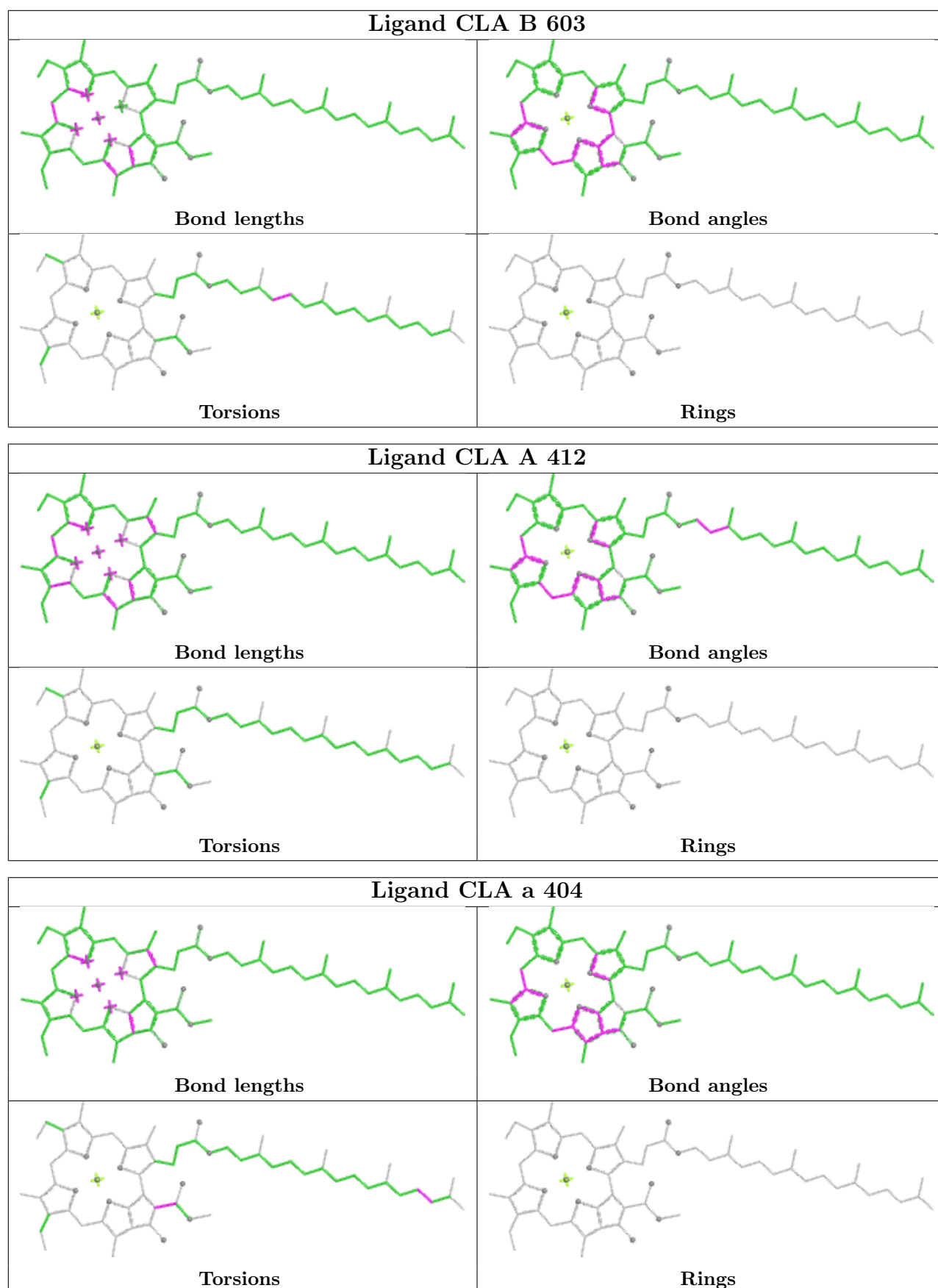


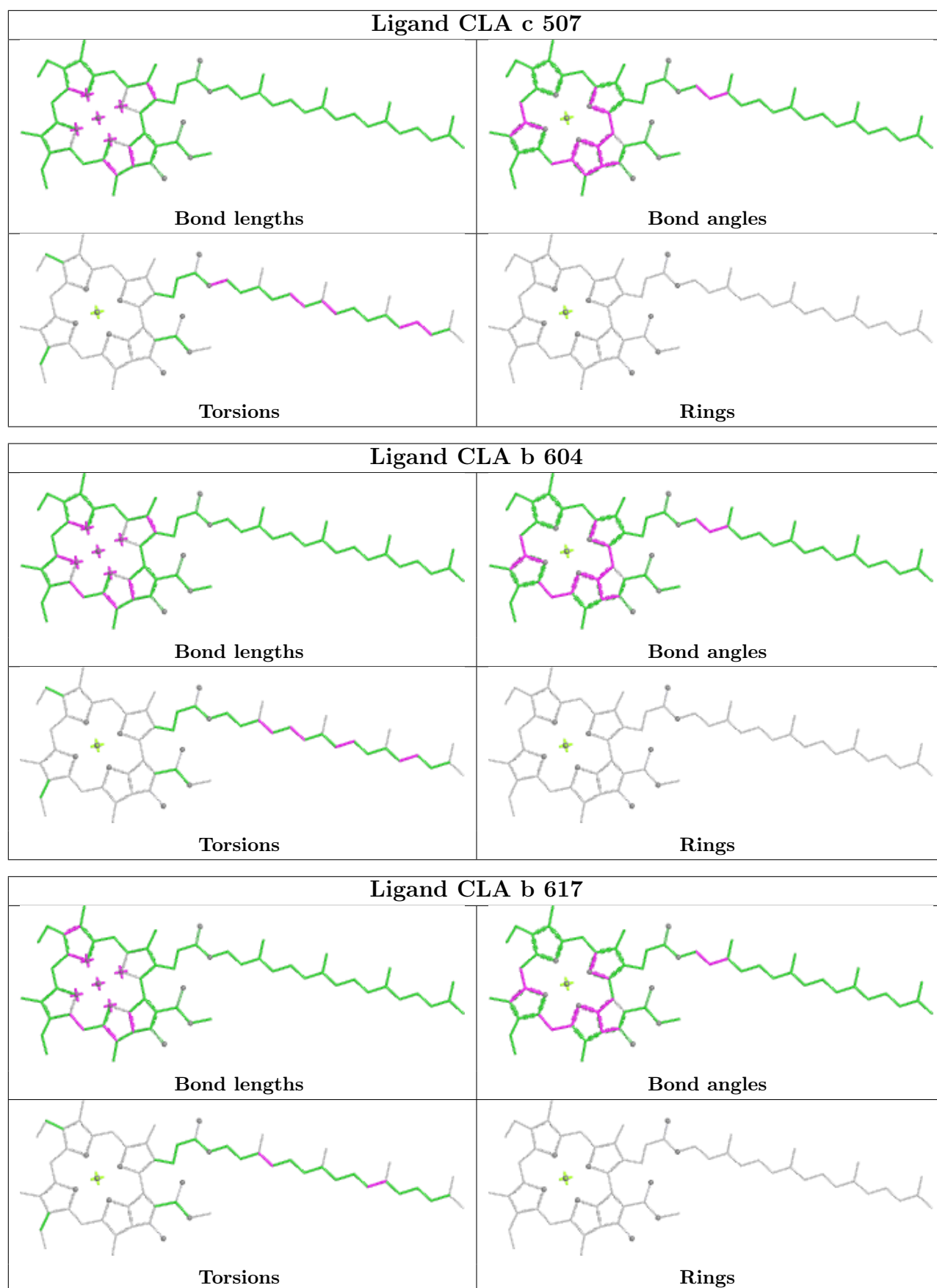


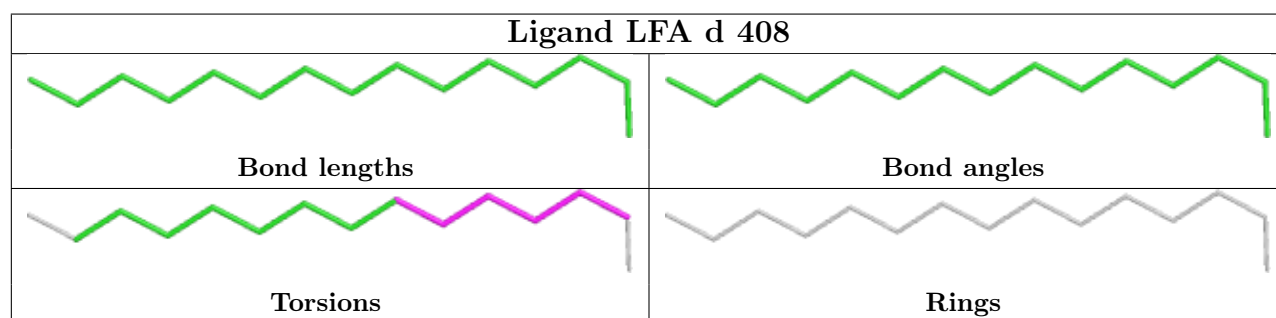
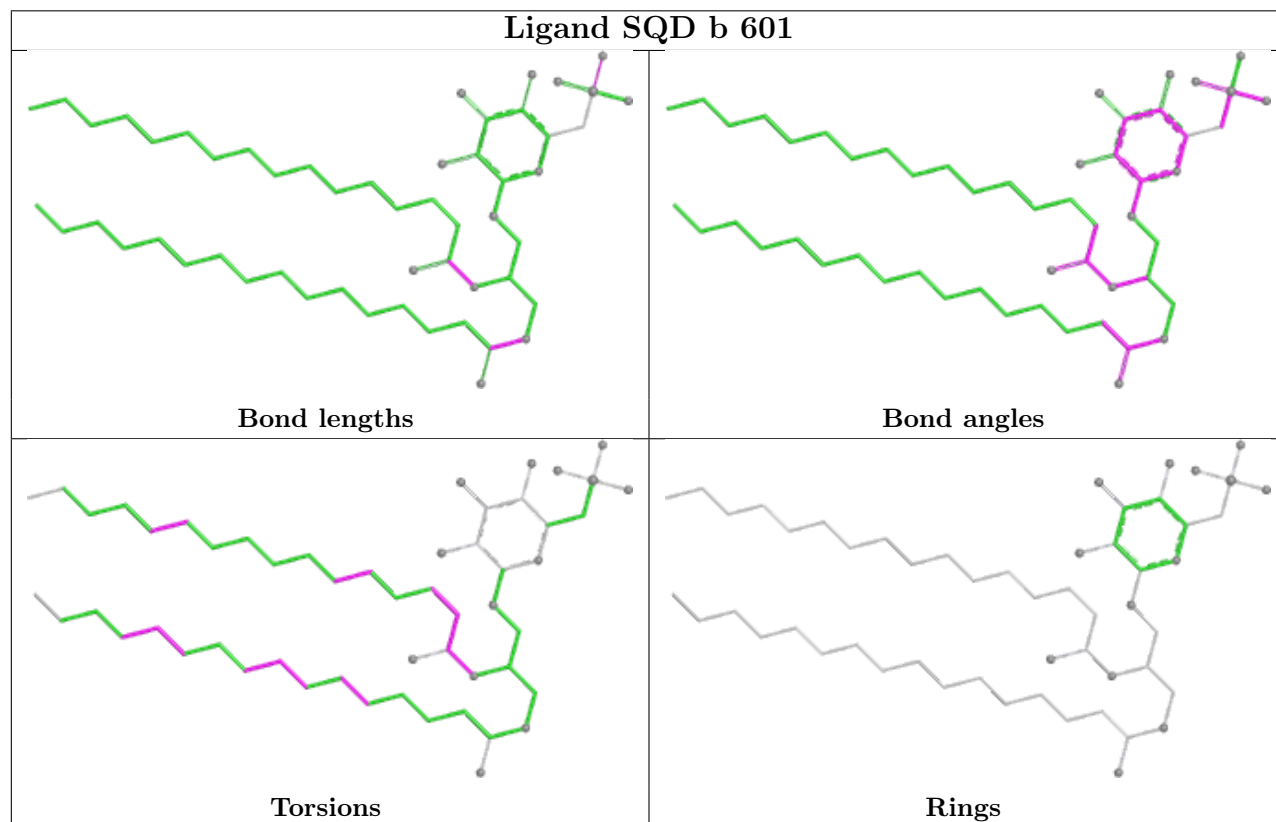
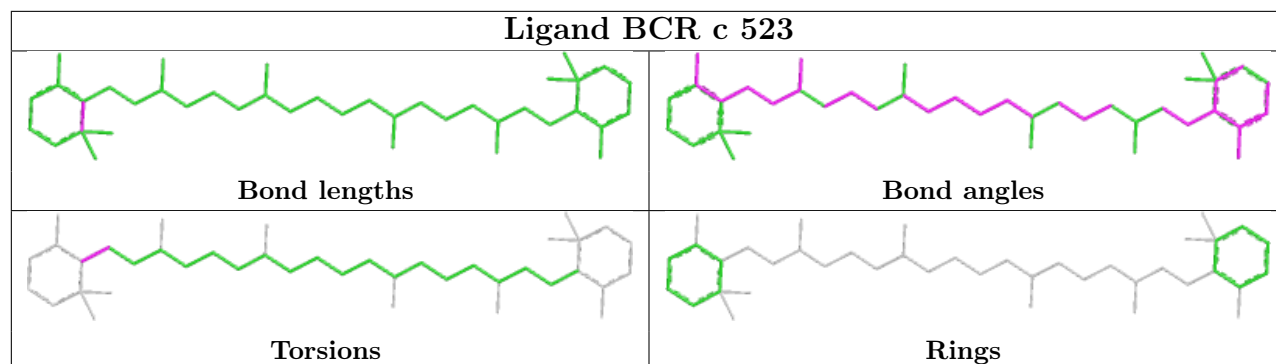


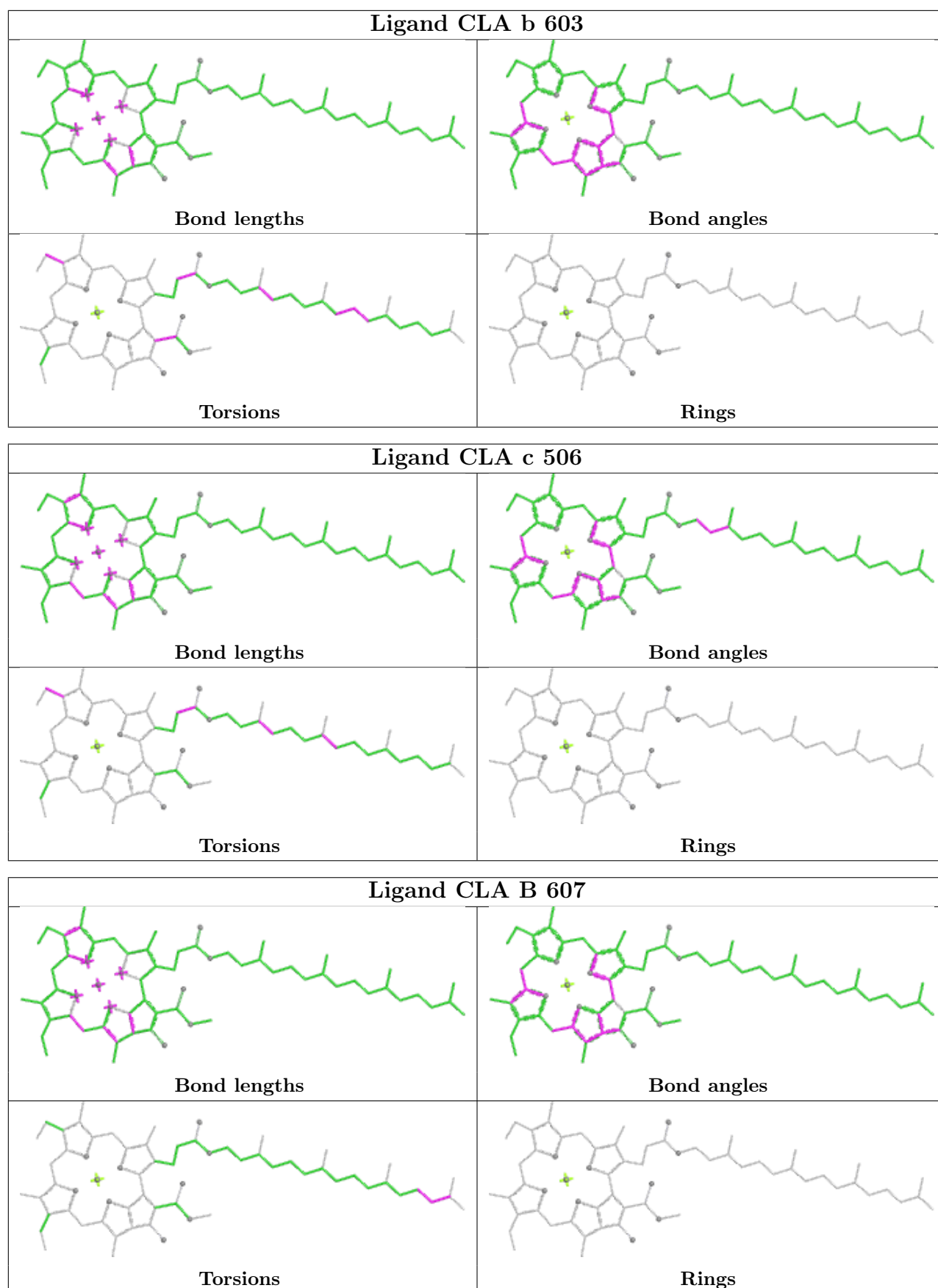


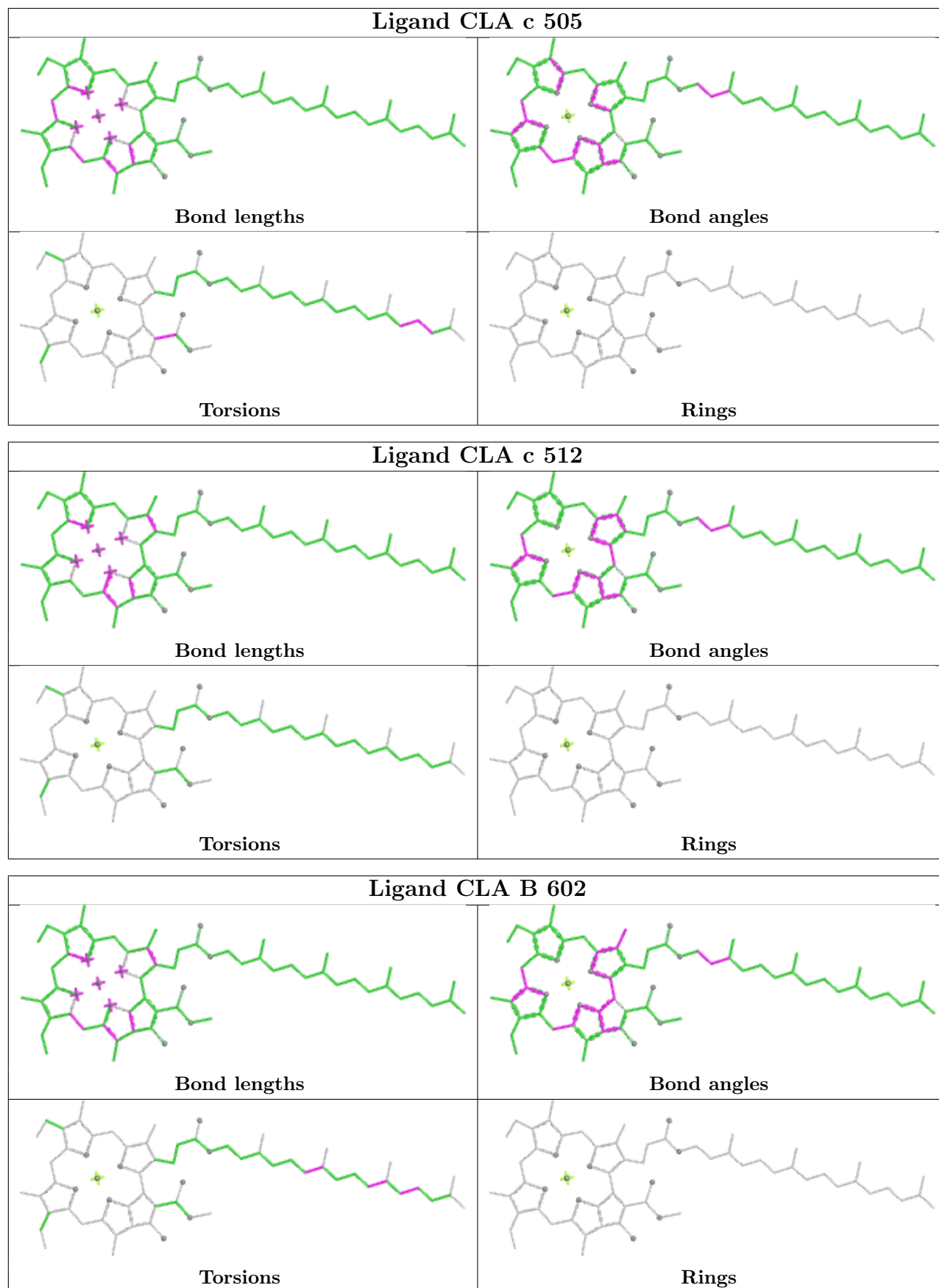


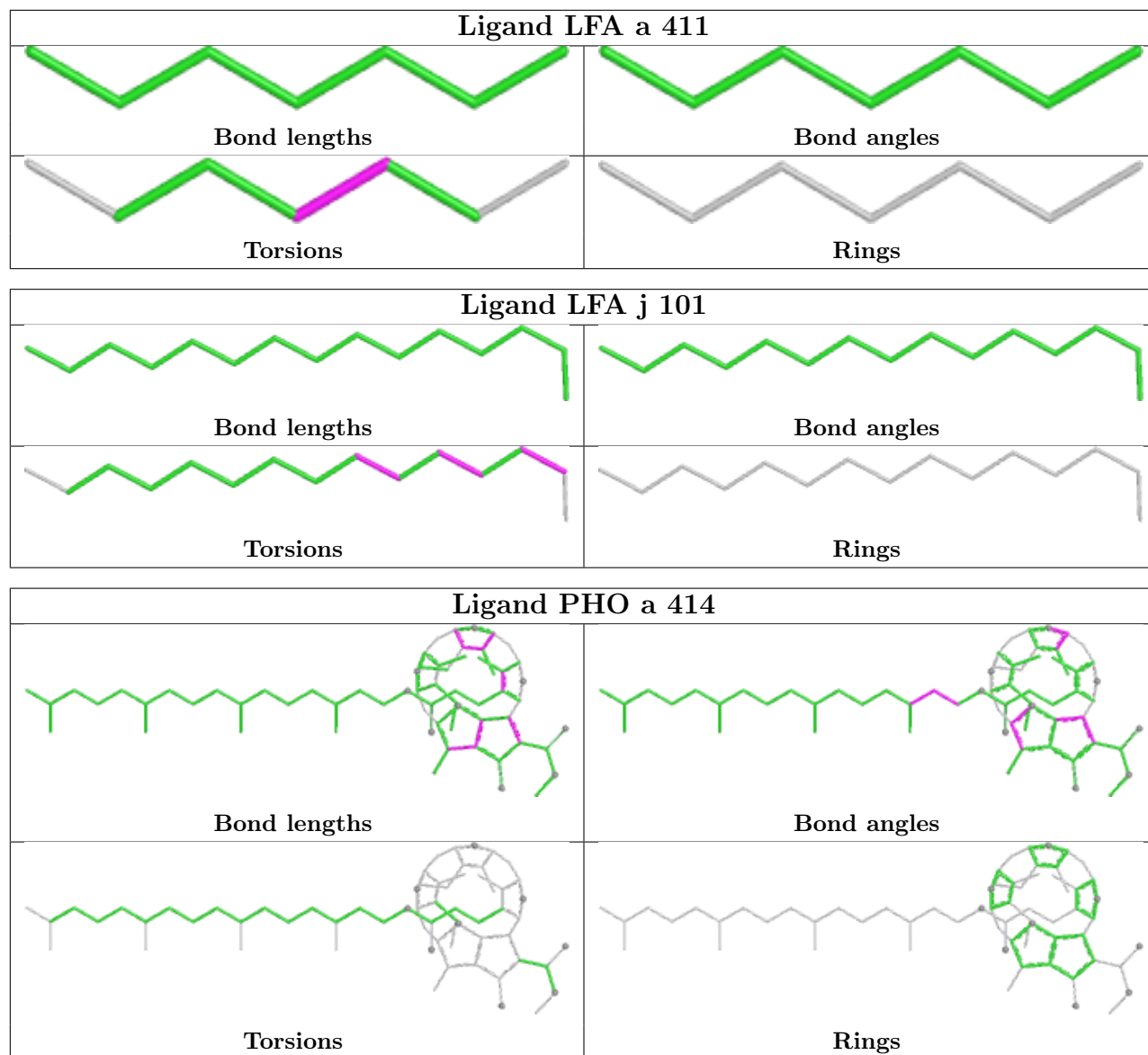


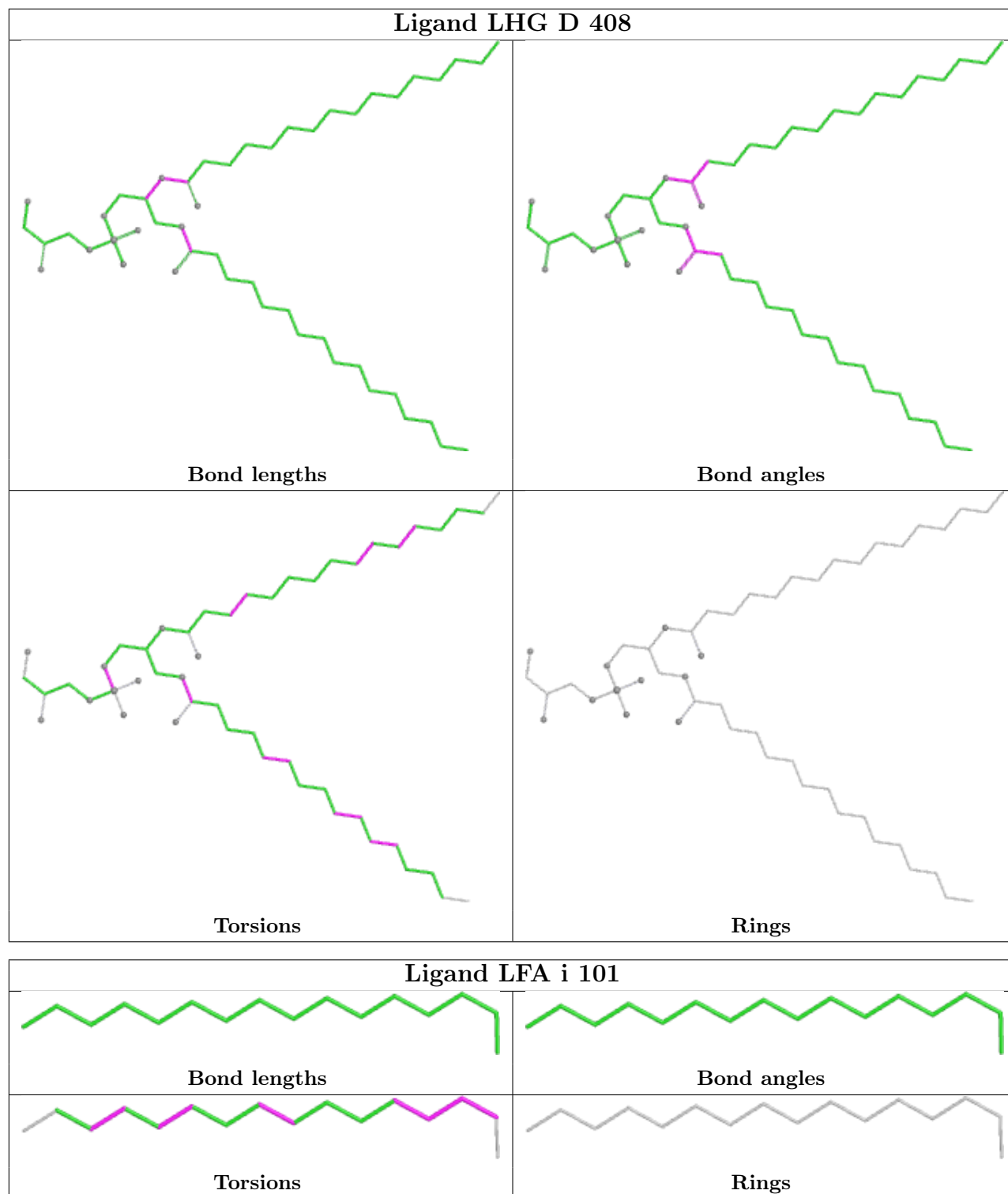


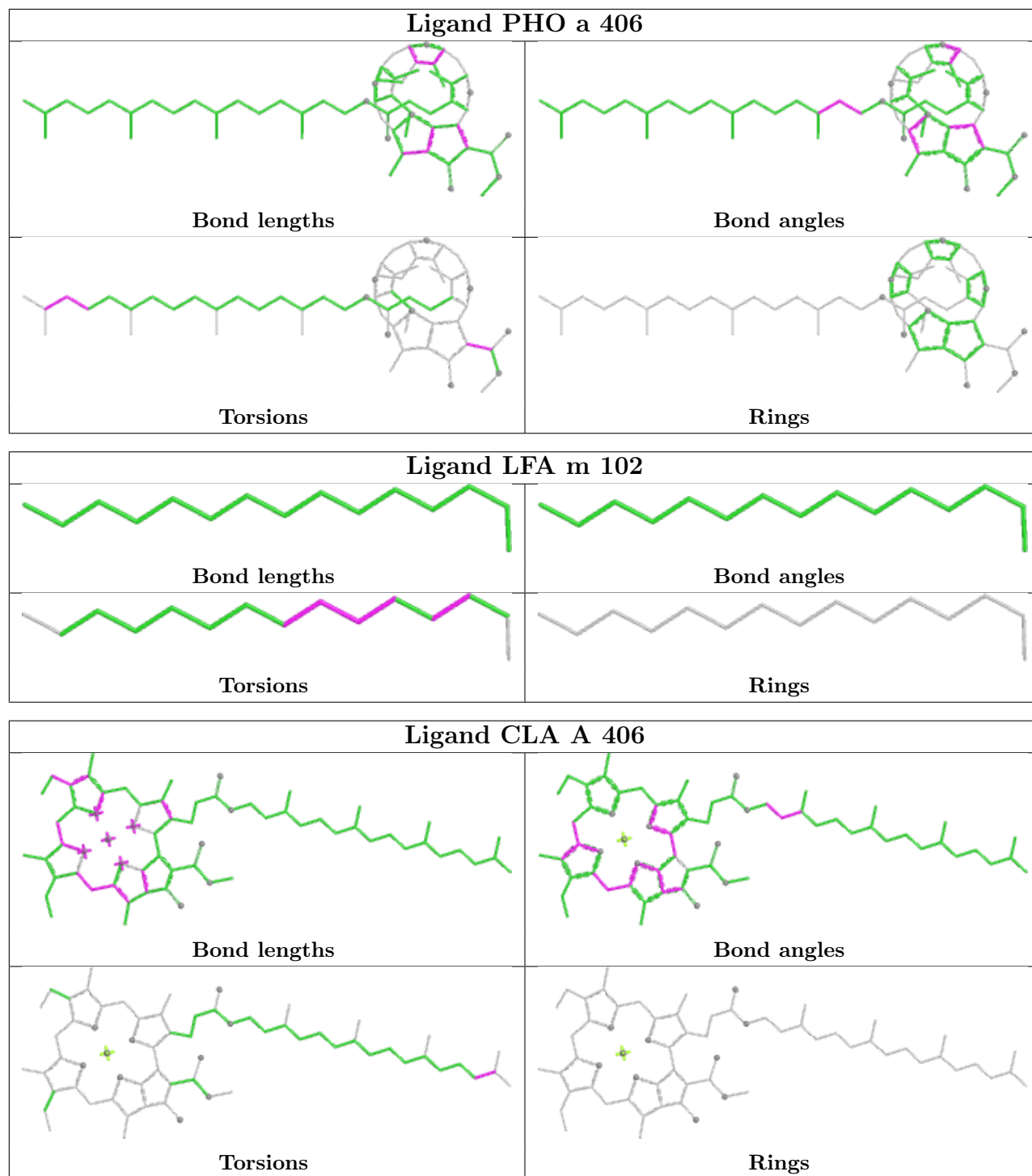


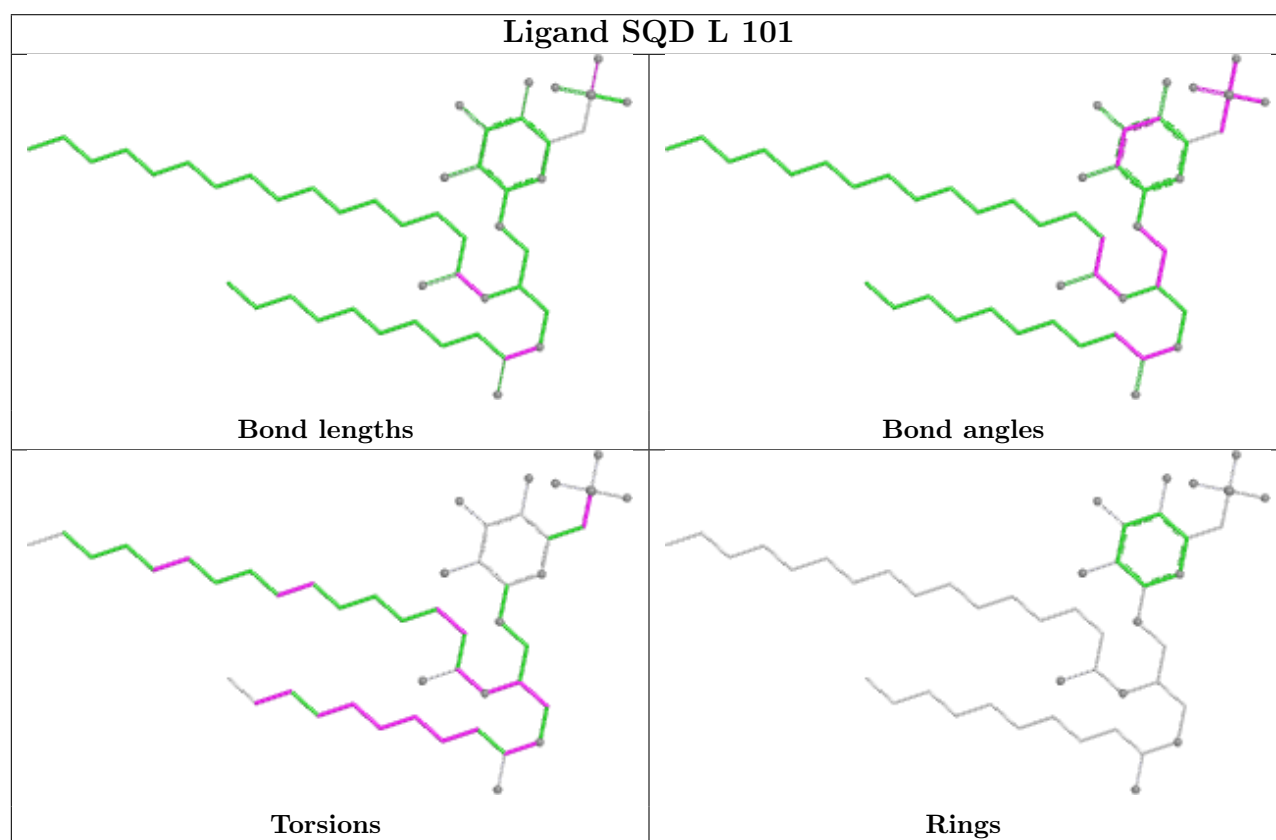
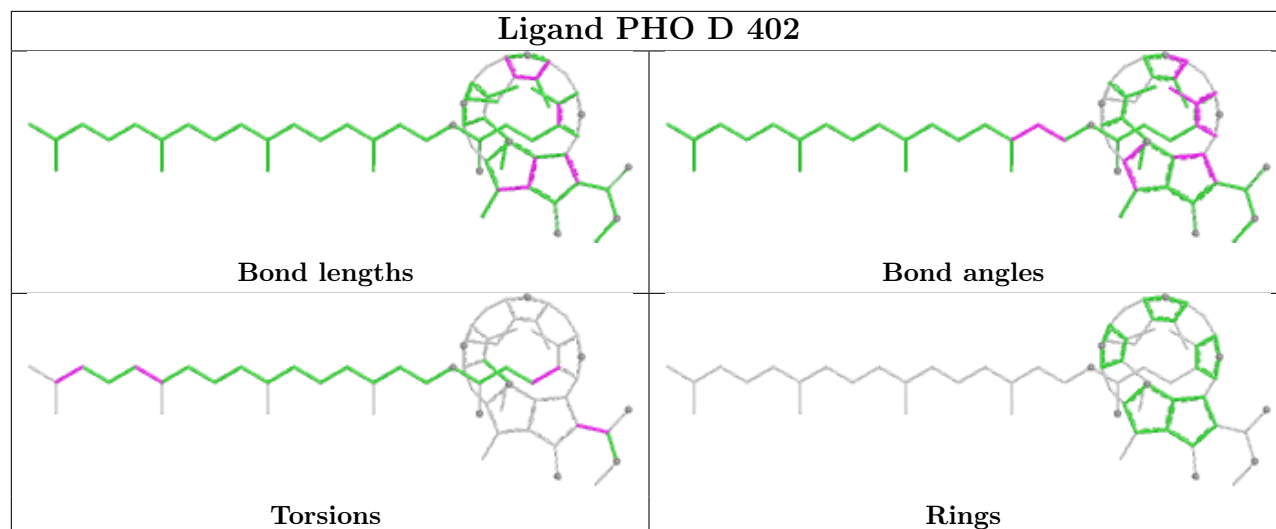


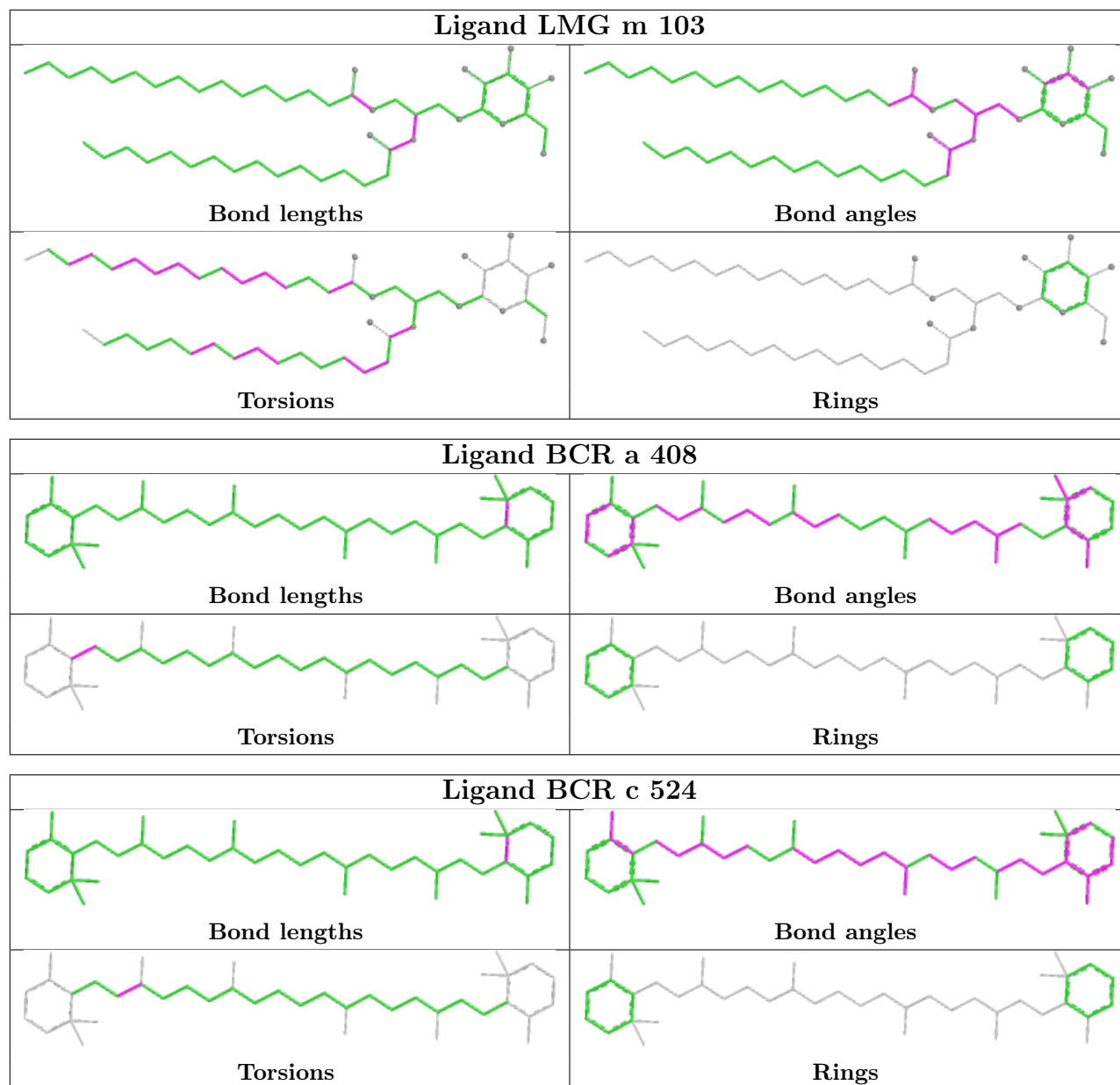


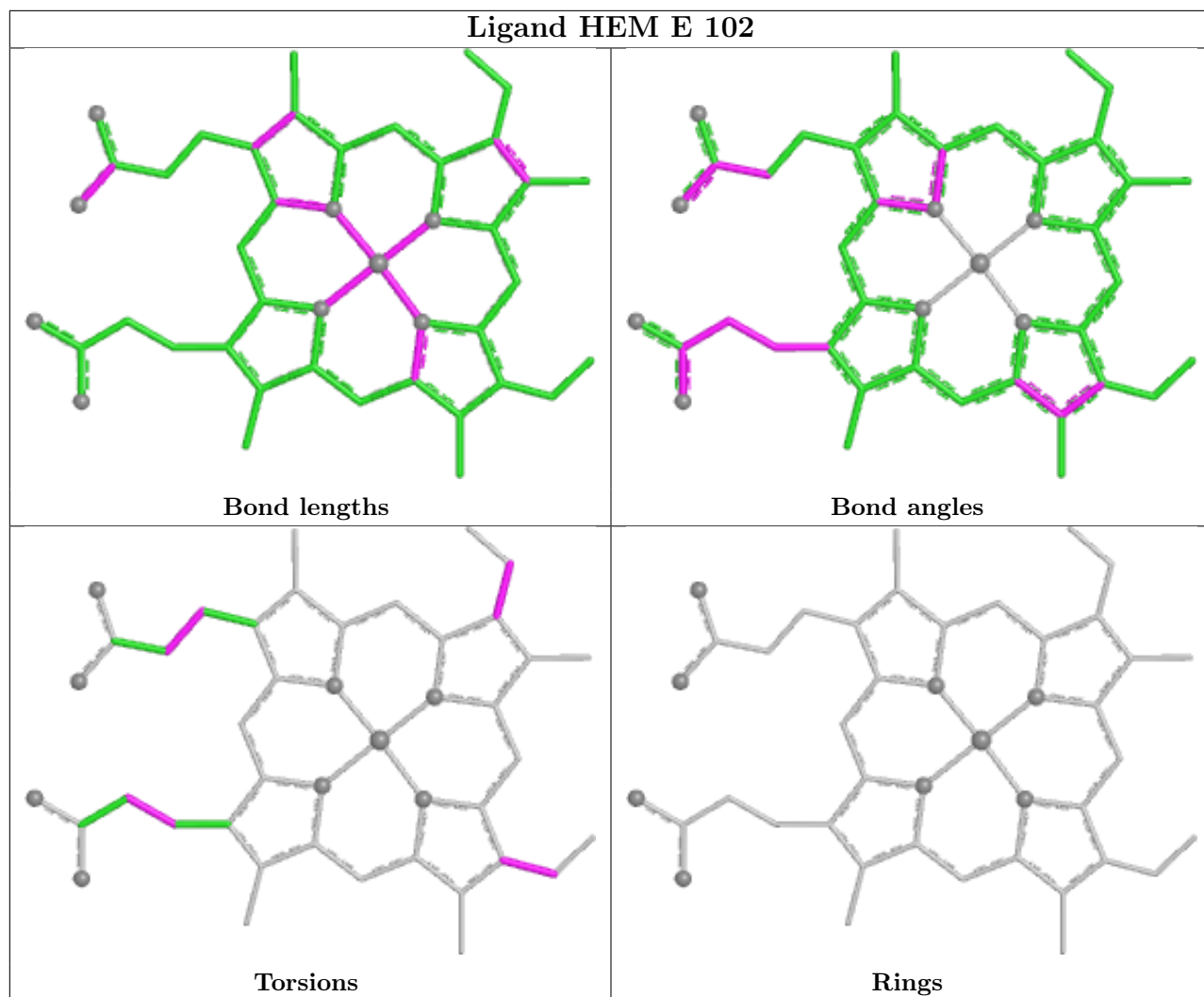


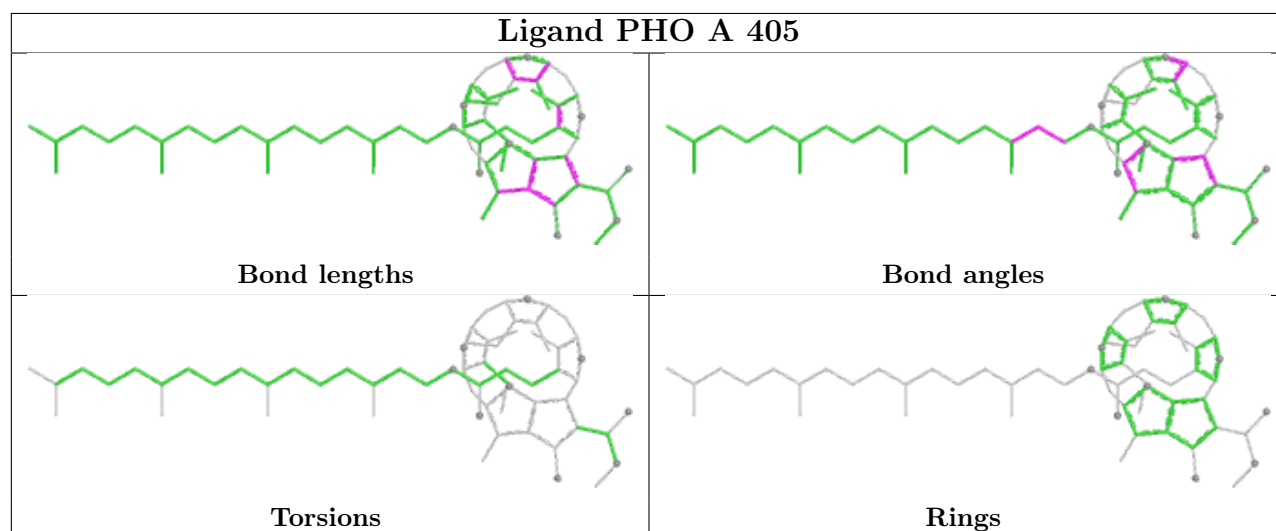
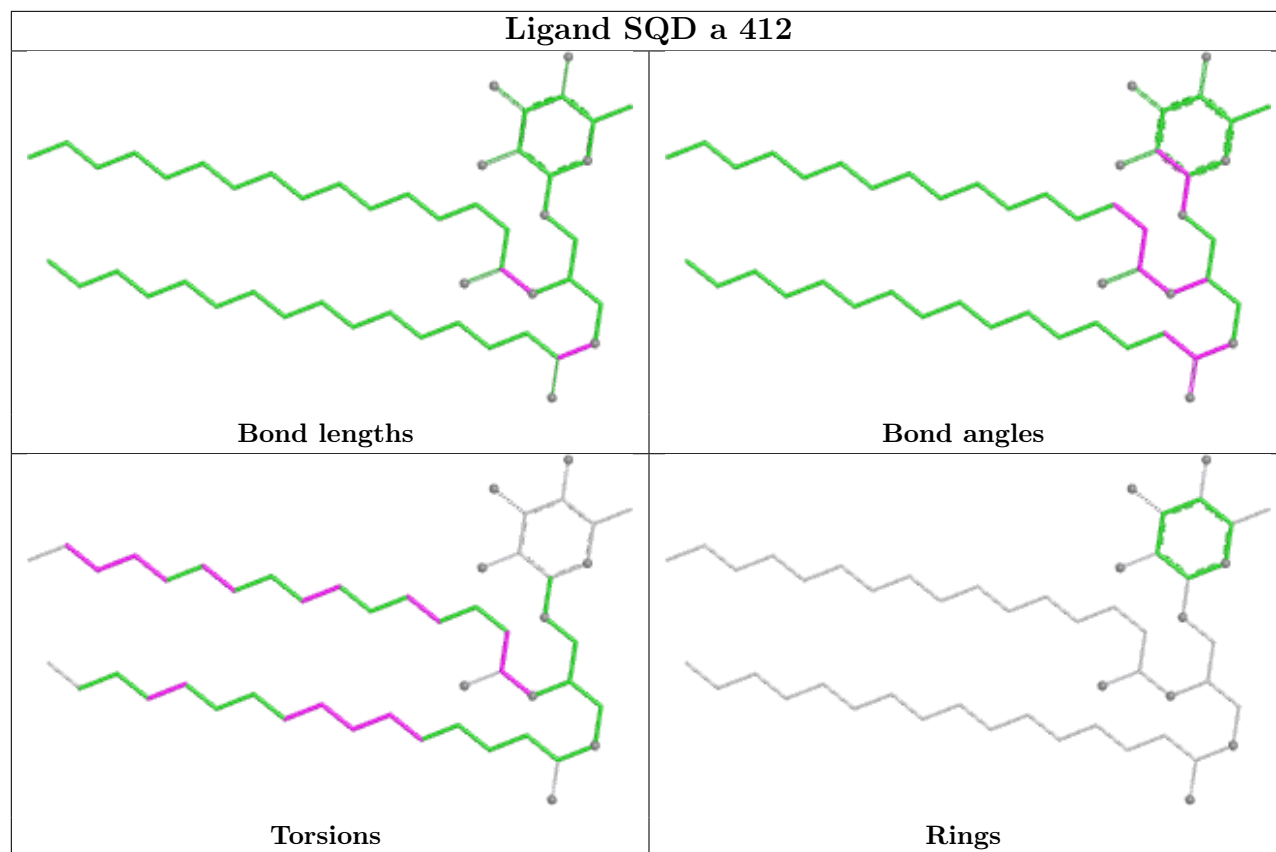


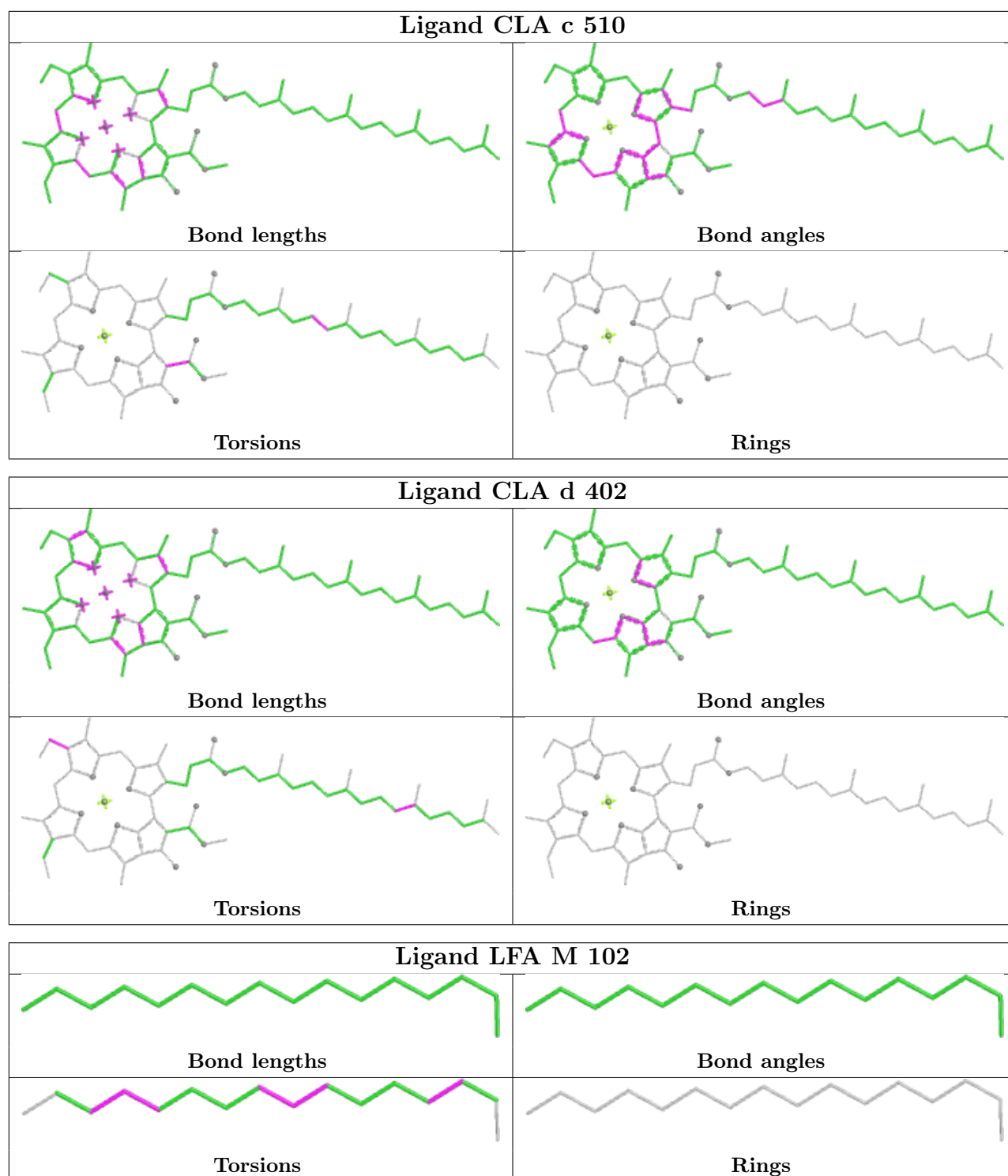


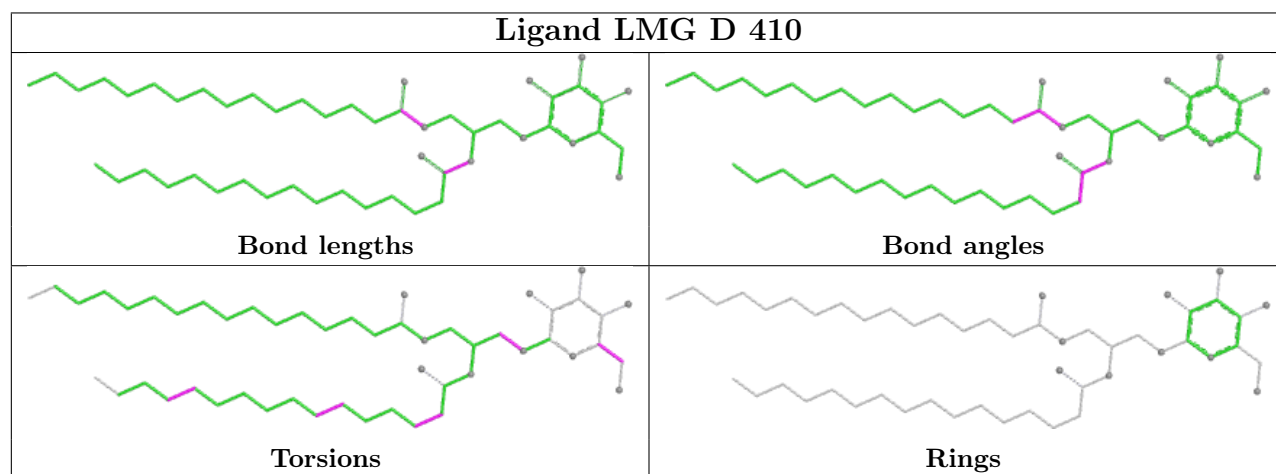
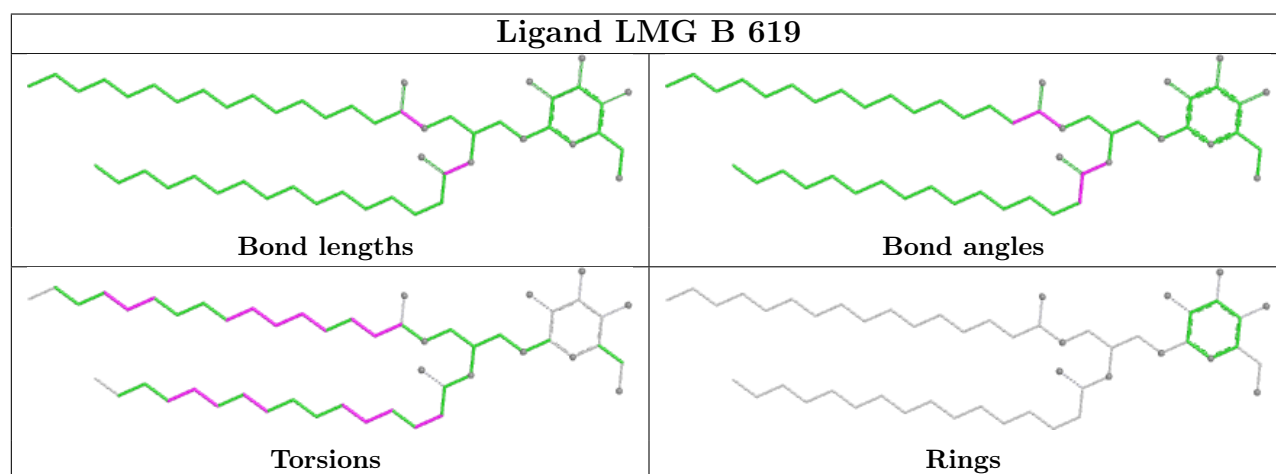
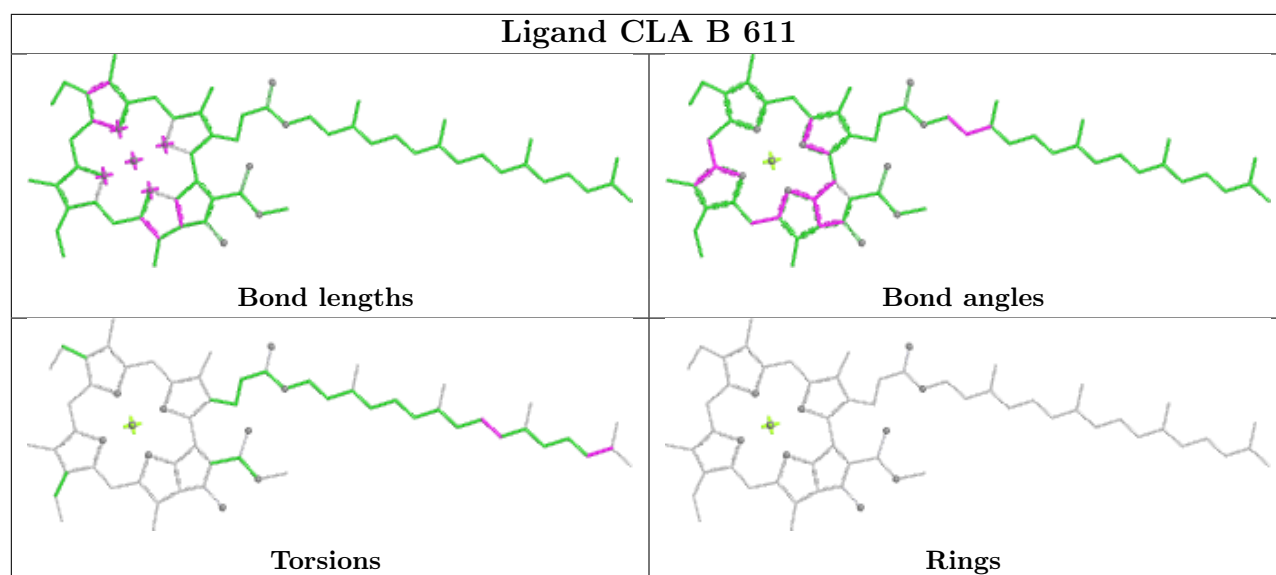


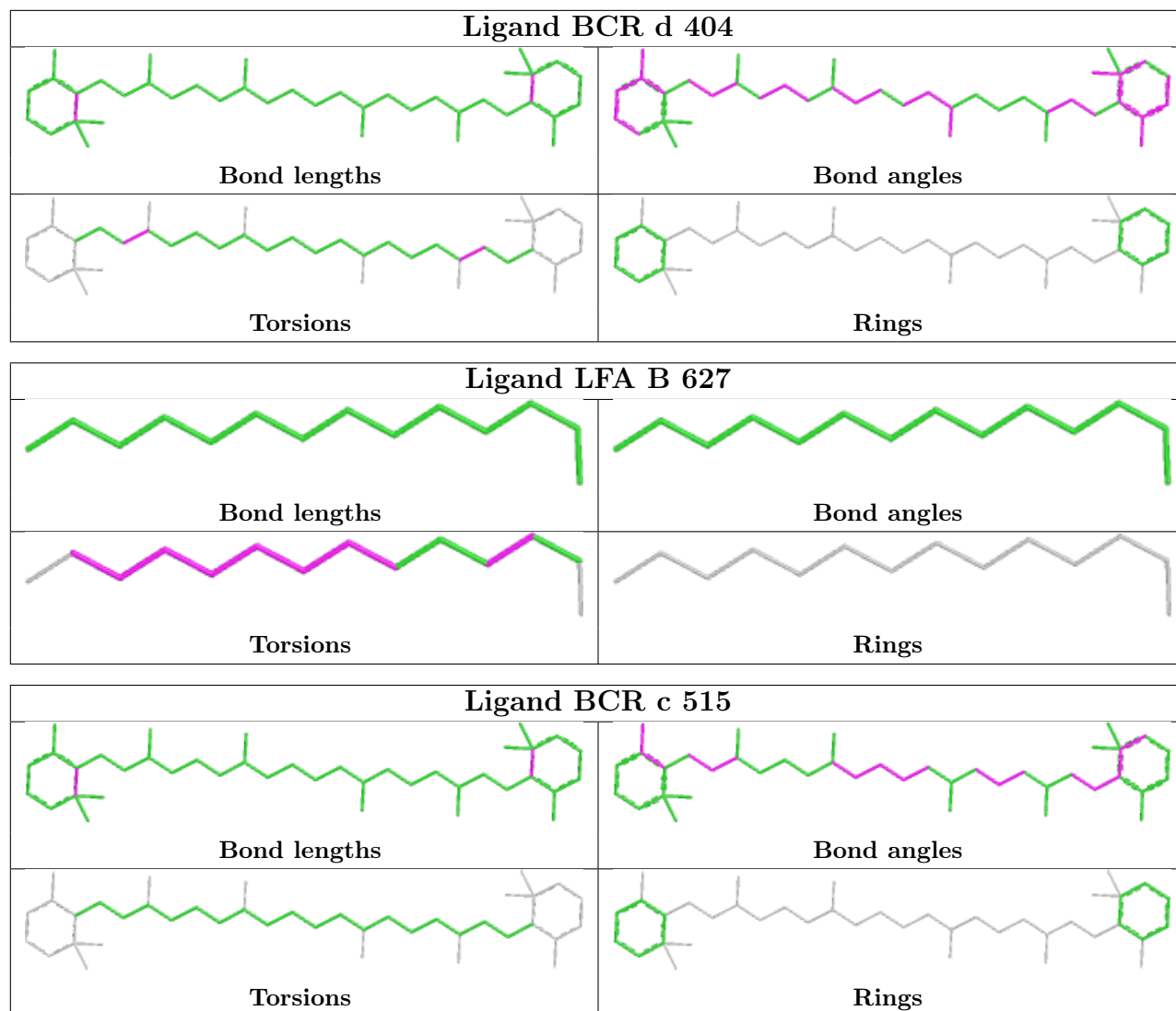


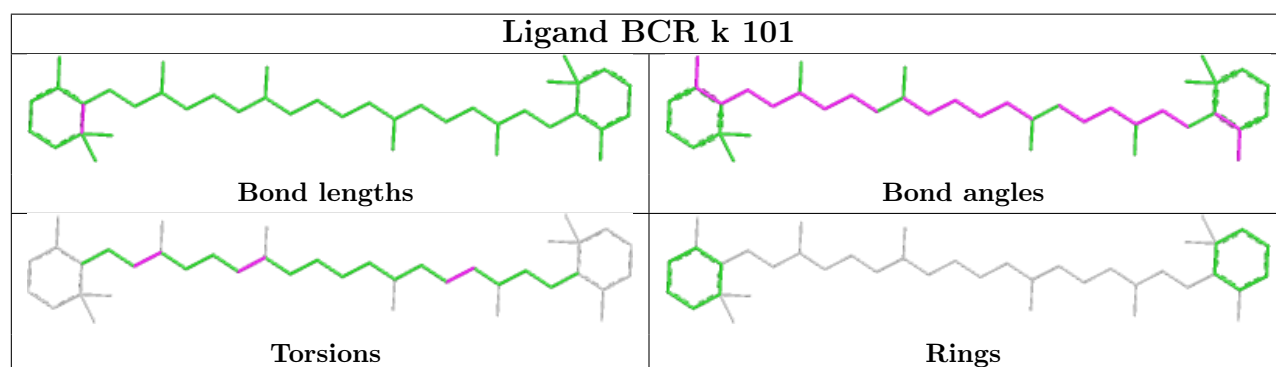
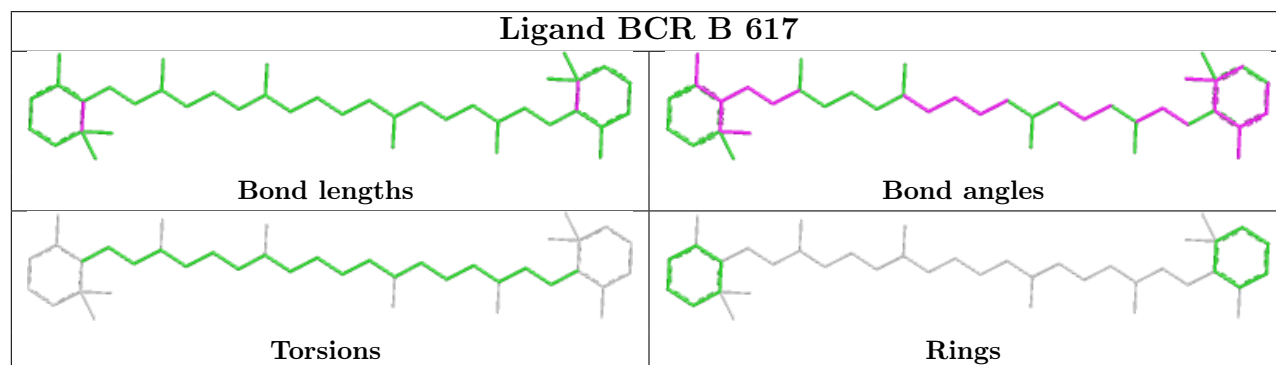
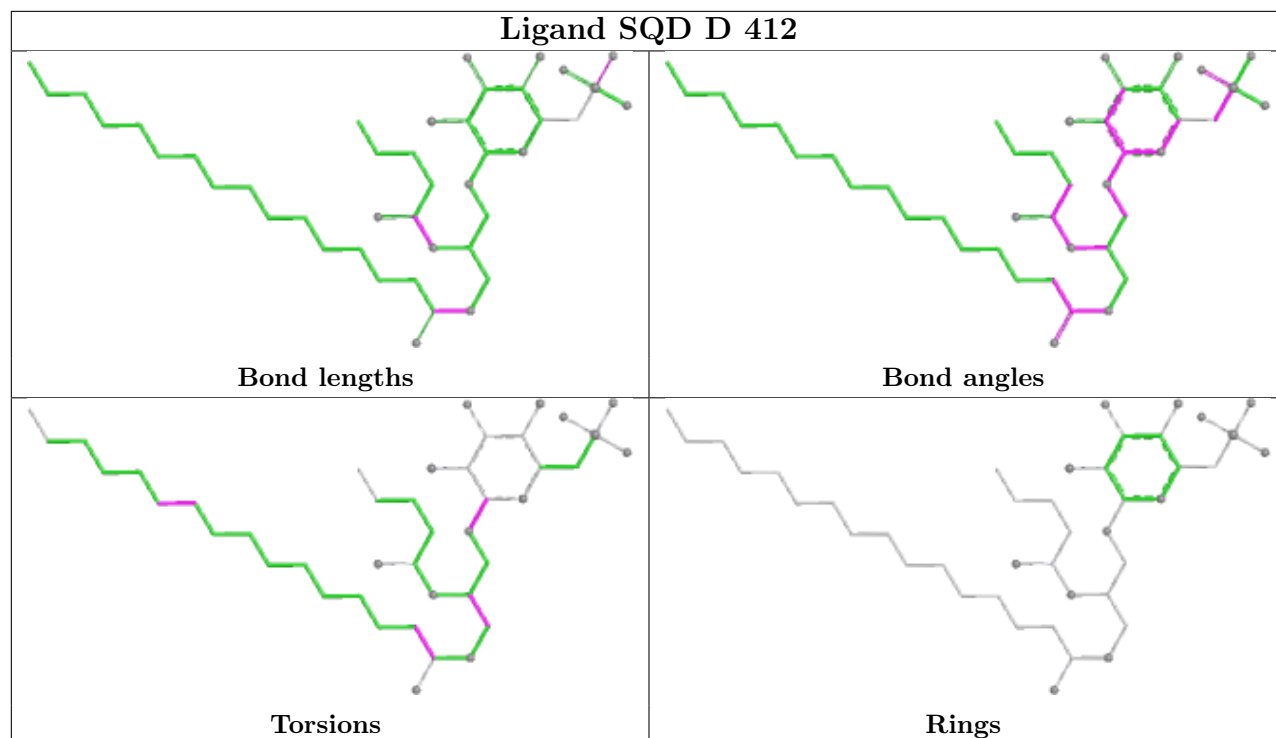


