



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:05 AM JST

PDB ID : 4YUU / pdb_00004yuu
Title : Crystal structure of oxygen-evolving photosystem II from a red alga
Authors : Ago, H.; Shen, J.-R.
Deposited on : 2015-03-19
Resolution : 2.77 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

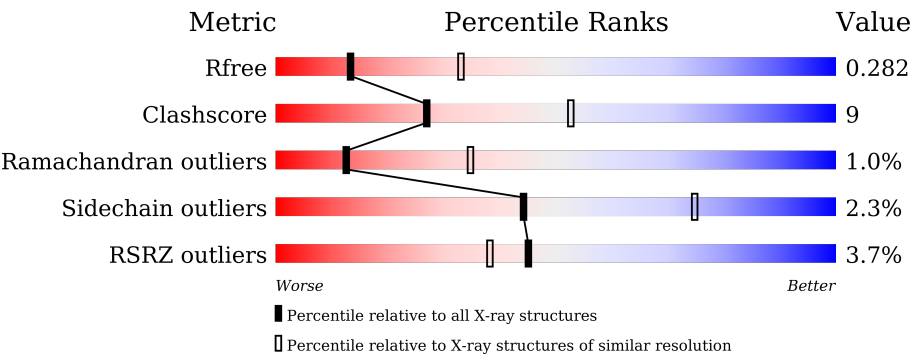
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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.



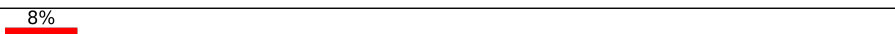
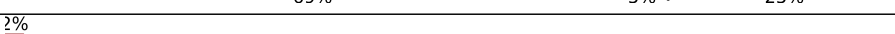
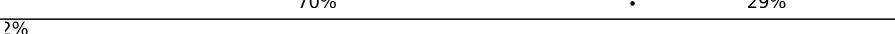
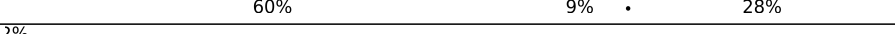
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	A1	344	%80%19%.
1	A2	344	2%81%15%..
1	a1	344	%78%18%..
1	a2	344	80%16%..
2	B1	509	%79%14%. 5%
2	B2	509	2%84%13%..

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Mol	Chain	Length	Quality of chain
2	b1	509	
2	b2	509	
3	C1	460	
3	C2	460	
3	c1	460	
3	c2	460	
4	D1	351	
4	D2	351	
4	d1	351	
4	d2	351	
5	E1	84	
5	E2	84	
5	e1	84	
5	e2	84	
6	F1	43	
6	F2	43	
6	f1	43	
6	f2	43	
7	H1	67	
7	H2	67	
7	h1	67	
7	h2	67	
8	I1	38	
8	I2	38	
8	i1	38	

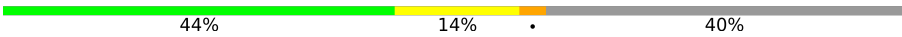
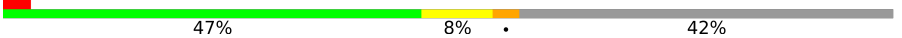
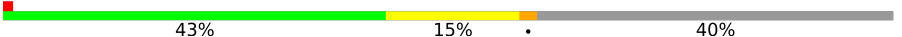
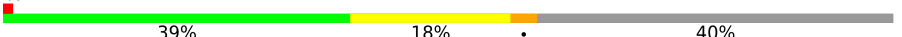
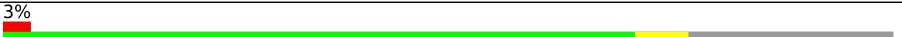
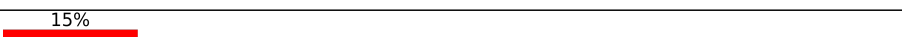
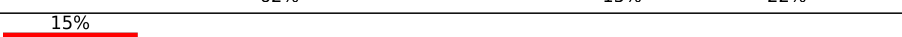
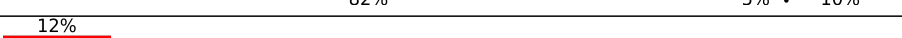
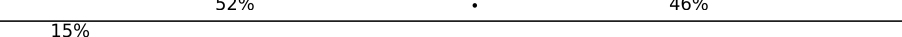
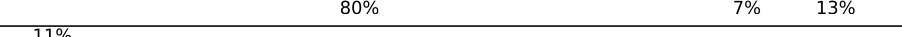
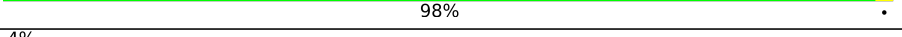
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Mol	Chain	Length	Quality of chain
8	i2	38	
9	J1	39	
9	J2	39	
9	j1	39	
9	j2	39	
10	K1	41	
10	K2	41	
10	k1	41	
10	k2	41	
11	L1	38	
11	L2	38	
11	l1	38	
11	l2	38	
12	M1	108	
12	M2	108	
12	m1	108	
12	m2	108	
13	O1	329	
13	O2	329	
13	o1	329	
13	o2	329	
14	T1	32	
14	T2	32	
14	t1	32	
14	t2	32	

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Mol	Chain	Length	Quality of chain
15	U1	155	
15	U2	155	
15	u1	155	
15	u2	155	
16	V1	155	
16	V2	155	
16	v1	155	
16	v2	155	
17	Y1	35	
17	Y2	35	
17	y1	35	
17	y2	35	
18	X1	40	
18	X2	40	
18	x1	40	
18	x2	40	
19	S1	46	
19	S2	46	
19	s1	46	
19	s2	46	
20	W1	25	
20	W2	25	
20	w1	25	
20	w2	25	
21	Q2	218	

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Mol	Chain	Length	Quality of chain
21	q1	218	8% 43% 5% 52%
22	Z2	62	21% 90% 5% 5%
22	z2	62	6% 82% 13% 5%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 92765 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	344	Total	C	N	O	S	0	0	0
			2609	1708	425	462	14			
1	a1	334	Total	C	N	O	S	0	0	0
			2564	1676	421	454	13			
1	A2	332	Total	C	N	O	S	0	1	0
			2475	1607	411	444	13			
1	a2	334	Total	C	N	O	S	0	0	0
			2513	1638	410	452	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B1	483	Total	C	N	O	S	0	0	0
			3703	2426	624	641	12			
2	b1	503	Total	C	N	O	S	0	1	0
			3881	2549	646	674	12			
2	B2	503	Total	C	N	O	S	0	0	0
			3770	2460	645	654	11			
2	b2	481	Total	C	N	O	S	0	0	0
			3681	2418	620	631	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C1	449	Total	C	N	O	S	0	0	0
			3392	2215	573	594	10			
3	c1	449	Total	C	N	O	S	0	2	0
			3439	2241	577	611	10			
3	C2	444	Total	C	N	O	S	0	0	0
			3145	2028	545	564	8			
3	c2	448	Total	C	N	O	S	0	0	0
			3386	2201	578	597	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D1	337	Total	C	N	O	S	0	0	0
			2615	1736	422	447	10			
4	d1	339	Total	C	N	O	S	0	0	0
			2678	1775	433	460	10			
4	D2	340	Total	C	N	O	S	0	0	0
			2585	1713	422	440	10			
4	d2	340	Total	C	N	O	S	0	0	0
			2643	1756	425	452	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E1	61	Total	C	N	O	0	0	0
			405	264	68	73			
5	e1	57	Total	C	N	O	0	0	0
			427	280	71	76			
5	E2	63	Total	C	N	O	0	0	0
			430	279	72	79			
5	e2	60	Total	C	N	O	0	0	0
			421	279	71	71			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F1	28	Total	C	N	O	S	0	0	0
			213	144	36	32	1			
6	f1	29	Total	C	N	O	S	0	0	0
			227	158	36	32	1			
6	F2	31	Total	C	N	O	S	0	0	0
			229	153	41	34	1			
6	f2	29	Total	C	N	O	S	0	0	0
			225	157	34	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H1	60	Total	C	N	O	S	0	0	0
			433	289	69	73	2			
7	h1	62	Total	C	N	O	S	0	0	0
			470	317	71	80	2			
7	H2	62	Total	C	N	O	S	0	0	0
			443	294	72	75	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	h2	62	Total	C	N	O	S	0	0	0
			450	302	69	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I1	34	Total	C	N	O	S	0	0	0
			274	184	42	45	3			
8	i1	34	Total	C	N	O	S	0	0	0
			280	188	44	45	3			
8	I2	35	Total	C	N	O	S	0	0	0
			265	177	41	45	2			
8	i2	33	Total	C	N	O	S	0	0	0
			261	174	40	44	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J1	32	Total	C	N	O	0	0	0
			220	148	33	39			
9	j1	32	Total	C	N	O	0	0	0
			224	152	33	39			
9	J2	35	Total	C	N	O	0	0	0
			231	154	36	41			
9	j2	33	Total	C	N	O	0	0	0
			228	153	34	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K1	37	Total	C	N	O	S	0	0	0
			279	195	39	44	1			
10	k1	37	Total	C	N	O	S	0	0	0
			280	198	39	42	1			
10	K2	37	Total	C	N	O		0	0	0
			250	171	39	40				
10	k2	37	Total	C	N	O	S	0	0	0
			269	185	40	43	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L1	37	Total	C	N	O	0	0	0
			292	197	46	49			
11	l1	37	Total	C	N	O	0	0	0
			299	203	47	49			
11	L2	37	Total	C	N	O	0	0	0
			299	202	46	51			
11	l2	37	Total	C	N	O	0	0	0
			299	202	46	51			

- Molecule 12 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	m1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	M2	40	Total	C	N	O	S	0	0	0
			284	188	46	48	2			
12	m2	40	Total	C	N	O	S	0	0	0
			287	189	46	50	2			

- Molecule 13 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O1	240	Total	C	N	O	S	0	0	0
			1674	1074	276	316	8			
13	o1	238	Total	C	N	O	S	0	0	0
			1692	1070	282	332	8			
13	O2	205	Total	C	N	O	S	0	0	0
			1376	870	237	262	7			
13	o2	245	Total	C	N	O	S	0	0	0
			1768	1123	296	341	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T1	30	Total	C	N	O	S	0	0	0
			241	168	36	36	1			
14	t1	30	Total	C	N	O	S	0	0	0
			246	173	36	36	1			
14	T2	30	Total	C	N	O	S	0	0	0
			240	170	33	36	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t2	29	Total	C	N	O	S	0	0	0
			235	167	32	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U1	93	Total	C	N	O	S	0	0	0
			691	445	116	129	1			
15	u1	93	Total	C	N	O	S	0	0	0
			703	449	119	134	1			
15	U2	90	Total	C	N	O	S	0	0	0
			577	355	103	118	1			
15	u2	93	Total	C	N	O	S	0	0	0
			708	455	120	132	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U1	-51	MET	-	initiating methionine	UNP Q9ZQS5
u1	-51	MET	-	initiating methionine	UNP Q9ZQS5
U2	-51	MET	-	initiating methionine	UNP Q9ZQS5
u2	-51	MET	-	initiating methionine	UNP Q9ZQS5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V1	129	Total	C	N	O	S	0	0	0
			917	579	159	175	4			
16	v1	129	Total	C	N	O	S	0	0	0
			921	577	163	177	4			
16	V2	129	Total	C	N	O	S	0	0	0
			845	521	152	168	4			
16	v2	129	Total	C	N	O	S	0	0	0
			963	608	168	183	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y1	27	Total	C	N	O	0	0	0
			170	111	29	30			
17	y1	27	Total	C	N	O	0	0	0
			195	133	30	32			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y2	25	Total	C	N	O	0	0	0
			159	104	27	28			
17	y2	27	Total	C	N	O	0	0	0
			188	126	30	32			

- Molecule 18 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X1	29	Total	C	N	O	0	0	0
			197	135	30	32			
18	x1	36	Total	C	N	O	0	0	0
			255	174	38	42			
18	X2	31	Total	C	N	O	0	0	0
			215	149	33	32			
18	x2	32	Total	C	N	O	0	0	0
			218	147	35	36			

- Molecule 19 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S1	25	Total	C	N	O	0	0	0
			164	113	26	25			
19	s1	40	Total	C	N	O	0	0	0
			263	182	41	40			
19	S2	30	Total	C	N	O	0	0	0
			191	130	31	30			
19	s2	46	Total	C	N	O	0	0	0
			281	188	47	46			

- Molecule 20 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	W1	21	Total	C	N	O	0	0	0
			134	91	21	22			
20	w1	25	Total	C	N	O	0	0	0
			152	101	25	26			
20	W2	21	Total	C	N	O	0	0	0
			129	86	21	22			
20	w2	20	Total	C	N	O	0	0	0
			127	86	20	21			

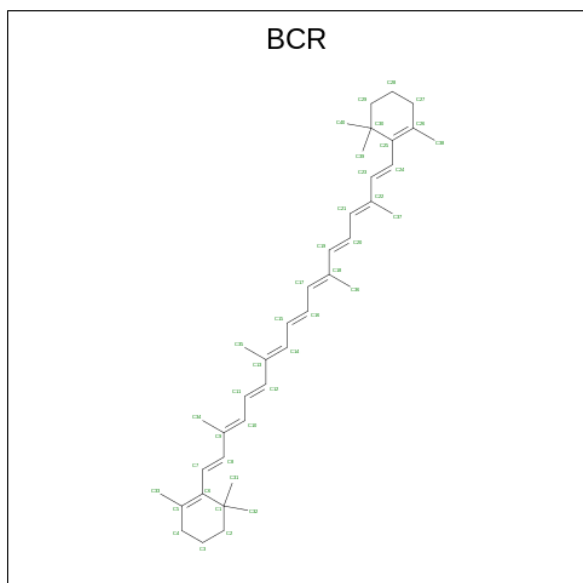
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	q1	105	Total	C	N	O	S	0	0	0
			645	399	115	127	4			
21	Q2	111	Total	C	N	O	S	0	0	0
			676	417	123	133	3			

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z2	59	Total	C	N	O	S	0	0	0
			351	224	61	65	1			
22	z2	59	Total	C	N	O	S	0	0	0
			381	250	63	67	1			

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D1	1	Total C 40 40	0	0
23	H1	1	Total C 22 22	0	0
23	J1	1	Total C 40 40	0	0
23	K1	1	Total C 31 31	0	0
23	a1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	d1	1	Total C 40 40	0	0
23	h1	1	Total C 40 40	0	0
23	k1	1	Total C 40 40	0	0
23	A2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	C2	1	Total C 40 40	0	0
23	F2	1	Total C 40 40	0	0
23	H2	1	Total C 24 24	0	0
23	K2	1	Total C 40 40	0	0

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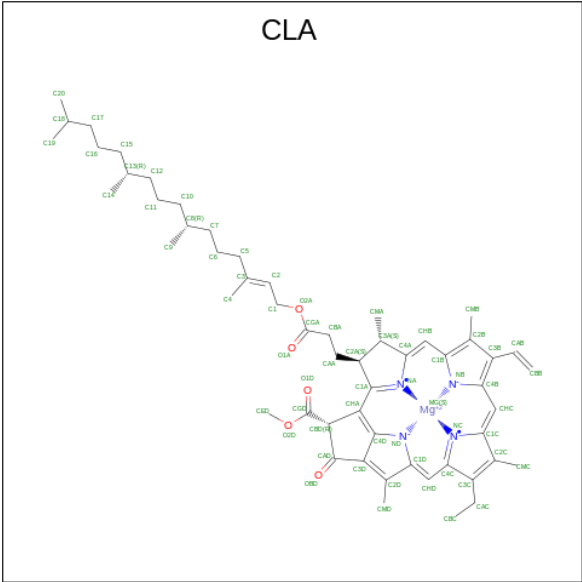
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	K2	1	Total C 29 29	0	0
23	a2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	c2	1	Total C 40 40	0	0
23	d2	1	Total C 40 40	0	0
23	h2	1	Total C 40 40	0	0
23	j2	1	Total C 40 40	0	0
23	k2	1	Total C 40 40	0	0
23	z2	1	Total C 40 40	0	0

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A1	1	Total Cl 1 1	0	0
24	a1	1	Total Cl 1 1	0	0
24	A2	1	Total Cl 1 1	0	0
24	a2	1	Total Cl 1 1	0	0

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	a1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	A2	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
25	B2	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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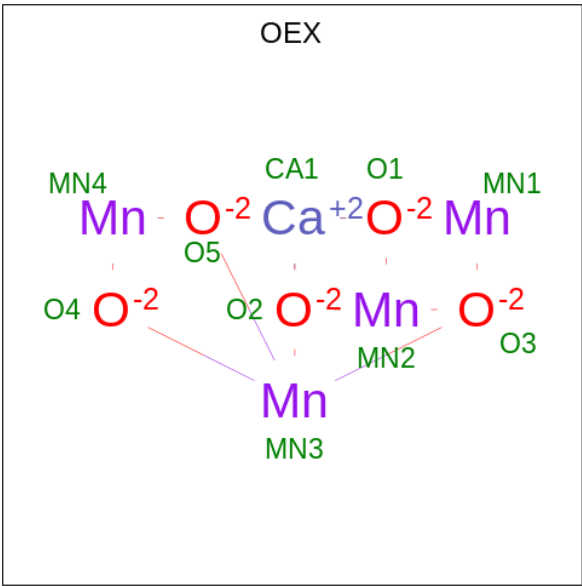
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C2	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
25	C2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	C2	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
25	D2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	D2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	K2	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
25	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	b2	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	b2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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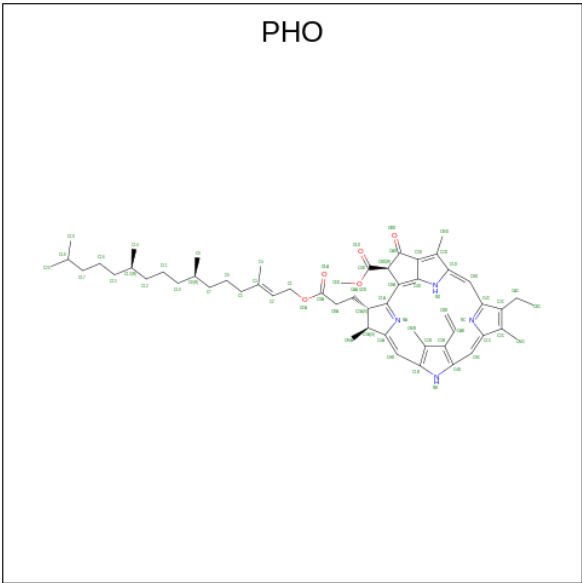
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	A2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A1	1	Total	C	N	O	0	0
			64	55	4	5		
27	D1	1	Total	C	N	O	0	0
			63	54	4	5		
27	a1	1	Total	C	N	O	0	0
			64	55	4	5		
27	d1	1	Total	C	N	O	0	0
			64	55	4	5		
27	A2	1	Total	C	N	O	0	0
			64	55	4	5		
27	D2	1	Total	C	N	O	0	0
			64	55	4	5		
27	a2	1	Total	C	N	O	0	0
			64	55	4	5		
27	d2	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 28 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

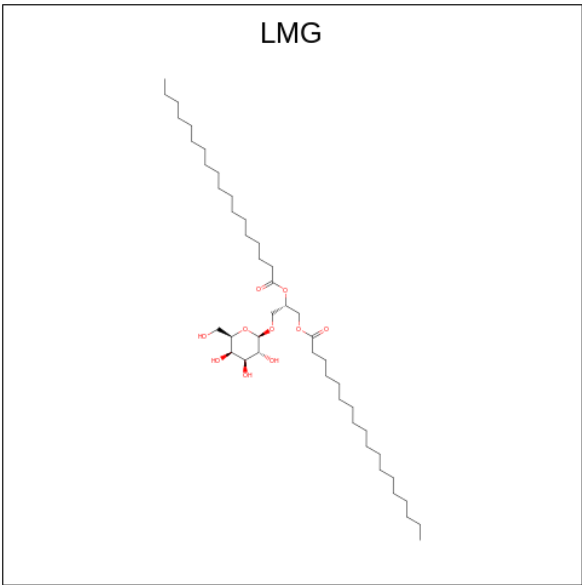
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A1	1	Total	C	0	0
			14	14		
28	B1	3	Total	C	0	0
			41	41		
28	D1	1	Total	C	0	0
			6	6		
28	a1	1	Total	C	0	0
			11	11		
28	b1	7	Total	C	0	0
			92	92		
28	d1	1	Total	C	0	0
			12	12		
28	j1	1	Total	C	0	0
			17	17		
28	l1	1	Total	C	0	0
			12	12		
28	m1	1	Total	C	0	0
			6	6		
28	t1	2	Total	C	0	0
			27	27		
28	x1	1	Total	C	0	0
			15	15		
28	A2	2	Total	C	0	0
			28	28		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B2	4	Total C 58 58	0	0
28	C2	2	Total C 24 24	0	0
28	F2	1	Total C 16 16	0	0
28	H2	1	Total C 5 5	0	0
28	I2	2	Total C 31 31	0	0
28	J2	1	Total C 10 10	0	0
28	K2	1	Total C 5 5	0	0
28	M2	1	Total C 11 11	0	0
28	X2	1	Total C 7 7	0	0
28	W2	1	Total C 9 9	0	0
28	a2	4	Total C 55 55	0	0
28	b2	1	Total C 12 12	0	0
28	c2	1	Total C 15 15	0	0
28	d2	2	Total C 25 25	0	0
28	i2	1	Total C 14 14	0	0
28	k2	4	Total C 30 30	0	0
28	m2	2	Total C 36 36	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A1	1	Total	C	O	0	0
			43	33	10		
29	A1	1	Total	C	O	0	0
			41	31	10		
29	B1	1	Total	C	O	0	0
			31	21	10		
29	B1	1	Total	C	O	0	0
			48	38	10		
29	C1	1	Total	C	O	0	0
			48	38	10		
29	D1	1	Total	C	O	0	0
			35	25	10		
29	M1	1	Total	C	O	0	0
			31	27	4		
29	a1	1	Total	C	O	0	0
			51	41	10		
29	b1	1	Total	C	O	0	0
			38	28	10		
29	b1	1	Total	C	O	0	0
			39	29	10		
29	b1	1	Total	C	O	0	0
			40	30	10		
29	c1	1	Total	C	O	0	0
			55	45	10		
29	d1	1	Total	C	O	0	0
			33	23	10		
29	d1	1	Total	C	O	0	0
			35	30	5		

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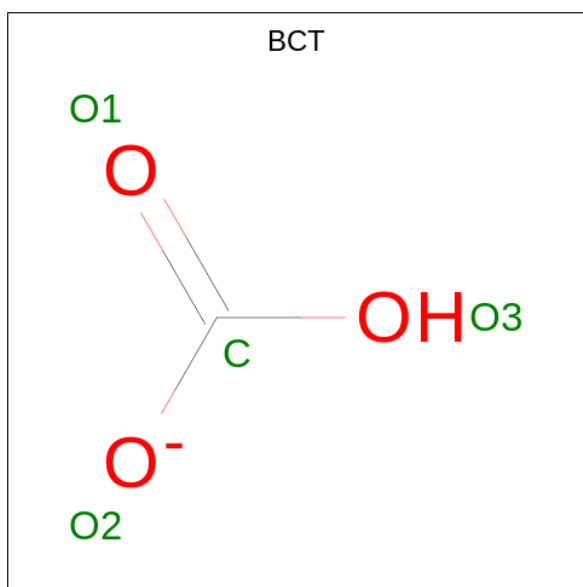
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A2	1	Total	C	O	0	0
			29	19	10		
29	B2	1	Total	C	O	0	0
			40	30	10		
29	B2	1	Total	C	O	0	0
			37	27	10		
29	C2	1	Total	C	O	0	0
			24	14	10		
29	F2	1	Total	C	O	0	0
			35	25	10		
29	I2	1	Total	C	O	0	0
			34	24	10		
29	a2	1	Total	C	O	0	0
			44	34	10		
29	b2	1	Total	C	O	0	0
			39	29	10		
29	c2	1	Total	C	O	0	0
			26	16	10		
29	d2	1	Total	C	O	0	0
			27	17	10		
29	j2	1	Total	C	O	0	0
			50	40	10		

- Molecule 30 is FE (III) ION (CCD ID: FE) (formula: Fe).

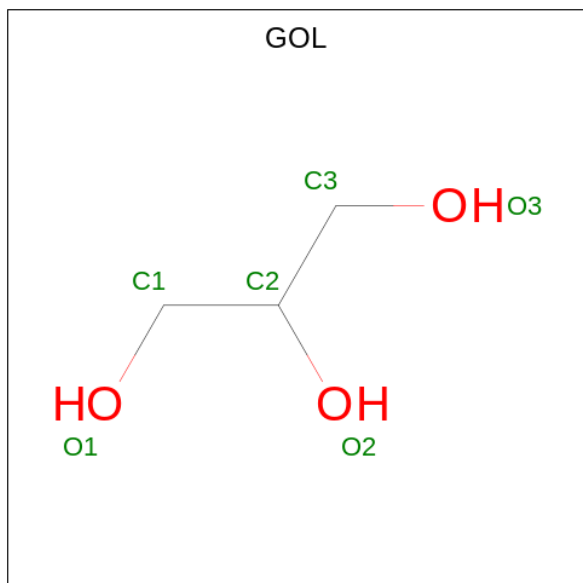
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A1	1	Total	Fe	0	0
			1	1		
30	a1	1	Total	Fe	0	0
			1	1		
30	A2	1	Total	Fe	0	0
			1	1		
30	a2	1	Total	Fe	0	0
			1	1		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



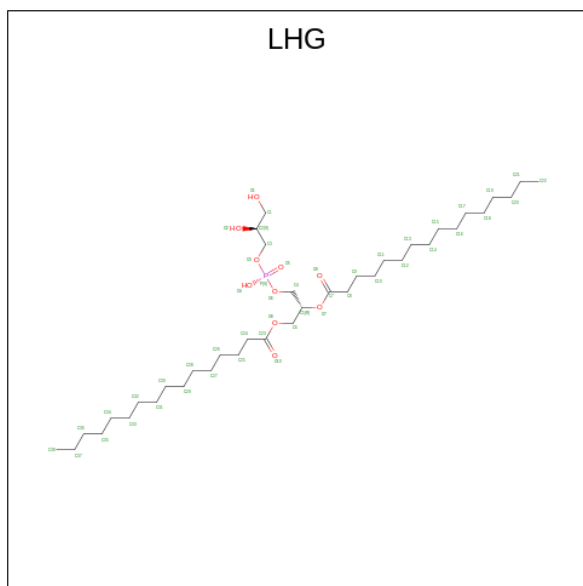
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A1	1	Total	C	O	0	0
			4	1	3		
31	a1	1	Total	C	O	0	0
			4	1	3		
31	A2	1	Total	C	O	0	0
			4	1	3		
31	a2	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B1	1	Total	C	O	0	0
			6	3	3		
32	C1	1	Total	C	O	0	0
			6	3	3		
32	a1	1	Total	C	O	0	0
			6	3	3		
32	b1	1	Total	C	O	0	0
			6	3	3		
32	c1	1	Total	C	O	0	0
			6	3	3		
32	i1	1	Total	C	O	0	0
			6	3	3		
32	C2	1	Total	C	O	0	0
			6	3	3		
32	a2	1	Total	C	O	0	0
			6	3	3		
32	c2	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



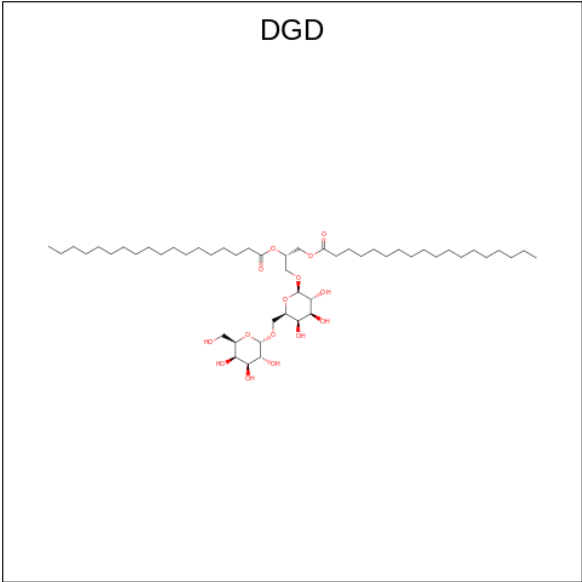
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B1	1	Total	C	O	P	0	0
			49	38	10	1		
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		

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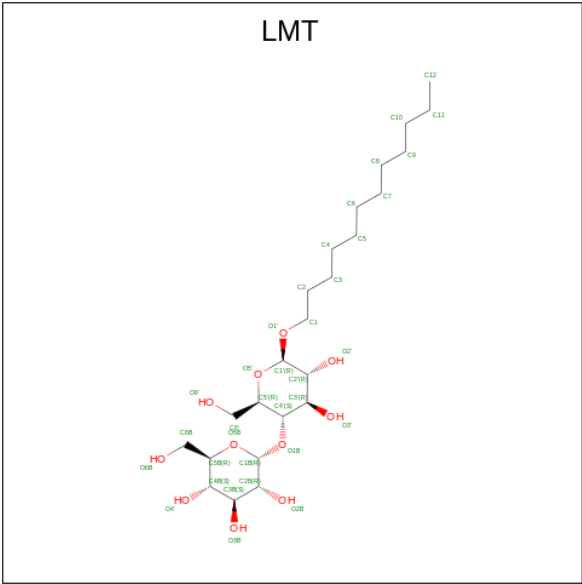
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		
33	L1	1	Total	C	O	P	0	0
			41	30	10	1		
33	a1	1	Total	C	O	P	0	0
			43	32	10	1		
33	b1	1	Total	C	O	P	0	0
			49	38	10	1		
33	d1	1	Total	C	O	P	0	0
			32	21	10	1		
33	d1	1	Total	C	O	P	0	0
			49	38	10	1		
33	l1	1	Total	C	O	P	0	0
			49	38	10	1		
33	A2	1	Total	C	O	P	0	0
			33	22	10	1		
33	B2	1	Total	C	O	P	0	0
			42	31	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	L2	1	Total	C	O	P	0	0
			49	38	10	1		
33	a2	1	Total	C	O	P	0	0
			30	19	10	1		
33	b2	1	Total	C	O	P	0	0
			43	32	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	l2	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C1	1	Total	C	O	0	0
			52	37	15		
34	C1	1	Total	C	O	0	0
			62	47	15		
34	C1	1	Total	C	O	0	0
			64	49	15		
34	H1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			51	36	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	h1	1	Total	C	O	0	0
			62	47	15		
34	C2	1	Total	C	O	0	0
			33	18	15		
34	H2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			52	37	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	h2	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



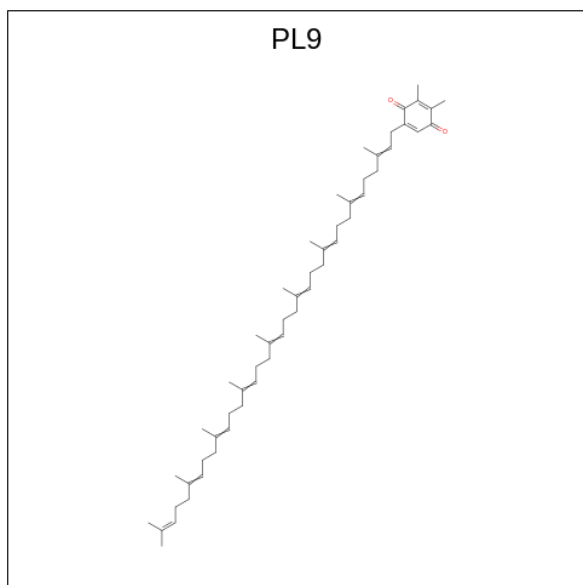
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C1	1	Total C O 35 24 11	0	0
35	L1	1	Total C 12 12	0	0
35	M1	1	Total C 11 11	0	0
35	M1	1	Total C O 24 18 6	0	0
35	T1	1	Total C 12 12	0	0
35	c1	1	Total C O 33 22 11	0	0
35	l1	1	Total C O 24 18 6	0	0
35	m1	1	Total C O 35 24 11	0	0
35	a2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	i2	1	Total C 7 7	0	0
35	m2	1	Total C O 30 19 11	0	0

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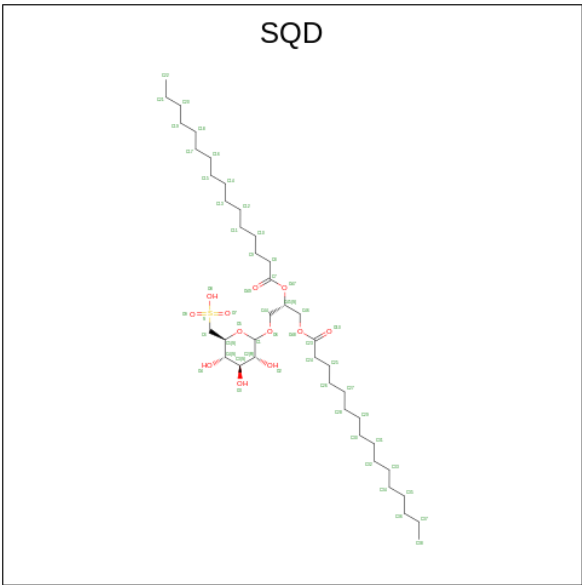
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	m2	1	Total	C	O	0	0
			29	18	11		

- Molecule 36 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).



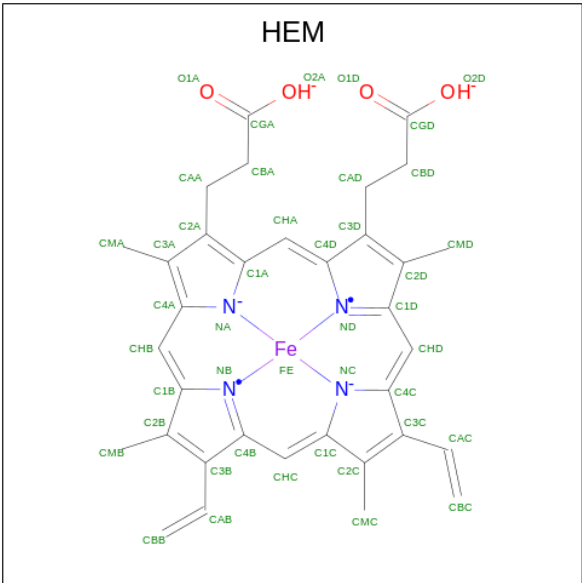
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D1	1	Total	C	O	0	0
			55	53	2		
36	d1	1	Total	C	O	0	0
			55	53	2		
36	D2	1	Total	C	O	0	0
			55	53	2		
36	d2	1	Total	C	O	0	0
			55	53	2		

- Molecule 37 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
37	D1	1	Total	C	O	S	0	0
			35	22	12	1		
37	B2	1	Total	C	O	S	0	0
			45	32	12	1		
37	D2	1	Total	C	O	S	0	0
			25	12	12	1		
37	b2	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	V1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	f1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	v1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	E2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	V2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	v2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O1	1	Total 1	Ca 1	0	0
39	o2	1	Total 1	Ca 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A1	2	Total 2	O 2	0	0
40	B1	1	Total 1	O 1	0	0
40	a1	4	Total 4	O 4	0	0
40	c1	2	Total 2	O 2	0	0
40	A2	2	Total 2	O 2	0	0
40	a2	4	Total 4	O 4	0	0
40	b2	1	Total 1	O 1	0	0
40	c2	1	Total 1	O 1	0	0

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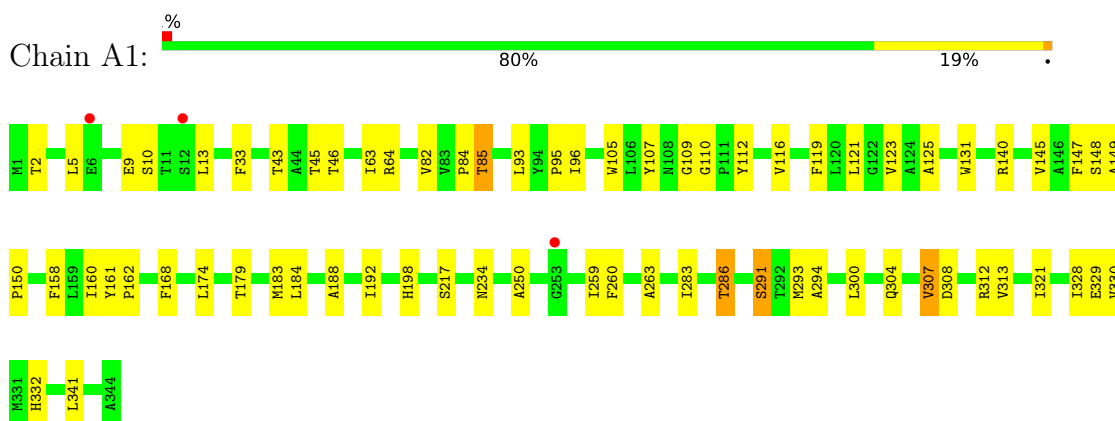
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d2	1	Total	O	0	0
			1	1		

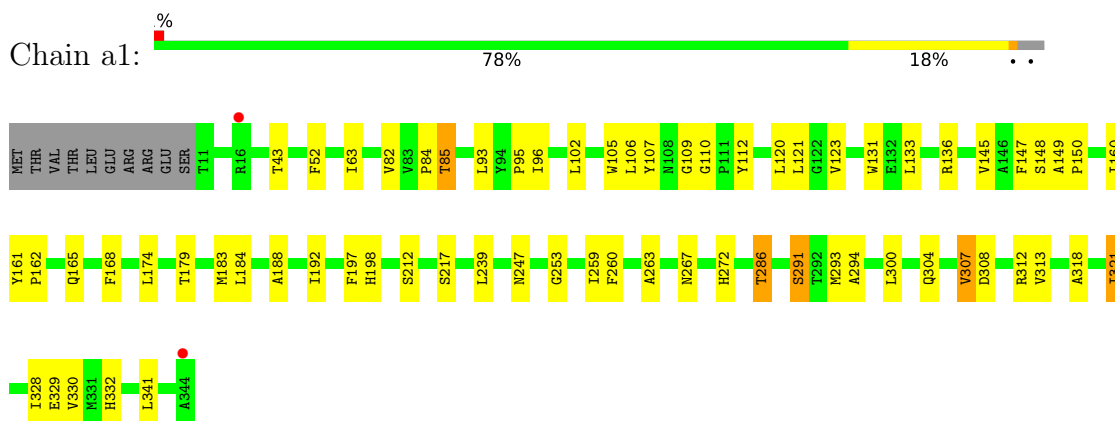
3 Residue-property plots

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

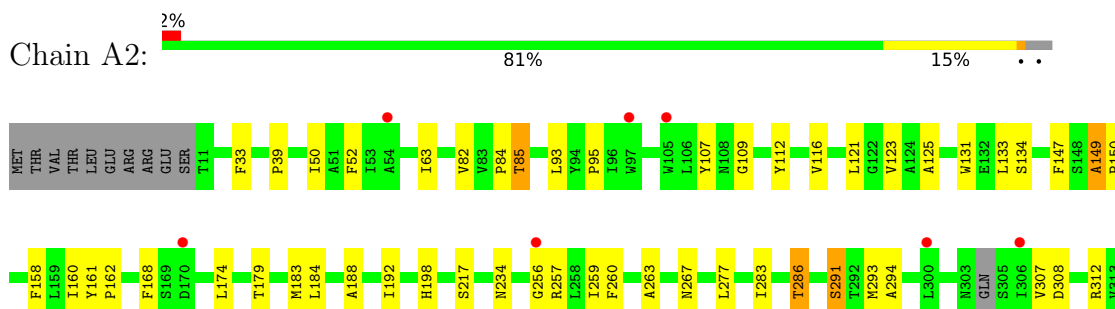
- Molecule 1: Photosystem II protein D1

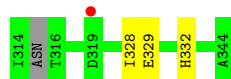


- Molecule 1: Photosystem II protein D1



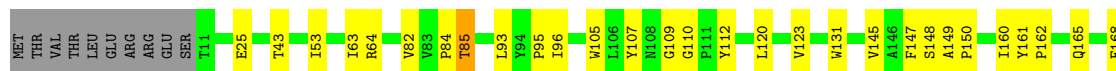
- Molecule 1: Photosystem II protein D1





- Molecule 1: Photosystem II protein D1

Chain a2: 80% 16% ..



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B1: % 79% 14% 5%



- Molecule 2: Photosystem II CP47 reaction center protein

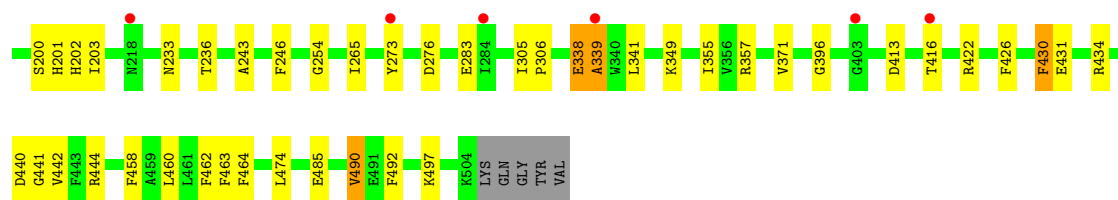
Chain b1: 83% 14% ..



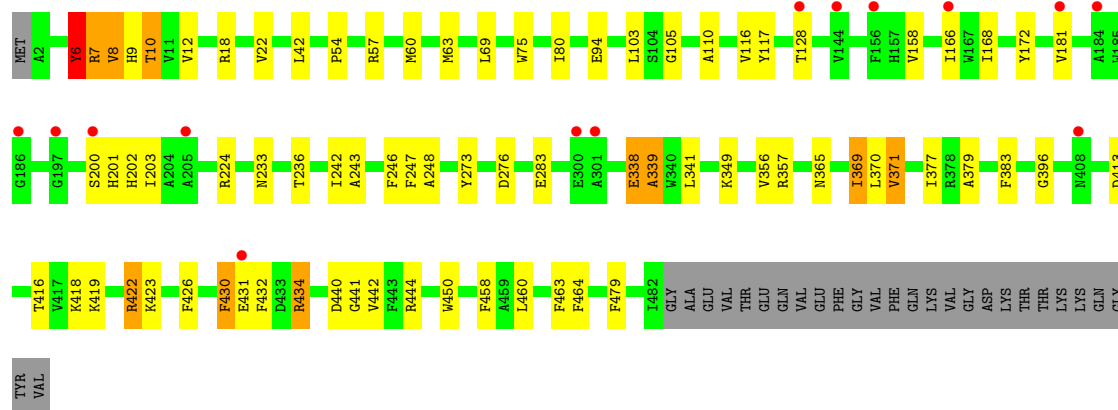
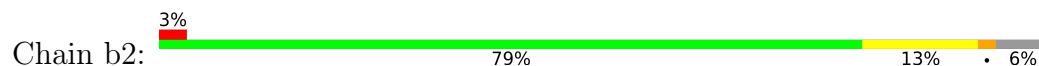
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B2: 2% 84% 13% ..

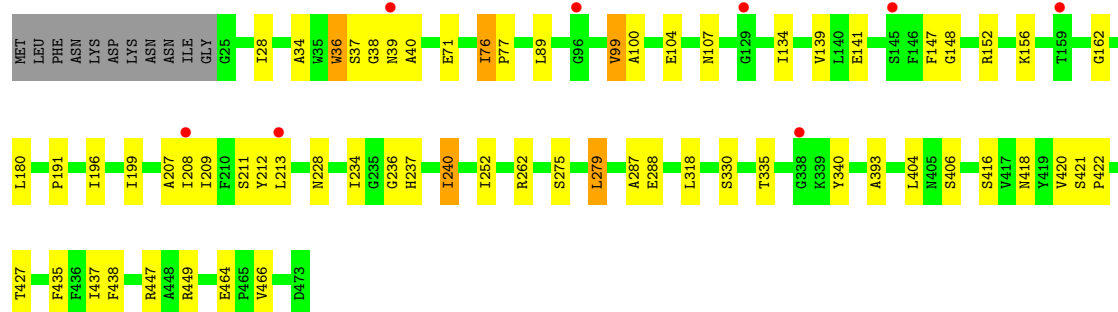
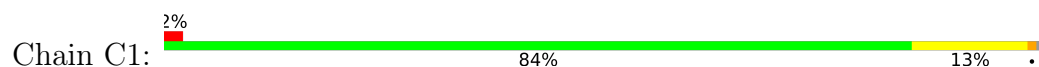




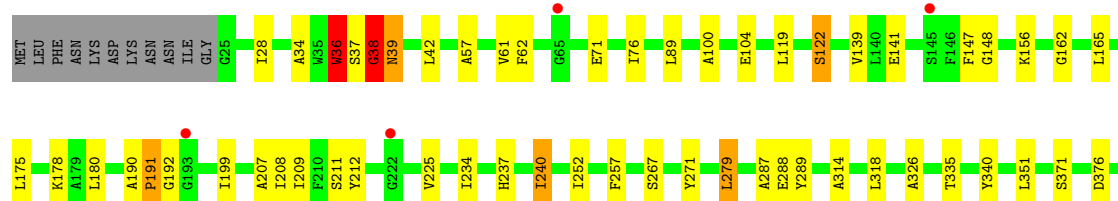
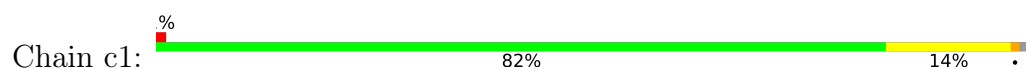
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

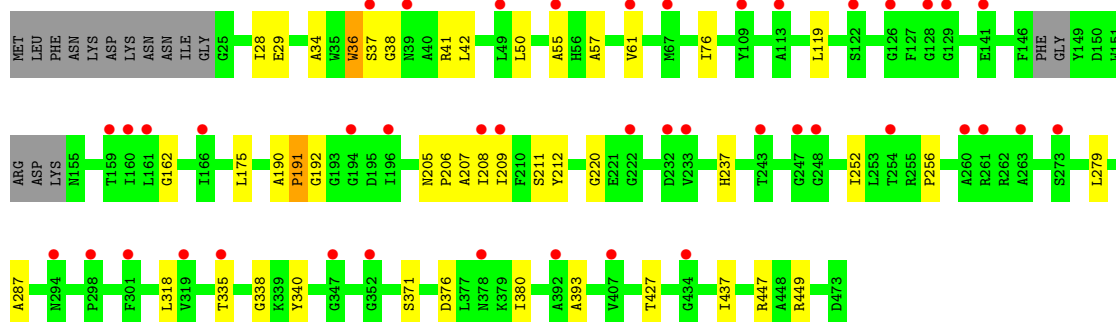
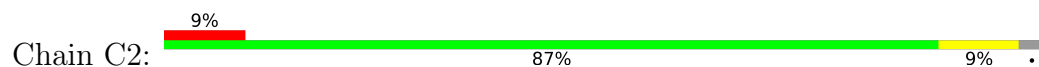


• Molecule 3: Photosystem II CP43 reaction center protein

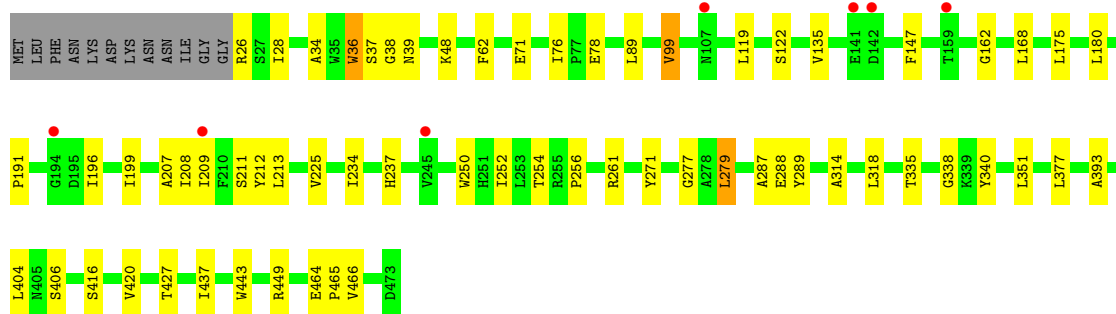
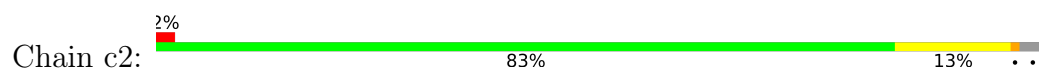




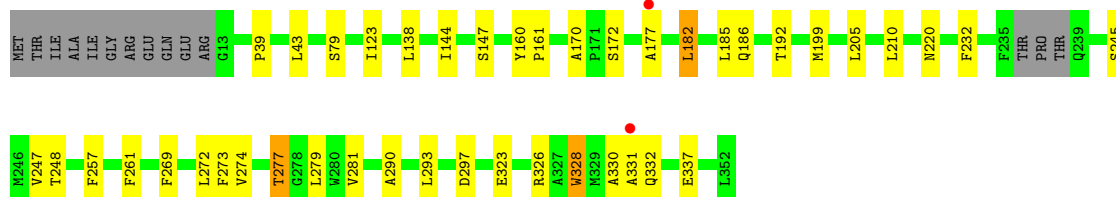
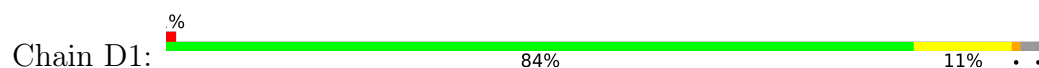
• Molecule 3: Photosystem II CP43 reaction center protein



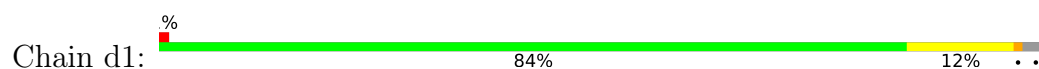
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

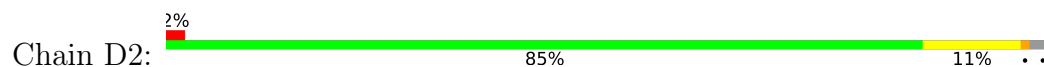


• Molecule 4: Photosystem II D2 protein

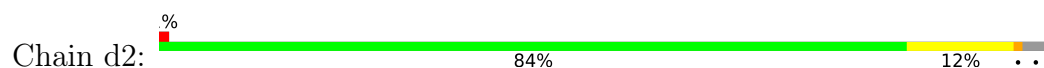




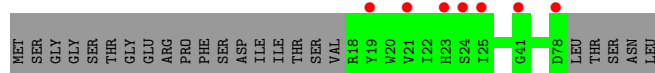
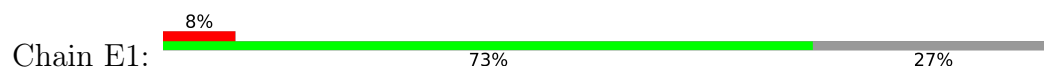
• Molecule 4: Photosystem II D2 protein



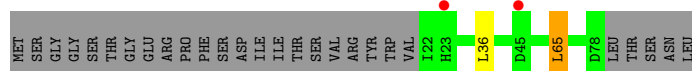
• Molecule 4: Photosystem II D2 protein



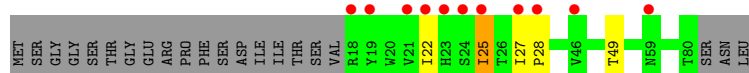
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

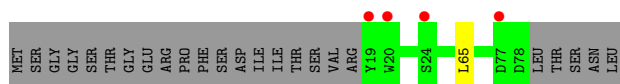


• Molecule 5: Cytochrome b559 subunit alpha

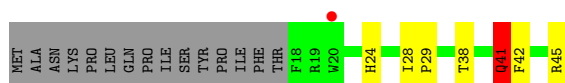


• Molecule 5: Cytochrome b559 subunit alpha

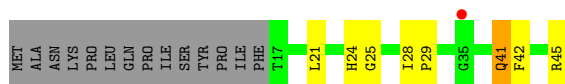




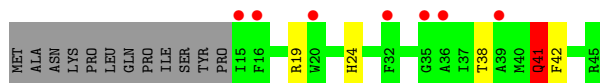
- Molecule 6: Cytochrome b559 subunit beta



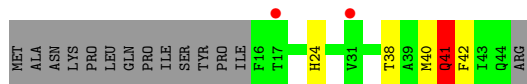
- Molecule 6: Cytochrome b559 subunit beta



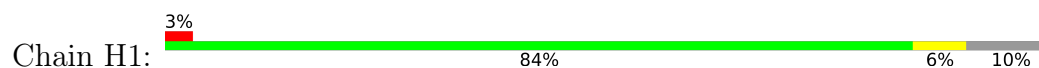
- Molecule 6: Cytochrome b559 subunit beta



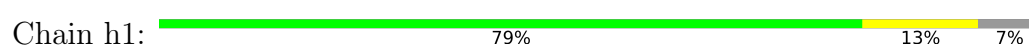
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

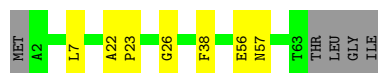


- Molecule 7: Photosystem II reaction center protein H



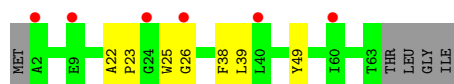
- Molecule 7: Photosystem II reaction center protein H

Chain H2:  82% 10% 7%



- Molecule 7: Photosystem II reaction center protein H

Chain h2:  9% 82% 10% 7%



- Molecule 8: Photosystem II reaction center protein I

Chain I1:  74% 16% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain i1:  68% 21% 11%



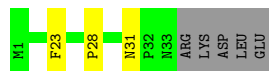
- Molecule 8: Photosystem II reaction center protein I

Chain I2:  3% 79% 13% 8%



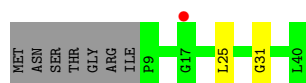
- Molecule 8: Photosystem II reaction center protein I

Chain i2:  79% 8% 13%



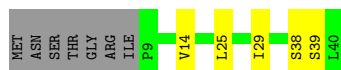
- Molecule 9: Photosystem II reaction center protein J

Chain J1:  3% 77% 5% 18%



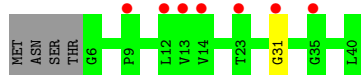
- Molecule 9: Photosystem II reaction center protein J

Chain j1:  69% 13% 18%



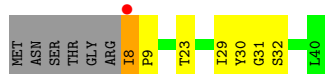
- Molecule 9: Photosystem II reaction center protein J

Chain J2:  18% 87% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j2:  3% 67% 15% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K1:  2% 56% 29% 5% 10%



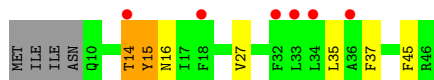
- Molecule 10: Photosystem II reaction center protein K

Chain k1:  61% 24% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K2:  15% 73% 12% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain k2:  5% 61% 27% 10%



- Molecule 11: Photosystem II reaction center protein L

Chain L1:  74% 24% .



- Molecule 11: Photosystem II reaction center protein L

Chain l1:  71% 26% .



- Molecule 11: Photosystem II reaction center protein L

Chain L2:  74% 24% .



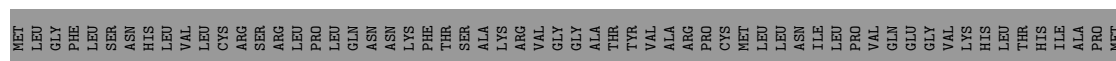
- Molecule 11: Photosystem II reaction center protein L

Chain l2:  71% 26% .



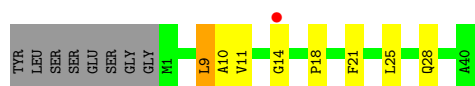
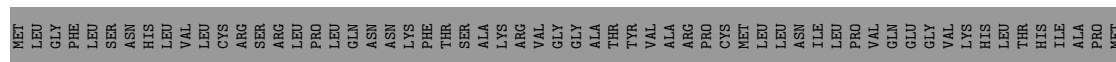
- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M1:  27% 10% 63%



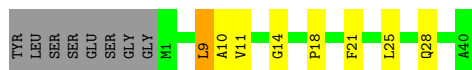
- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain m1:  30% 6% 63%

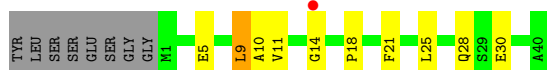


- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

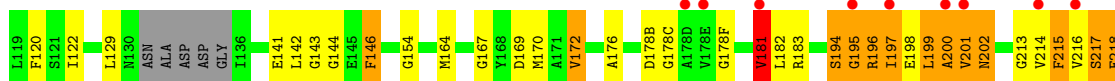
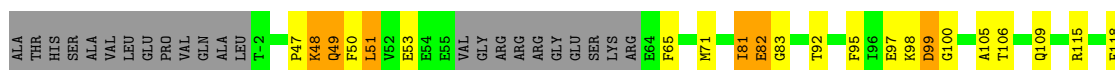
Chain M2:  30% 6% 63%



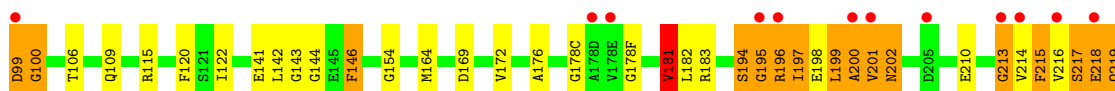
Chain m2:

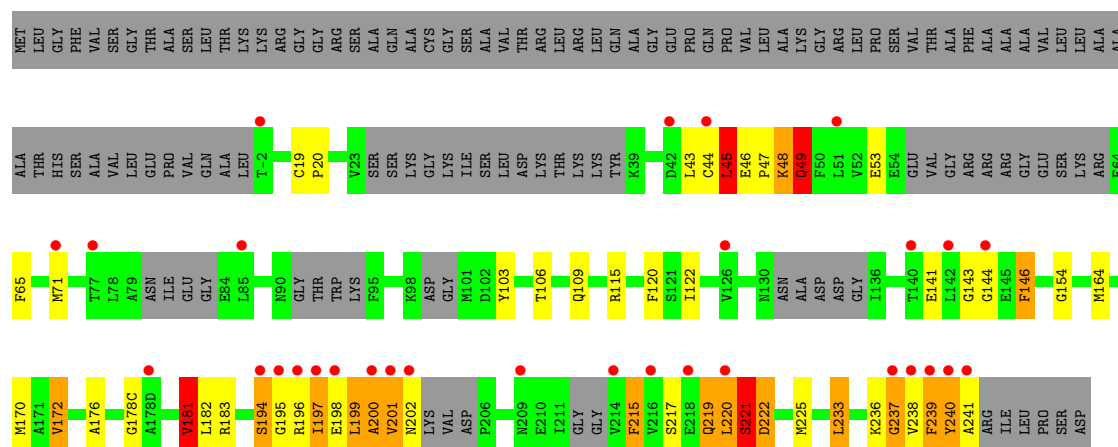


Chain Q1:

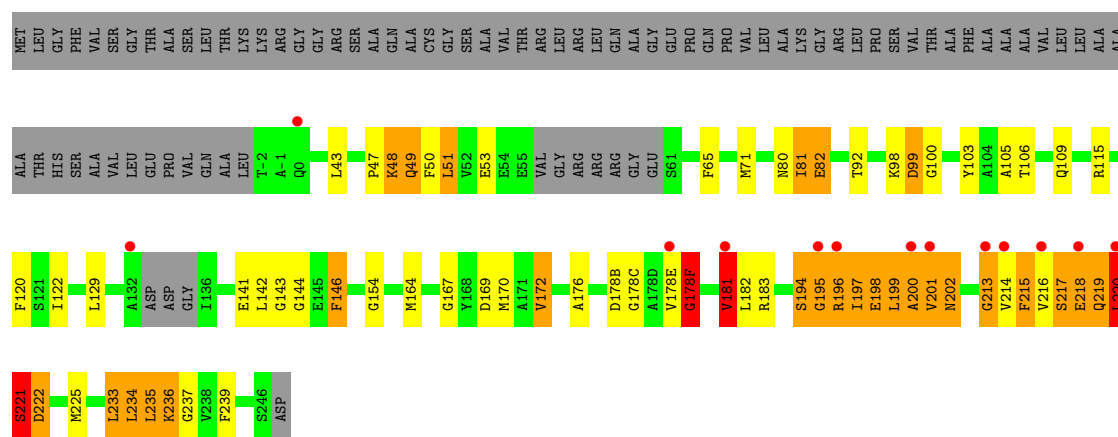


Chain 01: 5% 54% 9% 8% 28%

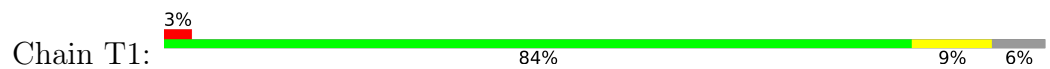




• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO



• Molecule 14: Photosystem II reaction center protein T

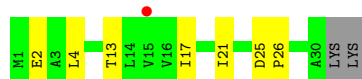


• Molecule 14: Photosystem II reaction center protein T



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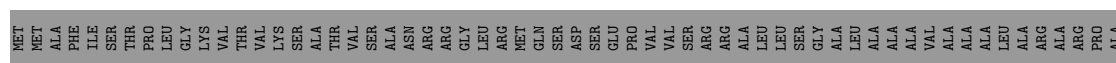




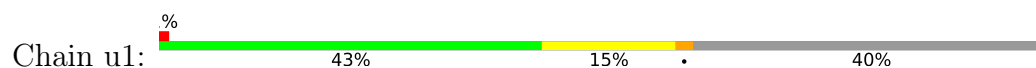
- Molecule 14: Photosystem II reaction center protein T



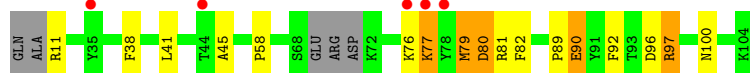
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



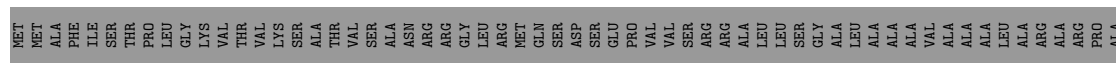
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



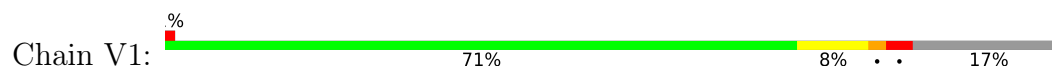
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



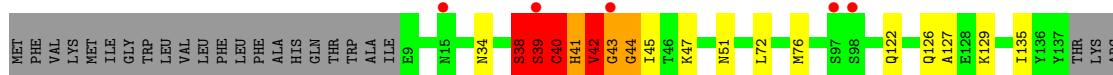
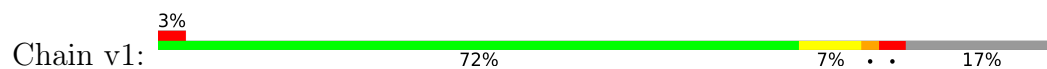
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



- Molecule 16: Cytochrome c-550

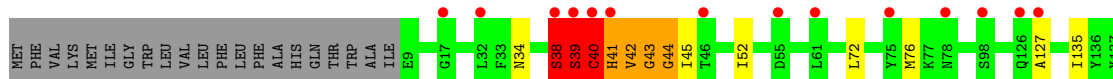
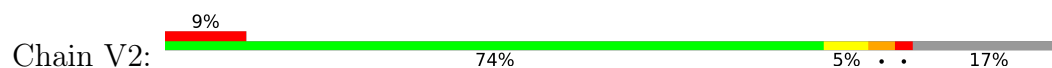


- Molecule 16: Cytochrome c-550



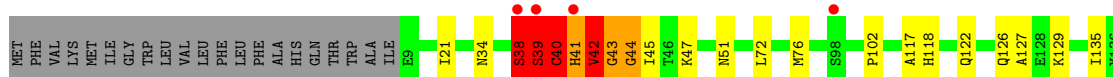
SER
MET

- Molecule 16: Cytochrome c-550



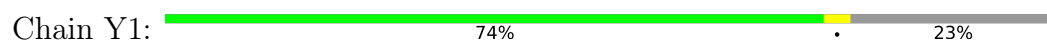
THR
LYS
ARG
SER
MET

- Molecule 16: Cytochrome c-550

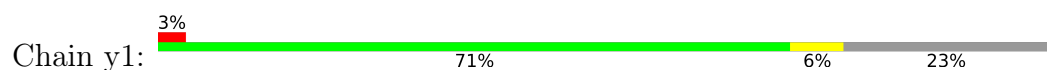


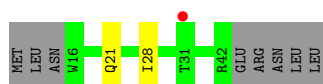
Y137
THR
LYS
ARG
SER
MET

- Molecule 17: Photosystem II reaction center protein Ycf12

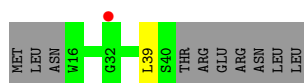


- Molecule 17: Photosystem II reaction center protein Ycf12





- Molecule 17: Photosystem II reaction center protein Ycf12



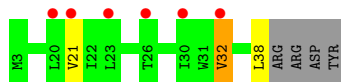
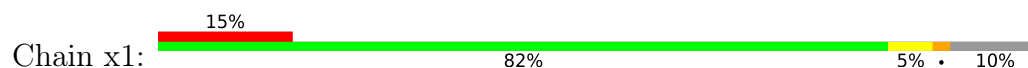
- Molecule 17: Photosystem II reaction center protein Ycf12



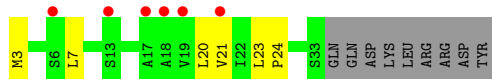
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



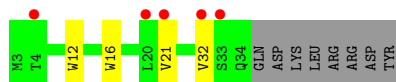
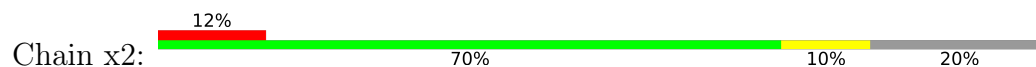
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

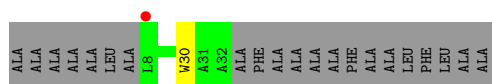


- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

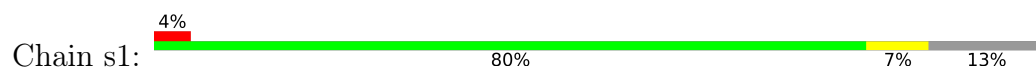


- Molecule 19: PEPTIDE CHAIN UNASSIGNED

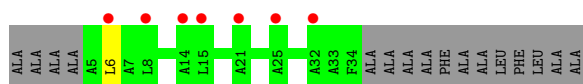




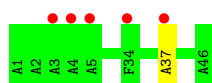
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



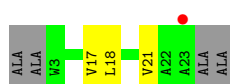
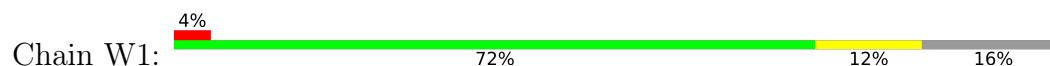
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



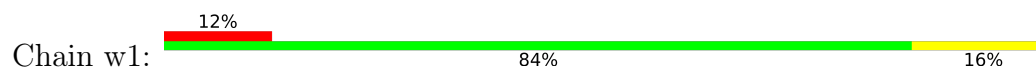
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



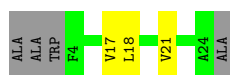
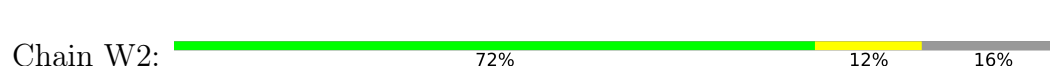
- Molecule 20: PEPTIDE CHAIN UNASSIGNED



- Molecule 20: PEPTIDE CHAIN UNASSIGNED

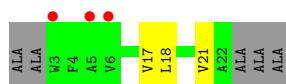


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

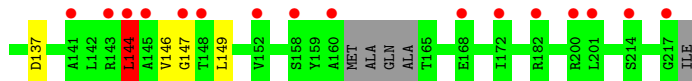
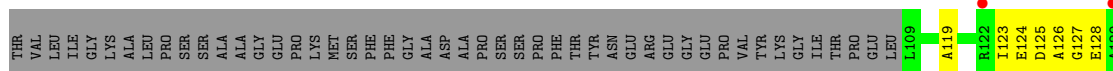
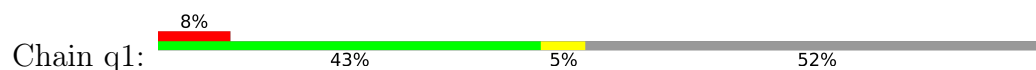


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

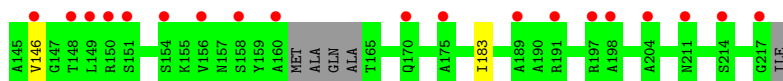
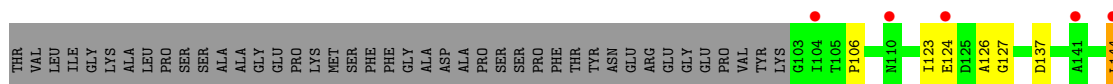




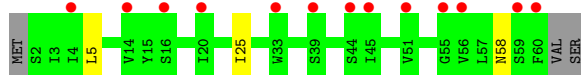
- Molecule 21: Extrinsic protein in photosystem II



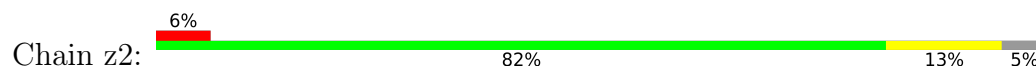
- Molecule 21: Extrinsic protein in photosystem II



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.44Å 240.31Å 300.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.77 10.00 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.77) 97.5 (10.00-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.249 , 0.278 0.255 , 0.282	Depositor DCC
R_{free} test set	19164 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	92765	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BCT, CA, PL9, PHO, OEX, UNL, FE, SQD, LMT, CLA, GOL, BCR, LHG, DGD, CL, LMG

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	A1	0.38	0/2685	0.77	1/3673 (0.0%)
1	A2	0.40	1/2548 (0.0%)	0.77	0/3481
1	a1	0.37	0/2642	0.76	0/3612
1	a2	0.37	0/2586	0.76	0/3538
2	B1	0.41	2/3830 (0.1%)	0.83	6/5227 (0.1%)
2	B2	0.41	2/3897 (0.1%)	0.83	6/5323 (0.1%)
2	b1	0.46	3/4015 (0.1%)	0.83	9/5473 (0.2%)
2	b2	0.41	2/3808 (0.1%)	0.83	6/5197 (0.1%)
3	C1	0.35	0/3501	0.77	2/4782 (0.0%)
3	C2	0.34	0/3242	0.79	2/4441 (0.0%)
3	c1	0.38	2/3555 (0.1%)	0.77	4/4850 (0.1%)
3	c2	0.34	0/3495	0.77	2/4773 (0.0%)
4	D1	0.44	1/2704 (0.0%)	0.77	2/3688 (0.1%)
4	D2	0.44	1/2675 (0.0%)	0.78	4/3655 (0.1%)
4	d1	0.44	1/2772 (0.0%)	0.78	2/3783 (0.1%)
4	d2	0.44	1/2736 (0.0%)	0.77	2/3734 (0.1%)
5	E1	0.33	0/418	0.74	0/577
5	E2	0.34	0/443	0.73	0/614
5	e1	0.32	0/440	0.69	0/603
5	e2	0.32	0/434	0.72	0/598
6	F1	0.67	0/220	0.95	3/299 (1.0%)
6	F2	0.61	0/236	0.95	3/320 (0.9%)
6	f1	0.64	0/235	0.92	3/319 (0.9%)
6	f2	0.63	0/234	0.92	3/318 (0.9%)
7	H1	0.29	0/443	0.70	0/606
7	H2	0.30	0/453	0.72	0/619
7	h1	0.29	0/481	0.71	0/657
7	h2	0.28	0/461	0.70	0/631
8	I1	0.30	0/283	0.68	0/381
8	I2	0.30	0/273	0.71	0/371
8	i1	0.29	0/289	0.69	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	i2	0.30	0/270	0.71	0/364
9	J1	0.27	0/225	0.70	0/307
9	J2	0.26	0/236	0.72	0/324
9	j1	0.26	0/229	0.70	0/313
9	j2	0.27	0/233	0.82	2/319 (0.6%)
10	K1	0.50	0/289	0.84	0/399
10	K2	0.54	0/258	0.87	0/359
10	k1	0.50	0/290	0.85	0/401
10	k2	0.53	0/278	0.85	0/385
11	L1	0.66	0/301	0.88	0/410
11	L2	0.64	0/308	0.87	0/419
11	l1	0.65	0/308	0.88	0/418
11	l2	0.65	0/308	0.87	0/418
12	M1	0.49	0/288	0.93	0/391
12	M2	0.48	0/287	0.93	0/390
12	m1	0.48	0/288	0.92	0/391
12	m2	0.46	0/290	0.93	0/394
13	O1	0.98	15/1700 (0.9%)	1.46	35/2315 (1.5%)
13	O2	0.89	9/1387 (0.6%)	1.35	27/1881 (1.4%)
13	o1	0.94	13/1716 (0.8%)	1.41	38/2330 (1.6%)
13	o2	0.95	14/1794 (0.8%)	1.46	40/2434 (1.6%)
14	T1	0.28	0/248	0.78	0/337
14	T2	0.28	0/247	0.77	0/337
14	t1	0.29	0/253	0.77	0/344
14	t2	0.29	0/242	0.77	0/330
15	U1	0.63	1/709 (0.1%)	1.03	7/970 (0.7%)
15	U2	0.67	2/588 (0.3%)	1.25	10/809 (1.2%)
15	u1	0.63	1/721 (0.1%)	1.02	5/981 (0.5%)
15	u2	0.62	2/726 (0.3%)	1.00	5/988 (0.5%)
16	V1	0.66	3/937 (0.3%)	0.98	8/1281 (0.6%)
16	V2	0.68	3/858 (0.3%)	0.98	8/1177 (0.7%)
16	v1	0.64	2/941 (0.2%)	0.98	8/1284 (0.6%)
16	v2	0.63	2/983 (0.2%)	0.96	8/1337 (0.6%)
17	Y1	0.61	0/171	1.00	0/236
17	Y2	0.62	0/159	1.05	0/219
17	y1	0.58	0/198	0.93	0/274
17	y2	0.59	0/191	0.98	0/264
18	X1	0.37	0/202	0.80	1/278 (0.4%)
18	X2	0.35	0/222	0.82	1/307 (0.3%)
18	x1	0.41	0/262	0.80	1/363 (0.3%)
18	x2	0.44	0/225	0.88	1/312 (0.3%)
19	S1	0.32	0/167	0.65	0/231
19	S2	0.32	0/194	0.66	0/268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	s1	0.32	0/269	0.63	0/371
19	s2	0.33	0/285	0.68	0/395
20	W1	0.34	0/134	0.77	0/186
20	W2	0.35	0/129	0.81	0/179
20	w1	0.34	0/152	0.77	0/211
20	w2	0.32	0/127	0.79	0/176
21	Q2	0.55	1/682 (0.1%)	0.85	0/937
21	q1	0.55	1/650 (0.2%)	0.84	0/893
22	Z2	0.33	0/353	0.81	0/487
22	z2	0.34	0/387	0.77	0/532
All	All	0.50	85/79929 (0.1%)	0.88	265/109188 (0.2%)

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
13	O1	0	2
13	O2	0	4
13	o1	0	3
13	o2	0	3
16	V1	0	3
16	V2	0	3
16	v1	0	3
16	v2	0	3
All	All	0	24

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V2	42	VAL	CA-C	-11.01	1.38	1.52
13	O1	220	LEU	N-CA	10.34	1.57	1.45
13	o2	220	LEU	N-CA	10.33	1.57	1.45
13	o1	220	LEU	N-CA	10.19	1.57	1.45
13	O1	221	SER	N-CA	9.74	1.58	1.46
13	o1	221	SER	N-CA	9.42	1.58	1.46
16	V1	42	VAL	CA-C	-8.98	1.41	1.52
16	v2	42	VAL	CA-C	-8.97	1.41	1.52
13	o2	221	SER	N-CA	8.93	1.58	1.46
16	v1	42	VAL	CA-C	-8.79	1.41	1.52
2	b1	422	ARG	C-O	8.08	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O2	221	SER	N-CA	8.08	1.57	1.46
13	O2	222	ASP	N-CA	7.82	1.56	1.46
13	O1	82	GLU	C-O	-7.78	1.14	1.23
13	o1	222	ASP	N-CA	7.61	1.55	1.46
13	o2	222	ASP	N-CA	7.54	1.55	1.46
13	o1	221	SER	CA-C	7.42	1.62	1.52
13	o1	218	GLU	N-CA	7.34	1.54	1.45
13	O1	222	ASP	N-CA	7.32	1.55	1.46
13	O2	194	SER	CA-C	-7.17	1.43	1.52
13	O1	221	SER	CA-C	7.12	1.62	1.52
13	o2	236	LYS	C-O	-7.04	1.16	1.24
13	O1	218	GLU	N-CA	6.95	1.54	1.45
13	O2	45	LEU	C-O	-6.94	1.14	1.23
13	O2	220	LEU	C-O	6.92	1.31	1.23
13	O1	236	LYS	C-O	-6.85	1.16	1.24
2	b1	6	TYR	C-O	6.80	1.32	1.24
13	o2	218	GLU	N-CA	6.76	1.53	1.45
13	o2	82	GLU	C-O	-6.75	1.15	1.23
13	O2	221	SER	CA-C	6.62	1.62	1.53
13	O2	197	ILE	CA-CB	6.55	1.63	1.54
13	o1	194	SER	CA-C	-6.47	1.46	1.53
13	o2	194	SER	CA-C	-6.45	1.46	1.53
13	o2	221	SER	CA-C	6.42	1.62	1.53
13	O1	197	ILE	C-O	-6.34	1.16	1.24
13	o1	197	ILE	C-O	-6.33	1.16	1.24
13	O1	146	PHE	C-O	6.31	1.31	1.23
4	d1	328	TRP	C-O	6.31	1.31	1.24
13	O2	240	TYR	N-CA	6.31	1.53	1.45
13	o2	146	PHE	C-O	6.26	1.31	1.23
13	o2	129	LEU	C-O	6.24	1.31	1.24
16	V1	42	VAL	N-CA	6.20	1.54	1.46
13	o2	197	ILE	C-O	-6.20	1.16	1.24
13	O1	129	LEU	C-O	6.15	1.31	1.24
13	o1	236	LYS	C-O	-6.15	1.16	1.24
13	O1	98	LYS	C-O	6.14	1.30	1.24
13	o1	146	PHE	C-O	6.12	1.31	1.23
16	v2	42	VAL	N-CA	6.06	1.53	1.46
16	v1	42	VAL	N-CA	6.04	1.53	1.46
4	D1	328	TRP	C-O	6.03	1.31	1.24
4	d2	328	TRP	C-O	6.02	1.31	1.24
15	U2	79	MET	CA-C	-5.98	1.45	1.52
15	u2	79	MET	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D2	328	TRP	C-O	5.87	1.30	1.24
15	U1	79	MET	CA-C	-5.86	1.45	1.52
13	o1	220	LEU	C-N	5.82	1.41	1.33
2	b2	422	ARG	C-O	5.82	1.30	1.24
13	O1	194	SER	CA-C	-5.82	1.47	1.53
13	O1	220	LEU	C-N	5.80	1.41	1.33
13	o1	195	GLY	C-O	-5.77	1.16	1.23
2	B2	422	ARG	C-O	5.66	1.30	1.24
1	A2	149	ALA	CA-C	5.64	1.58	1.52
13	o2	195	GLY	C-O	-5.64	1.16	1.23
15	u1	79	MET	CA-C	-5.62	1.45	1.52
2	B1	422	ARG	C-O	5.61	1.30	1.24
13	o2	220	LEU	C-N	5.59	1.41	1.33
21	q1	144	LEU	C-O	5.38	1.30	1.24
13	O1	195	GLY	C-O	-5.38	1.16	1.23
2	B2	338	GLU	CA-C	5.29	1.59	1.52
2	b2	338	GLU	CA-C	5.25	1.59	1.52
15	u2	77	LYS	C-O	5.24	1.30	1.24
21	Q2	144	LEU	C-O	5.23	1.30	1.24
16	V1	42	VAL	C-N	-5.23	1.26	1.33
2	B1	338	GLU	CA-C	5.21	1.59	1.52
13	O2	196	ARG	CA-C	5.21	1.58	1.52
13	O1	196	ARG	CA-C	5.18	1.58	1.52
13	o2	196	ARG	CA-C	5.17	1.58	1.52
16	V2	42	VAL	CA-CB	5.17	1.61	1.54
3	c1	39	ASN	CA-C	5.11	1.59	1.52
16	V2	42	VAL	N-CA	5.10	1.52	1.46
2	b1	338	GLU	CA-C	5.07	1.59	1.52
3	c1	36	TRP	C-O	5.05	1.30	1.24
15	U2	77	LYS	C-O	5.05	1.30	1.24
13	o1	197	ILE	N-CA	5.04	1.52	1.46
13	o1	196	ARG	CA-C	5.04	1.58	1.52

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O1	219	GLN	N-CA-C	12.94	128.74	109.07
13	o2	219	GLN	N-CA-C	12.93	128.73	109.07
13	o1	219	GLN	N-CA-C	12.60	128.22	109.07
13	O1	215	PHE	CA-C-N	-12.49	102.53	122.64
13	O1	215	PHE	C-N-CA	-12.49	102.53	122.64
13	o1	215	PHE	CA-C-N	-12.46	102.58	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o1	215	PHE	C-N-CA	-12.46	102.58	122.64
13	o2	215	PHE	CA-C-N	-12.44	102.61	122.64
13	o2	215	PHE	C-N-CA	-12.44	102.61	122.64
13	o1	195	GLY	CA-C-O	-11.59	105.69	122.62
13	o2	195	GLY	CA-C-O	-11.58	105.71	122.62
13	O1	195	GLY	CA-C-O	-11.50	105.83	122.62
13	O2	239	PHE	CA-C-N	-11.49	102.70	122.92
13	O2	239	PHE	C-N-CA	-11.49	102.70	122.92
13	o2	92	THR	CA-C-N	-11.20	107.88	122.77
13	o2	92	THR	C-N-CA	-11.20	107.88	122.77
15	U2	11	ARG	NE-CZ-NH2	11.01	129.11	119.20
2	b2	339	ALA	N-CA-C	11.01	125.06	110.53
13	o2	221	SER	N-CA-C	11.01	126.82	109.65
2	b1	339	ALA	N-CA-C	10.97	125.01	110.53
15	U2	11	ARG	NE-CZ-NH1	-10.95	110.56	121.50
2	B2	339	ALA	N-CA-C	10.86	124.86	110.53
13	O1	92	THR	CA-C-N	-10.78	107.85	122.72
13	O1	92	THR	C-N-CA	-10.78	107.85	122.72
2	B1	339	ALA	N-CA-C	10.65	124.92	110.55
13	O2	221	SER	N-CA-C	10.22	125.59	109.65
13	O1	194	SER	CA-C-N	-10.19	106.54	121.01
13	O1	194	SER	C-N-CA	-10.19	106.54	121.01
13	o1	194	SER	CA-C-N	-10.09	106.68	121.01
13	o1	194	SER	C-N-CA	-10.09	106.68	121.01
13	o2	194	SER	CA-C-N	-10.06	106.72	121.01
13	o2	194	SER	C-N-CA	-10.06	106.72	121.01
13	O2	144	GLY	N-CA-C	9.61	124.78	110.75
13	O2	219	GLN	N-CA-C	9.30	123.03	108.79
13	o2	217	SER	CA-C-N	-9.18	107.03	122.64
13	o2	217	SER	C-N-CA	-9.18	107.03	122.64
13	O1	217	SER	CA-C-N	-9.14	107.10	122.64
13	O1	217	SER	C-N-CA	-9.14	107.10	122.64
13	o2	219	GLN	CA-C-N	-9.06	107.25	122.64
13	o2	219	GLN	C-N-CA	-9.06	107.25	122.64
13	O1	219	GLN	CA-C-N	-9.04	107.27	122.64
13	O1	219	GLN	C-N-CA	-9.04	107.27	122.64
13	o1	219	GLN	CA-C-N	-8.91	107.50	122.64
13	o1	219	GLN	C-N-CA	-8.91	107.50	122.64
15	U2	11	ARG	CD-NE-CZ	8.74	136.64	124.40
2	B1	430	PHE	CA-C-N	-8.68	106.95	122.74
2	B1	430	PHE	C-N-CA	-8.68	106.95	122.74
16	v2	42	VAL	CA-C-O	8.62	131.55	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v2	42	VAL	N-CA-CB	8.61	125.44	111.23
16	V1	42	VAL	N-CA-CB	8.61	125.43	111.23
16	v1	42	VAL	CA-C-O	8.61	131.54	120.78
13	o1	217	SER	CA-C-N	-8.56	108.09	122.64
13	o1	217	SER	C-N-CA	-8.56	108.09	122.64
16	v1	42	VAL	N-CA-CB	8.55	125.35	111.23
16	V1	42	VAL	CA-C-O	8.52	131.43	120.78
13	o1	144	GLY	N-CA-C	8.47	123.11	110.75
2	b1	430	PHE	CA-C-N	-8.44	107.38	122.74
2	b1	430	PHE	C-N-CA	-8.44	107.38	122.74
13	O1	220	LEU	CA-C-N	8.40	137.59	121.54
13	O1	220	LEU	C-N-CA	8.40	137.59	121.54
13	o2	144	GLY	N-CA-C	8.36	122.95	110.75
13	O1	144	GLY	N-CA-C	8.22	122.75	110.75
13	o1	220	LEU	CA-C-N	8.15	137.10	121.54
13	o1	220	LEU	C-N-CA	8.15	137.10	121.54
13	o1	143	GLY	CA-C-N	-8.08	108.76	120.97
13	o1	143	GLY	C-N-CA	-8.08	108.76	120.97
13	o2	143	GLY	CA-C-N	-8.05	108.81	120.97
13	o2	143	GLY	C-N-CA	-8.05	108.81	120.97
13	O1	143	GLY	CA-C-N	-8.02	108.85	120.97
13	O1	143	GLY	C-N-CA	-8.02	108.85	120.97
2	b2	430	PHE	CA-C-N	-8.02	108.14	122.74
2	b2	430	PHE	C-N-CA	-8.02	108.14	122.74
2	B2	430	PHE	CA-C-N	-7.97	108.23	122.74
2	B2	430	PHE	C-N-CA	-7.97	108.23	122.74
13	o1	100	GLY	N-CA-C	7.83	121.73	111.70
13	O2	194	SER	CA-C-N	-7.80	109.03	121.05
13	O2	194	SER	C-N-CA	-7.80	109.03	121.05
13	O2	196	ARG	N-CA-C	7.75	121.05	108.34
15	U1	81	ARG	N-CA-C	7.67	122.27	113.15
15	u1	81	ARG	N-CA-C	7.66	122.26	113.15
16	v1	43	GLY	N-CA-C	-7.55	104.62	115.27
13	O1	221	SER	N-CA-C	7.50	126.78	110.80
16	v2	43	GLY	N-CA-C	-7.50	104.70	115.27
13	O2	220	LEU	CA-C-N	7.46	137.57	123.09
13	O2	220	LEU	C-N-CA	7.46	137.57	123.09
13	o2	220	LEU	CA-C-N	7.46	137.55	123.09
13	o2	220	LEU	C-N-CA	7.46	137.55	123.09
16	V1	43	GLY	N-CA-C	-7.41	104.34	115.00
13	O2	45	LEU	CA-C-O	-7.20	113.51	121.87
15	u2	81	ARG	N-CA-C	7.14	121.65	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	10	SER	N-CA-C	7.13	119.25	110.91
15	U2	79	MET	N-CA-C	-7.12	103.59	111.36
13	o1	221	SER	N-CA-C	7.12	125.96	110.80
13	O1	141	GLU	CA-C-N	-7.07	111.85	122.74
13	O1	141	GLU	C-N-CA	-7.07	111.85	122.74
13	O2	237	GLY	CA-C-N	-7.07	109.63	122.43
13	O2	237	GLY	C-N-CA	-7.07	109.63	122.43
13	o2	220	LEU	CA-C-O	-7.06	112.95	121.28
15	u2	79	MET	N-CA-C	-7.06	103.67	111.36
13	O2	220	LEU	O-C-N	7.04	131.20	123.10
13	O2	146	PHE	N-CA-C	7.04	119.89	108.76
13	o2	141	GLU	CA-C-N	-7.03	111.91	122.74
13	o2	141	GLU	C-N-CA	-7.03	111.91	122.74
13	o1	220	LEU	CA-C-O	-7.03	112.99	121.28
13	o1	141	GLU	CA-C-N	-7.02	111.93	122.74
13	o1	141	GLU	C-N-CA	-7.02	111.93	122.74
15	U2	81	ARG	N-CA-C	7.00	121.47	113.15
15	U1	79	MET	N-CA-C	-6.99	103.74	111.36
13	O1	220	LEU	CA-C-O	-6.97	113.05	121.28
16	V2	43	GLY	N-CA-C	-6.95	104.99	115.00
13	O2	141	GLU	CA-C-N	-6.77	112.31	122.74
13	O2	141	GLU	C-N-CA	-6.77	112.31	122.74
13	O2	220	LEU	CA-C-O	-6.73	113.34	121.28
15	u1	79	MET	N-CA-C	-6.71	104.05	111.36
2	b1	426	PHE	N-CA-C	6.64	121.05	113.15
13	o2	82	GLU	N-CA-C	6.60	119.93	109.50
15	U1	82	PHE	N-CA-C	6.57	120.23	109.72
15	u1	82	PHE	N-CA-C	6.56	120.21	109.72
15	u2	82	PHE	N-CA-C	6.54	120.19	109.72
13	O2	143	GLY	CA-C-N	-6.53	111.11	120.97
13	O2	143	GLY	C-N-CA	-6.53	111.11	120.97
13	o1	82	GLU	N-CA-C	6.51	120.12	109.24
15	U2	82	PHE	N-CA-C	6.43	120.01	109.72
15	U1	80	ASP	CA-C-N	-6.42	109.47	122.31
15	U1	80	ASP	C-N-CA	-6.42	109.47	122.31
13	O2	215	PHE	CA-C-N	-6.41	112.32	122.64
13	O2	215	PHE	C-N-CA	-6.41	112.32	122.64
15	u1	80	ASP	CA-C-N	-6.36	109.59	122.31
15	u1	80	ASP	C-N-CA	-6.36	109.59	122.31
3	c1	38	GLY	CA-C-N	-6.32	110.50	120.60
3	c1	38	GLY	C-N-CA	-6.32	110.50	120.60
15	u2	80	ASP	CA-C-N	-6.16	109.98	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	u2	80	ASP	C-N-CA	-6.16	109.98	122.31
3	c1	76	ILE	CA-C-N	6.15	125.64	119.24
3	c1	76	ILE	C-N-CA	6.15	125.64	119.24
3	c2	76	ILE	CA-C-N	6.15	125.64	119.24
3	c2	76	ILE	C-N-CA	6.15	125.64	119.24
13	o1	222	ASP	N-CA-C	6.14	119.14	110.23
13	o1	146	PHE	N-CA-C	6.09	118.56	108.99
3	C2	76	ILE	CA-C-N	6.09	125.57	119.24
3	C2	76	ILE	C-N-CA	6.09	125.57	119.24
13	O1	97	GLU	CA-C-N	6.08	131.23	122.23
13	O1	97	GLU	C-N-CA	6.08	131.23	122.23
13	o2	222	ASP	N-CA-C	6.07	119.03	110.23
13	o2	146	PHE	N-CA-C	6.05	118.49	108.99
13	o1	81	ILE	CA-C-N	-6.05	112.94	122.73
13	o1	81	ILE	C-N-CA	-6.05	112.94	122.73
15	U2	80	ASP	CA-C-N	-6.05	110.22	122.31
15	U2	80	ASP	C-N-CA	-6.05	110.22	122.31
3	C1	76	ILE	CA-C-N	6.04	125.52	119.24
3	C1	76	ILE	C-N-CA	6.04	125.52	119.24
13	O1	129	LEU	O-C-N	5.99	130.04	123.27
13	O1	146	PHE	N-CA-C	5.98	118.38	108.99
13	O2	222	ASP	N-CA-C	5.96	118.98	110.10
2	b1	8	VAL	CA-C-N	-5.94	109.43	121.18
2	b1	8	VAL	C-N-CA	-5.94	109.43	121.18
13	O1	222	ASP	N-CA-C	5.88	118.76	110.23
13	o2	129	LEU	O-C-N	5.87	130.22	123.29
2	b2	426	PHE	N-CA-C	5.87	120.13	113.15
4	d2	331	ALA	CA-C-N	-5.85	110.74	120.68
4	d2	331	ALA	C-N-CA	-5.85	110.74	120.68
2	B2	8	VAL	CA-C-N	-5.83	110.99	120.72
2	B2	8	VAL	C-N-CA	-5.83	110.99	120.72
2	B2	426	PHE	N-CA-C	5.82	120.08	113.15
16	V1	42	VAL	N-CA-C	-5.80	97.27	109.34
2	B1	8	VAL	CA-C-N	-5.80	111.03	120.72
2	B1	8	VAL	C-N-CA	-5.80	111.03	120.72
13	o2	234	LEU	CA-C-N	-5.80	115.00	123.00
13	o2	234	LEU	C-N-CA	-5.80	115.00	123.00
4	d1	331	ALA	CA-C-N	-5.79	110.83	120.68
4	d1	331	ALA	C-N-CA	-5.79	110.83	120.68
16	v2	42	VAL	N-CA-C	-5.78	97.31	109.34
2	b2	8	VAL	CA-C-N	-5.76	111.10	120.72
2	b2	8	VAL	C-N-CA	-5.76	111.10	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V2	42	VAL	CA-C-O	5.75	127.97	120.78
4	D2	331	ALA	CA-C-N	-5.74	110.92	120.68
4	D2	331	ALA	C-N-CA	-5.74	110.92	120.68
6	F1	41	GLN	CA-C-N	-5.73	113.48	122.65
6	F1	41	GLN	C-N-CA	-5.73	113.48	122.65
16	v1	42	VAL	N-CA-C	-5.73	97.43	109.34
4	D1	331	ALA	CA-C-N	-5.72	110.96	120.68
4	D1	331	ALA	C-N-CA	-5.72	110.96	120.68
6	f1	41	GLN	CA-C-N	-5.72	113.50	122.65
6	f1	41	GLN	C-N-CA	-5.72	113.50	122.65
13	o2	81	ILE	CA-C-N	-5.70	113.73	122.62
13	o2	81	ILE	C-N-CA	-5.70	113.73	122.62
13	O1	48	LYS	N-CA-C	-5.67	98.73	110.80
6	f2	41	GLN	CA-C-N	-5.66	113.60	122.65
6	f2	41	GLN	C-N-CA	-5.66	113.60	122.65
13	o2	221	SER	CB-CA-C	-5.65	100.73	112.44
13	O1	98	LYS	N-CA-C	-5.62	100.31	108.07
13	o2	48	LYS	N-CA-C	-5.62	98.84	110.80
13	O2	240	TYR	CA-C-N	5.61	131.81	121.70
13	O2	240	TYR	C-N-CA	5.61	131.81	121.70
2	b1	425	GLN	CA-C-N	-5.58	111.14	122.31
2	b1	425	GLN	C-N-CA	-5.58	111.14	122.31
18	X2	21	VAL	N-CA-C	-5.57	108.07	113.53
18	x1	21	VAL	N-CA-C	-5.55	108.09	113.53
6	F2	41	GLN	CA-C-N	-5.54	113.78	122.65
6	F2	41	GLN	C-N-CA	-5.54	113.78	122.65
16	v2	40	CYS	CA-C-O	5.53	128.41	120.51
13	o2	178(F)	GLY	N-CA-C	5.51	126.24	113.18
13	O2	221	SER	CB-CA-C	-5.49	101.08	112.44
9	j2	8	ILE	CA-C-N	5.49	125.80	119.93
9	j2	8	ILE	C-N-CA	5.49	125.80	119.93
13	O1	234	LEU	CA-C-N	-5.48	115.38	123.05
13	O1	234	LEU	C-N-CA	-5.48	115.38	123.05
16	V1	40	CYS	CA-C-O	5.48	128.35	120.51
13	o1	234	LEU	CA-C-N	-5.47	115.28	122.99
13	o1	234	LEU	C-N-CA	-5.47	115.28	122.99
13	o2	213	GLY	CA-C-N	-5.46	114.75	122.34
13	o2	213	GLY	C-N-CA	-5.46	114.75	122.34
16	V2	42	VAL	O-C-N	5.45	129.38	122.57
16	v1	40	CYS	CA-C-O	5.44	128.29	120.51
13	O1	217	SER	N-CA-C	5.44	117.77	108.90
13	o2	235	LEU	CA-C-N	-5.43	115.14	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o2	235	LEU	C-N-CA	-5.43	115.14	123.07
13	o1	234	LEU	N-CA-C	5.43	117.24	108.34
13	o2	236	LYS	CA-C-N	-5.42	111.80	121.93
13	o2	236	LYS	C-N-CA	-5.42	111.80	121.93
18	x2	21	VAL	N-CA-C	-5.41	108.23	113.53
16	v2	40	CYS	CA-C-N	-5.40	111.60	122.55
16	v2	40	CYS	C-N-CA	-5.40	111.60	122.55
13	O2	237	GLY	N-CA-C	5.36	118.97	111.19
13	o2	217	SER	N-CA-C	5.36	117.63	108.90
16	V1	40	CYS	CA-C-N	-5.33	111.72	122.55
16	V1	40	CYS	C-N-CA	-5.33	111.72	122.55
13	o1	48	LYS	N-CA-C	-5.32	99.46	110.80
6	f1	42	PHE	N-CA-C	5.31	119.45	112.92
16	v1	40	CYS	CA-C-N	-5.31	111.78	122.55
16	v1	40	CYS	C-N-CA	-5.31	111.78	122.55
18	X1	21	VAL	N-CA-C	-5.30	108.34	113.53
16	V2	40	CYS	CA-C-O	5.30	128.08	120.51
13	o1	217	SER	N-CA-C	5.28	117.50	108.90
13	o1	218	GLU	CA-C-O	-5.27	115.06	121.28
13	O1	197	ILE	CA-C-O	-5.27	114.20	120.78
13	o1	236	LYS	CA-C-N	-5.26	112.09	121.93
13	o1	236	LYS	C-N-CA	-5.26	112.09	121.93
6	F1	42	PHE	N-CA-C	5.26	119.39	112.92
2	B1	426	PHE	N-CA-C	5.20	119.34	113.15
13	o1	235	LEU	CA-C-N	-5.19	115.75	123.11
13	o1	235	LEU	C-N-CA	-5.19	115.75	123.11
6	F2	42	PHE	N-CA-C	5.18	119.29	112.92
6	f2	42	PHE	N-CA-C	5.14	119.25	112.92
15	U2	38	PHE	CA-C-N	5.14	125.43	119.93
15	U2	38	PHE	C-N-CA	5.14	125.43	119.93
13	o1	213	GLY	CA-C-N	-5.13	115.21	122.34
13	o1	213	GLY	C-N-CA	-5.13	115.21	122.34
4	D2	148	GLY	CA-C-N	5.12	125.16	119.32
4	D2	148	GLY	C-N-CA	5.12	125.16	119.32
13	o2	197	ILE	CA-C-O	-5.12	114.38	120.78
13	O1	81	ILE	CA-C-N	-5.12	114.44	122.73
13	O1	81	ILE	C-N-CA	-5.12	114.44	122.73
16	V1	127	ALA	CB-CA-C	-5.11	110.28	117.23
16	v2	127	ALA	CB-CA-C	-5.08	110.32	117.23
16	V2	40	CYS	CA-C-N	-5.07	112.25	122.55
16	V2	40	CYS	C-N-CA	-5.07	112.25	122.55
16	V2	127	ALA	CB-CA-C	-5.07	110.33	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b1	430	PHE	CA-C-O	-5.06	115.71	121.58
16	V2	42	VAL	N-CA-CB	5.06	119.58	111.23
16	v1	127	ALA	CB-CA-C	-5.05	110.36	117.23
15	U1	38	PHE	CA-C-N	5.04	125.33	119.93
15	U1	38	PHE	C-N-CA	5.04	125.33	119.93
13	O1	221	SER	CB-CA-C	-5.02	100.43	110.42
13	o1	197	ILE	CA-C-O	-5.02	114.51	120.78