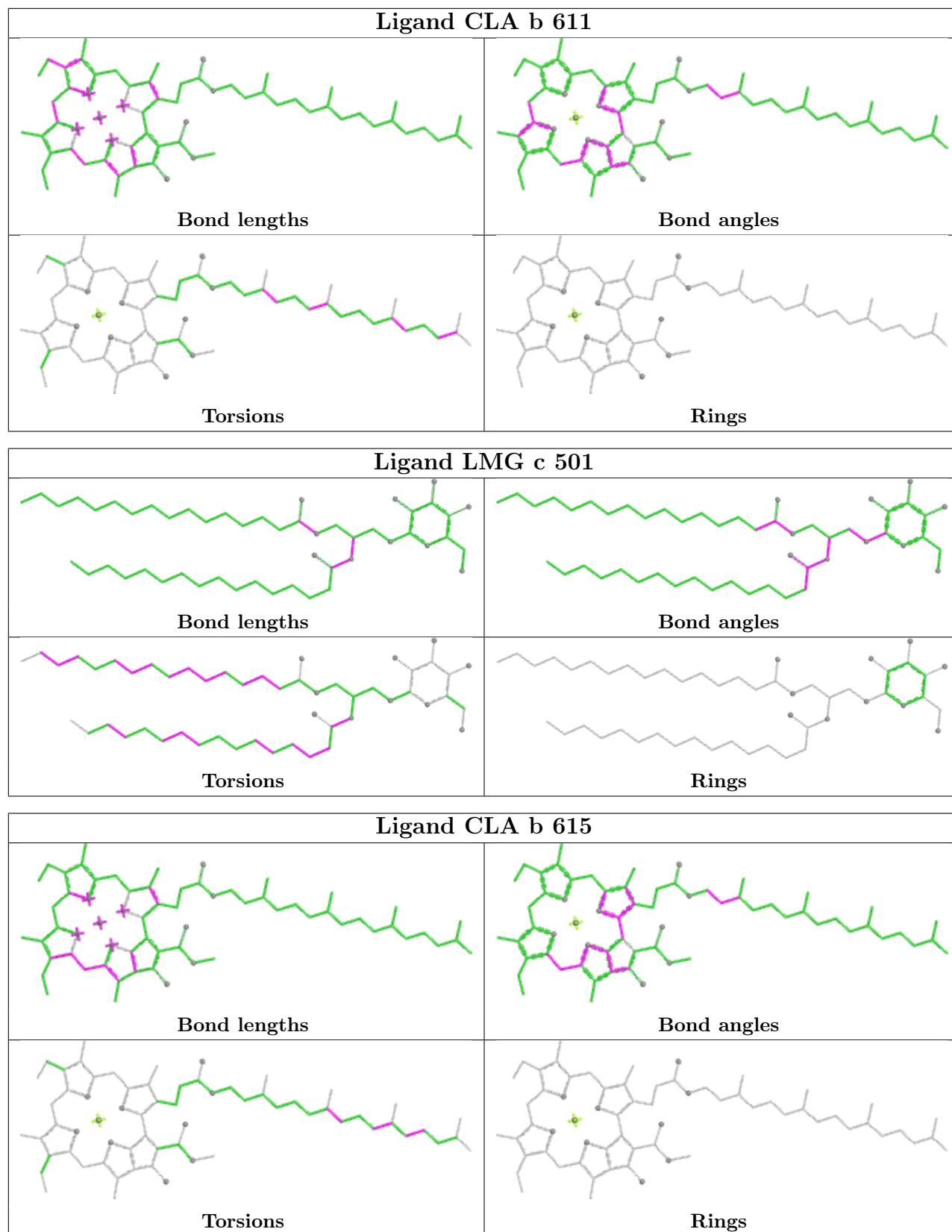


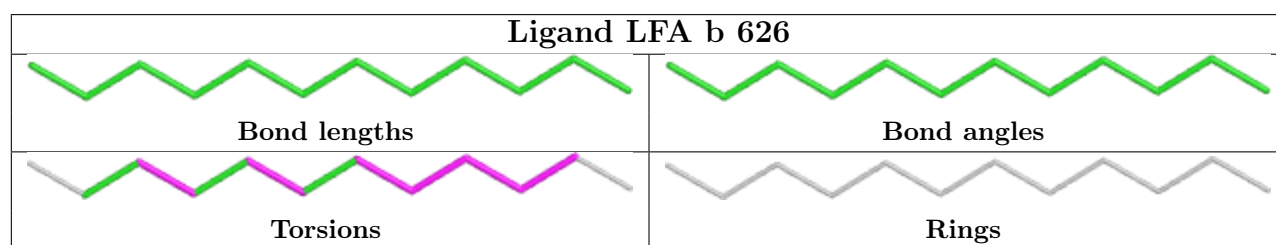
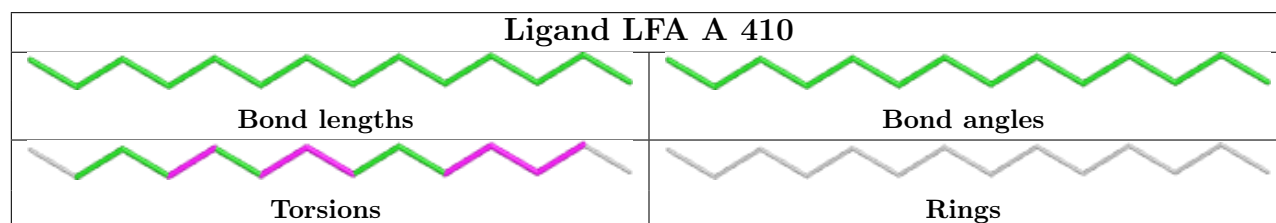
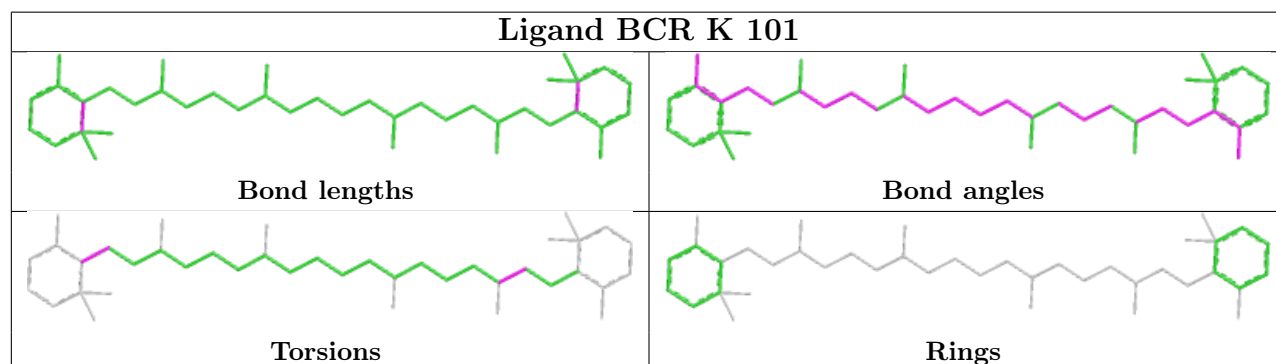
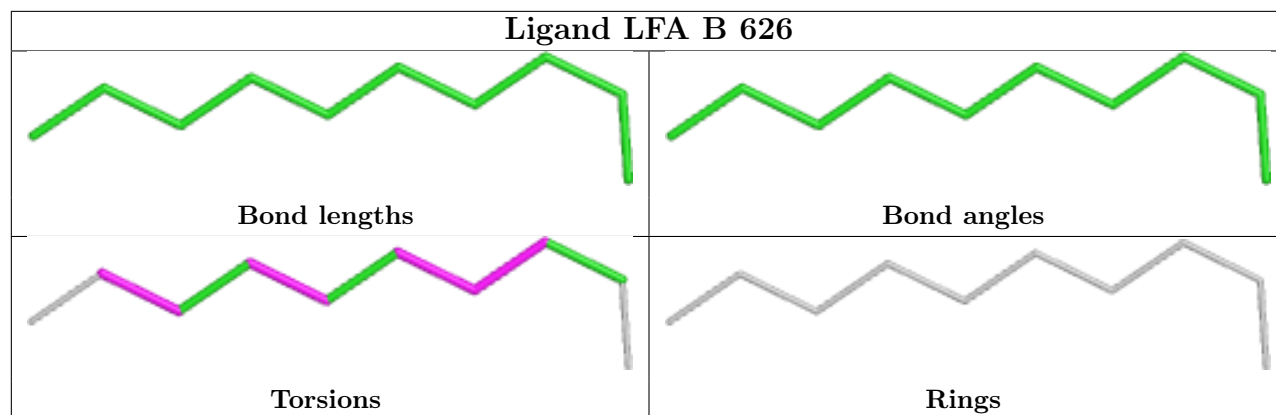


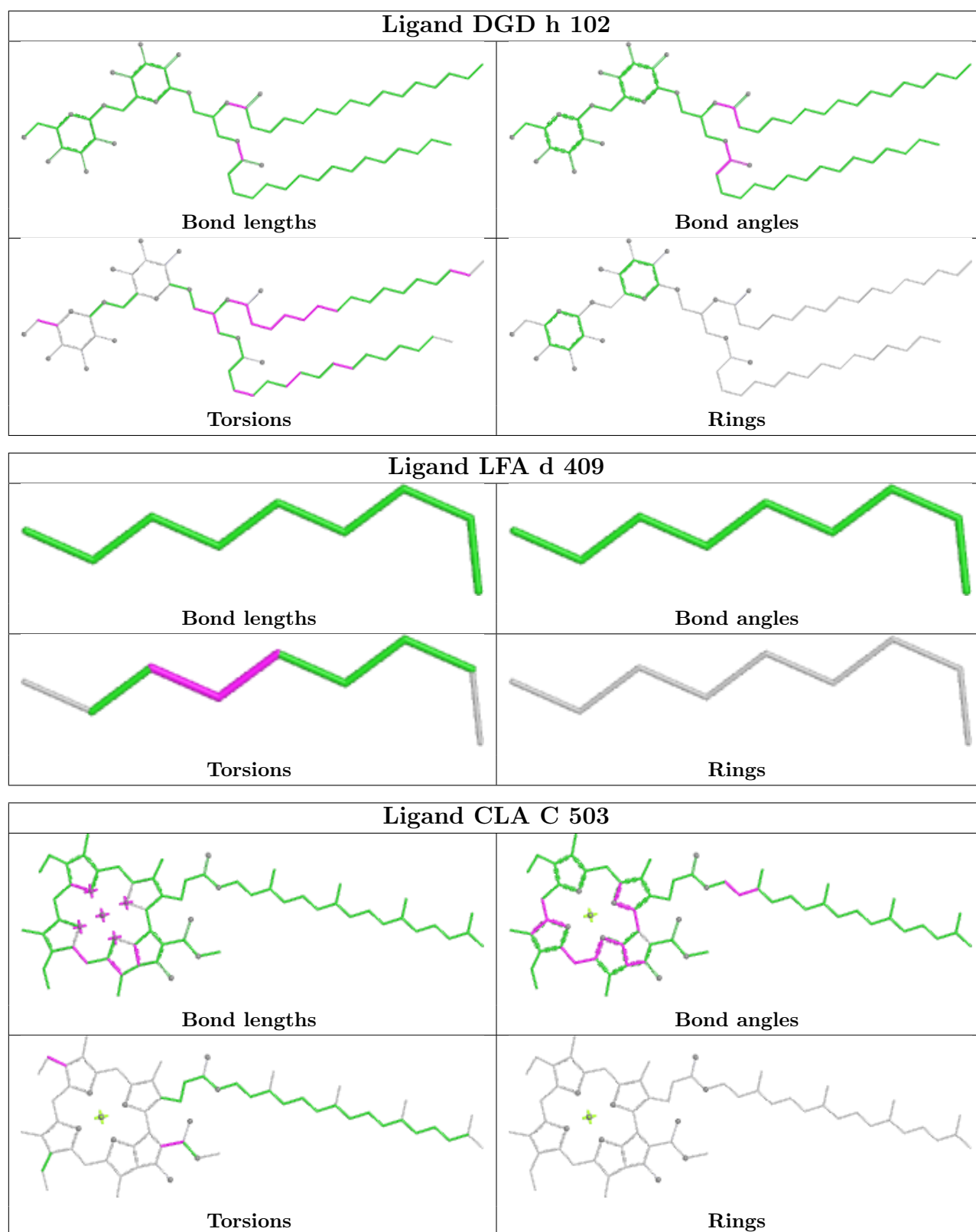


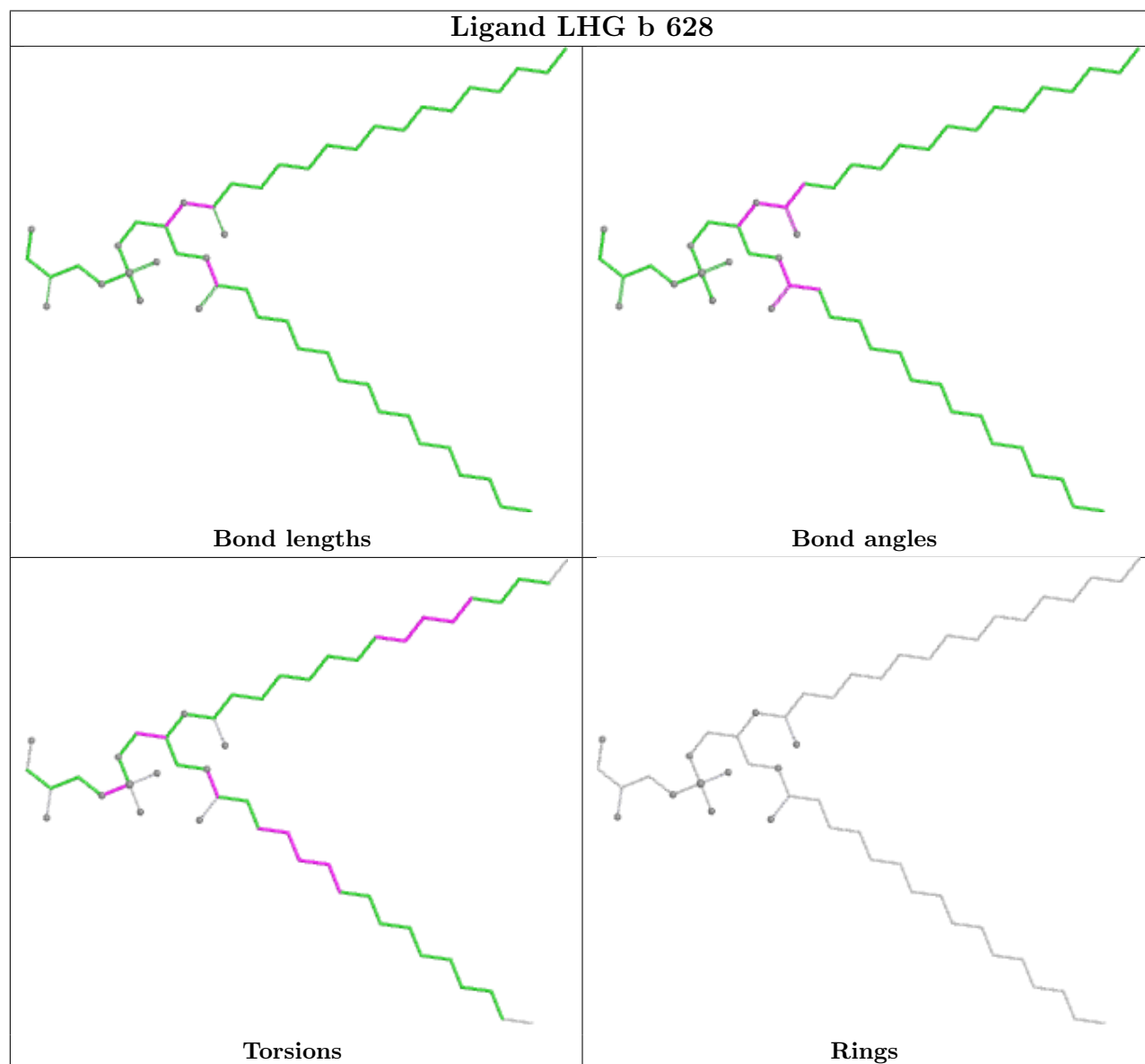
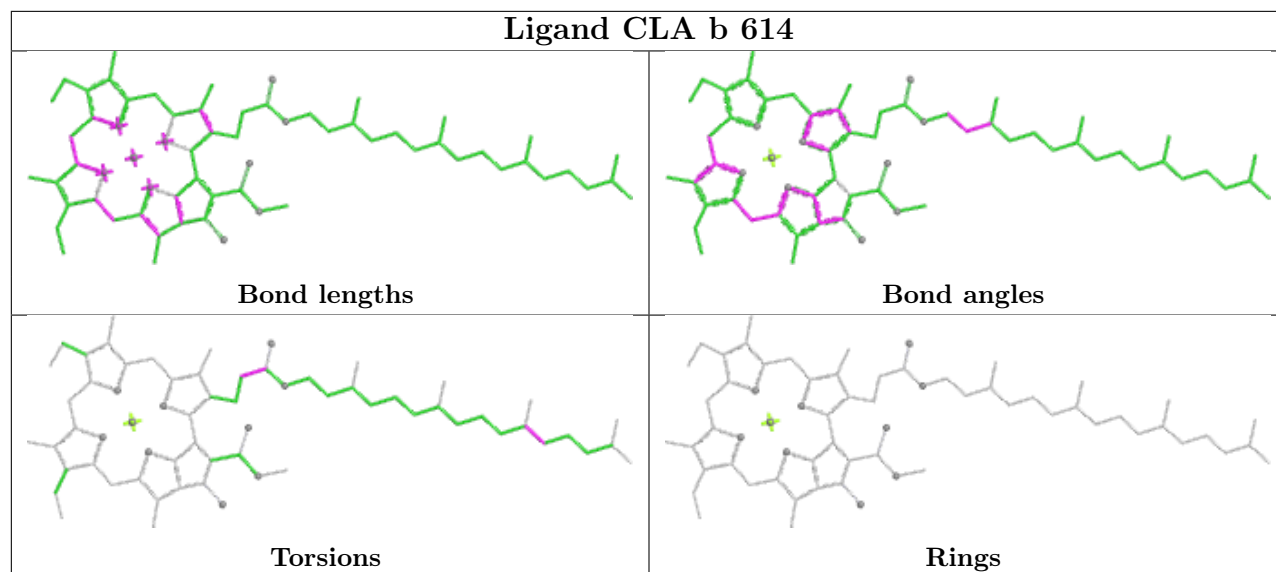


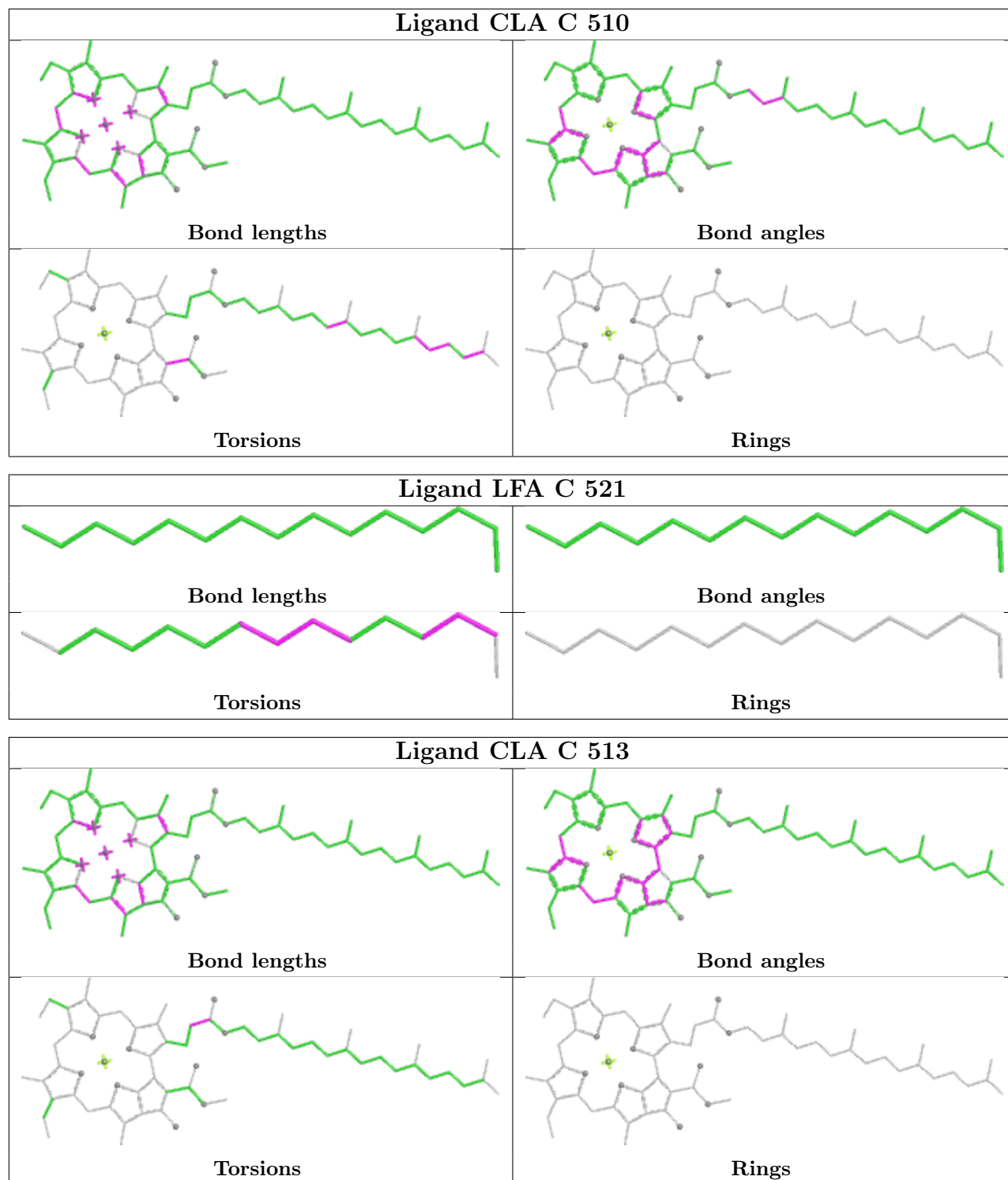


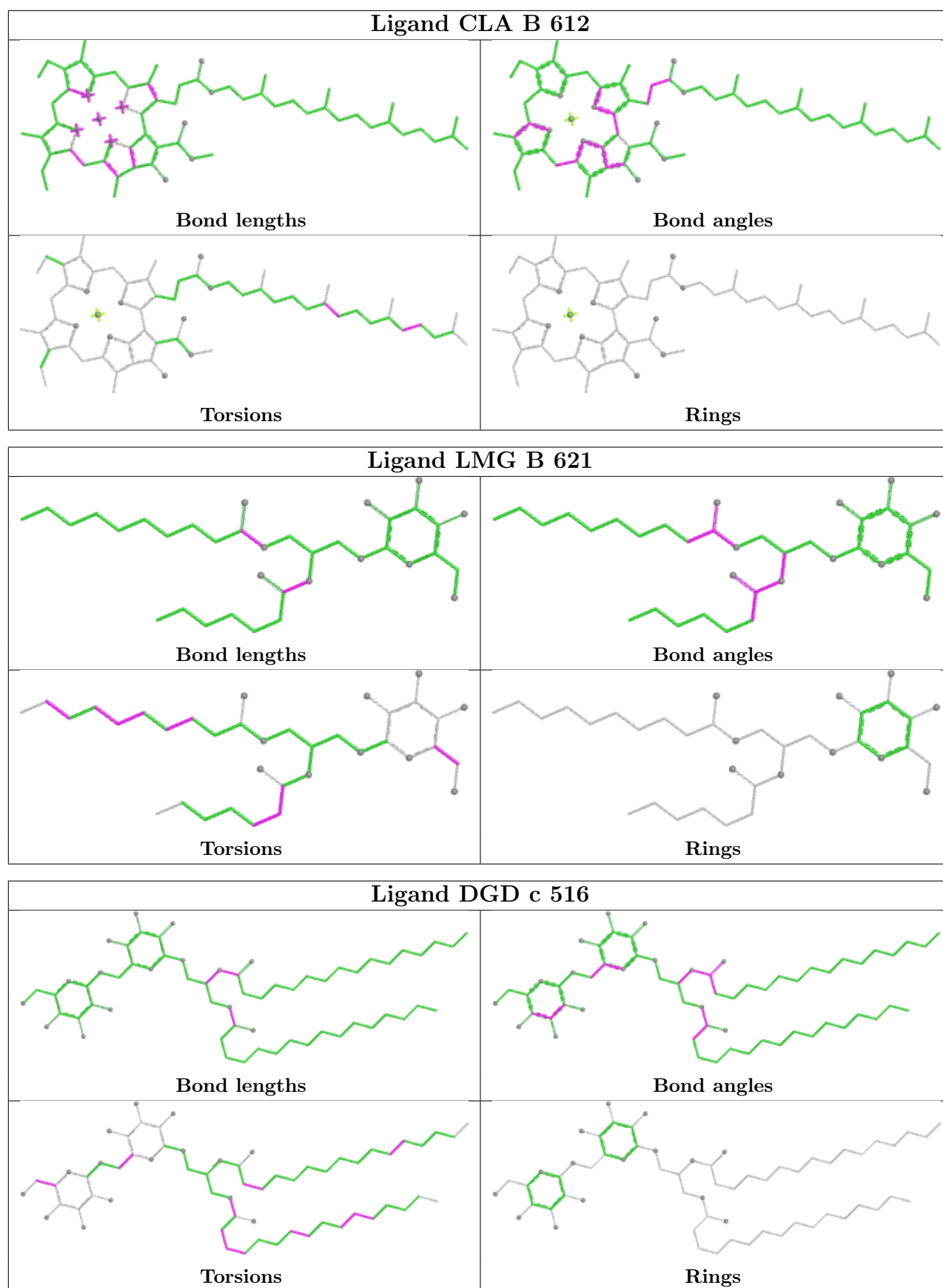


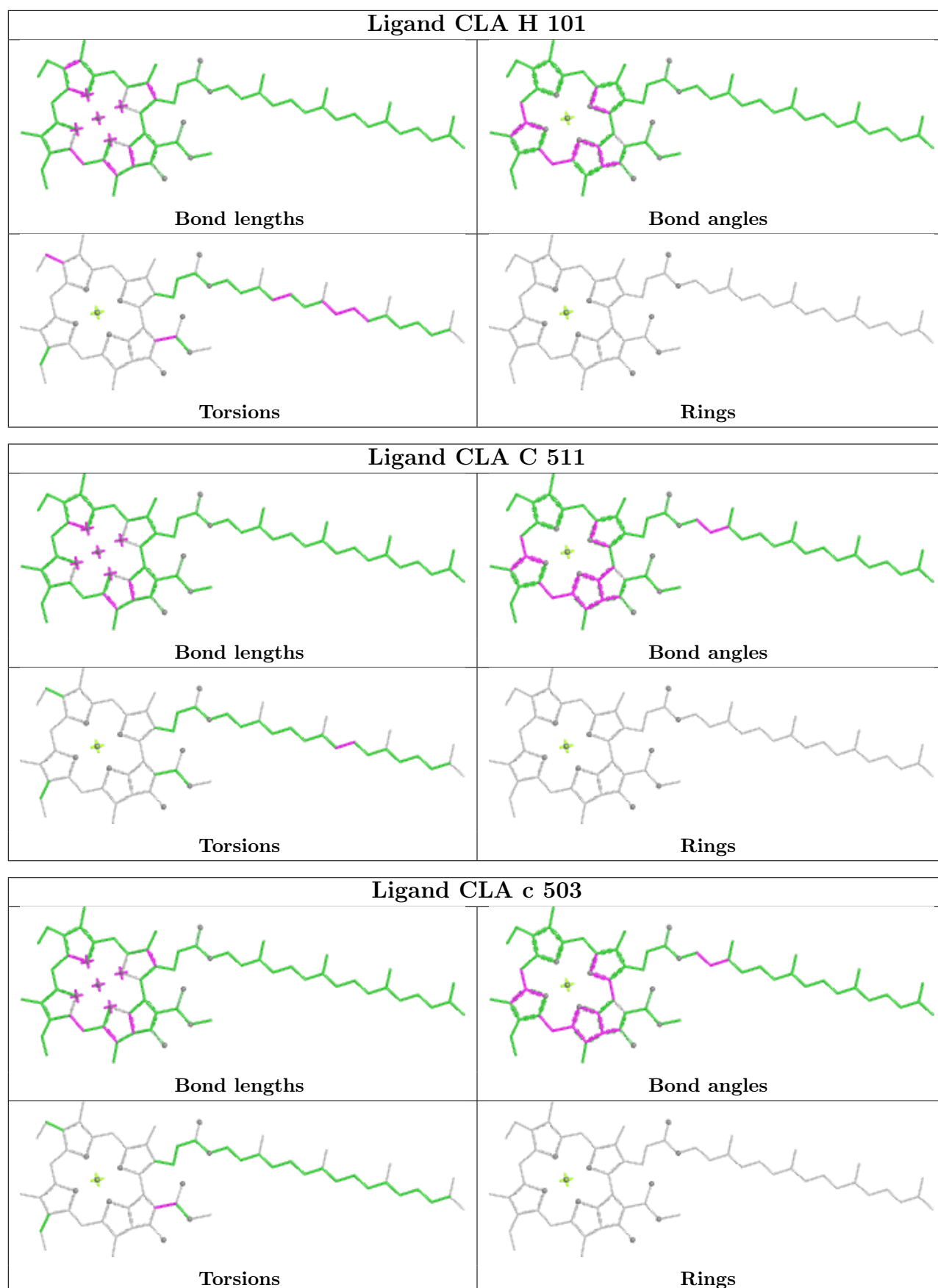


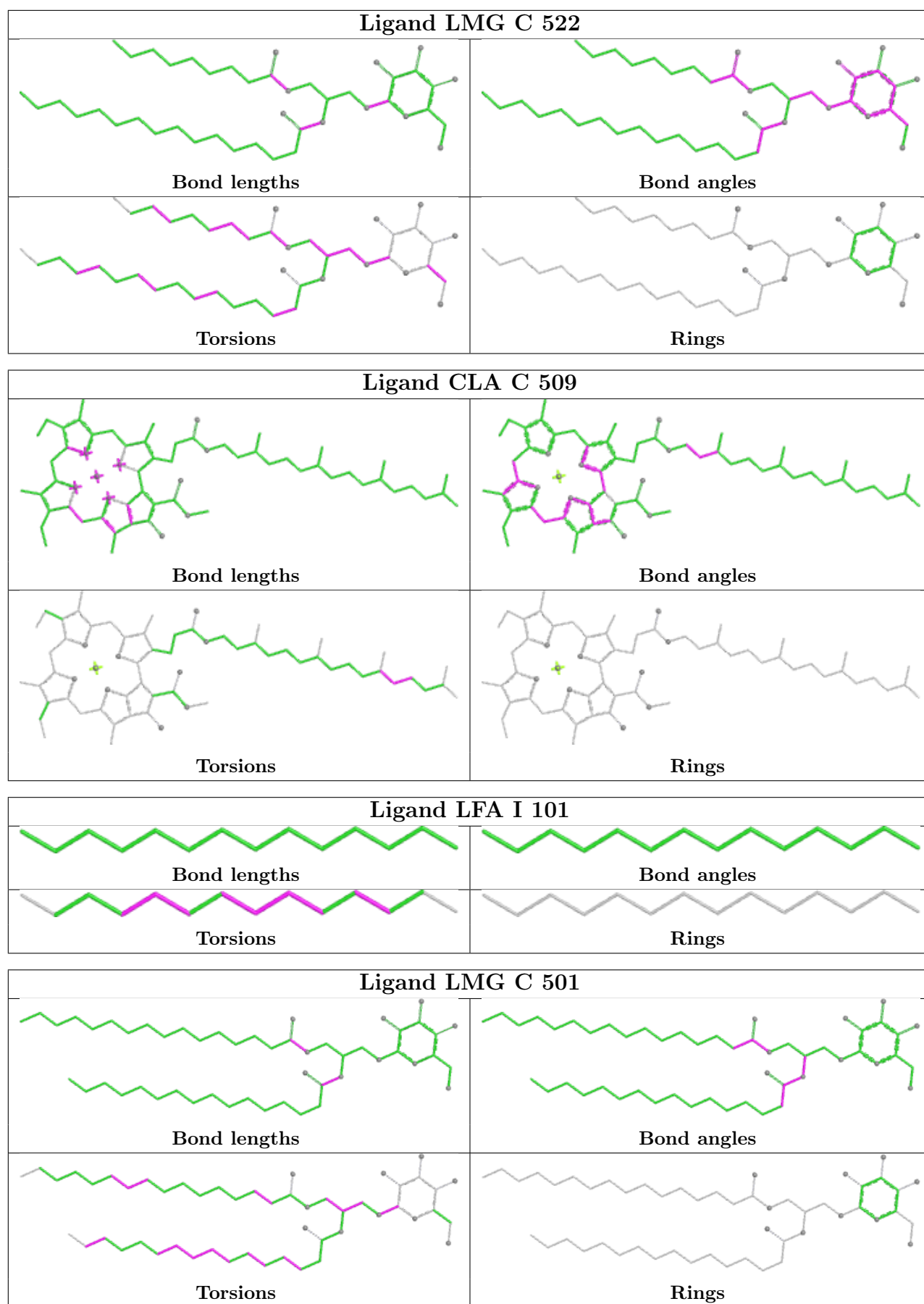


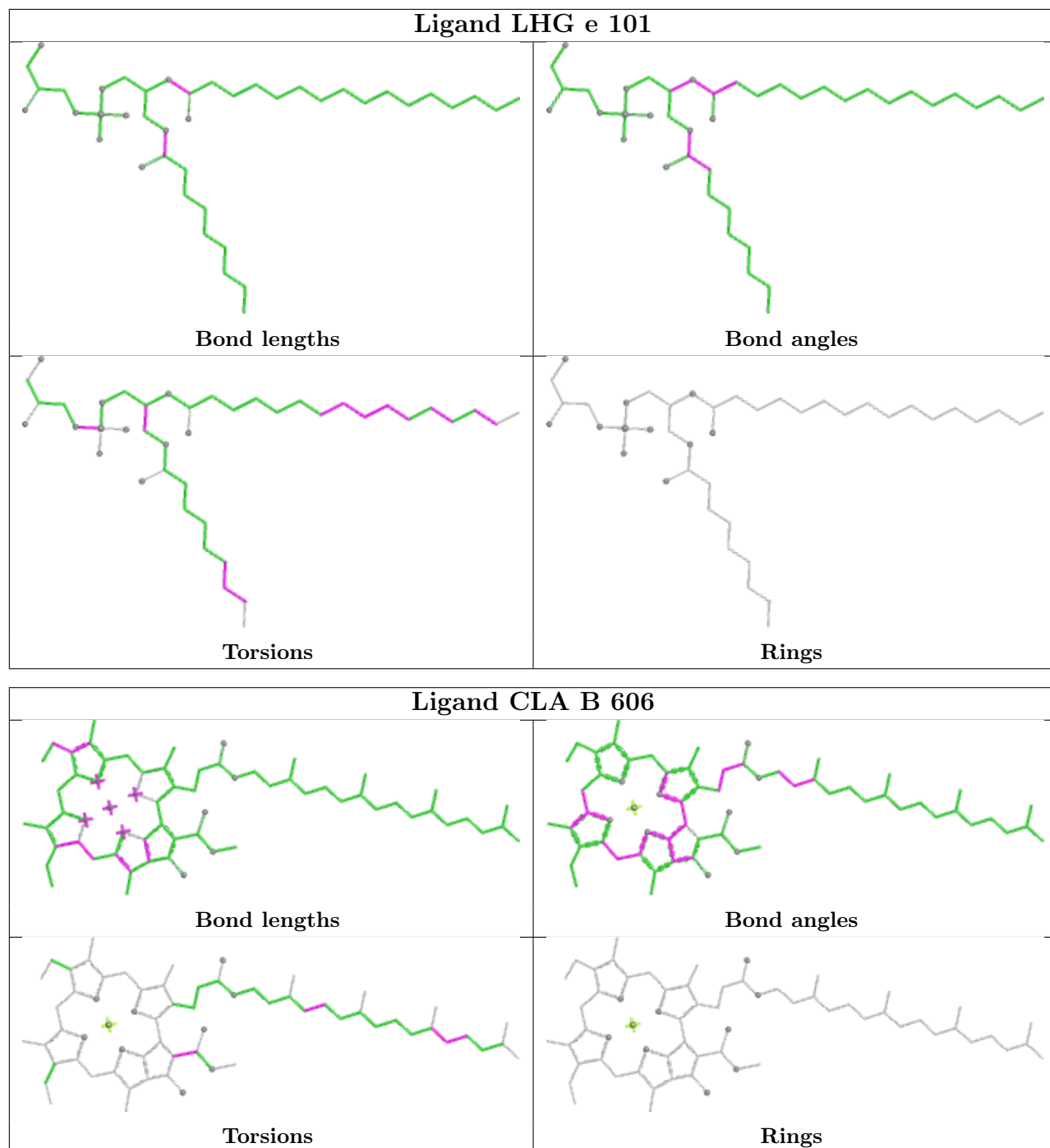


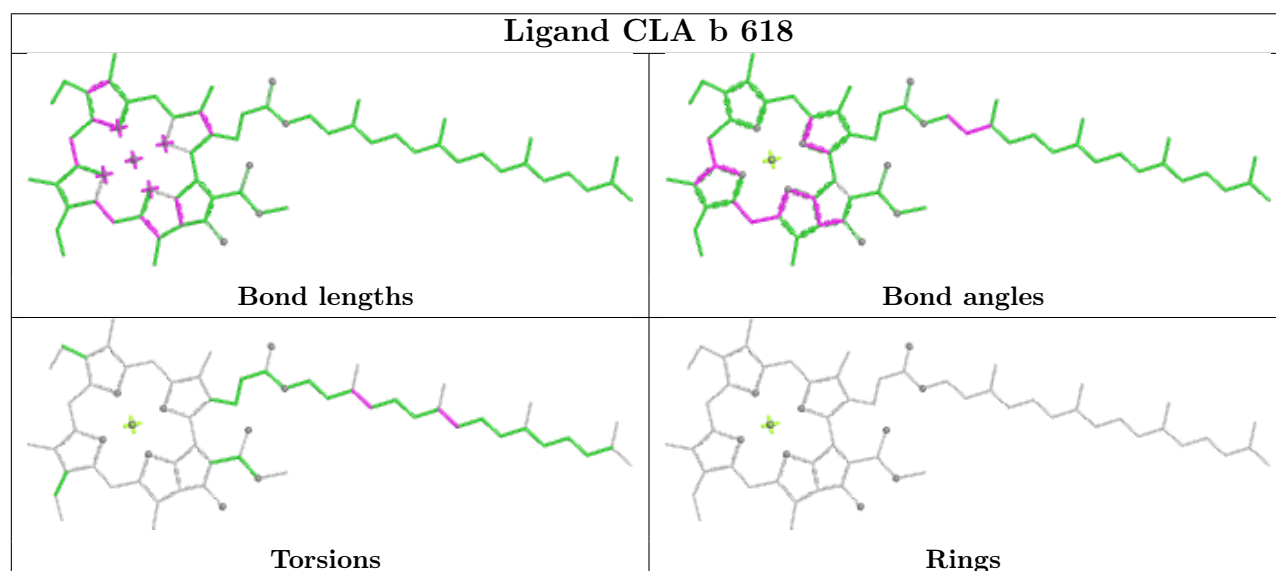
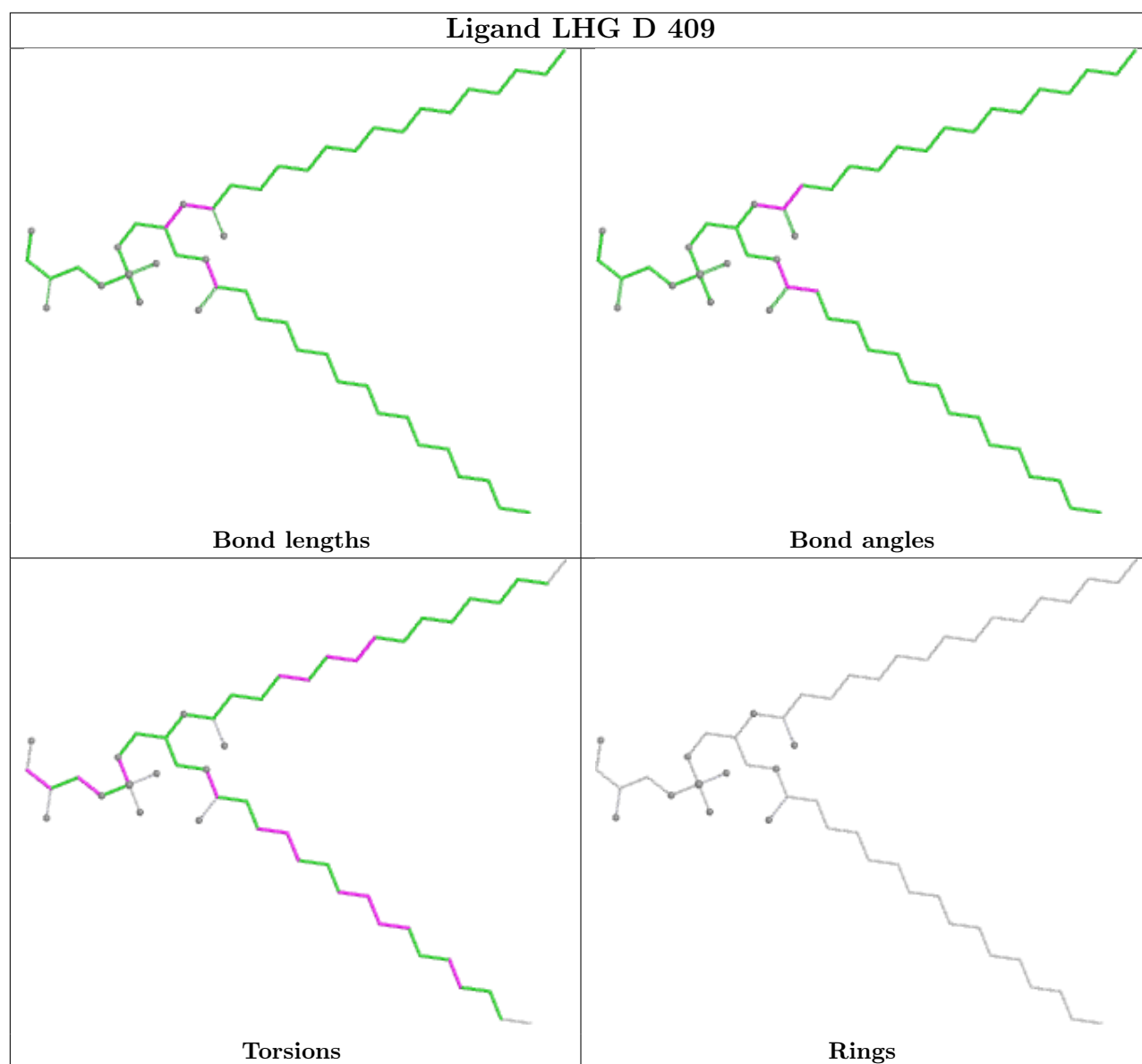


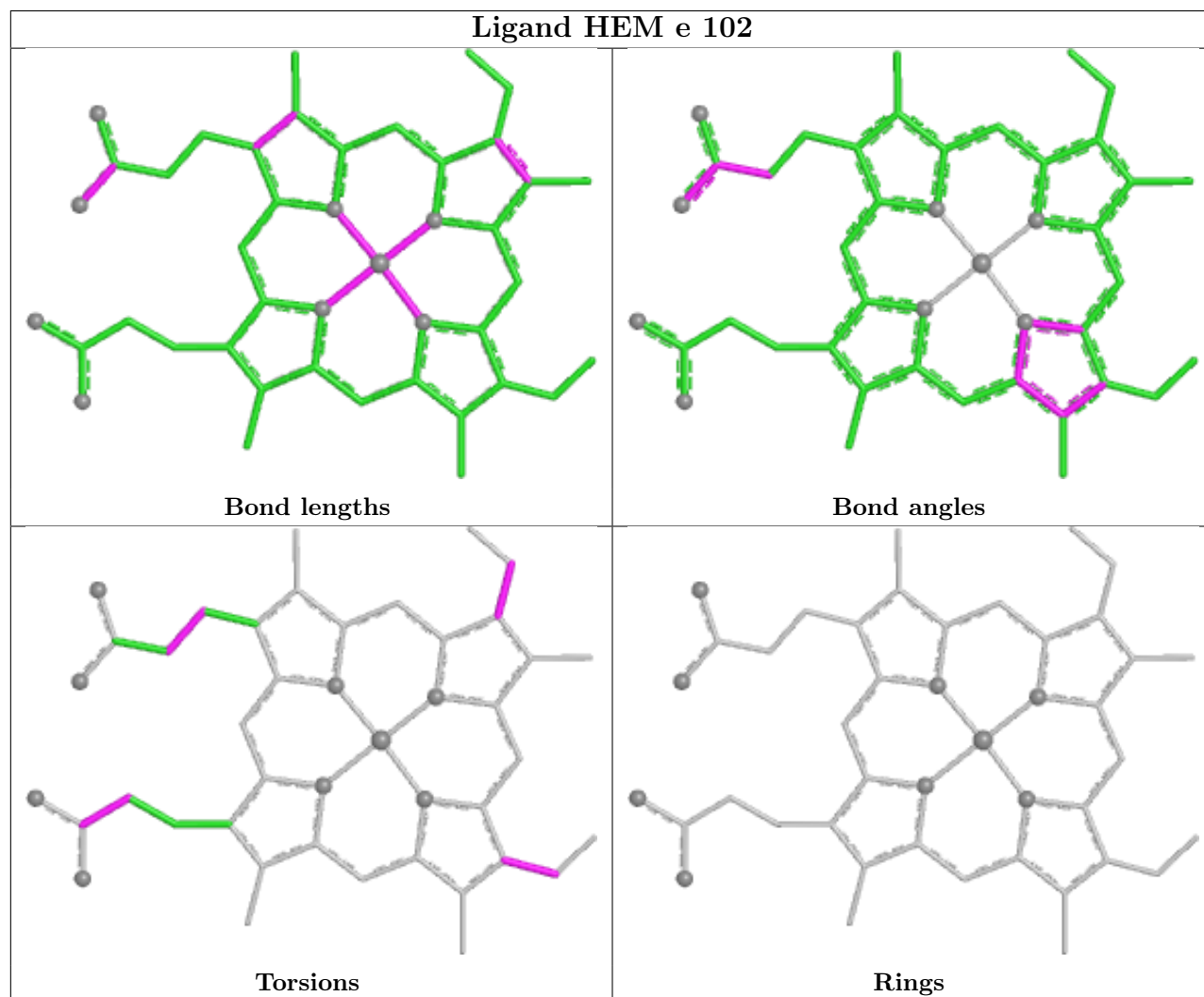
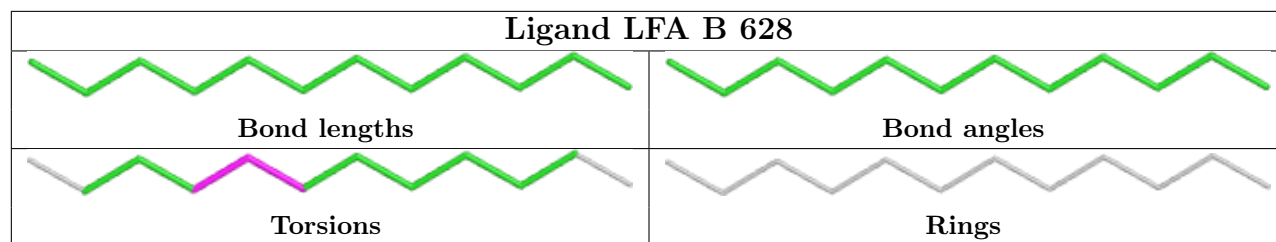


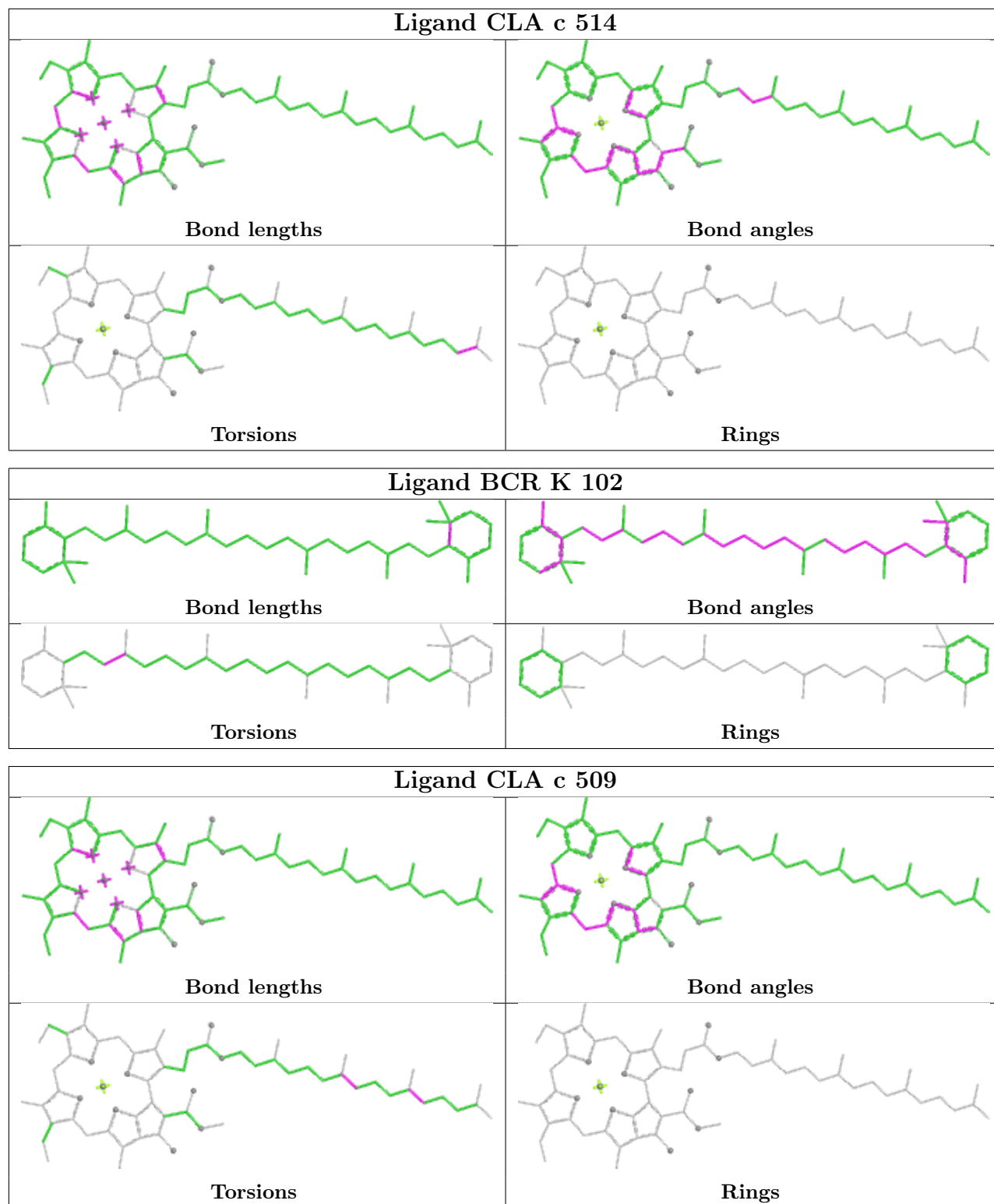


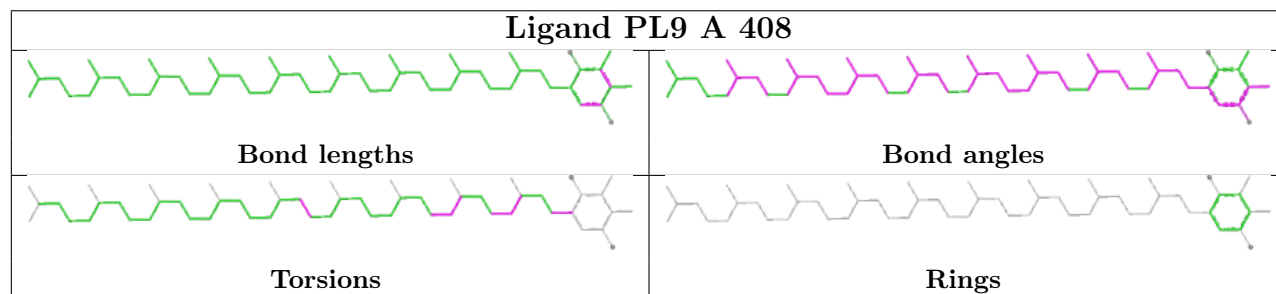
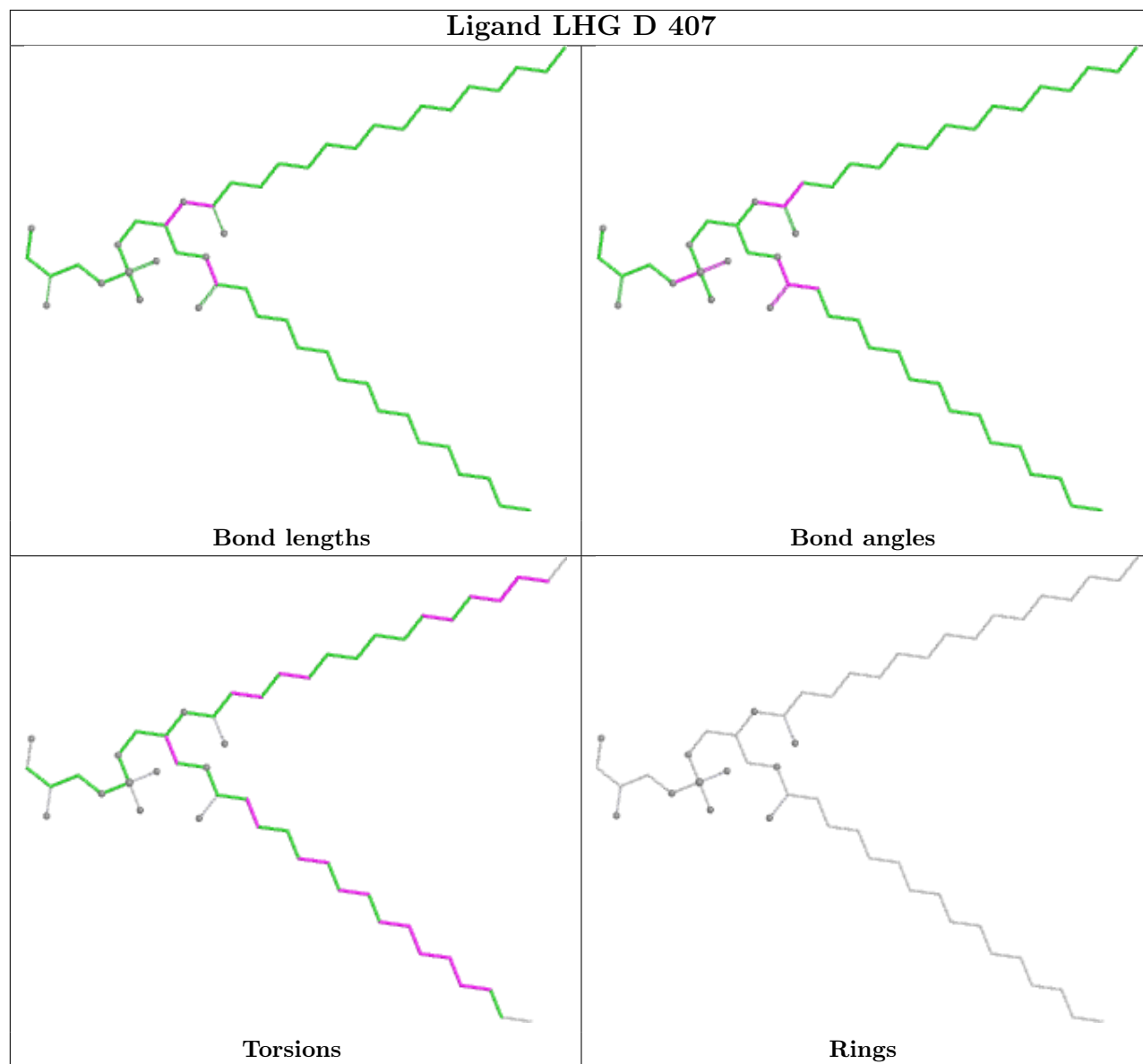