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O1	194	SER	Peptide
13	O1	220	LEU	Peptide
13	O2	194	SER	Peptide
13	O2	220	LEU	Mainchain
13	O2	45	LEU	Mainchain
13	O2	49	GLN	Peptide
16	V1	38	SER	Peptide
16	V1	41	HIS	Peptide
16	V1	44	GLY	Peptide
16	V2	38	SER	Peptide
16	V2	41	HIS	Peptide
16	V2	44	GLY	Peptide
13	o1	194	SER	Peptide
13	o1	220	LEU	Peptide
13	o1	98	LYS	Peptide
13	o2	178(E)	VAL	Peptide
13	o2	194	SER	Peptide
13	o2	220	LEU	Peptide
16	v1	38	SER	Peptide
16	v1	41	HIS	Peptide
16	v1	44	GLY	Peptide
16	v2	38	SER	Peptide
16	v2	41	HIS	Peptide
16	v2	44	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	2609	0	2500	51	0
1	A2	2475	0	2296	41	0
1	a1	2564	0	2462	54	0
1	a2	2513	0	2376	46	0
2	B1	3703	0	3485	59	0
2	B2	3770	0	3462	47	0
2	b1	3881	0	3672	64	0
2	b2	3681	0	3452	59	0
3	C1	3392	0	3206	54	0
3	C2	3145	0	2751	34	0
3	c1	3439	0	3293	57	0
3	c2	3386	0	3189	50	0
4	D1	2615	0	2465	42	0
4	D2	2585	0	2371	41	0
4	d1	2678	0	2544	39	0
4	d2	2643	0	2489	40	0
5	E1	405	0	304	0	0
5	E2	430	0	345	3	0
5	e1	427	0	374	1	0
5	e2	421	0	354	0	0
6	F1	213	0	198	5	0
6	F2	229	0	204	5	0
6	f1	227	0	221	4	0
6	f2	225	0	205	4	0
7	H1	433	0	407	3	0
7	H2	443	0	414	4	0
7	h1	470	0	474	4	0
7	h2	450	0	432	5	0
8	I1	274	0	262	4	0
8	I2	265	0	236	4	0
8	i1	280	0	276	6	0
8	i2	261	0	238	1	0
9	J1	220	0	209	2	0
9	J2	231	0	208	1	0
9	j1	224	0	223	4	0
9	j2	228	0	220	6	0
10	K1	279	0	268	15	0
10	K2	250	0	218	6	0
10	k1	280	0	280	12	0
10	k2	269	0	252	10	0
11	L1	292	0	284	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L2	299	0	297	11	0
11	l1	299	0	304	9	0
11	l2	299	0	294	12	0
12	M1	285	0	295	10	0
12	M2	284	0	296	9	0
12	m1	285	0	295	7	0
12	m2	287	0	298	9	0
13	O1	1674	0	1534	65	0
13	O2	1376	0	1198	57	0
13	o1	1692	0	1547	60	0
13	o2	1768	0	1663	71	0
14	T1	241	0	248	3	0
14	T2	240	0	253	6	0
14	t1	246	0	264	5	0
14	t2	235	0	248	4	0
15	U1	691	0	628	14	0
15	U2	577	0	435	10	0
15	u1	703	0	645	15	0
15	u2	708	0	671	19	0
16	V1	917	0	847	19	0
16	V2	845	0	719	15	0
16	v1	921	0	842	17	0
16	v2	963	0	937	22	0
17	Y1	170	0	141	1	0
17	Y2	159	0	148	1	0
17	y1	195	0	194	2	0
17	y2	188	0	174	7	0
18	X1	197	0	192	1	0
18	X2	215	0	197	3	0
18	x1	255	0	245	2	0
18	x2	218	0	191	1	0
19	S1	164	0	161	1	0
19	S2	191	0	184	1	0
19	s1	263	0	260	3	0
19	s2	281	0	276	1	0
20	W1	134	0	149	2	0
20	W2	129	0	136	3	0
20	w1	152	0	165	5	0
20	w2	127	0	137	2	0
21	Q2	676	0	484	4	0
21	q1	645	0	462	7	0
22	Z2	351	0	280	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	z2	381	0	335	6	0
23	A1	40	0	56	4	0
23	A2	40	0	56	6	0
23	B1	120	0	168	12	0
23	B2	120	0	168	13	0
23	C1	80	0	112	7	0
23	C2	40	0	56	3	0
23	D1	40	0	56	3	0
23	F2	40	0	56	4	0
23	H1	22	0	29	3	0
23	H2	24	0	30	4	0
23	J1	40	0	56	6	0
23	K1	31	0	40	4	0
23	K2	69	0	97	8	0
23	a1	40	0	56	7	0
23	a2	40	0	56	4	0
23	b1	120	0	168	10	0
23	b2	120	0	168	15	0
23	c1	80	0	112	11	0
23	c2	40	0	56	8	0
23	d1	40	0	56	4	0
23	d2	40	0	56	4	0
23	h1	40	0	56	3	0
23	h2	40	0	56	3	0
23	j2	40	0	56	9	0
23	k1	40	0	56	6	0
23	k2	40	0	56	8	0
23	z2	40	0	56	5	0
24	A1	1	0	0	0	0
24	A2	1	0	0	0	0
24	a1	1	0	0	0	0
24	a2	1	0	0	0	0
25	A1	236	0	234	16	0
25	A2	177	0	174	17	0
25	B1	1002	0	1072	45	0
25	B2	1000	0	1072	37	0
25	C1	816	0	873	34	0
25	C2	636	0	572	15	0
25	D1	116	0	113	3	0
25	D2	191	0	205	10	0
25	K2	55	0	49	4	0
25	a1	175	0	170	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	a2	180	0	183	9	0
25	b1	1034	0	1138	34	0
25	b2	997	0	1060	41	0
25	c1	815	0	867	36	0
25	c2	789	0	814	35	0
25	d1	195	0	216	16	0
25	d2	180	0	183	7	0
26	A1	10	0	0	0	0
26	A2	10	0	0	0	0
26	a1	10	0	0	0	0
26	a2	10	0	0	0	0
27	A1	64	0	74	2	0
27	A2	64	0	74	2	0
27	D1	63	0	70	1	0
27	D2	64	0	74	3	0
27	a1	64	0	74	4	0
27	a2	64	0	74	3	0
27	d1	64	0	74	2	0
27	d2	64	0	74	1	0
28	A1	14	0	0	0	0
28	A2	28	0	0	0	0
28	B1	41	0	0	0	0
28	B2	58	0	0	0	0
28	C2	24	0	0	1	0
28	D1	6	0	0	0	0
28	F2	16	0	0	0	0
28	H2	5	0	0	0	0
28	I2	31	0	0	0	0
28	J2	10	0	0	0	0
28	K2	5	0	0	0	0
28	M2	11	0	0	0	0
28	W2	9	0	0	0	0
28	X2	7	0	0	0	0
28	a1	11	0	0	0	0
28	a2	55	0	0	0	0
28	b1	92	0	0	0	0
28	b2	12	0	0	0	0
28	c2	15	0	0	0	0
28	d1	12	0	0	0	0
28	d2	25	0	0	0	0
28	i2	14	0	0	0	0
28	j1	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	k2	30	0	0	0	0
28	l1	12	0	0	0	0
28	m1	6	0	0	0	0
28	m2	36	0	0	0	0
28	t1	27	0	0	0	0
28	x1	15	0	0	0	0
29	A1	84	0	108	6	0
29	A2	29	0	28	1	0
29	B1	79	0	98	3	0
29	B2	77	0	94	3	0
29	C1	48	0	66	1	0
29	C2	24	0	18	0	0
29	D1	35	0	40	1	0
29	F2	35	0	40	1	0
29	I2	34	0	38	2	0
29	M1	31	0	43	2	0
29	a1	51	0	72	6	0
29	a2	44	0	58	0	0
29	b1	117	0	144	14	0
29	b2	39	0	48	3	0
29	c1	55	0	86	1	0
29	c2	26	0	24	0	0
29	d1	68	0	85	1	0
29	d2	27	0	24	2	0
29	j2	50	0	73	6	0
30	A1	1	0	0	0	0
30	A2	1	0	0	0	0
30	a1	1	0	0	0	0
30	a2	1	0	0	0	0
31	A1	4	0	0	0	0
31	A2	4	0	0	0	0
31	a1	4	0	0	0	0
31	a2	4	0	0	0	0
32	B1	6	0	8	0	0
32	C1	6	0	8	0	0
32	C2	6	0	8	0	0
32	a1	6	0	8	0	0
32	a2	6	0	8	0	0
32	b1	6	0	8	0	0
32	c1	6	0	8	0	0
32	c2	6	0	8	0	0
32	i1	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A2	33	0	36	3	0
33	B1	49	0	74	8	0
33	B2	42	0	57	2	0
33	D1	98	0	148	10	0
33	D2	98	0	148	16	0
33	L1	41	0	55	1	0
33	L2	49	0	74	5	0
33	a1	43	0	59	3	0
33	a2	30	0	32	4	0
33	b1	49	0	74	4	0
33	b2	43	0	56	0	0
33	d1	81	0	108	6	0
33	d2	98	0	148	9	0
33	l1	49	0	74	3	0
33	l2	44	0	61	5	0
34	C1	178	0	233	10	0
34	C2	33	0	26	0	0
34	H1	62	0	82	1	0
34	H2	62	0	82	3	0
34	c1	175	0	224	14	0
34	c2	176	0	226	6	0
34	h1	62	0	82	4	0
34	h2	62	0	82	5	0
35	C1	35	0	46	1	0
35	L1	12	0	23	1	0
35	M1	35	0	56	1	0
35	T1	12	0	23	0	0
35	a2	35	0	46	2	0
35	b2	70	0	92	2	0
35	c1	33	0	39	0	0
35	i2	7	0	10	0	0
35	l1	24	0	35	1	0
35	m1	35	0	46	1	0
35	m2	59	0	64	3	0
36	D1	55	0	80	9	0
36	D2	55	0	80	11	0
36	d1	55	0	80	12	0
36	d2	55	0	80	7	0
37	B2	45	0	57	2	0
37	D1	35	0	34	1	0
37	D2	25	0	15	0	0
37	b2	45	0	54	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	E1	43	0	30	3	0
38	E2	43	0	30	4	0
38	V1	43	0	30	3	0
38	V2	43	0	30	4	0
38	e2	43	0	30	3	0
38	f1	43	0	30	3	0
38	v1	43	0	30	3	0
38	v2	43	0	30	3	0
39	O1	1	0	0	0	0
39	o2	1	0	0	0	0
40	A1	2	0	0	0	0
40	A2	2	0	0	0	0
40	B1	1	0	0	0	0
40	a1	4	0	0	1	0
40	a2	4	0	0	2	0
40	b2	1	0	0	0	0
40	c1	2	0	0	1	0
40	c2	1	0	0	1	0
40	d2	1	0	0	0	0
All	All	92765	0	88715	1661	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 (1661) 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)
13:O2:44:CYS:O	13:O2:240:TYR:N	1.70	1.25
23:c2:501:BCR:H361	23:c2:501:BCR:H21C	1.37	1.06
13:O2:201:VAL:HG12	13:O2:202:ASN:H	1.31	0.92
13:o1:195:GLY:CA	13:o1:220:LEU:H	1.86	0.89
13:O1:195:GLY:CA	13:O1:220:LEU:H	1.86	0.87
13:o2:195:GLY:CA	13:o2:220:LEU:H	1.86	0.87
13:O2:46:GLU:N	13:O2:238:VAL:O	2.06	0.87
13:O2:44:CYS:N	13:O2:240:TYR:O	2.09	0.86
13:o1:199:LEU:HA	13:o1:215:PHE:HA	1.58	0.86
4:D2:186:GLN:HB2	25:D2:401:CLA:HBC1	1.58	0.86
13:o2:199:LEU:HA	13:o2:215:PHE:HA	1.58	0.86
16:V2:34:ASN:HA	16:V2:38:SER:HB3	1.59	0.85
16:V1:34:ASN:HA	16:V1:38:SER:HB3	1.60	0.84
16:v2:34:ASN:HA	16:v2:38:SER:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B1:611:CLA:H2	25:B1:612:CLA:HBB2	1.61	0.82
13:o2:51:LEU:HB2	13:o2:234:LEU:HB3	1.59	0.82
13:O1:199:LEU:HA	13:O1:215:PHE:HA	1.60	0.81
16:v1:34:ASN:HA	16:v1:38:SER:HB3	1.61	0.81
4:d2:186:GLN:HB2	25:d2:405:CLA:HBC1	1.63	0.81
13:o1:195:GLY:HA3	13:o1:219:GLN:HB2	1.63	0.81
3:c1:36:TRP:O	3:c1:38:GLY:N	2.14	0.81
13:O1:195:GLY:HA3	13:O1:219:GLN:HB2	1.63	0.81
13:o2:201:VAL:HG12	13:o2:202:ASN:H	1.46	0.81
13:o1:51:LEU:HB2	13:o1:234:LEU:HB3	1.61	0.80
2:b1:365:ASN:HD21	4:d1:323:GLU:HG2	1.45	0.80
3:C1:36:TRP:O	3:C1:38:GLY:N	2.15	0.80
4:d1:186:GLN:HB2	25:d1:401:CLA:HBC1	1.64	0.80
4:D1:186:GLN:HB2	25:D1:402:CLA:HBC1	1.62	0.79
13:O1:51:LEU:HB2	13:O1:234:LEU:HB3	1.64	0.79
13:o1:201:VAL:HG12	13:o1:202:ASN:H	1.47	0.79
13:O1:201:VAL:HG12	13:O1:202:ASN:H	1.47	0.79
13:o2:195:GLY:HA3	13:o2:219:GLN:HB2	1.63	0.79
3:c2:36:TRP:O	3:c2:38:GLY:N	2.16	0.79
23:j2:102:BCR:H10C	17:y2:28:ILE:HG23	1.64	0.79
4:D1:192:THR:HG23	25:D1:402:CLA:HBC2	1.66	0.78
2:B1:222:PRO:HD2	25:B1:611:CLA:HED3	1.66	0.78
25:A2:402:CLA:HBB1	4:D2:182:LEU:HD21	1.63	0.78
38:E2:101:HEM:HBB2	38:E2:101:HEM:HHC	1.66	0.78
3:C2:36:TRP:O	3:C2:38:GLY:N	2.17	0.77
23:b2:602:BCR:H372	35:b2:623:LMT:H123	1.65	0.77
33:D2:405:LHG:H311	14:T2:21:ILE:HD11	1.66	0.77
2:B1:339:ALA:H	2:B1:431:GLU:HB2	1.49	0.77
2:b1:339:ALA:H	2:b1:431:GLU:HB2	1.51	0.76
13:O2:46:GLU:O	13:O2:238:VAL:N	2.19	0.76
15:U2:76:LYS:O	15:U2:79:MET:HB2	1.84	0.76
15:u2:76:LYS:O	15:u2:79:MET:HB2	1.85	0.76
15:u1:76:LYS:O	15:u1:79:MET:HB2	1.86	0.76
25:B1:610:CLA:HBB1	25:B1:610:CLA:HHC	1.68	0.76
25:B2:606:CLA:HBB2	25:B2:608:CLA:H193	1.68	0.76
4:d2:192:THR:HG23	25:d2:405:CLA:HBC2	1.67	0.76
16:v2:34:ASN:HA	16:v2:38:SER:CB	2.16	0.75
2:B1:365:ASN:HD21	4:D1:323:GLU:HG2	1.51	0.75
4:D2:192:THR:HG23	25:D2:401:CLA:HBC2	1.68	0.75
16:V2:34:ASN:HA	16:V2:38:SER:CB	2.16	0.75
13:o2:221:SER:HB2	13:o2:233:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f1:101:HEM:HHC	38:f1:101:HEM:HBB2	1.69	0.75
13:o2:195:GLY:HA2	13:o2:220:LEU:H	1.51	0.75
38:E1:101:HEM:HHC	38:E1:101:HEM:HBB2	1.69	0.75
15:U1:76:LYS:O	15:U1:79:MET:HB2	1.87	0.75
13:o1:195:GLY:HA2	13:o1:220:LEU:H	1.50	0.75
38:V2:201:HEM:HBC2	38:V2:201:HEM:HHH	1.69	0.75
16:v1:34:ASN:HA	16:v1:38:SER:CB	2.17	0.74
21:q1:146:VAL:HA	21:q1:149:LEU:HB3	1.70	0.74
25:D2:406:CLA:HAA2	36:D2:408:PL9:H371	1.69	0.74
25:b2:614:CLA:H171	25:b2:615:CLA:HBB2	1.68	0.74
25:B1:619:CLA:HBB1	29:M1:101:LMG:H371	1.69	0.74
2:b2:365:ASN:HD21	4:d2:323:GLU:HG2	1.51	0.74
38:e2:101:HEM:HHC	38:e2:101:HEM:HBB2	1.67	0.74
16:V1:34:ASN:HA	16:V1:38:SER:CB	2.17	0.74
25:A2:404:CLA:HHC	25:A2:404:CLA:HBB1	1.70	0.74
25:B2:617:CLA:H121	20:W2:18:LEU:HD21	1.68	0.74
25:c2:502:CLA:H161	25:c2:508:CLA:H102	1.70	0.73
38:V1:201:HEM:HBC2	38:V1:201:HEM:HHH	1.71	0.73
13:O2:197:ILE:HG13	13:O2:217:SER:HB2	1.71	0.73
38:v2:201:HEM:HBC2	38:v2:201:HEM:HHH	1.71	0.73
13:O2:199:LEU:HA	13:O2:215:PHE:HA	1.70	0.72
25:a1:404:CLA:HHC	25:a1:404:CLA:HBB1	1.72	0.72
4:d1:192:THR:HG23	25:d1:401:CLA:HBC2	1.72	0.72
13:O2:221:SER:HB2	13:O2:233:LEU:HD11	1.70	0.72
25:A2:403:CLA:HHC	25:A2:403:CLA:HBB1	1.70	0.72
13:O1:195:GLY:HA2	13:O1:220:LEU:H	1.52	0.72
25:B1:617:CLA:H121	20:W1:18:LEU:HD21	1.72	0.72
25:c1:508:CLA:HBB2	25:c1:509:CLA:H51	1.72	0.71
25:d1:404:CLA:HHC	25:d1:404:CLA:HBB1	1.71	0.71
25:C1:512:CLA:H151	23:K1:101:BCR:H21C	1.70	0.71
29:b1:624:LMG:H112	20:w1:6:VAL:HG11	1.72	0.71
13:O1:221:SER:HB2	13:O1:233:LEU:HD11	1.72	0.71
25:c1:503:CLA:H202	25:c1:509:CLA:HBB1	1.71	0.70
1:A2:93:LEU:HG	1:A2:95:PRO:HD3	1.74	0.70
2:B1:339:ALA:N	2:B1:431:GLU:HB2	2.06	0.70
13:o1:82:GLU:N	13:o1:99:ASP:O	2.23	0.70
23:d1:405:BCR:H391	9:j1:25:LEU:HD11	1.74	0.70
23:A1:401:BCR:H16C	25:A1:405:CLA:HBC2	1.74	0.70
29:B1:626:LMG:H171	25:a1:404:CLA:HBC1	1.71	0.70
4:D2:123:ILE:HD11	34:H2:101:DGD:HAW2	1.73	0.69
13:O2:45:LEU:HA	13:O2:239:PHE:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a2:93:LEU:HG	1:a2:95:PRO:HD3	1.73	0.69
2:b1:339:ALA:N	2:b1:431:GLU:HB2	2.07	0.69
23:F2:401:BCR:H361	23:F2:401:BCR:H21C	1.72	0.69
33:a2:407:LHG:H162	3:c2:443:TRP:HH2	1.57	0.69
10:k2:23:ASP:OD2	17:y2:21:GLN:NE2	2.25	0.69
13:O2:195:GLY:HA3	13:O2:219:GLN:HB2	1.75	0.69
33:d2:406:LHG:H311	14:t2:21:ILE:HD11	1.74	0.69
13:o1:146:PHE:HE2	13:o1:197:ILE:N	1.90	0.69
13:O2:201:VAL:HG12	13:O2:202:ASN:N	2.07	0.69
1:a1:93:LEU:HG	1:a1:95:PRO:HD3	1.73	0.68
29:C1:520:LMG:H181	10:K1:27:VAL:HG11	1.75	0.68
2:B2:12:VAL:HG12	25:B2:614:CLA:HMC2	1.75	0.68
13:o1:195:GLY:HA2	13:o1:220:LEU:N	2.09	0.68
1:A1:93:LEU:HG	1:A1:95:PRO:HD3	1.74	0.68
23:B2:602:BCR:HC8	29:B2:621:LMG:H211	1.75	0.68
25:B1:606:CLA:HBB2	25:B1:608:CLA:H193	1.76	0.68
13:o1:195:GLY:CA	13:o1:220:LEU:N	2.57	0.68
15:u1:36:ARG:NH1	16:v1:51:ASN:O	2.26	0.68
13:O2:195:GLY:CA	13:O2:219:GLN:HA	2.23	0.68
13:o2:146:PHE:HE2	13:o2:197:ILE:N	1.92	0.68
13:O1:51:LEU:HB3	13:O1:65:PHE:HB3	1.74	0.68
13:O1:146:PHE:HE2	13:O1:197:ILE:N	1.92	0.68
13:O1:195:GLY:HA3	13:O1:219:GLN:CA	2.24	0.68
25:b1:608:CLA:H192	25:b1:611:CLA:HBB2	1.73	0.68
38:v1:201:HEM:HBC2	38:v1:201:HEM:HHD	1.75	0.68
13:o1:48:LYS:O	13:o1:236:LYS:O	2.12	0.68
23:K2:102:BCR:H21C	23:K2:102:BCR:H361	1.76	0.68
33:L2:101:LHG:H311	12:M2:18:PRO:HB3	1.75	0.68
1:a2:161:TYR:OH	40:a2:501:HOH:O	2.10	0.68
23:j2:102:BCR:H332	10:k2:25:MET:HE1	1.76	0.67
12:M1:14:GLY:O	12:M1:18:PRO:HD2	1.94	0.67
1:a1:160:ILE:HD11	34:c1:518:DGD:HBT1	1.75	0.67
3:C1:39:ASN:HB2	25:C1:509:CLA:CGA	2.24	0.67
12:m2:14:GLY:O	12:m2:18:PRO:HD2	1.94	0.67
13:o2:195:GLY:HA2	13:o2:220:LEU:N	2.09	0.67
16:V2:41:HIS:C	16:V2:43:GLY:H	2.03	0.67
13:O1:195:GLY:CA	13:O1:220:LEU:N	2.57	0.67
2:b1:6:TYR:O	2:b1:8:VAL:N	2.27	0.67
13:O1:195:GLY:CA	13:O1:219:GLN:HA	2.25	0.67
12:M2:14:GLY:O	12:M2:18:PRO:HD2	1.95	0.67
13:o2:195:GLY:CA	13:o2:220:LEU:N	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o1:195:GLY:HA3	13:o1:219:GLN:CA	2.26	0.66
36:d2:409:PL9:H352	11:l2:26:VAL:HG12	1.77	0.66
1:A1:107:TYR:HB2	13:O1:71:MET:HE3	1.78	0.66
13:O1:48:LYS:O	13:O1:49:GLN:HB2	1.94	0.66
1:a1:120:LEU:HB3	34:c1:518:DGD:HAW2	1.78	0.66
2:b1:91:TRP:CD1	29:b1:624:LMG:HC1	2.30	0.66
13:o1:197:ILE:HG13	13:o1:217:SER:HB2	1.77	0.66
13:o2:48:LYS:O	13:o2:49:GLN:HB2	1.95	0.66
3:c1:39:ASN:HB2	25:c1:510:CLA:CGA	2.25	0.66
1:A2:160:ILE:HG21	1:A2:291:SER:HB3	1.78	0.66
13:o2:48:LYS:O	13:o2:236:LYS:O	2.13	0.66
12:m1:14:GLY:O	12:m1:18:PRO:HD2	1.95	0.66
13:o1:195:GLY:CA	13:o1:219:GLN:HA	2.25	0.66
13:O2:199:LEU:HD12	13:O2:199:LEU:H	1.60	0.66
13:O1:195:GLY:HA2	13:O1:220:LEU:N	2.10	0.66
4:d2:199:MET:HB2	4:d2:281:VAL:HG11	1.78	0.66
23:c1:502:BCR:H361	23:c1:502:BCR:H21C	1.78	0.65
25:A1:406:CLA:HAA2	36:D1:408:PL9:H371	1.78	0.65
13:o2:195:GLY:CA	13:o2:219:GLN:HA	2.27	0.65
25:A2:402:CLA:CBB	4:D2:182:LEU:HD21	2.26	0.65
13:O1:199:LEU:HD12	13:O1:199:LEU:H	1.61	0.65
13:o2:47:PRO:O	13:o2:48:LYS:HG2	1.96	0.65
6:F2:41:GLN:HG3	9:J2:31:GLY:HA3	1.78	0.65
2:B1:341:LEU:HD11	13:O1:178(C):GLY:HA3	1.78	0.65
13:O1:48:LYS:O	13:O1:236:LYS:O	2.14	0.65
23:D1:401:BCR:H391	9:J1:25:LEU:HD11	1.78	0.65
2:b1:489:GLN:HE21	2:b1:501:LYS:HE2	1.62	0.65
13:o1:48:LYS:O	13:o1:49:GLN:HB2	1.96	0.65
2:b1:377:ILE:HD11	4:d1:340:VAL:HB	1.78	0.65
25:c1:504:CLA:HAB	25:c1:512:CLA:H141	1.79	0.65
3:c2:279:LEU:HD22	25:c2:510:CLA:HED2	1.79	0.65
3:c2:36:TRP:C	3:c2:38:GLY:H	2.05	0.64
4:D1:172:SER:HB2	4:D1:177:ALA:HB1	1.79	0.64
4:D1:199:MET:HB2	4:D1:281:VAL:HG11	1.78	0.64
33:D1:405:LHG:H311	14:T1:21:ILE:HD11	1.77	0.64
23:k1:101:BCR:H10C	17:y1:28:ILE:HG23	1.79	0.64
13:O2:195:GLY:HA2	13:O2:219:GLN:HA	1.77	0.64
3:c2:261:ARG:NH1	19:s2:37:ALA:O	2.31	0.64
13:O1:49:GLN:O	13:O1:235:LEU:HA	1.98	0.64
25:B2:608:CLA:HMA3	25:B2:609:CLA:H3A	1.80	0.64
2:B1:231:MET:HE1	25:B1:611:CLA:HED1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:422:ARG:NH1	13:O1:169:ASP:OD2	2.29	0.64
4:d2:172:SER:HB2	4:d2:177:ALA:HB1	1.79	0.64
1:A1:160:ILE:HG21	1:A1:291:SER:HB3	1.79	0.64
13:O1:47:PRO:O	13:O1:48:LYS:HG2	1.97	0.64
13:O1:154:GLY:HA2	13:O1:164:MET:HB2	1.79	0.64
13:o2:195:GLY:HA3	13:o2:219:GLN:CB	2.28	0.64
25:C1:506:CLA:H93	25:C1:506:CLA:HBB1	1.80	0.64
2:b1:12:VAL:HG12	25:b1:614:CLA:HMC2	1.77	0.64
13:o2:195:GLY:HA3	13:o2:219:GLN:CA	2.27	0.64
1:a1:247:ASN:HD21	2:b1:487:THR:HG23	1.62	0.64
1:a2:192:ILE:HG13	1:a2:293:MET:HE1	1.80	0.64
1:a2:165:GLN:NE2	40:a2:501:HOH:O	2.29	0.64
16:V1:41:HIS:C	16:V1:43:GLY:H	2.06	0.64
1:a2:107:TYR:HB2	13:o2:71:MET:HE3	1.79	0.64
33:b1:622:LHG:O4	4:d1:141:TYR:OH	2.13	0.63
36:d1:409:PL9:H353	11:l1:30:LEU:HD22	1.80	0.63
6:f1:24:HIS:NE2	38:f1:101:HEM:ND	2.45	0.63
13:o1:195:GLY:HA3	13:o1:219:GLN:CB	2.27	0.63
13:O2:197:ILE:HA	13:O2:217:SER:HA	1.80	0.63
13:o2:81:ILE:HA	13:o2:100:GLY:HA3	1.79	0.63
4:d1:172:SER:HB2	4:d1:177:ALA:HB1	1.79	0.63
13:o1:146:PHE:CE2	13:o1:197:ILE:N	2.66	0.63
2:b2:6:TYR:O	2:b2:8:VAL:N	2.31	0.63
2:B1:6:TYR:O	2:B1:8:VAL:N	2.31	0.63
3:C1:36:TRP:C	3:C1:38:GLY:H	2.06	0.63
1:A2:192:ILE:HG13	1:A2:293:MET:HE1	1.80	0.63
1:a2:341:LEU:HD11	16:v2:47:LYS:HD3	1.80	0.63
1:a1:106:LEU:HD11	23:a1:401:BCR:H402	1.80	0.63
1:a1:160:ILE:HG21	1:a1:291:SER:HB3	1.79	0.63
23:a1:401:BCR:H16C	25:a1:404:CLA:HBC2	1.79	0.63
3:c1:148:GLY:O	3:c1:156:LYS:NZ	2.29	0.63
13:o1:200:ALA:O	13:o1:201:VAL:O	2.17	0.63
16:v1:41:HIS:C	16:v1:43:GLY:H	2.06	0.63
1:a2:160:ILE:HG21	1:a2:291:SER:HB3	1.79	0.63
13:o2:49:GLN:O	13:o2:235:LEU:HA	1.98	0.63
1:A1:5:LEU:HD23	3:C1:262:ARG:HG2	1.81	0.63
25:A1:403:CLA:CBB	4:D1:182:LEU:HD21	2.29	0.63
13:O1:195:GLY:HA3	13:O1:219:GLN:CB	2.27	0.63
2:B2:458:PHE:CE2	25:B2:607:CLA:HBB1	2.34	0.63
13:O1:200:ALA:O	13:O1:201:VAL:O	2.16	0.63
2:B2:458:PHE:HB3	25:B2:607:CLA:HBC2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D2:332:GLN:N	4:D2:332:GLN:OE1	2.32	0.63
13:o2:197:ILE:HG13	13:o2:217:SER:HB2	1.79	0.63
3:c2:213:LEU:HD21	23:c2:501:BCR:H12C	1.80	0.63
3:C1:447:ARG:NE	33:D1:404:LHG:O2	2.31	0.63
13:o2:146:PHE:CE2	13:o2:197:ILE:N	2.67	0.63
15:u2:36:ARG:NH1	16:v2:51:ASN:O	2.30	0.63
1:A1:192:ILE:HG13	1:A1:293:MET:HE1	1.80	0.63
3:c1:209:ILE:HG23	23:c1:502:BCR:H403	1.80	0.63
4:d2:332:GLN:N	4:d2:332:GLN:OE1	2.31	0.63
1:A1:121:LEU:HD13	25:A1:405:CLA:HMB3	1.80	0.62
2:B1:434:ARG:NH2	13:O1:178(F):GLY:O	2.32	0.62
13:O1:197:ILE:HG13	13:O1:217:SER:HB2	1.79	0.62
25:a1:403:CLA:CBB	4:d1:182:LEU:HD21	2.28	0.62
16:v1:41:HIS:O	16:v1:43:GLY:N	2.31	0.62
13:o2:199:LEU:HD12	13:o2:199:LEU:H	1.63	0.62
13:o2:200:ALA:O	13:o2:201:VAL:O	2.16	0.62
2:B2:6:TYR:O	2:B2:8:VAL:N	2.31	0.62
4:d1:332:GLN:N	4:d1:332:GLN:OE1	2.32	0.62
3:c2:256:PRO:HA	25:c2:507:CLA:HED3	1.81	0.62
1:a1:192:ILE:HG13	1:a1:293:MET:HE1	1.82	0.62
3:c1:288:GLU:HG3	34:c1:518:DGD:HB32	1.81	0.62
13:O2:154:GLY:HA2	13:O2:164:MET:HB2	1.81	0.62
4:D1:332:GLN:N	4:D1:332:GLN:OE1	2.32	0.62
33:B1:621:LHG:H192	4:D1:277:THR:HG22	1.81	0.62
29:B1:626:LMG:HC3	1:a1:102:LEU:HB2	1.82	0.62
36:D1:408:PL9:H352	11:L1:26:VAL:HG12	1.80	0.62
36:D1:408:PL9:H353	11:L1:30:LEU:HD22	1.81	0.62
3:C2:36:TRP:C	3:C2:38:GLY:H	2.08	0.62
25:b2:620:CLA:H2	29:b2:622:LMG:H162	1.80	0.62
16:v2:41:HIS:O	16:v2:43:GLY:N	2.32	0.62
13:o2:154:GLY:HA2	13:o2:164:MET:HB2	1.80	0.62
3:c2:207:ALA:O	3:c2:211:SER:HB2	2.00	0.62
9:j2:30:TYR:HA	29:j2:101:LMG:H111	1.81	0.62
16:v2:41:HIS:C	16:v2:43:GLY:H	2.07	0.62
3:C1:466:VAL:HG21	4:D1:248:THR:HA	1.82	0.61
13:o1:82:GLU:HG2	13:o1:99:ASP:HB3	1.80	0.61
13:O1:146:PHE:CE2	13:O1:197:ILE:N	2.67	0.61
25:c1:512:CLA:H2	25:c1:512:CLA:HED2	1.81	0.61
13:o1:49:GLN:O	13:o1:235:LEU:HA	2.00	0.61
3:c2:39:ASN:HB2	25:c2:509:CLA:CGA	2.29	0.61
2:B1:116:VAL:HG21	23:B1:603:BCR:H292	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V1:41:HIS:C	16:V1:43:GLY:N	2.56	0.61
2:b1:370:LEU:HB2	2:b1:379:ALA:HB3	1.82	0.61
38:v1:201:HEM:HMB1	38:v1:201:HEM:HBB2	1.83	0.61
2:b1:422:ARG:NH1	13:o1:169:ASP:OD2	2.34	0.61
25:d1:404:CLA:HAA2	36:d1:409:PL9:H371	1.82	0.61
3:c1:267:SER:HB3	19:s1:42:LEU:HD22	1.83	0.61
2:b1:327:ALA:HB1	29:b1:631:LMG:HC8	1.83	0.60
3:C2:437:ILE:HA	25:C2:511:CLA:HMC2	1.83	0.60
3:c2:99:VAL:HG23	3:c2:196:ILE:HD11	1.83	0.60
9:j2:23:THR:HA	29:j2:101:LMG:H361	1.83	0.60
13:o1:195:GLY:N	13:o1:220:LEU:H	1.98	0.60
2:b2:370:LEU:HB2	2:b2:379:ALA:HB3	1.82	0.60
25:b2:608:CLA:H192	25:b2:610:CLA:HBB2	1.83	0.60
13:O1:195:GLY:N	13:O1:220:LEU:H	1.98	0.60
38:V1:201:HEM:HMB1	38:V1:201:HEM:HBB2	1.84	0.60
23:b1:601:BCR:H332	12:m1:9:LEU:HD23	1.82	0.60
3:c1:36:TRP:C	3:c1:38:GLY:H	2.07	0.60
1:A2:291:SER:O	1:A2:294:ALA:HB3	2.00	0.60
1:a1:107:TYR:HB2	13:o1:71:MET:HE3	1.81	0.60
16:v1:41:HIS:C	16:v1:43:GLY:N	2.56	0.60
3:C2:207:ALA:O	3:C2:211:SER:HB2	2.01	0.60
3:C1:209:ILE:HG23	23:C1:501:BCR:H403	1.84	0.60
3:c1:192:GLY:HA2	21:q1:146:VAL:C	2.26	0.60
13:o1:154:GLY:HA2	13:o1:164:MET:HB2	1.82	0.60
38:E2:101:HEM:O1A	6:F2:19:ARG:NH1	2.35	0.60
13:o2:195:GLY:N	13:o2:220:LEU:H	1.98	0.60
36:d1:409:PL9:H222	33:l1:102:LHG:H202	1.84	0.60
2:b2:158:VAL:HG22	2:b2:166:ILE:HD11	1.84	0.60
3:c1:36:TRP:C	3:c1:38:GLY:N	2.58	0.60
2:B2:158:VAL:HG22	2:B2:166:ILE:HD11	1.84	0.60
16:v2:41:HIS:C	16:v2:43:GLY:N	2.56	0.60
2:B1:370:LEU:HB2	2:B1:379:ALA:HB3	1.82	0.59
2:b1:168:ILE:HD11	2:b1:181:VAL:HG22	1.84	0.59
2:b2:341:LEU:HD11	13:o2:178(C):GLY:HA3	1.84	0.59
2:b2:434:ARG:NH2	13:o2:178(F):GLY:O	2.34	0.59
3:C1:207:ALA:O	3:C1:211:SER:HB2	2.01	0.59
3:C1:288:GLU:HG3	34:C1:516:DGD:HB31	1.83	0.59
3:c1:207:ALA:O	3:c1:211:SER:HB2	2.02	0.59
13:O2:146:PHE:HE2	13:O2:197:ILE:N	2.00	0.59
2:b2:458:PHE:HB3	25:b2:616:CLA:HBC2	1.83	0.59
16:V1:41:HIS:O	16:V1:43:GLY:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a2:404:CLA:CBB	4:d2:182:LEU:HD21	2.32	0.59
2:b2:18:ARG:HH22	37:b2:605:SQD:HO8	1.50	0.59
16:V2:41:HIS:C	16:V2:43:GLY:N	2.55	0.59
3:C1:99:VAL:HG23	3:C1:196:ILE:HD11	1.83	0.59
3:C1:107:ASN:ND2	35:C1:519:LMT:O4'	2.36	0.59
2:b1:458:PHE:HB3	25:b1:607:CLA:HBC2	1.84	0.59
25:b1:606:CLA:HBB2	25:b1:608:CLA:H193	1.85	0.59
23:A1:401:BCR:H373	29:A1:412:LMG:H301	1.83	0.59
25:B1:614:CLA:H171	25:B1:615:CLA:HBB2	1.83	0.59
25:b1:609:CLA:OBD	29:b1:624:LMG:O2	2.18	0.59
13:o1:201:VAL:HG12	13:o1:202:ASN:N	2.17	0.59
2:B1:458:PHE:HB3	25:B1:607:CLA:HBC2	1.83	0.59
2:b1:7:ARG:O	2:b1:10:THR:OG1	2.21	0.59
2:b1:158:VAL:HG22	2:b1:166:ILE:HD11	1.84	0.59
36:D2:408:PL9:H353	11:L2:30:LEU:HD22	1.85	0.58
1:a2:149:ALA:HB3	1:a2:150:PRO:HD3	1.86	0.58
1:a2:160:ILE:HD11	34:c2:514:DGD:HBT1	1.84	0.58
2:b1:75:TRP:HB3	29:b1:621:LMG:HC5	1.84	0.58
1:A2:149:ALA:HB3	1:A2:150:PRO:HD3	1.86	0.58
2:B2:497:LYS:NZ	4:D2:20:ASP:OD1	2.31	0.58
21:Q2:124:GLU:O	21:Q2:127:GLY:N	2.36	0.58
29:a1:412:LMG:H411	34:c1:518:DGD:HBE1	1.85	0.58
4:d1:326:ARG:O	4:d1:330:ALA:HB2	2.03	0.58
21:q1:124:GLU:O	21:q1:127:GLY:N	2.36	0.58
13:O2:221:SER:CB	13:O2:233:LEU:HD11	2.33	0.58
13:o2:197:ILE:HA	13:o2:217:SER:HA	1.85	0.58
1:a1:131:TRP:CH2	25:c1:507:CLA:HAA2	2.38	0.58
11:l1:25:PHE:HB3	14:t1:13:THR:HG22	1.86	0.58
1:A1:9:GLU:HG3	19:S1:30:TRP:CZ2	2.39	0.58
1:A1:149:ALA:HB3	1:A1:150:PRO:HD3	1.86	0.58
13:O1:201:VAL:HG12	13:O1:202:ASN:N	2.17	0.58
33:D2:403:LHG:H292	33:D2:403:LHG:H201	1.84	0.58
3:C1:36:TRP:C	3:C1:38:GLY:N	2.60	0.58
3:C1:275:SER:HB3	25:C1:510:CLA:HED2	1.85	0.58
23:a2:402:BCR:H16C	25:a2:405:CLA:HBC2	1.85	0.58
2:b2:349:LYS:HE3	2:b2:396:GLY:HA3	1.86	0.58
2:b2:377:ILE:HD11	4:d2:340:VAL:HB	1.83	0.58
2:b2:422:ARG:NH1	13:o2:169:ASP:OD2	2.36	0.58
4:D1:326:ARG:O	4:D1:330:ALA:HB2	2.03	0.58
13:O1:81:ILE:HA	13:O1:100:GLY:HA3	1.86	0.58
1:a1:121:LEU:HD13	25:a1:404:CLA:HMB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:349:LYS:HE3	2:b1:396:GLY:HA3	1.85	0.58
3:c1:452:ALA:HA	19:s1:42:LEU:HD12	1.86	0.58
3:C2:36:TRP:C	3:C2:38:GLY:N	2.61	0.58
38:V2:201:HEM:HHC	38:V2:201:HEM:HBB2	1.86	0.58
29:j2:101:LMG:H451	10:k2:31:LEU:HA	1.85	0.58
11:l2:25:PHE:HB3	14:t2:13:THR:HG22	1.85	0.58
25:C1:512:CLA:H152	25:C1:512:CLA:HMA2	1.84	0.58
25:A2:402:CLA:HBB1	25:A2:402:CLA:HHC	1.84	0.58
25:b2:613:CLA:H171	34:h2:102:DGD:HAE2	1.86	0.58
1:A1:291:SER:O	1:A1:294:ALA:HB3	2.02	0.58
2:b1:90:LEU:H	29:b1:624:LMG:HC4	1.69	0.58
4:D2:326:ARG:O	4:D2:330:ALA:HB2	2.04	0.58
36:D2:408:PL9:H352	11:L2:26:VAL:HG12	1.85	0.58
2:b2:7:ARG:O	2:b2:10:THR:OG1	2.22	0.58
13:O1:197:ILE:HA	13:O1:217:SER:HA	1.85	0.57
11:L2:25:PHE:HB3	14:T2:13:THR:HG22	1.85	0.57
25:C1:513:CLA:H2	23:C1:521:BCR:H281	1.86	0.57
1:a1:291:SER:O	1:a1:294:ALA:HB3	2.03	0.57
2:b1:458:PHE:CE2	25:b1:607:CLA:HBB1	2.39	0.57
3:c1:318:LEU:HD12	3:c1:340:TYR:HB3	1.86	0.57
13:o1:197:ILE:HA	13:o1:217:SER:HA	1.85	0.57
1:a2:291:SER:O	1:a2:294:ALA:HB3	2.03	0.57
16:V1:42:VAL:O	16:V1:42:VAL:HG13	2.03	0.57
2:b1:371:VAL:HG23	2:b1:377:ILE:HD13	1.84	0.57
2:B2:168:ILE:HD11	2:B2:181:VAL:HG22	1.85	0.57
18:X2:3:MET:HG3	18:X2:7:LEU:HD23	1.86	0.57
4:d2:326:ARG:O	4:d2:330:ALA:HB2	2.04	0.57
1:A2:50:ILE:HG22	23:A2:401:BCR:H271	1.85	0.57
13:O2:45:LEU:HD12	13:O2:45:LEU:H	1.69	0.57
16:v1:42:VAL:HG13	16:v1:42:VAL:O	2.03	0.57
33:A2:405:LHG:O2	3:C2:447:ARG:NE	2.37	0.57
38:E2:101:HEM:HMC2	38:E2:101:HEM:HBC2	1.86	0.57
27:A1:408:PHO:HAB	4:D1:205:LEU:HD13	1.85	0.57
14:T2:4:LEU:HG	35:b2:623:LMT:H32	1.87	0.57
2:b2:168:ILE:HD11	2:b2:181:VAL:HG22	1.86	0.57
2:B1:158:VAL:HG22	2:B1:166:ILE:HD11	1.85	0.57
23:B1:602:BCR:HC8	23:B1:602:BCR:H331	1.87	0.57
1:a1:149:ALA:HB3	1:a1:150:PRO:HD3	1.87	0.57
2:b1:341:LEU:HD11	13:o1:178(C):GLY:HA3	1.87	0.57
3:c1:147:PHE:CD2	25:c1:516:CLA:H3A	2.40	0.57
16:v1:126:GLN:HB3	16:v1:129:LYS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B2:601:BCR:H332	12:M2:9:LEU:HD23	1.87	0.57
1:A1:184:LEU:HD21	4:D1:186:GLN:HG2	1.86	0.57
3:C2:42:LEU:HD21	25:K2:101:CLA:H2A	1.85	0.57
25:a2:404:CLA:H41	25:d2:402:CLA:HBB1	1.87	0.57
25:b2:612:CLA:H18	25:b2:615:CLA:H8	1.86	0.57
13:o2:201:VAL:HG12	13:o2:202:ASN:N	2.17	0.57
2:B2:7:ARG:O	2:B2:10:THR:OG1	2.22	0.56
2:B2:349:LYS:HE3	2:B2:396:GLY:HA3	1.86	0.56
3:c2:119:LEU:HG	23:k2:501:BCR:H10C	1.86	0.56
29:A1:410:LMG:H121	25:C1:506:CLA:H203	1.88	0.56
13:o1:49:GLN:HB2	13:o1:236:LYS:HB2	1.86	0.56
4:D2:193:LEU:O	11:L2:34:TYR:OH	2.23	0.56
13:O2:146:PHE:CE2	13:O2:197:ILE:N	2.73	0.56
3:c2:318:LEU:HD12	3:c2:340:TYR:HB3	1.87	0.56
2:B1:7:ARG:O	2:B1:10:THR:OG1	2.22	0.56
33:b1:622:LHG:H101	33:b1:622:LHG:H332	1.86	0.56
25:B2:608:CLA:H192	25:B2:611:CLA:HBB2	1.87	0.56
3:C2:256:PRO:HA	25:C2:508:CLA:HED3	1.88	0.56
25:C2:503:CLA:C2D	25:C2:505:CLA:H2	2.35	0.56
33:D2:405:LHG:HC91	11:L2:19:TRP:HZ2	1.70	0.56
16:V2:41:HIS:O	16:V2:43:GLY:N	2.32	0.56
13:o2:200:ALA:N	13:o2:214:VAL:O	2.39	0.56
3:c1:257:PHE:HD2	25:c1:508:CLA:HED3	1.69	0.56
3:c1:406:SER:HA	3:c1:420:VAL:HG23	1.88	0.56
33:B2:627:LHG:H322	4:D2:36:LEU:HB2	1.87	0.56
13:O2:201:VAL:CG1	13:O2:202:ASN:H	2.12	0.56
25:b2:620:CLA:HBB1	29:b2:622:LMG:H191	1.87	0.56
3:c2:36:TRP:C	3:c2:38:GLY:N	2.60	0.56
33:B1:621:LHG:H292	33:B1:621:LHG:H201	1.88	0.56
2:B2:441:GLY:C	13:O2:176:ALA:HB3	2.30	0.56
13:o2:164:MET:HE3	13:o2:225:MET:HG2	1.88	0.56
2:B1:168:ILE:HD11	2:B1:181:VAL:HG22	1.86	0.56
2:B1:349:LYS:HE3	2:B1:396:GLY:HA3	1.86	0.56
13:O2:43:LEU:HD12	13:O2:240:TYR:O	2.05	0.56
13:o1:200:ALA:N	13:o1:214:VAL:O	2.38	0.56
1:a2:184:LEU:HD21	4:d2:186:GLN:HG2	1.88	0.56
2:b2:339:ALA:O	2:b2:431:GLU:N	2.39	0.56
25:c2:503:CLA:HBB2	25:c2:511:CLA:H151	1.88	0.56
25:d2:402:CLA:HAA2	36:d2:409:PL9:H371	1.87	0.56
16:v2:42:VAL:O	16:v2:42:VAL:HG13	2.04	0.56
2:B2:339:ALA:O	2:B2:430:PHE:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K2:35:LEU:HA	23:K2:102:BCR:H19C	1.86	0.56
1:a2:53:ILE:HD12	35:a2:406:LMT:H111	1.87	0.56
38:e2:101:HEM:HMC1	38:e2:101:HEM:HBC2	1.86	0.56
10:K1:23:ASP:OD2	17:Y1:21:GLN:NE2	2.38	0.56
3:c1:38:GLY:HA3	25:c1:513:CLA:HMD2	1.88	0.56
38:f1:101:HEM:HMC1	38:f1:101:HEM:HBC2	1.87	0.56
4:d2:160:TYR:HA	4:d2:290:ALA:HB2	1.87	0.56
33:D1:404:LHG:H132	33:D1:404:LHG:H321	1.88	0.55
3:C2:318:LEU:HD12	3:C2:340:TYR:HB3	1.87	0.55
38:v2:201:HEM:HBB2	38:v2:201:HEM:HMB1	1.87	0.55
11:L1:25:PHE:HB3	14:T1:13:THR:HG22	1.87	0.55
4:d1:123:ILE:HD11	34:h1:101:DGD:HAW2	1.87	0.55
23:k1:101:BCR:H361	23:k1:101:BCR:H21C	1.88	0.55
1:A2:131:TRP:CH2	25:C2:507:CLA:HAA2	2.41	0.55
1:A2:161:TYR:HA	1:A2:294:ALA:HB1	1.87	0.55
16:v2:21:ILE:HD13	16:v2:117:ALA:HB1	1.88	0.55
3:c1:192:GLY:C	21:q1:147:GLY:HA2	2.32	0.55
25:c1:503:CLA:C2D	25:c1:505:CLA:H2	2.36	0.55
13:o1:164:MET:HE3	13:o1:225:MET:HG2	1.89	0.55
33:B2:627:LHG:HC42	4:D2:134:ARG:HG2	1.88	0.55
2:b2:339:ALA:O	2:b2:430:PHE:HA	2.06	0.55
23:B1:601:BCR:H362	25:B1:616:CLA:H112	1.89	0.55
23:c1:502:BCR:H17C	25:c1:503:CLA:H101	1.89	0.55
36:d1:409:PL9:H352	11:l1:26:VAL:HG12	1.88	0.55
3:c2:288:GLU:HG3	34:c2:514:DGD:HB31	1.88	0.55
3:c2:406:SER:HA	3:c2:420:VAL:HG23	1.88	0.55
12:M2:25:LEU:O	12:M2:28:GLN:HG3	2.06	0.55
25:c2:509:CLA:H12	25:c2:512:CLA:HBC2	1.88	0.55
12:m2:25:LEU:O	12:m2:28:GLN:HG3	2.07	0.55
33:B1:621:LHG:H141	11:L1:23:LEU:HD21	1.87	0.55
3:C1:406:SER:HA	3:C1:420:VAL:HG23	1.88	0.55
1:a1:341:LEU:HD11	16:v1:47:LYS:HD3	1.88	0.55
3:c1:371:SER:HB3	3:c1:376:ASP:HB2	1.89	0.55
3:c1:437:ILE:HA	25:c1:510:CLA:HMC2	1.89	0.55
18:X2:23:LEU:HB3	18:X2:24:PRO:HD3	1.88	0.55
2:B1:339:ALA:O	2:B1:431:GLU:N	2.40	0.55
13:O1:195:GLY:HA3	13:O1:219:GLN:HA	1.88	0.55
16:V1:21:ILE:HD13	16:V1:117:ALA:HB1	1.89	0.55
2:B2:339:ALA:O	2:B2:431:GLU:N	2.39	0.55
25:C1:505:CLA:H43	34:C1:517:DGD:HB32	1.88	0.55
13:o1:51:LEU:HB3	13:o1:65:PHE:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:116:VAL:HG21	23:B2:603:BCR:H292	1.88	0.55
1:a2:43:THR:HG22	23:a2:402:BCR:H16C	1.89	0.55
1:a2:120:LEU:HB3	34:c2:514:DGD:HAW2	1.89	0.55
2:b2:371:VAL:HG23	2:b2:377:ILE:HD13	1.88	0.55
2:B1:339:ALA:O	2:B1:430:PHE:HA	2.07	0.55
13:O2:181:VAL:O	13:O2:183:ARG:N	2.40	0.55
33:a2:407:LHG:O1	4:d2:230:ASP:OD2	2.25	0.55
3:C1:318:LEU:HD12	3:C1:340:TYR:HB3	1.88	0.54
7:h1:46:LEU:HD11	34:h1:101:DGD:HA31	1.90	0.54
33:d2:406:LHG:HC92	36:d2:409:PL9:H111	1.89	0.54
16:v1:122:GLN:NE2	16:v1:126:GLN:OE1	2.40	0.54
23:c2:501:BCR:H353	25:c2:508:CLA:H91	1.89	0.54
25:d1:404:CLA:H13	36:d1:409:PL9:H452	1.89	0.54
1:A2:121:LEU:HD13	25:A2:403:CLA:HMB3	1.89	0.54
25:B1:619:CLA:HBA2	29:M1:101:LMG:H291	1.88	0.54
2:b1:488:GLU:HB2	4:D2:238:THR:HG21	1.90	0.54
3:c2:277:GLY:C	25:c2:506:CLA:HBC3	2.32	0.54
23:c2:501:BCR:H382	25:c2:507:CLA:H12	1.90	0.54
36:d2:409:PL9:H353	11:l2:30:LEU:HD22	1.89	0.54
1:A1:234:ASN:ND2	33:B1:621:LHG:O1	2.38	0.54
4:D1:160:TYR:HA	4:D1:290:ALA:HB2	1.88	0.54
1:a1:161:TYR:HA	1:a1:294:ALA:HB1	1.88	0.54
1:a1:184:LEU:HD21	4:d1:186:GLN:HG2	1.89	0.54
13:O1:181:VAL:O	13:O1:183:ARG:N	2.41	0.54
18:X1:23:LEU:HB3	18:X1:24:PRO:HD3	1.88	0.54
25:c1:510:CLA:H2	25:c1:512:CLA:H12	1.89	0.54
12:M1:27:ILE:HD13	35:l1:101:LMT:H21	1.90	0.54
2:b1:339:ALA:O	2:b1:431:GLU:N	2.40	0.54
23:b1:601:BCR:H313	29:b1:631:LMG:H111	1.89	0.54
23:b1:603:BCR:H342	25:b1:609:CLA:H71	1.90	0.54
2:b2:383:PHE:CZ	13:o2:167:GLY:HA2	2.43	0.54
13:o2:49:GLN:HB2	13:o2:236:LYS:HB2	1.90	0.54
25:B2:615:CLA:H51	33:D2:403:LHG:H352	1.89	0.54
33:D2:403:LHG:H141	11:L2:23:LEU:HD21	1.90	0.54
16:V2:39:SER:O	16:V2:40:CYS:C	2.49	0.54
33:d2:403:LHG:H111	33:l2:101:LHG:HC91	1.90	0.54
1:A1:160:ILE:HD11	34:C1:516:DGD:HBT2	1.89	0.54
3:C1:418:ASN:HD21	34:C1:515:DGD:HD4	1.72	0.54
38:E1:101:HEM:HMC1	38:E1:101:HEM:HBC2	1.89	0.54
3:c1:42:LEU:HD21	25:c1:513:CLA:H2A	1.89	0.54
23:j2:102:BCR:H12C	17:y2:28:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l2:23:LEU:HD23	33:l2:101:LHG:H291	1.89	0.54
16:v2:39:SER:O	16:v2:40:CYS:C	2.50	0.54
3:c1:28:ILE:HG13	10:k1:45:PHE:HE2	1.73	0.54
4:D2:160:TYR:HA	4:D2:290:ALA:HB2	1.89	0.54
13:O2:164:MET:HE3	13:O2:225:MET:HG2	1.89	0.54
23:D1:401:BCR:H372	29:D1:406:LMG:H301	1.89	0.53
1:a1:253:GLY:HA3	2:b1:490:VAL:HG22	1.90	0.53
3:c2:393:ALA:HB1	38:v2:201:HEM:HBC1	1.90	0.53
13:o2:221:SER:CB	13:o2:233:LEU:HD11	2.38	0.53
2:b1:339:ALA:O	2:b1:430:PHE:HA	2.08	0.53
2:b1:441:GLY:C	13:o1:176:ALA:HB3	2.33	0.53
2:B2:60:MET:HB3	2:B2:63:MET:HB2	1.90	0.53
13:O2:53:GLU:HA	13:O2:65:PHE:HA	1.89	0.53
29:j2:101:LMG:H453	23:j2:102:BCR:H363	1.88	0.53
1:A1:131:TRP:CH2	25:C1:506:CLA:HAA2	2.43	0.53
25:A1:403:CLA:HMC3	4:D1:182:LEU:HD22	1.88	0.53
3:C1:148:GLY:O	3:C1:156:LYS:NZ	2.41	0.53
12:M1:25:LEU:O	12:M1:28:GLN:HG3	2.07	0.53
1:a1:43:THR:HG22	23:a1:401:BCR:H16C	1.89	0.53
1:a2:161:TYR:HA	1:a2:294:ALA:HB1	1.90	0.53
4:D1:274:VAL:HG13	36:D1:408:PL9:H252	1.89	0.53
1:A1:84:PRO:HA	1:A1:112:TYR:CG	2.44	0.53
25:B1:607:CLA:HBB1	25:B1:619:CLA:HBB2	1.91	0.53
2:b1:60:MET:HB3	2:b1:63:MET:HB2	1.90	0.53
15:U2:96:ASP:HB3	15:U2:100:ASN:HA	1.91	0.53
1:a2:84:PRO:HA	1:a2:112:TYR:CG	2.43	0.53
3:c2:147:PHE:CD2	25:c2:515:CLA:H3A	2.43	0.53
4:d2:274:VAL:HG13	36:d2:409:PL9:H252	1.89	0.53
23:d1:405:BCR:H372	29:d1:408:LMG:H301	1.91	0.53
13:o1:201:VAL:C	13:o1:213:GLY:HA3	2.34	0.53
1:a2:85:THR:HA	1:a2:109:GLY:HA3	1.91	0.53
12:m2:5:GLU:OE1	35:m2:104:LMT:O2'	2.26	0.53
13:o2:195:GLY:HA2	13:o2:219:GLN:HA	1.89	0.53
1:A1:85:THR:HA	1:A1:109:GLY:HA3	1.91	0.53
13:O1:164:MET:HE3	13:O1:225:MET:HG2	1.91	0.53
15:U2:92:PHE:O	15:U2:97:ARG:NH1	2.41	0.53
25:b1:609:CLA:H121	20:w1:11:LEU:HD11	1.91	0.53
4:d1:160:TYR:HA	4:d1:290:ALA:HB2	1.89	0.53
13:o1:181:VAL:O	13:o1:183:ARG:N	2.42	0.53
13:O2:43:LEU:HA	13:O2:241:ALA:HA	1.91	0.53
13:O2:195:GLY:HA3	13:O2:219:GLN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o2:51:LEU:HB3	13:o2:65:PHE:HB3	1.91	0.53
1:A1:162:PRO:HB3	1:A1:168:PHE:HA	1.91	0.53
11:L1:28:ALA:O	11:L1:32:SER:HB3	2.09	0.53
16:V1:39:SER:O	16:V1:40:CYS:C	2.51	0.53
1:a1:85:THR:HA	1:a1:109:GLY:HA3	1.91	0.53
34:c1:514:DGD:HA22	9:j1:29:ILE:HG21	1.90	0.53
10:k1:23:ASP:OD2	17:y1:21:GLN:NE2	2.41	0.53
12:m1:25:LEU:O	12:m1:28:GLN:HG3	2.08	0.53
1:A2:85:THR:HA	1:A2:109:GLY:HA3	1.91	0.53
25:B2:616:CLA:H42	37:B2:623:SQD:H141	1.90	0.53
2:B1:60:MET:HB3	2:B1:63:MET:HB2	1.90	0.53
13:O1:200:ALA:N	13:O1:214:VAL:O	2.42	0.53
1:a1:84:PRO:HA	1:a1:112:TYR:CG	2.44	0.53
1:a2:131:TRP:CH2	25:c2:506:CLA:HAA2	2.44	0.53
1:A1:161:TYR:HA	1:A1:294:ALA:HB1	1.90	0.52
1:a1:52:PHE:CD1	36:d1:409:PL9:H48	2.45	0.52
13:o1:195:GLY:HA2	13:o1:219:GLN:HA	1.89	0.52
1:A2:162:PRO:HB3	1:A2:168:PHE:HA	1.91	0.52
25:A2:402:CLA:HMC3	4:D2:182:LEU:HD22	1.90	0.52
2:b2:105:GLY:HA3	23:b2:602:BCR:H282	1.90	0.52
25:b2:610:CLA:H191	25:b2:624:CLA:H18	1.91	0.52
4:d2:43:LEU:HD22	23:d2:401:BCR:H323	1.91	0.52
3:c1:119:LEU:HG	23:c1:501:BCR:H10C	1.91	0.52
4:d1:335:PRO:HG2	5:e1:65:LEU:HD21	1.90	0.52
16:v1:39:SER:O	16:v1:40:CYS:C	2.51	0.52
1:A2:277:LEU:HA	33:A2:405:LHG:H291	1.91	0.52
11:L2:28:ALA:O	11:L2:32:SER:HB3	2.10	0.52
27:a1:411:PHO:HAB	4:d1:205:LEU:HD13	1.91	0.52
4:d1:185:LEU:HD22	25:d1:401:CLA:HMD1	1.91	0.52
13:o1:195:GLY:CA	13:o1:219:GLN:CA	2.87	0.52
1:A2:107:TYR:HB2	13:O2:71:MET:HE3	1.91	0.52
25:A2:403:CLA:H43	29:I2:101:LMG:H111	1.92	0.52
23:b2:603:BCR:H311	25:b2:609:CLA:H72	1.92	0.52
17:y2:39:LEU:HD21	22:z2:25:ILE:HA	1.91	0.52
25:B1:613:CLA:H112	25:B1:615:CLA:H52	1.91	0.52
23:J1:101:BCR:H271	10:K1:37:PHE:HB3	1.91	0.52
3:C2:192:GLY:HA2	21:Q2:146:VAL:C	2.35	0.52
11:l2:28:ALA:O	11:l2:32:SER:HB3	2.10	0.52
3:C1:228:ASN:HB3	34:C1:516:DGD:HE62	1.90	0.52
3:C1:464:GLU:OE2	4:D1:245:SER:OG	2.20	0.52
13:O1:195:GLY:HA2	13:O1:219:GLN:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d1:401:CLA:H193	27:d1:403:PHO:H152	1.91	0.52
3:c2:437:ILE:HA	25:c2:509:CLA:HMC2	1.92	0.52
1:A1:341:LEU:HD11	16:V1:47:LYS:HD3	1.91	0.52
23:A2:401:BCR:H14C	25:A2:403:CLA:HBC2	1.90	0.52
13:O2:195:GLY:HA3	13:O2:219:GLN:CB	2.40	0.52
13:o2:181:VAL:O	13:o2:183:ARG:N	2.42	0.52
2:b1:357:ARG:NH2	4:d1:337:GLU:O	2.42	0.52
13:o1:43:LEU:HB3	13:o1:81:ILE:HB	1.91	0.52
25:B2:612:CLA:H122	25:B2:617:CLA:HAA1	1.92	0.52
4:D2:54:PHE:O	5:E2:49:THR:OG1	2.23	0.52
25:D2:404:CLA:HBC3	18:X2:20:LEU:HD13	1.91	0.52
15:U1:36:ARG:NH1	16:V1:51:ASN:O	2.36	0.52
25:a1:403:CLA:H143	27:a1:411:PHO:H72	1.91	0.52
11:l1:28:ALA:O	11:l1:32:SER:HB3	2.09	0.52
14:t1:2:GLU:CD	14:t1:2:GLU:H	2.18	0.52
15:u1:96:ASP:HB3	15:u1:100:ASN:HA	1.91	0.52
1:A2:84:PRO:HA	1:A2:112:TYR:CG	2.44	0.52
4:D2:279:LEU:HD11	27:D2:407:PHO:HMC2	1.91	0.52
36:D2:408:PL9:H513	36:D2:408:PL9:H451	1.91	0.52
11:L2:23:LEU:HD13	33:L2:101:LHG:H151	1.92	0.52
14:t2:2:GLU:CD	14:t2:2:GLU:H	2.18	0.52
3:C1:28:ILE:HG13	10:K1:45:PHE:HE2	1.75	0.52
2:b2:60:MET:HB3	2:b2:63:MET:HB2	1.90	0.52
14:T1:2:GLU:H	14:T1:2:GLU:CD	2.18	0.51
1:a1:162:PRO:HB3	1:a1:168:PHE:HA	1.92	0.51
29:a1:412:LMG:H141	25:c1:507:CLA:H172	1.92	0.51
16:V2:41:HIS:HA	16:V2:44:GLY:H	1.75	0.51
13:o2:195:GLY:CA	13:o2:219:GLN:CA	2.88	0.51
25:B1:611:CLA:HED2	25:B1:611:CLA:HAA1	1.91	0.51
13:O1:51:LEU:O	13:O1:234:LEU:N	2.43	0.51
13:O2:221:SER:OG	13:O2:222:ASP:N	2.43	0.51
23:b2:601:BCR:H332	12:m2:9:LEU:HD23	1.91	0.51
13:o2:51:LEU:O	13:o2:234:LEU:N	2.41	0.51
15:u2:22:GLY:O	15:u2:37:LYS:NZ	2.31	0.51
13:o1:51:LEU:O	13:o1:234:LEU:N	2.42	0.51
17:Y2:39:LEU:HD21	22:Z2:25:ILE:HA	1.92	0.51
13:o2:201:VAL:C	13:o2:213:GLY:HA3	2.35	0.51
2:B1:356:VAL:HG22	2:B1:370:LEU:HG	1.92	0.51
18:x1:38:LEU:HD13	3:C2:29:GLU:HG2	1.91	0.51
1:a2:63:ILE:HB	3:c2:335:THR:HG21	1.91	0.51
15:u2:96:ASP:HB3	15:u2:100:ASN:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:413:ASP:OD2	2:B1:416:THR:OG1	2.26	0.51
16:v2:122:GLN:NE2	16:v2:126:GLN:OE1	2.43	0.51
4:D1:185:LEU:HD22	25:D1:402:CLA:HMD1	1.93	0.51
16:V1:34:ASN:HA	16:V1:38:SER:OG	2.11	0.51
1:a1:131:TRP:HZ2	3:c1:449:ARG:HG3	1.75	0.51
1:a1:145:VAL:O	1:a1:148:SER:OG	2.26	0.51
16:v1:34:ASN:HA	16:v1:38:SER:OG	2.10	0.51
25:B2:618:CLA:HHC	25:B2:618:CLA:HBB1	1.93	0.51
3:C1:416:SER:HB2	16:V1:42:VAL:HG23	1.93	0.51
13:O1:82:GLU:N	13:O1:99:ASP:O	2.43	0.51
15:U1:96:ASP:HB3	15:U1:100:ASN:HA	1.92	0.51
25:A1:405:CLA:HHC	25:A1:405:CLA:HBB1	1.91	0.51
3:c1:34:ALA:O	3:c1:38:GLY:N	2.44	0.51
25:C2:503:CLA:H52	25:C2:505:CLA:H91	1.91	0.51
4:d1:261:PHE:CZ	33:d1:407:LHG:HC81	2.46	0.51
1:a2:64:ARG:NH1	13:o2:105:ALA:O	2.40	0.51
13:o2:82:GLU:N	13:o2:99:ASP:O	2.40	0.51
33:B1:621:LHG:H262	4:D1:277:THR:HG23	1.92	0.51
23:c1:501:BCR:H382	25:c1:513:CLA:HMB1	1.93	0.51
29:c1:519:LMG:H382	10:k1:30:ILE:HD11	1.92	0.51
23:k2:501:BCR:HC42	23:z2:101:BCR:HC42	1.91	0.51
13:o2:199:LEU:HA	13:o2:215:PHE:CA	2.37	0.51
25:C1:502:CLA:C2D	25:C1:504:CLA:H2	2.42	0.50
33:d1:407:LHG:HC91	11:l1:19:TRP:HZ2	1.76	0.50
3:C1:279:LEU:HD22	25:C1:510:CLA:HED3	1.92	0.50
15:U1:92:PHE:O	15:U1:97:ARG:NH1	2.40	0.50
15:u1:38:PHE:HB3	15:u1:78:TYR:CD1	2.46	0.50
1:A2:63:ILE:HB	3:C2:335:THR:HG21	1.91	0.50
1:a2:162:PRO:HB3	1:a2:168:PHE:HA	1.92	0.50
25:b2:624:CLA:H142	7:h2:39:LEU:HD21	1.93	0.50
4:d2:89:LEU:HD21	34:h2:102:DGD:HA42	1.93	0.50
9:j2:29:ILE:HD12	29:j2:101:LMG:H181	1.92	0.50
16:v2:34:ASN:HA	16:v2:38:SER:OG	2.11	0.50
3:C1:435:PHE:HD1	34:C1:516:DGD:HBH2	1.75	0.50
4:D1:232:PHE:CE2	33:D1:404:LHG:HC42	2.46	0.50
11:l1:23:LEU:HD13	33:l1:102:LHG:H162	1.92	0.50
3:C2:192:GLY:HA2	21:Q2:146:VAL:O	2.11	0.50
4:D2:161:PRO:HB3	4:D2:170:ALA:HB2	1.94	0.50
1:A1:308:ASP:OD1	1:A1:312:ARG:N	2.41	0.50
25:B1:617:CLA:H171	7:H1:7:LEU:HD21	1.92	0.50
4:D1:161:PRO:HB3	4:D1:170:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h1:7:LEU:HB2	20:w1:21:VAL:HG11	1.92	0.50
21:q1:123:ILE:O	21:q1:126:ALA:HB3	2.11	0.50
25:b2:618:CLA:H122	20:w2:18:LEU:HD21	1.93	0.50
3:c2:62:PHE:HD2	23:k2:501:BCR:H362	1.77	0.50
13:O1:199:LEU:HA	13:O1:215:PHE:CA	2.38	0.50
15:U1:38:PHE:HB3	15:U1:78:TYR:CD1	2.47	0.50
13:o1:53:GLU:HA	13:o1:65:PHE:HA	1.93	0.50
29:I2:101:LMG:HC71	19:S2:6:LEU:HB3	1.93	0.50
3:c2:175:LEU:HD23	3:c2:237:HIS:CD2	2.47	0.50
13:o2:53:GLU:HA	13:o2:65:PHE:HA	1.93	0.50
1:A1:43:THR:HG22	23:A1:401:BCR:H16C	1.94	0.50
2:B1:6:TYR:CD1	2:B1:7:ARG:HG3	2.46	0.50
2:b1:356:VAL:HG22	2:b1:370:LEU:HG	1.93	0.50
33:d1:407:LHG:H291	14:t1:17:ILE:HG23	1.94	0.50
4:D2:261:PHE:CZ	33:D2:405:LHG:HC81	2.46	0.50
13:O2:195:GLY:HA3	13:O2:219:GLN:CA	2.42	0.50
16:V2:34:ASN:HA	16:V2:38:SER:OG	2.11	0.50
2:b2:356:VAL:HG22	2:b2:370:LEU:HG	1.93	0.50
15:u2:38:PHE:HB3	15:u2:78:TYR:CD1	2.46	0.50
1:A1:2:THR:HA	3:C1:152:ARG:HH11	1.77	0.50
7:H1:38:PHE:HB2	23:H1:102:BCR:H10C	1.93	0.50
25:d1:404:CLA:HMA2	36:d1:409:PL9:H421	1.94	0.50
1:a2:308:ASP:OD1	1:a2:312:ARG:N	2.40	0.50
2:B1:103:LEU:HD21	25:B1:608:CLA:HMC2	1.93	0.50
23:B1:601:BCR:H361	25:B1:616:CLA:HBB1	1.94	0.50
2:b1:18:ARG:HH12	11:l1:7:LYS:HE2	1.77	0.50
3:C2:220:GLY:H	28:C2:517:UNL:C1	2.24	0.50
13:O1:201:VAL:C	13:O1:213:GLY:HA3	2.37	0.50
1:a1:217:SER:HA	4:d1:272:LEU:HD12	1.94	0.50
13:o1:82:GLU:CG	13:o1:99:ASP:HB3	2.42	0.50
25:b2:610:CLA:H202	25:b2:613:CLA:H101	1.94	0.50
3:c2:119:LEU:O	3:c2:122:SER:HB3	2.12	0.50
16:v2:126:GLN:HB3	16:v2:129:LYS:HB2	1.92	0.50
4:d1:161:PRO:HB3	4:d1:170:ALA:HB2	1.93	0.49
13:o1:210:GLU:HG2	13:o1:242:ARG:HG2	1.93	0.49
4:D2:73:PHE:CD1	29:F2:402:LMG:H291	2.47	0.49
14:T2:2:GLU:CD	14:T2:2:GLU:H	2.18	0.49
2:B1:91:TRP:HE1	29:B1:622:LMG:HC91	1.76	0.49
11:L2:26:VAL:HG11	33:L2:101:LHG:H201	1.94	0.49
25:b2:618:CLA:H172	25:b2:619:CLA:NC	2.26	0.49
25:c2:502:CLA:C2D	25:c2:504:CLA:H2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c2:512:CLA:HMB1	23:k2:501:BCR:H382	1.94	0.49
4:d2:161:PRO:HB3	4:d2:170:ALA:HB2	1.93	0.49
1:A1:2:THR:HA	3:C1:152:ARG:HD2	1.94	0.49
15:u1:92:PHE:O	15:u1:97:ARG:NH1	2.41	0.49
1:A2:308:ASP:OD1	1:A2:312:ARG:N	2.41	0.49
4:D2:286:ILE:HG13	25:D2:401:CLA:HED2	1.93	0.49
2:b2:6:TYR:CD1	2:b2:7:ARG:HG3	2.47	0.49
25:C1:509:CLA:H8	25:C1:511:CLA:H51	1.93	0.49
2:B2:6:TYR:CD1	2:B2:7:ARG:HG3	2.46	0.49
33:D2:403:LHG:H332	33:D2:403:LHG:H101	1.94	0.49
13:o2:43:LEU:HB3	13:o2:81:ILE:HB	1.94	0.49
3:C1:180:LEU:HD21	3:C1:234:ILE:HG21	1.95	0.49
10:k1:25:MET:HE1	23:k1:101:BCR:H332	1.95	0.49
15:U2:41:LEU:HA	15:U2:45:ALA:HB3	1.95	0.49
21:Q2:123:ILE:O	21:Q2:126:ALA:HB3	2.13	0.49
23:b2:601:BCR:HC31	29:b2:622:LMG:H302	1.94	0.49
3:c2:180:LEU:HD21	3:c2:234:ILE:HG21	1.94	0.49
25:c2:505:CLA:H43	34:c2:517:DGD:HB32	1.95	0.49
13:O1:221:SER:CB	13:O1:233:LEU:HD11	2.39	0.49
3:c1:178:LYS:HB2	25:c1:504:CLA:H203	1.94	0.49
3:c1:180:LEU:HD21	3:c1:234:ILE:HG21	1.94	0.49
2:B2:413:ASP:OD2	2:B2:416:THR:OG1	2.26	0.49
13:o2:221:SER:OG	13:o2:222:ASP:N	2.43	0.49
2:b1:103:LEU:HB2	25:b1:609:CLA:H62	1.95	0.49
4:D2:141:TYR:OH	33:D2:403:LHG:O4	2.27	0.49
25:b2:616:CLA:HBB1	25:b2:620:CLA:HBB2	1.94	0.49
3:C1:147:PHE:CD2	25:C1:514:CLA:H3A	2.47	0.49
16:v1:41:HIS:HA	16:v1:44:GLY:H	1.78	0.49
25:C2:509:CLA:HMA1	25:C2:509:CLA:H2	1.95	0.49
2:B1:244:ALA:HA	25:B1:606:CLA:H121	1.95	0.49
33:B1:621:LHG:HC12	4:D1:269:PHE:CD2	2.48	0.49
25:C1:504:CLA:H112	25:C1:504:CLA:H72	1.58	0.49
23:A2:401:BCR:H16C	25:A2:403:CLA:HBC2	1.95	0.49
13:o2:146:PHE:HE2	13:o2:197:ILE:H	1.52	0.49
1:A1:45:THR:HG23	25:A1:406:CLA:H201	1.95	0.48
1:a1:308:ASP:OD1	1:a1:312:ARG:N	2.40	0.48
2:b1:243:ALA:HA	2:b1:246:PHE:CE2	2.48	0.48
25:b1:612:CLA:H142	25:b1:614:CLA:H2	1.95	0.48
1:A2:183:MET:HB3	25:A2:402:CLA:HBC2	1.94	0.48
2:b2:116:VAL:HG21	23:b2:603:BCR:H292	1.94	0.48
4:d2:291:LEU:HD21	34:h2:102:DGD:HBF2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:j2:102:BCR:H12C	17:y2:28:ILE:CG2	2.43	0.48
1:A1:63:ILE:HB	3:C1:335:THR:HG21	1.95	0.48
1:A1:121:LEU:HG	34:C1:516:DGD:HAT2	1.93	0.48
15:U1:41:LEU:HA	15:U1:45:ALA:HB3	1.95	0.48
27:A2:407:PHO:HAB	4:D2:205:LEU:HD13	1.94	0.48
23:b2:603:BCR:H321	25:b2:609:CLA:H52	1.95	0.48
13:o2:201:VAL:CG1	13:o2:202:ASN:H	2.23	0.48
1:A1:198:HIS:HA	1:A1:286:THR:HG23	1.96	0.48
25:C1:509:CLA:H2	25:C1:511:CLA:H12	1.95	0.48
2:b1:6:TYR:CD1	2:b1:7:ARG:HG3	2.48	0.48
25:c1:507:CLA:H192	34:c1:518:DGD:HA72	1.95	0.48
13:o1:81:ILE:HA	13:o1:100:GLY:HA3	1.94	0.48
3:C2:119:LEU:HG	23:K2:104:BCR:H10C	1.95	0.48
1:a2:145:VAL:O	1:a2:148:SER:OG	2.27	0.48
2:B1:243:ALA:HA	2:B1:246:PHE:CE2	2.48	0.48
3:c1:393:ALA:HB1	38:v1:201:HEM:HBC1	1.96	0.48
3:C2:175:LEU:HD23	3:C2:237:HIS:CD2	2.48	0.48
23:B1:601:BCR:H12C	23:B1:602:BCR:HC7	1.95	0.48
4:D1:257:PHE:O	33:D1:405:LHG:H322	2.13	0.48
3:c1:175:LEU:HD23	3:c1:237:HIS:CD2	2.48	0.48
25:c2:509:CLA:H2	25:c2:511:CLA:H12	1.95	0.48
25:A1:405:CLA:H2	8:I1:12:VAL:HG11	1.95	0.48
2:B1:432:PHE:HD2	13:O1:178(B):ASP:HB3	1.78	0.48
25:C2:509:CLA:H91	25:C2:509:CLA:H111	1.65	0.48
13:o2:195:GLY:HA3	13:o2:219:GLN:HA	1.92	0.48
29:A1:412:LMG:HC1	8:I1:1:MET:HE2	1.96	0.48
3:C1:237:HIS:HA	3:C1:240:ILE:HG22	1.95	0.48
2:b1:7:ARG:O	2:b1:8:VAL:C	2.55	0.48
3:c1:119:LEU:O	3:c1:122:SER:HB3	2.14	0.48
25:c1:512:CLA:H152	25:c1:512:CLA:H112	1.67	0.48
1:A2:267:ASN:ND2	4:D2:232:PHE:O	2.46	0.48
2:b2:357:ARG:NH2	4:d2:337:GLU:O	2.47	0.48
1:A1:250:ALA:HB1	4:D1:138:LEU:HD21	1.96	0.48
1:a1:198:HIS:HA	1:a1:286:THR:HG23	1.96	0.48
15:u1:27:VAL:HG11	15:u1:61:ILE:HD11	1.96	0.48
1:A2:217:SER:HA	4:D2:272:LEU:HD12	1.96	0.48
3:C2:34:ALA:O	3:C2:38:GLY:N	2.47	0.48
10:K2:14:THR:O	10:K2:16:ASN:N	2.47	0.48
2:b2:450:TRP:NE1	25:b2:620:CLA:HBA1	2.29	0.48
1:A1:145:VAL:O	1:A1:148:SER:OG	2.27	0.48
25:C1:509:CLA:H12	25:C1:513:CLA:HBC2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:82:VAL:HB	1:A2:174:LEU:HB2	1.96	0.48
25:A2:402:CLA:H112	25:A2:402:CLA:H72	1.66	0.48
2:B2:243:ALA:HA	2:B2:246:PHE:CE2	2.48	0.48
16:v2:41:HIS:HA	16:v2:44:GLY:H	1.79	0.48
4:D1:210:LEU:HD21	36:D1:408:PL9:H13	1.96	0.48
2:b1:460:LEU:O	2:b1:463:PHE:HB3	2.14	0.48
27:a2:416:PHO:HAB	4:d2:205:LEU:HD13	1.95	0.48
23:B1:603:BCR:H321	25:B1:609:CLA:H52	1.96	0.47
13:O1:221:SER:OG	13:O1:222:ASP:N	2.42	0.47
15:u1:41:LEU:HA	15:u1:45:ALA:HB3	1.95	0.47
1:A2:184:LEU:HD21	4:D2:186:GLN:HG2	1.94	0.47
13:O2:44:CYS:O	13:O2:240:TYR:CA	2.61	0.47
3:c2:168:LEU:HD21	25:c2:510:CLA:H62	1.94	0.47
2:b1:149:LEU:HD23	25:b1:606:CLA:HBC1	1.96	0.47
25:c1:503:CLA:H162	25:c1:508:CLA:HBB1	1.96	0.47
36:d1:409:PL9:H222	36:d1:409:PL9:H201	1.72	0.47
37:B2:623:SQD:H1	35:m2:103:LMT:O3'	2.14	0.47
4:D2:210:LEU:HD21	36:D2:408:PL9:H13	1.96	0.47
25:b2:606:CLA:H192	25:b2:610:CLA:H152	1.95	0.47
1:A1:217:SER:HA	4:D1:272:LEU:HD12	1.96	0.47
13:O1:195:GLY:CA	13:O1:219:GLN:CA	2.87	0.47
16:V1:41:HIS:HA	16:V1:44:GLY:H	1.78	0.47
23:b1:601:BCR:H362	25:b1:616:CLA:H71	1.95	0.47
3:c1:237:HIS:HA	3:c1:240:ILE:HG22	1.95	0.47
13:o1:215:PHE:CE1	13:o1:237:GLY:HA3	2.49	0.47
1:A2:198:HIS:HA	1:A2:286:THR:HG23	1.96	0.47
1:A2:257:ARG:NH1	2:B2:490:VAL:O	2.34	0.47
3:c2:34:ALA:O	3:c2:38:GLY:N	2.48	0.47
4:d2:269:PHE:CG	33:d2:403:LHG:HC12	2.49	0.47
1:A1:300:LEU:HD23	3:C1:404:LEU:HB3	1.95	0.47
2:B1:419:LYS:HG2	2:B1:423:LYS:HE2	1.96	0.47
15:U1:27:VAL:HG11	15:U1:61:ILE:HD11	1.97	0.47
3:c1:165:LEU:HD21	25:c1:508:CLA:HAB	1.95	0.47
13:o1:201:VAL:CG1	13:o1:202:ASN:H	2.24	0.47
19:s1:39:PHE:CE1	19:s1:44:LEU:HB2	2.49	0.47
33:D2:405:LHG:O1	33:L2:101:LHG:O4	2.23	0.47
13:O2:44:CYS:H	13:O2:240:TYR:C	2.17	0.47
13:O2:197:ILE:CG1	13:O2:198:GLU:H	2.27	0.47
25:C1:505:CLA:C4D	34:C1:515:DGD:HB21	2.45	0.47
23:J1:101:BCR:H21C	23:J1:101:BCR:H361	1.96	0.47
25:b1:604:CLA:H171	25:b1:604:CLA:H13	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b2:243:ALA:HA	2:b2:246:PHE:CE2	2.48	0.47
33:d2:406:LHG:O1	33:l2:101:LHG:O4	2.24	0.47
10:K1:11:LEU:HD11	10:K1:22:ILE:HD12	1.97	0.47
10:K1:14:THR:O	10:K1:16:ASN:N	2.48	0.47
13:O1:146:PHE:HE2	13:O1:197:ILE:H	1.52	0.47
13:O1:198:GLU:N	13:O1:216:VAL:O	2.46	0.47
1:a1:179:THR:O	1:a1:183:MET:HG3	2.15	0.47
29:a1:412:LMG:H402	34:c1:518:DGD:HB92	1.97	0.47
2:b1:485[A]:GLU:HG3	4:D2:239:GLN:HA	1.95	0.47
1:a2:198:HIS:HA	1:a2:286:THR:HG23	1.97	0.47
23:d2:401:BCR:H372	29:d2:407:LMG:H301	1.96	0.47
25:C1:502:CLA:H151	25:C1:508:CLA:HMB3	1.96	0.47
34:H1:101:DGD:HBE2	34:H1:101:DGD:HBF1	1.74	0.47
13:O1:118:PHE:CD1	13:O1:233:LEU:HD22	2.50	0.47
13:o1:234:LEU:C	13:o1:235:LEU:HD23	2.40	0.47
25:B2:606:CLA:H152	7:H2:38:PHE:HE2	1.80	0.47
33:D2:405:LHG:H292	14:T2:17:ILE:HG23	1.96	0.47
13:O2:19:CYS:SG	13:O2:45:LEU:O	2.72	0.47
1:a2:179:THR:O	1:a2:183:MET:HG3	2.14	0.47
1:a2:273:PHE:CZ	33:a2:407:LHG:H111	2.49	0.47
25:a2:404:CLA:H192	25:a2:404:CLA:H161	1.67	0.47
25:b2:615:CLA:H143	25:b2:615:CLA:H111	1.70	0.47
12:m2:30:GLU:OE1	35:m2:103:LMT:O6B	2.33	0.47
13:o2:215:PHE:CE1	13:o2:237:GLY:HA3	2.49	0.47
1:a1:330:VAL:HG21	4:d1:328:TRP:CE2	2.50	0.47
3:c1:287:ALA:HB1	3:c1:427:THR:HG23	1.97	0.47
15:u1:92:PHE:HA	15:u1:97:ARG:HD3	1.97	0.47
13:O2:197:ILE:HG13	13:O2:217:SER:CB	2.43	0.47
2:b2:460:LEU:O	2:b2:463:PHE:HB3	2.15	0.47
13:O1:196:ARG:N	13:O1:218:GLU:O	2.48	0.47
2:B2:254:GLY:HA2	34:H2:101:DGD:HBW1	1.97	0.47
3:C2:371:SER:HB3	3:C2:376:ASP:HB2	1.96	0.47
10:k2:14:THR:O	10:k2:16:ASN:N	2.47	0.47
15:u2:38:PHE:HB2	15:u2:41:LEU:HD12	1.97	0.47
15:u2:92:PHE:O	15:u2:97:ARG:NH1	2.41	0.47
23:B1:602:BCR:H11C	23:B1:602:BCR:H341	1.79	0.47
2:B2:460:LEU:O	2:B2:463:PHE:HB3	2.15	0.47
25:B2:617:CLA:H101	25:B2:617:CLA:H13	1.66	0.47
2:b2:413:ASP:OD2	2:b2:416:THR:OG1	2.26	0.47
3:c2:287:ALA:HB1	3:c2:427:THR:HG23	1.98	0.47
25:C1:511:CLA:H203	10:K1:33:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J1:101:BCR:H24C	23:J1:101:BCR:H371	1.70	0.46
2:b1:434:ARG:NH2	13:o1:178(F):GLY:O	2.48	0.46
25:b1:606:CLA:H62	25:b1:606:CLA:H41	1.78	0.46
8:i1:30:ARG:HD3	32:i1:101:GOL:H32	1.97	0.46
4:D2:43:LEU:HD22	23:F2:401:BCR:H323	1.97	0.46
1:a2:82:VAL:HB	1:a2:174:LEU:HB2	1.97	0.46
2:b2:441:GLY:C	13:o2:176:ALA:HB3	2.39	0.46
13:o2:198:GLU:N	13:o2:216:VAL:O	2.44	0.46
1:A1:283:ILE:HG13	27:A1:408:PHO:HBC3	1.96	0.46
36:d1:409:PL9:H352	11:l1:26:VAL:CG1	2.46	0.46
13:o1:199:LEU:HA	13:o1:215:PHE:CA	2.37	0.46
10:k2:11:LEU:HD11	10:k2:22:ILE:HD12	1.97	0.46
15:u2:41:LEU:HA	15:u2:45:ALA:HB3	1.95	0.46
15:u2:70:ARG:O	15:u2:74:VAL:HG23	2.14	0.46
22:z2:24:PRO:O	22:z2:28:SER:OG	2.29	0.46
25:C1:508:CLA:H41	25:C1:508:CLA:H62	1.64	0.46
6:F1:41:GLN:HG3	9:J1:31:GLY:HA3	1.98	0.46
13:O1:83:GLY:HA3	13:O1:95:PHE:CE1	2.49	0.46
2:b1:117:TYR:HA	11:l1:1:SER:HB2	1.97	0.46
23:b1:603:BCR:H11C	23:b1:603:BCR:H341	1.79	0.46
1:A2:179:THR:O	1:A2:183:MET:HG3	2.16	0.46
33:A2:405:LHG:HC42	4:D2:232:PHE:CE2	2.50	0.46
25:C2:505:CLA:H8	25:C2:505:CLA:H51	1.62	0.46
4:d2:123:ILE:HD11	34:h2:102:DGD:HAW2	1.97	0.46
3:C1:40:ALA:N	25:C1:509:CLA:HAA2	2.31	0.46
33:D1:405:LHG:O1	33:L1:101:LHG:O4	2.20	0.46
10:k1:11:LEU:HD11	10:k1:22:ILE:HD12	1.96	0.46
1:A1:82:VAL:HB	1:A1:174:LEU:HB2	1.97	0.46
3:C1:437:ILE:HA	25:C1:509:CLA:HMC2	1.97	0.46
2:b1:369:ILE:HD11	4:d1:345:VAL:HG21	1.97	0.46
1:A2:131:TRP:HZ2	3:C2:449:ARG:HG3	1.80	0.46
23:a2:402:BCR:H15C	23:a2:402:BCR:H351	1.84	0.46
7:h2:38:PHE:HB2	23:h2:101:BCR:H21C	1.97	0.46
2:B1:441:GLY:C	13:O1:176:ALA:HB3	2.41	0.46
25:B1:604:CLA:HAB	23:H1:102:BCR:H15C	1.98	0.46
25:B1:610:CLA:HBB2	4:D1:123:ILE:HG12	1.98	0.46
25:C1:503:CLA:H72	25:C1:504:CLA:NB	2.30	0.46
11:l2:24:ILE:HD11	33:l2:101:LHG:H292	1.98	0.46
15:u2:27:VAL:HG11	15:u2:61:ILE:HD11	1.96	0.46
15:u2:92:PHE:HA	15:u2:97:ARG:HD3	1.98	0.46
3:C1:34:ALA:O	3:C1:38:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:273:PHE:CZ	4:D1:277:THR:HG21	2.50	0.46
23:F2:401:BCR:H11C	23:F2:401:BCR:H341	1.81	0.46
25:b1:608:CLA:H62	25:b1:608:CLA:H41	1.55	0.46
25:b1:609:CLA:NC	29:b1:624:LMG:H291	2.31	0.46
25:c1:508:CLA:HMC2	25:c1:509:CLA:H101	1.98	0.46
6:f1:28:ILE:HB	6:f1:29:PRO:HD3	1.98	0.46
23:h1:102:BCR:H15C	23:h1:102:BCR:H351	1.85	0.46
15:u1:38:PHE:HB2	15:u1:41:LEU:HD12	1.98	0.46
25:B2:613:CLA:H142	25:B2:613:CLA:H111	1.69	0.46
15:U2:92:PHE:HA	15:U2:97:ARG:HD3	1.98	0.46
2:b2:369:ILE:HD11	4:d2:345:VAL:HG21	1.96	0.46
2:b2:419:LYS:HG2	2:b2:423:LYS:HE2	1.98	0.46
29:A1:410:LMG:H352	34:C1:516:DGD:HB41	1.98	0.46
2:B1:460:LEU:O	2:B1:463:PHE:HB3	2.15	0.46
3:c1:418:ASN:HD21	34:c1:514:DGD:HD4	1.80	0.46
10:k1:22:ILE:HA	10:k1:25:MET:HG2	1.97	0.46
25:D2:404:CLA:H112	25:D2:404:CLA:H91	1.65	0.46
1:A1:330:VAL:HG21	4:D1:328:TRP:CE2	2.51	0.46
25:C1:504:CLA:H51	25:C1:504:CLA:H8	1.83	0.46
16:V1:41:HIS:C	16:V1:44:GLY:H	2.24	0.46
1:a1:82:VAL:HB	1:a1:174:LEU:HB2	1.97	0.46
3:c1:279:LEU:HD22	25:c1:511:CLA:HED2	1.97	0.46
20:w1:17:VAL:O	20:w1:21:VAL:HG23	2.16	0.46
10:k2:22:ILE:HA	10:k2:25:MET:HG2	1.98	0.46
13:o2:82:GLU:O	13:o2:98:LYS:O	2.34	0.46
2:B1:237:VAL:HG22	25:B1:612:CLA:HBC2	1.98	0.45
10:K1:22:ILE:HA	10:K1:25:MET:HG2	1.98	0.45
25:c1:507:CLA:H101	25:c1:507:CLA:H61	1.69	0.45
10:k1:14:THR:O	10:k1:16:ASN:N	2.48	0.45
23:B2:601:BCR:H15C	23:B2:601:BCR:H351	1.75	0.45
3:C2:41:ARG:NH1	25:K2:101:CLA:OBD	2.47	0.45
3:C2:287:ALA:HB1	3:C2:427:THR:HG23	1.98	0.45
3:c2:416:SER:HB2	16:v2:42:VAL:HG23	1.99	0.45
20:w2:17:VAL:O	20:w2:21:VAL:HG23	2.16	0.45
1:A1:179:THR:O	1:A1:183:MET:HG3	2.16	0.45
23:K1:101:BCR:H11C	23:K1:101:BCR:H341	1.85	0.45
15:U1:76:LYS:O	15:U1:77:LYS:C	2.60	0.45
23:b1:602:BCR:H15C	23:b1:602:BCR:H351	1.78	0.45
34:h1:101:DGD:HBE2	34:h1:101:DGD:HBF1	1.68	0.45
25:B2:614:CLA:H171	25:B2:615:CLA:HBB2	1.97	0.45
23:K2:102:BCR:H24C	23:K2:102:BCR:H371	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a2:416:PHO:H43	33:d2:406:LHG:H341	1.98	0.45
2:b2:242:ILE:HG12	25:b2:612:CLA:HBB1	1.97	0.45
2:b2:338:GLU:HB2	2:b2:431:GLU:CB	2.46	0.45
1:a1:329:GLU:O	1:a1:332:HIS:ND1	2.49	0.45
1:A2:256:GLY:HA3	2:B2:492:PHE:HZ	1.81	0.45
4:D2:348:ARG:HH12	16:V2:135:ILE:HD11	1.81	0.45
25:B1:606:CLA:H72	25:B1:606:CLA:H112	1.54	0.45
23:J1:101:BCR:HC31	10:K1:21:ILE:HD11	1.98	0.45
25:c1:506:CLA:H11	34:c1:514:DGD:HB32	1.99	0.45
2:B2:338:GLU:HB2	2:B2:431:GLU:CB	2.46	0.45
4:D2:121:GLY:HA3	27:D2:407:PHO:H41	1.97	0.45
13:O2:200:ALA:O	13:O2:201:VAL:O	2.33	0.45
25:c2:505:CLA:H61	34:c2:516:DGD:HB72	1.98	0.45
23:B1:601:BCR:HC8	23:B1:602:BCR:HC42	1.98	0.45
12:M1:13:LEU:HD23	12:M1:13:LEU:HA	1.78	0.45
20:W1:17:VAL:O	20:W1:21:VAL:HG23	2.17	0.45
1:a1:304:GLN:HG2	1:a1:313:VAL:HG11	1.99	0.45
25:b1:616:CLA:H62	25:b1:616:CLA:H41	1.80	0.45
33:d2:403:LHG:H141	11:l2:23:LEU:HD21	1.98	0.45
25:a1:404:CLA:H2	8:i1:12:VAL:HG11	1.98	0.45
23:b1:603:BCR:H15C	23:b1:603:BCR:H351	1.79	0.45
14:t1:25:ASP:HA	14:t1:26:PRO:HD3	1.85	0.45
25:B2:604:CLA:HAB	23:H2:103:BCR:H15C	1.99	0.45
16:v2:41:HIS:C	16:v2:44:GLY:H	2.25	0.45
3:C1:208:ILE:O	3:C1:211:SER:HB3	2.17	0.45
4:D1:144:ILE:O	4:D1:147:SER:N	2.48	0.45
1:a1:105:TRP:NE1	1:a1:110:GLY:HA3	2.32	0.45
13:o1:82:GLU:O	13:o1:98:LYS:C	2.60	0.45
13:o1:200:ALA:O	13:o1:214:VAL:N	2.49	0.45
25:b2:612:CLA:H121	25:b2:612:CLA:H161	1.49	0.45
3:c2:271:TYR:O	40:c2:601:HOH:O	2.21	0.45
13:O1:234:LEU:C	13:O1:235:LEU:HD23	2.41	0.45
25:a1:405:CLA:HAB	25:d1:401:CLA:H72	1.98	0.45
4:d1:18:LEU:HA	18:x1:32:VAL:HG21	1.98	0.45
20:W2:17:VAL:O	20:W2:21:VAL:HG23	2.17	0.45
25:a2:404:CLA:H112	25:a2:404:CLA:H72	1.77	0.45
35:a2:406:LMT:H31	35:a2:406:LMT:H62	1.73	0.45
37:b2:605:SQD:H292	37:b2:605:SQD:H122	1.99	0.45
25:b2:606:CLA:C2D	25:b2:608:CLA:H2	2.46	0.45
3:c2:135:VAL:HG22	22:z2:27:LEU:O	2.17	0.45
25:c2:504:CLA:H72	25:c2:504:CLA:H112	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d2:348:ARG:HH12	16:v2:135:ILE:HD11	1.81	0.45
11:l2:23:LEU:HD13	33:l2:101:LHG:H142	1.97	0.45
2:B1:462:PHE:HA	25:B1:613:CLA:HMC2	1.98	0.45
2:b1:273:TYR:HA	2:b1:276:ASP:HB2	1.99	0.45
2:B2:440:ASP:OD2	2:B2:444:ARG:NH2	2.37	0.45
25:C2:503:CLA:H61	25:C2:503:CLA:H41	1.77	0.45
1:a2:217:SER:HA	4:d2:272:LEU:HD12	1.98	0.45
2:b2:110:ALA:HB2	23:b2:603:BCR:H17C	1.99	0.45
23:b2:603:BCR:H24C	23:b2:603:BCR:H371	1.82	0.45
3:c2:38:GLY:HA3	25:c2:512:CLA:HMD2	1.99	0.45
6:f2:41:GLN:HG3	9:j2:31:GLY:HA3	1.98	0.45
13:o2:196:ARG:N	13:o2:218:GLU:O	2.50	0.45
1:A1:131:TRP:HZ2	3:C1:449:ARG:HG3	1.82	0.45
25:B1:616:CLA:H202	25:B1:616:CLA:H162	1.79	0.45
3:C1:393:ALA:HB1	38:V1:201:HEM:HBC1	1.98	0.45
16:V1:72:LEU:O	16:V1:76:MET:HG3	2.17	0.45
33:a1:407:LHG:H372	33:a1:407:LHG:H112	1.99	0.45
3:c1:100:ALA:HB3	3:c1:104:GLU:HB3	1.99	0.45
25:d1:404:CLA:H203	25:d1:404:CLA:H162	1.77	0.45
13:o1:109:GLN:NE2	13:o1:115:ARG:HE	2.15	0.45
4:D2:273:PHE:CD1	33:D2:403:LHG:H242	2.52	0.45
13:O2:197:ILE:HG12	13:O2:198:GLU:H	1.82	0.45
13:o2:201:VAL:O	13:o2:202:ASN:CG	2.60	0.45
25:B1:612:CLA:H203	25:B1:612:CLA:H161	1.87	0.44
3:C1:435:PHE:CD1	34:C1:516:DGD:HBH2	2.51	0.44
4:D1:261:PHE:CZ	33:D1:405:LHG:HC81	2.52	0.44
33:D1:405:LHG:HC92	36:D1:408:PL9:H111	1.99	0.44
36:D1:408:PL9:H352	11:L1:26:VAL:CG1	2.46	0.44
23:c1:502:BCR:H24C	23:c1:502:BCR:H371	1.72	0.44
25:B2:613:CLA:H61	25:B2:613:CLA:H2	1.79	0.44
16:v2:39:SER:HB2	16:v2:40:CYS:H	1.36	0.44
22:z2:23:VAL:HB	22:z2:24:PRO:HD3	1.99	0.44
1:A1:64:ARG:NH1	13:O1:105:ALA:O	2.48	0.44
25:A1:405:CLA:H42	8:I1:9:TYR:CE2	2.52	0.44
15:U1:38:PHE:HB2	15:U1:41:LEU:HD12	1.98	0.44
25:a1:403:CLA:H193	25:a1:403:CLA:H161	1.82	0.44
25:a1:404:CLA:HMB2	29:a1:412:LMG:H151	1.99	0.44
2:b1:26:HIS:CE1	25:b1:614:CLA:HMA2	2.53	0.44
23:h1:102:BCR:H24C	23:h1:102:BCR:H371	1.76	0.44
1:A2:283:ILE:HG13	27:A2:407:PHO:HBC3	1.98	0.44
1:A2:329:GLU:O	1:A2:332:HIS:ND1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A2:403:CLA:H11	8:I2:9:TYR:CE1	2.52	0.44
23:B2:602:BCR:H20C	23:B2:602:BCR:H361	1.85	0.44
12:M2:18:PRO:O	12:M2:21:PHE:HB3	2.17	0.44
25:b2:615:CLA:H112	25:b2:615:CLA:H72	1.77	0.44
13:o2:200:ALA:O	13:o2:214:VAL:N	2.49	0.44
23:B1:603:BCR:H11C	23:B1:603:BCR:H341	1.81	0.44
4:D1:199:MET:HG2	36:D1:408:PL9:H311	1.99	0.44
6:F1:28:ILE:HB	6:F1:29:PRO:HD3	1.99	0.44
1:a1:197:PHE:CE2	34:c1:514:DGD:HBN2	2.53	0.44
25:a1:404:CLA:H42	8:i1:9:TYR:CE2	2.52	0.44
33:a1:407:LHG:H141	33:a1:407:LHG:H322	1.99	0.44
2:b1:440:ASP:OD2	2:b1:444:ARG:NH2	2.36	0.44
2:B2:103:LEU:HD21	25:B2:608:CLA:HMC3	2.00	0.44
3:C2:55:ALA:HB1	23:K2:104:BCR:H373	1.98	0.44
3:C2:208:ILE:O	3:C2:211:SER:HB3	2.17	0.44
7:H2:7:LEU:HB2	20:W2:21:VAL:HG11	2.00	0.44
25:a2:404:CLA:HMC3	4:d2:182:LEU:HD22	1.99	0.44
23:b2:601:BCR:H15C	23:b2:601:BCR:H351	1.75	0.44
25:c2:502:CLA:H202	25:c2:508:CLA:HBB1	2.00	0.44
23:k2:501:BCR:H11C	23:k2:501:BCR:H341	1.81	0.44
15:u2:14:TYR:O	15:u2:17:ILE:HG13	2.18	0.44
2:B1:80:ILE:H	2:B1:80:ILE:HG13	1.59	0.44
2:B1:357:ARG:NH2	4:D1:337:GLU:O	2.51	0.44
15:U1:14:TYR:O	15:U1:17:ILE:HG13	2.17	0.44
1:a1:239:LEU:HD22	14:t1:27:PRO:HB2	1.99	0.44
23:d1:405:BCR:H15C	23:d1:405:BCR:H351	1.87	0.44
25:a2:405:CLA:H141	25:a2:405:CLA:H161	1.68	0.44
2:B1:273:TYR:HA	2:B1:276:ASP:HB2	2.00	0.44
13:O1:200:ALA:O	13:O1:214:VAL:N	2.51	0.44
15:U1:92:PHE:HA	15:U1:97:ARG:HD3	1.98	0.44
29:b1:621:LMG:H372	29:b1:621:LMG:H341	1.81	0.44
36:d1:409:PL9:H472	36:d1:409:PL9:H451	1.68	0.44
13:o1:201:VAL:O	13:o1:202:ASN:CG	2.61	0.44
25:c2:506:CLA:H62	25:c2:506:CLA:H102	1.67	0.44
12:m2:18:PRO:O	12:m2:21:PHE:HB3	2.18	0.44
17:y2:28:ILE:O	17:y2:31:THR:HB	2.17	0.44
22:z2:23:VAL:HG22	22:z2:40:ILE:HG23	2.00	0.44
1:A1:188:ALA:HB2	1:A1:328:ILE:HB	2.00	0.44
1:A1:307:VAL:HB	6:F1:45:ARG:HD2	1.99	0.44
3:c1:39:ASN:HB2	25:c1:510:CLA:O1A	2.17	0.44
16:v1:41:HIS:C	16:v1:44:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:259:ILE:HG22	1:A2:260:PHE:CD2	2.52	0.44
2:B2:273:TYR:HA	2:B2:276:ASP:HB2	2.00	0.44
13:O2:45:LEU:HD12	13:O2:45:LEU:N	2.31	0.44
1:a2:340:PRO:HD3	15:u2:103:TYR:CZ	2.53	0.44
2:b2:248:ALA:HB2	25:b2:606:CLA:H61	2.00	0.44
2:b2:413:ASP:OD1	2:b2:413:ASP:N	2.51	0.44
25:b2:610:CLA:H92	25:b2:610:CLA:H62	1.75	0.44
25:C1:512:CLA:H161	25:C1:512:CLA:H121	1.62	0.44
1:a1:96:ILE:HG12	1:a1:105:TRP:CE2	2.53	0.44
2:b1:221:PRO:HA	25:b1:611:CLA:HED3	2.00	0.44
3:c1:139:VAL:HG13	3:c1:141:GLU:OE2	2.18	0.44
25:B2:606:CLA:H62	25:B2:606:CLA:H41	1.71	0.44
13:O2:197:ILE:CG1	13:O2:217:SER:HB2	2.45	0.44
16:V2:52:ILE:HB	38:V2:201:HEM:HAD2	2.00	0.44
2:b2:440:ASP:OD2	2:b2:444:ARG:NH2	2.39	0.44
25:b2:610:CLA:C2B	23:h2:101:BCR:H402	2.48	0.44
23:c2:501:BCR:H361	23:c2:501:BCR:C21	2.27	0.44
23:c2:501:BCR:H341	23:c2:501:BCR:H11C	1.73	0.44
10:k2:20:PRO:O	10:k2:23:ASP:HB2	2.17	0.44
1:A1:105:TRP:NE1	1:A1:110:GLY:HA3	2.33	0.44
10:K1:20:PRO:O	10:K1:23:ASP:HB2	2.17	0.44
23:K1:101:BCR:H321	23:K1:101:BCR:HC8	2.00	0.44
13:O1:48:LYS:O	13:O1:49:GLN:CB	2.65	0.44
1:a1:131:TRP:CZ2	3:c1:449:ARG:HG3	2.53	0.44
10:k1:20:PRO:O	10:k1:23:ASP:HB2	2.18	0.44
23:B2:601:BCR:H12C	23:B2:602:BCR:HC7	2.00	0.44
25:B2:608:CLA:H61	25:B2:608:CLA:H41	1.77	0.44
25:d2:402:CLA:H91	36:d2:409:PL9:H402	2.00	0.44
1:A1:96:ILE:HG12	1:A1:105:TRP:CE2	2.53	0.44
2:B1:247:PHE:HE1	25:B1:605:CLA:H8	1.83	0.44
25:B1:611:CLA:H42	7:H1:35:MET:HE1	2.00	0.44
1:a1:259:ILE:HG22	1:a1:260:PHE:CD2	2.52	0.44
3:c1:62:PHE:HD2	23:c1:501:BCR:H362	1.83	0.44
3:c1:257:PHE:CD2	25:c1:508:CLA:HED3	2.51	0.44
16:v1:39:SER:HB2	16:v1:40:CYS:H	1.34	0.44
23:K2:102:BCR:H11C	23:K2:102:BCR:H341	1.82	0.44
1:a2:105:TRP:NE1	1:a2:110:GLY:HA3	2.32	0.44
1:a2:300:LEU:HD23	3:c2:404:LEU:HB3	1.99	0.44
1:a2:329:GLU:O	1:a2:332:HIS:ND1	2.49	0.44
25:b2:608:CLA:H61	25:b2:608:CLA:H41	1.72	0.44
25:c2:506:CLA:H42	25:c2:506:CLA:NC	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d2:409:PL9:C35	11:l2:30:LEU:HD22	2.48	0.44
14:t2:25:ASP:HA	14:t2:26:PRO:HD3	1.85	0.44
1:A1:259:ILE:HG22	1:A1:260:PHE:CD2	2.52	0.43
25:B1:619:CLA:H93	25:B1:619:CLA:H111	1.85	0.43
3:C1:287:ALA:HB1	3:C1:427:THR:HG23	1.99	0.43
1:a1:165:GLN:NE2	40:a1:501:HOH:O	2.51	0.43
15:u1:14:TYR:O	15:u1:17:ILE:HG13	2.18	0.43
1:A2:188:ALA:HB2	1:A2:328:ILE:HB	1.99	0.43
2:B2:202:HIS:O	2:B2:203:ILE:C	2.61	0.43
2:B2:305:ILE:HA	2:B2:306:PRO:HD3	1.85	0.43
25:C2:513:CLA:HMB2	25:C2:516:CLA:HAA1	1.99	0.43
13:O2:109:GLN:NE2	13:O2:115:ARG:HE	2.16	0.43
16:V2:39:SER:O	16:V2:41:HIS:N	2.51	0.43
4:d2:53:THR:HG22	6:f2:40:MET:HE1	2.00	0.43
9:j2:8:ILE:HA	9:j2:9:PRO:HD3	1.87	0.43
1:A1:329:GLU:O	1:A1:332:HIS:ND1	2.49	0.43
25:B1:617:CLA:H92	25:B1:617:CLA:H61	1.87	0.43
3:C1:134:ILE:HD13	25:C1:513:CLA:H43	1.99	0.43
13:O1:109:GLN:NE2	13:O1:115:ARG:HE	2.16	0.43
25:b1:613:CLA:H61	25:b1:613:CLA:H2	1.80	0.43
13:o1:196:ARG:N	13:o1:218:GLU:O	2.51	0.43
13:o1:221:SER:OG	13:o1:222:ASP:N	2.48	0.43
23:H2:103:BCR:H15C	23:H2:103:BCR:H351	1.85	0.43
13:O2:48:LYS:C	13:O2:236:LYS:O	2.61	0.43
3:c2:39:ASN:HB2	25:c2:509:CLA:O1A	2.18	0.43
7:h2:22:ALA:HA	7:h2:23:PRO:HD3	1.91	0.43
23:k2:501:BCR:H24C	23:k2:501:BCR:H371	1.76	0.43
3:C1:71:GLU:OE1	3:C1:89:LEU:HG	2.19	0.43
23:C2:502:BCR:H351	23:C2:502:BCR:H15C	1.73	0.43
4:D2:144:ILE:O	4:D2:147:SER:N	2.49	0.43
16:V2:41:HIS:C	16:V2:44:GLY:H	2.25	0.43
22:Z2:5:LEU:HD11	22:Z2:58:ASN:HA	2.00	0.43
1:a2:96:ILE:HG12	1:a2:105:TRP:CE2	2.54	0.43
25:a2:404:CLA:HBB1	25:d2:405:CLA:NC	2.33	0.43
2:b2:464:PHE:HB2	4:d2:280:TRP:CH2	2.53	0.43
25:c2:511:CLA:H112	25:c2:511:CLA:H152	1.82	0.43
23:h2:101:BCR:H15C	23:h2:101:BCR:H351	1.73	0.43
13:o2:214:VAL:O	13:o2:239:PHE:HE1	2.00	0.43
22:z2:5:LEU:HD11	22:z2:58:ASN:HA	2.00	0.43
25:B1:610:CLA:H42	25:B1:611:CLA:H72	2.00	0.43
3:C1:38:GLY:HA3	25:C1:513:CLA:HMD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:100:ALA:HB3	3:C1:104:GLU:HB3	1.99	0.43
16:V1:135:ILE:H	16:V1:135:ILE:HG12	1.70	0.43
23:b1:602:BCR:H361	23:b1:602:BCR:H20C	1.83	0.43
4:d1:42:TYR:OH	6:f1:25:GLY:O	2.28	0.43
23:d1:405:BCR:H11C	23:d1:405:BCR:H341	1.80	0.43
23:A2:401:BCR:H16C	25:A2:403:CLA:CBC	2.47	0.43
2:B2:26:HIS:CE1	25:B2:614:CLA:HMA2	2.53	0.43
10:K2:14:THR:HB	10:K2:15:TYR:H	1.68	0.43
10:K2:37:PHE:HB3	23:K2:102:BCR:H271	2.00	0.43
27:a2:416:PHO:H61	27:a2:416:PHO:H2	1.85	0.43
3:c2:162:GLY:HA3	3:c2:252:ILE:HG13	2.01	0.43
16:v2:72:LEU:O	16:v2:76:MET:HG3	2.18	0.43
25:A1:406:CLA:H52	36:D1:408:PL9:H171	2.00	0.43
3:C1:236:GLY:C	23:C1:501:BCR:H383	2.43	0.43
13:O1:201:VAL:O	13:O1:202:ASN:CG	2.61	0.43
25:B2:614:CLA:H102	25:B2:614:CLA:H13	1.82	0.43
3:C2:393:ALA:HB1	38:V2:201:HEM:HBC1	2.00	0.43
16:V2:72:LEU:O	16:V2:76:MET:HG3	2.19	0.43
23:b2:603:BCR:H15C	23:b2:603:BCR:H351	1.78	0.43
3:c2:208:ILE:O	3:c2:211:SER:HB3	2.18	0.43
13:o2:181:VAL:C	13:o2:183:ARG:H	2.26	0.43
13:O1:181:VAL:C	13:O1:183:ARG:H	2.26	0.43
23:a1:401:BCR:H11C	23:a1:401:BCR:H341	1.79	0.43
2:b1:326:ARG:HH21	4:d1:297:ASP:CG	2.25	0.43
25:c1:504:CLA:H61	25:c1:515:CLA:H42	2.01	0.43
4:d1:297:ASP:OD1	4:d1:297:ASP:N	2.52	0.43
25:d1:406:CLA:H61	25:d1:406:CLA:H41	1.73	0.43
7:h1:22:ALA:HA	7:h1:23:PRO:HD3	1.92	0.43
23:k1:101:BCR:H11C	23:k1:101:BCR:H341	1.83	0.43
13:o1:181:VAL:C	13:o1:183:ARG:H	2.26	0.43
3:C2:338:GLY:HA2	13:O2:103:TYR:OH	2.19	0.43
2:b2:224:ARG:HD3	7:h2:25:TRP:CE2	2.54	0.43
13:o2:198:GLU:O	13:o2:216:VAL:N	2.44	0.43
2:B1:248:ALA:HA	25:B1:606:CLA:H42	2.00	0.43
25:C1:511:CLA:HED3	10:K1:33:LEU:HD13	2.01	0.43
12:M1:18:PRO:O	12:M1:21:PHE:HB3	2.19	0.43
2:b1:67:ALA:O	2:b1:178:ILE:HD11	2.19	0.43
3:c1:162:GLY:HA3	3:c1:252:ILE:HG13	2.01	0.43
2:B2:357:ARG:NH2	4:D2:337:GLU:O	2.52	0.43
3:C2:50:LEU:HD11	25:C2:510:CLA:HBB1	2.01	0.43
4:D2:39:PRO:HB2	25:D2:404:CLA:HAB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b2:603:BCR:H20C	23:b2:603:BCR:H361	1.89	0.43
23:b2:603:BCR:H12C	25:b2:619:CLA:H143	2.00	0.43
25:b2:620:CLA:H193	11:l2:28:ALA:HA	2.01	0.43
3:c2:466:VAL:HG21	4:d2:248:THR:HA	2.01	0.43
13:o2:109:GLN:NE2	13:o2:115:ARG:HE	2.16	0.43
2:B1:67:ALA:O	2:B1:178:ILE:HD11	2.18	0.43
3:C1:180:LEU:HD22	3:C1:199:ILE:O	2.19	0.43
1:a1:267:ASN:ND2	4:d1:232:PHE:O	2.44	0.43
2:b1:254:GLY:HA2	34:h1:101:DGD:HBW1	2.00	0.43
25:b1:609:CLA:HMD2	29:b1:624:LMG:O9	2.19	0.43
15:u1:76:LYS:O	15:u1:77:LYS:C	2.60	0.43
1:A2:259:ILE:HD11	27:D2:407:PHO:HED2	2.01	0.43
23:A2:401:BCR:H341	23:A2:401:BCR:H11C	1.75	0.43
2:B2:341:LEU:HD11	13:O2:178(C):GLY:HA3	2.00	0.43
12:M2:18:PRO:HA	12:M2:21:PHE:HB3	2.01	0.43
1:a2:188:ALA:HB2	1:a2:328:ILE:HB	1.99	0.43
4:d2:262:ALA:N	33:d2:406:LHG:O5	2.43	0.43
2:B1:326:ARG:HH21	4:D1:297:ASP:CG	2.26	0.43
1:a1:300:LEU:HD23	3:c1:404:LEU:HB3	2.00	0.43
25:a1:403:CLA:H72	25:a1:403:CLA:H112	1.71	0.43
25:b1:606:CLA:H161	25:b1:606:CLA:H141	1.60	0.43
25:b1:613:CLA:H143	25:b1:613:CLA:H111	1.69	0.43
4:d1:348:ARG:HH12	16:v1:135:ILE:HD11	1.84	0.43
13:o1:198:GLU:O	13:o1:216:VAL:N	2.46	0.43
25:K2:101:CLA:HMB1	23:K2:104:BCR:H382	2.01	0.43
23:b2:602:BCR:H11C	23:b2:602:BCR:H341	1.87	0.43
25:b2:610:CLA:H162	25:b2:610:CLA:H141	1.80	0.43
23:c2:501:BCR:H24C	23:c2:501:BCR:H371	1.34	0.43
23:d2:401:BCR:H11C	23:d2:401:BCR:H341	1.83	0.43
8:i2:28:PRO:O	8:i2:31:ASN:ND2	2.52	0.43
23:z2:101:BCR:H11C	23:z2:101:BCR:H341	1.83	0.43
25:A1:404:CLA:C4A	25:A1:404:CLA:HBA2	2.49	0.43
2:B1:173:GLY:HA3	2:B1:265:ILE:HD11	2.01	0.43
25:B1:608:CLA:H192	25:B1:608:CLA:H162	1.83	0.43
25:c1:506:CLA:HMB1	25:c1:506:CLA:HBB1	2.00	0.43
23:B2:601:BCR:H11C	23:B2:601:BCR:H341	1.85	0.43
25:C2:505:CLA:H72	25:C2:505:CLA:H112	1.42	0.43
13:O2:46:GLU:C	13:O2:47:PRO:O	2.62	0.43
13:O2:197:ILE:HG12	13:O2:198:GLU:N	2.34	0.43
15:U2:89:PRO:HA	15:U2:92:PHE:HB3	2.01	0.43
2:b2:273:TYR:HA	2:b2:276:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:133:LEU:HD23	4:d1:256:ILE:HG12	2.01	0.42
2:b1:305:ILE:HA	2:b1:306:PRO:HD3	1.86	0.42
23:k1:101:BCR:H371	23:k1:101:BCR:H24C	1.74	0.42
13:o1:81:ILE:HD13	13:o1:122:ILE:HG21	2.00	0.42
2:B2:67:ALA:O	2:B2:178:ILE:HD11	2.19	0.42
23:B2:601:BCR:H24C	23:B2:601:BCR:H371	1.83	0.42
25:B2:608:CLA:H192	25:B2:608:CLA:H162	1.79	0.42
23:C2:502:BCR:H24C	23:C2:502:BCR:H371	1.86	0.42
1:a2:304:GLN:HG2	1:a2:313:VAL:HG11	2.01	0.42
2:b2:202:HIS:O	2:b2:203:ILE:C	2.61	0.42
13:o2:82:GLU:O	13:o2:98:LYS:C	2.62	0.42
4:D1:79:SER:HA	4:D1:172:SER:HB3	2.00	0.42
12:M1:18:PRO:HA	12:M1:21:PHE:HB3	2.01	0.42
15:U1:55:TYR:HB3	15:U1:60:ASP:HB2	2.01	0.42
3:c1:208:ILE:O	3:c1:211:SER:HB3	2.19	0.42
34:c1:514:DGD:HBF1	34:c1:514:DGD:HBE2	1.56	0.42
25:d1:401:CLA:HBA2	25:d1:401:CLA:H3A	1.78	0.42
29:A2:412:LMG:HC5	2:b2:75:TRP:HB3	2.00	0.42
3:C2:162:GLY:HA3	3:C2:252:ILE:HG13	2.01	0.42
33:D2:403:LHG:H383	33:D2:403:LHG:HC81	2.00	0.42
33:D2:405:LHG:H151	25:D2:406:CLA:H61	2.01	0.42
5:E2:22:ILE:O	5:E2:25:ILE:HG22	2.19	0.42
2:b2:247:PHE:HB2	25:b2:624:CLA:HBC1	2.00	0.42
25:b2:611:CLA:H203	25:b2:611:CLA:H161	1.80	0.42
25:c2:502:CLA:C1B	25:c2:502:CLA:H2	2.48	0.42
29:d2:407:LMG:O3	9:j2:32:SER:HA	2.19	0.42
23:j2:102:BCR:C10	17:y2:28:ILE:HG23	2.41	0.42
18:x2:12:TRP:HD1	18:x2:16:TRP:HE1	1.66	0.42
23:A1:401:BCR:H11C	23:A1:401:BCR:H341	1.85	0.42
2:B1:464:PHE:CE2	33:B1:621:LHG:H252	2.54	0.42
25:B1:616:CLA:HMD1	12:M1:21:PHE:HE1	1.83	0.42
3:C1:139:VAL:HG13	3:C1:141:GLU:OE2	2.18	0.42
1:a1:63:ILE:HB	3:c1:335:THR:HG21	2.01	0.42
25:c1:512:CLA:H91	25:c1:512:CLA:H111	1.71	0.42
1:A2:52:PHE:CD1	36:D2:408:PL9:H48	2.54	0.42
23:B2:603:BCR:H15C	23:B2:603:BCR:H351	1.76	0.42
13:O2:181:VAL:C	13:O2:183:ARG:H	2.26	0.42
14:T2:25:ASP:HA	14:T2:26:PRO:HD3	1.85	0.42
1:a2:196:PRO:HB2	34:c2:517:DGD:HBT1	2.00	0.42
1:a2:330:VAL:HG21	4:d2:328:TRP:CE2	2.54	0.42
3:c2:209:ILE:O	3:c2:212:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e2:101:HEM:ND	6:f2:24:HIS:NE2	2.66	0.42
2:B1:202:HIS:O	2:B1:203:ILE:C	2.61	0.42
13:O1:53:GLU:HA	13:O1:65:PHE:HA	2.01	0.42
23:a1:401:BCR:H20C	23:a1:401:BCR:H361	1.89	0.42
23:c1:501:BCR:H20C	23:c1:501:BCR:H361	1.86	0.42
16:v1:72:LEU:O	16:v1:76:MET:HG3	2.19	0.42
6:F2:38:THR:O	6:F2:41:GLN:HB2	2.20	0.42
15:U2:90:GLU:H	15:U2:90:GLU:HG3	1.48	0.42
4:d2:79:SER:HA	4:d2:172:SER:HB3	2.00	0.42
2:B1:247:PHE:CD2	25:B1:606:CLA:H122	2.54	0.42
23:C1:501:BCR:H15C	23:C1:501:BCR:H351	1.76	0.42
13:O1:201:VAL:CG1	13:O1:202:ASN:H	2.24	0.42
1:a1:188:ALA:HB2	1:a1:328:ILE:HB	2.00	0.42
2:b1:204:ALA:CB	25:b1:605:CLA:HAB	2.49	0.42
3:c1:71:GLU:OE1	3:c1:89:LEU:HG	2.19	0.42
12:m1:18:PRO:O	12:m1:21:PHE:HB3	2.19	0.42
23:B2:602:BCR:H15C	23:B2:602:BCR:H351	1.82	0.42
4:D2:274:VAL:HG13	36:D2:408:PL9:H252	2.00	0.42
15:U2:76:LYS:O	15:U2:77:LYS:C	2.63	0.42
1:a2:250:ALA:HB1	4:d2:138:LEU:HD21	2.01	0.42
2:b2:464:PHE:CD1	2:b2:464:PHE:C	2.98	0.42
25:b2:606:CLA:H62	25:b2:606:CLA:H41	1.91	0.42
33:d2:403:LHG:H332	33:d2:403:LHG:H362	1.86	0.42
12:m2:18:PRO:HA	12:m2:21:PHE:HB3	2.00	0.42
15:u2:89:PRO:HA	15:u2:92:PHE:HB3	2.02	0.42
1:A1:260:PHE:CE1	1:A1:263:ALA:HB2	2.55	0.42
9:j1:14:VAL:HG12	23:k1:101:BCR:H383	2.02	0.42
25:B2:613:CLA:H72	25:B2:613:CLA:H112	1.82	0.42
23:H2:103:BCR:H11C	23:H2:103:BCR:H341	1.94	0.42
1:a2:147:PHE:O	1:a2:150:PRO:HD2	2.20	0.42
23:b2:601:BCR:H11C	23:b2:601:BCR:H341	1.79	0.42
3:c2:28:ILE:HG13	10:k2:45:PHE:HE2	1.85	0.42
4:d2:144:ILE:O	4:d2:147:SER:N	2.50	0.42
25:C1:514:CLA:HMC1	23:K1:101:BCR:H373	2.02	0.42
1:a1:136:ARG:NH1	8:i1:27:ASP:OD1	2.48	0.42
25:d1:401:CLA:H142	27:d1:403:PHO:HBA2	2.02	0.42
1:A2:234:ASN:HD21	33:D2:403:LHG:HC11	1.85	0.42
25:B2:616:CLA:HMD3	12:M2:21:PHE:HE1	1.84	0.42
25:C2:507:CLA:CMD	25:C2:509:CLA:HAB	2.49	0.42
13:O2:48:LYS:O	13:O2:49:GLN:HB2	2.20	0.42
2:b2:339:ALA:H	2:b2:431:GLU:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b2:608:CLA:HBB1	25:b2:609:CLA:H51	2.02	0.42
3:c2:78:GLU:HB3	16:v2:102:PRO:O	2.20	0.42
13:o2:50:PHE:CD1	13:o2:235:LEU:HD22	2.54	0.42
13:o2:122:ILE:HD12	13:o2:122:ILE:HA	1.91	0.42
15:u2:104:LYS:HE2	15:u2:104:LYS:HA	2.01	0.42
33:B1:621:LHG:H332	33:B1:621:LHG:H101	2.02	0.42
10:K1:22:ILE:HA	10:K1:25:MET:CG	2.50	0.42
13:O1:50:PHE:CD1	13:O1:235:LEU:HD22	2.55	0.42
1:a1:212:SER:OG	4:d1:271:LEU:HB2	2.20	0.42
2:b1:200:SER:O	2:b1:201:HIS:C	2.62	0.42
23:c1:501:BCR:H24C	23:c1:501:BCR:H371	1.77	0.42
7:h1:29:PRO:O	7:h1:33:ILE:HG13	2.20	0.42
1:A2:39:PRO:HB2	25:A2:403:CLA:HBB1	2.01	0.42
25:A2:403:CLA:H62	8:I2:12:VAL:HG12	2.02	0.42
2:B2:91:TRP:HE1	29:B2:620:LMG:HC91	1.84	0.42
3:c2:250:TRP:O	3:c2:254:THR:OG1	2.30	0.42
3:c2:338:GLY:HA2	13:o2:103:TYR:OH	2.19	0.42
4:D1:273:PHE:O	4:D1:277:THR:OG1	2.30	0.42
15:U1:89:PRO:HA	15:U1:92:PHE:HB3	2.02	0.42
1:a1:260:PHE:CE1	1:a1:263:ALA:HB2	2.55	0.42
1:a1:307:VAL:HB	6:f1:45:ARG:HD2	2.02	0.42
25:b1:612:CLA:H8	25:b1:612:CLA:H51	1.82	0.42
25:c1:506:CLA:H43	34:c1:520:DGD:HB32	2.01	0.42
4:d1:79:SER:HA	4:d1:172:SER:HB3	2.02	0.42
15:u1:32:VAL:HG23	15:u1:97:ARG:O	2.20	0.42
25:B2:609:CLA:H91	25:B2:609:CLA:H112	1.75	0.42
3:C2:205:ASN:HA	3:C2:206:PRO:HD3	1.94	0.42
13:O2:47:PRO:HA	13:O2:237:GLY:HA3	2.01	0.42
25:b2:606:CLA:H93	25:b2:606:CLA:H112	1.84	0.42
15:u2:55:TYR:HB3	15:u2:60:ASP:HB2	2.02	0.42
1:A1:304:GLN:HG2	1:A1:313:VAL:HG11	2.02	0.42
1:a1:183:MET:HB3	25:a1:403:CLA:HBC2	2.01	0.42
23:a1:401:BCR:H24C	23:a1:401:BCR:H371	1.87	0.42
3:c1:190:ALA:HA	3:c1:191:PRO:HD3	1.91	0.42
25:c1:509:CLA:H91	25:c1:509:CLA:H111	1.69	0.42
25:B2:612:CLA:H51	25:B2:612:CLA:H8	1.83	0.42
23:C2:502:BCR:H11C	23:C2:502:BCR:H341	1.84	0.42
38:E2:101:HEM:ND	6:F2:24:HIS:NE2	2.67	0.42
13:O2:122:ILE:HD12	13:O2:122:ILE:HA	1.93	0.42
2:b2:117:TYR:HA	11:l2:1:SER:HB2	2.02	0.42
25:b2:612:CLA:H2	25:b2:612:CLA:H61	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c2:180:LEU:HD22	3:c2:199:ILE:O	2.20	0.42
23:j2:102:BCR:H361	23:j2:102:BCR:H21C	2.01	0.42
15:u2:48:LYS:HD3	15:u2:67:LEU:HD23	2.01	0.42
2:B1:7:ARG:O	2:B1:8:VAL:C	2.62	0.41
25:B1:605:CLA:H141	25:B1:605:CLA:H161	1.79	0.41
25:B1:610:CLA:H91	25:B1:610:CLA:H111	1.73	0.41
2:b1:464:PHE:C	2:b1:464:PHE:CD1	2.98	0.41
25:c1:506:CLA:C4D	34:c1:514:DGD:HB21	2.50	0.41
4:d1:230:ASP:OD2	33:d1:402:LHG:O1	2.28	0.41
10:k1:22:ILE:HA	10:k1:25:MET:CG	2.50	0.41
21:q1:119:ALA:O	21:q1:123:ILE:HG13	2.20	0.41
2:B2:42:LEU:HD13	2:B2:94:GLU:HG3	2.02	0.41
2:B2:200:SER:O	2:B2:201:HIS:C	2.63	0.41
25:D2:406:CLA:HMA1	36:D2:408:PL9:H421	2.02	0.41
2:b2:69:LEU:HD21	25:b2:606:CLA:HMD1	2.01	0.41
25:c2:515:CLA:C4B	23:z2:101:BCR:H383	2.50	0.41
4:d2:279:LEU:HD22	27:d2:408:PHO:HBC3	2.01	0.41
13:o2:234:LEU:C	13:o2:235:LEU:HD23	2.45	0.41
15:u2:90:GLU:H	15:u2:90:GLU:HG3	1.48	0.41
1:A1:147:PHE:O	1:A1:150:PRO:HD2	2.20	0.41
2:B1:383:PHE:CZ	13:O1:167:GLY:HA2	2.55	0.41
25:B1:610:CLA:CBB	4:D1:123:ILE:HG12	2.50	0.41
23:C1:521:BCR:H15C	23:C1:521:BCR:H351	1.77	0.41
4:D1:279:LEU:HD11	27:D1:407:PHO:HMC2	2.02	0.41
23:J1:101:BCR:H19C	10:K1:35:LEU:HA	2.02	0.41
12:M1:10:ALA:O	12:M1:11:VAL:C	2.63	0.41
15:U1:32:VAL:HG23	15:U1:97:ARG:O	2.20	0.41
1:a1:147:PHE:O	1:a1:150:PRO:HD2	2.20	0.41
33:a1:407:LHG:H111	33:d1:402:LHG:HC81	2.01	0.41
29:b1:624:LMG:H112	20:w1:6:VAL:CG1	2.48	0.41
3:c1:464:GLU:HA	3:c1:465:PRO:HD3	1.88	0.41
10:k1:14:THR:HB	10:k1:15:TYR:H	1.69	0.41
2:B2:173:GLY:HA3	2:B2:265:ILE:HD11	2.02	0.41
2:B2:339:ALA:H	2:B2:431:GLU:CB	2.33	0.41
4:d2:198:MET:SD	25:d2:402:CLA:HED2	2.60	0.41
12:m2:10:ALA:O	12:m2:11:VAL:C	2.63	0.41
1:A1:46:THR:HG21	29:b1:621:LMG:H321	2.01	0.41
3:C1:279:LEU:HD13	25:C1:510:CLA:HED1	2.02	0.41
16:V1:42:VAL:O	16:V1:42:VAL:CG1	2.69	0.41
25:b1:620:CLA:H41	25:b1:620:CLA:H62	1.68	0.41
12:m1:10:ALA:O	12:m1:11:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:m1:101:LMT:H5'	35:m1:101:LMT:H1B	1.66	0.41
1:A2:33:PHE:O	1:A2:125:ALA:HB1	2.21	0.41
1:A2:147:PHE:O	1:A2:150:PRO:HD2	2.20	0.41
1:A2:260:PHE:CE1	1:A2:263:ALA:HB2	2.55	0.41
2:B2:33:TRP:HE1	25:B2:619:CLA:C3C	2.33	0.41
23:B2:602:BCR:H341	23:B2:602:BCR:H11C	1.77	0.41
1:a2:267:ASN:ND2	4:d2:232:PHE:O	2.51	0.41
2:b2:200:SER:O	2:b2:201:HIS:C	2.64	0.41
3:c2:71:GLU:OE1	3:c2:89:LEU:HG	2.19	0.41
3:C1:76:ILE:HA	3:C1:77:PRO:HD3	1.89	0.41
23:D1:401:BCR:H11C	23:D1:401:BCR:H341	1.77	0.41
29:a1:412:LMG:H352	34:c1:518:DGD:HB51	2.01	0.41
2:b1:91:TRP:HD1	29:b1:624:LMG:HC1	1.80	0.41
2:b1:172:TYR:CE1	2:b1:283:GLU:HB2	2.55	0.41
3:c1:57:ALA:O	3:c1:61:VAL:HG23	2.21	0.41
25:c1:506:CLA:H143	25:c1:506:CLA:H112	1.80	0.41
8:i1:28:PRO:O	8:i1:31:ASN:ND2	2.51	0.41
12:m1:18:PRO:HA	12:m1:21:PHE:HB3	2.01	0.41
13:o1:40:VAL:HB	13:o1:95:PHE:CE1	2.55	0.41
23:B2:603:BCR:H341	23:B2:603:BCR:H11C	1.79	0.41
2:b2:103:LEU:HB2	25:b2:609:CLA:H62	2.01	0.41
3:c2:464:GLU:HA	3:c2:465:PRO:HD3	1.88	0.41
25:c2:502:CLA:H41	25:c2:502:CLA:H61	1.90	0.41
7:h2:49:TYR:CD2	34:h2:102:DGD:HB22	2.55	0.41
13:o2:170:MET:HE3	13:o2:172:VAL:HG23	2.02	0.41
23:z2:101:BCR:H24C	23:z2:101:BCR:H371	1.86	0.41
25:A1:406:CLA:C4A	25:A1:406:CLA:HBA2	2.51	0.41
29:A1:412:LMG:H352	29:A1:412:LMG:H381	1.91	0.41
2:B1:172:TYR:CE1	2:B1:283:GLU:HB2	2.56	0.41
2:B1:413:ASP:OD1	2:B1:413:ASP:N	2.51	0.41
23:B1:601:BCR:H24C	23:B1:601:BCR:H371	1.82	0.41
25:B1:604:CLA:CAB	23:H1:102:BCR:H15C	2.50	0.41
3:C1:162:GLY:HA3	3:C1:252:ILE:HG13	2.01	0.41
23:C1:521:BCR:H24C	23:C1:521:BCR:H371	1.78	0.41
8:I1:28:PRO:O	8:I1:31:ASN:ND2	2.54	0.41
1:a1:161:TYR:HA	1:a1:294:ALA:CB	2.51	0.41
1:a1:161:TYR:HB3	1:a1:162:PRO:HD3	2.02	0.41
2:b1:243:ALA:HA	2:b1:246:PHE:CD2	2.55	0.41
25:b1:609:CLA:H161	25:b1:609:CLA:H192	1.77	0.41
3:c1:209:ILE:O	3:c1:212:TYR:HB2	2.21	0.41
3:c1:326:ALA:HB2	15:u1:98:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j1:38:SER:O	9:j1:39:SER:OG	2.35	0.41
15:u1:89:PRO:HA	15:u1:92:PHE:HB3	2.01	0.41
2:B2:462:PHE:HA	25:B2:613:CLA:HMC2	2.02	0.41
25:C2:513:CLA:H3A	25:C2:513:CLA:HBA1	1.82	0.41
6:F2:38:THR:O	6:F2:41:GLN:N	2.53	0.41
3:c2:48:LYS:HD2	25:c2:512:CLA:HED3	2.02	0.41
25:c2:503:CLA:HBA2	25:c2:504:CLA:H42	2.02	0.41
25:c2:505:CLA:H111	25:c2:505:CLA:H93	1.81	0.41
4:d2:39:PRO:O	4:d2:43:LEU:HG	2.21	0.41
6:f2:38:THR:O	6:f2:41:GLN:HB2	2.21	0.41
13:o2:48:LYS:O	13:o2:49:GLN:CB	2.66	0.41
2:B1:243:ALA:HA	2:B1:246:PHE:CD2	2.56	0.41
25:C1:507:CLA:H61	25:C1:507:CLA:H92	1.75	0.41
6:F1:38:THR:O	6:F1:41:GLN:HB2	2.21	0.41
13:O1:122:ILE:HD12	13:O1:122:ILE:HA	1.91	0.41
2:b1:233:ASN:O	2:b1:236:THR:HG22	2.20	0.41
25:b1:604:CLA:H2	25:b1:604:CLA:H61	1.76	0.41
25:c1:507:CLA:H91	25:c1:507:CLA:H111	1.66	0.41
13:o1:198:GLU:N	13:o1:216:VAL:O	2.44	0.41
25:A2:403:CLA:H11	8:I2:9:TYR:CZ	2.55	0.41
3:C2:209:ILE:O	3:C2:212:TYR:HB2	2.20	0.41
7:H2:56:GLU:HG3	7:H2:57:ASN:H	1.86	0.41
12:M2:10:ALA:O	12:M2:11:VAL:C	2.63	0.41
2:b2:172:TYR:CE1	2:b2:283:GLU:HB2	2.56	0.41
3:c2:377:LEU:HD12	13:o2:80:ASN:HB2	2.03	0.41
25:c2:503:CLA:HBA2	25:c2:503:CLA:HBD	2.03	0.41
23:j2:102:BCR:H333	23:k2:501:BCR:C13	2.51	0.41
2:B1:68:ARG:HB3	2:B1:69:LEU:HD12	2.03	0.41
33:D1:405:LHG:HC91	11:L1:19:TRP:HZ2	1.86	0.41
10:K1:14:THR:C	10:K1:16:ASN:H	2.29	0.41
13:O1:170:MET:HE3	13:O1:172:VAL:HG23	2.02	0.41
23:a1:401:BCR:H15C	23:a1:401:BCR:H351	1.86	0.41
2:b1:202:HIS:O	2:b1:203:ILE:C	2.63	0.41
4:d1:329:MET:HE3	4:d1:329:MET:HB2	1.90	0.41
21:q1:125:ASP:O	21:q1:128:GLU:N	2.54	0.41
2:B2:7:ARG:O	2:B2:8:VAL:C	2.63	0.41
2:B2:125:ASP:HA	2:B2:126:PRO:HD3	1.88	0.41
23:B2:602:BCR:HC41	29:B2:621:LMG:H181	2.02	0.41
25:B2:611:CLA:H141	25:B2:611:CLA:H162	1.65	0.41
25:D2:406:CLA:H13	36:D2:408:PL9:H452	2.03	0.41
1:a2:273:PHE:CD1	33:a2:407:LHG:H161	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b2:432:PHE:HD2	13:o2:178(B):ASP:HB3	1.86	0.41
3:c2:213:LEU:HD11	23:c2:501:BCR:C12	2.50	0.41
4:d2:199:MET:CB	4:d2:281:VAL:HG11	2.48	0.41
23:j2:102:BCR:H351	23:j2:102:BCR:H15C	1.80	0.41
1:A1:140:ARG:HB2	4:D1:220:ASN:HA	2.03	0.41
2:B1:97:ALA:O	2:B1:101:ILE:HG12	2.21	0.41
11:L1:18:PHE:HE1	35:L1:102:LMT:H72	1.85	0.41
23:b1:603:BCR:H24C	23:b1:603:BCR:H371	1.90	0.41
25:b1:606:CLA:H18	25:b1:611:CLA:H8	2.02	0.41
3:c1:271:TYR:O	40:c1:601:HOH:O	2.22	0.41
23:c1:501:BCR:H313	10:k1:18:PHE:CD2	2.56	0.41
1:A2:161:TYR:HB3	1:A2:162:PRO:HD3	2.02	0.41
23:A2:401:BCR:H15C	23:A2:401:BCR:H351	1.85	0.41
2:B2:233:ASN:O	2:B2:236:THR:HG22	2.21	0.41
25:C2:503:CLA:CHA	25:C2:503:CLA:HBA1	2.47	0.41
4:D2:273:PHE:HD1	33:D2:403:LHG:H242	1.86	0.41
7:H2:22:ALA:HA	7:H2:23:PRO:HD3	1.91	0.41
2:b2:243:ALA:HA	2:b2:246:PHE:CD2	2.56	0.41
1:A1:33:PHE:O	1:A1:125:ALA:HB1	2.21	0.41
25:A1:405:CLA:H43	29:A1:410:LMG:H111	2.02	0.41
25:A1:406:CLA:H92	25:A1:406:CLA:H62	1.89	0.41
2:B1:99:THR:HB	25:B1:609:CLA:H61	2.01	0.41
2:B1:440:ASP:OD2	2:B1:444:ARG:NH2	2.38	0.41
23:B1:601:BCR:H15C	23:B1:601:BCR:H351	1.81	0.41
23:B1:602:BCR:H24C	23:B1:602:BCR:H371	1.81	0.41
3:C1:209:ILE:O	3:C1:212:TYR:HB2	2.20	0.41
3:C1:213:LEU:HD11	23:C1:501:BCR:C20	2.51	0.41
4:D1:293:LEU:HD12	4:D1:293:LEU:HA	1.95	0.41
23:J1:101:BCR:H351	23:J1:101:BCR:H15C	1.80	0.41
12:M1:23:ILE:HD13	35:M1:102:LMT:H101	2.03	0.41
27:a1:411:PHO:H61	27:a1:411:PHO:H2	1.78	0.41
29:a1:412:LMG:H192	8:i1:16:CYS:SG	2.60	0.41
2:b1:42:LEU:HD13	2:b1:94:GLU:HG3	2.03	0.41
23:b1:601:BCR:H11C	23:b1:601:BCR:H341	1.83	0.41
25:b1:612:CLA:C14	25:b1:614:CLA:H2	2.51	0.41
3:c1:34:ALA:HB2	4:d1:230:ASP:OD2	2.21	0.41
3:c1:180:LEU:HD22	3:c1:199:ILE:O	2.20	0.41
3:c1:225:VAL:HG13	3:c1:289:TYR:HA	2.03	0.41
4:d1:39:PRO:O	4:d1:43:LEU:HG	2.20	0.41
4:d1:257:PHE:HE2	33:d1:407:LHG:H112	1.84	0.41
25:d1:404:CLA:HED1	36:d1:409:PL9:H361	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o1:48:LYS:O	13:o1:49:GLN:CB	2.66	0.41
1:A2:116:VAL:HG13	1:A2:158:PHE:HB3	2.03	0.41
1:A2:131:TRP:O	1:A2:134:SER:OG	2.32	0.41
1:A2:133:LEU:HD23	4:D2:256:ILE:HG12	2.02	0.41
2:B2:97:ALA:O	2:B2:101:ILE:HG12	2.21	0.41
2:B2:172:TYR:CE1	2:B2:283:GLU:HB2	2.56	0.41
2:B2:474:LEU:HD11	25:B2:610:CLA:HAA2	2.03	0.41
25:B2:605:CLA:H91	25:B2:605:CLA:H111	1.85	0.41
25:B2:611:CLA:NC	23:H2:103:BCR:H332	2.36	0.41
25:B2:614:CLA:H171	25:B2:614:CLA:H13	1.81	0.41
25:B2:616:CLA:H92	33:L2:101:LHG:H372	2.02	0.41
10:K2:14:THR:C	10:K2:16:ASN:H	2.29	0.41
15:U2:58:PRO:HB2	15:U2:79:MET:HE1	2.03	0.41
1:a2:161:TYR:HB3	1:a2:162:PRO:HD3	2.02	0.41
1:a2:212:SER:OG	4:d2:271:LEU:HB2	2.20	0.41
25:a2:404:CLA:H141	25:a2:404:CLA:H162	1.71	0.41
3:c2:314:ALA:HB3	3:c2:351:LEU:HD13	2.03	0.41
25:c2:515:CLA:NB	23:z2:101:BCR:H383	2.35	0.41
4:d2:193:LEU:O	11:l2:34:TYR:OH	2.31	0.41
29:j2:101:LMG:H392	29:j2:101:LMG:H421	1.82	0.41
16:v2:38:SER:C	16:v2:39:SER:O	2.63	0.41
16:v2:118:HIS:O	16:v2:122:GLN:HG2	2.21	0.41
1:A1:119:PHE:HE1	25:A1:403:CLA:H121	1.86	0.41
1:A1:161:TYR:HB3	1:A1:162:PRO:HD3	2.02	0.41
2:B1:200:SER:O	2:B1:201:HIS:C	2.64	0.41
25:B1:610:CLA:H142	25:B1:610:CLA:H112	1.79	0.41
38:E1:101:HEM:ND	6:F1:24:HIS:NE2	2.69	0.41
12:M1:25:LEU:HD23	12:M1:25:LEU:HA	1.90	0.41
16:V1:39:SER:HB2	16:V1:40:CYS:H	1.33	0.41
2:b1:242:ILE:HG12	25:b1:613:CLA:HBB1	2.03	0.41
33:b1:622:LHG:H292	33:b1:622:LHG:H201	2.02	0.41
3:c1:314:ALA:HB3	3:c1:351:LEU:HD13	2.03	0.41
3:c1:433:LEU:HD22	25:c1:504:CLA:HMC3	2.02	0.41
4:d1:144:ILE:O	4:d1:147:SER:N	2.51	0.41
10:k1:14:THR:C	10:k1:16:ASN:H	2.29	0.41
33:l1:102:LHG:H292	33:l1:102:LHG:H261	1.89	0.41
2:B2:243:ALA:HA	2:B2:246:PHE:CD2	2.56	0.41
25:B2:610:CLA:H8	25:B2:611:CLA:H13	2.03	0.41
3:C2:28:ILE:HG13	10:K2:45:PHE:HE2	1.85	0.41
3:C2:190:ALA:HA	3:C2:191:PRO:HD3	1.91	0.41
33:D2:405:LHG:HC92	36:D2:408:PL9:H111	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:F2:401:BCR:H15C	23:F2:401:BCR:H351	1.77	0.41
13:O2:170:MET:HE3	13:O2:172:VAL:HG23	2.02	0.41
16:V2:38:SER:C	16:V2:39:SER:O	2.63	0.41
1:a2:161:TYR:HA	1:a2:294:ALA:CB	2.51	0.41
25:c2:504:CLA:H121	25:c2:510:CLA:H43	2.03	0.41
12:m2:9:LEU:O	12:m2:10:ALA:C	2.63	0.41
2:B1:242:ILE:HG12	25:B1:613:CLA:HBB1	2.02	0.40
25:B1:617:CLA:H101	25:B1:617:CLA:H13	1.60	0.40
25:B1:617:CLA:H191	25:B1:617:CLA:C1B	2.52	0.40
25:C1:509:CLA:H162	25:C1:509:CLA:H122	1.36	0.40
33:D1:404:LHG:H162	33:D1:404:LHG:H191	1.85	0.40
16:V1:118:HIS:O	16:V1:122:GLN:HG2	2.21	0.40
25:b1:613:CLA:H111	25:b1:613:CLA:H72	1.80	0.40
25:b1:619:CLA:H162	25:b1:619:CLA:H202	1.71	0.40
3:c1:421:SER:HA	3:c1:422:PRO:HD3	1.99	0.40
4:d1:199:MET:HG2	36:d1:409:PL9:H311	2.03	0.40
3:C2:38:GLY:HA3	25:K2:101:CLA:HMD2	2.02	0.40
3:C2:57:ALA:O	3:C2:61:VAL:HG23	2.21	0.40
36:D2:408:PL9:H352	11:L2:26:VAL:CG1	2.49	0.40
5:E2:27:ILE:HB	5:E2:28:PRO:HD3	2.03	0.40
13:O2:181:VAL:C	13:O2:183:ARG:N	2.79	0.40
1:a2:131:TRP:HZ2	3:c2:449:ARG:HG3	1.86	0.40
23:a2:402:BCR:H24C	23:a2:402:BCR:H371	1.92	0.40
2:b2:6:TYR:C	2:b2:8:VAL:H	2.29	0.40
13:o2:214:VAL:O	13:o2:239:PHE:CE1	2.74	0.40
15:u2:32:VAL:HG23	15:u2:97:ARG:O	2.20	0.40
2:B1:464:PHE:C	2:B1:464:PHE:CD1	2.98	0.40
3:C1:438:PHE:CZ	25:C1:506:CLA:HAB	2.56	0.40
1:a1:318:ALA:O	1:a1:321:ILE:HG22	2.22	0.40
2:b1:91:TRP:HD1	29:b1:624:LMG:HC3	1.87	0.40
2:b1:464:PHE:CE2	33:b1:622:LHG:H252	2.56	0.40
2:b1:464:PHE:HB2	4:d1:280:TRP:CZ2	2.57	0.40
2:B2:464:PHE:CD1	2:B2:464:PHE:C	2.98	0.40
4:D2:195:PRO:HD3	11:L2:34:TYR:CZ	2.56	0.40
34:H2:101:DGD:HBE2	34:H2:101:DGD:HBF1	1.82	0.40
13:O2:48:LYS:O	13:O2:236:LYS:O	2.39	0.40
15:U2:76:LYS:O	15:U2:79:MET:N	2.49	0.40
2:b2:42:LEU:HD13	2:b2:94:GLU:HG3	2.03	0.40
2:b2:54:PRO:HD2	2:b2:57:ARG:HG3	2.04	0.40
23:d2:401:BCR:H15C	23:d2:401:BCR:H351	1.84	0.40
1:A1:116:VAL:HG13	1:A1:158:PHE:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:42:LEU:HD13	2:B1:94:GLU:HG3	2.03	0.40
3:C1:466:VAL:HG11	4:D1:247:VAL:HG12	2.02	0.40
37:D1:409:SQD:H301	10:K1:37:PHE:CZ	2.56	0.40
25:d1:406:CLA:H143	25:d1:406:CLA:H161	1.94	0.40
23:h1:102:BCR:H20C	23:h1:102:BCR:H361	1.89	0.40
12:m1:9:LEU:O	12:m1:10:ALA:C	2.64	0.40
2:B2:6:TYR:C	2:B2:8:VAL:H	2.30	0.40
13:O2:46:GLU:O	13:O2:47:PRO:O	2.38	0.40
13:O2:197:ILE:CG1	13:O2:198:GLU:N	2.85	0.40
25:b2:608:CLA:HMA3	25:b2:609:CLA:H3A	2.03	0.40
3:c2:225:VAL:HG13	3:c2:289:TYR:HA	2.03	0.40
10:k2:22:ILE:HA	10:k2:25:MET:CG	2.50	0.40
25:A1:403:CLA:H192	25:A1:403:CLA:H161	1.83	0.40
2:B1:6:TYR:C	2:B1:8:VAL:H	2.30	0.40
2:B1:233:ASN:O	2:B1:236:THR:HG22	2.21	0.40
3:C1:330:SER:OG	13:O1:100:GLY:O	2.31	0.40
25:C1:503:CLA:H43	25:C1:504:CLA:H61	2.03	0.40
13:O1:181:VAL:C	13:O1:183:ARG:N	2.79	0.40
1:a1:272:HIS:CD2	4:d1:218:VAL:HG21	2.57	0.40
2:b1:173:GLY:HA3	2:b1:265:ILE:HD11	2.02	0.40
25:b1:616:CLA:CGA	25:b1:616:CLA:C1A	3.00	0.40
3:C2:376:ASP:O	3:C2:380:ILE:HG12	2.22	0.40
4:D2:293:LEU:HD12	4:D2:293:LEU:HA	1.96	0.40
8:I2:28:PRO:O	8:I2:31:ASN:ND2	2.53	0.40
16:V2:39:SER:HB2	16:V2:40:CYS:H	1.39	0.40
1:a2:318:ALA:O	1:a2:321:ILE:HG22	2.22	0.40
2:b2:247:PHE:CD2	25:b2:606:CLA:H101	2.57	0.40
2:b2:450:TRP:CE2	25:b2:620:CLA:HBA1	2.56	0.40
25:c2:503:CLA:H2A	25:c2:503:CLA:CED	2.51	0.40
10:k2:14:THR:C	10:k2:16:ASN:H	2.29	0.40
2:B1:418:LYS:O	2:B1:422:ARG:HG3	2.22	0.40
25:B1:616:CLA:H41	25:B1:616:CLA:H62	1.89	0.40
3:C1:421:SER:HA	3:C1:422:PRO:HD3	1.99	0.40
4:D1:39:PRO:O	4:D1:43:LEU:HG	2.21	0.40
4:D1:297:ASP:OD1	4:D1:297:ASP:N	2.53	0.40
27:a1:411:PHO:H192	25:d1:404:CLA:C1B	2.52	0.40
2:b1:6:TYR:C	2:b1:8:VAL:N	2.79	0.40
23:c1:501:BCR:H351	23:c1:501:BCR:H15C	1.75	0.40
13:o1:122:ILE:HD12	13:o1:122:ILE:HA	1.93	0.40
15:u1:55:TYR:HB3	15:u1:60:ASP:HB2	2.02	0.40
25:B2:605:CLA:H101	25:B2:611:CLA:H193	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D2:39:PRO:O	4:D2:43:LEU:HG	2.21	0.40
12:M2:9:LEU:O	12:M2:10:ALA:C	2.64	0.40
13:O2:19:CYS:HA	13:O2:20:PRO:HD3	1.92	0.40
2:b2:9:HIS:CG	25:b2:612:CLA:O1A	2.75	0.40
2:b2:233:ASN:O	2:b2:236:THR:HG22	2.21	0.40
2:b2:418:LYS:O	2:b2:422:ARG:HG3	2.22	0.40
23:k2:501:BCR:H15C	23:k2:501:BCR:H351	1.77	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	A1	342/344 (99%)	328 (96%)	14 (4%)	0	100	100
1	A2	327/344 (95%)	318 (97%)	9 (3%)	0	100	100
1	a1	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a2	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B1	481/509 (94%)	456 (95%)	23 (5%)	2 (0%)	30	57
2	B2	501/509 (98%)	474 (95%)	26 (5%)	1 (0%)	43	70
2	b1	502/509 (99%)	474 (94%)	26 (5%)	2 (0%)	30	57
2	b2	479/509 (94%)	454 (95%)	23 (5%)	2 (0%)	30	57
3	C1	447/460 (97%)	424 (95%)	20 (4%)	3 (1%)	18	44
3	C2	438/460 (95%)	416 (95%)	19 (4%)	3 (1%)	18	44
3	c1	449/460 (98%)	426 (95%)	19 (4%)	4 (1%)	14	37
3	c2	446/460 (97%)	424 (95%)	19 (4%)	3 (1%)	18	44
4	D1	333/351 (95%)	318 (96%)	15 (4%)	0	100	100
4	D2	338/351 (96%)	322 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d1	337/351 (96%)	321 (95%)	16 (5%)	0	100	100
4	d2	338/351 (96%)	323 (96%)	15 (4%)	0	100	100
5	E1	59/84 (70%)	57 (97%)	2 (3%)	0	100	100
5	E2	61/84 (73%)	59 (97%)	2 (3%)	0	100	100
5	e1	55/84 (66%)	54 (98%)	1 (2%)	0	100	100
5	e2	58/84 (69%)	57 (98%)	1 (2%)	0	100	100
6	F1	26/43 (60%)	26 (100%)	0	0	100	100
6	F2	29/43 (67%)	29 (100%)	0	0	100	100
6	f1	27/43 (63%)	27 (100%)	0	0	100	100
6	f2	27/43 (63%)	26 (96%)	1 (4%)	0	100	100
7	H1	56/67 (84%)	53 (95%)	2 (4%)	1 (2%)	6	21
7	H2	60/67 (90%)	54 (90%)	5 (8%)	1 (2%)	7	22
7	h1	60/67 (90%)	57 (95%)	2 (3%)	1 (2%)	7	22
7	h2	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	7	22
8	I1	32/38 (84%)	32 (100%)	0	0	100	100
8	I2	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i1	32/38 (84%)	32 (100%)	0	0	100	100
8	i2	31/38 (82%)	31 (100%)	0	0	100	100
9	J1	30/39 (77%)	30 (100%)	0	0	100	100
9	J2	33/39 (85%)	33 (100%)	0	0	100	100
9	j1	30/39 (77%)	30 (100%)	0	0	100	100
9	j2	31/39 (80%)	31 (100%)	0	0	100	100
10	K1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	K2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	k1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	k2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
11	L1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
11	L2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
11	l1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
11	l2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
12	M1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
13	O1	234/329 (71%)	210 (90%)	14 (6%)	10 (4%)	2	6
13	O2	187/329 (57%)	165 (88%)	14 (8%)	8 (4%)	2	6
13	o1	230/329 (70%)	204 (89%)	16 (7%)	10 (4%)	2	6
13	o2	239/329 (73%)	212 (89%)	15 (6%)	12 (5%)	1	4
14	T1	28/32 (88%)	28 (100%)	0	0	100	100
14	T2	28/32 (88%)	28 (100%)	0	0	100	100
14	t1	28/32 (88%)	28 (100%)	0	0	100	100
14	t2	27/32 (84%)	27 (100%)	0	0	100	100
15	U1	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
15	U2	86/155 (56%)	81 (94%)	5 (6%)	0	100	100
15	u1	91/155 (59%)	87 (96%)	4 (4%)	0	100	100
15	u2	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
16	V1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	V2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	v1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	v2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
17	Y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	Y2	23/35 (66%)	22 (96%)	1 (4%)	0	100	100
17	y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	y2	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
18	X1	27/40 (68%)	27 (100%)	0	0	100	100
18	X2	29/40 (72%)	29 (100%)	0	0	100	100
18	x1	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
18	x2	30/40 (75%)	30 (100%)	0	0	100	100
19	S1	23/46 (50%)	23 (100%)	0	0	100	100
19	S2	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
19	s1	38/46 (83%)	34 (90%)	4 (10%)	0	100	100
19	s2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	W1	19/25 (76%)	19 (100%)	0	0	100	100
20	W2	19/25 (76%)	19 (100%)	0	0	100	100
20	w1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
20	w2	18/25 (72%)	18 (100%)	0	0	100	100
21	Q2	107/218 (49%)	102 (95%)	3 (3%)	2 (2%)	6	19
21	q1	101/218 (46%)	97 (96%)	3 (3%)	1 (1%)	12	35
22	Z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
22	z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
All	All	10304/12316 (84%)	9726 (94%)	479 (5%)	99 (1%)	12	35

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C1	36	TRP
3	C1	37	SER
10	K1	14	THR
13	O1	49	GLN
13	O1	99	ASP
13	O1	199	LEU
13	O1	201	VAL
13	O1	202	ASN
16	V1	39	SER
16	V1	40	CYS
3	c1	36	TRP
3	c1	37	SER
10	k1	14	THR
13	o1	49	GLN
13	o1	99	ASP
13	o1	199	LEU
13	o1	201	VAL
13	o1	202	ASN
16	v1	39	SER
16	v1	40	CYS
3	C2	36	TRP
3	C2	37	SER
10	K2	14	THR
13	O2	49	GLN
13	O2	199	LEU
13	O2	200	ALA

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Mol	Chain	Res	Type
13	O2	201	VAL
16	V2	39	SER
16	V2	40	CYS
16	V2	42	VAL
21	Q2	106	PRO
3	c2	36	TRP
3	c2	37	SER
10	k2	14	THR
13	o2	49	GLN
13	o2	99	ASP
13	o2	178(F)	GLY
13	o2	199	LEU
13	o2	201	VAL
13	o2	202	ASN
16	v2	39	SER
16	v2	40	CYS
2	B1	7	ARG
10	K1	15	TYR
13	O1	51	LEU
13	O1	181	VAL
13	O1	182	LEU
13	O1	200	ALA
16	V1	42	VAL
2	b1	7	ARG
10	k1	15	TYR
13	o1	51	LEU
13	o1	181	VAL
13	o1	182	LEU
13	o1	200	ALA
16	v1	42	VAL
2	B2	7	ARG
10	K2	15	TYR
13	O2	48	LYS
13	O2	181	VAL
13	O2	182	LEU
2	b2	7	ARG
10	k2	15	TYR
13	o2	51	LEU
13	o2	181	VAL
13	o2	182	LEU
13	o2	200	ALA
16	v2	42	VAL

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Mol	Chain	Res	Type
13	O1	120	PHE
16	V1	45	ILE
13	o1	120	PHE
16	v1	45	ILE
21	q1	144	LEU
13	O2	120	PHE
16	V2	45	ILE
21	Q2	144	LEU
13	o2	120	PHE
16	V1	38	SER
16	v1	38	SER
16	V2	38	SER
16	v2	38	SER
16	v2	45	ILE
2	B1	6	TYR
7	H1	26	GLY
7	h1	26	GLY
7	H2	26	GLY
2	b2	6	TYR
7	h2	26	GLY
3	C1	191	PRO
2	b1	6	TYR
3	c1	191	PRO
3	C2	191	PRO
3	c2	191	PRO
13	o2	198	GLU
11	l1	29	VAL
11	L2	29	VAL
11	l2	29	VAL
11	L1	29	VAL
3	c1	38	GLY

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	261/282 (93%)	254 (97%)	7 (3%)	39	71
1	A2	239/282 (85%)	234 (98%)	5 (2%)	47	76
1	a1	261/282 (93%)	255 (98%)	6 (2%)	44	75
1	a2	249/282 (88%)	242 (97%)	7 (3%)	38	70
2	B1	360/415 (87%)	350 (97%)	10 (3%)	38	70
2	B2	351/415 (85%)	339 (97%)	12 (3%)	32	65
2	b1	380/415 (92%)	368 (97%)	12 (3%)	34	67
2	b2	352/415 (85%)	341 (97%)	11 (3%)	35	68
3	C1	320/364 (88%)	317 (99%)	3 (1%)	70	87
3	C2	261/364 (72%)	260 (100%)	1 (0%)	84	93
3	c1	338/364 (93%)	335 (99%)	3 (1%)	70	87
3	c2	323/364 (89%)	320 (99%)	3 (1%)	70	87
4	D1	255/283 (90%)	253 (99%)	2 (1%)	73	89
4	D2	238/283 (84%)	236 (99%)	2 (1%)	73	89
4	d1	267/283 (94%)	266 (100%)	1 (0%)	84	93
4	d2	258/283 (91%)	257 (100%)	1 (0%)	84	93
5	E1	28/75 (37%)	28 (100%)	0	100	100
5	E2	34/75 (45%)	33 (97%)	1 (3%)	37	70
5	e1	38/75 (51%)	36 (95%)	2 (5%)	20	49
5	e2	33/75 (44%)	32 (97%)	1 (3%)	36	69
6	F1	18/36 (50%)	17 (94%)	1 (6%)	19	46
6	F2	17/36 (47%)	16 (94%)	1 (6%)	18	44
6	f1	20/36 (56%)	18 (90%)	2 (10%)	7	21
6	f2	19/36 (53%)	18 (95%)	1 (5%)	20	49
7	H1	39/58 (67%)	39 (100%)	0	100	100
7	H2	38/58 (66%)	38 (100%)	0	100	100
7	h1	47/58 (81%)	45 (96%)	2 (4%)	26	57
7	h2	42/58 (72%)	42 (100%)	0	100	100
8	I1	30/36 (83%)	29 (97%)	1 (3%)	33	66
8	I2	26/36 (72%)	25 (96%)	1 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i1	32/36 (89%)	31 (97%)	1 (3%)	35	68
8	i2	28/36 (78%)	27 (96%)	1 (4%)	31	63
9	J1	20/32 (62%)	20 (100%)	0	100	100
9	J2	19/32 (59%)	19 (100%)	0	100	100
9	j1	22/32 (69%)	22 (100%)	0	100	100
9	j2	22/32 (69%)	22 (100%)	0	100	100
10	K1	26/36 (72%)	25 (96%)	1 (4%)	29	61
10	K2	18/36 (50%)	17 (94%)	1 (6%)	19	46
10	k1	27/36 (75%)	26 (96%)	1 (4%)	30	62
10	k2	24/36 (67%)	21 (88%)	3 (12%)	4	13
11	L1	31/35 (89%)	31 (100%)	0	100	100
11	L2	33/35 (94%)	33 (100%)	0	100	100
11	l1	33/35 (94%)	33 (100%)	0	100	100
11	l2	32/35 (91%)	32 (100%)	0	100	100
12	M1	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	M2	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	m1	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	m2	27/88 (31%)	26 (96%)	1 (4%)	30	62
13	O1	148/266 (56%)	141 (95%)	7 (5%)	23	54
13	O2	110/266 (41%)	105 (96%)	5 (4%)	24	55
13	o1	156/266 (59%)	150 (96%)	6 (4%)	29	61
13	o2	168/266 (63%)	161 (96%)	7 (4%)	26	58
14	T1	24/28 (86%)	24 (100%)	0	100	100
14	T2	25/28 (89%)	25 (100%)	0	100	100
14	t1	26/28 (93%)	26 (100%)	0	100	100
14	t2	25/28 (89%)	24 (96%)	1 (4%)	28	60
15	U1	63/122 (52%)	59 (94%)	4 (6%)	16	41
15	U2	40/122 (33%)	37 (92%)	3 (8%)	12	34
15	u1	66/122 (54%)	62 (94%)	4 (6%)	17	43
15	u2	69/122 (57%)	64 (93%)	5 (7%)	13	35
16	V1	88/132 (67%)	86 (98%)	2 (2%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V2	70/132 (53%)	68 (97%)	2 (3%)	37	70
16	v1	88/132 (67%)	86 (98%)	2 (2%)	44	75
16	v2	100/132 (76%)	99 (99%)	1 (1%)	68	86
17	Y1	11/33 (33%)	11 (100%)	0	100	100
17	Y2	13/33 (39%)	13 (100%)	0	100	100
17	y1	18/33 (54%)	18 (100%)	0	100	100
17	y2	16/33 (48%)	16 (100%)	0	100	100
18	X1	17/34 (50%)	16 (94%)	1 (6%)	18	44
18	X2	16/34 (47%)	16 (100%)	0	100	100
18	x1	23/34 (68%)	22 (96%)	1 (4%)	26	57
18	x2	17/34 (50%)	16 (94%)	1 (6%)	18	44
19	S1	10/20 (50%)	10 (100%)	0	100	100
19	S2	10/20 (50%)	10 (100%)	0	100	100
19	s1	15/20 (75%)	15 (100%)	0	100	100
19	s2	13/20 (65%)	13 (100%)	0	100	100
20	W1	12/13 (92%)	12 (100%)	0	100	100
20	W2	10/13 (77%)	10 (100%)	0	100	100
20	w1	11/13 (85%)	11 (100%)	0	100	100
20	w2	11/13 (85%)	11 (100%)	0	100	100
21	Q2	35/175 (20%)	33 (94%)	2 (6%)	18	46
21	q1	33/175 (19%)	31 (94%)	2 (6%)	17	43
22	Z2	22/54 (41%)	22 (100%)	0	100	100
22	z2	28/54 (52%)	28 (100%)	0	100	100
All	All	7221/10010 (72%)	7054 (98%)	167 (2%)	44	75

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	13	LEU
1	A1	85	THR
1	A1	123	VAL
1	A1	286	THR
1	A1	291	SER
1	A1	307	VAL

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Mol	Chain	Res	Type
1	A1	321	ILE
2	B1	6	TYR
2	B1	10	THR
2	B1	12	VAL
2	B1	22	VAL
2	B1	80	ILE
2	B1	128	THR
2	B1	369	ILE
2	B1	371	VAL
2	B1	434	ARG
2	B1	442	VAL
3	C1	99	VAL
3	C1	240	ILE
3	C1	279	LEU
4	D1	182	LEU
4	D1	277	THR
6	F1	41	GLN
8	I1	23	PHE
10	K1	27	VAL
12	M1	9	LEU
13	O1	106	THR
13	O1	142	LEU
13	O1	172	VAL
13	O1	181	VAL
13	O1	220	LEU
13	O1	221	SER
13	O1	233	LEU
15	U1	57	THR
15	U1	80	ASP
15	U1	90	GLU
15	U1	97	ARG
16	V1	39	SER
16	V1	40	CYS
18	X1	32	VAL
1	a1	85	THR
1	a1	123	VAL
1	a1	286	THR
1	a1	291	SER
1	a1	307	VAL
1	a1	321	ILE
2	b1	6	TYR
2	b1	10	THR

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Mol	Chain	Res	Type
2	b1	12	VAL
2	b1	22	VAL
2	b1	80	ILE
2	b1	128	THR
2	b1	369	ILE
2	b1	371	VAL
2	b1	434	ARG
2	b1	442	VAL
2	b1	479	PHE
2	b1	490	VAL
3	c1	122	SER
3	c1	240	ILE
3	c1	279	LEU
4	d1	182	LEU
5	e1	36	LEU
5	e1	65	LEU
6	f1	21	LEU
6	f1	41	GLN
7	h1	56	GLU
7	h1	60	ILE
8	i1	23	PHE
10	k1	27	VAL
12	m1	9	LEU
13	o1	106	THR
13	o1	142	LEU
13	o1	172	VAL
13	o1	181	VAL
13	o1	220	LEU
13	o1	221	SER
15	u1	57	THR
15	u1	80	ASP
15	u1	90	GLU
15	u1	97	ARG
16	v1	39	SER
16	v1	40	CYS
18	x1	32	VAL
21	q1	137	ASP
21	q1	144	LEU
1	A2	85	THR
1	A2	123	VAL
1	A2	286	THR
1	A2	291	SER

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Mol	Chain	Res	Type
1	A2	307	VAL
2	B2	6	TYR
2	B2	10	THR
2	B2	12	VAL
2	B2	22	VAL
2	B2	80	ILE
2	B2	128	THR
2	B2	355	ILE
2	B2	371	VAL
2	B2	434	ARG
2	B2	442	VAL
2	B2	485	GLU
2	B2	490	VAL
3	C2	279	LEU
4	D2	182	LEU
4	D2	238	THR
5	E2	25	ILE
6	F2	41	GLN
8	I2	23	PHE
10	K2	27	VAL
12	M2	9	LEU
13	O2	106	THR
13	O2	172	VAL
13	O2	181	VAL
13	O2	221	SER
13	O2	233	LEU
15	U2	80	ASP
15	U2	90	GLU
15	U2	97	ARG
16	V2	39	SER
16	V2	40	CYS
21	Q2	137	ASP
21	Q2	183	ILE
1	a2	25	GLU
1	a2	85	THR
1	a2	123	VAL
1	a2	286	THR
1	a2	291	SER
1	a2	307	VAL
1	a2	321	ILE
2	b2	6	TYR
2	b2	10	THR

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Mol	Chain	Res	Type
2	b2	12	VAL
2	b2	22	VAL
2	b2	80	ILE
2	b2	128	THR
2	b2	369	ILE
2	b2	371	VAL
2	b2	434	ARG
2	b2	442	VAL
2	b2	479	PHE
3	c2	26	ARG
3	c2	99	VAL
3	c2	279	LEU
4	d2	182	LEU
5	e2	65	LEU
6	f2	41	GLN
8	i2	23	PHE
10	k2	14	THR
10	k2	27	VAL
10	k2	38	VAL
12	m2	9	LEU
13	o2	106	THR
13	o2	142	LEU
13	o2	172	VAL
13	o2	181	VAL
13	o2	220	LEU
13	o2	221	SER
13	o2	233	LEU
14	t2	29	ILE
15	u2	57	THR
15	u2	80	ASP
15	u2	90	GLU
15	u2	97	ARG
15	u2	104	LYS
16	v2	39	SER
18	x2	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	75	ASN
1	A1	165	GLN
1	A1	181	ASN

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Mol	Chain	Res	Type
1	A1	234	ASN
2	B1	26	HIS
2	B1	114	HIS
2	B1	216	HIS
2	B1	223	GLN
2	B1	365	ASN
3	C1	56	HIS
3	C1	107	ASN
3	C1	155	ASN
3	C1	385	GLN
3	C1	418	ASN
4	D1	334	GLN
13	O1	109	GLN
13	O1	191	GLN
1	a1	75	ASN
1	a1	165	GLN
1	a1	181	ASN
1	a1	247	ASN
2	b1	26	HIS
2	b1	114	HIS
2	b1	216	HIS
2	b1	223	GLN
2	b1	365	ASN
2	b1	489	GLN
3	c1	53	HIS
3	c1	56	HIS
3	c1	107	ASN
3	c1	155	ASN
3	c1	284	GLN
3	c1	418	ASN
4	d1	334	GLN
5	e1	71	ASN
11	l1	8	GLN
12	m1	4	GLN
13	o1	49	GLN
13	o1	191	GLN
21	q1	170	GLN
1	A2	75	ASN
1	A2	165	GLN
1	A2	234	ASN
2	B2	26	HIS
2	B2	114	HIS

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Mol	Chain	Res	Type
2	B2	216	HIS
3	C2	56	HIS
3	C2	107	ASN
3	C2	155	ASN
3	C2	385	GLN
4	D2	197	HIS
4	D2	334	GLN
13	O2	90	ASN
13	O2	191	GLN
16	V2	122	GLN
1	a2	75	ASN
1	a2	165	GLN
1	a2	181	ASN
2	b2	26	HIS
2	b2	114	HIS
2	b2	216	HIS
2	b2	365	ASN
3	c2	53	HIS
3	c2	56	HIS
3	c2	107	ASN
3	c2	385	GLN
4	d2	334	GLN
13	o2	49	GLN
13	o2	109	GLN
13	o2	191	GLN
18	x2	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 353 ligands modelled in this entry, 10 are monoatomic and 52 are unknown - leaving 291 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
25	CLA	a1	403	1	69,73,73	1.32	8 (11%)	83,113,113	1.27	7 (8%)
32	GOL	c2	518	-	5,5,5	0.37	0	5,5,5	0.26	0
25	CLA	b1	610	2	69,73,73	1.27	8 (11%)	83,113,113	1.26	8 (9%)
27	PHO	d2	408	-	58,69,69	2.76	12 (20%)	56,99,99	2.62	16 (28%)
34	DGD	c2	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.84	2 (2%)
25	CLA	B1	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.33	6 (7%)
23	BCR	k2	501	-	41,41,41	0.68	0	56,56,56	2.04	16 (28%)
25	CLA	c1	513	3	64,68,73	1.32	7 (10%)	77,107,113	1.32	6 (7%)
25	CLA	c1	508	3	54,58,73	1.45	8 (14%)	65,95,113	1.41	9 (13%)
25	CLA	c1	512	3	69,73,73	1.28	8 (11%)	83,113,113	1.29	6 (7%)
25	CLA	A1	405	1	59,63,73	1.40	7 (11%)	71,101,113	1.37	8 (11%)
25	CLA	b2	610	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	b1	612	-	69,73,73	1.27	6 (8%)	83,113,113	1.31	7 (8%)
29	LMG	M1	101	-	30,30,55	1.20	3 (10%)	32,32,63	1.33	3 (9%)
25	CLA	b2	618	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	c2	513	3	58,62,73	1.38	8 (13%)	69,99,113	1.37	6 (8%)
25	CLA	B1	607	2	64,68,73	1.33	8 (12%)	77,107,113	1.29	6 (7%)
23	BCR	A2	401	-	41,41,41	0.69	0	56,56,56	2.02	16 (28%)
32	GOL	a2	415	-	5,5,5	0.36	0	5,5,5	0.39	0
25	CLA	d1	406	4	69,73,73	1.26	6 (8%)	83,113,113	1.30	7 (8%)
25	CLA	C2	511	3	54,58,73	1.42	9 (16%)	65,95,113	1.49	8 (12%)
29	LMG	a2	412	-	44,44,55	1.01	2 (4%)	52,52,63	1.11	5 (9%)
25	CLA	c1	516	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
29	LMG	C1	520	-	48,48,55	0.97	2 (4%)	56,56,63	1.00	3 (5%)
34	DGD	H2	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PHO	D1	407	-	57,68,69	2.78	12 (21%)	54,97,99	2.69	16 (29%)
25	CLA	B1	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
25	CLA	a2	404	1	69,73,73	1.29	8 (11%)	83,113,113	1.28	7 (8%)
35	LMT	M1	103	-	24,24,36	0.46	0	29,29,47	0.56	0
25	CLA	B2	605	2	69,73,73	1.27	6 (8%)	83,113,113	1.27	5 (6%)
36	PL9	d2	409	-	55,55,55	0.64	1 (1%)	68,69,69	1.72	16 (23%)
25	CLA	b2	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
35	LMT	m2	104	-	30,30,36	0.47	0	41,41,47	0.81	1 (2%)
25	CLA	C1	502	3	69,73,73	1.25	6 (8%)	83,113,113	1.31	7 (8%)
26	OEX	a1	408	3,40,1	0,14,14	-	-	-	-	-
25	CLA	c1	510	3	69,73,73	1.27	8 (11%)	83,113,113	1.34	6 (7%)
38	HEM	v1	201	16	50,50,50	1.92	7 (14%)	66,82,82	1.43	6 (9%)
33	LHG	l1	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
31	BCT	A1	413	30	2,3,3	0.94	0	2,3,3	0.26	0
32	GOL	i1	101	-	5,5,5	0.41	0	5,5,5	0.20	0
29	LMG	B2	621	-	37,37,55	0.95	3 (8%)	45,45,63	1.11	3 (6%)
29	LMG	B1	622	-	31,31,55	1.20	2 (6%)	39,39,63	1.19	4 (10%)
33	LHG	d1	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
25	CLA	B1	617	2	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
23	BCR	B2	601	-	41,41,41	0.70	0	56,56,56	1.92	15 (26%)
25	CLA	c2	503	3	69,73,73	1.27	8 (11%)	83,113,113	1.29	4 (4%)
25	CLA	C1	506	3	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
25	CLA	B2	607	2	69,73,73	1.29	8 (11%)	83,113,113	1.30	8 (9%)
25	CLA	C2	508	3	54,58,73	1.43	6 (11%)	65,95,113	1.42	7 (10%)
23	BCR	b2	601	-	41,41,41	0.70	0	56,56,56	1.97	16 (28%)
25	CLA	B1	608	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	b2	624	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	8 (9%)
26	OEX	a2	408	3,40,1	0,14,14	-	-	-	-	-
29	LMG	d1	411	-	34,34,55	1.10	2 (5%)	36,36,63	1.14	3 (8%)
29	LMG	j2	101	-	50,50,55	0.94	2 (4%)	58,58,63	1.03	2 (3%)
34	DGD	C1	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
25	CLA	C2	510	3	49,53,73	1.49	7 (14%)	59,89,113	1.47	5 (8%)
37	SQD	B2	623	-	44,45,54	1.31	4 (9%)	53,56,65	1.22	6 (11%)
25	CLA	D1	402	4	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
25	CLA	B2	608	2	69,73,73	1.25	6 (8%)	83,113,113	1.29	7 (8%)
23	BCR	b1	602	-	41,41,41	0.69	0	56,56,56	2.05	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c2	507	3	58,62,73	1.39	8 (13%)	69,99,113	1.35	5 (7%)
23	BCR	z2	101	-	41,41,41	0.70	0	56,56,56	1.76	10 (17%)
23	BCR	c2	501	-	41,41,41	0.80	1 (2%)	56,56,56	3.50	20 (35%)
38	HEM	V2	201	16	50,50,50	1.96	7 (14%)	66,82,82	1.51	8 (12%)
23	BCR	H2	103	-	24,24,41	0.71	0	31,31,56	1.67	8 (25%)
25	CLA	C2	516	3	50,54,73	1.47	7 (14%)	60,90,113	1.43	6 (10%)
33	LHG	l2	101	-	43,43,48	1.00	2 (4%)	46,49,54	1.07	4 (8%)
25	CLA	D2	401	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
25	CLA	C1	511	3	69,73,73	1.28	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	B1	612	-	69,73,73	1.28	6 (8%)	83,113,113	1.29	7 (8%)
25	CLA	D2	404	4	65,69,73	1.31	7 (10%)	78,108,113	1.30	7 (8%)
29	LMG	C2	515	-	24,24,55	1.18	2 (8%)	32,32,63	1.05	2 (6%)
33	LHG	D1	405	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
29	LMG	b1	631	-	40,40,55	1.08	2 (5%)	48,48,63	1.23	5 (10%)
25	CLA	B2	604	-	45,49,73	1.55	6 (13%)	54,84,113	1.47	7 (12%)
29	LMG	c2	519	-	26,26,55	1.60	3 (11%)	32,33,63	1.30	2 (6%)
25	CLA	a1	404	1	64,68,73	1.34	7 (10%)	77,107,113	1.29	8 (10%)
25	CLA	B2	615	2	69,73,73	1.26	7 (10%)	83,113,113	1.25	6 (7%)
29	LMG	A2	412	-	29,29,55	1.07	2 (6%)	37,37,63	1.10	2 (5%)
23	BCR	K1	101	-	31,31,41	0.70	0	40,40,56	2.32	14 (35%)
27	PHO	a1	411	-	58,69,69	2.72	12 (20%)	56,99,99	2.56	16 (28%)
25	CLA	b2	615	2	64,68,73	1.31	7 (10%)	77,107,113	1.31	6 (7%)
37	SQD	D1	409	-	34,35,54	1.53	4 (11%)	43,46,65	1.41	6 (13%)
25	CLA	b2	611	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	7 (8%)
25	CLA	b2	617	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	7 (8%)
25	CLA	B2	611	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	D1	403	4	55,59,73	1.42	7 (12%)	66,96,113	1.34	5 (7%)
23	BCR	b2	603	-	41,41,41	0.70	0	56,56,56	1.91	13 (23%)
29	LMG	b1	621	-	38,38,55	1.11	2 (5%)	46,46,63	1.07	2 (4%)
26	OEX	A1	407	3,40,1	0,14,14	-	-	-	-	-
33	LHG	D2	405	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	4 (7%)
23	BCR	c1	501	-	41,41,41	0.70	0	56,56,56	2.10	13 (23%)
23	BCR	K2	102	-	41,41,41	0.72	0	56,56,56	2.07	16 (28%)
25	CLA	B2	606	2	69,73,73	1.28	7 (10%)	83,113,113	1.26	6 (7%)
35	LMT	C1	519	-	36,36,36	0.35	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c2	502	3	69,73,73	1.27	6 (8%)	83,113,113	1.27	6 (7%)
25	CLA	B2	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	7 (8%)
33	LHG	a1	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.09	3 (6%)
34	DGD	c1	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	2 (2%)
25	CLA	c2	508	40	69,73,73	1.27	6 (8%)	83,113,113	1.24	5 (6%)
27	PHO	A2	407	-	58,69,69	2.72	12 (20%)	56,99,99	2.61	15 (26%)
32	GOL	b1	618	-	5,5,5	0.35	0	5,5,5	0.39	0
25	CLA	b1	604	-	69,73,73	1.29	7 (10%)	83,113,113	1.21	6 (7%)
23	BCR	b1	601	-	41,41,41	0.69	0	56,56,56	1.83	14 (25%)
25	CLA	c1	509	40	69,73,73	1.27	7 (10%)	83,113,113	1.27	4 (4%)
25	CLA	c2	505	-	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
25	CLA	B1	605	2	69,73,73	1.27	6 (8%)	83,113,113	1.23	6 (7%)
23	BCR	a2	402	-	41,41,41	0.67	0	56,56,56	1.64	12 (21%)
25	CLA	d1	401	4	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
25	CLA	B2	612	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	8 (9%)
29	LMG	A1	412	-	41,41,55	1.06	2 (4%)	49,49,63	1.02	3 (6%)
25	CLA	C1	510	3	69,73,73	1.29	8 (11%)	83,113,113	1.23	6 (7%)
29	LMG	A1	410	-	43,43,55	1.03	2 (4%)	51,51,63	1.11	4 (7%)
33	LHG	A2	405	-	32,32,48	1.13	2 (6%)	35,38,54	1.07	2 (5%)
25	CLA	B1	610	2	69,73,73	1.28	8 (11%)	83,113,113	1.25	7 (8%)
33	LHG	B2	627	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	3 (6%)
33	LHG	B1	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
25	CLA	c2	506	3	65,69,73	1.30	8 (12%)	78,108,113	1.37	7 (8%)
29	LMG	b1	624	-	39,39,55	1.08	2 (5%)	47,47,63	1.31	5 (10%)
35	LMT	L1	102	-	11,11,36	0.25	0	10,10,47	0.56	0
25	CLA	B1	615	2	69,73,73	1.27	6 (8%)	83,113,113	1.25	5 (6%)
25	CLA	b1	611	2	69,73,73	1.27	7 (10%)	83,113,113	1.22	5 (6%)
25	CLA	C2	506	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
25	CLA	B2	617	2	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
25	CLA	C1	514	3	49,53,73	1.50	7 (14%)	59,89,113	1.44	6 (10%)
27	PHO	A1	408	-	58,69,69	2.71	12 (20%)	56,99,99	2.61	16 (28%)
38	HEM	v2	201	16	50,50,50	1.92	7 (14%)	66,82,82	1.45	7 (10%)
23	BCR	d2	401	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
29	LMG	D1	406	-	35,35,55	1.11	2 (5%)	43,43,63	1.07	3 (6%)
23	BCR	K2	104	-	29,29,41	0.56	0	40,41,56	1.67	10 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	a2	406	-	36,36,36	0.45	0	47,47,47	0.66	1 (2%)
38	HEM	E2	101	5	50,50,50	1.89	8 (16%)	66,82,82	1.43	6 (9%)
25	CLA	b2	608	2	69,73,73	1.28	7 (10%)	83,113,113	1.22	7 (8%)
25	CLA	C1	509	3	69,73,73	1.27	8 (11%)	83,113,113	1.38	8 (9%)
25	CLA	b2	616	2	64,68,73	1.34	8 (12%)	77,107,113	1.33	7 (9%)
23	BCR	j2	102	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
25	CLA	B1	604	-	46,50,73	1.54	6 (13%)	55,85,113	1.43	5 (9%)
25	CLA	B1	619	40	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
25	CLA	b1	619	2	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
25	CLA	C1	508	-	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
23	BCR	a1	401	-	41,41,41	0.69	0	56,56,56	1.73	14 (25%)
23	BCR	B1	603	-	41,41,41	0.68	0	56,56,56	1.72	11 (19%)
25	CLA	c2	511	3	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
36	PL9	D1	408	-	55,55,55	0.64	2 (3%)	68,69,69	1.76	16 (23%)
25	CLA	B2	619	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
25	CLA	C1	503	3	64,68,73	1.31	7 (10%)	77,107,113	1.29	5 (6%)
25	CLA	B2	609	2	69,73,73	1.25	7 (10%)	83,113,113	1.33	7 (8%)
23	BCR	C1	521	-	41,41,41	0.69	0	56,56,56	1.94	13 (23%)
23	BCR	F2	401	-	41,41,41	0.72	0	56,56,56	2.18	18 (32%)
29	LMG	B2	620	-	40,40,55	1.07	3 (7%)	48,48,63	1.05	4 (8%)
25	CLA	C2	513	3	57,61,73	1.42	8 (14%)	68,98,113	1.34	6 (8%)
23	BCR	k1	101	-	41,41,41	0.71	0	56,56,56	2.03	15 (26%)
25	CLA	b1	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.34	6 (7%)
29	LMG	I2	101	-	34,34,55	1.15	2 (5%)	42,42,63	1.13	3 (7%)
25	CLA	c1	504	3	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
25	CLA	B1	611	2	66,70,73	1.31	6 (9%)	79,109,113	1.27	7 (8%)
25	CLA	b1	617	2	69,73,73	1.28	8 (11%)	83,113,113	1.27	5 (6%)
25	CLA	b1	607	2	69,73,73	1.30	7 (10%)	83,113,113	1.29	7 (8%)
29	LMG	d1	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.10	3 (7%)
32	GOL	B1	620	-	5,5,5	0.35	0	5,5,5	0.32	0
23	BCR	b2	602	-	41,41,41	0.70	0	56,56,56	2.13	16 (28%)
25	CLA	b1	608	2	69,73,73	1.28	7 (10%)	83,113,113	1.30	7 (8%)
23	BCR	B2	602	-	41,41,41	0.68	0	56,56,56	2.02	14 (25%)
27	PHO	a2	416	-	58,69,69	2.71	12 (20%)	56,99,99	2.62	16 (28%)
25	CLA	c1	515	3	59,63,73	1.38	6 (10%)	71,101,113	1.34	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	GOL	a1	406	-	5,5,5	0.35	0	5,5,5	0.28	0
33	LHG	d2	403	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
38	HEM	V1	201	16	50,50,50	1.93	7 (14%)	66,82,82	1.47	9 (13%)
31	BCT	a2	417	30	2,3,3	0.67	0	2,3,3	0.77	0
25	CLA	B1	618	2	62,66,73	1.34	8 (12%)	74,104,113	1.32	5 (6%)
25	CLA	B1	614	2	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
25	CLA	A2	402	1	69,73,73	1.32	8 (11%)	83,113,113	1.28	7 (8%)
23	BCR	B2	603	-	41,41,41	0.69	0	56,56,56	1.84	12 (21%)
32	GOL	C2	514	-	5,5,5	0.36	0	5,5,5	0.31	0
34	DGD	c1	514	-	52,52,67	0.96	2 (3%)	66,66,81	1.04	4 (6%)
25	CLA	c1	506	40	69,73,73	1.26	6 (8%)	83,113,113	1.31	8 (9%)
33	LHG	D1	404	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	4 (7%)
34	DGD	c1	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.00	5 (6%)
25	CLA	B2	616	2	58,62,73	1.38	7 (12%)	69,99,113	1.39	7 (10%)
25	CLA	B1	609	2	69,73,73	1.26	7 (10%)	83,113,113	1.51	10 (12%)
31	BCT	A2	413	30	2,3,3	0.68	0	2,3,3	0.74	0
34	DGD	H1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.92	3 (3%)
25	CLA	c2	504	3	69,73,73	1.27	6 (8%)	83,113,113	1.27	6 (7%)
34	DGD	c2	516	-	53,53,67	0.96	2 (3%)	67,67,81	1.03	3 (4%)
29	LMG	B1	626	-	48,48,55	0.98	2 (4%)	56,56,63	1.18	3 (5%)
23	BCR	H1	102	-	22,22,41	0.69	0	29,29,56	1.72	6 (20%)
25	CLA	d1	404	40	69,73,73	1.31	7 (10%)	83,113,113	1.31	7 (8%)
25	CLA	b2	619	2	63,67,73	1.34	7 (11%)	75,105,113	1.31	5 (6%)
25	CLA	a1	405	-	54,58,73	1.42	7 (12%)	65,95,113	1.49	8 (12%)
25	CLA	b2	612	2	69,73,73	1.29	10 (14%)	83,113,113	1.34	6 (7%)
27	PHO	d1	403	-	58,69,69	2.76	12 (20%)	56,99,99	2.66	14 (25%)
32	GOL	c1	521	-	5,5,5	0.36	0	5,5,5	0.31	0
25	CLA	C1	504	3	69,73,73	1.29	7 (10%)	83,113,113	1.23	6 (7%)
25	CLA	b2	609	2	65,69,73	1.30	8 (12%)	78,108,113	1.33	5 (6%)
23	BCR	B1	601	-	41,41,41	0.69	0	56,56,56	1.90	15 (26%)
25	CLA	c2	512	3	69,73,73	1.27	6 (8%)	83,113,113	1.25	6 (7%)
33	LHG	L2	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)
25	CLA	A2	404	-	55,59,73	1.46	8 (14%)	66,96,113	1.37	8 (12%)
25	CLA	b1	609	2	69,73,73	1.27	7 (10%)	83,113,113	1.26	6 (7%)
25	CLA	b1	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	7 (8%)
37	SQD	D2	402	-	24,25,54	1.94	4 (16%)	31,35,65	1.66	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	l1	101	-	24,24,36	0.47	0	29,29,47	0.83	2 (6%)
25	CLA	C2	504	3	50,54,73	1.48	7 (14%)	60,90,113	1.40	4 (6%)
25	CLA	C2	505	3	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	C1	512	3	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
34	DGD	c2	514	-	63,63,67	0.87	2 (3%)	77,77,81	0.97	4 (5%)
35	LMT	i2	102	-	6,6,36	0.28	0	5,5,47	0.44	0
32	GOL	C1	518	-	5,5,5	0.37	0	5,5,5	0.23	0
35	LMT	T1	101	-	11,11,36	0.25	0	10,10,47	0.58	0
25	CLA	B1	616	2	69,73,73	1.29	8 (11%)	83,113,113	1.26	7 (8%)
23	BCR	b1	603	-	41,41,41	0.72	0	56,56,56	1.75	11 (19%)
25	CLA	A1	403	1	69,73,73	1.31	9 (13%)	83,113,113	1.28	7 (8%)
35	LMT	c1	517	-	34,34,36	0.43	0	45,45,47	0.68	1 (2%)
25	CLA	c2	509	3	69,73,73	1.26	8 (11%)	83,113,113	1.37	9 (10%)
25	CLA	B2	618	2	64,68,73	1.34	7 (10%)	77,107,113	1.32	5 (6%)
25	CLA	d2	402	-	69,73,73	1.27	7 (10%)	83,113,113	1.34	8 (9%)
33	LHG	D2	403	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
37	SQD	b2	605	-	44,45,54	1.30	4 (9%)	53,56,65	1.16	4 (7%)
25	CLA	b2	613	2	69,73,73	1.27	6 (8%)	83,113,113	1.24	5 (6%)
25	CLA	d2	405	4	69,73,73	1.26	7 (10%)	83,113,113	1.23	6 (7%)
25	CLA	c1	503	3	69,73,73	1.24	7 (10%)	83,113,113	1.32	6 (7%)
23	BCR	J1	101	-	41,41,41	0.75	0	56,56,56	2.10	16 (28%)
23	BCR	h1	102	-	41,41,41	0.68	0	56,56,56	1.89	17 (30%)
25	CLA	C1	513	3	65,69,73	1.31	7 (10%)	78,108,113	1.28	5 (6%)
34	DGD	h2	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.91	2 (2%)
25	CLA	C2	518	3	45,49,73	1.53	6 (13%)	54,84,113	1.52	6 (11%)
38	HEM	f1	101	6	50,50,50	1.93	7 (14%)	66,82,82	1.43	6 (9%)
25	CLA	d2	404	4	54,58,73	1.43	6 (11%)	65,95,113	1.41	7 (10%)
29	LMG	a1	412	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
33	LHG	b2	625	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
25	CLA	c1	505	3	69,73,73	1.27	7 (10%)	83,113,113	1.25	5 (6%)
27	PHO	D2	407	-	58,69,69	2.77	12 (20%)	56,99,99	2.64	15 (26%)
25	CLA	b2	620	40	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
35	LMT	m1	101	-	36,36,36	0.42	0	47,47,47	0.68	0
33	LHG	d2	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	4 (7%)
23	BCR	B1	602	-	41,41,41	0.69	0	56,56,56	1.95	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c2	515	3	50,54,73	1.46	7 (14%)	60,90,113	1.43	6 (10%)
25	CLA	b1	605	2	69,73,73	1.27	7 (10%)	83,113,113	1.29	4 (4%)
25	CLA	b1	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
26	OEX	A2	406	3,40,1	0,14,14	-	-	-		
33	LHG	b1	622	-	48,48,48	0.92	2 (4%)	51,54,54	1.04	5 (9%)
35	LMT	M1	102	-	10,10,36	0.24	0	9,9,47	0.57	0
33	LHG	d1	402	-	31,31,48	1.16	2 (6%)	34,37,54	1.35	3 (8%)
36	PL9	d1	409	-	55,55,55	0.64	2 (3%)	68,69,69	1.78	20 (29%)
23	BCR	c1	502	-	41,41,41	0.75	0	56,56,56	2.09	14 (25%)
25	CLA	c2	510	3	58,62,73	1.40	7 (12%)	69,99,113	1.32	6 (8%)
23	BCR	C1	501	-	41,41,41	0.70	0	56,56,56	1.80	14 (25%)
36	PL9	D2	408	-	55,55,55	0.62	1 (1%)	68,69,69	1.73	19 (27%)
23	BCR	A1	401	-	41,41,41	0.68	0	56,56,56	1.74	11 (19%)
25	CLA	A1	406	-	69,73,73	1.29	7 (10%)	83,113,113	1.35	8 (9%)
25	CLA	a2	405	1	69,73,73	1.24	6 (8%)	83,113,113	1.29	8 (9%)
29	LMG	F2	402	-	35,35,55	1.13	2 (5%)	43,43,63	1.03	3 (6%)
34	DGD	C1	517	-	65,65,67	0.86	2 (3%)	79,79,81	0.85	3 (3%)
33	LHG	L1	101	-	40,40,48	1.01	2 (5%)	43,46,54	1.10	4 (9%)
29	LMG	c1	519	-	55,55,55	0.91	2 (3%)	63,63,63	0.95	2 (3%)
38	HEM	E1	101	5,6	50,50,50	1.93	8 (16%)	66,82,82	1.43	6 (9%)
25	CLA	A2	403	1	65,69,73	1.32	6 (9%)	78,108,113	1.27	7 (8%)
25	CLA	b1	616	2	69,73,73	1.26	6 (8%)	83,113,113	1.30	7 (8%)
25	CLA	c1	507	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	B2	610	2	69,73,73	1.27	7 (10%)	83,113,113	1.25	8 (9%)
25	CLA	K2	101	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	6 (8%)
23	BCR	D1	401	-	41,41,41	0.72	0	56,56,56	1.98	13 (23%)
25	CLA	b2	604	-	46,50,73	1.52	6 (13%)	55,85,113	1.43	4 (7%)
23	BCR	h2	101	-	41,41,41	0.68	0	56,56,56	1.79	14 (25%)
34	DGD	C2	512	-	34,34,67	1.16	2 (5%)	46,47,81	1.06	2 (4%)
35	LMT	m2	103	-	31,31,36	0.44	0	42,42,47	0.91	1 (2%)
33	LHG	a2	407	-	29,29,48	1.09	2 (6%)	30,34,54	1.02	1 (3%)
25	CLA	D2	406	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	7 (8%)
35	LMT	b2	621	-	36,36,36	0.41	0	47,47,47	0.69	0
25	CLA	B2	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.36	8 (9%)
25	CLA	b1	620	-	69,73,73	1.28	6 (8%)	83,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C2	507	3	49,53,73	1.50	7 (14%)	59,89,113	1.43	4 (6%)
25	CLA	c1	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
23	BCR	C2	502	-	41,41,41	0.70	0	56,56,56	1.88	12 (21%)
34	DGD	h1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
25	CLA	b1	615	2	63,67,73	1.31	7 (11%)	75,105,113	1.32	7 (9%)
35	LMT	b2	623	-	36,36,36	0.38	0	47,47,47	0.84	0
25	CLA	C1	505	-	69,73,73	1.25	6 (8%)	83,113,113	1.31	5 (6%)
23	BCR	d1	405	-	41,41,41	0.71	0	56,56,56	1.86	12 (21%)
25	CLA	C2	509	-	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	a2	413	-	54,58,73	1.44	7 (12%)	65,95,113	1.38	9 (13%)
29	LMG	b2	622	-	39,39,55	1.07	2 (5%)	47,47,63	1.01	3 (6%)
34	DGD	C1	515	-	53,53,67	0.96	2 (3%)	67,67,81	1.02	4 (5%)
38	HEM	e2	101	5,6	50,50,50	1.92	8 (16%)	66,82,82	1.45	7 (10%)
29	LMG	d2	407	-	27,27,55	1.36	2 (7%)	35,35,63	1.29	3 (8%)
25	CLA	C1	507	3	69,73,73	1.28	9 (13%)	83,113,113	1.25	8 (9%)
25	CLA	A1	404	-	55,59,73	1.42	8 (14%)	66,96,113	1.42	7 (10%)
25	CLA	b2	606	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
25	CLA	C2	503	3	69,73,73	1.26	6 (8%)	83,113,113	1.32	5 (6%)
31	BCT	a1	413	30	2,3,3	0.67	0	2,3,3	0.72	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
25	CLA	a1	403	1	-	6/39/115/115	-
32	GOL	c2	518	-	-	2/4/4/4	-
25	CLA	b1	610	2	-	2/39/115/115	-
27	PHO	d2	408	-	-	0/37/103/103	0/5/6/6
34	DGD	c2	517	-	-	7/51/91/95	0/2/2/2
25	CLA	B1	613	2	-	15/39/115/115	-
23	BCR	k2	501	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	513	3	-	5/33/109/115	-
25	CLA	c1	508	3	-	7/21/97/115	-
25	CLA	c1	512	3	-	15/39/115/115	-
25	CLA	A1	405	1	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b2	610	2	-	9/39/115/115	-
25	CLA	b1	612	-	-	12/39/115/115	-
29	LMG	M1	101	-	-	4/31/31/70	-
25	CLA	b2	618	2	-	6/39/115/115	-
25	CLA	c2	513	3	-	7/26/102/115	-
25	CLA	B1	607	2	-	9/33/109/115	-
23	BCR	A2	401	-	-	0/29/63/63	0/2/2/2
32	GOL	a2	415	-	-	2/4/4/4	-
25	CLA	d1	406	4	-	15/39/115/115	-
25	CLA	C2	511	3	-	4/21/97/115	-
29	LMG	a2	412	-	-	6/39/59/70	0/1/1/1
25	CLA	c1	516	3	-	11/39/115/115	-
29	LMG	C1	520	-	-	8/43/63/70	0/1/1/1
34	DGD	H2	101	-	-	7/51/91/95	0/2/2/2
27	PHO	D1	407	-	-	3/35/101/103	0/5/6/6
25	CLA	B1	606	2	-	20/39/115/115	-
25	CLA	a2	404	1	-	7/39/115/115	-
35	LMT	M1	103	-	-	3/15/35/61	0/1/1/2
25	CLA	B2	605	2	-	9/39/115/115	-
36	PL9	d2	409	-	-	8/53/73/73	0/1/1/1
25	CLA	b2	614	2	-	17/39/115/115	-
35	LMT	m2	104	-	-	4/15/55/61	0/2/2/2
25	CLA	C1	502	3	-	17/39/115/115	-
25	CLA	c1	510	3	-	10/39/115/115	-
38	HEM	v1	201	16	-	4/14/54/54	-
33	LHG	l1	102	-	-	18/53/53/53	-
32	GOL	i1	101	-	-	2/4/4/4	-
29	LMG	B2	621	-	-	8/31/51/70	0/1/1/1
29	LMG	B1	622	-	-	2/26/46/70	0/1/1/1
33	LHG	d1	407	-	-	14/53/53/53	-
25	CLA	B1	617	2	-	12/39/115/115	-
23	BCR	B2	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c2	503	3	-	15/39/115/115	-
25	CLA	C1	506	3	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B2	607	2	-	7/39/115/115	-
25	CLA	C2	508	3	-	7/21/97/115	-
23	BCR	b2	601	-	-	0/29/63/63	0/2/2/2
25	CLA	B1	608	2	-	16/39/115/115	-
25	CLA	b2	624	2	-	9/39/115/115	-
29	LMG	d1	411	-	-	2/36/36/70	-
29	LMG	j2	101	-	-	7/45/65/70	0/1/1/1
34	DGD	C1	516	-	-	9/51/91/95	0/2/2/2
25	CLA	C2	510	3	-	6/15/91/115	-
37	SQD	B2	623	-	-	2/40/60/69	0/1/1/1
25	CLA	D1	402	4	-	9/39/115/115	-
25	CLA	B2	608	2	-	20/39/115/115	-
23	BCR	b1	602	-	-	3/29/63/63	0/2/2/2
25	CLA	c2	507	3	-	5/26/102/115	-
23	BCR	z2	101	-	-	0/29/63/63	0/2/2/2
23	BCR	c2	501	-	-	14/29/63/63	0/2/2/2
38	HEM	V2	201	16	-	3/14/54/54	-
23	BCR	H2	103	-	-	3/17/34/63	0/1/1/2
25	CLA	C2	516	3	-	8/17/93/115	-
33	LHG	l2	101	-	-	20/48/48/53	-
25	CLA	D2	401	4	-	7/39/115/115	-
25	CLA	C1	511	3	-	12/39/115/115	-
25	CLA	B1	612	-	-	10/39/115/115	-
25	CLA	D2	404	4	-	11/35/111/115	-
29	LMG	C2	515	-	-	0/18/38/70	0/1/1/1
33	LHG	D1	405	-	-	14/53/53/53	-
29	LMG	b1	631	-	-	7/35/55/70	0/1/1/1
25	CLA	B2	604	-	-	6/10/86/115	-
29	LMG	c2	519	-	-	3/20/40/70	0/1/1/1
25	CLA	a1	404	1	-	7/33/109/115	-
25	CLA	B2	615	2	-	11/39/115/115	-
29	LMG	A2	412	-	-	5/23/43/70	0/1/1/1
23	BCR	K1	101	-	-	5/26/43/63	0/1/1/2
27	PHO	a1	411	-	-	5/37/103/103	0/5/6/6
25	CLA	b2	615	2	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SQD	D1	409	-	-	2/29/49/69	0/1/1/1
25	CLA	b2	611	-	-	7/39/115/115	-
25	CLA	b2	617	2	-	18/39/115/115	-
25	CLA	B2	611	2	-	10/39/115/115	-
25	CLA	D1	403	4	-	4/23/99/115	-
23	BCR	b2	603	-	-	0/29/63/63	0/2/2/2
29	LMG	b1	621	-	-	6/33/53/70	0/1/1/1
33	LHG	D2	405	-	-	16/53/53/53	-
23	BCR	c1	501	-	-	0/29/63/63	0/2/2/2
23	BCR	K2	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B2	606	2	-	13/39/115/115	-
35	LMT	C1	519	-	-	2/21/61/61	0/2/2/2
25	CLA	c2	502	3	-	13/39/115/115	-
25	CLA	B2	614	2	-	12/39/115/115	-
33	LHG	a1	407	-	-	14/47/47/53	-
34	DGD	c1	520	-	-	8/51/91/95	0/2/2/2
25	CLA	c2	508	40	-	16/39/115/115	-
27	PHO	A2	407	-	-	8/37/103/103	0/5/6/6
32	GOL	b1	618	-	-	4/4/4/4	-
25	CLA	b1	604	-	-	16/39/115/115	-
23	BCR	b1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	509	40	-	17/39/115/115	-
25	CLA	c2	505	-	-	16/39/115/115	-
25	CLA	B1	605	2	-	11/39/115/115	-
23	BCR	a2	402	-	-	3/29/63/63	0/2/2/2
25	CLA	d1	401	4	-	12/39/115/115	-
25	CLA	B2	612	-	-	9/39/115/115	-
29	LMG	A1	412	-	-	7/36/56/70	0/1/1/1
25	CLA	C1	510	3	-	8/39/115/115	-
29	LMG	A1	410	-	-	4/38/58/70	0/1/1/1
33	LHG	A2	405	-	-	10/37/37/53	-
25	CLA	B1	610	2	-	13/39/115/115	-
33	LHG	B2	627	-	-	8/46/46/53	-
33	LHG	B1	621	-	-	11/53/53/53	-
25	CLA	c2	506	3	-	13/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	b1	624	-	-	3/34/54/70	0/1/1/1
35	LMT	L1	102	-	-	1/9/9/61	-
25	CLA	B1	615	2	-	15/39/115/115	-
25	CLA	b1	611	2	-	8/39/115/115	-
25	CLA	C2	506	-	-	14/39/115/115	-
25	CLA	B2	617	2	-	9/39/115/115	-
25	CLA	C1	514	3	-	4/15/91/115	-
27	PHO	A1	408	-	-	7/37/103/103	0/5/6/6
38	HEM	v2	201	16	-	2/14/54/54	-
23	BCR	d2	401	-	-	8/29/63/63	0/2/2/2
29	LMG	D1	406	-	-	4/30/50/70	0/1/1/1
23	BCR	K2	104	-	-	2/12/46/63	0/2/2/2
35	LMT	a2	406	-	-	5/21/61/61	0/2/2/2
38	HEM	E2	101	5	-	1/14/54/54	-
25	CLA	b2	608	2	-	14/39/115/115	-
25	CLA	C1	509	3	-	20/39/115/115	-
25	CLA	b2	616	2	-	11/33/109/115	-
23	BCR	j2	102	-	-	9/29/63/63	0/2/2/2
25	CLA	B1	604	-	-	6/12/88/115	-
25	CLA	B1	619	40	-	18/39/115/115	-
25	CLA	b1	619	2	-	17/39/115/115	-
25	CLA	C1	508	-	-	13/39/115/115	-
23	BCR	a1	401	-	-	2/29/63/63	0/2/2/2
23	BCR	B1	603	-	-	1/29/63/63	0/2/2/2
25	CLA	c2	511	3	-	16/39/115/115	-
36	PL9	D1	408	-	-	7/53/73/73	0/1/1/1
25	CLA	B2	619	-	-	17/39/115/115	-
25	CLA	C1	503	3	-	13/33/109/115	-
25	CLA	B2	609	2	-	11/39/115/115	-
23	BCR	C1	521	-	-	0/29/63/63	0/2/2/2
23	BCR	F2	401	-	-	9/29/63/63	0/2/2/2
29	LMG	B2	620	-	-	8/35/55/70	0/1/1/1
25	CLA	C2	513	3	-	2/25/101/115	-
23	BCR	k1	101	-	-	5/29/63/63	0/2/2/2
25	CLA	b1	613	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	I2	101	-	-	3/29/49/70	0/1/1/1
25	CLA	c1	504	3	-	7/39/115/115	-
25	CLA	B1	611	2	-	11/36/112/115	-
25	CLA	b1	617	2	-	5/39/115/115	-
25	CLA	b1	607	2	-	10/39/115/115	-
29	LMG	d1	408	-	-	2/28/48/70	0/1/1/1
32	GOL	B1	620	-	-	2/4/4/4	-
23	BCR	b2	602	-	-	6/29/63/63	0/2/2/2
25	CLA	b1	608	2	-	17/39/115/115	-
23	BCR	B2	602	-	-	2/29/63/63	0/2/2/2
27	PHO	a2	416	-	-	6/37/103/103	0/5/6/6
25	CLA	c1	515	3	-	9/27/103/115	-
32	GOL	a1	406	-	-	2/4/4/4	-
33	LHG	d2	403	-	-	13/53/53/53	-
38	HEM	V1	201	16	-	4/14/54/54	-
25	CLA	B1	618	2	-	3/31/107/115	-
25	CLA	B1	614	2	-	12/39/115/115	-
25	CLA	A2	402	1	-	10/39/115/115	-
23	BCR	B2	603	-	-	2/29/63/63	0/2/2/2
32	GOL	C2	514	-	-	2/4/4/4	-
34	DGD	c1	514	-	-	9/40/80/95	0/2/2/2
25	CLA	c1	506	40	-	15/39/115/115	-
33	LHG	D1	404	-	-	11/53/53/53	-
34	DGD	c1	518	-	-	10/51/91/95	0/2/2/2
25	CLA	B2	616	2	-	9/26/102/115	-
25	CLA	B1	609	2	-	12/39/115/115	-
34	DGD	H1	101	-	-	12/51/91/95	0/2/2/2
25	CLA	c2	504	3	-	12/39/115/115	-
34	DGD	c2	516	-	-	6/41/81/95	0/2/2/2
29	LMG	B1	626	-	-	12/43/63/70	0/1/1/1
23	BCR	H1	102	-	-	3/15/32/63	0/1/1/2
25	CLA	d1	404	40	-	8/39/115/115	-
25	CLA	b2	619	2	-	10/32/108/115	-
25	CLA	a1	405	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b2	612	2	-	12/39/115/115	-
27	PHO	d1	403	-	-	3/37/103/103	0/5/6/6
32	GOL	c1	521	-	-	2/4/4/4	-
25	CLA	C1	504	3	-	8/39/115/115	-
25	CLA	b2	609	2	-	12/35/111/115	-
23	BCR	B1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c2	512	3	-	15/39/115/115	-
25	CLA	A2	404	-	-	9/23/99/115	-
25	CLA	b1	609	2	-	13/39/115/115	-
25	CLA	b1	614	2	-	14/39/115/115	-
37	SQD	D2	402	-	-	4/18/38/69	0/1/1/1
35	LMT	l1	101	-	-	3/15/35/61	0/1/1/2
25	CLA	C2	504	3	-	8/17/93/115	-
25	CLA	C2	505	3	-	17/39/115/115	-
25	CLA	C1	512	3	-	14/39/115/115	-
34	DGD	c2	514	-	-	16/51/91/95	0/2/2/2
35	LMT	i2	102	-	-	0/4/4/61	-
32	GOL	C1	518	-	-	2/4/4/4	-
35	LMT	T1	101	-	-	0/9/9/61	-
25	CLA	B1	616	2	-	10/39/115/115	-
23	BCR	b1	603	-	-	4/29/63/63	0/2/2/2
25	CLA	A1	403	1	-	10/39/115/115	-
35	LMT	c1	517	-	-	1/19/59/61	0/2/2/2
25	CLA	c2	509	3	-	11/39/115/115	-
25	CLA	B2	618	2	-	4/33/109/115	-
25	CLA	d2	402	-	-	12/39/115/115	-
33	LHG	D2	403	-	-	10/53/53/53	-
37	SQD	b2	605	-	-	10/40/60/69	0/1/1/1
25	CLA	b2	613	2	-	6/39/115/115	-
25	CLA	d2	405	4	-	11/39/115/115	-
25	CLA	c1	503	3	-	16/39/115/115	-
23	BCR	J1	101	-	-	9/29/63/63	0/2/2/2
23	BCR	h1	102	-	-	5/29/63/63	0/2/2/2
25	CLA	C1	513	3	-	15/35/111/115	-
34	DGD	h2	102	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C2	518	3	-	4/10/86/115	-
38	HEM	f1	101	6	-	5/14/54/54	-
25	CLA	d2	404	4	-	4/21/97/115	-
29	LMG	a1	412	-	-	12/46/66/70	0/1/1/1
33	LHG	b2	625	-	-	5/47/47/53	-
25	CLA	c1	505	3	-	5/39/115/115	-
27	PHO	D2	407	-	-	6/37/103/103	0/5/6/6
25	CLA	b2	620	40	-	22/39/115/115	-
35	LMT	m1	101	-	-	8/21/61/61	0/2/2/2
33	LHG	d2	406	-	-	10/53/53/53	-
23	BCR	B1	602	-	-	5/29/63/63	0/2/2/2
25	CLA	c2	515	3	-	6/17/93/115	-
25	CLA	b1	605	2	-	7/39/115/115	-
25	CLA	b1	606	2	-	19/39/115/115	-
35	LMT	M1	102	-	-	1/8/8/61	-
33	LHG	b1	622	-	-	14/53/53/53	-
33	LHG	d1	402	-	-	12/36/36/53	-
36	PL9	d1	409	-	-	9/53/73/73	0/1/1/1
23	BCR	c1	502	-	-	5/29/63/63	0/2/2/2
25	CLA	c2	510	3	-	8/26/102/115	-
23	BCR	C1	501	-	-	4/29/63/63	0/2/2/2
36	PL9	D2	408	-	-	7/53/73/73	0/1/1/1
23	BCR	A1	401	-	-	2/29/63/63	0/2/2/2
25	CLA	A1	406	-	-	11/39/115/115	-
25	CLA	a2	405	1	-	15/39/115/115	-
29	LMG	F2	402	-	-	2/30/50/70	0/1/1/1
34	DGD	C1	517	-	-	6/53/93/95	0/2/2/2
33	LHG	L1	101	-	-	14/45/45/53	-
29	LMG	c1	519	-	-	9/50/70/70	0/1/1/1
38	HEM	E1	101	5,6	-	3/14/54/54	-
25	CLA	A2	403	1	-	7/35/111/115	-
25	CLA	b1	616	2	-	15/39/115/115	-
25	CLA	c1	507	3	-	18/39/115/115	-
25	CLA	B2	610	2	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	K2	101	-	-	13/27/103/115	-
23	BCR	D1	401	-	-	8/29/63/63	0/2/2/2
25	CLA	b2	604	-	-	6/12/88/115	-
23	BCR	h2	101	-	-	4/29/63/63	0/2/2/2
34	DGD	C2	512	-	-	1/20/60/95	0/2/2/2
35	LMT	m2	103	-	-	5/16/56/61	0/2/2/2
33	LHG	a2	407	-	-	11/33/33/53	-
25	CLA	D2	406	-	-	14/39/115/115	-
35	LMT	b2	621	-	-	1/21/61/61	0/2/2/2
25	CLA	B2	613	2	-	12/39/115/115	-
25	CLA	b1	620	-	-	18/39/115/115	-
25	CLA	C2	507	3	-	6/15/91/115	-
25	CLA	c1	511	3	-	10/39/115/115	-
23	BCR	C2	502	-	-	0/29/63/63	0/2/2/2
34	DGD	h1	101	-	-	9/51/91/95	0/2/2/2
25	CLA	b1	615	2	-	7/32/108/115	-
35	LMT	b2	623	-	-	1/21/61/61	0/2/2/2
25	CLA	C1	505	-	-	11/39/115/115	-
23	BCR	d1	405	-	-	8/29/63/63	0/2/2/2
25	CLA	C2	509	-	-	16/39/115/115	-
25	CLA	a2	413	-	-	7/21/97/115	-
29	LMG	b2	622	-	-	0/34/54/70	0/1/1/1
34	DGD	C1	515	-	-	10/41/81/95	0/2/2/2
38	HEM	e2	101	5,6	-	2/14/54/54	-
29	LMG	d2	407	-	-	3/21/41/70	0/1/1/1
25	CLA	C1	507	3	-	22/39/115/115	-
25	CLA	A1	404	-	-	9/23/99/115	-
25	CLA	b2	606	2	-	14/39/115/115	-
25	CLA	C2	503	3	-	16/39/115/115	-
33	LHG	L2	101	-	-	16/53/53/53	-

All (1291) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d2	408	PHO	C1D-C2D	10.10	1.50	1.39
27	D1	407	PHO	C1D-C2D	10.06	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D2	407	PHO	C1D-C2D	9.97	1.50	1.39
27	d1	403	PHO	C1D-C2D	9.94	1.50	1.39
27	A2	407	PHO	C1D-C2D	9.92	1.50	1.39
27	a2	416	PHO	C1D-C2D	9.91	1.50	1.39
27	A1	408	PHO	C1D-C2D	9.86	1.50	1.39
27	a1	411	PHO	C1D-C2D	9.84	1.50	1.39
27	D2	407	PHO	C1B-C2B	8.92	1.49	1.39
27	a1	411	PHO	C1B-C2B	8.87	1.49	1.39
27	A2	407	PHO	C1B-C2B	8.86	1.49	1.39
27	d2	408	PHO	C1B-C2B	8.83	1.49	1.39
27	A1	408	PHO	C1B-C2B	8.82	1.49	1.39
27	d1	403	PHO	C1B-C2B	8.60	1.49	1.39
27	a2	416	PHO	C1B-C2B	8.58	1.49	1.39
27	D1	407	PHO	C1B-C2B	8.57	1.49	1.39
38	E1	101	HEM	C3D-C2D	8.07	1.53	1.36
38	e2	101	HEM	C3D-C2D	8.07	1.53	1.36
38	E2	101	HEM	C3D-C2D	8.05	1.53	1.36
38	V1	201	HEM	C3D-C2D	8.04	1.53	1.36
38	V2	201	HEM	C3D-C2D	8.04	1.53	1.36
38	f1	101	HEM	C3D-C2D	8.03	1.53	1.36
38	v1	201	HEM	C3D-C2D	8.01	1.53	1.36
38	v2	201	HEM	C3D-C2D	7.99	1.53	1.36
37	D2	402	SQD	O7-S	6.36	1.63	1.45
27	D1	407	PHO	C3B-C4B	6.35	1.48	1.41
27	d1	403	PHO	C3B-C4B	6.32	1.48	1.41
27	D2	407	PHO	C3B-C4B	6.24	1.48	1.41
27	a2	416	PHO	C3B-C4B	6.22	1.48	1.41
27	d2	408	PHO	C3B-C4B	6.19	1.48	1.41
27	a1	411	PHO	C3B-C4B	6.06	1.48	1.41
27	A2	407	PHO	C3B-C4B	6.01	1.48	1.41
27	A1	408	PHO	C3B-C4B	5.87	1.48	1.41
27	D2	407	PHO	C4D-CHA	5.73	1.48	1.39
27	A1	408	PHO	C4D-CHA	5.69	1.48	1.39
27	A2	407	PHO	C4D-CHA	5.62	1.48	1.39
27	d2	408	PHO	C4D-CHA	5.62	1.48	1.39
29	c2	519	LMG	O7-C10	5.61	1.45	1.33
27	D1	407	PHO	C4D-CHA	5.61	1.48	1.39
27	a1	411	PHO	C4D-CHA	5.54	1.48	1.39
27	D2	407	PHO	C3C-C2C	5.51	1.48	1.36
27	a1	411	PHO	C3C-C2C	5.51	1.48	1.36
27	a2	416	PHO	C3C-C2C	5.51	1.48	1.36
27	D1	407	PHO	C3C-C2C	5.50	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d1	403	PHO	C4D-CHA	5.48	1.48	1.39
27	D1	407	PHO	C3B-C2B	5.47	1.48	1.40
27	A1	408	PHO	C3C-C2C	5.42	1.48	1.36
27	d1	403	PHO	C3B-C2B	5.42	1.47	1.40
27	D2	407	PHO	C3B-C2B	5.41	1.47	1.40
27	a2	416	PHO	C4D-CHA	5.38	1.48	1.39
27	A2	407	PHO	C3C-C2C	5.38	1.48	1.36
27	d1	403	PHO	C3C-C2C	5.37	1.48	1.36
27	d2	408	PHO	C3C-C2C	5.37	1.48	1.36
27	d2	408	PHO	C3B-C2B	5.37	1.47	1.40
27	a1	411	PHO	C3B-C2B	5.29	1.47	1.40
27	d2	408	PHO	O2D-CGD	5.29	1.46	1.33
38	f1	101	HEM	FE-ND	5.25	2.11	1.94
27	D1	407	PHO	O2D-CGD	5.22	1.45	1.33
27	d1	403	PHO	O2D-CGD	5.21	1.45	1.33
27	D2	407	PHO	O2D-CGD	5.18	1.45	1.33
27	a2	416	PHO	O2D-CGD	5.16	1.45	1.33
27	a1	411	PHO	O2D-CGD	5.15	1.45	1.33
27	A2	407	PHO	O2D-CGD	5.12	1.45	1.33
38	E1	101	HEM	FE-ND	5.10	2.10	1.94
38	e2	101	HEM	FE-ND	5.09	2.10	1.94
27	A1	408	PHO	C3B-C2B	5.08	1.47	1.40
27	A2	407	PHO	C3B-C2B	5.07	1.47	1.40
27	a2	416	PHO	C3B-C2B	5.04	1.47	1.40
27	A1	408	PHO	O2D-CGD	5.03	1.45	1.33
27	a1	411	PHO	C3D-C4D	-4.91	1.34	1.41
27	d1	403	PHO	C3D-C4D	-4.89	1.34	1.41
27	d1	403	PHO	OBD-CAD	4.86	1.29	1.22
29	d2	407	LMG	O7-C10	4.85	1.46	1.35
38	v2	201	HEM	FE-ND	4.85	2.09	1.94
38	V1	201	HEM	FE-ND	4.83	2.09	1.94
38	V2	201	HEM	FE-ND	4.83	2.09	1.94
27	D2	407	PHO	OBD-CAD	4.81	1.29	1.22
34	C2	512	DGD	O2G-C1B	4.80	1.46	1.35
27	A2	407	PHO	C3D-C4D	-4.79	1.34	1.41
37	D2	402	SQD	O47-C7	4.77	1.46	1.35
27	D1	407	PHO	OBD-CAD	4.75	1.28	1.22
37	D1	409	SQD	O47-C7	4.73	1.45	1.35
38	v1	201	HEM	FE-ND	4.72	2.09	1.94
27	d2	408	PHO	OBD-CAD	4.68	1.28	1.22
27	A1	408	PHO	C3D-C4D	-4.68	1.34	1.41
37	B2	623	SQD	O8-S	4.66	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d2	408	PHO	C3D-C4D	-4.65	1.34	1.41
38	V2	201	HEM	FE-NB	4.64	2.09	1.94
37	D1	409	SQD	O8-S	4.63	1.64	1.47
27	a2	416	PHO	OBD-CAD	4.63	1.28	1.22
27	D2	407	PHO	C3D-C4D	-4.62	1.34	1.41
37	b2	605	SQD	O8-S	4.62	1.63	1.47
27	A2	407	PHO	OBD-CAD	4.61	1.28	1.22
27	A1	408	PHO	OBD-CAD	4.58	1.28	1.22
27	a2	416	PHO	C3D-C4D	-4.58	1.34	1.41
27	D1	407	PHO	C3D-C4D	-4.55	1.34	1.41
38	E2	101	HEM	FE-ND	4.49	2.08	1.94
27	a1	411	PHO	OBD-CAD	4.41	1.28	1.22
29	a1	412	LMG	O8-C28	4.39	1.46	1.33
29	B1	626	LMG	O8-C28	4.38	1.46	1.33
29	A1	412	LMG	O8-C28	4.38	1.46	1.33
29	b1	621	LMG	O8-C28	4.38	1.46	1.33
29	b1	621	LMG	O7-C10	4.38	1.46	1.34
34	c1	514	DGD	O1G-C1A	4.37	1.46	1.33
29	b2	622	LMG	O8-C28	4.33	1.46	1.33
33	B2	627	LHG	O8-C23	4.33	1.46	1.33
34	c2	517	DGD	O1G-C1A	4.32	1.46	1.33
29	A1	410	LMG	O8-C28	4.31	1.45	1.33
34	c1	520	DGD	O1G-C1A	4.30	1.45	1.33
34	C1	515	DGD	O1G-C1A	4.30	1.45	1.33
29	b1	624	LMG	O8-C28	4.30	1.45	1.33
29	I2	101	LMG	O8-C28	4.29	1.45	1.33
29	b1	631	LMG	O7-C10	4.29	1.46	1.34
37	B2	623	SQD	O48-C23	4.29	1.45	1.33
29	d2	407	LMG	O8-C28	4.29	1.45	1.33
29	j2	101	LMG	O8-C28	4.28	1.45	1.33
38	v2	201	HEM	FE-NC	4.28	2.09	1.95
29	b1	631	LMG	O8-C28	4.28	1.45	1.33
29	d1	408	LMG	O8-C28	4.28	1.45	1.33
34	h1	101	DGD	O1G-C1A	4.28	1.45	1.33
29	c2	519	LMG	O8-C28	4.27	1.45	1.33
29	C1	520	LMG	O8-C28	4.26	1.45	1.33
37	b2	605	SQD	O47-C7	4.26	1.46	1.34
29	d1	411	LMG	O8-C28	4.26	1.45	1.33
33	b2	625	LHG	O8-C23	4.26	1.45	1.33
29	F2	402	LMG	O8-C28	4.26	1.45	1.33
27	d1	403	PHO	O2A-CGA	4.25	1.45	1.33
33	a1	407	LHG	O8-C23	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d1	402	LHG	O8-C23	4.25	1.45	1.33
33	a1	407	LHG	O7-C7	4.25	1.46	1.34
29	b1	624	LMG	O7-C10	4.25	1.46	1.34
29	c1	519	LMG	O8-C28	4.24	1.45	1.33
33	a2	407	LHG	O7-C7	4.24	1.46	1.34
29	B1	622	LMG	O8-C28	4.24	1.45	1.33
27	d1	403	PHO	C3D-C2D	4.24	1.47	1.39
29	M1	101	LMG	O8-C28	4.24	1.45	1.33
37	D1	409	SQD	O48-C23	4.24	1.45	1.33
29	c1	519	LMG	O7-C10	4.24	1.46	1.34
34	c2	516	DGD	O1G-C1A	4.24	1.45	1.33
37	b2	605	SQD	O48-C23	4.24	1.45	1.33
29	B1	626	LMG	O7-C10	4.23	1.46	1.34
33	l1	102	LHG	O8-C23	4.23	1.45	1.33
34	C1	517	DGD	O1G-C1A	4.23	1.45	1.33
38	V1	201	HEM	FE-NC	4.22	2.09	1.95
33	d2	403	LHG	O8-C23	4.22	1.45	1.33
34	h2	102	DGD	O1G-C1A	4.22	1.45	1.33
33	D1	405	LHG	O8-C23	4.21	1.45	1.33
27	d2	408	PHO	O2A-CGA	4.21	1.45	1.33
33	A2	405	LHG	O7-C7	4.21	1.46	1.34
34	H2	101	DGD	O1G-C1A	4.21	1.45	1.33
29	B2	620	LMG	O8-C28	4.21	1.45	1.33
34	c2	514	DGD	O1G-C1A	4.21	1.45	1.33
33	D1	404	LHG	O8-C23	4.20	1.45	1.33
29	D1	406	LMG	O8-C28	4.20	1.45	1.33
33	L2	101	LHG	O8-C23	4.20	1.45	1.33
34	H1	101	DGD	O2G-C1B	4.20	1.46	1.34
34	c1	518	DGD	O1G-C1A	4.20	1.45	1.33
29	A2	412	LMG	O7-C10	4.20	1.46	1.34
27	D1	407	PHO	C3D-C2D	4.20	1.47	1.39
34	H1	101	DGD	O1G-C1A	4.20	1.45	1.33
29	a2	412	LMG	O8-C28	4.19	1.45	1.33
29	B2	620	LMG	O7-C10	4.19	1.46	1.34
29	M1	101	LMG	O7-C10	4.19	1.46	1.34
29	F2	402	LMG	O7-C10	4.19	1.46	1.34
27	a2	416	PHO	O2A-CGA	4.19	1.45	1.33
29	d1	411	LMG	O7-C10	4.18	1.46	1.34
25	b1	608	CLA	C1D-ND	4.18	1.42	1.37
27	D1	407	PHO	O2A-CGA	4.18	1.45	1.33
34	H2	101	DGD	O2G-C1B	4.17	1.46	1.34
33	B1	621	LHG	O8-C23	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	l2	101	LHG	O8-C23	4.17	1.45	1.33
29	C2	515	LMG	O7-C10	4.17	1.46	1.34
29	I2	101	LMG	O7-C10	4.16	1.46	1.34
34	c2	516	DGD	O2G-C1B	4.16	1.46	1.34
33	d1	402	LHG	O7-C7	4.15	1.46	1.34
34	C1	516	DGD	O1G-C1A	4.15	1.45	1.33
29	a1	412	LMG	O7-C10	4.15	1.46	1.34
33	b2	625	LHG	O7-C7	4.14	1.46	1.34
25	B1	611	CLA	C1D-ND	4.14	1.42	1.37
33	D2	405	LHG	O8-C23	4.14	1.45	1.33
38	V1	201	HEM	FE-NB	4.14	2.07	1.94
33	d2	406	LHG	O8-C23	4.14	1.45	1.33
33	l2	101	LHG	O7-C7	4.14	1.46	1.34
29	a2	412	LMG	O7-C10	4.14	1.46	1.34
33	A2	405	LHG	O8-C23	4.14	1.45	1.33
37	B2	623	SQD	O47-C7	4.13	1.46	1.34
33	L1	101	LHG	O8-C23	4.13	1.45	1.33
34	c2	514	DGD	O2G-C1B	4.13	1.45	1.34
34	h2	102	DGD	O2G-C1B	4.13	1.45	1.34
33	D2	403	LHG	O8-C23	4.13	1.45	1.33
29	C1	520	LMG	O7-C10	4.13	1.45	1.34
33	B2	627	LHG	O7-C7	4.13	1.45	1.34
34	c1	518	DGD	O2G-C1B	4.12	1.45	1.34
27	D2	407	PHO	C3D-C2D	4.12	1.46	1.39
29	A1	410	LMG	O7-C10	4.11	1.45	1.34
25	B1	616	CLA	C1D-ND	4.11	1.42	1.37
29	b2	622	LMG	O7-C10	4.11	1.45	1.34
34	c2	517	DGD	O2G-C1B	4.11	1.45	1.34
29	A1	412	LMG	O7-C10	4.11	1.45	1.34
25	c2	502	CLA	C1D-ND	4.11	1.42	1.37
29	B1	622	LMG	O7-C10	4.11	1.45	1.34
38	f1	101	HEM	FE-NB	4.10	2.07	1.94
25	B2	611	CLA	C1D-ND	4.10	1.42	1.37
34	c1	514	DGD	O2G-C1B	4.09	1.45	1.34
34	C1	515	DGD	O2G-C1B	4.09	1.45	1.34
25	c1	510	CLA	C1D-ND	4.09	1.42	1.37
27	A1	408	PHO	O2A-CGA	4.09	1.45	1.33
34	h1	101	DGD	O2G-C1B	4.09	1.45	1.34
29	B2	621	LMG	O7-C10	4.08	1.45	1.34
33	D1	404	LHG	O7-C7	4.08	1.45	1.34
27	d2	408	PHO	C3D-C2D	4.08	1.46	1.39
38	V2	201	HEM	FE-NC	4.08	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a1	411	PHO	C3D-C2D	4.08	1.46	1.39
25	d1	404	CLA	C1D-ND	4.08	1.42	1.37
38	v1	201	HEM	FE-NB	4.08	2.07	1.94
33	d1	407	LHG	O8-C23	4.07	1.45	1.33
33	b1	622	LHG	O8-C23	4.07	1.45	1.33
25	B1	604	CLA	C1D-ND	4.06	1.42	1.37
29	j2	101	LMG	O7-C10	4.06	1.45	1.34
33	d2	403	LHG	O7-C7	4.06	1.45	1.34
25	a1	404	CLA	C1D-ND	4.06	1.42	1.37
25	C2	504	CLA	C1D-ND	4.06	1.42	1.37
25	C1	502	CLA	C1D-ND	4.06	1.42	1.37
25	B2	607	CLA	C1D-ND	4.06	1.42	1.37
34	C1	517	DGD	O2G-C1B	4.05	1.45	1.34
34	C1	516	DGD	O2G-C1B	4.05	1.45	1.34
29	D1	406	LMG	O7-C10	4.04	1.45	1.34
25	A2	404	CLA	C1D-ND	4.04	1.42	1.37
27	A1	408	PHO	C3D-C2D	4.04	1.46	1.39
27	A2	407	PHO	O2A-CGA	4.04	1.45	1.33
25	a1	405	CLA	C1D-ND	4.03	1.42	1.37
34	c1	520	DGD	O2G-C1B	4.03	1.45	1.34
25	a1	403	CLA	C1D-ND	4.03	1.42	1.37
25	c2	503	CLA	C1D-ND	4.03	1.42	1.37
33	D1	405	LHG	O7-C7	4.03	1.45	1.34
25	B2	606	CLA	C1D-ND	4.03	1.42	1.37
25	c1	503	CLA	C1D-ND	4.03	1.42	1.37
27	D2	407	PHO	O2A-CGA	4.02	1.45	1.33
25	C2	508	CLA	C1D-ND	4.02	1.42	1.37
25	b2	617	CLA	C1D-ND	4.02	1.42	1.37
33	b1	622	LHG	O7-C7	4.02	1.45	1.34
25	b1	607	CLA	C1D-ND	4.02	1.42	1.37
25	c2	504	CLA	C1D-ND	4.02	1.42	1.37
33	L1	101	LHG	O7-C7	4.02	1.45	1.34
38	E2	101	HEM	FE-NB	4.01	2.07	1.94
25	D1	403	CLA	C1D-ND	4.01	1.42	1.37
25	c1	515	CLA	C1D-ND	4.00	1.42	1.37
25	B2	619	CLA	C1D-ND	4.00	1.42	1.37
25	b2	613	CLA	C1D-ND	4.00	1.42	1.37
25	b2	611	CLA	C1D-ND	4.00	1.42	1.37
27	a1	411	PHO	O2A-CGA	4.00	1.45	1.33
25	C2	503	CLA	C1D-ND	3.99	1.42	1.37
25	C1	514	CLA	C1D-ND	3.99	1.42	1.37
25	b1	606	CLA	C1D-ND	3.99	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B2	604	CLA	C1D-ND	3.98	1.42	1.37
25	C2	511	CLA	C1D-ND	3.98	1.42	1.37
25	A1	405	CLA	C1D-ND	3.98	1.42	1.37
25	c2	515	CLA	C1D-ND	3.98	1.42	1.37
25	a2	404	CLA	C1D-ND	3.98	1.42	1.37
25	A1	404	CLA	C1D-ND	3.98	1.42	1.37
33	D2	403	LHG	O7-C7	3.98	1.45	1.34
33	L2	101	LHG	O7-C7	3.98	1.45	1.34
27	a2	416	PHO	C3D-C2D	3.97	1.46	1.39
25	B1	615	CLA	C1D-ND	3.97	1.42	1.37
25	c2	507	CLA	C1D-ND	3.97	1.42	1.37
25	b1	604	CLA	C1D-ND	3.97	1.42	1.37
25	C1	508	CLA	C1D-ND	3.97	1.42	1.37
25	C2	510	CLA	C1D-ND	3.97	1.42	1.37
25	C2	509	CLA	C1D-ND	3.97	1.42	1.37
25	C2	518	CLA	C1D-ND	3.97	1.42	1.37
25	b2	610	CLA	C1D-ND	3.96	1.42	1.37
25	b2	608	CLA	C1D-ND	3.96	1.42	1.37
25	b2	616	CLA	C1D-ND	3.96	1.42	1.37
25	b1	620	CLA	C1D-ND	3.96	1.42	1.37
25	c1	504	CLA	C1D-ND	3.96	1.42	1.37
25	d2	402	CLA	C1D-ND	3.96	1.42	1.37
25	c1	516	CLA	C1D-ND	3.96	1.42	1.37
25	c2	505	CLA	C1D-ND	3.96	1.42	1.37
33	d1	407	LHG	O7-C7	3.95	1.45	1.34
25	B1	608	CLA	C1D-ND	3.95	1.42	1.37
29	d1	408	LMG	O7-C10	3.95	1.45	1.34
25	b1	611	CLA	C1D-ND	3.95	1.42	1.37
25	b1	616	CLA	C1D-ND	3.95	1.42	1.37
25	c2	508	CLA	C1D-ND	3.95	1.42	1.37
25	B1	617	CLA	C1D-ND	3.94	1.42	1.37
25	C2	513	CLA	C1D-ND	3.94	1.42	1.37
25	b2	620	CLA	C1D-ND	3.94	1.42	1.37
25	C1	513	CLA	C1D-ND	3.94	1.42	1.37
25	b1	617	CLA	C1D-ND	3.94	1.42	1.37
25	C1	504	CLA	C1D-ND	3.94	1.42	1.37
25	b2	604	CLA	C1D-ND	3.94	1.42	1.37
33	B1	621	LHG	O7-C7	3.94	1.45	1.34
25	a2	405	CLA	C1D-ND	3.94	1.42	1.37
25	C2	505	CLA	C1D-ND	3.94	1.42	1.37
25	A2	402	CLA	C1D-ND	3.94	1.42	1.37
25	b1	613	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c1	506	CLA	C1D-ND	3.93	1.42	1.37
25	c1	513	CLA	C1D-ND	3.93	1.42	1.37
25	B2	605	CLA	C1D-ND	3.93	1.42	1.37
25	B2	618	CLA	C1D-ND	3.93	1.42	1.37
25	A2	403	CLA	C1D-ND	3.93	1.42	1.37
25	d2	404	CLA	C1D-ND	3.93	1.42	1.37
33	D2	405	LHG	O7-C7	3.93	1.45	1.34
25	A1	406	CLA	C1D-ND	3.93	1.42	1.37
25	b2	618	CLA	C1D-ND	3.92	1.42	1.37
25	b2	609	CLA	C1D-ND	3.92	1.42	1.37
25	B1	607	CLA	C1D-ND	3.92	1.42	1.37
25	d1	404	CLA	C4B-NB	3.92	1.42	1.37
33	d2	406	LHG	O7-C7	3.91	1.45	1.34
25	A1	403	CLA	C1D-ND	3.91	1.42	1.37
25	B2	612	CLA	C1D-ND	3.91	1.42	1.37
25	A2	402	CLA	C4B-NB	3.91	1.42	1.37
25	c1	509	CLA	C1D-ND	3.90	1.42	1.37
25	c2	511	CLA	C1D-ND	3.90	1.42	1.37
25	C1	503	CLA	C1D-ND	3.90	1.42	1.37
25	b1	610	CLA	C1D-ND	3.90	1.42	1.37
25	b1	619	CLA	C1D-ND	3.90	1.42	1.37
25	a2	413	CLA	C1D-ND	3.90	1.42	1.37
25	D2	404	CLA	C1D-ND	3.90	1.42	1.37
25	b1	605	CLA	C1D-ND	3.90	1.42	1.37
33	l1	102	LHG	O7-C7	3.89	1.45	1.34
25	c1	511	CLA	C1D-ND	3.89	1.42	1.37
25	b2	606	CLA	C1D-ND	3.89	1.42	1.37
25	b1	612	CLA	C1D-ND	3.89	1.42	1.37
25	B1	612	CLA	C1D-ND	3.89	1.42	1.37
25	A2	404	CLA	C4B-NB	3.89	1.42	1.37
25	B2	616	CLA	C1D-ND	3.88	1.42	1.37
25	c2	512	CLA	C1D-ND	3.88	1.42	1.37
27	A2	407	PHO	C3D-C2D	3.88	1.46	1.39
25	d1	406	CLA	C1D-ND	3.88	1.42	1.37
38	E1	101	HEM	FE-NB	3.88	2.06	1.94
25	B1	610	CLA	C1D-ND	3.88	1.42	1.37
25	b2	619	CLA	C1D-ND	3.88	1.42	1.37
25	B2	610	CLA	C1D-ND	3.88	1.42	1.37
25	c1	508	CLA	C1D-ND	3.87	1.42	1.37
25	C1	511	CLA	C1D-ND	3.87	1.42	1.37
25	c1	505	CLA	C1D-ND	3.87	1.42	1.37
25	c2	509	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	605	CLA	C1D-ND	3.86	1.42	1.37
25	b1	615	CLA	C1D-ND	3.86	1.42	1.37
25	b2	615	CLA	C1D-ND	3.86	1.42	1.37
25	c1	507	CLA	C1D-ND	3.86	1.42	1.37
25	c1	512	CLA	C1D-ND	3.85	1.42	1.37
25	b1	609	CLA	C1D-ND	3.85	1.42	1.37
25	b1	607	CLA	C4B-NB	3.85	1.42	1.37
25	B1	618	CLA	C1D-ND	3.85	1.42	1.37
25	B2	617	CLA	C1D-ND	3.84	1.42	1.37
25	D2	406	CLA	C1D-ND	3.84	1.42	1.37
25	c2	513	CLA	C1D-ND	3.84	1.42	1.37
25	K2	101	CLA	C1D-ND	3.83	1.42	1.37
25	A1	406	CLA	C4B-NB	3.83	1.42	1.37
25	b2	624	CLA	C1D-ND	3.82	1.42	1.37
25	C1	505	CLA	C1D-ND	3.82	1.42	1.37
38	v2	201	HEM	FE-NB	3.81	2.06	1.94
25	C2	506	CLA	C1D-ND	3.81	1.42	1.37
25	B2	608	CLA	C1D-ND	3.80	1.42	1.37
25	C2	507	CLA	C1D-ND	3.80	1.42	1.37
25	c2	510	CLA	C1D-ND	3.80	1.42	1.37
25	B1	619	CLA	C1D-ND	3.79	1.42	1.37
25	B1	613	CLA	C1D-ND	3.79	1.42	1.37
25	C1	507	CLA	C1D-ND	3.78	1.42	1.37
25	C1	506	CLA	C1D-ND	3.78	1.42	1.37
25	C1	510	CLA	C1D-ND	3.78	1.42	1.37
38	e2	101	HEM	FE-NB	3.77	2.06	1.94
25	B2	618	CLA	C4B-NB	3.77	1.42	1.37
25	B1	606	CLA	C1D-ND	3.77	1.42	1.37
25	C2	516	CLA	C1D-ND	3.77	1.42	1.37
25	c2	506	CLA	C1D-ND	3.77	1.42	1.37
25	B2	615	CLA	C1D-ND	3.75	1.42	1.37
25	C1	509	CLA	C1D-ND	3.73	1.42	1.37
25	B1	616	CLA	C4B-NB	3.73	1.42	1.37
25	B2	609	CLA	C1D-ND	3.72	1.42	1.37
25	C1	512	CLA	C1D-ND	3.69	1.42	1.37
25	B2	613	CLA	C1D-ND	3.69	1.42	1.37
25	a1	404	CLA	C4B-NB	3.69	1.42	1.37
25	c2	510	CLA	C4B-NB	3.69	1.42	1.37
25	d2	405	CLA	C1D-ND	3.68	1.42	1.37
25	B1	612	CLA	C4B-NB	3.67	1.42	1.37
25	D1	402	CLA	C1D-ND	3.67	1.42	1.37
25	A2	402	CLA	C3B-C4B	3.67	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	614	CLA	C1D-ND	3.67	1.42	1.37
25	b2	608	CLA	C4B-NB	3.66	1.42	1.37
25	b1	604	CLA	C4B-NB	3.66	1.42	1.37
25	C2	513	CLA	C4B-NB	3.65	1.42	1.37
25	A1	405	CLA	C4B-NB	3.65	1.42	1.37
25	B1	609	CLA	C1D-ND	3.65	1.42	1.37
25	a1	403	CLA	C4B-NB	3.65	1.42	1.37
25	b2	612	CLA	C1D-ND	3.64	1.42	1.37
25	b2	612	CLA	C4B-NB	3.64	1.42	1.37
25	A2	403	CLA	C4B-NB	3.63	1.42	1.37
25	B1	611	CLA	C4B-NB	3.62	1.42	1.37
25	A1	403	CLA	C4B-NB	3.61	1.42	1.37
25	B2	614	CLA	C1D-ND	3.61	1.42	1.37
25	b1	619	CLA	C4B-NB	3.61	1.42	1.37
25	b2	614	CLA	C1D-ND	3.60	1.42	1.37
25	C1	507	CLA	C4B-NB	3.59	1.42	1.37
25	C1	504	CLA	C4B-NB	3.58	1.42	1.37
25	b1	620	CLA	C4B-NB	3.58	1.42	1.37
25	b2	616	CLA	C4B-NB	3.58	1.42	1.37
25	b2	619	CLA	C4B-NB	3.58	1.42	1.37
25	D2	401	CLA	C1D-ND	3.57	1.42	1.37
25	B2	607	CLA	C4B-NB	3.57	1.42	1.37
25	B1	613	CLA	C4B-NB	3.56	1.42	1.37
25	d1	401	CLA	C4B-NB	3.56	1.42	1.37
25	b1	614	CLA	C1D-ND	3.56	1.42	1.37
25	D2	406	CLA	C4B-NB	3.55	1.42	1.37
25	c2	506	CLA	C4B-NB	3.54	1.42	1.37
25	b1	609	CLA	C4B-NB	3.54	1.42	1.37
25	B2	613	CLA	C4B-NB	3.53	1.42	1.37
25	C1	510	CLA	C4B-NB	3.53	1.42	1.37
25	B2	616	CLA	C4B-NB	3.53	1.42	1.37
27	d1	403	PHO	C3A-C2A	-3.53	1.51	1.54
25	d1	404	CLA	C3B-C4B	3.52	1.51	1.42
25	B1	604	CLA	C4B-NB	3.51	1.42	1.37
25	B1	619	CLA	C4B-NB	3.51	1.42	1.37
38	E1	101	HEM	FE-NC	3.51	2.07	1.95
25	C2	507	CLA	C4B-NB	3.51	1.42	1.37
25	d1	406	CLA	C4B-NB	3.51	1.42	1.37
25	B1	618	CLA	C4B-NB	3.51	1.42	1.37
25	C1	511	CLA	C4B-NB	3.50	1.42	1.37
25	b2	615	CLA	C4B-NB	3.49	1.42	1.37
25	B2	615	CLA	C4B-NB	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c1	506	CLA	C4B-NB	3.49	1.42	1.37
25	c1	508	CLA	C4B-NB	3.49	1.42	1.37
38	v1	201	HEM	FE-NC	3.49	2.06	1.95
25	a1	404	CLA	C3B-C4B	3.48	1.50	1.42
25	c2	503	CLA	C4B-NB	3.48	1.42	1.37
25	b2	620	CLA	C4B-NB	3.48	1.42	1.37
25	B1	607	CLA	C4B-NB	3.48	1.42	1.37
25	d2	402	CLA	C4B-NB	3.48	1.42	1.37
25	b1	617	CLA	C4B-NB	3.47	1.42	1.37
25	D2	404	CLA	C4B-NB	3.47	1.42	1.37
25	a1	403	CLA	C3B-C4B	3.47	1.50	1.42
25	c1	515	CLA	C4B-NB	3.46	1.42	1.37
25	c2	508	CLA	C4B-NB	3.46	1.42	1.37
25	b2	618	CLA	C4B-NB	3.46	1.42	1.37
25	d2	404	CLA	C4B-NB	3.46	1.42	1.37
25	B1	610	CLA	C4B-NB	3.45	1.42	1.37
25	C2	505	CLA	C4B-NB	3.45	1.42	1.37
25	A2	404	CLA	C3B-C4B	3.45	1.50	1.42
25	d1	401	CLA	C1D-ND	3.45	1.42	1.37
25	c2	502	CLA	C4B-NB	3.45	1.42	1.37
25	C1	513	CLA	C4B-NB	3.45	1.42	1.37
25	A1	403	CLA	C3B-C4B	3.44	1.50	1.42
25	B1	610	CLA	C3B-C4B	3.44	1.50	1.42
25	c1	513	CLA	C4B-NB	3.43	1.42	1.37
25	A1	405	CLA	C3B-C4B	3.43	1.50	1.42
25	C2	518	CLA	C4B-NB	3.43	1.42	1.37
25	C1	508	CLA	C4B-NB	3.43	1.42	1.37
25	B1	605	CLA	C4B-NB	3.43	1.42	1.37
25	c1	505	CLA	C4B-NB	3.43	1.42	1.37
25	B2	610	CLA	C4B-NB	3.43	1.42	1.37
25	b2	613	CLA	C4B-NB	3.43	1.42	1.37
25	b2	604	CLA	C4B-NB	3.42	1.42	1.37
25	C2	503	CLA	C4B-NB	3.42	1.42	1.37
25	B1	614	CLA	C4B-NB	3.42	1.42	1.37
25	c2	507	CLA	C4B-NB	3.40	1.42	1.37
25	A1	404	CLA	C4B-NB	3.40	1.42	1.37
25	c2	511	CLA	C4B-NB	3.40	1.42	1.37
25	b1	610	CLA	C4B-NB	3.40	1.42	1.37
25	b1	608	CLA	C4B-NB	3.39	1.42	1.37
25	B2	604	CLA	C4B-NB	3.39	1.42	1.37
25	c2	504	CLA	C4B-NB	3.39	1.42	1.37
25	B2	606	CLA	C4B-NB	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C2	508	CLA	C4B-NB	3.39	1.42	1.37
25	B2	614	CLA	C4B-NB	3.39	1.41	1.37
25	c2	513	CLA	C4B-NB	3.39	1.41	1.37
25	b1	605	CLA	C4B-NB	3.39	1.41	1.37
25	B2	617	CLA	C4B-NB	3.38	1.41	1.37
25	A2	403	CLA	C3B-C4B	3.38	1.50	1.42
25	C2	509	CLA	C4B-NB	3.38	1.41	1.37
25	b2	617	CLA	C4B-NB	3.38	1.41	1.37
25	d2	405	CLA	C4B-NB	3.38	1.41	1.37
25	B2	605	CLA	C4B-NB	3.38	1.41	1.37
25	b1	612	CLA	C4B-NB	3.38	1.41	1.37
25	a2	413	CLA	C4B-NB	3.37	1.41	1.37
25	c2	512	CLA	C4B-NB	3.37	1.41	1.37
25	B2	611	CLA	C4B-NB	3.36	1.41	1.37
38	v1	201	HEM	FE-NA	3.36	2.06	1.95
25	B1	615	CLA	C4B-NB	3.36	1.41	1.37
25	c1	512	CLA	C4B-NB	3.36	1.41	1.37
25	B2	609	CLA	C4B-NB	3.36	1.41	1.37
25	D2	401	CLA	C4B-NB	3.36	1.41	1.37
25	c1	507	CLA	C4B-NB	3.35	1.41	1.37
25	B2	612	CLA	C4B-NB	3.35	1.41	1.37
25	c1	510	CLA	C4B-NB	3.35	1.41	1.37
25	K2	101	CLA	C4B-NB	3.35	1.41	1.37
25	b2	606	CLA	C4B-NB	3.34	1.41	1.37
25	B1	609	CLA	C4B-NB	3.34	1.41	1.37
25	c1	509	CLA	C4B-NB	3.33	1.41	1.37
25	C1	514	CLA	C4B-NB	3.33	1.41	1.37
25	C2	506	CLA	C4B-NB	3.33	1.41	1.37
25	C2	511	CLA	C4B-NB	3.33	1.41	1.37
25	B1	608	CLA	C4B-NB	3.33	1.41	1.37
38	e2	101	HEM	FE-NA	3.33	2.06	1.95
25	B2	619	CLA	C4B-NB	3.33	1.41	1.37
25	b2	610	CLA	C4B-NB	3.32	1.41	1.37
25	b2	611	CLA	C4B-NB	3.32	1.41	1.37
25	a2	404	CLA	C3B-C4B	3.32	1.50	1.42
27	D1	407	PHO	C3A-C2A	-3.31	1.51	1.54
25	C1	506	CLA	C4B-NB	3.31	1.41	1.37
25	b1	614	CLA	C4B-NB	3.31	1.41	1.37
25	b2	614	CLA	C4B-NB	3.31	1.41	1.37
25	a2	404	CLA	C4B-NB	3.31	1.41	1.37
25	B2	608	CLA	C4B-NB	3.31	1.41	1.37
25	C1	509	CLA	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b1	611	CLA	C4B-NB	3.30	1.41	1.37
25	D1	403	CLA	C4B-NB	3.30	1.41	1.37
25	c2	515	CLA	C4B-NB	3.30	1.41	1.37
25	c2	509	CLA	C4B-NB	3.29	1.41	1.37
25	B1	617	CLA	C4B-NB	3.29	1.41	1.37
38	f1	101	HEM	FE-NA	3.29	2.06	1.95
25	b2	624	CLA	C4B-NB	3.29	1.41	1.37
38	E1	101	HEM	FE-NA	3.29	2.06	1.95
25	c1	516	CLA	C4B-NB	3.29	1.41	1.37
25	b1	606	CLA	C4B-NB	3.28	1.41	1.37
25	b1	613	CLA	C4B-NB	3.28	1.41	1.37
25	C2	504	CLA	C4B-NB	3.28	1.41	1.37
25	C2	516	CLA	C4B-NB	3.28	1.41	1.37
25	b1	607	CLA	C3B-C4B	3.28	1.50	1.42
25	C1	505	CLA	C4B-NB	3.27	1.41	1.37
25	b2	609	CLA	C4B-NB	3.27	1.41	1.37
25	A1	406	CLA	C3B-C4B	3.27	1.50	1.42
34	C2	512	DGD	O1G-C1A	3.27	1.46	1.33
38	E2	101	HEM	FE-NA	3.26	2.06	1.95
25	b1	616	CLA	C4B-NB	3.26	1.41	1.37
25	B1	606	CLA	C4B-NB	3.26	1.41	1.37
37	D2	402	SQD	O48-C23	3.26	1.45	1.33
25	B2	607	CLA	C3B-C4B	3.26	1.50	1.42
25	C1	512	CLA	C4B-NB	3.26	1.41	1.37
25	C2	510	CLA	C4B-NB	3.25	1.41	1.37
25	a1	405	CLA	C4B-NB	3.25	1.41	1.37
25	c2	505	CLA	C4B-NB	3.25	1.41	1.37
25	C1	503	CLA	C4B-NB	3.24	1.41	1.37
33	a2	407	LHG	O8-C23	3.24	1.45	1.33
25	C1	510	CLA	C3B-C4B	3.23	1.50	1.42
25	b1	615	CLA	C4B-NB	3.23	1.41	1.37
25	C1	502	CLA	C4B-NB	3.22	1.41	1.37
25	c1	511	CLA	C4B-NB	3.22	1.41	1.37
38	e2	101	HEM	FE-NC	3.21	2.06	1.95
25	B1	618	CLA	C3B-C4B	3.20	1.50	1.42
29	c2	519	LMG	O7-C8	-3.19	1.43	1.46
25	D1	402	CLA	C4B-NB	3.18	1.41	1.37
25	d2	402	CLA	C3B-C4B	3.18	1.50	1.42
25	b1	620	CLA	C3B-C4B	3.17	1.50	1.42
25	c1	504	CLA	C4B-NB	3.17	1.41	1.37
25	B2	613	CLA	C4D-ND	-3.16	1.33	1.37
25	B2	618	CLA	C3B-C4B	3.16	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a2	413	CLA	C3B-C4B	3.16	1.50	1.42
38	f1	101	HEM	FE-NC	3.15	2.05	1.95
25	c2	510	CLA	C3B-C4B	3.15	1.50	1.42
25	D1	402	CLA	C4D-ND	-3.14	1.33	1.37
38	V2	201	HEM	FE-NA	3.13	2.05	1.95
25	b2	619	CLA	C3B-C4B	3.13	1.50	1.42
25	B1	612	CLA	C3B-C4B	3.12	1.50	1.42
25	C2	513	CLA	C3B-C4B	3.12	1.50	1.42
38	v2	201	HEM	CAB-C3B	3.12	1.55	1.47
25	B2	610	CLA	C3B-C4B	3.12	1.50	1.42
25	b1	616	CLA	C3B-C4B	3.11	1.50	1.42
25	D2	406	CLA	C3B-C4B	3.10	1.50	1.42
25	B1	611	CLA	C3B-C4B	3.10	1.50	1.42
25	B2	619	CLA	C3B-C4B	3.10	1.50	1.42
25	d2	404	CLA	C3B-C4B	3.10	1.50	1.42
25	B1	604	CLA	C3B-C4B	3.09	1.50	1.42
25	c2	502	CLA	C3B-C4B	3.09	1.50	1.42
25	c1	508	CLA	C4D-ND	-3.09	1.33	1.37
27	a2	416	PHO	C3A-C2A	-3.09	1.51	1.54
25	b1	604	CLA	C3B-C4B	3.09	1.50	1.42
25	b1	610	CLA	C3B-C4B	3.08	1.50	1.42
25	b1	619	CLA	C3B-C4B	3.08	1.50	1.42
25	B2	606	CLA	C3B-C4B	3.08	1.50	1.42
27	D2	407	PHO	C3A-C2A	-3.08	1.51	1.54
27	A2	407	PHO	C3A-C2A	-3.08	1.51	1.54
25	B1	619	CLA	C3B-C4B	3.08	1.50	1.42
25	a2	405	CLA	C4B-NB	3.08	1.41	1.37
25	B2	612	CLA	C3B-C4B	3.07	1.50	1.42
25	b2	624	CLA	C3B-C4B	3.07	1.50	1.42
25	B1	608	CLA	C3B-C4B	3.07	1.49	1.42
38	e2	101	HEM	CAC-C3C	3.07	1.55	1.47
25	b1	608	CLA	C3B-C4B	3.07	1.49	1.42
25	b1	605	CLA	C3B-C4B	3.06	1.49	1.42
38	V1	201	HEM	CAB-C3B	3.06	1.55	1.47
25	d1	401	CLA	C4D-ND	-3.06	1.33	1.37
25	A1	404	CLA	C4D-ND	-3.05	1.33	1.37
27	d2	408	PHO	C3A-C2A	-3.05	1.51	1.54
38	v1	201	HEM	CAB-C3B	3.05	1.55	1.47
25	B2	604	CLA	C3B-C4B	3.05	1.49	1.42
38	E2	101	HEM	CAC-C3C	3.05	1.55	1.47
25	d1	406	CLA	C3B-C4B	3.05	1.49	1.42
25	B1	616	CLA	C3B-C4B	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E1	101	HEM	CAC-C3C	3.04	1.55	1.47
25	B1	607	CLA	C3B-C4B	3.04	1.49	1.42
25	c1	506	CLA	C3B-C4B	3.04	1.49	1.42
25	c2	509	CLA	C4D-ND	-3.03	1.33	1.37
25	C1	507	CLA	C3B-C4B	3.03	1.49	1.42
25	D1	403	CLA	C3B-C4B	3.03	1.49	1.42
25	A1	404	CLA	C3B-C4B	3.02	1.49	1.42
25	B2	616	CLA	C3B-C4B	3.02	1.49	1.42
25	B1	619	CLA	C4D-ND	-3.02	1.33	1.37
38	v2	201	HEM	CAC-C3C	3.02	1.55	1.47
25	c1	503	CLA	C4B-NB	3.02	1.41	1.37
25	B2	606	CLA	C4D-ND	-3.02	1.33	1.37
25	B2	615	CLA	C3B-C4B	3.02	1.49	1.42
25	A1	403	CLA	C4D-ND	-3.01	1.33	1.37
25	b2	616	CLA	C3B-C4B	3.01	1.49	1.42
38	v1	201	HEM	CAC-C3C	3.01	1.55	1.47
25	A1	406	CLA	C4D-ND	-3.00	1.33	1.37
38	f1	101	HEM	CAC-C3C	3.00	1.55	1.47
25	b2	608	CLA	C3B-C4B	3.00	1.49	1.42
25	C2	506	CLA	C4D-ND	-3.00	1.33	1.37
25	B2	613	CLA	C3B-C4B	3.00	1.49	1.42
25	b1	612	CLA	C3B-C4B	2.99	1.49	1.42
38	V2	201	HEM	CAC-C3C	2.99	1.55	1.47
25	c2	507	CLA	C4D-ND	-2.98	1.33	1.37
25	b1	609	CLA	C4D-ND	-2.98	1.33	1.37
25	b2	611	CLA	C3B-C4B	2.98	1.49	1.42
38	E2	101	HEM	FE-NC	2.98	2.05	1.95
25	c1	512	CLA	C3B-C4B	2.97	1.49	1.42
25	C1	505	CLA	C4D-ND	-2.97	1.33	1.37
25	C1	504	CLA	C4D-ND	-2.97	1.33	1.37
25	A2	402	CLA	C4D-ND	-2.97	1.33	1.37
25	D2	404	CLA	C3B-C4B	2.97	1.49	1.42
37	D1	409	SQD	C6-S	-2.96	1.66	1.77
25	b2	604	CLA	C3B-C4B	2.96	1.49	1.42
25	B2	618	CLA	C4D-ND	-2.96	1.33	1.37
25	C1	504	CLA	C3B-C4B	2.96	1.49	1.42
25	b2	617	CLA	C3B-C4B	2.96	1.49	1.42
25	c1	512	CLA	C4D-ND	-2.96	1.33	1.37
25	B1	612	CLA	C4D-ND	-2.96	1.33	1.37
25	B1	606	CLA	C4D-ND	-2.96	1.33	1.37
25	C1	512	CLA	C3B-C4B	2.96	1.49	1.42
25	b2	620	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	e2	101	HEM	CAB-C3B	2.96	1.55	1.47
25	C2	507	CLA	C3B-C4B	2.95	1.49	1.42
25	b2	613	CLA	C4D-ND	-2.95	1.33	1.37
27	a1	411	PHO	C3A-C2A	-2.95	1.52	1.54
25	c2	515	CLA	C3B-C4B	2.95	1.49	1.42
25	b1	612	CLA	C4D-ND	-2.95	1.33	1.37
38	V1	201	HEM	CAC-C3C	2.95	1.55	1.47
25	C2	506	CLA	C3B-C4B	2.94	1.49	1.42
25	c1	515	CLA	C3B-C4B	2.94	1.49	1.42
25	C2	518	CLA	C3B-C4B	2.94	1.49	1.42
25	c2	505	CLA	C3B-C4B	2.94	1.49	1.42
25	d2	404	CLA	C4D-ND	-2.94	1.33	1.37
25	C2	504	CLA	C3B-C4B	2.94	1.49	1.42
25	B2	609	CLA	C4D-ND	-2.94	1.33	1.37
25	C1	510	CLA	C4D-ND	-2.94	1.33	1.37
25	c1	504	CLA	C3B-C4B	2.94	1.49	1.42
25	b1	613	CLA	C4D-ND	-2.94	1.33	1.37
25	B1	617	CLA	C3B-C4B	2.93	1.49	1.42
25	C1	514	CLA	C3B-C4B	2.93	1.49	1.42
25	c1	505	CLA	C4D-ND	-2.93	1.33	1.37
25	c1	504	CLA	C4D-ND	-2.93	1.33	1.37
25	C1	503	CLA	C3B-C4B	2.93	1.49	1.42
25	C1	506	CLA	C4D-ND	-2.93	1.33	1.37
25	C1	511	CLA	C4D-ND	-2.93	1.33	1.37
25	B1	605	CLA	C3B-C4B	2.93	1.49	1.42
25	c1	513	CLA	C3B-C4B	2.93	1.49	1.42
38	E1	101	HEM	CAB-C3B	2.93	1.55	1.47
25	B2	614	CLA	C1B-C2B	2.92	1.50	1.43
25	c1	516	CLA	C3B-C4B	2.92	1.49	1.42
25	B1	615	CLA	C3B-C4B	2.92	1.49	1.42
25	c1	510	CLA	C4D-ND	-2.92	1.33	1.37
25	C1	511	CLA	C3B-C4B	2.92	1.49	1.42
25	b2	619	CLA	C4D-ND	-2.92	1.33	1.37
25	b2	609	CLA	C4D-ND	-2.92	1.33	1.37
25	D1	403	CLA	C4D-ND	-2.92	1.33	1.37
25	C2	503	CLA	C3B-C4B	2.92	1.49	1.42
25	d1	404	CLA	C4D-ND	-2.92	1.33	1.37
25	b2	611	CLA	C4D-ND	-2.92	1.33	1.37
25	a1	405	CLA	C4D-ND	-2.92	1.33	1.37
25	B2	611	CLA	C3B-C4B	2.92	1.49	1.42
25	c2	511	CLA	C3B-C4B	2.92	1.49	1.42
25	B2	619	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a2	405	CLA	C3B-C4B	2.91	1.49	1.42
25	b2	610	CLA	C3B-C4B	2.91	1.49	1.42
25	b2	613	CLA	C3B-C4B	2.91	1.49	1.42
38	E2	101	HEM	CAB-C3B	2.91	1.55	1.47
25	B2	608	CLA	C3B-C4B	2.91	1.49	1.42
25	B1	613	CLA	C4D-ND	-2.91	1.33	1.37
27	A1	408	PHO	C3A-C2A	-2.91	1.52	1.54
25	d2	405	CLA	C4D-ND	-2.91	1.33	1.37
25	c2	506	CLA	C4D-ND	-2.91	1.33	1.37
25	c1	515	CLA	C4D-ND	-2.91	1.33	1.37
37	B2	623	SQD	C6-S	-2.91	1.66	1.77
25	B2	608	CLA	C4D-ND	-2.91	1.33	1.37
25	c1	508	CLA	C3B-C4B	2.91	1.49	1.42
25	b1	611	CLA	C4D-ND	-2.90	1.33	1.37
25	B1	609	CLA	C3B-C4B	2.90	1.49	1.42
25	b1	609	CLA	C3B-C4B	2.90	1.49	1.42
25	a2	404	CLA	C4D-ND	-2.90	1.33	1.37
25	a2	413	CLA	C4D-ND	-2.90	1.33	1.37
25	b2	617	CLA	C4D-ND	-2.90	1.33	1.37
25	B2	615	CLA	C4D-ND	-2.90	1.33	1.37
25	B2	605	CLA	C4D-ND	-2.90	1.33	1.37
25	B2	605	CLA	C3B-C4B	2.90	1.49	1.42
25	c2	507	CLA	C3B-C4B	2.90	1.49	1.42
37	D2	402	SQD	C6-S	-2.90	1.66	1.77
25	c2	504	CLA	C3B-C4B	2.90	1.49	1.42
25	C2	508	CLA	C3B-C4B	2.90	1.49	1.42
25	B1	606	CLA	C3B-C4B	2.90	1.49	1.42
25	C1	507	CLA	C4D-ND	-2.90	1.33	1.37
25	b2	608	CLA	C4D-ND	-2.90	1.33	1.37
25	c1	511	CLA	C3B-C4B	2.90	1.49	1.42
25	C2	505	CLA	C3B-C4B	2.89	1.49	1.42
25	a2	405	CLA	C4D-ND	-2.89	1.33	1.37
25	d2	402	CLA	C4D-ND	-2.89	1.33	1.37
25	B2	609	CLA	C3B-C4B	2.89	1.49	1.42
25	C2	510	CLA	C4D-ND	-2.89	1.33	1.37
25	b1	605	CLA	C4D-ND	-2.89	1.33	1.37
25	K2	101	CLA	C3B-C4B	2.89	1.49	1.42
25	C2	516	CLA	C4D-ND	-2.89	1.33	1.37
25	B2	610	CLA	C4D-ND	-2.89	1.33	1.37
25	b1	614	CLA	C3B-C4B	2.89	1.49	1.42
25	B1	611	CLA	C4D-ND	-2.89	1.33	1.37
25	C2	511	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b1	615	CLA	C3B-C4B	2.89	1.49	1.42
25	d1	401	CLA	C3B-C4B	2.88	1.49	1.42
25	c2	513	CLA	C3B-C4B	2.88	1.49	1.42
25	b2	612	CLA	C3B-C4B	2.88	1.49	1.42
25	A2	402	CLA	CHC-C1C	2.88	1.44	1.38
25	b2	606	CLA	C3B-C4B	2.88	1.49	1.42
25	B1	614	CLA	C3B-C4B	2.88	1.49	1.42
25	c1	505	CLA	C3B-C4B	2.88	1.49	1.42
25	b2	614	CLA	C4D-ND	-2.88	1.33	1.37
25	B1	610	CLA	C4D-ND	-2.87	1.33	1.37
25	B1	615	CLA	C4D-ND	-2.87	1.33	1.37
25	C1	502	CLA	C4D-ND	-2.87	1.33	1.37
25	B1	608	CLA	C4D-ND	-2.87	1.33	1.37
25	c2	506	CLA	C3B-C4B	2.87	1.49	1.42
25	c2	509	CLA	C3B-C4B	2.87	1.49	1.42
25	B1	609	CLA	C4D-ND	-2.87	1.33	1.37
25	C2	503	CLA	C4D-ND	-2.87	1.33	1.37
25	b1	611	CLA	C3B-C4B	2.87	1.49	1.42
25	c2	503	CLA	C3B-C4B	2.87	1.49	1.42
25	D2	401	CLA	C4D-ND	-2.87	1.33	1.37
25	b1	617	CLA	C3B-C4B	2.87	1.49	1.42
38	f1	101	HEM	CAB-C3B	2.86	1.55	1.47
25	a1	403	CLA	CHC-C1C	2.86	1.44	1.38
25	C1	513	CLA	C4D-ND	-2.86	1.33	1.37
25	C2	510	CLA	C3B-C4B	2.86	1.49	1.42
25	B1	605	CLA	C4D-ND	-2.86	1.33	1.37
25	C2	507	CLA	C4D-ND	-2.86	1.33	1.37
25	c2	511	CLA	C4D-ND	-2.86	1.33	1.37
38	V2	201	HEM	CAB-C3B	2.86	1.55	1.47
25	c2	512	CLA	C3B-C4B	2.86	1.49	1.42
25	b1	608	CLA	C4D-ND	-2.86	1.33	1.37
25	B2	616	CLA	C4D-ND	-2.86	1.33	1.37
25	b1	617	CLA	C4D-ND	-2.86	1.33	1.37
25	c1	506	CLA	C4D-ND	-2.86	1.33	1.37
25	c2	513	CLA	C4D-ND	-2.86	1.33	1.37
25	b1	616	CLA	C4D-ND	-2.86	1.33	1.37
25	c1	510	CLA	C3B-C4B	2.86	1.49	1.42
25	B2	617	CLA	C3B-C4B	2.86	1.49	1.42
25	b2	606	CLA	C4D-ND	-2.85	1.33	1.37
25	b2	612	CLA	C4D-ND	-2.85	1.33	1.37
25	b2	615	CLA	C3B-C4B	2.85	1.49	1.42
25	b2	614	CLA	C1B-C2B	2.85	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A1	405	CLA	C4D-ND	-2.85	1.33	1.37
25	c2	512	CLA	C4D-ND	-2.85	1.33	1.37
25	c1	516	CLA	C4D-ND	-2.85	1.33	1.37
25	B2	611	CLA	C4D-ND	-2.85	1.33	1.37
25	C1	506	CLA	C1B-C2B	2.85	1.50	1.43
25	C1	509	CLA	C4D-ND	-2.84	1.33	1.37
25	C1	514	CLA	C4D-ND	-2.84	1.33	1.37
25	b1	614	CLA	C4D-ND	-2.84	1.33	1.37
25	C2	516	CLA	C3B-C4B	2.84	1.49	1.42
25	c1	507	CLA	C4D-ND	-2.84	1.33	1.37
25	c1	503	CLA	C4D-ND	-2.84	1.33	1.37
25	b1	610	CLA	C4D-ND	-2.83	1.33	1.37
25	c2	515	CLA	C4D-ND	-2.83	1.33	1.37
25	b1	606	CLA	C3B-C4B	2.83	1.49	1.42
25	a1	403	CLA	C4D-ND	-2.83	1.33	1.37
25	A2	403	CLA	C4D-ND	-2.83	1.33	1.37
25	D2	406	CLA	C4D-ND	-2.83	1.33	1.37
25	b1	613	CLA	C3B-C4B	2.82	1.49	1.42
25	c2	512	CLA	C1B-C2B	2.82	1.49	1.43
25	c1	513	CLA	C4D-ND	-2.82	1.33	1.37
25	d2	405	CLA	C3B-C4B	2.82	1.49	1.42
25	b2	618	CLA	C4D-ND	-2.82	1.33	1.37
25	b2	604	CLA	C4D-ND	-2.82	1.33	1.37
25	c2	508	CLA	C1B-C2B	2.82	1.49	1.43
25	B2	604	CLA	C4D-ND	-2.82	1.33	1.37
25	b2	624	CLA	C4D-ND	-2.82	1.33	1.37
25	c2	502	CLA	C4D-ND	-2.82	1.33	1.37
25	b1	604	CLA	C4D-ND	-2.81	1.33	1.37
25	b2	618	CLA	C3B-C4B	2.81	1.49	1.42
25	b2	609	CLA	C3B-C4B	2.81	1.49	1.42
25	d1	406	CLA	C4D-ND	-2.81	1.33	1.37
37	b2	605	SQD	C6-S	-2.81	1.67	1.77
25	C1	512	CLA	C4D-ND	-2.81	1.33	1.37
25	b1	620	CLA	C4D-ND	-2.81	1.33	1.37
25	b2	615	CLA	C4D-ND	-2.81	1.33	1.37
25	A1	403	CLA	CHC-C1C	2.81	1.44	1.38
25	C2	508	CLA	C4D-ND	-2.81	1.33	1.37
25	B2	617	CLA	C4D-ND	-2.80	1.33	1.37
25	D2	404	CLA	C4D-ND	-2.80	1.33	1.37
25	B1	615	CLA	C1B-C2B	2.80	1.49	1.43
25	c1	511	CLA	C1B-C2B	2.80	1.49	1.43
25	D2	401	CLA	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a1	404	CLA	C4D-ND	-2.80	1.33	1.37
25	b1	619	CLA	C4D-ND	-2.80	1.33	1.37
25	C2	511	CLA	C3B-C4B	2.80	1.49	1.42
25	C1	505	CLA	C3B-C4B	2.80	1.49	1.42
25	B1	616	CLA	C4D-ND	-2.80	1.33	1.37
25	A2	404	CLA	C4D-ND	-2.80	1.33	1.37
25	C2	513	CLA	C4D-ND	-2.80	1.33	1.37
25	b1	615	CLA	C4D-ND	-2.79	1.33	1.37
25	c2	510	CLA	C4D-ND	-2.79	1.33	1.37
25	D2	401	CLA	C1B-C2B	2.79	1.49	1.43
25	C1	513	CLA	C1B-C2B	2.79	1.49	1.43
25	C2	509	CLA	C3B-C4B	2.79	1.49	1.42
25	b2	620	CLA	C3B-C4B	2.79	1.49	1.42
25	b1	620	CLA	C1B-C2B	2.79	1.49	1.43
25	c1	509	CLA	C3B-C4B	2.79	1.49	1.42
25	C1	513	CLA	C3B-C4B	2.79	1.49	1.42
25	b1	606	CLA	C4D-ND	-2.78	1.33	1.37
25	B2	612	CLA	C4D-ND	-2.78	1.33	1.37
25	c2	508	CLA	C4D-ND	-2.78	1.33	1.37
25	c1	509	CLA	C1B-C2B	2.78	1.49	1.43
25	a1	405	CLA	C3B-C4B	2.78	1.49	1.42
25	C1	503	CLA	C4D-ND	-2.77	1.33	1.37
25	c1	505	CLA	C1B-C2B	2.77	1.49	1.43
25	c2	504	CLA	C4D-ND	-2.77	1.33	1.37
25	B1	613	CLA	C3B-C4B	2.77	1.49	1.42
25	b2	618	CLA	C1B-C2B	2.77	1.49	1.43
25	b2	614	CLA	C3B-C4B	2.77	1.49	1.42
25	B1	614	CLA	C4D-ND	-2.77	1.33	1.37
25	B1	614	CLA	C1B-C2B	2.76	1.49	1.43
25	C1	502	CLA	C1B-C2B	2.76	1.49	1.43
25	D1	402	CLA	C1B-C2B	2.76	1.49	1.43
25	B1	607	CLA	C1B-C2B	2.76	1.49	1.43
25	C1	511	CLA	C1B-C2B	2.76	1.49	1.43
25	c2	511	CLA	C1B-C2B	2.76	1.49	1.43
25	b2	609	CLA	C1B-C2B	2.76	1.49	1.43
25	B1	618	CLA	C4D-ND	-2.76	1.33	1.37
25	c1	515	CLA	C1B-C2B	2.76	1.49	1.43
25	c2	502	CLA	C1B-C2B	2.76	1.49	1.43
25	C1	502	CLA	C3B-C4B	2.76	1.49	1.42
25	C2	505	CLA	C1B-C2B	2.76	1.49	1.43
25	C2	516	CLA	C1B-C2B	2.75	1.49	1.43
25	c1	513	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c2	503	CLA	C4D-ND	-2.74	1.33	1.37
25	c1	503	CLA	C3B-C4B	2.74	1.49	1.42
25	c1	512	CLA	C1B-C2B	2.74	1.49	1.43
25	b2	616	CLA	C4D-ND	-2.74	1.33	1.37
25	c2	508	CLA	C3B-C4B	2.74	1.49	1.42
25	D1	402	CLA	C3B-C4B	2.74	1.49	1.42
25	B1	617	CLA	C1B-C2B	2.74	1.49	1.43
25	c1	507	CLA	C3B-C4B	2.74	1.49	1.42
25	C1	504	CLA	C1B-C2B	2.74	1.49	1.43
25	c2	504	CLA	C1B-C2B	2.74	1.49	1.43
25	a2	404	CLA	CHC-C1C	2.74	1.44	1.38
25	C2	510	CLA	C1B-C2B	2.74	1.49	1.43
25	b1	617	CLA	C1B-C2B	2.74	1.49	1.43
25	c1	511	CLA	C4D-ND	-2.73	1.33	1.37
25	C2	505	CLA	C4D-ND	-2.73	1.33	1.37
25	B1	605	CLA	C1B-C2B	2.73	1.49	1.43
25	C1	503	CLA	C1B-C2B	2.73	1.49	1.43
25	C2	504	CLA	C1B-C2B	2.73	1.49	1.43
25	K2	101	CLA	C4D-ND	-2.73	1.33	1.37
25	C1	512	CLA	C1B-C2B	2.73	1.49	1.43
25	B2	615	CLA	C1B-C2B	2.73	1.49	1.43
25	B1	604	CLA	C1B-C2B	2.73	1.49	1.43
25	C2	518	CLA	C1B-C2B	2.72	1.49	1.43
25	B2	618	CLA	C1B-C2B	2.72	1.49	1.43
25	B2	608	CLA	C1B-C2B	2.72	1.49	1.43
25	b1	608	CLA	C1B-C2B	2.72	1.49	1.43
25	B2	617	CLA	C1B-C2B	2.72	1.49	1.43
25	C2	503	CLA	C1B-C2B	2.72	1.49	1.43
25	C1	505	CLA	C1B-C2B	2.72	1.49	1.43
25	b2	610	CLA	C4D-ND	-2.72	1.34	1.37
25	C2	507	CLA	C1B-C2B	2.72	1.49	1.43
25	C2	518	CLA	C4D-ND	-2.72	1.34	1.37
25	C1	506	CLA	C3B-C4B	2.72	1.49	1.42
25	b2	604	CLA	C1B-C2B	2.72	1.49	1.43
25	C1	508	CLA	C4D-ND	-2.72	1.34	1.37
25	c2	505	CLA	C1B-C2B	2.72	1.49	1.43
25	b1	615	CLA	C1B-C2B	2.72	1.49	1.43
25	c1	510	CLA	C1B-C2B	2.71	1.49	1.43
25	C2	509	CLA	C4D-ND	-2.71	1.34	1.37
25	b1	609	CLA	C1B-C2B	2.71	1.49	1.43
25	d2	405	CLA	C1B-C2B	2.71	1.49	1.43
25	C1	508	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c2	505	CLA	C4D-ND	-2.71	1.34	1.37
25	B2	614	CLA	C3B-C4B	2.71	1.49	1.42
25	c1	509	CLA	C4D-ND	-2.71	1.34	1.37
25	C1	508	CLA	C3B-C4B	2.70	1.49	1.42
25	B1	619	CLA	C1B-C2B	2.70	1.49	1.43
25	B2	614	CLA	C4D-ND	-2.70	1.34	1.37
25	C1	509	CLA	C3B-C4B	2.70	1.49	1.42
25	D2	404	CLA	C1B-C2B	2.69	1.49	1.43
25	c2	503	CLA	C1B-C2B	2.69	1.49	1.43
25	B2	604	CLA	C1B-C2B	2.69	1.49	1.43
25	B1	604	CLA	C4D-ND	-2.69	1.34	1.37
25	d1	401	CLA	C1B-C2B	2.69	1.49	1.43
25	K2	101	CLA	C1B-C2B	2.69	1.49	1.43
25	b2	610	CLA	C1B-C2B	2.69	1.49	1.43
25	C1	509	CLA	CMB-C2B	-2.69	1.45	1.50
25	b1	607	CLA	C4D-ND	-2.68	1.34	1.37
25	C1	514	CLA	C1B-C2B	2.68	1.49	1.43
25	c1	507	CLA	C1B-C2B	2.68	1.49	1.43
25	C2	509	CLA	C1B-C2B	2.68	1.49	1.43
25	c1	504	CLA	C1B-C2B	2.68	1.49	1.43
25	b2	615	CLA	C1B-C2B	2.67	1.49	1.43
25	B2	619	CLA	C1B-C2B	2.67	1.49	1.43
25	c2	510	CLA	C1B-C2B	2.67	1.49	1.43
25	b2	613	CLA	C1B-C2B	2.67	1.49	1.43
25	b2	619	CLA	C1B-C2B	2.67	1.49	1.43
25	b2	616	CLA	C1B-C2B	2.67	1.49	1.43
25	a1	405	CLA	C1B-C2B	2.67	1.49	1.43
25	b1	604	CLA	C1B-C2B	2.66	1.49	1.43
25	B1	609	CLA	C1B-C2B	2.66	1.49	1.43
25	C2	508	CLA	C1B-C2B	2.66	1.49	1.43
25	B2	609	CLA	C1B-C2B	2.66	1.49	1.43
25	b1	612	CLA	C1B-C2B	2.65	1.49	1.43
25	d1	406	CLA	C1B-C2B	2.65	1.49	1.43
25	b1	611	CLA	C1B-C2B	2.65	1.49	1.43
25	c1	516	CLA	C1B-C2B	2.65	1.49	1.43
25	B2	605	CLA	C1B-C2B	2.65	1.49	1.43
25	b2	612	CLA	CMB-C2B	-2.65	1.45	1.50
25	c2	513	CLA	C1B-C2B	2.65	1.49	1.43
25	c2	515	CLA	C1B-C2B	2.65	1.49	1.43
25	c2	507	CLA	C1B-C2B	2.65	1.49	1.43
25	b1	614	CLA	C1B-C2B	2.64	1.49	1.43
25	B1	608	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	617	CLA	C4D-ND	-2.64	1.34	1.37
25	C2	504	CLA	C4D-ND	-2.64	1.34	1.37
25	C2	511	CLA	C1B-C2B	2.63	1.49	1.43
25	b1	606	CLA	C1B-C2B	2.62	1.49	1.43
25	C2	506	CLA	C1B-C2B	2.62	1.49	1.43
25	B1	606	CLA	C1B-C2B	2.62	1.49	1.43
25	c2	506	CLA	C1B-C2B	2.62	1.49	1.43
25	b1	605	CLA	C1B-C2B	2.62	1.49	1.43
25	B1	607	CLA	C4D-ND	-2.62	1.34	1.37
25	B2	607	CLA	C4D-ND	-2.62	1.34	1.37
25	B2	611	CLA	C1B-C2B	2.61	1.49	1.43
25	b2	606	CLA	C1B-C2B	2.61	1.49	1.43
25	B2	612	CLA	C1B-C2B	2.61	1.49	1.43
25	c1	508	CLA	C1B-C2B	2.61	1.49	1.43
25	B2	607	CLA	C1B-C2B	2.59	1.49	1.43
25	D2	406	CLA	C1B-C2B	2.59	1.49	1.43
25	a2	405	CLA	C1B-C2B	2.59	1.49	1.43
25	b2	608	CLA	C1B-C2B	2.59	1.49	1.43
25	c1	503	CLA	C1B-C2B	2.59	1.49	1.43
25	b1	616	CLA	C1B-C2B	2.58	1.49	1.43
36	D2	408	PL9	C6-C5	2.58	1.48	1.35
25	A1	404	CLA	C1B-C2B	2.58	1.49	1.43
25	C1	510	CLA	C1B-C2B	2.58	1.49	1.43
25	b2	620	CLA	C1B-C2B	2.57	1.49	1.43
25	A1	405	CLA	CHC-C1C	2.57	1.43	1.38
25	d2	402	CLA	C1B-C2B	2.57	1.49	1.43
25	a2	413	CLA	C1B-C2B	2.57	1.49	1.43
25	D1	403	CLA	C1B-C2B	2.57	1.49	1.43
25	b2	611	CLA	C1B-C2B	2.57	1.49	1.43
25	B1	611	CLA	C1B-C2B	2.56	1.49	1.43
25	C2	513	CLA	C1B-C2B	2.56	1.49	1.43
25	B2	606	CLA	C1B-C2B	2.56	1.49	1.43
25	B1	618	CLA	C1B-C2B	2.55	1.49	1.43
25	c1	506	CLA	C1B-C2B	2.55	1.49	1.43
29	C2	515	LMG	O8-C28	2.55	1.45	1.33
36	D1	408	PL9	C6-C5	2.54	1.48	1.35
29	A2	412	LMG	O8-C28	2.54	1.45	1.33
25	B1	616	CLA	C1B-C2B	2.54	1.49	1.43
25	b1	607	CLA	CHC-C1C	2.54	1.43	1.38
36	d1	409	PL9	C6-C5	2.54	1.48	1.35
25	B1	613	CLA	C1B-C2B	2.54	1.49	1.43
25	a1	404	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	v2	201	HEM	FE-NA	2.53	2.03	1.95
36	d2	409	PL9	C6-C5	2.52	1.48	1.35
25	b1	613	CLA	CMB-C2B	-2.52	1.45	1.50
25	B1	612	CLA	C1B-C2B	2.52	1.49	1.43
25	B2	610	CLA	C1B-C2B	2.52	1.49	1.43
25	B2	616	CLA	C1B-C2B	2.52	1.49	1.43
25	C1	507	CLA	C1B-C2B	2.52	1.49	1.43
25	b1	604	CLA	CHC-C1C	2.51	1.43	1.38
25	b2	617	CLA	C1B-C2B	2.51	1.49	1.43
25	b1	610	CLA	C1B-C2B	2.51	1.49	1.43
29	B2	621	LMG	O8-C28	2.51	1.45	1.33
25	B1	613	CLA	CMB-C2B	-2.50	1.45	1.50
25	A2	404	CLA	C1B-C2B	2.49	1.49	1.43
25	d2	404	CLA	CHC-C1C	2.49	1.43	1.38
25	B2	610	CLA	CHC-C1C	2.48	1.43	1.38
25	b1	619	CLA	C1B-C2B	2.48	1.49	1.43
25	A2	403	CLA	C1B-C2B	2.48	1.49	1.43
25	b1	605	CLA	CHC-C1C	2.47	1.43	1.38
25	d1	404	CLA	C1B-C2B	2.47	1.49	1.43
25	B1	616	CLA	CHC-C1C	2.46	1.43	1.38
25	a2	413	CLA	CHC-C1C	2.46	1.43	1.38
25	a1	404	CLA	CHC-C1C	2.46	1.43	1.38
25	d2	404	CLA	C1B-C2B	2.46	1.49	1.43
25	b1	620	CLA	CHC-C1C	2.45	1.43	1.38
25	b2	624	CLA	C1B-C2B	2.45	1.49	1.43
25	b2	624	CLA	CHC-C1C	2.45	1.43	1.38
25	b2	612	CLA	C1B-C2B	2.45	1.49	1.43
25	C1	507	CLA	CHC-C1C	2.43	1.43	1.38
25	A2	404	CLA	CHC-C1C	2.43	1.43	1.38
25	C2	513	CLA	CHC-C1C	2.43	1.43	1.38
38	V1	201	HEM	FE-NA	2.43	2.03	1.95
25	B1	619	CLA	CHC-C1C	2.42	1.43	1.38
25	B2	606	CLA	CHC-C1C	2.42	1.43	1.38
25	c2	509	CLA	C1B-C2B	2.40	1.48	1.43
25	B2	616	CLA	CHC-C1C	2.40	1.43	1.38
25	b1	607	CLA	C1B-C2B	2.40	1.48	1.43
25	B1	606	CLA	CHC-C1C	2.39	1.43	1.38
25	c1	506	CLA	CHC-C1C	2.39	1.43	1.38
25	b2	617	CLA	CHC-C1C	2.39	1.43	1.38
25	d1	406	CLA	CHC-C1C	2.39	1.43	1.38
25	B2	613	CLA	C1B-C2B	2.39	1.48	1.43
25	A1	406	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b1	616	CLA	CHC-C1C	2.37	1.43	1.38
25	B2	619	CLA	CHC-C1C	2.37	1.43	1.38
25	A1	404	CLA	CHC-C1C	2.37	1.43	1.38
25	b1	613	CLA	C1B-C2B	2.37	1.48	1.43
25	b1	608	CLA	CHC-C1C	2.37	1.43	1.38
25	B2	607	CLA	CHC-C1C	2.37	1.43	1.38
25	b1	609	CLA	CHC-C1C	2.37	1.43	1.38
25	b1	606	CLA	CHC-C1C	2.36	1.43	1.38
25	B2	613	CLA	CMB-C2B	-2.36	1.45	1.50
25	B2	604	CLA	CHC-C1C	2.35	1.43	1.38
25	b2	606	CLA	CHC-C1C	2.35	1.43	1.38
25	B1	612	CLA	CHC-C1C	2.34	1.43	1.38
25	B1	610	CLA	CHC-C1C	2.34	1.43	1.38
23	c2	501	BCR	C19-C18	2.34	1.51	1.45
25	A2	403	CLA	CHC-C1C	2.34	1.43	1.38
25	b2	604	CLA	CHC-C1C	2.33	1.43	1.38
25	b2	615	CLA	CHC-C1C	2.33	1.43	1.38
25	C2	507	CLA	CHC-C1C	2.33	1.43	1.38
25	c1	504	CLA	CHC-C1C	2.33	1.43	1.38
25	B2	609	CLA	CHC-C1C	2.33	1.43	1.38
25	C1	510	CLA	CHC-C1C	2.32	1.43	1.38
25	b1	610	CLA	CHC-C1C	2.32	1.43	1.38
25	a2	404	CLA	C1B-C2B	2.32	1.48	1.43
25	D1	403	CLA	CHC-C1C	2.32	1.43	1.38
25	c2	506	CLA	CHC-C1C	2.32	1.43	1.38
25	c1	515	CLA	CHC-C1C	2.32	1.43	1.38
25	C1	504	CLA	CHC-C1C	2.32	1.43	1.38
25	C2	504	CLA	CHC-C1C	2.32	1.43	1.38
25	C2	506	CLA	CHC-C1C	2.32	1.43	1.38
25	d1	404	CLA	CHC-C1C	2.32	1.43	1.38
25	B1	604	CLA	CHC-C1C	2.31	1.43	1.38
25	D2	404	CLA	CHC-C1C	2.31	1.43	1.38
25	c2	510	CLA	CHC-C1C	2.31	1.43	1.38
25	B1	615	CLA	CHC-C1C	2.30	1.43	1.38
25	d2	402	CLA	CHC-C1C	2.30	1.43	1.38
25	C2	508	CLA	CHC-C1C	2.30	1.43	1.38
25	b2	616	CLA	CHC-C1C	2.30	1.43	1.38
25	D1	402	CLA	MG-NB	-2.30	2.01	2.05
25	b1	607	CLA	CMB-C2B	-2.30	1.45	1.50
25	C1	509	CLA	MG-NB	-2.30	2.01	2.05
25	B1	617	CLA	CHC-C1C	2.30	1.43	1.38
25	c2	515	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A1	406	CLA	CHC-C1C	2.30	1.43	1.38
25	B1	618	CLA	CHC-C1C	2.29	1.43	1.38
25	b2	608	CLA	CHC-C1C	2.29	1.43	1.38
25	c1	505	CLA	CHC-C1C	2.29	1.43	1.38
25	A1	403	CLA	CMD-C2D	-2.29	1.46	1.50
25	C1	514	CLA	CHC-C1C	2.29	1.43	1.38
25	B2	605	CLA	CHC-C1C	2.28	1.43	1.38
25	B1	614	CLA	CHC-C1C	2.28	1.43	1.38
25	B1	610	CLA	C1B-C2B	2.28	1.48	1.43
25	B1	605	CLA	CHC-C1C	2.28	1.43	1.38
25	a1	403	CLA	C1B-C2B	2.28	1.48	1.43
25	D2	406	CLA	CHC-C1C	2.28	1.43	1.38
25	B1	611	CLA	CHC-C1C	2.27	1.43	1.38
25	c1	507	CLA	CHC-C1C	2.27	1.43	1.38
25	c1	513	CLA	CHC-C1C	2.27	1.43	1.38
25	B1	609	CLA	CHC-C1C	2.26	1.43	1.38
25	d1	401	CLA	CHC-C1C	2.26	1.43	1.38
25	c1	512	CLA	CHC-C1C	2.26	1.43	1.38
25	C1	506	CLA	CMD-C2D	-2.26	1.46	1.50
25	C2	518	CLA	CHC-C1C	2.26	1.43	1.38
25	C2	503	CLA	CHC-C1C	2.26	1.43	1.38
25	b2	611	CLA	CHC-C1C	2.26	1.43	1.38
25	c1	508	CLA	CHC-C1C	2.26	1.43	1.38
25	C2	505	CLA	CHC-C1C	2.26	1.43	1.38
25	B1	607	CLA	CHC-C1C	2.26	1.43	1.38
25	B2	608	CLA	CHC-C1C	2.25	1.43	1.38
25	K2	101	CLA	CHC-C1C	2.25	1.43	1.38
25	b1	612	CLA	CHC-C1C	2.25	1.43	1.38
25	A1	403	CLA	C1B-C2B	2.25	1.48	1.43
25	C1	509	CLA	C1B-C2B	2.25	1.48	1.43
25	b2	613	CLA	CHC-C1C	2.25	1.43	1.38
25	C1	511	CLA	CHC-C1C	2.25	1.43	1.38
25	b2	618	CLA	CHC-C1C	2.25	1.43	1.38
25	b2	619	CLA	CHC-C1C	2.24	1.43	1.38
25	c2	509	CLA	CHC-C1C	2.24	1.43	1.38
25	b1	615	CLA	CHC-C1C	2.24	1.43	1.38
25	B2	611	CLA	CHC-C1C	2.24	1.43	1.38
25	c2	504	CLA	CHC-C1C	2.24	1.43	1.38
25	c2	508	CLA	CHC-C1C	2.24	1.43	1.38
25	b2	620	CLA	CHC-C1C	2.24	1.43	1.38
25	b1	617	CLA	CHC-C1C	2.23	1.43	1.38
25	B2	613	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C2	511	CLA	CMB-C2B	-2.23	1.46	1.50
25	b1	619	CLA	CHC-C1C	2.23	1.43	1.38
25	B1	608	CLA	CHC-C1C	2.23	1.43	1.38
25	c1	511	CLA	CHC-C1C	2.23	1.43	1.38
25	D2	401	CLA	CHC-C1C	2.23	1.43	1.38
25	A1	405	CLA	C1B-C2B	2.23	1.48	1.43
25	c2	513	CLA	CHC-C1C	2.23	1.43	1.38
25	B2	615	CLA	CHC-C1C	2.22	1.43	1.38
25	c2	503	CLA	CHC-C1C	2.22	1.43	1.38
25	C1	512	CLA	CHC-C1C	2.22	1.43	1.38
25	c1	516	CLA	CHC-C1C	2.22	1.43	1.38
25	b1	611	CLA	CHC-C1C	2.22	1.43	1.38
25	c2	509	CLA	CMB-C2B	-2.21	1.46	1.50
25	b1	614	CLA	CHC-C1C	2.21	1.43	1.38
25	C1	508	CLA	CHC-C1C	2.21	1.43	1.38
25	C2	510	CLA	CHC-C1C	2.21	1.43	1.38
25	b2	614	CLA	CMD-C2D	-2.21	1.46	1.50
25	B2	617	CLA	CHC-C1C	2.21	1.43	1.38
25	c2	505	CLA	CHC-C1C	2.21	1.43	1.38
25	C1	503	CLA	CHC-C1C	2.21	1.43	1.38
25	C1	506	CLA	CHC-C1C	2.21	1.43	1.38
25	c2	507	CLA	CHC-C1C	2.20	1.43	1.38
25	a2	413	CLA	CMD-C2D	-2.20	1.46	1.50
25	c1	510	CLA	CHC-C1C	2.20	1.43	1.38
25	D2	401	CLA	MG-NB	-2.20	2.01	2.05
25	a2	405	CLA	CHC-C1C	2.20	1.43	1.38
25	c2	511	CLA	CHC-C1C	2.19	1.43	1.38
25	b2	610	CLA	CHC-C1C	2.19	1.43	1.38
25	c1	509	CLA	CHC-C1C	2.19	1.43	1.38
25	c1	508	CLA	CMB-C2B	-2.19	1.46	1.50
25	b1	614	CLA	CMD-C2D	-2.19	1.46	1.50
25	B2	612	CLA	CHC-C1C	2.19	1.43	1.38
25	b2	619	CLA	CMC-C2C	-2.18	1.46	1.50
29	M1	101	LMG	O7-C8	-2.18	1.43	1.47
25	b2	616	CLA	CMB-C2B	-2.18	1.46	1.50
25	C1	505	CLA	CHC-C1C	2.18	1.42	1.38
25	c2	502	CLA	CHC-C1C	2.18	1.42	1.38
25	b2	609	CLA	CHC-C1C	2.17	1.42	1.38
25	A1	403	CLA	CMC-C2C	-2.17	1.46	1.50
25	B2	614	CLA	CHC-C1C	2.17	1.42	1.38
25	A2	402	CLA	C1B-C2B	2.17	1.48	1.43
25	c1	507	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	613	CLA	CHC-C1C	2.16	1.42	1.38
25	a1	405	CLA	CHC-C1C	2.15	1.42	1.38
25	c2	512	CLA	CHC-C1C	2.15	1.42	1.38
25	c1	512	CLA	CMD-C2D	-2.15	1.46	1.50
25	C1	512	CLA	CMD-C2D	-2.14	1.46	1.50
25	a2	404	CLA	CMD-C2D	-2.14	1.46	1.50
25	C2	509	CLA	CHC-C1C	2.14	1.42	1.38
25	a1	403	CLA	CMD-C2D	-2.14	1.46	1.50
25	c1	511	CLA	CMD-C2D	-2.14	1.46	1.50
25	K2	101	CLA	CMD-C2D	-2.14	1.46	1.50
25	B2	618	CLA	CHC-C1C	2.14	1.42	1.38
25	C1	513	CLA	CHC-C1C	2.14	1.42	1.38
25	b1	614	CLA	MG-NB	-2.14	2.01	2.05
25	d2	405	CLA	MG-NB	-2.14	2.01	2.05
25	C2	516	CLA	CHC-C1C	2.13	1.42	1.38
25	b2	612	CLA	MG-NB	-2.13	2.01	2.05
25	B2	618	CLA	CMC-C2C	-2.13	1.46	1.50
25	B1	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	A2	402	CLA	CMC-C2C	-2.13	1.46	1.50
25	C2	507	CLA	CMD-C2D	-2.13	1.46	1.50
25	c2	509	CLA	MG-NB	-2.12	2.01	2.05
25	c1	509	CLA	CMB-C2B	-2.12	1.46	1.50
25	A2	402	CLA	CMB-C2B	-2.12	1.46	1.50
25	C1	514	CLA	MG-NB	-2.12	2.01	2.05
25	c2	506	CLA	CMD-C2D	-2.12	1.46	1.50
25	B2	615	CLA	MG-NB	-2.12	2.01	2.05
25	C1	507	CLA	C3C-C2C	2.11	1.41	1.36
25	B2	607	CLA	CMD-C2D	-2.11	1.46	1.50
25	c1	513	CLA	CMD-C2D	-2.11	1.46	1.50
25	A1	404	CLA	CMD-C2D	-2.11	1.46	1.50
25	C1	509	CLA	CHC-C1C	2.10	1.42	1.38
25	d1	401	CLA	MG-NB	-2.10	2.01	2.05
25	c1	503	CLA	CHC-C1C	2.10	1.42	1.38
25	B2	614	CLA	CMD-C2D	-2.10	1.46	1.50
25	b2	624	CLA	MG-NB	-2.10	2.01	2.05
25	B1	614	CLA	CMD-C2D	-2.09	1.46	1.50
25	B1	613	CLA	CMD-C2D	-2.09	1.46	1.50
25	c1	510	CLA	CMB-C2B	-2.09	1.46	1.50
25	b2	612	CLA	CHC-C1C	2.09	1.42	1.38
25	B1	607	CLA	MG-NB	-2.09	2.01	2.05
25	b1	611	CLA	MG-NB	-2.09	2.01	2.05
25	b2	616	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C1	507	CLA	MG-NB	-2.09	2.01	2.05
25	C2	516	CLA	MG-NB	-2.09	2.01	2.05
25	c1	516	CLA	MG-NB	-2.09	2.01	2.05
25	c2	511	CLA	MG-NB	-2.08	2.01	2.05
25	C2	511	CLA	CHC-C1C	2.08	1.42	1.38
25	B2	607	CLA	CMB-C2B	-2.08	1.46	1.50
25	B1	606	CLA	MG-NB	-2.08	2.01	2.05
25	c2	507	CLA	CMB-C2B	-2.08	1.46	1.50
25	C1	510	CLA	MG-NB	-2.08	2.01	2.05
25	b2	618	CLA	MG-NB	-2.07	2.01	2.05
25	B2	610	CLA	MG-NB	-2.07	2.01	2.05
25	B1	610	CLA	MG-NB	-2.07	2.01	2.05
25	B1	607	CLA	CMB-C2B	-2.07	1.46	1.50
25	C1	511	CLA	CMD-C2D	-2.07	1.46	1.50
25	b1	613	CLA	CHC-C1C	2.07	1.42	1.38
25	b2	614	CLA	CHC-C1C	2.07	1.42	1.38
25	B2	609	CLA	CMC-C2C	-2.07	1.46	1.50
25	C2	510	CLA	MG-NB	-2.07	2.01	2.05
25	B1	618	CLA	CMC-C2C	-2.07	1.46	1.50
25	c1	508	CLA	MG-NB	-2.07	2.01	2.05
25	b2	617	CLA	MG-NB	-2.06	2.01	2.05
25	B1	613	CLA	MG-NB	-2.06	2.01	2.05
25	C1	502	CLA	CHC-C1C	2.06	1.42	1.38
36	D1	408	PL9	C2-C3	2.06	1.40	1.34
25	C2	511	CLA	MG-NB	-2.06	2.01	2.05
25	d2	405	CLA	CHC-C1C	2.06	1.42	1.38
25	b1	610	CLA	CMB-C2B	-2.06	1.46	1.50
25	A2	404	CLA	CMB-C2B	-2.06	1.46	1.50
25	A1	405	CLA	CMB-C2B	-2.06	1.46	1.50
25	C1	512	CLA	MG-NB	-2.06	2.01	2.05
25	A1	404	CLA	MG-NB	-2.06	2.01	2.05
25	c2	513	CLA	MG-NB	-2.06	2.01	2.05
25	A1	403	CLA	CMB-C2B	-2.06	1.46	1.50
25	D1	403	CLA	MG-NB	-2.05	2.01	2.05
29	B2	620	LMG	O1-C1	2.05	1.43	1.40
25	B2	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	C1	510	CLA	CMD-C2D	-2.05	1.46	1.50
25	B2	611	CLA	MG-NB	-2.05	2.01	2.05
25	c2	513	CLA	CMD-C2D	-2.05	1.46	1.50
25	b1	619	CLA	CMC-C2C	-2.05	1.46	1.50
25	c1	504	CLA	MG-NB	-2.05	2.01	2.05
25	c1	512	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C1	508	CLA	MG-NB	-2.05	2.01	2.05
25	b2	608	CLA	MG-NB	-2.05	2.01	2.05
25	c2	503	CLA	CMB-C2B	-2.05	1.46	1.50
25	b1	619	CLA	CMB-C2B	-2.05	1.46	1.50
25	c2	510	CLA	CMD-C2D	-2.04	1.46	1.50
25	c1	505	CLA	MG-NB	-2.04	2.01	2.05
25	d1	404	CLA	CMB-C2B	-2.04	1.46	1.50
25	C1	503	CLA	MG-NB	-2.04	2.01	2.05
38	e2	101	HEM	CMC-C2C	2.04	1.55	1.50
25	b2	609	CLA	CMC-C2C	-2.04	1.46	1.50
25	d2	402	CLA	CMB-C2B	-2.04	1.46	1.50
25	a2	404	CLA	MG-NB	-2.04	2.01	2.05
25	b1	613	CLA	CMC-C2C	-2.04	1.46	1.50
25	C2	511	CLA	CMC-C2C	-2.04	1.46	1.50
25	B2	613	CLA	MG-NB	-2.04	2.01	2.05
25	b2	620	CLA	MG-NB	-2.04	2.01	2.05
25	c1	510	CLA	CMC-C2C	-2.04	1.46	1.50
25	c1	503	CLA	MG-NB	-2.04	2.01	2.05
25	b2	606	CLA	MG-NB	-2.04	2.01	2.05
25	B1	616	CLA	CMB-C2B	-2.04	1.46	1.50
25	c2	506	CLA	MG-NB	-2.04	2.01	2.05
38	E2	101	HEM	CMC-C2C	2.04	1.55	1.50
25	c2	503	CLA	MG-NB	-2.04	2.01	2.05
25	C2	513	CLA	MG-NB	-2.03	2.01	2.05
25	c2	515	CLA	MG-NB	-2.03	2.01	2.05
25	C1	507	CLA	CMB-C2B	-2.03	1.46	1.50
25	b2	612	CLA	CMD-C2D	-2.03	1.46	1.50
25	b2	620	CLA	CMB-C2B	-2.03	1.46	1.50
25	b1	617	CLA	MG-NB	-2.03	2.01	2.05
25	b2	614	CLA	MG-NB	-2.03	2.01	2.05
25	C2	504	CLA	MG-NB	-2.03	2.01	2.05
25	b2	610	CLA	MG-NB	-2.03	2.01	2.05
25	b1	610	CLA	MG-NB	-2.03	2.01	2.05
25	a1	403	CLA	CMC-C2C	-2.03	1.46	1.50
25	D1	402	CLA	CHC-C1C	2.03	1.42	1.38
25	B2	606	CLA	CMB-C2B	-2.03	1.46	1.50
36	d1	409	PL9	C2-C3	2.02	1.40	1.34
25	B1	616	CLA	CMD-C2D	-2.02	1.46	1.50
25	a1	405	CLA	MG-NB	-2.02	2.01	2.05
25	C2	513	CLA	CMB-C2B	-2.02	1.46	1.50
25	D2	401	CLA	CMD-C2D	-2.02	1.46	1.50
25	b1	604	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E1	101	HEM	CMC-C2C	2.02	1.55	1.50
25	K2	101	CLA	CMB-C2B	-2.02	1.46	1.50
25	C1	513	CLA	CMD-C2D	-2.02	1.46	1.50
25	B1	609	CLA	MG-NB	-2.01	2.01	2.05
25	B2	616	CLA	CMD-C2D	-2.01	1.46	1.50
25	b2	609	CLA	MG-NB	-2.01	2.01	2.05
25	b1	615	CLA	CMD-C2D	-2.01	1.46	1.50
25	b2	615	CLA	MG-NB	-2.01	2.01	2.05
25	B2	614	CLA	MG-NB	-2.01	2.01	2.05
25	C2	509	CLA	CMB-C2B	-2.01	1.46	1.50
25	a1	404	CLA	CMB-C2B	-2.01	1.46	1.50
25	C2	505	CLA	MG-NB	-2.01	2.01	2.05
25	A2	404	CLA	CMD-C2D	-2.01	1.46	1.50
25	D2	404	CLA	CMB-C2B	-2.01	1.46	1.50
25	B2	617	CLA	MG-NB	-2.01	2.01	2.05
25	c2	507	CLA	MG-NB	-2.01	2.01	2.05
25	b1	613	CLA	CMD-C2D	-2.01	1.46	1.50
25	b1	609	CLA	MG-NB	-2.01	2.01	2.05
29	B2	621	LMG	O1-C1	2.01	1.43	1.40
25	b1	617	CLA	CMD-C2D	-2.01	1.46	1.50
25	A1	406	CLA	CMB-C2B	-2.01	1.46	1.50
25	b1	608	CLA	MG-NB	-2.01	2.01	2.05
25	b1	605	CLA	CMD-C2D	-2.00	1.46	1.50
25	b1	606	CLA	CMD-C2D	-2.00	1.46	1.50
25	B1	608	CLA	MG-NB	-2.00	2.01	2.05
25	b2	612	CLA	CMC-C2C	-2.00	1.46	1.50
25	C1	504	CLA	CMB-C2B	-2.00	1.46	1.50
25	B1	618	CLA	CMD-C2D	-2.00	1.46	1.50
25	b2	606	CLA	CMD-C2D	-2.00	1.46	1.50