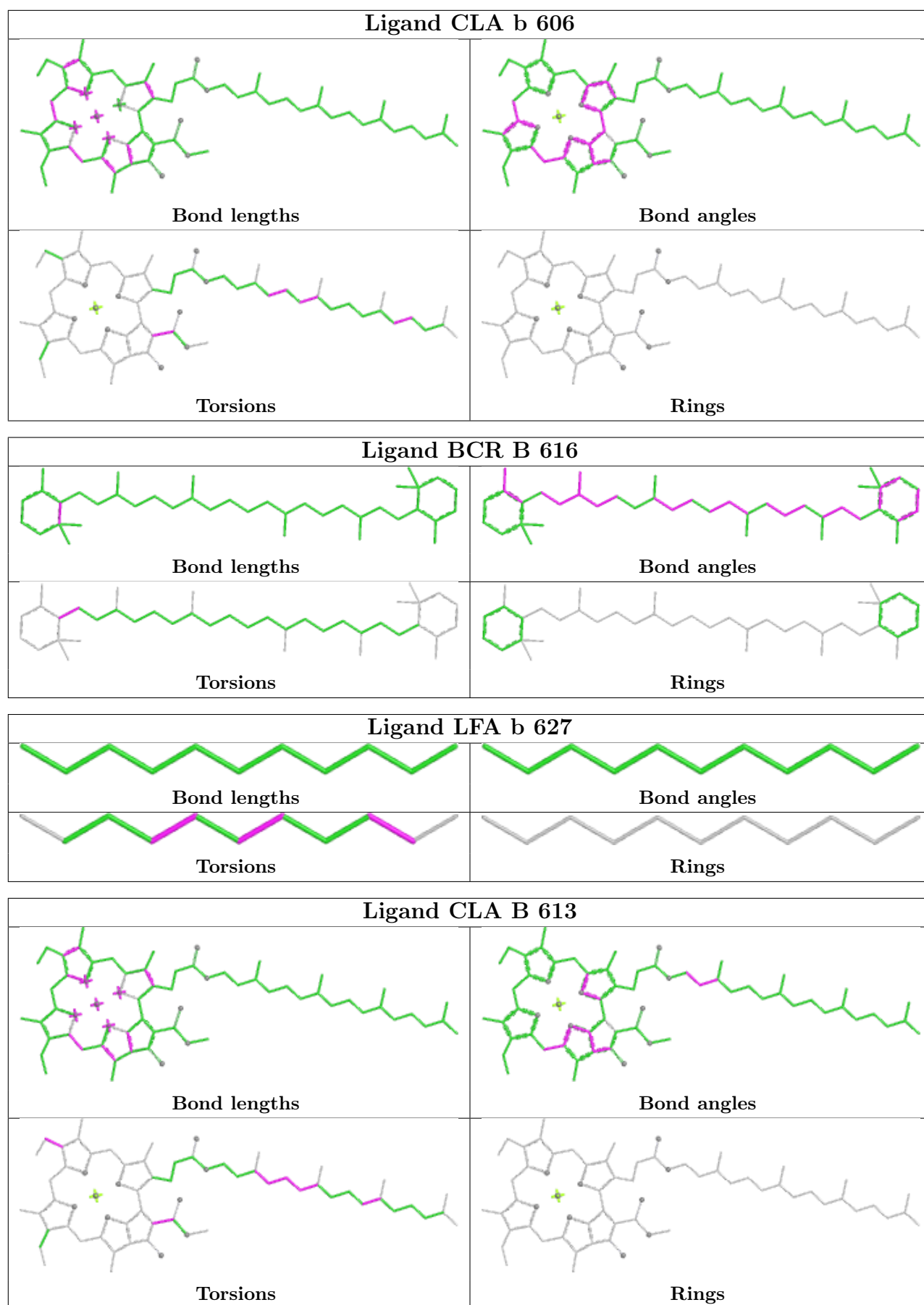


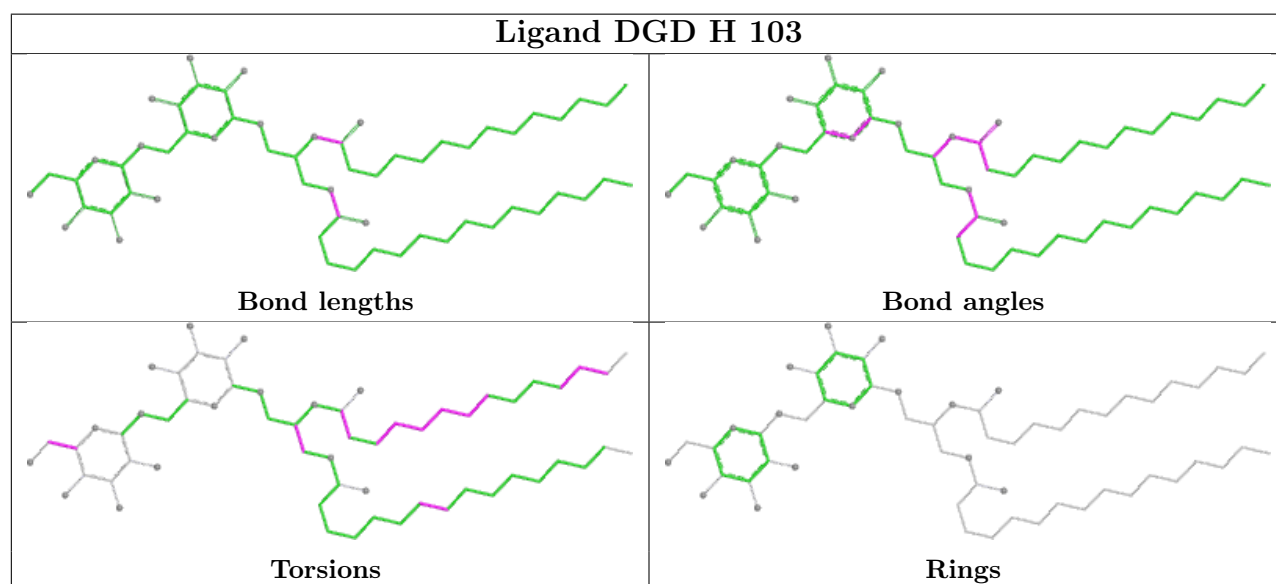
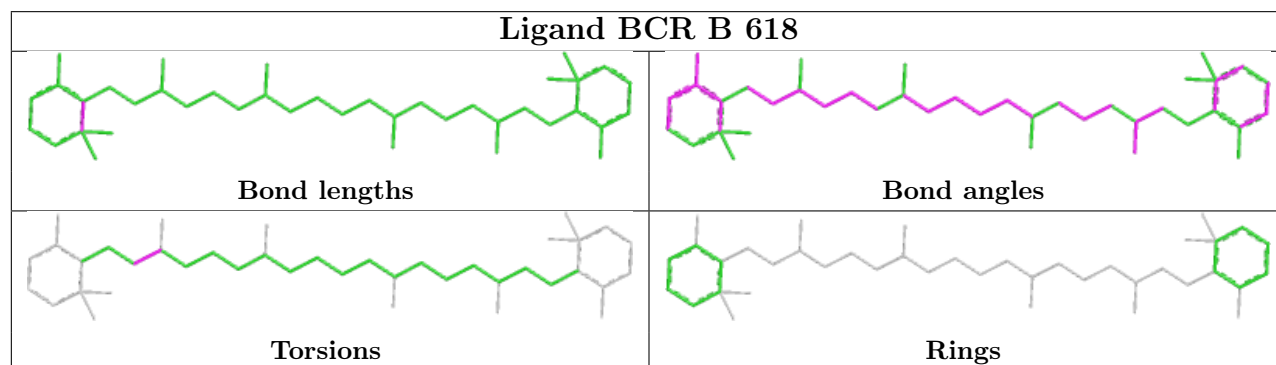
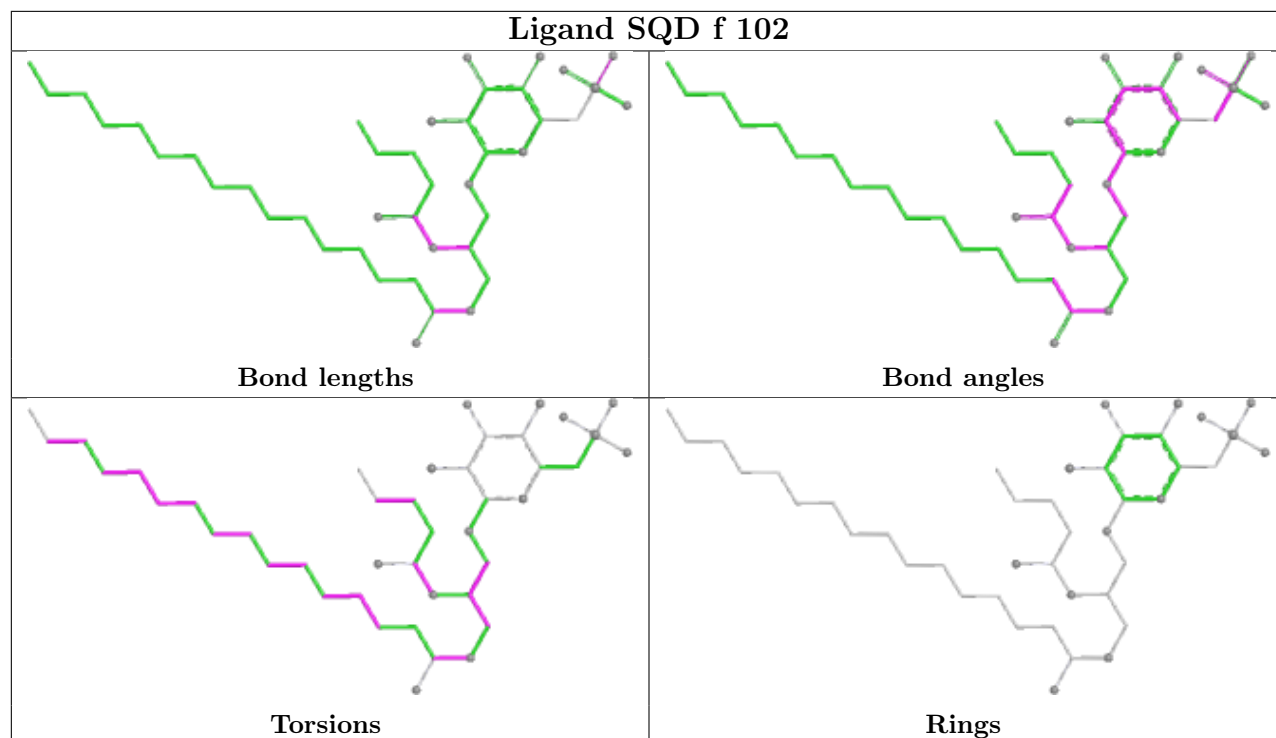


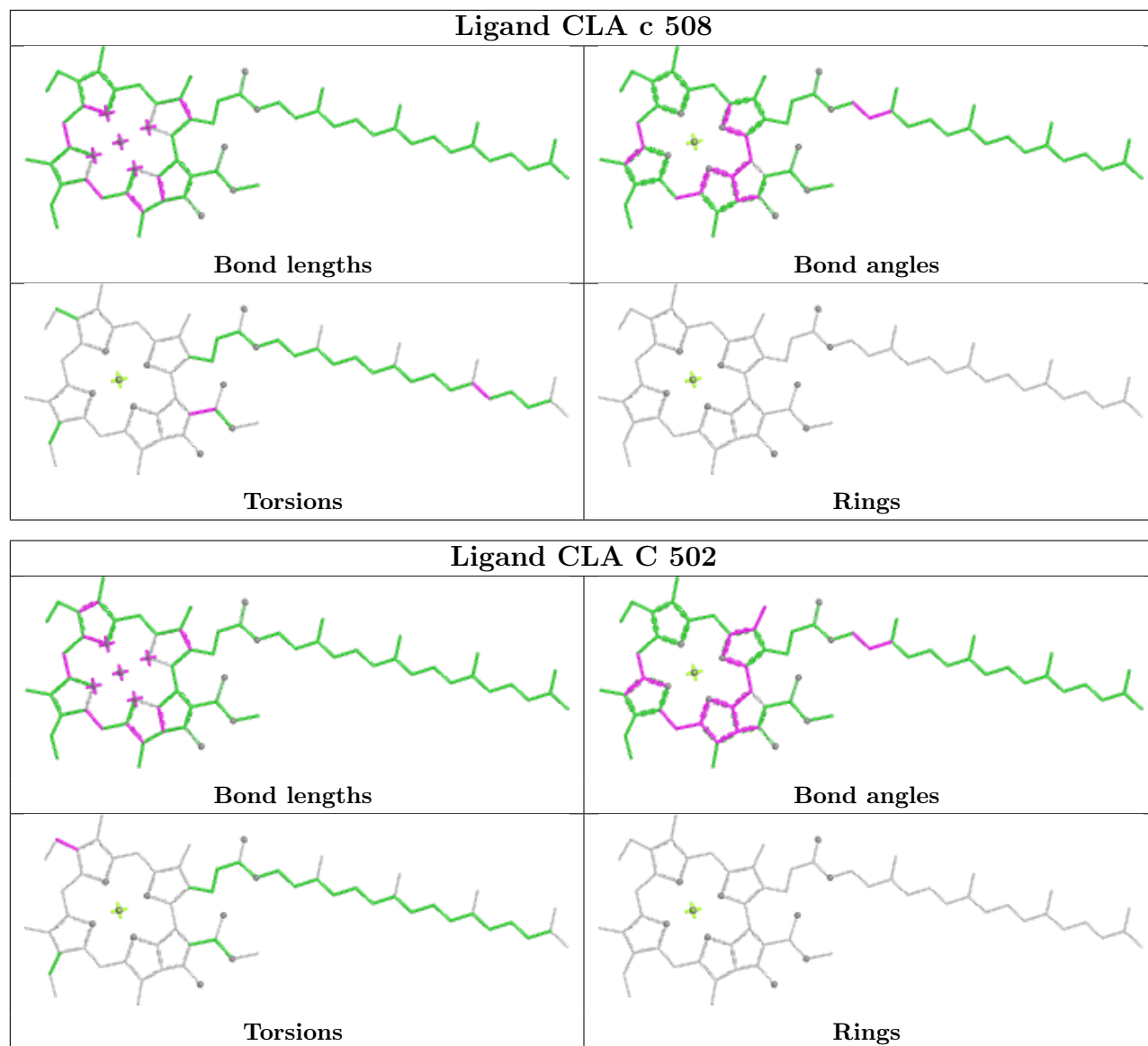


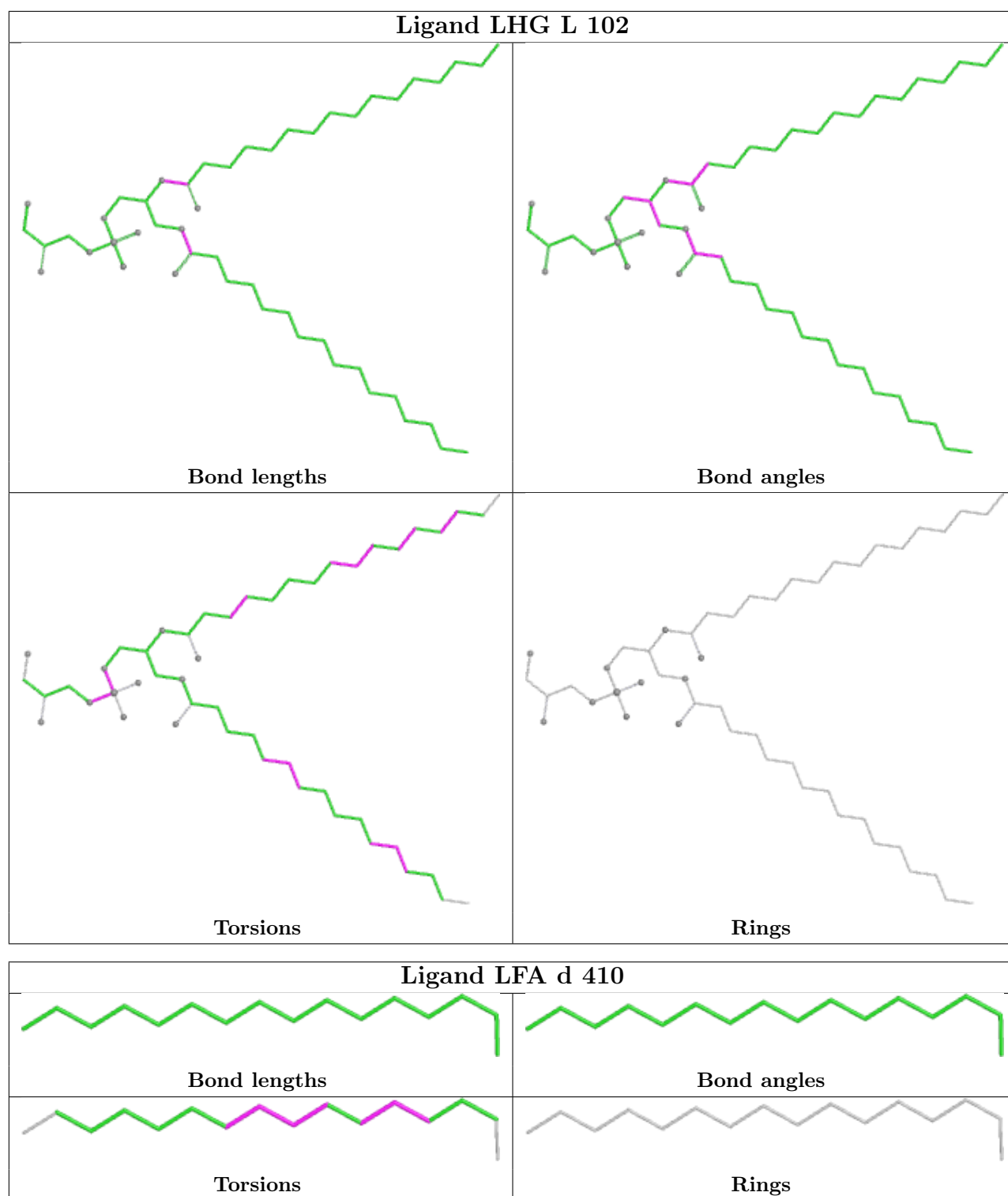


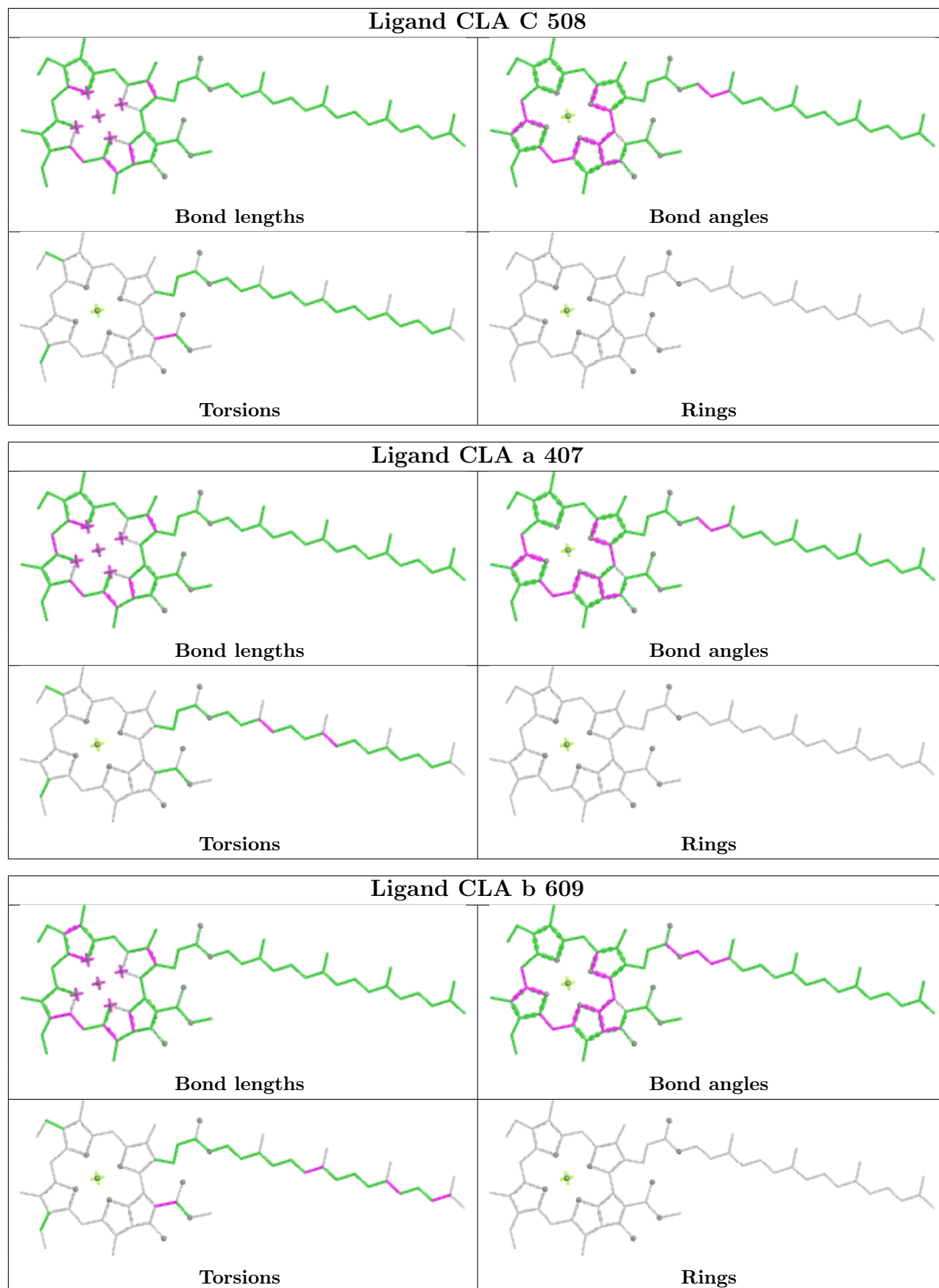


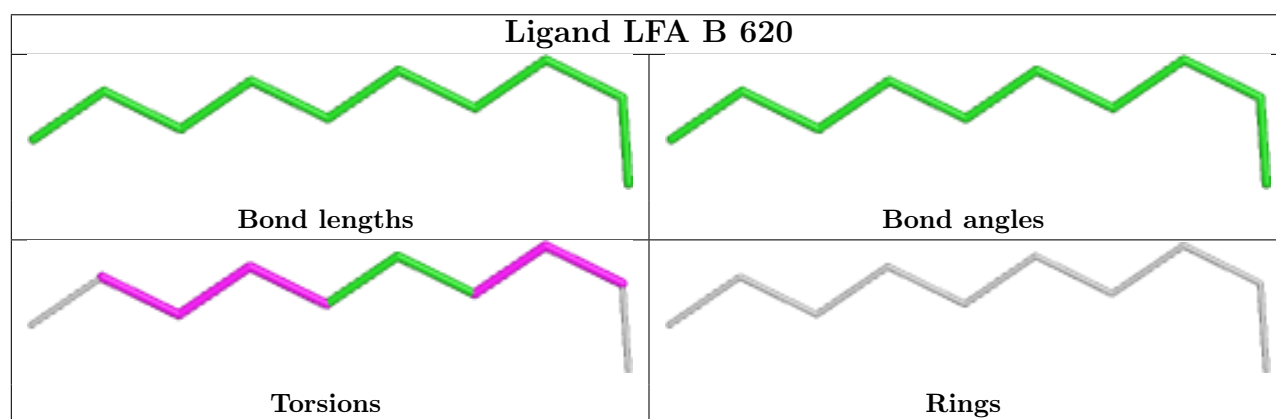
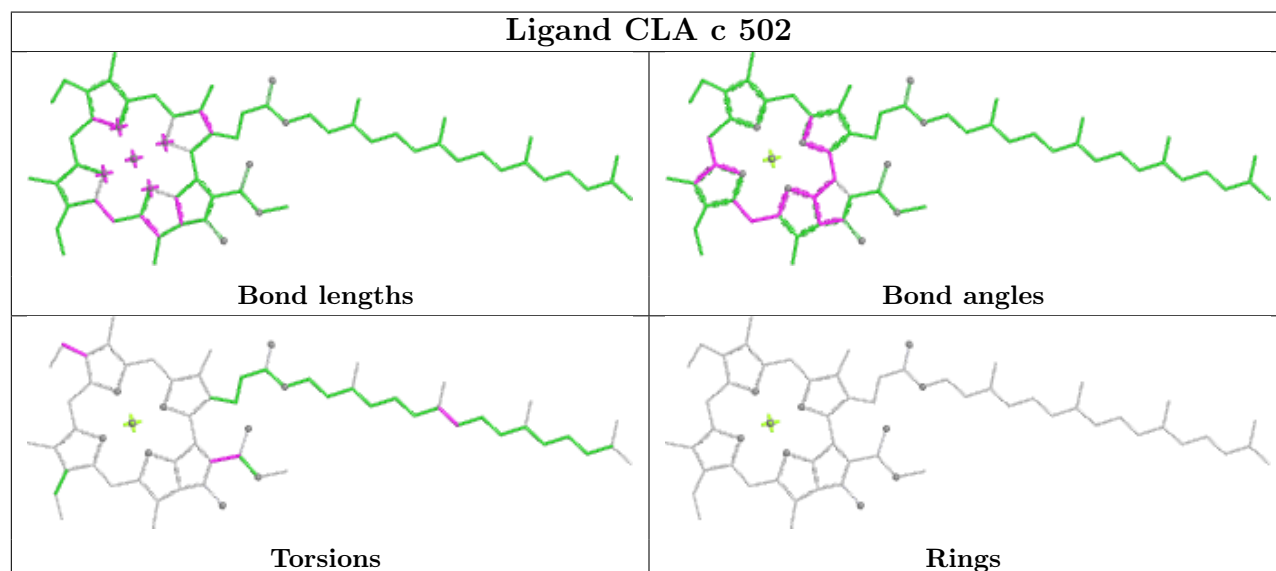
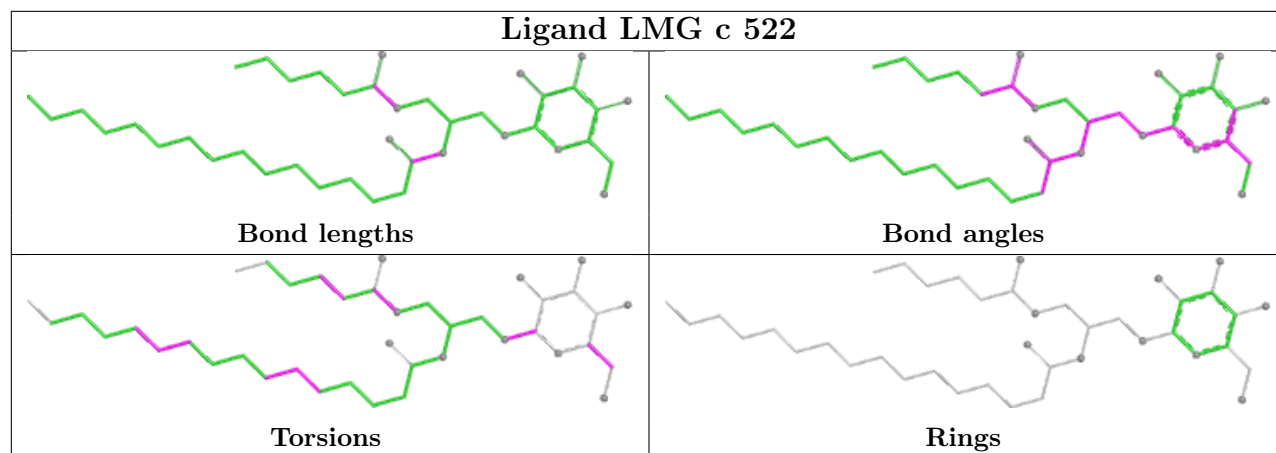


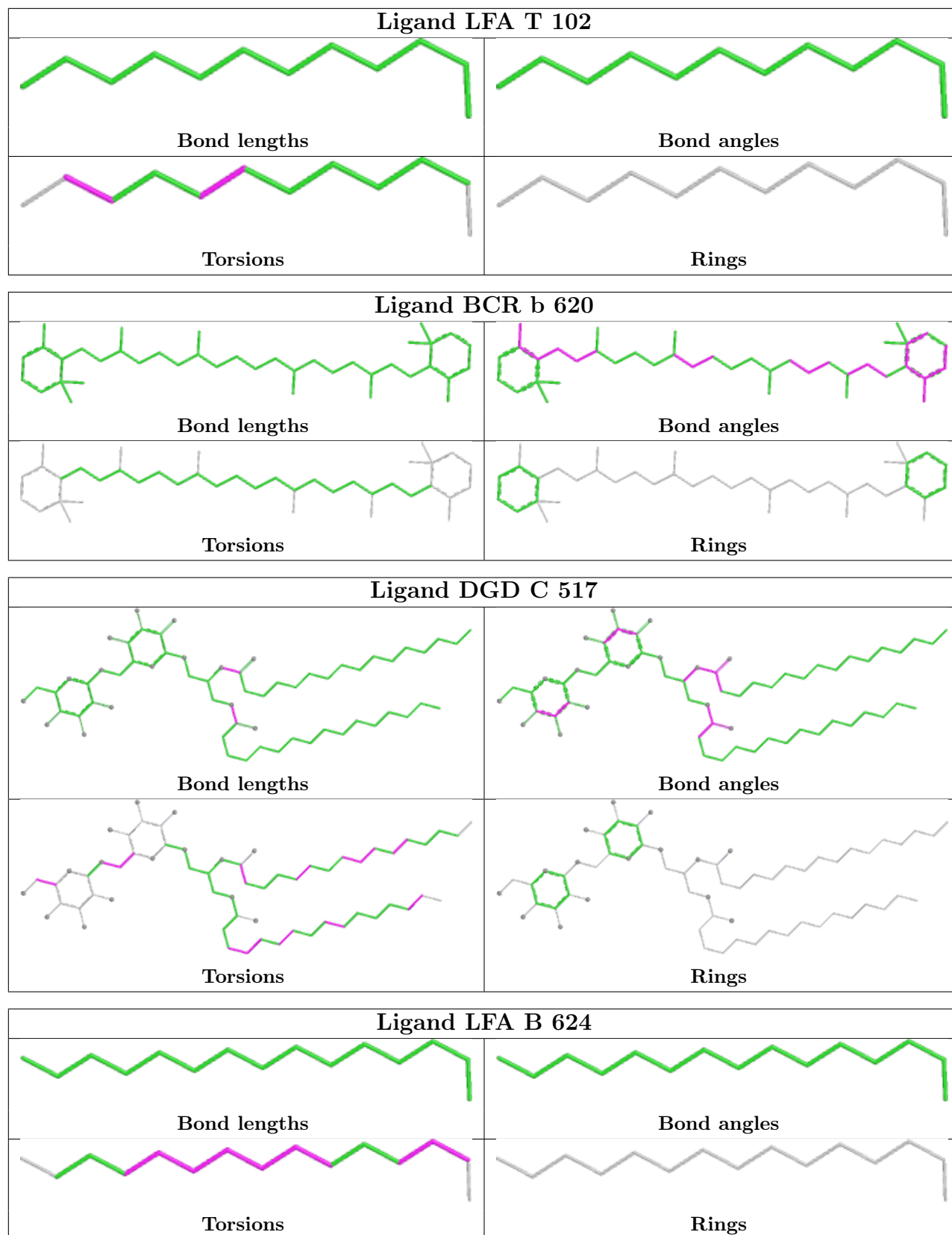


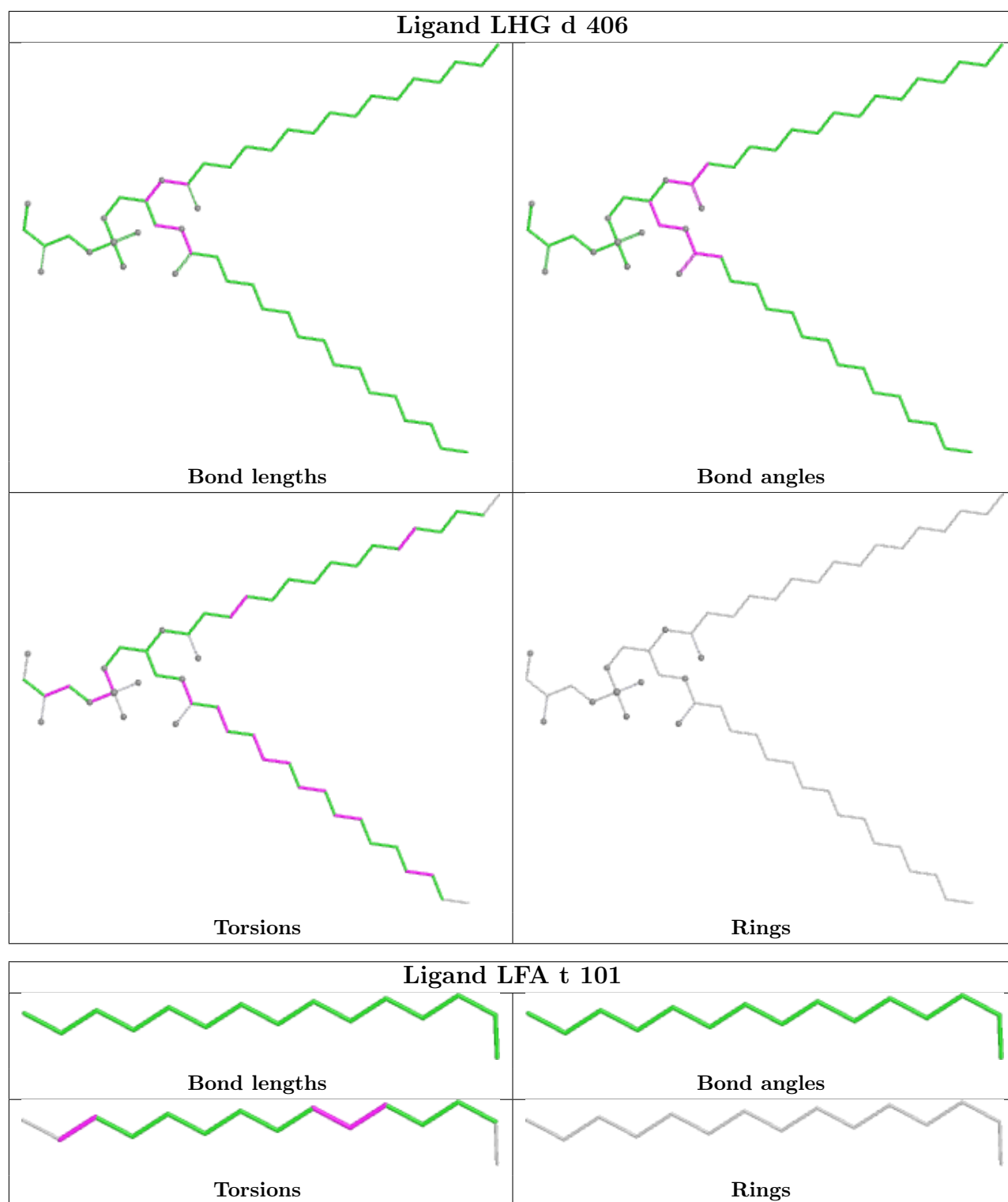


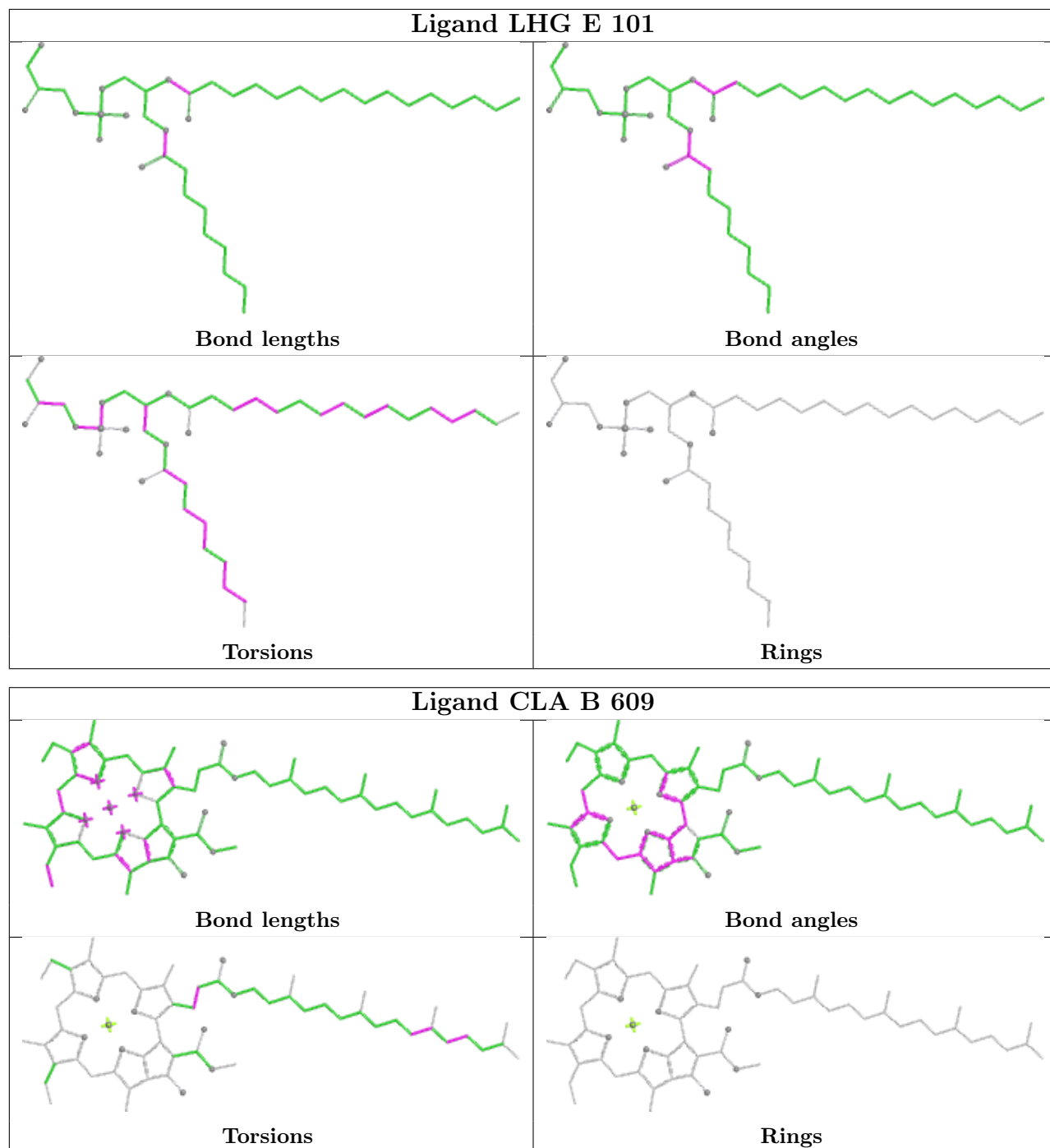


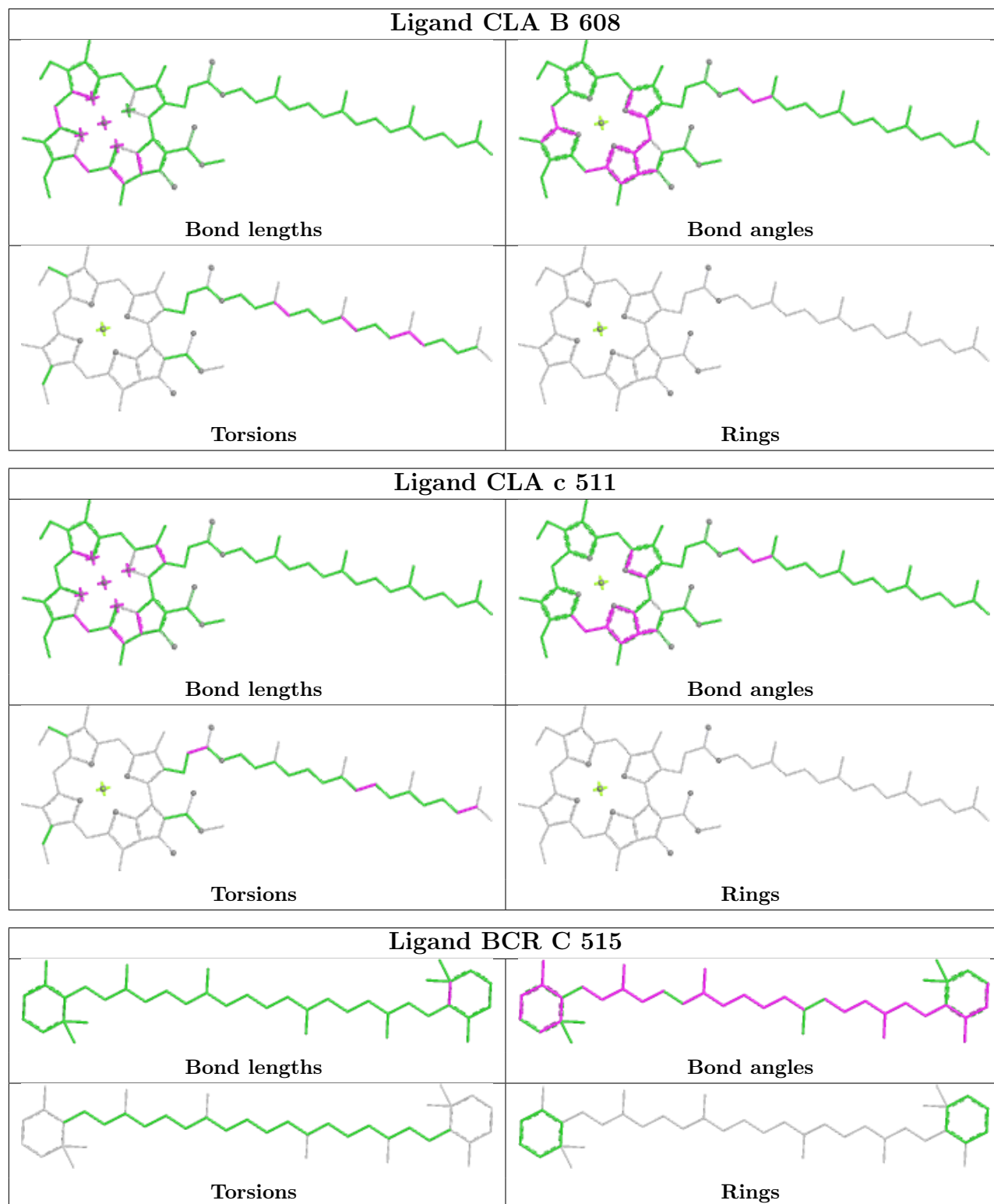


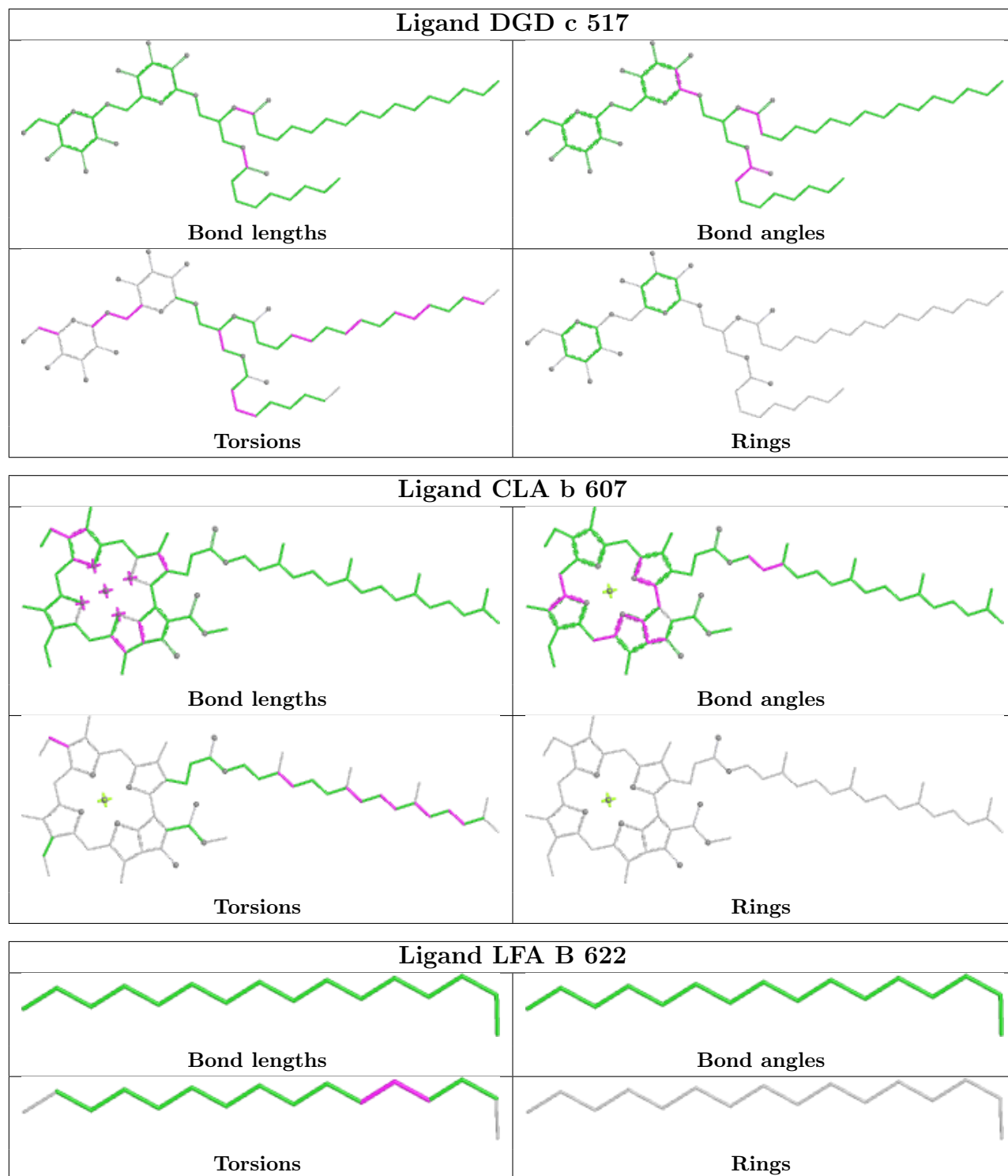


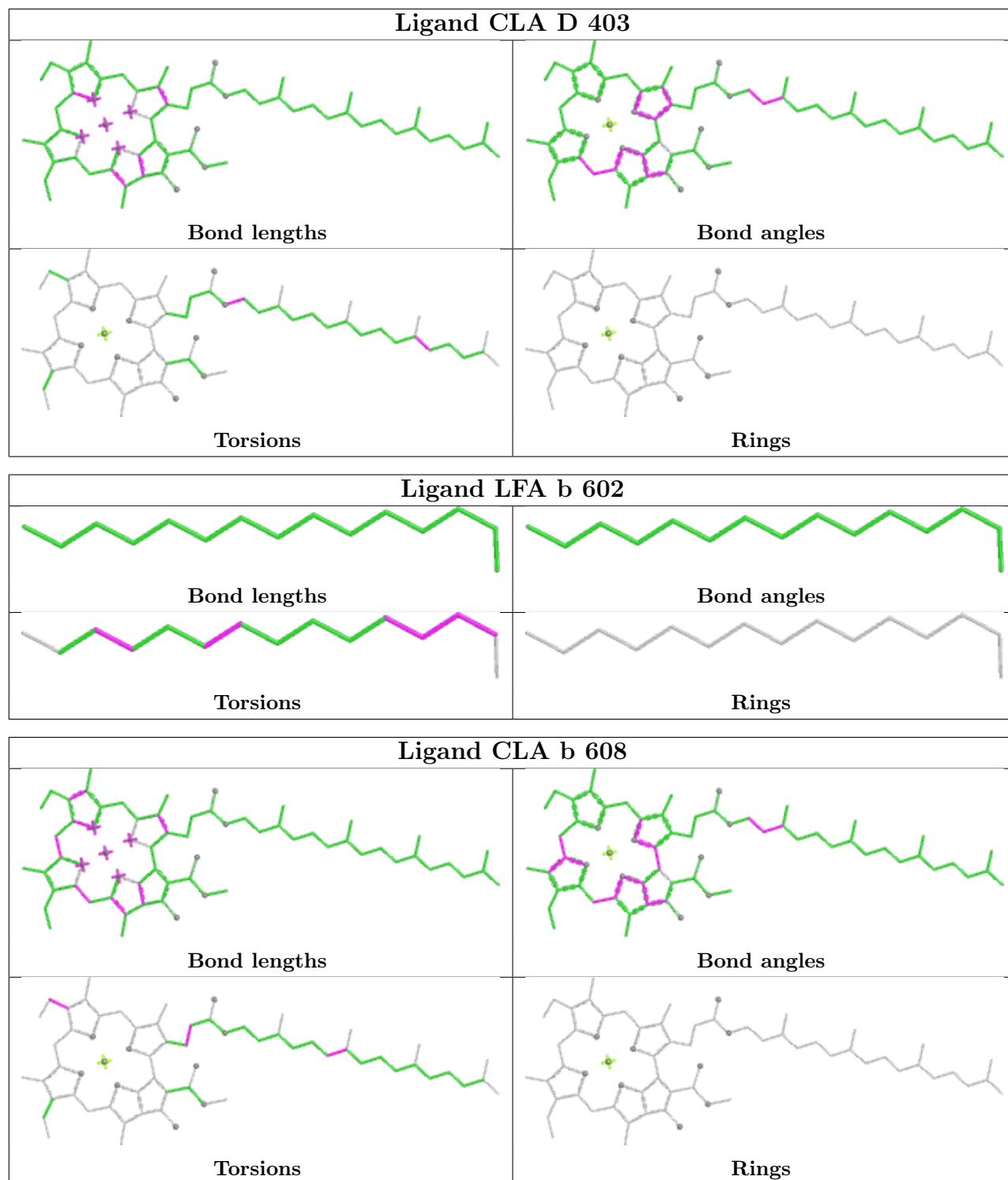


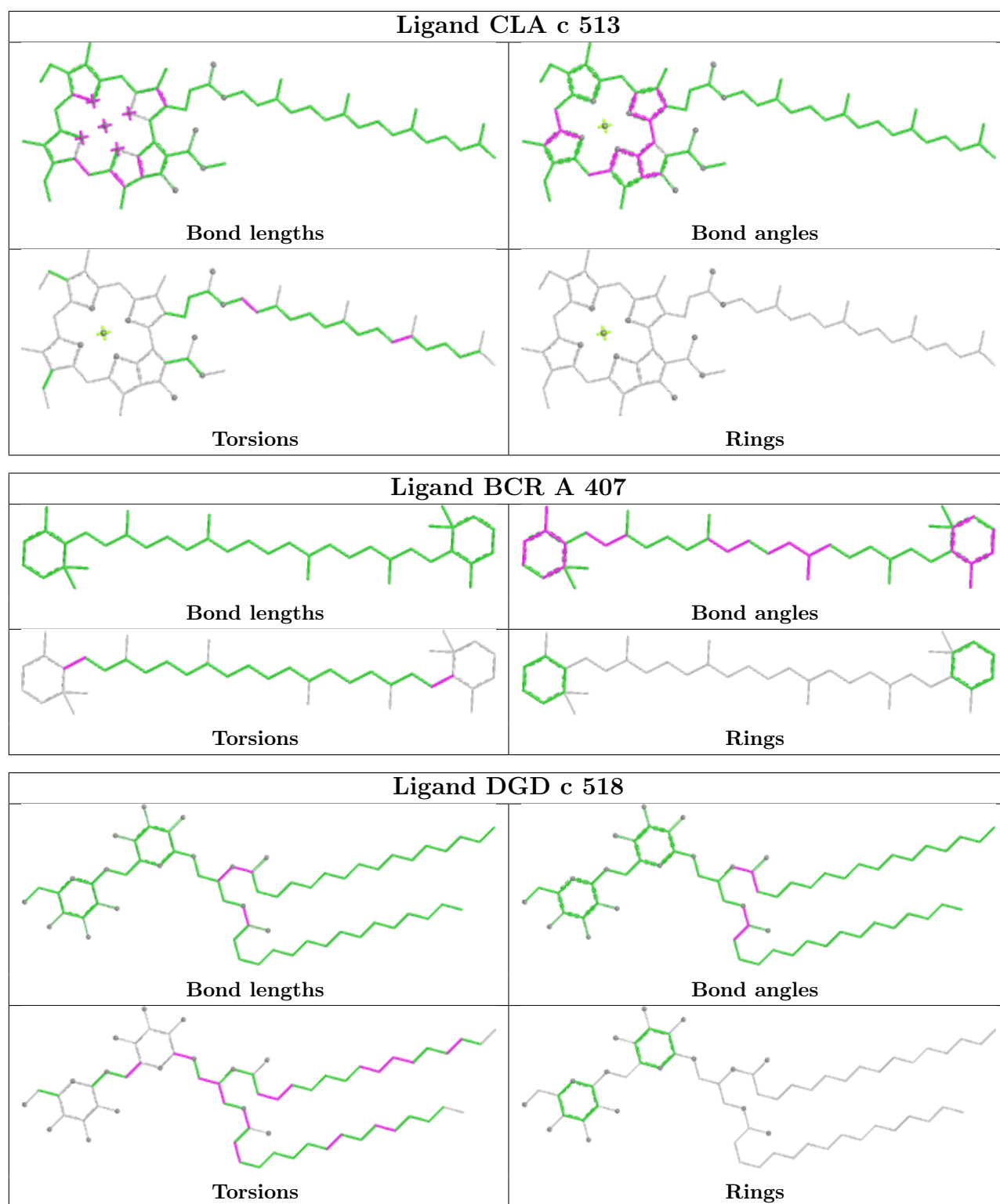


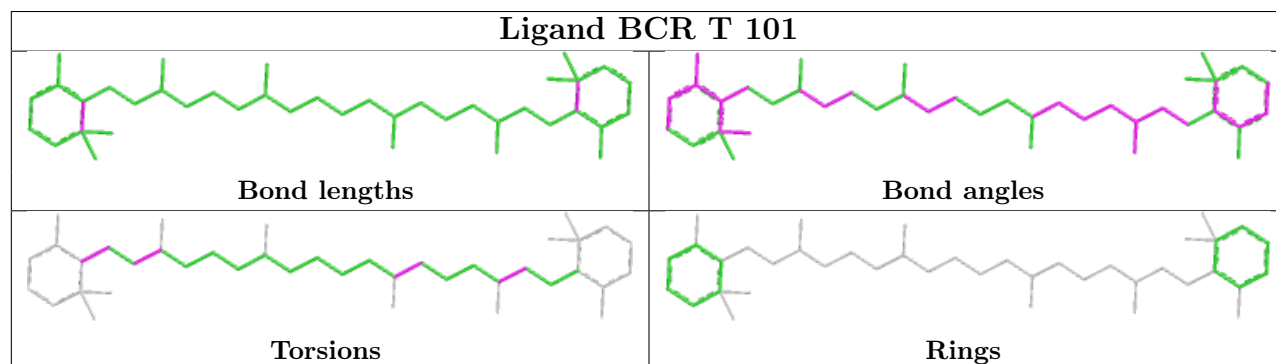
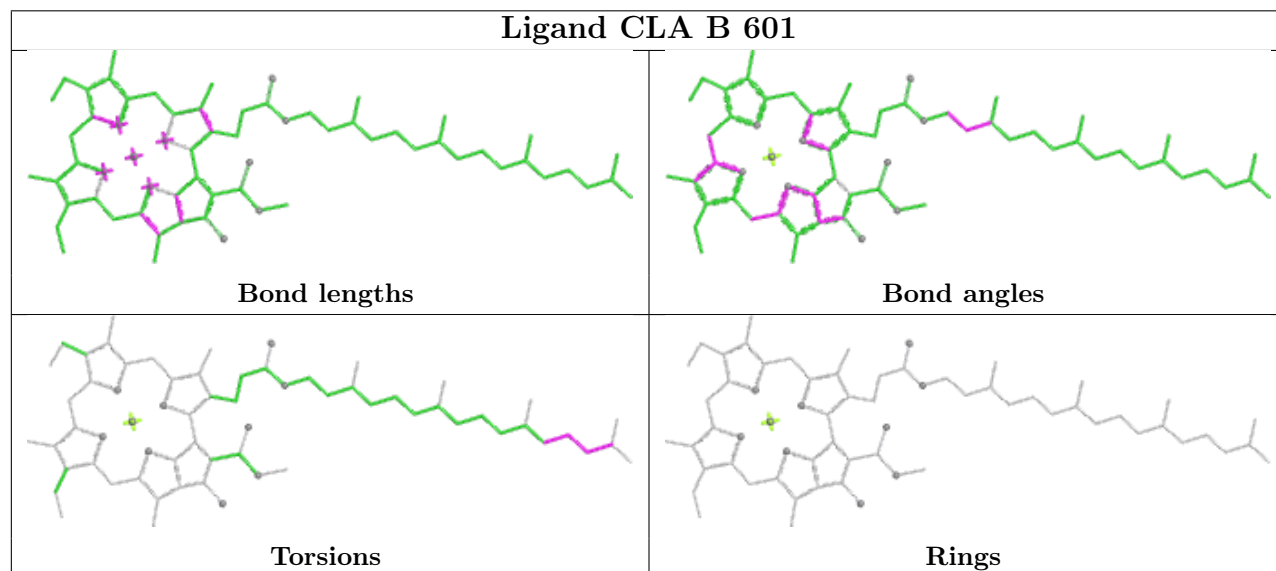
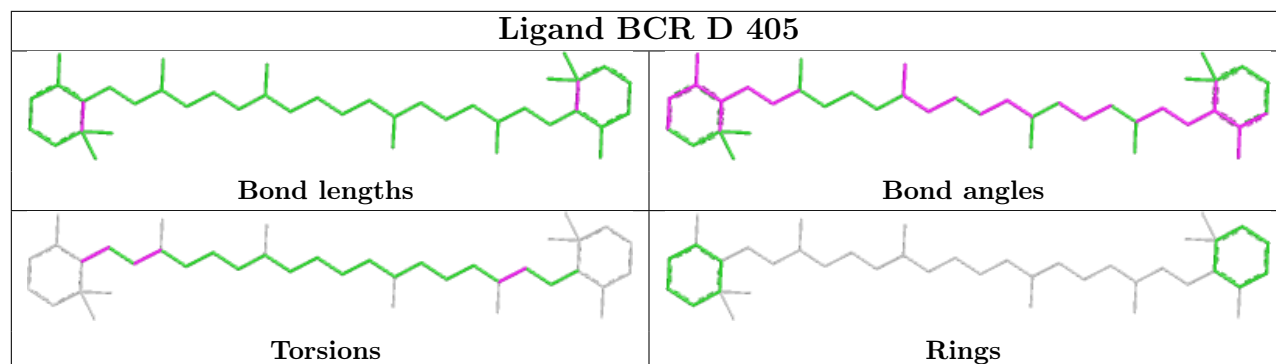


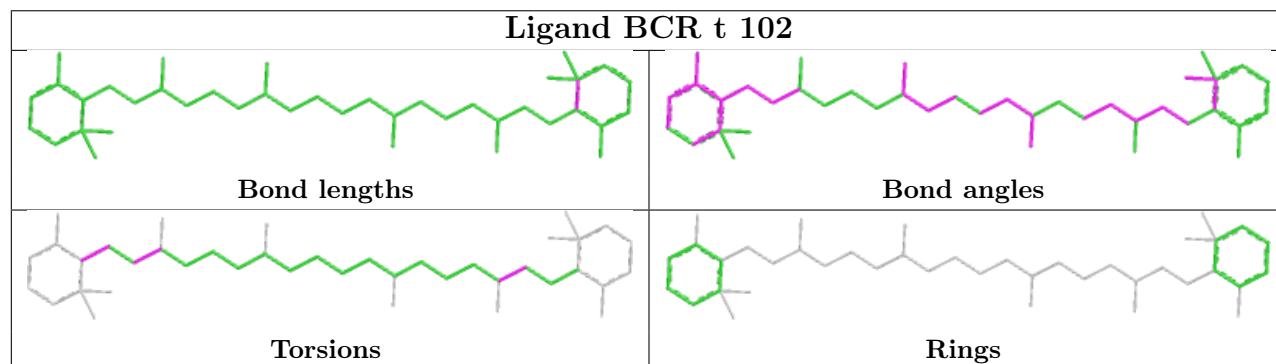
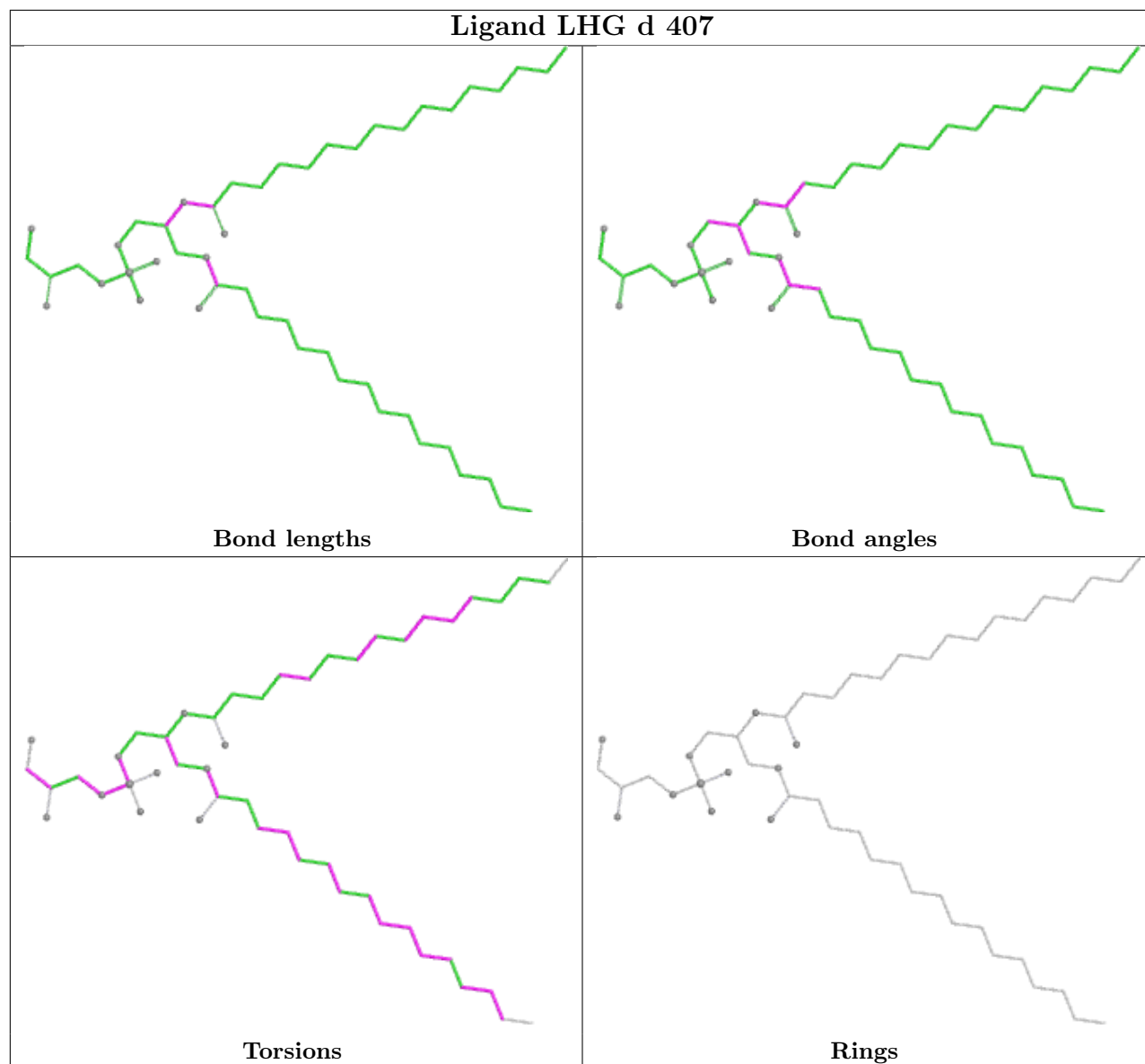


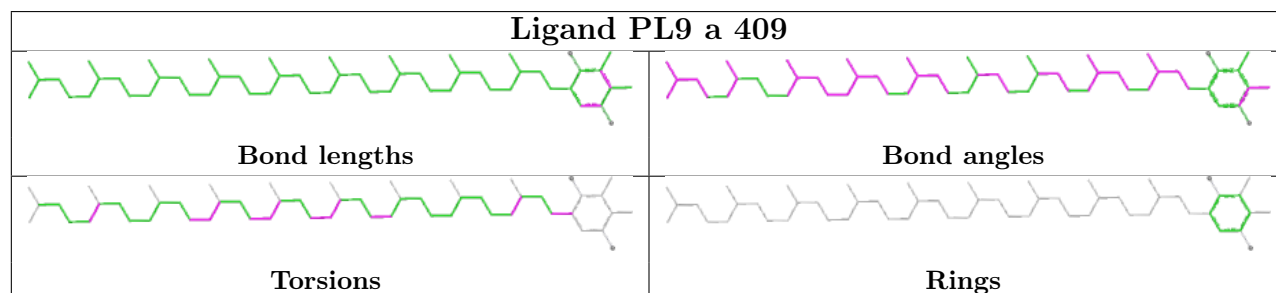
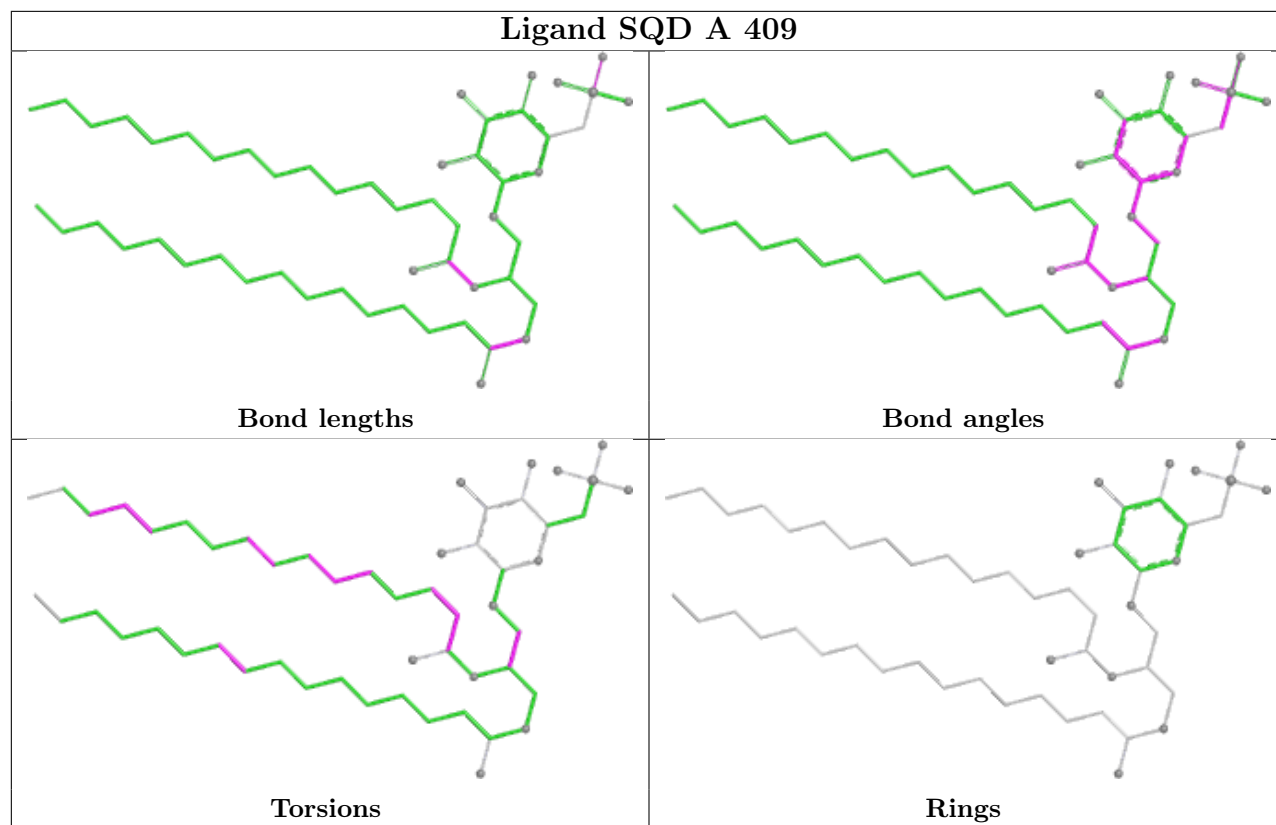