All (1879) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c2	501	BCR	C36-C18-C17	-10.87	107.70	122.92
23	c2	501	BCR	C24-C23-C22	-9.36	112.09	126.23
23	c2	501	BCR	C16-C17-C18	9.01	140.16	127.31
27	d1	403	PHO	C2B-C1B-NB	8.29	115.25	109.53
27	d2	408	PHO	C2B-C1B-NB	8.22	115.20	109.53
27	a2	416	PHO	C2B-C1B-NB	8.15	115.15	109.53
27	D1	407	PHO	C2B-C1B-NB	8.09	115.11	109.53
27	D2	407	PHO	C2B-C1B-NB	7.97	115.03	109.53
27	A2	407	PHO	C2B-C1B-NB	7.94	115.01	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A1	408	PHO	C2B-C1B-NB	7.82	114.92	109.53
27	a1	411	PHO	C2B-C1B-NB	7.70	114.84	109.53
27	a1	411	PHO	O2D-CGD-CBD	7.32	120.27	111.00
27	A1	408	PHO	O2D-CGD-CBD	7.29	120.24	111.00
27	D1	407	PHO	O2D-CGD-CBD	7.29	120.23	111.00
27	d1	403	PHO	O2D-CGD-CBD	7.28	120.22	111.00
27	D2	407	PHO	O2D-CGD-CBD	7.27	120.21	111.00
23	c2	501	BCR	C16-C15-C14	-7.18	108.77	123.47
27	A2	407	PHO	O2D-CGD-CBD	7.17	120.08	111.00
27	a2	416	PHO	O2D-CGD-CBD	7.15	120.06	111.00
25	c1	509	CLA	C4A-NA-C1A	7.10	109.90	106.71
25	C1	506	CLA	C4A-NA-C1A	7.06	109.88	106.71
25	b2	609	CLA	C4A-NA-C1A	6.98	109.84	106.71
27	a2	416	PHO	C2D-C1D-ND	6.98	114.34	109.53
25	C1	512	CLA	C4A-NA-C1A	6.97	109.84	106.71
25	c1	507	CLA	C4A-NA-C1A	6.95	109.83	106.71
25	C1	502	CLA	C4A-NA-C1A	6.95	109.83	106.71
25	B1	606	CLA	C4A-NA-C1A	6.93	109.82	106.71
25	B2	608	CLA	C4A-NA-C1A	6.93	109.82	106.71
25	D1	402	CLA	C4A-NA-C1A	6.92	109.81	106.71
27	d2	408	PHO	C2D-C1D-ND	6.89	114.28	109.53
25	b2	616	CLA	C4A-NA-C1A	6.88	109.80	106.71
25	b2	606	CLA	C4A-NA-C1A	6.88	109.80	106.71
25	D2	401	CLA	C4A-NA-C1A	6.87	109.79	106.71
25	d1	401	CLA	C4A-NA-C1A	6.84	109.78	106.71
25	B2	614	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	B2	618	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	C2	510	CLA	C4A-NA-C1A	6.82	109.77	106.71
27	D1	407	PHO	C2D-C1D-ND	6.81	114.23	109.53
25	c2	504	CLA	C4A-NA-C1A	6.79	109.76	106.71
27	A1	408	PHO	C2D-C1D-ND	6.79	114.21	109.53
25	C2	503	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	C2	505	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	C1	505	CLA	C4A-NA-C1A	6.76	109.75	106.71
25	C2	511	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	C2	516	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	B2	602	BCR	C7-C8-C9	-6.73	116.06	126.23
25	b1	616	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	c2	501	BCR	C23-C22-C21	6.73	129.27	118.94
25	B1	608	CLA	C4A-NA-C1A	6.73	109.73	106.71
27	d2	408	PHO	O2D-CGD-CBD	6.73	119.52	111.00
25	c2	503	CLA	C4A-NA-C1A	6.72	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C2	509	CLA	C4A-NA-C1A	6.72	109.73	106.71
25	d2	402	CLA	C4A-NA-C1A	6.72	109.72	106.71
25	C2	507	CLA	C4A-NA-C1A	6.71	109.72	106.71
27	D2	407	PHO	C2D-C1D-ND	6.70	114.15	109.53
25	B2	616	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	C2	518	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	b2	619	CLA	C4A-NA-C1A	6.69	109.71	106.71
27	A2	407	PHO	C2D-C1D-ND	6.68	114.14	109.53
25	K2	101	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	a2	416	PHO	C4D-ND-C1D	-6.67	102.04	108.83
27	d1	403	PHO	C2D-C1D-ND	6.67	114.13	109.53
25	b2	615	CLA	C4A-NA-C1A	6.67	109.70	106.71
25	B2	609	CLA	C4A-NA-C1A	6.66	109.70	106.71
25	A1	406	CLA	C4A-NA-C1A	6.66	109.70	106.71
25	c1	503	CLA	C4A-NA-C1A	6.66	109.70	106.71
25	c2	502	CLA	C4A-NA-C1A	6.66	109.70	106.71
25	c1	506	CLA	C4A-NA-C1A	6.65	109.70	106.71
25	c1	513	CLA	C4A-NA-C1A	6.65	109.70	106.71
25	c1	510	CLA	C4A-NA-C1A	6.65	109.69	106.71
25	c2	508	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	c1	505	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	c1	515	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	b1	606	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	B2	615	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	D2	406	CLA	C4A-NA-C1A	6.60	109.67	106.71
27	A2	407	PHO	C1C-C2C-C3C	-6.60	103.12	108.61
27	A1	408	PHO	C4D-ND-C1D	-6.60	102.12	108.83
25	c2	513	CLA	C4A-NA-C1A	6.59	109.67	106.71
25	b2	618	CLA	C4A-NA-C1A	6.58	109.66	106.71
25	a1	405	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	c2	506	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	b2	614	CLA	C4A-NA-C1A	6.56	109.65	106.71
38	V1	201	HEM	C4D-ND-C1D	6.55	111.84	105.07
27	a1	411	PHO	C2D-C1D-ND	6.55	114.05	109.53
25	B1	615	CLA	C4A-NA-C1A	6.54	109.65	106.71
25	B2	606	CLA	C4A-NA-C1A	6.54	109.65	106.71
25	b1	617	CLA	C4A-NA-C1A	6.54	109.65	106.71
25	B1	614	CLA	C4A-NA-C1A	6.54	109.64	106.71
25	B1	619	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	b1	620	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	c1	511	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	b2	620	CLA	C4A-NA-C1A	6.50	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E2	101	HEM	C4D-ND-C1D	6.49	111.78	105.07
27	A2	407	PHO	C4D-ND-C1D	-6.49	102.23	108.83
25	B1	604	CLA	C4A-NA-C1A	6.48	109.62	106.71
38	e2	101	HEM	C4D-ND-C1D	6.47	111.76	105.07
27	d2	408	PHO	C4D-ND-C1D	-6.47	102.25	108.83
25	C1	504	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	d1	403	PHO	C4D-ND-C1D	-6.45	102.26	108.83
25	c1	512	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	b2	602	BCR	C7-C8-C9	-6.45	116.49	126.23
25	B1	613	CLA	C4A-NA-C1A	6.45	109.60	106.71
25	A1	404	CLA	C4A-NA-C1A	6.44	109.60	106.71
25	b1	609	CLA	C4A-NA-C1A	6.44	109.60	106.71
25	C2	508	CLA	C4A-NA-C1A	6.44	109.60	106.71
38	V2	201	HEM	C4D-ND-C1D	6.44	111.72	105.07
25	c2	515	CLA	C4A-NA-C1A	6.43	109.59	106.71
25	C1	508	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	b2	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	c2	511	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	D1	407	PHO	C4D-ND-C1D	-6.40	102.31	108.83
25	b1	614	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	c2	505	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	A1	408	PHO	C1C-C2C-C3C	-6.39	103.30	108.61
25	B2	604	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	b1	619	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	C1	503	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	b1	607	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	B2	613	CLA	C4A-NA-C1A	6.36	109.57	106.71
38	v1	201	HEM	C4D-ND-C1D	6.36	111.64	105.07
38	E1	101	HEM	C4D-ND-C1D	6.35	111.63	105.07
25	b1	608	CLA	C4A-NA-C1A	6.34	109.56	106.71
27	D2	407	PHO	C4D-ND-C1D	-6.34	102.38	108.83
25	b1	615	CLA	C4A-NA-C1A	6.34	109.56	106.71
25	B2	617	CLA	C4A-NA-C1A	6.34	109.56	106.71
25	B2	619	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	b1	612	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	c1	504	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	a1	411	PHO	C1C-C2C-C3C	-6.32	103.36	108.61
25	C1	511	CLA	C4A-NA-C1A	6.31	109.54	106.71
38	v2	201	HEM	C4D-ND-C1D	6.30	111.58	105.07
25	C2	504	CLA	C4A-NA-C1A	6.30	109.54	106.71
27	a1	411	PHO	C4D-ND-C1D	-6.29	102.43	108.83
25	C1	513	CLA	C4A-NA-C1A	6.28	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B2	607	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	c2	510	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	d2	405	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	C1	510	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	b2	617	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	c1	516	CLA	C4A-NA-C1A	6.27	109.52	106.71
25	c2	507	CLA	C4A-NA-C1A	6.26	109.52	106.71
25	A2	404	CLA	C4A-NA-C1A	6.25	109.52	106.71
25	d1	406	CLA	C4A-NA-C1A	6.23	109.51	106.71
27	D1	407	PHO	C1C-C2C-C3C	-6.23	103.43	108.61
25	C1	514	CLA	C4A-NA-C1A	6.22	109.50	106.71
25	b2	613	CLA	C4A-NA-C1A	6.22	109.50	106.71
25	D2	404	CLA	C4A-NA-C1A	6.21	109.50	106.71
27	a2	416	PHO	C1C-C2C-C3C	-6.21	103.44	108.61
25	B1	607	CLA	C4A-NA-C1A	6.21	109.50	106.71
27	d2	408	PHO	C1C-C2C-C3C	-6.21	103.44	108.61
23	b1	602	BCR	C7-C8-C9	-6.21	116.85	126.23
25	b1	605	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	B1	605	CLA	C4A-NA-C1A	6.20	109.49	106.71
25	c2	509	CLA	C4A-NA-C1A	6.20	109.49	106.71
25	b2	610	CLA	C4A-NA-C1A	6.17	109.48	106.71
38	f1	101	HEM	C4D-ND-C1D	6.16	111.44	105.07
25	B2	612	CLA	C4A-NA-C1A	6.16	109.48	106.71
27	D2	407	PHO	C1C-C2C-C3C	-6.15	103.50	108.61
25	C2	506	CLA	C4A-NA-C1A	6.15	109.47	106.71
25	B1	609	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	b2	611	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	b2	612	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	B1	616	CLA	C4A-NA-C1A	6.12	109.46	106.71
27	d1	403	PHO	C1C-C2C-C3C	-6.11	103.53	108.61
25	B1	618	CLA	C4A-NA-C1A	6.09	109.45	106.71
25	d1	404	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	b2	608	CLA	C4A-NA-C1A	6.07	109.44	106.71
25	c2	512	CLA	C4A-NA-C1A	6.06	109.43	106.71
25	B2	605	CLA	C4A-NA-C1A	6.06	109.43	106.71
25	B1	617	CLA	C4A-NA-C1A	6.05	109.43	106.71
25	b2	624	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	b1	610	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	C2	513	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	a2	405	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	B1	612	CLA	C4A-NA-C1A	5.94	109.38	106.71
25	b1	604	CLA	C4A-NA-C1A	5.94	109.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B1	611	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	c2	501	BCR	C20-C21-C22	5.89	135.72	127.31
25	C1	509	CLA	C4A-NA-C1A	5.89	109.35	106.71
25	D1	403	CLA	C4A-NA-C1A	5.89	109.35	106.71
25	d2	404	CLA	C4A-NA-C1A	5.86	109.34	106.71
25	B2	610	CLA	C4A-NA-C1A	5.83	109.33	106.71
25	B2	611	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	b1	611	CLA	C4A-NA-C1A	5.77	109.30	106.71
23	K1	101	BCR	C24-C23-C22	-5.75	120.52	126.59
23	c2	501	BCR	C37-C22-C21	-5.74	114.88	122.92
25	B1	609	CLA	CAC-C3C-C4C	5.73	132.25	124.81
27	d1	403	PHO	C3D-C4D-ND	5.72	115.51	107.72
25	c1	508	CLA	C4A-NA-C1A	5.67	109.25	106.71
27	a2	416	PHO	C3D-C4D-ND	5.66	115.44	107.72
25	b1	613	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	A2	403	CLA	C4A-NA-C1A	5.60	109.22	106.71
23	J1	101	BCR	C20-C21-C22	-5.60	119.32	127.31
27	D1	407	PHO	C3D-C4D-ND	5.59	115.34	107.72
23	B1	602	BCR	C7-C8-C9	-5.57	117.82	126.23
27	d2	408	PHO	C3D-C4D-ND	5.56	115.29	107.72
27	A1	408	PHO	C3D-C4D-ND	5.55	115.28	107.72
23	k1	101	BCR	C20-C21-C22	-5.54	119.41	127.31
25	C1	507	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	B1	602	BCR	C11-C10-C9	-5.53	119.42	127.31
23	c2	501	BCR	C15-C16-C17	5.51	134.76	123.47
23	j2	102	BCR	C33-C5-C6	-5.51	118.34	124.53
25	A2	402	CLA	C4A-NA-C1A	5.48	109.17	106.71
27	A2	407	PHO	C3D-C4D-ND	5.48	115.19	107.72
23	F2	401	BCR	C20-C21-C22	-5.47	119.51	127.31
23	D1	401	BCR	C7-C8-C9	-5.47	117.97	126.23
27	D2	407	PHO	C3D-C4D-ND	5.46	115.17	107.72
29	c2	519	LMG	O7-C10-O9	-5.46	118.62	125.57
25	B1	610	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	K1	101	BCR	C15-C14-C13	-5.44	119.54	127.31
23	c2	501	BCR	C19-C18-C17	5.43	127.28	118.94
27	a1	411	PHO	C3D-C4D-ND	5.40	115.08	107.72
25	a2	413	CLA	C4A-NA-C1A	5.39	109.13	106.71
23	J1	101	BCR	C33-C5-C6	-5.34	118.53	124.53
25	A1	403	CLA	C4A-NA-C1A	5.34	109.11	106.71
23	B2	602	BCR	C11-C10-C9	-5.30	119.74	127.31
23	j2	102	BCR	C20-C21-C22	-5.29	119.76	127.31
23	F2	401	BCR	C7-C8-C9	-5.26	118.28	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c1	502	BCR	C15-C14-C13	-5.21	119.88	127.31
23	c1	501	BCR	C11-C10-C9	-5.16	119.95	127.31
25	A1	405	CLA	C4A-NA-C1A	5.14	109.02	106.71
23	d1	405	BCR	C7-C8-C9	-5.10	118.52	126.23
23	k1	101	BCR	C33-C5-C6	-5.10	118.80	124.53
25	a1	404	CLA	C4A-NA-C1A	5.08	108.99	106.71
25	a2	404	CLA	C4A-NA-C1A	5.05	108.98	106.71
23	c1	501	BCR	C15-C14-C13	-5.01	120.16	127.31
37	D1	409	SQD	O47-C7-C8	5.00	120.29	111.09
37	D2	402	SQD	O47-C7-C8	5.00	120.28	111.09
23	c1	501	BCR	C16-C17-C18	-4.98	120.21	127.31
23	c1	502	BCR	C24-C23-C22	-4.93	118.78	126.23
23	b2	602	BCR	C20-C21-C22	-4.93	120.27	127.31
29	b1	624	LMG	O7-C10-C11	4.92	122.10	111.50
23	d2	401	BCR	C16-C17-C18	-4.91	120.30	127.31
29	d2	407	LMG	O7-C10-C11	4.91	120.12	111.09
25	a1	403	CLA	C4A-NA-C1A	4.90	108.91	106.71
23	c1	502	BCR	C20-C21-C22	-4.90	120.32	127.31
23	H1	102	BCR	C15-C14-C13	-4.89	120.33	127.31
23	D1	401	BCR	C11-C10-C9	-4.89	120.33	127.31
34	C2	512	DGD	O2G-C1B-C2B	4.88	120.07	111.09
23	j2	102	BCR	C15-C14-C13	-4.88	120.35	127.31
23	C2	502	BCR	C15-C14-C13	-4.87	120.36	127.31
23	h2	101	BCR	C15-C14-C13	-4.86	120.38	127.31
23	D1	401	BCR	C16-C17-C18	-4.81	120.45	127.31
23	k2	501	BCR	C24-C23-C22	-4.78	119.01	126.23
23	J1	101	BCR	C24-C23-C22	-4.77	119.03	126.23
23	A2	401	BCR	C28-C27-C26	-4.71	105.66	114.08
23	F2	401	BCR	C15-C14-C13	-4.70	120.60	127.31
23	k2	501	BCR	C20-C21-C22	-4.70	120.60	127.31
23	h1	102	BCR	C16-C17-C18	-4.69	120.61	127.31
27	D2	407	PHO	C1-C2-C3	-4.69	117.93	126.04
23	K2	102	BCR	C24-C23-C22	-4.68	119.16	126.23
23	K2	102	BCR	C20-C21-C22	-4.68	120.63	127.31
23	k2	501	BCR	C15-C14-C13	-4.67	120.64	127.31
23	C1	521	BCR	C11-C10-C9	-4.66	120.66	127.31
33	d1	402	LHG	O7-C7-C8	4.64	121.50	111.50
36	D1	408	PL9	C7-C8-C9	-4.63	119.08	126.79
23	A2	401	BCR	C7-C8-C9	-4.62	119.25	126.23
36	D2	408	PL9	C7-C8-C9	-4.62	119.11	126.79
23	A2	401	BCR	C16-C17-C18	-4.62	120.72	127.31
23	B2	601	BCR	C28-C27-C26	-4.60	105.86	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c1	501	BCR	C20-C21-C22	-4.60	120.75	127.31
23	C1	501	BCR	C15-C14-C13	-4.58	120.77	127.31
23	B2	601	BCR	C15-C14-C13	-4.54	120.84	127.31
37	b2	605	SQD	O47-C7-C8	4.52	121.23	111.50
23	c1	502	BCR	C36-C18-C19	4.52	125.19	118.08
23	b2	601	BCR	C28-C27-C26	-4.52	106.01	114.08
36	d2	409	PL9	C7-C8-C9	-4.50	119.30	126.79
36	d1	409	PL9	C7-C8-C9	-4.50	119.30	126.79
23	c2	501	BCR	C38-C26-C25	-4.50	119.48	124.53
23	A2	401	BCR	C11-C10-C9	-4.49	120.90	127.31
23	F2	401	BCR	C36-C18-C19	4.48	125.14	118.08
23	h1	102	BCR	C20-C21-C22	-4.48	120.92	127.31
23	B1	601	BCR	C28-C27-C26	-4.48	106.08	114.08
23	c1	502	BCR	C7-C8-C9	-4.47	119.48	126.23
23	b2	601	BCR	C15-C14-C13	-4.46	120.95	127.31
23	K1	101	BCR	C33-C5-C6	-4.42	119.56	124.53
29	M1	101	LMG	O7-C10-C11	4.42	121.03	111.50
34	c2	516	DGD	O2G-C1B-C2B	4.42	121.02	111.50
23	j2	102	BCR	C24-C23-C22	-4.41	119.57	126.23
23	C2	502	BCR	C20-C21-C22	-4.40	121.03	127.31
23	c2	501	BCR	C36-C18-C19	4.40	125.00	118.08
23	c2	501	BCR	C7-C8-C9	-4.39	119.59	126.23
23	K1	101	BCR	C16-C17-C18	-4.39	121.04	127.31
23	K2	104	BCR	C28-C27-C26	-4.39	106.24	114.08
34	c1	518	DGD	O2G-C1B-C2B	4.39	120.95	111.50
23	B2	603	BCR	C15-C14-C13	-4.37	121.07	127.31
29	B1	626	LMG	O7-C10-C11	4.37	120.92	111.50
23	B1	601	BCR	C7-C8-C9	-4.37	119.64	126.23
23	d2	401	BCR	C20-C21-C22	-4.36	121.09	127.31
23	k2	501	BCR	C16-C17-C18	-4.36	121.09	127.31
23	C1	521	BCR	C15-C14-C13	-4.35	121.10	127.31
23	b2	603	BCR	C15-C14-C13	-4.34	121.12	127.31
23	K2	102	BCR	C36-C18-C19	4.33	124.90	118.08
23	b2	603	BCR	C7-C8-C9	-4.33	119.69	126.23
29	b1	621	LMG	O7-C10-C11	4.32	120.82	111.50
29	b1	631	LMG	O7-C10-C11	4.30	120.77	111.50
23	b1	602	BCR	C35-C13-C12	4.27	124.80	118.08
23	J1	101	BCR	C15-C14-C13	-4.25	121.24	127.31
23	K2	102	BCR	C15-C14-C13	-4.25	121.24	127.31
23	b2	603	BCR	C11-C10-C9	-4.24	121.25	127.31
37	B2	623	SQD	O47-C7-C8	4.23	120.62	111.50
23	J1	101	BCR	C36-C18-C19	4.22	124.73	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b2	602	BCR	C15-C14-C13	-4.22	121.29	127.31
29	A2	412	LMG	O7-C10-C11	4.22	120.59	111.50
34	c1	514	DGD	O2G-C1B-C2B	4.21	120.56	111.50
34	C1	515	DGD	O2G-C1B-C2B	4.20	120.56	111.50
23	d2	401	BCR	C38-C26-C25	-4.19	119.82	124.53
23	z2	101	BCR	C15-C14-C13	-4.18	121.34	127.31
23	c1	502	BCR	C33-C5-C6	-4.18	119.84	124.53
23	k1	101	BCR	C24-C23-C22	-4.17	119.93	126.23
23	h1	102	BCR	C28-C27-C26	-4.17	106.62	114.08
23	b1	601	BCR	C28-C27-C26	-4.16	106.64	114.08
23	d2	401	BCR	C11-C10-C9	-4.15	121.38	127.31
34	H1	101	DGD	O2G-C1B-C2B	4.15	120.44	111.50
29	j2	101	LMG	O7-C10-C11	4.15	120.44	111.50
23	z2	101	BCR	C16-C17-C18	-4.15	121.39	127.31
33	L2	101	LHG	O7-C7-C8	4.13	120.41	111.50
34	C1	516	DGD	O2G-C1B-C2B	4.13	120.40	111.50
23	D1	401	BCR	C24-C23-C22	-4.13	120.00	126.23
23	c1	501	BCR	C24-C23-C22	-4.13	120.00	126.23
29	I2	101	LMG	O7-C10-C11	4.12	120.39	111.50
23	A2	401	BCR	C33-C5-C6	-4.12	119.90	124.53
34	c2	514	DGD	O2G-C1B-C2B	4.12	120.37	111.50
23	B1	602	BCR	C28-C27-C26	-4.11	106.75	114.08
23	C1	521	BCR	C16-C17-C18	-4.09	121.47	127.31
23	k1	101	BCR	C36-C18-C19	4.08	124.50	118.08
25	a1	403	CLA	C3B-C4B-NB	-4.07	106.74	110.52
23	j2	102	BCR	C36-C18-C19	4.07	124.49	118.08
23	B2	602	BCR	C16-C17-C18	-4.07	121.50	127.31
29	C1	520	LMG	O7-C10-C11	4.07	120.27	111.50
23	C2	502	BCR	C16-C17-C18	-4.07	121.50	127.31
29	d1	408	LMG	O7-C10-C11	4.06	120.26	111.50
33	l2	101	LHG	O7-C7-C8	4.06	120.26	111.50
23	B2	603	BCR	C7-C8-C9	-4.06	120.10	126.23
23	D1	401	BCR	C33-C5-C6	-4.04	119.99	124.53
33	a2	407	LHG	O7-C7-C8	4.04	120.22	111.50
23	B2	603	BCR	C11-C10-C9	-4.04	121.55	127.31
23	b2	601	BCR	C7-C8-C9	-4.03	120.14	126.23
33	B2	627	LHG	O7-C7-C8	4.02	120.17	111.50
34	h1	101	DGD	O2G-C1B-C2B	4.02	120.16	111.50
33	l1	102	LHG	O7-C7-C8	4.00	120.12	111.50
23	K1	101	BCR	C3-C4-C5	-3.99	106.94	114.08
23	h2	101	BCR	C11-C10-C9	-3.99	121.61	127.31
23	b2	602	BCR	C24-C23-C22	-3.99	120.21	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b2	625	LHG	O7-C7-C8	3.99	120.09	111.50
29	F2	402	LMG	O7-C10-C11	3.98	120.09	111.50
25	A2	402	CLA	C3B-C4B-NB	-3.98	106.82	110.52
23	c2	501	BCR	C11-C10-C9	-3.98	121.63	127.31
23	d2	401	BCR	C24-C23-C22	-3.98	120.22	126.23
23	b2	603	BCR	C24-C23-C22	-3.97	120.23	126.23
29	A1	412	LMG	O7-C10-C11	3.97	120.06	111.50
23	k2	501	BCR	C11-C10-C9	-3.97	121.64	127.31
23	a1	401	BCR	C33-C5-C6	-3.96	120.08	124.53
23	b2	601	BCR	C11-C10-C9	-3.96	121.66	127.31
33	a1	407	LHG	O7-C7-C8	3.95	120.02	111.50
23	B1	601	BCR	C24-C23-C22	-3.95	120.27	126.23
27	D1	407	PHO	C1-C2-C3	-3.95	119.22	126.04
23	k1	101	BCR	C15-C14-C13	-3.94	121.68	127.31
29	B2	621	LMG	O7-C10-C11	3.94	120.00	111.50
23	D1	401	BCR	C15-C14-C13	-3.94	121.69	127.31
23	d1	405	BCR	C33-C5-C6	-3.94	120.11	124.53
23	d2	401	BCR	C15-C14-C13	-3.93	121.70	127.31
33	d1	407	LHG	O7-C7-C8	3.93	119.97	111.50
23	K1	101	BCR	C11-C10-C9	-3.92	121.71	127.31
23	b1	603	BCR	C15-C14-C13	-3.92	121.71	127.31
23	A1	401	BCR	C16-C17-C18	-3.91	121.73	127.31
23	d2	401	BCR	C1-C6-C5	-3.91	117.11	122.61
23	C1	521	BCR	C24-C23-C22	-3.91	120.33	126.23
23	h1	102	BCR	C24-C23-C22	-3.90	120.34	126.23
23	F2	401	BCR	C11-C10-C9	-3.90	121.75	127.31
25	A1	403	CLA	C3B-C4B-NB	-3.90	106.90	110.52
25	a2	404	CLA	C3B-C4B-NB	-3.90	106.90	110.52
25	b1	613	CLA	O2A-CGA-O1A	-3.89	113.77	123.59
23	b1	603	BCR	C11-C10-C9	-3.89	121.76	127.31
33	D1	404	LHG	O7-C7-C8	3.89	119.88	111.50
23	d2	401	BCR	C3-C4-C5	-3.89	107.14	114.08
27	d2	408	PHO	C1-C2-C3	-3.88	119.33	126.04
23	F2	401	BCR	C24-C23-C22	-3.88	120.37	126.23
29	a2	412	LMG	O7-C10-C11	3.88	119.85	111.50
33	D2	405	LHG	O7-C7-C8	3.87	119.85	111.50
23	c1	502	BCR	C11-C10-C9	-3.86	121.80	127.31
29	A1	410	LMG	O7-C10-C11	3.86	119.82	111.50
23	b1	603	BCR	C7-C8-C9	-3.86	120.41	126.23
33	L1	101	LHG	O7-C7-C8	3.86	119.81	111.50
23	B2	602	BCR	C38-C26-C25	-3.85	120.20	124.53
23	A1	401	BCR	C7-C8-C9	-3.84	120.43	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b1	622	LHG	O7-C7-C8	3.84	119.78	111.50
36	d2	409	PL9	C22-C23-C24	-3.84	118.42	127.66
29	D1	406	LMG	O7-C10-C11	3.84	119.77	111.50
23	b2	602	BCR	C16-C17-C18	-3.84	121.84	127.31
23	a2	402	BCR	C38-C26-C25	-3.84	120.22	124.53
34	C1	517	DGD	O2G-C1B-C2B	3.83	119.77	111.50
29	b1	624	LMG	O1-C1-C2	3.83	114.28	108.30
23	d1	405	BCR	C24-C23-C22	-3.83	120.45	126.23
29	d1	411	LMG	O7-C10-C11	3.82	119.74	111.50
34	H2	101	DGD	O2G-C1B-C2B	3.82	119.74	111.50
33	D1	405	LHG	O7-C7-C8	3.82	119.73	111.50
27	d1	403	PHO	C1-C2-C3	-3.82	119.44	126.04
23	d1	405	BCR	C11-C10-C9	-3.82	121.86	127.31
23	a1	401	BCR	C11-C10-C9	-3.82	121.86	127.31
23	B1	603	BCR	C15-C14-C13	-3.82	121.86	127.31
23	C1	521	BCR	C7-C8-C9	-3.80	120.49	126.23
36	D1	408	PL9	C22-C23-C24	-3.80	118.50	127.66
23	b1	601	BCR	C15-C14-C13	-3.80	121.88	127.31
23	C2	502	BCR	C7-C8-C9	-3.80	120.50	126.23
23	K2	104	BCR	C33-C5-C6	-3.80	120.26	124.53
23	c1	501	BCR	C7-C8-C9	-3.79	120.51	126.23
29	B1	622	LMG	O7-C10-C11	3.79	119.66	111.50
23	B2	601	BCR	C20-C21-C22	-3.79	121.91	127.31
23	B1	603	BCR	C7-C8-C9	-3.78	120.53	126.23
23	c2	501	BCR	C3-C4-C5	-3.77	107.34	114.08
29	a1	412	LMG	O7-C10-C11	3.76	119.60	111.50
23	b2	603	BCR	C38-C26-C25	-3.75	120.31	124.53
23	B1	601	BCR	C15-C14-C13	-3.75	121.95	127.31
23	a1	401	BCR	C38-C26-C25	-3.75	120.32	124.53
23	b1	601	BCR	C7-C8-C9	-3.74	120.58	126.23
23	b2	602	BCR	C11-C10-C9	-3.73	121.99	127.31
23	A1	401	BCR	C33-C5-C6	-3.73	120.34	124.53
23	b2	602	BCR	C38-C26-C25	-3.73	120.34	124.53
23	b1	602	BCR	C28-C27-C26	-3.73	107.42	114.08
23	B2	603	BCR	C20-C21-C22	-3.72	122.00	127.31
33	d2	406	LHG	O7-C7-C8	3.72	119.51	111.50
23	B1	602	BCR	C16-C17-C18	-3.72	122.01	127.31
23	a1	401	BCR	C7-C8-C9	-3.71	120.62	126.23
23	C1	501	BCR	C7-C8-C9	-3.71	120.64	126.23
23	A1	401	BCR	C15-C14-C13	-3.70	122.03	127.31
23	b2	603	BCR	C16-C17-C18	-3.70	122.03	127.31
23	K2	104	BCR	C7-C8-C9	-3.69	120.65	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J1	101	BCR	C11-C10-C9	-3.69	122.04	127.31
23	d2	401	BCR	C4-C5-C6	-3.69	117.37	122.73
23	c2	501	BCR	C33-C5-C6	-3.69	120.38	124.53
25	c2	506	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	B2	602	BCR	C15-C14-C13	-3.68	122.06	127.31
29	c1	519	LMG	O7-C10-C11	3.68	119.43	111.50
33	d2	403	LHG	O7-C7-C8	3.68	119.42	111.50
23	d1	405	BCR	C16-C17-C18	-3.68	122.06	127.31
36	d1	409	PL9	C22-C23-C24	-3.68	118.81	127.66
29	B2	620	LMG	O7-C10-C11	3.67	119.40	111.50
23	z2	101	BCR	C11-C10-C9	-3.66	122.08	127.31
23	B1	601	BCR	C33-C5-C6	-3.66	120.42	124.53
23	C2	502	BCR	C11-C10-C9	-3.66	122.09	127.31
23	K2	102	BCR	C3-C4-C5	-3.65	107.55	114.08
23	b2	601	BCR	C33-C5-C6	-3.65	120.43	124.53
23	K2	102	BCR	C16-C17-C18	-3.65	122.10	127.31
23	b1	602	BCR	C16-C17-C18	-3.65	122.11	127.31
36	d1	409	PL9	C42-C43-C44	-3.65	118.88	127.66
23	A1	401	BCR	C38-C26-C25	-3.64	120.44	124.53
23	B1	603	BCR	C11-C10-C9	-3.64	122.12	127.31
29	b2	622	LMG	O7-C10-C11	3.63	119.33	111.50
23	F2	401	BCR	C33-C5-C6	-3.62	120.46	124.53
23	B2	603	BCR	C38-C26-C25	-3.62	120.46	124.53
34	h2	102	DGD	O2G-C1B-C2B	3.62	119.30	111.50
34	c2	517	DGD	O2G-C1B-C2B	3.62	119.29	111.50
23	k2	501	BCR	C7-C8-C9	-3.61	120.78	126.23
33	D2	403	LHG	O7-C7-C8	3.61	119.27	111.50
25	a1	405	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
23	B1	601	BCR	C11-C10-C9	-3.60	122.17	127.31
23	B2	603	BCR	C24-C23-C22	-3.60	120.79	126.23
36	D2	408	PL9	C42-C43-C44	-3.60	119.00	127.66
23	k1	101	BCR	C11-C10-C9	-3.59	122.18	127.31
23	b2	601	BCR	C16-C17-C18	-3.59	122.18	127.31
23	B2	601	BCR	C33-C5-C6	-3.58	120.50	124.53
23	B1	603	BCR	C16-C17-C18	-3.58	122.20	127.31
23	h2	101	BCR	C16-C17-C18	-3.57	122.21	127.31
23	K1	101	BCR	C7-C8-C9	-3.55	120.87	126.23
23	b1	601	BCR	C33-C5-C6	-3.54	120.55	124.53
36	D1	408	PL9	C37-C38-C39	-3.54	119.14	127.66
23	K2	102	BCR	C11-C10-C9	-3.53	122.27	127.31
25	A1	405	CLA	C3B-C4B-NB	-3.52	107.25	110.52
23	b2	603	BCR	C20-C21-C22	-3.51	122.30	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B1	611	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
23	B2	602	BCR	C20-C21-C22	-3.50	122.31	127.31
23	B1	602	BCR	C24-C23-C22	-3.50	120.95	126.23
23	C1	501	BCR	C11-C10-C9	-3.50	122.32	127.31
25	B2	607	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
23	B2	601	BCR	C7-C8-C9	-3.49	120.96	126.23
23	B2	603	BCR	C16-C17-C18	-3.49	122.33	127.31
36	D2	408	PL9	C22-C23-C24	-3.48	119.28	127.66
25	b1	606	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
33	B1	621	LHG	O7-C7-C8	3.48	119.00	111.50
25	b2	612	CLA	O2A-CGA-O1A	-3.48	114.82	123.59
23	d1	405	BCR	C15-C14-C13	-3.47	122.36	127.31
23	K2	102	BCR	C33-C5-C6	-3.47	120.63	124.53
23	k2	501	BCR	C3-C4-C5	-3.46	107.89	114.08
34	c1	520	DGD	O2G-C1B-C2B	3.46	118.97	111.50
23	B2	601	BCR	C16-C17-C18	-3.46	122.38	127.31
23	C1	521	BCR	C20-C21-C22	-3.45	122.38	127.31
23	F2	401	BCR	C16-C17-C18	-3.45	122.39	127.31
25	C1	509	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
23	C2	502	BCR	C24-C23-C22	-3.45	121.02	126.23
23	b1	602	BCR	C20-C21-C22	-3.45	122.39	127.31
23	b1	601	BCR	C16-C17-C18	-3.44	122.40	127.31
23	a1	401	BCR	C16-C17-C18	-3.42	122.42	127.31
23	b2	603	BCR	C33-C5-C6	-3.42	120.69	124.53
23	b1	603	BCR	C38-C26-C25	-3.42	120.69	124.53
36	d2	409	PL9	C30-C29-C31	3.41	121.02	115.27
25	b1	608	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
23	a2	402	BCR	C11-C10-C9	-3.40	122.46	127.31
23	b1	603	BCR	C16-C17-C18	-3.40	122.46	127.31
25	B1	609	CLA	CAC-C3C-C2C	-3.39	121.73	127.53
25	B2	613	CLA	O2A-CGA-O1A	-3.38	115.07	123.59
23	a2	402	BCR	C7-C8-C9	-3.37	121.15	126.23
23	z2	101	BCR	C33-C5-C6	-3.37	120.75	124.53
23	h2	101	BCR	C7-C8-C9	-3.36	121.16	126.23
36	D1	408	PL9	C15-C14-C16	3.35	120.91	115.27
23	K2	102	BCR	C36-C18-C17	-3.35	118.23	122.92
25	B1	619	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
25	B2	605	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
25	b1	614	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
29	C2	515	LMG	O7-C10-C11	3.34	120.11	110.80
23	H2	103	BCR	C15-C14-C13	-3.34	122.55	127.31
25	A1	406	CLA	O2D-CGD-O1D	-3.33	117.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b2	602	BCR	C28-C27-C26	-3.33	108.14	114.08
23	b1	601	BCR	C11-C10-C9	-3.31	122.58	127.31
36	d1	409	PL9	C20-C19-C21	3.31	120.84	115.27
23	B1	602	BCR	C20-C21-C22	-3.30	122.59	127.31
33	d1	402	LHG	C5-O7-C7	-3.30	109.67	117.79
25	c1	507	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
25	D2	404	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
25	A2	403	CLA	C3B-C4B-NB	-3.30	107.46	110.52
23	h2	101	BCR	C3-C4-C5	-3.30	108.19	114.08
23	C1	521	BCR	C38-C26-C25	-3.29	120.83	124.53
25	a1	404	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	C2	518	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	C2	502	BCR	C38-C26-C25	-3.29	120.83	124.53
36	D1	408	PL9	C30-C29-C31	3.28	120.79	115.27
25	c1	510	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	B2	601	BCR	C24-C23-C22	-3.28	121.28	126.23
23	d2	401	BCR	C33-C5-C4	3.28	119.91	113.62
25	c2	505	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
34	C1	516	DGD	C2G-O2G-C1B	-3.27	109.73	117.79
25	B1	610	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	d1	401	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
25	b1	607	CLA	C3B-C4B-NB	-3.26	107.49	110.52
23	k2	501	BCR	C28-C27-C26	-3.26	108.25	114.08
23	b1	602	BCR	C35-C13-C14	-3.26	118.35	122.92
25	B2	616	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
25	B1	610	CLA	C3B-C4B-NB	-3.24	107.50	110.52
23	b2	601	BCR	C20-C21-C22	-3.24	122.68	127.31
36	d2	409	PL9	C25-C24-C26	3.24	120.73	115.27
25	d2	402	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
23	A2	401	BCR	C15-C14-C13	-3.24	122.68	127.31
23	c1	501	BCR	C33-C5-C6	-3.24	120.89	124.53
25	b2	612	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
25	d1	406	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	b2	617	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	c2	509	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
25	C1	507	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	B2	609	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
25	B1	616	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	B1	613	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
25	A1	406	CLA	C3B-C4B-NB	-3.23	107.52	110.52
23	z2	101	BCR	C7-C8-C9	-3.23	121.36	126.23
25	b1	605	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b1	609	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
23	d1	405	BCR	C38-C26-C25	-3.22	120.92	124.53
23	h1	102	BCR	C15-C14-C13	-3.21	122.72	127.31
23	B2	601	BCR	C11-C10-C9	-3.21	122.72	127.31
25	B2	619	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
25	b1	616	CLA	C3B-C4B-NB	-3.21	107.53	110.52
23	A1	401	BCR	C11-C10-C9	-3.21	122.73	127.31
29	B1	626	LMG	O8-C28-C29	3.21	121.97	111.91
25	C2	511	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
23	B1	601	BCR	C16-C17-C18	-3.20	122.74	127.31
25	B1	618	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	C2	502	BCR	C33-C5-C6	-3.20	120.93	124.53
27	d1	403	PHO	CMB-C2B-C3B	3.19	130.65	124.68
25	b2	624	CLA	C3B-C4B-NB	-3.19	107.56	110.52
23	B1	602	BCR	C15-C14-C13	-3.19	122.76	127.31
23	k2	501	BCR	C38-C26-C25	-3.18	120.95	124.53
23	J1	101	BCR	C16-C17-C18	-3.18	122.77	127.31
25	A2	402	CLA	CHB-C1B-NB	3.18	127.62	124.26
27	d1	403	PHO	C4D-CHA-CBD	3.17	109.95	108.52
23	b2	601	BCR	C24-C23-C22	-3.16	121.46	126.23
23	C1	521	BCR	C3-C4-C5	-3.16	108.44	114.08
25	b2	620	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
25	C2	507	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
25	c1	508	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
25	B2	618	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
33	d1	402	LHG	O8-C23-C24	3.15	119.65	111.38
23	z2	101	BCR	C20-C21-C22	-3.15	122.81	127.31
23	b1	602	BCR	C24-C23-C22	-3.15	121.48	126.23
25	B1	608	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
36	d1	409	PL9	C15-C14-C16	3.15	120.56	115.27
25	d2	404	CLA	C3B-C4B-NB	-3.14	107.60	110.52
23	a2	402	BCR	C15-C14-C13	-3.14	122.83	127.31
23	a2	402	BCR	C16-C17-C18	-3.14	122.83	127.31
23	d2	401	BCR	C28-C27-C26	-3.14	108.47	114.08
36	D1	408	PL9	C25-C24-C26	3.14	120.55	115.27
23	B2	602	BCR	C24-C23-C22	-3.13	121.50	126.23
23	C1	501	BCR	C3-C4-C5	-3.13	108.49	114.08
33	A2	405	LHG	O7-C7-C8	3.13	119.53	110.80
37	D2	402	SQD	C45-O47-C7	-3.13	112.06	117.90
25	B2	607	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	b1	616	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	z2	101	BCR	C24-C23-C22	-3.12	121.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F2	401	BCR	C36-C18-C17	-3.12	118.55	122.92
25	A1	404	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	c1	515	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	a2	402	BCR	C33-C5-C6	-3.12	121.03	124.53
23	c1	501	BCR	C33-C5-C4	3.11	119.60	113.62
25	B2	611	CLA	C1-C2-C3	-3.11	120.66	126.04
25	C1	506	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	C2	503	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	c1	506	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	B1	607	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
23	k1	101	BCR	C38-C26-C25	-3.10	121.05	124.53
25	D2	406	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
33	l1	102	LHG	C5-O7-C7	-3.09	110.18	117.79
36	d1	409	PL9	C27-C28-C29	-3.09	120.21	127.66
23	k2	501	BCR	C33-C5-C6	-3.09	121.06	124.53
23	h2	101	BCR	C33-C5-C6	-3.09	121.06	124.53
23	z2	101	BCR	C38-C26-C25	-3.09	121.06	124.53
25	d2	404	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
23	C1	501	BCR	C16-C17-C18	-3.08	122.91	127.31
25	a1	403	CLA	CHB-C1B-NB	3.08	127.52	124.26
25	b1	607	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	A2	404	CLA	C3B-C4B-NB	-3.08	107.66	110.52
27	D1	407	PHO	C4-C3-C5	3.08	120.45	115.27
25	a2	404	CLA	CHB-C1B-NB	3.08	127.52	124.26
25	b2	617	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	c1	503	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
33	L2	101	LHG	C5-O7-C7	-3.07	110.23	117.79
36	d2	409	PL9	C17-C18-C19	-3.07	120.27	127.66
25	A1	405	CLA	CHB-C1B-NB	3.07	127.50	124.26
25	c2	502	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	B1	616	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	d1	404	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	c1	502	BCR	C15-C16-C17	-3.06	117.21	123.47
25	c2	503	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
36	D2	408	PL9	C15-C14-C16	3.06	120.42	115.27
25	C1	507	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
36	D1	408	PL9	C32-C33-C34	-3.05	120.31	127.66
25	C1	502	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
23	k1	101	BCR	C16-C17-C18	-3.05	122.95	127.31
23	a1	401	BCR	C24-C23-C22	-3.05	121.62	126.23
25	B1	612	CLA	C3B-C4B-NB	-3.05	107.69	110.52
23	C1	501	BCR	C24-C23-C22	-3.05	121.63	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a2	416	PHO	CBA-CAA-C2A	-3.05	104.91	113.81
23	c1	501	BCR	C3-C4-C5	-3.05	108.64	114.08
38	e2	101	HEM	C1B-NB-C4B	3.04	108.22	105.07
25	C2	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	B2	616	CLA	C3B-C4B-NB	-3.04	107.69	110.52
25	d1	404	CLA	C3B-C4B-NB	-3.04	107.70	110.52
38	f1	101	HEM	C1B-NB-C4B	3.04	108.21	105.07
27	D1	407	PHO	CMB-C2B-C3B	3.03	130.35	124.68
25	C2	513	CLA	C3B-C4B-NB	-3.03	107.70	110.52
25	b2	606	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	j2	102	BCR	C11-C10-C9	-3.03	122.99	127.31
29	B1	622	LMG	O8-C28-C29	3.03	121.41	111.91
36	d2	409	PL9	C37-C38-C39	-3.03	120.37	127.66
36	d1	409	PL9	C17-C18-C19	-3.03	120.38	127.66
25	D1	402	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
23	H1	102	BCR	C33-C5-C6	-3.02	121.13	124.53
23	b1	601	BCR	C3-C4-C5	-3.02	108.68	114.08
25	B1	609	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	C2	508	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	C1	508	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	c2	501	BCR	C33-C5-C4	3.02	119.41	113.62
23	c1	501	BCR	C38-C26-C25	-3.02	121.14	124.53
27	d2	408	PHO	CMB-C2B-C3B	3.01	130.31	124.68
25	C1	514	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	B1	603	BCR	C33-C5-C6	-3.01	121.15	124.53
25	D1	403	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	b1	602	BCR	C15-C14-C13	-3.01	123.02	127.31
23	b1	603	BCR	C24-C23-C22	-3.01	121.69	126.23
25	B1	614	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
23	b1	602	BCR	C34-C9-C10	-3.00	118.72	122.92
25	C2	504	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	C1	509	CLA	O2A-CGA-O1A	-3.00	116.03	123.59
27	a2	416	PHO	CMB-C2B-C3B	2.99	130.28	124.68
25	C2	505	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	C1	510	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	A1	403	CLA	CHB-C1B-NB	2.99	127.42	124.26
25	B1	606	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	b1	620	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
25	A2	404	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
25	B2	610	CLA	C3B-C4B-NB	-2.98	107.75	110.52
36	D2	408	PL9	C37-C38-C39	-2.98	120.48	127.66
23	F2	401	BCR	C28-C27-C26	-2.98	108.75	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B1	617	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	b1	611	CLA	C3B-C4B-NB	-2.98	107.75	110.52
25	b1	604	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	b1	612	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	K2	102	BCR	C38-C26-C25	-2.97	121.19	124.53
29	a1	412	LMG	O8-C28-C29	2.97	121.22	111.91
23	j2	102	BCR	C30-C25-C26	-2.97	118.43	122.61
25	B2	617	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
38	E2	101	HEM	C1B-NB-C4B	2.97	108.14	105.07
27	A2	407	PHO	CBC-CAC-C3C	-2.96	108.54	112.88
25	C1	509	CLA	CHB-C1B-NB	2.96	127.39	124.26
25	b2	611	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	c2	504	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
38	V2	201	HEM	C3B-C2B-C1B	2.96	108.68	106.49
23	J1	101	BCR	C38-C26-C25	-2.96	121.20	124.53
25	B2	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	c2	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	B2	604	CLA	C3B-C4B-NB	-2.96	107.77	110.52
25	B2	606	CLA	C3B-C4B-NB	-2.96	107.77	110.52
23	b1	602	BCR	C33-C5-C6	-2.95	121.21	124.53
25	C1	505	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
38	v2	201	HEM	C4A-NA-C1A	2.95	108.24	105.35
23	F2	401	BCR	C38-C26-C27	2.95	119.28	113.62
23	B1	603	BCR	C38-C26-C25	-2.95	121.22	124.53
23	B1	603	BCR	C20-C21-C22	-2.95	123.10	127.31
38	E1	101	HEM	C1B-NB-C4B	2.95	108.12	105.07
25	c2	515	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	a2	413	CLA	C3B-C4B-NB	-2.95	107.78	110.52
23	c2	501	BCR	C34-C9-C10	-2.95	118.80	122.92
25	d1	401	CLA	C3B-C4B-NB	-2.95	107.78	110.52
34	c1	518	DGD	C2G-O2G-C1B	-2.95	110.54	117.79
23	B2	601	BCR	C29-C30-C25	2.94	115.01	110.48
36	D2	408	PL9	C27-C28-C29	-2.94	120.58	127.66
23	K2	104	BCR	C3-C4-C5	-2.94	108.83	114.08
23	A2	401	BCR	C38-C26-C27	2.94	119.26	113.62
23	B1	603	BCR	C28-C27-C26	-2.94	108.83	114.08
23	a1	401	BCR	C15-C14-C13	-2.94	123.12	127.31
25	C1	513	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
23	b1	601	BCR	C29-C30-C25	2.93	115.00	110.48
25	c1	516	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	K2	101	CLA	C3B-C4B-NB	-2.93	107.80	110.52
23	C1	501	BCR	C38-C26-C25	-2.93	121.24	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A2	403	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	d2	402	CLA	C3B-C4B-NB	-2.92	107.81	110.52
25	b2	610	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	C1	521	BCR	C33-C5-C6	-2.91	121.26	124.53
25	B2	611	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	C1	501	BCR	C33-C5-C6	-2.91	121.26	124.53
34	C2	512	DGD	C2G-O2G-C1B	-2.91	112.47	117.90
25	B1	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	A1	406	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	c2	503	CLA	C3B-C4B-NB	-2.91	107.81	110.52
25	c2	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	B1	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	C1	514	CLA	C3B-C4B-NB	-2.91	107.82	110.52
36	D2	408	PL9	C20-C19-C21	2.91	120.16	115.27
27	A2	407	PHO	C4-C3-C5	2.91	120.16	115.27
25	C1	503	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	b2	610	CLA	C1-C2-C3	-2.90	121.02	126.04
25	B1	606	CLA	C3B-C4B-NB	-2.90	107.82	110.52
25	c2	515	CLA	C3B-C4B-NB	-2.90	107.82	110.52
25	d2	405	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	a2	413	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	B2	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	B1	607	CLA	C3B-C4B-NB	-2.90	107.83	110.52
25	b1	610	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
36	D1	408	PL9	C20-C19-C21	2.89	120.14	115.27
27	A1	408	PHO	C4-C3-C5	2.89	120.13	115.27
23	A1	401	BCR	C20-C21-C22	-2.89	123.19	127.31
23	A2	401	BCR	C23-C24-C25	-2.89	119.10	127.20
25	b1	613	CLA	CHB-C1B-NB	2.88	127.31	124.26
25	a2	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	b1	603	BCR	C28-C27-C26	-2.88	108.93	114.08
25	B1	605	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	c1	502	BCR	C38-C26-C25	-2.88	121.29	124.53
29	b1	631	LMG	O1-C1-C2	2.88	112.80	108.30
25	b2	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	B1	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	b2	618	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	c2	510	CLA	C3B-C4B-NB	-2.88	107.85	110.52
25	a2	405	CLA	C3B-C4B-NB	-2.87	107.85	110.52
36	d1	409	PL9	C53-C6-C1	2.87	120.87	114.99
23	b2	602	BCR	C1-C6-C5	-2.87	118.57	122.61
25	d1	406	CLA	C3B-C4B-NB	-2.87	107.85	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b2	608	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	a1	404	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
38	e2	101	HEM	C3B-C2B-C1B	2.86	108.61	106.49
29	B1	622	LMG	C8-O7-C10	-2.86	110.74	117.79
27	d1	403	PHO	O2D-CGD-O1D	-2.86	118.24	123.84
36	d1	409	PL9	C32-C33-C34	-2.86	120.77	127.66
34	c2	516	DGD	O1G-C1A-C2A	2.86	120.88	111.91
25	D2	401	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	A1	403	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	j2	102	BCR	C38-C26-C25	-2.86	121.32	124.53
29	A1	410	LMG	C8-O7-C10	-2.86	110.75	117.79
33	D2	403	LHG	O8-C23-C24	2.86	120.87	111.91
36	d2	409	PL9	C32-C33-C34	-2.86	120.78	127.66
29	a2	412	LMG	O8-C28-C29	2.86	120.87	111.91
25	C2	513	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
27	a2	416	PHO	O1D-CGD-CBD	-2.85	119.98	124.74
25	b2	616	CLA	C3B-C4B-NB	-2.85	107.87	110.52
23	H2	103	BCR	C11-C10-C9	-2.85	123.24	127.31
23	C1	501	BCR	C15-C16-C17	-2.85	117.63	123.47
25	b2	613	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	d2	409	PL9	C53-C6-C1	2.85	120.81	114.99
25	b1	609	CLA	C3B-C4B-NB	-2.84	107.88	110.52
25	B1	618	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	A2	401	BCR	C29-C30-C25	2.84	114.86	110.48
33	b2	625	LHG	O8-C23-C24	2.84	120.82	111.91
23	A2	401	BCR	C20-C21-C22	-2.84	123.26	127.31
25	A1	406	CLA	O2D-CGD-CBD	2.84	116.31	111.27
38	V2	201	HEM	C1B-NB-C4B	2.84	108.00	105.07
25	c2	511	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
27	D2	407	PHO	O2A-CGA-CBA	2.83	120.80	111.91
25	b2	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	d2	407	LMG	C8-O7-C10	-2.83	112.62	117.90
29	B2	620	LMG	O8-C28-C29	2.83	120.79	111.91
33	a1	407	LHG	O8-C23-C24	2.83	120.79	111.91
25	c2	507	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
38	V1	201	HEM	C4A-NA-C1A	2.83	108.12	105.35
25	A1	405	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	b2	616	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	C1	503	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	B1	608	CLA	C3B-C4B-NB	-2.82	107.89	110.52
36	d2	409	PL9	C15-C14-C16	2.82	120.02	115.27
25	B1	604	CLA	C3B-C4B-NB	-2.82	107.90	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A1	408	PHO	C4D-CHA-CBD	2.82	109.79	108.52
23	K2	102	BCR	C33-C5-C4	2.82	119.03	113.62
38	v2	201	HEM	CHD-C1D-ND	2.82	127.48	124.42
25	C1	504	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	b1	619	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	B1	609	CLA	CBC-CAC-C3C	2.82	120.20	112.43
25	c2	513	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	b2	601	BCR	C38-C26-C25	-2.82	121.36	124.53
25	B2	606	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	b2	614	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	a2	416	PHO	C1-C2-C3	-2.81	121.18	126.04
38	f1	101	HEM	C3B-C2B-C1B	2.81	108.57	106.49
36	D2	408	PL9	C40-C39-C41	2.81	120.00	115.27
25	A1	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	C2	504	CLA	C3B-C4B-NB	-2.80	107.91	110.52
23	B1	601	BCR	C29-C30-C25	2.80	114.80	110.48
38	v2	201	HEM	CAD-C3D-C4D	2.80	129.56	124.66
33	B2	627	LHG	O8-C23-C24	2.80	120.70	111.91
25	b1	612	CLA	C3B-C4B-NB	-2.80	107.92	110.52
29	M1	101	LMG	O8-C28-C29	2.79	120.67	111.91
25	b1	610	CLA	C3B-C4B-NB	-2.79	107.92	110.52
38	E1	101	HEM	C3B-C2B-C1B	2.79	108.56	106.49
25	C2	509	CLA	CHB-C4A-NA	2.79	128.37	124.51
36	d2	409	PL9	C20-C19-C21	2.79	119.96	115.27
23	b1	603	BCR	C20-C21-C22	-2.79	123.33	127.31
25	C2	510	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
38	V2	201	HEM	C4C-NC-C1C	2.79	108.08	105.35
25	b1	604	CLA	C3B-C4B-NB	-2.78	107.93	110.52
37	D1	409	SQD	O48-C23-C24	2.78	120.64	111.91
23	K1	101	BCR	C20-C21-C22	-2.78	123.34	127.31
25	C2	516	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	k1	101	BCR	C7-C8-C9	-2.78	122.03	126.23
23	b2	602	BCR	C3-C4-C5	-2.78	109.11	114.08
25	c2	504	CLA	C3B-C4B-NB	-2.78	107.94	110.52
38	e2	101	HEM	C4A-NA-C1A	2.78	108.07	105.35
25	b2	604	CLA	C3B-C4B-NB	-2.78	107.94	110.52
37	D1	409	SQD	C45-O47-C7	-2.77	112.72	117.90
25	B1	610	CLA	CHB-C1B-NB	2.77	127.19	124.26
38	E2	101	HEM	C4A-NA-C1A	2.77	108.06	105.35
23	B2	603	BCR	C33-C5-C6	-2.77	121.42	124.53
25	b1	613	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	c2	511	CLA	C3B-C4B-NB	-2.77	107.95	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f1	101	HEM	C4A-NA-C1A	2.77	108.06	105.35
27	a2	416	PHO	C4-C3-C5	2.77	119.92	115.27
23	h2	101	BCR	C38-C26-C25	-2.77	121.42	124.53
25	b1	615	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
27	D2	407	PHO	CAA-CBA-CGA	-2.76	105.17	113.25
25	C1	509	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
25	B2	610	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
38	V2	201	HEM	C4A-NA-C1A	2.76	108.05	105.35
25	c1	513	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b1	602	BCR	C11-C10-C9	-2.76	123.37	127.31
23	b2	601	BCR	C38-C26-C27	2.76	118.91	113.62
23	b1	602	BCR	C8-C9-C10	2.76	123.17	118.94
25	C2	510	CLA	C3B-C4B-NB	-2.76	107.96	110.52
25	b2	606	CLA	C3B-C4B-NB	-2.75	107.96	110.52
25	B2	614	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
38	E1	101	HEM	C4A-NA-C1A	2.75	108.04	105.35
23	b2	603	BCR	C28-C27-C26	-2.75	109.17	114.08
25	C1	512	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	K2	104	BCR	C33-C5-C4	2.75	118.89	113.62
25	B1	615	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	b1	601	BCR	C24-C23-C22	-2.75	122.09	126.23
25	B1	617	CLA	C3B-C4B-NB	-2.75	107.97	110.52
36	D2	408	PL9	C30-C29-C31	2.75	119.89	115.27
29	b1	624	LMG	C8-O7-C10	-2.74	111.03	117.79
25	B2	609	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	D2	406	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	C1	512	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	c1	504	CLA	C3B-C4B-NB	-2.74	107.97	110.52
25	c1	509	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	d2	402	CLA	CHB-C4A-NA	2.74	128.31	124.51
27	D2	407	PHO	CMB-C2B-C3B	2.74	129.80	124.68
27	a1	411	PHO	O2D-CGD-O1D	-2.74	118.48	123.84
25	B1	613	CLA	C3B-C4B-NB	-2.74	107.98	110.52
25	c1	504	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
25	D2	406	CLA	CHB-C4A-NA	2.73	128.29	124.51
34	h2	102	DGD	O1G-C1A-C2A	2.73	120.48	111.91
36	D1	408	PL9	C27-C28-C29	-2.73	121.08	127.66
23	b2	601	BCR	C29-C30-C25	2.73	114.68	110.48
33	b1	622	LHG	O8-C23-C24	2.73	120.46	111.91
25	A1	404	CLA	CHB-C4A-NA	2.72	128.28	124.51
27	d2	408	PHO	C4-C3-C5	2.72	119.85	115.27
25	b2	615	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b1	617	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	c2	510	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
23	c1	502	BCR	C37-C22-C21	-2.72	119.12	122.92
29	d1	411	LMG	O8-C28-C29	2.72	120.43	111.91
25	B2	613	CLA	CHB-C1B-NB	2.71	127.13	124.26
37	D1	409	SQD	O8-S-C6	2.71	110.06	105.74
34	h1	101	DGD	O1G-C1A-C2A	2.71	120.41	111.91
38	v1	201	HEM	C4C-NC-C1C	2.71	108.00	105.35
23	b1	602	BCR	C3-C4-C5	-2.70	109.25	114.08
27	A1	408	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
25	B2	607	CLA	O2D-CGD-CBD	2.70	116.07	111.27
25	b2	615	CLA	C3B-C4B-NB	-2.70	108.01	110.52
33	d1	407	LHG	C5-O7-C7	-2.70	111.14	117.79
33	D1	404	LHG	O8-C23-C24	2.70	120.37	111.91
25	K2	101	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
25	c2	509	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
25	b1	615	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	B2	613	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
36	d2	409	PL9	C25-C24-C23	-2.70	116.76	123.68
25	C1	510	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	b1	608	CLA	C3B-C4B-NB	-2.69	108.02	110.52
36	D2	408	PL9	C53-C6-C1	2.69	120.50	114.99
36	D1	408	PL9	C17-C18-C19	-2.69	121.18	127.66
25	K2	101	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	b1	601	BCR	C20-C21-C22	-2.69	123.47	127.31
25	b2	619	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	b2	612	CLA	CHB-C1B-NB	2.69	127.11	124.26
23	B1	601	BCR	C38-C26-C27	2.69	118.78	113.62
25	A2	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	b2	602	BCR	C33-C5-C4	2.69	118.78	113.62
25	b2	612	CLA	C3B-C4B-NB	-2.69	108.02	110.52
34	H1	101	DGD	O1G-C1A-C2A	2.69	120.34	111.91
23	C1	521	BCR	C33-C5-C4	2.69	118.78	113.62
23	c1	502	BCR	C36-C18-C17	-2.69	119.16	122.92
25	b1	617	CLA	C3B-C4B-NB	-2.69	108.02	110.52
25	a1	405	CLA	CHB-C4A-NA	2.69	128.23	124.51
27	a1	411	PHO	C1-C2-C3	-2.69	121.40	126.04
25	d2	402	CLA	O2D-CGD-CBD	2.68	116.04	111.27
36	D2	408	PL9	C25-C24-C26	2.68	119.78	115.27
23	h1	102	BCR	C33-C5-C6	-2.68	121.52	124.53
27	a1	411	PHO	CMB-C2B-C3B	2.68	129.69	124.68
25	c2	502	CLA	C3B-C4B-NB	-2.68	108.03	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b1	601	BCR	C38-C26-C25	-2.68	121.52	124.53
33	L2	101	LHG	O8-C23-C24	2.68	120.31	111.91
25	C2	505	CLA	C3B-C4B-NB	-2.68	108.03	110.52
36	D2	408	PL9	C32-C33-C34	-2.68	121.22	127.66
36	D1	408	PL9	C53-C6-C1	2.68	120.46	114.99
29	A1	410	LMG	O8-C28-C29	2.68	120.31	111.91
25	b1	617	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
29	c2	519	LMG	O8-C28-C29	2.68	120.30	111.91
23	h1	102	BCR	C29-C30-C25	2.67	114.59	110.48
23	K2	104	BCR	C29-C30-C25	2.67	114.59	110.48
27	D2	407	PHO	C4-C3-C5	2.67	119.76	115.27
23	d2	401	BCR	C16-C15-C14	-2.67	118.01	123.47
33	l1	102	LHG	O8-C23-C24	2.67	120.28	111.91
36	d1	409	PL9	C37-C38-C39	-2.67	121.24	127.66
25	D2	404	CLA	C3B-C4B-NB	-2.67	108.04	110.52
27	A1	408	PHO	C1-C2-C3	-2.66	121.44	126.04
25	B2	615	CLA	C3B-C4B-NB	-2.66	108.04	110.52
25	B2	612	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
25	a1	403	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
33	d2	406	LHG	O8-C23-C24	2.66	120.25	111.91
25	c1	516	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	B2	608	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	b2	610	CLA	C3B-C4B-NB	-2.66	108.05	110.52
29	B1	626	LMG	C8-O7-C10	-2.66	111.25	117.79
25	B2	617	CLA	CHB-C4A-NA	2.66	128.18	124.51
25	c1	511	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
23	j2	102	BCR	C37-C22-C21	-2.65	119.20	122.92
25	c1	512	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	c1	503	CLA	C3B-C4B-NB	-2.65	108.05	110.52
33	l2	101	LHG	O8-C23-C24	2.65	120.23	111.91
27	d1	403	PHO	O2A-CGA-CBA	2.65	120.23	111.91
27	d2	408	PHO	O2A-CGA-CBA	2.65	120.23	111.91
25	b2	619	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	a2	402	BCR	C23-C24-C25	-2.65	119.76	127.20
23	J1	101	BCR	C36-C18-C17	-2.65	119.21	122.92
27	d1	403	PHO	C4-C3-C5	2.65	119.73	115.27
25	c1	505	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	C2	509	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
38	v1	201	HEM	C4A-NA-C1A	2.65	107.94	105.35
27	A1	408	PHO	CMB-C2B-C3B	2.65	129.63	124.68
25	c1	505	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	B2	612	CLA	C3B-C4B-NB	-2.65	108.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j2	101	LMG	O8-C28-C29	2.65	120.21	111.91
25	c1	508	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	b2	611	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	D1	403	CLA	C3B-C4B-NB	-2.64	108.06	110.52
36	D1	408	PL9	C25-C24-C23	-2.64	116.90	123.68
29	B2	620	LMG	C8-O7-C10	-2.64	111.28	117.79
34	c2	514	DGD	C2G-O2G-C1B	-2.64	111.29	117.79
25	b2	624	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	a1	405	CLA	C3B-C4B-NB	-2.64	108.07	110.52
25	b1	619	CLA	C3B-C4B-NB	-2.64	108.07	110.52
25	a1	404	CLA	CHB-C1B-NB	2.64	127.05	124.26
23	h1	102	BCR	C11-C10-C9	-2.64	123.55	127.31
25	B1	609	CLA	C3B-C4B-NB	-2.64	108.07	110.52
23	B1	602	BCR	C38-C26-C25	-2.64	121.57	124.53
23	a1	401	BCR	C40-C30-C25	-2.64	106.03	110.30
25	b1	620	CLA	C3B-C4B-NB	-2.63	108.07	110.52
25	c2	509	CLA	C3B-C4B-NB	-2.63	108.07	110.52
25	C1	505	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	d1	404	CLA	CHB-C4A-NA	2.63	128.15	124.51
36	D1	408	PL9	C10-C9-C11	2.63	119.70	115.27
23	D1	401	BCR	C38-C26-C25	-2.63	121.58	124.53
27	a1	411	PHO	C4D-CHA-CBD	2.63	109.71	108.52
23	A2	401	BCR	C16-C15-C14	-2.63	118.09	123.47
25	B2	615	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
27	D2	407	PHO	O1D-CGD-CBD	-2.62	120.37	124.74
25	B2	611	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	b2	618	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	c2	513	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	B2	619	CLA	C3B-C4B-NB	-2.62	108.08	110.52
36	d1	409	PL9	C30-C29-C31	2.62	119.68	115.27
23	a1	401	BCR	C20-C21-C22	-2.62	123.57	127.31
29	B2	621	LMG	O1-C1-C2	2.62	112.39	108.30
25	B2	613	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	b2	616	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	c2	509	CLA	CHB-C1B-NB	2.62	127.03	124.26
23	H2	103	BCR	C33-C5-C6	-2.62	121.59	124.53
25	b1	605	CLA	C3B-C4B-NB	-2.62	108.09	110.52
25	C2	503	CLA	C3B-C4B-NB	-2.62	108.09	110.52
23	h2	101	BCR	C21-C20-C19	-2.62	115.06	123.22
29	B2	621	LMG	C7-O1-C1	-2.61	108.63	113.74
36	d1	409	PL9	C25-C24-C26	2.61	119.67	115.27
23	B1	601	BCR	C38-C26-C25	-2.61	121.59	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c2	508	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	j2	102	BCR	C16-C17-C18	-2.61	123.58	127.31
33	d2	403	LHG	O8-C23-C24	2.61	120.10	111.91
25	B1	611	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	b2	608	CLA	C3B-C4B-NB	-2.61	108.09	110.52
34	C1	515	DGD	O1G-C1A-C2A	2.61	120.09	111.91
33	D2	405	LHG	C5-O7-C7	-2.61	111.37	117.79
25	c2	512	CLA	C3B-C4B-NB	-2.61	108.10	110.52
23	K1	101	BCR	C33-C5-C4	2.61	118.62	113.62
27	A1	408	PHO	CBA-CAA-C2A	-2.61	106.20	113.81
23	A2	401	BCR	C33-C5-C4	2.61	118.62	113.62
33	B1	621	LHG	O8-C23-C24	2.60	120.08	111.91
25	c1	503	CLA	CHB-C4A-NA	2.60	128.11	124.51
36	d1	409	PL9	C40-C39-C41	2.60	119.65	115.27
29	a2	412	LMG	O1-C1-C2	2.60	112.36	108.30
23	c1	501	BCR	C8-C7-C6	-2.60	119.89	127.20
29	b2	622	LMG	O8-C28-C29	2.60	120.07	111.91
23	b1	603	BCR	C1-C6-C5	-2.60	118.95	122.61
25	B1	611	CLA	O2D-CGD-CBD	2.60	115.89	111.27
29	I2	101	LMG	O8-C28-C29	2.60	120.06	111.91
23	A1	401	BCR	C24-C23-C22	-2.60	122.31	126.23
29	b1	631	LMG	C8-O7-C10	-2.60	111.39	117.79
23	a2	402	BCR	C20-C21-C22	-2.60	123.60	127.31
25	B1	615	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	C2	518	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	B2	617	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	b1	612	CLA	C1-C2-C3	-2.59	121.56	126.04
25	A1	405	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	b2	609	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	b2	618	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	b1	620	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	b2	609	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	B2	615	CLA	CHB-C4A-NA	2.59	128.09	124.51
33	L1	101	LHG	O8-C23-C24	2.59	120.02	111.91
23	K2	102	BCR	C37-C22-C21	-2.58	119.30	122.92
25	b1	607	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	c1	510	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	c1	510	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
25	b1	619	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	B2	619	CLA	CHD-C1D-ND	-2.58	122.08	124.45
37	B2	623	SQD	C45-O47-C7	-2.58	111.44	117.79
23	h1	102	BCR	C10-C11-C12	-2.58	115.16	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A2	407	PHO	CMB-C2B-C3B	2.58	129.51	124.68
23	A1	401	BCR	C3-C4-C5	-2.58	109.47	114.08
25	b2	606	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	C1	511	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
38	E2	101	HEM	C3B-C2B-C1B	2.58	108.40	106.49
29	b1	631	LMG	C7-O1-C1	-2.58	108.70	113.74
25	C2	511	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	J1	101	BCR	C7-C8-C9	-2.58	122.34	126.23
23	d2	401	BCR	C38-C26-C27	2.57	118.56	113.62
33	A2	405	LHG	O8-C23-C24	2.57	119.98	111.91
27	A2	407	PHO	C1-C2-C3	-2.57	121.59	126.04
25	C2	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	A1	405	CLA	CAC-C3C-C4C	2.57	128.15	124.81
37	B2	623	SQD	O9-S-C6	2.57	109.99	106.94
35	c1	517	LMT	C1B-O1B-C4'	-2.57	111.61	117.96
23	H2	103	BCR	C7-C8-C9	-2.57	122.36	126.23
34	c2	514	DGD	O1G-C1A-C2A	2.57	119.96	111.91
25	B2	604	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
25	b1	610	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	B1	602	BCR	C34-C9-C10	-2.56	119.33	122.92
23	J1	101	BCR	C8-C7-C6	-2.56	120.01	127.20
25	C2	508	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	B2	618	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	a1	405	CLA	O2D-CGD-CBD	2.56	115.82	111.27
23	A2	401	BCR	C24-C23-C22	-2.56	122.37	126.23
25	C2	516	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	B2	609	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
23	F2	401	BCR	C38-C26-C25	-2.56	121.66	124.53
25	B1	619	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	b2	620	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	k1	101	BCR	C37-C22-C21	-2.55	119.34	122.92
34	H2	101	DGD	O1G-C1A-C2A	2.55	119.92	111.91
23	B1	601	BCR	C20-C21-C22	-2.55	123.67	127.31
25	d2	404	CLA	CHB-C4A-NA	2.55	128.04	124.51
34	c1	514	DGD	O1G-C1A-C2A	2.55	119.92	111.91
36	d2	409	PL9	C10-C9-C11	2.55	119.56	115.27
33	l2	101	LHG	C5-O7-C7	-2.55	111.51	117.79
25	a2	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	C2	506	CLA	C3B-C4B-NB	-2.55	108.15	110.52
33	D2	405	LHG	O8-C23-C24	2.55	119.91	111.91
25	B2	616	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	C2	509	CLA	C3B-C4B-NB	-2.55	108.15	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b1	607	CLA	CHB-C1B-NB	2.55	126.95	124.26
25	b1	606	CLA	C3B-C4B-NB	-2.54	108.15	110.52
27	a1	411	PHO	C4-C3-C5	2.54	119.55	115.27
29	a1	412	LMG	C8-O7-C10	-2.54	111.53	117.79
25	B2	607	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	c2	513	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	b2	615	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	d1	404	CLA	CHB-C1B-NB	2.54	126.95	124.26
23	b2	602	BCR	C38-C26-C27	2.54	118.50	113.62
23	A2	401	BCR	C38-C26-C25	-2.54	121.67	124.53
27	A2	407	PHO	CBA-CAA-C2A	-2.54	106.39	113.81
23	F2	401	BCR	C27-C26-C25	-2.54	119.04	122.73
29	M1	101	LMG	C8-O7-C10	-2.54	114.61	117.88
25	c2	503	CLA	CHB-C4A-NA	2.54	128.02	124.51
34	c1	518	DGD	O1G-C1A-C2A	2.54	119.87	111.91
25	C1	503	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	A2	401	BCR	C27-C26-C25	-2.54	119.05	122.73
25	c1	506	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	C1	520	LMG	O8-C28-C29	2.54	119.86	111.91
25	B1	606	CLA	CHB-C4A-NA	2.53	128.02	124.51
36	d2	409	PL9	C27-C28-C29	-2.53	121.56	127.66
25	c2	505	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	d2	405	CLA	C3B-C4B-NB	-2.53	108.17	110.52
25	c1	512	CLA	C3B-C4B-NB	-2.53	108.17	110.52
29	a2	412	LMG	C8-O7-C10	-2.53	111.56	117.79
25	b1	614	CLA	C3B-C4B-NB	-2.53	108.17	110.52
27	D1	407	PHO	O2A-CGA-CBA	2.53	119.84	111.91
25	b1	613	CLA	C3B-C4B-NB	-2.53	108.17	110.52
33	L1	101	LHG	C5-O7-C7	-2.53	111.57	117.79
27	D1	407	PHO	O1D-CGD-CBD	-2.53	120.53	124.74
25	b2	617	CLA	CHB-C4A-NA	2.53	128.00	124.51
25	c1	516	CLA	CHD-C1D-ND	-2.52	122.13	124.45
25	c1	512	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	B2	602	BCR	C34-C9-C10	-2.52	119.39	122.92
37	D2	402	SQD	O9-S-C6	2.52	109.93	106.94
27	A2	407	PHO	O1D-CGD-CBD	-2.52	120.55	124.74
23	C1	501	BCR	C21-C20-C19	-2.52	115.36	123.22
23	B2	602	BCR	C28-C27-C26	-2.52	109.59	114.08
35	C1	519	LMT	C1B-O1B-C4'	-2.51	111.74	117.96
25	d1	404	CLA	O2D-CGD-CBD	2.51	115.74	111.27
23	k1	101	BCR	C33-C5-C4	2.51	118.44	113.62
37	B2	623	SQD	O48-C23-C24	2.51	119.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	m2	104	LMT	O1B-C1B-C2B	2.51	114.61	108.10
25	d1	401	CLA	CHD-C1D-ND	-2.51	122.14	124.45
25	C2	511	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	D1	401	BCR	C16-C15-C14	-2.51	118.33	123.47
25	C2	513	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	b1	602	BCR	C29-C30-C25	2.51	114.34	110.48
25	C2	503	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	c2	512	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	A2	403	CLA	CHB-C1B-NB	2.51	126.91	124.26
25	b1	616	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	d2	405	CLA	CHD-C1D-ND	-2.51	122.15	124.45
25	B2	610	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
36	D1	408	PL9	C51-C49-C50	2.51	120.14	114.60
23	b2	602	BCR	C4-C5-C6	-2.51	119.09	122.73
25	B1	619	CLA	C3B-C4B-NB	-2.50	108.19	110.52
29	b1	631	LMG	O8-C28-C29	2.50	119.76	111.91
25	c1	511	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	b1	606	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	a1	404	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	b1	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	B2	619	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	A1	401	BCR	C23-C24-C25	-2.50	120.19	127.20
25	C2	518	CLA	C3B-C4B-NB	-2.50	108.20	110.52
25	a2	404	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
25	c2	511	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	C1	502	CLA	C3B-C4B-NB	-2.49	108.20	110.52
25	B2	604	CLA	CAA-C2A-C3A	-2.49	110.28	116.10
23	h1	102	BCR	C38-C26-C25	-2.49	121.73	124.53
25	C1	508	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	A1	412	LMG	O8-C28-C29	2.49	119.72	111.91
25	c2	515	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	c2	502	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	H1	102	BCR	C7-C8-C9	-2.49	122.47	126.23
25	a1	404	CLA	CAC-C3C-C4C	2.49	128.04	124.81
25	c2	505	CLA	C3B-C4B-NB	-2.49	108.21	110.52
25	c2	506	CLA	O2D-CGD-CBD	2.49	115.69	111.27
23	h1	102	BCR	C3-C4-C5	-2.49	109.64	114.08
29	I2	101	LMG	C8-O7-C10	-2.49	111.67	117.79
25	b1	609	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	B1	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	B2	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	C1	508	CLA	C3B-C4B-NB	-2.48	108.21	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b1	602	BCR	C38-C26-C25	-2.48	121.74	124.53
23	k1	101	BCR	C36-C18-C17	-2.48	119.45	122.92
25	C1	511	CLA	C3B-C4B-NB	-2.48	108.21	110.52
25	A2	403	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	C2	507	CLA	C3B-C4B-NB	-2.48	108.22	110.52
25	B2	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	c2	510	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	c1	506	CLA	C3B-C4B-NB	-2.48	108.22	110.52
23	a2	402	BCR	C24-C23-C22	-2.48	122.49	126.23
23	B1	603	BCR	C24-C23-C22	-2.47	122.50	126.23
23	D1	401	BCR	C28-C27-C26	-2.47	109.66	114.08
29	c1	519	LMG	O8-C28-C29	2.47	119.67	111.91
37	b2	605	SQD	O48-C23-C24	2.47	119.67	111.91
25	C1	512	CLA	C3B-C4B-NB	-2.47	108.22	110.52
27	a1	411	PHO	O2A-CGA-CBA	2.47	119.66	111.91
25	b1	611	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
27	D1	407	PHO	CBC-CAC-C3C	-2.47	109.26	112.88
25	B1	608	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	c2	508	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	b1	621	LMG	O8-C28-C29	2.47	119.65	111.91
25	B2	604	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	C1	511	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	c1	504	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	c2	506	CLA	C3B-C4B-NB	-2.47	108.23	110.52
25	D1	403	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	b2	614	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	A2	404	CLA	CHB-C1B-NB	2.46	126.86	124.26
25	B1	609	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	C2	510	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	b2	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	C1	502	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	C2	502	BCR	C3-C4-C5	-2.46	109.69	114.08
25	a2	413	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
23	F2	401	BCR	C30-C25-C26	-2.45	119.16	122.61
25	a1	405	CLA	C1-C2-C3	-2.45	122.78	126.75
23	a2	402	BCR	C3-C4-C5	-2.45	109.70	114.08
25	c1	513	CLA	C3B-C4B-NB	-2.45	108.24	110.52
25	C2	504	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	c2	509	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	b1	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	C2	505	CLA	CHB-C4A-NA	2.45	127.90	124.51
36	D2	408	PL9	C10-C9-C11	2.45	119.39	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C1	510	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	b2	619	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	c1	515	CLA	CHB-C4A-NA	2.45	127.89	124.51
36	d1	409	PL9	C12-C13-C14	-2.44	121.77	127.66
25	c1	510	CLA	O2D-CGD-CBD	2.44	115.61	111.27
25	A2	404	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
23	J1	101	BCR	C33-C5-C4	2.44	118.31	113.62
25	b2	617	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	a1	404	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	B2	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	B2	612	CLA	C1-C2-C3	-2.44	121.83	126.04
25	B2	612	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	C2	516	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	B2	605	CLA	C3B-C4B-NB	-2.44	108.25	110.52
23	a1	401	BCR	C28-C27-C26	-2.44	109.73	114.08
23	c2	501	BCR	C28-C27-C26	-2.44	109.73	114.08
25	D2	404	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	b1	608	CLA	C1-C2-C3	-2.43	121.83	126.04
25	b2	624	CLA	CHB-C1B-NB	2.43	126.83	124.26
25	b2	611	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	b2	620	CLA	C3B-C4B-NB	-2.43	108.26	110.52
36	d1	409	PL9	C25-C24-C23	-2.43	117.44	123.68
29	A2	412	LMG	C8-O7-C10	-2.43	111.81	117.79
25	B2	619	CLA	O2D-CGD-CBD	2.43	115.58	111.27
25	C2	503	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	C1	514	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	A2	404	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	a2	413	CLA	CHB-C4A-NA	2.43	127.87	124.51
34	h1	101	DGD	C2G-O2G-C1B	-2.43	111.82	117.79
25	b1	615	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B1	612	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B2	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	d2	404	CLA	CHB-C1B-NB	2.42	126.82	124.26
25	B2	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
36	D2	408	PL9	C45-C44-C46	2.42	119.35	115.27
38	V1	201	HEM	CHD-C1D-ND	2.42	127.05	124.42
23	B2	603	BCR	C28-C27-C26	-2.42	109.75	114.08
25	B1	610	CLA	CHD-C1D-ND	-2.42	122.23	124.45
25	c2	507	CLA	C3B-C4B-NB	-2.42	108.27	110.52
23	d1	405	BCR	C20-C21-C22	-2.42	123.86	127.31
36	D2	408	PL9	C17-C18-C19	-2.42	121.84	127.66
25	c1	509	CLA	C3B-C4B-NB	-2.42	108.27	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b2	614	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	B1	617	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	B1	614	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	B1	615	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	c1	506	CLA	CHD-C1D-ND	-2.41	122.23	124.45
25	c2	507	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	B1	602	BCR	C38-C26-C27	2.41	118.25	113.62
25	D2	401	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	c1	515	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
25	A1	406	CLA	CHB-C1B-NB	2.41	126.81	124.26
25	d1	406	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	j2	102	BCR	C38-C26-C27	2.41	118.25	113.62
25	B1	610	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	B1	605	CLA	C3B-C4B-NB	-2.41	108.28	110.52
25	B1	618	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	b1	620	CLA	CHD-C1D-ND	-2.41	122.24	124.45
23	d1	405	BCR	C16-C15-C14	-2.41	118.55	123.47
25	C1	504	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
25	C1	506	CLA	C3B-C4B-NB	-2.41	108.28	110.52
25	b2	613	CLA	C3B-C4B-NB	-2.40	108.28	110.52
25	c1	507	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	c1	508	CLA	C1-C2-C3	-2.40	122.87	126.75
25	c1	508	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	a1	403	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	b1	612	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	b1	615	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
25	D2	401	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	c1	516	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	B1	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	c1	510	CLA	C3B-C4B-NB	-2.40	108.29	110.52
35	l1	101	LMT	O1'-C1'-C2'	2.40	112.05	108.30
25	C1	504	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	C1	513	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	b2	601	BCR	C3-C4-C5	-2.39	109.80	114.08
23	d2	401	BCR	C8-C7-C6	-2.39	120.48	127.20
38	V1	201	HEM	CAD-CBD-CGD	-2.39	108.45	113.60
25	B1	616	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	c2	509	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
23	H2	103	BCR	C3-C4-C5	-2.39	109.81	114.08
38	V2	201	HEM	CHD-C1D-ND	2.39	127.02	124.42
25	b1	610	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
33	D1	405	LHG	C5-O7-C7	-2.39	111.91	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C1	507	CLA	CHB-C1B-NB	2.39	126.78	124.26
38	f1	101	HEM	C4C-NC-C1C	2.38	107.68	105.35
23	h1	102	BCR	C7-C8-C9	-2.38	122.63	126.23
23	J1	101	BCR	C37-C22-C21	-2.38	119.58	122.92
25	B1	616	CLA	CHB-C4A-NA	2.38	127.81	124.51
38	E2	101	HEM	C4C-NC-C1C	2.38	107.68	105.35
25	b2	613	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	A1	404	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	c2	504	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	b2	610	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	b2	605	SQD	O9-S-C6	2.38	109.77	106.94
38	V1	201	HEM	C4C-NC-C1C	2.38	107.68	105.35
25	C1	509	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	k2	501	BCR	C38-C26-C27	2.38	118.18	113.62
25	a2	413	CLA	CHB-C1B-NB	2.38	126.77	124.26
25	B1	605	CLA	CHB-C4A-NA	2.37	127.80	124.51
25	b2	624	CLA	CHB-C4A-NA	2.37	127.79	124.51
33	B2	627	LHG	C5-O7-C7	-2.37	111.95	117.79
23	C1	521	BCR	C15-C16-C17	-2.37	118.61	123.47
25	B1	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	c1	513	CLA	CHB-C4A-NA	2.37	127.79	124.51
38	e2	101	HEM	C4C-NC-C1C	2.37	107.67	105.35
25	B2	618	CLA	C3B-C4B-NB	-2.37	108.32	110.52
25	b2	611	CLA	C1-C2-C3	-2.37	121.95	126.04
25	C1	510	CLA	CHD-C1D-ND	-2.37	122.28	124.45
37	b2	605	SQD	O7-S-C6	2.37	109.75	106.94
23	B1	601	BCR	C3-C4-C5	-2.37	109.85	114.08
23	c2	501	BCR	C38-C26-C27	2.36	118.16	113.62
25	b2	620	CLA	O2D-CGD-CBD	2.36	115.47	111.27
25	c1	515	CLA	C3B-C4B-NB	-2.36	108.33	110.52
25	b1	604	CLA	CHB-C4A-NA	2.36	127.78	124.51
35	a2	406	LMT	C1B-O1B-C4'	-2.36	112.12	117.96
38	V2	201	HEM	CAD-CBD-CGD	-2.36	108.53	113.60
34	C1	515	DGD	C2G-O2G-C1B	-2.36	111.99	117.79
27	D1	407	PHO	O2D-CGD-O1D	-2.36	119.23	123.84
25	c2	509	CLA	O2D-CGD-CBD	2.36	115.45	111.27
25	A1	406	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
25	d1	401	CLA	O2D-CGD-CBD	2.36	115.45	111.27
33	D1	405	LHG	O8-C23-C24	2.35	119.30	111.91
25	c1	509	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
38	V1	201	HEM	C3B-C2B-C1B	2.35	108.23	106.49
27	d2	408	PHO	CMA-C3A-C4A	-2.35	109.22	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b1	609	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	H1	102	BCR	C11-C10-C9	-2.35	123.95	127.31
25	d1	401	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	B2	605	CLA	CHB-C4A-NA	2.35	127.76	124.51
36	d2	409	PL9	C51-C49-C50	2.34	119.78	114.60
25	C2	508	CLA	C1-C2-C3	-2.34	122.96	126.75
25	C1	507	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	h1	102	BCR	C16-C15-C14	-2.34	118.68	123.47
25	A1	403	CLA	CHB-C4A-NA	2.34	127.75	124.51
36	D1	408	PL9	C45-C44-C46	2.34	119.20	115.27
25	C2	507	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	B1	613	CLA	CHB-C1B-NB	2.34	126.73	124.26
23	j2	102	BCR	C36-C18-C17	-2.34	119.65	122.92
25	d1	401	CLA	CHB-C4A-NA	2.34	127.74	124.51
23	B2	602	BCR	C3-C4-C5	-2.34	109.91	114.08
25	d2	404	CLA	C1-C2-C3	-2.34	122.97	126.75
23	h2	101	BCR	C23-C24-C25	-2.34	120.64	127.20
23	K2	104	BCR	C38-C26-C27	2.34	118.10	113.62
25	C2	508	CLA	C3B-C4B-NB	-2.33	108.35	110.52
25	b1	616	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	B2	614	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	B1	617	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	A1	406	CLA	CHD-C1D-ND	-2.33	122.31	124.45
29	d1	408	LMG	C8-O7-C10	-2.33	112.05	117.79
25	B2	608	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	B2	616	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	K1	101	BCR	C7-C6-C5	-2.33	115.82	121.46
23	a2	402	BCR	C21-C20-C19	-2.33	115.95	123.22
23	K2	102	BCR	C7-C8-C9	-2.33	122.72	126.23
25	d2	402	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	C1	513	CLA	C3B-C4B-NB	-2.33	108.36	110.52
25	D1	402	CLA	CHB-C4A-NA	2.32	127.73	124.51
25	d2	402	CLA	CHB-C1B-NB	2.32	126.72	124.26
25	C2	511	CLA	C3B-C4B-NB	-2.32	108.36	110.52
37	D2	402	SQD	O6-C1-C2	2.32	111.93	108.30
25	B1	606	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
36	d1	409	PL9	C45-C44-C46	2.32	119.17	115.27
25	B1	611	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	b1	606	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
25	b1	611	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	c1	507	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	a2	413	CLA	C1-C2-C3	-2.31	123.01	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c1	505	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	C2	518	CLA	O2D-CGD-CBD	2.31	115.37	111.27
25	D1	402	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	d1	408	LMG	O8-C28-C29	2.31	119.15	111.91
25	B1	616	CLA	CHB-C1B-NB	2.31	126.70	124.26
23	C1	501	BCR	C23-C24-C25	-2.31	120.72	127.20
25	A2	402	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	c2	505	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	B2	607	CLA	CHB-C1B-NB	2.31	126.70	124.26
23	b2	602	BCR	C37-C22-C21	-2.31	119.69	122.92
25	B1	613	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	C1	509	CLA	O2D-CGD-CBD	2.30	115.36	111.27
25	b1	608	CLA	CHB-C4A-NA	2.30	127.70	124.51
33	b1	622	LHG	C5-O7-C7	-2.30	112.12	117.79
25	d1	406	CLA	CHD-C1D-ND	-2.30	122.34	124.45
38	v2	201	HEM	C2A-C1A-NA	-2.30	107.58	110.15
25	a2	404	CLA	CHD-C1D-ND	-2.30	122.34	124.45
23	k1	101	BCR	C8-C7-C6	-2.30	120.75	127.20
23	b2	601	BCR	C23-C24-C25	-2.30	120.76	127.20
23	B2	601	BCR	C38-C26-C27	2.30	118.03	113.62
25	B2	607	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
34	c2	517	DGD	O1G-C1A-C2A	2.29	119.11	111.91
25	b2	616	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	A1	404	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	C1	510	CLA	CHB-C1B-NB	2.29	126.68	124.26
25	D2	406	CLA	O2D-CGD-CBD	2.29	115.34	111.27
35	m2	103	LMT	C1B-O5B-C5B	-2.29	109.19	113.69
27	A2	407	PHO	O2A-CGA-CBA	2.29	119.09	111.91
25	b1	610	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	a1	401	BCR	C23-C24-C25	-2.29	120.78	127.20
25	b2	624	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
25	B1	612	CLA	CHB-C1B-NB	2.29	126.68	124.26
25	B2	610	CLA	CHB-C1B-NB	2.29	126.68	124.26
27	A2	407	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
25	A2	402	CLA	CHB-C4A-NA	2.29	127.67	124.51
25	c2	506	CLA	CHB-C4A-NA	2.29	127.67	124.51
25	B2	616	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
25	C1	505	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	B2	611	CLA	CHB-C4A-NA	2.28	127.67	124.51
36	D2	408	PL9	C35-C34-C36	2.28	119.11	115.27
29	F2	402	LMG	C8-O7-C10	-2.28	112.18	117.79
25	A1	405	CLA	CHD-C1D-ND	-2.28	122.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b2	620	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	a2	413	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	b2	601	BCR	C33-C5-C4	2.28	117.99	113.62
34	c1	520	DGD	O1G-C1A-C2A	2.28	119.05	111.91
23	B1	603	BCR	C29-C30-C25	2.28	113.99	110.48
23	D1	401	BCR	C21-C20-C19	-2.28	116.11	123.22
25	a1	405	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
25	b2	608	CLA	CHB-C4A-NA	2.27	127.66	124.51
23	c1	502	BCR	C16-C17-C18	-2.27	124.06	127.31
25	c2	515	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	c1	508	CLA	CHB-C1B-NB	2.27	126.66	124.26
23	b1	602	BCR	C38-C26-C27	2.27	117.98	113.62
25	C2	513	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	C1	504	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
38	V1	201	HEM	CAD-C3D-C4D	2.27	128.62	124.66
25	b1	616	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	B2	613	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	h1	102	BCR	C38-C26-C27	2.26	117.97	113.62
23	B2	601	BCR	C3-C4-C5	-2.26	110.04	114.08
27	D2	407	PHO	O2D-CGD-O1D	-2.26	119.42	123.84
25	c1	511	CLA	C3B-C4B-NB	-2.26	108.42	110.52
25	c1	512	CLA	CHD-C1D-ND	-2.26	122.38	124.45
25	B2	618	CLA	O2D-CGD-CBD	2.26	115.28	111.27
38	v1	201	HEM	C1B-NB-C4B	2.26	107.40	105.07
23	B1	602	BCR	C1-C6-C5	-2.26	119.44	122.61
25	b2	617	CLA	CHB-C1B-NB	2.25	126.64	124.26
29	C2	515	LMG	C8-O7-C10	-2.25	112.24	117.79
25	C1	506	CLA	O2D-CGD-CBD	2.25	115.27	111.27
27	d2	408	PHO	O1D-CGD-CBD	-2.25	120.99	124.74
25	d2	405	CLA	CHB-C4A-NA	2.25	127.63	124.51
33	d2	403	LHG	C5-O7-C7	-2.25	112.25	117.79
29	A1	412	LMG	C8-O7-C10	-2.25	112.25	117.79
25	b2	615	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	b1	607	CLA	O2D-CGD-CBD	2.25	115.27	111.27
27	A2	407	PHO	C4B-NB-C1B	-2.25	105.34	108.83
23	B2	602	BCR	C23-C24-C25	-2.25	120.88	127.20
25	D2	404	CLA	C1-C2-C3	-2.25	122.15	126.04
25	a2	404	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	h2	101	BCR	C15-C16-C17	-2.25	118.87	123.47
25	C1	506	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	c1	506	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
25	c1	507	CLA	O2D-CGD-CBD	2.24	115.26	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A1	408	PHO	O2A-CGA-CBA	2.24	118.95	111.91
25	B2	612	CLA	CHB-C1B-NB	2.24	126.63	124.26
27	a1	411	PHO	CMA-C3A-C4A	-2.24	109.47	114.38
34	c1	518	DGD	O6D-C5D-C6D	2.24	111.19	106.67
25	b2	611	CLA	CHB-C1B-NB	2.24	126.63	124.26
23	k2	501	BCR	C8-C7-C6	-2.24	120.92	127.20
25	d1	404	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	b2	601	BCR	C15-C16-C17	-2.23	118.90	123.47
25	b1	608	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	c2	512	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	b2	618	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
27	a1	411	PHO	CBC-CAC-C3C	-2.23	109.61	112.88
23	B2	601	BCR	C15-C16-C17	-2.23	118.90	123.47
23	z2	101	BCR	C28-C27-C26	-2.23	110.09	114.08
29	D1	406	LMG	O8-C28-C29	2.23	118.91	111.91
25	C1	506	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	b1	603	BCR	C33-C5-C6	-2.23	122.02	124.53
25	B2	615	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	F2	401	BCR	C15-C16-C17	-2.23	118.91	123.47
25	C2	518	CLA	CAA-C2A-C3A	-2.23	110.90	116.10
25	c1	504	CLA	CHB-C1B-NB	2.23	126.61	124.26
25	B2	611	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	c1	501	BCR	C4-C5-C6	-2.22	119.50	122.73
25	B1	607	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
27	D1	407	PHO	CMA-C3A-C4A	-2.22	109.50	114.38
23	j2	102	BCR	C8-C7-C6	-2.22	120.96	127.20
27	d2	408	PHO	O2D-CGD-O1D	-2.22	119.49	123.84
38	E1	101	HEM	C4C-NC-C1C	2.22	107.52	105.35
25	C1	505	CLA	C3B-C4B-NB	-2.22	108.45	110.52
25	b1	610	CLA	CHB-C1B-NB	2.22	126.61	124.26
25	c1	505	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	B1	616	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
25	A1	404	CLA	CHD-C1D-ND	-2.22	122.42	124.45
23	h2	101	BCR	C33-C5-C4	2.22	117.87	113.62
36	d1	409	PL9	C51-C49-C50	2.22	119.50	114.60
25	C2	516	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	b2	624	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
25	B1	615	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
23	K1	101	BCR	C1-C6-C7	2.21	122.04	115.78
34	C1	516	DGD	O1G-C1A-C2A	2.21	118.85	111.91
29	d1	411	LMG	C8-O7-C10	-2.21	112.34	117.79
23	k2	501	BCR	C33-C5-C4	2.21	117.86	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A1	403	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
25	B1	619	CLA	CHD-C1D-ND	-2.21	122.42	124.45
33	b1	622	LHG	O8-C23-O10	-2.21	118.02	123.59
25	B1	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	h1	102	BCR	C39-C30-C25	-2.21	106.72	110.30
23	b1	601	BCR	C38-C26-C27	2.21	117.85	113.62
23	B2	603	BCR	C3-C4-C5	-2.20	110.14	114.08
23	b2	602	BCR	C33-C5-C6	-2.20	122.05	124.53
38	v2	201	HEM	C4C-NC-C1C	2.20	107.50	105.35
37	D2	402	SQD	O8-S-C6	2.20	109.25	105.74
25	C1	514	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	c1	503	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	a1	412	LMG	O1-C1-C2	2.20	111.74	108.30
25	a2	405	CLA	CAC-C3C-C4C	2.20	127.67	124.81
33	d1	407	LHG	O8-C23-C24	2.20	118.81	111.91
25	a2	404	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	K1	101	BCR	C16-C15-C14	-2.20	118.97	123.47
23	j2	102	BCR	C33-C5-C4	2.20	117.84	113.62
25	c1	508	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
23	b2	603	BCR	C33-C5-C4	2.19	117.83	113.62
25	b2	606	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	C1	504	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	D2	406	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	c1	513	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	c2	513	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	B2	613	CLA	O2D-CGD-CBD	2.19	115.16	111.27
38	E2	101	HEM	C2A-C1A-NA	-2.19	107.70	110.15
23	J1	101	BCR	C38-C26-C27	2.19	117.82	113.62
25	b1	614	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	C1	521	BCR	C8-C7-C6	-2.18	121.07	127.20
23	K1	101	BCR	C35-C13-C14	-2.18	119.86	122.92
25	c2	510	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	b1	612	CLA	CHB-C1B-NB	2.18	126.56	124.26
27	a2	416	PHO	C4D-CHA-CBD	2.18	109.50	108.52
34	H1	101	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
23	B2	602	BCR	C38-C26-C27	2.18	117.80	113.62
36	D1	408	PL9	C42-C43-C44	-2.18	122.42	127.66
36	D2	408	PL9	C12-C13-C14	-2.18	122.42	127.66
23	C2	502	BCR	C28-C27-C26	-2.18	110.19	114.08
34	C1	517	DGD	O1G-C1A-C2A	2.18	118.74	111.91
25	b2	609	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	H1	102	BCR	C3-C4-C5	-2.18	110.19	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c1	502	BCR	C20-C19-C18	2.17	132.53	126.42
29	D1	406	LMG	C8-O7-C10	-2.17	112.44	117.79
25	a2	405	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	b2	612	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	h1	102	BCR	C36-C18-C17	-2.17	119.88	122.92
23	C1	501	BCR	C20-C21-C22	-2.17	124.21	127.31
25	b2	608	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	c1	506	CLA	CHB-C1B-NB	2.17	126.56	124.26
33	L2	101	LHG	O7-C7-O9	-2.17	118.45	123.70
33	D1	404	LHG	C5-O7-C7	-2.17	112.45	117.79
25	C2	506	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	F2	401	BCR	C33-C5-C4	2.17	117.78	113.62
25	b1	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
27	A1	408	PHO	CMA-C3A-C4A	-2.17	109.63	114.38
38	e2	101	HEM	C2A-C1A-NA	-2.17	107.72	110.15
25	D2	404	CLA	CHD-C1D-ND	-2.17	122.46	124.45
33	d2	406	LHG	C5-O7-C7	-2.17	112.46	117.79
34	c1	518	DGD	O2G-C1B-O1B	-2.17	118.47	123.70
27	a2	416	PHO	CBC-CAC-C3C	-2.17	109.71	112.88
25	c1	508	CLA	CHD-C1D-ND	-2.17	122.46	124.45
34	C1	517	DGD	C2G-O2G-C1B	-2.16	112.46	117.79
23	K2	104	BCR	C8-C7-C6	-2.16	121.12	127.20
25	c1	512	CLA	CHB-C1B-NB	2.16	126.55	124.26
27	d1	403	PHO	C4B-NB-C1B	-2.16	105.48	108.83
25	B2	609	CLA	C1-C2-C3	-2.16	122.31	126.04
29	a2	412	LMG	C7-O1-C1	-2.16	109.52	113.74
25	A2	402	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	B2	601	BCR	C33-C5-C4	2.16	117.77	113.62
23	B1	601	BCR	C27-C26-C25	-2.16	119.60	122.73
23	K2	102	BCR	C8-C7-C6	-2.16	121.14	127.20
27	d2	408	PHO	C4D-CHA-CBD	2.16	109.49	108.52
25	b1	615	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
29	b2	622	LMG	C8-O7-C10	-2.16	112.48	117.79
27	a2	416	PHO	CED-O2D-CGD	2.15	120.81	115.94
23	b2	603	BCR	C34-C9-C10	-2.15	119.91	122.92
25	B1	614	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	b1	611	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	b1	607	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	B1	602	BCR	C29-C30-C25	2.15	113.79	110.48
23	C2	502	BCR	C15-C16-C17	-2.15	119.07	123.47
25	b1	619	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
33	l1	102	LHG	O7-C7-O9	-2.15	118.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J1	101	BCR	C28-C27-C26	-2.15	110.24	114.08
38	V1	201	HEM	C1B-NB-C4B	2.15	107.29	105.07
23	c1	502	BCR	C19-C18-C17	-2.15	115.64	118.94
23	k2	501	BCR	C11-C12-C13	-2.15	120.38	126.42
23	a1	401	BCR	C21-C20-C19	-2.15	116.52	123.22
25	c2	511	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	A1	408	PHO	C4B-NB-C1B	-2.14	105.51	108.83
25	a2	405	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
25	c2	509	CLA	CHD-C1D-ND	-2.14	122.48	124.45
38	v2	201	HEM	C1B-NB-C4B	2.14	107.29	105.07
33	a1	407	LHG	O8-C23-O10	-2.14	118.19	123.59
23	B2	602	BCR	C2-C1-C6	2.14	113.78	110.48
25	b1	614	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
27	d2	408	PHO	C4B-NB-C1B	-2.14	105.51	108.83
25	C2	513	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	b2	610	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	C1	512	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	B1	618	CLA	CHB-C1B-NB	2.14	126.52	124.26
23	b2	603	BCR	C38-C26-C27	2.14	117.73	113.62
25	B2	610	CLA	CMB-C2B-C3B	2.14	131.77	126.59
36	D2	408	PL9	C25-C24-C23	-2.14	118.19	123.68
25	C1	507	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	B2	617	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
38	E1	101	HEM	C2A-C1A-NA	-2.14	107.76	110.15
29	b1	624	LMG	O8-C28-C29	2.14	118.61	111.91
25	B1	608	CLA	CHD-C1D-ND	-2.13	122.49	124.45
25	b2	608	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	j2	102	BCR	C7-C8-C9	-2.13	123.01	126.23
25	b1	619	CLA	CHB-C1B-NB	2.13	126.52	124.26
25	b1	620	CLA	O2D-CGD-CBD	2.13	115.05	111.27
23	h2	101	BCR	C28-C27-C26	-2.13	110.27	114.08
23	a1	401	BCR	C38-C26-C27	2.13	117.71	113.62
25	d2	404	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	B2	601	BCR	C38-C26-C25	-2.13	122.14	124.53
23	K2	104	BCR	C27-C26-C25	-2.13	119.64	122.73
29	d2	407	LMG	O8-C28-C29	2.13	118.59	111.91
25	B2	616	CLA	CHB-C1B-NB	2.13	126.51	124.26
36	d1	409	PL9	C12-C11-C9	-2.13	105.98	112.98
27	D2	407	PHO	CBC-CAC-C3C	-2.13	109.77	112.88
25	c1	503	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
25	C2	506	CLA	CHB-C1B-NB	2.12	126.51	124.26
25	B1	609	CLA	CHD-C1D-ND	-2.12	122.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b1	616	CLA	CHD-C1D-ND	-2.12	122.50	124.45
25	C1	511	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	b1	601	BCR	C33-C5-C4	2.12	117.69	113.62
27	A1	408	PHO	O1D-CGD-CBD	-2.12	121.21	124.74
25	B2	612	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	C1	521	BCR	C28-C27-C26	-2.12	110.30	114.08
23	K2	102	BCR	C38-C26-C27	2.12	117.68	113.62
37	B2	623	SQD	O8-S-C6	2.12	109.11	105.74
23	C1	501	BCR	C33-C5-C4	2.12	117.68	113.62
25	b1	612	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	D2	401	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
37	D1	409	SQD	O48-C23-O10	-2.12	118.25	123.59
25	B2	609	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	H2	103	BCR	C16-C15-C14	-2.11	119.14	123.47
25	C2	505	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
23	H2	103	BCR	C10-C11-C12	-2.11	116.62	123.22
25	B2	610	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
33	l2	101	LHG	O8-C23-O10	-2.11	118.26	123.59
25	A2	404	CLA	O2D-CGD-CBD	2.11	115.02	111.27
25	d2	405	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	b1	610	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	B2	604	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	b1	604	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	b1	608	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	c1	513	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	h1	102	BCR	C8-C7-C6	-2.11	121.28	127.20
23	b2	602	BCR	C10-C11-C12	-2.11	116.64	123.22
25	c2	508	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
37	D2	402	SQD	O7-S-C6	2.11	109.44	106.94
25	b2	613	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
25	c2	504	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
25	a2	413	CLA	C2D-C1D-ND	-2.10	108.55	110.10
25	C2	511	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	j2	102	BCR	C15-C16-C17	-2.10	119.16	123.47
25	B2	608	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	h2	101	BCR	C8-C7-C6	-2.10	121.29	127.20
23	A2	401	BCR	C3-C4-C5	-2.10	110.32	114.08
25	a1	403	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	C2	510	CLA	CHD-C1D-ND	-2.10	122.52	124.45
33	D1	404	LHG	O8-C23-O10	-2.10	118.29	123.59
25	b2	611	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
27	a2	416	PHO	C4B-NB-C1B	-2.10	105.58	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H2	101	DGD	O6D-C5D-C6D	2.10	110.90	106.67
29	b1	624	LMG	O7-C10-O9	-2.10	118.63	123.70
23	H2	103	BCR	C16-C17-C18	-2.10	120.73	124.69
23	F2	401	BCR	C3-C4-C5	-2.10	110.33	114.08
27	D1	407	PHO	CED-O2D-CGD	2.10	120.68	115.94
25	b2	624	CLA	CHD-C1D-ND	-2.10	122.53	124.45
33	D2	403	LHG	O8-C23-O10	-2.10	118.30	123.59
27	d1	403	PHO	CBC-CAC-C3C	-2.10	109.81	112.88
27	a1	411	PHO	O1D-CGD-CBD	-2.10	121.25	124.74
25	B1	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	c2	516	DGD	O1G-C1A-O1A	-2.09	118.31	123.59
23	d1	405	BCR	C3-C4-C5	-2.09	110.34	114.08
25	d1	406	CLA	CHB-C1B-NB	2.09	126.47	124.26
38	V2	201	HEM	C2A-C1A-NA	-2.09	107.81	110.15
23	b2	601	BCR	C27-C26-C25	-2.09	119.69	122.73
23	c1	501	BCR	C15-C16-C17	-2.09	119.19	123.47
25	b2	616	CLA	CHB-C1B-NB	2.09	126.47	124.26
23	d1	405	BCR	C21-C20-C19	-2.09	116.69	123.22
23	d1	405	BCR	C34-C9-C10	-2.09	119.99	122.92
23	C2	502	BCR	C33-C5-C4	2.09	117.63	113.62
23	D1	401	BCR	C3-C4-C5	-2.09	110.34	114.08
23	k1	101	BCR	C28-C27-C26	-2.09	110.34	114.08
23	B1	601	BCR	C21-C20-C19	-2.09	116.69	123.22
36	d2	409	PL9	C35-C34-C36	2.09	118.79	115.27
25	B2	606	CLA	CHD-C1D-ND	-2.09	122.53	124.45
25	A2	404	CLA	CHD-C1D-ND	-2.09	122.53	124.45
34	C1	515	DGD	O2G-C1B-O1B	-2.09	118.66	123.70
25	B2	607	CLA	C1-C2-C3	-2.09	122.43	126.04
25	D1	402	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	b1	614	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	b1	617	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	d2	401	BCR	C37-C22-C21	-2.09	120.00	122.92
37	D1	409	SQD	O9-S-C6	2.08	109.42	106.94
29	F2	402	LMG	O8-C28-C29	2.08	118.45	111.91
25	c1	515	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	B1	611	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	C1	507	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	B2	612	CLA	CHD-C1D-ND	-2.08	122.54	124.45
38	e2	101	HEM	CAA-CBA-CGA	-2.08	109.12	113.60
25	C1	503	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	B1	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
33	b1	622	LHG	O7-C7-O9	-2.08	118.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d2	408	PHO	CBC-CAC-C3C	-2.08	109.84	112.88
25	c2	512	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	D1	402	CLA	CHC-C4B-NB	2.08	126.45	124.26
23	B1	601	BCR	C33-C5-C4	2.08	117.60	113.62
38	V1	201	HEM	C2A-C1A-NA	-2.07	107.83	110.15
38	f1	101	HEM	C2A-C1A-NA	-2.07	107.83	110.15
25	C1	502	CLA	O2D-CGD-CBD	2.07	114.95	111.27
25	A1	403	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	a1	401	BCR	C34-C9-C10	-2.07	120.02	122.92
23	h2	101	BCR	C37-C22-C23	2.07	121.34	118.08
34	c1	514	DGD	C1E-O6E-C5E	-2.07	109.62	113.69
23	K2	102	BCR	C28-C27-C26	-2.07	110.38	114.08
23	B2	603	BCR	C11-C12-C13	-2.07	120.60	126.42
33	B1	621	LHG	C5-O7-C7	-2.07	112.70	117.79
25	c1	516	CLA	CHB-C1B-NB	2.07	126.45	124.26
23	d2	401	BCR	C20-C19-C18	-2.07	120.61	126.42
23	F2	401	BCR	C23-C24-C25	-2.07	121.39	127.20
25	B2	614	CLA	C3B-C4B-NB	-2.07	108.60	110.52
25	B1	607	CLA	CHB-C1B-NB	2.07	126.44	124.26
25	c2	506	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
23	J1	101	BCR	C15-C16-C17	-2.07	119.24	123.47
36	d2	409	PL9	C45-C44-C46	2.06	118.74	115.27
25	b2	616	CLA	O2D-CGD-CBD	2.06	114.94	111.27
25	c2	506	CLA	CBC-CAC-C3C	2.06	118.12	112.43
25	C1	507	CLA	CBC-CAC-C3C	2.06	118.12	112.43
25	B2	605	CLA	O1D-CGD-CBD	2.06	128.70	124.48
25	c2	507	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	C2	511	CLA	O2D-CGD-CBD	2.06	114.93	111.27
25	c1	516	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	c2	513	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	B2	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
37	B2	623	SQD	O6-C1-C2	2.06	111.52	108.30
25	B1	614	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	c1	511	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
35	l1	101	LMT	C1-O1'-C1'	-2.06	110.43	113.84
25	c1	511	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
25	c1	504	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b1	602	BCR	C11-C12-C13	2.06	132.19	126.42
25	a1	404	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	C2	516	CLA	CHC-C4B-NB	2.06	126.43	124.26
33	d2	406	LHG	O8-C23-O10	-2.06	118.41	123.59
25	C1	509	CLA	CHB-C4A-NA	2.06	127.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C2	506	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
25	C1	513	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B1	617	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	B2	620	LMG	O8-C28-O10	-2.05	118.41	123.59
25	B2	608	CLA	C1-C2-C3	-2.05	122.49	126.04
25	d1	406	CLA	O2D-CGD-CBD	2.05	114.91	111.27
25	B2	614	CLA	CHC-C4B-NB	2.05	126.43	124.26
23	B1	603	BCR	C3-C4-C5	-2.05	110.42	114.08
25	C1	502	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	c2	515	CLA	CHB-C1B-NB	2.05	126.43	124.26
38	v1	201	HEM	C2A-C1A-NA	-2.05	107.86	110.15
25	c2	502	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	d2	402	CLA	C1-C2-C3	-2.05	122.50	126.04
25	B1	605	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	a1	405	CLA	CHB-C1B-NB	2.05	126.42	124.26
23	a2	402	BCR	C16-C15-C14	-2.05	119.28	123.47
23	k1	101	BCR	C20-C19-C18	2.05	132.17	126.42
25	b1	613	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	c2	501	BCR	C1-C6-C7	2.05	121.57	115.78
25	b1	609	CLA	O2D-CGD-CBD	2.05	114.90	111.27
23	K1	101	BCR	C36-C18-C17	-2.05	120.06	122.92
25	b2	615	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B1	619	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	b1	606	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	C1	508	CLA	CHC-C4B-NB	2.04	126.42	124.26
33	L1	101	LHG	O7-C7-O9	-2.04	118.77	123.70
25	D1	402	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	b2	617	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
34	c2	514	DGD	O6D-C5D-C6D	2.04	110.79	106.67
25	a2	405	CLA	CHB-C1B-NB	2.04	126.42	124.26
36	D2	408	PL9	C51-C49-C50	2.04	119.11	114.60
25	D2	406	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	c2	504	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b2	603	BCR	C3-C4-C5	-2.04	110.43	114.08
27	a1	411	PHO	C4B-NB-C1B	-2.04	105.67	108.83
33	D2	405	LHG	O7-C7-O9	-2.04	118.77	123.70
25	b2	614	CLA	CHC-C4B-NB	2.04	126.42	124.26
25	B2	615	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
23	B2	602	BCR	C16-C15-C14	-2.04	119.30	123.47
25	B1	609	CLA	CHB-C1B-NB	2.04	126.41	124.26
23	A1	401	BCR	C33-C5-C4	2.04	117.53	113.62
27	D1	407	PHO	C4B-NB-C1B	-2.04	105.68	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B1	612	CLA	CHD-C1D-ND	-2.03	122.58	124.45
23	j2	102	BCR	C19-C18-C17	-2.03	115.82	118.94
25	A2	403	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	A2	403	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	b1	603	BCR	C35-C13-C14	-2.03	120.08	122.92
25	B1	606	CLA	C1-C2-C3	-2.03	122.53	126.04
23	B2	603	BCR	C33-C5-C4	2.03	117.52	113.62
25	A1	405	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	c1	511	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	b2	618	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	C1	514	CLA	CHB-C1B-NB	2.03	126.41	124.26
29	A1	410	LMG	C7-O1-C1	-2.03	109.78	113.74
25	C2	508	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	c2	505	CLA	O2D-CGD-CBD	2.03	114.87	111.27
25	C1	512	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	K2	101	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
34	c1	514	DGD	O2G-C1B-O1B	-2.03	118.81	123.70
25	b2	619	CLA	CHB-C1B-NB	2.03	126.40	124.26
29	C1	520	LMG	C8-O7-C10	-2.02	112.81	117.79
25	C2	508	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	C2	511	CLA	CHB-C1B-NB	2.02	126.40	124.26
34	h1	101	DGD	O2G-C1B-O1B	-2.02	118.81	123.70
25	c2	502	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	B1	622	LMG	O8-C28-O10	-2.02	118.49	123.59
23	K2	104	BCR	C38-C26-C25	-2.02	122.26	124.53
23	z2	101	BCR	C8-C7-C6	-2.02	121.53	127.20
23	C1	501	BCR	C36-C18-C19	2.02	121.26	118.08
33	b2	625	LHG	C5-O7-C7	-2.02	112.82	117.79
23	j2	102	BCR	C10-C11-C12	-2.02	116.92	123.22
25	D2	401	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	k2	501	BCR	C20-C19-C18	-2.02	120.75	126.42
36	d1	409	PL9	C47-C46-C44	-2.02	106.35	112.98
25	C2	509	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	a1	403	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	B1	612	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	K2	101	CLA	CHB-C1B-NB	2.01	126.39	124.26
23	D1	401	BCR	C34-C9-C10	-2.01	120.10	122.92
23	b1	601	BCR	C35-C13-C14	-2.01	120.10	122.92
23	k2	501	BCR	C37-C22-C21	-2.01	120.10	122.92
25	B1	614	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
25	b2	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	D2	407	PHO	C4B-NB-C1B	-2.01	105.72	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c1	504	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
25	b1	615	CLA	CHD-C1D-ND	-2.01	122.61	124.45
38	v1	201	HEM	C3B-C2B-C1B	2.01	107.98	106.49
25	D1	403	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	c1	506	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	D2	404	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	B1	605	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	C1	502	CLA	CHC-C4B-NB	2.01	126.38	124.26
25	c2	510	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	c1	508	CLA	CAC-C3C-C4C	2.01	127.41	124.81
25	b2	608	CLA	CHB-C1B-NB	2.01	126.38	124.26
36	d1	409	PL9	C10-C9-C11	2.01	118.65	115.27
25	B2	606	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	B2	619	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	B2	614	CLA	C1-C2-C3	-2.01	122.58	126.04
23	D1	401	BCR	C33-C5-C4	2.01	117.47	113.62
23	B2	601	BCR	C27-C26-C25	-2.00	119.82	122.73
23	b1	602	BCR	C39-C30-C25	-2.00	107.05	110.30
23	H1	102	BCR	C8-C7-C6	-2.00	121.58	127.20
27	a2	416	PHO	O2A-CGA-CBA	2.00	118.19	111.91
25	B1	604	CLA	CHB-C1B-NB	2.00	126.38	124.26
34	C1	516	DGD	O2G-C1B-O1B	-2.00	118.86	123.70

There are no chirality outliers.