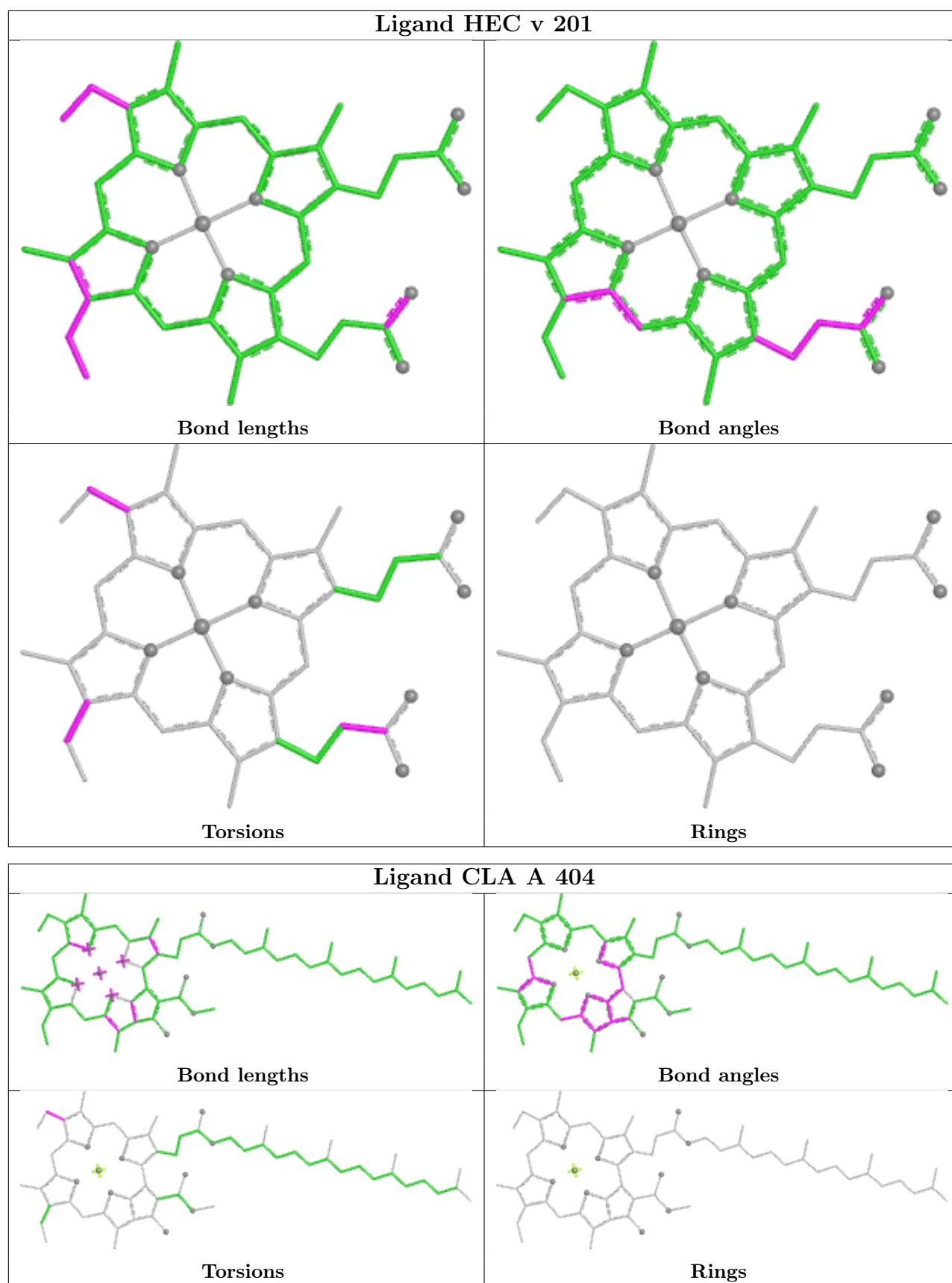


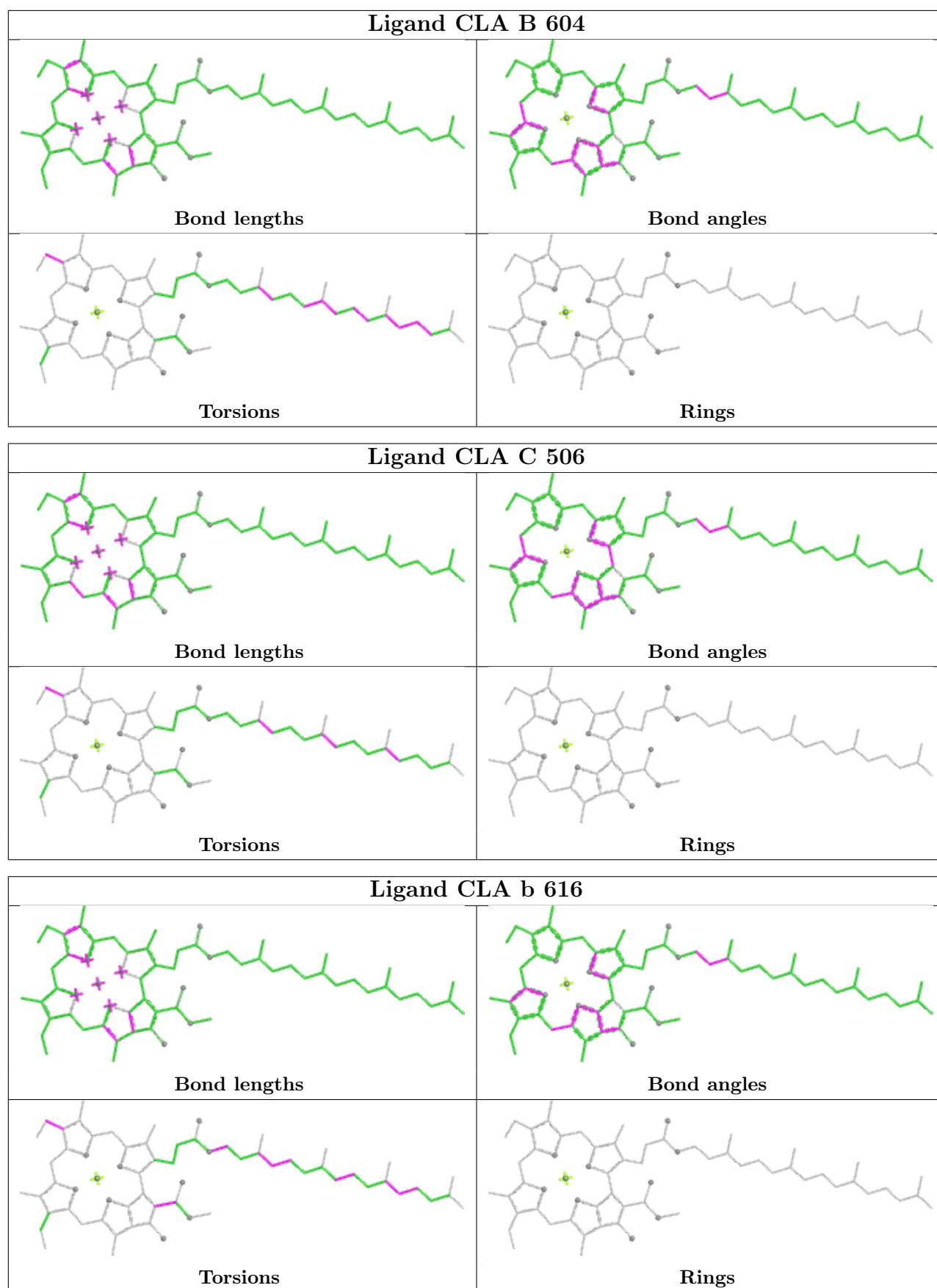


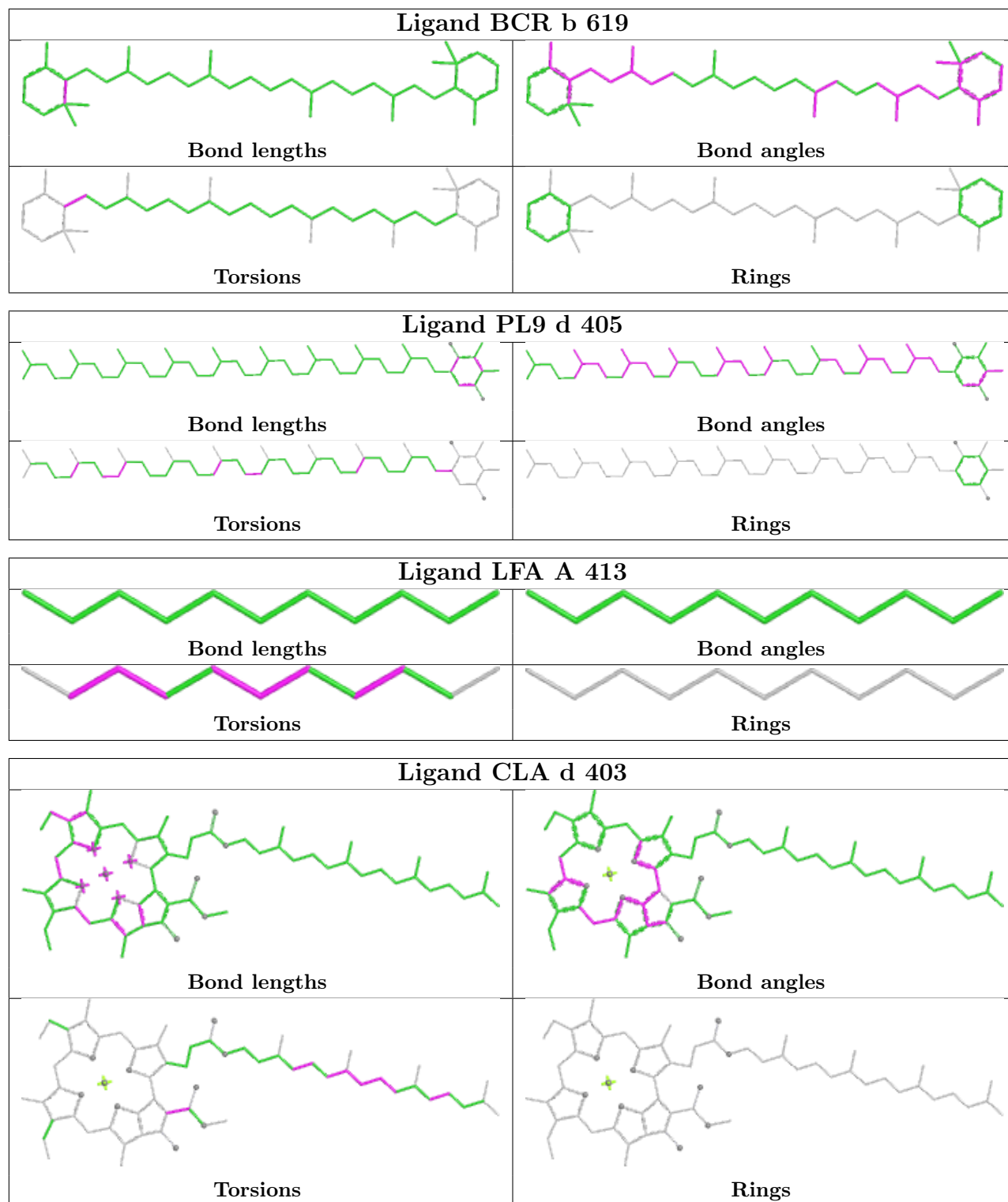


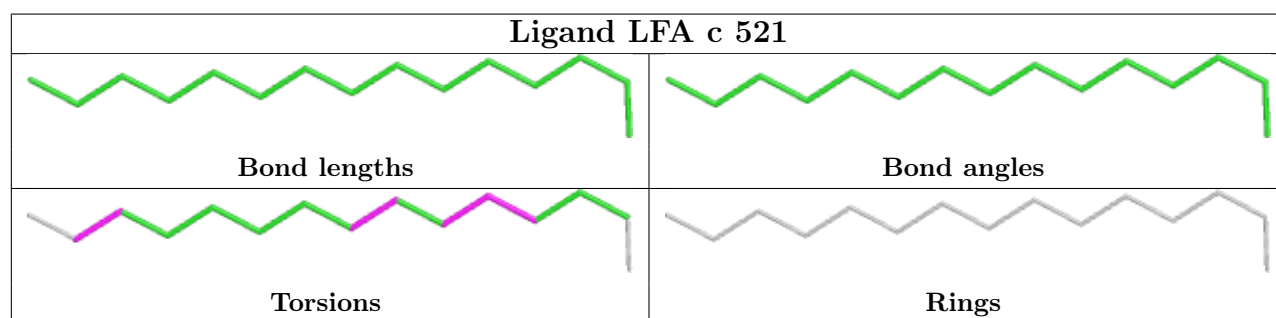
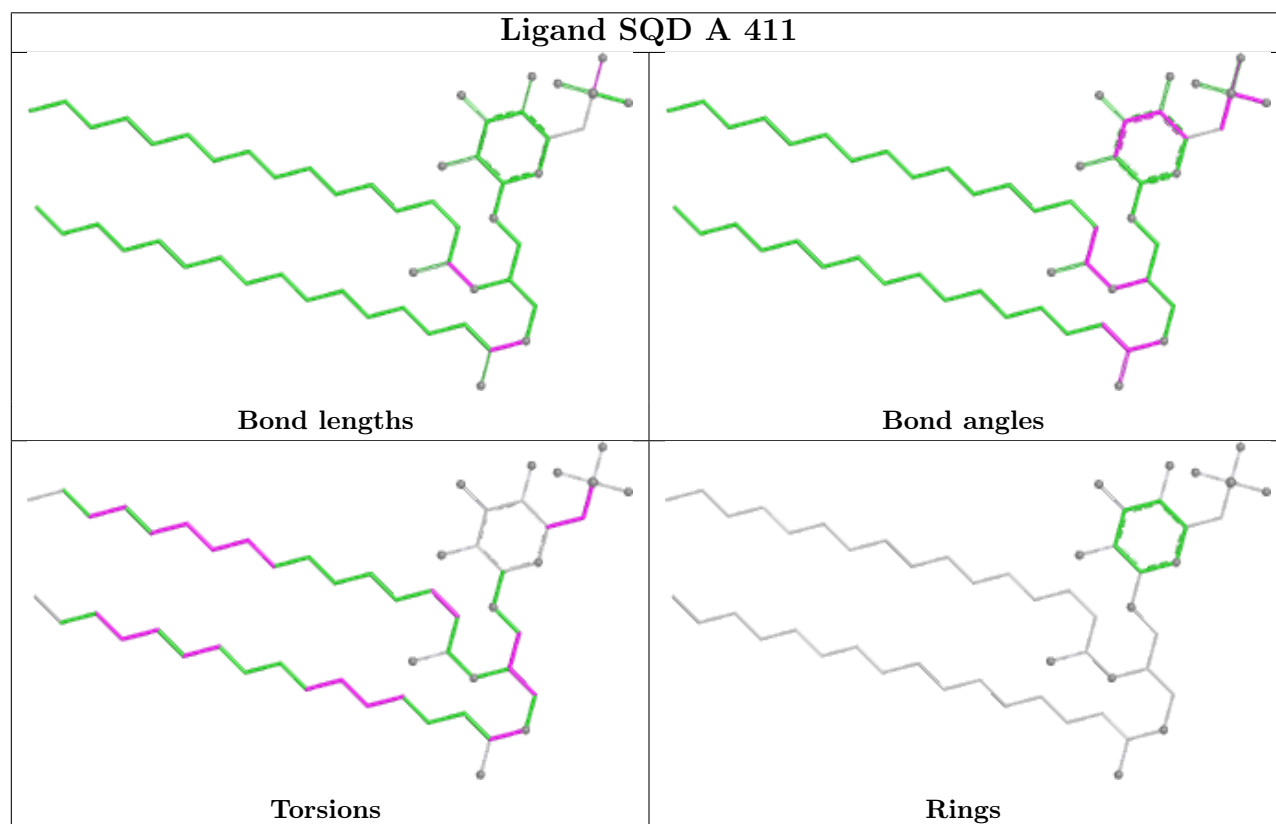
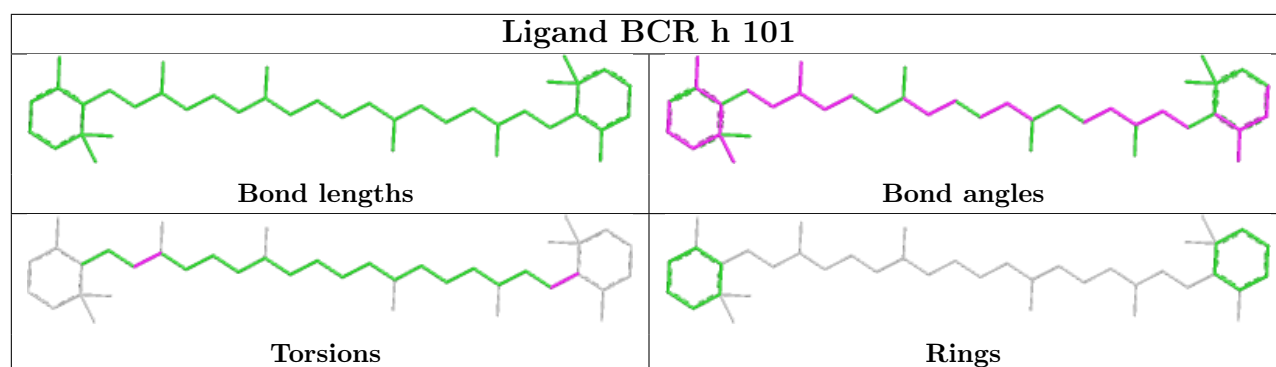


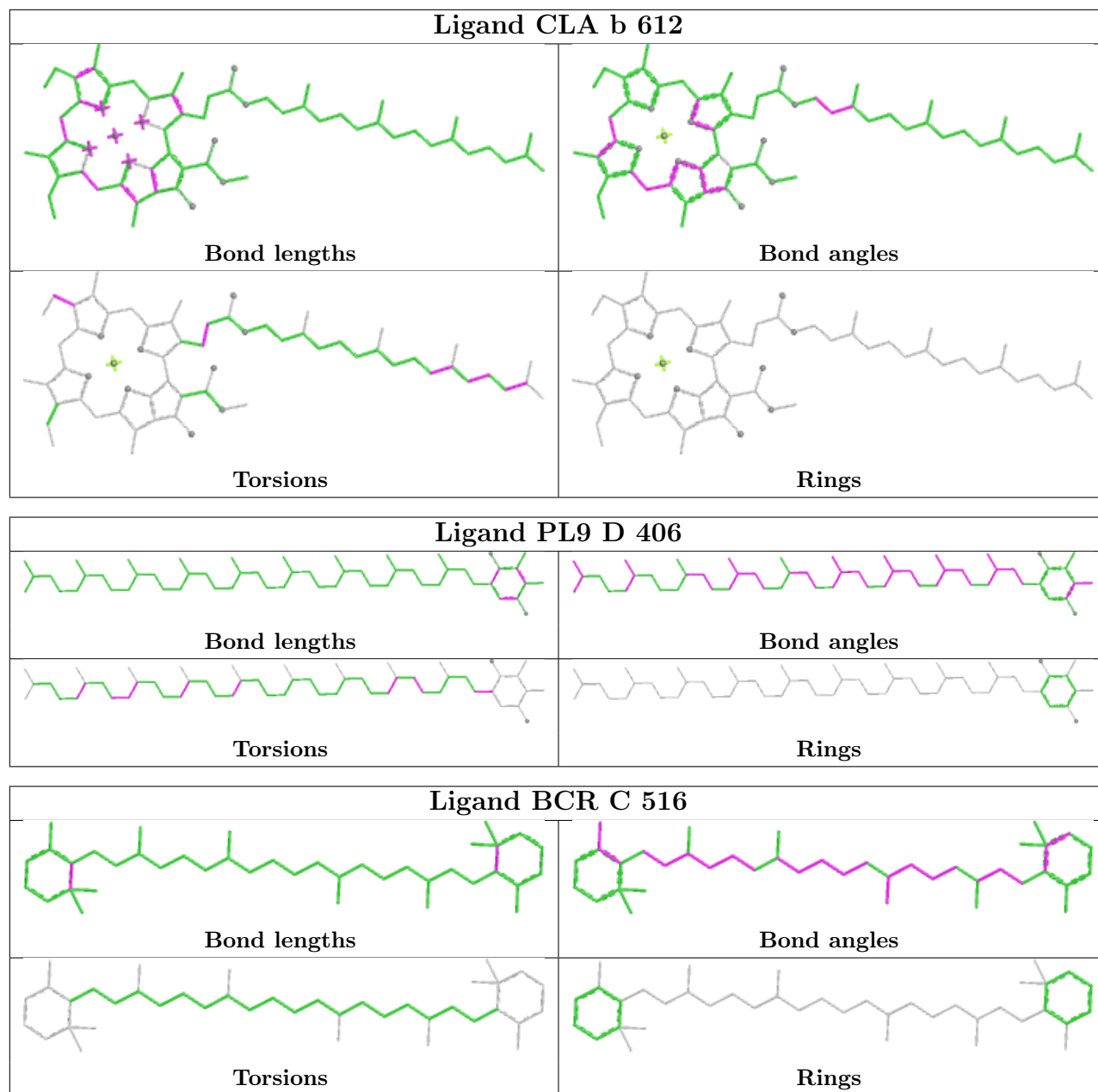


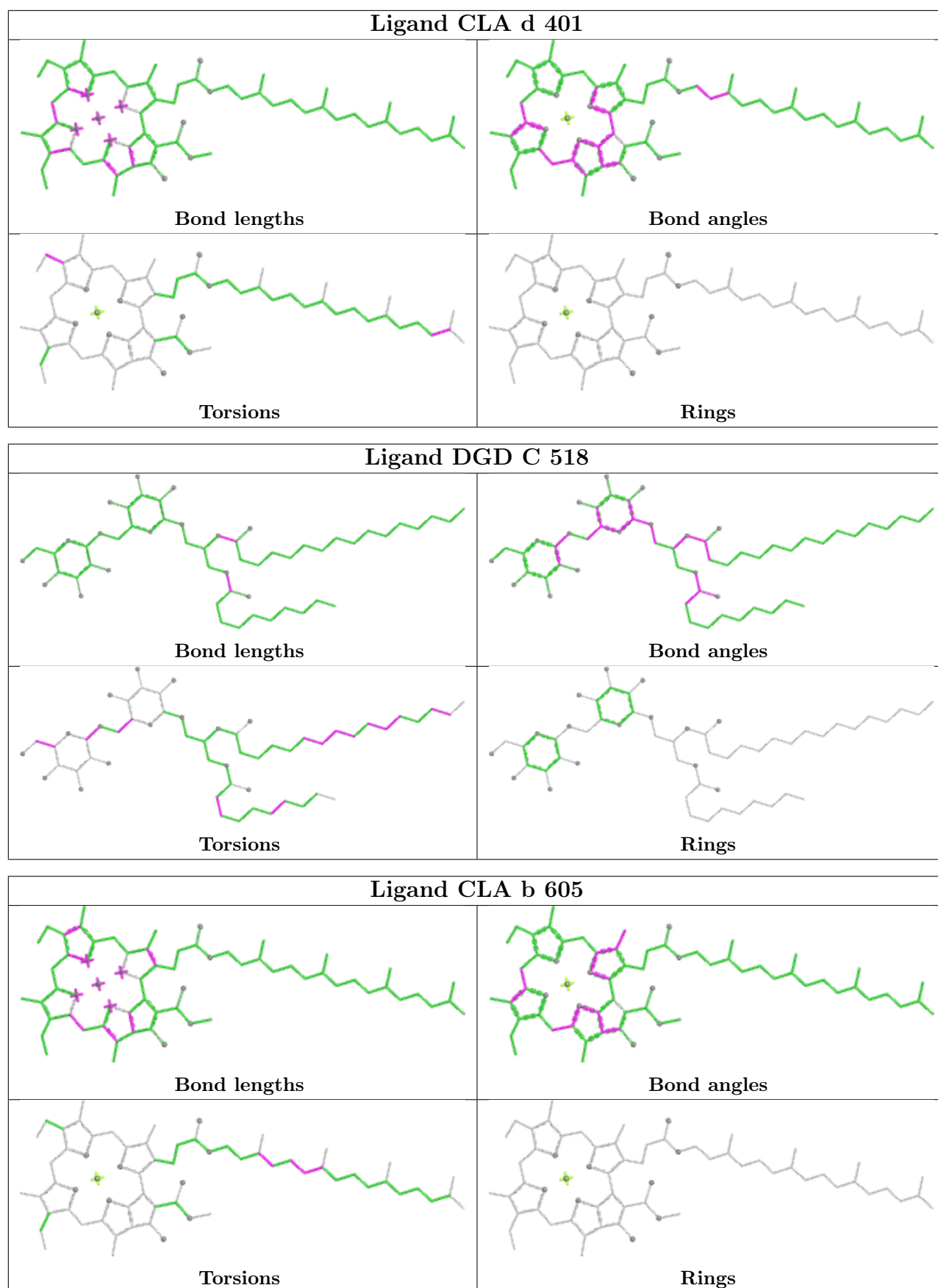


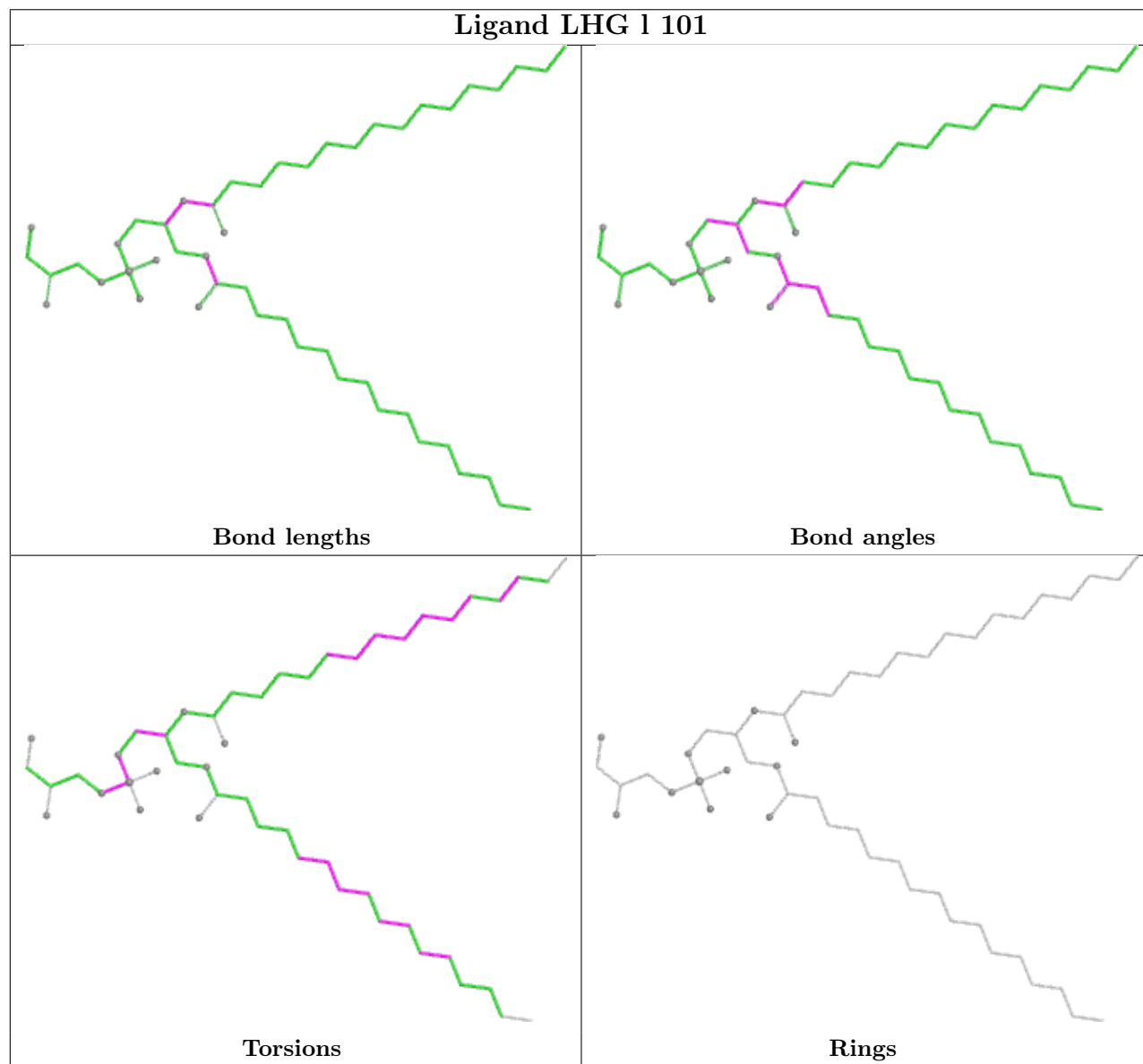
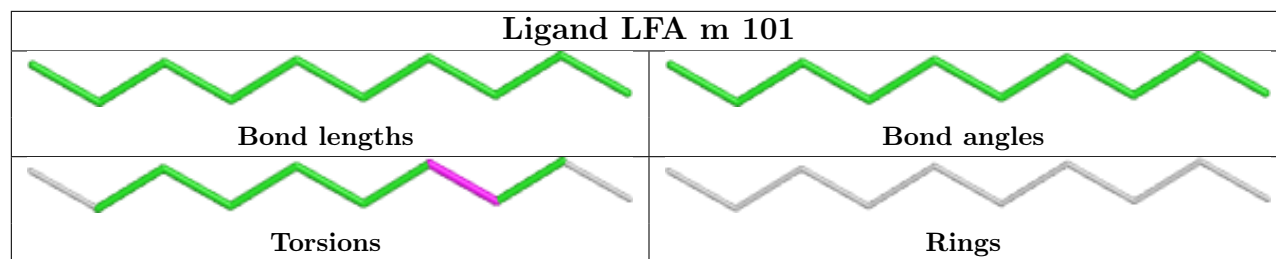


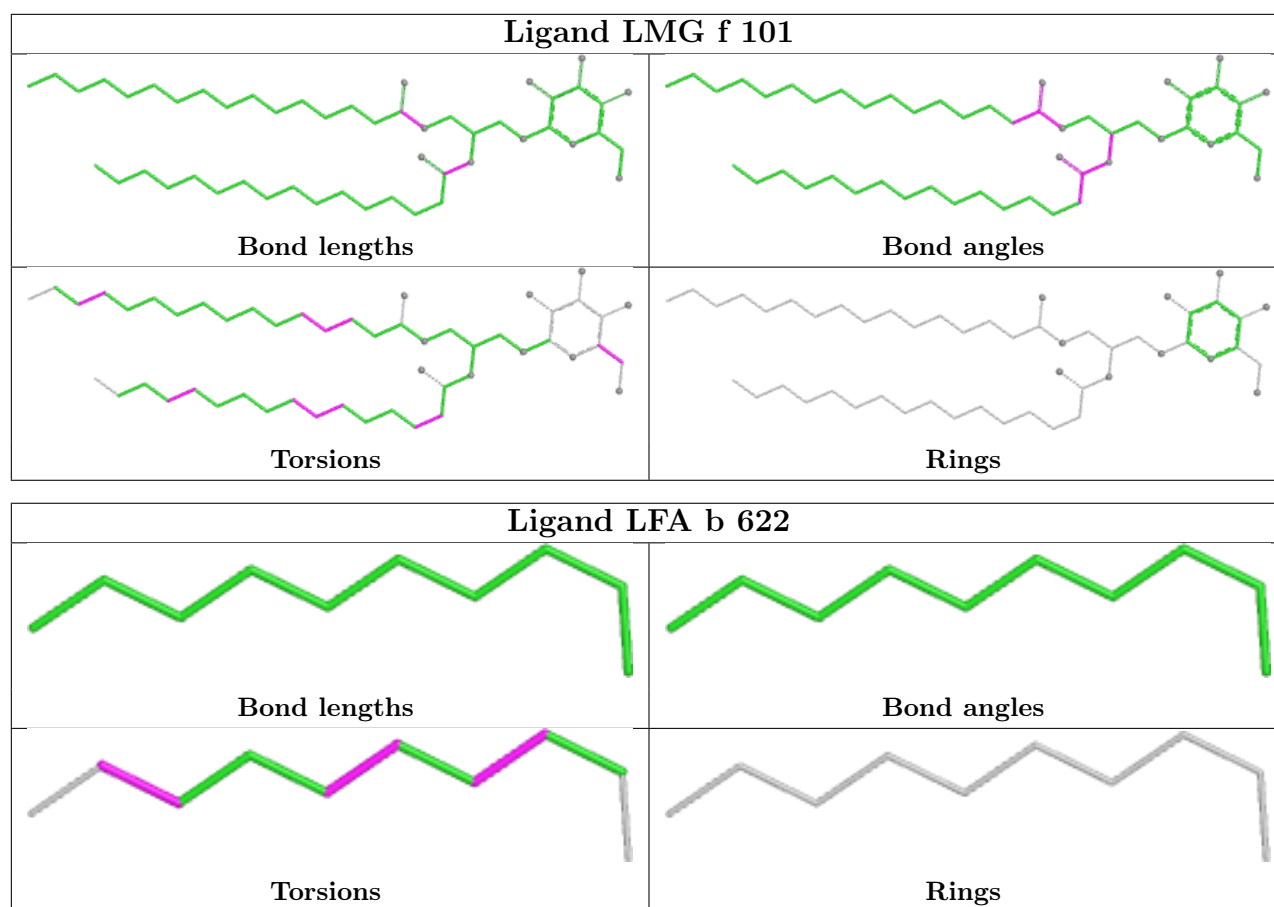












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	c	1
5	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	399:ALA	C	400:PRO	N	1.19
1	e	63:ILE	C	64:PRO	N	1.13

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/344 (96%)	-0.18	10 (3%) 52 49	17, 24, 47, 70	0
1	a	333/344 (96%)	-0.23	4 (1%) 76 74	16, 24, 48, 66	0
2	B	505/510 (99%)	-0.16	12 (2%) 59 56	16, 25, 55, 73	0
2	b	503/510 (98%)	-0.05	10 (1%) 65 62	19, 30, 59, 90	0
3	C	447/461 (96%)	-0.01	6 (1%) 75 73	20, 32, 50, 83	0
3	c	448/461 (97%)	-0.10	0 100 100	21, 32, 46, 67	0
4	D	340/352 (96%)	-0.28	3 (0%) 81 79	16, 25, 42, 62	0
4	d	340/352 (96%)	-0.15	2 (0%) 85 83	17, 28, 48, 67	0
5	E	81/84 (96%)	0.48	1 (1%) 76 74	29, 46, 59, 76	0
5	e	79/84 (94%)	0.74	5 (6%) 26 23	34, 50, 68, 87	0
6	F	33/45 (73%)	0.23	0 100 100	32, 39, 49, 58	0
6	f	33/45 (73%)	0.50	1 (3%) 52 49	39, 44, 61, 63	0
7	H	62/66 (93%)	-0.16	1 (1%) 70 67	25, 30, 36, 45	0
7	h	63/66 (95%)	0.35	2 (3%) 50 47	34, 39, 50, 55	0
8	I	33/38 (86%)	-0.24	0 100 100	23, 28, 35, 43	0
8	i	33/38 (86%)	-0.32	1 (3%) 52 49	21, 28, 39, 45	0
9	J	33/40 (82%)	0.27	1 (3%) 52 49	33, 41, 49, 54	0
9	j	33/40 (82%)	0.53	1 (3%) 52 49	33, 41, 49, 56	0
10	K	35/46 (76%)	0.72	4 (11%) 10 7	41, 47, 69, 76	0
10	k	36/46 (78%)	0.56	2 (5%) 30 27	35, 45, 66, 77	0
11	L	36/37 (97%)	-0.44	0 100 100	18, 22, 46, 54	0
11	l	36/37 (97%)	-0.53	0 100 100	17, 23, 43, 55	0
12	M	32/36 (88%)	-0.38	0 100 100	19, 24, 45, 51	0
12	m	32/36 (88%)	-0.22	0 100 100	20, 25, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.39	14 (5%) 29 25	24, 43, 69, 124	0
13	o	241/272 (88%)	0.31	10 (4%) 41 38	25, 39, 68, 122	0
14	T	28/32 (87%)	-0.39	0 100 100	19, 23, 42, 72	0
14	t	29/32 (90%)	-0.15	2 (6%) 23 20	20, 24, 46, 57	0
15	U	96/134 (71%)	1.07	11 (11%) 9 7	45, 61, 83, 90	0
15	u	96/134 (71%)	0.13	0 100 100	32, 40, 51, 54	0
16	V	137/163 (84%)	0.14	2 (1%) 72 69	32, 40, 50, 61	0
16	v	137/163 (84%)	0.34	0 100 100	34, 43, 59, 75	0
17	Y	21/46 (45%)	1.49	6 (28%) 1 1	54, 65, 81, 85	0
17	y	23/46 (50%)	1.26	2 (8%) 16 13	50, 58, 79, 82	0
18	X	37/41 (90%)	-0.01	1 (2%) 56 53	32, 38, 53, 65	0
18	x	38/41 (92%)	0.65	1 (2%) 57 54	38, 49, 68, 84	0
19	Z	61/62 (98%)	1.64	18 (29%) 1 1	50, 64, 121, 133	0
19	z	61/62 (98%)	1.78	21 (34%) 1 0	51, 72, 114, 128	0
20	R	35/41 (85%)	1.29	7 (20%) 3 2	49, 61, 81, 84	0
20	r	32/41 (78%)	1.71	10 (31%) 1 1	56, 65, 90, 97	0
All	All	5253/5700 (92%)	0.08	171 (3%) 49 46	16, 33, 65, 133	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	5.7
1	A	344	ALA	5.6
3	C	29	GLU	4.9
19	z	39	LEU	4.8
13	O	59	LYS	4.5
19	Z	42	LEU	4.5
13	o	56	PRO	4.4
19	Z	30	PRO	4.4
13	O	58	ASN	4.3
3	C	354	GLU	4.1
19	z	61	VAL	4.1
19	z	3	ILE	4.0
19	Z	39	LEU	4.0
3	C	30	SER	3.8
13	O	191	SER	3.8

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Mol	Chain	Res	Type	RSRZ
19	Z	31	GLN	3.8
19	z	33	TRP	3.8
13	O	63	ALA	3.8
5	e	5	THR	3.7
5	e	78	THR	3.6
19	z	42	LEU	3.6
2	b	499	VAL	3.5
19	Z	61	VAL	3.5
1	A	343	LEU	3.5
13	O	56	PRO	3.4
20	r	34	LEU	3.4
13	o	60	ARG	3.4
19	z	32	ASP	3.3
15	U	87	VAL	3.3
13	o	58	ASN	3.2
10	k	11	LEU	3.2
17	Y	26	ALA	3.2
19	z	36	SER	3.2
19	Z	41	PHE	3.1
10	K	17	ILE	3.1
19	z	4	LEU	3.1
13	o	57	LYS	3.1
5	e	83	LEU	3.1
9	j	8	ILE	3.1
3	C	31	SER	3.0
1	A	332	HIS	3.0
19	Z	1	MET	3.0
19	Z	37	LYS	3.0
2	b	479	PHE	3.0
15	U	74	ILE	3.0
17	y	24	MET	3.0
1	A	336	ALA	2.9
19	Z	34	ASP	2.9
20	r	9	LEU	2.9
17	y	25	ILE	2.9
13	O	245	PRO	2.9
17	Y	27	MET	2.9
19	z	1	MET	2.9
1	A	339	PHE	2.8
3	C	27	ASP	2.8
7	h	64	ALA	2.8
15	U	10	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	488	PRO	2.8
19	z	41	PHE	2.8
13	O	25	THR	2.8
17	Y	41	VAL	2.8
19	Z	60	PHE	2.8
10	K	11	LEU	2.8
2	b	503	THR	2.8
13	o	59	LYS	2.8
1	A	341	LEU	2.7
2	B	486	LEU	2.7
2	B	504	THR	2.7
19	z	37	LYS	2.7
20	R	27	ALA	2.7
1	a	230	THR	2.7
2	B	84	THR	2.7
15	U	61	VAL	2.7
20	R	28	VAL	2.7
2	b	495	PHE	2.7
5	e	79	PHE	2.7
7	h	41	PHE	2.7
13	o	63	ALA	2.7
19	z	31	GLN	2.7
13	o	25	THR	2.7
1	A	189	GLU	2.7
5	E	3	GLY	2.7
18	x	2	THR	2.6
13	O	57	LYS	2.6
2	B	85	GLY	2.6
20	r	33	LYS	2.6
10	K	16	ALA	2.6
15	U	75	LEU	2.6
10	k	17	ILE	2.5
2	B	487	SER	2.5
20	r	3	TRP	2.5
15	U	40	GLY	2.5
19	z	48	ILE	2.5
20	R	31	VAL	2.5
20	R	10	LEU	2.5
20	r	24	LEU	2.5
19	z	60	PHE	2.5
15	U	65	PRO	2.4
19	z	7	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
13	o	61	GLN	2.4
14	t	28	ARG	2.4
19	z	10	ALA	2.4
1	A	230	THR	2.4
15	U	62	LEU	2.4
17	Y	39	LEU	2.4
2	B	479	PHE	2.4
19	Z	40	ILE	2.4
16	V	35	TYR	2.3
20	r	26	TYR	2.3
20	r	6	LEU	2.3
2	B	127	ARG	2.3
7	H	41	PHE	2.3
17	Y	30	ILE	2.3
19	z	2	THR	2.3
3	C	28	GLN	2.3
19	z	11	ALA	2.3
17	Y	45	ASN	2.3
19	Z	35	ARG	2.3
15	U	82	PHE	2.3
2	B	86	ILE	2.3
14	t	29	ILE	2.3
2	B	490	GLN	2.3
19	Z	2	THR	2.3
13	O	133	VAL	2.3
13	o	132	ASN	2.3
15	U	66	GLY	2.3
4	D	236	ASN	2.2
1	a	342	ASP	2.2
19	z	34	ASP	2.2
18	X	2	THR	2.2
2	b	485	GLU	2.2
19	Z	38	GLN	2.2
4	d	238	THR	2.2
19	Z	25	VAL	2.2
1	a	343	LEU	2.2
13	O	192	LEU	2.2
20	r	10	LEU	2.2
6	f	15	ILE	2.1
2	B	386	ALA	2.1
4	D	233	ARG	2.1
19	z	35	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
8	i	33	LYS	2.1
1	A	243	GLU	2.1
2	b	504	THR	2.1
19	z	47	TRP	2.1
9	J	8	ILE	2.1
1	a	344	ALA	2.1
13	o	191	SER	2.1
19	Z	4	LEU	2.1
20	R	6	LEU	2.1
2	b	130	GLU	2.1
10	K	19	ASP	2.1
13	O	36	GLN	2.1
2	B	496	TYR	2.1
13	O	60	ARG	2.1
2	b	494	GLY	2.1
5	e	6	GLY	2.1
19	Z	59	PHE	2.1
20	r	20	VAL	2.1
20	r	31	VAL	2.1
4	d	240	ALA	2.1
15	U	20	ALA	2.1
20	R	35	LEU	2.0
2	b	126	PRO	2.0
13	O	190	PHE	2.0
13	O	182	LEU	2.0
20	R	24	LEU	2.0
1	A	228	THR	2.0
2	B	503	THR	2.0
4	D	237	PRO	2.0
16	V	16	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
27	LFA	A	410	14/20	0.68	0.17	37,39,43,45	0
27	LFA	B	624	15/20	0.70	0.20	28,37,47,48	0
27	LFA	b	623	12/20	0.73	0.16	25,36,38,39	0
27	LFA	b	626	12/20	0.75	0.15	29,36,43,47	0
27	LFA	m	101	10/20	0.76	0.14	28,36,44,50	0
27	LFA	i	102	7/20	0.78	0.13	26,32,34,39	0
27	LFA	b	629	9/20	0.78	0.14	29,31,33,39	0
27	LFA	b	627	11/20	0.79	0.15	36,46,49,53	0
29	LMG	c	522	41/55	0.79	0.14	21,46,54,60	0
29	LMG	B	621	36/55	0.80	0.14	28,50,59,63	0
27	LFA	b	630	15/20	0.80	0.15	31,39,42,42	0
29	LMG	C	522	44/55	0.81	0.14	32,42,53,58	0
29	LMG	C	520	48/55	0.81	0.15	38,53,67,71	0
27	LFA	B	626	10/20	0.82	0.13	20,29,38,40	0
27	LFA	a	411	7/20	0.82	0.13	26,32,35,35	0
27	LFA	A	413	11/20	0.82	0.14	27,32,46,47	0
27	LFA	d	409	9/20	0.82	0.14	24,35,40,46	0
29	LMG	b	624	39/55	0.82	0.14	34,53,60,66	0
22	CLA	b	603	65/65	0.82	0.14	33,57,78,85	0
25	PL9	A	408	55/55	0.83	0.13	34,43,53,56	0
26	SQD	A	411	54/54	0.83	0.14	27,47,71,83	0
27	LFA	b	625	16/20	0.83	0.12	27,32,41,45	0
27	LFA	D	411	15/20	0.83	0.12	23,28,40,47	0
27	LFA	D	413	8/20	0.83	0.14	25,30,37,40	0
27	LFA	B	623	13/20	0.84	0.12	21,31,34,36	0
29	LMG	C	501	51/55	0.84	0.12	26,40,50,53	0
27	LFA	B	628	12/20	0.84	0.11	23,28,37,37	0
27	LFA	i	101	16/20	0.84	0.12	23,32,40,41	0
27	LFA	b	622	10/20	0.84	0.11	27,31,37,38	0
26	SQD	b	601	54/54	0.84	0.11	25,39,62,65	0
27	LFA	B	627	14/20	0.85	0.12	20,31,36,39	0
27	LFA	j	101	15/20	0.85	0.15	41,45,51,56	0
29	LMG	c	519	51/55	0.85	0.15	38,52,64,67	0
26	SQD	L	101	48/54	0.85	0.11	21,42,66,69	0
32	LHG	E	101	42/49	0.85	0.12	31,54,67,71	0
32	LHG	e	101	42/49	0.85	0.14	40,62,80,94	0
27	LFA	d	408	15/20	0.86	0.11	25,32,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LFA	b	602	15/20	0.86	0.12	29,33,42,42	0
26	SQD	a	412	50/54	0.86	0.13	28,43,70,76	0
27	LFA	M	102	16/20	0.86	0.12	25,27,46,47	0
25	PL9	a	409	55/55	0.86	0.14	38,48,59,65	0
27	LFA	J	101	11/20	0.87	0.12	38,43,49,49	0
26	SQD	f	102	43/54	0.87	0.16	51,66,77,86	0
27	LFA	d	410	16/20	0.87	0.11	28,35,44,45	0
27	LFA	T	102	12/20	0.87	0.09	22,28,32,32	0
24	BCR	c	524	40/40	0.88	0.12	36,43,53,53	0
27	LFA	I	101	14/20	0.88	0.10	21,29,32,32	0
22	CLA	H	101	65/65	0.88	0.10	30,45,64,72	0
24	BCR	K	101	40/40	0.88	0.12	37,48,53,55	0
29	LMG	c	501	51/55	0.88	0.10	25,39,51,60	0
27	LFA	c	520	9/20	0.88	0.11	31,39,46,47	0
27	LFA	c	521	15/20	0.88	0.10	31,35,41,41	0
29	LMG	B	619	51/55	0.88	0.10	15,31,42,47	0
27	LFA	B	625	9/20	0.88	0.11	20,25,27,33	0
27	LFA	B	622	16/20	0.89	0.09	27,32,36,37	0
27	LFA	m	102	15/20	0.89	0.10	25,29,37,37	0
27	LFA	t	101	15/20	0.89	0.11	25,31,42,43	0
26	SQD	D	412	43/54	0.89	0.12	38,50,58,69	0
24	BCR	h	101	40/40	0.89	0.10	28,40,45,49	0
29	LMG	m	103	51/55	0.89	0.10	17,30,41,45	0
26	SQD	a	410	54/54	0.89	0.12	30,48,58,62	0
24	BCR	T	101	40/40	0.89	0.09	22,29,34,37	0
27	LFA	C	521	15/20	0.90	0.10	26,34,39,42	0
22	CLA	C	514	65/65	0.90	0.11	37,49,63,67	0
21	CL	A	401	1/1	0.90	0.11	57,57,57,57	0
27	LFA	D	414	10/20	0.90	0.09	22,23,26,28	0
22	CLA	C	511	65/65	0.90	0.09	25,34,41,49	0
24	BCR	C	515	40/40	0.90	0.10	36,45,52,55	0
30	DGD	h	102	62/66	0.90	0.10	23,33,40,45	0
27	LFA	B	620	10/20	0.90	0.10	22,24,28,33	0
22	CLA	C	513	65/65	0.90	0.10	34,41,54,63	0
24	BCR	c	523	40/40	0.91	0.10	39,46,52,55	0
22	CLA	c	514	65/65	0.91	0.11	33,45,61,67	0
30	DGD	C	518	56/66	0.91	0.10	29,38,48,53	0
24	BCR	d	404	40/40	0.91	0.10	25,36,53,56	0
22	CLA	c	513	65/65	0.91	0.10	36,42,55,62	0
24	BCR	k	101	40/40	0.91	0.10	29,43,51,54	0
24	BCR	C	516	40/40	0.92	0.08	21,30,37,38	0
24	BCR	D	405	40/40	0.92	0.09	23,33,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	t	102	40/40	0.92	0.09	21,26,38,40	0
22	CLA	b	608	65/65	0.92	0.09	22,29,42,53	0
25	PL9	D	406	55/55	0.92	0.09	12,21,26,28	0
24	BCR	K	102	40/40	0.92	0.10	39,44,47,48	0
29	LMG	f	101	51/55	0.92	0.10	31,38,55,61	0
26	SQD	A	409	54/54	0.92	0.11	24,42,54,56	0
22	CLA	b	618	65/65	0.92	0.11	23,32,58,64	0
30	DGD	H	103	60/66	0.92	0.09	22,29,40,45	0
22	CLA	C	507	65/65	0.92	0.09	22,30,55,57	0
32	LHG	D	409	49/49	0.92	0.11	16,33,53,57	0
22	CLA	C	503	65/65	0.92	0.08	24,32,36,38	0
22	CLA	C	504	65/65	0.92	0.08	20,35,38,42	0
29	LMG	D	410	51/55	0.93	0.10	25,36,51,54	0
24	BCR	B	616	40/40	0.93	0.07	19,25,31,32	0
24	BCR	B	617	40/40	0.93	0.07	15,24,30,30	0
24	BCR	B	618	40/40	0.93	0.07	18,26,34,36	0
22	CLA	C	512	65/65	0.93	0.09	35,44,52,56	0
22	CLA	c	504	65/65	0.93	0.08	26,34,39,40	0
22	CLA	c	507	65/65	0.93	0.09	25,32,52,58	0
24	BCR	H	102	40/40	0.93	0.08	22,28,42,43	0
30	DGD	C	519	62/66	0.93	0.09	27,33,46,60	0
22	CLA	c	510	65/65	0.93	0.09	22,31,38,40	0
30	DGD	c	517	55/66	0.93	0.09	25,34,50,63	0
30	DGD	c	518	62/66	0.93	0.09	26,32,52,58	0
22	CLA	B	615	65/65	0.93	0.10	19,25,70,79	0
22	CLA	C	505	65/65	0.93	0.09	28,35,48,61	0
24	BCR	b	619	40/40	0.93	0.08	18,28,34,35	0
32	LHG	d	407	49/49	0.93	0.12	21,37,60,63	0
24	BCR	b	620	40/40	0.93	0.07	18,25,30,32	0
22	CLA	b	611	65/65	0.94	0.08	23,30,40,52	0
22	CLA	b	616	65/65	0.94	0.08	20,26,39,42	0
22	CLA	C	508	65/65	0.94	0.07	21,26,35,45	0
22	CLA	c	502	65/65	0.94	0.08	17,28,35,38	0
22	CLA	C	509	65/65	0.94	0.09	22,31,62,66	0
25	PL9	d	405	55/55	0.94	0.07	16,23,27,30	0
22	CLA	c	505	65/65	0.94	0.09	21,33,49,53	0
22	CLA	C	510	65/65	0.94	0.08	25,31,39,40	0
22	CLA	c	508	65/65	0.94	0.07	22,30,34,37	0
30	DGD	C	517	62/66	0.94	0.09	20,26,49,52	0
22	CLA	B	605	65/65	0.94	0.07	17,25,38,44	0
22	CLA	c	511	65/65	0.94	0.07	27,32,38,44	0
22	CLA	c	512	65/65	0.94	0.08	28,39,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	DGD	c	516	62/66	0.94	0.09	23,28,49,52	0
27	LFA	M	101	10/20	0.94	0.08	26,31,41,42	0
24	BCR	b	621	40/40	0.94	0.08	23,34,42,47	0
24	BCR	c	515	40/40	0.94	0.07	19,29,38,41	0
31	BCT	D	401	4/4	0.94	0.08	25,29,31,32	0
32	LHG	D	407	49/49	0.94	0.08	17,24,30,33	0
22	CLA	b	604	65/65	0.94	0.08	25,30,41,46	0
22	CLA	C	502	65/65	0.94	0.08	18,24,33,35	0
32	LHG	b	628	49/49	0.94	0.08	22,27,35,49	0
22	CLA	d	403	65/65	0.94	0.09	22,30,57,63	0
22	CLA	b	610	65/65	0.94	0.08	22,28,37,45	0
32	LHG	l	101	49/49	0.94	0.07	17,25,34,39	0
33	HEM	E	102	43/43	0.94	0.11	34,43,52,54	0
33	HEM	e	102	43/43	0.94	0.11	37,48,57,60	0
22	CLA	a	404	65/65	0.95	0.07	14,20,27,36	0
22	CLA	a	405	65/65	0.95	0.07	14,19,25,31	0
22	CLA	c	506	65/65	0.95	0.07	21,26,37,40	0
22	CLA	B	613	65/65	0.95	0.08	18,25,46,57	0
24	BCR	a	408	40/40	0.95	0.06	18,22,29,31	0
22	CLA	A	412	65/65	0.95	0.06	16,20,25,27	0
22	CLA	c	509	65/65	0.95	0.09	24,30,59,66	0
22	CLA	b	606	65/65	0.95	0.07	16,23,38,45	0
22	CLA	b	607	65/65	0.95	0.07	18,23,30,32	0
22	CLA	B	602	65/65	0.95	0.07	18,21,35,38	0
22	CLA	B	604	65/65	0.95	0.06	15,21,25,29	0
22	CLA	A	404	65/65	0.95	0.08	15,23,61,72	0
22	CLA	d	401	65/65	0.95	0.09	18,27,63,69	0
22	CLA	d	402	65/65	0.95	0.07	17,20,37,40	0
22	CLA	b	613	65/65	0.95	0.07	18,23,29,31	0
31	BCT	a	413	4/4	0.95	0.08	31,33,34,40	0
23	PHO	A	405	64/64	0.95	0.06	15,21,28,31	0
23	PHO	a	406	64/64	0.95	0.06	13,17,25,27	0
24	BCR	A	407	40/40	0.95	0.06	14,23,30,31	0
32	LHG	L	102	49/49	0.95	0.07	18,24,31,34	0
22	CLA	b	614	65/65	0.95	0.07	16,23,28,32	0
22	CLA	b	615	65/65	0.95	0.07	16,21,36,39	0
22	CLA	B	610	65/65	0.95	0.06	12,18,24,29	0
22	CLA	b	617	65/65	0.95	0.07	21,27,39,50	0
22	CLA	C	506	65/65	0.95	0.07	17,27,32,40	0
22	CLA	B	611	65/65	0.95	0.07	14,19,25,28	0
22	CLA	D	403	65/65	0.96	0.06	13,18,26,35	0
22	CLA	D	404	65/65	0.96	0.09	17,24,62,66	0

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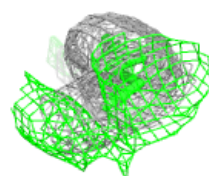
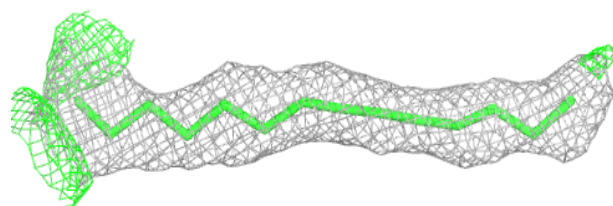
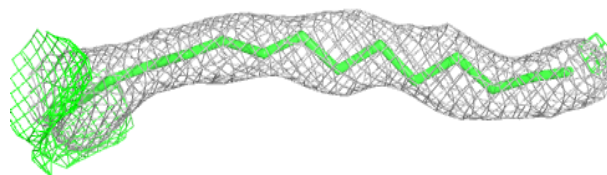
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	609	65/65	0.96	0.06	15,20,27,29	0
21	CL	A	402	1/1	0.96	0.12	57,57,57,57	0
22	CLA	B	603	65/65	0.96	0.06	14,21,35,44	0
22	CLA	a	407	65/65	0.96	0.08	13,19,56,60	0
23	PHO	D	402	64/64	0.96	0.06	14,18,25,28	0
22	CLA	B	612	65/65	0.96	0.06	13,18,40,43	0
23	PHO	a	414	64/64	0.96	0.06	21,28,33,39	0
22	CLA	c	503	65/65	0.96	0.06	23,30,38,39	0
32	LHG	D	408	49/49	0.96	0.07	18,24,30,37	0
22	CLA	A	403	65/65	0.96	0.06	12,18,23,30	0
22	CLA	b	605	65/65	0.96	0.07	18,22,37,49	0
22	CLA	B	614	65/65	0.96	0.06	15,22,32,47	0
22	CLA	B	601	65/65	0.96	0.07	17,26,32,36	0
32	LHG	d	406	49/49	0.96	0.07	18,24,32,36	0
22	CLA	B	606	65/65	0.96	0.06	10,18,33,37	0
22	CLA	b	609	65/65	0.96	0.06	11,21,29,32	0
22	CLA	B	607	65/65	0.96	0.06	13,19,26,34	0
22	CLA	B	608	65/65	0.96	0.06	15,24,33,36	0
22	CLA	b	612	65/65	0.96	0.07	16,25,31,33	0
34	HEC	V	201	43/43	0.96	0.09	28,36,41,45	0
22	CLA	A	406	65/65	0.97	0.08	11,20,54,60	0
21	CL	a	402	1/1	0.97	0.08	52,52,52,52	0
21	CL	a	403	1/1	0.97	0.11	40,40,40,40	0
34	HEC	v	201	43/43	0.97	0.07	28,34,38,41	0
28	FE	A	414	1/1	0.98	0.03	26,26,26,26	0
28	FE	a	401	1/1	0.99	0.05	39,39,39,39	0

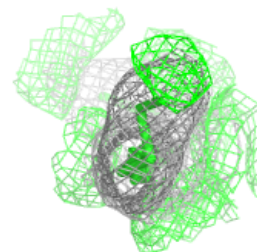
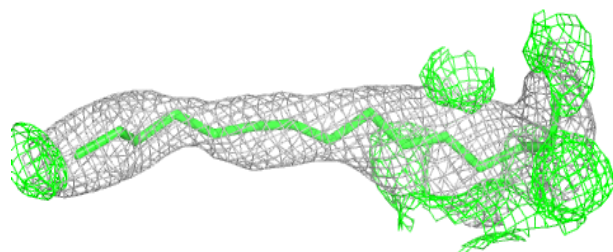
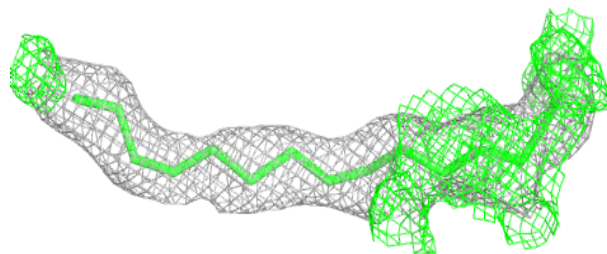
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA A 410:

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

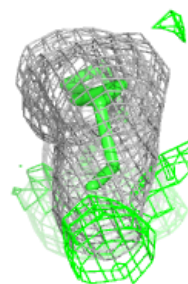
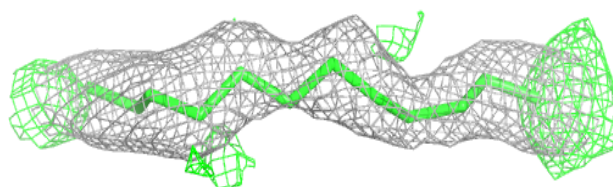
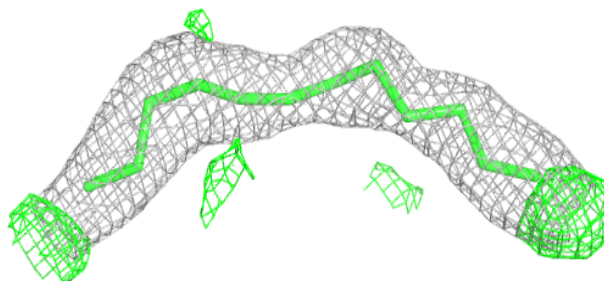
**Electron density around LFA B 624:**

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

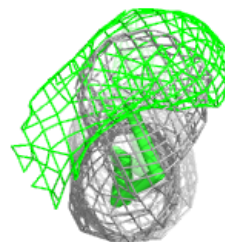
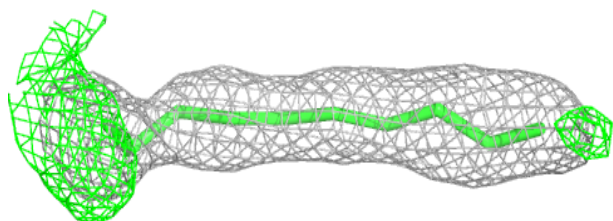
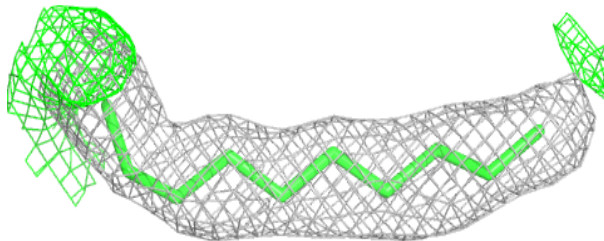


Electron density around LFA b 626:

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

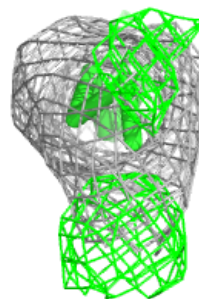
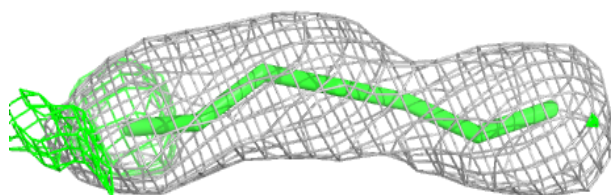
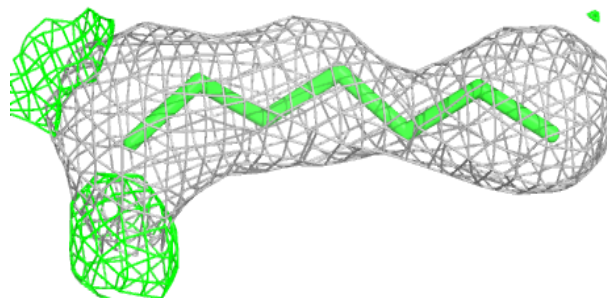
**Electron density around LFA m 101:**

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

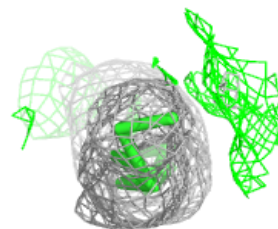
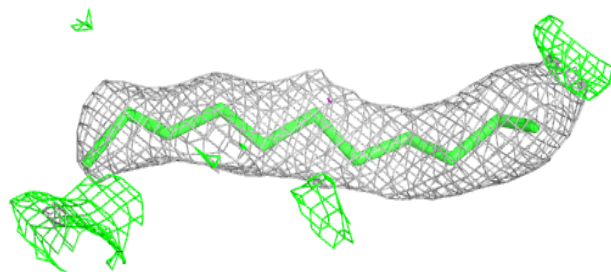
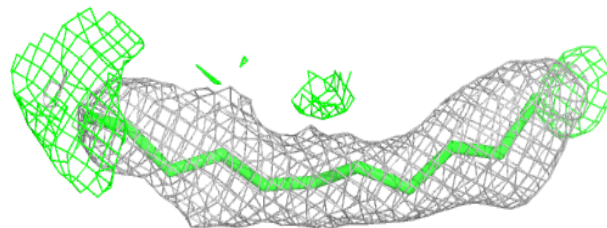


Electron density around LFA i 102:

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

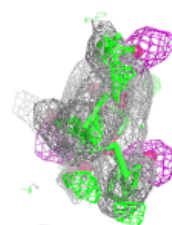
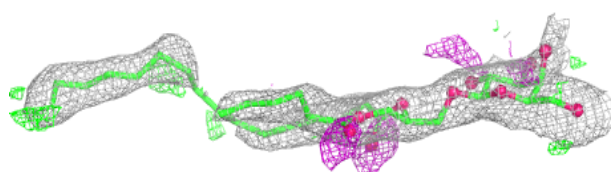
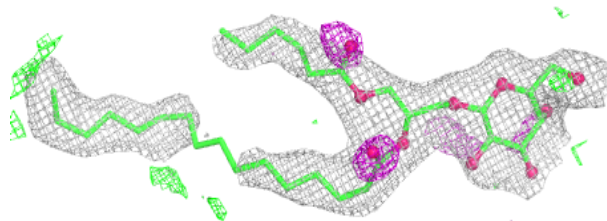
**Electron density around LFA b 627:**

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

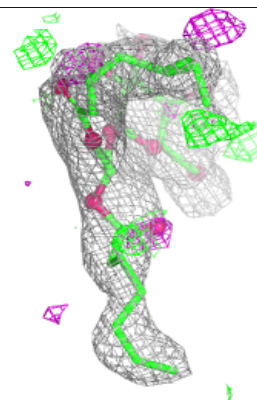
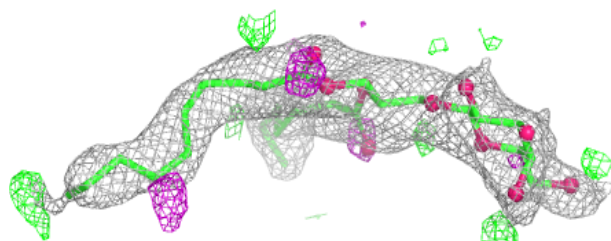
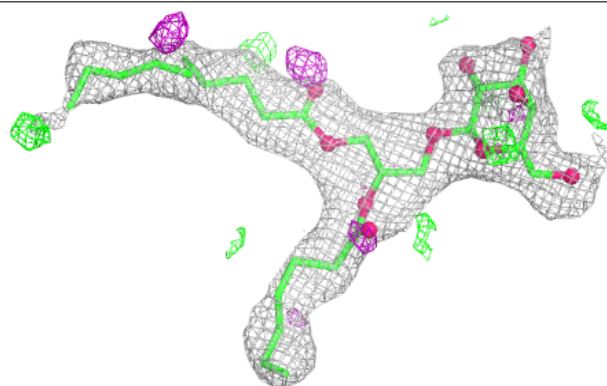


Electron density around LMG c 522:

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

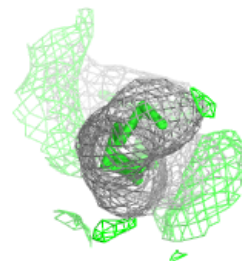
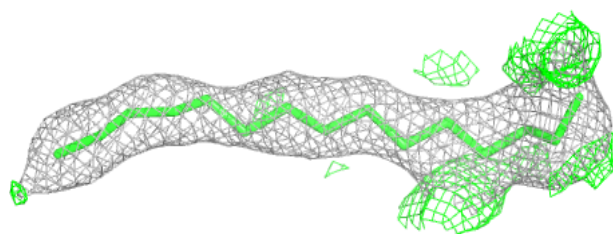
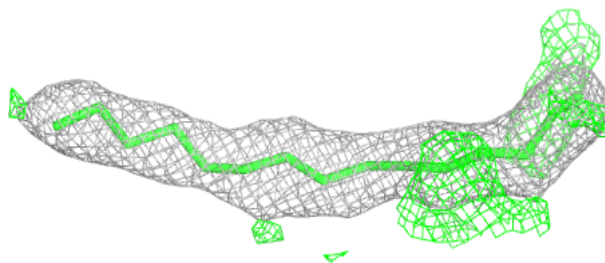
**Electron density around LMG B 621:**