All (2327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C1	501	BCR	C7-C8-C9-C10
23	C1	501	BCR	C7-C8-C9-C34
23	D1	401	BCR	C7-C8-C9-C10
23	D1	401	BCR	C7-C8-C9-C34
23	K1	101	BCR	C1-C6-C7-C8
23	K1	101	BCR	C5-C6-C7-C8
23	K1	101	BCR	C36-C18-C19-C20
23	c1	502	BCR	C7-C8-C9-C34
23	d1	405	BCR	C7-C8-C9-C10
23	d1	405	BCR	C7-C8-C9-C34
23	d1	405	BCR	C21-C22-C23-C24
23	d1	405	BCR	C37-C22-C23-C24
23	B2	602	BCR	C7-C8-C9-C10
23	B2	602	BCR	C7-C8-C9-C34
23	F2	401	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	F2	401	BCR	C7-C8-C9-C34
23	F2	401	BCR	C21-C22-C23-C24
23	F2	401	BCR	C37-C22-C23-C24
23	K2	102	BCR	C5-C6-C7-C8
23	K2	102	BCR	C7-C8-C9-C10
23	K2	102	BCR	C7-C8-C9-C34
23	b2	602	BCR	C1-C6-C7-C8
23	b2	602	BCR	C5-C6-C7-C8
23	c2	501	BCR	C1-C6-C7-C8
23	c2	501	BCR	C5-C6-C7-C8
23	c2	501	BCR	C7-C8-C9-C10
23	c2	501	BCR	C7-C8-C9-C34
23	c2	501	BCR	C11-C12-C13-C14
23	c2	501	BCR	C11-C12-C13-C35
23	d2	401	BCR	C7-C8-C9-C10
23	d2	401	BCR	C7-C8-C9-C34
23	d2	401	BCR	C23-C24-C25-C26
23	j2	102	BCR	C1-C6-C7-C8
23	j2	102	BCR	C5-C6-C7-C8
23	j2	102	BCR	C7-C8-C9-C10
23	j2	102	BCR	C7-C8-C9-C34
25	A1	404	CLA	C1A-C2A-CAA-CBA
25	A1	404	CLA	C3A-C2A-CAA-CBA
25	A1	404	CLA	C2B-C3B-CAB-CBB
25	A1	404	CLA	C4B-C3B-CAB-CBB
25	A1	404	CLA	CHA-CBD-CGD-O1D
25	A1	404	CLA	CHA-CBD-CGD-O2D
25	A1	406	CLA	CHA-CBD-CGD-O1D
25	A1	406	CLA	CHA-CBD-CGD-O2D
25	B1	604	CLA	CHA-CBD-CGD-O1D
25	B1	604	CLA	CHA-CBD-CGD-O2D
25	B1	606	CLA	C2B-C3B-CAB-CBB
25	B1	606	CLA	C4B-C3B-CAB-CBB
25	B1	607	CLA	C2B-C3B-CAB-CBB
25	B1	607	CLA	C4B-C3B-CAB-CBB
25	B1	609	CLA	C2C-C3C-CAC-CBC
25	B1	609	CLA	C4C-C3C-CAC-CBC
25	B1	611	CLA	CHA-CBD-CGD-O1D
25	B1	611	CLA	CHA-CBD-CGD-O2D
25	B1	611	CLA	CBD-CGD-O2D-CED
25	B1	612	CLA	CBD-CGD-O2D-CED
25	B1	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B1	613	CLA	C4B-C3B-CAB-CBB
25	B1	613	CLA	C11-C12-C13-C14
25	B1	616	CLA	CHA-CBD-CGD-O1D
25	B1	616	CLA	CHA-CBD-CGD-O2D
25	B1	616	CLA	CAD-CBD-CGD-O1D
25	B1	618	CLA	CBD-CGD-O2D-CED
25	B1	619	CLA	C2B-C3B-CAB-CBB
25	B1	619	CLA	C4B-C3B-CAB-CBB
25	B1	619	CLA	CBD-CGD-O2D-CED
25	C1	503	CLA	CHA-CBD-CGD-O1D
25	C1	503	CLA	CHA-CBD-CGD-O2D
25	C1	507	CLA	C2B-C3B-CAB-CBB
25	C1	507	CLA	C4B-C3B-CAB-CBB
25	C1	507	CLA	CHA-CBD-CGD-O1D
25	C1	507	CLA	CHA-CBD-CGD-O2D
25	C1	508	CLA	C2B-C3B-CAB-CBB
25	C1	508	CLA	C4B-C3B-CAB-CBB
25	C1	508	CLA	C2-C3-C5-C6
25	C1	508	CLA	C4-C3-C5-C6
25	C1	509	CLA	CHA-CBD-CGD-O1D
25	C1	509	CLA	CHA-CBD-CGD-O2D
25	C1	512	CLA	C12-C13-C15-C16
25	a1	405	CLA	C1A-C2A-CAA-CBA
25	a1	405	CLA	C3A-C2A-CAA-CBA
25	a1	405	CLA	C2B-C3B-CAB-CBB
25	a1	405	CLA	C4B-C3B-CAB-CBB
25	b1	606	CLA	C2B-C3B-CAB-CBB
25	b1	606	CLA	C4B-C3B-CAB-CBB
25	b1	606	CLA	C2-C3-C5-C6
25	b1	606	CLA	C4-C3-C5-C6
25	b1	608	CLA	C2-C3-C5-C6
25	b1	608	CLA	C4-C3-C5-C6
25	b1	609	CLA	C2B-C3B-CAB-CBB
25	b1	609	CLA	C4B-C3B-CAB-CBB
25	b1	611	CLA	C2B-C3B-CAB-CBB
25	b1	611	CLA	C4B-C3B-CAB-CBB
25	b1	613	CLA	C2B-C3B-CAB-CBB
25	b1	613	CLA	C4B-C3B-CAB-CBB
25	b1	616	CLA	CAD-CBD-CGD-O1D
25	b1	616	CLA	CAD-CBD-CGD-O2D
25	b1	619	CLA	CBD-CGD-O2D-CED
25	b1	620	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b1	620	CLA	C4-C3-C5-C6
25	b1	620	CLA	C11-C10-C8-C9
25	c1	503	CLA	CHA-CBD-CGD-O1D
25	c1	503	CLA	CHA-CBD-CGD-O2D
25	c1	503	CLA	CAD-CBD-CGD-O1D
25	c1	504	CLA	CHA-CBD-CGD-O1D
25	c1	504	CLA	CHA-CBD-CGD-O2D
25	c1	504	CLA	CAD-CBD-CGD-O1D
25	c1	508	CLA	C2B-C3B-CAB-CBB
25	c1	508	CLA	C4B-C3B-CAB-CBB
25	c1	508	CLA	CHA-CBD-CGD-O1D
25	c1	508	CLA	CHA-CBD-CGD-O2D
25	c1	508	CLA	CBD-CGD-O2D-CED
25	c1	510	CLA	CHA-CBD-CGD-O1D
25	c1	510	CLA	CHA-CBD-CGD-O2D
25	c1	515	CLA	CHA-CBD-CGD-O1D
25	c1	515	CLA	CHA-CBD-CGD-O2D
25	d1	404	CLA	CHA-CBD-CGD-O1D
25	d1	404	CLA	CHA-CBD-CGD-O2D
25	A2	404	CLA	CHA-CBD-CGD-O1D
25	A2	404	CLA	CHA-CBD-CGD-O2D
25	A2	404	CLA	C4-C3-C5-C6
25	B2	604	CLA	CHA-CBD-CGD-O1D
25	B2	604	CLA	CHA-CBD-CGD-O2D
25	B2	604	CLA	CAD-CBD-CGD-O1D
25	B2	605	CLA	CHA-CBD-CGD-O1D
25	B2	605	CLA	CBD-CGD-O2D-CED
25	B2	606	CLA	CBD-CGD-O2D-CED
25	B2	606	CLA	C2-C3-C5-C6
25	B2	606	CLA	C4-C3-C5-C6
25	B2	606	CLA	C11-C10-C8-C9
25	B2	608	CLA	C2-C3-C5-C6
25	B2	608	CLA	C4-C3-C5-C6
25	B2	616	CLA	CHA-CBD-CGD-O1D
25	B2	616	CLA	CAD-CBD-CGD-O1D
25	B2	616	CLA	CAD-CBD-CGD-O2D
25	B2	618	CLA	CBD-CGD-O2D-CED
25	C2	503	CLA	C1A-C2A-CAA-CBA
25	C2	504	CLA	CHA-CBD-CGD-O1D
25	C2	504	CLA	CHA-CBD-CGD-O2D
25	C2	504	CLA	CAD-CBD-CGD-O1D
25	C2	505	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C2	505	CLA	CHA-CBD-CGD-O2D
25	C2	507	CLA	CBD-CGD-O2D-CED
25	C2	508	CLA	CBD-CGD-O2D-CED
25	C2	509	CLA	C2B-C3B-CAB-CBB
25	C2	509	CLA	C4B-C3B-CAB-CBB
25	C2	510	CLA	C1A-C2A-CAA-CBA
25	C2	510	CLA	C2A-CAA-CBA-CGA
25	K2	101	CLA	C4B-C3B-CAB-CBB
25	a2	413	CLA	CHA-CBD-CGD-O1D
25	a2	413	CLA	CHA-CBD-CGD-O2D
25	b2	604	CLA	CHA-CBD-CGD-O1D
25	b2	604	CLA	CAD-CBD-CGD-O1D
25	b2	604	CLA	CAD-CBD-CGD-O2D
25	b2	609	CLA	C2B-C3B-CAB-CBB
25	b2	609	CLA	C4B-C3B-CAB-CBB
25	b2	610	CLA	C6-C7-C8-C9
25	b2	612	CLA	CHA-CBD-CGD-O1D
25	b2	612	CLA	CHA-CBD-CGD-O2D
25	b2	614	CLA	C6-C7-C8-C10
25	b2	614	CLA	C11-C10-C8-C9
25	b2	616	CLA	C4B-C3B-CAB-CBB
25	b2	617	CLA	CHA-CBD-CGD-O1D
25	b2	617	CLA	CHA-CBD-CGD-O2D
25	b2	619	CLA	CBD-CGD-O2D-CED
25	b2	620	CLA	C2B-C3B-CAB-CBB
25	b2	620	CLA	C4B-C3B-CAB-CBB
25	b2	620	CLA	CBD-CGD-O2D-CED
25	b2	624	CLA	C11-C10-C8-C9
25	c2	503	CLA	C1A-C2A-CAA-CBA
25	c2	503	CLA	C3A-C2A-CAA-CBA
25	c2	503	CLA	C2B-C3B-CAB-CBB
25	c2	503	CLA	C4B-C3B-CAB-CBB
25	c2	507	CLA	CBD-CGD-O2D-CED
25	c2	508	CLA	C2B-C3B-CAB-CBB
25	c2	508	CLA	C4B-C3B-CAB-CBB
25	c2	508	CLA	C11-C10-C8-C9
25	c2	508	CLA	C11-C12-C13-C14
25	c2	509	CLA	CHA-CBD-CGD-O1D
25	c2	509	CLA	CHA-CBD-CGD-O2D
25	c2	511	CLA	CBD-CGD-O2D-CED
25	c2	511	CLA	C2-C3-C5-C6
25	c2	511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c2	512	CLA	C2B-C3B-CAB-CBB
25	d2	402	CLA	CHA-CBD-CGD-O1D
25	d2	402	CLA	CHA-CBD-CGD-O2D
25	d2	405	CLA	C4B-C3B-CAB-CBB
29	A1	410	LMG	O1-C7-C8-O7
29	M1	101	LMG	C11-C10-O7-C8
29	a1	412	LMG	O1-C7-C8-O7
29	b1	621	LMG	C11-C10-O7-C8
29	c2	519	LMG	O9-C10-O7-C8
32	C1	518	GOL	O1-C1-C2-C3
32	b1	618	GOL	O1-C1-C2-C3
32	b1	618	GOL	C1-C2-C3-O3
32	c1	521	GOL	O1-C1-C2-C3
32	C2	514	GOL	O1-C1-C2-C3
32	a2	415	GOL	O1-C1-C2-C3
32	c2	518	GOL	O1-C1-C2-C3
33	B1	621	LHG	C3-O3-P-O4
33	B1	621	LHG	C3-O3-P-O5
33	B1	621	LHG	C3-O3-P-O6
33	D1	404	LHG	C3-O3-P-O5
33	D1	404	LHG	C4-O6-P-O4
33	D1	404	LHG	C4-O6-P-O5
33	D1	405	LHG	C4-O6-P-O3
33	D1	405	LHG	C4-O6-P-O4
33	D1	405	LHG	C4-O6-P-O5
33	L1	101	LHG	C3-O3-P-O4
33	L1	101	LHG	C4-O6-P-O4
33	L1	101	LHG	C4-O6-P-O5
33	a1	407	LHG	C3-O3-P-O5
33	a1	407	LHG	C4-O6-P-O4
33	b1	622	LHG	C3-O3-P-O5
33	b1	622	LHG	C4-O6-P-O5
33	d1	402	LHG	C1-C2-C3-O3
33	d1	402	LHG	C3-O3-P-O5
33	d1	402	LHG	C4-O6-P-O3
33	d1	407	LHG	C4-O6-P-O3
33	d1	407	LHG	C4-O6-P-O4
33	d1	407	LHG	C4-O6-P-O5
33	l1	102	LHG	C3-O3-P-O4
33	l1	102	LHG	C3-O3-P-O5
33	l1	102	LHG	C3-O3-P-O6
33	l1	102	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	l1	102	LHG	C4-O6-P-O5
33	A2	405	LHG	C3-O3-P-O5
33	A2	405	LHG	C4-O6-P-O3
33	A2	405	LHG	C4-O6-P-O5
33	B2	627	LHG	C4-O6-P-O5
33	D2	403	LHG	O1-C1-C2-C3
33	D2	403	LHG	C3-O3-P-O4
33	D2	405	LHG	C3-O3-P-O5
33	D2	405	LHG	C4-O6-P-O3
33	D2	405	LHG	C4-O6-P-O5
33	L2	101	LHG	C3-O3-P-O4
33	L2	101	LHG	C4-O6-P-O5
33	a2	407	LHG	C4-O6-P-O3
33	a2	407	LHG	C4-O6-P-O4
33	a2	407	LHG	C4-O6-P-O5
33	b2	625	LHG	C4-O6-P-O3
33	b2	625	LHG	C4-O6-P-O5
33	b2	625	LHG	C8-C7-O7-C5
33	d2	403	LHG	O1-C1-C2-C3
33	d2	403	LHG	C3-O3-P-O4
33	d2	403	LHG	C4-O6-P-O3
33	d2	406	LHG	C4-O6-P-O4
33	d2	406	LHG	C4-O6-P-O5
33	l2	101	LHG	C3-O3-P-O4
33	l2	101	LHG	C3-O3-P-O5
33	l2	101	LHG	C4-O6-P-O3
33	l2	101	LHG	C4-O6-P-O4
33	l2	101	LHG	C4-O6-P-O5
35	m1	101	LMT	C2'-C1'-O1'-C1
35	m1	101	LMT	O5'-C1'-O1'-C1
35	b2	623	LMT	C2-C1-O1'-C1'
36	D1	408	PL9	C34-C36-C37-C38
36	d1	409	PL9	C34-C36-C37-C38
36	D2	408	PL9	C34-C36-C37-C38
36	d2	409	PL9	C34-C36-C37-C38
37	D2	402	SQD	O10-C23-O48-C46
37	b2	605	SQD	O5-C1-O6-C44
37	b2	605	SQD	C8-C7-O47-C45
25	C1	507	CLA	O1D-CGD-O2D-CED
25	b1	619	CLA	O1D-CGD-O2D-CED
25	c1	508	CLA	O1D-CGD-O2D-CED
25	b2	619	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	m1	101	LMT	C5'-C4'-O1B-C1B
25	B1	618	CLA	O1D-CGD-O2D-CED
25	B1	605	CLA	CBD-CGD-O2D-CED
25	B1	606	CLA	CBD-CGD-O2D-CED
25	C1	502	CLA	CBD-CGD-O2D-CED
25	C1	507	CLA	CBD-CGD-O2D-CED
25	b1	606	CLA	CBD-CGD-O2D-CED
25	b1	612	CLA	CBD-CGD-O2D-CED
25	c1	503	CLA	CBD-CGD-O2D-CED
25	B2	619	CLA	CBD-CGD-O2D-CED
25	C2	503	CLA	CBD-CGD-O2D-CED
25	C2	504	CLA	CBD-CGD-O2D-CED
25	C2	516	CLA	CBD-CGD-O2D-CED
25	b2	606	CLA	CBD-CGD-O2D-CED
25	c2	502	CLA	CBD-CGD-O2D-CED
25	c2	503	CLA	CBD-CGD-O2D-CED
25	B1	611	CLA	O1D-CGD-O2D-CED
35	m2	104	LMT	O5B-C1B-O1B-C4'
25	B1	606	CLA	O1D-CGD-O2D-CED
25	B1	619	CLA	O1D-CGD-O2D-CED
25	b1	606	CLA	O1D-CGD-O2D-CED
25	B2	618	CLA	O1D-CGD-O2D-CED
25	b2	606	CLA	O1D-CGD-O2D-CED
25	c2	511	CLA	O1D-CGD-O2D-CED
25	B1	607	CLA	CBD-CGD-O2D-CED
25	B1	608	CLA	CBD-CGD-O2D-CED
25	C1	503	CLA	CBD-CGD-O2D-CED
25	c1	504	CLA	CBD-CGD-O2D-CED
25	B2	607	CLA	CBD-CGD-O2D-CED
25	K2	101	CLA	CBD-CGD-O2D-CED
25	b2	613	CLA	CBD-CGD-O2D-CED
25	c2	504	CLA	CBD-CGD-O2D-CED
25	c2	512	CLA	CBD-CGD-O2D-CED
25	b1	620	CLA	O1D-CGD-O2D-CED
25	B2	606	CLA	O1D-CGD-O2D-CED
25	C2	507	CLA	O1D-CGD-O2D-CED
25	C2	508	CLA	O1D-CGD-O2D-CED
25	b2	620	CLA	O1D-CGD-O2D-CED
25	c2	506	CLA	C4C-C3C-CAC-CBC
25	B1	612	CLA	O1D-CGD-O2D-CED
25	B2	605	CLA	O1D-CGD-O2D-CED
25	C1	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b1	614	CLA	CBD-CGD-O2D-CED
25	A2	402	CLA	CBD-CGD-O2D-CED
25	C2	518	CLA	CBD-CGD-O2D-CED
25	b2	610	CLA	CBD-CGD-O2D-CED
25	C2	504	CLA	O1D-CGD-O2D-CED
25	c2	507	CLA	O1D-CGD-O2D-CED
29	M1	101	LMG	O9-C10-O7-C8
29	b1	621	LMG	O9-C10-O7-C8
33	b2	625	LHG	O9-C7-O7-C5
37	b2	605	SQD	O49-C7-O47-C45
35	m2	104	LMT	C2B-C1B-O1B-C4'
25	C1	502	CLA	O1D-CGD-O2D-CED
25	B1	611	CLA	C3-C5-C6-C7
25	B1	613	CLA	C3-C5-C6-C7
25	b1	620	CLA	C3-C5-C6-C7
25	A2	403	CLA	C3-C5-C6-C7
25	B2	607	CLA	C3-C5-C6-C7
25	b2	617	CLA	C3-C5-C6-C7
25	b2	619	CLA	C3-C5-C6-C7
25	c2	507	CLA	C3-C5-C6-C7
25	c2	510	CLA	C3-C5-C6-C7
25	c2	512	CLA	C3-C5-C6-C7
25	c2	503	CLA	CBA-CGA-O2A-C1
25	c2	506	CLA	CBA-CGA-O2A-C1
25	c2	506	CLA	C2C-C3C-CAC-CBC
25	c2	503	CLA	O1D-CGD-O2D-CED
25	D1	403	CLA	CBD-CGD-O2D-CED
25	C2	516	CLA	CBA-CGA-O2A-C1
25	c1	509	CLA	C4-C3-C5-C6
25	C2	503	CLA	C4-C3-C5-C6
25	C2	506	CLA	C4-C3-C5-C6
25	C2	509	CLA	C4-C3-C5-C6
36	d1	409	PL9	C20-C19-C21-C22
25	b1	620	CLA	C2-C3-C5-C6
25	C1	511	CLA	CBD-CGD-O2D-CED
25	a1	403	CLA	C2A-CAA-CBA-CGA
25	b1	609	CLA	C2A-CAA-CBA-CGA
25	B2	609	CLA	C2A-CAA-CBA-CGA
25	b2	611	CLA	C2A-CAA-CBA-CGA
25	B1	610	CLA	C3-C5-C6-C7
25	B1	619	CLA	C3-C5-C6-C7
25	B2	619	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	c2	506	CLA	C3-C5-C6-C7
25	c1	507	CLA	CBA-CGA-O2A-C1
25	C2	506	CLA	CBA-CGA-O2A-C1
29	B1	626	LMG	C29-C28-O8-C9
25	b1	612	CLA	O1D-CGD-O2D-CED
25	C1	509	CLA	CBD-CGD-O2D-CED
25	c1	513	CLA	CBD-CGD-O2D-CED
25	C2	505	CLA	CBD-CGD-O2D-CED
25	B1	605	CLA	O1D-CGD-O2D-CED
25	C2	516	CLA	O1D-CGD-O2D-CED
25	C2	506	CLA	O1A-CGA-O2A-C1
29	B1	626	LMG	O10-C28-O8-C9
23	K1	101	BCR	C19-C20-C21-C22
25	B1	610	CLA	CBD-CGD-O2D-CED
25	C1	505	CLA	CBD-CGD-O2D-CED
25	d1	406	CLA	CBD-CGD-O2D-CED
25	D2	406	CLA	CBD-CGD-O2D-CED
25	b2	617	CLA	CBD-CGD-O2D-CED
25	C2	503	CLA	O1D-CGD-O2D-CED
33	d1	402	LHG	O2-C2-C3-O3
25	C1	507	CLA	C3-C5-C6-C7
25	B2	613	CLA	C3-C5-C6-C7
25	c2	503	CLA	O1A-CGA-O2A-C1
25	c2	506	CLA	O1A-CGA-O2A-C1
29	F2	402	LMG	C11-C10-O7-C8
25	b1	607	CLA	CBD-CGD-O2D-CED
25	b1	615	CLA	CBD-CGD-O2D-CED
25	D2	404	CLA	CBD-CGD-O2D-CED
25	b2	616	CLA	CBD-CGD-O2D-CED
25	d2	404	CLA	CBD-CGD-O2D-CED
29	B1	626	LMG	O6-C5-C6-O5
25	c2	502	CLA	O1D-CGD-O2D-CED
25	c1	510	CLA	CBD-CGD-O2D-CED
25	C1	506	CLA	CBA-CGA-O2A-C1
25	B2	619	CLA	O1D-CGD-O2D-CED
29	A2	412	LMG	C4-C5-C6-O5
25	c1	507	CLA	O1A-CGA-O2A-C1
38	V1	201	HEM	C3D-CAD-CBD-CGD
25	B1	606	CLA	C4-C3-C5-C6
25	B1	608	CLA	C4-C3-C5-C6
25	B1	606	CLA	C2-C3-C5-C6
25	B1	608	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	d1	409	PL9	C18-C19-C21-C22
25	C2	511	CLA	CBD-CGD-O2D-CED
25	B1	609	CLA	C2A-CAA-CBA-CGA
25	A2	402	CLA	C2A-CAA-CBA-CGA
25	C1	506	CLA	O1A-CGA-O2A-C1
29	I2	101	LMG	O6-C1-O1-C7
36	D1	408	PL9	C14-C16-C17-C18
36	d1	409	PL9	C19-C21-C22-C23
36	d1	409	PL9	C29-C31-C32-C33
36	D2	408	PL9	C29-C31-C32-C33
36	D2	408	PL9	C44-C46-C47-C48
36	d2	409	PL9	C9-C11-C12-C13
36	d2	409	PL9	C14-C16-C17-C18
25	C2	516	CLA	O1A-CGA-O2A-C1
25	c1	507	CLA	C3-C5-C6-C7
25	B1	619	CLA	CBA-CGA-O2A-C1
25	C2	506	CLA	CBD-CGD-O2D-CED
35	m2	103	LMT	C4'-C5'-C6'-O6'
25	c1	503	CLA	O1D-CGD-O2D-CED
25	B1	608	CLA	O1D-CGD-O2D-CED
33	a2	407	LHG	C1-C2-C3-O3
29	F2	402	LMG	O9-C10-O7-C8
25	K2	101	CLA	O1D-CGD-O2D-CED
34	C1	516	DGD	O6E-C5E-C6E-O5E
34	c1	520	DGD	O6E-C5E-C6E-O5E
35	m1	101	LMT	O5B-C5B-C6B-O6B
29	B1	626	LMG	C4-C5-C6-O5
35	m1	101	LMT	C4B-C5B-C6B-O6B
25	b1	613	CLA	C15-C16-C17-C18
25	b1	619	CLA	C10-C11-C12-C13
25	a2	404	CLA	C8-C10-C11-C12
34	c1	520	DGD	C4E-C5E-C6E-O5E
25	b2	615	CLA	C8-C10-C11-C12
25	b2	618	CLA	C10-C11-C12-C13
29	A2	412	LMG	O6-C5-C6-O5
25	d1	406	CLA	C4-C3-C5-C6
25	c1	509	CLA	C2-C3-C5-C6
25	C2	503	CLA	C2-C3-C5-C6
25	C2	509	CLA	C2-C3-C5-C6
25	B1	606	CLA	C14-C13-C15-C16
25	B1	611	CLA	C11-C12-C13-C14
25	B1	612	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B1	614	CLA	C11-C10-C8-C9
25	B1	619	CLA	C6-C7-C8-C9
25	C1	503	CLA	C6-C7-C8-C9
25	C1	506	CLA	C11-C12-C13-C14
25	C1	510	CLA	C14-C13-C15-C16
25	b1	608	CLA	C11-C10-C8-C9
25	b1	611	CLA	C6-C7-C8-C9
25	b1	612	CLA	C11-C12-C13-C14
25	c1	506	CLA	C11-C12-C13-C14
25	c1	507	CLA	C11-C10-C8-C9
25	c1	509	CLA	C11-C10-C8-C9
25	c1	509	CLA	C11-C12-C13-C14
25	B2	611	CLA	C6-C7-C8-C9
25	B2	612	CLA	C11-C12-C13-C14
25	B2	613	CLA	C11-C12-C13-C14
25	B2	619	CLA	C6-C7-C8-C9
25	C2	509	CLA	C11-C12-C13-C14
25	D2	404	CLA	C11-C10-C8-C9
25	b2	606	CLA	C11-C10-C8-C9
25	b2	608	CLA	C11-C10-C8-C9
25	b2	609	CLA	C11-C12-C13-C14
25	b2	612	CLA	C11-C12-C13-C14
25	b2	613	CLA	C14-C13-C15-C16
25	b2	617	CLA	C6-C7-C8-C9
25	b2	617	CLA	C11-C10-C8-C9
25	b2	619	CLA	C11-C10-C8-C9
25	b2	620	CLA	C6-C7-C8-C9
25	c2	502	CLA	C11-C12-C13-C14
25	c2	505	CLA	C11-C12-C13-C14
25	d2	405	CLA	C11-C10-C8-C9
25	B1	607	CLA	O1D-CGD-O2D-CED
25	c2	504	CLA	O1D-CGD-O2D-CED
25	A1	403	CLA	CBD-CGD-O2D-CED
25	C1	507	CLA	C2C-C3C-CAC-CBC
25	C1	511	CLA	C10-C11-C12-C13
25	D2	404	CLA	C8-C10-C11-C12
25	C2	507	CLA	C2A-CAA-CBA-CGA
23	B1	602	BCR	C7-C8-C9-C34
23	D1	401	BCR	C37-C22-C23-C24
23	J1	101	BCR	C7-C8-C9-C34
23	J1	101	BCR	C36-C18-C19-C20
23	d2	401	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	j2	102	BCR	C36-C18-C19-C20
23	B1	602	BCR	C7-C8-C9-C10
23	D1	401	BCR	C21-C22-C23-C24
23	d2	401	BCR	C21-C22-C23-C24
25	B1	610	CLA	C8-C10-C11-C12
25	C1	505	CLA	C5-C6-C7-C8
25	b1	614	CLA	C10-C11-C12-C13
25	C2	509	CLA	C8-C10-C11-C12
25	b2	606	CLA	C10-C11-C12-C13
25	c2	505	CLA	C8-C10-C11-C12
25	c2	512	CLA	O1D-CGD-O2D-CED
25	c1	516	CLA	CBA-CGA-O2A-C1
25	B1	607	CLA	C8-C10-C11-C12
25	B1	609	CLA	C8-C10-C11-C12
25	B1	615	CLA	C8-C10-C11-C12
25	C1	507	CLA	C5-C6-C7-C8
25	a1	404	CLA	C8-C10-C11-C12
25	b1	612	CLA	C15-C16-C17-C18
25	B2	608	CLA	C10-C11-C12-C13
25	B2	608	CLA	C15-C16-C17-C18
25	B2	613	CLA	C13-C15-C16-C17
25	a2	404	CLA	C15-C16-C17-C18
25	b2	615	CLA	C10-C11-C12-C13
25	b2	620	CLA	C15-C16-C17-C18
25	d2	405	CLA	C10-C11-C12-C13
25	B1	606	CLA	C8-C10-C11-C12
25	B1	613	CLA	C10-C11-C12-C13
25	B1	619	CLA	C15-C16-C17-C18
25	C1	504	CLA	C8-C10-C11-C12
25	C1	507	CLA	C8-C10-C11-C12
25	C1	511	CLA	C5-C6-C7-C8
25	a1	403	CLA	C8-C10-C11-C12
25	b1	604	CLA	C15-C16-C17-C18
25	b1	606	CLA	C13-C15-C16-C17
25	b1	607	CLA	C13-C15-C16-C17
25	b1	609	CLA	C15-C16-C17-C18
25	b1	620	CLA	C5-C6-C7-C8
25	c1	507	CLA	C10-C11-C12-C13
25	c1	511	CLA	C10-C11-C12-C13
25	d1	406	CLA	C8-C10-C11-C12
25	A2	402	CLA	C8-C10-C11-C12
25	B2	609	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B2	615	CLA	C8-C10-C11-C12
25	a2	405	CLA	C13-C15-C16-C17
25	a2	405	CLA	C15-C16-C17-C18
25	b2	620	CLA	C10-C11-C12-C13
25	c2	511	CLA	C13-C15-C16-C17
25	c2	512	CLA	C8-C10-C11-C12
25	C1	503	CLA	O1D-CGD-O2D-CED
25	c1	504	CLA	O1D-CGD-O2D-CED
25	b2	613	CLA	O1D-CGD-O2D-CED
32	i1	101	GOL	O1-C1-C2-O2
37	D1	409	SQD	C23-C24-C25-C26
25	a2	405	CLA	CBD-CGD-O2D-CED
25	B2	607	CLA	O1D-CGD-O2D-CED
25	C1	509	CLA	C10-C11-C12-C13
25	b1	605	CLA	C13-C15-C16-C17
25	b1	608	CLA	C15-C16-C17-C18
25	b1	614	CLA	C8-C10-C11-C12
25	d1	406	CLA	C15-C16-C17-C18
25	B2	608	CLA	C5-C6-C7-C8
25	B2	612	CLA	C15-C16-C17-C18
25	B2	619	CLA	C15-C16-C17-C18
27	D2	407	PHO	C15-C16-C17-C18
34	c2	514	DGD	O6E-C5E-C6E-O5E
25	C1	507	CLA	C15-C16-C17-C18
25	C1	509	CLA	C13-C15-C16-C17
25	b1	615	CLA	C8-C10-C11-C12
25	c1	506	CLA	C8-C10-C11-C12
25	c2	506	CLA	C10-C11-C12-C13
25	c1	512	CLA	CBD-CGD-O2D-CED
35	m2	103	LMT	C4B-C5B-C6B-O6B
38	v1	201	HEM	C3D-CAD-CBD-CGD
25	B1	613	CLA	C13-C15-C16-C17
25	C1	505	CLA	C8-C10-C11-C12
25	b1	614	CLA	C13-C15-C16-C17
25	c1	507	CLA	C8-C10-C11-C12
25	c1	509	CLA	C8-C10-C11-C12
25	a2	404	CLA	C13-C15-C16-C17
25	B1	606	CLA	C11-C10-C8-C7
25	B1	609	CLA	C12-C13-C15-C16
25	B1	614	CLA	C6-C7-C8-C10
25	B1	615	CLA	C11-C10-C8-C7
25	B1	615	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C1	506	CLA	C11-C12-C13-C15
25	C1	507	CLA	C12-C13-C15-C16
25	C1	509	CLA	C12-C13-C15-C16
25	b1	607	CLA	C6-C7-C8-C10
25	b1	615	CLA	C11-C10-C8-C7
25	C2	505	CLA	C6-C7-C8-C10
25	C2	505	CLA	C11-C10-C8-C7
25	b2	612	CLA	C12-C13-C15-C16
25	b2	620	CLA	C3-C5-C6-C7
25	c2	513	CLA	CBA-CGA-O2A-C1
25	A1	403	CLA	C2A-CAA-CBA-CGA
25	B2	605	CLA	C2A-CAA-CBA-CGA
25	K2	101	CLA	C2A-CAA-CBA-CGA
25	A2	402	CLA	O1D-CGD-O2D-CED
25	C2	518	CLA	O1D-CGD-O2D-CED
25	b2	610	CLA	O1D-CGD-O2D-CED
25	B1	615	CLA	C5-C6-C7-C8
25	C1	505	CLA	C15-C16-C17-C18
25	b1	620	CLA	C15-C16-C17-C18
25	b2	618	CLA	C13-C15-C16-C17
25	C1	506	CLA	CBD-CGD-O2D-CED
25	b1	609	CLA	CBD-CGD-O2D-CED
25	B2	606	CLA	C5-C6-C7-C8
25	B2	613	CLA	C10-C11-C12-C13
25	b2	624	CLA	C10-C11-C12-C13
25	b1	614	CLA	O1D-CGD-O2D-CED
36	D1	408	PL9	C9-C11-C12-C13
36	D2	408	PL9	C14-C16-C17-C18
29	D1	406	LMG	C10-C11-C12-C13
33	a2	407	LHG	O2-C2-C3-O3
25	B1	611	CLA	C13-C15-C16-C17
25	B1	611	CLA	C5-C6-C7-C8
25	C2	505	CLA	C8-C10-C11-C12
25	C2	506	CLA	C10-C11-C12-C13
25	b2	619	CLA	C5-C6-C7-C8
25	c2	509	CLA	C10-C11-C12-C13
25	C1	513	CLA	O1D-CGD-O2D-CED
25	B1	619	CLA	O1A-CGA-O2A-C1
25	c1	516	CLA	O1A-CGA-O2A-C1
25	c2	515	CLA	CBA-CGA-O2A-C1
35	a2	406	LMT	O1'-C1-C2-C3
25	C1	505	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	C1	509	CLA	C15-C16-C17-C18
25	b1	606	CLA	C10-C11-C12-C13
25	c1	505	CLA	C5-C6-C7-C8
35	m2	103	LMT	O5'-C5'-C6'-O6'
29	c1	519	LMG	C11-C10-O7-C8
25	B1	606	CLA	C5-C6-C7-C8
25	C1	507	CLA	C10-C11-C12-C13
25	D1	402	CLA	C15-C16-C17-C18
25	b1	604	CLA	C8-C10-C11-C12
25	b1	606	CLA	C5-C6-C7-C8
25	b1	620	CLA	C8-C10-C11-C12
25	B2	615	CLA	C13-C15-C16-C17
25	c2	504	CLA	C8-C10-C11-C12
25	c2	505	CLA	C10-C11-C12-C13
25	c2	506	CLA	C5-C6-C7-C8
25	c2	512	CLA	C15-C16-C17-C18
33	D1	404	LHG	C3-O3-P-O6
33	D1	404	LHG	C4-O6-P-O3
33	L1	101	LHG	C4-O6-P-O3
33	a1	407	LHG	C3-O3-P-O6
33	a1	407	LHG	C4-O6-P-O3
33	d1	402	LHG	C3-O3-P-O6
33	l1	102	LHG	C4-O6-P-O3
33	A2	405	LHG	C3-O3-P-O6
33	B2	627	LHG	C4-O6-P-O3
33	d2	406	LHG	C4-O6-P-O3
33	l2	101	LHG	C3-O3-P-O6
25	b2	609	CLA	C3-C5-C6-C7
25	B1	617	CLA	C10-C11-C12-C13
25	C1	512	CLA	C13-C15-C16-C17
25	D1	403	CLA	O1D-CGD-O2D-CED
29	c1	519	LMG	O9-C10-O7-C8
25	b1	616	CLA	C4-C3-C5-C6
25	K2	101	CLA	C4-C3-C5-C6
25	b2	608	CLA	C4-C3-C5-C6
25	C2	506	CLA	C2-C3-C5-C6
25	C1	508	CLA	C5-C6-C7-C8
25	C2	509	CLA	C10-C11-C12-C13
34	C1	516	DGD	C6A-C7A-C8A-C9A
25	B1	605	CLA	C2A-CAA-CBA-CGA
25	B1	612	CLA	C2A-CAA-CBA-CGA
25	b1	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c1	503	CLA	C2A-CAA-CBA-CGA
25	c1	507	CLA	C2A-CAA-CBA-CGA
25	C2	503	CLA	C2A-CAA-CBA-CGA
25	b2	609	CLA	C2A-CAA-CBA-CGA
25	c2	508	CLA	C2A-CAA-CBA-CGA
25	b1	620	CLA	C16-C17-C18-C20
25	C2	503	CLA	C16-C17-C18-C19
25	b2	620	CLA	C16-C17-C18-C20
25	b1	613	CLA	C3-C5-C6-C7
25	B2	619	CLA	CBA-CGA-O2A-C1
25	K2	101	CLA	CBA-CGA-O2A-C1
25	c1	511	CLA	C8-C10-C11-C12
34	c2	514	DGD	C7A-C8A-C9A-CAA
29	A1	410	LMG	C11-C10-O7-C8
29	a1	412	LMG	C11-C10-O7-C8
29	b1	631	LMG	C11-C10-O7-C8
29	a2	412	LMG	C11-C10-O7-C8
25	c1	511	CLA	C13-C15-C16-C17
33	D1	405	LHG	C9-C10-C11-C12
33	a2	407	LHG	C9-C10-C11-C12
34	c1	518	DGD	C7A-C8A-C9A-CAA
25	C1	502	CLA	C16-C17-C18-C19
25	b1	616	CLA	C16-C17-C18-C19
25	B2	615	CLA	C16-C17-C18-C20
25	d2	405	CLA	C16-C17-C18-C19
29	a1	412	LMG	C14-C15-C16-C17
29	c1	519	LMG	C41-C42-C43-C44
33	l2	101	LHG	C11-C10-C9-C8
25	C1	509	CLA	O1D-CGD-O2D-CED
25	c1	513	CLA	O1D-CGD-O2D-CED
29	A1	410	LMG	O9-C10-O7-C8
29	a1	412	LMG	O9-C10-O7-C8
29	b1	631	LMG	O9-C10-O7-C8
25	c2	509	CLA	CBD-CGD-O2D-CED
33	L1	101	LHG	C10-C11-C12-C13
33	l2	101	LHG	C9-C10-C11-C12
34	c2	514	DGD	C4B-C5B-C6B-C7B
25	C1	511	CLA	O1D-CGD-O2D-CED
25	C2	505	CLA	O1D-CGD-O2D-CED
33	D2	405	LHG	C10-C11-C12-C13
34	h2	102	DGD	CBB-CCB-CDB-CEB
25	C1	505	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	l1	102	LHG	O2-C2-C3-O3
38	V2	201	HEM	C3D-CAD-CBD-CGD
25	B1	607	CLA	C3-C5-C6-C7
34	C1	515	DGD	C2E-C1E-O5D-C6D
34	c1	514	DGD	C2E-C1E-O5D-C6D
34	c2	516	DGD	C2E-C1E-O5D-C6D
33	A2	405	LHG	C29-C30-C31-C32
25	C1	506	CLA	C5-C6-C7-C8
25	B2	619	CLA	O1A-CGA-O2A-C1
25	C1	505	CLA	C16-C17-C18-C20
25	b1	606	CLA	C16-C17-C18-C20
25	c1	509	CLA	C16-C17-C18-C20
25	K2	101	CLA	C6-C7-C8-C10
25	c2	505	CLA	C16-C17-C18-C20
25	b1	604	CLA	C4-C3-C5-C6
33	d2	406	LHG	C30-C31-C32-C33
25	K2	101	CLA	C2-C3-C5-C6
25	A1	406	CLA	C11-C12-C13-C14
25	B1	608	CLA	C11-C12-C13-C14
25	B1	611	CLA	C6-C7-C8-C9
25	C1	508	CLA	C11-C10-C8-C9
25	C1	512	CLA	C14-C13-C15-C16
25	C1	513	CLA	C11-C12-C13-C14
25	b1	610	CLA	C11-C12-C13-C14
25	c1	503	CLA	C14-C13-C15-C16
25	c1	504	CLA	C6-C7-C8-C9
25	c1	510	CLA	C11-C10-C8-C9
25	B2	619	CLA	C11-C12-C13-C14
25	C2	509	CLA	C11-C10-C8-C9
25	b2	614	CLA	C6-C7-C8-C9
25	c2	511	CLA	C14-C13-C15-C16
27	A2	407	PHO	C11-C10-C8-C9
25	c2	510	CLA	C5-C6-C7-C8
33	l1	102	LHG	C11-C12-C13-C14
25	C1	513	CLA	C10-C11-C12-C13
25	c1	505	CLA	C8-C10-C11-C12
25	b2	610	CLA	C5-C6-C7-C8
25	c2	513	CLA	O1A-CGA-O2A-C1
23	b2	602	BCR	C7-C8-C9-C34
34	C1	515	DGD	C3B-C4B-C5B-C6B
32	B1	620	GOL	O1-C1-C2-C3
32	i1	101	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	c1	502	BCR	C7-C8-C9-C10
23	b2	602	BCR	C7-C8-C9-C10
25	b1	604	CLA	C3-C5-C6-C7
29	a2	412	LMG	O9-C10-O7-C8
25	B1	615	CLA	C13-C15-C16-C17
25	B1	618	CLA	C8-C10-C11-C12
25	c1	510	CLA	C15-C16-C17-C18
29	a1	412	LMG	C17-C18-C19-C20
34	c1	518	DGD	C5B-C6B-C7B-C8B
29	a1	412	LMG	C13-C14-C15-C16
33	b1	622	LHG	C17-C18-C19-C20
33	L2	101	LHG	C14-C15-C16-C17
25	B1	609	CLA	C4B-C3B-CAB-CBB
25	C1	506	CLA	C4B-C3B-CAB-CBB
25	C1	513	CLA	C4B-C3B-CAB-CBB
25	D1	402	CLA	C4B-C3B-CAB-CBB
25	b1	617	CLA	C4B-C3B-CAB-CBB
25	C2	516	CLA	C4B-C3B-CAB-CBB
25	a2	413	CLA	C4B-C3B-CAB-CBB
25	b2	610	CLA	C4B-C3B-CAB-CBB
25	b2	612	CLA	C4B-C3B-CAB-CBB
25	b2	617	CLA	C4B-C3B-CAB-CBB
25	c2	504	CLA	C4B-C3B-CAB-CBB
25	c2	512	CLA	C4B-C3B-CAB-CBB
25	C1	503	CLA	C11-C12-C13-C14
25	C1	503	CLA	C11-C12-C13-C15
25	b1	616	CLA	C16-C17-C18-C20
25	c1	503	CLA	C16-C17-C18-C19
25	C2	503	CLA	C16-C17-C18-C20
25	b2	620	CLA	C16-C17-C18-C19
25	c2	502	CLA	C16-C17-C18-C19
25	c2	502	CLA	C16-C17-C18-C20
34	C1	515	DGD	O6E-C1E-O5D-C6D
34	c1	514	DGD	O6E-C1E-O5D-C6D
34	c2	516	DGD	O6E-C1E-O5D-C6D
25	C1	510	CLA	C10-C11-C12-C13
33	l2	101	LHG	C11-C12-C13-C14
25	c2	510	CLA	CBD-CGD-O2D-CED
25	D2	406	CLA	O1D-CGD-O2D-CED
29	B2	620	LMG	C10-C11-C12-C13
25	B2	615	CLA	C15-C16-C17-C18
29	c1	519	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
33	l1	102	LHG	C25-C26-C27-C28
25	B2	605	CLA	C3-C5-C6-C7
35	m2	104	LMT	O5'-C5'-C6'-O6'
25	b2	617	CLA	O1D-CGD-O2D-CED
25	C1	512	CLA	C3A-C2A-CAA-CBA
25	c1	515	CLA	C3A-C2A-CAA-CBA
25	C2	510	CLA	C3A-C2A-CAA-CBA
25	D2	401	CLA	C3A-C2A-CAA-CBA
25	C1	507	CLA	C4C-C3C-CAC-CBC
23	H1	102	BCR	C14-C15-C16-C17
23	H2	103	BCR	C16-C17-C18-C19
25	B1	615	CLA	C16-C17-C18-C20
25	C1	505	CLA	C16-C17-C18-C19
25	b1	606	CLA	C16-C17-C18-C19
25	c1	510	CLA	C16-C17-C18-C19
25	B2	615	CLA	C16-C17-C18-C19
29	A1	412	LMG	C39-C40-C41-C42
29	B2	621	LMG	C7-C8-C9-O8
25	C1	508	CLA	CBD-CGD-O2D-CED
25	C1	511	CLA	C3-C5-C6-C7
34	h1	101	DGD	C1A-C2A-C3A-C4A
25	c1	512	CLA	C5-C6-C7-C8
27	a1	411	PHO	C4-C3-C5-C6
27	A2	407	PHO	C4-C3-C5-C6
25	b1	608	CLA	CBA-CGA-O2A-C1
25	B2	613	CLA	C2-C3-C5-C6
25	b2	612	CLA	C2-C3-C5-C6
27	A2	407	PHO	C2-C3-C5-C6
29	B1	622	LMG	C11-C10-O7-C8
29	d1	411	LMG	C11-C10-O7-C8
33	D1	405	LHG	C33-C34-C35-C36
35	M1	103	LMT	C7-C8-C9-C10
25	c1	509	CLA	C2A-CAA-CBA-CGA
25	a2	404	CLA	C2A-CAA-CBA-CGA
32	b1	618	GOL	O1-C1-C2-O2
32	C2	514	GOL	O1-C1-C2-O2
33	D2	403	LHG	O1-C1-C2-O2
33	d1	407	LHG	C30-C31-C32-C33
25	c1	506	CLA	C16-C17-C18-C20
25	B1	609	CLA	C2B-C3B-CAB-CBB
25	C1	506	CLA	C2B-C3B-CAB-CBB
25	C1	513	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	D1	402	CLA	C2B-C3B-CAB-CBB
25	b1	617	CLA	C2B-C3B-CAB-CBB
25	C2	516	CLA	C2B-C3B-CAB-CBB
25	K2	101	CLA	C2B-C3B-CAB-CBB
25	a2	413	CLA	C2B-C3B-CAB-CBB
25	b2	604	CLA	C2B-C3B-CAB-CBB
25	b2	610	CLA	C2B-C3B-CAB-CBB
25	b2	612	CLA	C2B-C3B-CAB-CBB
25	b2	616	CLA	C2B-C3B-CAB-CBB
25	b2	617	CLA	C2B-C3B-CAB-CBB
25	c2	504	CLA	C2B-C3B-CAB-CBB
25	d2	405	CLA	C2B-C3B-CAB-CBB
33	B1	621	LHG	O2-C2-C3-O3
25	c2	505	CLA	CBA-CGA-O2A-C1
25	K2	101	CLA	O1A-CGA-O2A-C1
29	B1	622	LMG	O9-C10-O7-C8
29	d1	411	LMG	O9-C10-O7-C8
25	c2	513	CLA	C2-C1-O2A-CGA
34	c2	514	DGD	O6D-C5D-C6D-O5D
34	c2	514	DGD	C5B-C6B-C7B-C8B
25	B1	615	CLA	C10-C11-C12-C13
25	B2	617	CLA	C15-C16-C17-C18
25	b2	617	CLA	C10-C11-C12-C13
34	c2	517	DGD	CAA-CBA-CCA-CDA
23	C1	501	BCR	C1-C6-C7-C8
23	C1	501	BCR	C5-C6-C7-C8
23	D1	401	BCR	C1-C6-C7-C8
23	D1	401	BCR	C5-C6-C7-C8
23	D1	401	BCR	C23-C24-C25-C30
23	J1	101	BCR	C1-C6-C7-C8
23	J1	101	BCR	C5-C6-C7-C8
23	b1	603	BCR	C5-C6-C7-C8
23	d1	405	BCR	C1-C6-C7-C8
23	d1	405	BCR	C5-C6-C7-C8
23	k1	101	BCR	C1-C6-C7-C8
23	k1	101	BCR	C5-C6-C7-C8
23	F2	401	BCR	C1-C6-C7-C8
23	F2	401	BCR	C5-C6-C7-C8
23	K2	102	BCR	C1-C6-C7-C8
23	c2	501	BCR	C23-C24-C25-C26
23	c2	501	BCR	C23-C24-C25-C30
23	d2	401	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	d2	401	BCR	C23-C24-C25-C30
23	h2	101	BCR	C1-C6-C7-C8
23	h2	101	BCR	C5-C6-C7-C8
25	B1	607	CLA	CBA-CGA-O2A-C1
25	c1	506	CLA	CBA-CGA-O2A-C1
25	d1	404	CLA	CBA-CGA-O2A-C1
25	B1	619	CLA	C10-C11-C12-C13
25	b1	616	CLA	C13-C15-C16-C17
25	C2	503	CLA	C5-C6-C7-C8
29	B2	620	LMG	C11-C10-O7-C8
33	D1	405	LHG	C32-C33-C34-C35
33	l2	101	LHG	C10-C11-C12-C13
25	b1	608	CLA	C10-C11-C12-C13
25	B2	606	CLA	C10-C11-C12-C13
25	C2	506	CLA	C5-C6-C7-C8
25	C1	506	CLA	C4-C3-C5-C6
25	c2	512	CLA	C4-C3-C5-C6
25	d2	404	CLA	O1D-CGD-O2D-CED
25	A1	403	CLA	C11-C10-C8-C7
25	A1	406	CLA	C11-C12-C13-C15
25	B1	608	CLA	C11-C12-C13-C15
25	C1	504	CLA	C11-C10-C8-C7
25	C1	507	CLA	C11-C12-C13-C15
25	C1	509	CLA	C11-C10-C8-C7
25	C1	512	CLA	C11-C10-C8-C7
25	b1	604	CLA	C2-C3-C5-C6
25	b1	608	CLA	C11-C12-C13-C15
25	b1	609	CLA	C6-C7-C8-C10
25	b1	610	CLA	C11-C12-C13-C15
25	b1	612	CLA	C11-C10-C8-C7
25	c1	507	CLA	C6-C7-C8-C10
25	c1	510	CLA	C11-C10-C8-C7
25	d1	406	CLA	C2-C3-C5-C6
25	B2	608	CLA	C11-C12-C13-C15
25	B2	609	CLA	C11-C12-C13-C15
25	B2	611	CLA	C2-C3-C5-C6
25	B2	613	CLA	C11-C10-C8-C7
25	B2	615	CLA	C12-C13-C15-C16
25	B2	617	CLA	C11-C12-C13-C15
25	B2	619	CLA	C11-C12-C13-C15
25	b2	606	CLA	C11-C10-C8-C7
25	b2	608	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b2	620	CLA	C11-C12-C13-C15
25	c2	504	CLA	C12-C13-C15-C16
25	c2	511	CLA	C12-C13-C15-C16
27	A1	408	PHO	C2-C3-C5-C6
27	a1	411	PHO	C2-C3-C5-C6
27	a2	416	PHO	C2-C3-C5-C6
36	D1	408	PL9	C38-C39-C41-C42
25	a1	404	CLA	C2C-C3C-CAC-CBC
25	C1	502	CLA	C5-C6-C7-C8
25	C1	513	CLA	C8-C10-C11-C12
25	B1	610	CLA	C16-C17-C18-C20
25	b1	620	CLA	C16-C17-C18-C19
25	c1	509	CLA	C16-C17-C18-C19
25	c2	505	CLA	C16-C17-C18-C19
25	B1	610	CLA	O1D-CGD-O2D-CED
25	d1	406	CLA	O1D-CGD-O2D-CED
29	B2	620	LMG	O9-C10-O7-C8
34	C1	517	DGD	C1A-C2A-C3A-C4A
25	D1	403	CLA	CBA-CGA-O2A-C1
25	c1	505	CLA	CBA-CGA-O2A-C1
25	B1	612	CLA	C15-C16-C17-C18
25	b1	615	CLA	O1D-CGD-O2D-CED
25	C1	505	CLA	C13-C15-C16-C17
25	b1	608	CLA	O1A-CGA-O2A-C1
25	c2	505	CLA	O1A-CGA-O2A-C1
25	a1	403	CLA	CBD-CGD-O2D-CED
25	B1	619	CLA	C16-C17-C18-C20
25	C2	509	CLA	C16-C17-C18-C20
25	b1	620	CLA	C10-C11-C12-C13
25	b2	609	CLA	C8-C10-C11-C12
33	l1	102	LHG	C7-C8-C9-C10
33	d1	402	LHG	C8-C7-O7-C5
33	B2	627	LHG	C8-C7-O7-C5
25	D2	404	CLA	O1D-CGD-O2D-CED
29	B1	626	LMG	C36-C37-C38-C39
33	l1	102	LHG	C11-C10-C9-C8
25	K2	101	CLA	C3-C5-C6-C7
34	C1	517	DGD	CAA-CBA-CCA-CDA
34	H2	101	DGD	CBB-CCB-CDB-CEB
35	m2	103	LMT	O1'-C1-C2-C3
25	c1	510	CLA	O1D-CGD-O2D-CED
25	d2	405	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
33	L1	101	LHG	C16-C17-C18-C19
29	D1	406	LMG	O6-C5-C6-O5
25	B1	616	CLA	C10-C11-C12-C13
25	B2	611	CLA	C4-C3-C5-C6
25	B2	613	CLA	C4-C3-C5-C6
25	b2	612	CLA	C4-C3-C5-C6
27	A1	408	PHO	C4-C3-C5-C6
27	a2	416	PHO	C4-C3-C5-C6
36	D1	408	PL9	C40-C39-C41-C42
25	b1	616	CLA	C2-C3-C5-C6
25	b2	608	CLA	C2-C3-C5-C6
25	c2	512	CLA	C2-C3-C5-C6
25	b1	615	CLA	C10-C11-C12-C13
25	B1	606	CLA	C11-C12-C13-C14
25	B1	609	CLA	C14-C13-C15-C16
25	B1	617	CLA	C11-C12-C13-C14
25	C1	507	CLA	C11-C12-C13-C14
25	C1	507	CLA	C14-C13-C15-C16
25	C1	509	CLA	C11-C10-C8-C9
25	C1	509	CLA	C14-C13-C15-C16
25	C1	510	CLA	C11-C12-C13-C14
25	b1	604	CLA	C11-C12-C13-C14
25	b1	607	CLA	C6-C7-C8-C9
25	b1	608	CLA	C11-C12-C13-C14
25	b1	609	CLA	C6-C7-C8-C9
25	d1	401	CLA	C6-C7-C8-C9
25	B2	609	CLA	C11-C12-C13-C14
25	B2	614	CLA	C14-C13-C15-C16
25	B2	617	CLA	C11-C12-C13-C14
25	C2	505	CLA	C6-C7-C8-C9
25	b2	620	CLA	C11-C12-C13-C14
25	c2	505	CLA	C6-C7-C8-C9
25	c2	512	CLA	C11-C12-C13-C14
27	a1	411	PHO	C14-C13-C15-C16
27	A2	407	PHO	C6-C7-C8-C9
25	B1	607	CLA	O1A-CGA-O2A-C1
34	c1	518	DGD	C4B-C5B-C6B-C7B
25	b1	607	CLA	C3-C5-C6-C7
25	C2	511	CLA	O1D-CGD-O2D-CED
25	b2	616	CLA	O1D-CGD-O2D-CED
25	b2	613	CLA	C2A-CAA-CBA-CGA
29	c2	519	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	C2	506	CLA	C8-C10-C11-C12
25	c1	506	CLA	O1A-CGA-O2A-C1
25	b1	607	CLA	O1D-CGD-O2D-CED
25	B1	619	CLA	C1A-C2A-CAA-CBA
25	C1	502	CLA	C1A-C2A-CAA-CBA
25	C1	512	CLA	C1A-C2A-CAA-CBA
25	a1	404	CLA	C1A-C2A-CAA-CBA
25	c1	503	CLA	C1A-C2A-CAA-CBA
25	c1	505	CLA	C1A-C2A-CAA-CBA
25	c1	515	CLA	C1A-C2A-CAA-CBA
25	A2	403	CLA	C1A-C2A-CAA-CBA
25	A2	404	CLA	C1A-C2A-CAA-CBA
25	a2	405	CLA	C1A-C2A-CAA-CBA
25	b2	620	CLA	C1A-C2A-CAA-CBA
25	c2	502	CLA	C1A-C2A-CAA-CBA
25	B1	610	CLA	C16-C17-C18-C19
25	B1	615	CLA	C16-C17-C18-C19
25	B1	619	CLA	C16-C17-C18-C19
25	C1	502	CLA	C16-C17-C18-C20
25	c1	506	CLA	C16-C17-C18-C19
25	c1	510	CLA	C16-C17-C18-C20
34	c2	514	DGD	C2B-C1B-O2G-C2G
29	j2	101	LMG	C41-C42-C43-C44
33	D2	405	LHG	C13-C14-C15-C16
25	c1	513	CLA	C5-C6-C7-C8
25	b2	611	CLA	C15-C16-C17-C18
35	m2	104	LMT	C1-C2-C3-C4
33	B2	627	LHG	C3-O3-P-O6
33	D2	403	LHG	C3-O3-P-O6
33	d1	407	LHG	C14-C15-C16-C17
33	D2	405	LHG	C11-C12-C13-C14
34	c2	517	DGD	C4A-C5A-C6A-C7A
25	d1	406	CLA	C10-C11-C12-C13
25	B2	609	CLA	C10-C11-C12-C13
25	D2	406	CLA	C10-C11-C12-C13
25	C2	505	CLA	CBA-CGA-O2A-C1
33	D2	405	LHG	O6-C4-C5-C6
25	A1	403	CLA	O1D-CGD-O2D-CED
34	H1	101	DGD	O6E-C5E-C6E-O5E
38	v2	201	HEM	C3D-CAD-CBD-CGD
25	c1	503	CLA	C16-C17-C18-C20
25	C2	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	D2	403	LHG	C7-C8-C9-C10
25	c2	509	CLA	CBA-CGA-O2A-C1
29	d1	408	LMG	O6-C5-C6-O5
33	B1	621	LHG	C1-C2-C3-O3
29	b1	621	LMG	C4-C5-C6-O5
25	A1	403	CLA	C15-C16-C17-C18
25	B1	605	CLA	C13-C15-C16-C17
34	h1	101	DGD	CAA-CBA-CCA-CDA
25	D1	403	CLA	O1A-CGA-O2A-C1
25	d1	404	CLA	O1A-CGA-O2A-C1
33	d1	407	LHG	C33-C34-C35-C36
25	B1	606	CLA	C16-C17-C18-C19
29	a2	412	LMG	C7-C8-C9-O8
33	A2	405	LHG	C4-C5-C6-O8
35	a2	406	LMT	C3-C4-C5-C6
25	B1	617	CLA	C8-C10-C11-C12
29	b1	631	LMG	C15-C16-C17-C18
33	L2	101	LHG	C11-C10-C9-C8
29	j2	101	LMG	O6-C5-C6-O5
35	m2	103	LMT	O5B-C5B-C6B-O6B
25	b2	617	CLA	C15-C16-C17-C18
25	c2	509	CLA	C8-C10-C11-C12
35	a2	406	LMT	O5B-C5B-C6B-O6B
25	c1	505	CLA	O1A-CGA-O2A-C1
25	C2	504	CLA	CBA-CGA-O2A-C1
25	B1	612	CLA	C13-C15-C16-C17
34	c1	518	DGD	O6E-C5E-C6E-O5E
32	B1	620	GOL	O1-C1-C2-O2
32	C1	518	GOL	O1-C1-C2-O2
32	b1	618	GOL	O2-C2-C3-O3
32	a2	415	GOL	O1-C1-C2-O2
34	c1	514	DGD	C6B-C7B-C8B-C9B
25	b2	608	CLA	C10-C11-C12-C13
33	l1	102	LHG	C9-C10-C11-C12
25	b1	604	CLA	C13-C15-C16-C17
25	B2	615	CLA	C10-C11-C12-C13
29	a1	412	LMG	O6-C5-C6-O5
29	d2	407	LMG	O6-C5-C6-O5
34	h2	102	DGD	O6E-C5E-C6E-O5E
35	M1	103	LMT	O5'-C5'-C6'-O6'
25	c2	515	CLA	O1A-CGA-O2A-C1
25	b1	611	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A1	412	LMG	C28-C29-C30-C31
33	L2	101	LHG	C23-C24-C25-C26
25	C2	509	CLA	C16-C17-C18-C19
25	B1	617	CLA	CBD-CGD-O2D-CED
25	c1	511	CLA	CBD-CGD-O2D-CED
25	C1	511	CLA	C8-C10-C11-C12
25	a2	405	CLA	C10-C11-C12-C13
34	c2	514	DGD	C4D-C5D-C6D-O5D
35	b2	621	LMT	O5'-C5'-C6'-O6'
25	C1	514	CLA	C2A-CAA-CBA-CGA
25	B2	612	CLA	C2A-CAA-CBA-CGA
25	C1	507	CLA	C2-C1-O2A-CGA
34	C1	515	DGD	C6B-C7B-C8B-C9B
25	c1	512	CLA	O1D-CGD-O2D-CED
33	d2	403	LHG	C31-C32-C33-C34
25	C1	513	CLA	CBA-CGA-O2A-C1
25	A2	404	CLA	CBA-CGA-O2A-C1
25	D2	406	CLA	CBA-CGA-O2A-C1
25	c2	509	CLA	O1A-CGA-O2A-C1
25	a2	405	CLA	O1D-CGD-O2D-CED
25	a2	405	CLA	C8-C10-C11-C12
25	b1	609	CLA	C3-C5-C6-C7
25	B1	619	CLA	C5-C6-C7-C8
29	b1	631	LMG	C2-C1-O1-C7
29	B2	621	LMG	O7-C8-C9-O8
35	M1	103	LMT	O1'-C1-C2-C3
33	B2	627	LHG	O9-C7-O7-C5
25	C2	505	CLA	O1A-CGA-O2A-C1
33	B1	621	LHG	C7-C8-C9-C10
33	b1	622	LHG	C7-C8-C9-C10
25	B1	613	CLA	C4-C3-C5-C6
36	d2	409	PL9	C40-C39-C41-C42
25	A1	405	CLA	C2C-C3C-CAC-CBC
33	b1	622	LHG	C12-C13-C14-C15
25	B1	606	CLA	C11-C12-C13-C15
25	B1	613	CLA	C11-C10-C8-C7
25	B1	617	CLA	C11-C12-C13-C15
25	B1	617	CLA	C12-C13-C15-C16
25	C1	506	CLA	C12-C13-C15-C16
25	C1	510	CLA	C11-C12-C13-C15
25	b1	604	CLA	C6-C7-C8-C10
25	b1	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b1	608	CLA	C11-C10-C8-C7
25	b1	614	CLA	C11-C12-C13-C15
25	b1	616	CLA	C12-C13-C15-C16
25	b1	620	CLA	C12-C13-C15-C16
25	c1	503	CLA	C12-C13-C15-C16
25	c1	506	CLA	C11-C12-C13-C15
25	c1	511	CLA	C11-C10-C8-C7
25	c1	512	CLA	C6-C7-C8-C10
25	B2	614	CLA	C11-C12-C13-C15
25	B2	614	CLA	C12-C13-C15-C16
25	B2	619	CLA	C6-C7-C8-C10
25	C2	503	CLA	C12-C13-C15-C16
25	C2	509	CLA	C11-C12-C13-C15
25	a2	405	CLA	C6-C7-C8-C10
25	b2	612	CLA	C11-C12-C13-C15
25	b2	618	CLA	C12-C13-C15-C16
25	b2	619	CLA	C11-C10-C8-C7
25	c2	505	CLA	C11-C12-C13-C15
25	c2	509	CLA	C11-C12-C13-C15
25	c2	512	CLA	C11-C12-C13-C15
27	A2	407	PHO	C6-C7-C8-C10
25	C1	505	CLA	C3-C5-C6-C7
25	C2	509	CLA	C3-C5-C6-C7
25	b2	612	CLA	C3-C5-C6-C7
25	B1	606	CLA	C6-C7-C8-C9
25	B1	608	CLA	C11-C10-C8-C9
25	B1	615	CLA	C11-C10-C8-C9
25	B1	617	CLA	C14-C13-C15-C16
25	C1	502	CLA	C11-C12-C13-C14
25	C1	506	CLA	C14-C13-C15-C16
25	C1	511	CLA	C14-C13-C15-C16
25	b1	604	CLA	C6-C7-C8-C9
25	b1	607	CLA	C11-C12-C13-C14
25	b1	614	CLA	C11-C12-C13-C14
25	b1	620	CLA	C14-C13-C15-C16
25	c1	507	CLA	C14-C13-C15-C16
25	c1	511	CLA	C11-C10-C8-C9
25	c1	512	CLA	C6-C7-C8-C9
25	B2	608	CLA	C11-C12-C13-C14
25	B2	614	CLA	C11-C12-C13-C14
25	C2	503	CLA	C14-C13-C15-C16
25	C2	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	D2	406	CLA	C11-C10-C8-C9
25	D2	406	CLA	C11-C12-C13-C14
25	b2	611	CLA	C14-C13-C15-C16
25	b2	618	CLA	C14-C13-C15-C16
25	c2	502	CLA	C14-C13-C15-C16
25	c2	509	CLA	C11-C12-C13-C14
33	L1	101	LHG	C11-C12-C13-C14
33	d1	407	LHG	C9-C10-C11-C12
25	A1	404	CLA	CBA-CGA-O2A-C1
25	C2	503	CLA	C8-C10-C11-C12
25	C1	506	CLA	C2A-CAA-CBA-CGA
34	h2	102	DGD	C3B-C4B-C5B-C6B
25	B1	606	CLA	C16-C17-C18-C20
33	L1	101	LHG	C11-C10-C9-C8
25	C1	503	CLA	C3-C5-C6-C7
25	B1	608	CLA	C15-C16-C17-C18
25	B2	617	CLA	C10-C11-C12-C13
29	j2	101	LMG	C11-C10-O7-C8
25	c2	513	CLA	C6-C7-C8-C9
37	b2	605	SQD	C11-C10-C9-C8
25	A1	406	CLA	CBA-CGA-O2A-C1
25	B2	619	CLA	C10-C11-C12-C13
25	c2	509	CLA	C15-C16-C17-C18
34	h1	101	DGD	O2G-C1B-C2B-C3B
25	b1	604	CLA	C4B-C3B-CAB-CBB
25	B2	604	CLA	C4B-C3B-CAB-CBB
25	C2	510	CLA	C4B-C3B-CAB-CBB
25	a2	405	CLA	C4B-C3B-CAB-CBB
25	b2	604	CLA	C4B-C3B-CAB-CBB
25	b2	608	CLA	C4B-C3B-CAB-CBB
25	b2	618	CLA	C4B-C3B-CAB-CBB
25	c1	516	CLA	C16-C17-C18-C19
25	b1	604	CLA	C5-C6-C7-C8
25	b2	616	CLA	C10-C11-C12-C13
33	L1	101	LHG	O6-C4-C5-C6
33	d1	407	LHG	O6-C4-C5-C6
33	l1	102	LHG	O6-C4-C5-C6
33	a2	407	LHG	O6-C4-C5-C6
33	d2	403	LHG	O6-C4-C5-C6
33	l2	101	LHG	O6-C4-C5-C6
35	a2	406	LMT	C4-C5-C6-C7
25	c2	504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C1	510	CLA	C13-C15-C16-C17
25	A2	403	CLA	C10-C11-C12-C13
25	B1	613	CLA	C2-C3-C5-C6
25	C1	506	CLA	C2-C3-C5-C6
36	d2	409	PL9	C38-C39-C41-C42
38	f1	101	HEM	C1A-C2A-CAA-CBA
25	C1	506	CLA	O1D-CGD-O2D-CED
33	a1	407	LHG	O2-C2-C3-O3
33	d1	402	LHG	O9-C7-O7-C5
25	C1	513	CLA	C14-C13-C15-C16
25	D2	404	CLA	C14-C13-C15-C16
33	b1	622	LHG	C18-C19-C20-C21
25	C1	512	CLA	CBA-CGA-O2A-C1
25	a2	413	CLA	CBA-CGA-O2A-C1
29	c1	519	LMG	C10-C11-C12-C13
25	C1	513	CLA	O1A-CGA-O2A-C1
25	A1	406	CLA	C3A-C2A-CAA-CBA
25	C1	507	CLA	C3A-C2A-CAA-CBA
25	A2	404	CLA	C3A-C2A-CAA-CBA
25	D2	406	CLA	C3A-C2A-CAA-CBA
25	b2	620	CLA	C3A-C2A-CAA-CBA
33	L2	101	LHG	C11-C12-C13-C14
34	C1	516	DGD	C4B-C5B-C6B-C7B
37	b2	605	SQD	C24-C25-C26-C27
25	c1	506	CLA	C10-C11-C12-C13
25	d2	402	CLA	CBA-CGA-O2A-C1
29	a1	412	LMG	C7-C8-C9-O8
33	d1	402	LHG	C4-C5-C6-O8
34	H1	101	DGD	O1G-C1G-C2G-C3G
34	h2	102	DGD	O1G-C1G-C2G-C3G
37	b2	605	SQD	C44-C45-C46-O48
33	D2	405	LHG	C30-C31-C32-C33
25	D1	402	CLA	O2A-C1-C2-C3
25	B2	614	CLA	C13-C15-C16-C17
34	C1	516	DGD	O6D-C5D-C6D-O5D
29	b1	631	LMG	O8-C28-C29-C30
25	B1	615	CLA	C4-C3-C5-C6
25	K2	101	CLA	C6-C7-C8-C9
25	b1	611	CLA	C2-C3-C5-C6
25	C1	508	CLA	O1D-CGD-O2D-CED
34	c1	518	DGD	O6D-C5D-C6D-O5D
27	A1	408	PHO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	L1	101	LHG	C3-O3-P-O6
35	m1	101	LMT	O1'-C1-C2-C3
25	b1	609	CLA	O1D-CGD-O2D-CED
25	D2	406	CLA	C3-C5-C6-C7
33	d2	403	LHG	O1-C1-C2-O2
25	b1	619	CLA	C15-C16-C17-C18
33	D2	405	LHG	C32-C33-C34-C35
33	A2	405	LHG	O6-C4-C5-O7
33	D2	405	LHG	O6-C4-C5-O7
33	a2	407	LHG	O6-C4-C5-O7
33	d2	403	LHG	O6-C4-C5-O7
25	b2	624	CLA	CBA-CGA-O2A-C1
33	L2	101	LHG	C10-C11-C12-C13
25	b2	615	CLA	C11-C12-C13-C15
25	B2	604	CLA	C2B-C3B-CAB-CBB
25	a2	405	CLA	C2B-C3B-CAB-CBB
34	c1	518	DGD	C3B-C4B-C5B-C6B
25	b2	620	CLA	C5-C6-C7-C8
25	A2	404	CLA	O1A-CGA-O2A-C1
25	D2	406	CLA	O1A-CGA-O2A-C1
29	A1	412	LMG	O7-C8-C9-O8
29	B1	626	LMG	O7-C8-C9-O8
29	a2	412	LMG	O7-C8-C9-O8
33	A2	405	LHG	O7-C5-C6-O8
25	b2	609	CLA	CBD-CGD-O2D-CED
27	a1	411	PHO	C13-C15-C16-C17
25	B2	619	CLA	C8-C10-C11-C12
33	B1	621	LHG	C31-C32-C33-C34
34	c2	514	DGD	O1B-C1B-O2G-C2G
25	c1	507	CLA	C2-C1-O2A-CGA
25	c2	507	CLA	C2-C1-O2A-CGA
33	L2	101	LHG	C15-C16-C17-C18
25	c1	512	CLA	C10-C11-C12-C13
25	B1	605	CLA	C14-C13-C15-C16
25	B1	609	CLA	C11-C10-C8-C9
25	B1	614	CLA	C6-C7-C8-C9
25	C1	509	CLA	C6-C7-C8-C9
25	b1	606	CLA	C14-C13-C15-C16
25	b1	613	CLA	C11-C12-C13-C14
25	b1	615	CLA	C11-C10-C8-C9
25	c1	507	CLA	C11-C12-C13-C14
25	d1	406	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B2	607	CLA	C6-C7-C8-C9
25	b2	609	CLA	C11-C10-C8-C9
25	b2	616	CLA	C6-C7-C8-C9
25	b2	620	CLA	C14-C13-C15-C16
25	d2	402	CLA	C11-C10-C8-C9
33	D1	404	LHG	C30-C31-C32-C33
25	b1	613	CLA	C5-C6-C7-C8
25	b2	611	CLA	C13-C15-C16-C17
25	A1	404	CLA	C4-C3-C5-C6
25	C2	509	CLA	C2A-CAA-CBA-CGA
25	A1	403	CLA	C16-C17-C18-C19
25	C1	509	CLA	C16-C17-C18-C19
23	A1	401	BCR	C23-C24-C25-C26
23	D1	401	BCR	C23-C24-C25-C26
23	H1	102	BCR	C1-C6-C7-C8
23	H1	102	BCR	C5-C6-C7-C8
23	b1	603	BCR	C1-C6-C7-C8
23	d1	405	BCR	C23-C24-C25-C26
23	h1	102	BCR	C23-C24-C25-C26
23	B2	603	BCR	C23-C24-C25-C26
23	a2	402	BCR	C23-C24-C25-C26
23	a2	402	BCR	C23-C24-C25-C30
23	d2	401	BCR	C1-C6-C7-C8
25	C1	503	CLA	C8-C10-C11-C12
25	B2	617	CLA	C8-C10-C11-C12
25	b2	624	CLA	C13-C15-C16-C17
25	c1	508	CLA	C2C-C3C-CAC-CBC
29	b1	621	LMG	C34-C35-C36-C37
29	b1	624	LMG	C32-C33-C34-C35
25	a1	403	CLA	O1D-CGD-O2D-CED
25	c2	509	CLA	O1D-CGD-O2D-CED
23	K1	101	BCR	C17-C18-C19-C20
25	B1	604	CLA	C1A-C2A-CAA-CBA
25	B1	615	CLA	C15-C16-C17-C18
25	c2	510	CLA	O1D-CGD-O2D-CED
34	h1	101	DGD	C6B-C7B-C8B-C9B
25	c1	513	CLA	C11-C12-C13-C15
25	b2	608	CLA	C5-C6-C7-C8
34	H1	101	DGD	C3B-C4B-C5B-C6B
25	C1	510	CLA	C8-C10-C11-C12
25	b2	606	CLA	C8-C10-C11-C12
33	D1	405	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	d1	402	LHG	O6-C4-C5-C6
29	d2	407	LMG	C28-C29-C30-C31
33	l2	101	LHG	C25-C26-C27-C28
25	A1	403	CLA	C11-C12-C13-C15
25	B1	606	CLA	C6-C7-C8-C10
25	B1	613	CLA	C11-C12-C13-C15
25	B1	614	CLA	C11-C10-C8-C7
25	B1	614	CLA	C11-C12-C13-C15
25	B1	617	CLA	C11-C10-C8-C7
25	B1	619	CLA	C12-C13-C15-C16
25	C1	508	CLA	C6-C7-C8-C10
25	C1	511	CLA	C12-C13-C15-C16
25	b1	607	CLA	C11-C12-C13-C15
25	b1	620	CLA	C11-C10-C8-C7
25	c1	506	CLA	C12-C13-C15-C16
25	c1	507	CLA	C12-C13-C15-C16
25	c1	509	CLA	C11-C12-C13-C15
25	c1	511	CLA	C11-C12-C13-C15
25	d1	406	CLA	C11-C12-C13-C15
25	A2	403	CLA	C11-C12-C13-C15
25	B2	606	CLA	C11-C10-C8-C7
25	B2	607	CLA	C6-C7-C8-C10
25	B2	610	CLA	C12-C13-C15-C16
25	B2	613	CLA	C11-C12-C13-C15
25	B2	619	CLA	C12-C13-C15-C16
25	C2	506	CLA	C12-C13-C15-C16
25	b2	608	CLA	C11-C12-C13-C15
25	b2	609	CLA	C11-C10-C8-C7
25	b2	614	CLA	C11-C10-C8-C7
25	b2	614	CLA	C11-C12-C13-C15
25	b2	617	CLA	C11-C10-C8-C7
25	b2	620	CLA	C6-C7-C8-C10
25	b2	620	CLA	C12-C13-C15-C16
25	b2	624	CLA	C11-C10-C8-C7
25	c2	505	CLA	C12-C13-C15-C16
25	c2	508	CLA	C11-C10-C8-C7
25	c2	508	CLA	C11-C12-C13-C15
25	c2	511	CLA	C6-C7-C8-C10
25	c2	512	CLA	C12-C13-C15-C16
29	C1	520	LMG	C30-C31-C32-C33
33	D2	405	LHG	C11-C10-C9-C8
33	a2	407	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	c2	501	BCR	C15-C16-C17-C18
25	c1	516	CLA	C16-C17-C18-C20
25	b2	615	CLA	C11-C12-C13-C14
27	a2	416	PHO	C16-C17-C18-C19
29	j2	101	LMG	O9-C10-O7-C8
34	c2	516	DGD	C1A-C2A-C3A-C4A
25	A1	404	CLA	O1A-CGA-O2A-C1
25	c1	516	CLA	C2A-CAA-CBA-CGA
25	c2	506	CLA	C2A-CAA-CBA-CGA
34	h1	101	DGD	CBB-CCB-CDB-CEB
25	A1	405	CLA	CBA-CGA-O2A-C1
25	B2	611	CLA	CBA-CGA-O2A-C1
25	b2	614	CLA	CBA-CGA-O2A-C1
25	B2	613	CLA	C8-C10-C11-C12
25	b2	606	CLA	C5-C6-C7-C8
25	B1	615	CLA	CAD-CBD-CGD-O2D
25	B1	616	CLA	CAD-CBD-CGD-O2D
25	C1	513	CLA	CAD-CBD-CGD-O2D
25	b1	614	CLA	CAD-CBD-CGD-O2D
25	c1	512	CLA	CAD-CBD-CGD-O2D
25	c1	516	CLA	CAD-CBD-CGD-O2D
25	B2	606	CLA	CAD-CBD-CGD-O2D
25	C2	504	CLA	CAD-CBD-CGD-O2D
25	C2	506	CLA	CAD-CBD-CGD-O2D
25	C2	510	CLA	CAD-CBD-CGD-O2D
25	b2	615	CLA	CAD-CBD-CGD-O2D
25	c2	502	CLA	CAD-CBD-CGD-O2D
27	d1	403	PHO	CAD-CBD-CGD-O2D
29	c1	519	LMG	C9-C8-O7-C10
34	C1	517	DGD	C6B-C7B-C8B-C9B
25	B1	616	CLA	C8-C10-C11-C12
25	B2	608	CLA	C16-C17-C18-C19
29	b1	631	LMG	O6-C1-O1-C7
29	B2	621	LMG	O6-C1-O1-C7
37	B2	623	SQD	O5-C1-O6-C44
25	c1	512	CLA	C8-C10-C11-C12
36	D2	408	PL9	C9-C11-C12-C13
29	A1	410	LMG	O1-C7-C8-C9
29	B1	626	LMG	O1-C7-C8-C9
29	C1	520	LMG	C7-C8-C9-O8
29	a1	412	LMG	O1-C7-C8-C9
29	c1	519	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	D1	404	LHG	C4-C5-C6-O8
33	D1	405	LHG	O6-C4-C5-O7
33	l1	102	LHG	O6-C4-C5-O7
25	B1	610	CLA	C13-C15-C16-C17
25	b1	619	CLA	C5-C6-C7-C8
34	c1	514	DGD	CBB-CCB-CDB-CEB
38	E1	101	HEM	C4B-C3B-CAB-CBB
38	V1	201	HEM	C4C-C3C-CAC-CBC
38	f1	101	HEM	C4B-C3B-CAB-CBB
38	v1	201	HEM	C4C-C3C-CAC-CBC
38	E2	101	HEM	C4B-C3B-CAB-CBB
38	V2	201	HEM	C4B-C3B-CAB-CBB
38	V2	201	HEM	C4C-C3C-CAC-CBC
38	e2	101	HEM	C4B-C3B-CAB-CBB
38	v2	201	HEM	C4C-C3C-CAC-CBC
25	C1	509	CLA	C16-C17-C18-C20
25	B1	605	CLA	CHA-CBD-CGD-O1D
25	B1	605	CLA	CHA-CBD-CGD-O2D
25	B1	608	CLA	CHA-CBD-CGD-O1D
25	C1	502	CLA	CHA-CBD-CGD-O1D
25	C1	512	CLA	CHA-CBD-CGD-O1D
25	C1	512	CLA	CHA-CBD-CGD-O2D
25	a1	405	CLA	CHA-CBD-CGD-O1D
25	a1	405	CLA	CHA-CBD-CGD-O2D
25	b1	609	CLA	CHA-CBD-CGD-O1D
25	b1	609	CLA	CHA-CBD-CGD-O2D
25	c1	506	CLA	CHA-CBD-CGD-O1D
25	c1	506	CLA	CHA-CBD-CGD-O2D
25	B2	605	CLA	CHA-CBD-CGD-O2D
25	B2	608	CLA	CHA-CBD-CGD-O1D
25	B2	608	CLA	CHA-CBD-CGD-O2D
25	C2	506	CLA	CHA-CBD-CGD-O1D
25	C2	508	CLA	CHA-CBD-CGD-O1D
25	C2	508	CLA	CHA-CBD-CGD-O2D
25	C2	511	CLA	CHA-CBD-CGD-O1D
25	C2	511	CLA	CHA-CBD-CGD-O2D
25	b2	604	CLA	CHA-CBD-CGD-O2D
25	b2	613	CLA	CHA-CBD-CGD-O1D
25	b2	613	CLA	CHA-CBD-CGD-O2D
25	b2	614	CLA	CHA-CBD-CGD-O1D
25	b2	616	CLA	CHA-CBD-CGD-O1D
25	c2	503	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	c2	503	CLA	CHA-CBD-CGD-O2D
25	c2	504	CLA	CHA-CBD-CGD-O1D
25	c2	504	CLA	CHA-CBD-CGD-O2D
25	c2	508	CLA	CHA-CBD-CGD-O1D
25	c2	508	CLA	CHA-CBD-CGD-O2D
25	A1	406	CLA	O1A-CGA-O2A-C1
25	C1	512	CLA	O1A-CGA-O2A-C1
25	a2	413	CLA	O1A-CGA-O2A-C1
25	b2	624	CLA	O1A-CGA-O2A-C1
25	c2	504	CLA	O1A-CGA-O2A-C1
34	C1	515	DGD	C7B-C8B-C9B-CAB
34	h2	102	DGD	O1G-C1G-C2G-O2G
29	B1	626	LMG	C14-C15-C16-C17
25	d2	402	CLA	O1A-CGA-O2A-C1
32	a1	406	GOL	O1-C1-C2-O2
32	c1	521	GOL	O1-C1-C2-O2
32	c2	518	GOL	O1-C1-C2-O2
34	c2	514	DGD	C2B-C3B-C4B-C5B
25	A1	403	CLA	C11-C12-C13-C14
25	B1	614	CLA	C11-C12-C13-C14
25	B1	619	CLA	C14-C13-C15-C16
25	c1	511	CLA	C11-C12-C13-C14
25	c1	516	CLA	C11-C12-C13-C14
25	B2	619	CLA	C14-C13-C15-C16
25	b2	614	CLA	C11-C12-C13-C14
25	c2	503	CLA	C14-C13-C15-C16
25	c2	505	CLA	C14-C13-C15-C16
34	C1	516	DGD	C4D-C5D-C6D-O5D
25	B2	611	CLA	O1A-CGA-O2A-C1
25	b2	616	CLA	C8-C10-C11-C12
23	J1	101	BCR	C17-C18-C19-C20
35	l1	101	LMT	O1'-C1-C2-C3
25	C1	514	CLA	C1A-C2A-CAA-CBA
25	c1	516	CLA	C1A-C2A-CAA-CBA
25	D2	401	CLA	C1A-C2A-CAA-CBA
25	D2	406	CLA	C1A-C2A-CAA-CBA
25	c2	515	CLA	C1A-C2A-CAA-CBA
34	c1	518	DGD	C4D-C5D-C6D-O5D
25	C1	512	CLA	C2-C1-O2A-CGA
25	B2	609	CLA	CBD-CGD-O2D-CED
25	c1	512	CLA	CBA-CGA-O2A-C1
29	B2	621	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	d1	404	CLA	C15-C16-C17-C18
33	D2	405	LHG	C3-O3-P-O6
33	L2	101	LHG	C4-O6-P-O3
33	a2	407	LHG	C3-O3-P-O6
33	b2	625	LHG	C3-O3-P-O6
33	d2	403	LHG	C3-O3-P-O6
34	c2	517	DGD	C2B-C3B-C4B-C5B
34	C1	516	DGD	C4E-C5E-C6E-O5E
25	B1	617	CLA	O1D-CGD-O2D-CED
25	B1	604	CLA	C4B-C3B-CAB-CBB
25	B1	608	CLA	C4B-C3B-CAB-CBB
25	b1	608	CLA	C4B-C3B-CAB-CBB
25	b1	620	CLA	C4B-C3B-CAB-CBB
25	B2	606	CLA	C4B-C3B-CAB-CBB
25	B2	616	CLA	C4B-C3B-CAB-CBB
25	C2	513	CLA	C4B-C3B-CAB-CBB
25	b2	611	CLA	C4B-C3B-CAB-CBB
25	d2	404	CLA	C4B-C3B-CAB-CBB
33	D1	404	LHG	C3-O3-P-O4
33	L1	101	LHG	C3-O3-P-O5
33	a1	407	LHG	C3-O3-P-O4
33	a1	407	LHG	C4-O6-P-O5
33	d1	402	LHG	C3-O3-P-O4
33	d1	402	LHG	C4-O6-P-O4
33	A2	405	LHG	C3-O3-P-O4
33	B2	627	LHG	C4-O6-P-O4
33	D2	403	LHG	C3-O3-P-O5
33	d2	403	LHG	C4-O6-P-O4
25	C1	508	CLA	C16-C17-C18-C19
25	b1	617	CLA	C16-C17-C18-C20
25	a2	405	CLA	C16-C17-C18-C19
25	c2	508	CLA	C16-C17-C18-C20
25	B2	605	CLA	C8-C10-C11-C12
25	B1	613	CLA	CBA-CGA-O2A-C1
25	b1	619	CLA	CBA-CGA-O2A-C1
36	d1	409	PL9	C9-C11-C12-C13
36	d1	409	PL9	C44-C46-C47-C48
25	c2	507	CLA	C6-C7-C8-C9
25	C1	502	CLA	C2A-CAA-CBA-CGA
25	c1	515	CLA	C3-C5-C6-C7
25	C1	502	CLA	C15-C16-C17-C18
25	b2	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b2	614	CLA	O1A-CGA-O2A-C1
25	A1	403	CLA	C16-C17-C18-C20
34	c1	514	DGD	C8B-C9B-CAB-CBB
25	B1	604	CLA	CAD-CBD-CGD-O1D
25	C1	503	CLA	CAD-CBD-CGD-O1D
25	C1	507	CLA	CAD-CBD-CGD-O1D
25	b1	611	CLA	CAD-CBD-CGD-O1D
25	c1	506	CLA	CAD-CBD-CGD-O1D
25	A2	404	CLA	C2-C3-C5-C6
25	B2	608	CLA	CAD-CBD-CGD-O1D
25	C2	508	CLA	CAD-CBD-CGD-O1D
25	b2	617	CLA	CAD-CBD-CGD-O1D
34	C1	515	DGD	C1A-C2A-C3A-C4A
33	d2	406	LHG	C14-C15-C16-C17
34	H1	101	DGD	CCB-CDB-CEB-CFB
25	B1	613	CLA	O1A-CGA-O2A-C1
33	l1	102	LHG	C1-C2-C3-O3
33	D2	403	LHG	C1-C2-C3-O3
25	b1	615	CLA	C11-C12-C13-C14
25	C1	512	CLA	C16-C17-C18-C20
25	b1	607	CLA	C16-C17-C18-C19
25	a2	404	CLA	C16-C17-C18-C19
25	b2	606	CLA	C16-C17-C18-C19
25	B1	610	CLA	C6-C7-C8-C10
25	B1	611	CLA	C11-C12-C13-C15
25	B1	616	CLA	C11-C10-C8-C7
25	B1	619	CLA	C6-C7-C8-C10
25	C1	509	CLA	C11-C12-C13-C15
25	C1	511	CLA	C6-C7-C8-C10
25	D1	402	CLA	C11-C12-C13-C15
25	b1	608	CLA	C6-C7-C8-C10
25	c1	507	CLA	C11-C10-C8-C7
25	d1	401	CLA	C11-C12-C13-C15
25	d1	406	CLA	C6-C7-C8-C10
25	B2	610	CLA	C11-C12-C13-C15
25	B2	611	CLA	C6-C7-C8-C10
25	B2	617	CLA	C11-C10-C8-C7
25	D2	404	CLA	C11-C10-C8-C7
25	b2	624	CLA	C3A-C2A-CAA-CBA
25	c2	502	CLA	C11-C12-C13-C15
25	c2	504	CLA	C11-C10-C8-C7
25	c2	508	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	c2	508	CLA	C12-C13-C15-C16
25	d2	405	CLA	C11-C10-C8-C7
33	L1	101	LHG	O6-C4-C5-O7
33	d1	402	LHG	O6-C4-C5-O7
33	d1	407	LHG	O6-C4-C5-O7
33	l2	101	LHG	O6-C4-C5-O7
34	H1	101	DGD	C8A-C9A-CAA-CBA
25	C1	513	CLA	C3-C5-C6-C7
25	A1	405	CLA	O1A-CGA-O2A-C1
33	D1	405	LHG	C11-C10-C9-C8
25	b1	620	CLA	C13-C15-C16-C17
34	c2	517	DGD	CCB-CDB-CEB-CFB
25	b2	620	CLA	C2A-CAA-CBA-CGA
25	A1	406	CLA	C16-C17-C18-C19
25	b1	608	CLA	C16-C17-C18-C19
25	c2	503	CLA	C3-C5-C6-C7
29	B1	626	LMG	O1-C7-C8-O7
29	b1	624	LMG	O1-C7-C8-O7
29	c1	519	LMG	O1-C7-C8-O7
37	b2	605	SQD	O47-C45-C46-O48
29	C1	520	LMG	C33-C34-C35-C36
34	c1	520	DGD	C8A-C9A-CAA-CBA
25	B2	610	CLA	CBA-CGA-O2A-C1
34	C1	516	DGD	C3B-C4B-C5B-C6B
25	B1	609	CLA	C15-C16-C17-C18
25	c1	511	CLA	O1D-CGD-O2D-CED
25	b2	609	CLA	O1D-CGD-O2D-CED
25	b1	619	CLA	O1A-CGA-O2A-C1
25	c1	512	CLA	O1A-CGA-O2A-C1
25	B1	606	CLA	C11-C10-C8-C9
25	C1	508	CLA	C6-C7-C8-C9
25	b1	606	CLA	C11-C10-C8-C9
25	b1	612	CLA	C14-C13-C15-C16
25	b1	616	CLA	C14-C13-C15-C16
25	c1	506	CLA	C11-C10-C8-C9
25	c1	506	CLA	C14-C13-C15-C16
25	d1	404	CLA	C11-C12-C13-C14
25	B2	612	CLA	C14-C13-C15-C16
25	b2	608	CLA	C11-C12-C13-C14
25	c2	511	CLA	C6-C7-C8-C9
25	c2	512	CLA	C14-C13-C15-C16
27	a2	416	PHO	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c2	513	CLA	C3-C5-C6-C7
29	B2	620	LMG	C30-C31-C32-C33
25	B2	610	CLA	O1A-CGA-O2A-C1
23	J1	101	BCR	C18-C19-C20-C21
23	b1	602	BCR	C10-C11-C12-C13
23	c1	502	BCR	C18-C19-C20-C21
23	k1	101	BCR	C18-C19-C20-C21
23	F2	401	BCR	C18-C19-C20-C21
23	K2	102	BCR	C18-C19-C20-C21
23	c2	501	BCR	C18-C19-C20-C21
23	j2	102	BCR	C18-C19-C20-C21
23	J1	101	BCR	C7-C8-C9-C10
25	C1	503	CLA	C2B-C3B-CAB-CBB
25	C1	509	CLA	C2B-C3B-CAB-CBB
25	C1	514	CLA	C2B-C3B-CAB-CBB
25	b1	604	CLA	C2B-C3B-CAB-CBB
25	b1	620	CLA	C2B-C3B-CAB-CBB
25	c1	507	CLA	C2B-C3B-CAB-CBB
25	C2	510	CLA	C2B-C3B-CAB-CBB
25	b2	608	CLA	C2B-C3B-CAB-CBB
25	b2	618	CLA	C2B-C3B-CAB-CBB
25	d2	404	CLA	C2B-C3B-CAB-CBB
27	D2	407	PHO	C4-C3-C5-C6
25	B2	608	CLA	CBD-CGD-O2D-CED
33	d1	407	LHG	C11-C10-C9-C8
25	b2	614	CLA	C16-C17-C18-C19
25	c1	516	CLA	C5-C6-C7-C8
25	B2	619	CLA	C5-C6-C7-C8
37	b2	605	SQD	C46-C45-O47-C7
25	C1	509	CLA	O1A-CGA-O2A-C1
25	A2	402	CLA	CBA-CGA-O2A-C1
25	B2	608	CLA	O1D-CGD-O2D-CED
25	B2	607	CLA	C8-C10-C11-C12
25	d1	401	CLA	C2-C1-O2A-CGA
25	b2	614	CLA	C2-C1-O2A-CGA
27	A1	408	PHO	C2-C1-O2A-CGA
27	D2	407	PHO	C2-C1-O2A-CGA
25	C2	504	CLA	O1A-CGA-O2A-C1
25	K2	101	CLA	C2C-C3C-CAC-CBC
29	j2	101	LMG	C38-C39-C40-C41
34	C1	517	DGD	O6D-C5D-C6D-O5D
25	c2	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B2	612	CLA	CBA-CGA-O2A-C1
25	A2	402	CLA	O1A-CGA-O2A-C1
25	A2	402	CLA	C16-C17-C18-C19
25	B2	619	CLA	C13-C15-C16-C17
25	b1	619	CLA	C4-C3-C5-C6
23	A1	401	BCR	C23-C24-C25-C30
23	B1	602	BCR	C23-C24-C25-C26
23	d1	405	BCR	C23-C24-C25-C30
23	h1	102	BCR	C1-C6-C7-C8
23	h1	102	BCR	C23-C24-C25-C30
23	b2	602	BCR	C23-C24-C25-C26
23	h2	101	BCR	C23-C24-C25-C30
29	M1	101	LMG	C31-C32-C33-C34
33	b1	622	LHG	C11-C12-C13-C14
34	H2	101	DGD	C2B-C3B-C4B-C5B
25	C1	508	CLA	C16-C17-C18-C20
25	B2	612	CLA	O1A-CGA-O2A-C1
34	H1	101	DGD	O1G-C1G-C2G-O2G
34	h2	102	DGD	C4B-C5B-C6B-C7B
33	D1	405	LHG	C3-O3-P-O6
33	b1	622	LHG	C3-O3-P-O6
33	d1	407	LHG	C3-O3-P-O6
33	d2	406	LHG	C3-O3-P-O6
29	B1	626	LMG	C7-C8-C9-O8
33	L1	101	LHG	C12-C13-C14-C15
25	B1	612	CLA	C5-C6-C7-C8
25	b1	609	CLA	C11-C12-C13-C15
25	c1	516	CLA	C11-C12-C13-C15
25	D2	406	CLA	C11-C12-C13-C15
25	b2	611	CLA	C12-C13-C15-C16
25	b2	616	CLA	C6-C7-C8-C10
25	c2	502	CLA	C12-C13-C15-C16
25	B1	610	CLA	C6-C7-C8-C9
25	B1	615	CLA	C14-C13-C15-C16
25	B1	617	CLA	C11-C10-C8-C9
25	d1	406	CLA	C6-C7-C8-C9
25	A2	403	CLA	C11-C12-C13-C14
25	B2	610	CLA	C11-C12-C13-C14
25	C2	506	CLA	C14-C13-C15-C16
25	A1	406	CLA	C16-C17-C18-C20
25	b1	614	CLA	C16-C17-C18-C19
25	c2	508	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	A2	407	PHO	C16-C17-C18-C19
25	C2	505	CLA	C5-C6-C7-C8
33	B1	621	LHG	C25-C26-C27-C28
25	b2	617	CLA	C2A-CAA-CBA-CGA
33	D2	405	LHG	C12-C13-C14-C15
34	H2	101	DGD	C3B-C4B-C5B-C6B
25	b1	607	CLA	C16-C17-C18-C20
27	A1	408	PHO	C16-C17-C18-C19
33	a1	407	LHG	C12-C13-C14-C15
29	A1	412	LMG	C29-C28-O8-C9
34	C1	516	DGD	CBA-CCA-CDA-CEA
25	c1	516	CLA	C8-C10-C11-C12
25	C1	513	CLA	C12-C13-C15-C16
25	c2	506	CLA	C12-C13-C15-C16
29	I2	101	LMG	C11-C10-O7-C8
25	D2	404	CLA	C4-C3-C5-C6
25	b2	620	CLA	C4-C3-C5-C6
25	B1	615	CLA	C2-C3-C5-C6
33	b1	622	LHG	C13-C14-C15-C16
25	b1	617	CLA	C16-C17-C18-C19
25	C1	509	CLA	CBA-CGA-O2A-C1
25	a1	405	CLA	CBA-CGA-O2A-C1
34	c1	520	DGD	O6D-C5D-C6D-O5D
25	b1	616	CLA	O1A-CGA-O2A-C1
25	b1	616	CLA	CBA-CGA-O2A-C1
37	b2	605	SQD	C14-C15-C16-C17
25	C1	502	CLA	C4B-C3B-CAB-CBB
25	C1	503	CLA	C4B-C3B-CAB-CBB
25	C1	504	CLA	C4B-C3B-CAB-CBB
25	C1	509	CLA	C4B-C3B-CAB-CBB
25	C1	514	CLA	C4B-C3B-CAB-CBB
25	b1	612	CLA	C4B-C3B-CAB-CBB
25	c1	503	CLA	C4B-C3B-CAB-CBB
25	c1	507	CLA	C4B-C3B-CAB-CBB
25	d1	401	CLA	C4B-C3B-CAB-CBB
25	B2	609	CLA	C4B-C3B-CAB-CBB
25	c2	511	CLA	C4B-C3B-CAB-CBB
25	b1	609	CLA	C16-C17-C18-C19
25	a2	405	CLA	C16-C17-C18-C20
25	b2	606	CLA	C16-C17-C18-C20
25	c1	503	CLA	C15-C16-C17-C18
33	D2	403	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	I2	101	LMG	O9-C10-O7-C8
33	d2	406	LHG	O6-C4-C5-C6
34	C1	515	DGD	O1A-C1A-O1G-C1G
25	c1	515	CLA	CAA-CBA-CGA-O2A
25	c1	515	CLA	C5-C6-C7-C8
25	b2	612	CLA	C10-C11-C12-C13
33	b1	622	LHG	C28-C29-C30-C31
34	h1	101	DGD	C5B-C6B-C7B-C8B
29	B2	621	LMG	C19-C20-C21-C22
25	b2	608	CLA	CBA-CGA-O2A-C1
33	d2	403	LHG	C13-C14-C15-C16
33	l2	101	LHG	C26-C27-C28-C29
34	c2	517	DGD	CBB-CCB-CDB-CEB
34	H2	101	DGD	CCB-CDB-CEB-CFB
25	C1	511	CLA	C4-C3-C5-C6
25	B2	616	CLA	C4-C3-C5-C6
27	d1	403	PHO	C15-C16-C17-C18
25	b2	608	CLA	O1A-CGA-O2A-C1
25	A1	403	CLA	C2-C1-O2A-CGA
25	c1	515	CLA	C2-C1-O2A-CGA
25	a2	404	CLA	C2-C1-O2A-CGA
25	b2	615	CLA	C2-C1-O2A-CGA
34	c1	518	DGD	C8B-C9B-CAB-CBB
34	c1	514	DGD	CDB-CEB-CFB-CGB
25	C1	512	CLA	C10-C11-C12-C13
25	C1	510	CLA	C2A-CAA-CBA-CGA
25	b1	605	CLA	C2A-CAA-CBA-CGA
25	c2	502	CLA	C2A-CAA-CBA-CGA
33	L2	101	LHG	O7-C5-C6-O8
34	c1	514	DGD	C7B-C8B-C9B-CAB
25	d2	402	CLA	C3A-C2A-CAA-CBA
25	c1	513	CLA	C11-C12-C13-C14
34	c1	520	DGD	CBA-CCA-CDA-CEA
25	B1	614	CLA	CBA-CGA-O2A-C1
34	H1	101	DGD	C7A-C8A-C9A-CAA
34	H1	101	DGD	C6B-C7B-C8B-C9B
34	c2	514	DGD	CAA-CBA-CCA-CDA
25	B1	605	CLA	C6-C7-C8-C9
25	C1	505	CLA	C11-C12-C13-C14
25	C1	512	CLA	C6-C7-C8-C9
25	a1	404	CLA	C11-C10-C8-C9
25	b1	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B2	608	CLA	C11-C10-C8-C9
25	B2	611	CLA	C14-C13-C15-C16
25	B2	614	CLA	C11-C10-C8-C9
25	B2	615	CLA	C14-C13-C15-C16
25	a2	405	CLA	C11-C10-C8-C9
25	b2	606	CLA	C14-C13-C15-C16
25	c2	505	CLA	C11-C10-C8-C9
27	A1	408	PHO	C11-C10-C8-C9
25	B2	605	CLA	C13-C15-C16-C17
29	B1	626	LMG	C33-C34-C35-C36
34	H1	101	DGD	C9B-CAB-CBB-CCB
25	d2	405	CLA	C15-C16-C17-C18
23	J1	101	BCR	C20-C21-C22-C37
23	b1	602	BCR	C11-C10-C9-C34
23	c1	502	BCR	C20-C21-C22-C37
23	k1	101	BCR	C20-C21-C22-C37
23	F2	401	BCR	C20-C21-C22-C37
23	K2	102	BCR	C20-C21-C22-C37
23	c2	501	BCR	C16-C17-C18-C36
23	c2	501	BCR	C20-C21-C22-C37
23	j2	102	BCR	C20-C21-C22-C37
34	H2	101	DGD	O1G-C1G-C2G-C3G
38	v1	201	HEM	CAD-CBD-CGD-O2D
25	C1	508	CLA	C2A-CAA-CBA-CGA
33	L1	101	LHG	C9-C10-C11-C12
25	A2	402	CLA	C16-C17-C18-C20
25	d2	405	CLA	O2A-C1-C2-C3
33	D2	403	LHG	O2-C2-C3-O3
25	a1	404	CLA	CBA-CGA-O2A-C1
34	C1	515	DGD	C2A-C1A-O1G-C1G
35	C1	519	LMT	O5'-C1'-O1'-C1
25	B2	609	CLA	O1D-CGD-O2D-CED
29	B2	620	LMG	C29-C30-C31-C32
25	B1	610	CLA	C4-C3-C5-C6
25	A1	406	CLA	C1A-C2A-CAA-CBA
25	C1	504	CLA	C1A-C2A-CAA-CBA
25	C1	507	CLA	C1A-C2A-CAA-CBA
25	d1	406	CLA	C1A-C2A-CAA-CBA
25	B1	616	CLA	C12-C13-C15-C16
25	C1	503	CLA	C6-C7-C8-C10
25	C1	506	CLA	C11-C10-C8-C7
25	b1	611	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b1	619	CLA	C12-C13-C15-C16
25	d1	401	CLA	C12-C13-C15-C16
25	B2	613	CLA	C12-C13-C15-C16
25	B2	614	CLA	C6-C7-C8-C10
25	B2	619	CLA	C11-C10-C8-C7
25	c2	503	CLA	C6-C7-C8-C10
25	c2	512	CLA	C6-C7-C8-C10
25	b2	620	CLA	C8-C10-C11-C12
23	B1	602	BCR	C9-C10-C11-C12
23	h1	102	BCR	C9-C10-C11-C12
34	c1	520	DGD	CAA-CBA-CCA-CDA
33	b1	622	LHG	C4-O6-P-O3
33	L2	101	LHG	C3-O3-P-O6
25	b1	605	CLA	CAA-CBA-CGA-O2A
25	a1	405	CLA	O1A-CGA-O2A-C1
35	m1	101	LMT	C2-C3-C4-C5
25	C2	505	CLA	C2A-CAA-CBA-CGA
25	B1	614	CLA	C10-C11-C12-C13
25	c2	502	CLA	C15-C16-C17-C18
25	d2	402	CLA	C15-C16-C17-C18
38	v1	201	HEM	CAD-CBD-CGD-O1D
33	b1	622	LHG	C31-C32-C33-C34
29	j2	101	LMG	C15-C16-C17-C18
34	h1	101	DGD	C9B-CAB-CBB-CCB
33	A2	405	LHG	O6-C4-C5-C6
25	c2	508	CLA	C8-C10-C11-C12
25	C1	513	CLA	C4-C3-C5-C6
25	B1	606	CLA	C13-C15-C16-C17
25	b2	617	CLA	C8-C10-C11-C12
25	B1	604	CLA	C2B-C3B-CAB-CBB
25	B1	605	CLA	C2B-C3B-CAB-CBB
25	B1	608	CLA	C2B-C3B-CAB-CBB
25	C1	502	CLA	C2B-C3B-CAB-CBB
25	C1	504	CLA	C2B-C3B-CAB-CBB
25	b1	608	CLA	C2B-C3B-CAB-CBB
25	c1	509	CLA	C2B-C3B-CAB-CBB
25	d1	401	CLA	C2B-C3B-CAB-CBB
25	B2	606	CLA	C2B-C3B-CAB-CBB
25	B2	608	CLA	C2B-C3B-CAB-CBB
25	B2	609	CLA	C2B-C3B-CAB-CBB
25	B2	611	CLA	C2B-C3B-CAB-CBB
25	B2	616	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B2	617	CLA	C2B-C3B-CAB-CBB
25	C2	513	CLA	C2B-C3B-CAB-CBB
25	b2	611	CLA	C2B-C3B-CAB-CBB
25	c2	505	CLA	C2B-C3B-CAB-CBB
33	L2	101	LHG	C12-C13-C14-C15
23	J1	101	BCR	C20-C21-C22-C23
23	b1	602	BCR	C11-C10-C9-C8
23	c1	502	BCR	C20-C21-C22-C23
23	k1	101	BCR	C20-C21-C22-C23
23	F2	401	BCR	C20-C21-C22-C23
23	K2	102	BCR	C20-C21-C22-C23
23	c2	501	BCR	C16-C17-C18-C19
23	c2	501	BCR	C20-C21-C22-C23
23	j2	102	BCR	C20-C21-C22-C23
29	b1	621	LMG	O1-C7-C8-O7
37	D1	409	SQD	O6-C44-C45-O47
37	B2	623	SQD	O6-C44-C45-O47
34	c1	520	DGD	C9A-CAA-CBA-CCA
34	C1	516	DGD	CAA-CBA-CCA-CDA
25	d1	406	CLA	C13-C15-C16-C17
33	b1	622	LHG	C10-C11-C12-C13
25	B1	614	CLA	O1A-CGA-O2A-C1
33	a1	407	LHG	C1-C2-C3-O3
25	c2	504	CLA	C15-C16-C17-C18
36	D1	408	PL9	C35-C34-C36-C37
36	d1	409	PL9	C45-C44-C46-C47
36	d2	409	PL9	C35-C34-C36-C37
25	a1	403	CLA	C2-C1-O2A-CGA
25	b1	604	CLA	C2-C1-O2A-CGA
25	d1	406	CLA	C2-C1-O2A-CGA
27	A2	407	PHO	C2-C1-O2A-CGA
25	c2	511	CLA	C5-C6-C7-C8
25	b1	606	CLA	C11-C12-C13-C14
25	c1	512	CLA	C14-C13-C15-C16
25	b2	606	CLA	C11-C12-C13-C14
25	b2	617	CLA	C11-C12-C13-C14
35	l1	101	LMT	C1-C2-C3-C4
33	D1	405	LHG	C14-C15-C16-C17
34	H1	101	DGD	CBB-CCB-CDB-CEB
25	B2	616	CLA	C2A-CAA-CBA-CGA
25	B2	614	CLA	C16-C17-C18-C19
38	E1	101	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
34	h1	101	DGD	O1B-C1B-C2B-C3B
23	B1	602	BCR	C23-C24-C25-C30
23	B1	603	BCR	C23-C24-C25-C30
23	a1	401	BCR	C23-C24-C25-C30
23	b1	603	BCR	C23-C24-C25-C30
23	h1	102	BCR	C5-C6-C7-C8
23	B2	603	BCR	C23-C24-C25-C30
23	H2	103	BCR	C1-C6-C7-C8
23	K2	104	BCR	C23-C24-C25-C30
23	a2	402	BCR	C1-C6-C7-C8
23	b2	602	BCR	C23-C24-C25-C30
23	h2	101	BCR	C23-C24-C25-C26
33	B1	621	LHG	C11-C12-C13-C14
34	H1	101	DGD	O2G-C1B-C2B-C3B
33	d2	403	LHG	C16-C17-C18-C19
32	a1	406	GOL	O1-C1-C2-C3
29	a1	412	LMG	C12-C13-C14-C15
34	H1	101	DGD	C5B-C6B-C7B-C8B
23	j2	102	BCR	C17-C18-C19-C20
27	D2	407	PHO	C2-C3-C5-C6
25	B1	617	CLA	C5-C6-C7-C8
25	b1	606	CLA	C8-C10-C11-C12
29	d2	407	LMG	C8-C7-O1-C1
35	M1	102	LMT	C2-C3-C4-C5
25	b2	619	CLA	C11-C12-C13-C14
29	A1	412	LMG	O10-C28-O8-C9
25	B1	607	CLA	C11-C12-C13-C15
25	A1	406	CLA	C15-C16-C17-C18
33	L2	101	LHG	O6-C4-C5-O7
34	c2	514	DGD	C6A-C7A-C8A-C9A
25	B2	608	CLA	C2A-CAA-CBA-CGA
25	B2	605	CLA	CAA-CBA-CGA-O2A
25	C2	508	CLA	CBA-CGA-O2A-C1
34	C2	512	DGD	O6D-C5D-C6D-O5D
25	D2	404	CLA	C3-C5-C6-C7
25	B1	605	CLA	C4B-C3B-CAB-CBB
25	c1	509	CLA	C4B-C3B-CAB-CBB
25	d1	406	CLA	C4B-C3B-CAB-CBB
25	B2	608	CLA	C4B-C3B-CAB-CBB
25	B2	611	CLA	C4B-C3B-CAB-CBB
25	B2	617	CLA	C4B-C3B-CAB-CBB
25	C2	505	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	D2	401	CLA	C4B-C3B-CAB-CBB
25	c2	505	CLA	C4B-C3B-CAB-CBB
25	c2	506	CLA	C4B-C3B-CAB-CBB
25	c2	515	CLA	C4B-C3B-CAB-CBB
33	L2	101	LHG	O6-C4-C5-C6
25	C2	508	CLA	O1A-CGA-O2A-C1
36	D2	408	PL9	C25-C24-C26-C27
25	b1	612	CLA	C12-C13-C15-C16
25	c1	512	CLA	C12-C13-C15-C16
25	d1	404	CLA	C11-C12-C13-C15
25	B2	612	CLA	C11-C12-C13-C15
25	B2	612	CLA	C12-C13-C15-C16
25	C2	505	CLA	C12-C13-C15-C16
25	C2	509	CLA	C5-C6-C7-C8
33	d2	406	LHG	C33-C34-C35-C36
34	h1	101	DGD	C3B-C4B-C5B-C6B
33	a1	407	LHG	C28-C29-C30-C31
34	C1	517	DGD	C3B-C4B-C5B-C6B
38	f1	101	HEM	C3A-C2A-CAA-CBA
33	D2	405	LHG	O7-C7-C8-C9
34	h2	102	DGD	O2G-C1B-C2B-C3B
33	l1	102	LHG	C27-C28-C29-C30
29	j2	101	LMG	C42-C43-C44-C45
33	D1	404	LHG	O7-C5-C6-O8
37	D2	402	SQD	O47-C45-C46-O48
29	C1	520	LMG	C29-C28-O8-C9
25	b1	616	CLA	C15-C16-C17-C18
25	C1	502	CLA	C3-C5-C6-C7
25	C2	507	CLA	CAA-CBA-CGA-O2A
25	C2	516	CLA	CAA-CBA-CGA-O2A
34	c1	514	DGD	O2G-C1B-C2B-C3B
34	h2	102	DGD	C8A-C9A-CAA-CBA
25	B2	614	CLA	O1A-CGA-O2A-C1
33	d1	407	LHG	O7-C7-C8-C9
25	b2	619	CLA	C4-C3-C5-C6
36	D1	408	PL9	C25-C24-C26-C27
25	d2	402	CLA	C10-C11-C12-C13
25	d2	405	CLA	C5-C6-C7-C8
25	C1	513	CLA	C2-C3-C5-C6
25	b2	620	CLA	C2-C3-C5-C6
25	A2	403	CLA	C12-C13-C15-C16
25	D2	404	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C1	507	CLA	C6-C7-C8-C9
25	C1	509	CLA	C11-C12-C13-C14
25	C1	511	CLA	C6-C7-C8-C9
25	D1	402	CLA	C11-C12-C13-C14
25	b1	608	CLA	C6-C7-C8-C9
25	B2	610	CLA	C14-C13-C15-C16
25	B2	617	CLA	C11-C10-C8-C9
25	D2	404	CLA	C11-C12-C13-C14
25	a2	405	CLA	C14-C13-C15-C16
25	b2	614	CLA	C14-C13-C15-C16
25	c2	503	CLA	C11-C10-C8-C9
25	c2	508	CLA	C6-C7-C8-C9
25	c2	508	CLA	C14-C13-C15-C16
25	c2	512	CLA	C6-C7-C8-C9
38	V1	201	HEM	CAD-CBD-CGD-O2D
25	d1	401	CLA	C3A-C2A-CAA-CBA
25	C2	503	CLA	C3A-C2A-CAA-CBA
25	a2	413	CLA	C3A-C2A-CAA-CBA
34	H2	101	DGD	C6B-C7B-C8B-C9B
25	b2	610	CLA	O1A-CGA-O2A-C1
29	C1	520	LMG	O10-C28-O8-C9
25	B1	614	CLA	CAA-CBA-CGA-O2A
29	C1	520	LMG	O7-C10-C11-C12
29	B2	621	LMG	O7-C10-C11-C12
34	h2	102	DGD	C6B-C7B-C8B-C9B
25	B1	606	CLA	CAD-CBD-CGD-O2D
25	B1	609	CLA	CAD-CBD-CGD-O2D
25	B1	610	CLA	CAD-CBD-CGD-O2D
25	B1	619	CLA	CAD-CBD-CGD-O2D
25	C1	506	CLA	CAD-CBD-CGD-O2D
25	b1	606	CLA	CAD-CBD-CGD-O2D
25	b1	612	CLA	CAD-CBD-CGD-O2D
25	c1	503	CLA	CAD-CBD-CGD-O2D
25	c1	504	CLA	CAD-CBD-CGD-O2D
25	c1	507	CLA	CAD-CBD-CGD-O2D
25	A2	402	CLA	CAD-CBD-CGD-O2D
25	B2	604	CLA	CAD-CBD-CGD-O2D
25	B2	607	CLA	CAD-CBD-CGD-O2D
25	B2	609	CLA	CAD-CBD-CGD-O2D
25	B2	611	CLA	CAD-CBD-CGD-O2D
25	B2	612	CLA	CAD-CBD-CGD-O2D
25	B2	618	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	C2	507	CLA	CAD-CBD-CGD-O2D
25	b2	606	CLA	CAD-CBD-CGD-O2D
25	b2	608	CLA	CAD-CBD-CGD-O2D
25	b2	619	CLA	CAD-CBD-CGD-O2D
25	c2	515	CLA	CAD-CBD-CGD-O2D
27	A1	408	PHO	CAD-CBD-CGD-O2D
27	a2	416	PHO	CAD-CBD-CGD-O2D
25	b1	613	CLA	C10-C11-C12-C13
25	B2	606	CLA	C2A-CAA-CBA-CGA
25	c2	510	CLA	C2A-CAA-CBA-CGA
25	b1	605	CLA	C8-C10-C11-C12
25	c2	511	CLA	C2-C1-O2A-CGA
25	c1	512	CLA	CAA-CBA-CGA-O2A
25	D2	401	CLA	CAA-CBA-CGA-O2A
25	c2	511	CLA	CAA-CBA-CGA-O2A
33	l1	102	LHG	O7-C7-C8-C9
29	B2	621	LMG	C18-C19-C20-C21
25	b2	610	CLA	CBA-CGA-O2A-C1
34	c2	514	DGD	C3B-C4B-C5B-C6B
29	A2	412	LMG	O6-C1-O1-C7
25	A2	403	CLA	C14-C13-C15-C16
25	b2	609	CLA	C14-C13-C15-C16
29	A1	412	LMG	C7-C8-C9-O8
29	b1	624	LMG	O1-C7-C8-C9
33	d2	403	LHG	C28-C29-C30-C31
25	B2	614	CLA	CBA-CGA-O2A-C1
34	c2	517	DGD	O6D-C5D-C6D-O5D
29	A2	412	LMG	O7-C10-C11-C12
38	E1	101	HEM	CAA-CBA-CGA-O1A
35	m1	101	LMT	C7-C8-C9-C10
25	c1	515	CLA	O2A-C1-C2-C3
25	d1	401	CLA	O2A-C1-C2-C3
25	D2	401	CLA	O2A-C1-C2-C3
25	a2	404	CLA	O2A-C1-C2-C3
33	B1	621	LHG	C15-C16-C17-C18
33	B1	621	LHG	C28-C29-C30-C31
34	C1	517	DGD	C4A-C5A-C6A-C7A
25	b1	606	CLA	C2A-CAA-CBA-CGA
25	c2	515	CLA	C2A-CAA-CBA-CGA
25	B2	614	CLA	C10-C11-C12-C13
27	A2	407	PHO	C8-C10-C11-C12
25	C2	507	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	b1	614	CLA	C16-C17-C18-C20
25	B2	609	CLA	C16-C17-C18-C19
34	c1	520	DGD	CBB-CCB-CDB-CEB
29	b1	631	LMG	O10-C28-C29-C30
25	a1	404	CLA	O1A-CGA-O2A-C1
25	B1	608	CLA	CHA-CBD-CGD-O2D
25	B1	612	CLA	CHA-CBD-CGD-O1D
25	B1	613	CLA	CHA-CBD-CGD-O1D
25	B1	613	CLA	CHA-CBD-CGD-O2D
25	C1	502	CLA	CHA-CBD-CGD-O2D
25	b1	605	CLA	CHA-CBD-CGD-O2D
25	b1	611	CLA	CHA-CBD-CGD-O1D
25	b1	616	CLA	CHA-CBD-CGD-O1D
25	b1	616	CLA	CHA-CBD-CGD-O2D
25	b1	619	CLA	CHA-CBD-CGD-O2D
25	c1	509	CLA	CHA-CBD-CGD-O1D
25	c1	509	CLA	CHA-CBD-CGD-O2D
25	c1	511	CLA	CHA-CBD-CGD-O1D
25	B2	606	CLA	CHA-CBD-CGD-O2D
25	B2	613	CLA	CHA-CBD-CGD-O1D
25	B2	613	CLA	CHA-CBD-CGD-O2D
25	B2	616	CLA	CHA-CBD-CGD-O2D
25	C2	509	CLA	CHA-CBD-CGD-O1D
25	C2	509	CLA	CHA-CBD-CGD-O2D
25	C2	518	CLA	CHA-CBD-CGD-O1D
25	C2	518	CLA	CHA-CBD-CGD-O2D
25	D2	406	CLA	CHA-CBD-CGD-O1D
25	D2	406	CLA	CHA-CBD-CGD-O2D
25	b2	616	CLA	CHA-CBD-CGD-O2D
25	c2	505	CLA	CHA-CBD-CGD-O1D
25	c2	510	CLA	CHA-CBD-CGD-O1D
25	c2	510	CLA	CHA-CBD-CGD-O2D
25	c2	511	CLA	CHA-CBD-CGD-O1D
25	c2	511	CLA	CHA-CBD-CGD-O2D
25	c2	513	CLA	CHA-CBD-CGD-O1D
38	V1	201	HEM	CAD-CBD-CGD-O1D
38	f1	101	HEM	CAA-CBA-CGA-O2A
25	c2	503	CLA	C4-C3-C5-C6
25	b2	614	CLA	CAA-CBA-CGA-O2A
25	B1	609	CLA	C16-C17-C18-C20
25	B1	605	CLA	CAA-CBA-CGA-O2A
33	D1	404	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	a2	412	LMG	O1-C7-C8-O7
33	B2	627	LHG	O7-C5-C6-O8
34	C1	515	DGD	O1G-C1G-C2G-O2G
33	D2	403	LHG	C31-C32-C33-C34
25	B1	617	CLA	C15-C16-C17-C18
25	C2	505	CLA	C15-C16-C17-C18
27	D2	407	PHO	C13-C15-C16-C17
25	a1	404	CLA	C4C-C3C-CAC-CBC
25	b1	614	CLA	CAA-CBA-CGA-O2A
29	D1	406	LMG	O7-C10-C11-C12
33	d2	406	LHG	O7-C7-C8-C9
25	B2	608	CLA	C16-C17-C18-C20
27	D1	407	PHO	CHA-CBD-CGD-O1D
27	D1	407	PHO	CHA-CBD-CGD-O2D
27	d1	403	PHO	CHA-CBD-CGD-O1D
27	D2	407	PHO	CHA-CBD-CGD-O1D
33	a1	407	LHG	O1-C1-C2-O2
25	c1	503	CLA	CAA-CBA-CGA-O2A
25	C1	502	CLA	C4-C3-C5-C6
29	A1	412	LMG	C36-C37-C38-C39
33	d1	407	LHG	O9-C7-C8-C9
29	B2	620	LMG	C31-C32-C33-C34
33	l2	101	LHG	C12-C13-C14-C15
25	b1	606	CLA	C11-C12-C13-C15
25	b1	613	CLA	C11-C12-C13-C15
25	c1	506	CLA	C11-C10-C8-C7
25	c1	509	CLA	C11-C10-C8-C7
25	b2	606	CLA	C11-C12-C13-C15
25	b2	609	CLA	C11-C12-C13-C15
25	b2	610	CLA	C6-C7-C8-C10
29	M1	101	LMG	C11-C12-C13-C14
34	c2	514	DGD	O6E-C1E-O5D-C6D
25	D1	402	CLA	CAA-CBA-CGA-O2A
33	a1	407	LHG	O8-C23-C24-C25
25	C1	504	CLA	C11-C10-C8-C9
25	b1	612	CLA	C11-C10-C8-C9
25	b1	619	CLA	C11-C12-C13-C14
25	b1	619	CLA	C14-C13-C15-C16
25	d1	401	CLA	C11-C12-C13-C14
25	C2	516	CLA	CAA-CBA-CGA-O1A
23	H2	103	BCR	C9-C10-C11-C12
25	C2	505	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c2	506	CLA	C2B-C3B-CAB-CBB
29	B2	620	LMG	C11-C12-C13-C14
25	C2	503	CLA	CAA-CBA-CGA-O2A
25	b2	615	CLA	CAA-CBA-CGA-O2A
33	l2	101	LHG	O7-C7-C8-C9
37	D2	402	SQD	C5-C6-S-O8
25	B1	614	CLA	C16-C17-C18-C19
25	B1	608	CLA	C2A-CAA-CBA-CGA
25	b2	606	CLA	C2A-CAA-CBA-CGA
33	d1	407	LHG	C7-C8-C9-C10
34	c2	514	DGD	C8B-C9B-CAB-CBB
34	c2	516	DGD	O2G-C1B-C2B-C3B
25	b1	619	CLA	C2-C3-C5-C6
36	D2	408	PL9	C23-C24-C26-C27
29	b1	621	LMG	O6-C5-C6-O5
25	c1	512	CLA	CAA-CBA-CGA-O1A
29	B2	621	LMG	O9-C10-C11-C12
34	c1	514	DGD	O1B-C1B-C2B-C3B
34	c2	516	DGD	O1B-C1B-C2B-C3B
25	b1	619	CLA	C13-C15-C16-C17
25	c2	502	CLA	C5-C6-C7-C8
33	D1	405	LHG	C12-C13-C14-C15
25	d1	401	CLA	C1A-C2A-CAA-CBA
25	C2	506	CLA	C1A-C2A-CAA-CBA
25	b2	624	CLA	C1A-C2A-CAA-CBA
25	d2	402	CLA	C1A-C2A-CAA-CBA
25	b2	615	CLA	CAA-CBA-CGA-O1A
25	c2	511	CLA	CAA-CBA-CGA-O1A
25	c1	512	CLA	C2-C1-O2A-CGA
25	b2	619	CLA	C2-C1-O2A-CGA
25	a2	405	CLA	C2C-C3C-CAC-CBC
25	C1	504	CLA	CBA-CGA-O2A-C1
29	c2	519	LMG	C29-C28-O8-C9
25	B1	614	CLA	CAA-CBA-CGA-O1A
25	b2	614	CLA	CAA-CBA-CGA-O1A
33	D2	405	LHG	O9-C7-C8-C9
33	D1	405	LHG	O7-C7-C8-C9
29	B1	626	LMG	C34-C35-C36-C37
25	b1	605	CLA	C16-C17-C18-C20
25	b1	619	CLA	C16-C17-C18-C20
25	d1	404	CLA	C16-C17-C18-C20
29	C1	520	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B1	608	CLA	C13-C15-C16-C17
34	c1	518	DGD	CBA-CCA-CDA-CEA
25	d1	401	CLA	CAA-CBA-CGA-O2A
25	B2	615	CLA	CAA-CBA-CGA-O2A
25	B1	608	CLA	C5-C6-C7-C8
33	l2	101	LHG	O9-C7-O7-C5
33	l1	102	LHG	O9-C7-C8-C9
33	l2	101	LHG	O9-C7-C8-C9
34	c2	514	DGD	C2E-C1E-O5D-C6D
35	C1	519	LMT	C2'-C1'-O1'-C1
25	C2	503	CLA	C13-C15-C16-C17
35	l1	101	LMT	C7-C8-C9-C10
25	B1	611	CLA	C4B-C3B-CAB-CBB
25	B1	612	CLA	C4B-C3B-CAB-CBB
25	B1	616	CLA	C4B-C3B-CAB-CBB
25	A2	404	CLA	C4B-C3B-CAB-CBB
25	d2	402	CLA	C4B-C3B-CAB-CBB
33	B2	627	LHG	C3-O3-P-O4
33	L2	101	LHG	C3-O3-P-O5
33	d2	403	LHG	C3-O3-P-O5
27	a1	411	PHO	C16-C17-C18-C19
29	a1	412	LMG	O7-C8-C9-O8
25	D1	402	CLA	CAA-CBA-CGA-O1A
25	C2	503	CLA	CAA-CBA-CGA-O1A
29	A2	412	LMG	O9-C10-C11-C12
33	a1	407	LHG	O10-C23-C24-C25
29	C1	520	LMG	C37-C38-C39-C40
38	f1	101	HEM	CAA-CBA-CGA-O1A
23	a1	401	BCR	C23-C24-C25-C26
23	b1	603	BCR	C23-C24-C25-C26
23	K2	104	BCR	C23-C24-C25-C26
25	c1	509	CLA	C10-C11-C12-C13
25	D2	401	CLA	CAA-CBA-CGA-O1A
27	a2	416	PHO	C16-C17-C18-C20
25	B1	606	CLA	C2A-CAA-CBA-CGA
25	B1	616	CLA	C2A-CAA-CBA-CGA
25	b1	616	CLA	C2A-CAA-CBA-CGA
33	L2	101	LHG	C9-C10-C11-C12
25	C1	511	CLA	C2-C3-C5-C6
33	a1	407	LHG	C32-C33-C34-C35
25	B1	608	CLA	CAD-CBD-CGD-O1D
25	B1	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B1	613	CLA	CAD-CBD-CGD-O1D
25	C1	502	CLA	CAD-CBD-CGD-O1D
25	b1	608	CLA	CAD-CBD-CGD-O1D
25	c1	509	CLA	C3-C5-C6-C7
25	b2	614	CLA	CAD-CBD-CGD-O1D
25	b2	616	CLA	CAD-CBD-CGD-O1D
25	c2	505	CLA	CAD-CBD-CGD-O1D
25	c2	506	CLA	CAD-CBD-CGD-O1D
37	D2	402	SQD	C5-C6-S-O9
37	b2	605	SQD	C44-C45-O47-C7
25	C1	504	CLA	O1A-CGA-O2A-C1
25	c1	503	CLA	CAA-CBA-CGA-O1A
29	D1	406	LMG	O9-C10-C11-C12
33	d2	406	LHG	O9-C7-C8-C9
33	D2	405	LHG	C33-C34-C35-C36
35	a2	406	LMT	C5-C6-C7-C8
25	B2	608	CLA	C13-C15-C16-C17
25	B1	610	CLA	C11-C12-C13-C14
25	b1	604	CLA	C14-C13-C15-C16
25	d1	401	CLA	C14-C13-C15-C16
25	B2	608	CLA	C14-C13-C15-C16
25	b2	612	CLA	C14-C13-C15-C16
25	d2	402	CLA	C6-C7-C8-C9
29	a1	412	LMG	C18-C19-C20-C21
34	c2	517	DGD	CBA-CCA-CDA-CEA
25	c2	506	CLA	C14-C13-C15-C16
25	B2	618	CLA	O1A-CGA-O2A-C1
25	b1	614	CLA	CAA-CBA-CGA-O1A
29	B2	620	LMG	C29-C28-O8-C9
25	C1	502	CLA	CAA-CBA-CGA-O2A
33	l2	101	LHG	C29-C30-C31-C32
25	c2	510	CLA	C6-C7-C8-C9
36	d2	409	PL9	C25-C24-C26-C27
25	B1	610	CLA	C2-C3-C5-C6
25	C1	510	CLA	C12-C13-C15-C16
25	a1	403	CLA	C11-C10-C8-C7
25	b1	604	CLA	C12-C13-C15-C16
25	b1	606	CLA	C11-C10-C8-C7
25	b1	614	CLA	C12-C13-C15-C16
25	b1	617	CLA	C12-C13-C15-C16
25	b1	619	CLA	C11-C12-C13-C15
25	A2	402	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B2	614	CLA	C11-C10-C8-C7
25	B2	615	CLA	C11-C10-C8-C7
25	B2	616	CLA	C2-C3-C5-C6
25	D2	401	CLA	C12-C13-C15-C16
25	D2	404	CLA	C2-C3-C5-C6
25	b2	614	CLA	C12-C13-C15-C16
25	b2	617	CLA	C6-C7-C8-C10
25	b2	617	CLA	C12-C13-C15-C16
25	b2	624	CLA	C6-C7-C8-C10
25	d2	402	CLA	C6-C7-C8-C10
25	d2	405	CLA	C12-C13-C15-C16
25	c1	507	CLA	CAA-CBA-CGA-O2A
29	d1	408	LMG	O7-C10-C11-C12
29	c1	519	LMG	C33-C34-C35-C36
25	c1	507	CLA	CAA-CBA-CGA-O1A
33	D1	405	LHG	O9-C7-C8-C9
38	e2	101	HEM	CAA-CBA-CGA-O2A
34	c1	518	DGD	C2A-C3A-C4A-C5A
35	L1	102	LMT	C3-C4-C5-C6
25	B1	615	CLA	CAA-CBA-CGA-O2A
25	C1	506	CLA	CAA-CBA-CGA-O2A
33	D1	404	LHG	O8-C23-C24-C25
34	C1	515	DGD	O2G-C1B-C2B-C3B
34	c2	516	DGD	C3B-C4B-C5B-C6B
35	c1	517	LMT	O5'-C1'-O1'-C1
25	b1	612	CLA	C13-C15-C16-C17
27	D1	407	PHO	C8-C10-C11-C12
34	c2	514	DGD	CBA-CCA-CDA-CEA
36	d1	409	PL9	C14-C16-C17-C18
36	d2	409	PL9	C29-C31-C32-C33
25	b1	619	CLA	C8-C10-C11-C12
25	c1	509	CLA	C5-C6-C7-C8
25	D2	406	CLA	C15-C16-C17-C18
25	b2	614	CLA	C13-C15-C16-C17
33	l2	101	LHG	O2-C2-C3-O3
29	a2	412	LMG	O8-C28-C29-C30
33	a2	407	LHG	O7-C7-C8-C9
34	H2	101	DGD	O2G-C1B-C2B-C3B
33	b1	622	LHG	C25-C26-C27-C28
25	D1	402	CLA	C5-C6-C7-C8
25	B2	615	CLA	CAA-CBA-CGA-O1A
25	b1	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b1	608	CLA	C13-C15-C16-C17
25	c1	510	CLA	C13-C15-C16-C17

There are no ring outliers.

250 monomers are involved in 721 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a1	403	CLA	5	0
27	d2	408	PHO	1	0
34	c2	517	DGD	2	0
25	B1	613	CLA	3	0
23	k2	501	BCR	8	0
25	c1	513	CLA	3	0
25	c1	508	CLA	6	0
25	c1	512	CLA	5	0
25	A1	405	CLA	6	0
25	b2	610	CLA	7	0
25	b1	612	CLA	3	0
29	M1	101	LMG	2	0
25	b2	618	CLA	2	0
25	B1	607	CLA	2	0
23	A2	401	BCR	6	0
25	d1	406	CLA	2	0
25	C2	511	CLA	1	0
25	c1	516	CLA	1	0
29	C1	520	LMG	1	0
34	H2	101	DGD	3	0
27	D1	407	PHO	1	0
25	B1	606	CLA	5	0
25	a2	404	CLA	7	0
25	B2	605	CLA	2	0
36	d2	409	PL9	7	0
25	b2	614	CLA	1	0
35	m2	104	LMT	1	0
25	C1	502	CLA	2	0
25	c1	510	CLA	4	0
38	v1	201	HEM	3	0
33	l1	102	LHG	3	0
32	i1	101	GOL	1	0
29	B2	621	LMG	2	0
29	B1	622	LMG	1	0
33	d1	407	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B1	617	CLA	5	0
23	B2	601	BCR	5	0
25	c2	503	CLA	4	0
25	C1	506	CLA	4	0
25	B2	607	CLA	2	0
25	C2	508	CLA	1	0
23	b2	601	BCR	4	0
25	B1	608	CLA	3	0
25	b2	624	CLA	3	0
29	j2	101	LMG	6	0
34	C1	516	DGD	7	0
25	C2	510	CLA	1	0
37	B2	623	SQD	2	0
25	D1	402	CLA	3	0
25	B2	608	CLA	6	0
23	b1	602	BCR	2	0
25	c2	507	CLA	2	0
23	z2	101	BCR	5	0
23	c2	501	BCR	8	0
38	V2	201	HEM	4	0
23	H2	103	BCR	4	0
25	C2	516	CLA	1	0
33	l2	101	LHG	5	0
25	D2	401	CLA	3	0
25	C1	511	CLA	4	0
25	B1	612	CLA	3	0
25	D2	404	CLA	3	0
33	D1	405	LHG	6	0
29	b1	631	LMG	2	0
25	B2	604	CLA	1	0
25	a1	404	CLA	7	0
25	B2	615	CLA	2	0
29	A2	412	LMG	1	0
23	K1	101	BCR	4	0
27	a1	411	PHO	4	0
25	b2	615	CLA	4	0
37	D1	409	SQD	1	0
25	b2	611	CLA	1	0
25	B2	611	CLA	5	0
23	b2	603	BCR	8	0
29	b1	621	LMG	3	0
33	D2	405	LHG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c1	501	BCR	7	0
23	K2	102	BCR	5	0
25	B2	606	CLA	3	0
35	C1	519	LMT	1	0
25	c2	502	CLA	5	0
25	B2	614	CLA	5	0
33	a1	407	LHG	3	0
34	c1	520	DGD	1	0
25	c2	508	CLA	3	0
27	A2	407	PHO	2	0
25	b1	604	CLA	2	0
23	b1	601	BCR	4	0
25	c1	509	CLA	4	0
25	c2	505	CLA	3	0
25	B1	605	CLA	2	0
23	a2	402	BCR	4	0
25	d1	401	CLA	7	0
25	B2	612	CLA	2	0
29	A1	412	LMG	3	0
25	C1	510	CLA	3	0
29	A1	410	LMG	3	0
33	A2	405	LHG	3	0
25	B1	610	CLA	6	0
33	B2	627	LHG	2	0
33	B1	621	LHG	8	0
25	c2	506	CLA	4	0
29	b1	624	LMG	9	0
35	L1	102	LMT	1	0
25	B1	615	CLA	2	0
25	b1	611	CLA	3	0
25	B2	617	CLA	3	0
25	C1	514	CLA	2	0
27	A1	408	PHO	2	0
38	v2	201	HEM	3	0
23	d2	401	BCR	4	0
29	D1	406	LMG	1	0
23	K2	104	BCR	3	0
35	a2	406	LMT	2	0
38	E2	101	HEM	4	0
25	b2	608	CLA	5	0
25	C1	509	CLA	7	0
25	b2	616	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	j2	102	BCR	9	0
25	B1	604	CLA	2	0
25	B1	619	CLA	4	0
25	b1	619	CLA	1	0
25	C1	508	CLA	2	0
23	a1	401	BCR	7	0
23	B1	603	BCR	3	0
25	c2	511	CLA	3	0
36	D1	408	PL9	9	0
25	B2	619	CLA	1	0
25	C1	503	CLA	2	0
25	B2	609	CLA	2	0
23	C1	521	BCR	3	0
23	F2	401	BCR	4	0
29	B2	620	LMG	1	0
25	C2	513	CLA	2	0
23	k1	101	BCR	6	0
25	b1	613	CLA	4	0
29	I2	101	LMG	2	0
25	c1	504	CLA	4	0
25	B1	611	CLA	6	0
25	b1	607	CLA	2	0
29	d1	408	LMG	1	0
23	b2	602	BCR	3	0
25	b1	608	CLA	3	0
23	B2	602	BCR	6	0
27	a2	416	PHO	3	0
25	c1	515	CLA	1	0
33	d2	403	LHG	4	0
38	V1	201	HEM	3	0
25	B1	614	CLA	1	0
25	A2	402	CLA	6	0
23	B2	603	BCR	3	0
34	c1	514	DGD	6	0
25	c1	506	CLA	5	0
33	D1	404	LHG	4	0
34	c1	518	DGD	7	0
25	B2	616	CLA	3	0
25	B1	609	CLA	2	0
34	H1	101	DGD	1	0
25	c2	504	CLA	4	0
34	c2	516	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B1	626	LMG	2	0
23	H1	102	BCR	3	0
25	d1	404	CLA	7	0
25	b2	619	CLA	2	0
25	a1	405	CLA	1	0
25	b2	612	CLA	5	0
27	d1	403	PHO	2	0
25	C1	504	CLA	5	0
25	b2	609	CLA	5	0
23	B1	601	BCR	6	0
25	c2	512	CLA	4	0
33	L2	101	LHG	5	0
25	A2	404	CLA	1	0
25	b1	609	CLA	7	0
25	b1	614	CLA	4	0
35	l1	101	LMT	1	0
25	C2	505	CLA	4	0
25	C1	512	CLA	3	0
34	c2	514	DGD	3	0
25	B1	616	CLA	5	0
23	b1	603	BCR	4	0
25	A1	403	CLA	4	0
25	c2	509	CLA	5	0
25	B2	618	CLA	1	0
25	d2	402	CLA	4	0
33	D2	403	LHG	9	0
37	b2	605	SQD	2	0
25	b2	613	CLA	2	0
25	d2	405	CLA	3	0
25	c1	503	CLA	4	0
23	J1	101	BCR	6	0
23	h1	102	BCR	3	0
25	C1	513	CLA	4	0
34	h2	102	DGD	5	0
38	f1	101	HEM	3	0
29	a1	412	LMG	6	0
25	c1	505	CLA	1	0
27	D2	407	PHO	3	0
25	b2	620	CLA	6	0
35	m1	101	LMT	1	0
33	d2	406	LHG	5	0
23	B1	602	BCR	5	0

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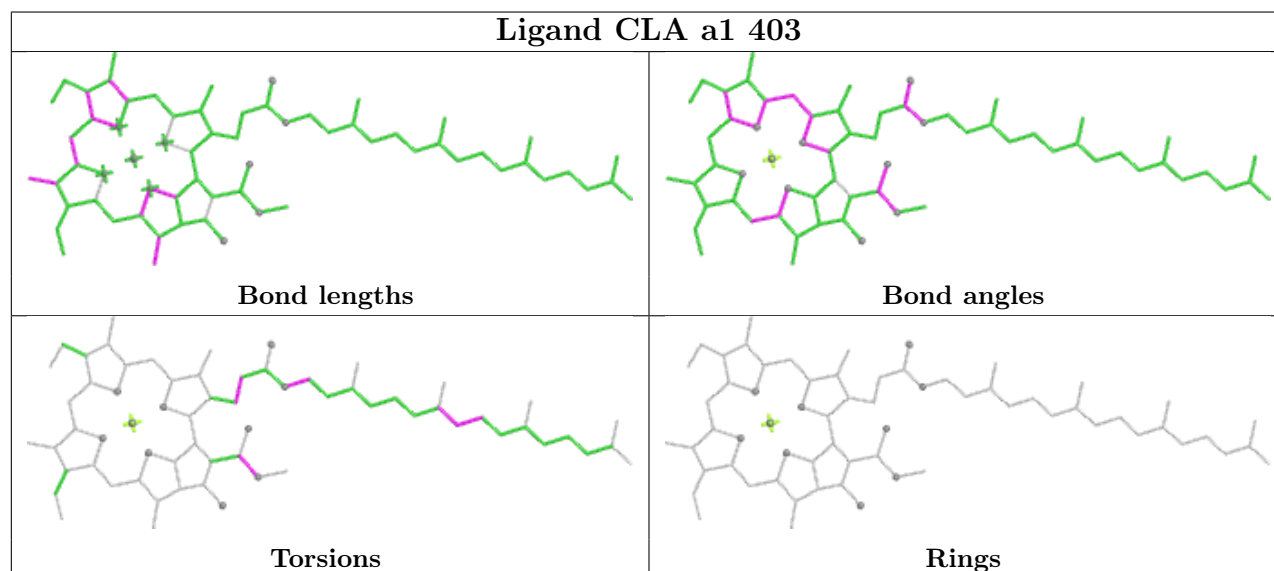
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25	c2	515	CLA	3	0
25	b1	605	CLA	1	0
25	b1	606	CLA	5	0
33	b1	622	LHG	4	0
35	M1	102	LMT	1	0
33	d1	402	LHG	2	0
36	d1	409	PL9	12	0
23	c1	502	BCR	4	0
25	c2	510	CLA	3	0
23	C1	501	BCR	4	0
36	D2	408	PL9	11	0
23	A1	401	BCR	4	0
25	A1	406	CLA	5	0
25	a2	405	CLA	2	0
29	F2	402	LMG	1	0
34	C1	517	DGD	1	0
33	L1	101	LHG	1	0
29	c1	519	LMG	1	0
38	E1	101	HEM	3	0
25	A2	403	CLA	10	0
25	b1	616	CLA	3	0
25	c1	507	CLA	5	0
25	B2	610	CLA	2	0
25	K2	101	CLA	4	0
23	D1	401	BCR	3	0
23	h2	101	BCR	3	0
35	m2	103	LMT	2	0
33	a2	407	LHG	4	0
25	D2	406	CLA	4	0
25	B2	613	CLA	4	0
25	b1	620	CLA	1	0
25	C2	507	CLA	2	0
25	c1	511	CLA	1	0
23	C2	502	BCR	3	0
34	h1	101	DGD	4	0
35	b2	623	LMT	2	0
25	C1	505	CLA	2	0
23	d1	405	BCR	4	0
25	C2	509	CLA	3	0
29	b2	622	LMG	3	0
34	C1	515	DGD	2	0
38	e2	101	HEM	3	0

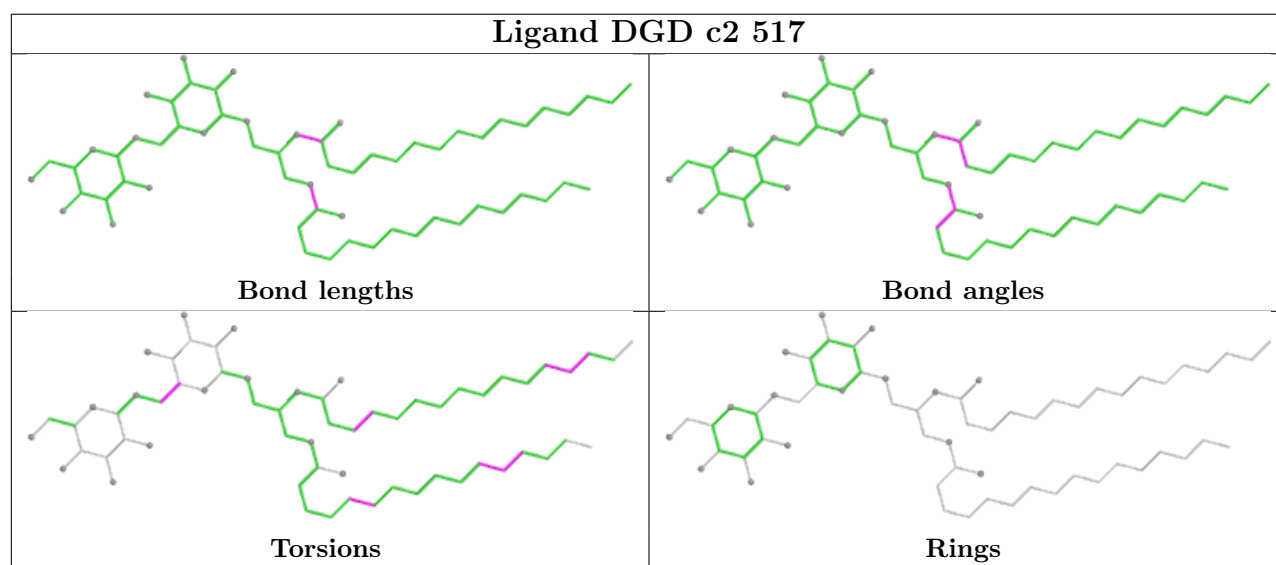
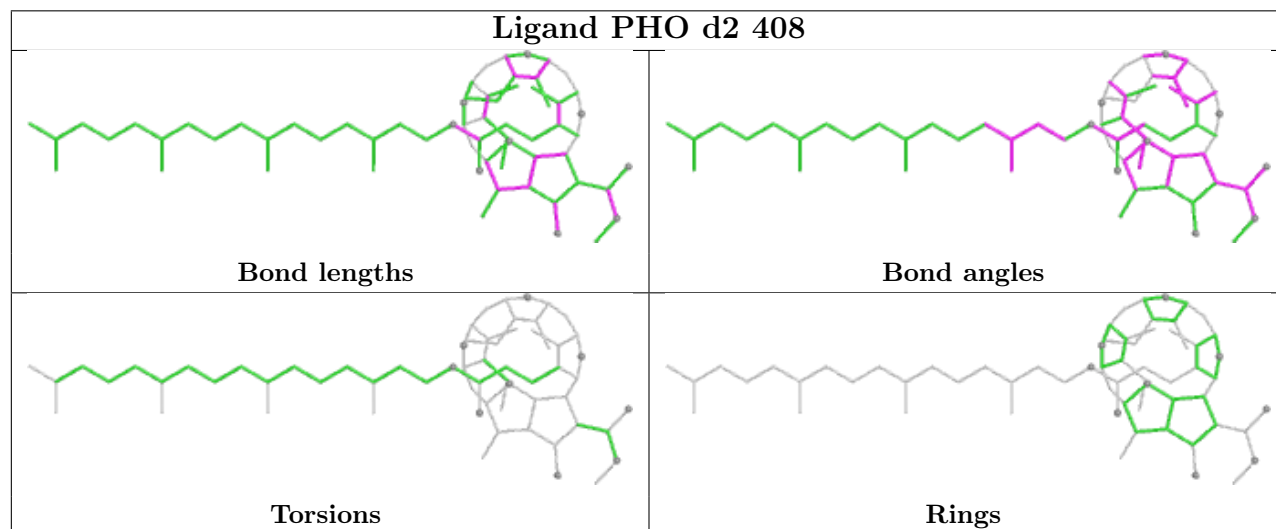
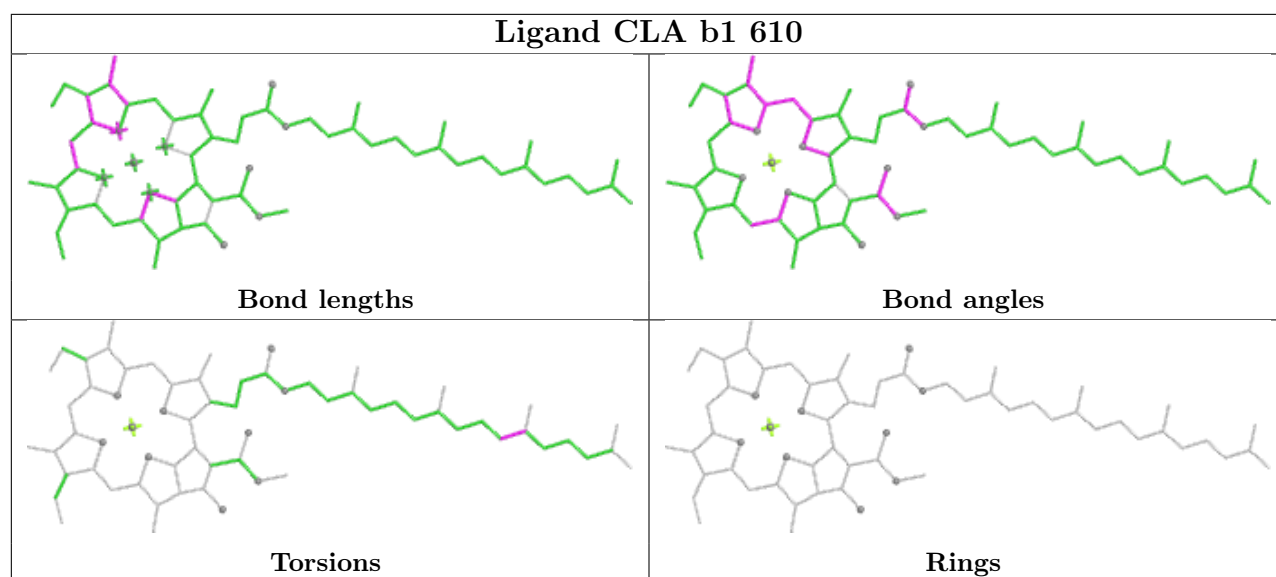
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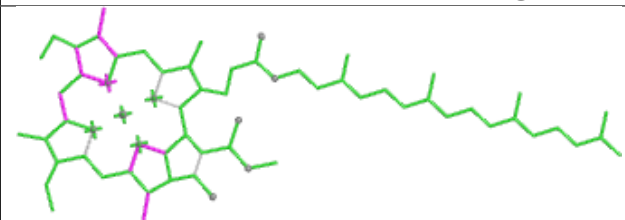
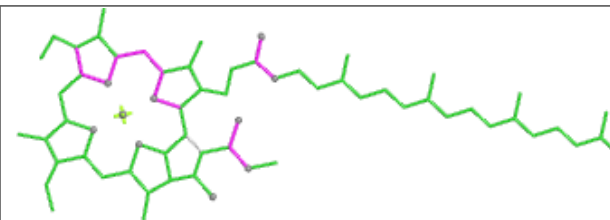
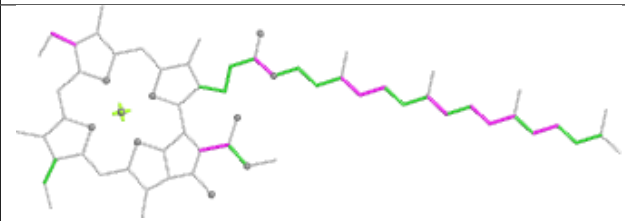
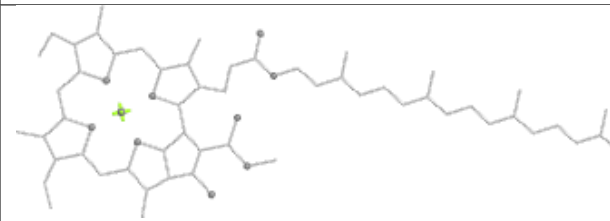
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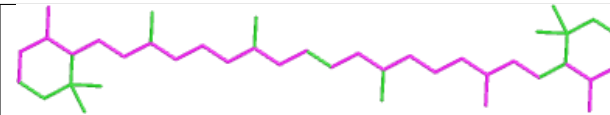
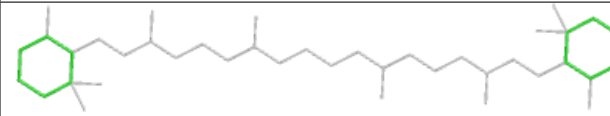
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d2	407	LMG	2	0
25	C1	507	CLA	1	0
25	A1	404	CLA	1	0
25	b2	606	CLA	7	0
25	C2	503	CLA	4	0

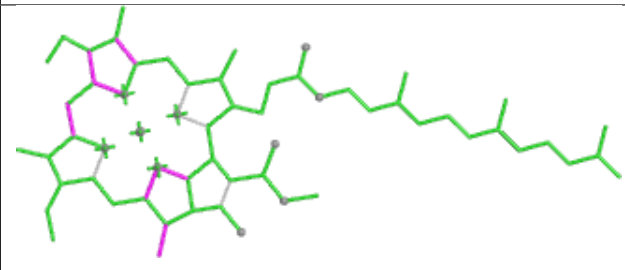
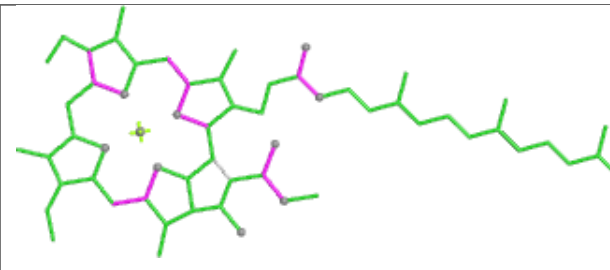
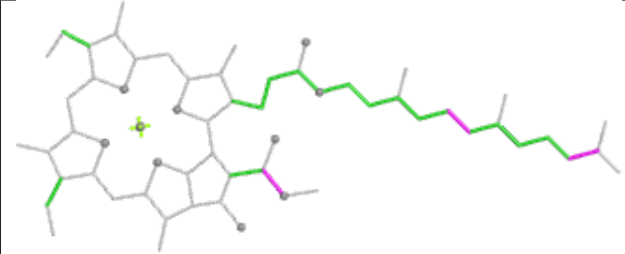
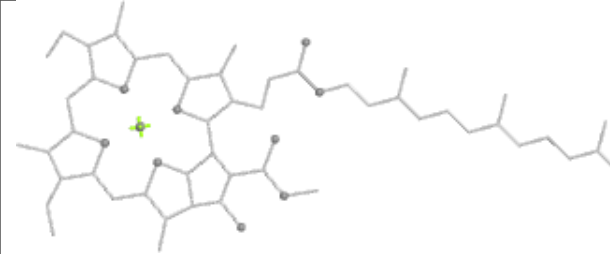
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

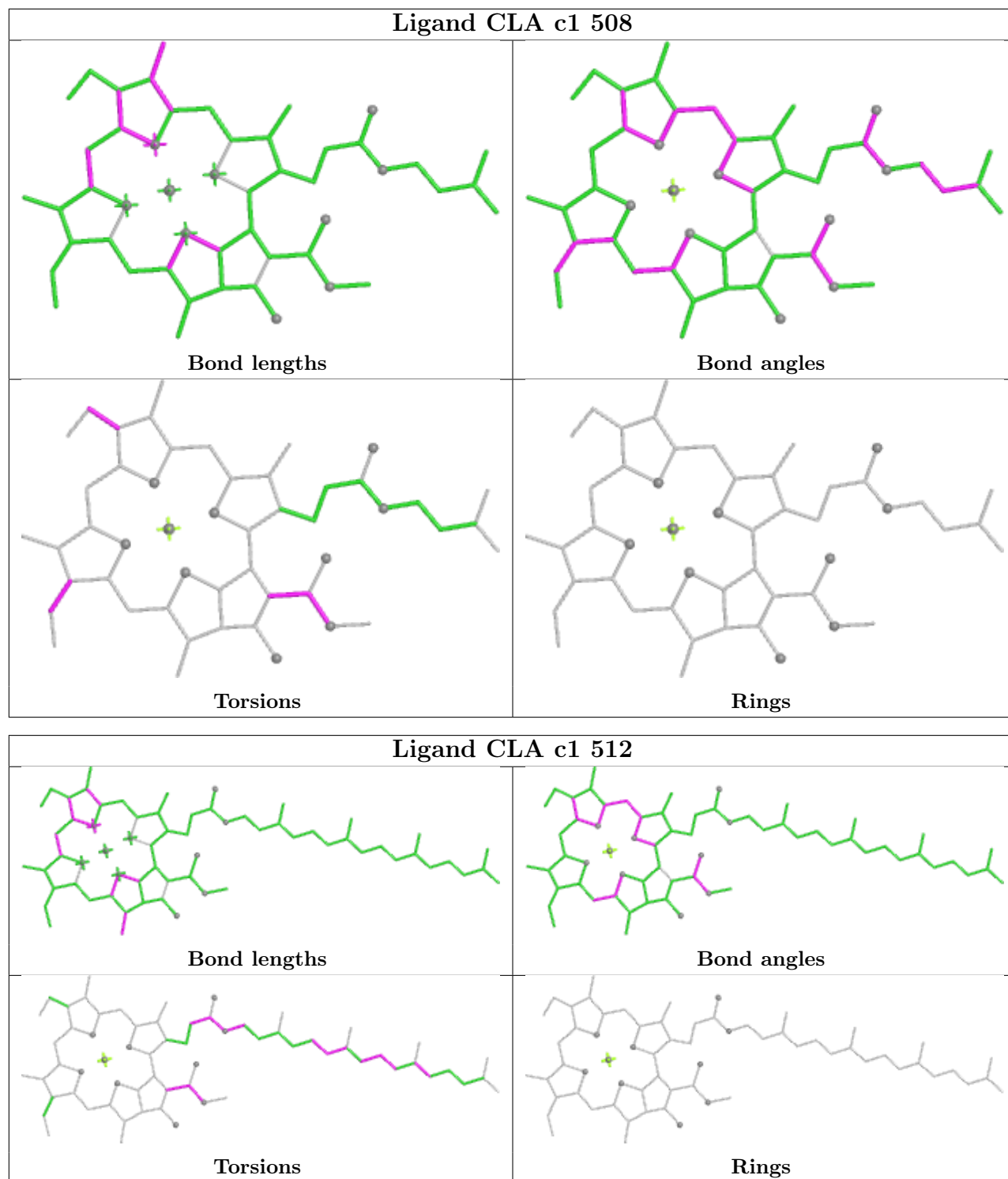




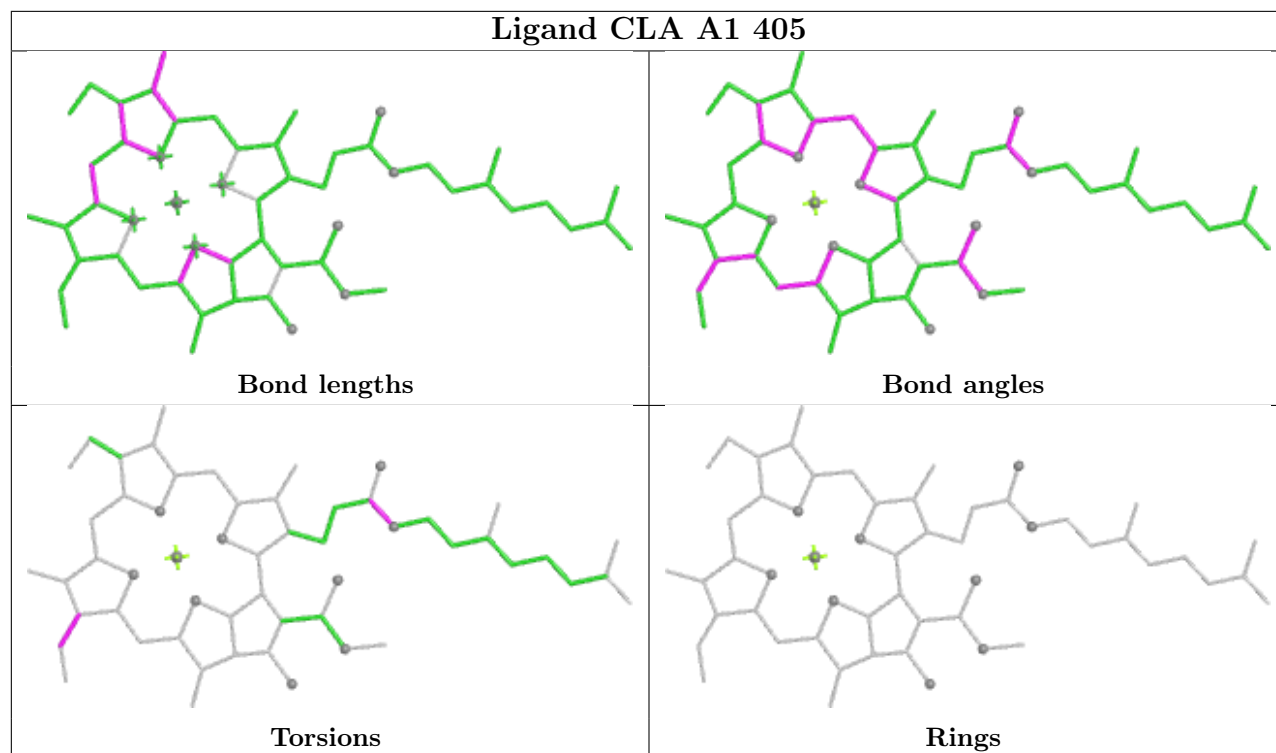
Ligand CLA B1 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR k2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

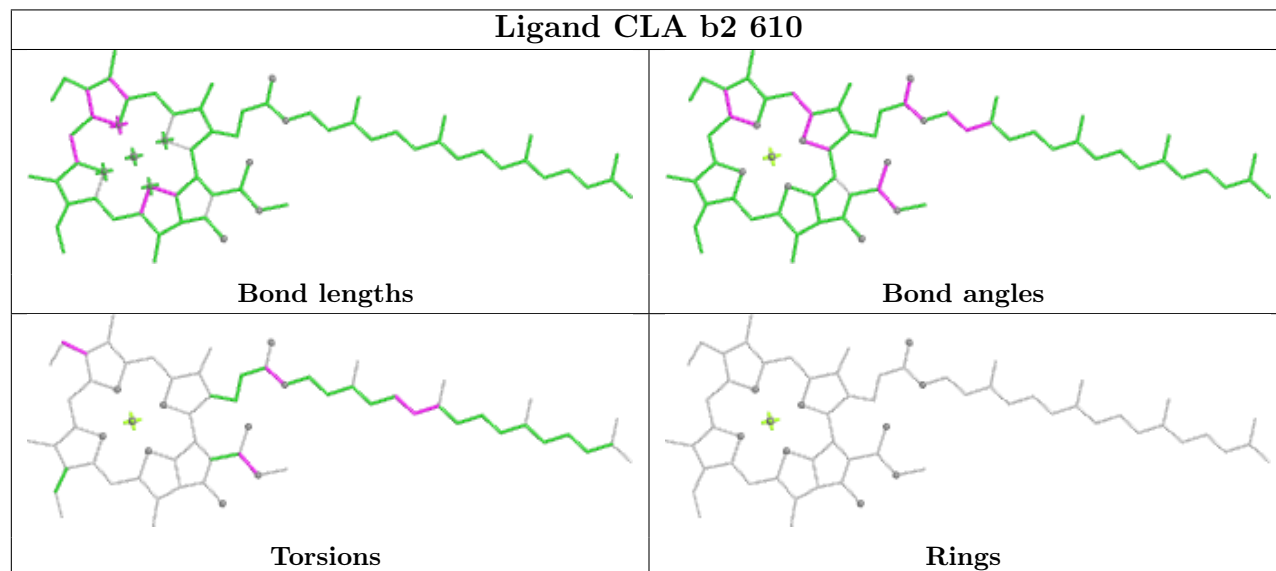
Ligand CLA c1 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

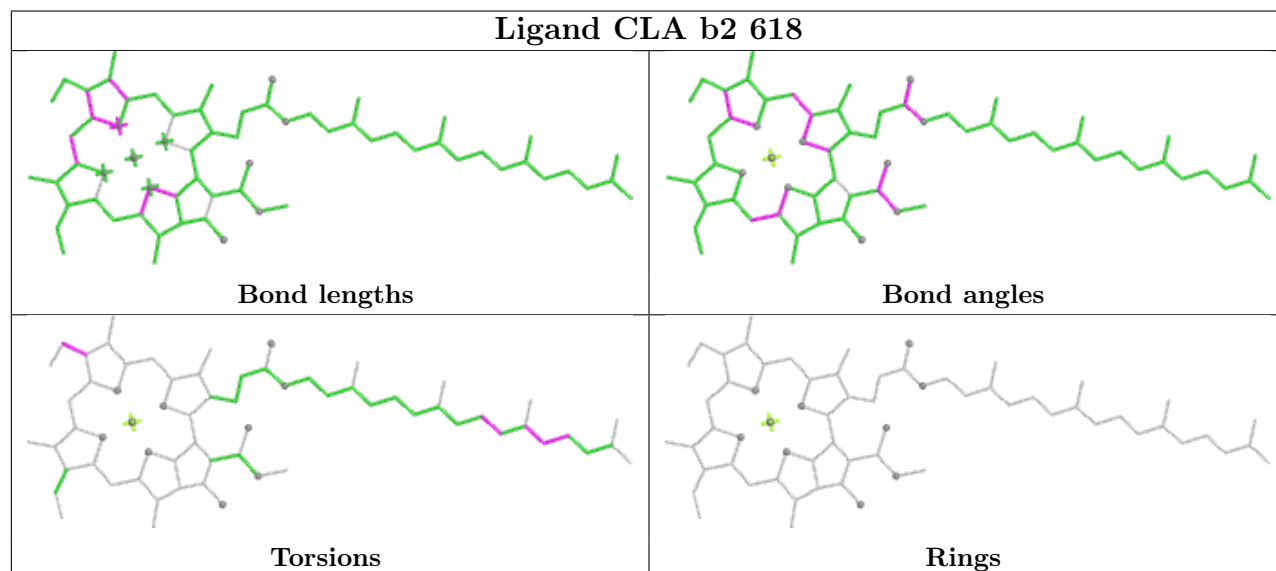
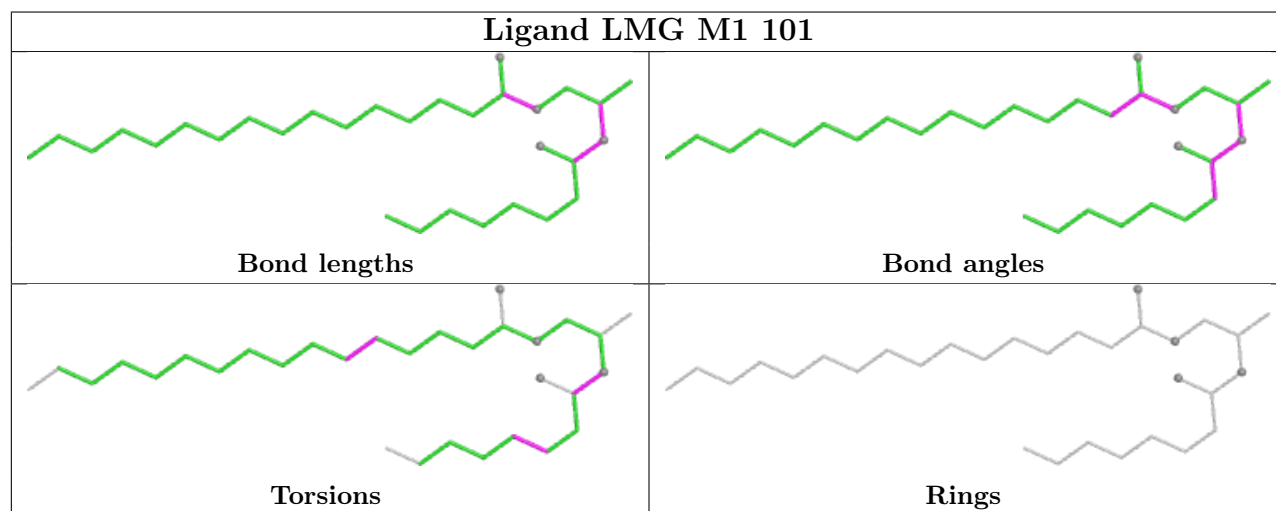
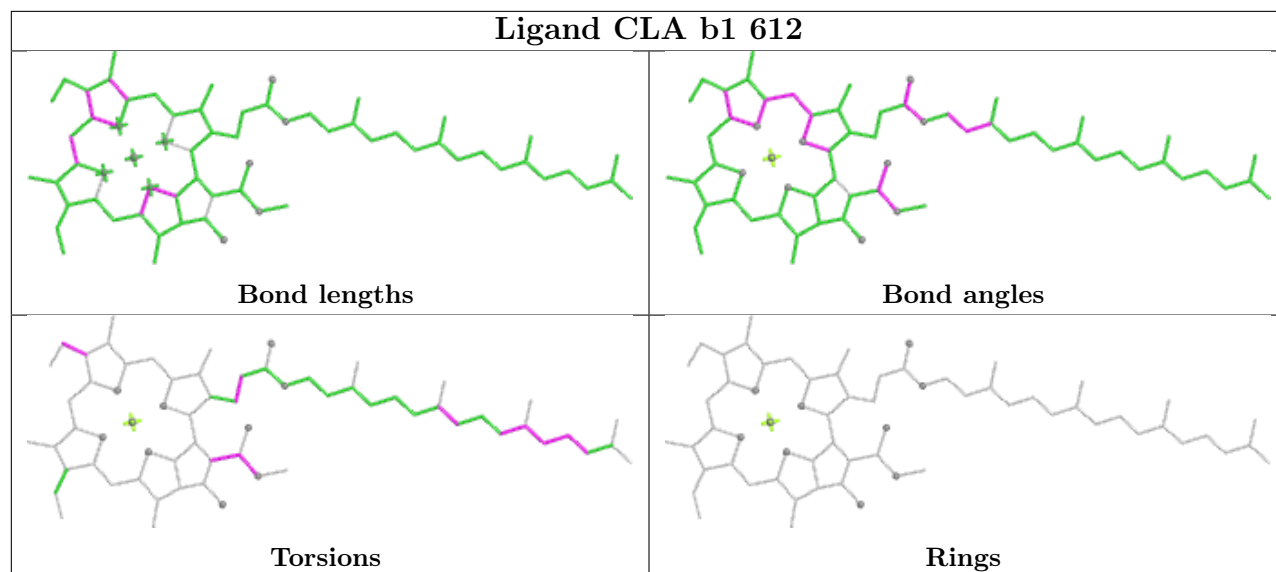


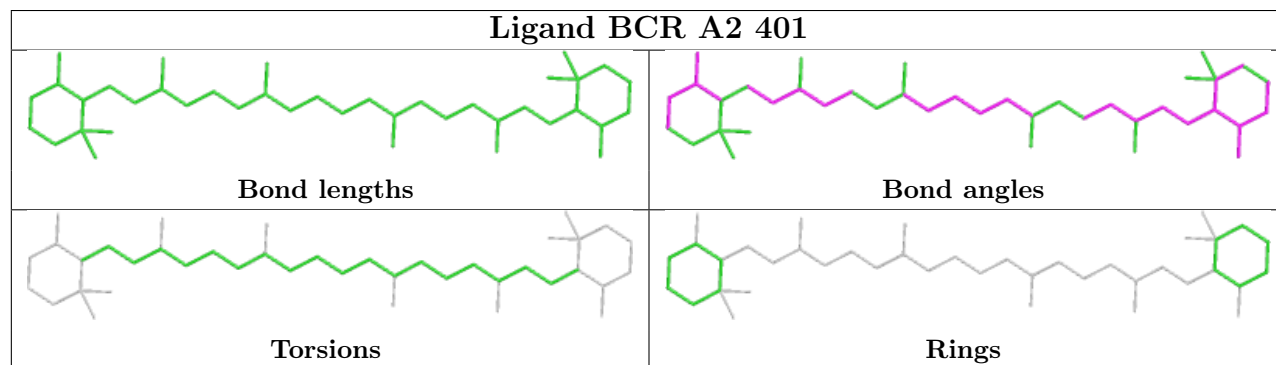
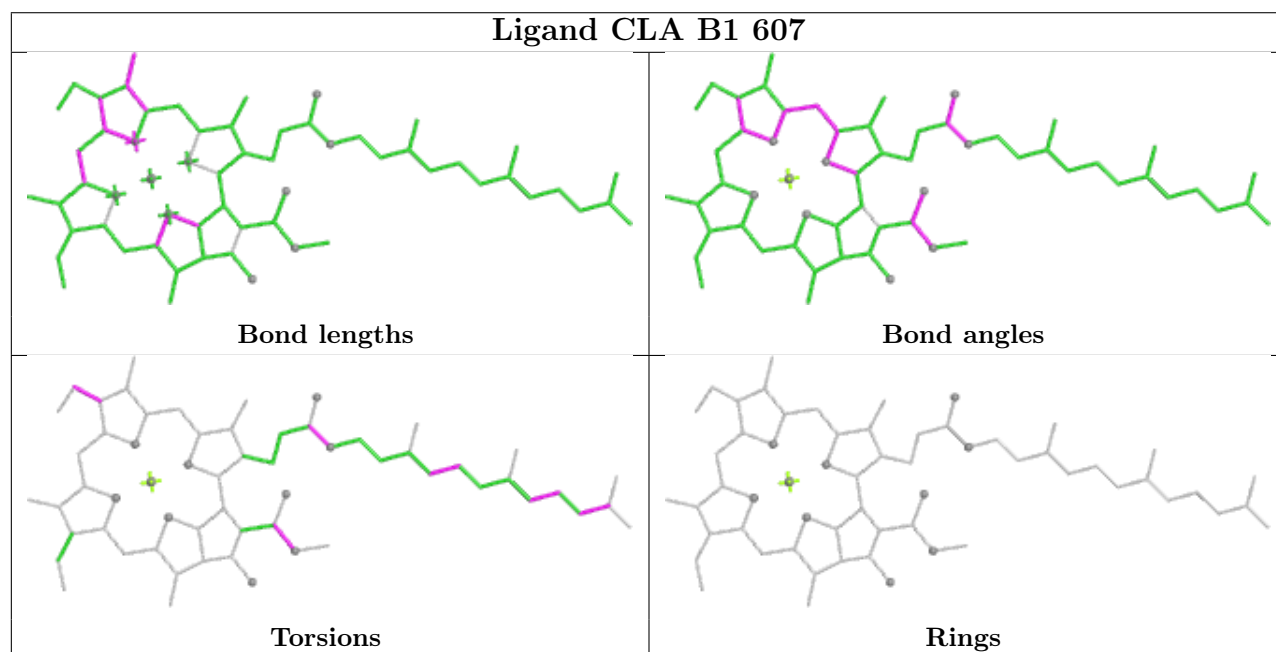
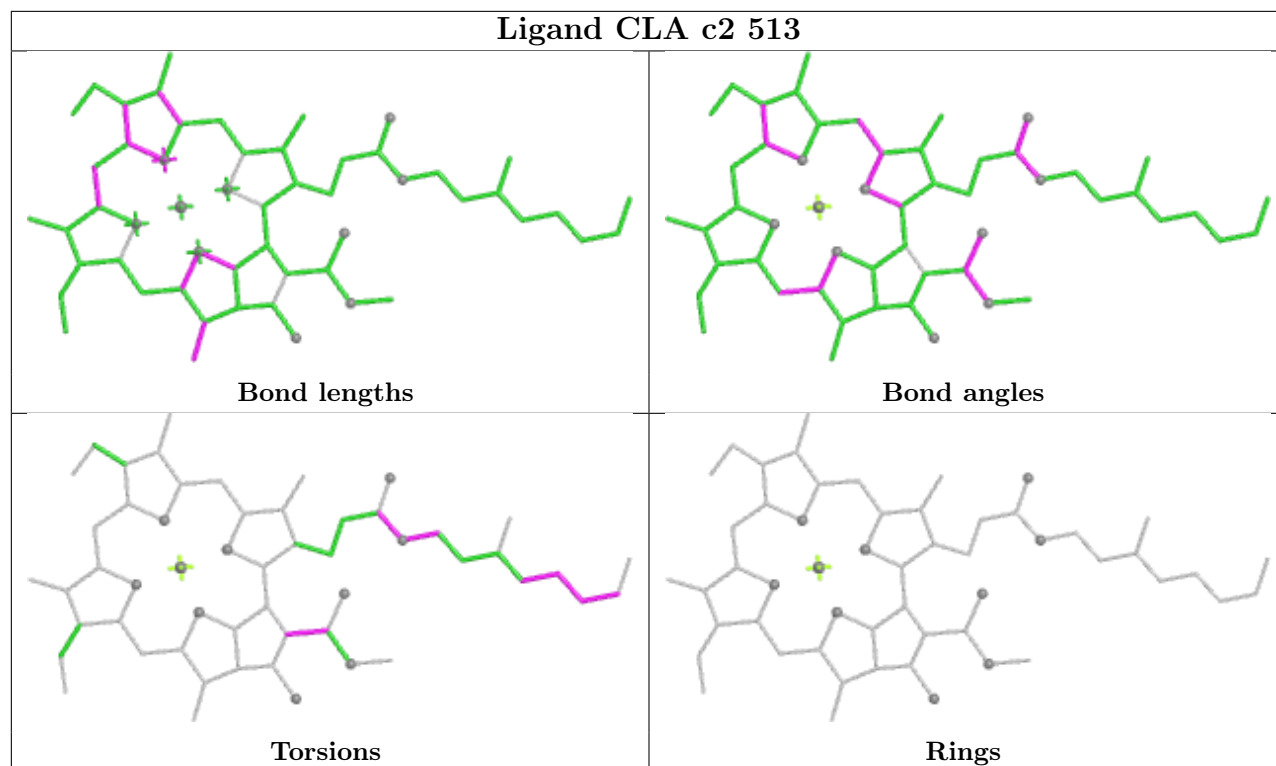
Ligand CLA A1 405

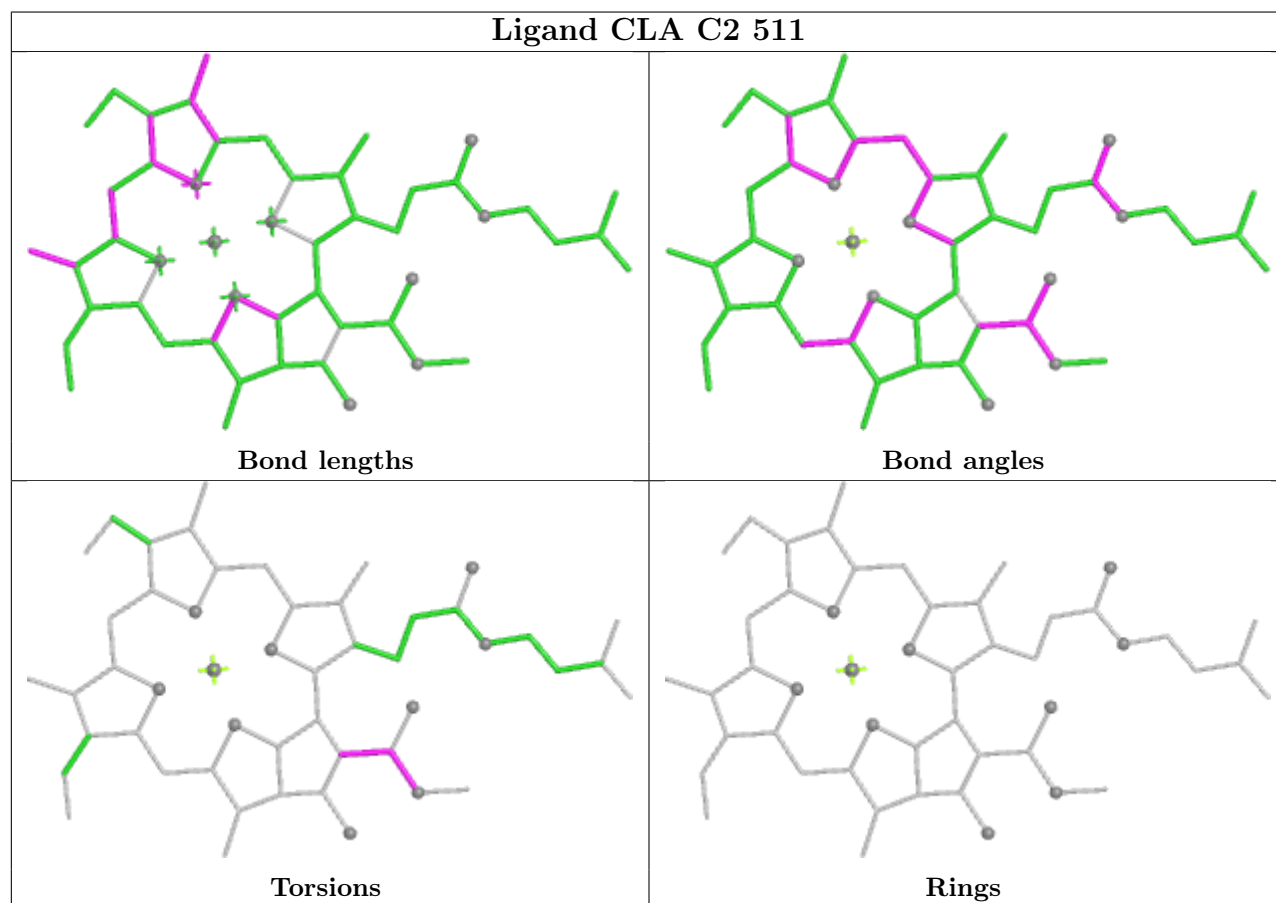
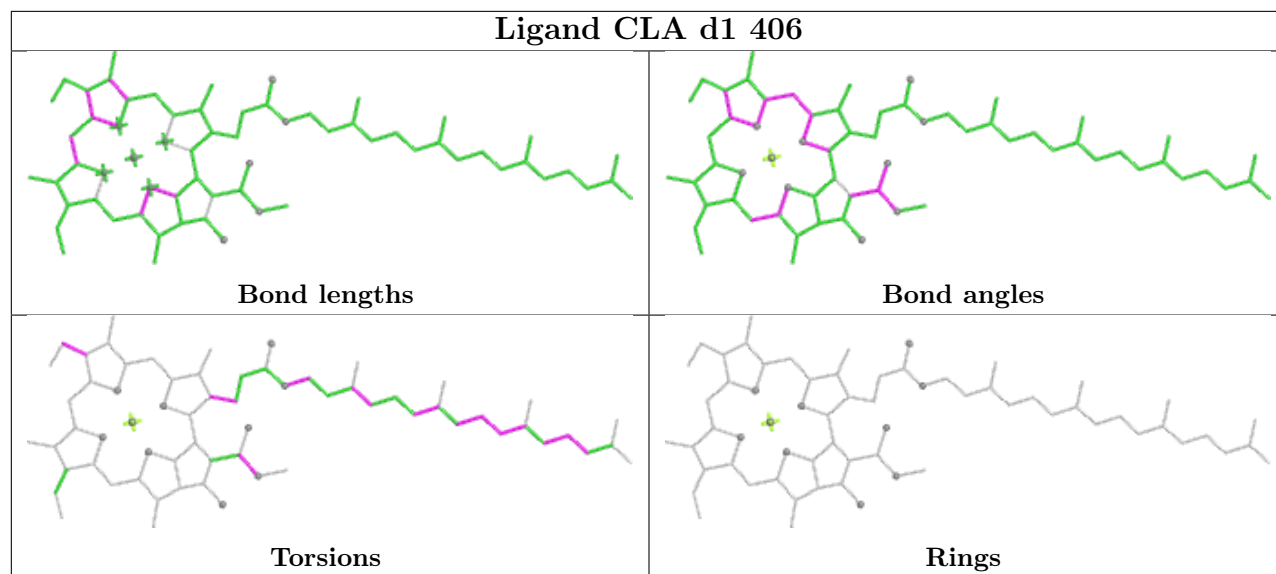


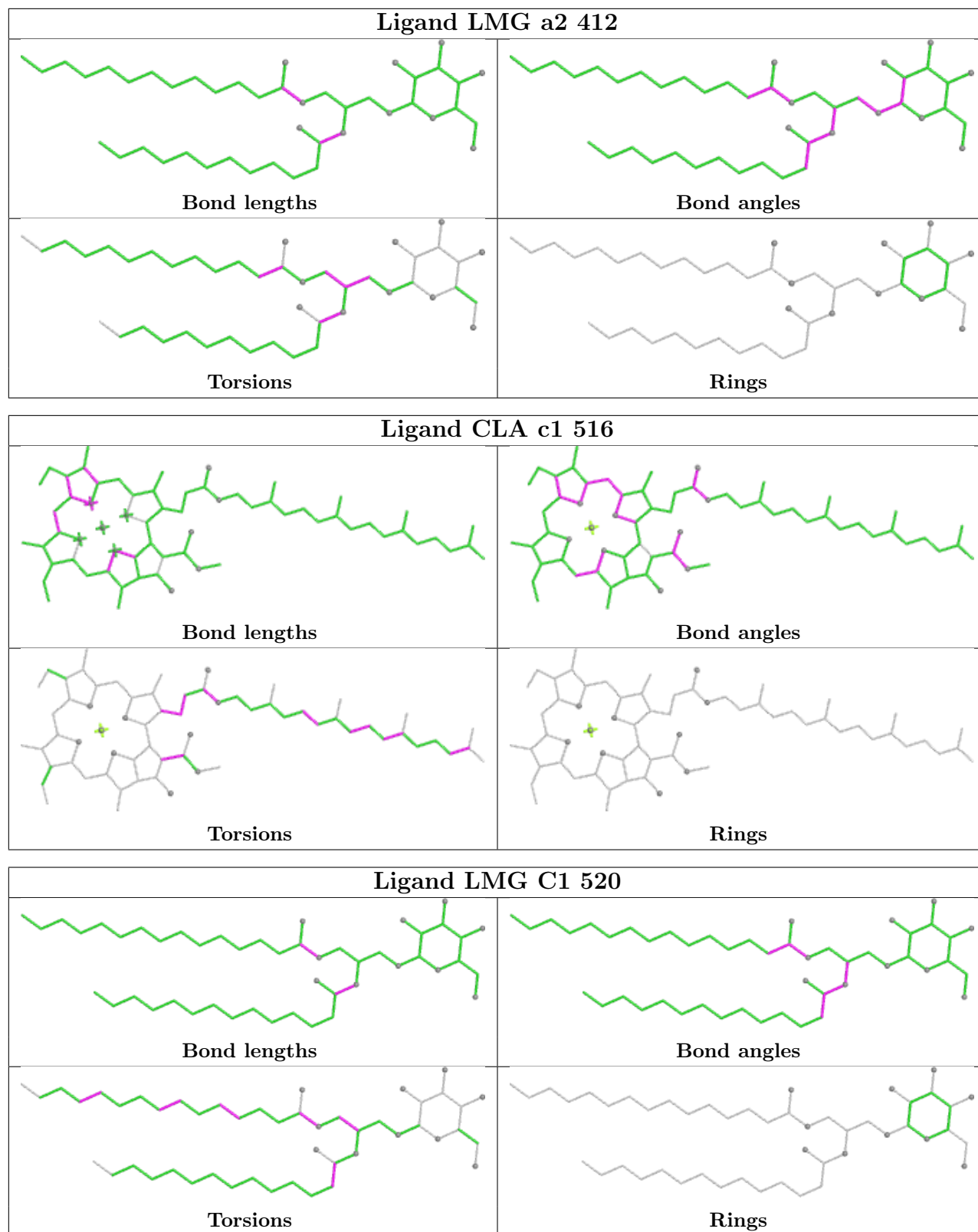
Ligand CLA b2 610



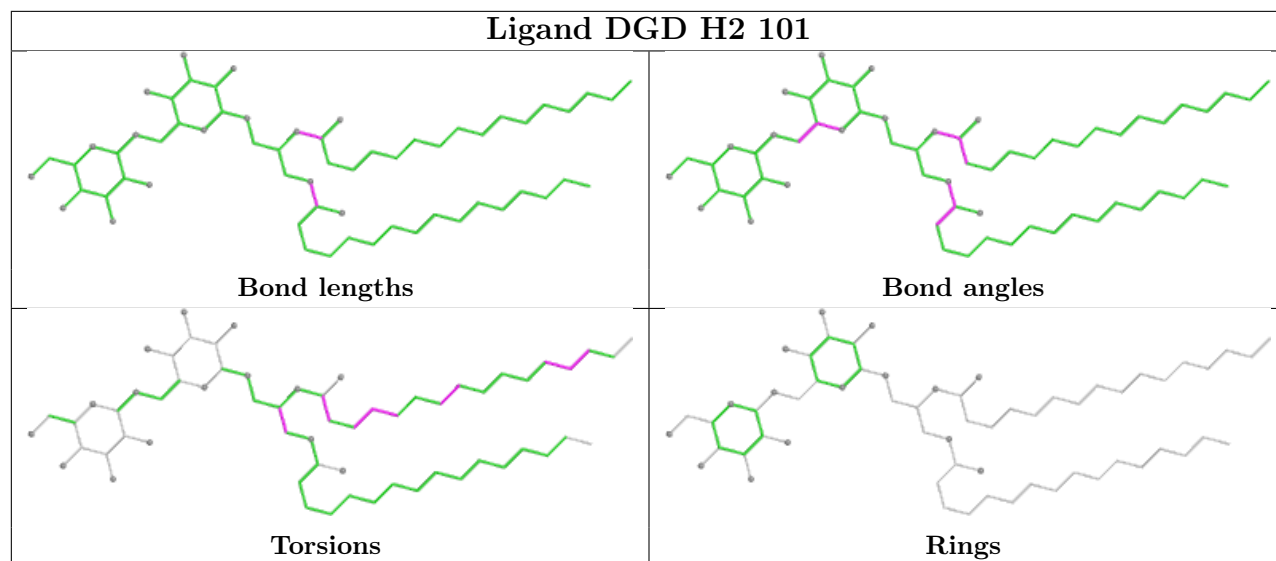




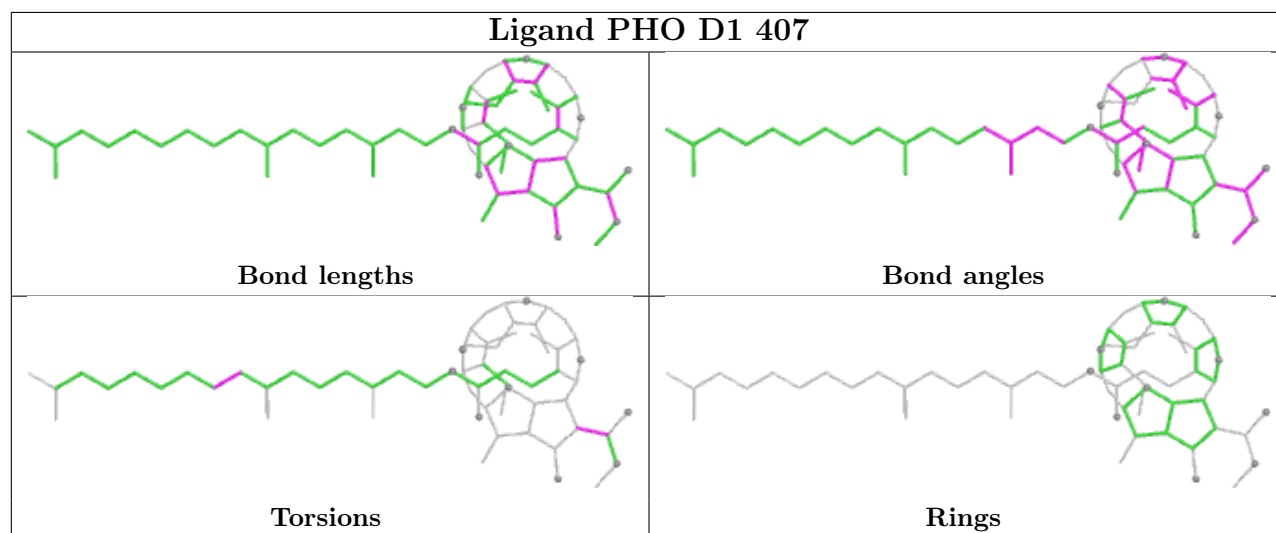




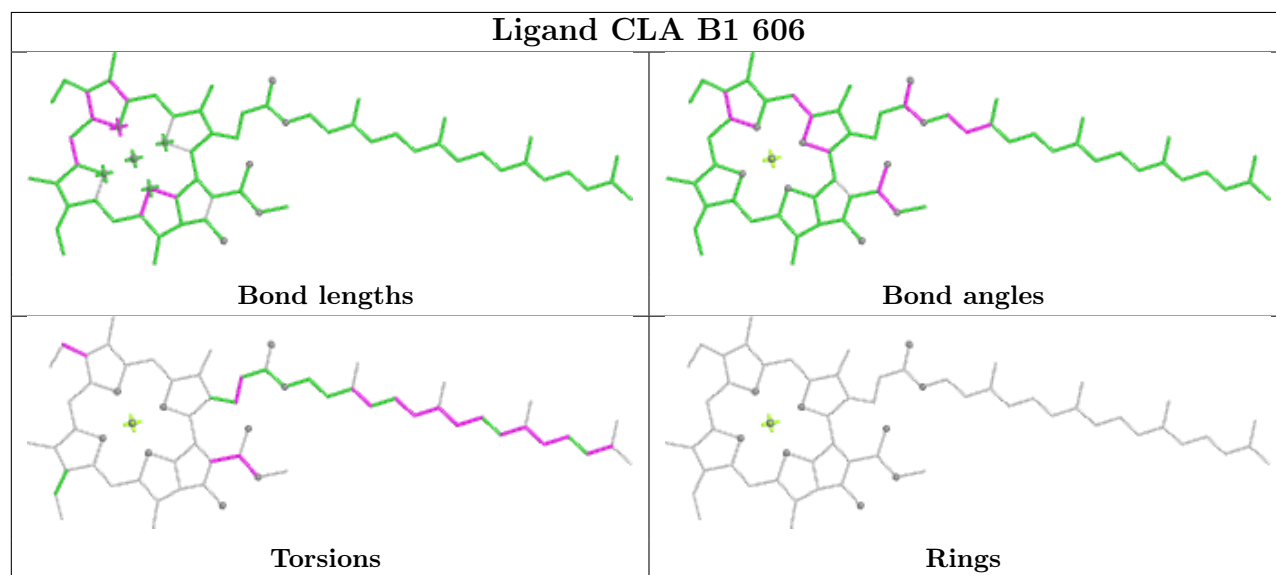
Ligand DGD H2 101

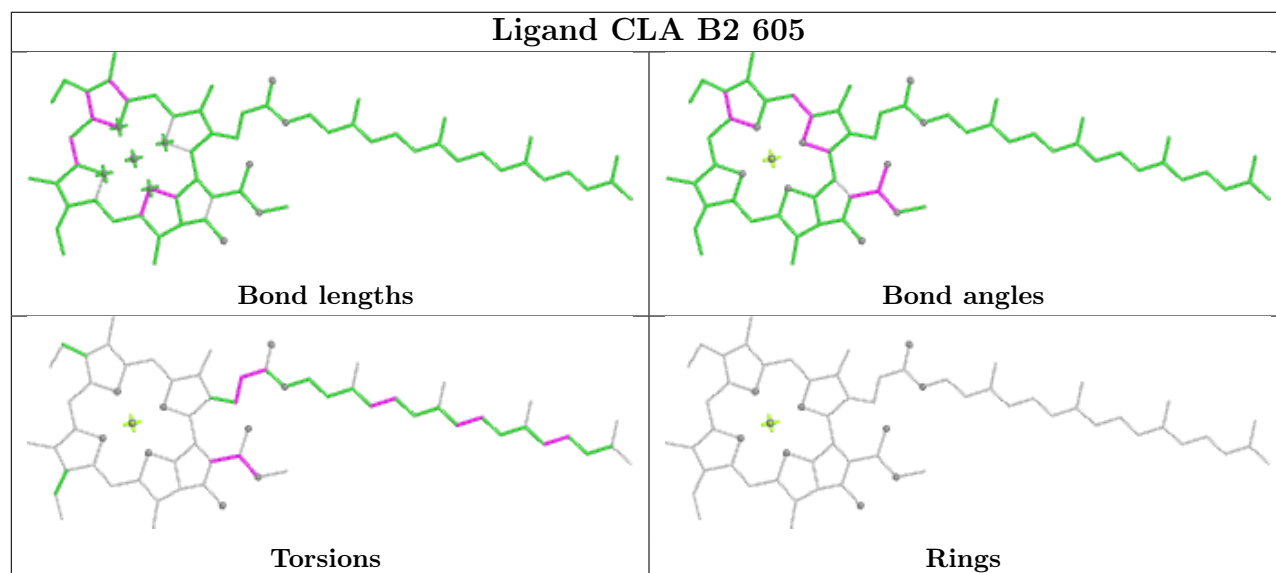
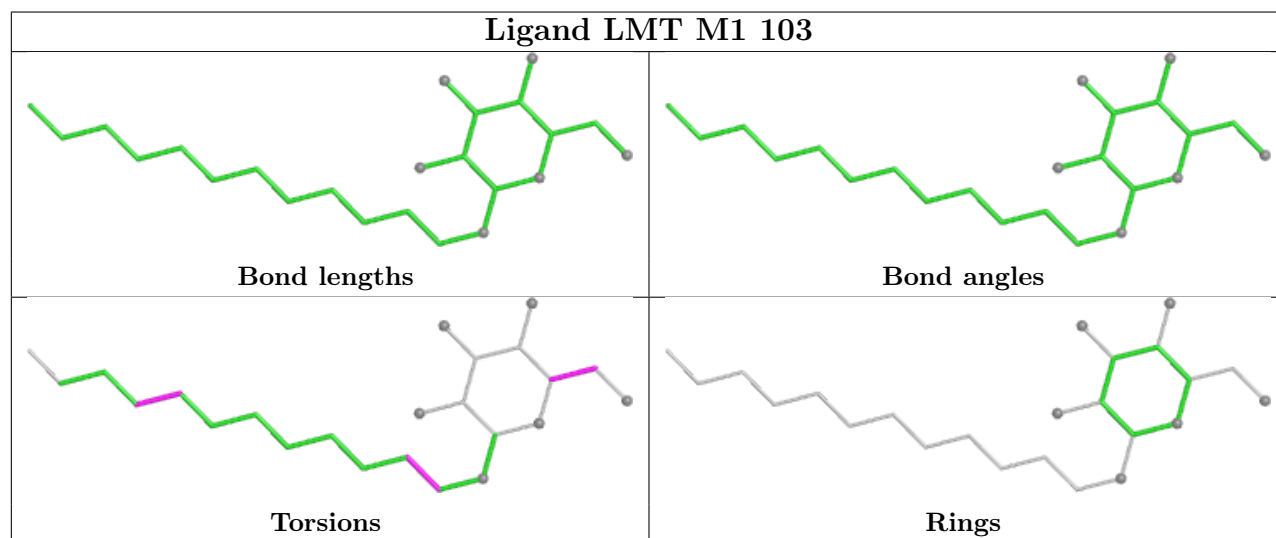
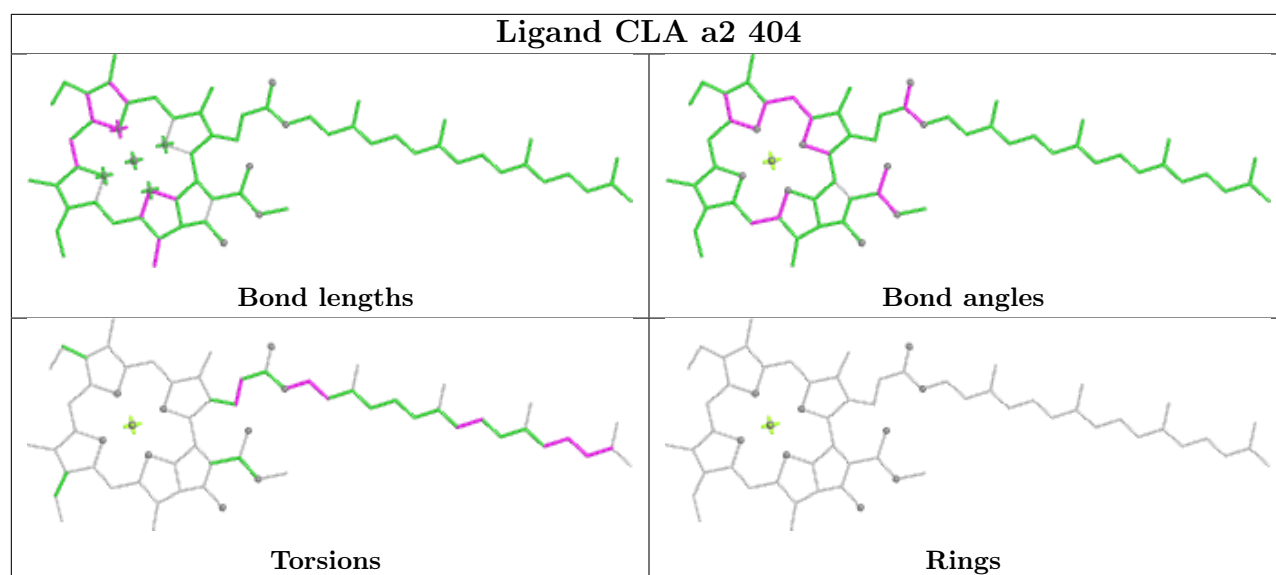


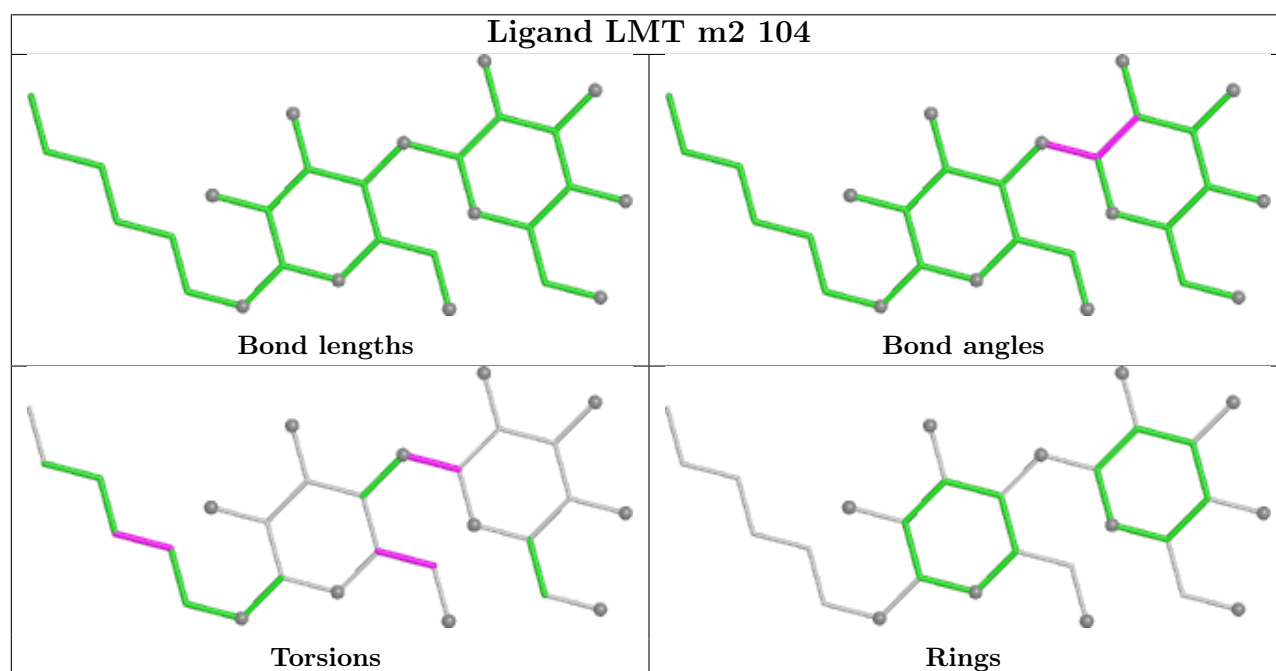
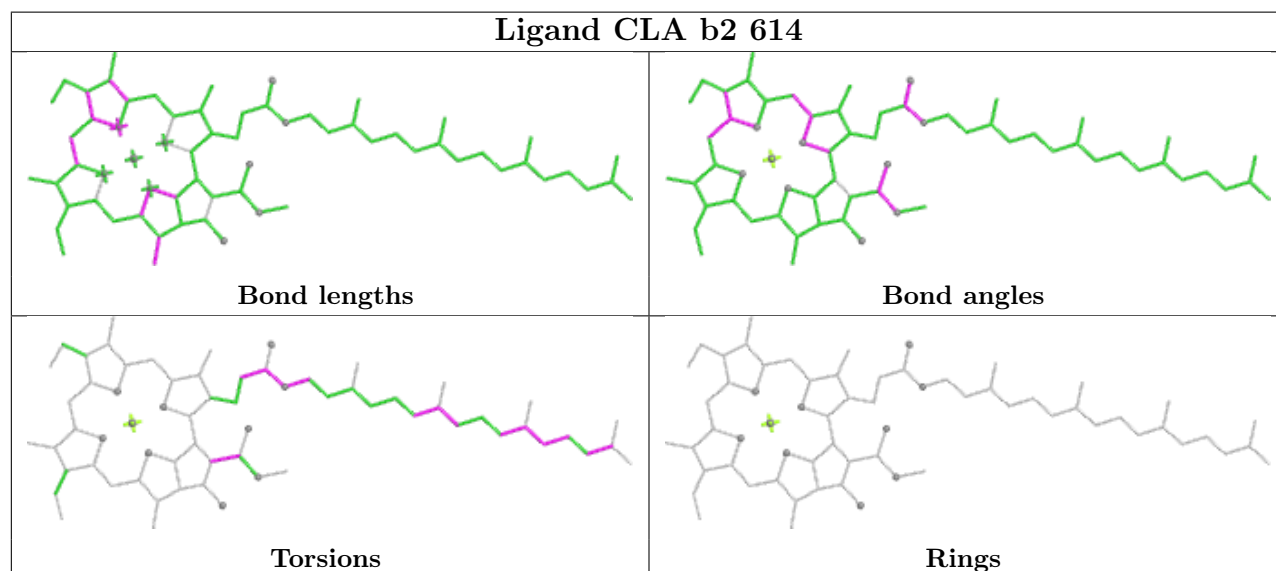
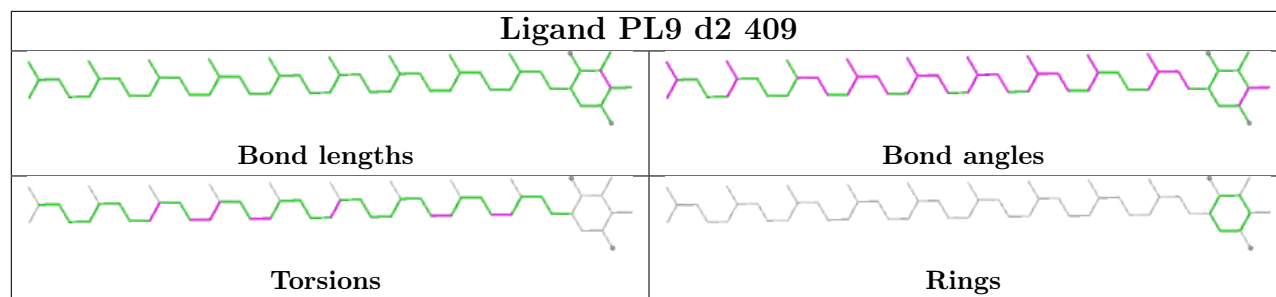
Ligand PHO D1 407

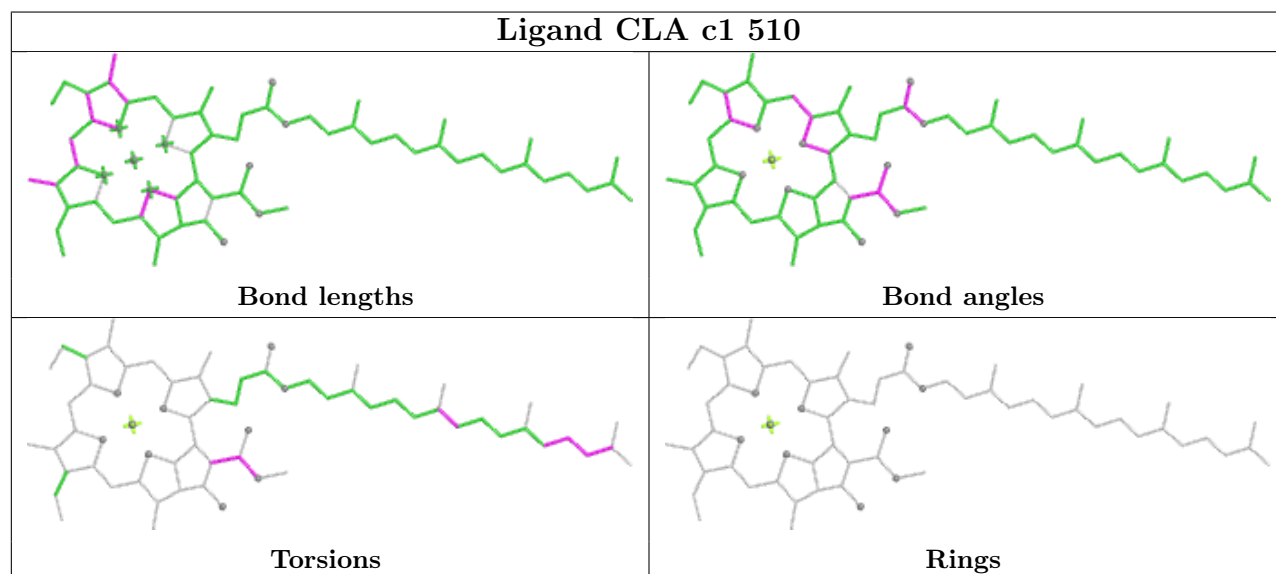
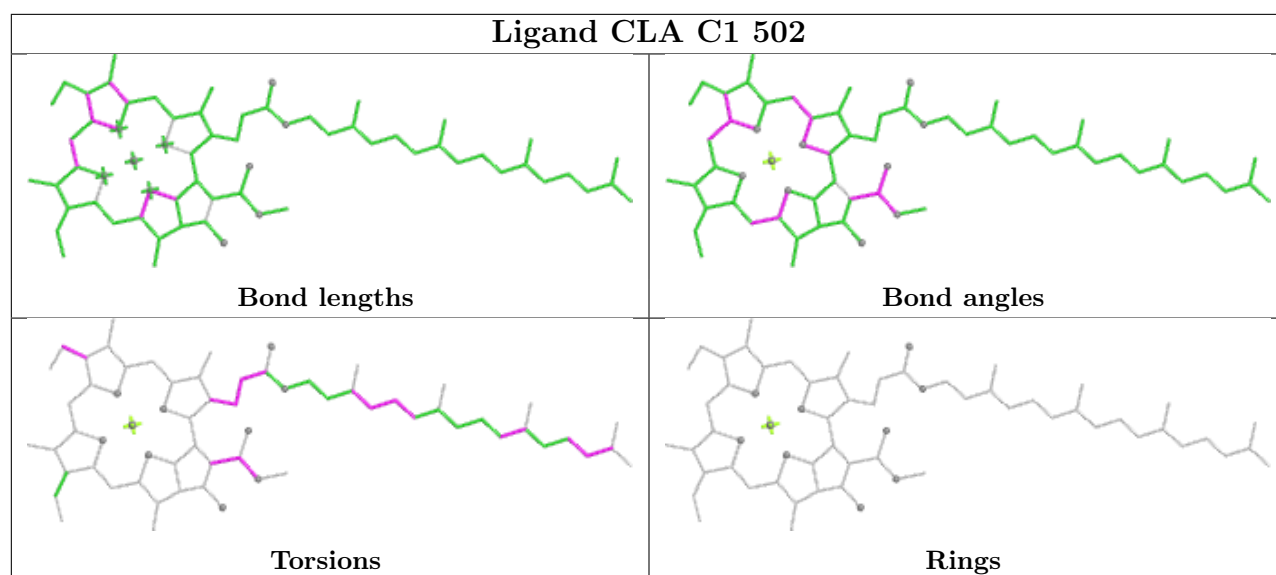


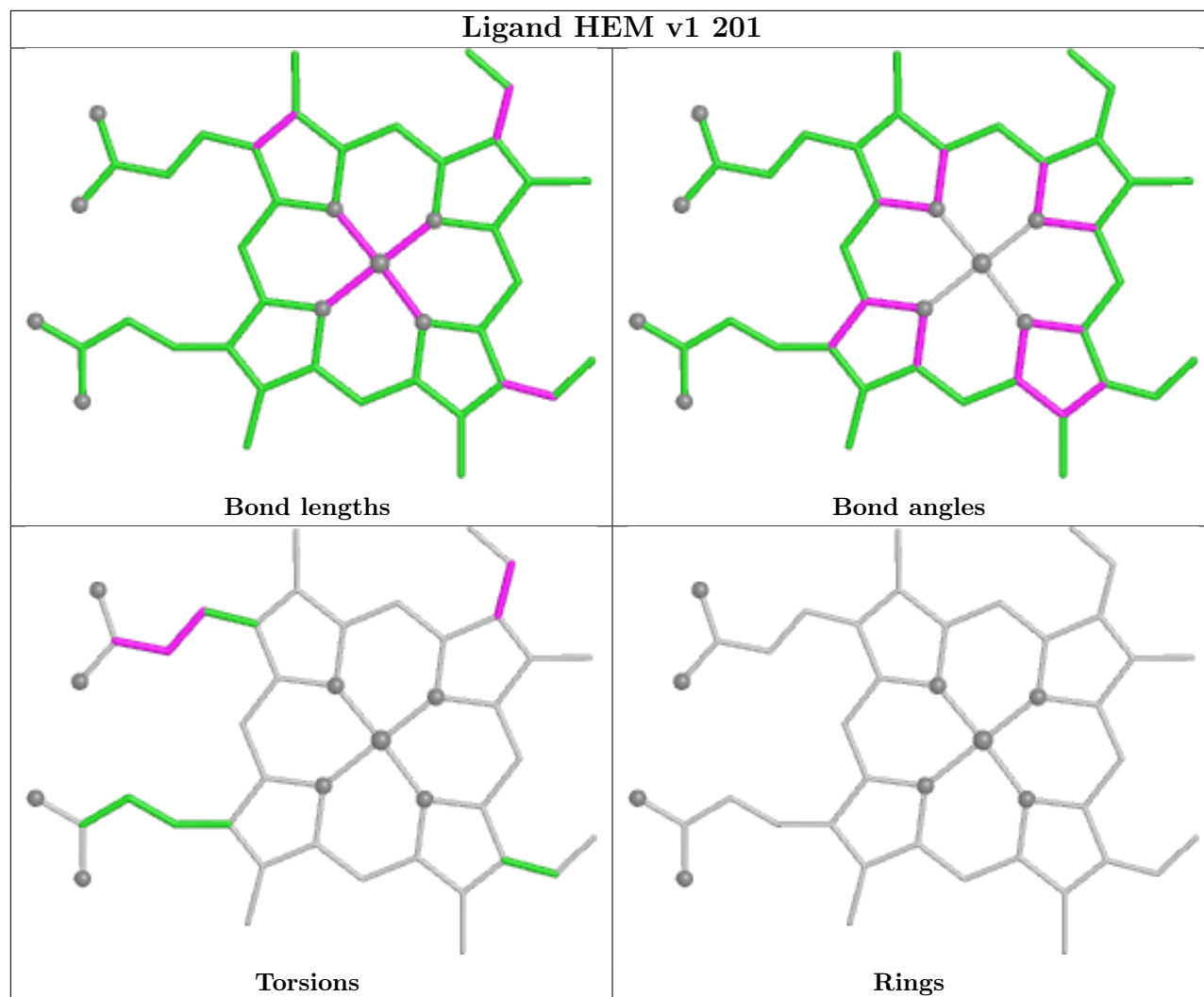
Ligand CLA B1 606

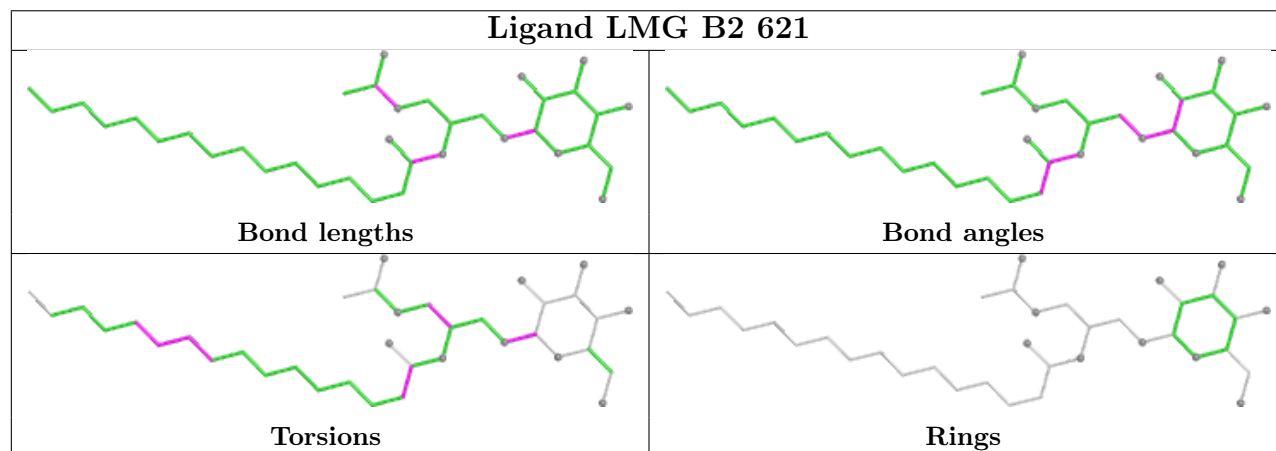
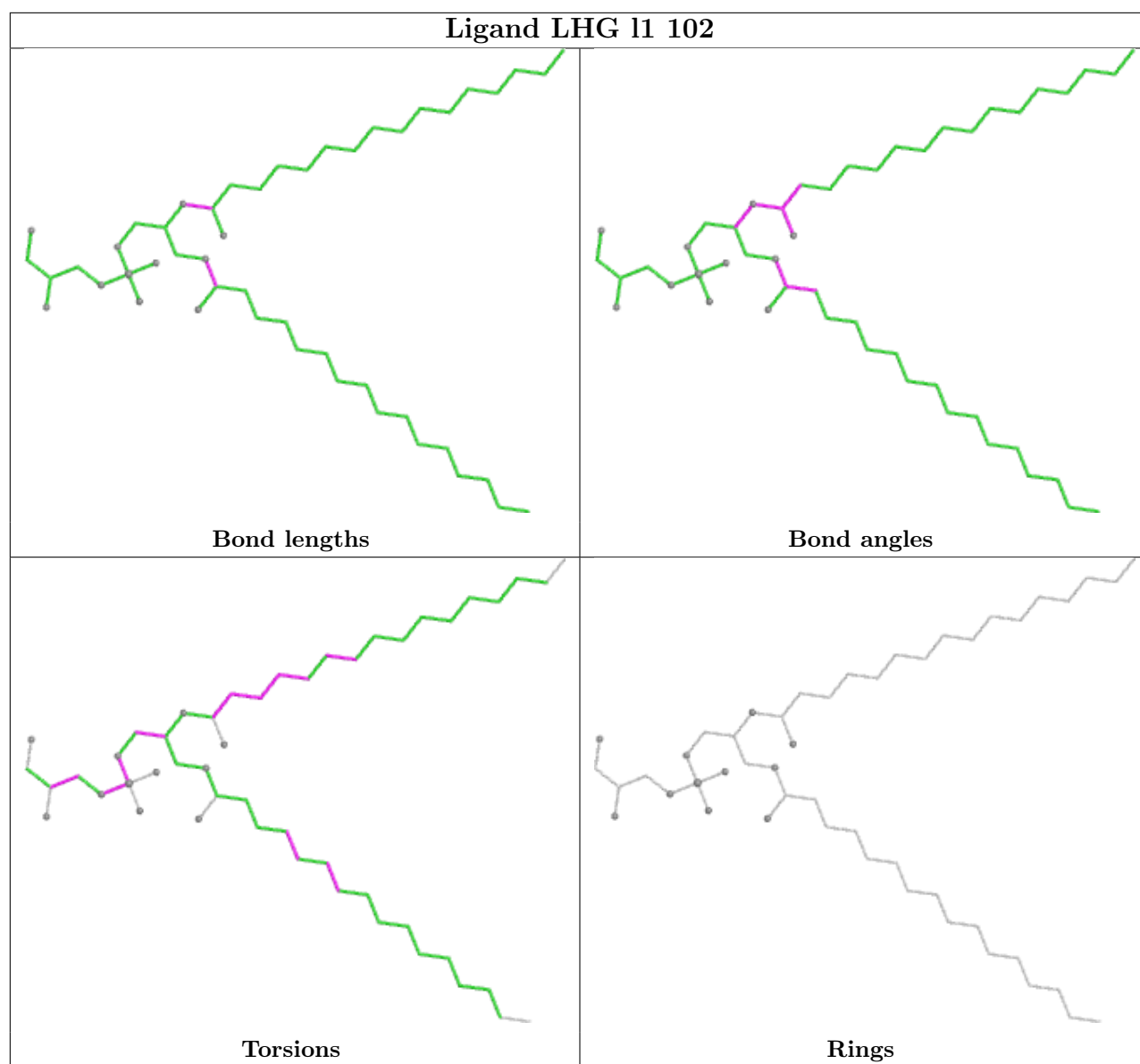


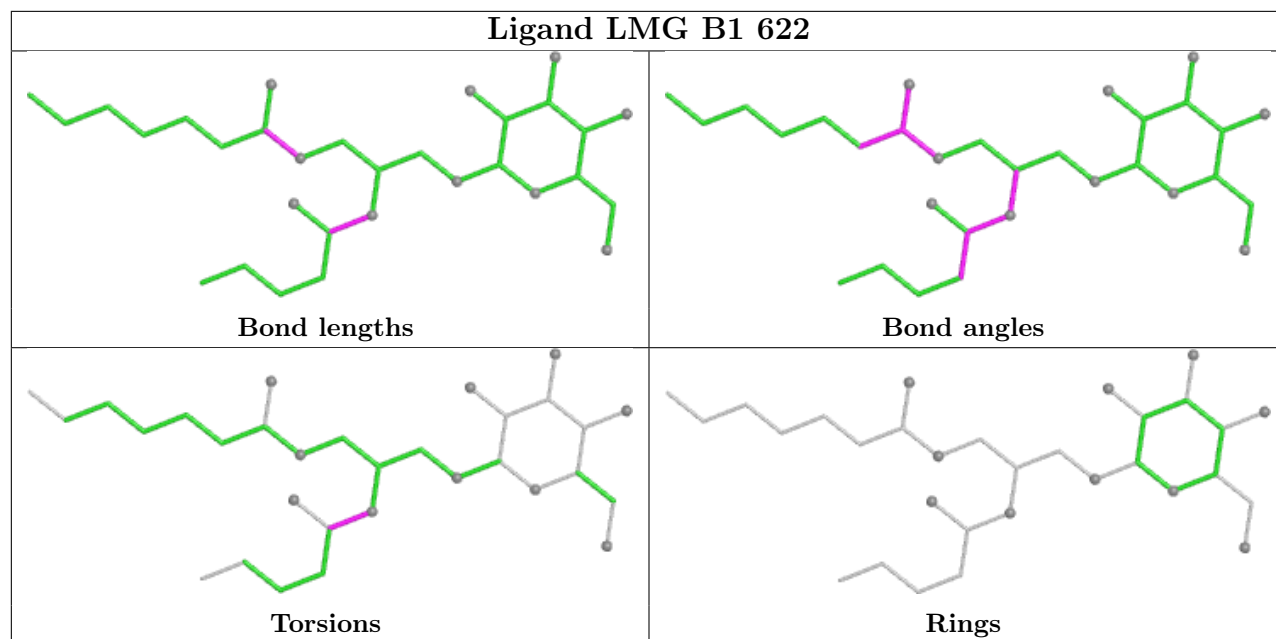


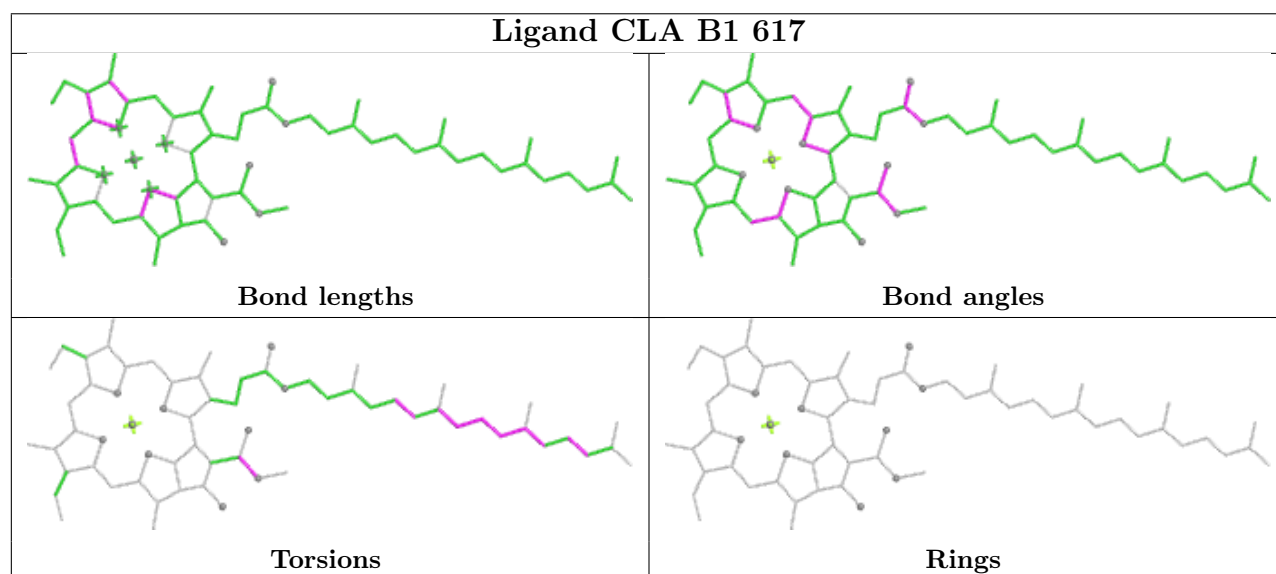
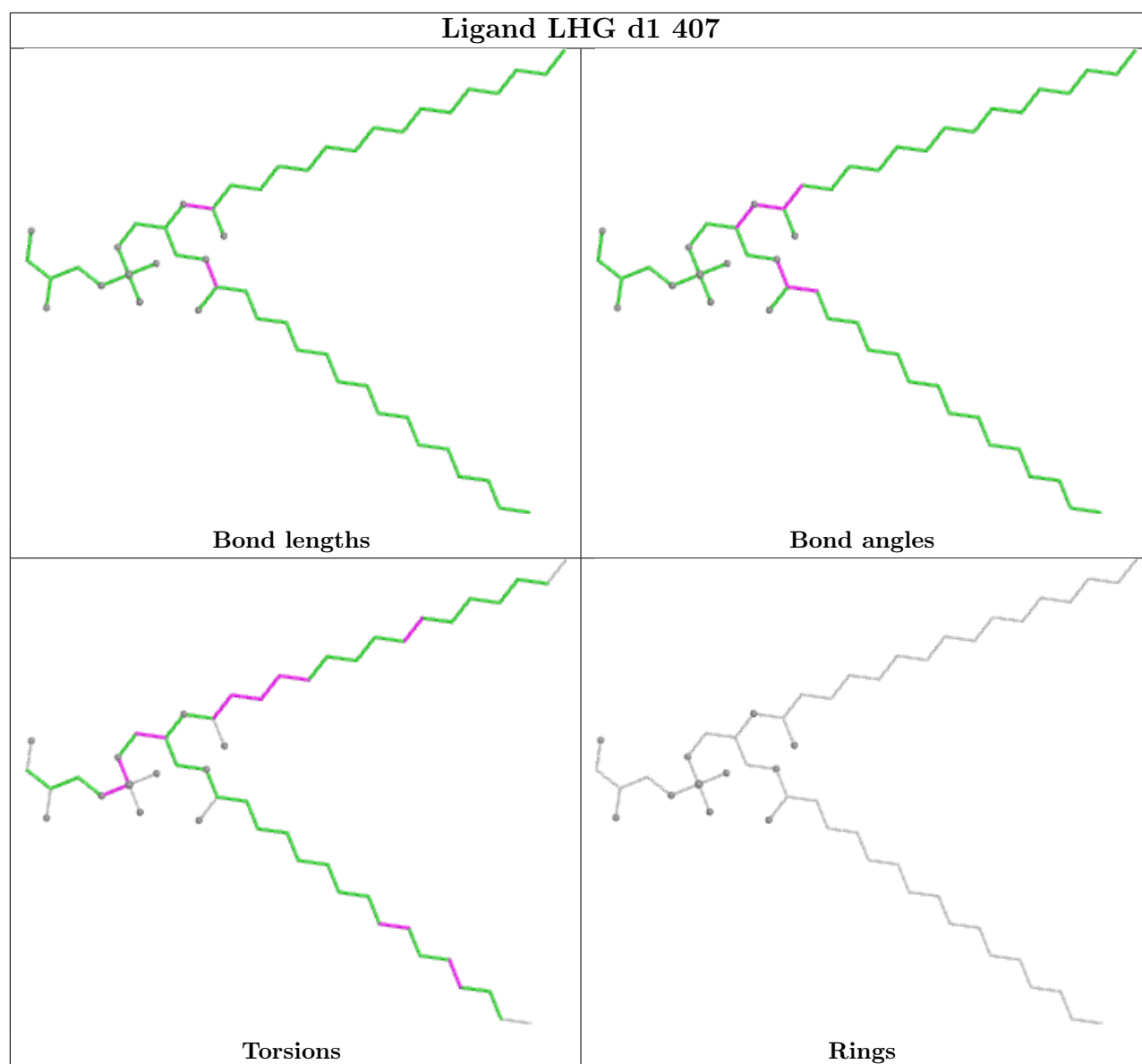


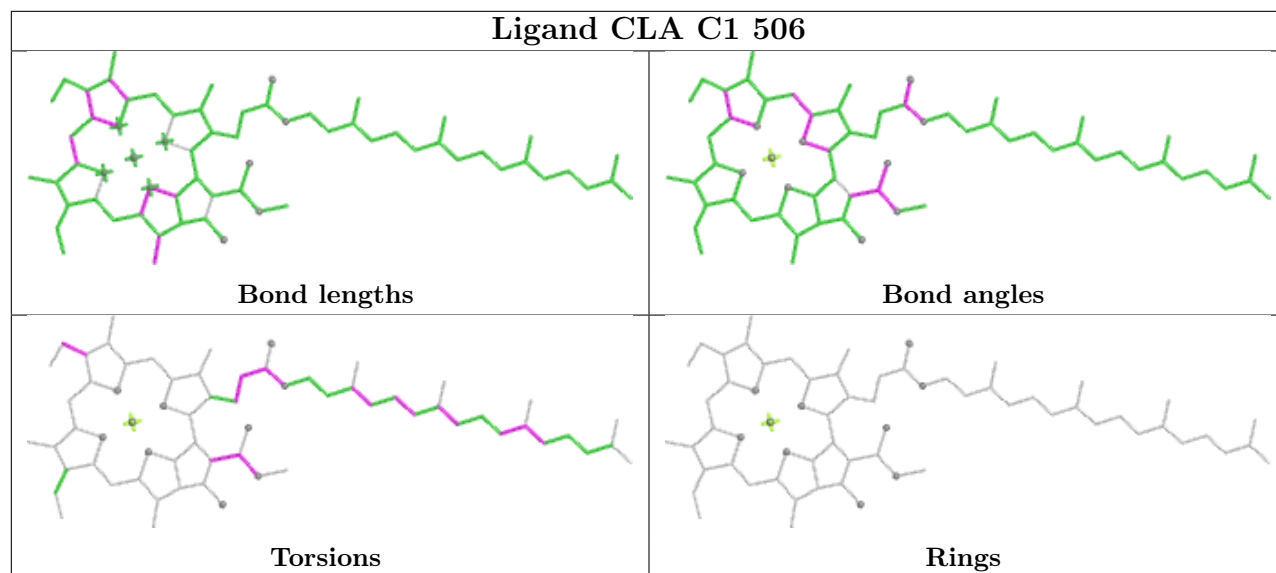
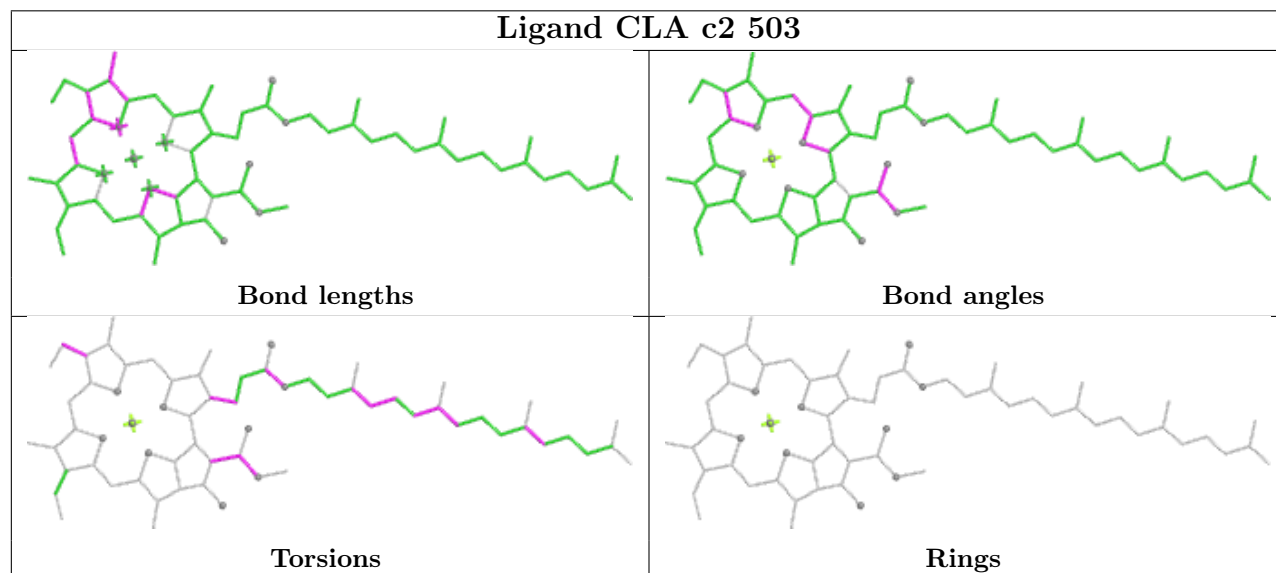
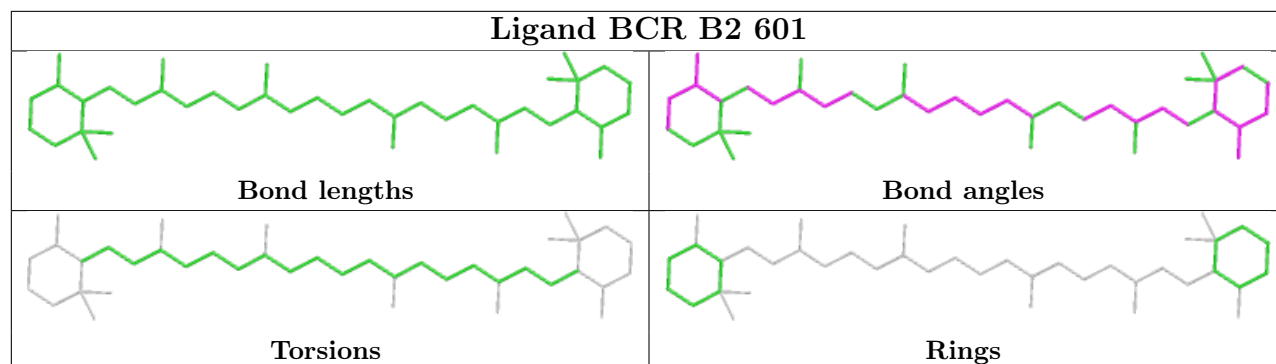




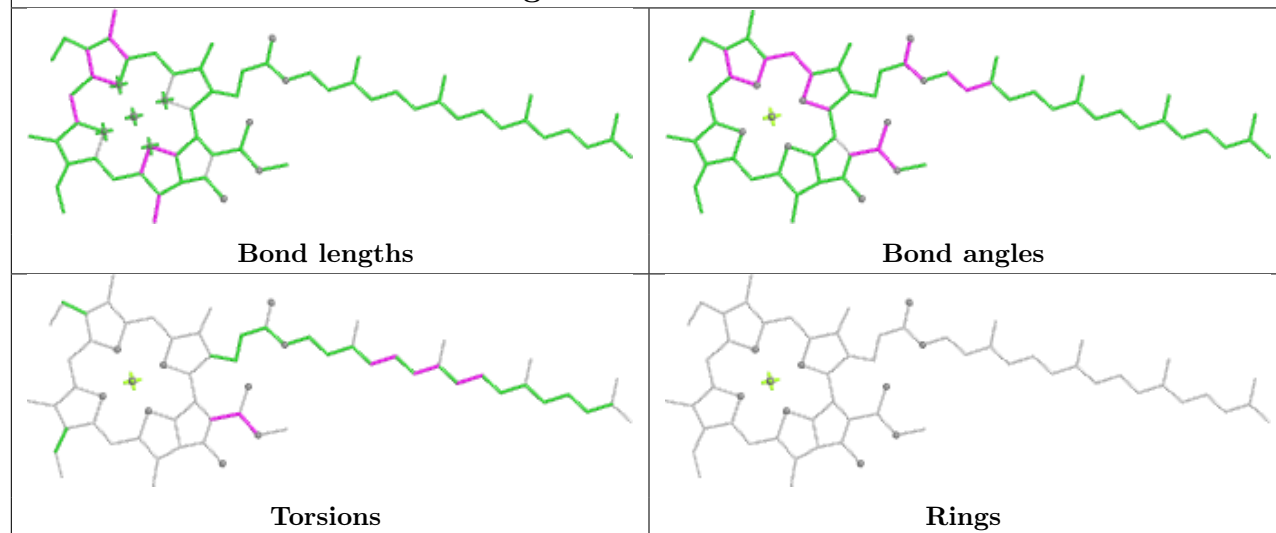




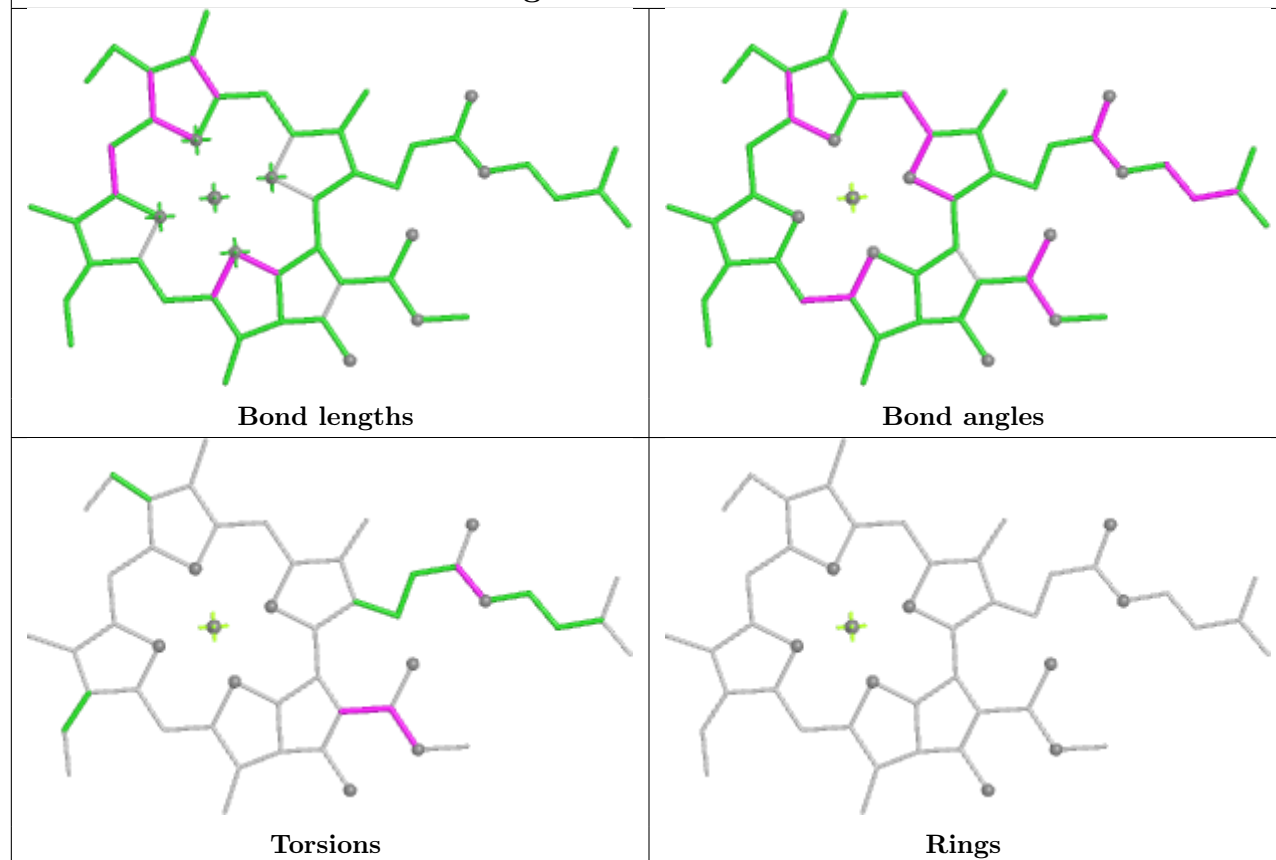


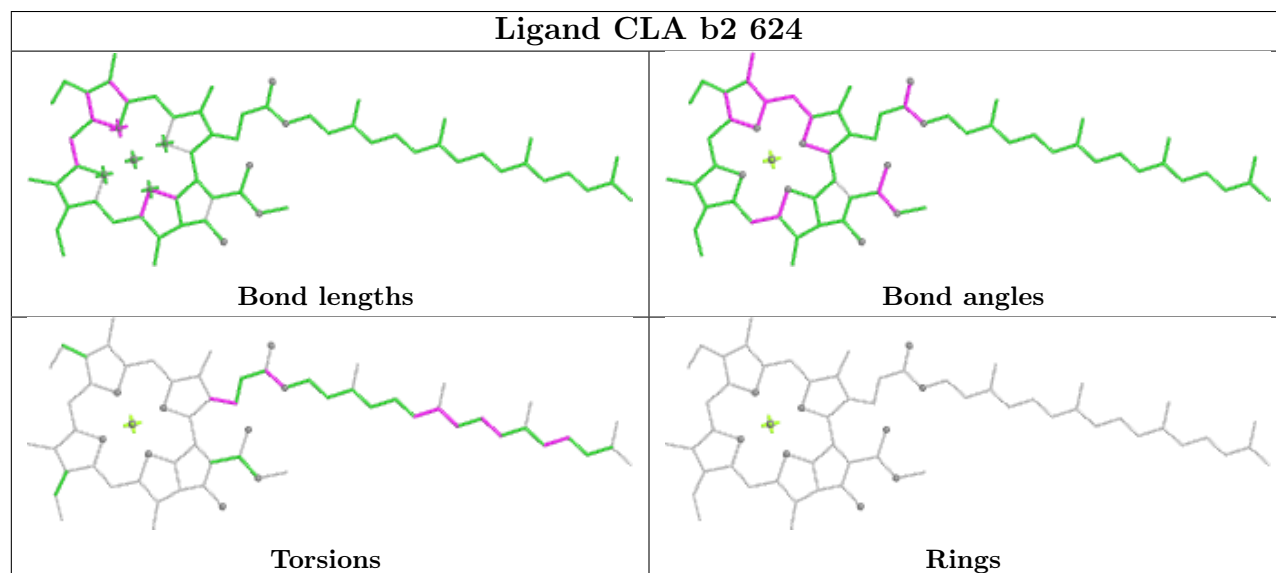
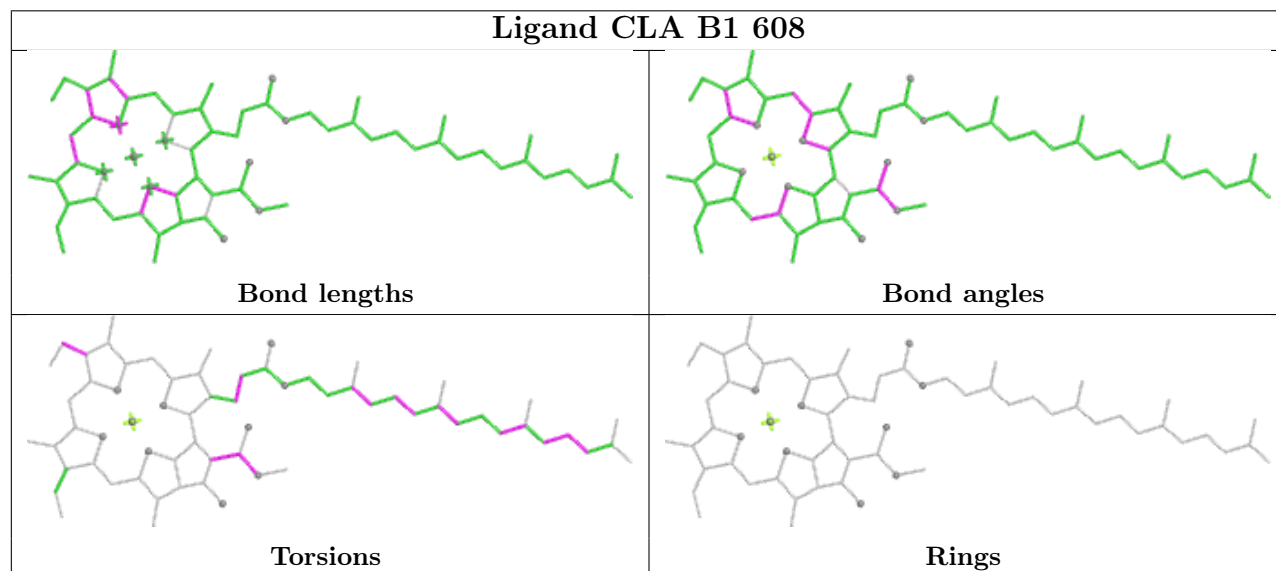
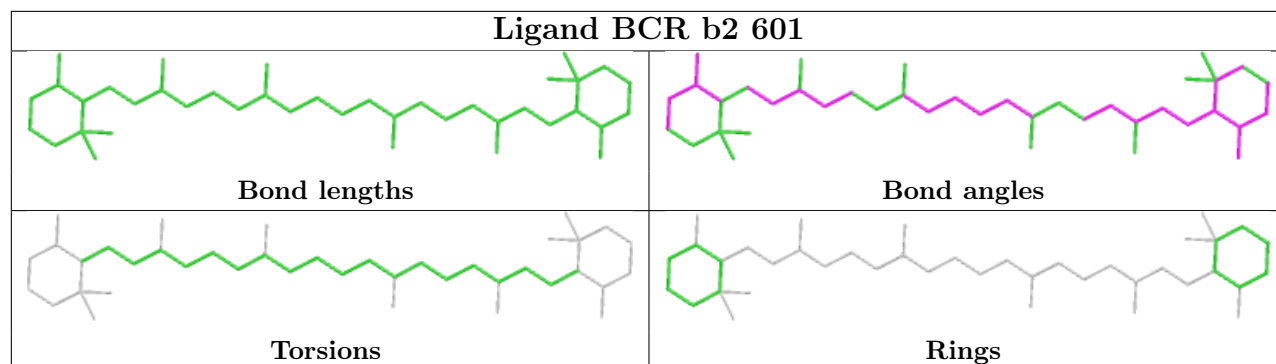