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

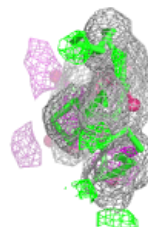
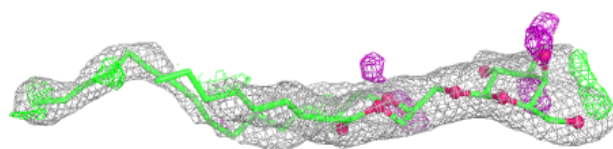
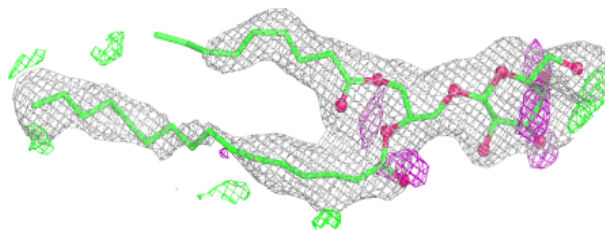


Electron density around LFA b 630:

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

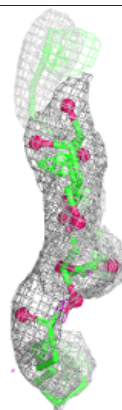
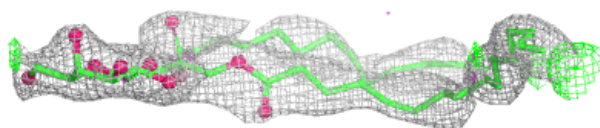
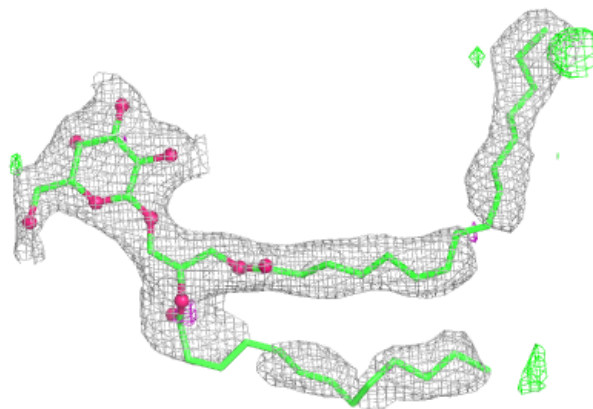
**Electron density around LMG C 522:**

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

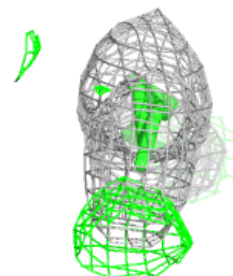
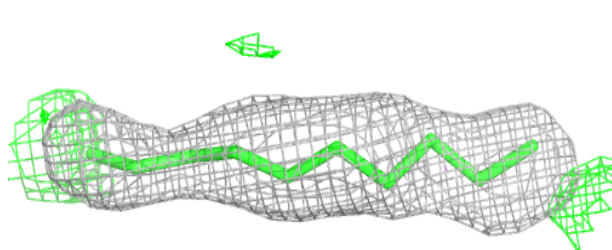
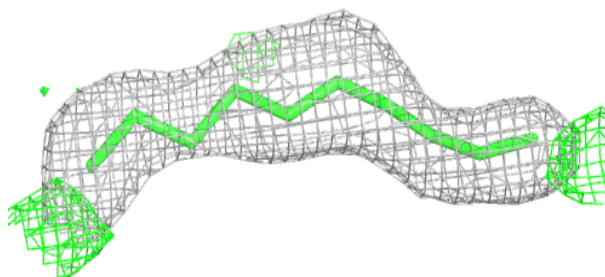


Electron density around LMG C 520:

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

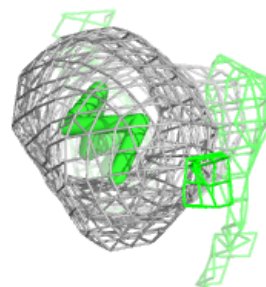
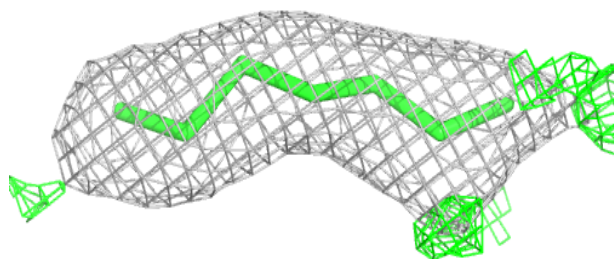
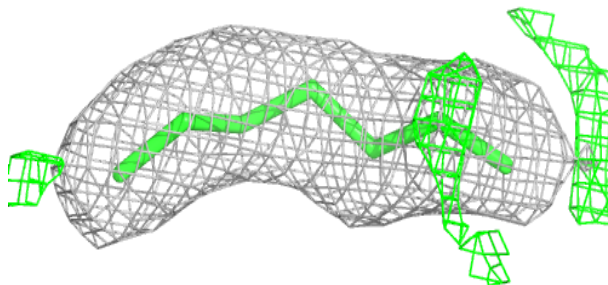
**Electron density around LFA B 626:**

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

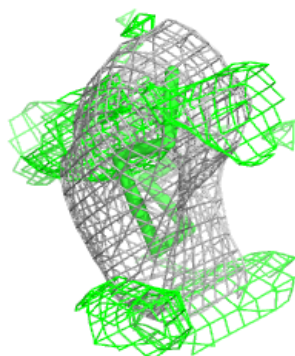
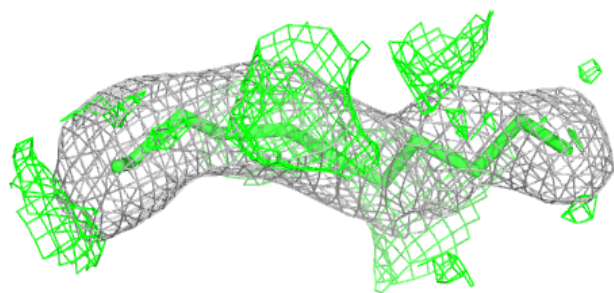
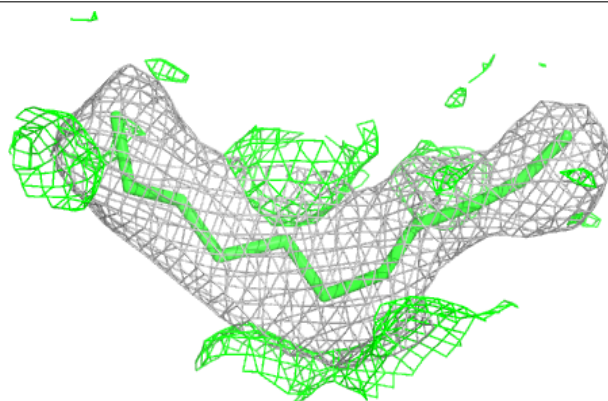


Electron density around LFA a 411:

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

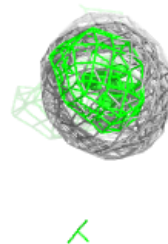
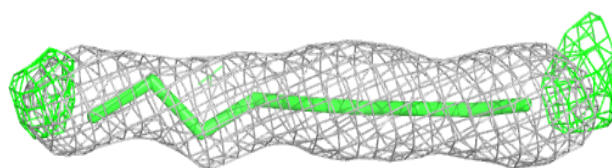
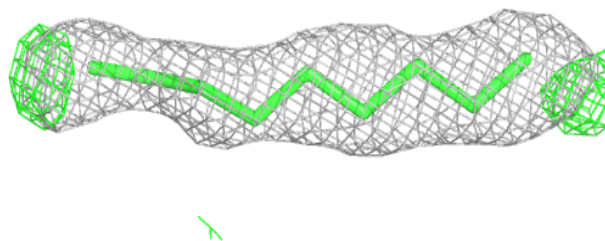
**Electron density around LFA A 413:**

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

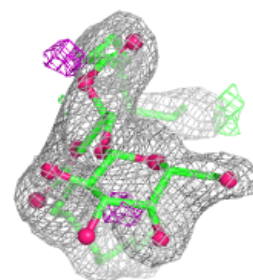
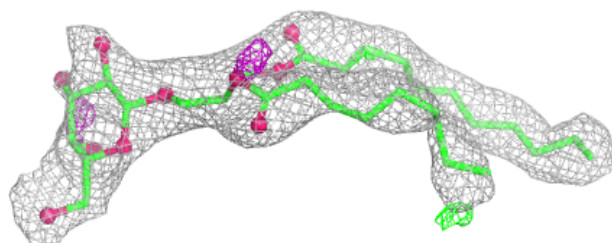
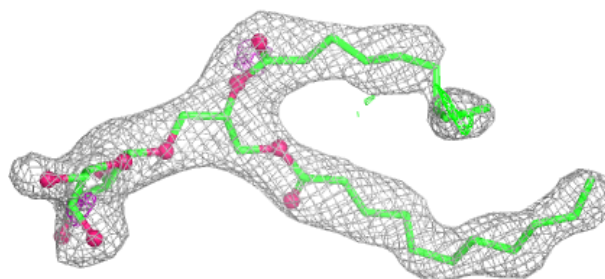


Electron density around LFA d 409:

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

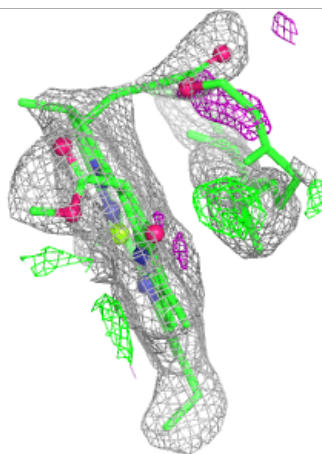
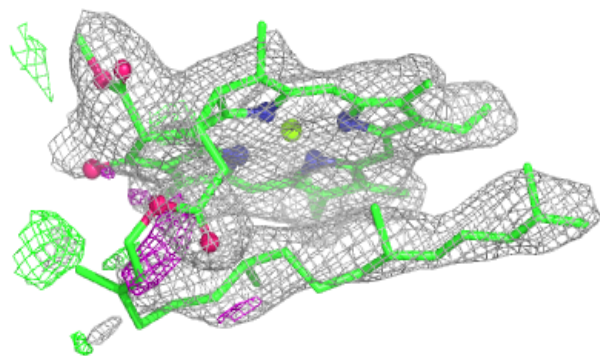
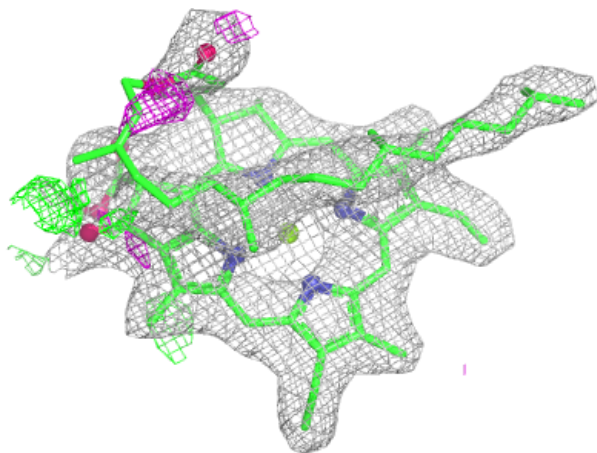
**Electron density around LMG b 624:**

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



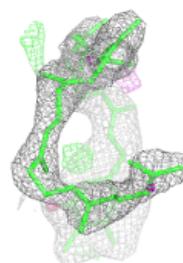
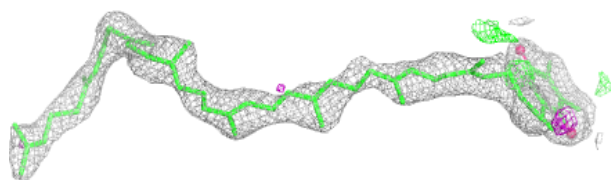
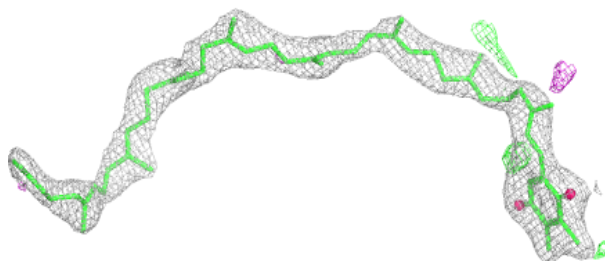
Electron density around CLA b 603:

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

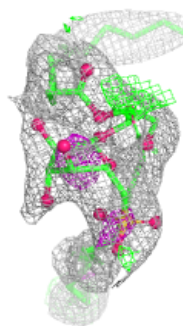
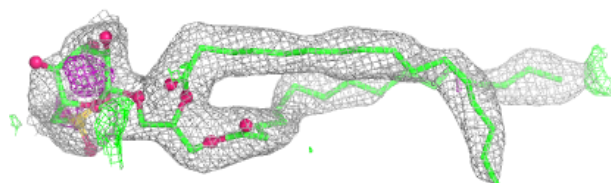
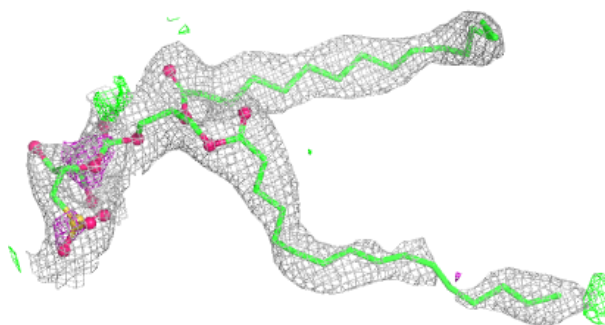


Electron density around PL9 A 408:

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

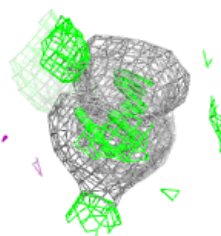
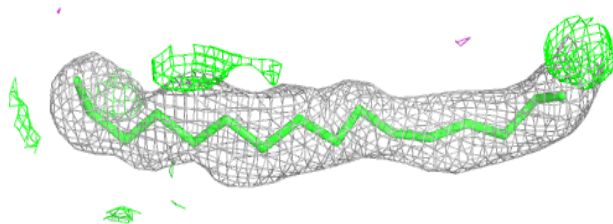
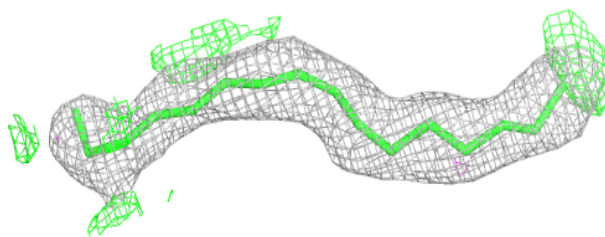
**Electron density around SQD A 411:**

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

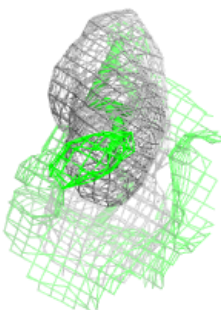
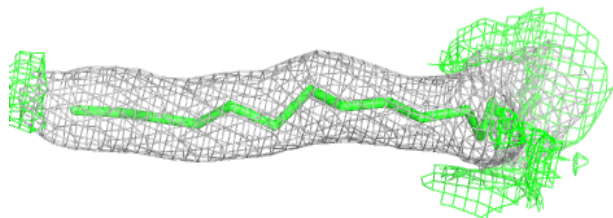
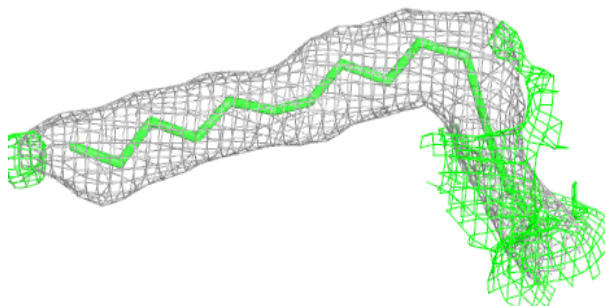


Electron density around LFA b 625:

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

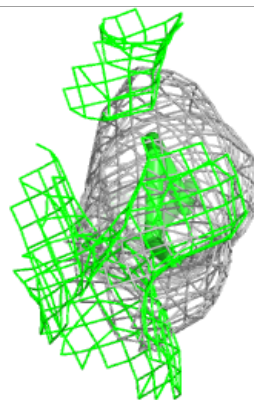
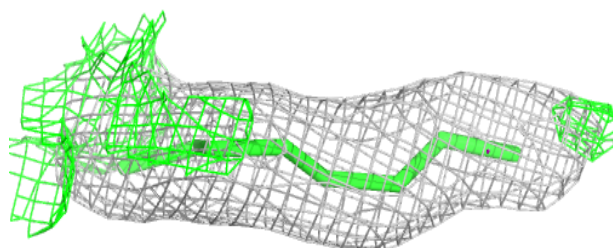
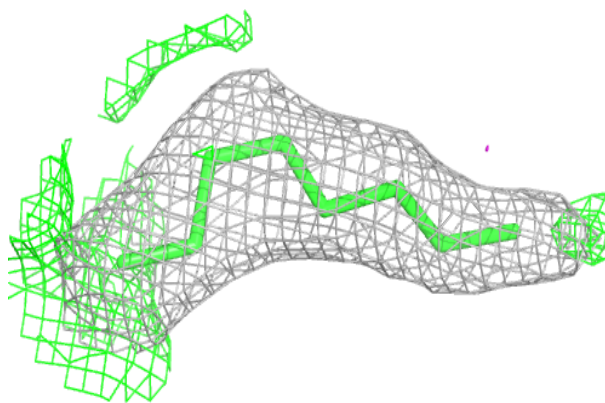
**Electron density around LFA D 411:**

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

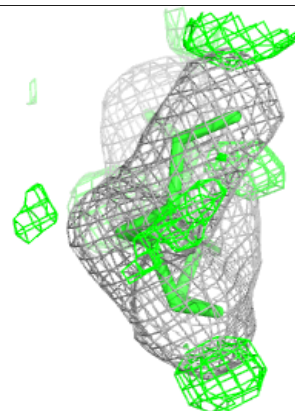
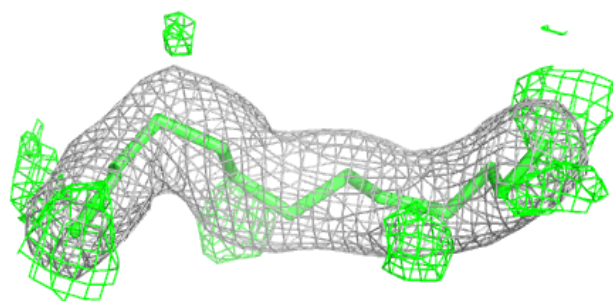
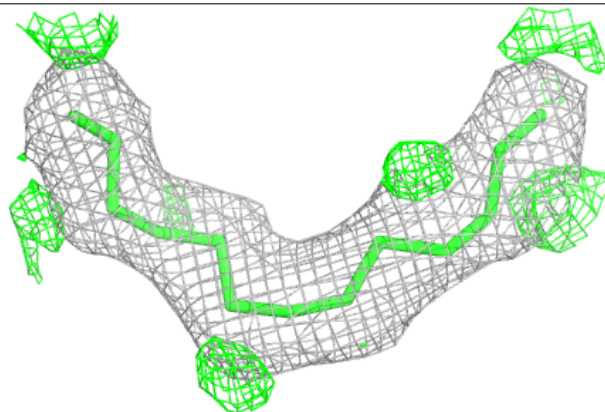


Electron density around LFA D 413:

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

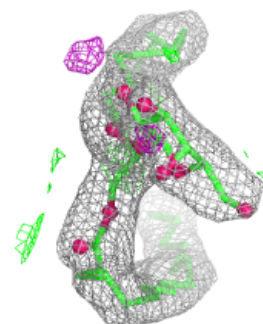
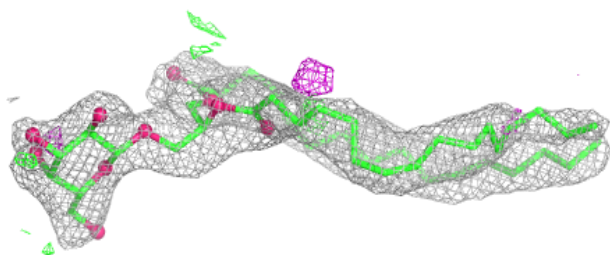
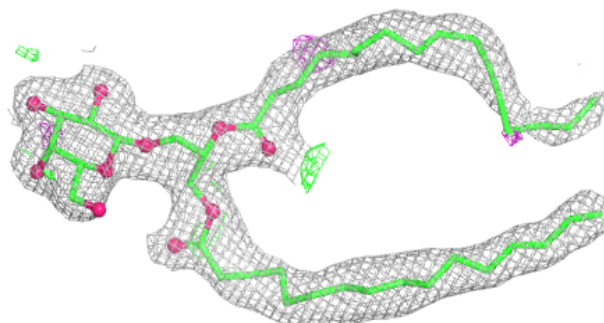
**Electron density around LFA B 623:**

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

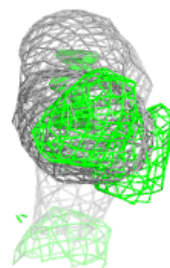
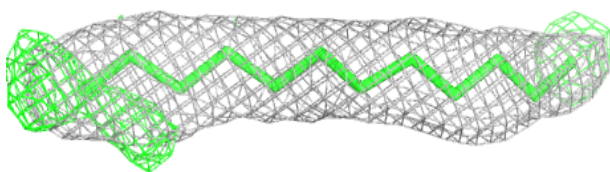
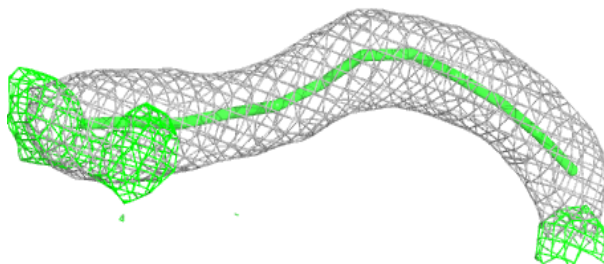


Electron density around LMG C 501:

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

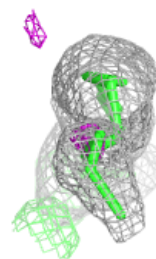
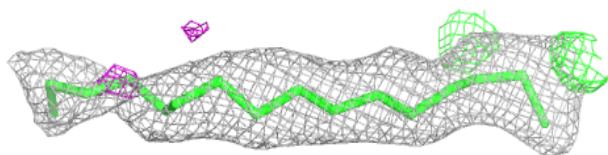
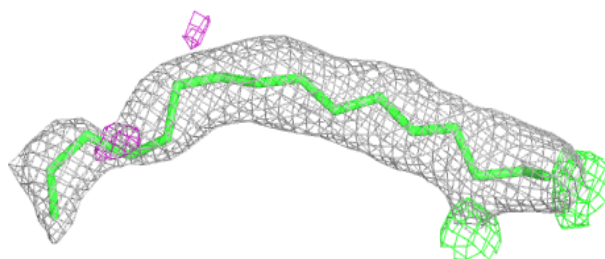
**Electron density around LFA B 628:**

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

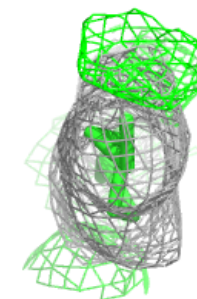
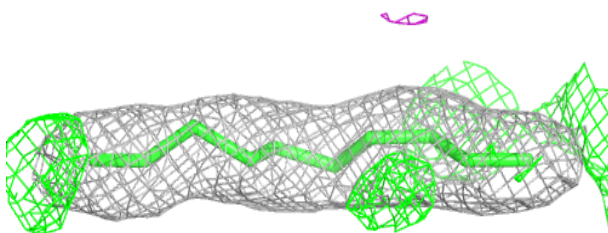
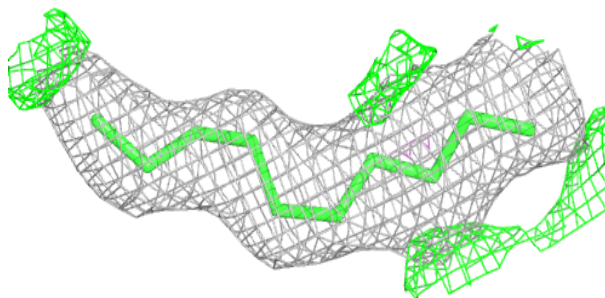


Electron density around LFA i 101:

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

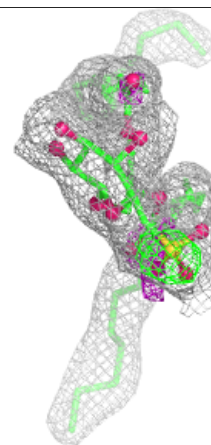
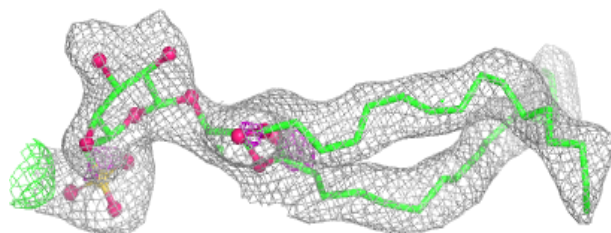
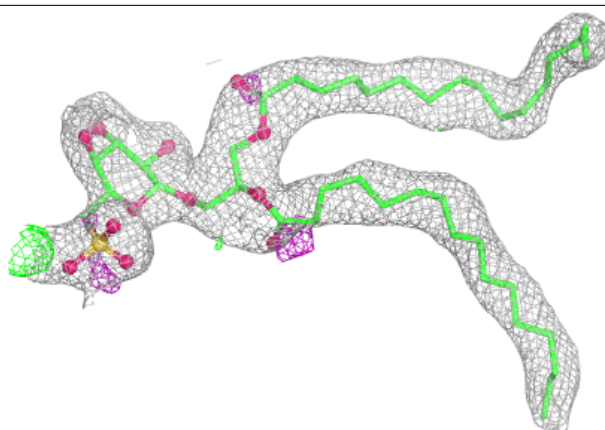
**Electron density around LFA b 622:**

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

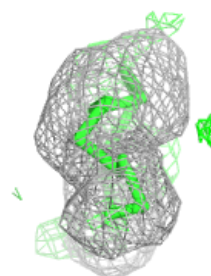
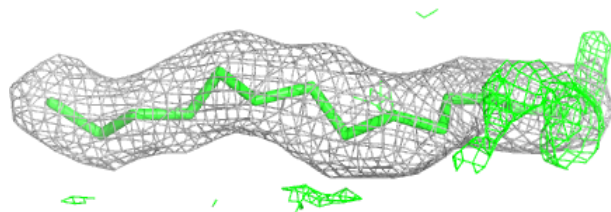


Electron density around SQD b 601:

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

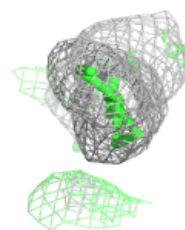
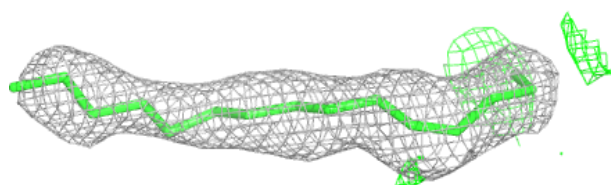
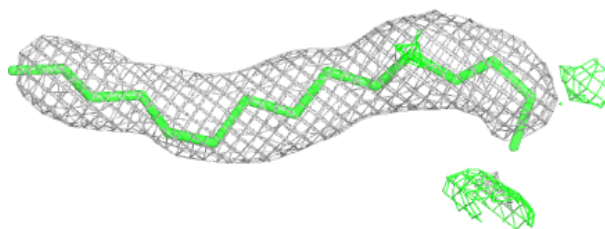
**Electron density around LFA B 627:**

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



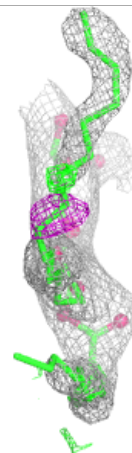
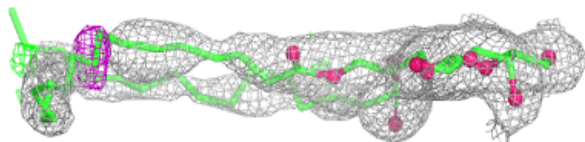
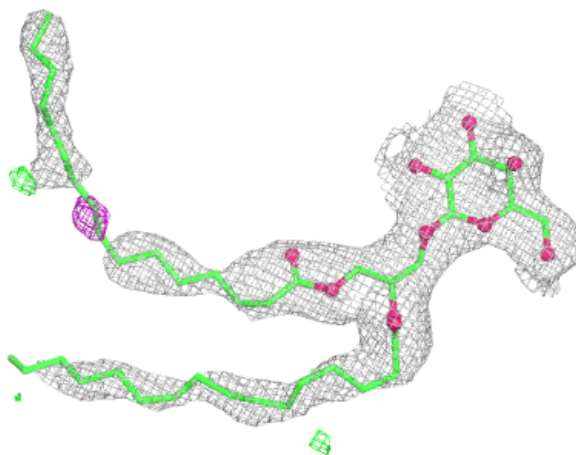
Electron density around LFA j 101:

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



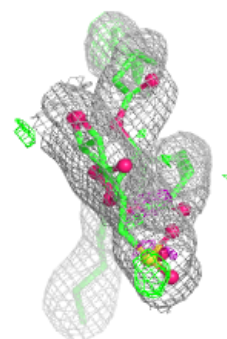
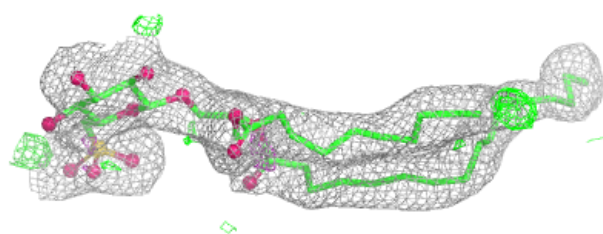
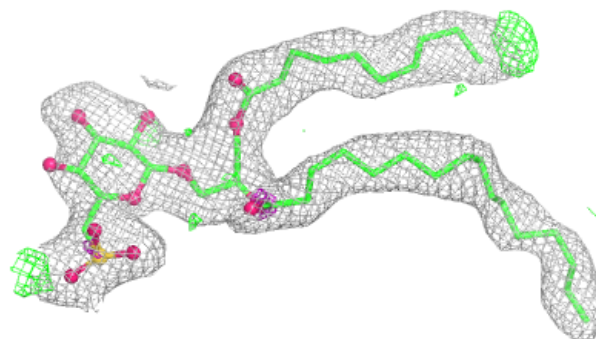
Electron density around LMG c 519:

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

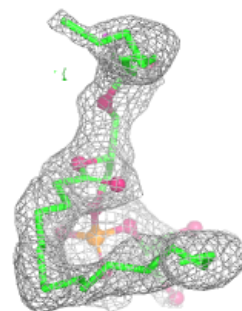
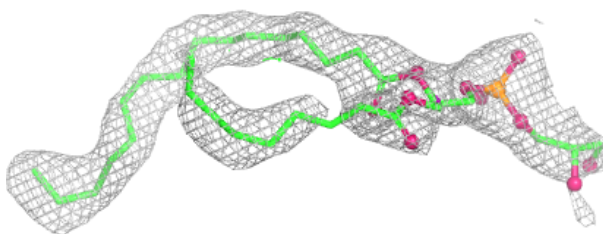
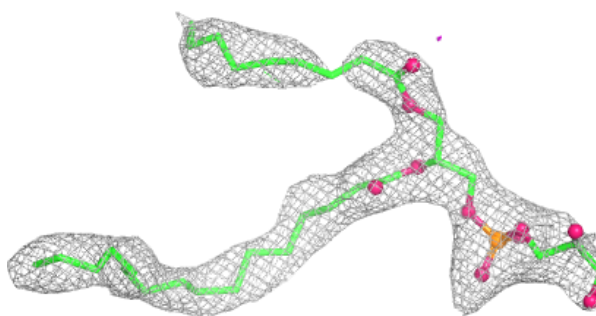


Electron density around SQD L 101:

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

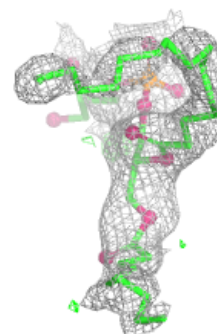
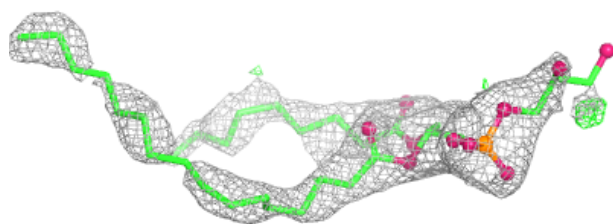
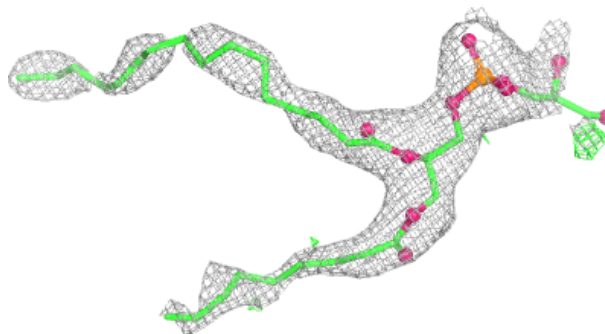
**Electron density around LHG E 101:**

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

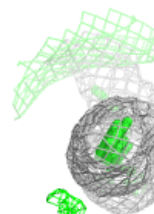
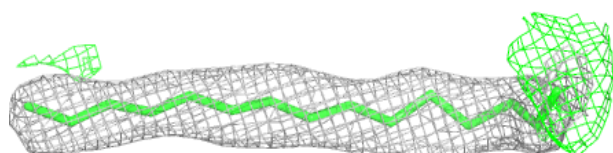
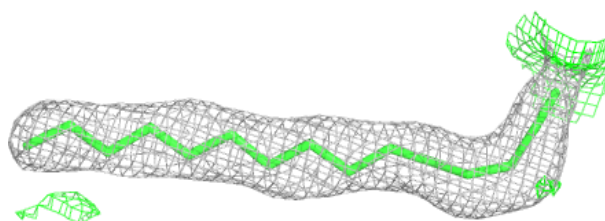


Electron density around LHG e 101:

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

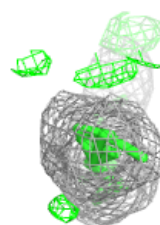
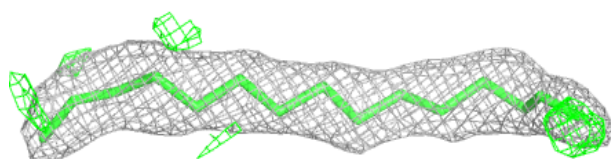
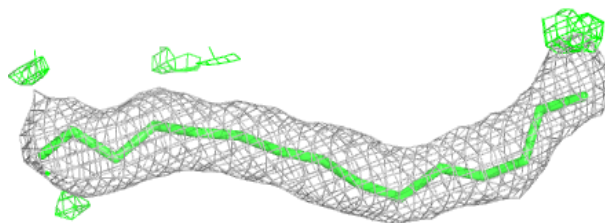
**Electron density around LFA d 408:**

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

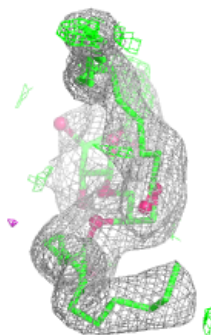
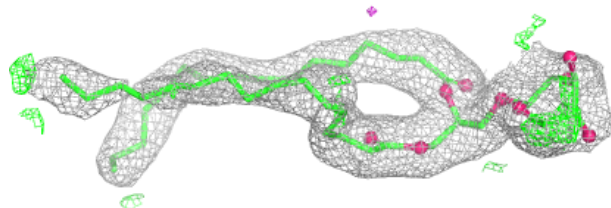
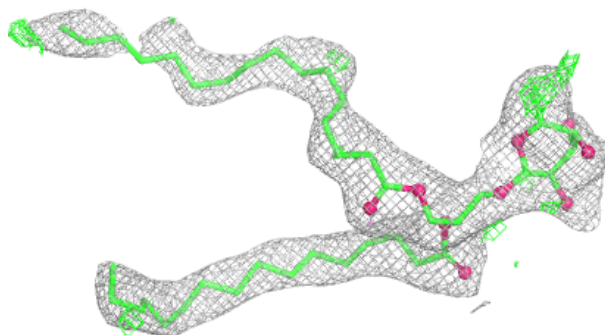


Electron density around LFA b 602:

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

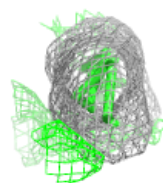
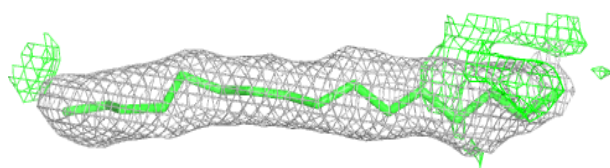
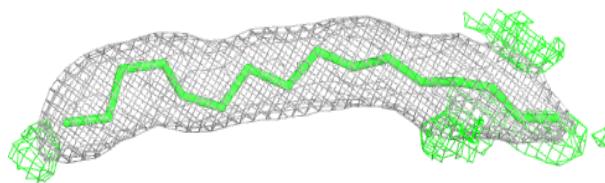
**Electron density around SQD a 412:**

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

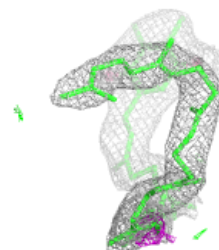
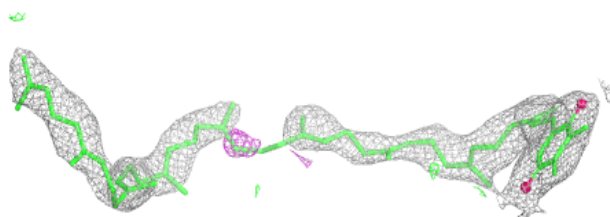
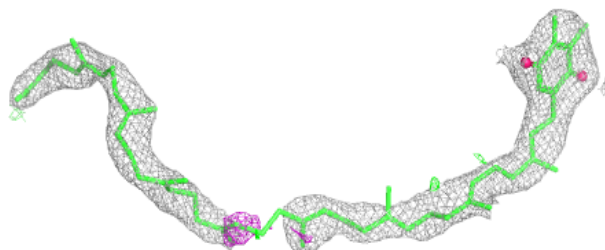


Electron density around LFA M 102:

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

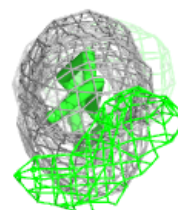
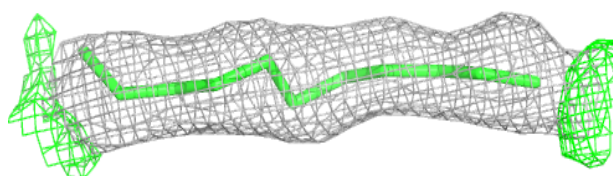
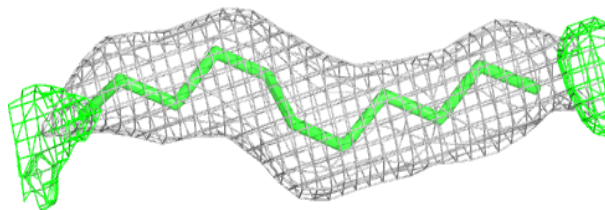
**Electron density around PL9 a 409:**

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

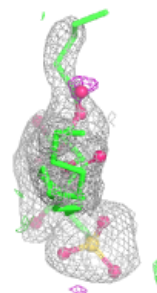
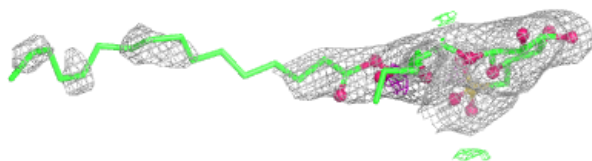
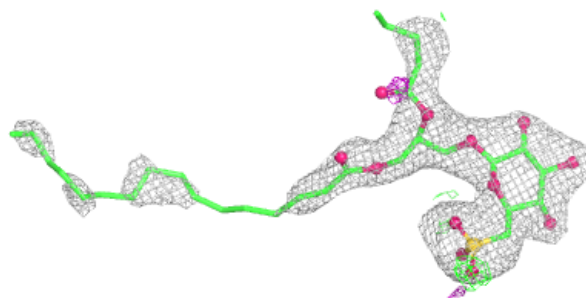


Electron density around LFA J 101:

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

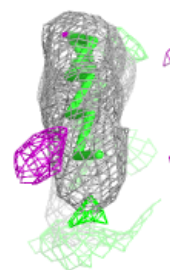
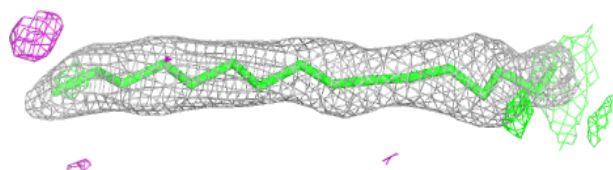
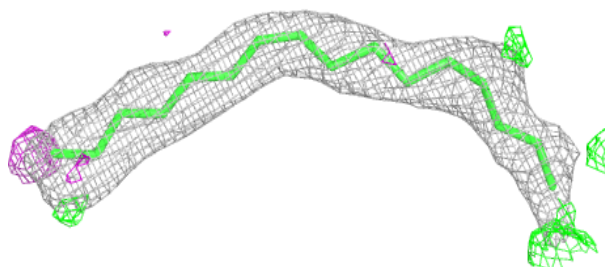
**Electron density around SQD f 102:**

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

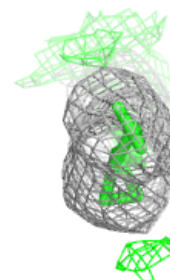
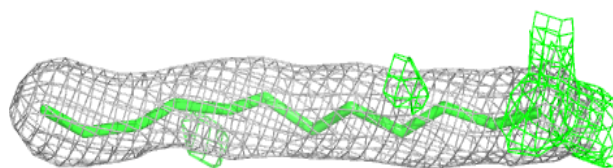
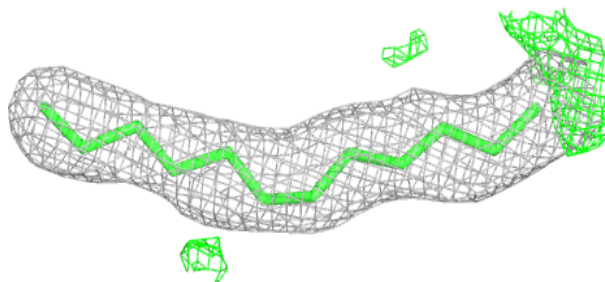


Electron density around LFA d 410:

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

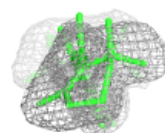
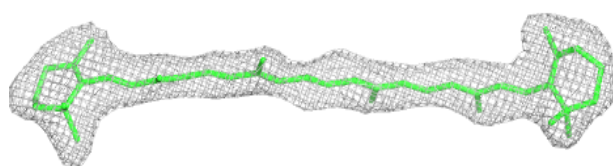
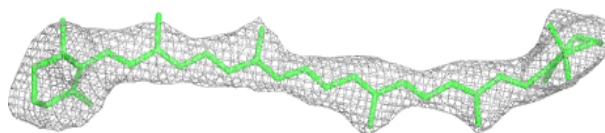
**Electron density around LFA T 102:**

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

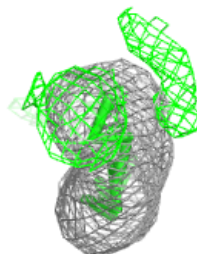
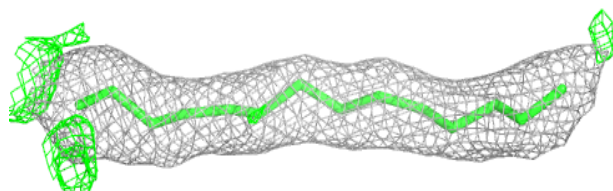
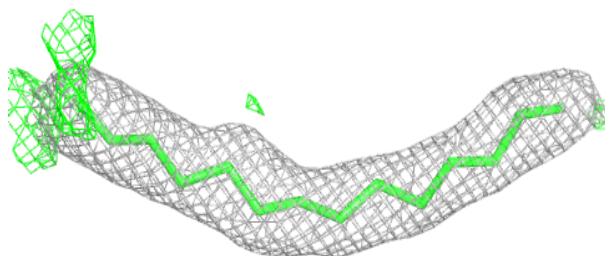


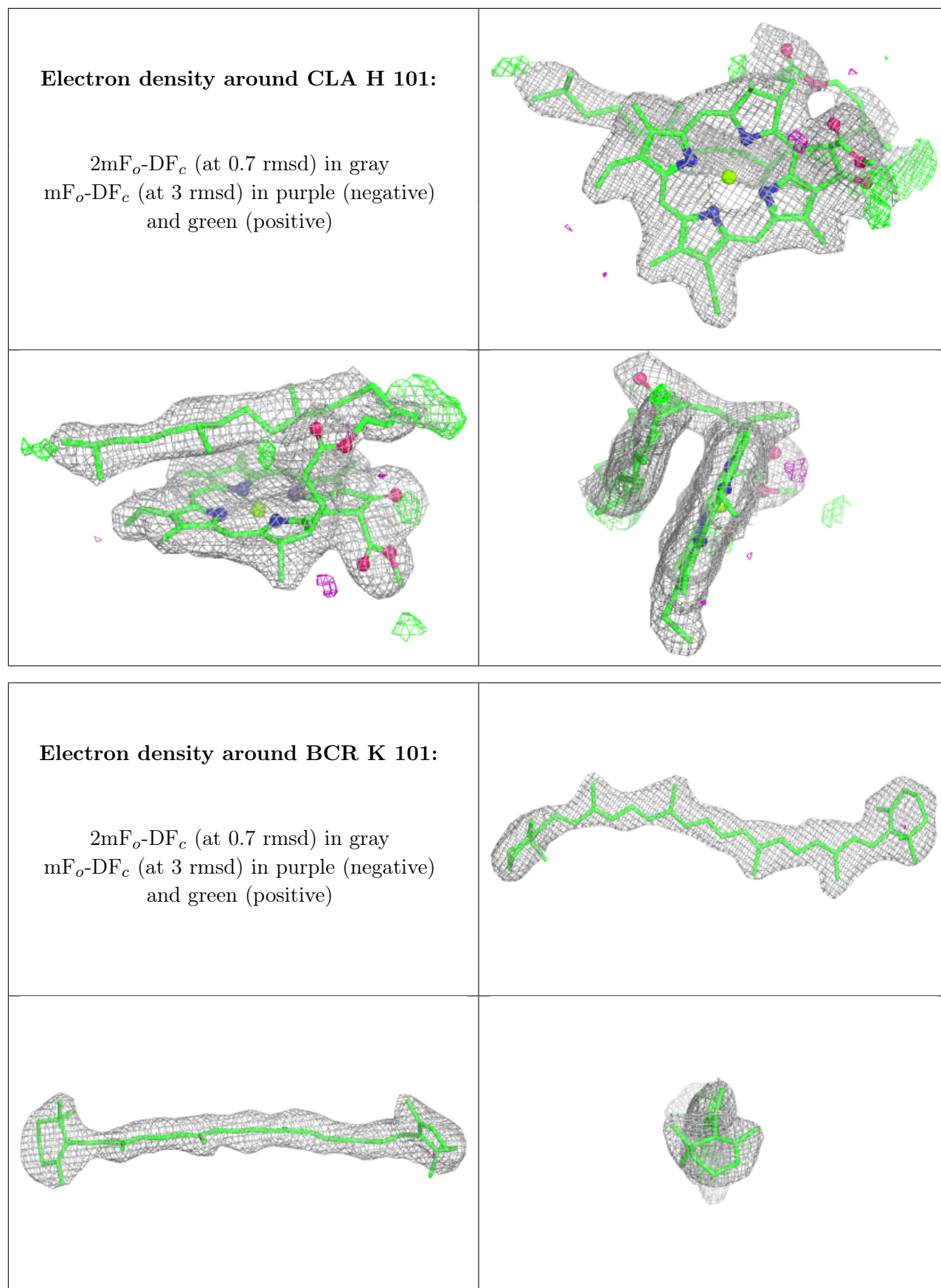
Electron density around BCR c 524:

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

**Electron density around LFA I 101:**

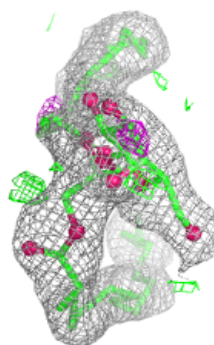
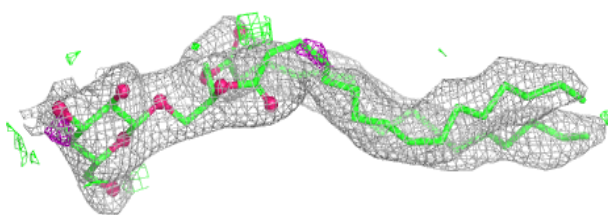
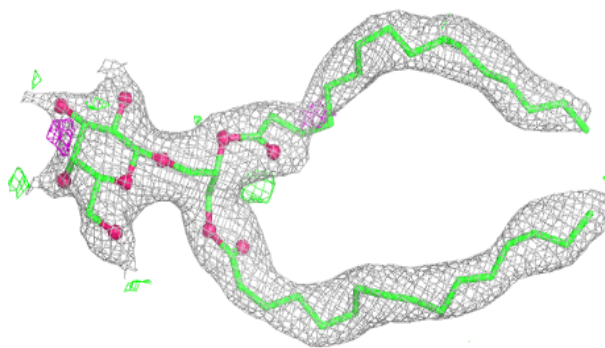
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



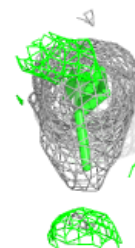
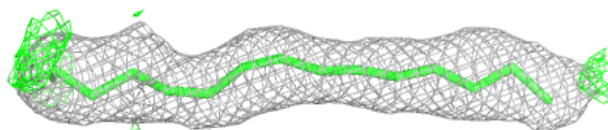
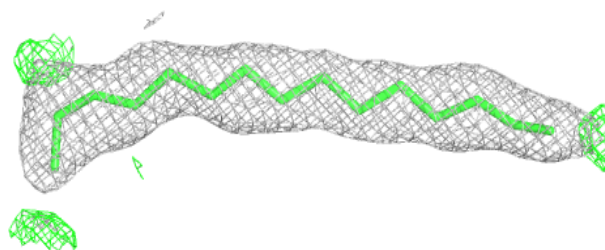


Electron density around LMG c 501:

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

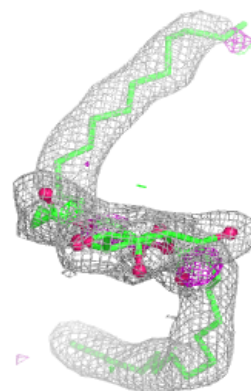
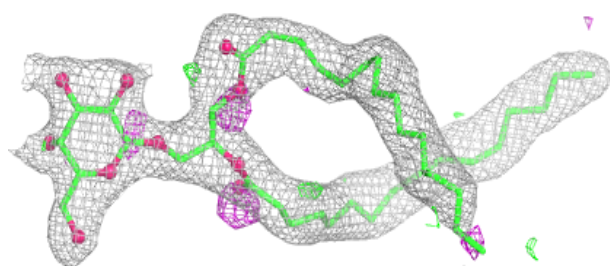
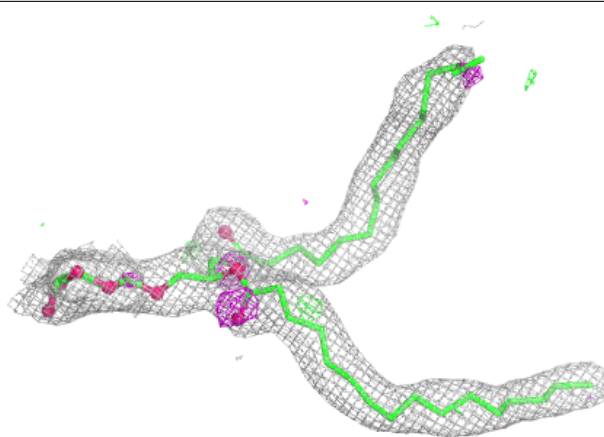
**Electron density around LFA c 521:**

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

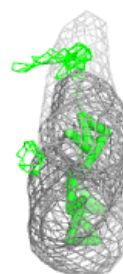
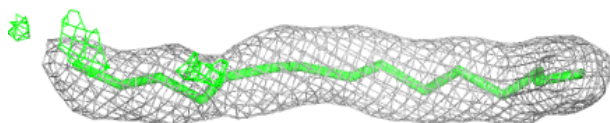
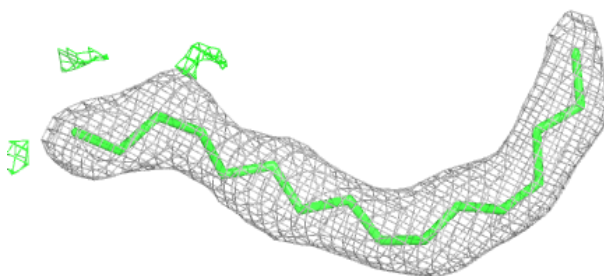


Electron density around LMG B 619:

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

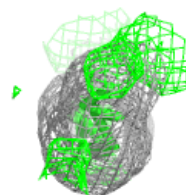
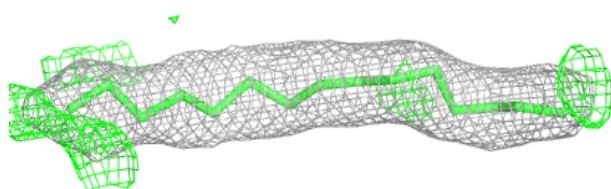
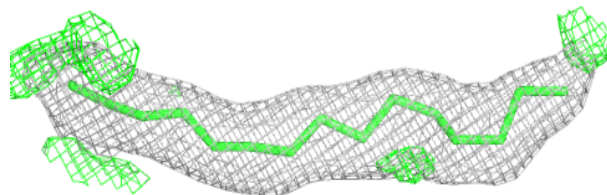
**Electron density around LFA B 622:**

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

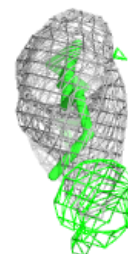
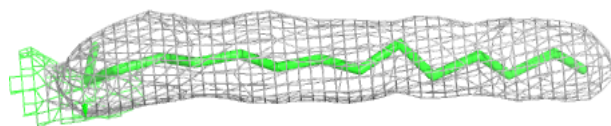
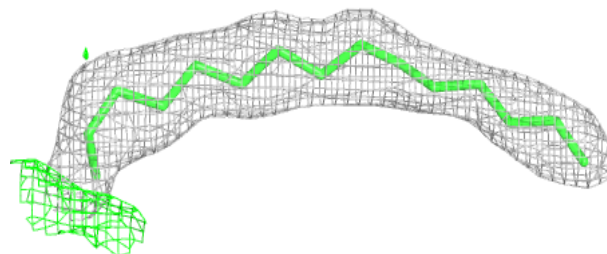


Electron density around LFA m 102:

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

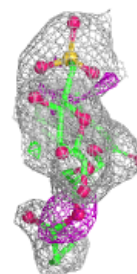
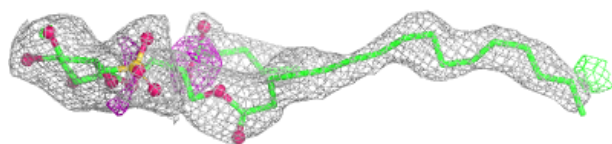
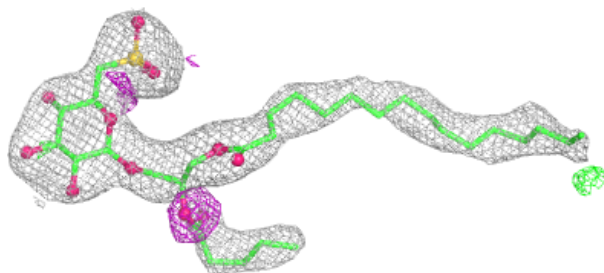
**Electron density around LFA t 101:**

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

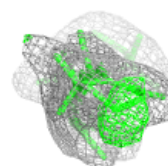
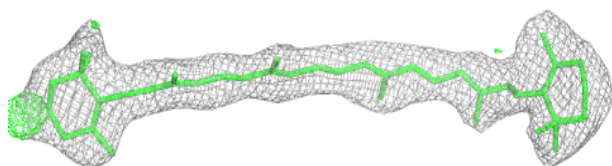
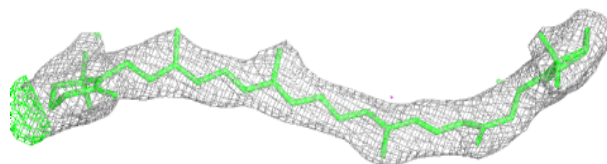


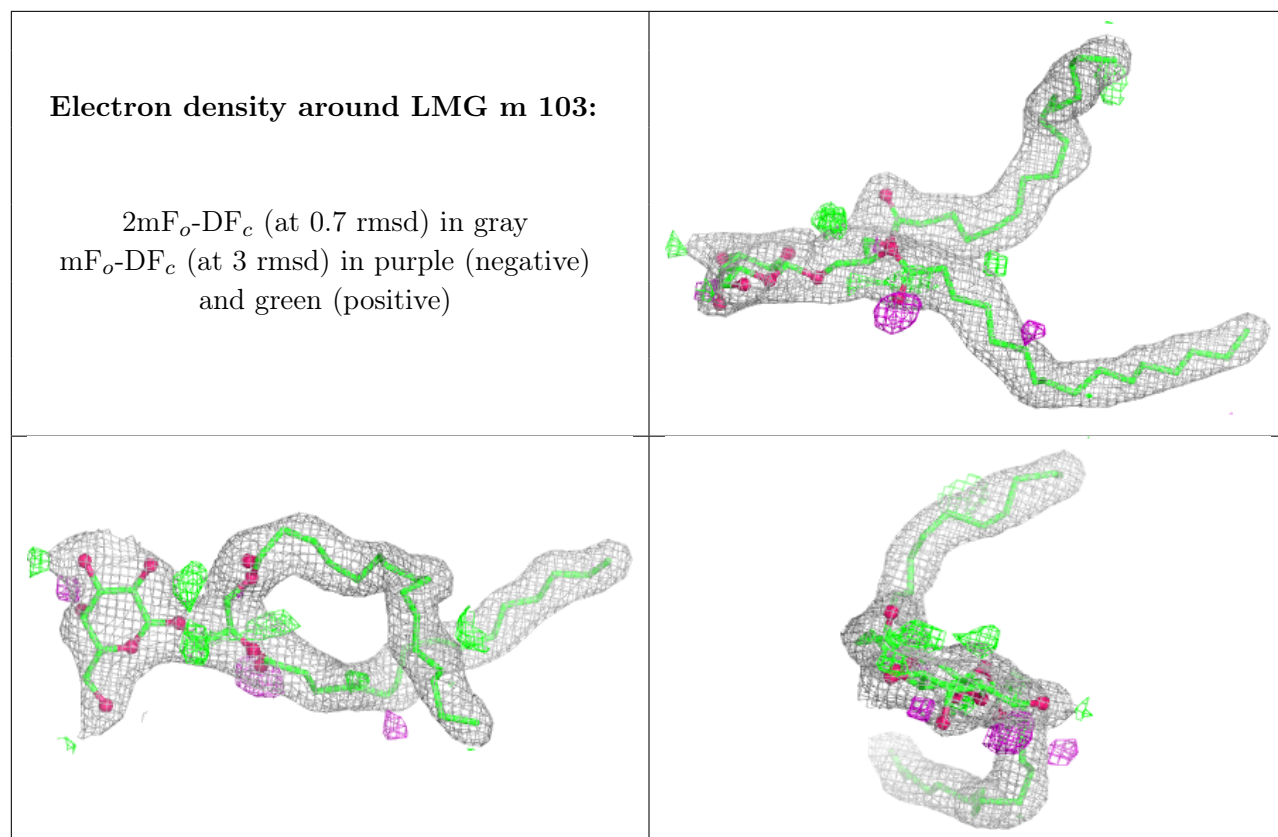
Electron density around SQD D 412:

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

**Electron density around BCR h 101:**

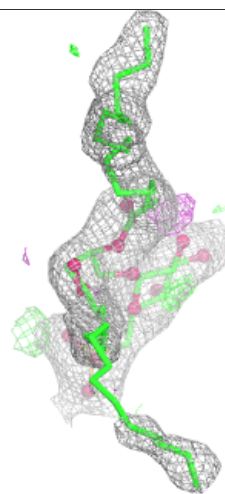
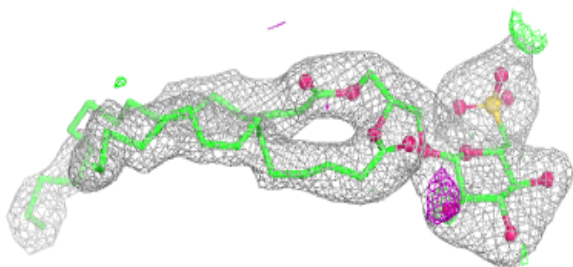
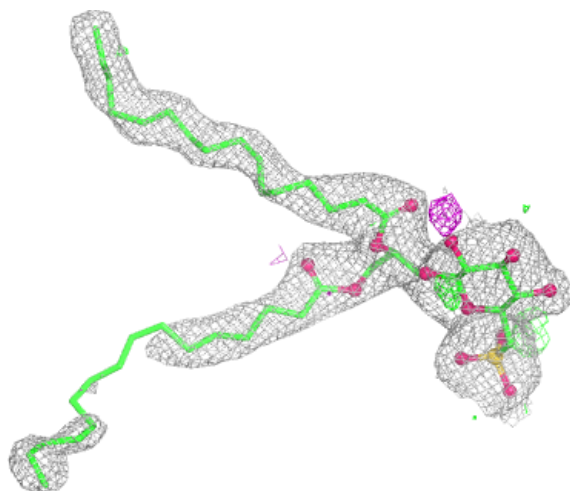
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