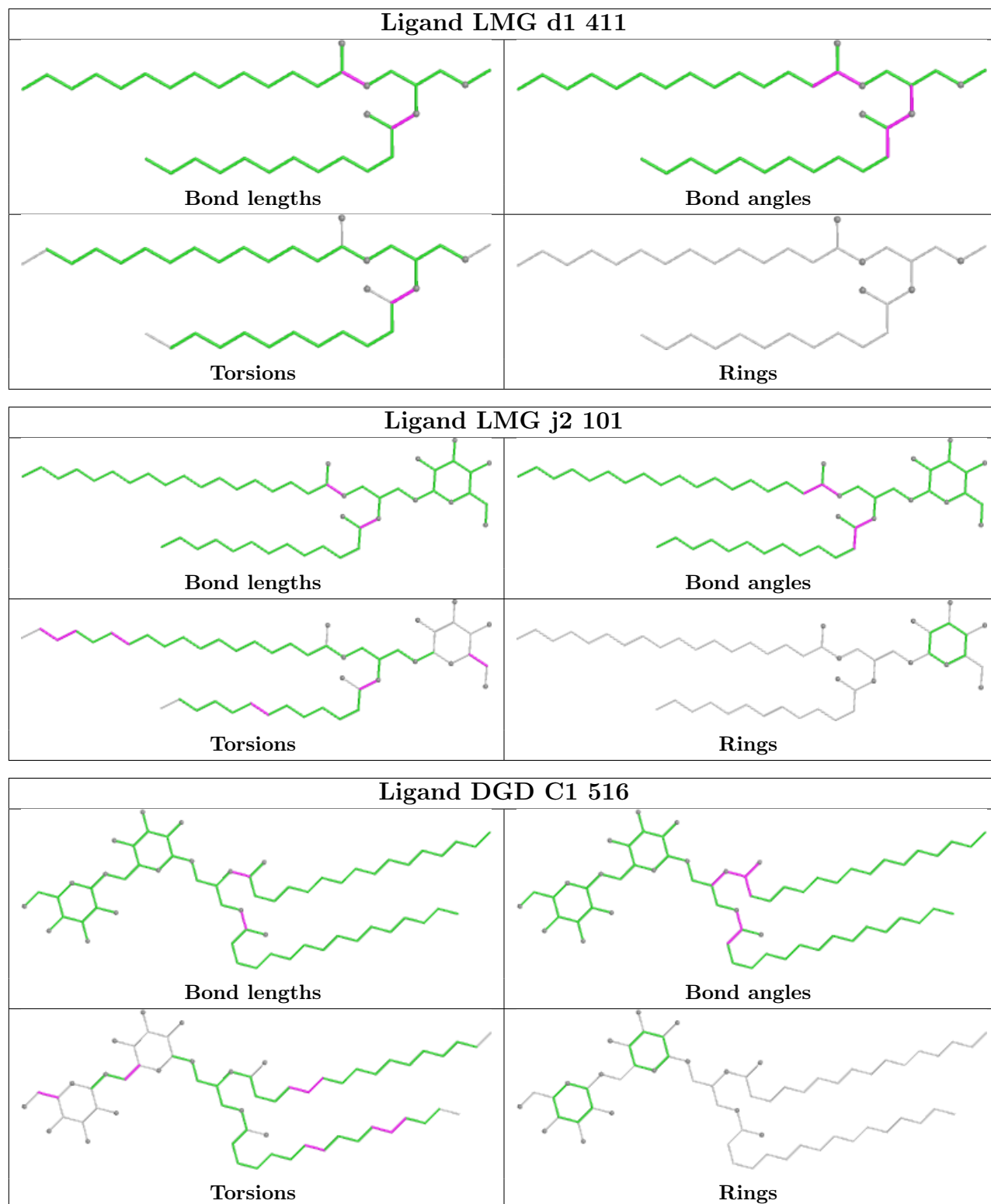
Ligand CLA B2 607



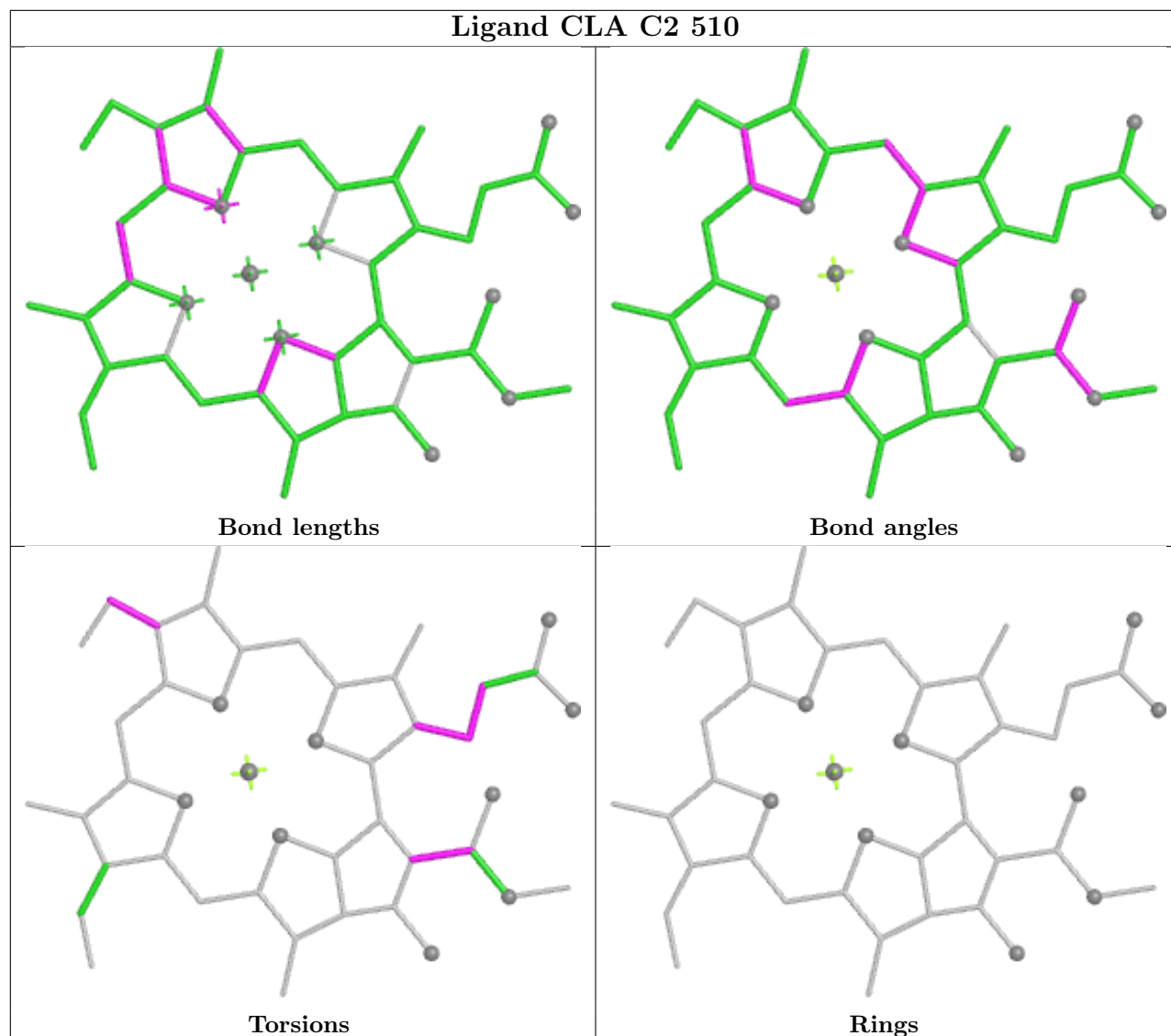
Ligand CLA C2 508

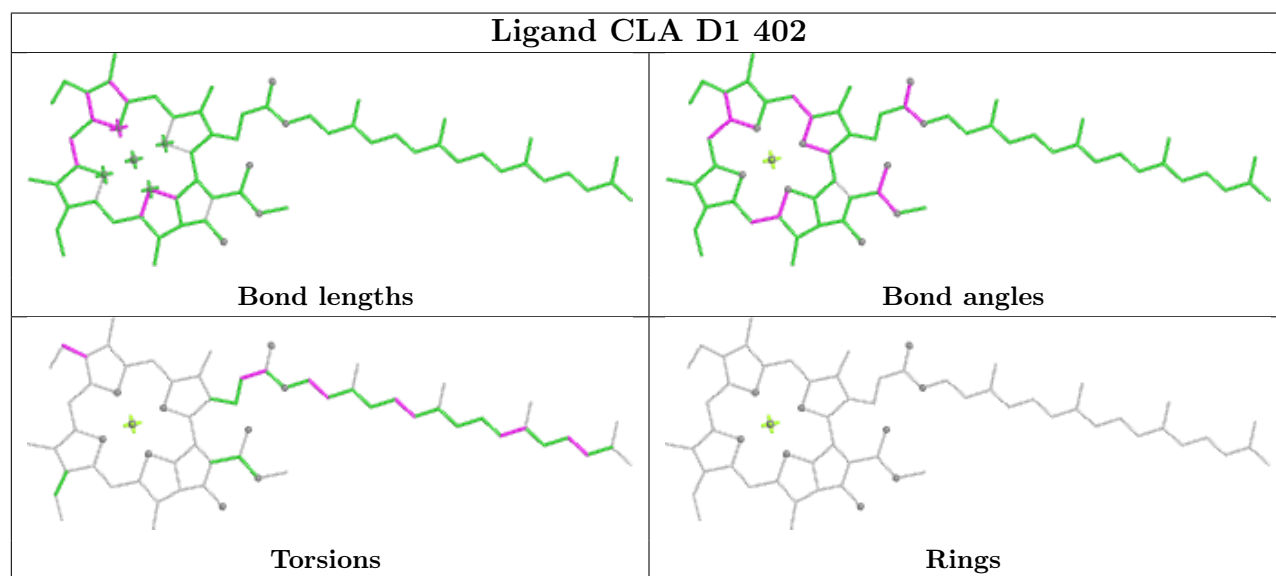
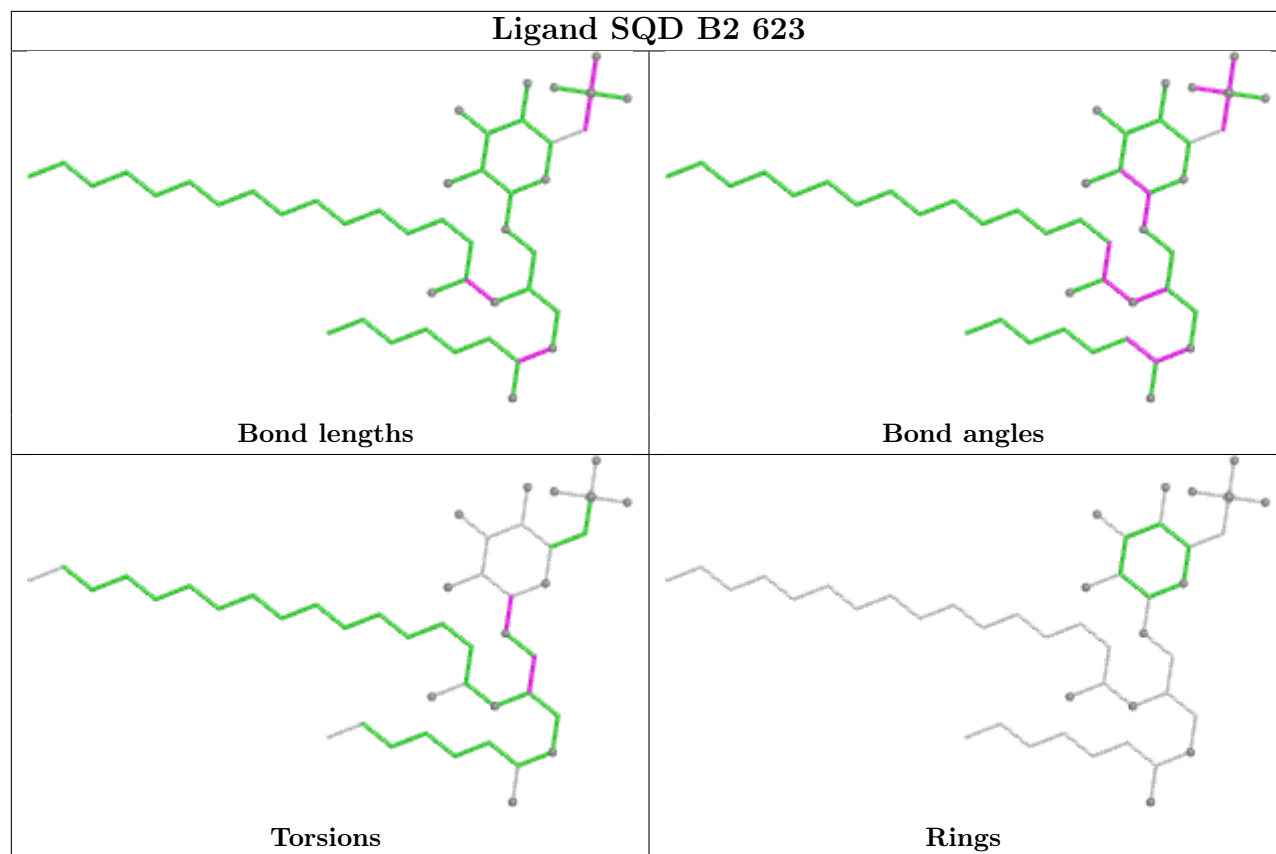


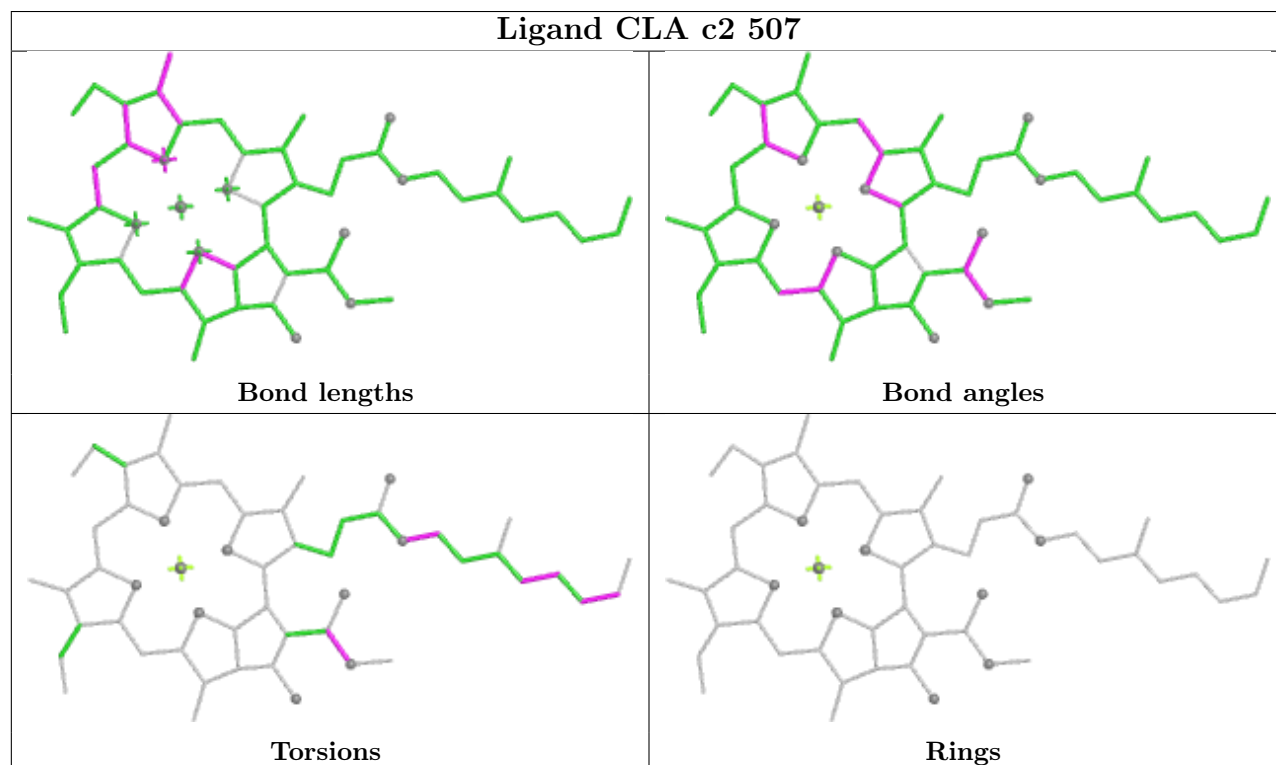
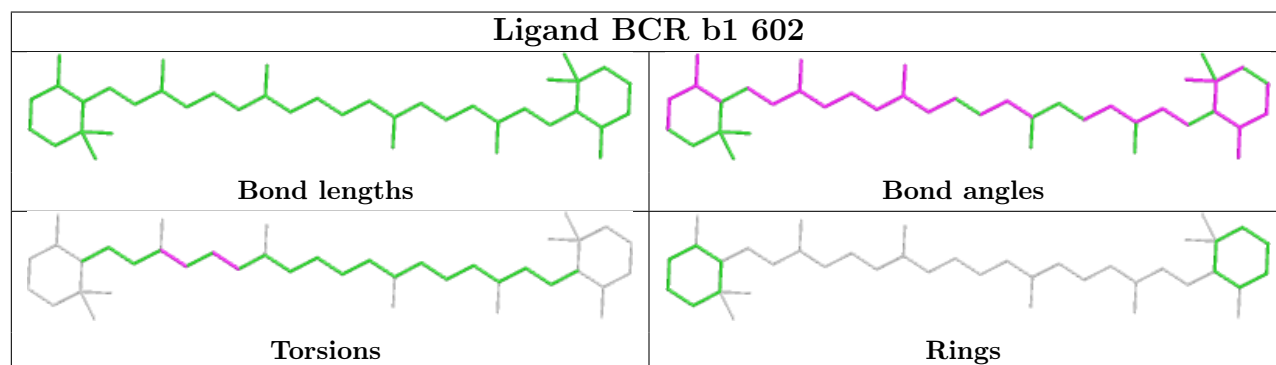
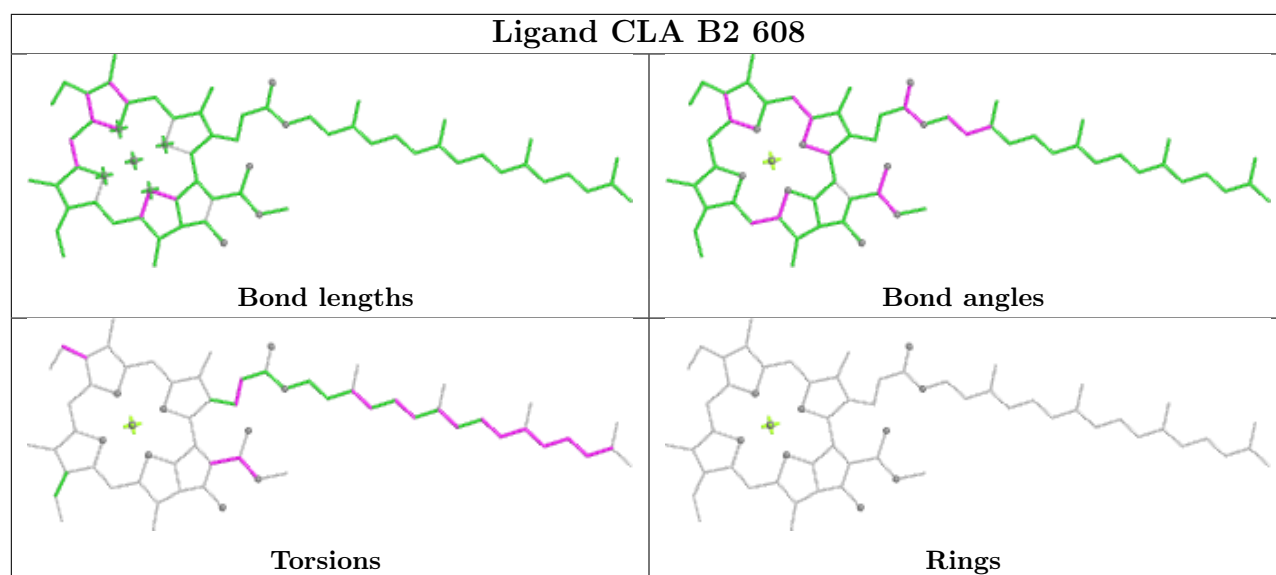


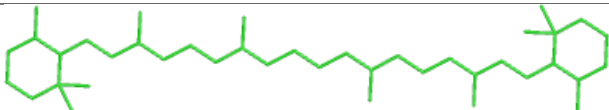
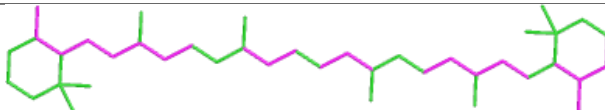
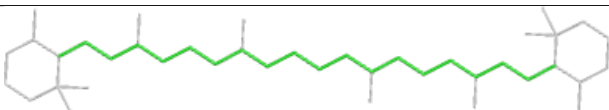
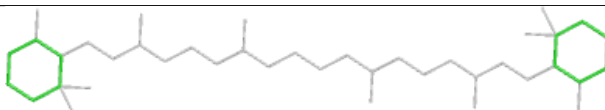


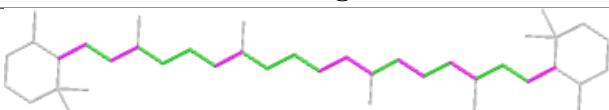
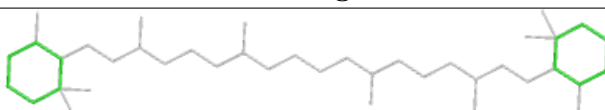
Ligand CLA C2 510



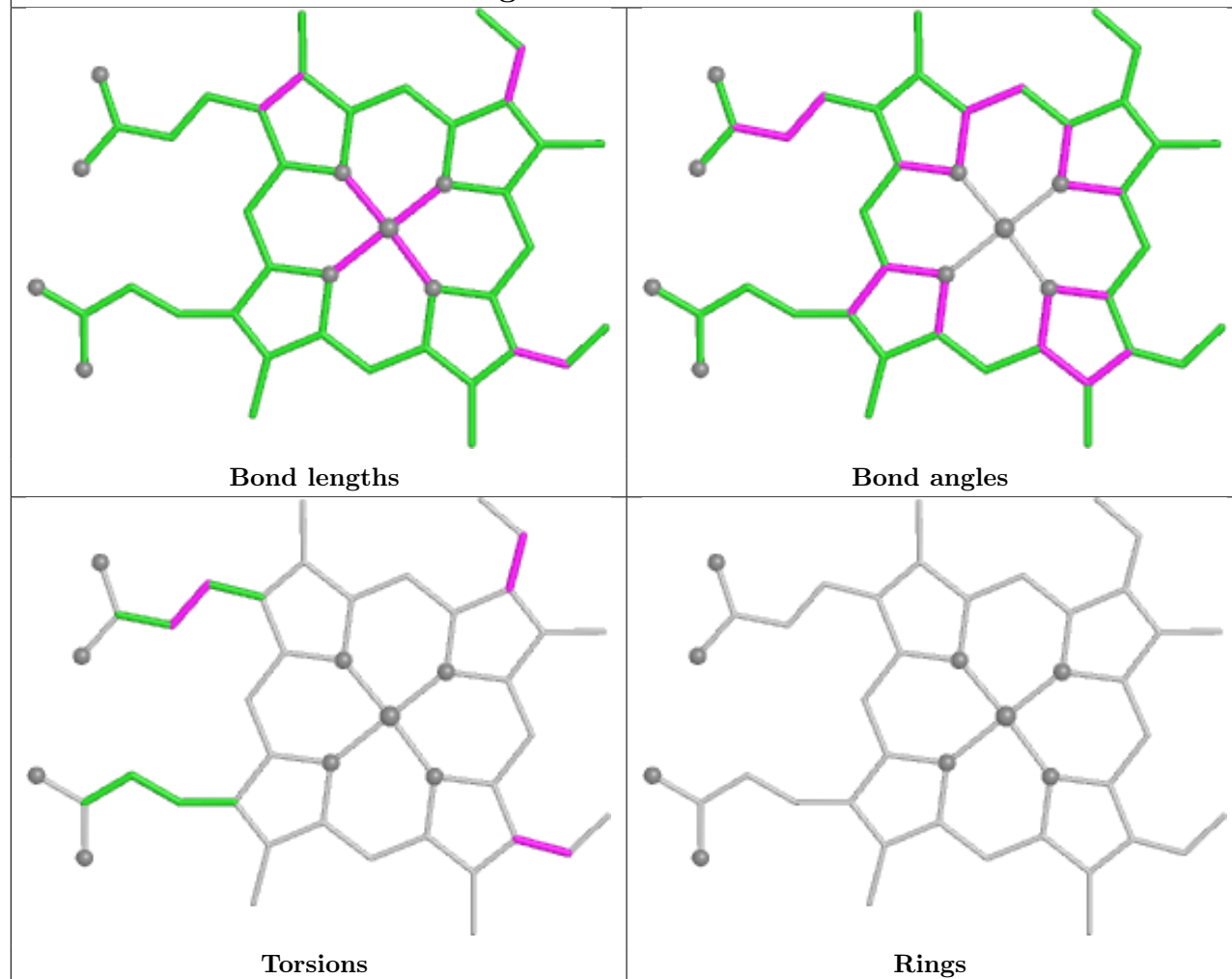




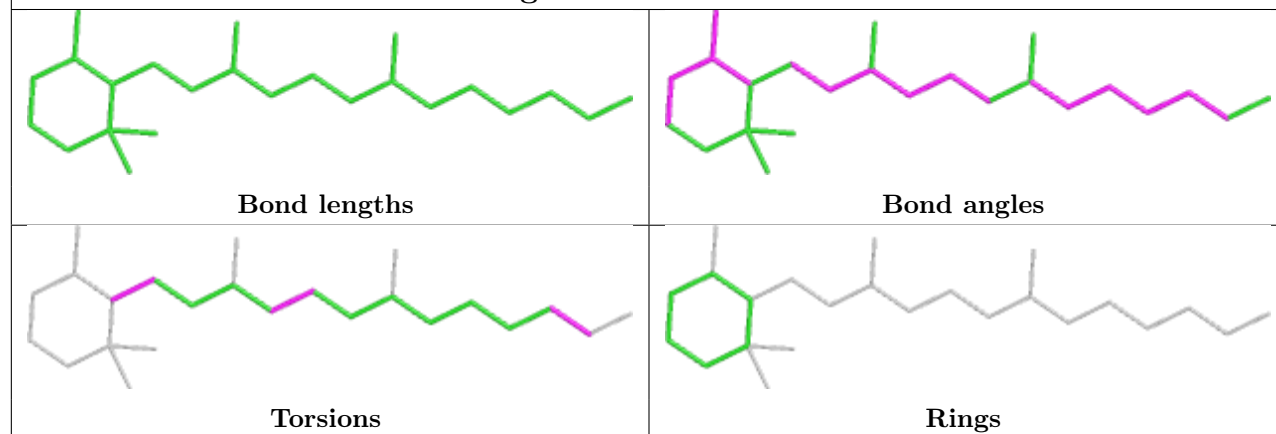
Ligand BCR z2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

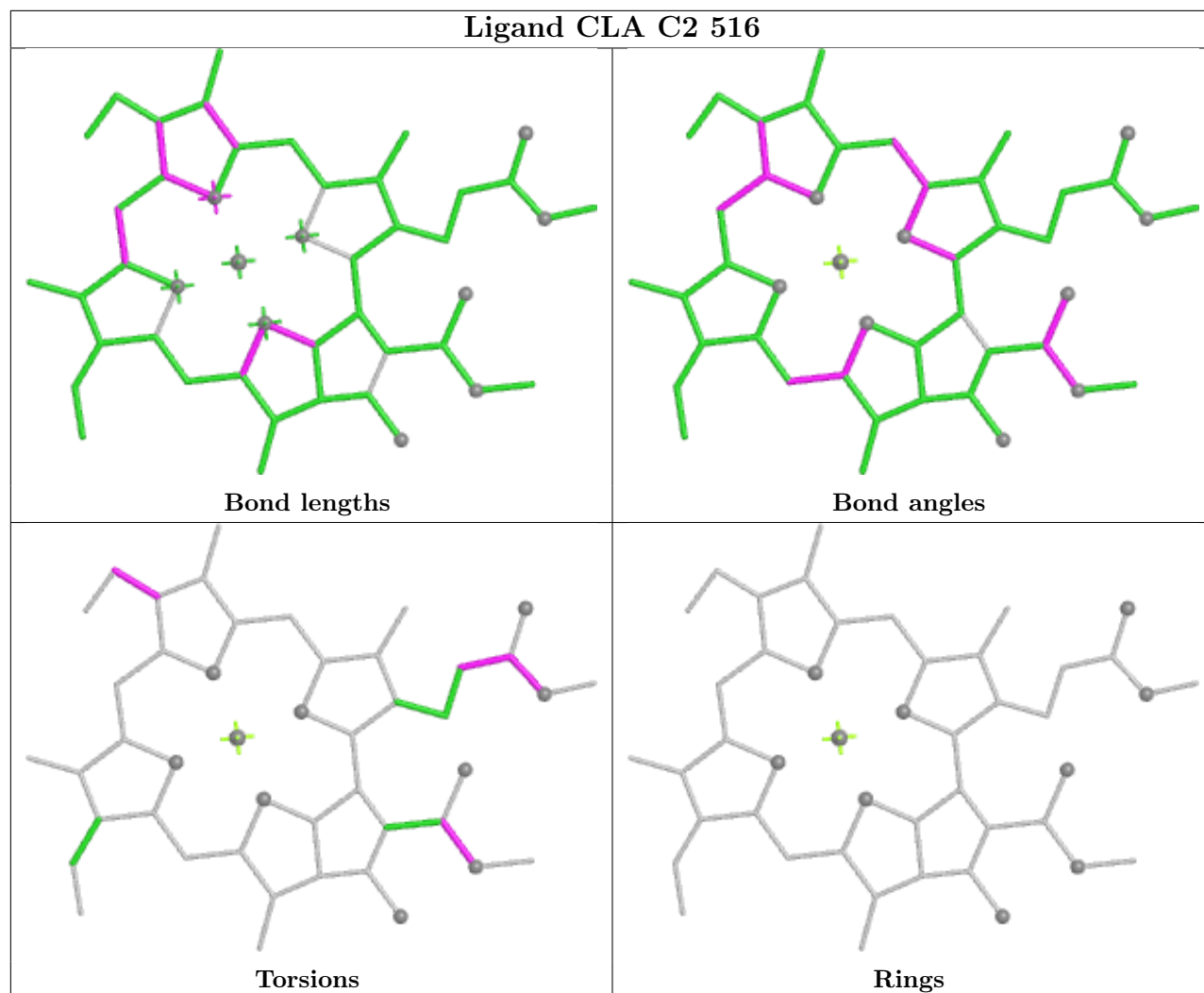
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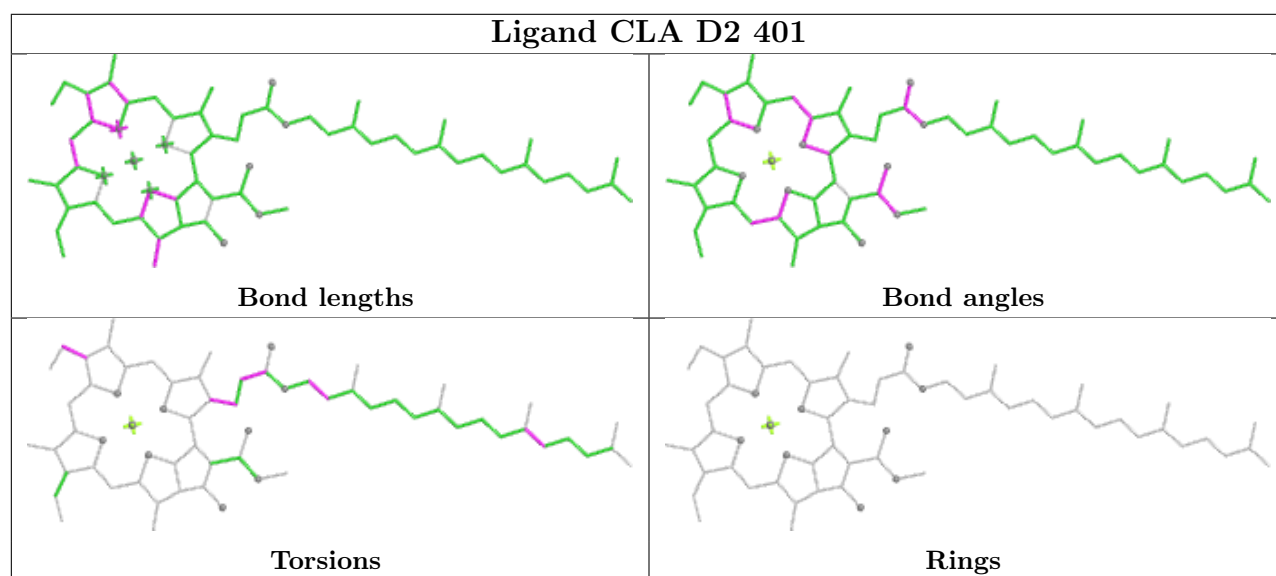
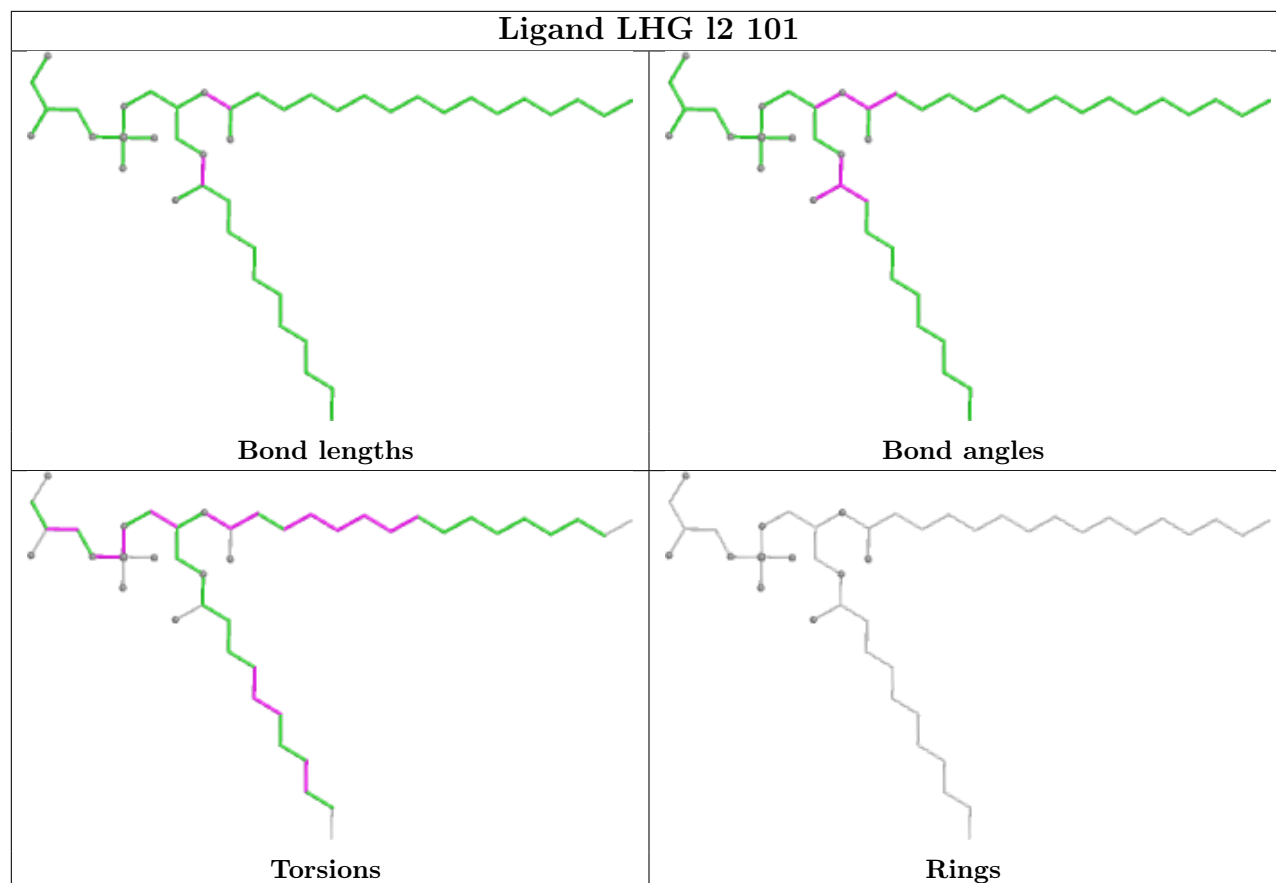


Ligand BCR H2 103

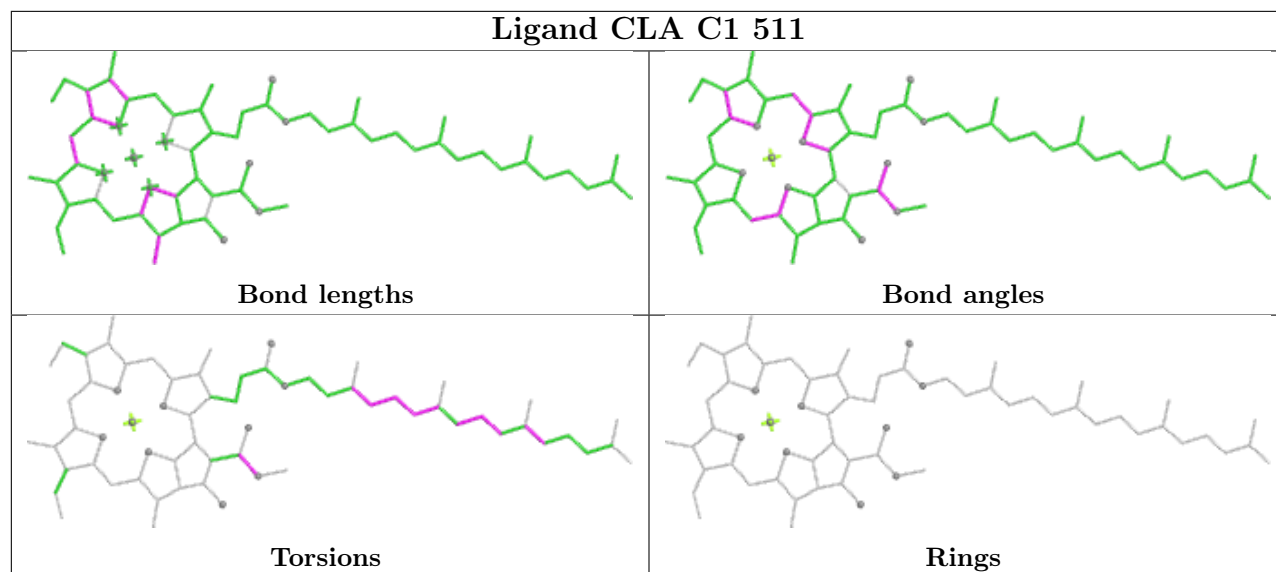


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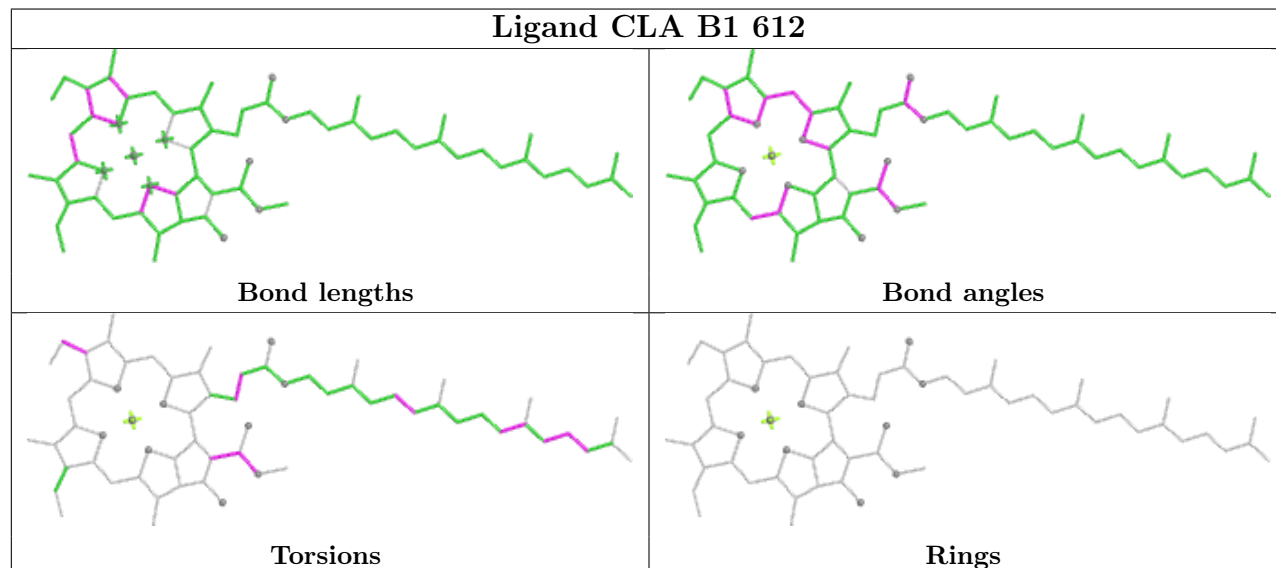




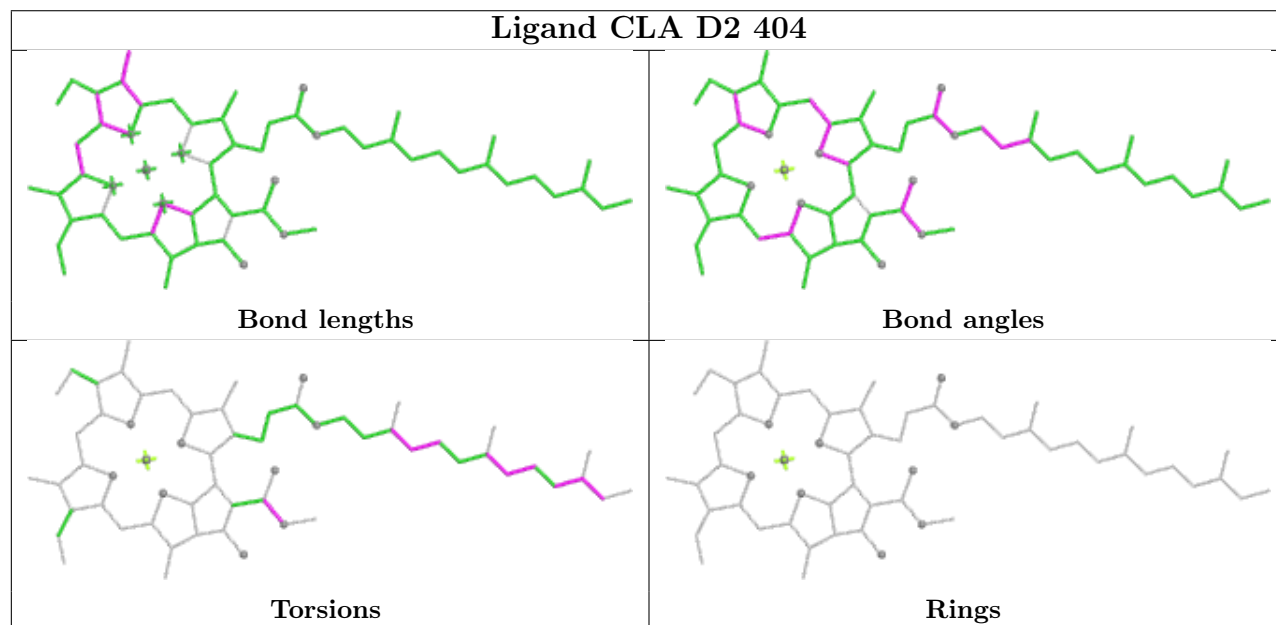
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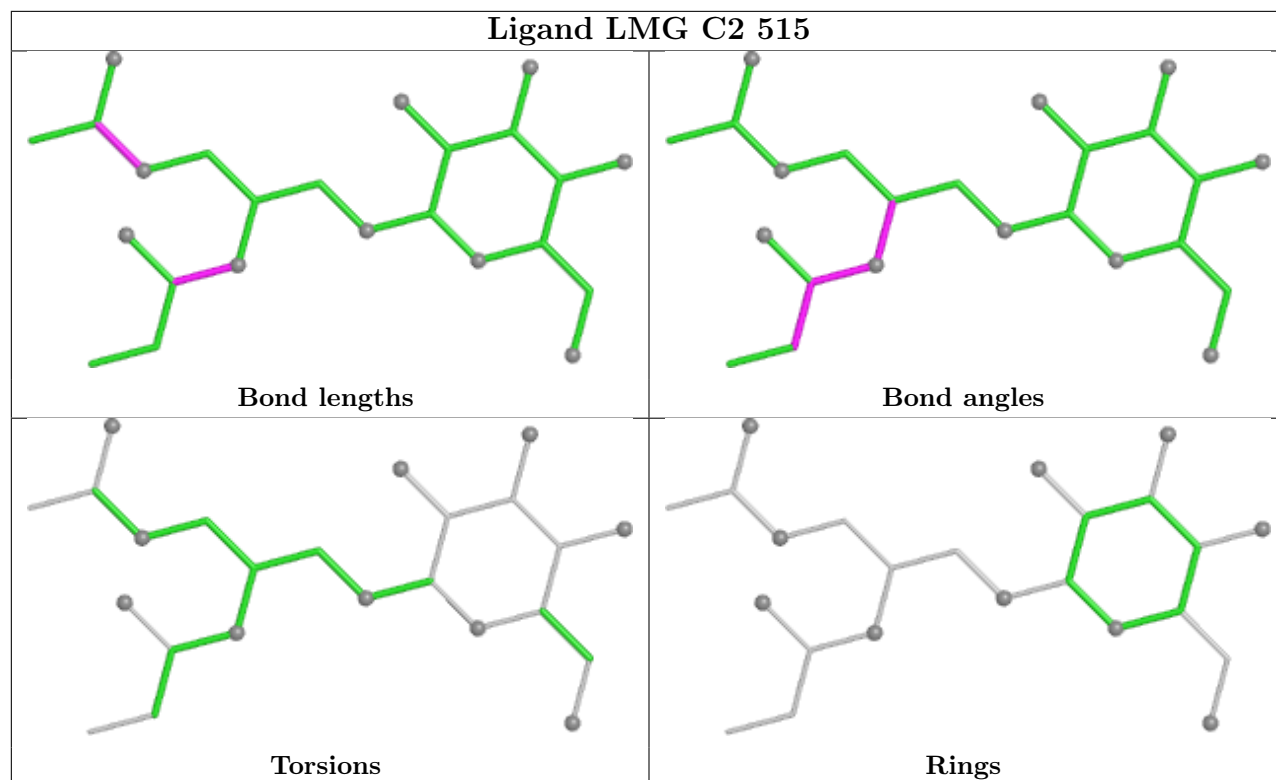


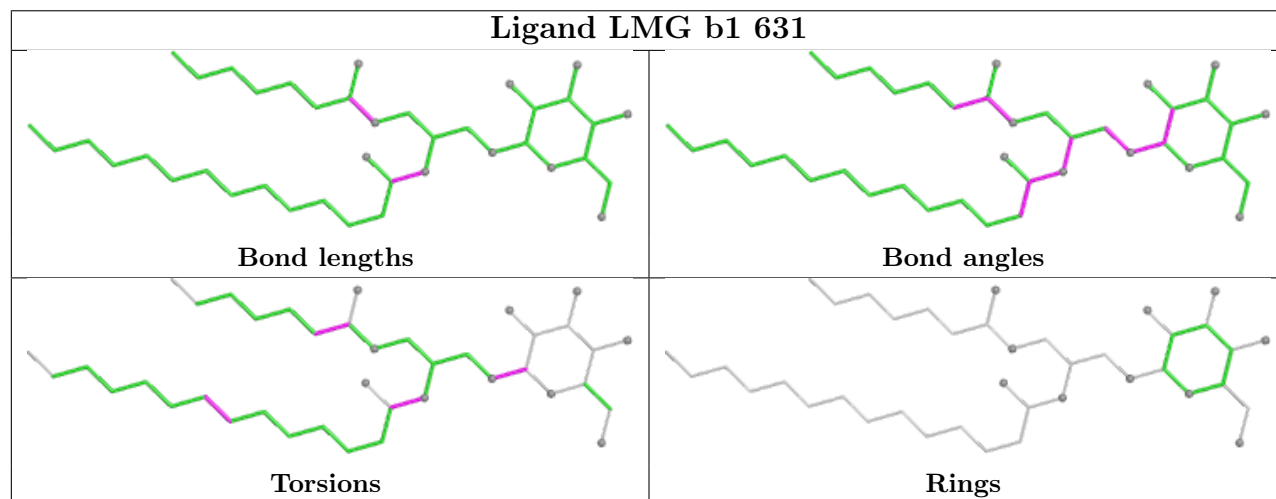
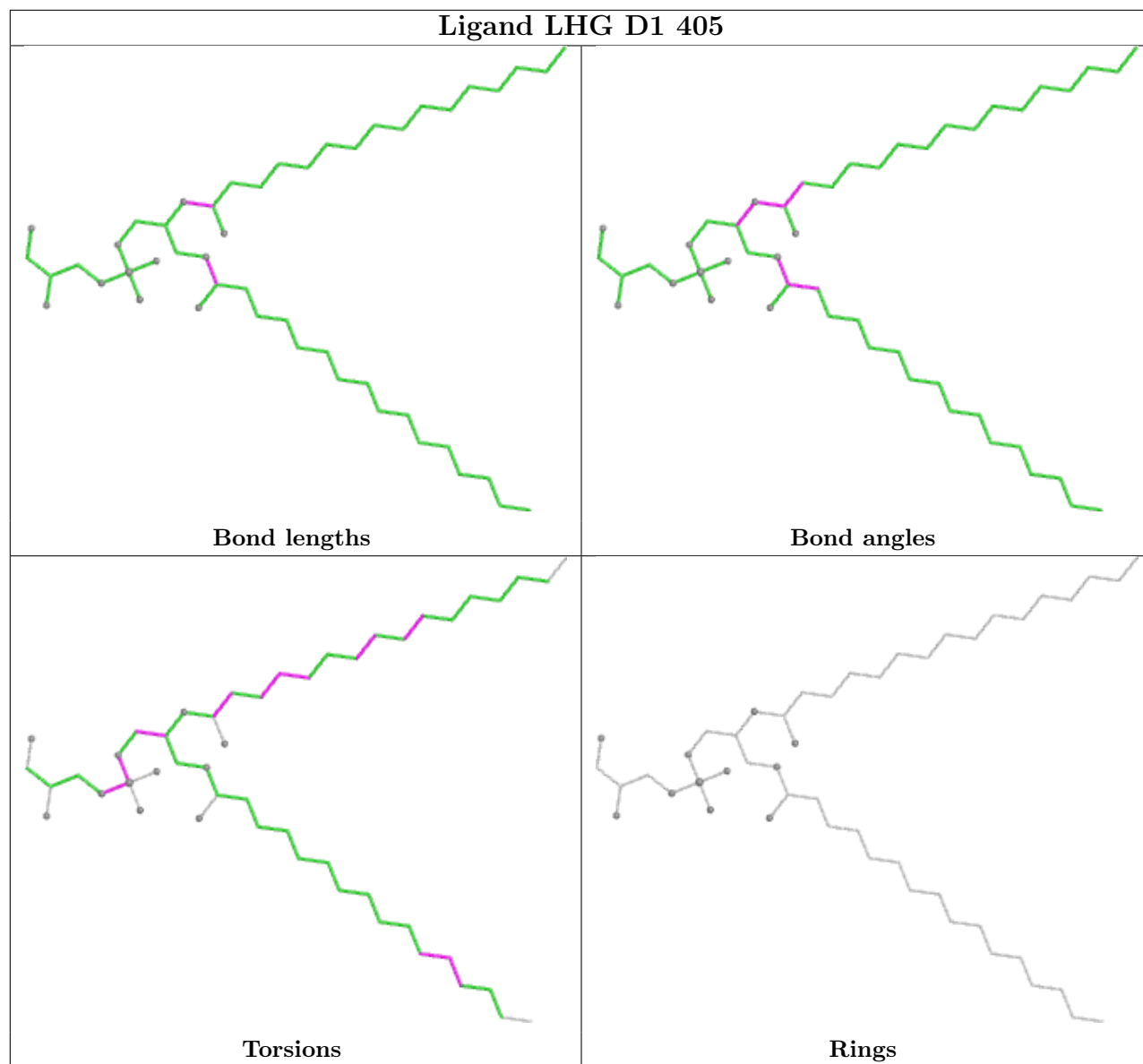
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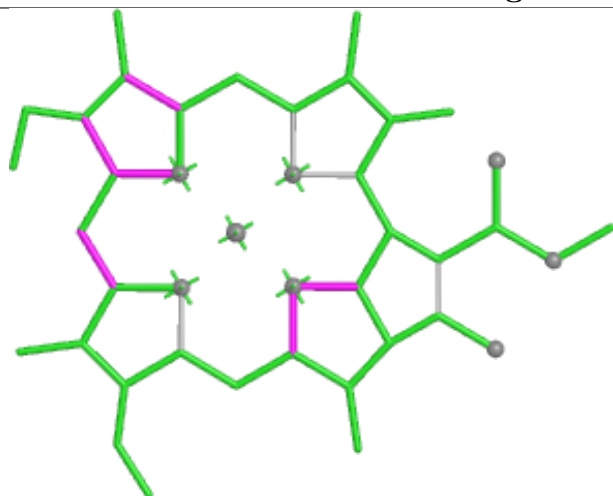
Ligand CLA D2 404



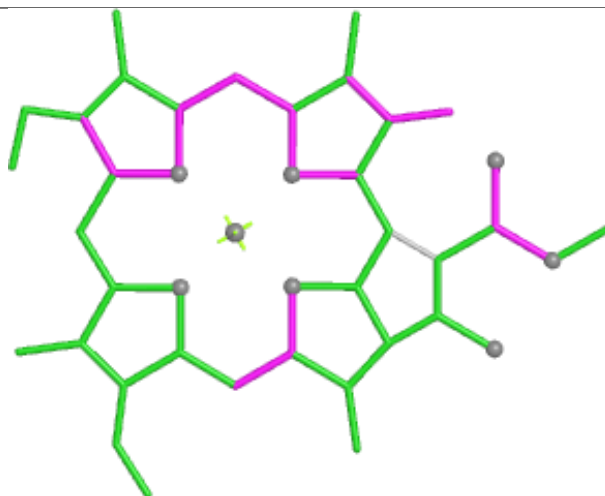




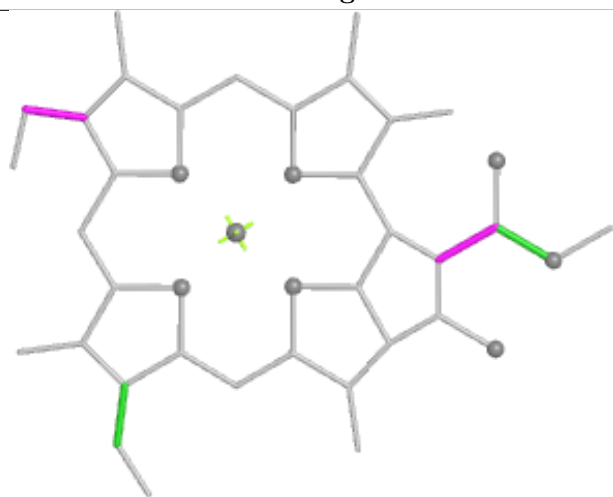
Ligand CLA B2 604



Bond lengths



Bond angles

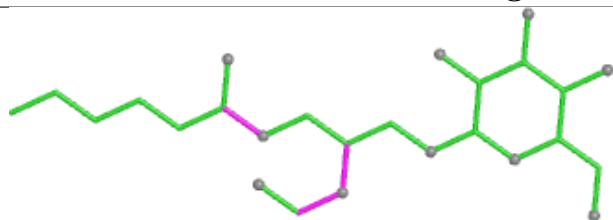


Torsions

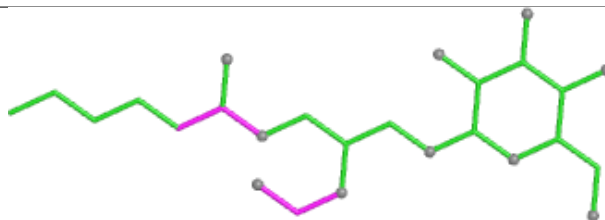


Rings

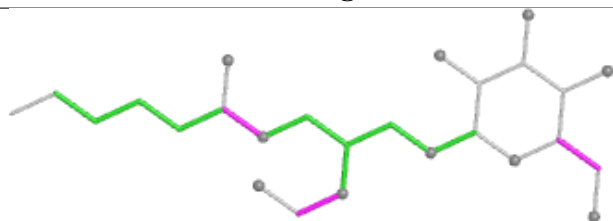
Ligand LMG c2 519



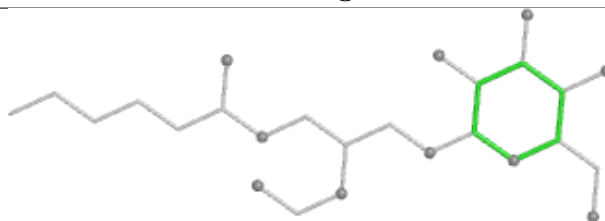
Bond lengths



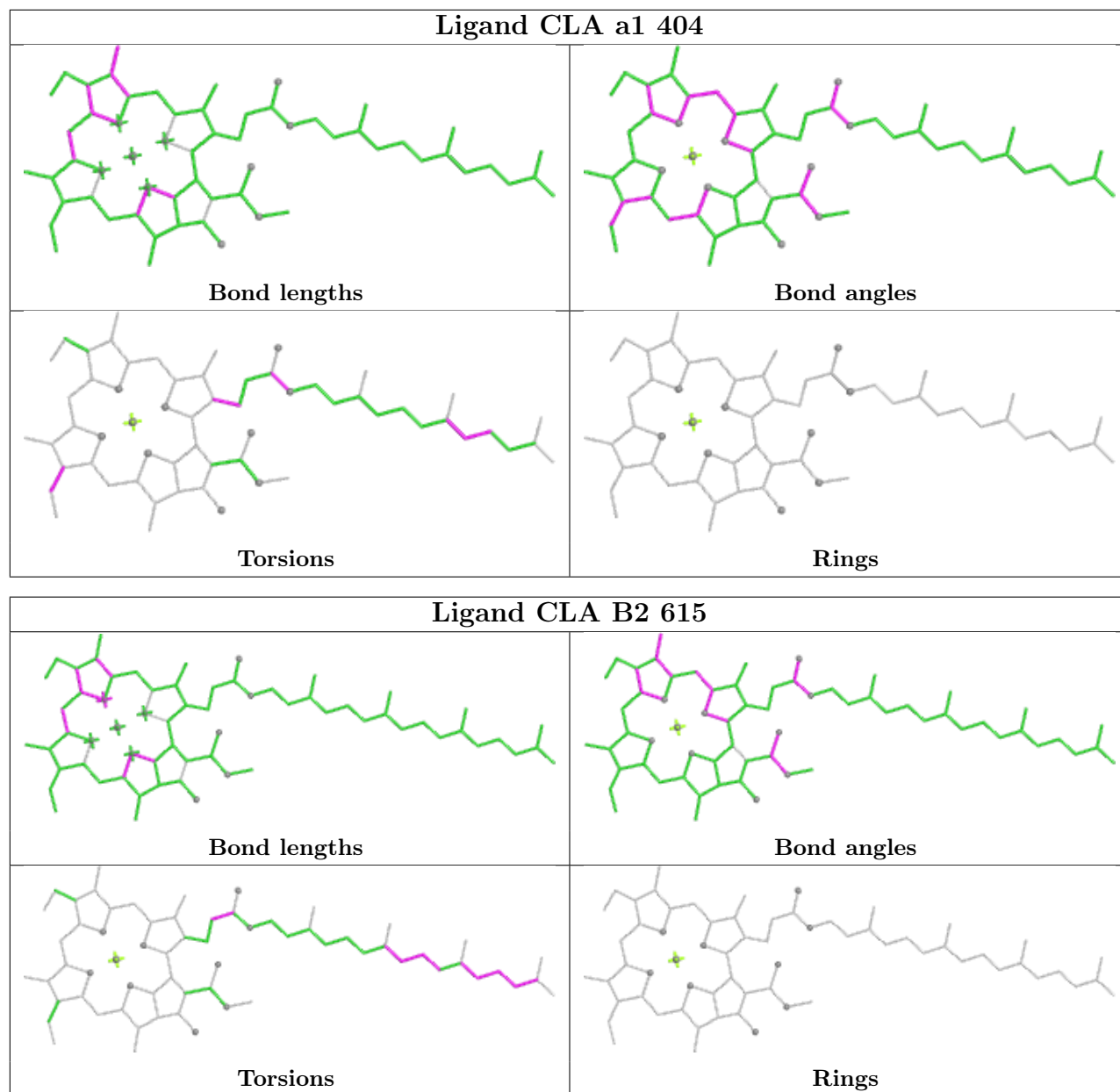
Bond angles

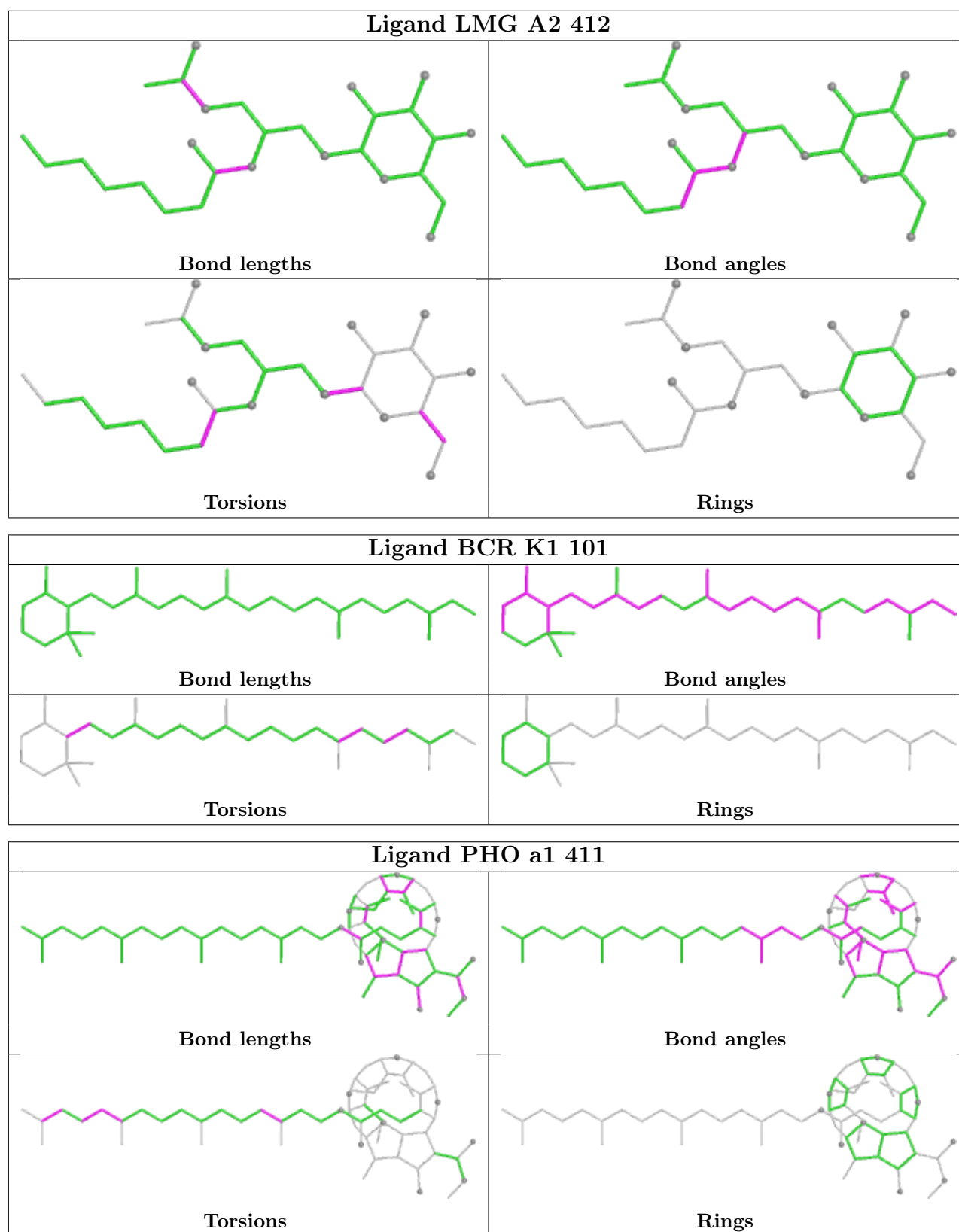


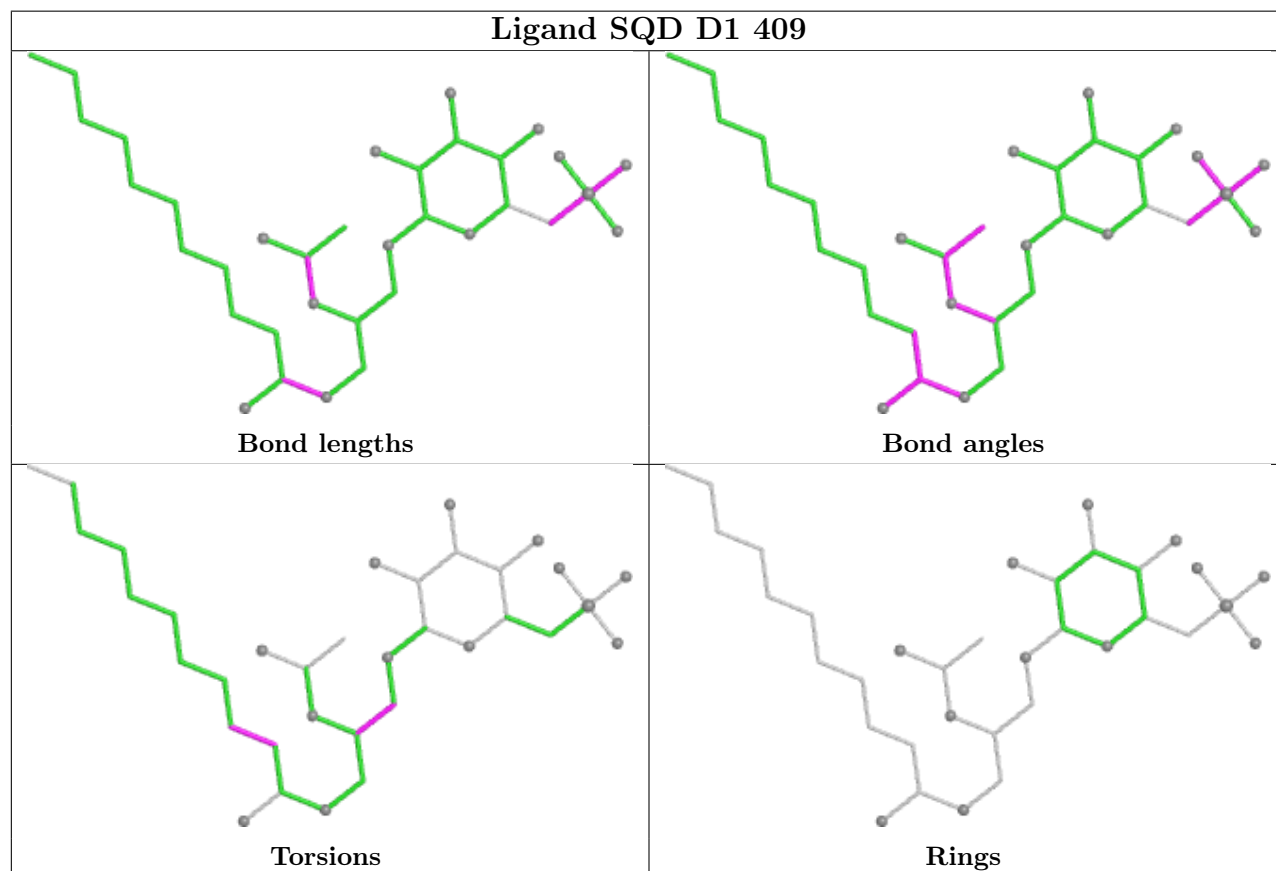
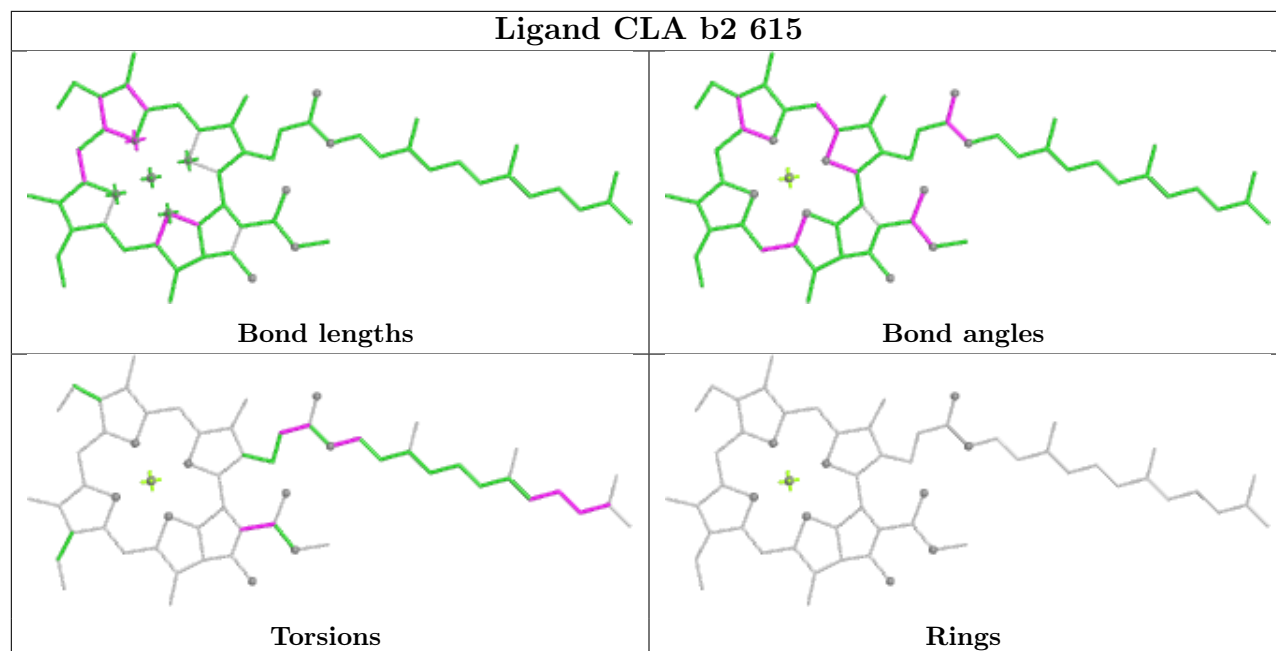
Torsions

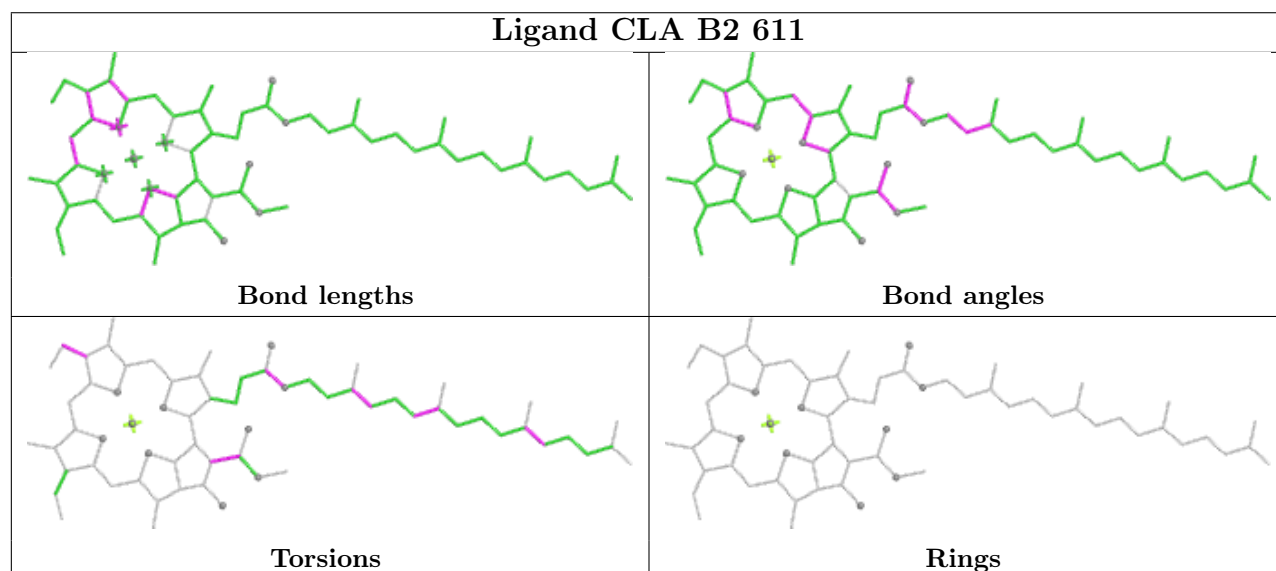
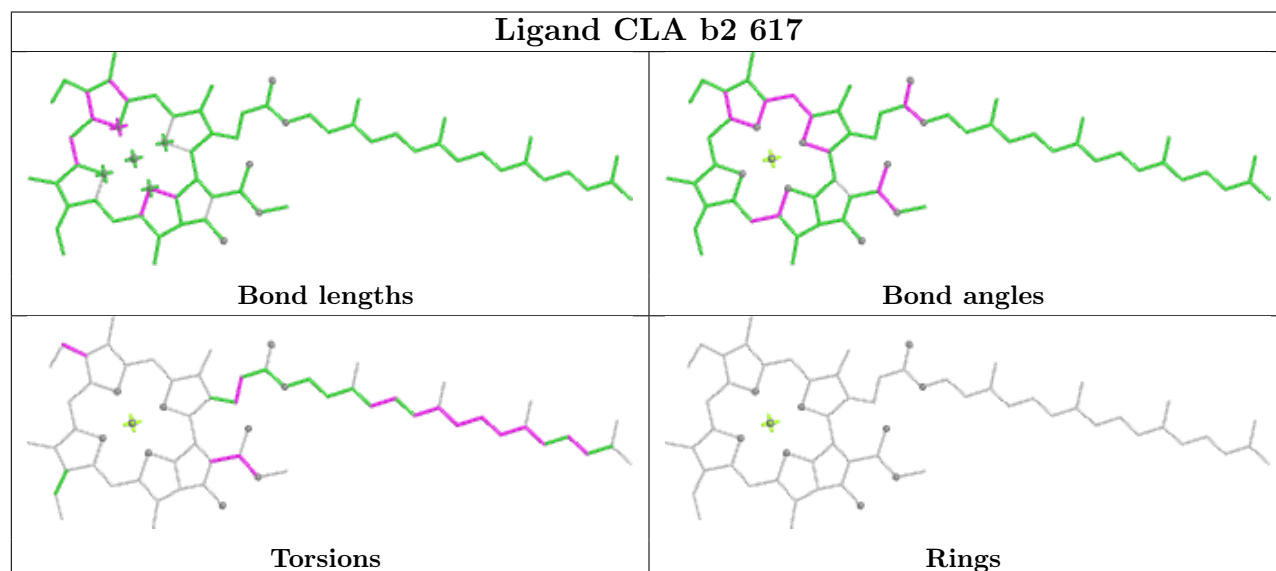
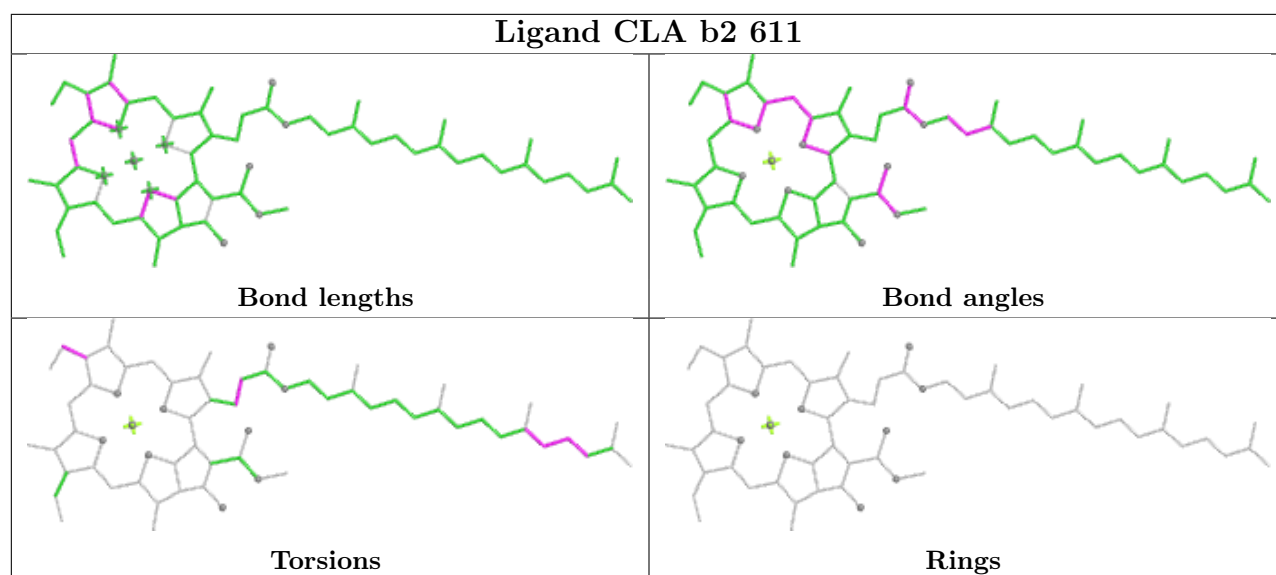


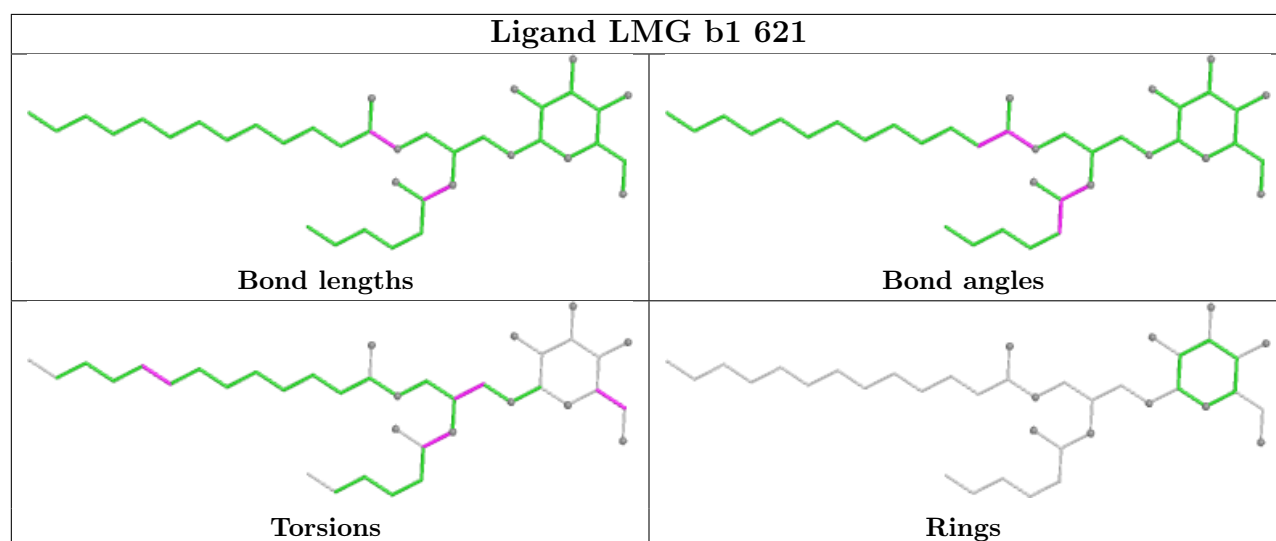
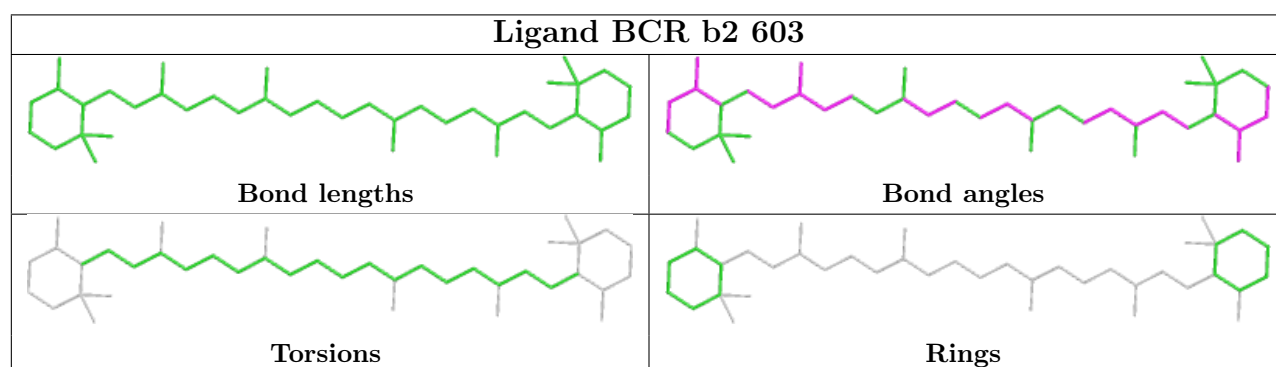
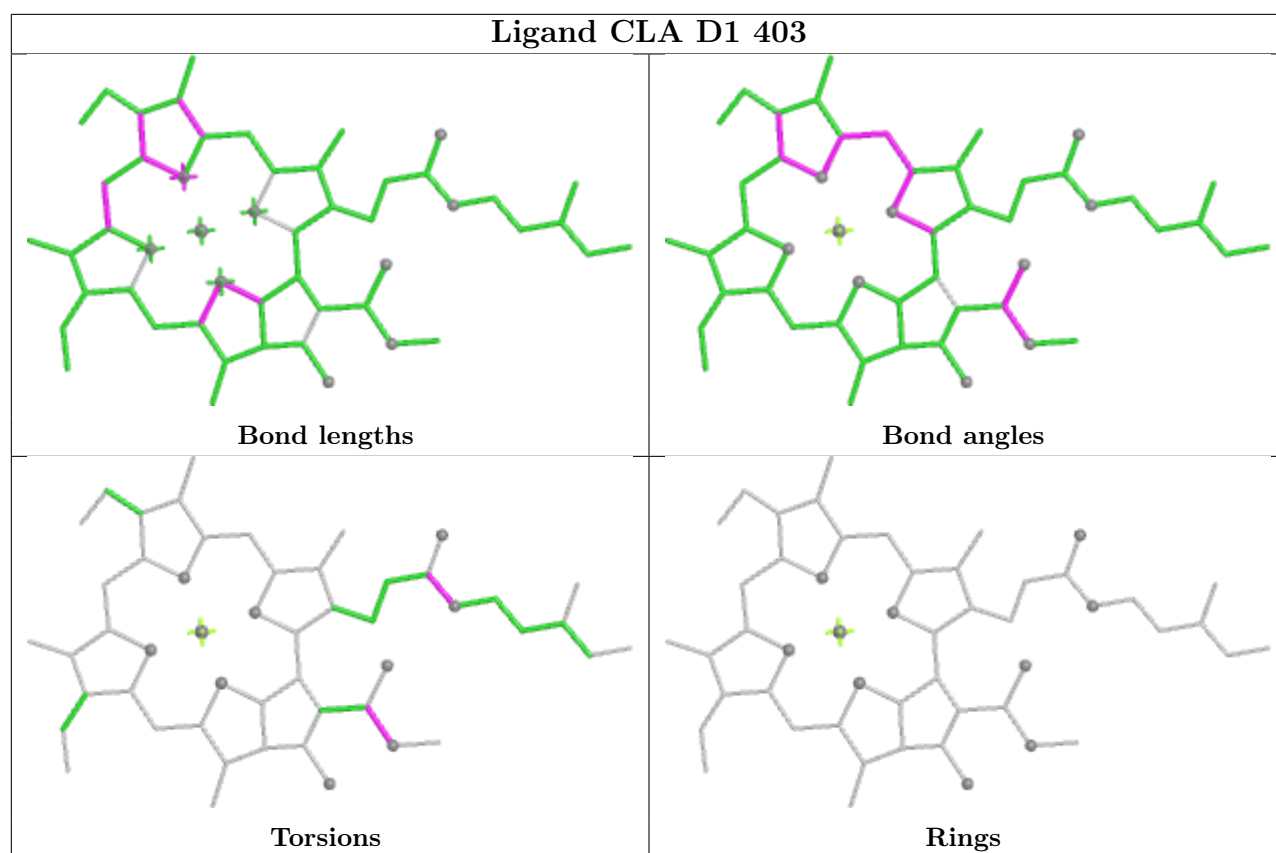
Rings

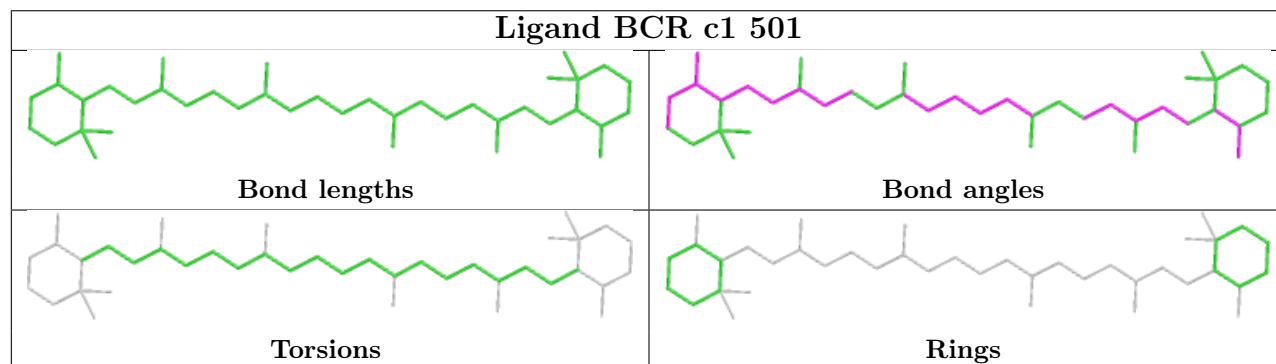
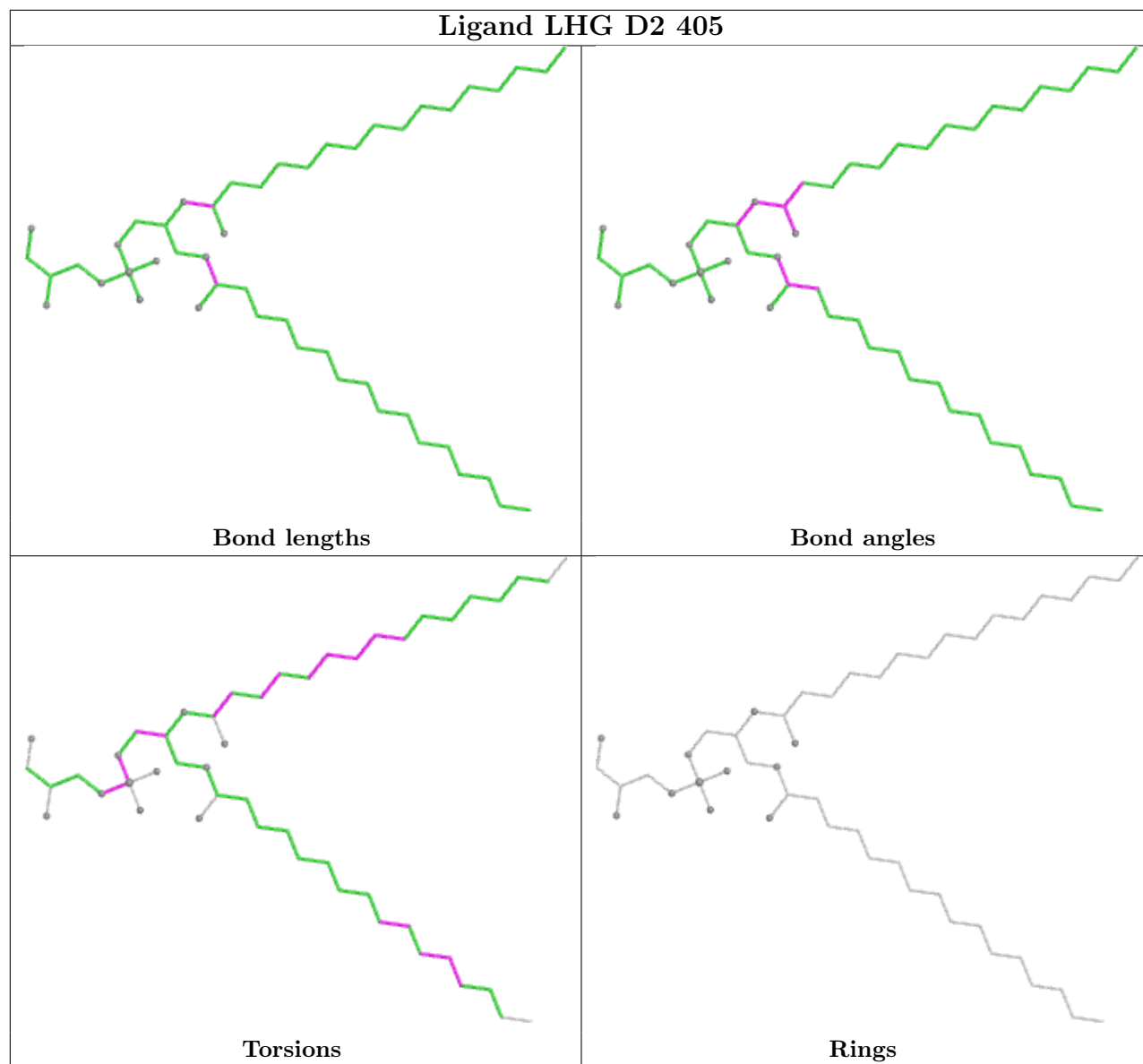


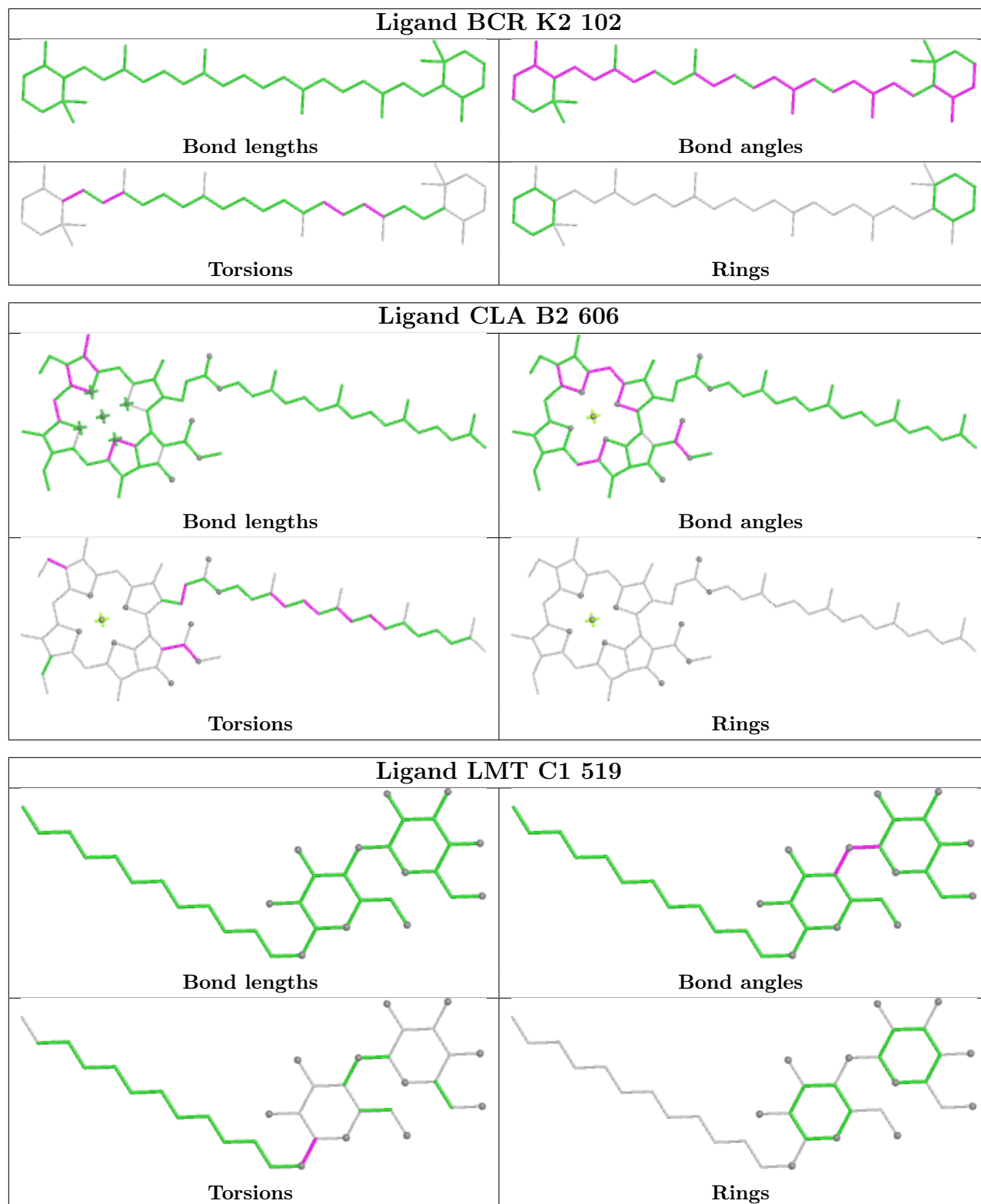


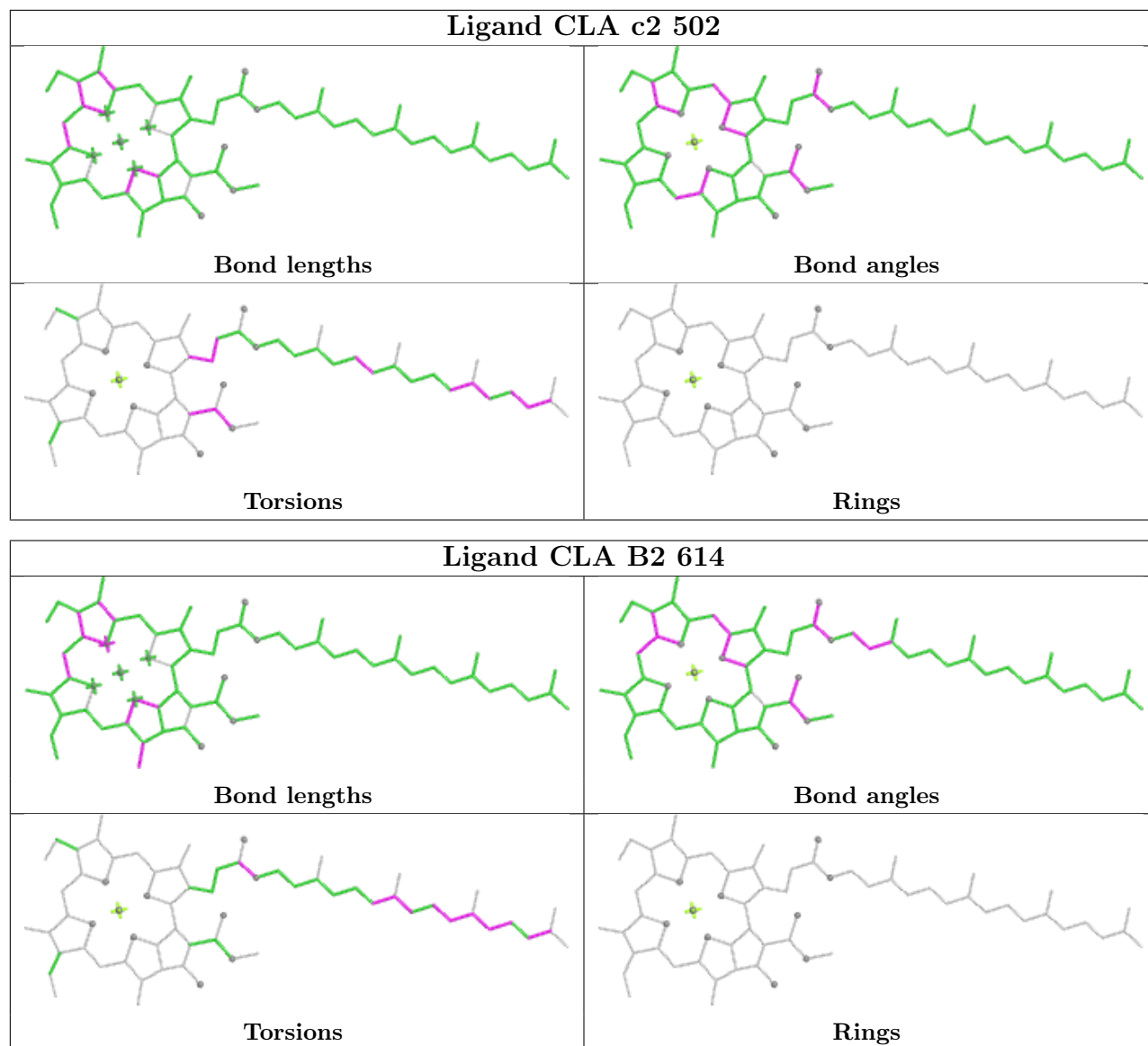


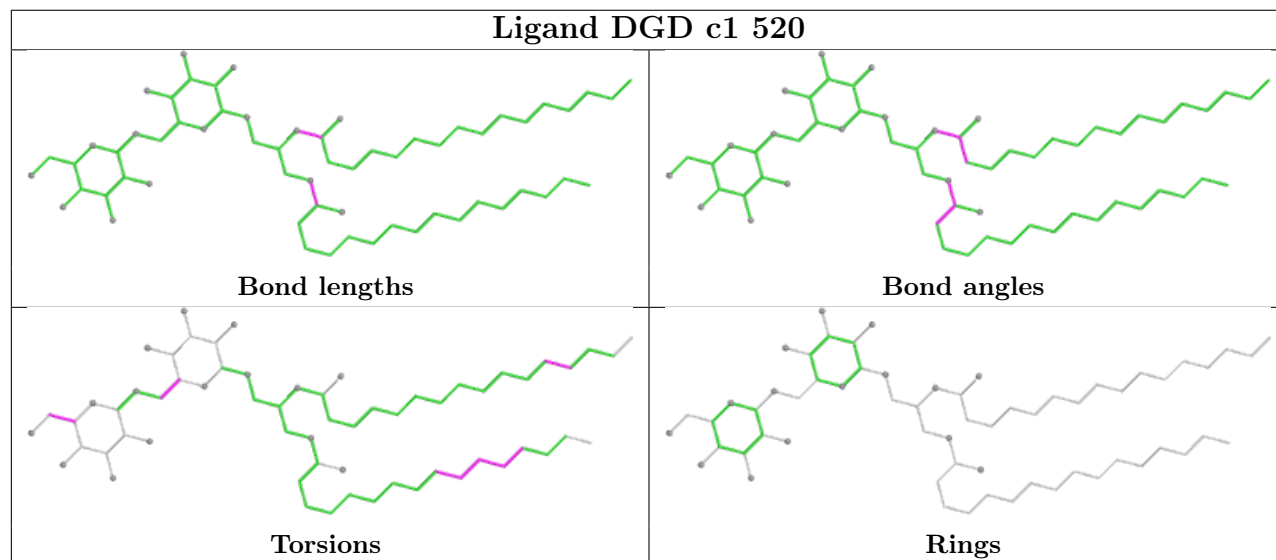
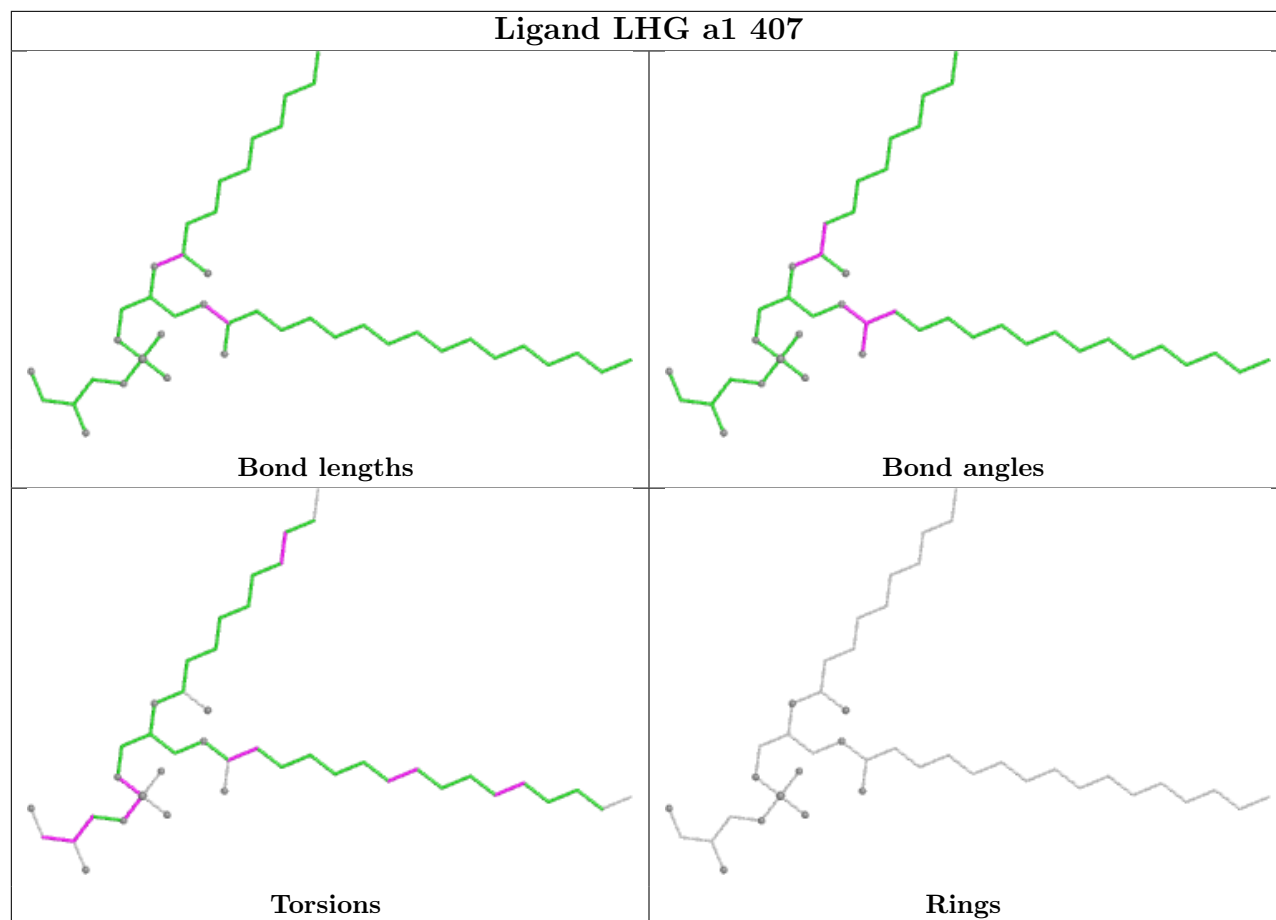


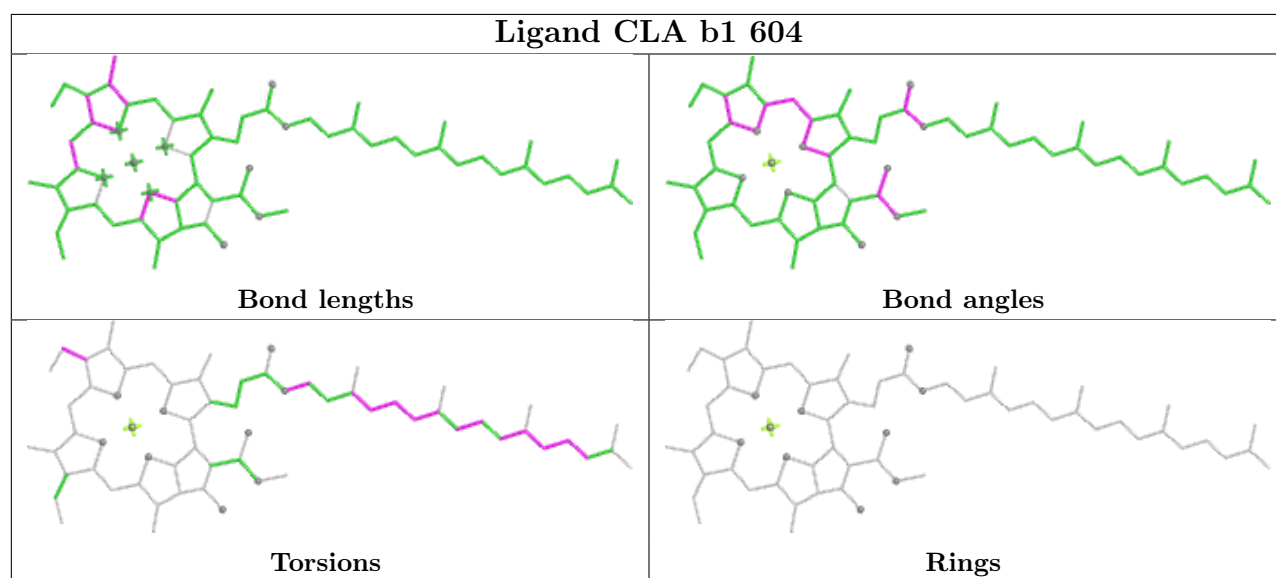
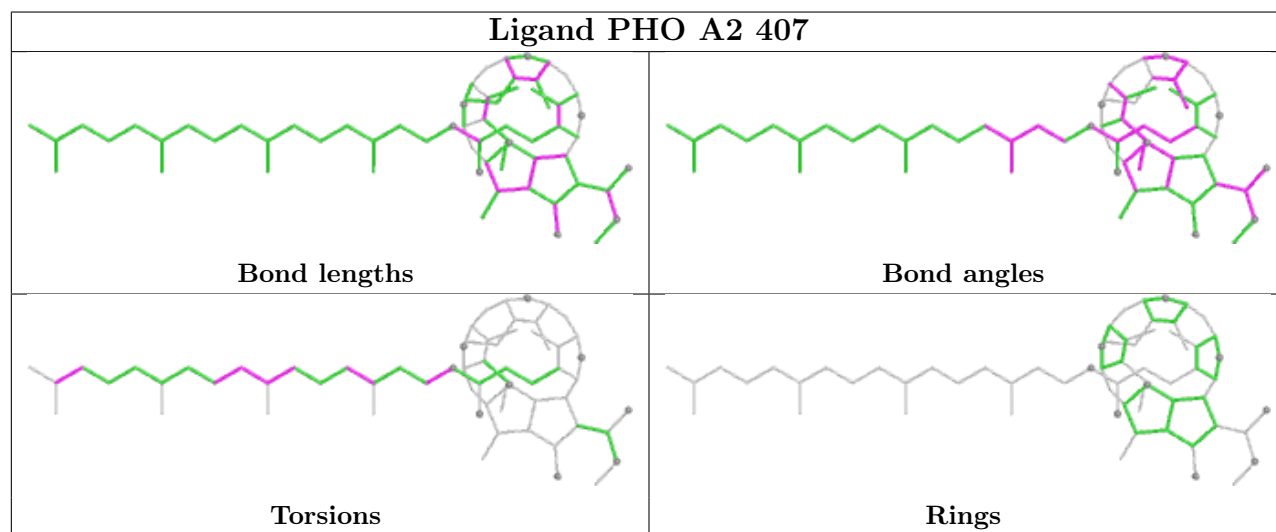
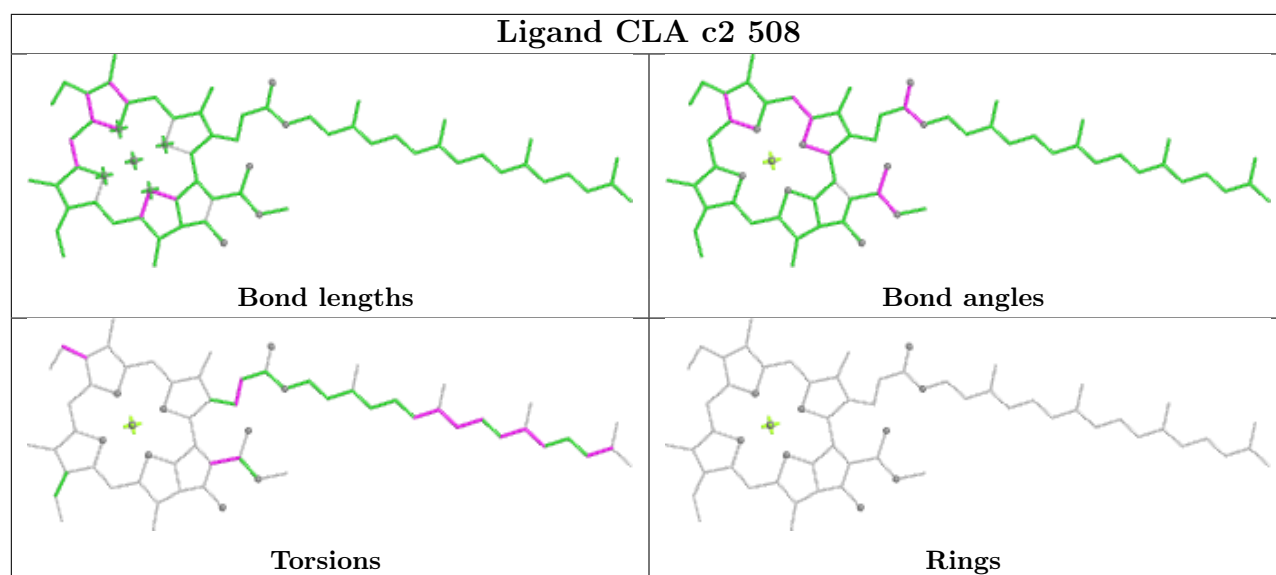


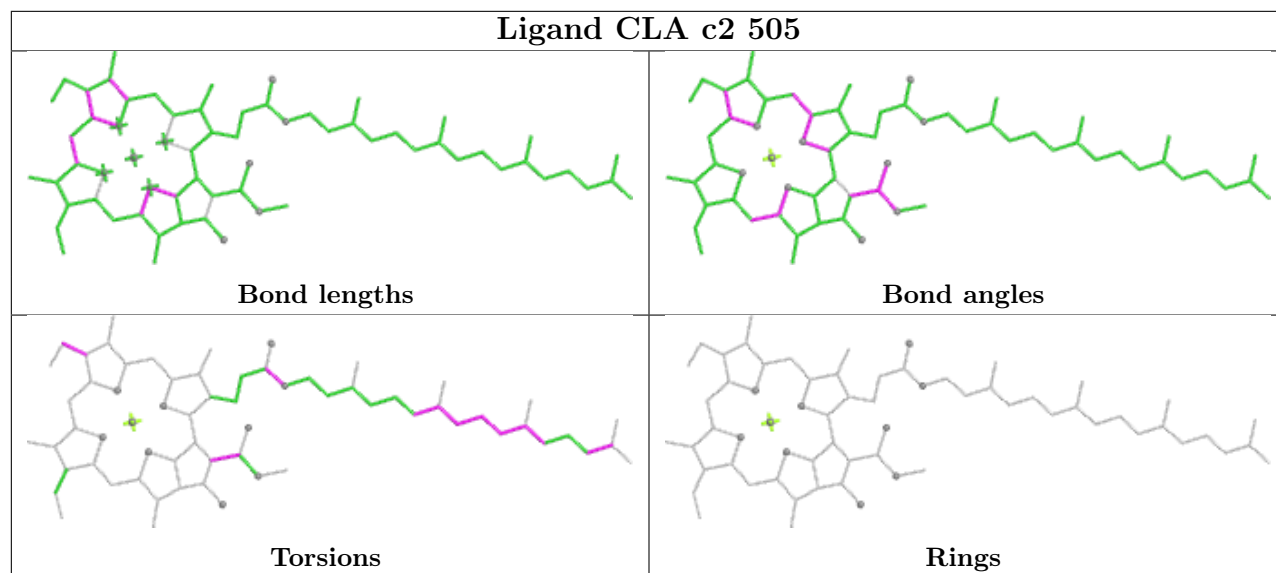
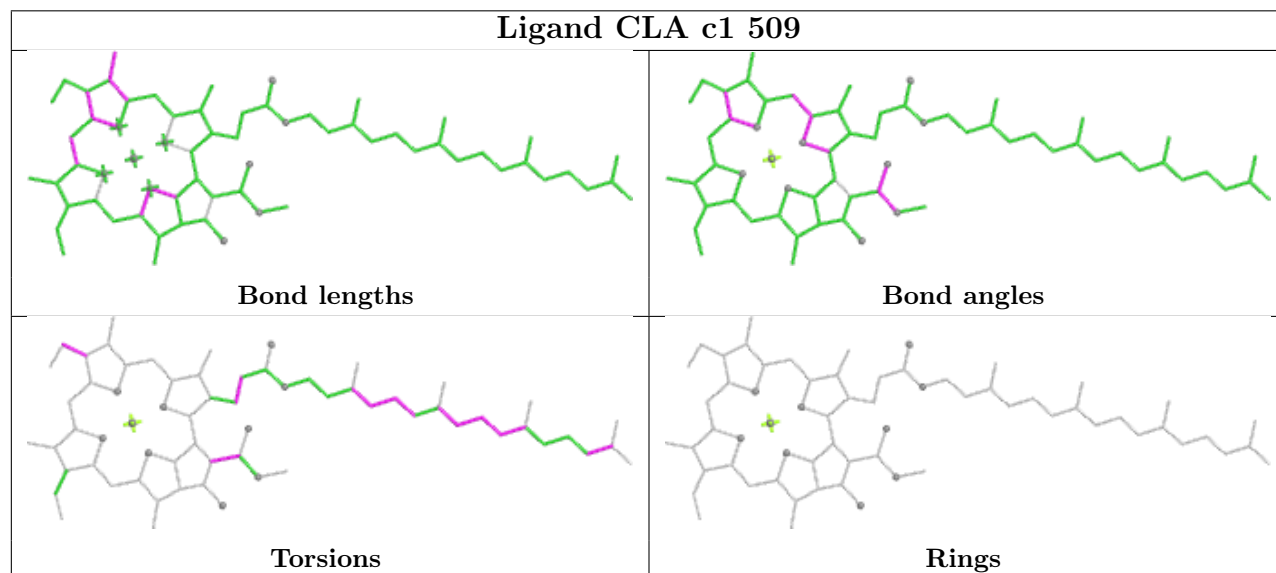
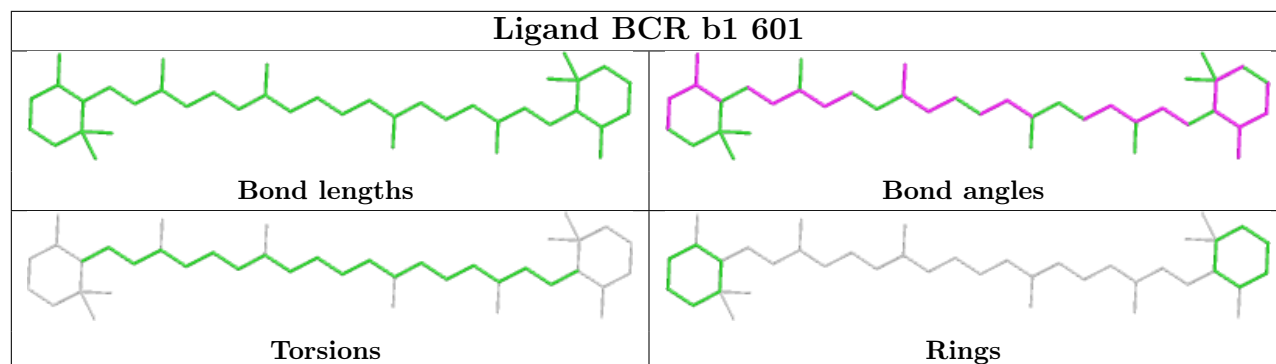


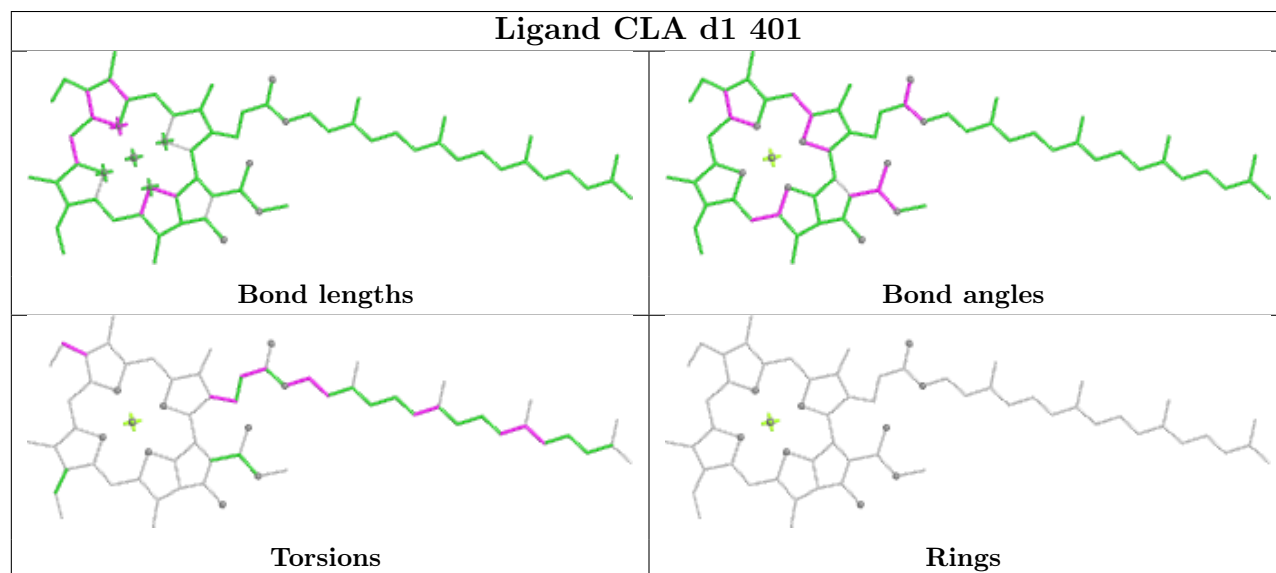
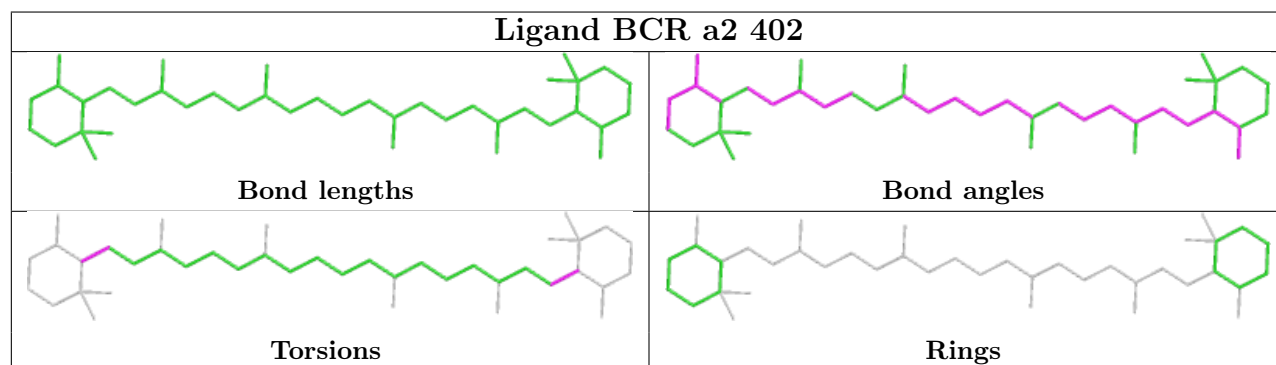
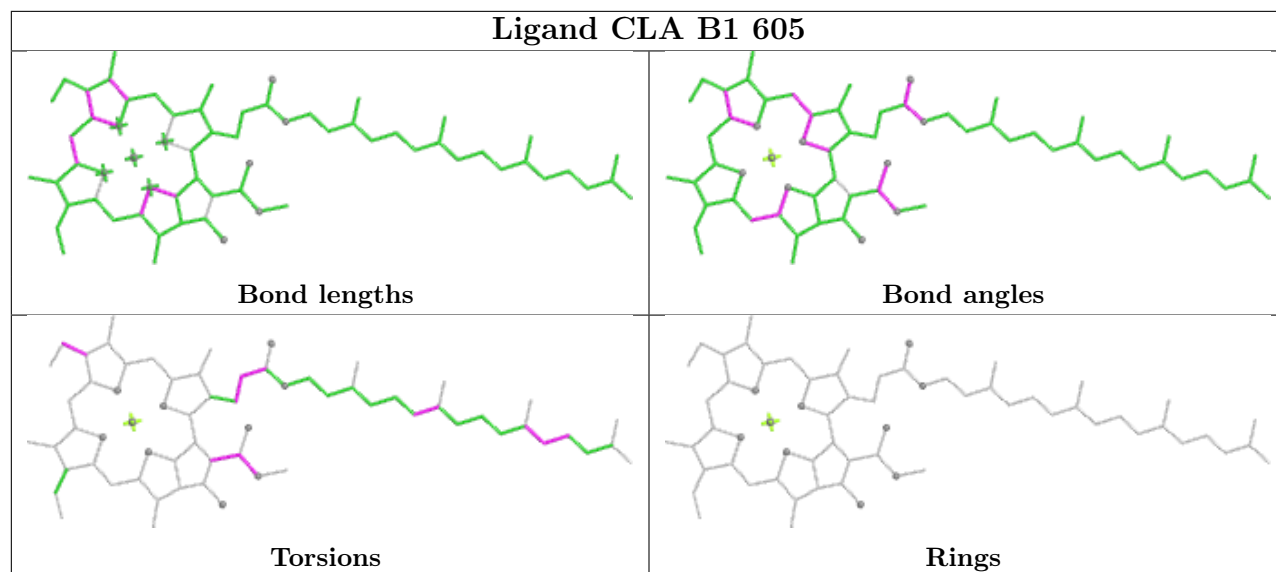


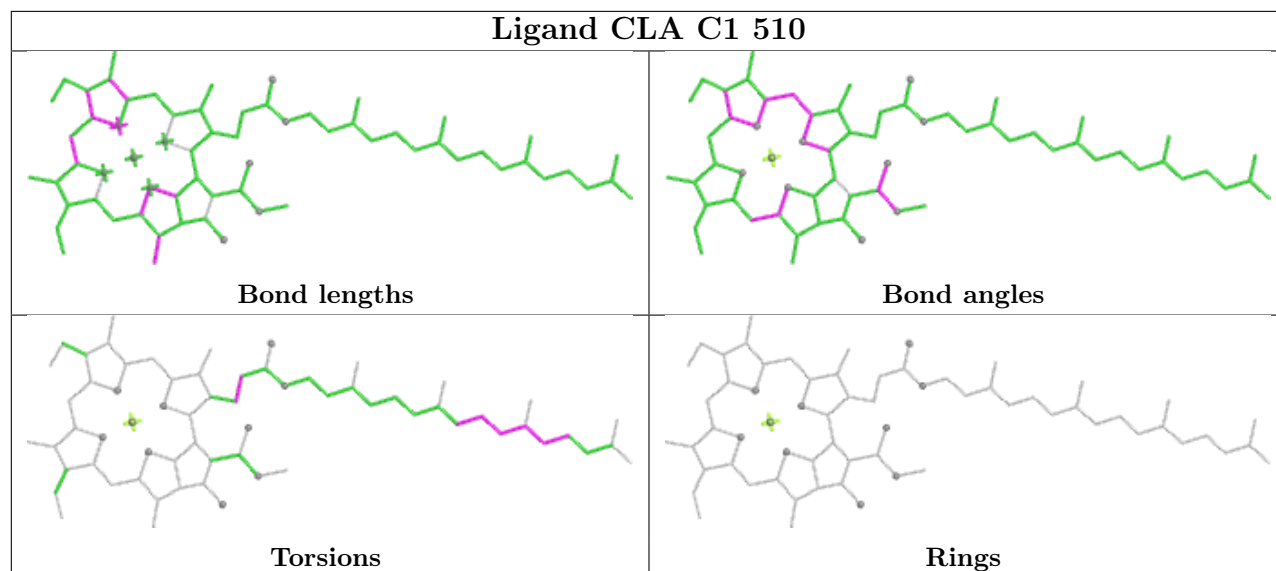
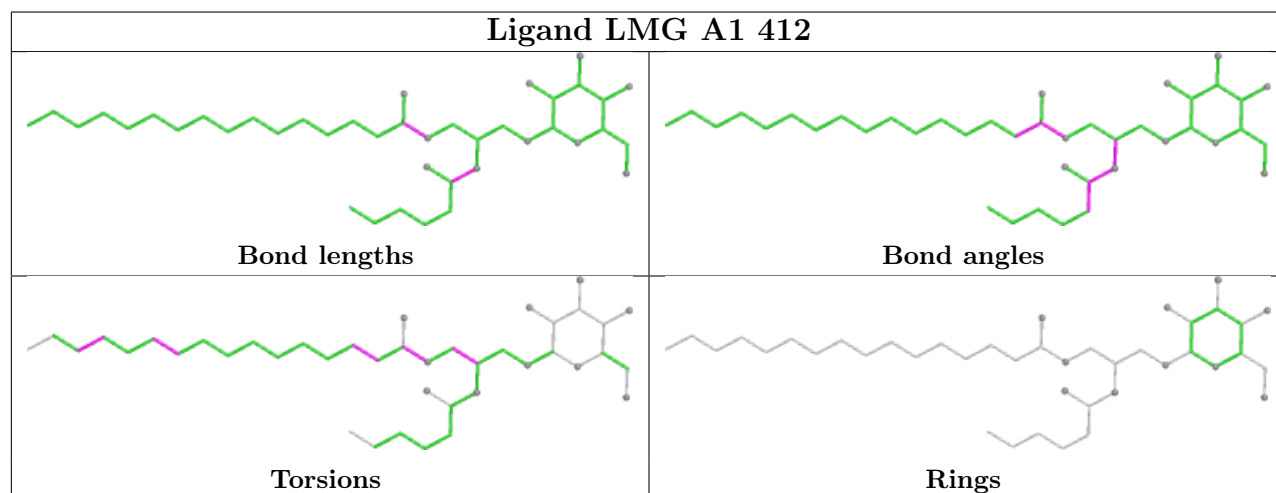
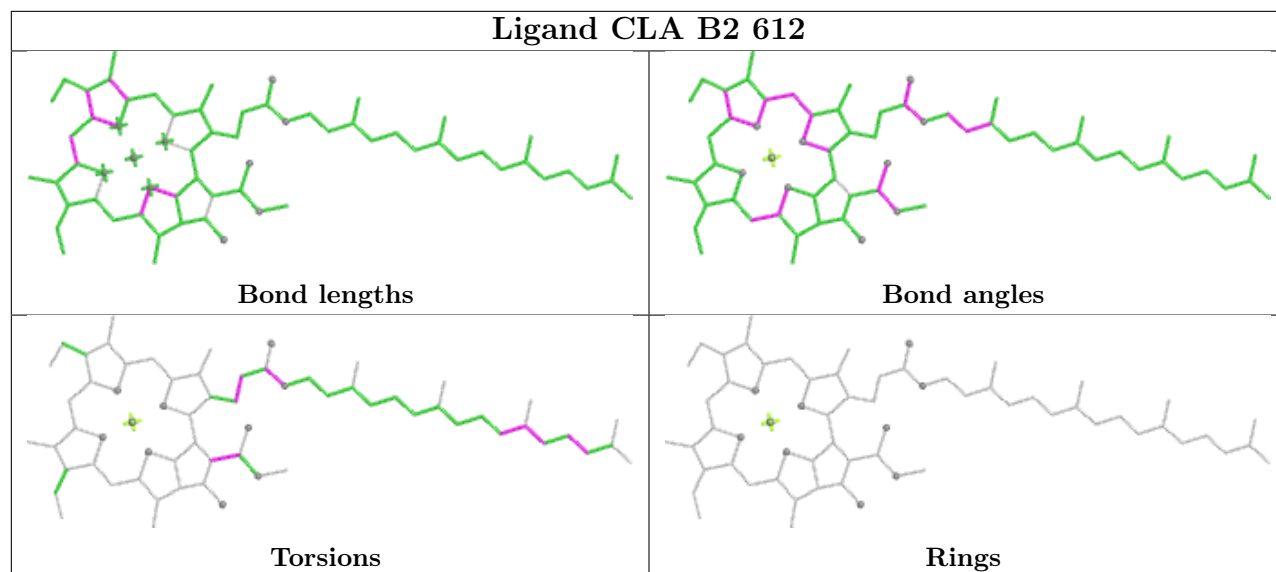


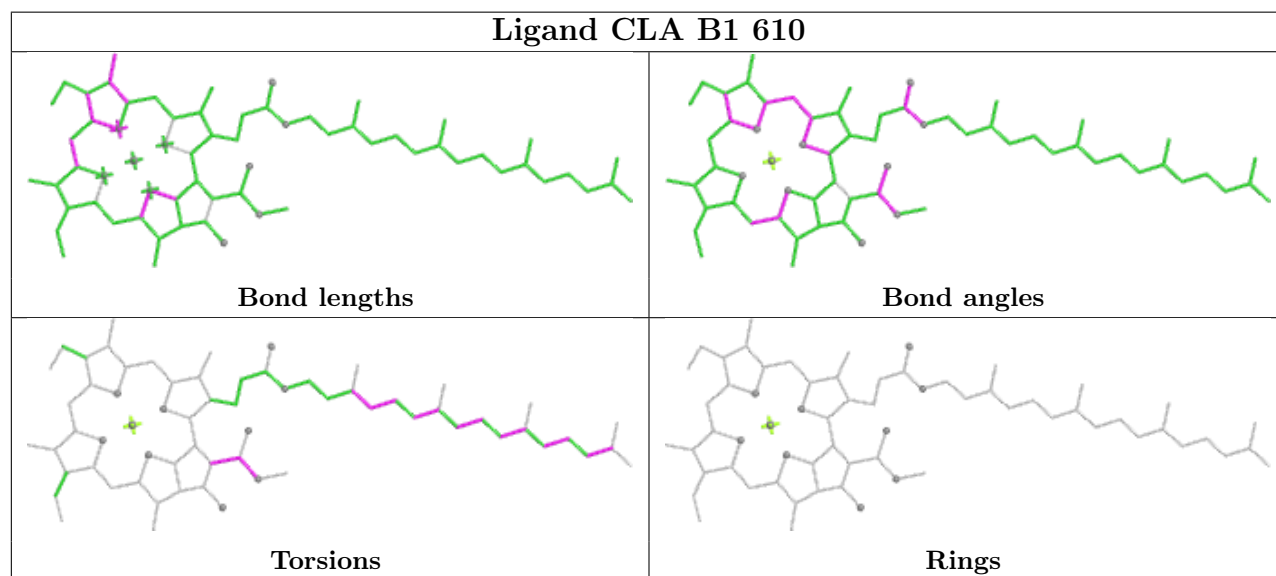
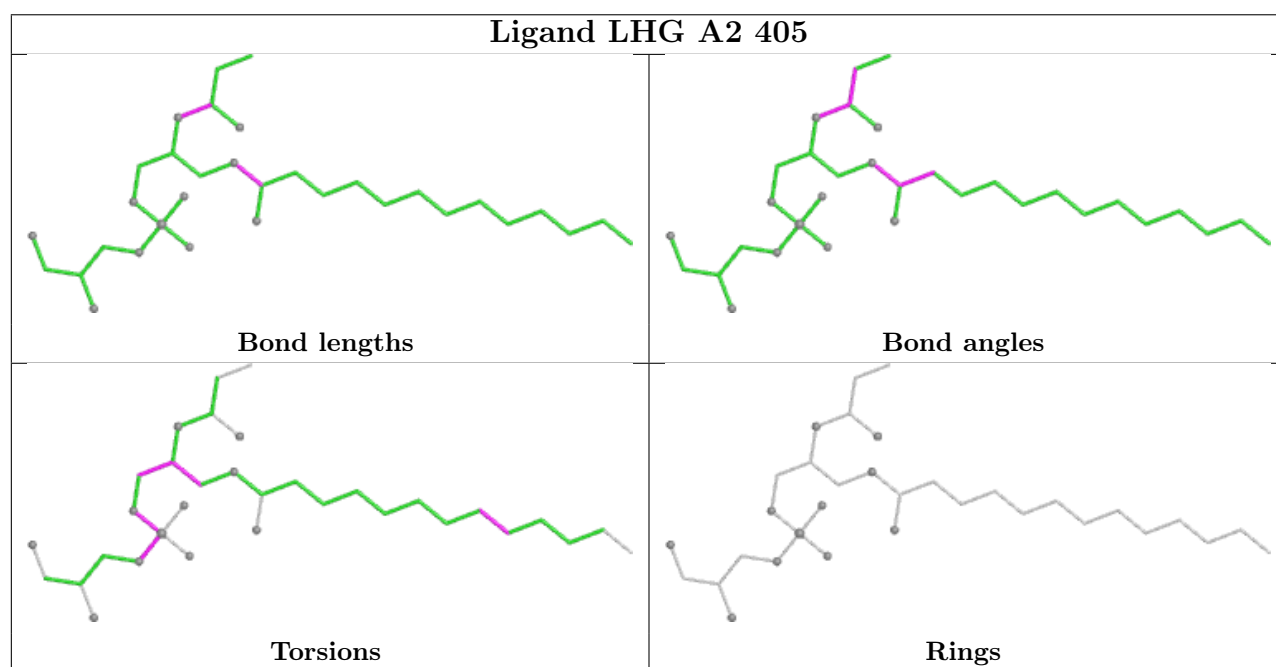
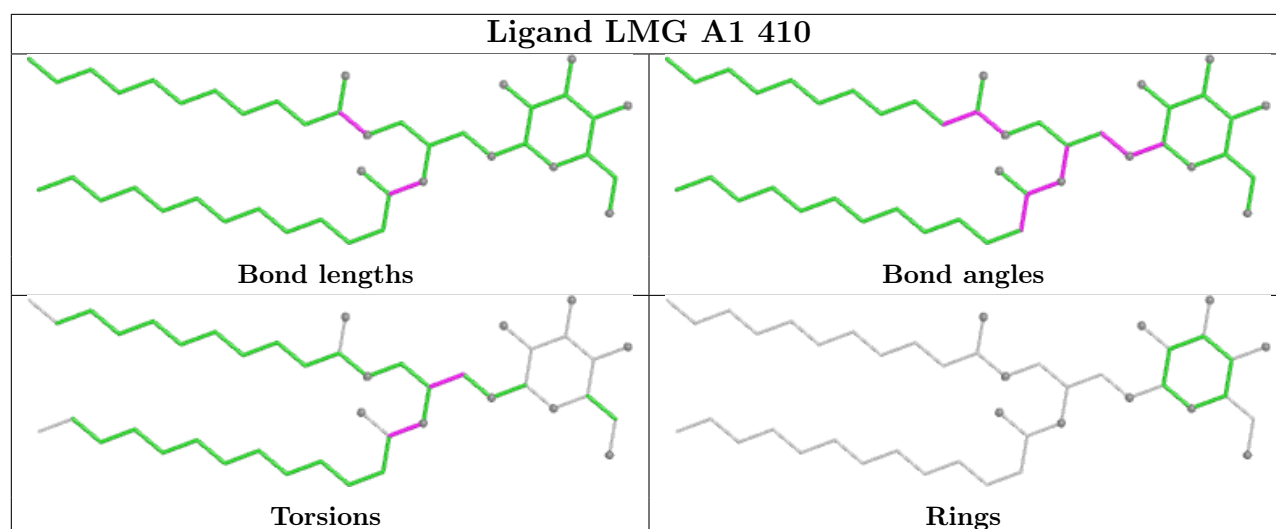