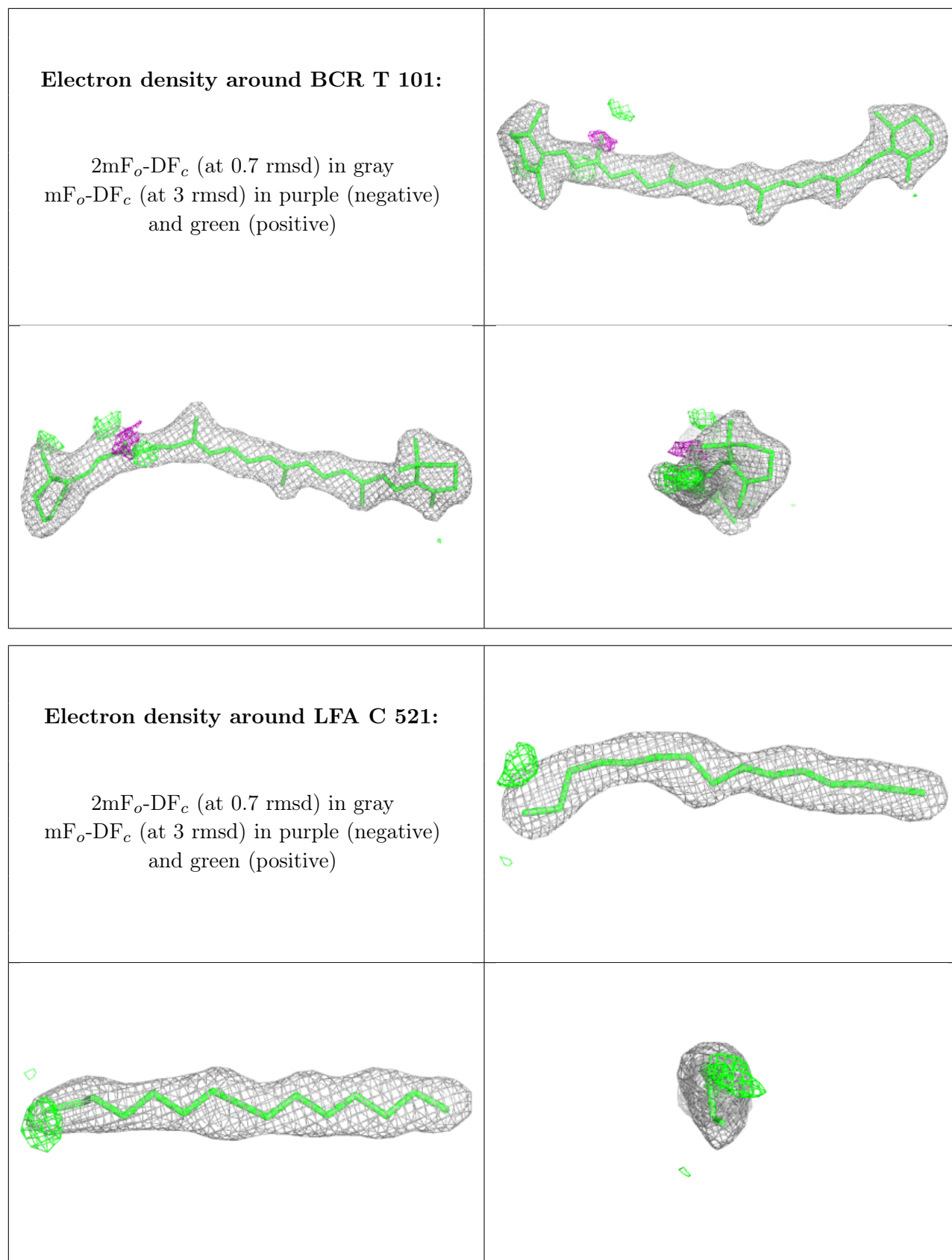


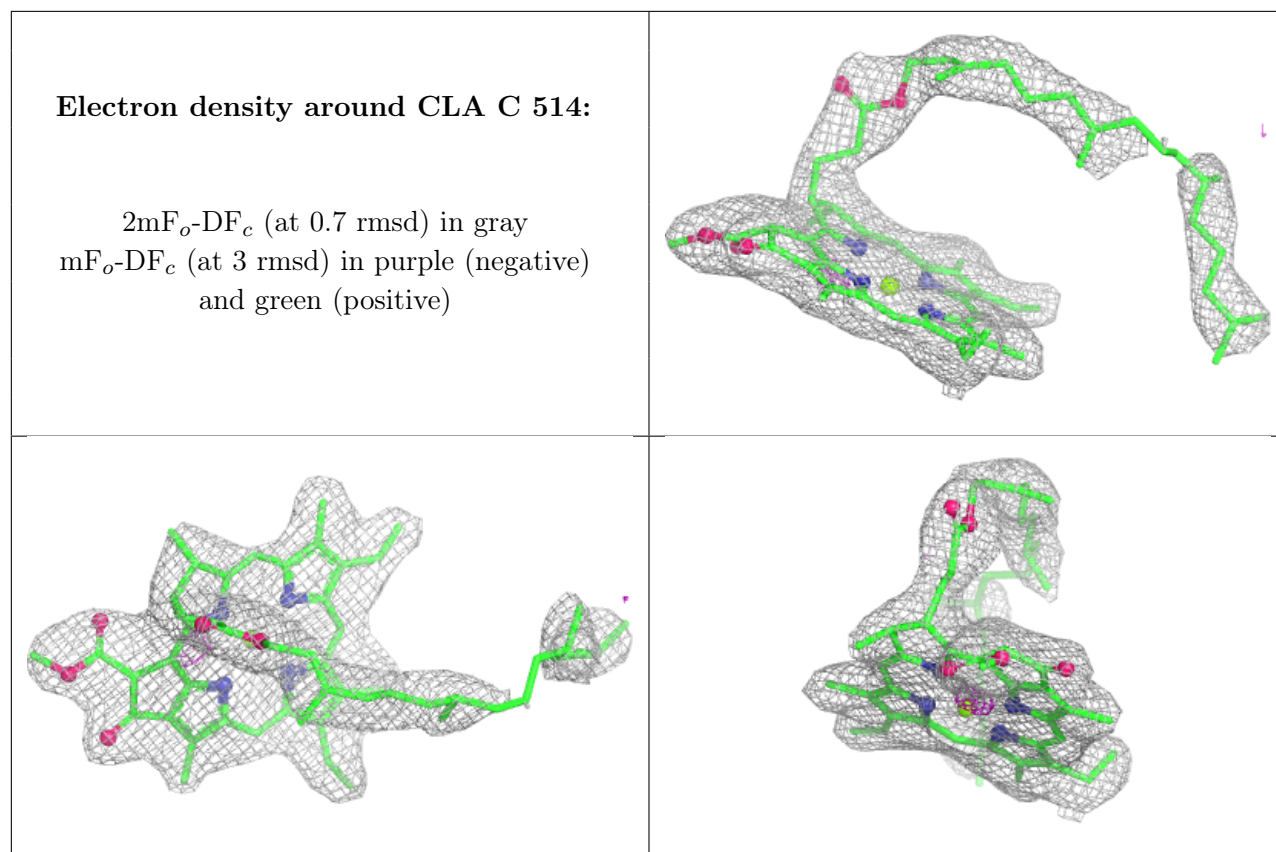


Electron density around SQD a 410:

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

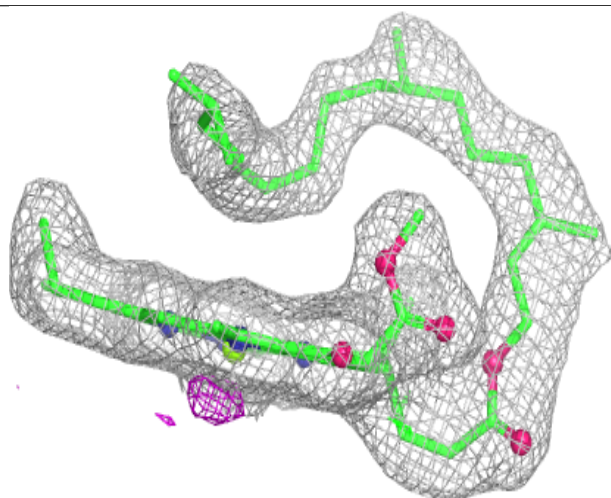
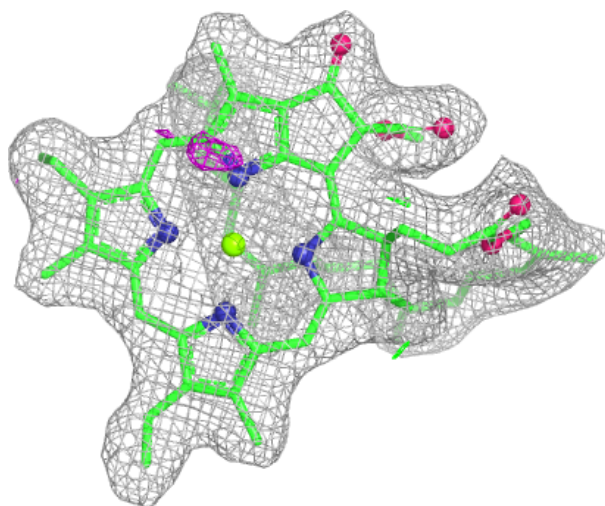


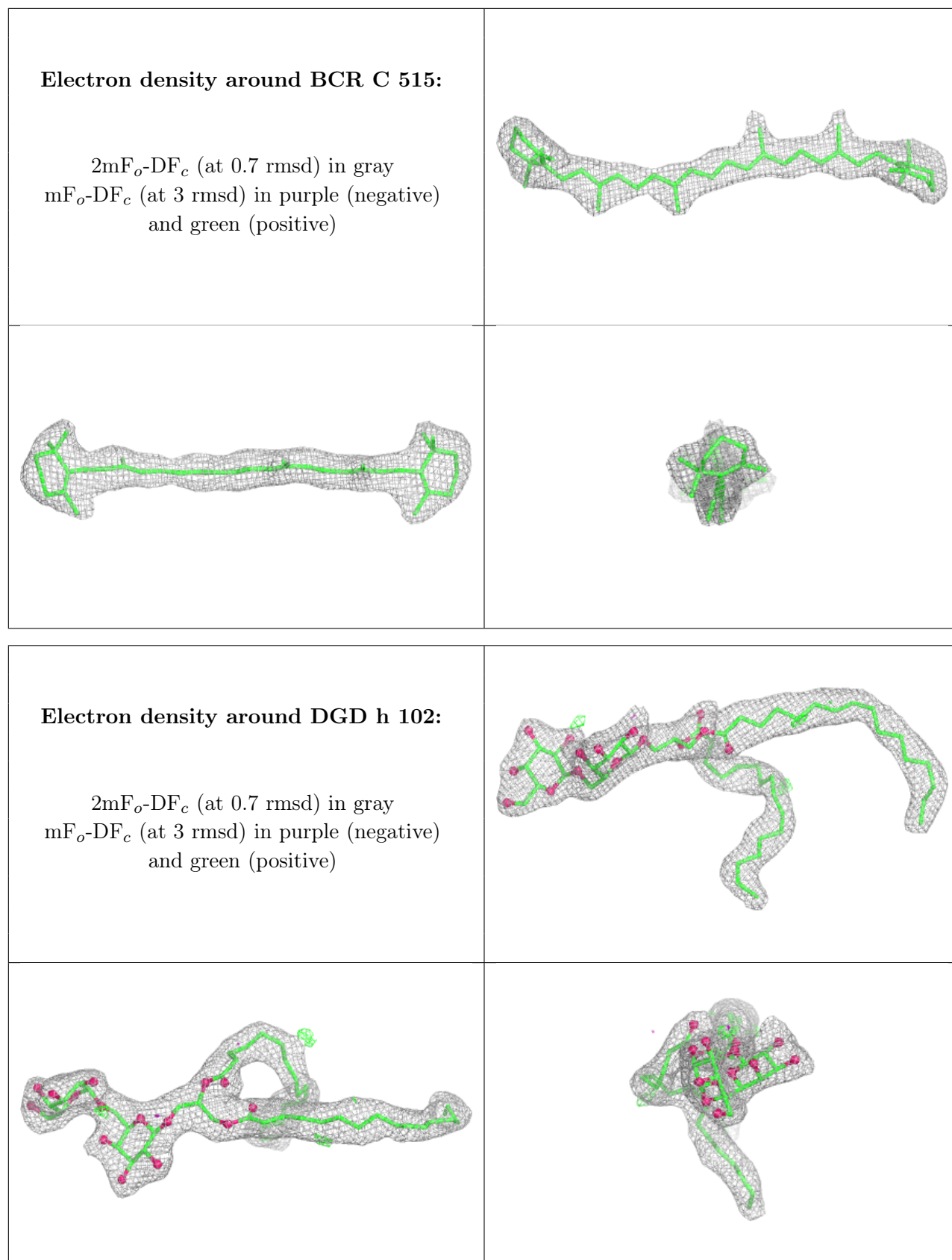




Electron density around CLA C 511:

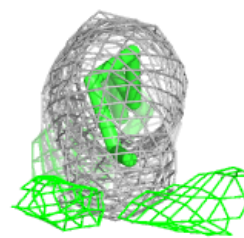
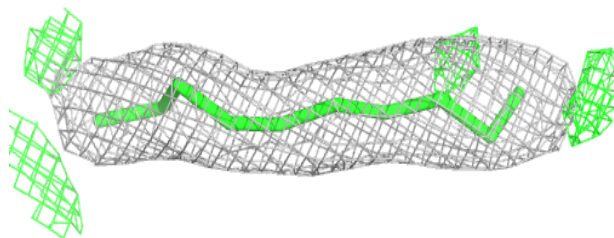
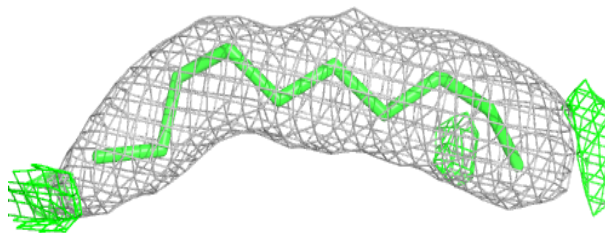
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





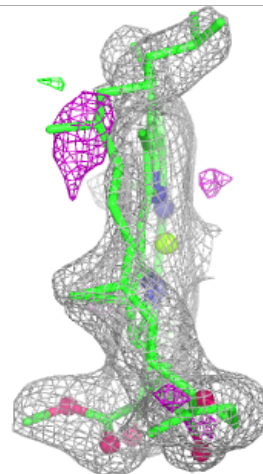
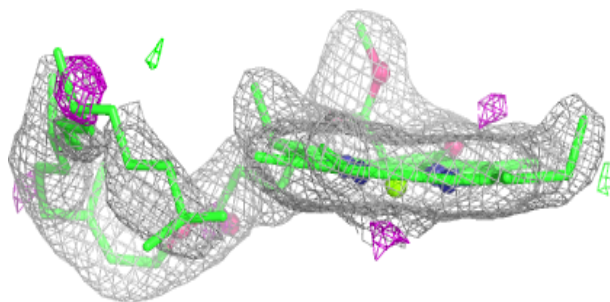
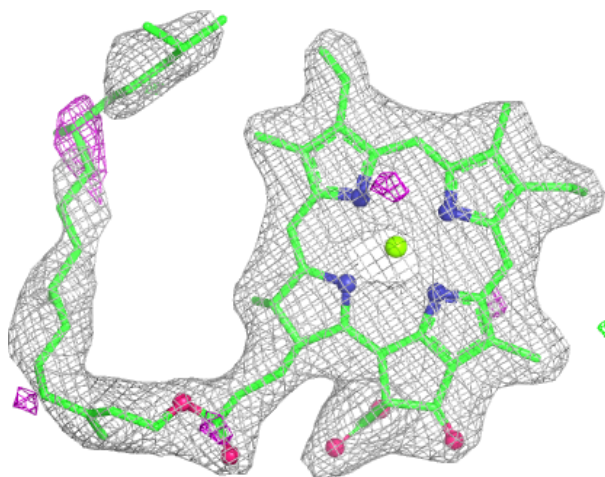
Electron density around LFA B 620:

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



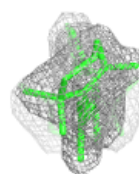
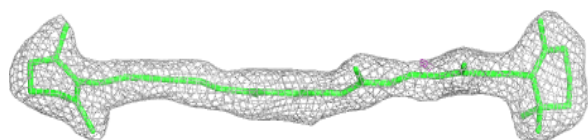
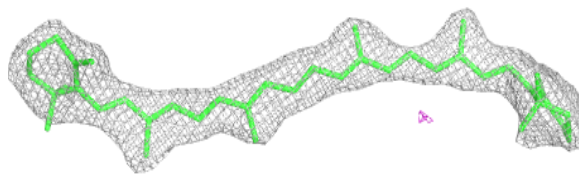
Electron density around CLA C 513:

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

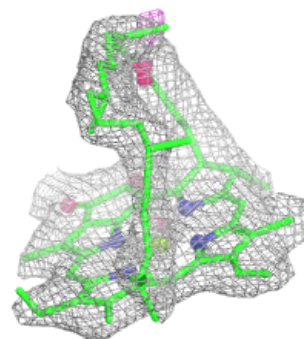
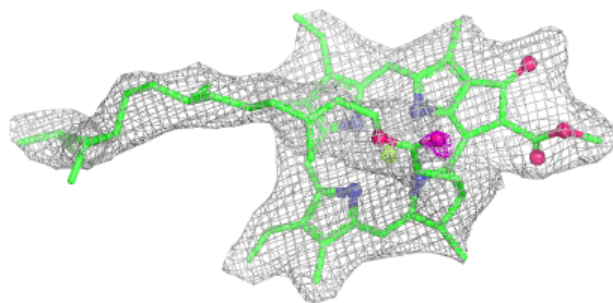
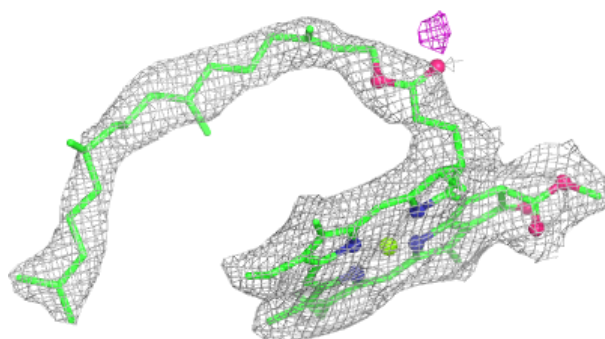


Electron density around BCR c 523:

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

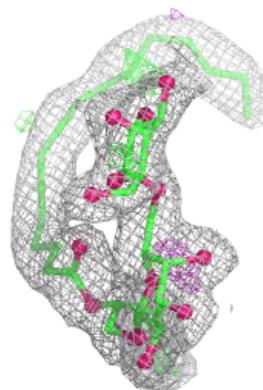
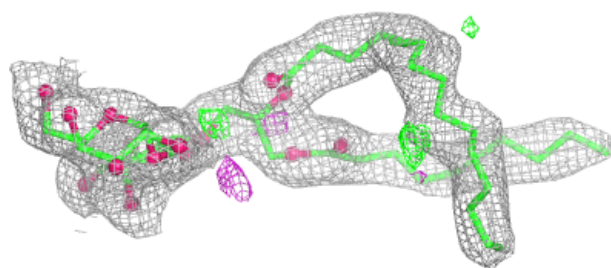
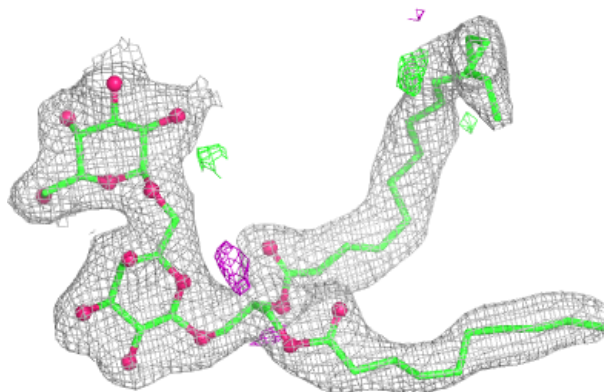
**Electron density around CLA c 514:**

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

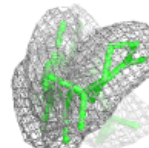
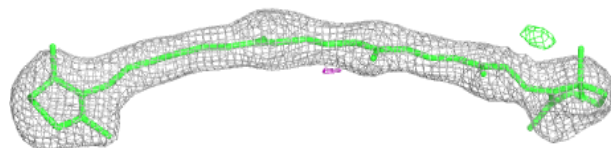


Electron density around DGD C 518:

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

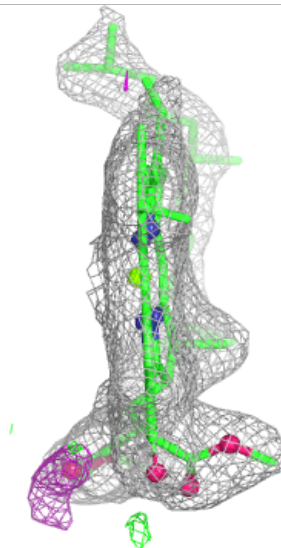
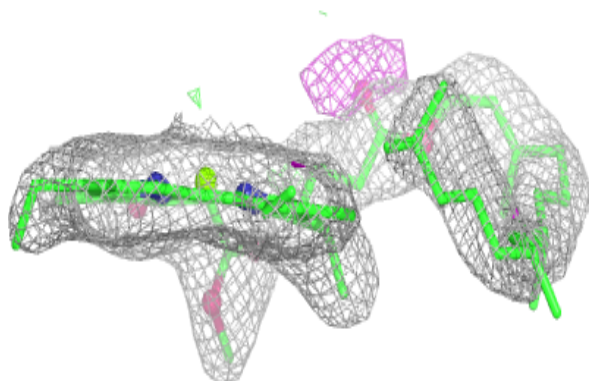
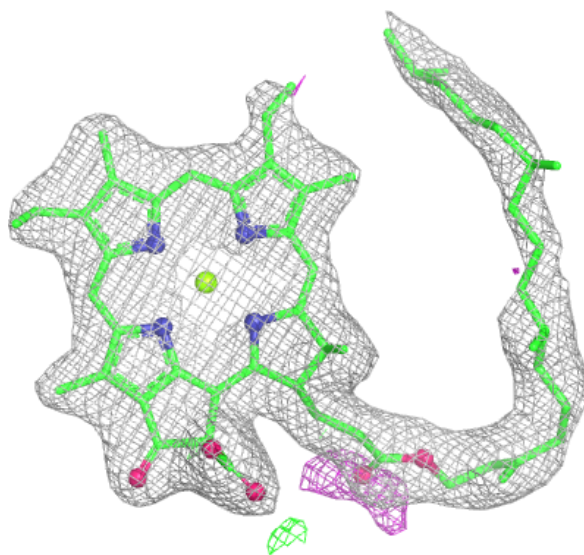
**Electron density around BCR d 404:**

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



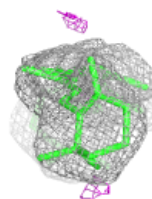
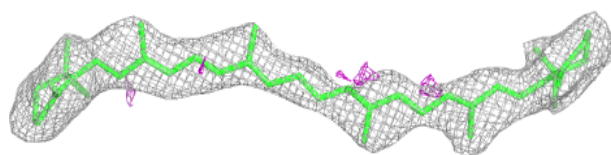
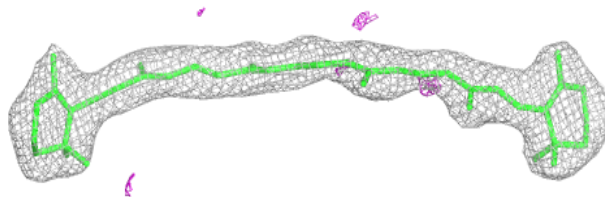
Electron density around CLA c 513:

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

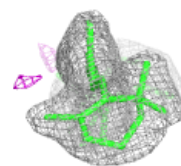
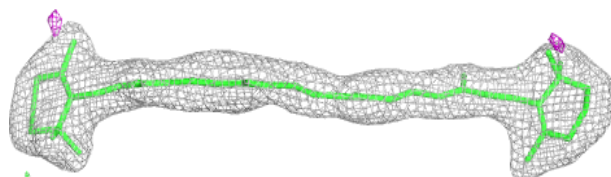
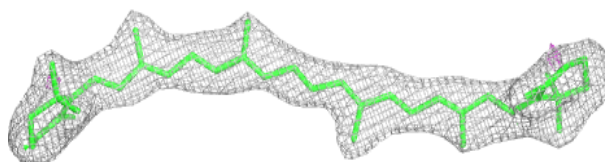


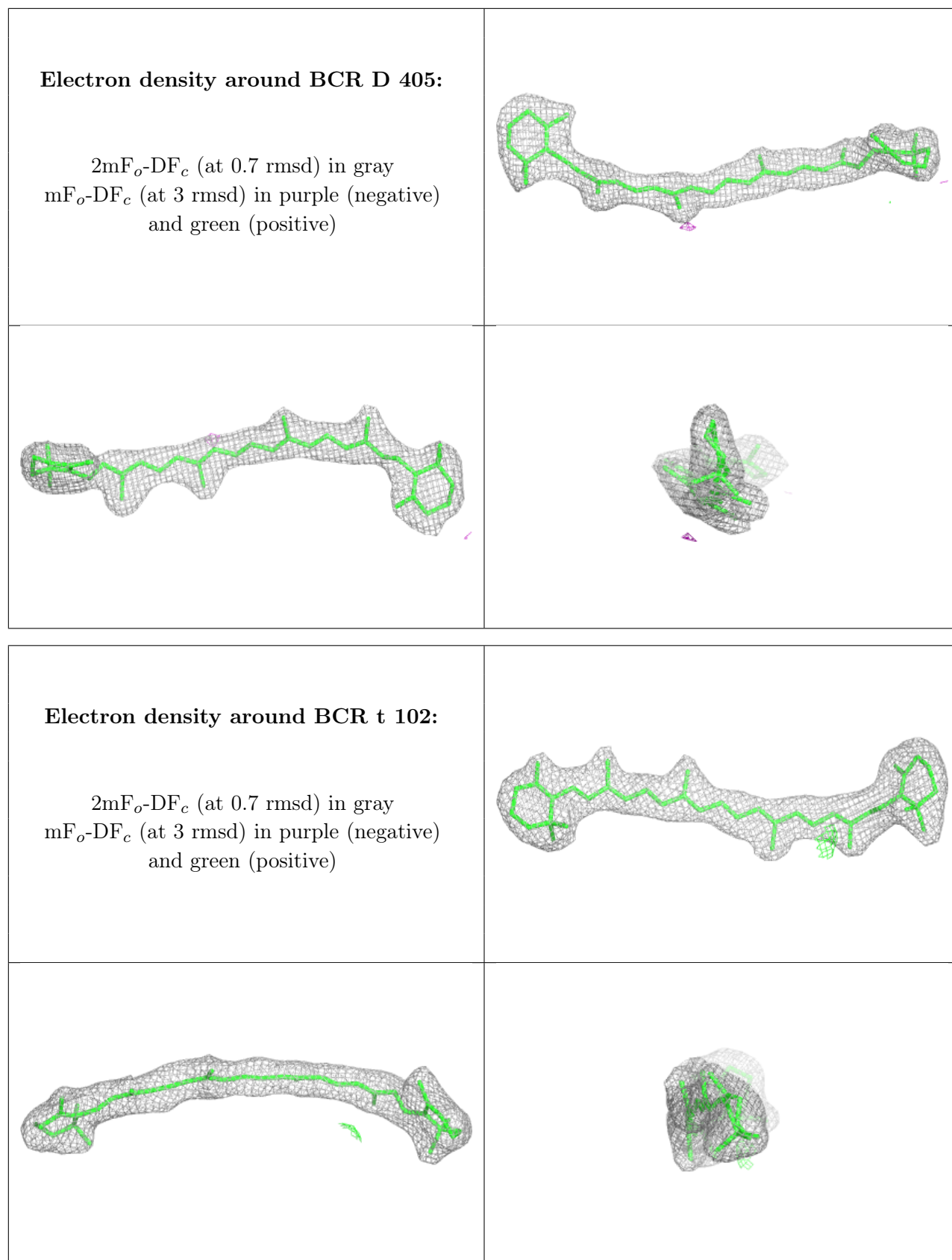
Electron density around BCR k 101:

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

**Electron density around BCR C 516:**

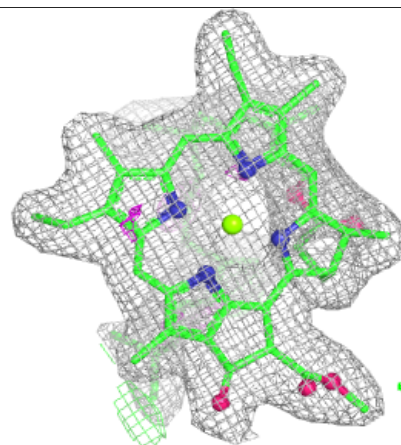
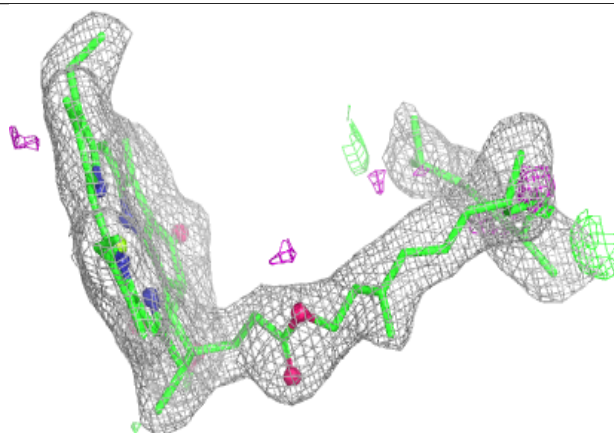
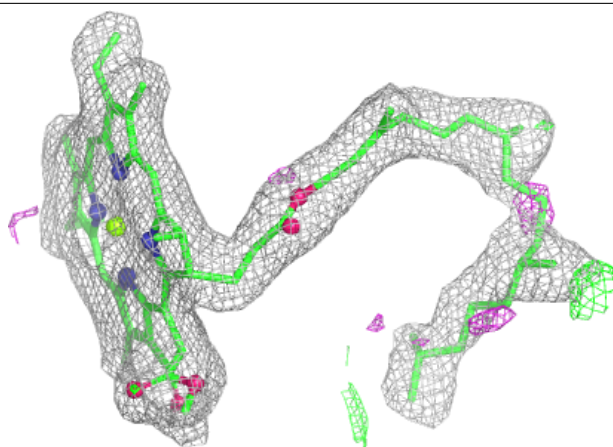
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



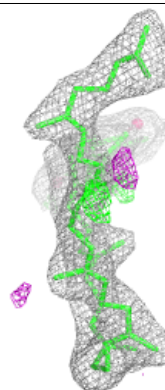
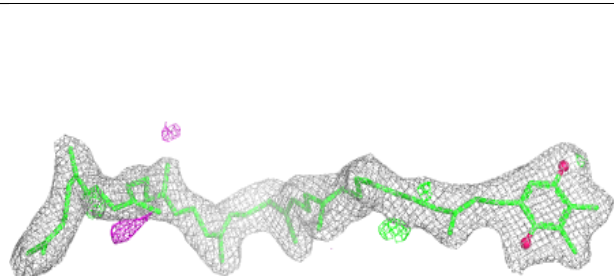
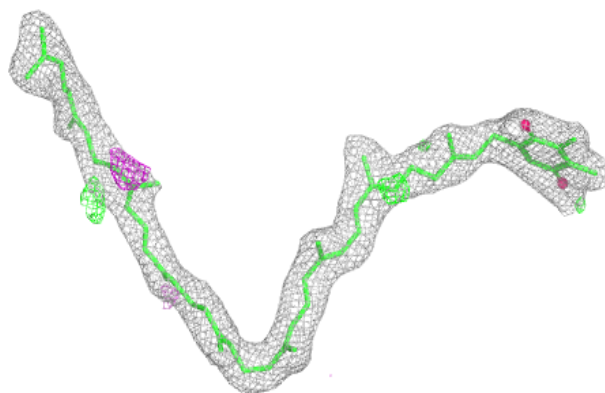


Electron density around CLA b 608:

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

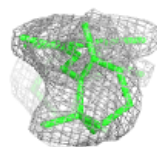
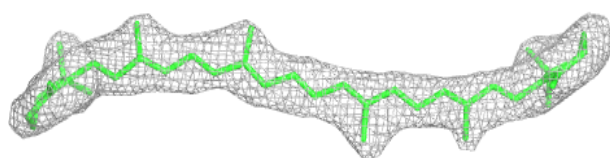
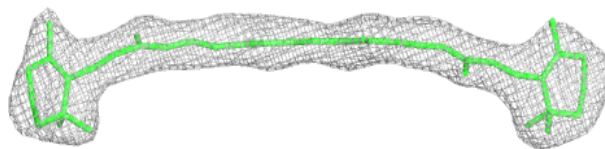
**Electron density around PL9 D 406:**

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

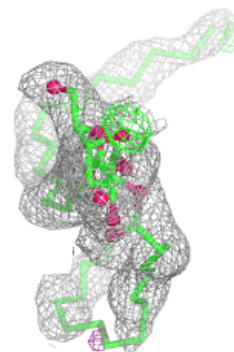
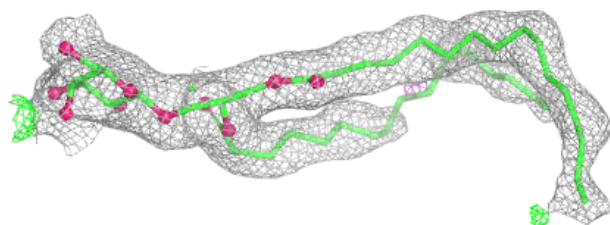
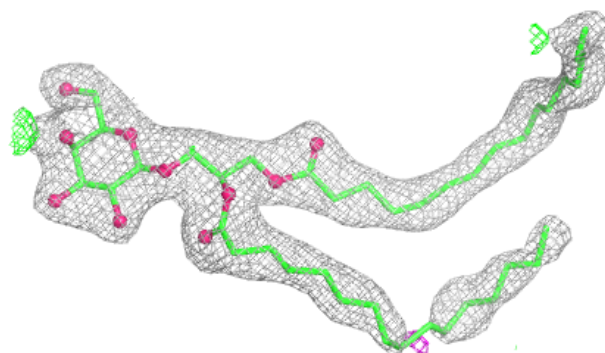


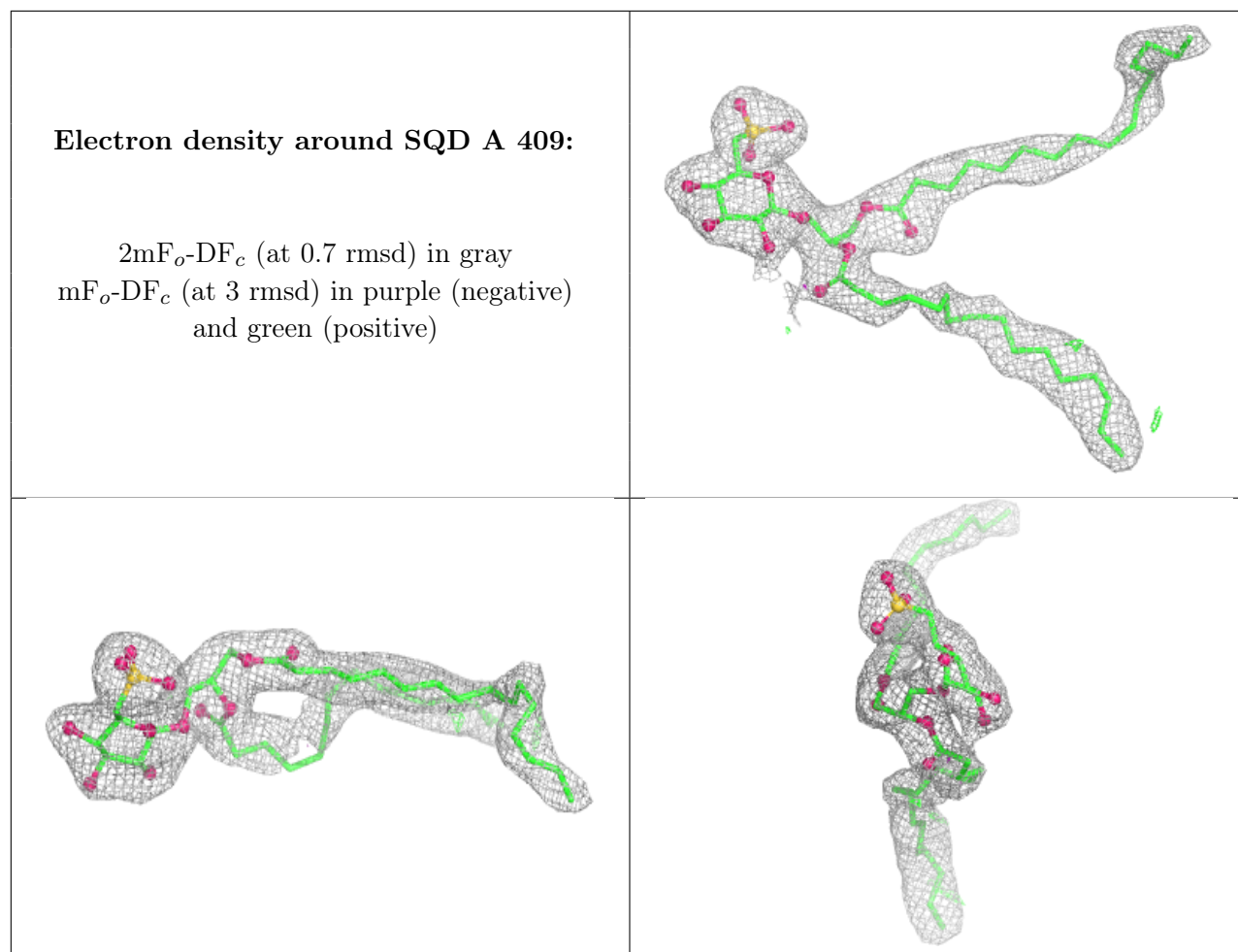
Electron density around BCR K 102:

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

**Electron density around LMG f 101:**

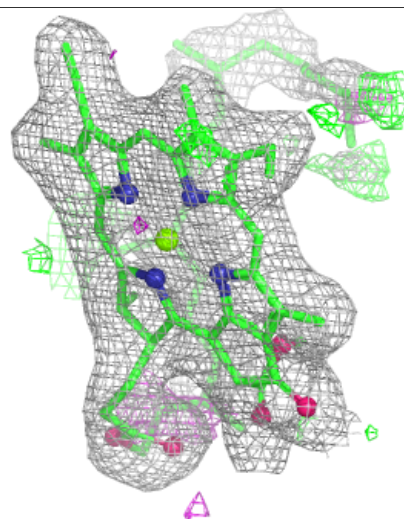
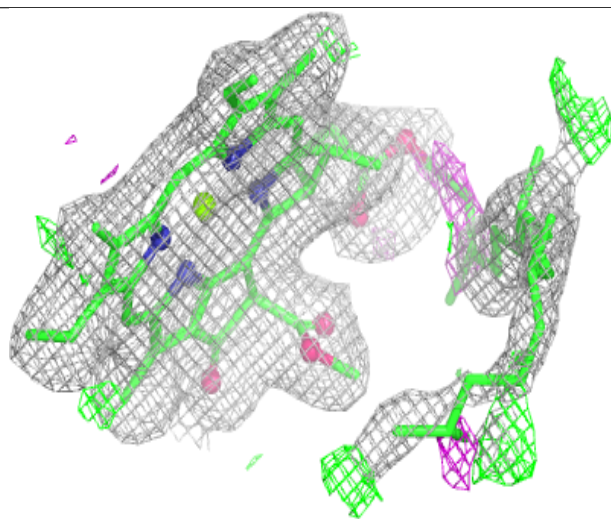
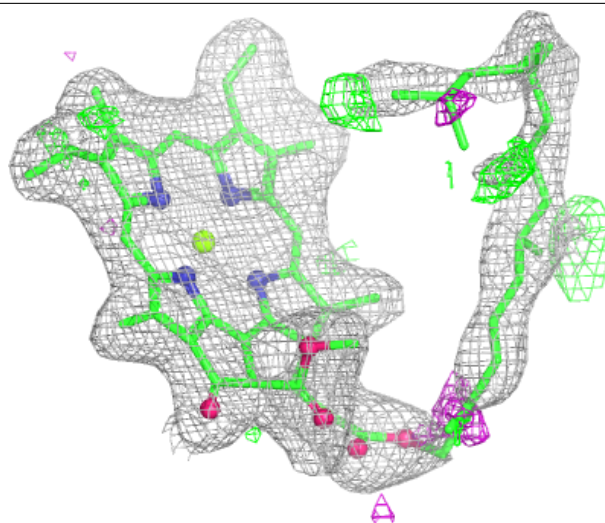
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





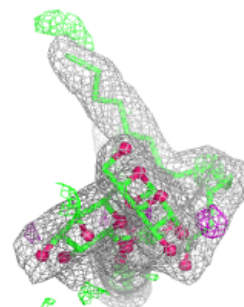
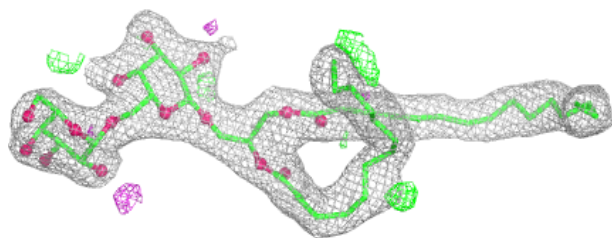
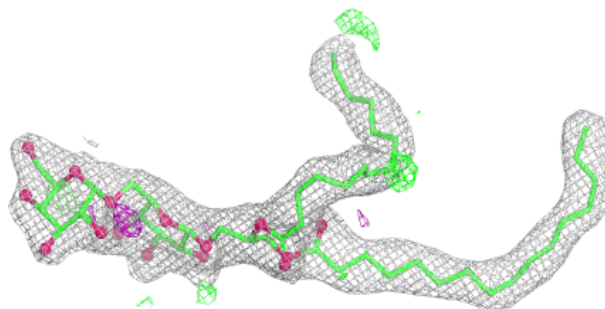
Electron density around CLA b 618:

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

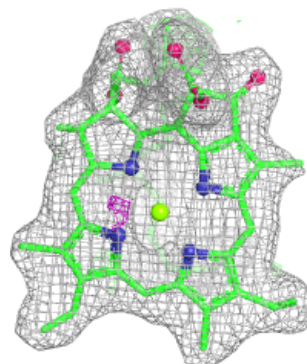
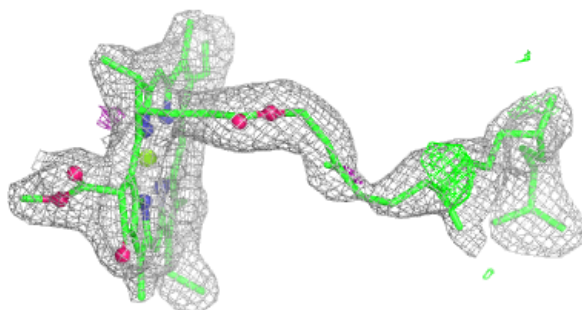
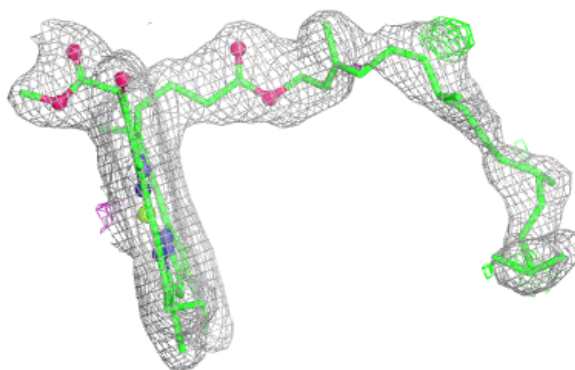


Electron density around DGD H 103:

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

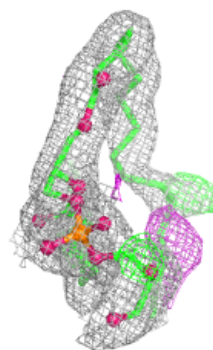
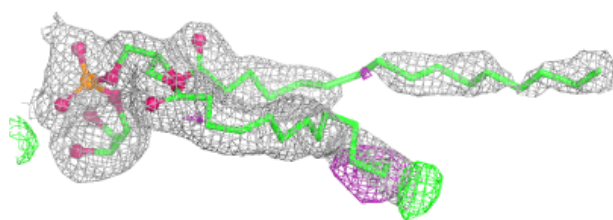
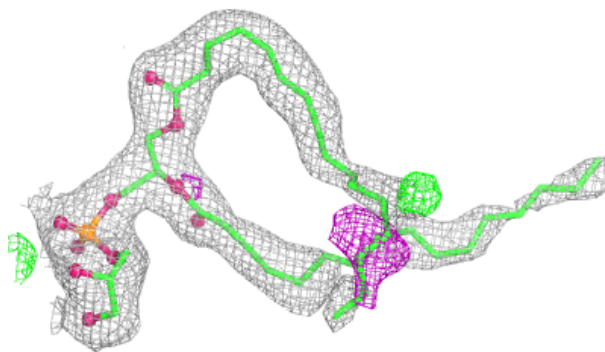
**Electron density around CLA C 507:**

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

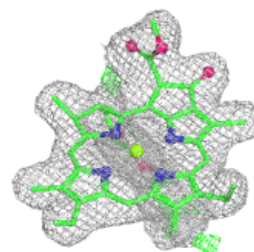
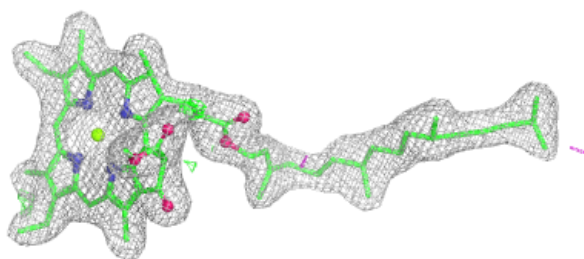
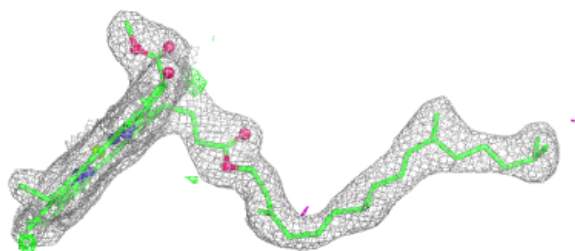


Electron density around LHG D 409:

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

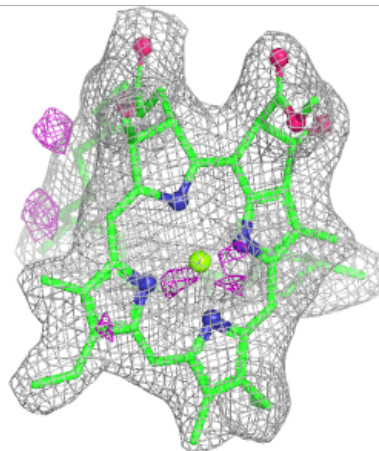
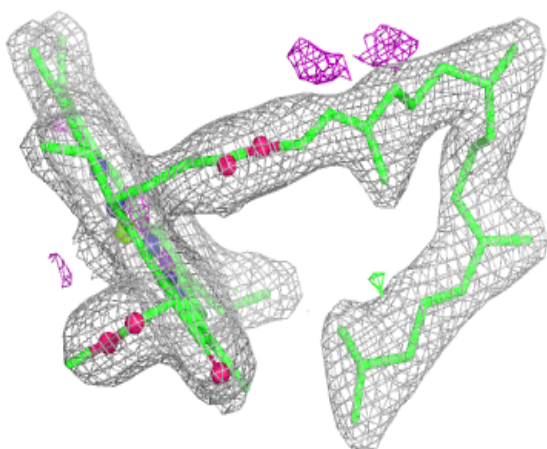
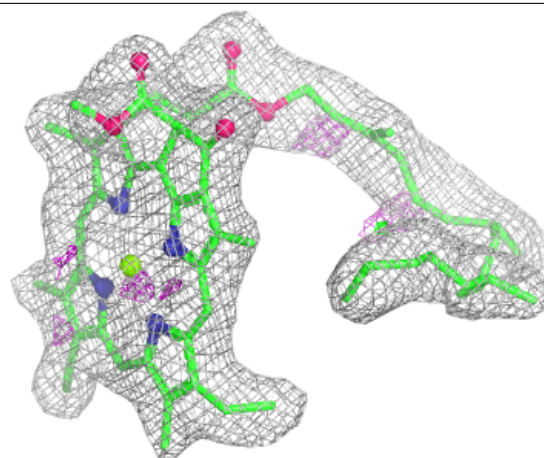
**Electron density around CLA C 503:**

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



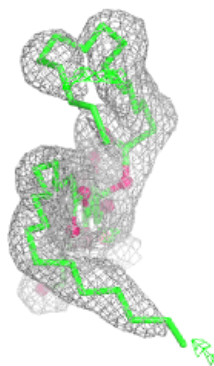
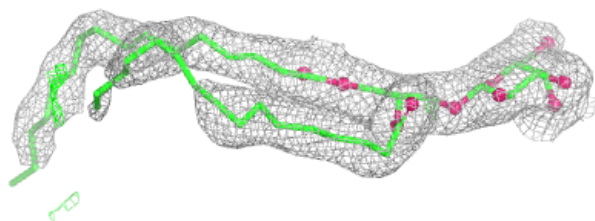
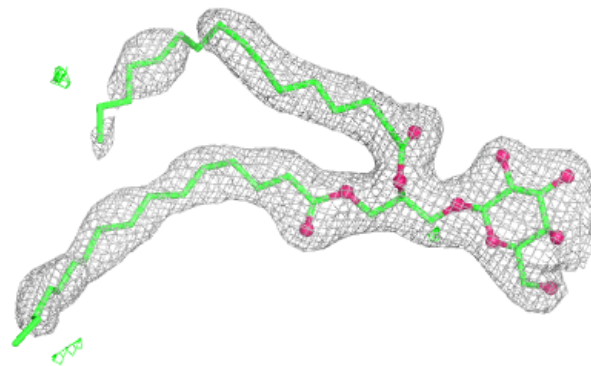
Electron density around CLA C 504:

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

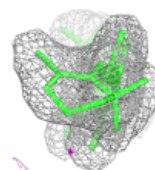
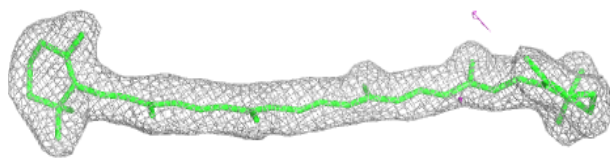
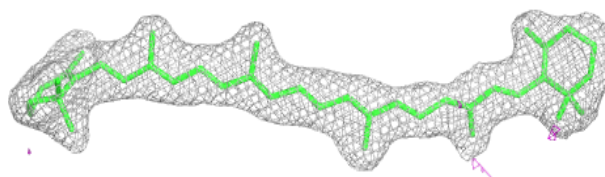


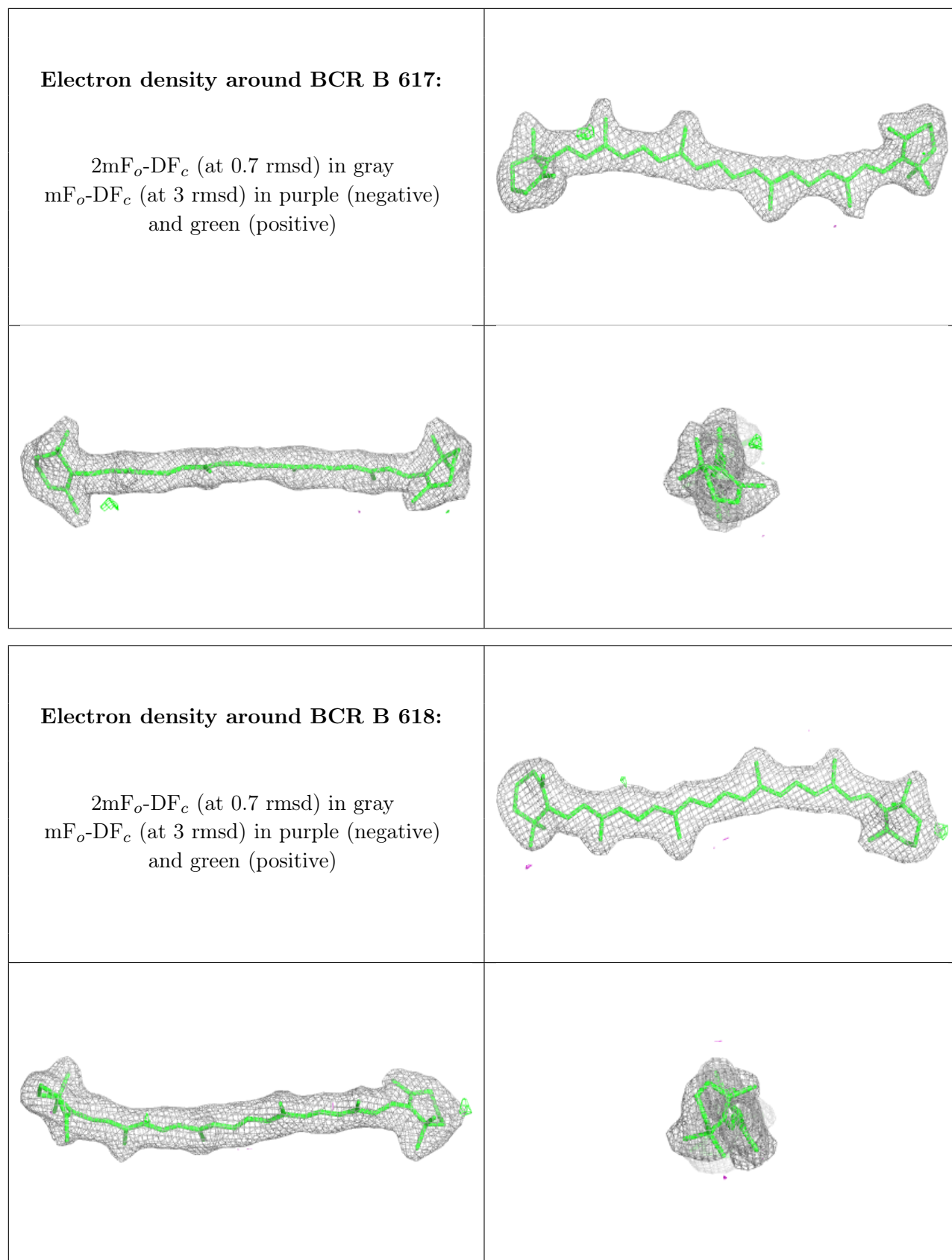
Electron density around LMG D 410:

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

**Electron density around BCR B 616:**

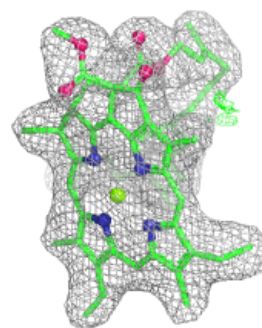
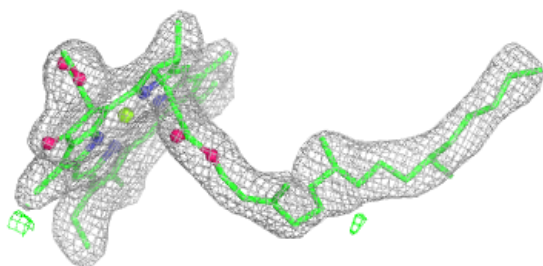
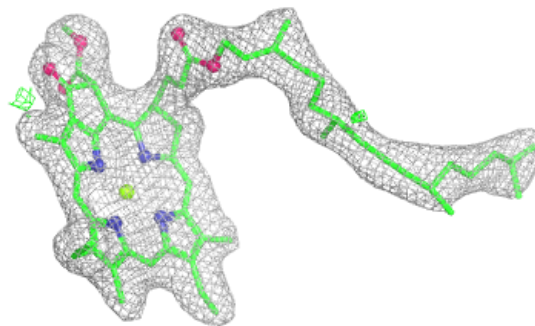
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





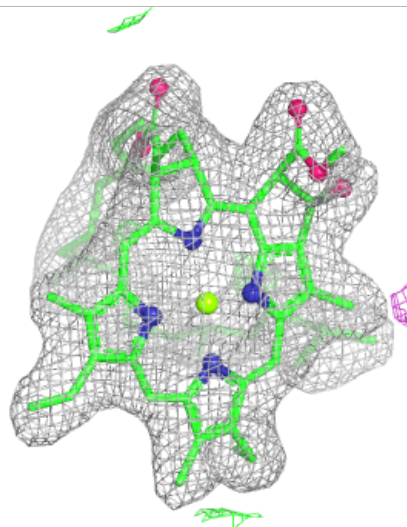
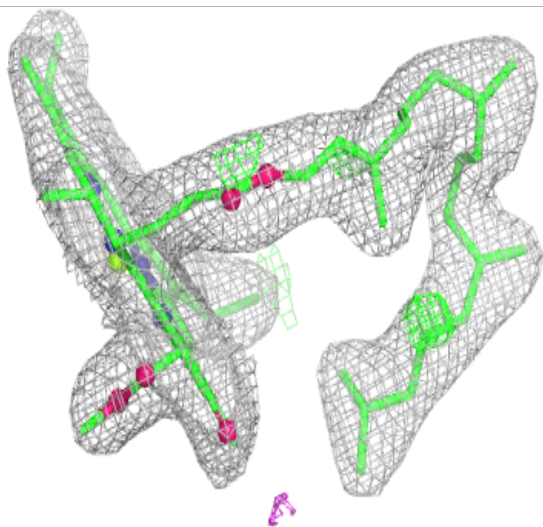
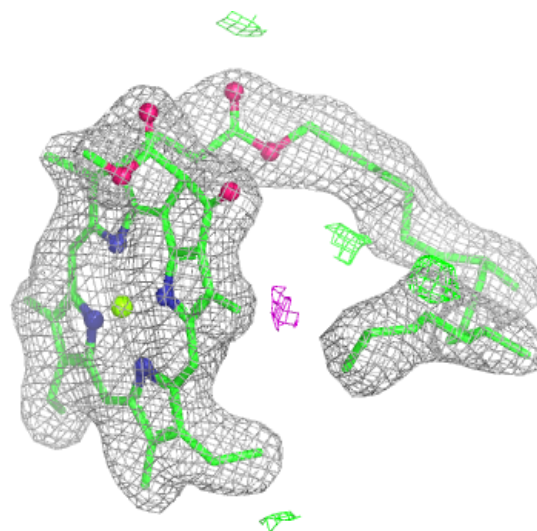
Electron density around CLA C 512:

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



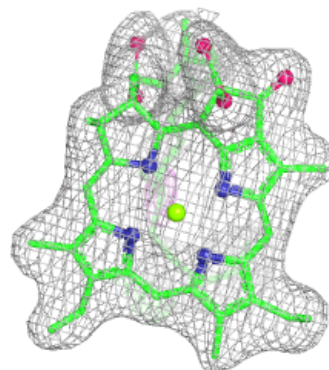
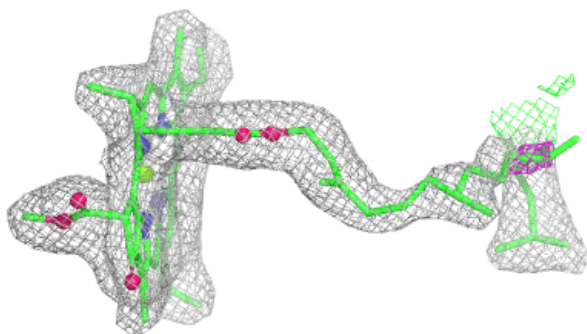
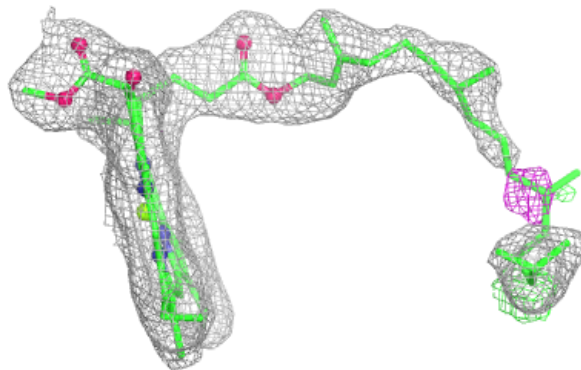
Electron density around CLA c 504:

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

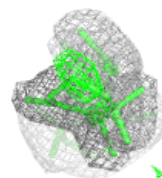
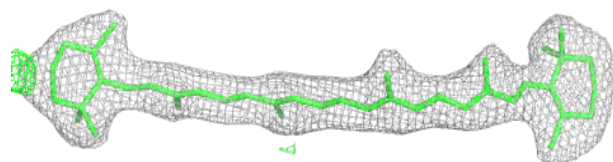
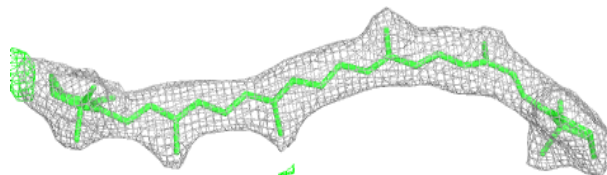


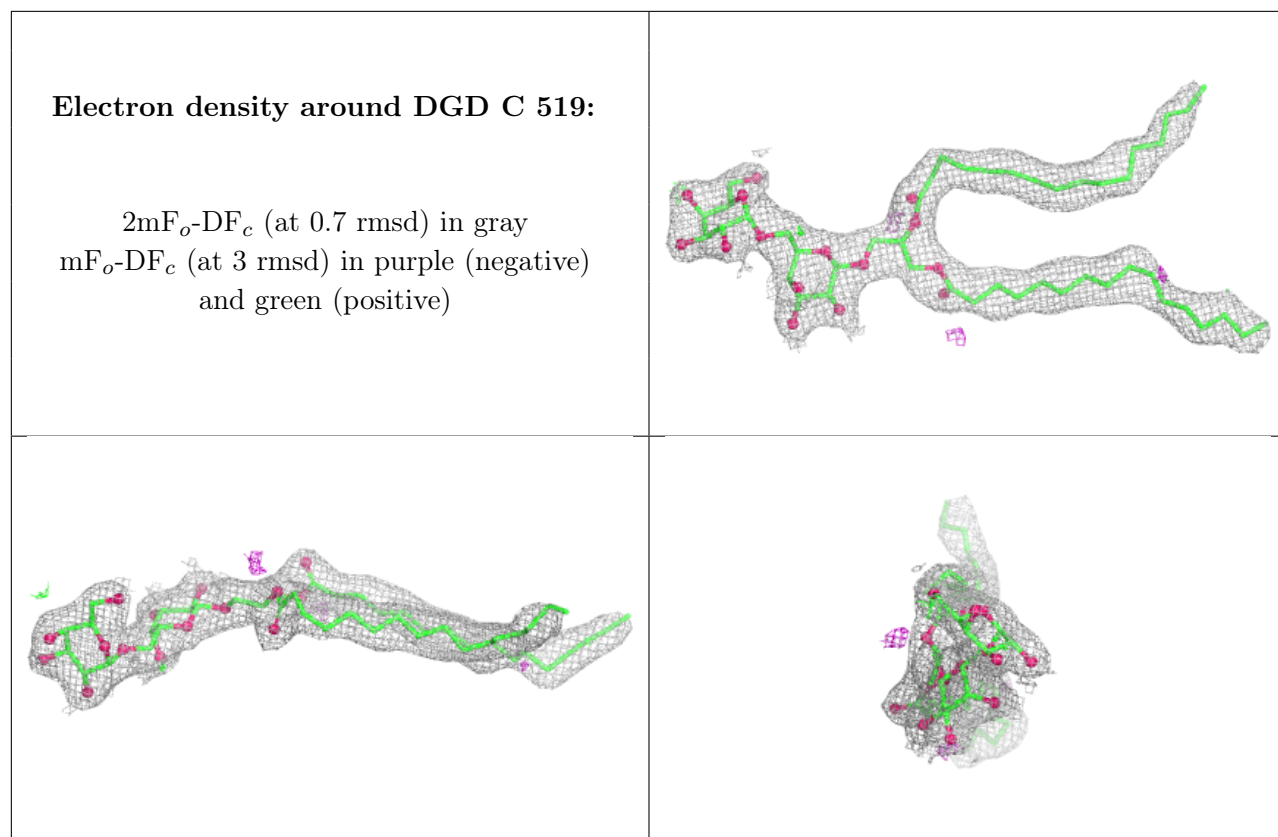
Electron density around CLA c 507:

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

**Electron density around BCR H 102:**

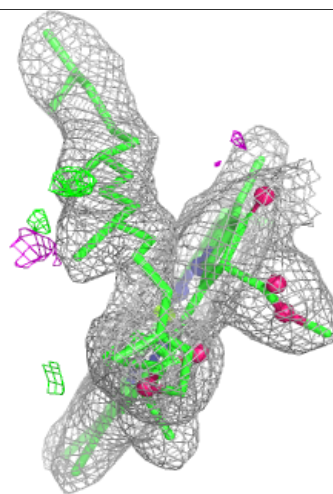
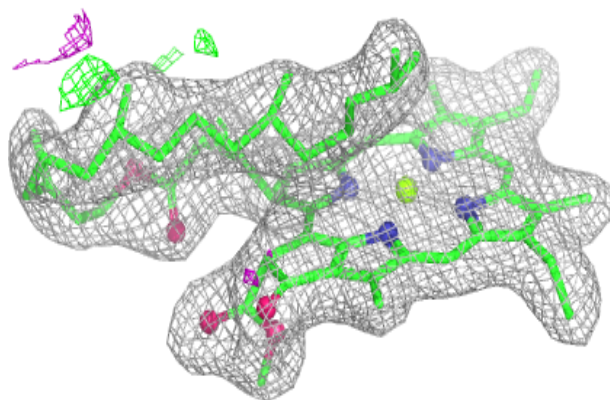
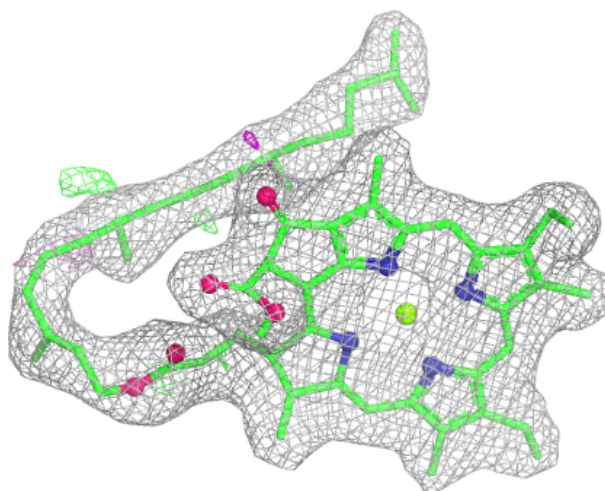
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





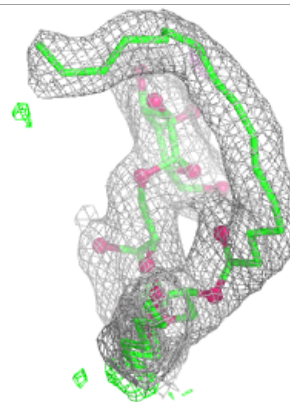
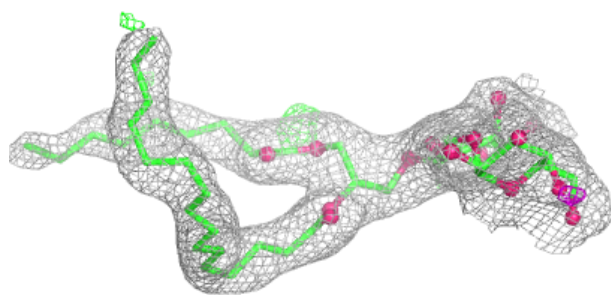
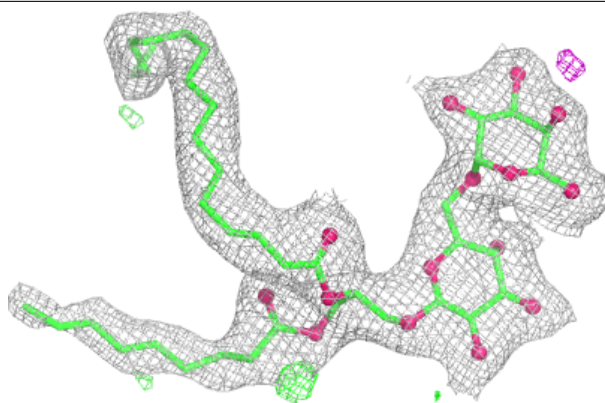
Electron density around CLA c 510:

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

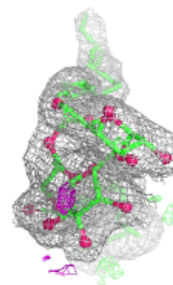
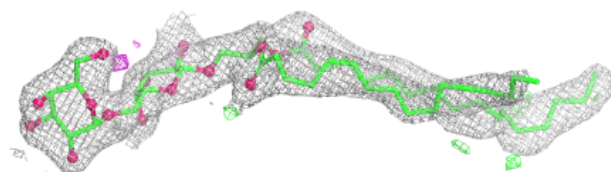
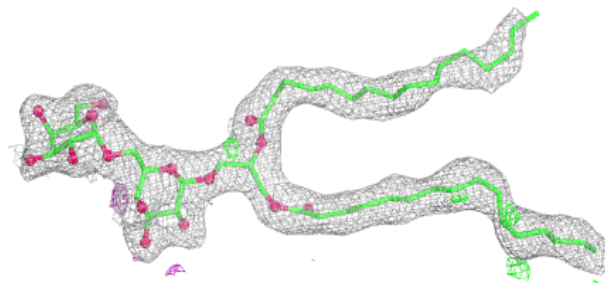


Electron density around DGD c 517:

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

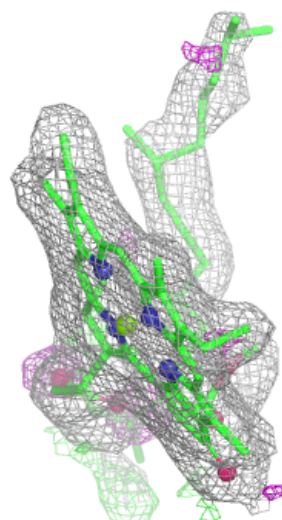
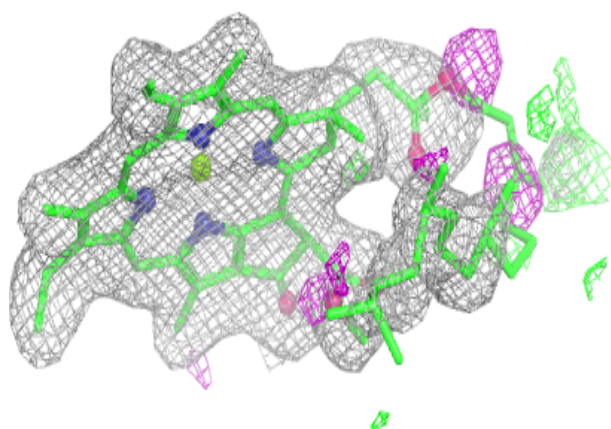
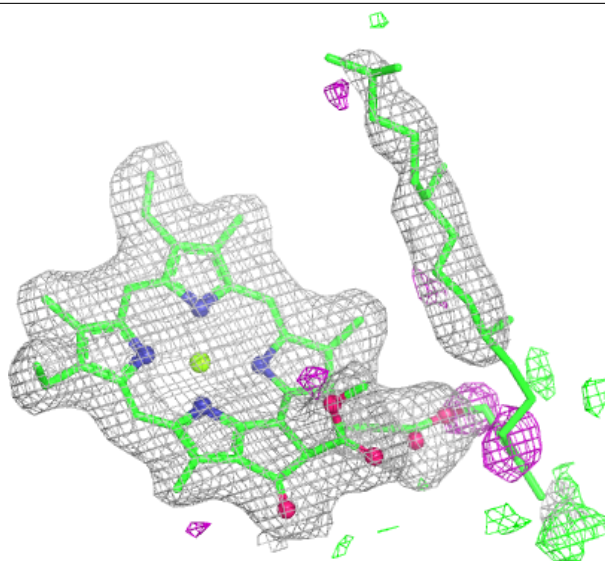
**Electron density around DGD c 518:**

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



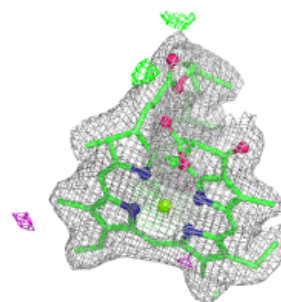
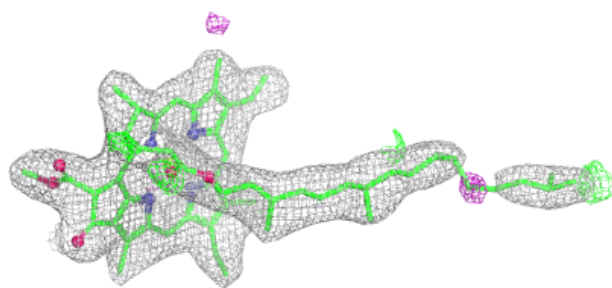
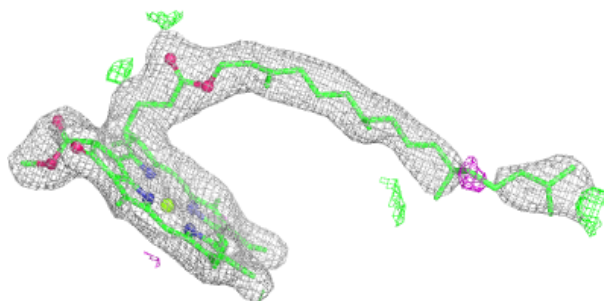
Electron density around CLA B 615:

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

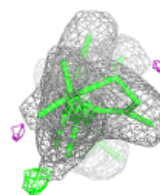
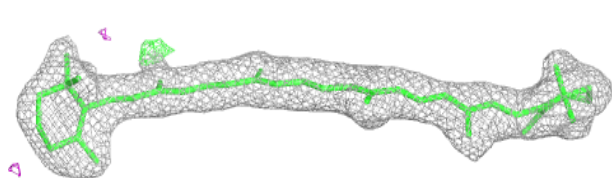
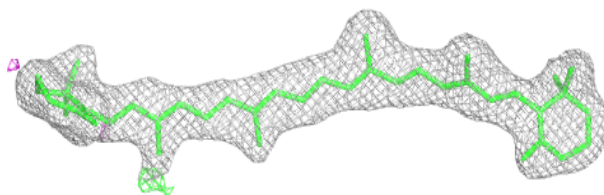


Electron density around CLA C 505:

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

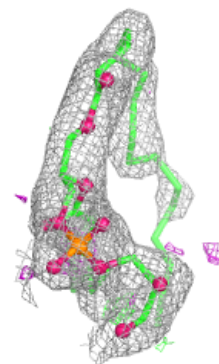
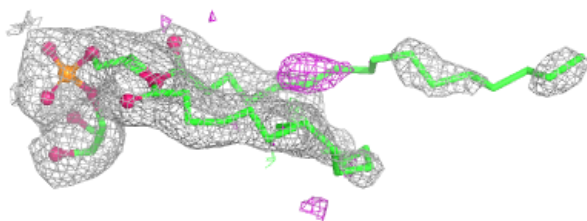
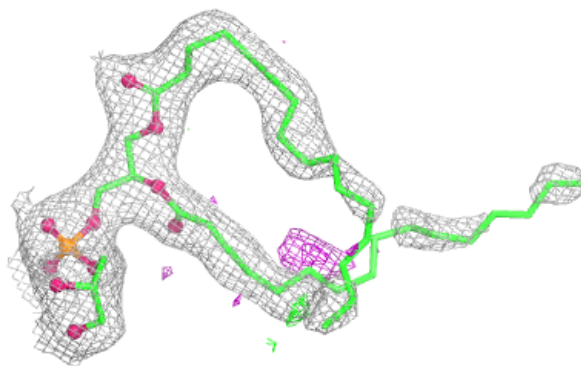
**Electron density around BCR b 619:**

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

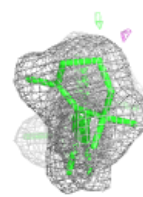
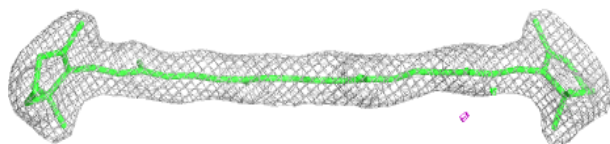
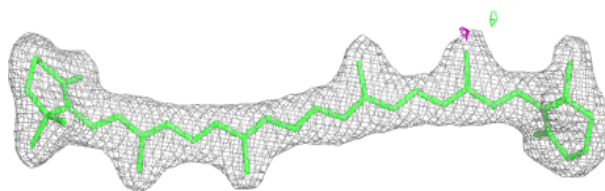


Electron density around LHG d 407:

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

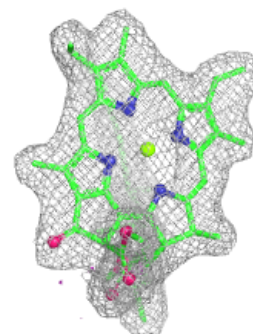
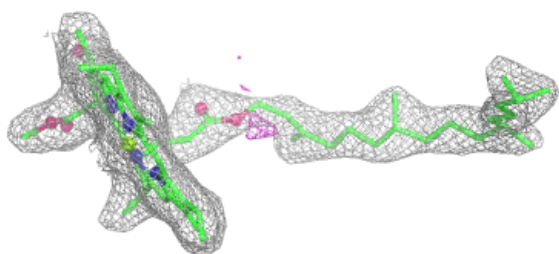
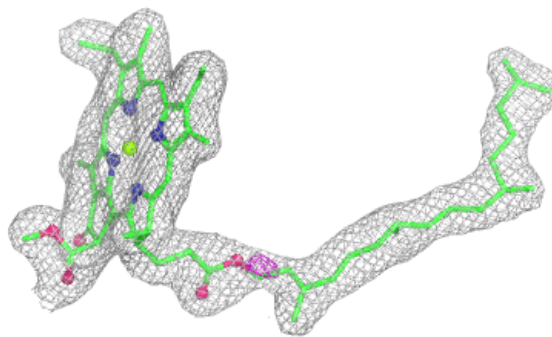
**Electron density around BCR b 620:**

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

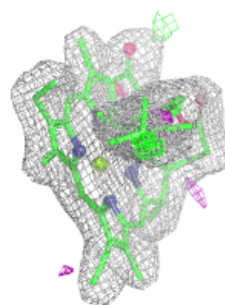
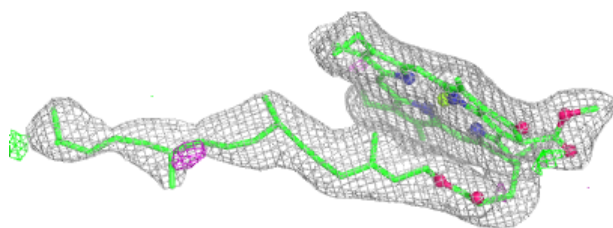
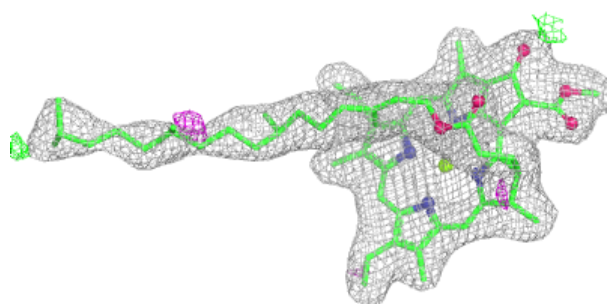


Electron density around CLA b 611:

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

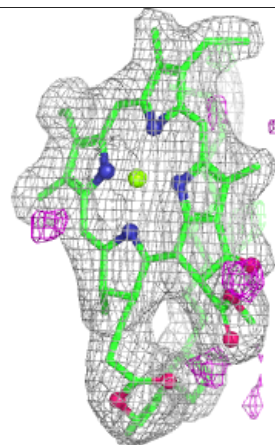
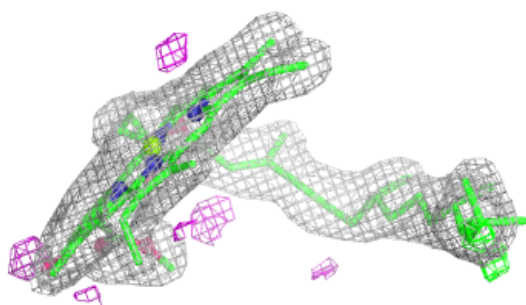
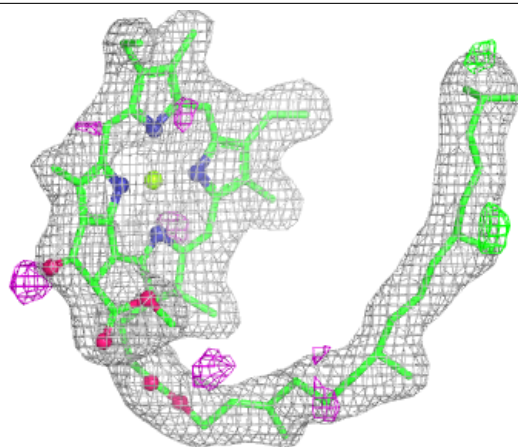
**Electron density around CLA b 616:**

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



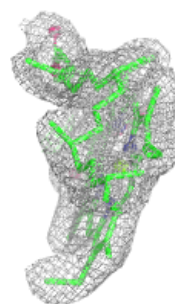
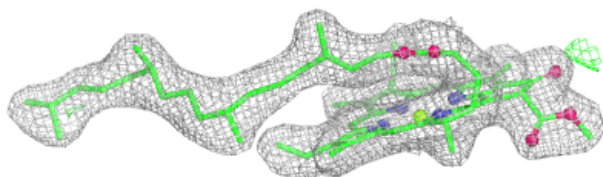
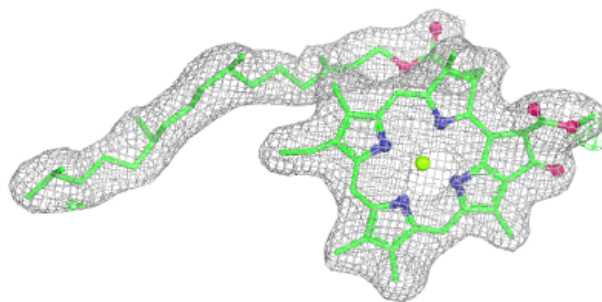
Electron density around CLA C 508:

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

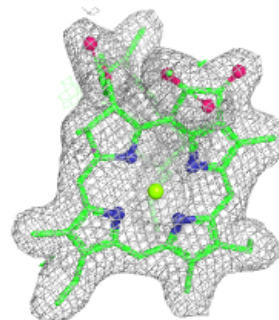
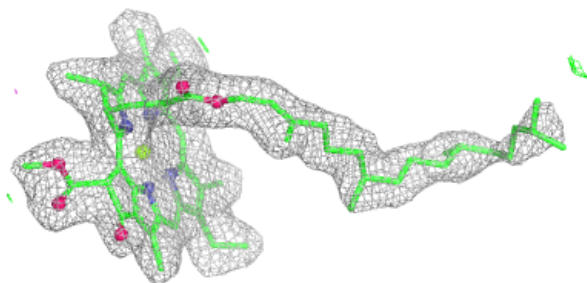
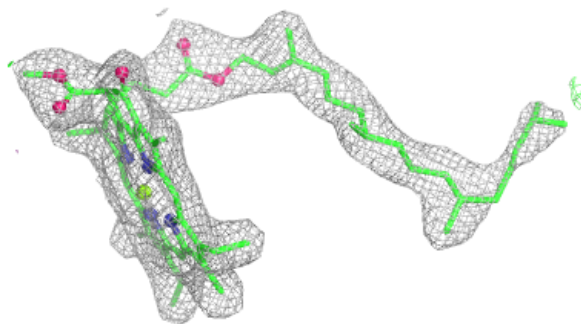


Electron density around CLA c 502:

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

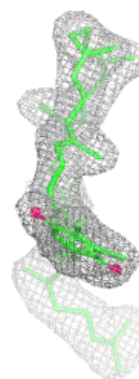
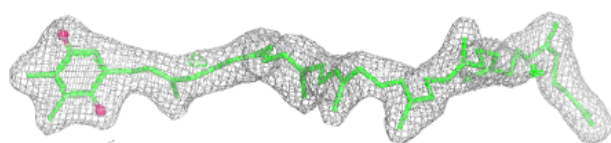
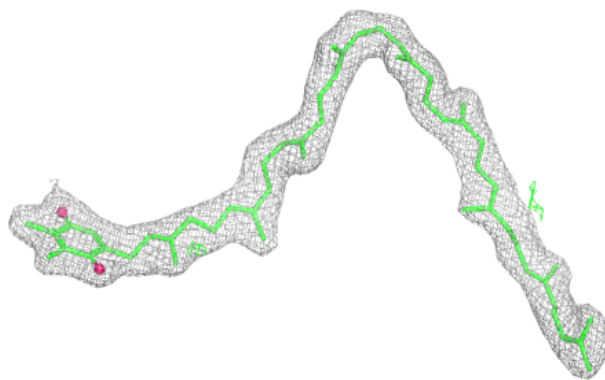
**Electron density around CLA C 509:**

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

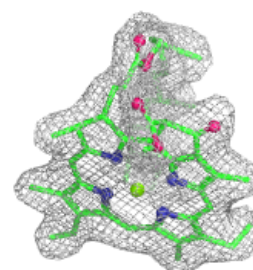
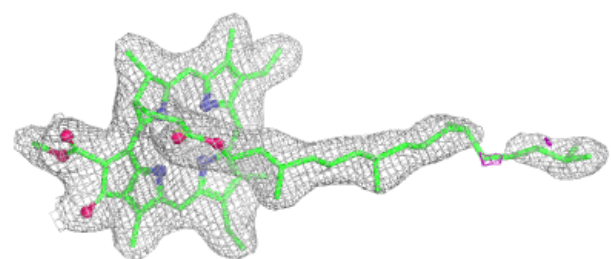
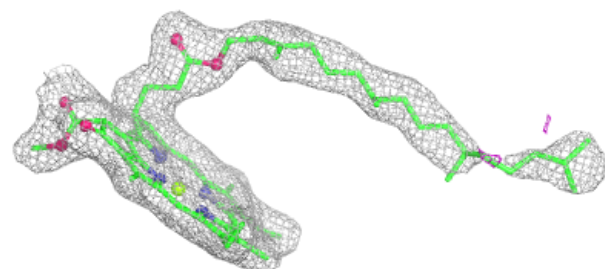


Electron density around PL9 d 405:

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

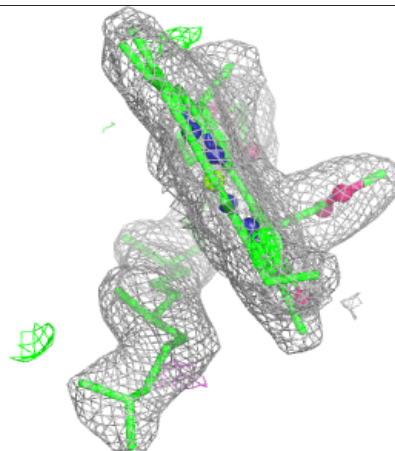
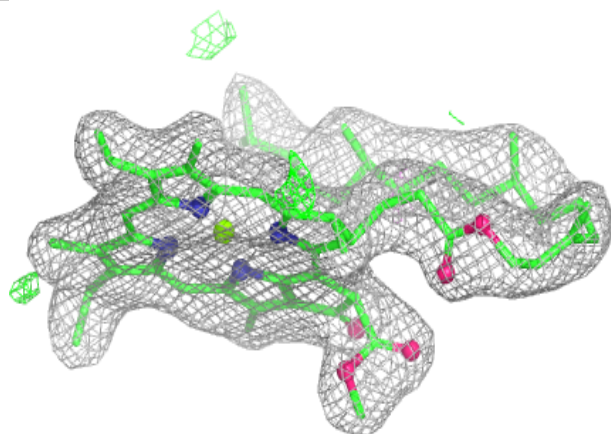
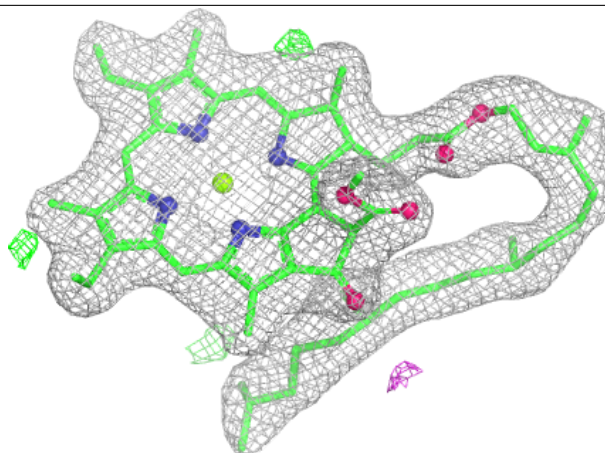
**Electron density around CLA c 505:**

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



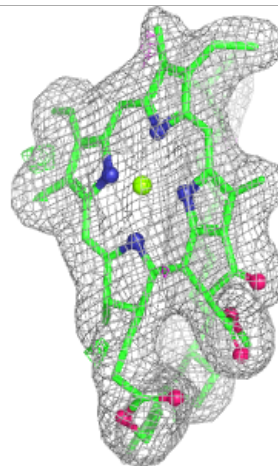
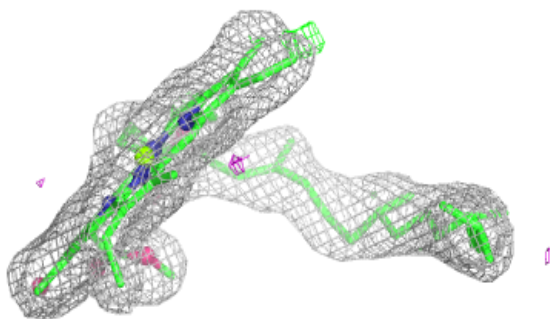
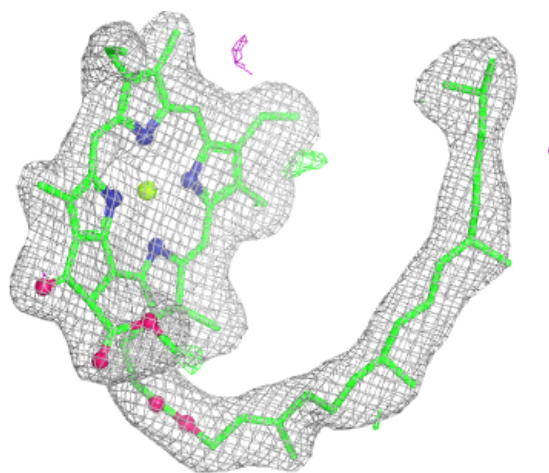
Electron density around CLA C 510:

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



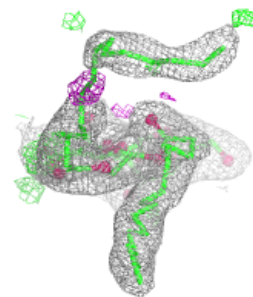
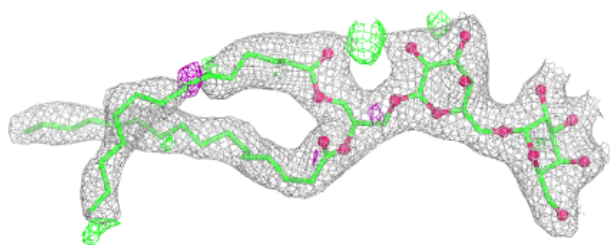
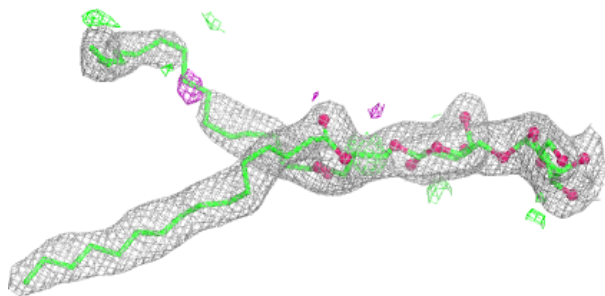
Electron density around CLA c 508:

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



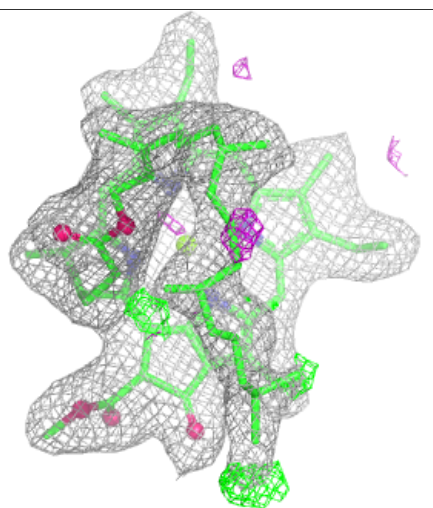
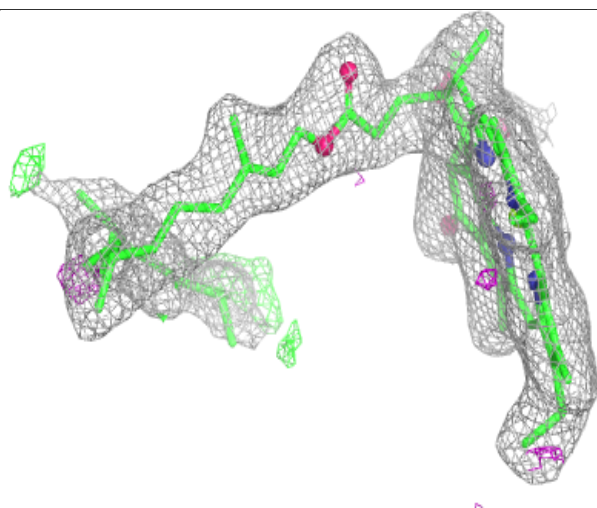
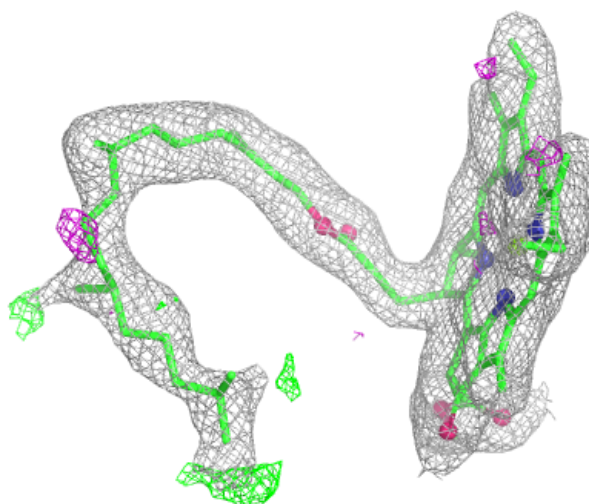
Electron density around DGD C 517:

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



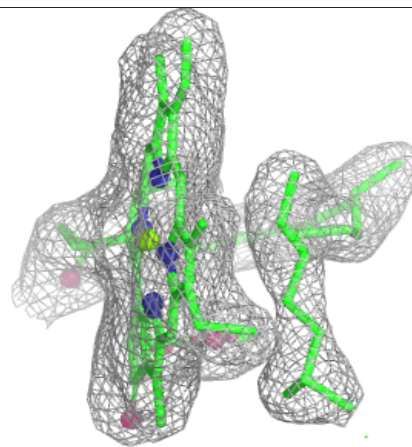
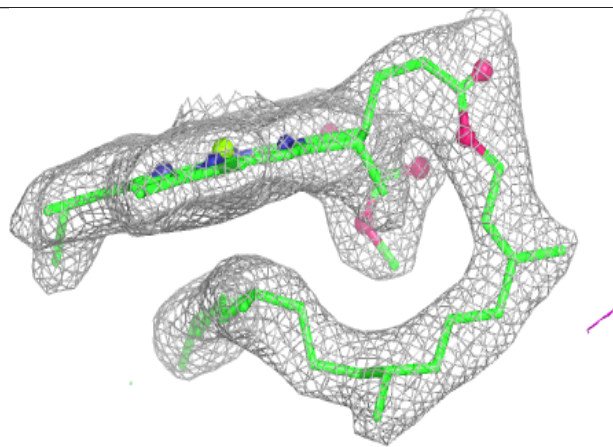
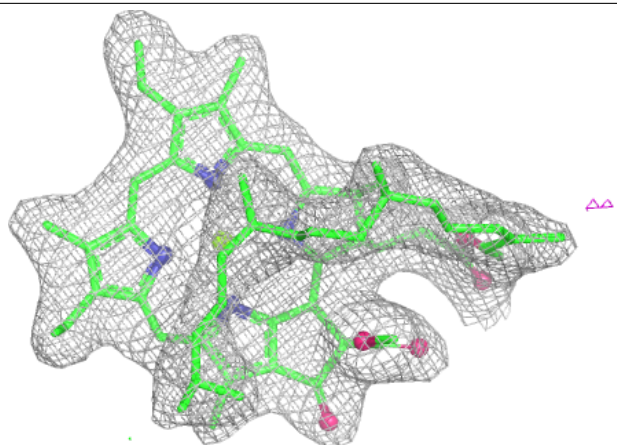
Electron density around CLA B 605:

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



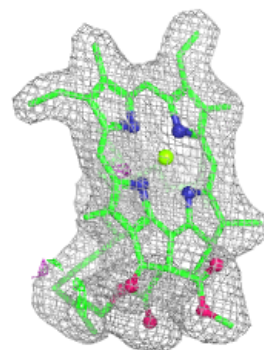
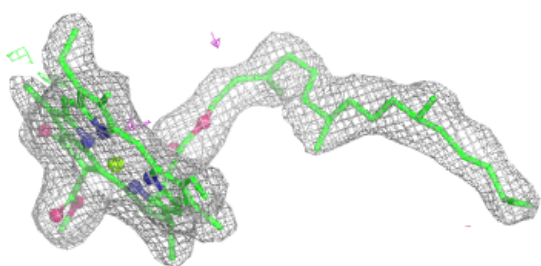
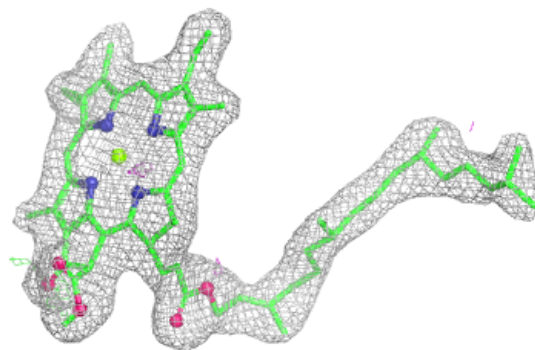
Electron density around CLA c 511:

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

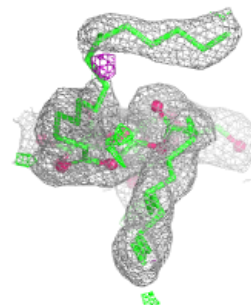
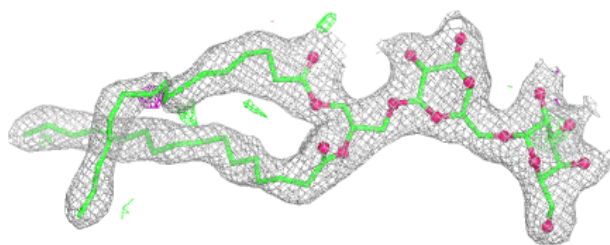
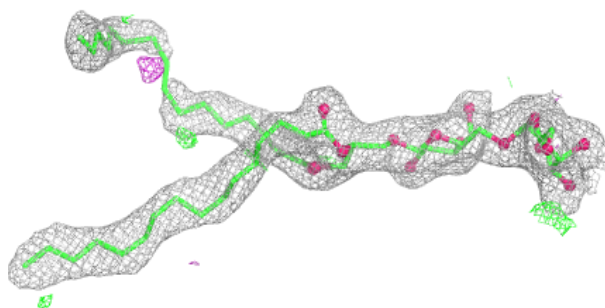


Electron density around CLA c 512:

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

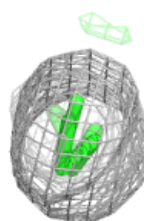
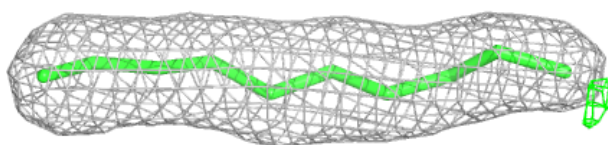
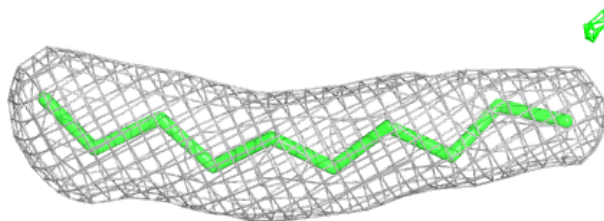
**Electron density around DGD c 516:**

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

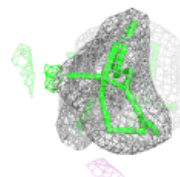
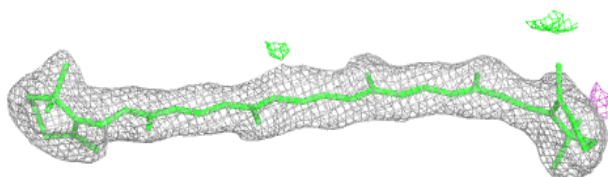
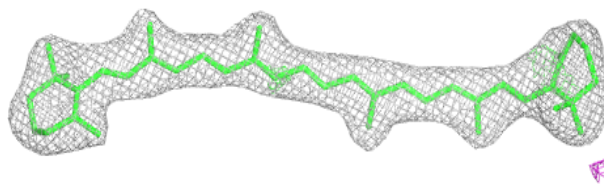


Electron density around LFA M 101:

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

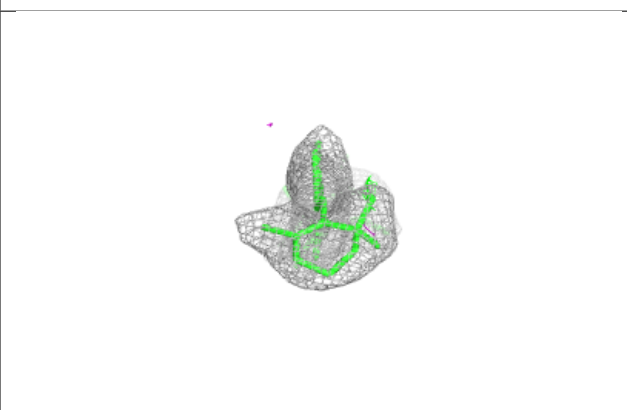
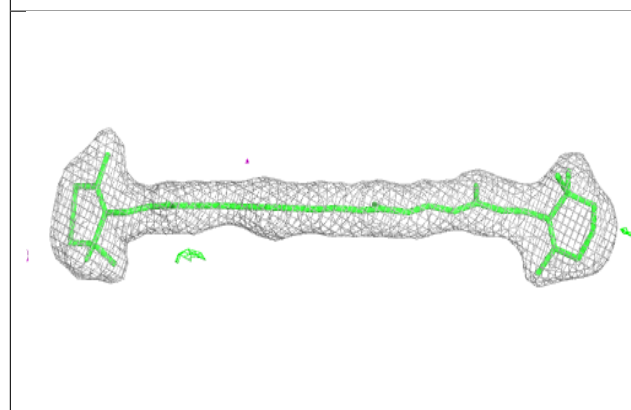
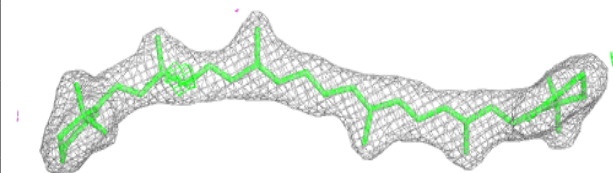
**Electron density around BCR b 621:**

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

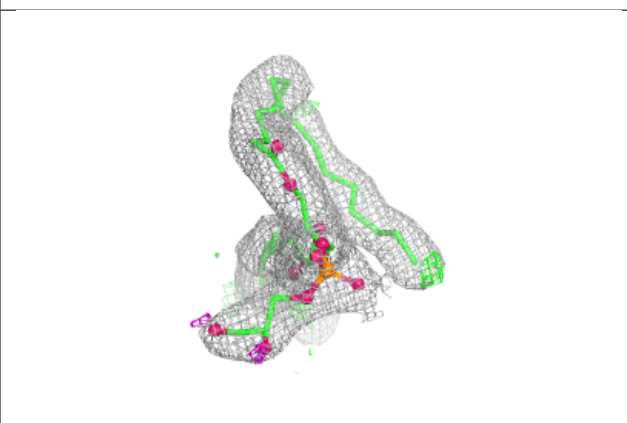
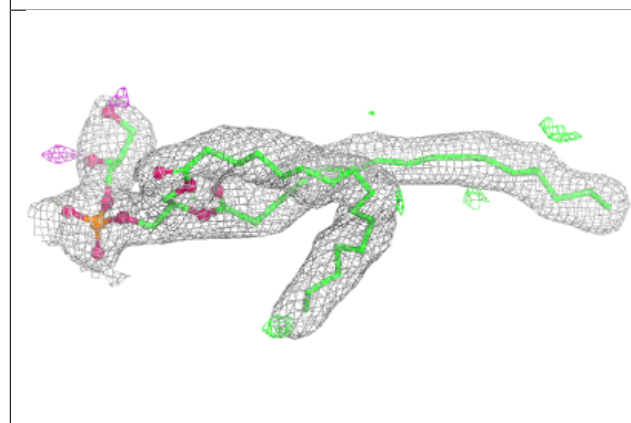
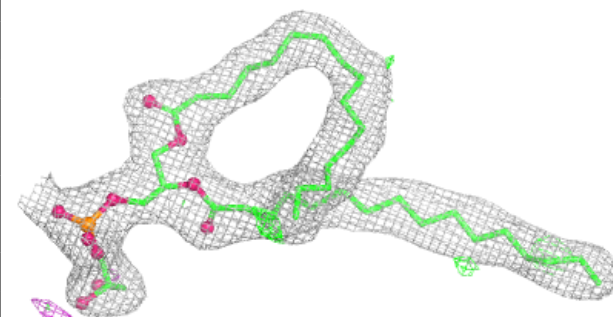


Electron density around BCR c 515:

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

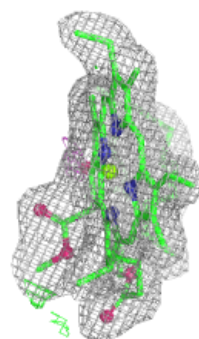
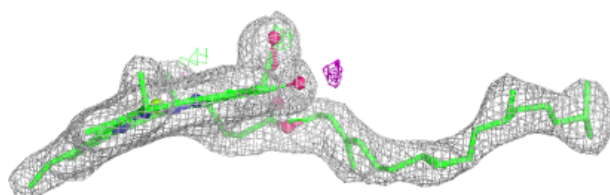
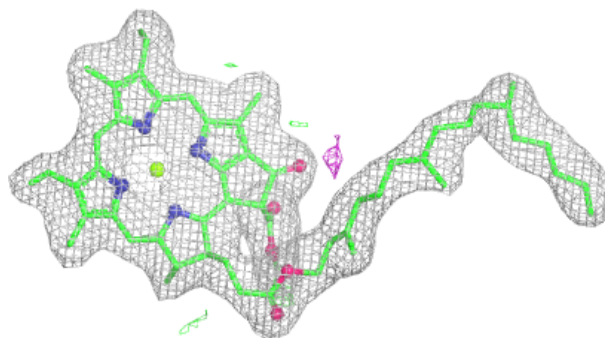
**Electron density around LHG D 407:**

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

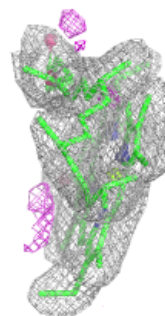
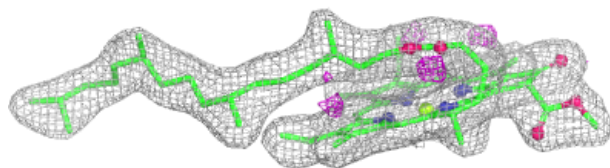
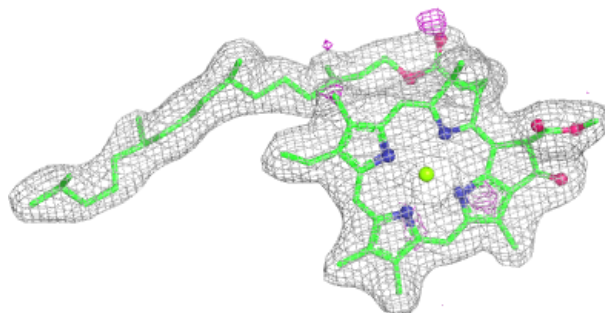


Electron density around CLA b 604:

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

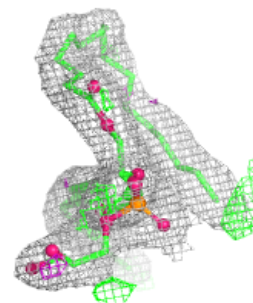
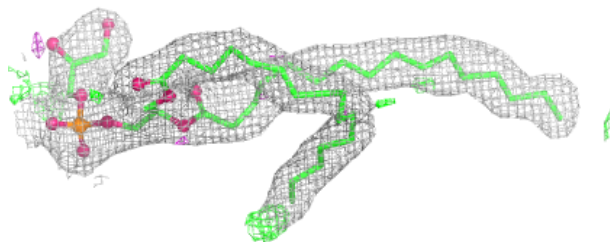
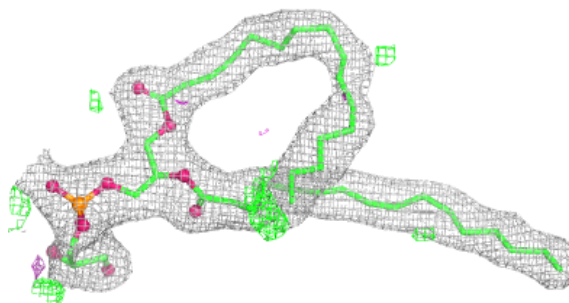
**Electron density around CLA C 502:**

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

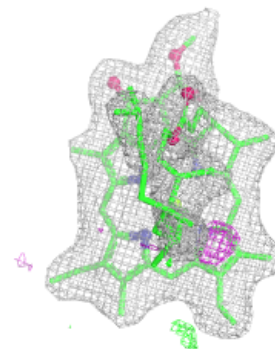
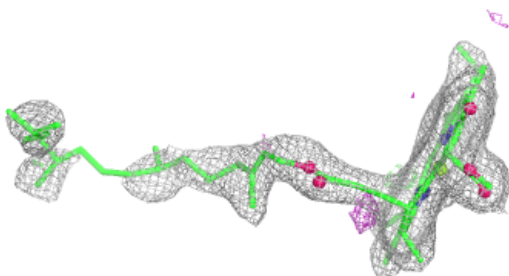
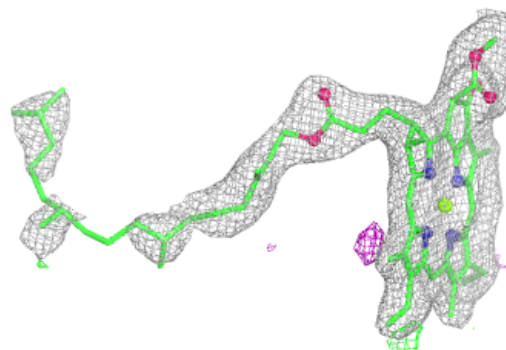


Electron density around LHG b 628:

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

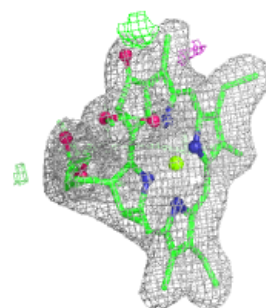
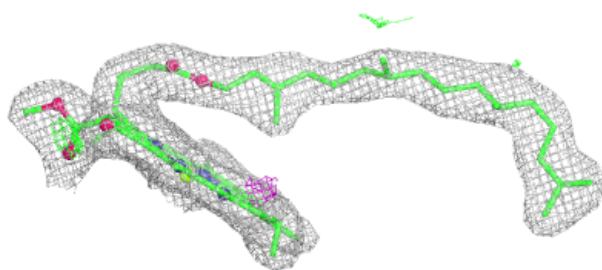
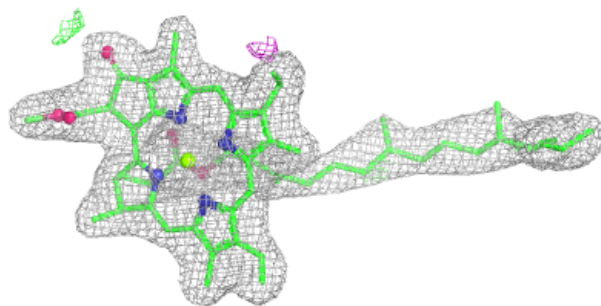
**Electron density around CLA d 403:**

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



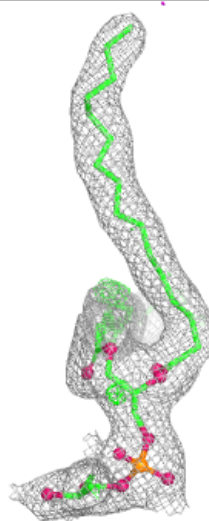
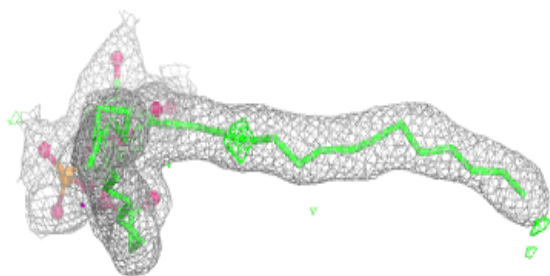
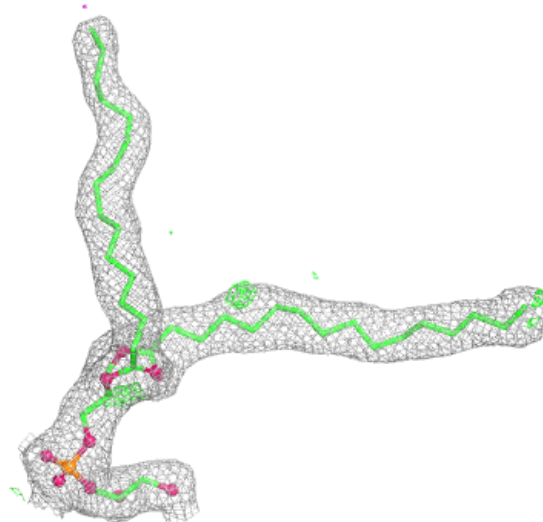
Electron density around CLA b 610:

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



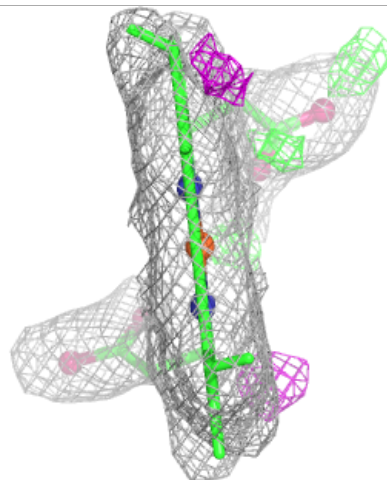
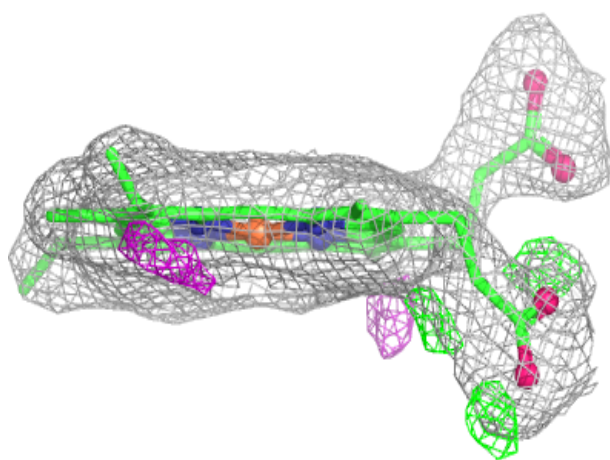
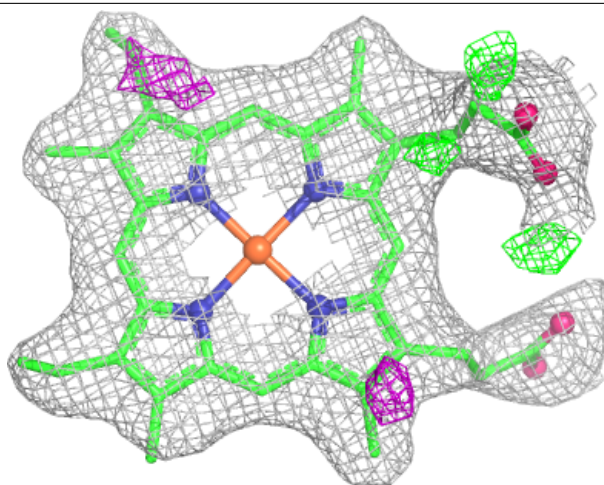
Electron density around LHG 1 101:

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



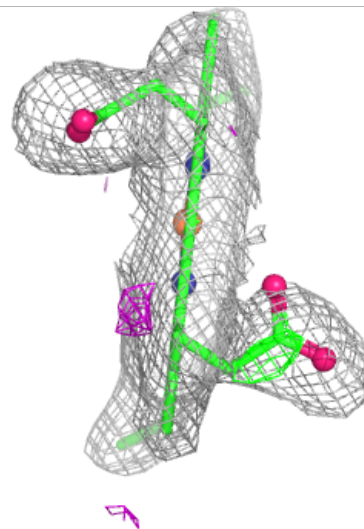
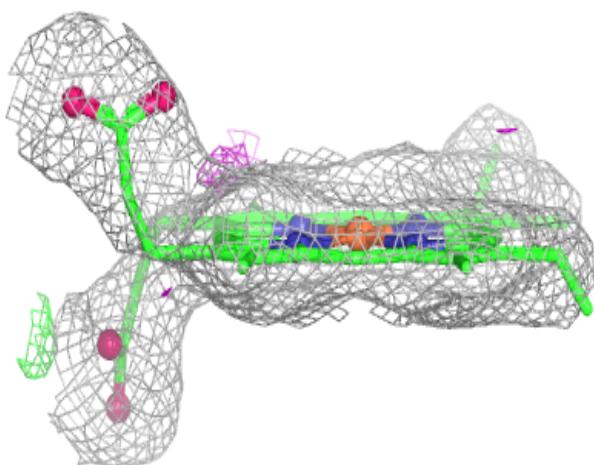
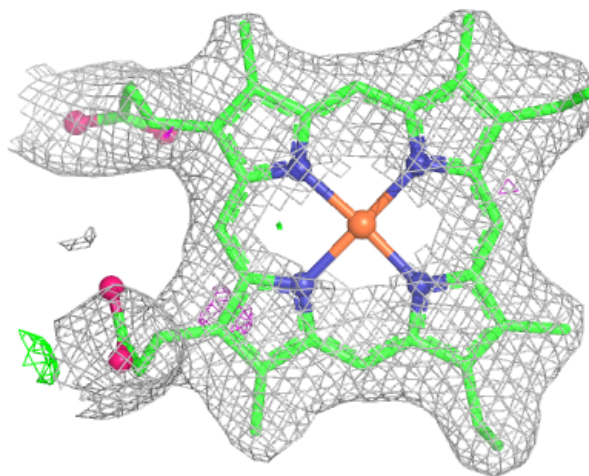
Electron density around HEM E 102:

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



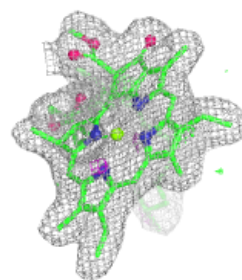
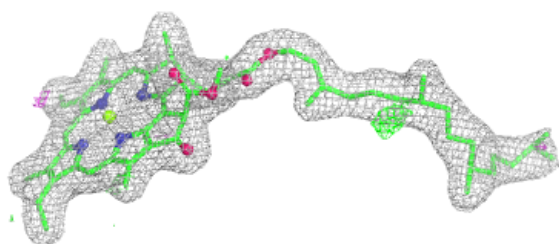
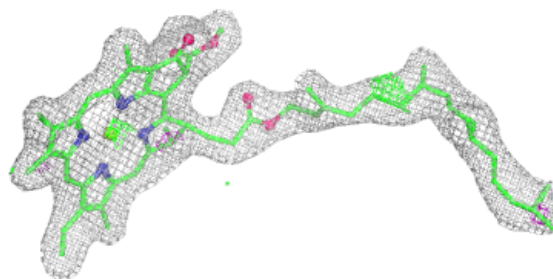
Electron density around HEM e 102:

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

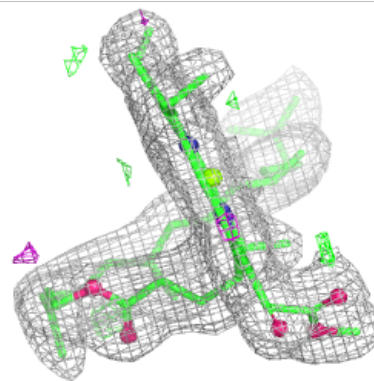
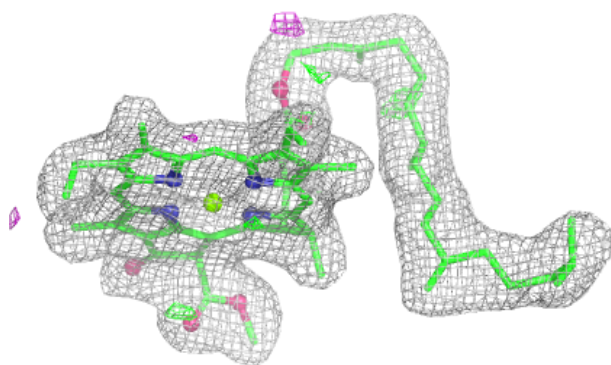
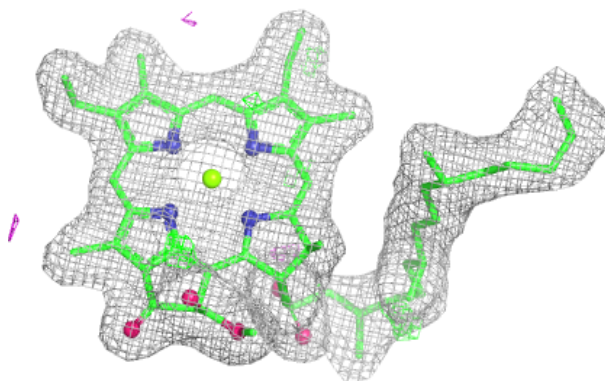


Electron density around CLA a 404:

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

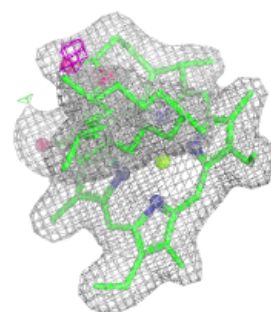
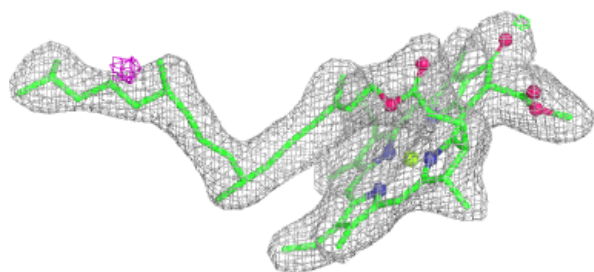
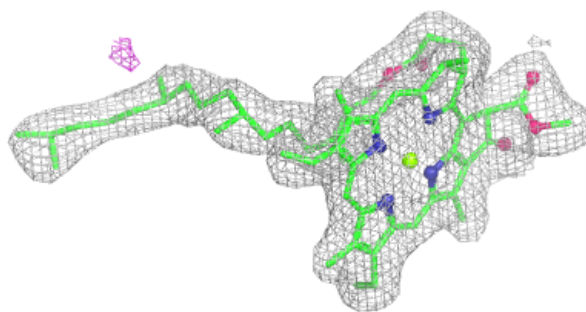
**Electron density around CLA a 405:**

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

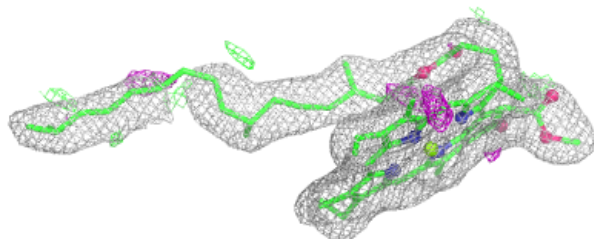
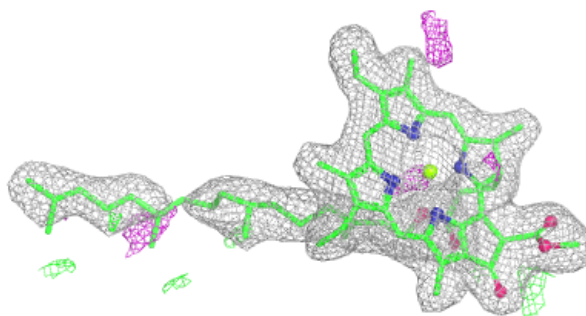


Electron density around CLA c 506:

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

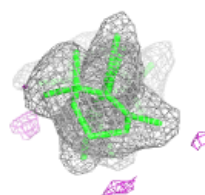
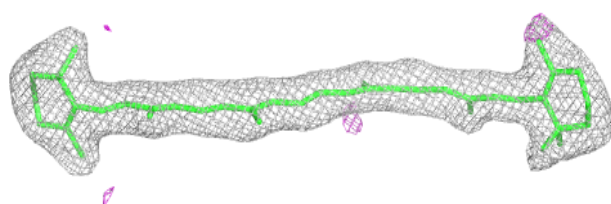
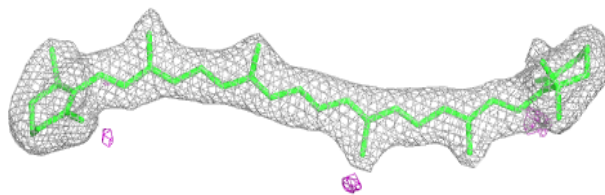
**Electron density around CLA B 613:**

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

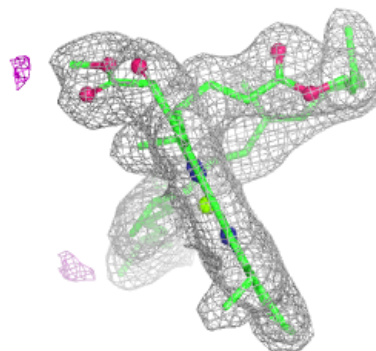
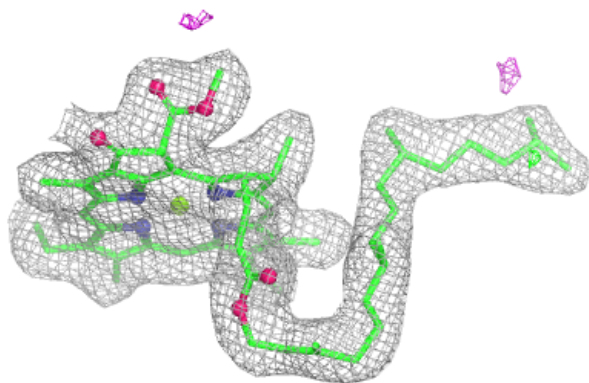
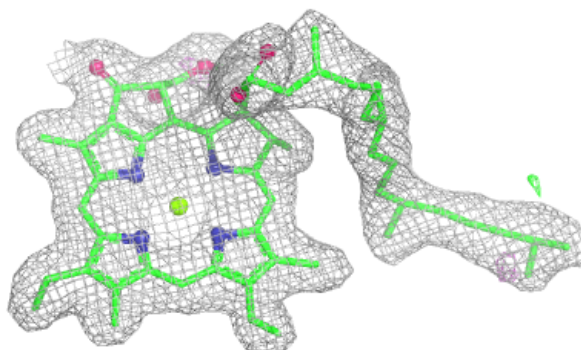


Electron density around BCR a 408:

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

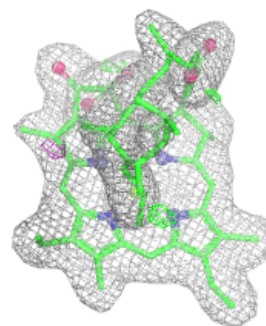
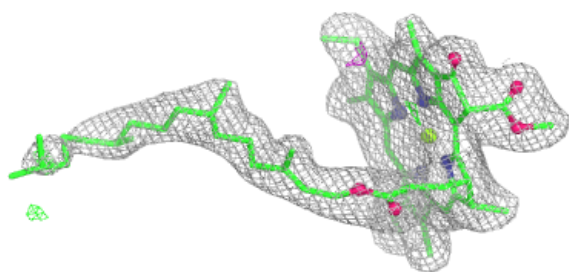
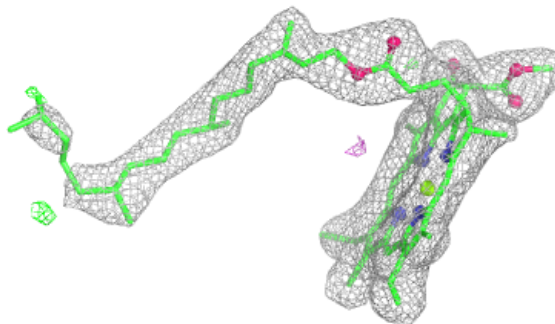
**Electron density around CLA A 412:**

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

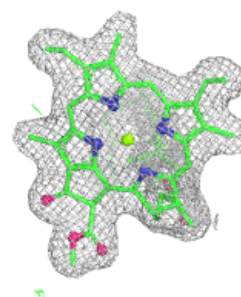
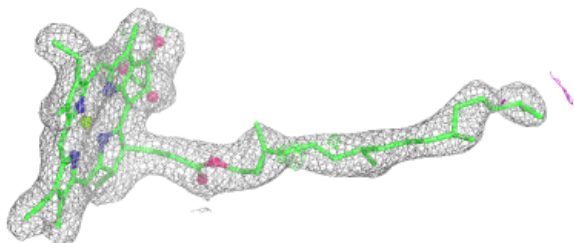
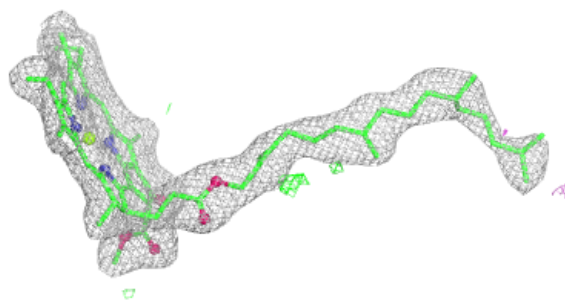


Electron density around CLA c 509:

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

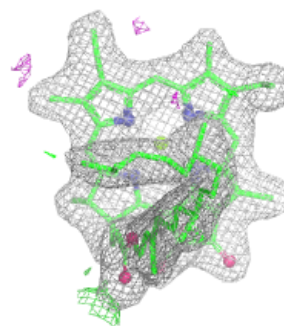
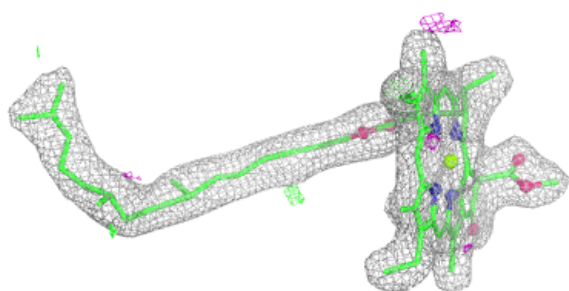
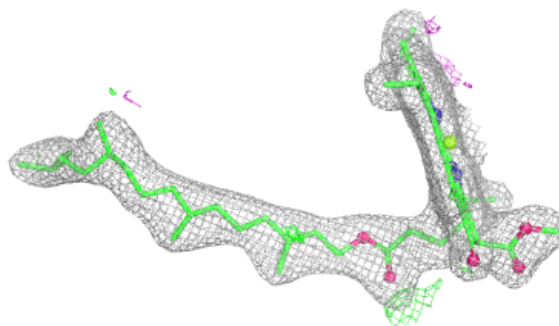
**Electron density around CLA b 606:**

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

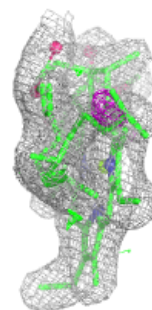
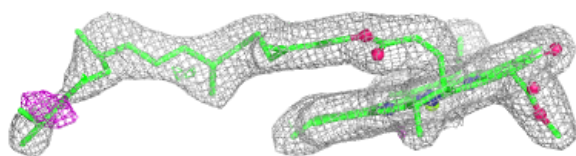
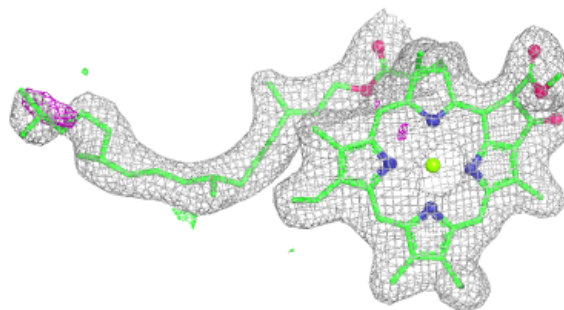


Electron density around CLA b 607:

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

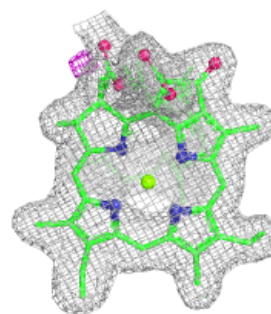
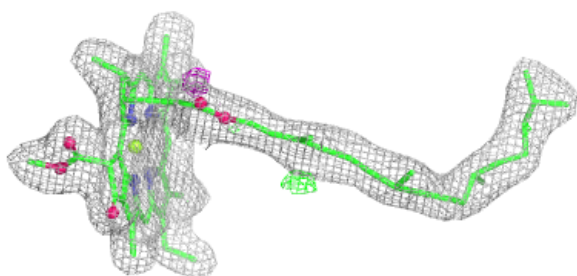
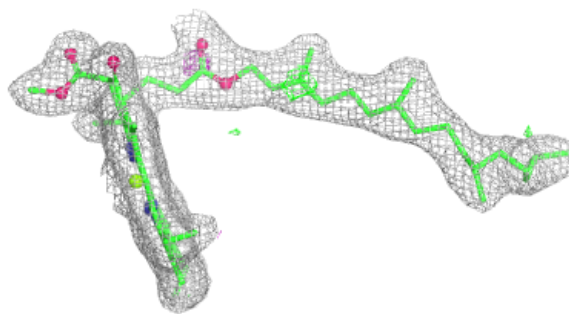
**Electron density around CLA B 602:**

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

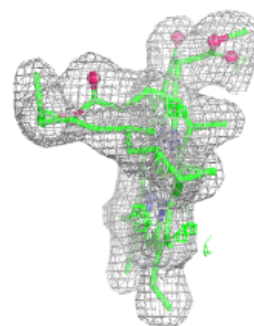
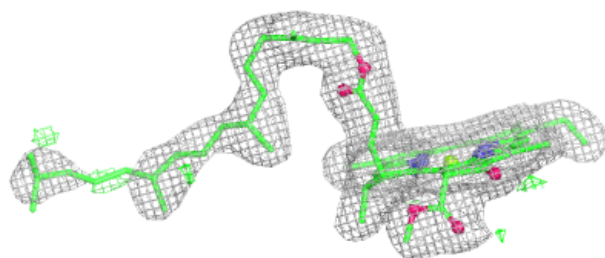
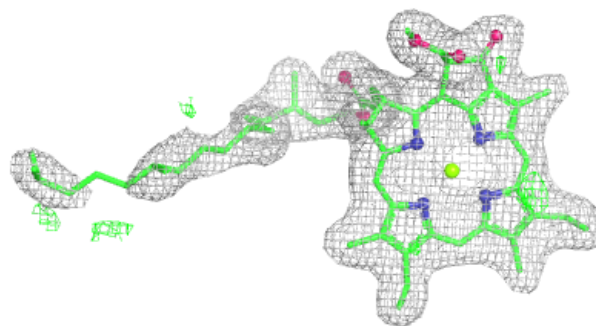


Electron density around CLA B 604:

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

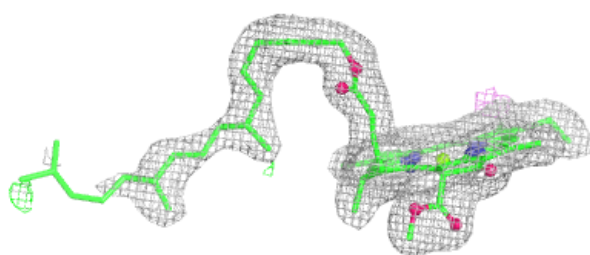
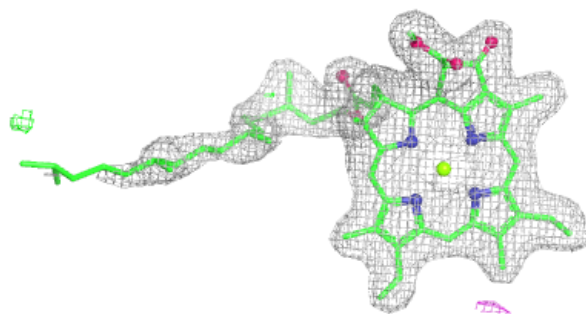
**Electron density around CLA A 404:**

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

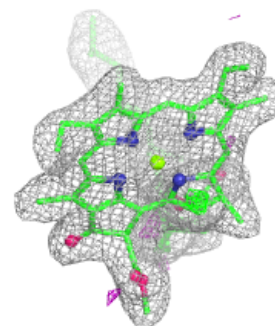
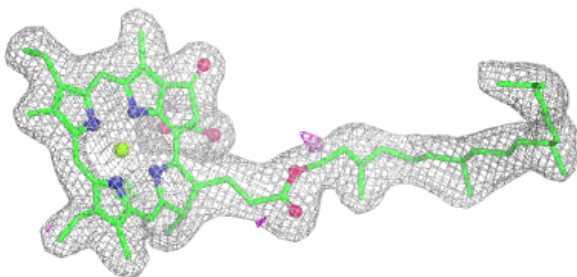
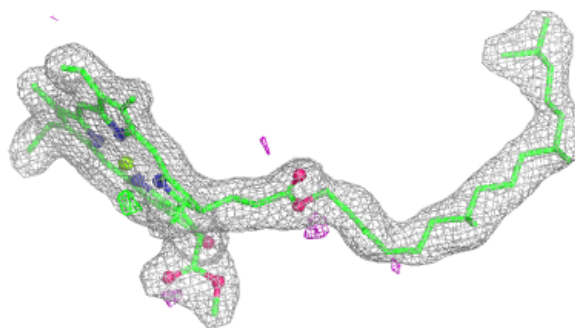


Electron density around CLA d 401:

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

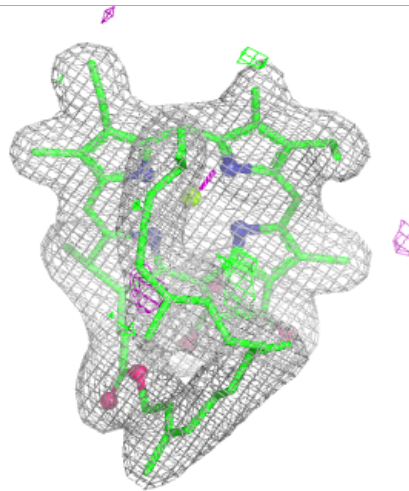
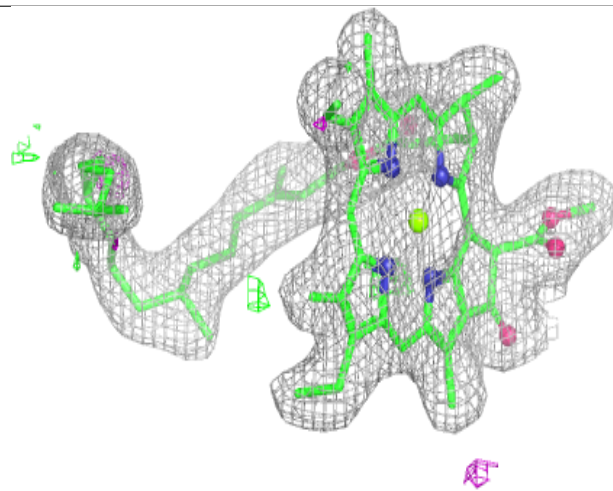
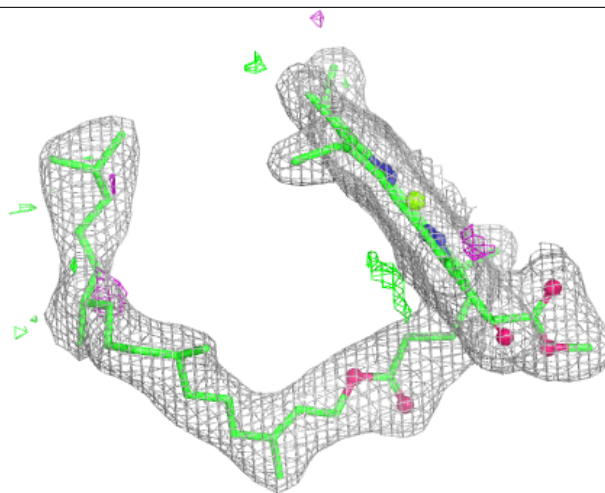
**Electron density around CLA d 402:**

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



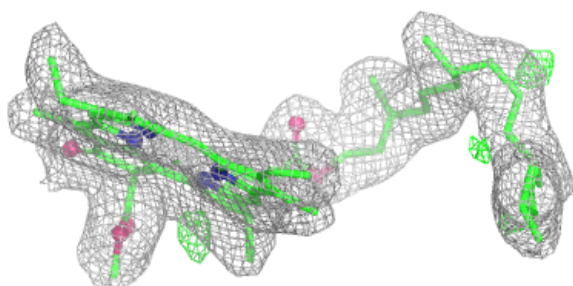
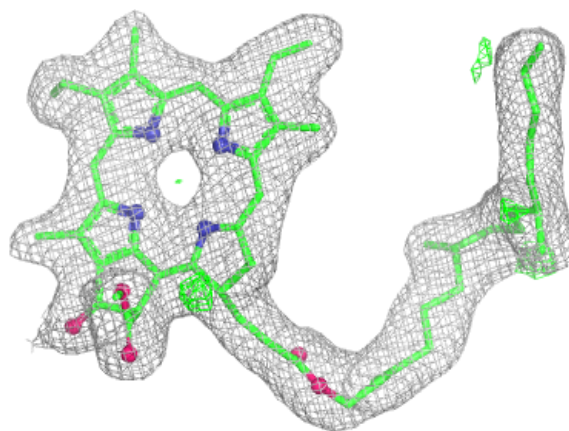
Electron density around CLA b 613:

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



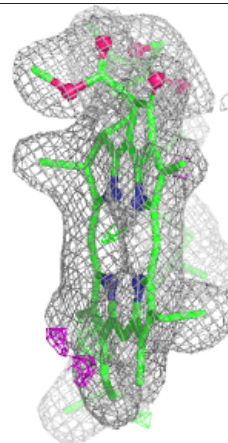
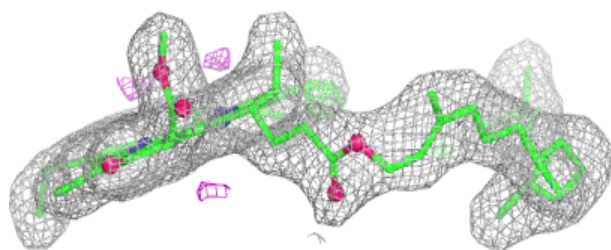
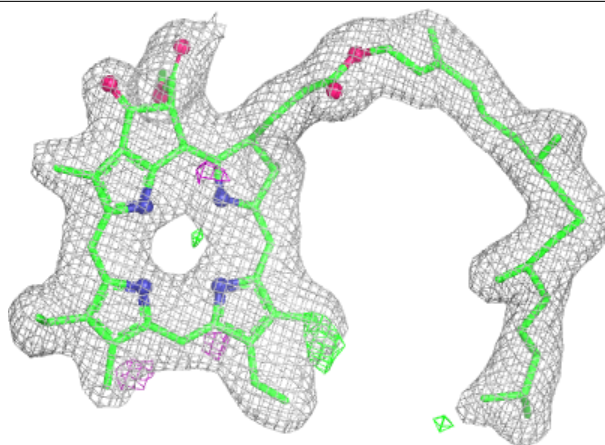
Electron density around PHO A 405:

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

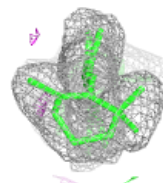
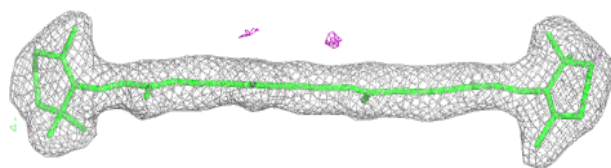
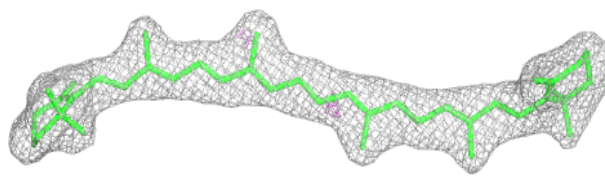


Electron density around PHO a 406:

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

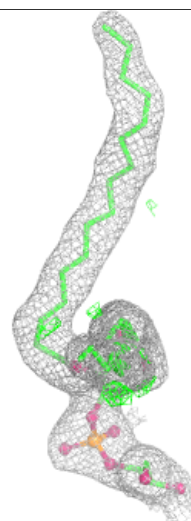
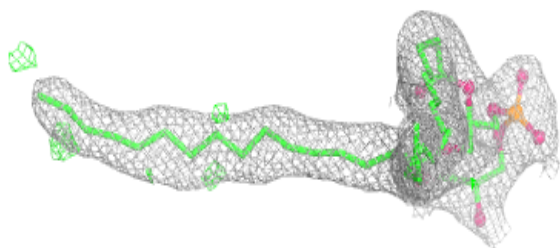
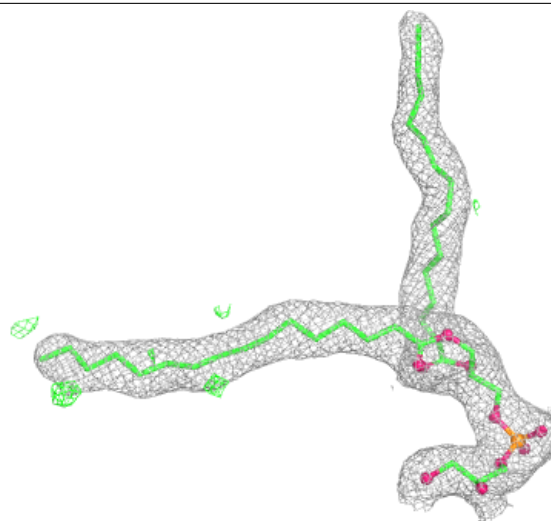
**Electron density around BCR A 407:**

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



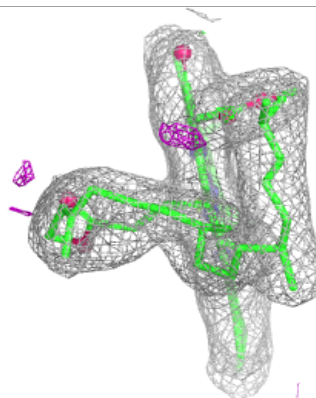
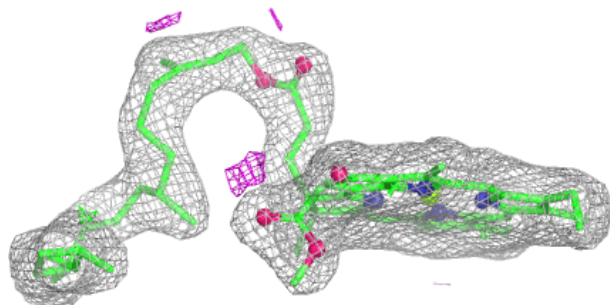
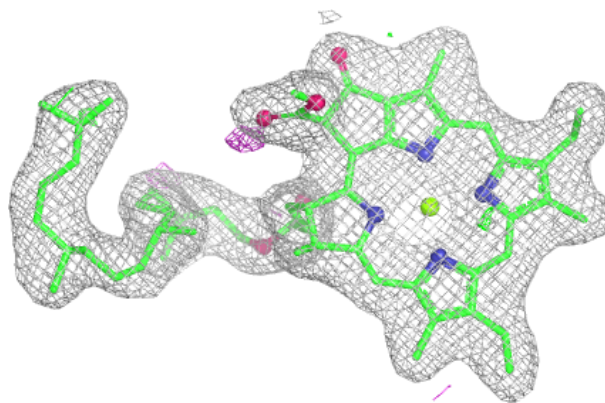
Electron density around LHG L 102:

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



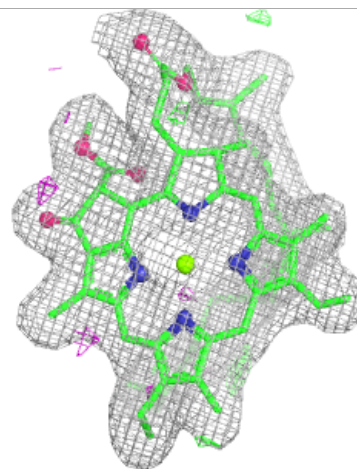
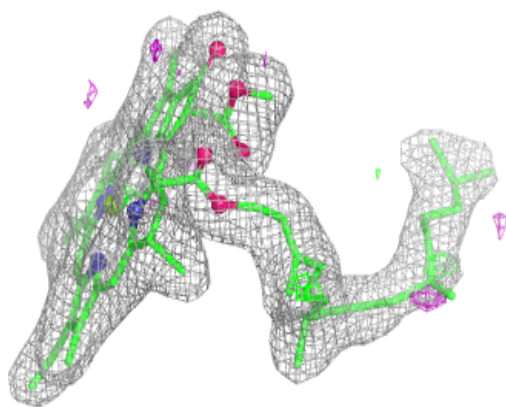
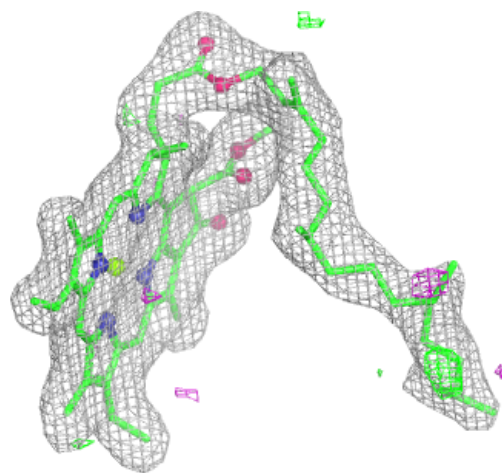
Electron density around CLA b 614:

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



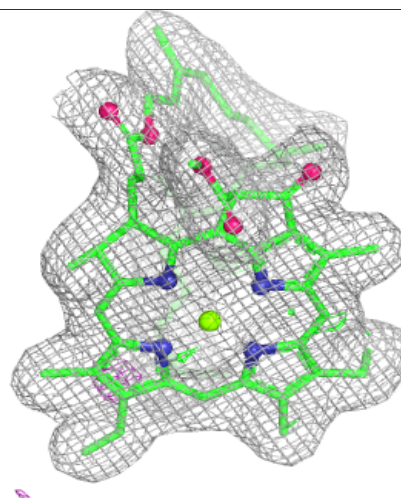
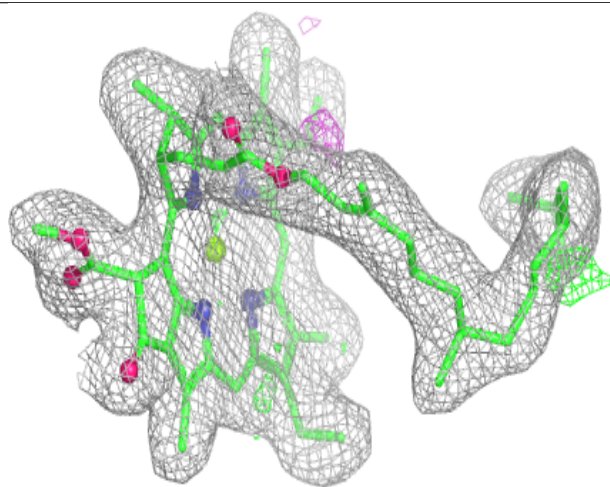
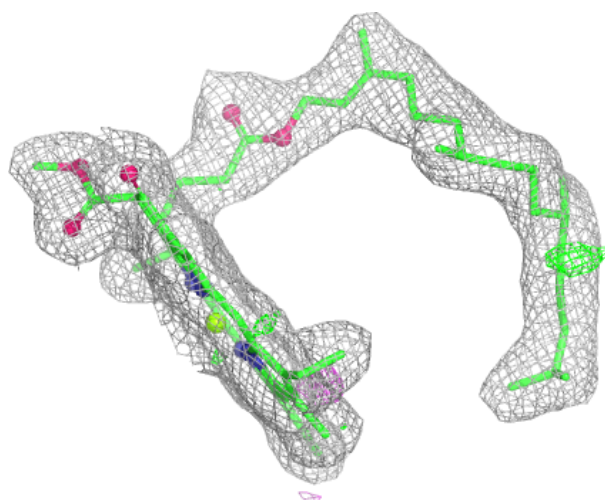
Electron density around CLA b 615:

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



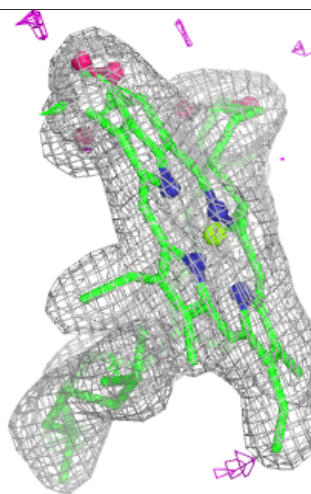
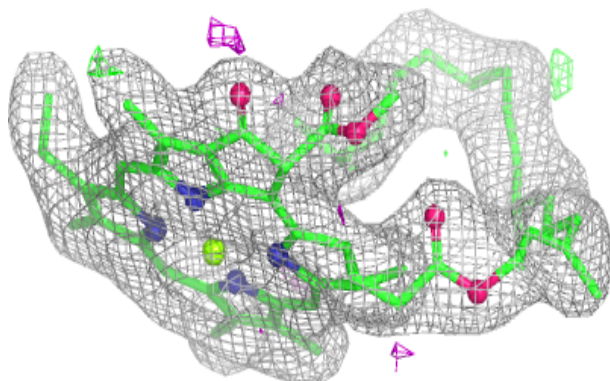
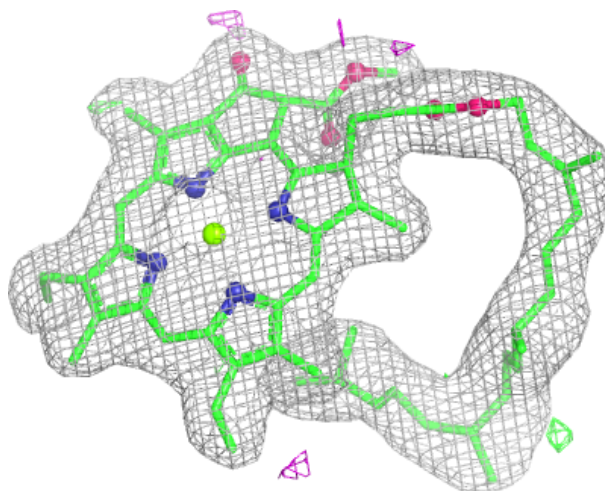
Electron density around CLA B 610:

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



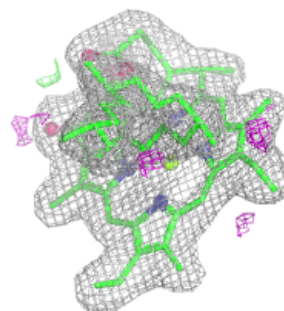
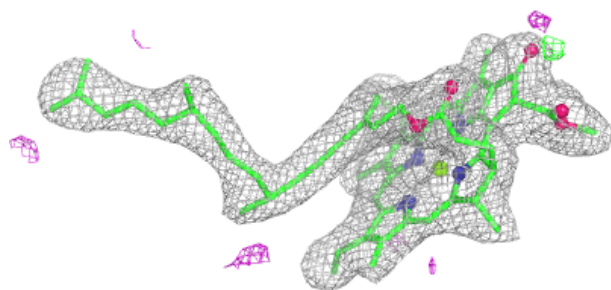
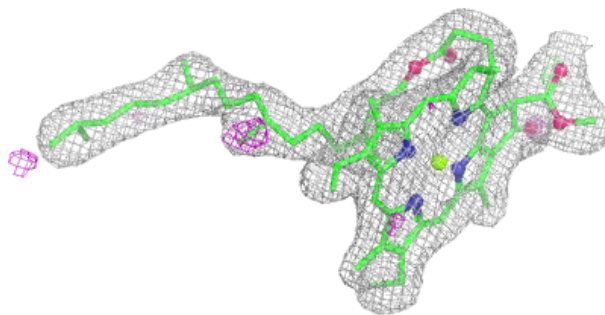
Electron density around CLA b 617:

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

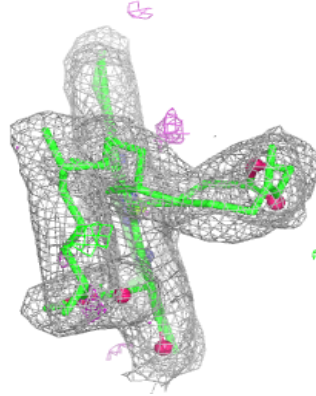
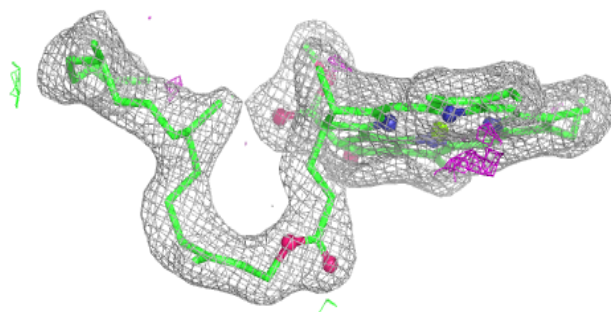
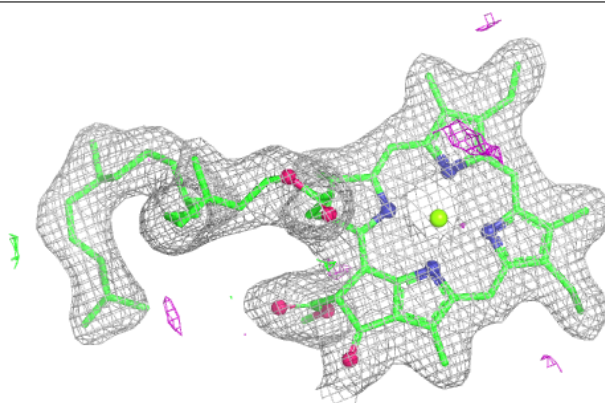


Electron density around CLA C 506:

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

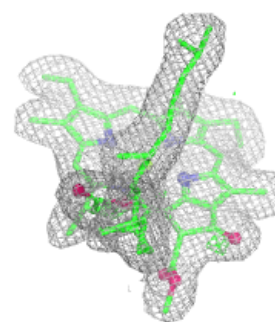
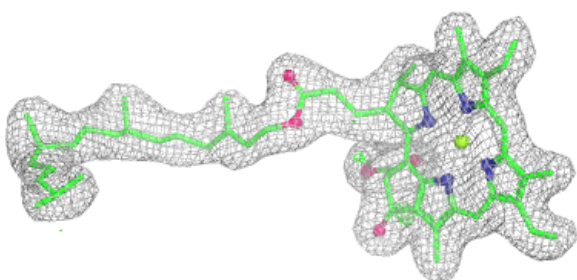
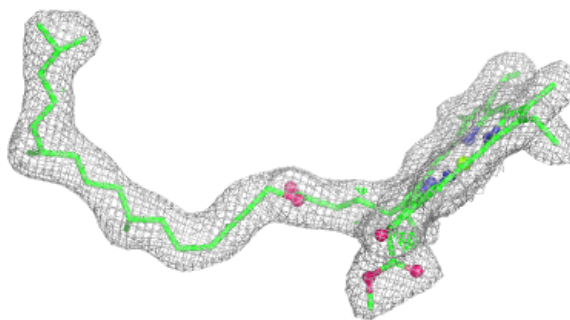
**Electron density around CLA B 611:**

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

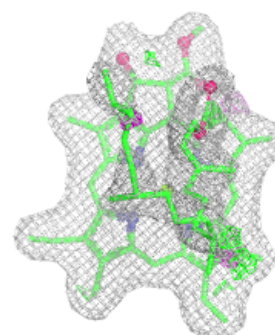
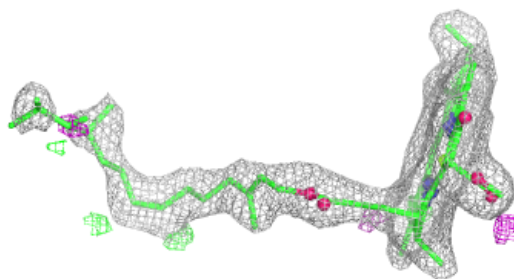
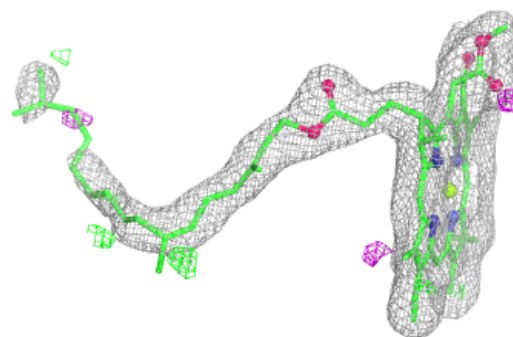


Electron density around CLA D 403:

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

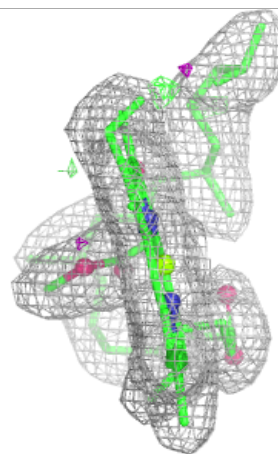
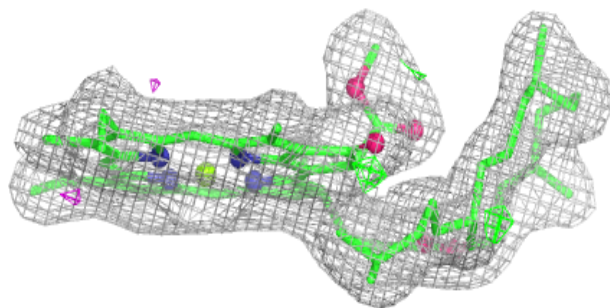
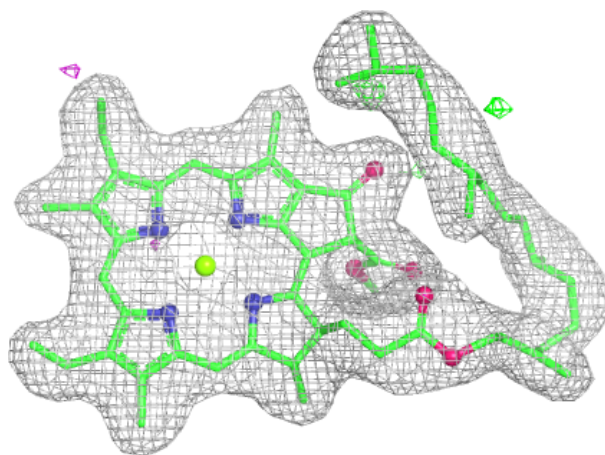
**Electron density around CLA D 404:**

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



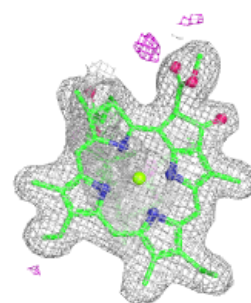
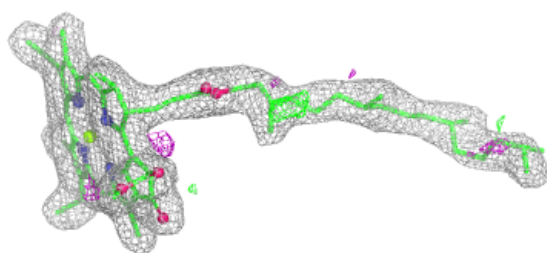
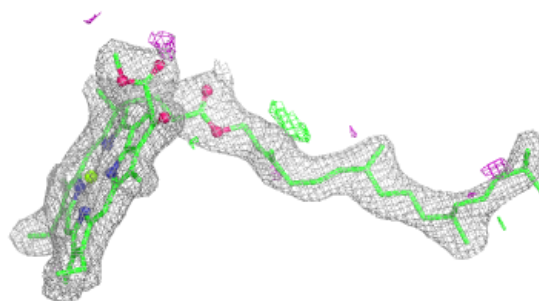
Electron density around CLA B 609:

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

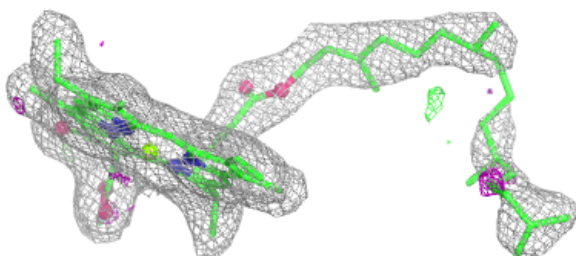
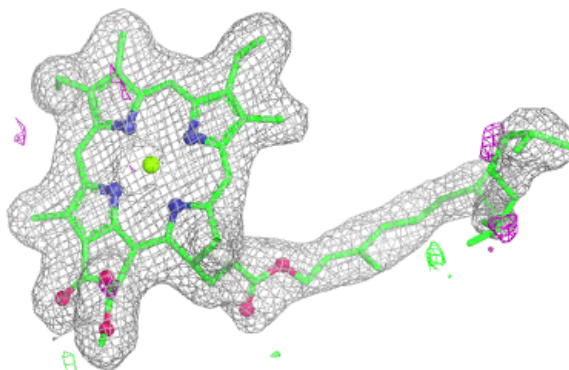


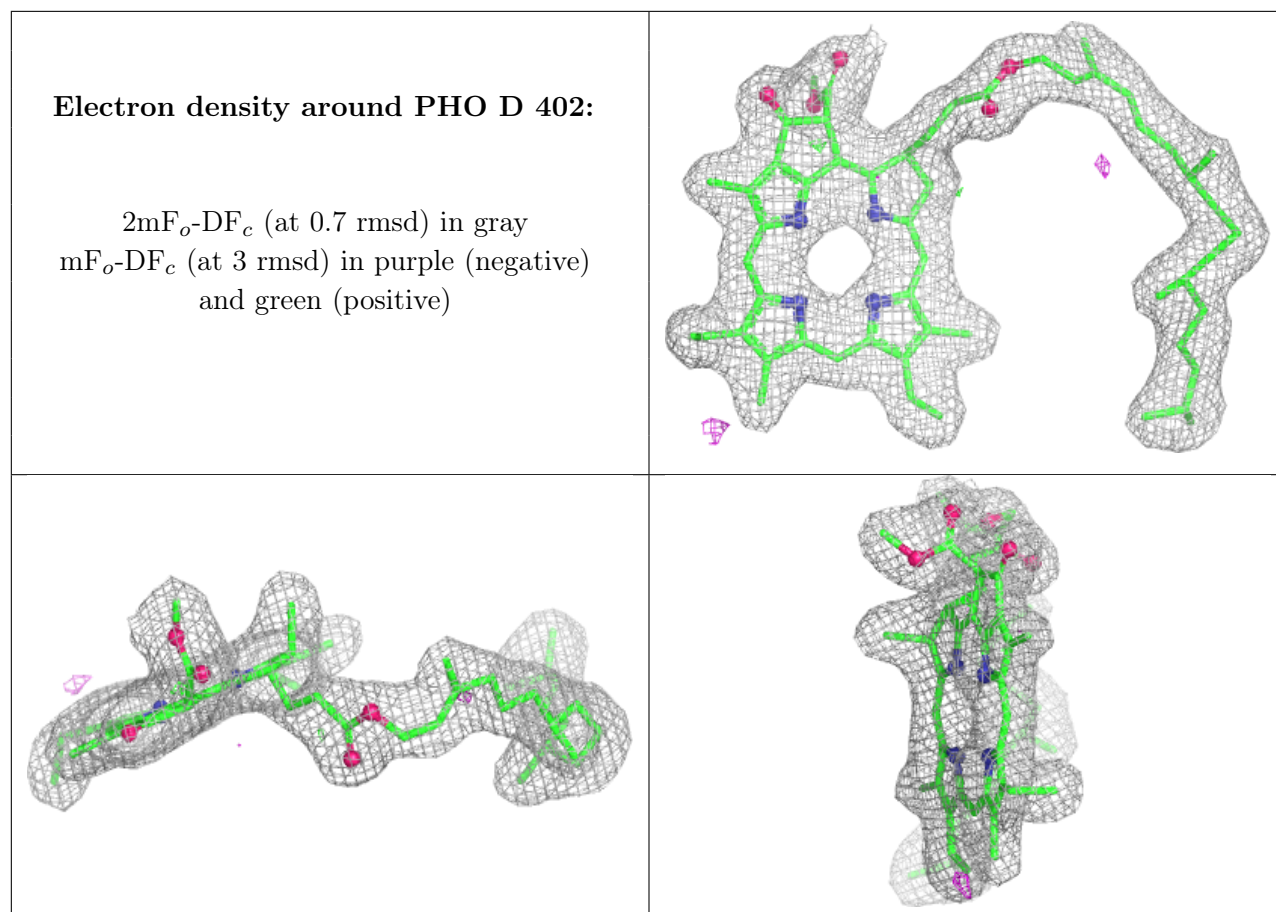
Electron density around CLA B 603:

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

**Electron density around CLA a 407:**

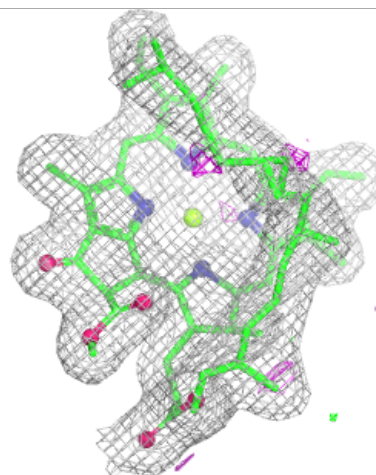
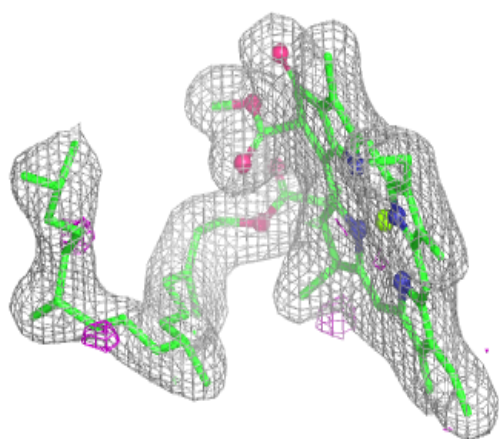
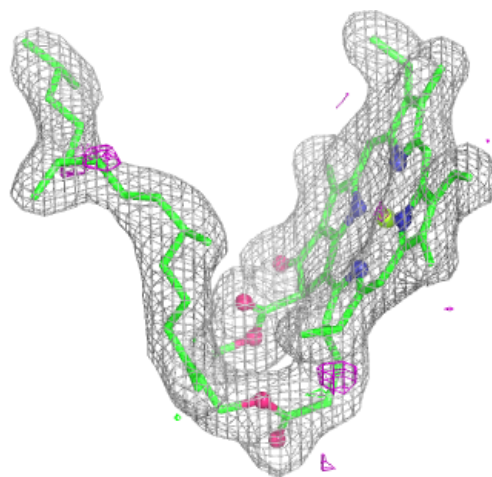
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





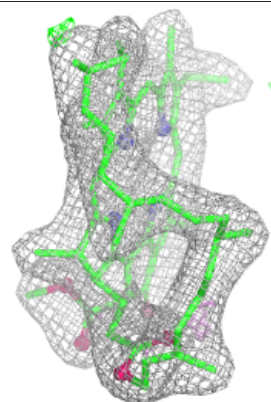
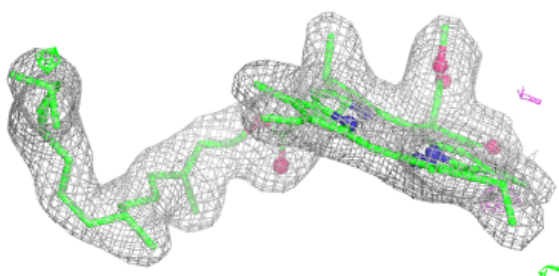
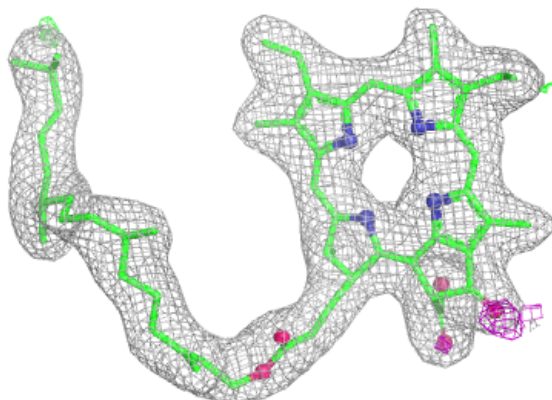
Electron density around CLA B 612:

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

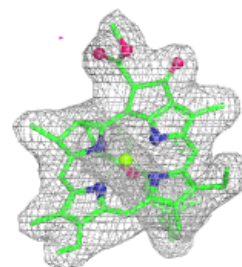
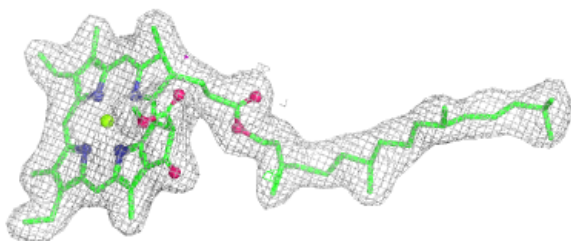
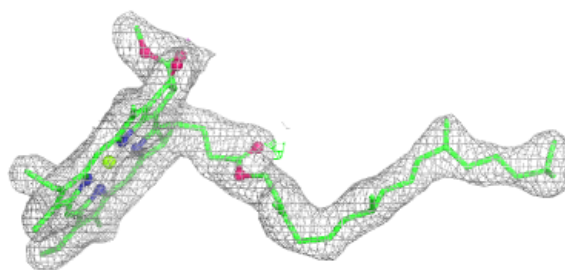


Electron density around PHO a 414:

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

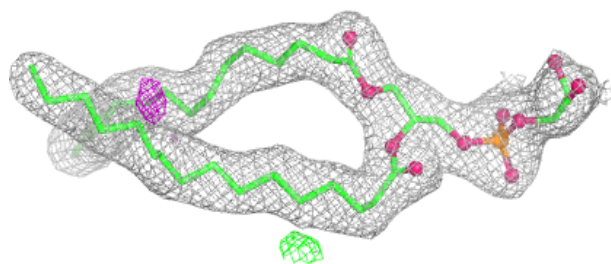
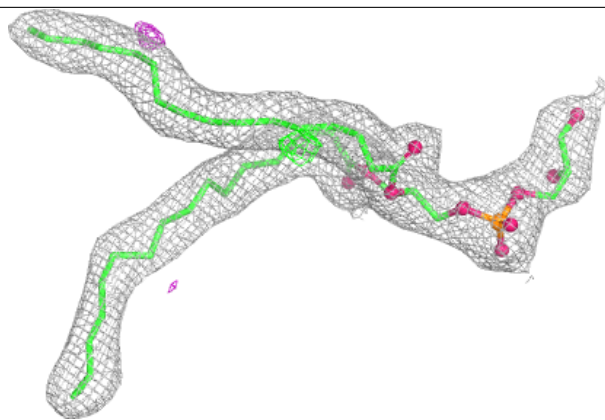
**Electron density around CLA c 503:**

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

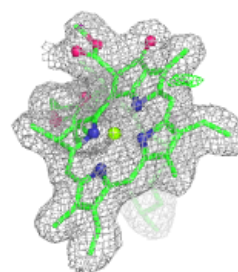
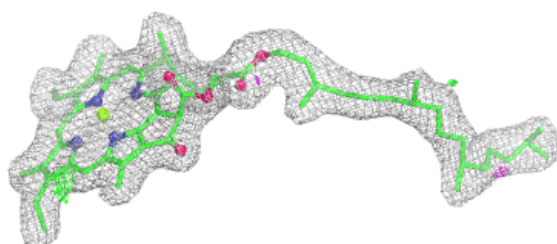
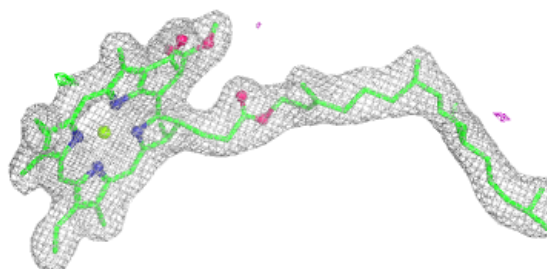


Electron density around LHG D 408:

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

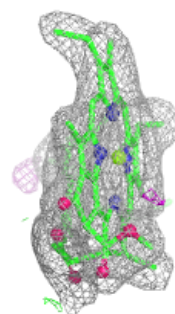
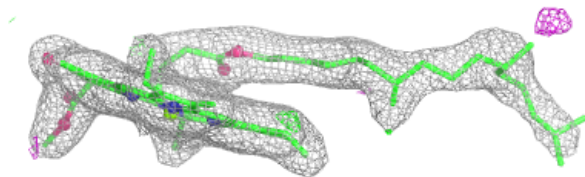
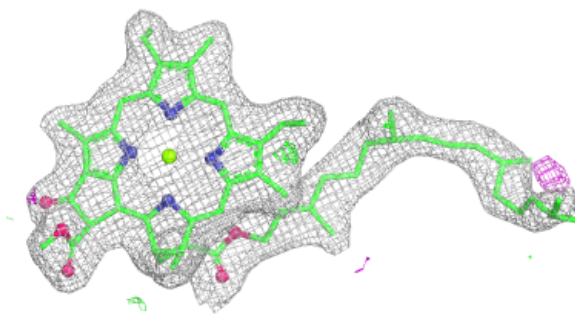
**Electron density around CLA A 403:**

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



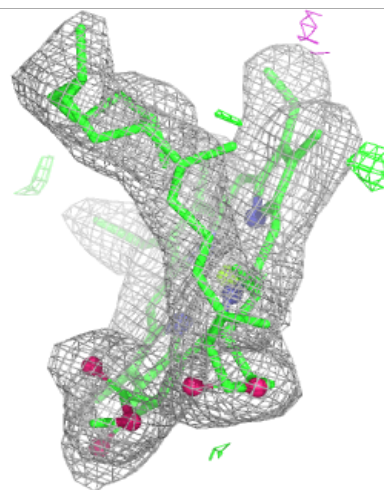
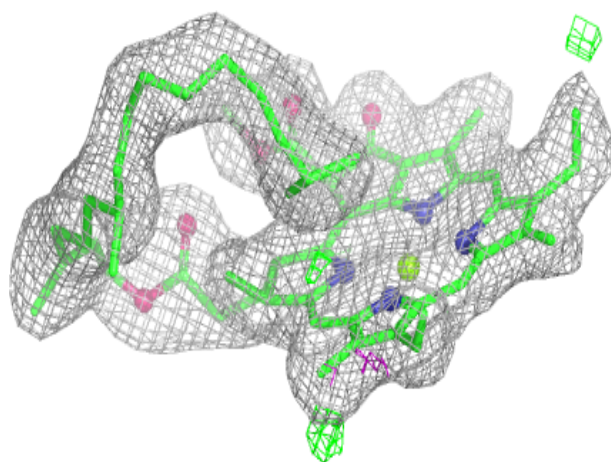
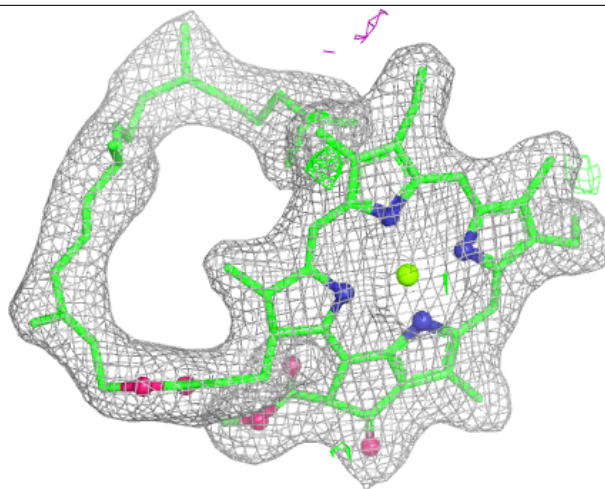
Electron density around CLA b 605:

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



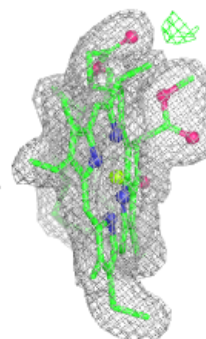
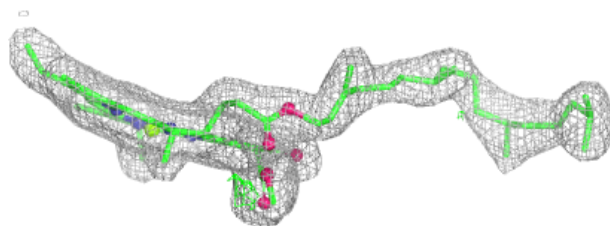
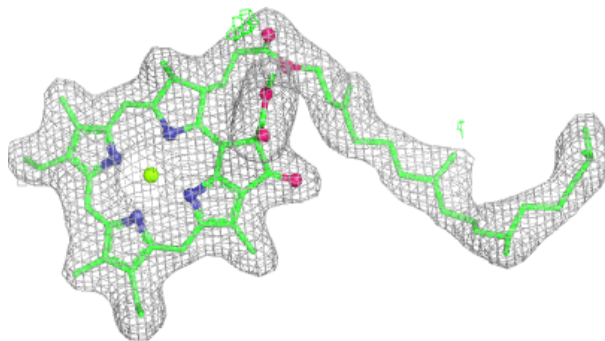
Electron density around CLA B 614:

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

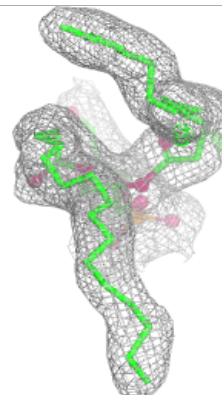
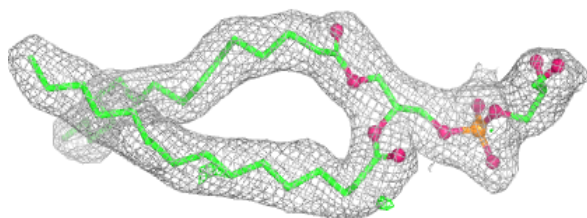
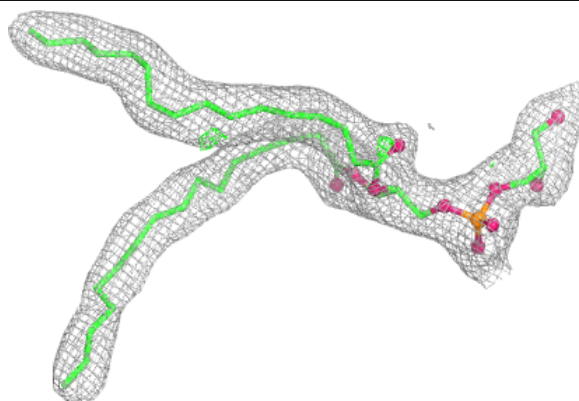


Electron density around CLA B 601:

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

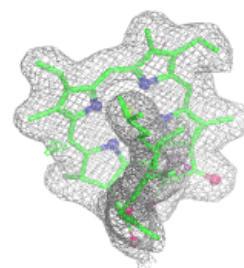
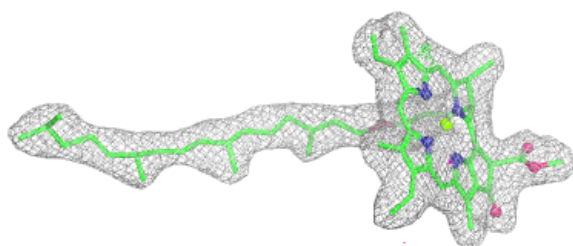
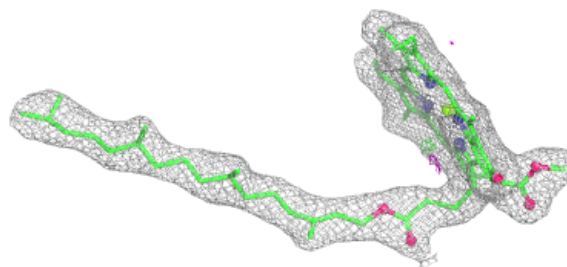
**Electron density around LHG d 406:**

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

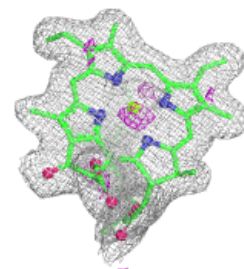
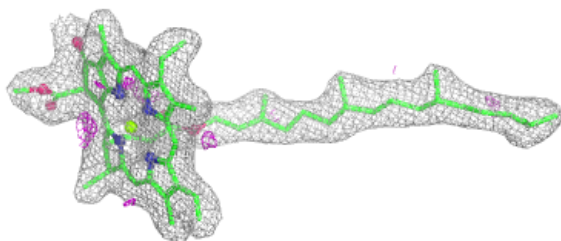
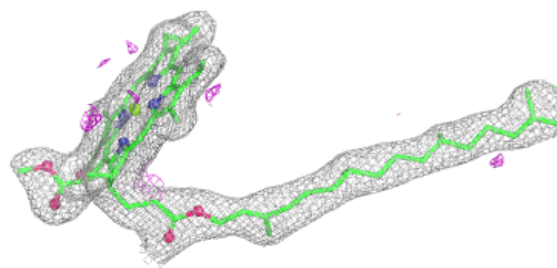


Electron density around CLA B 606:

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

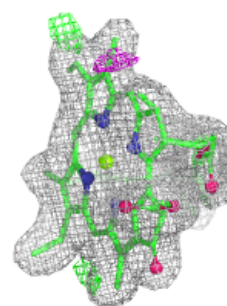
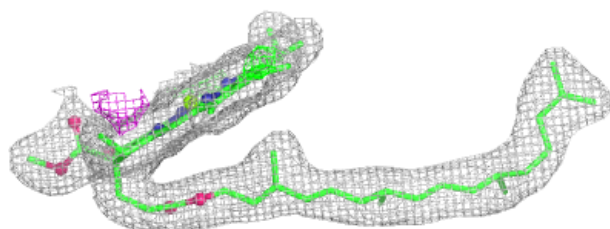
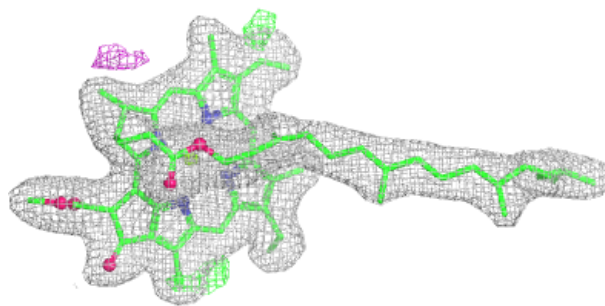
**Electron density around CLA b 609:**

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

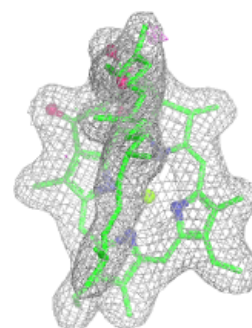
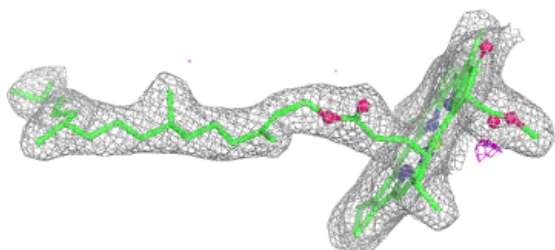
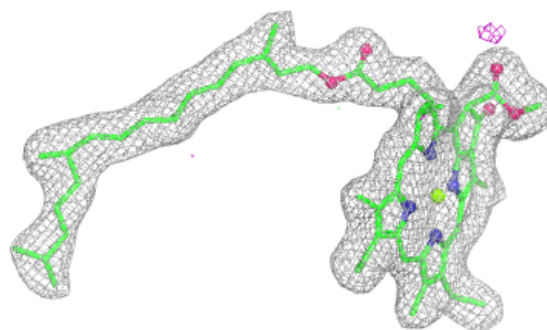


Electron density around CLA B 607:

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

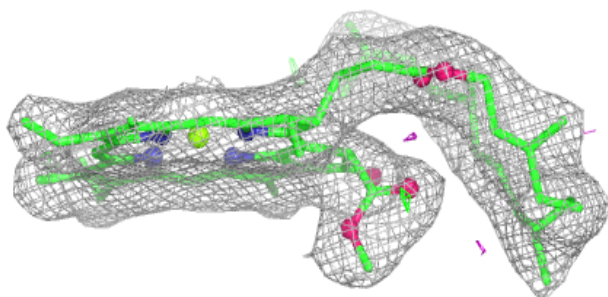
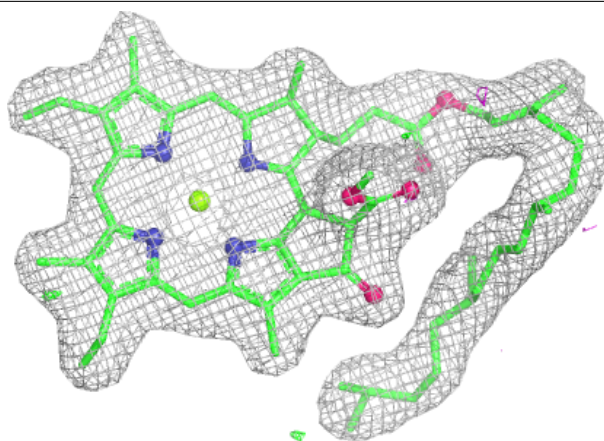
**Electron density around CLA B 608:**

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



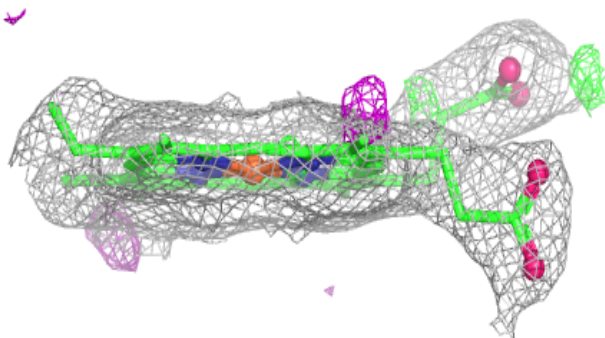
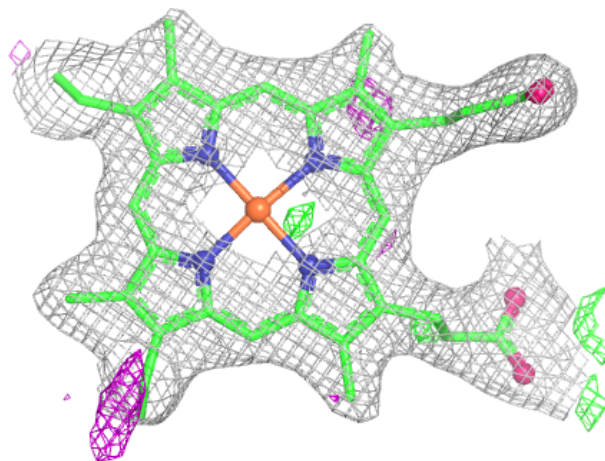
Electron density around CLA b 612:

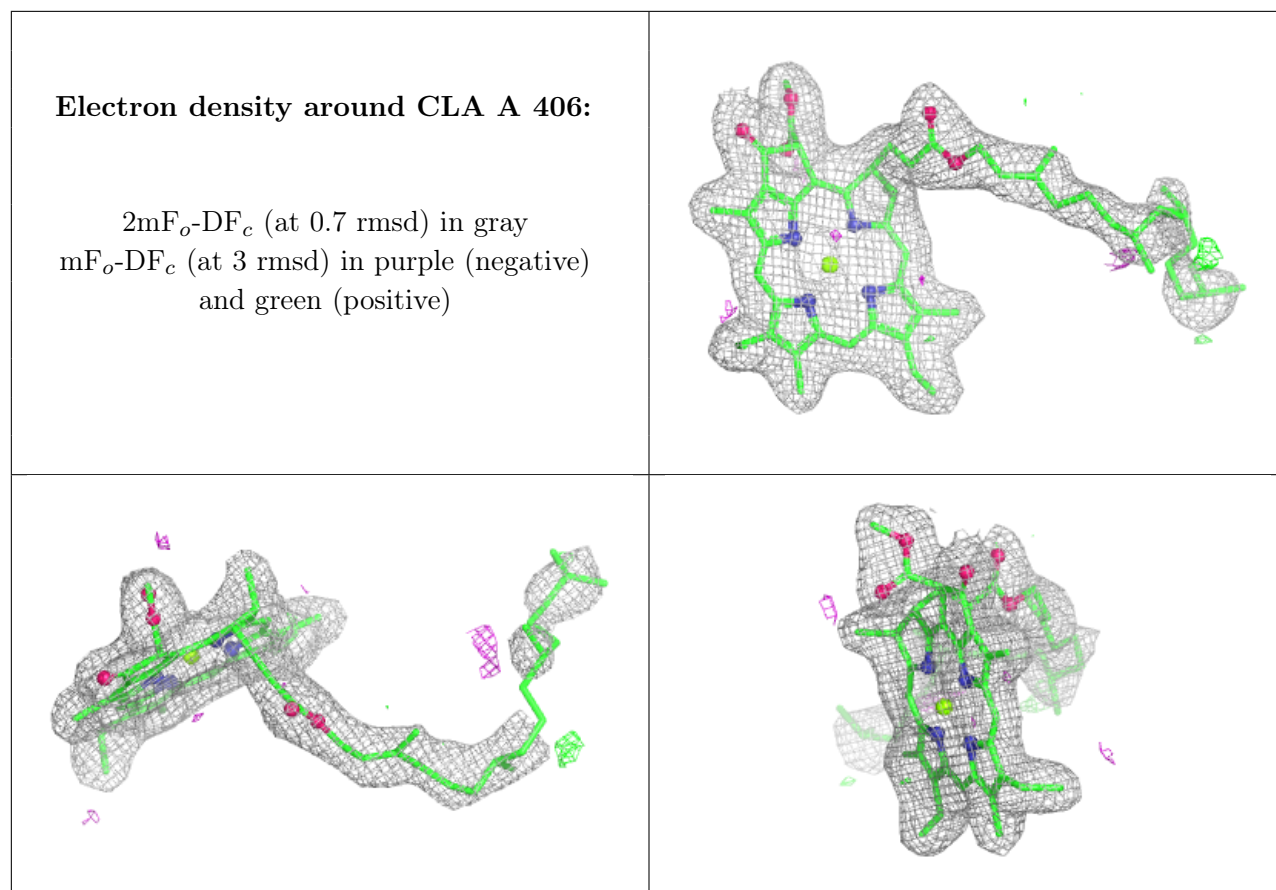
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

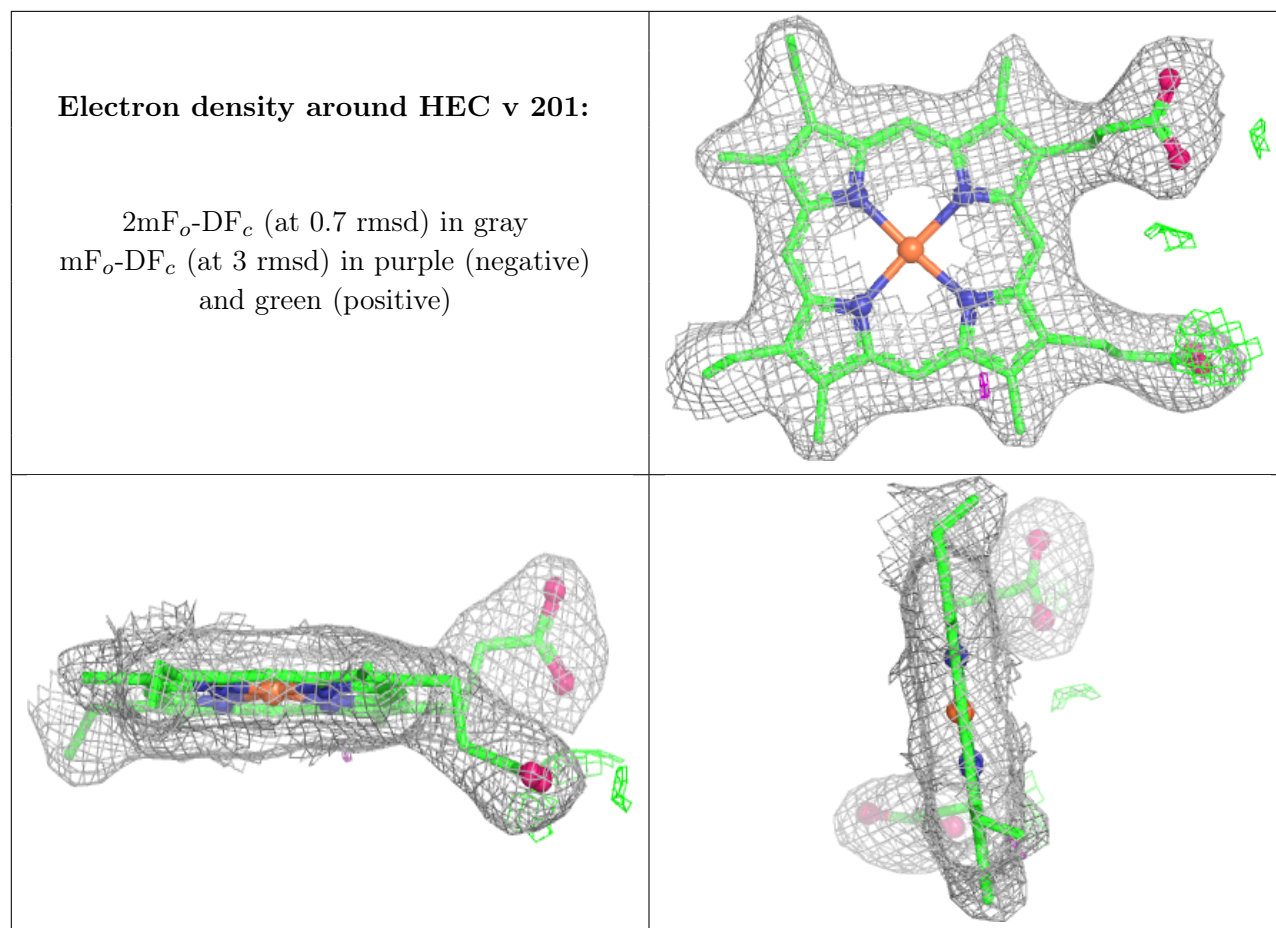


Electron density around HEC V 201:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.