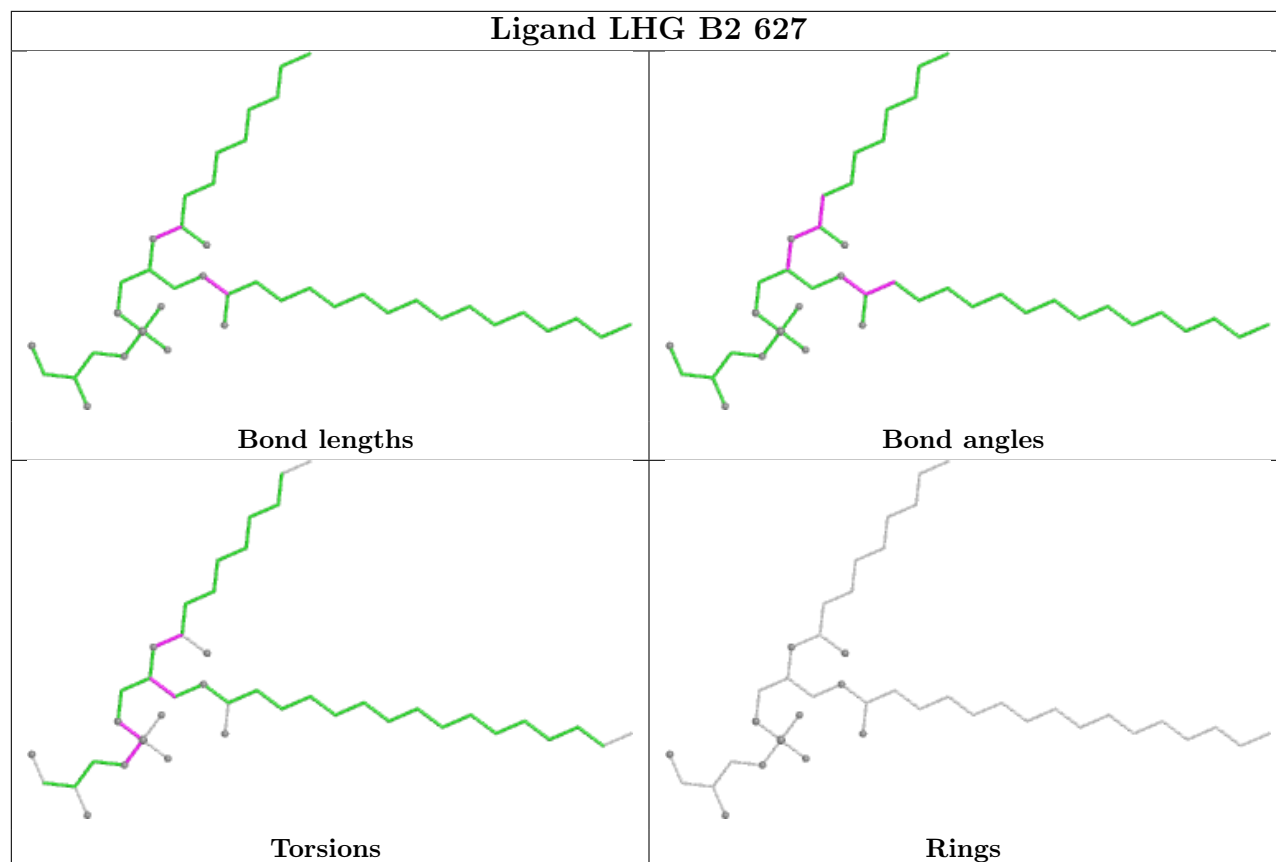


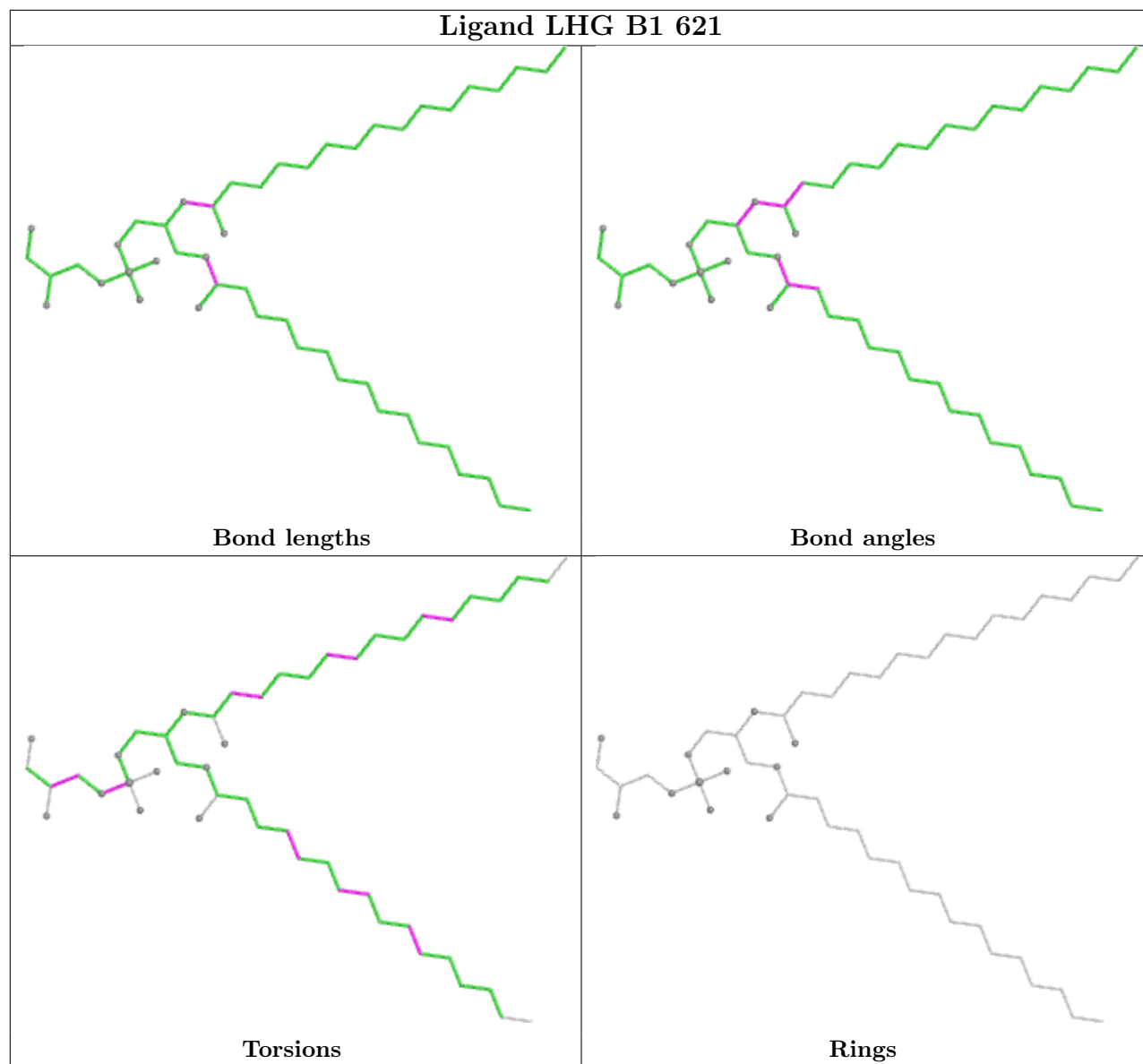


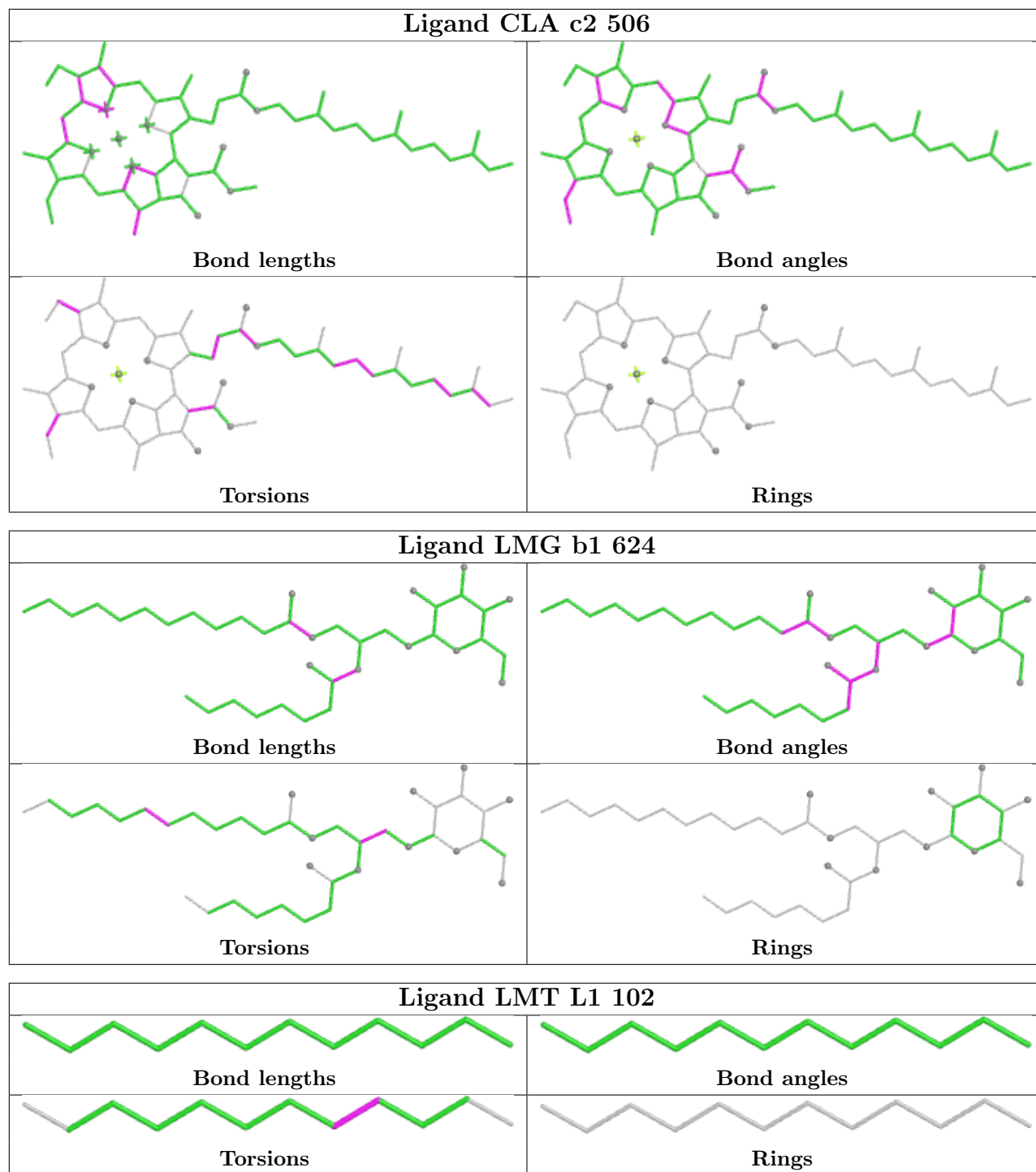


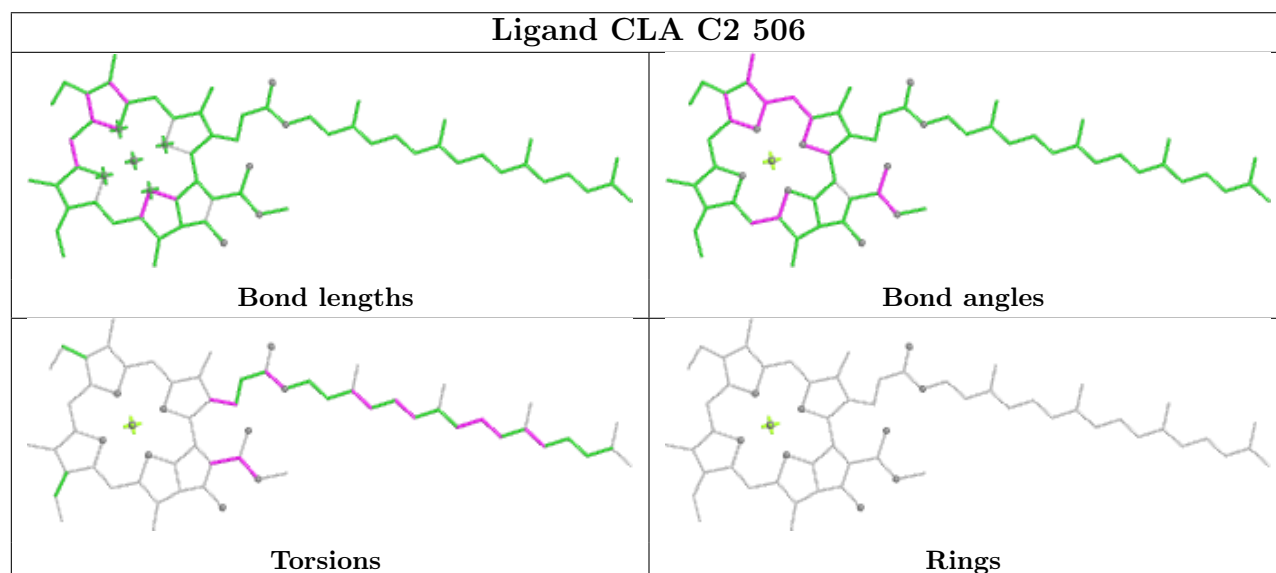
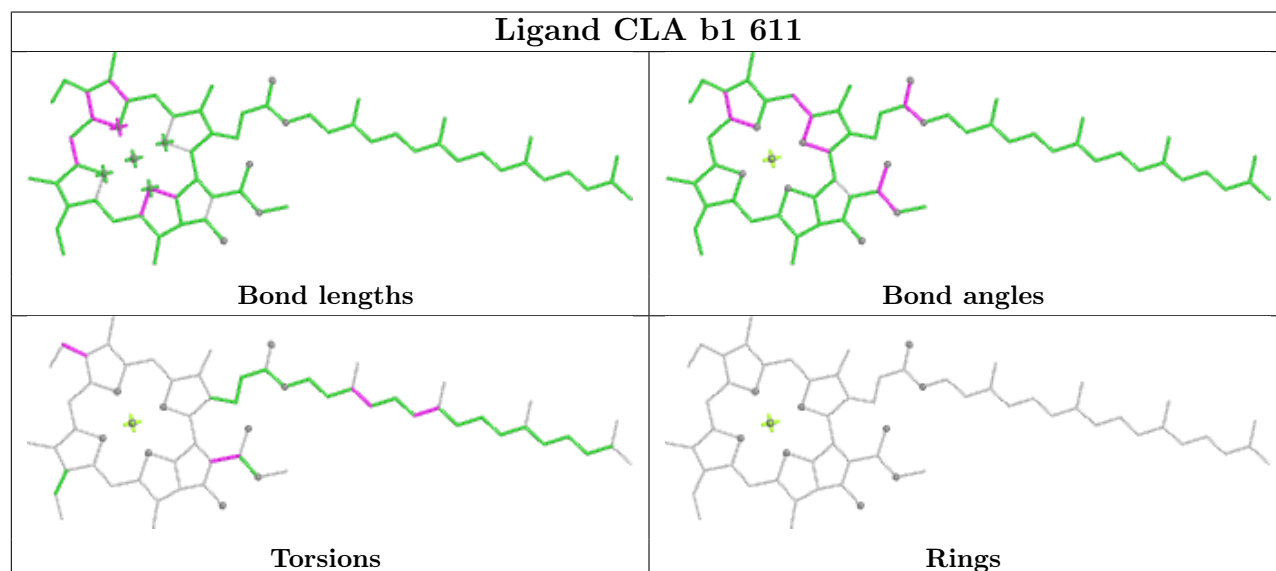
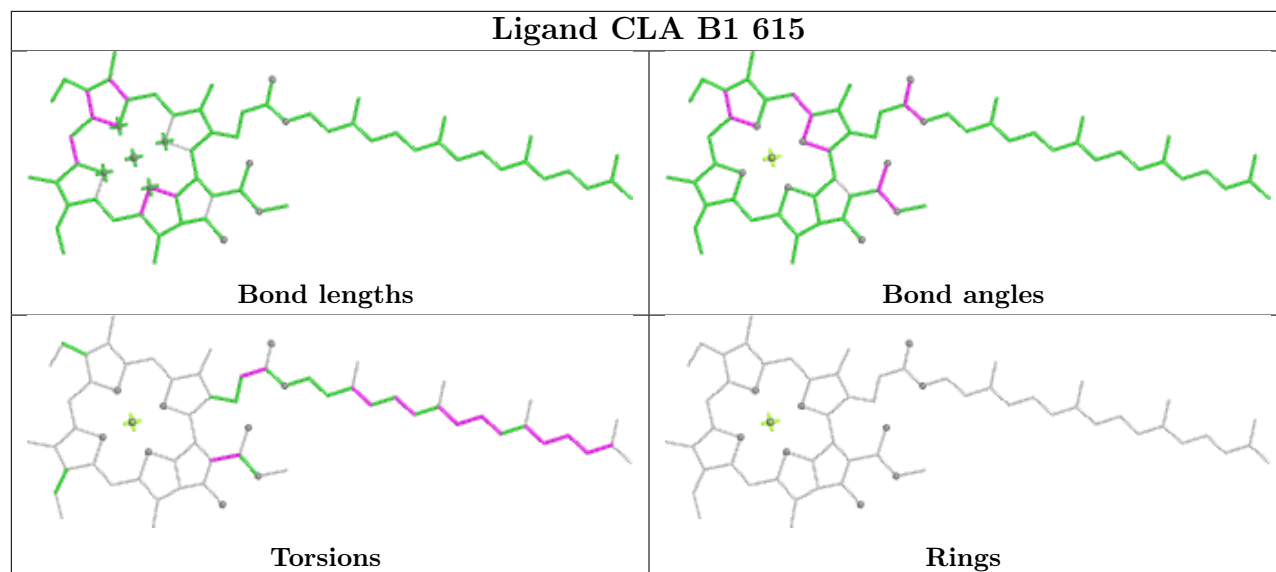


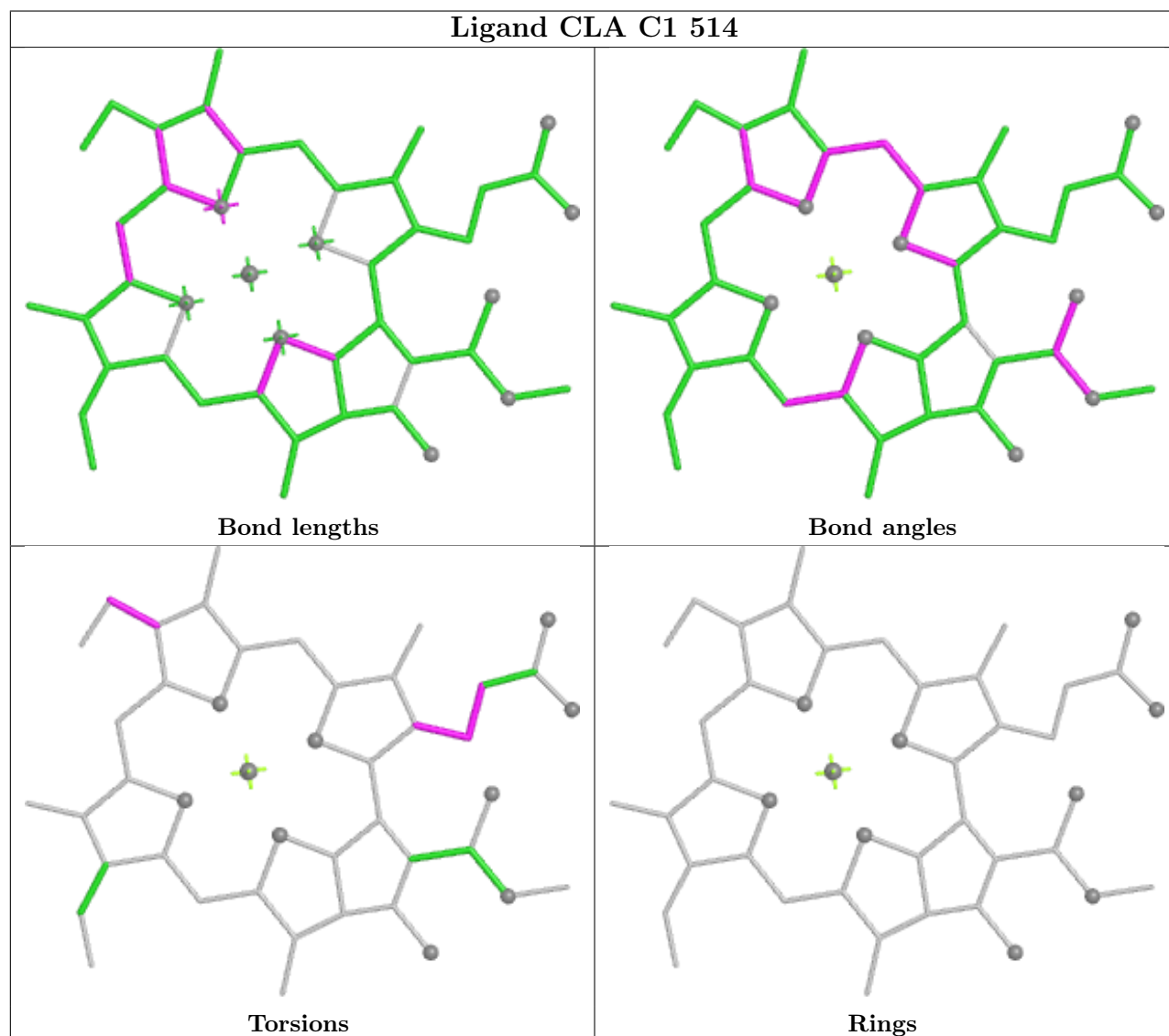
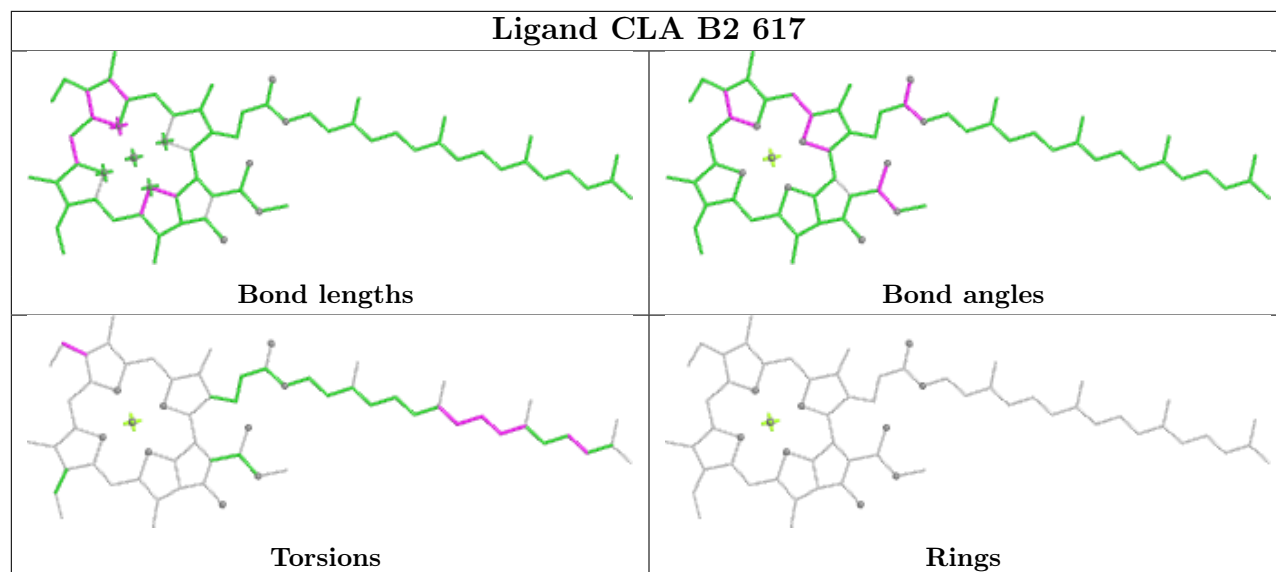




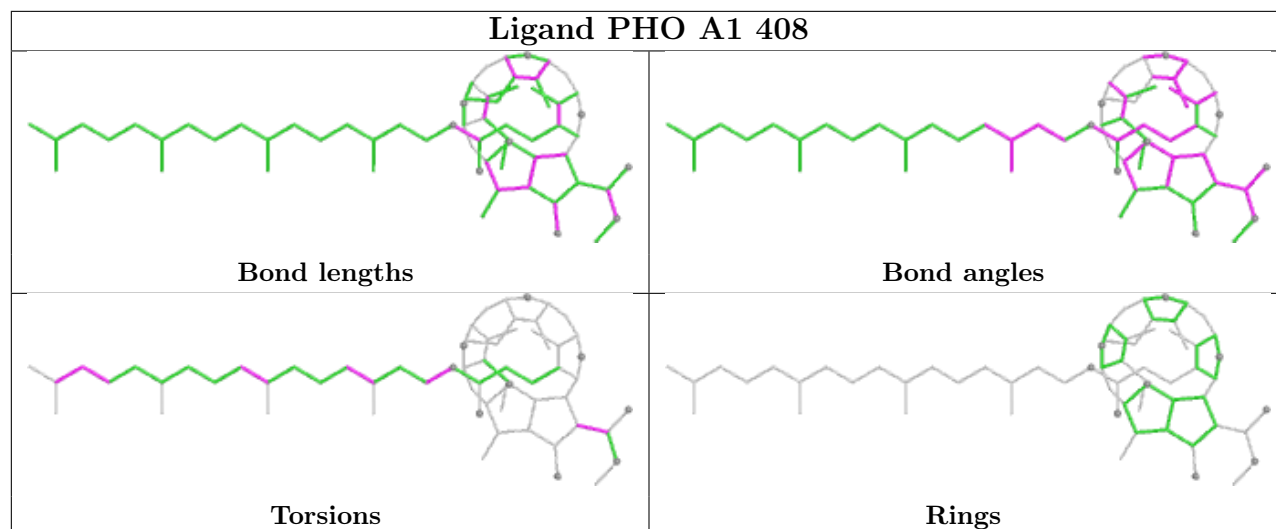




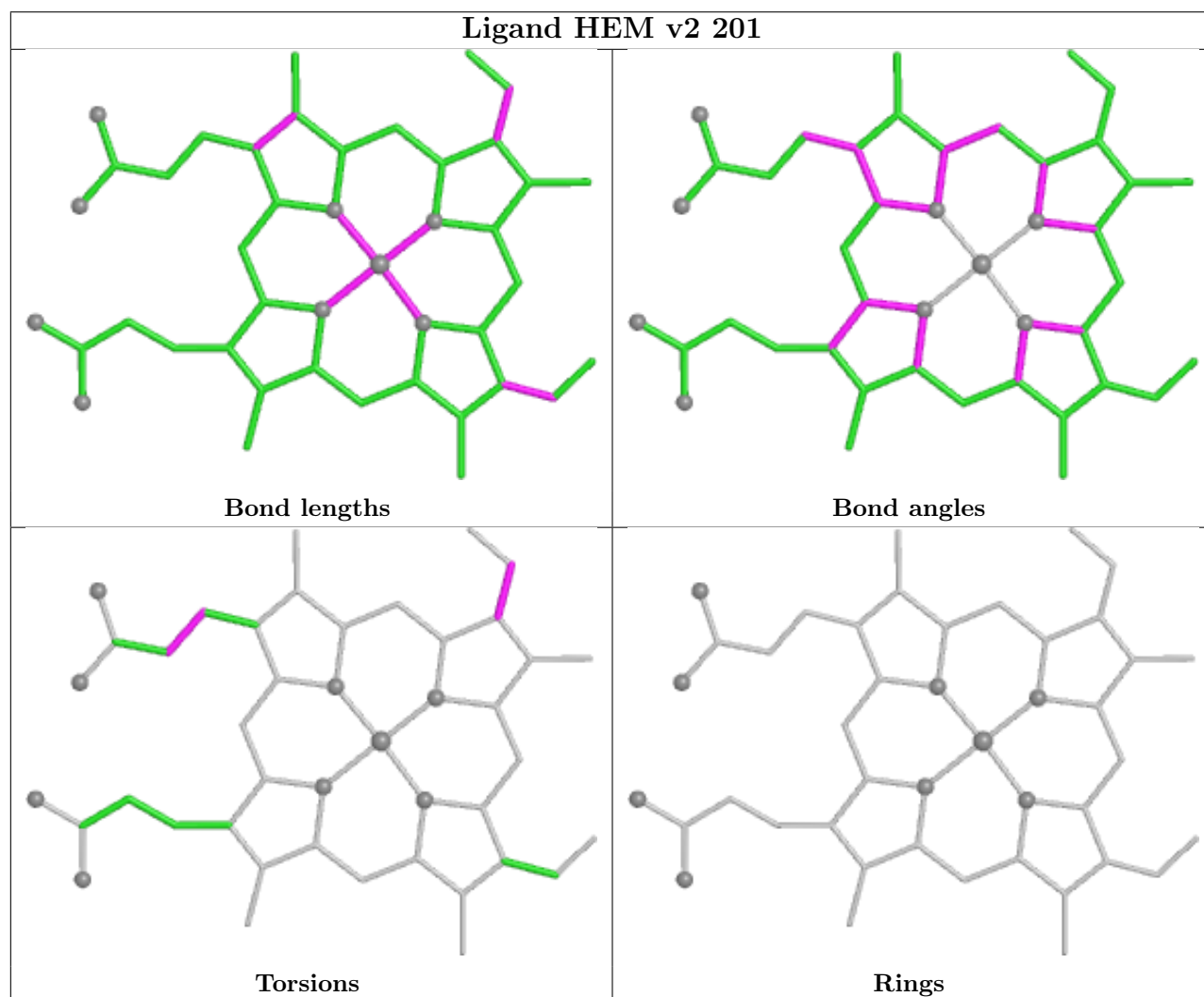


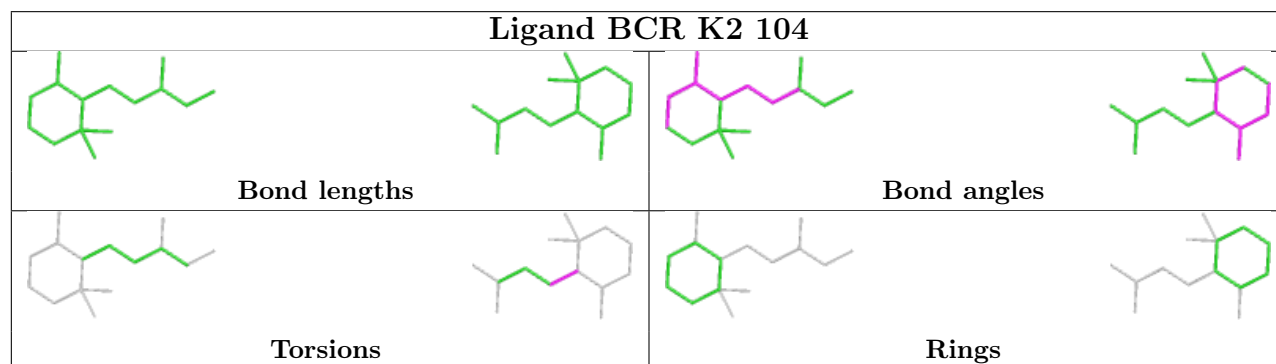
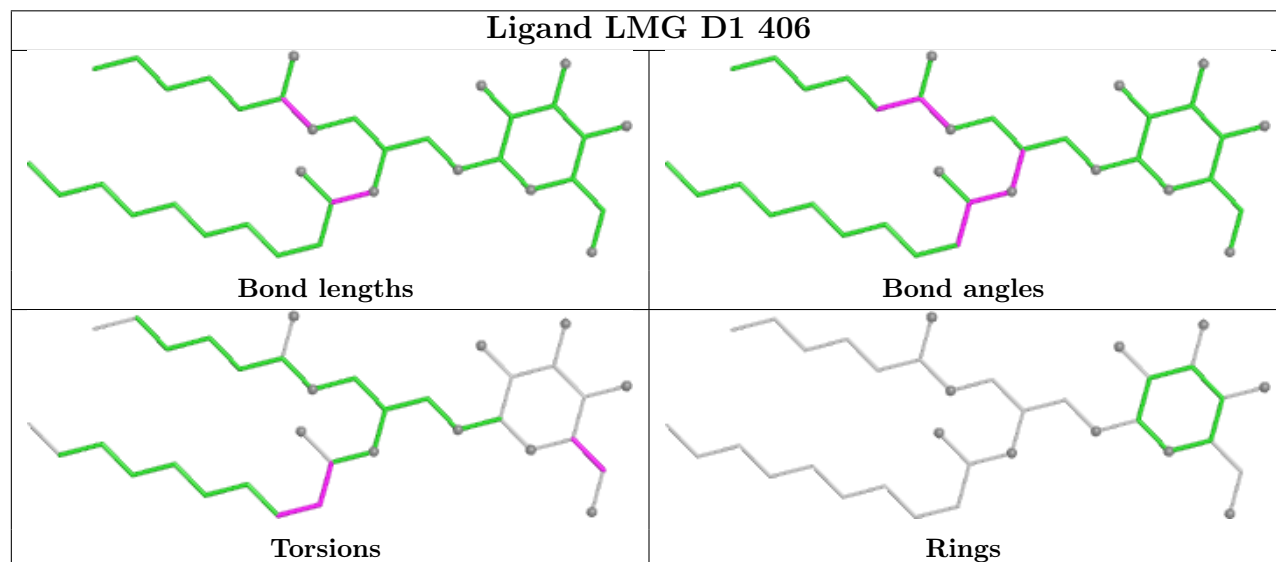
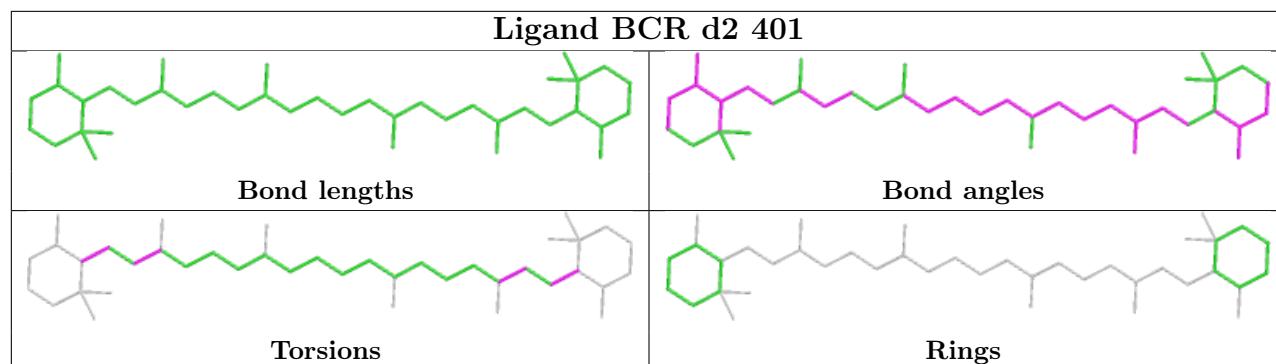


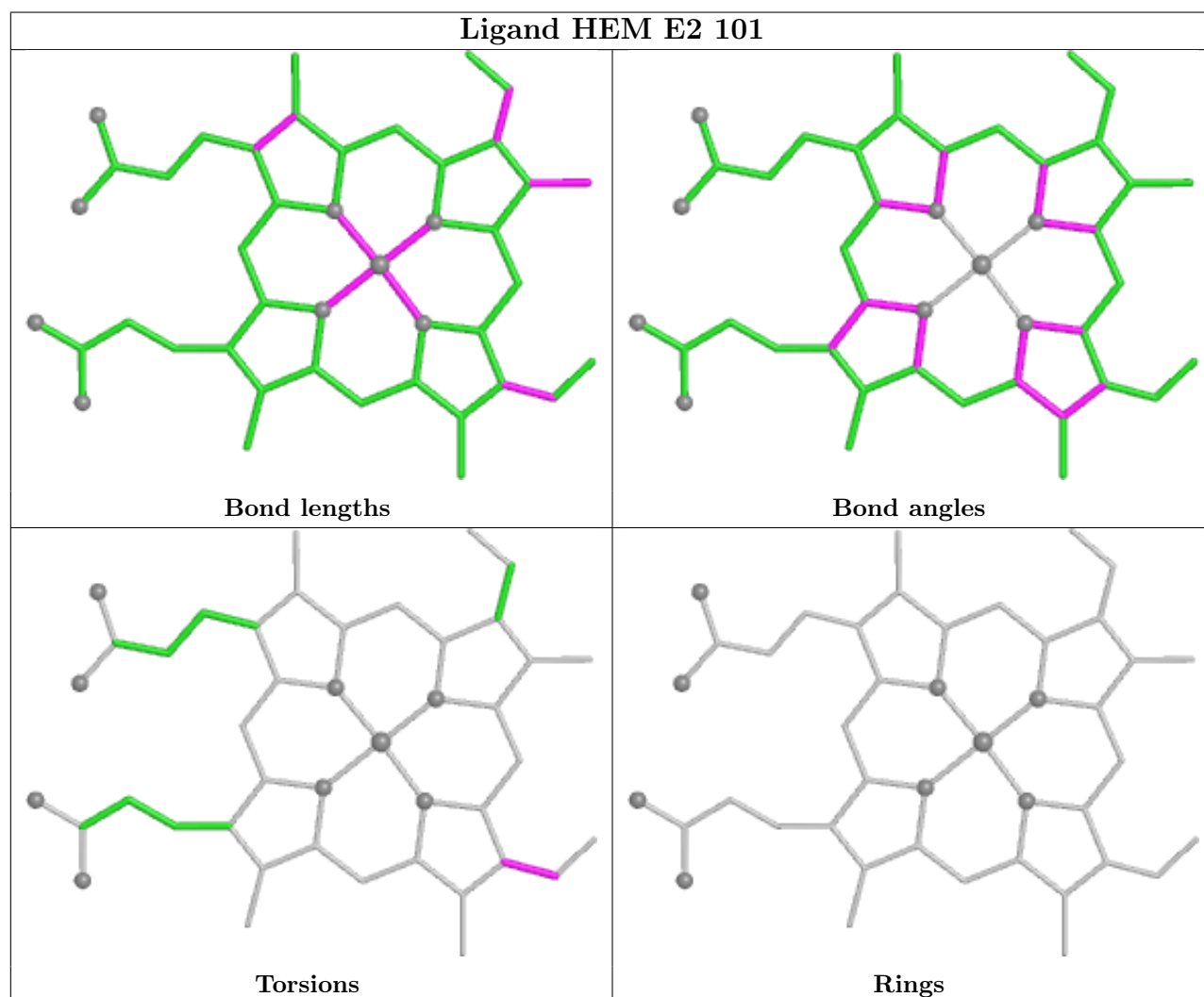
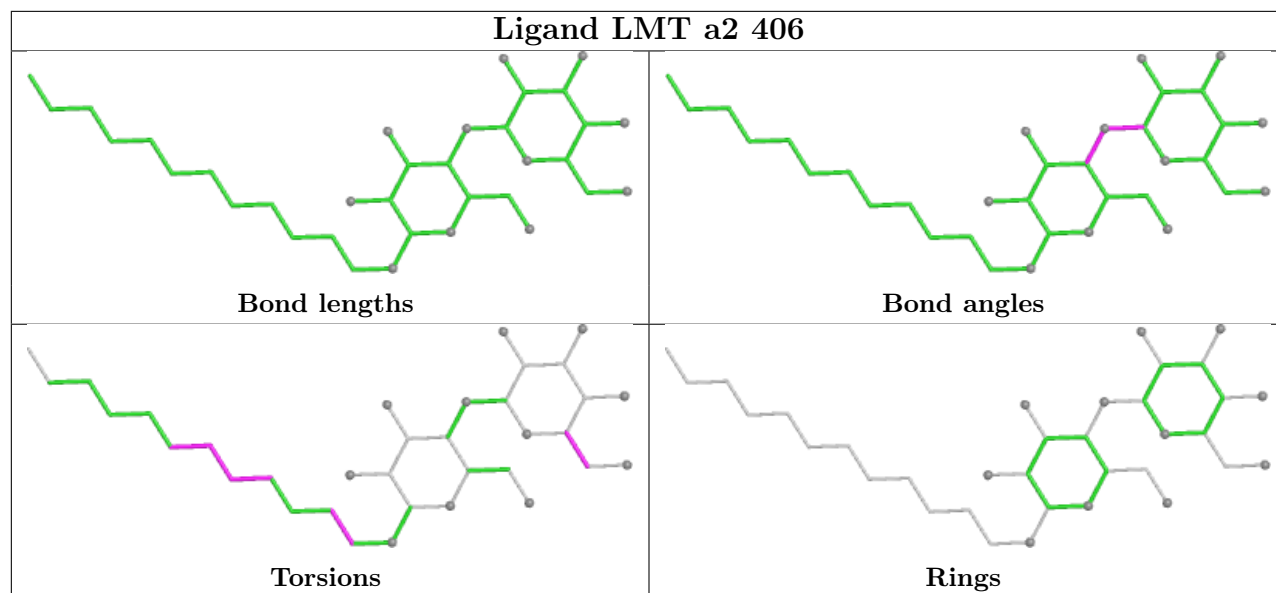
Ligand PHO A1 408

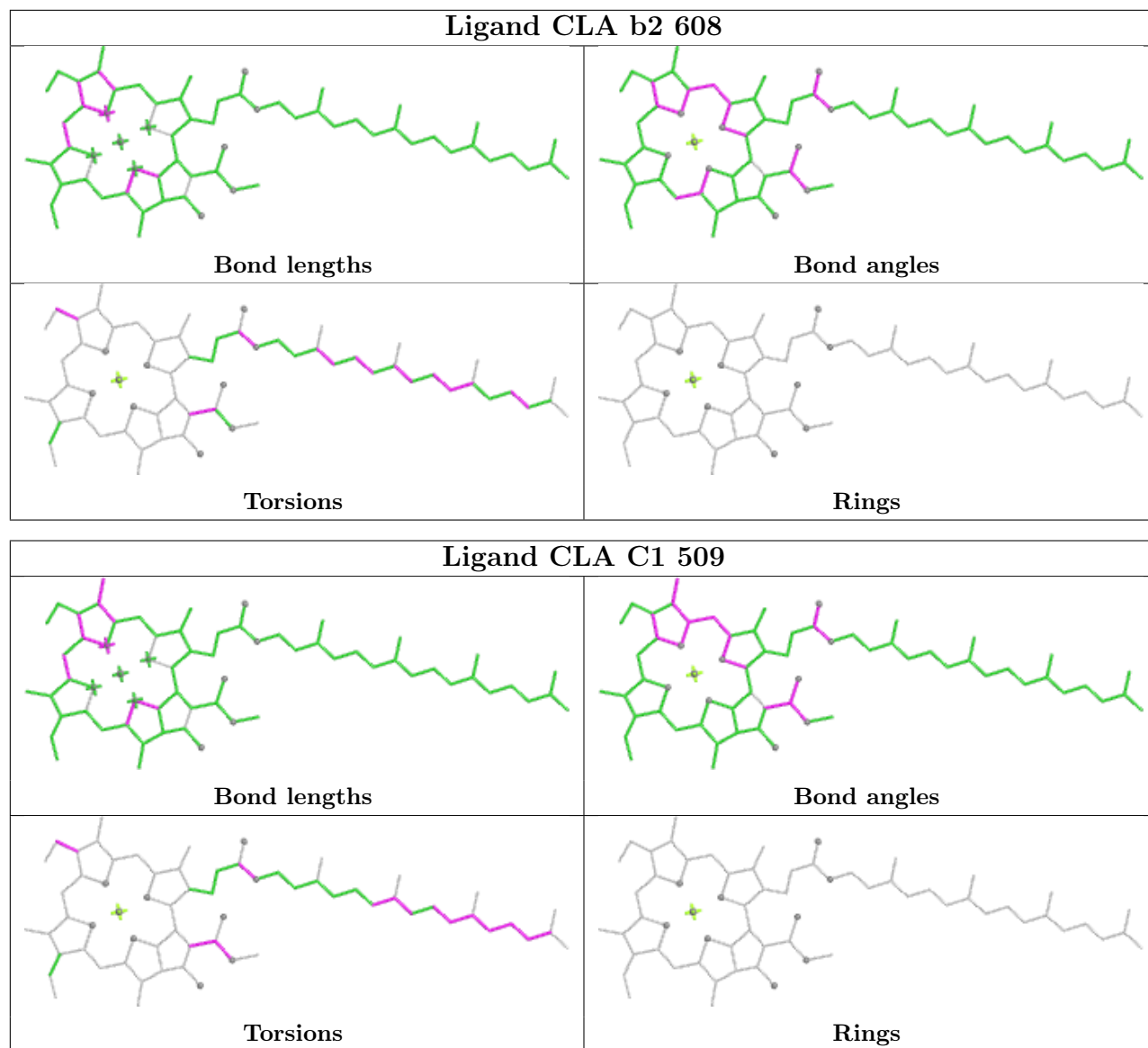


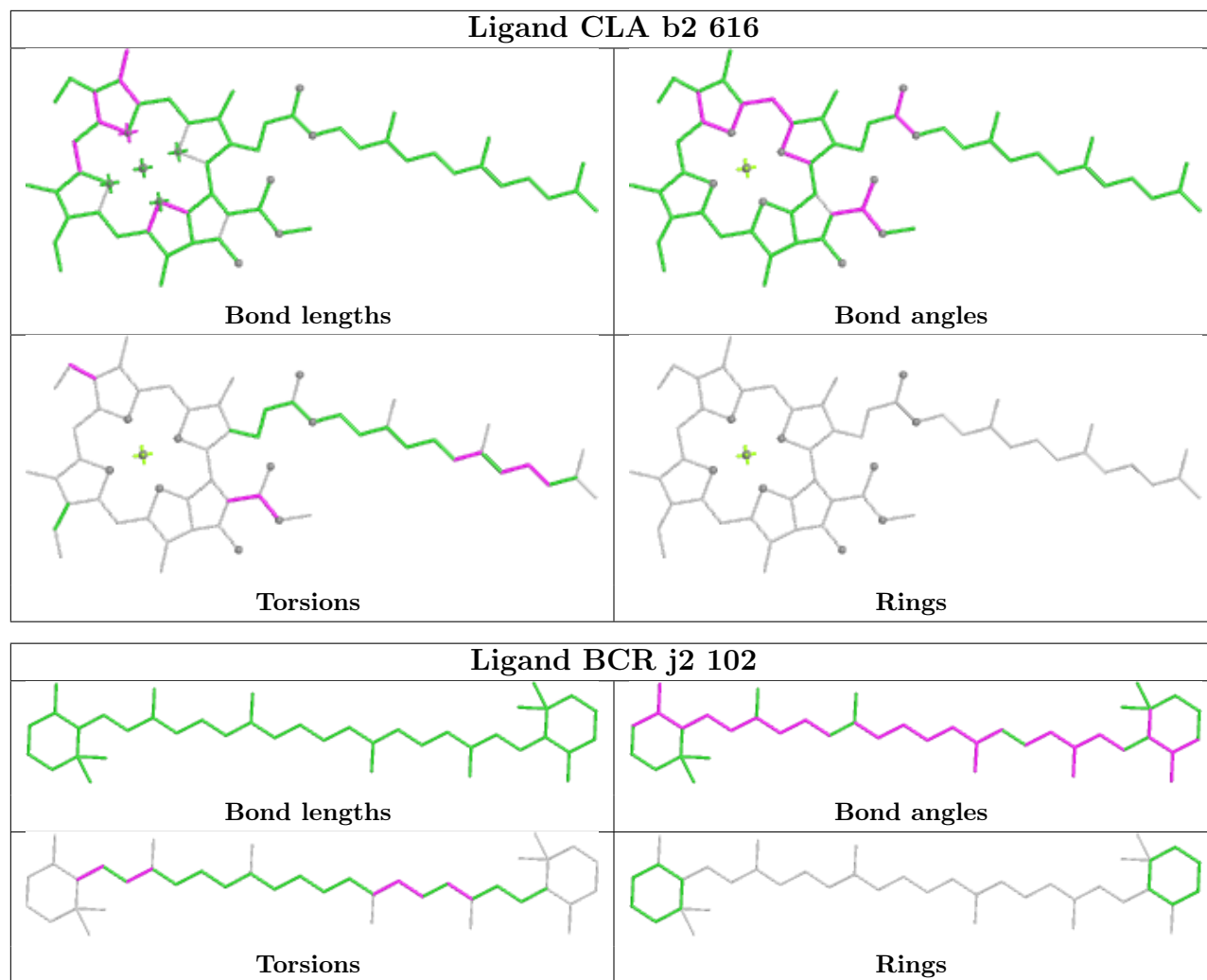
Ligand HEM v2 201



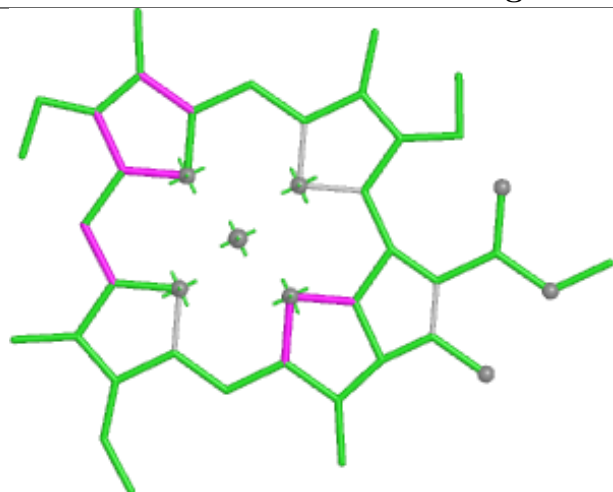




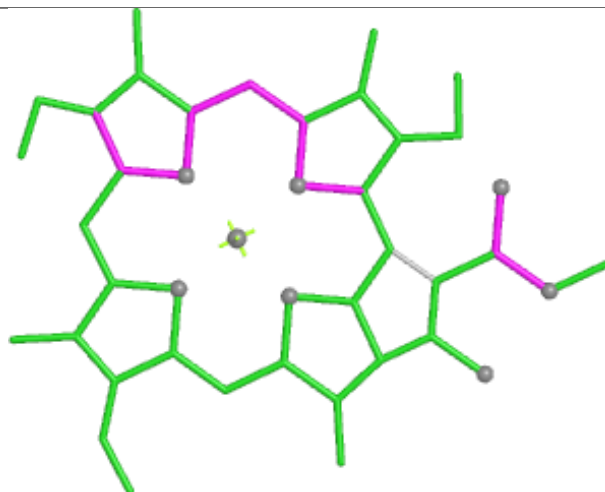




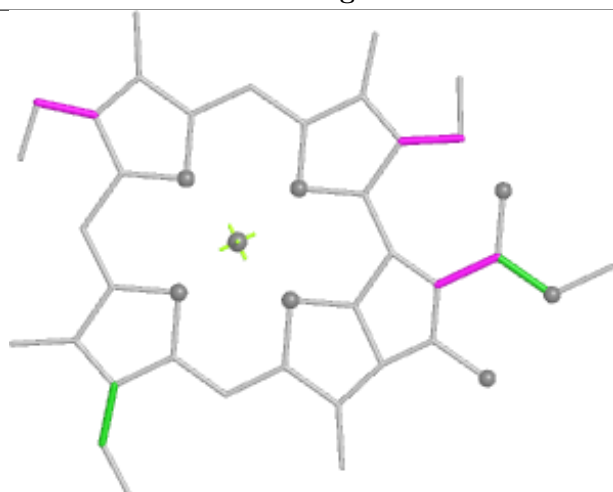
Ligand CLA B1 604



Bond lengths



Bond angles

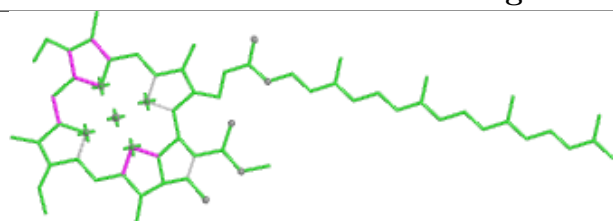


Torsions

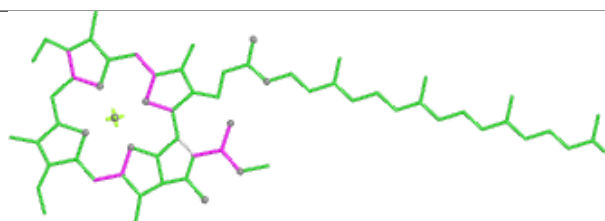


Rings

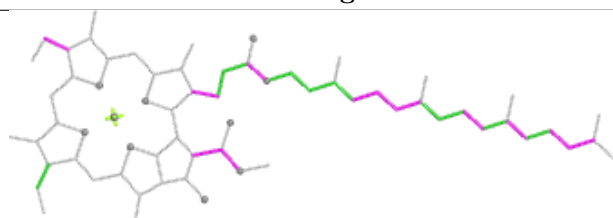
Ligand CLA B1 619



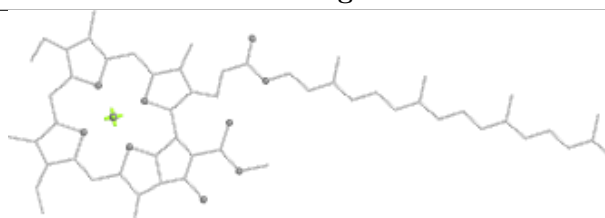
Bond lengths



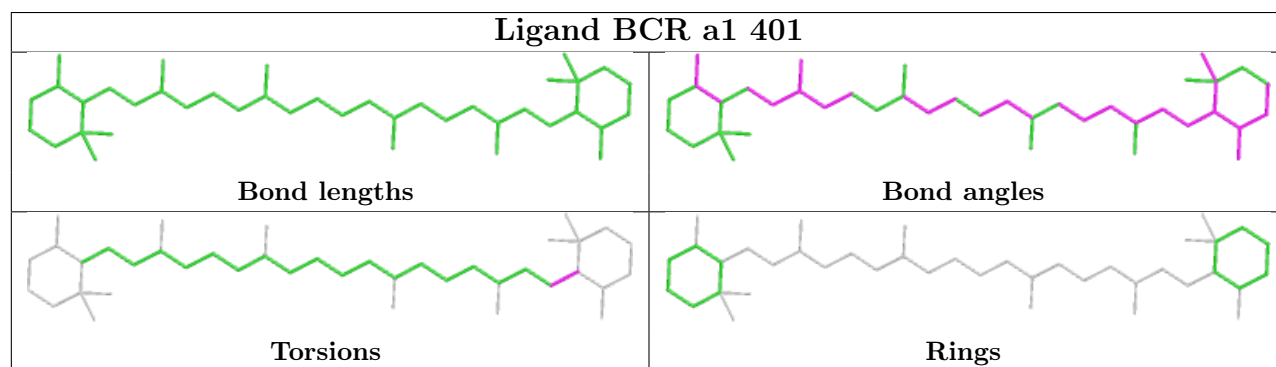
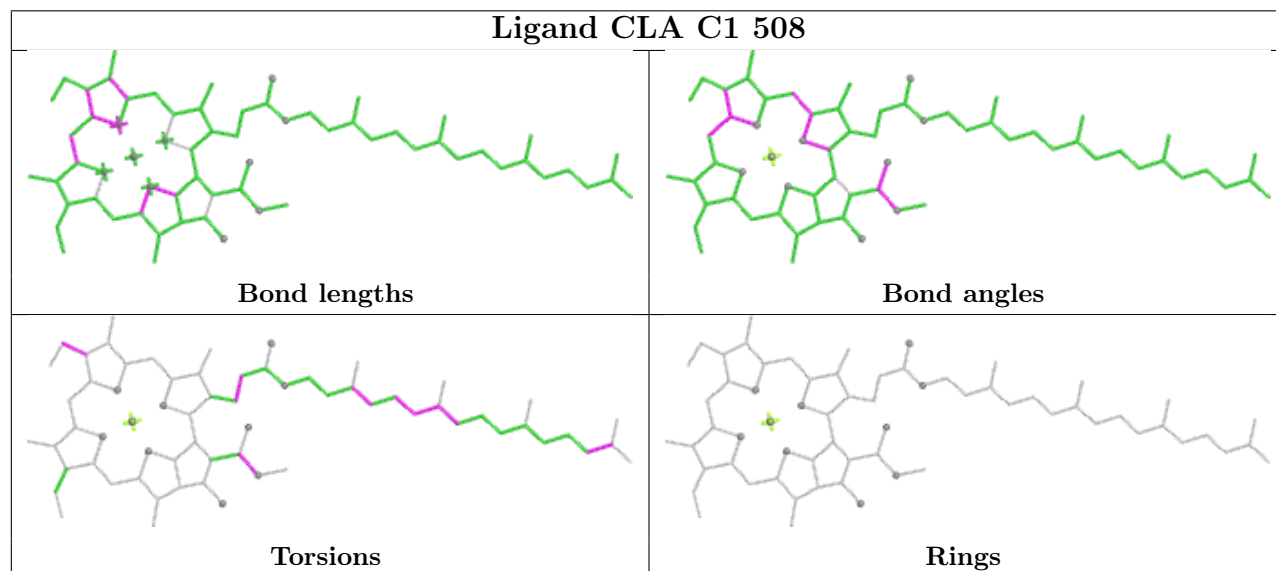
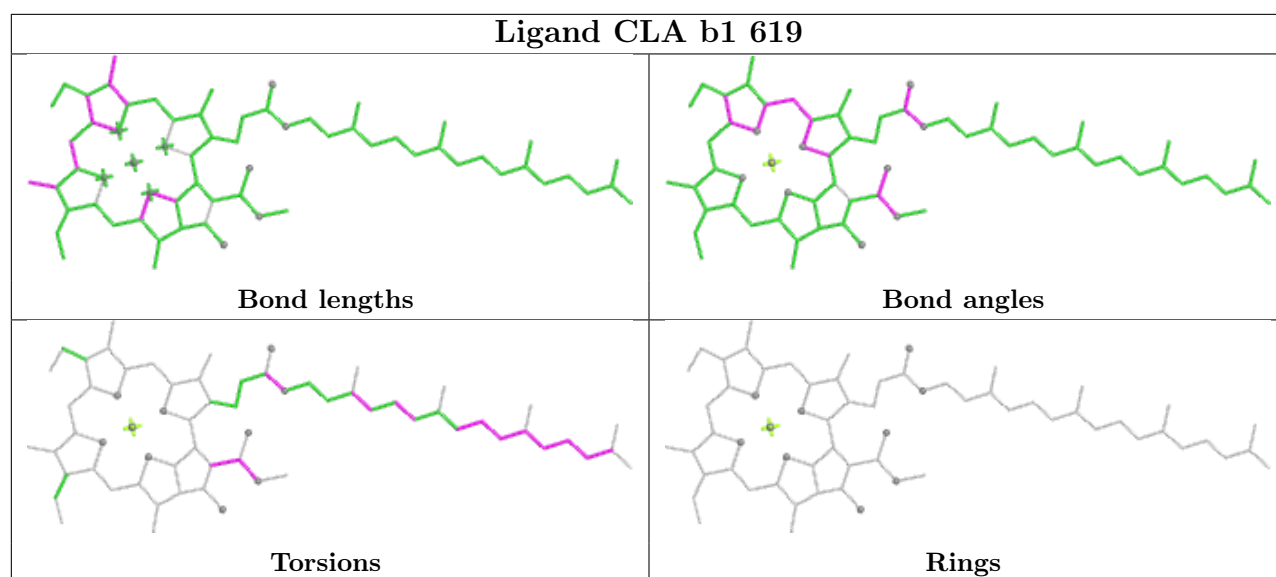
Bond angles

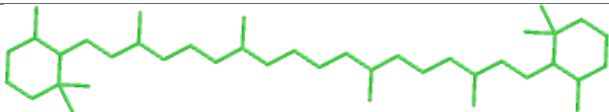
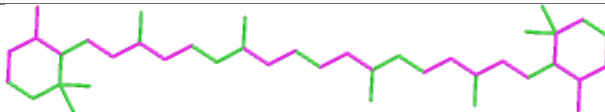
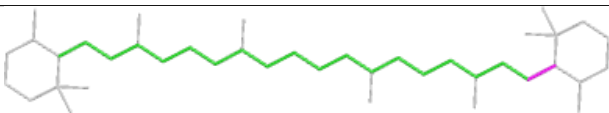
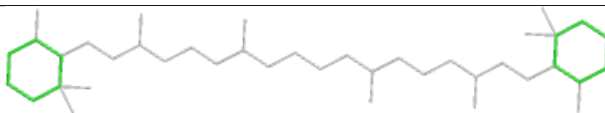


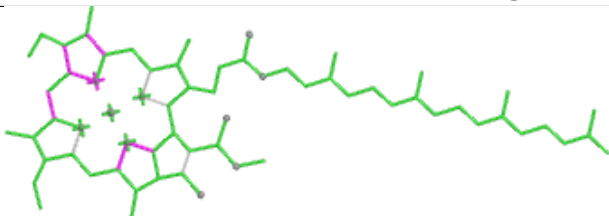
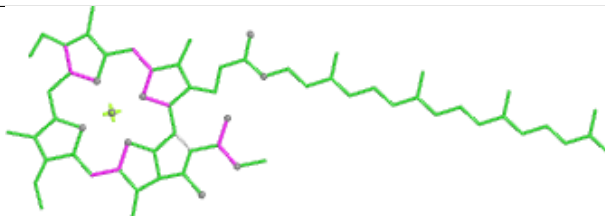
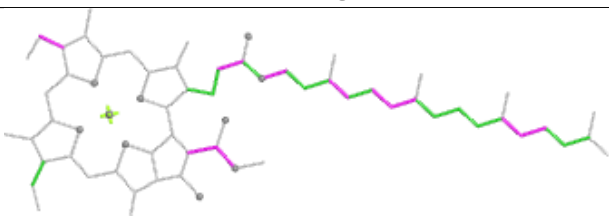
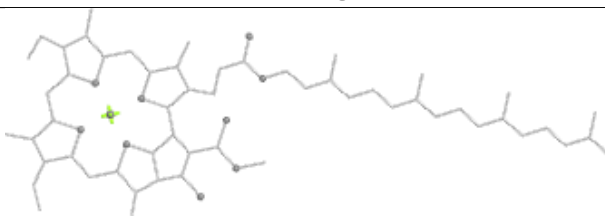
Torsions

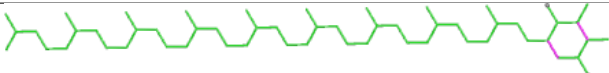
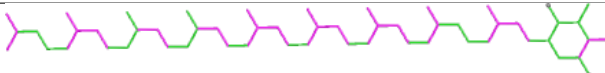
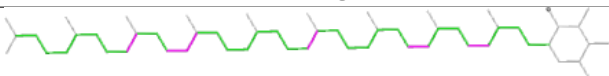


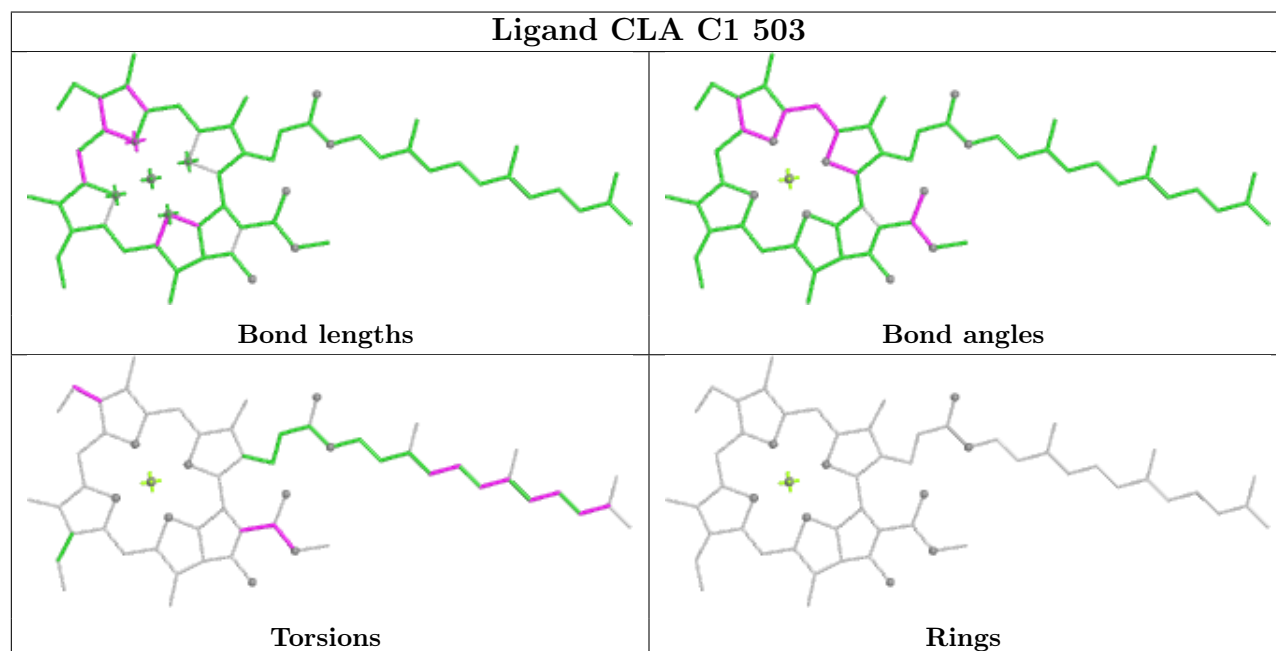
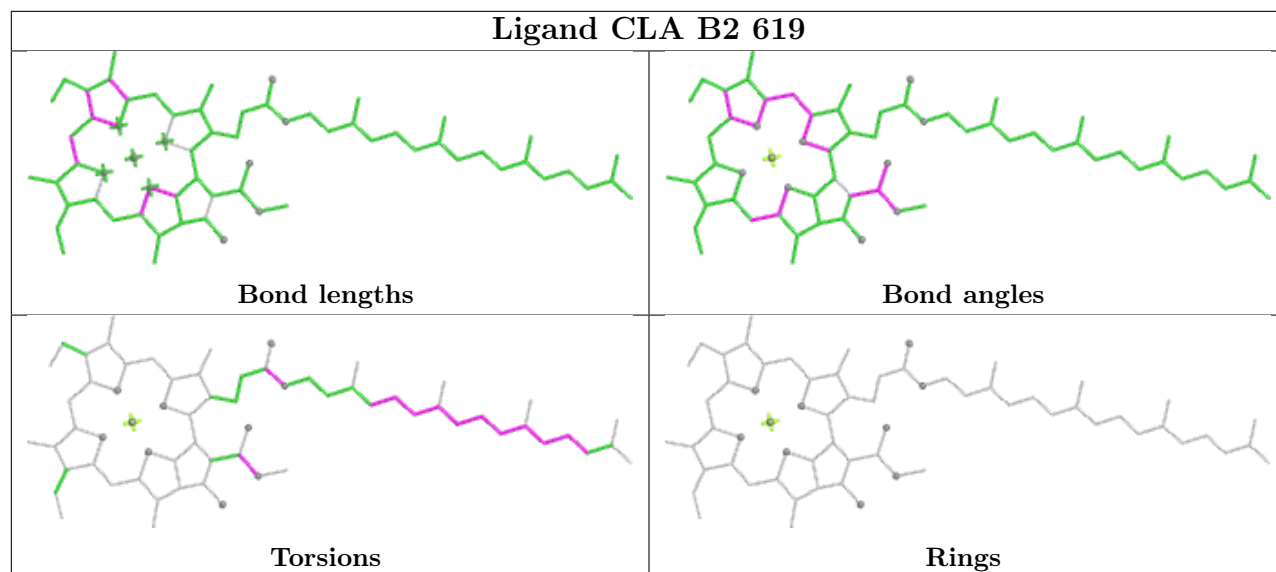
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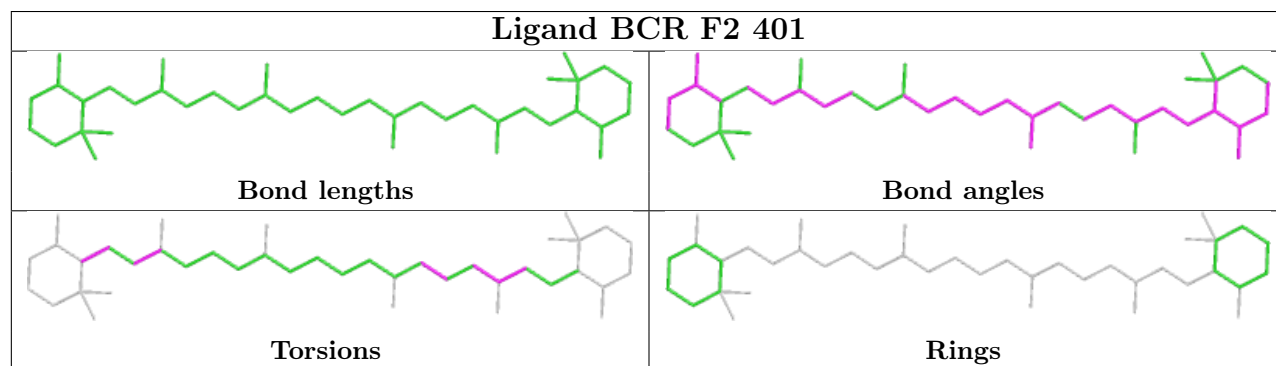
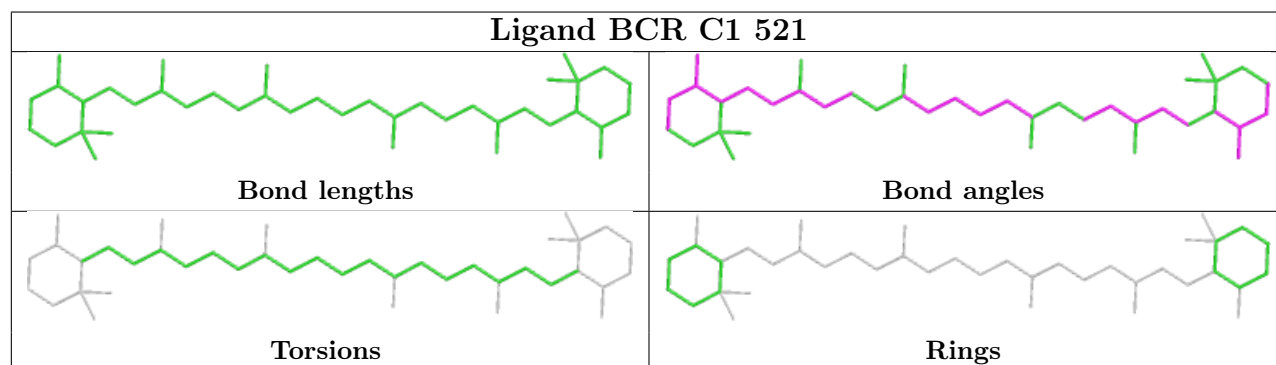
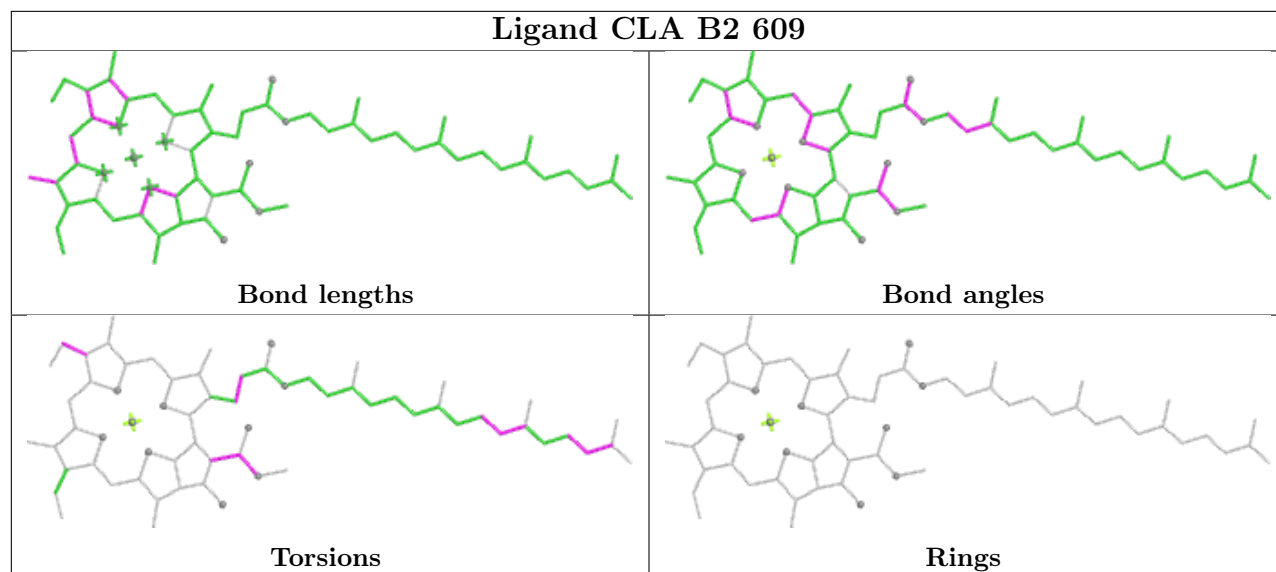


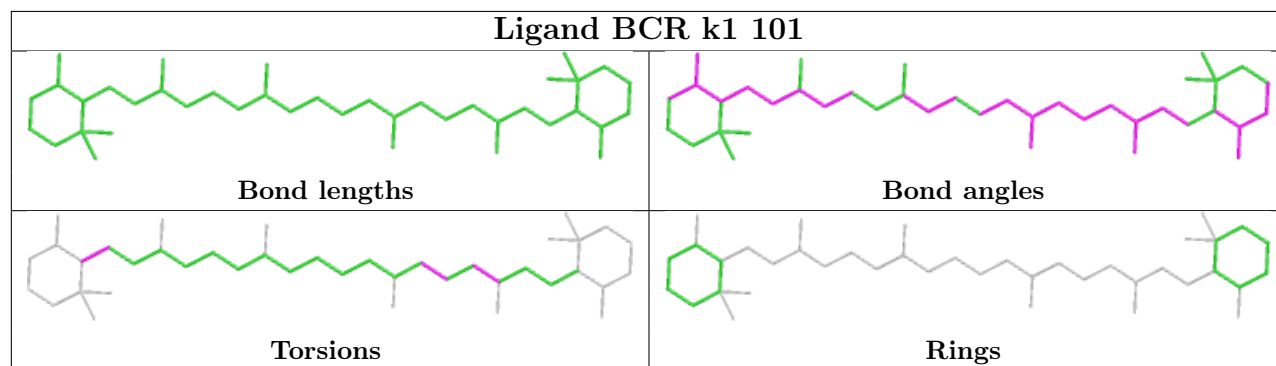
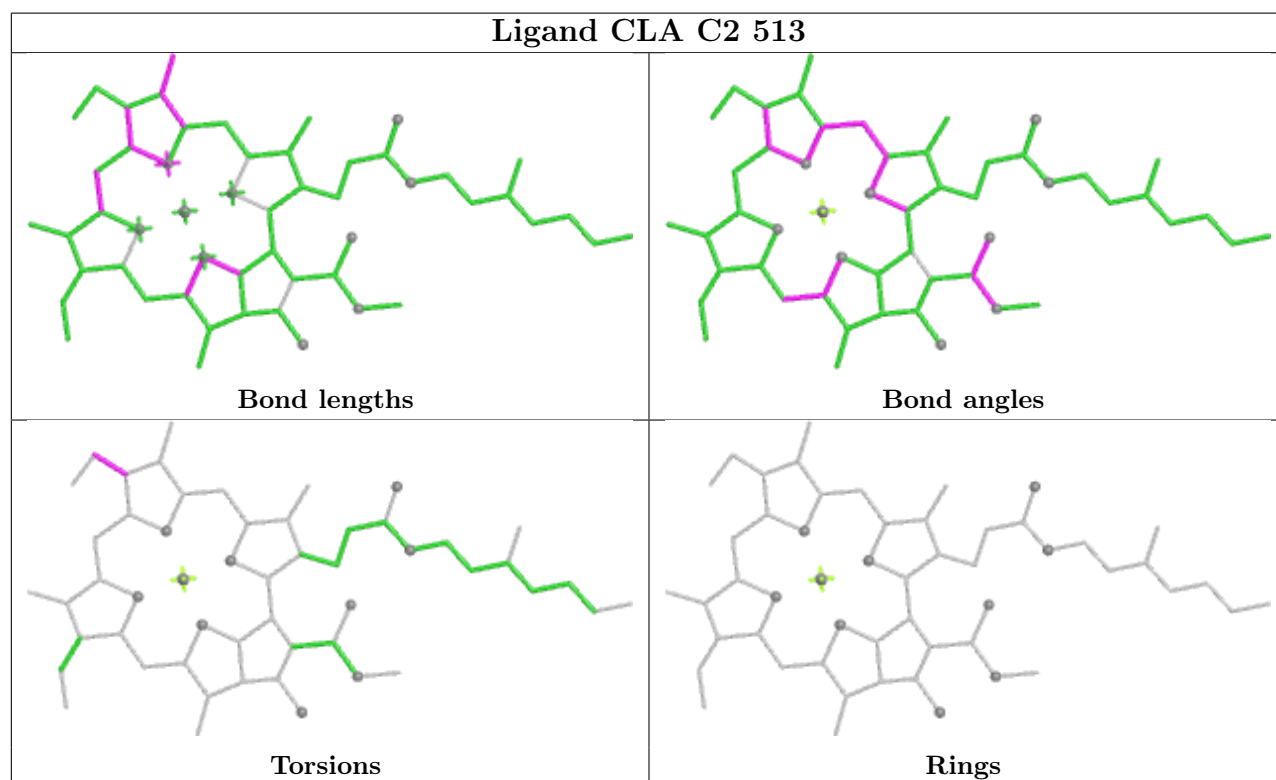
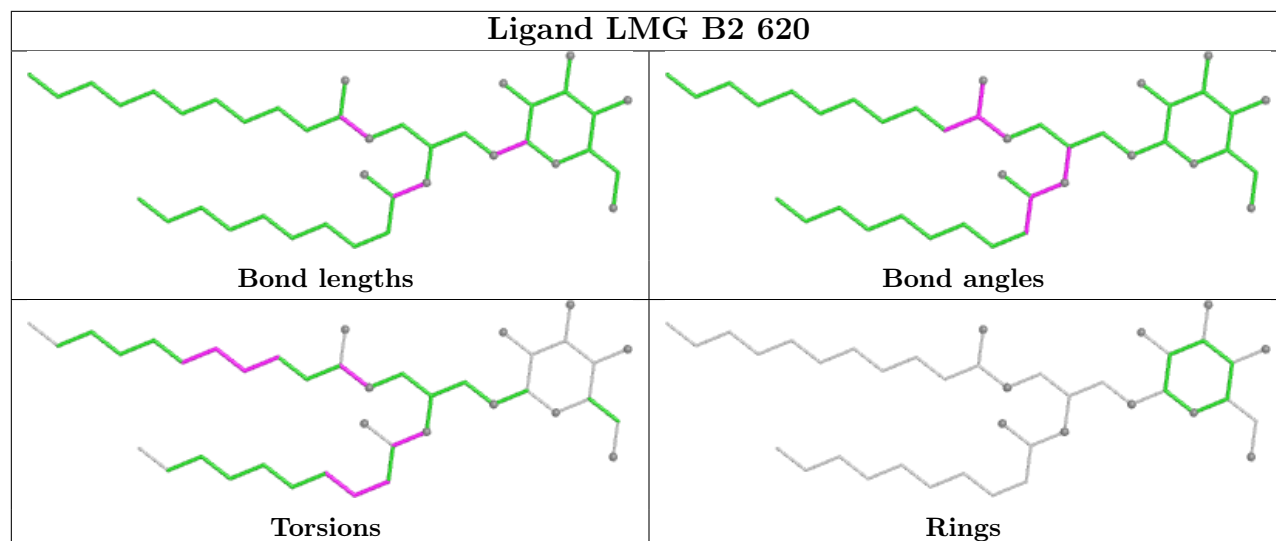
Ligand BCR B1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

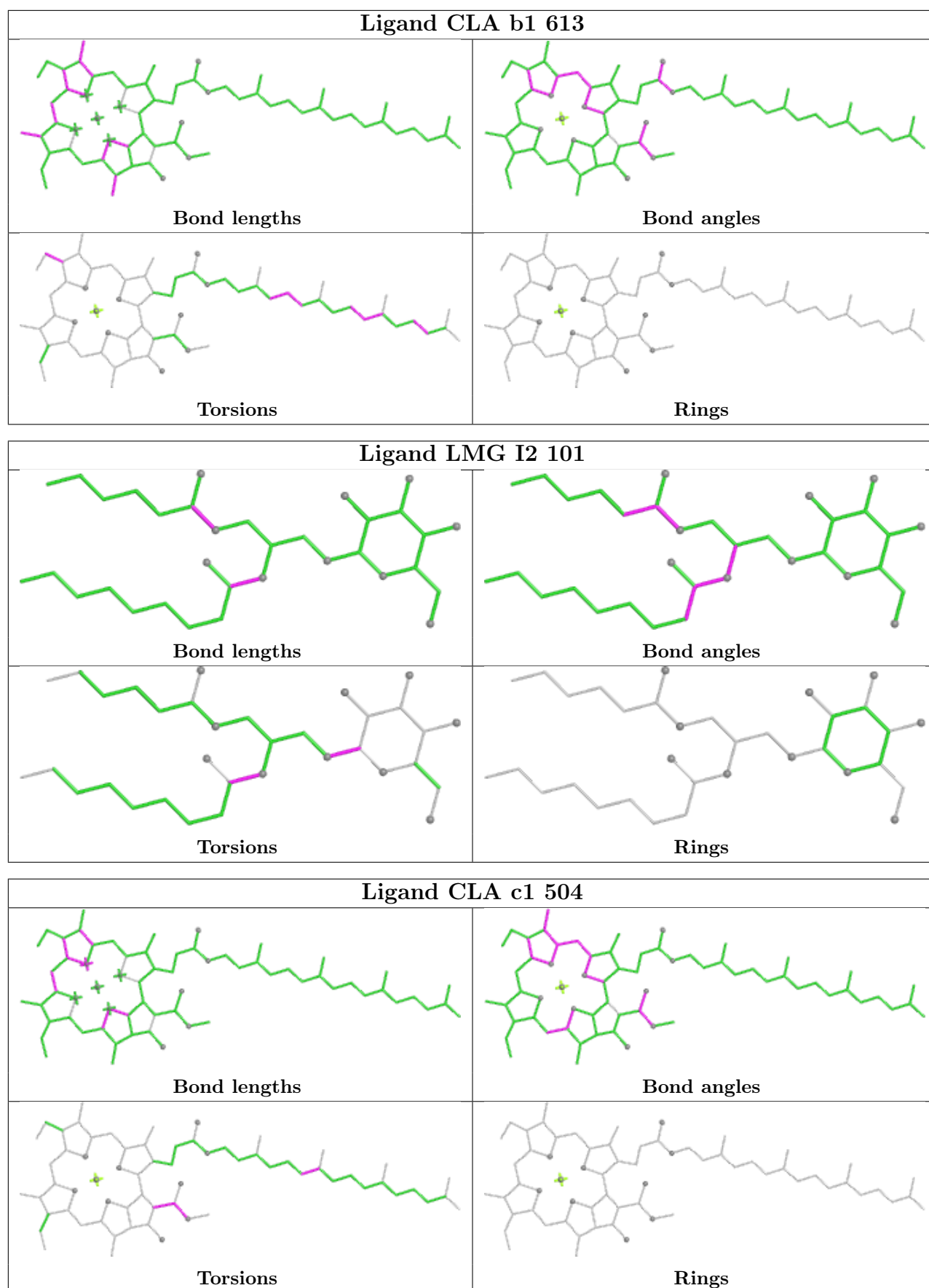
Ligand CLA c2 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

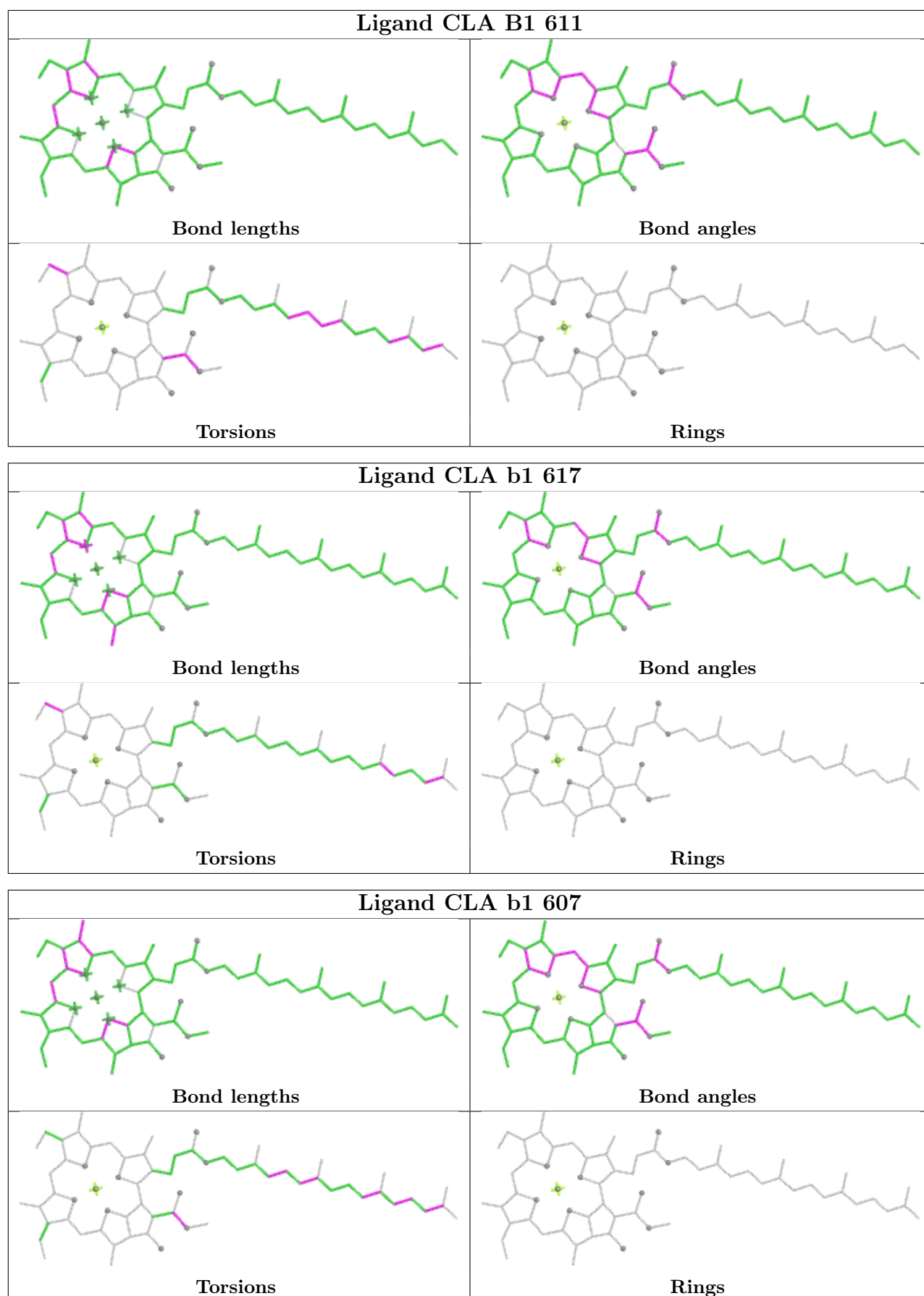
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Bond lengths	Bond angles
	
Torsions	Rings

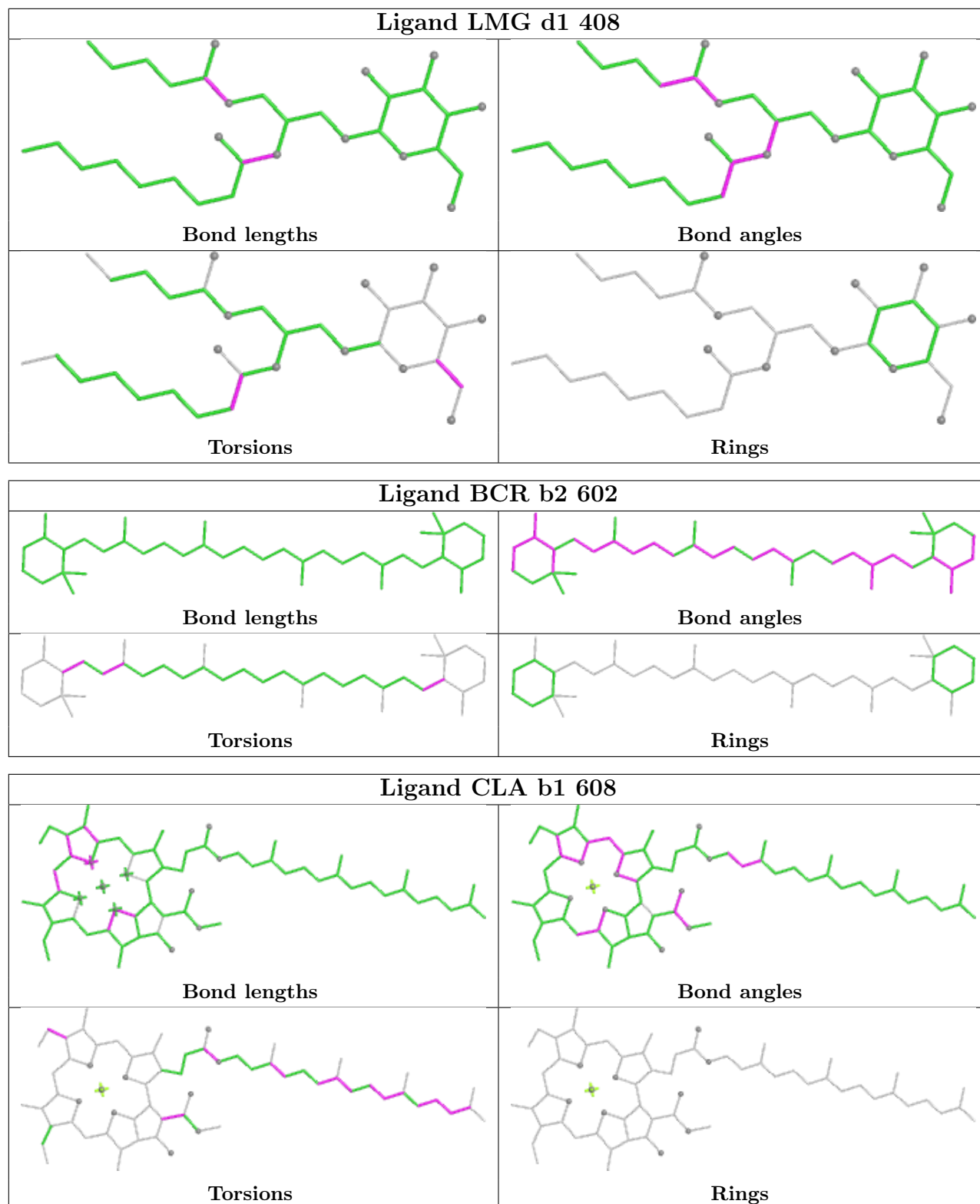


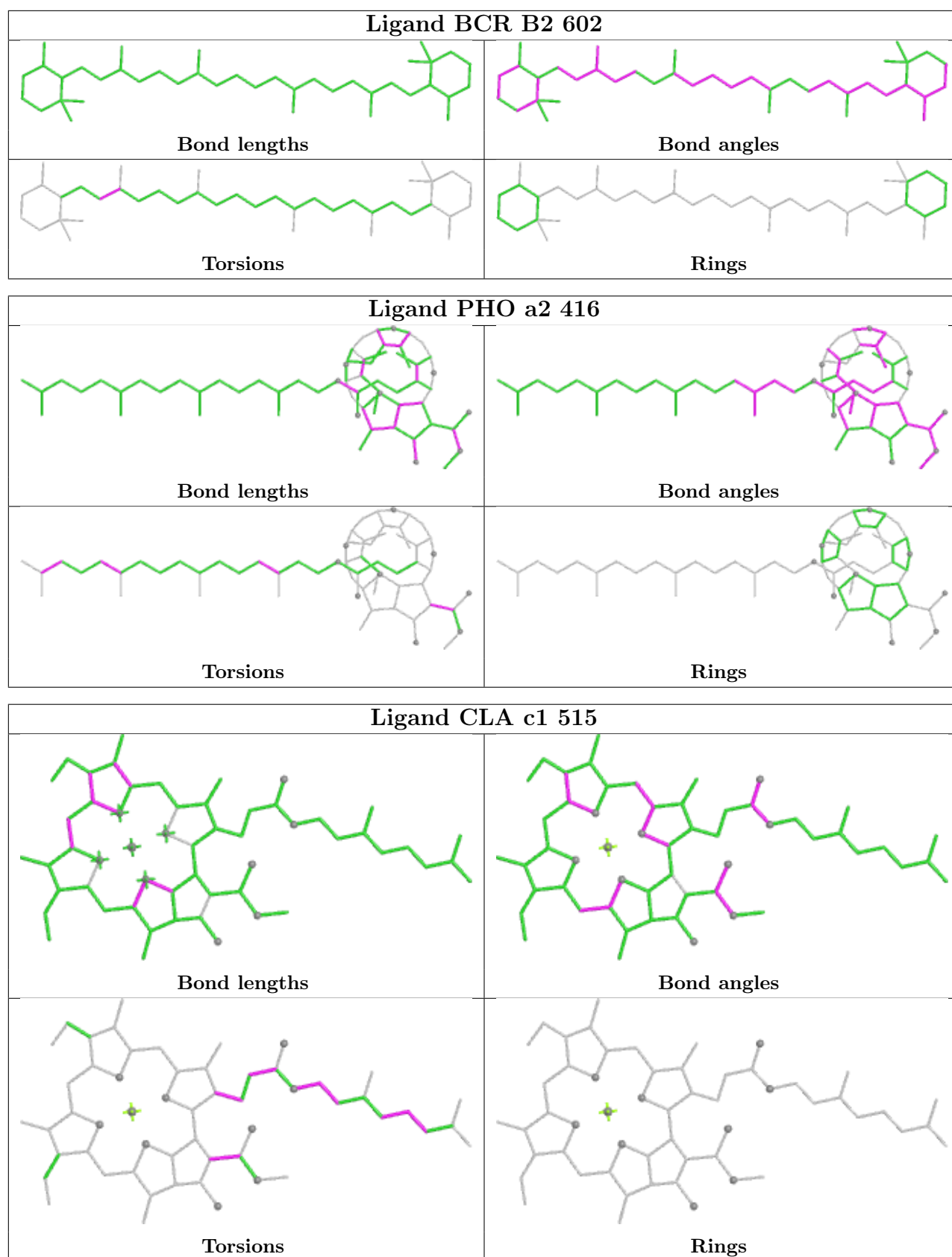


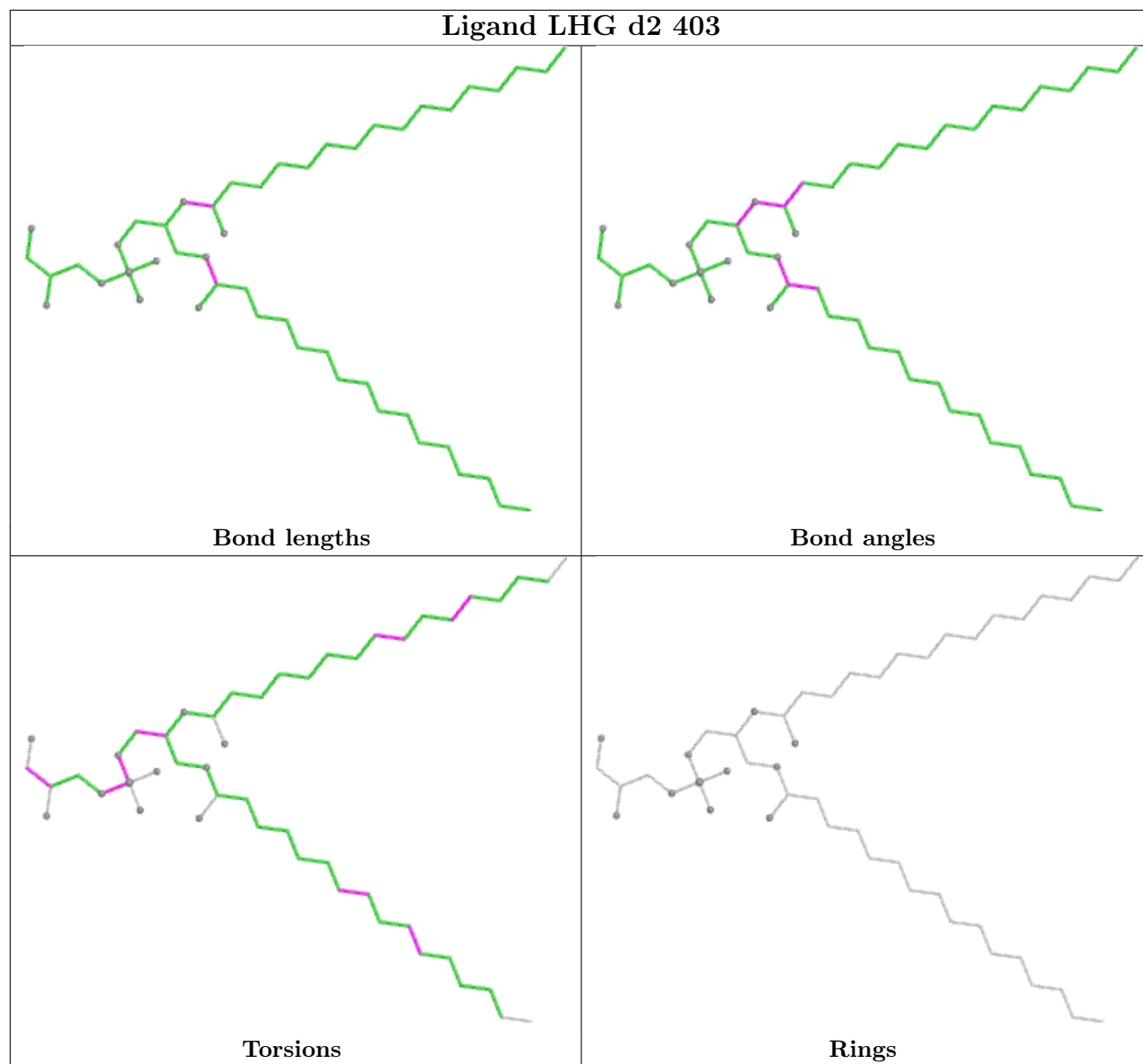




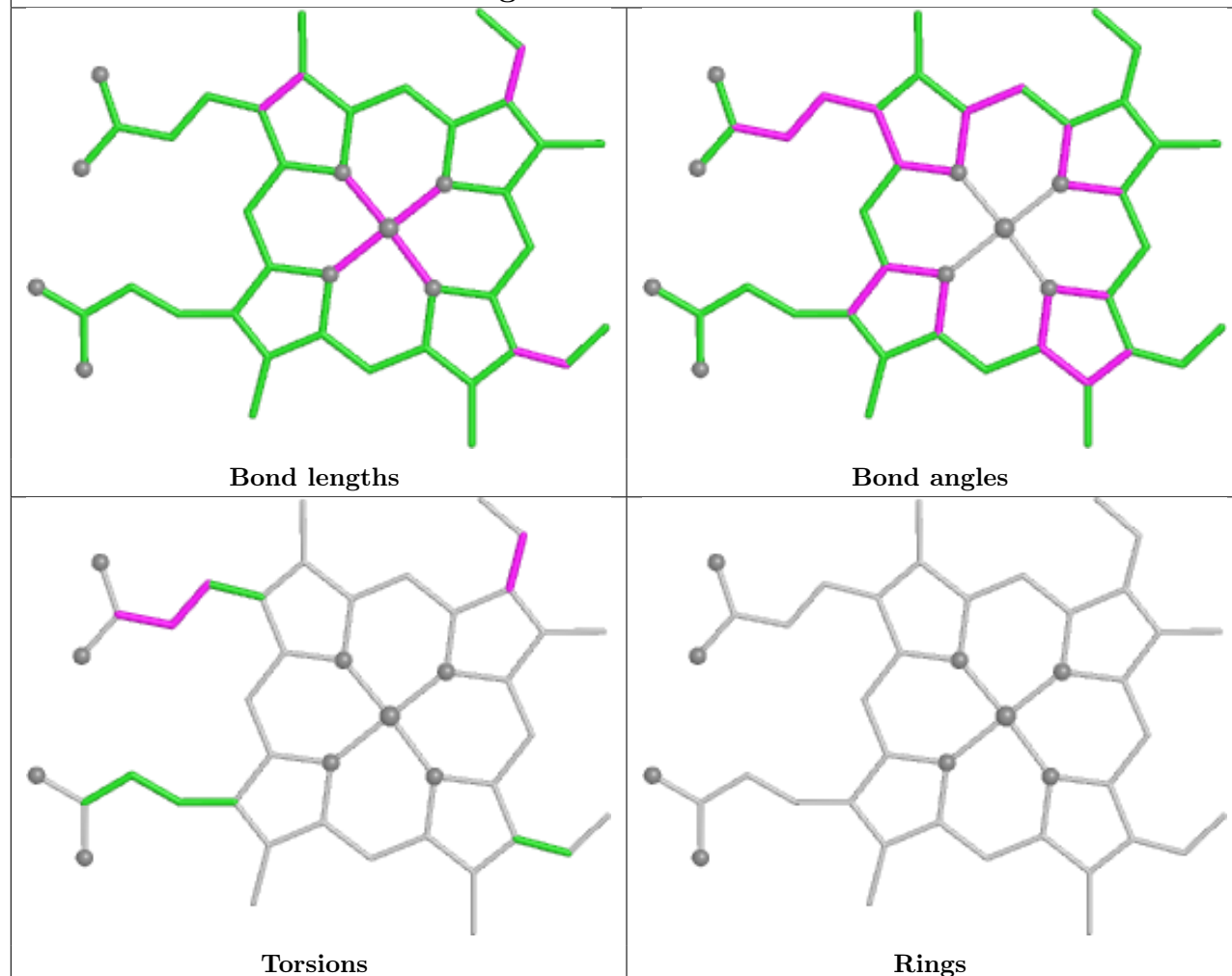




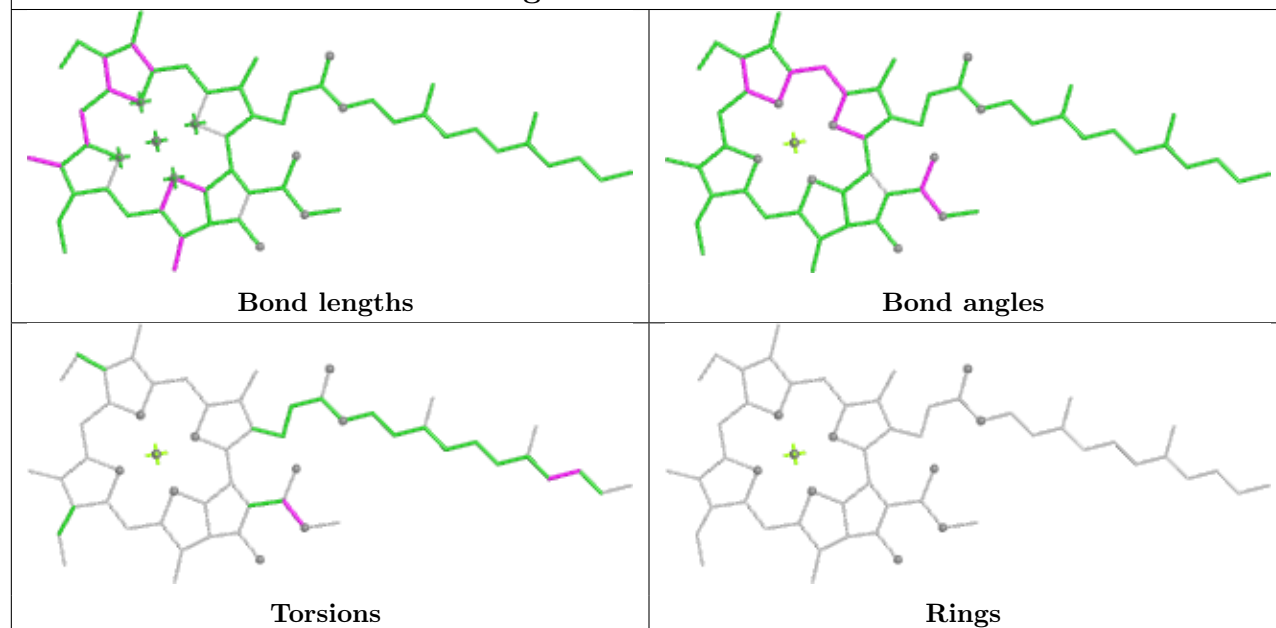


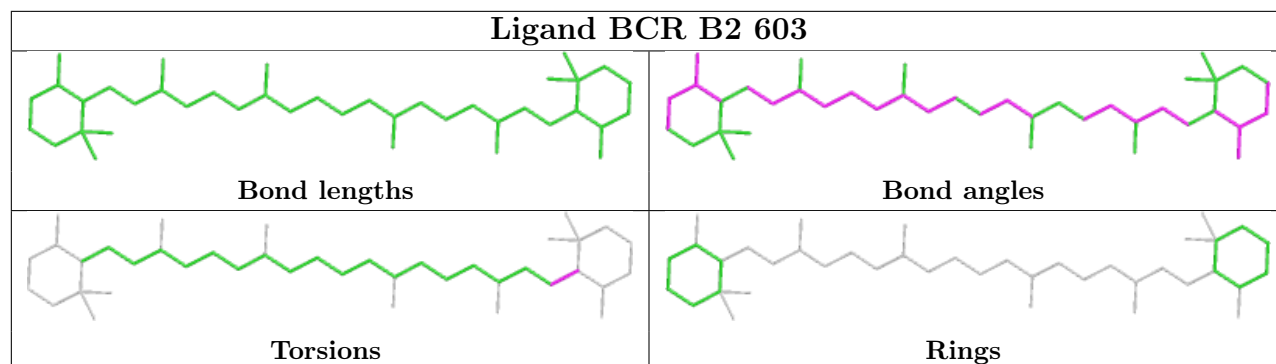
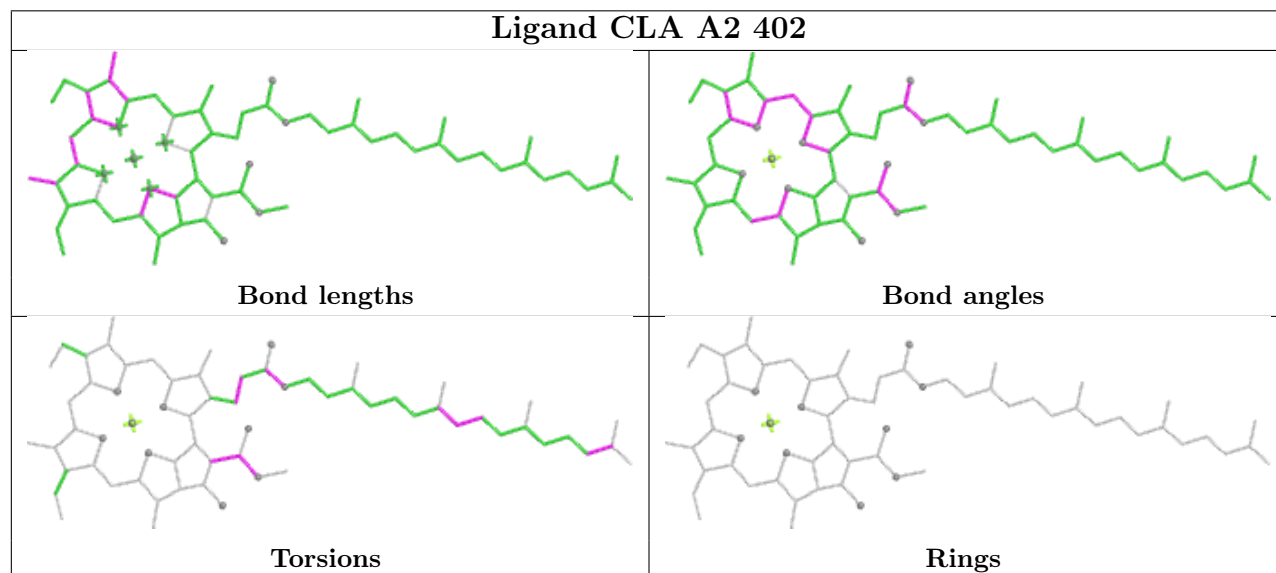
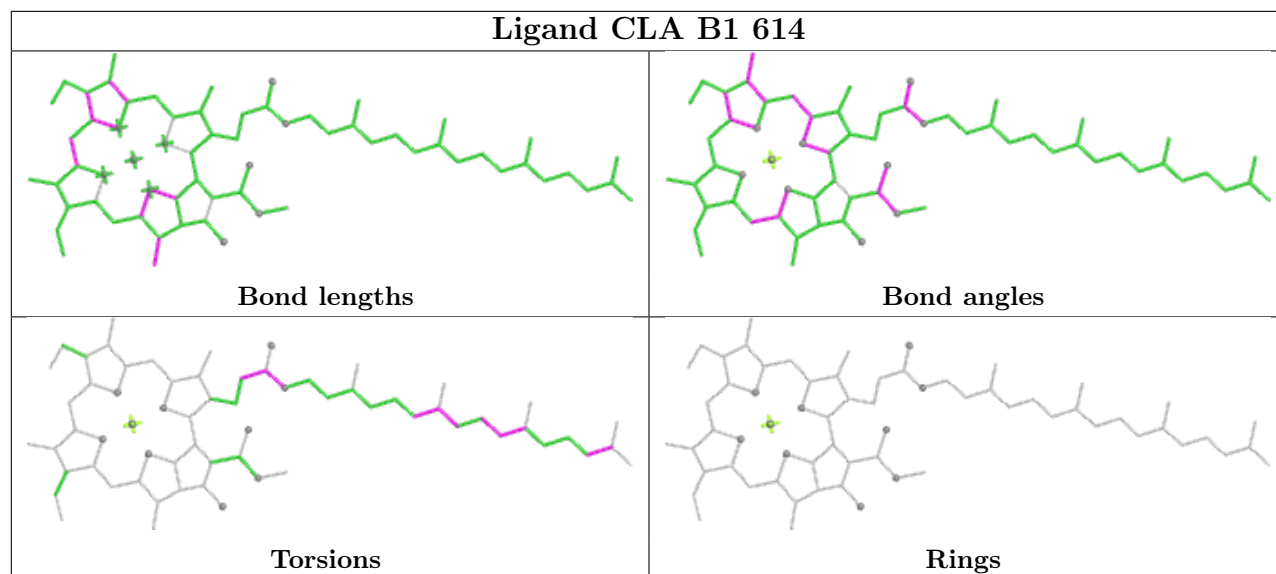


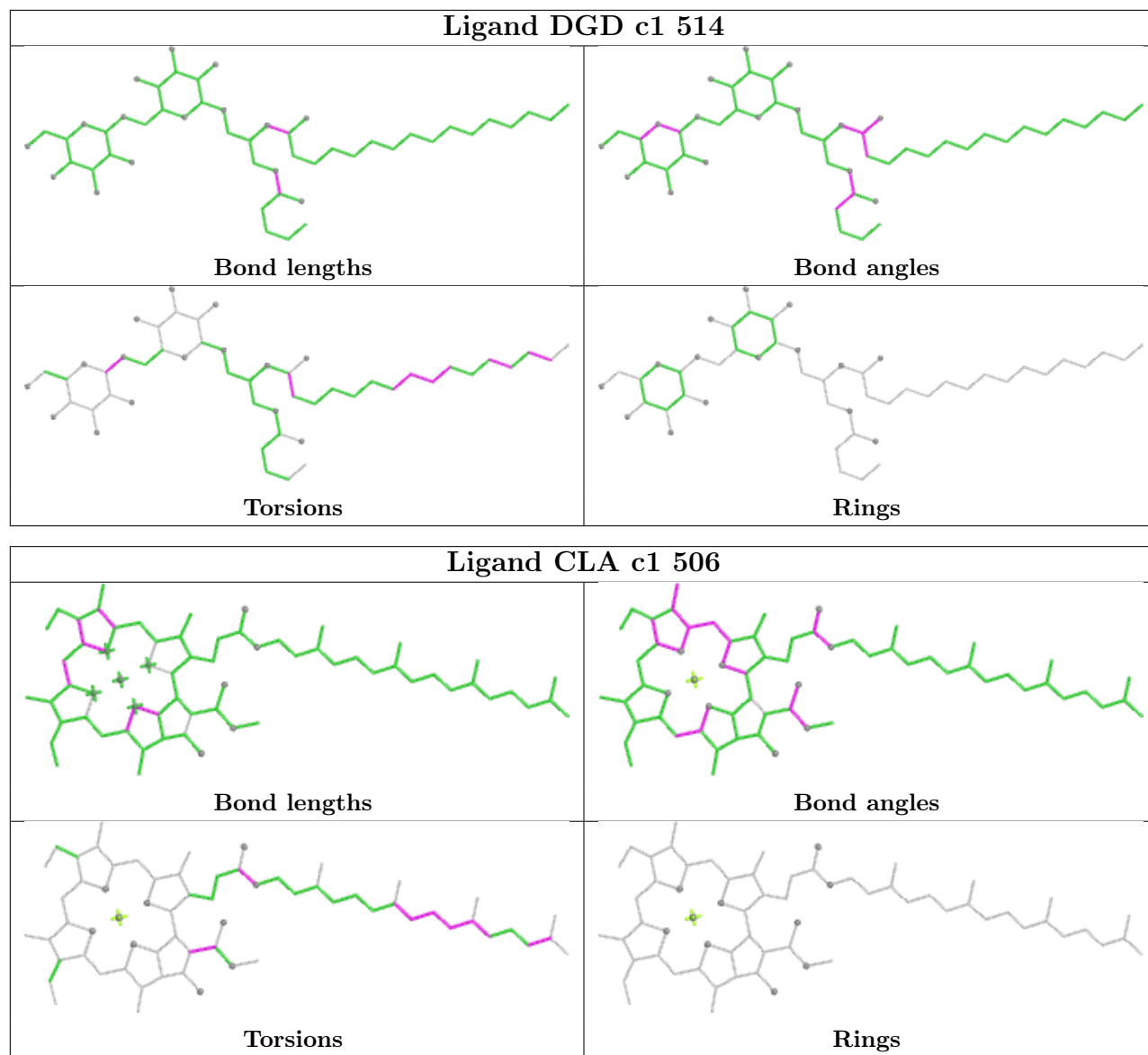
Ligand HEM V1 201

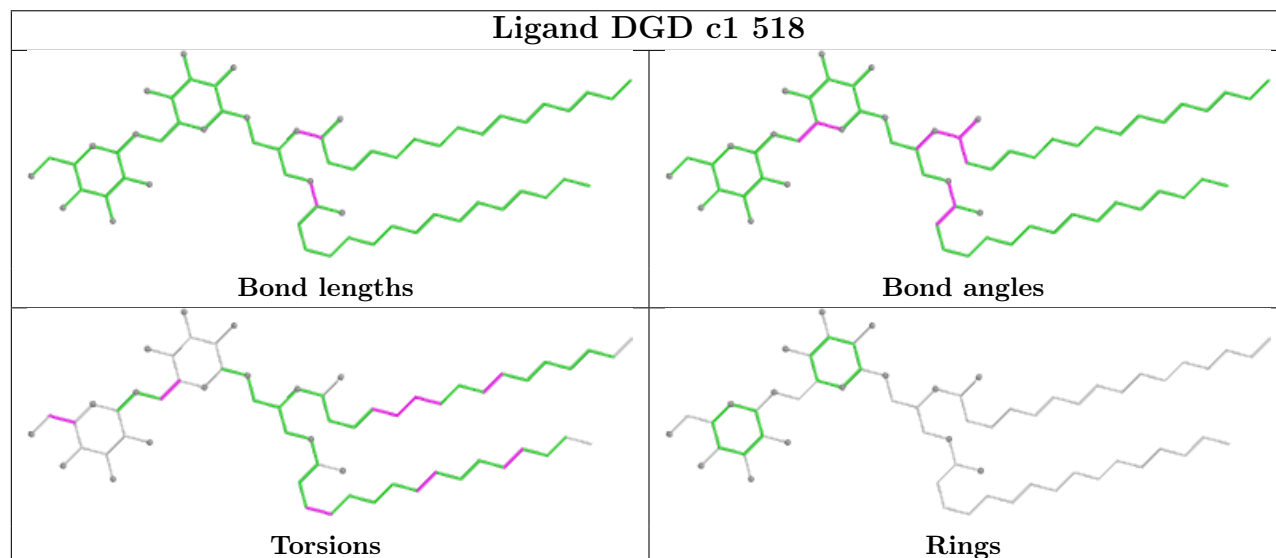
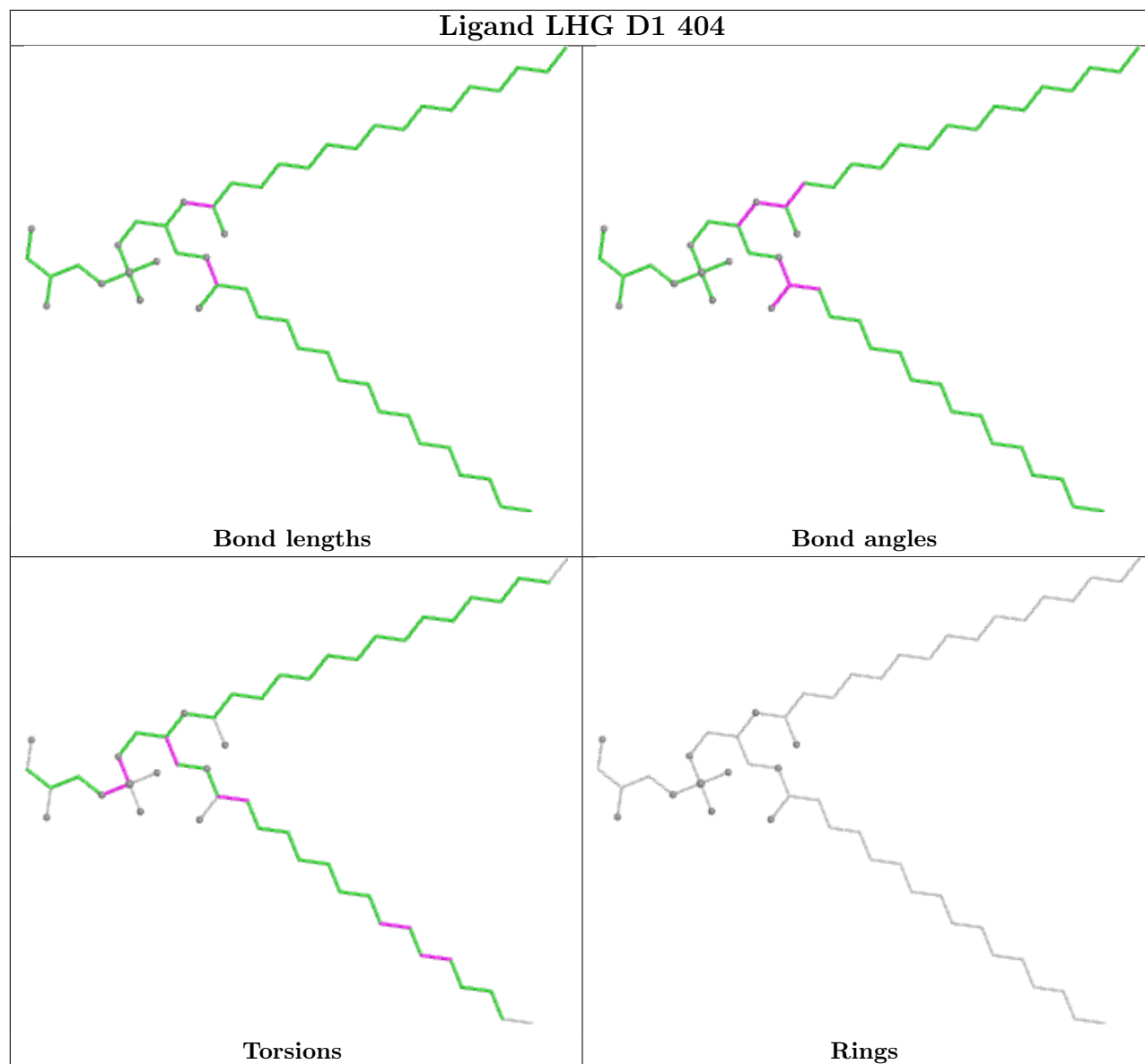


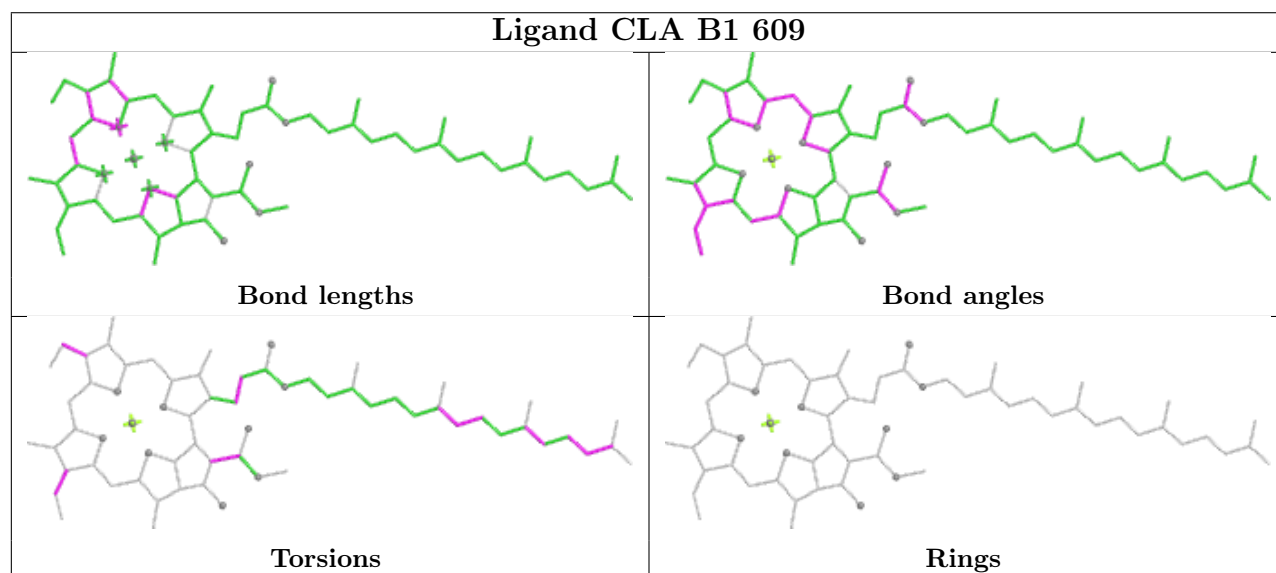
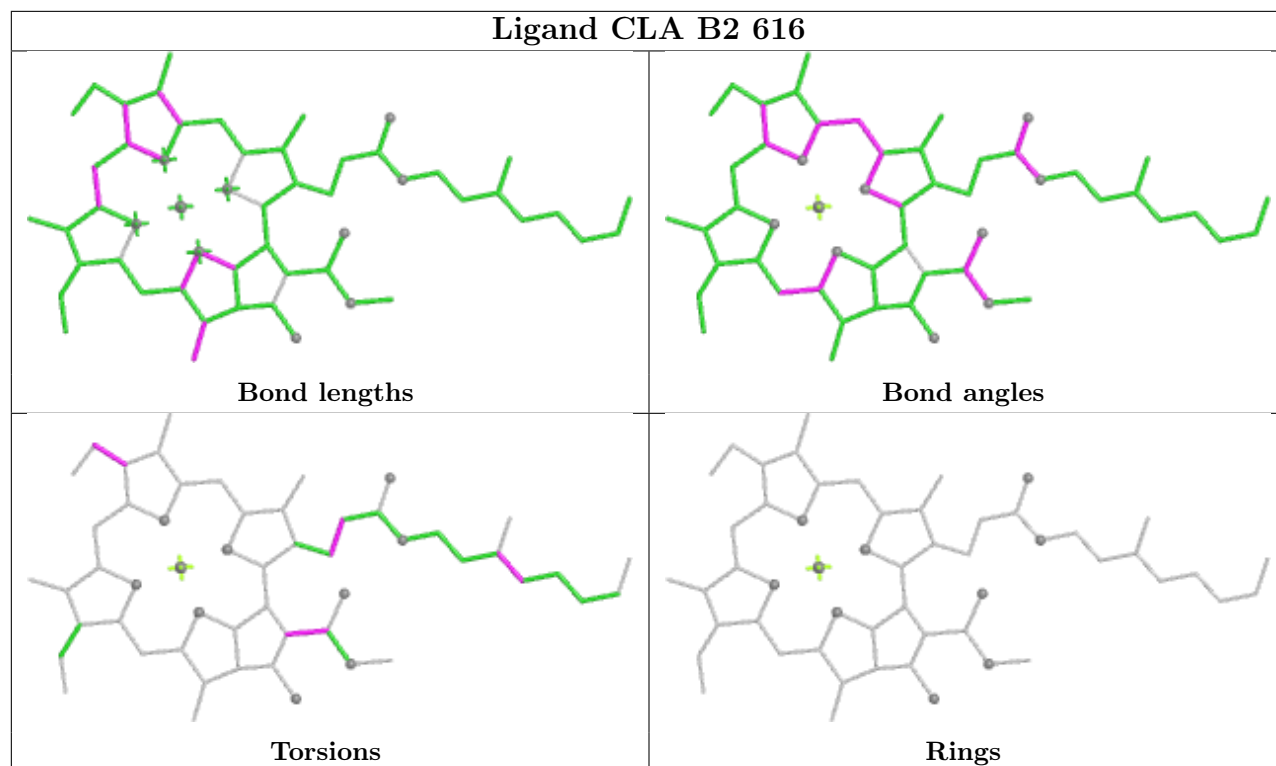
Ligand CLA B1 618



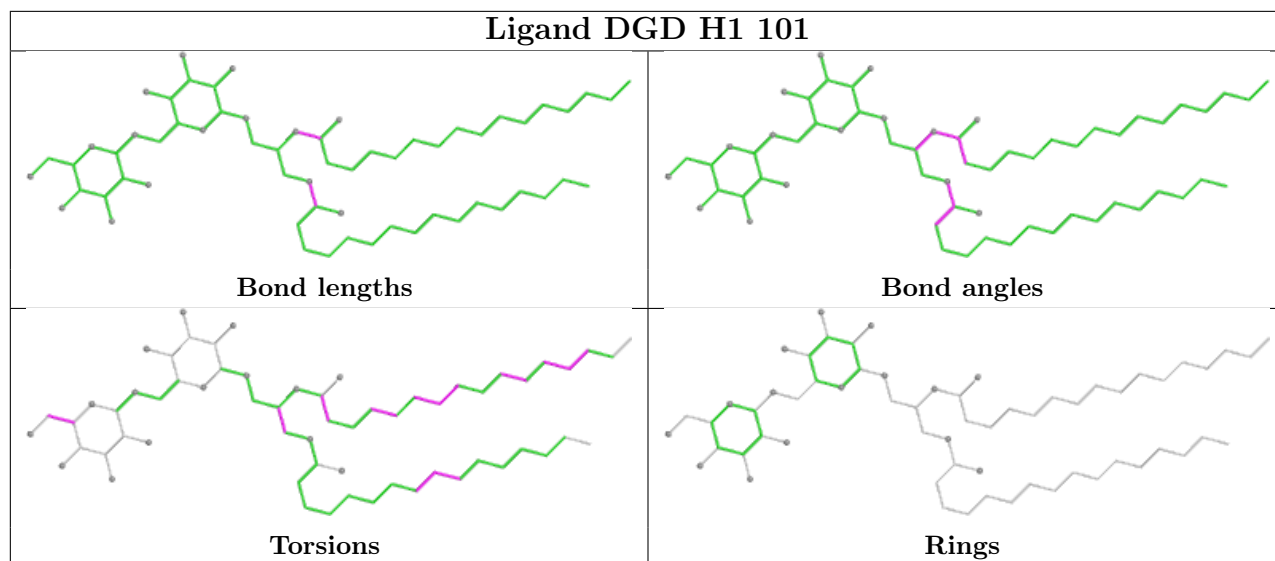




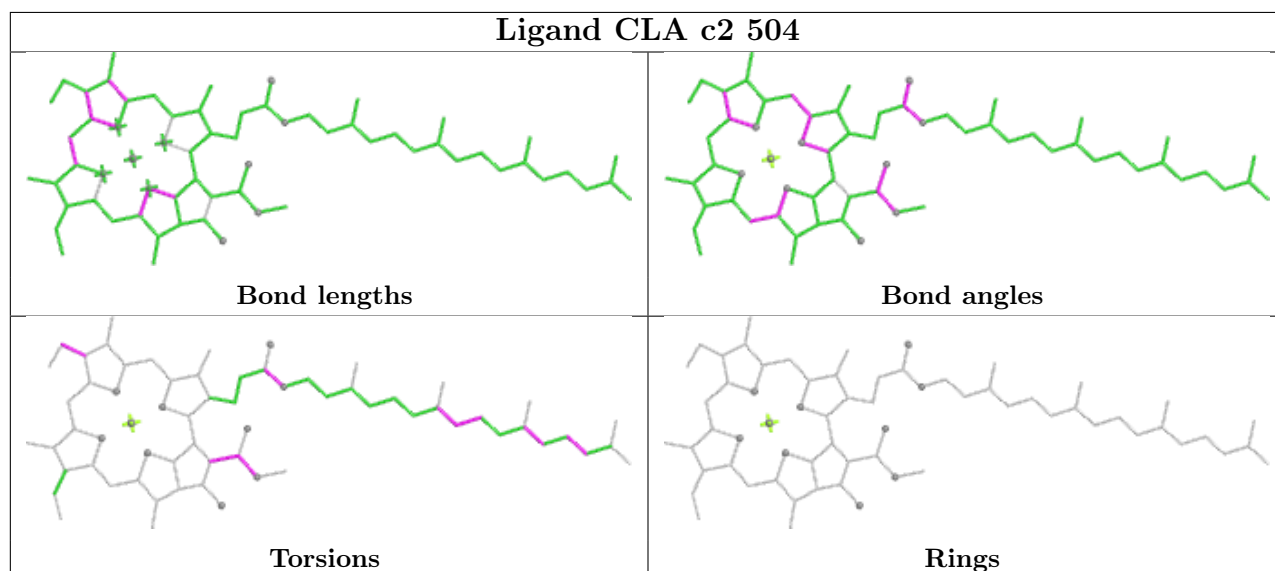




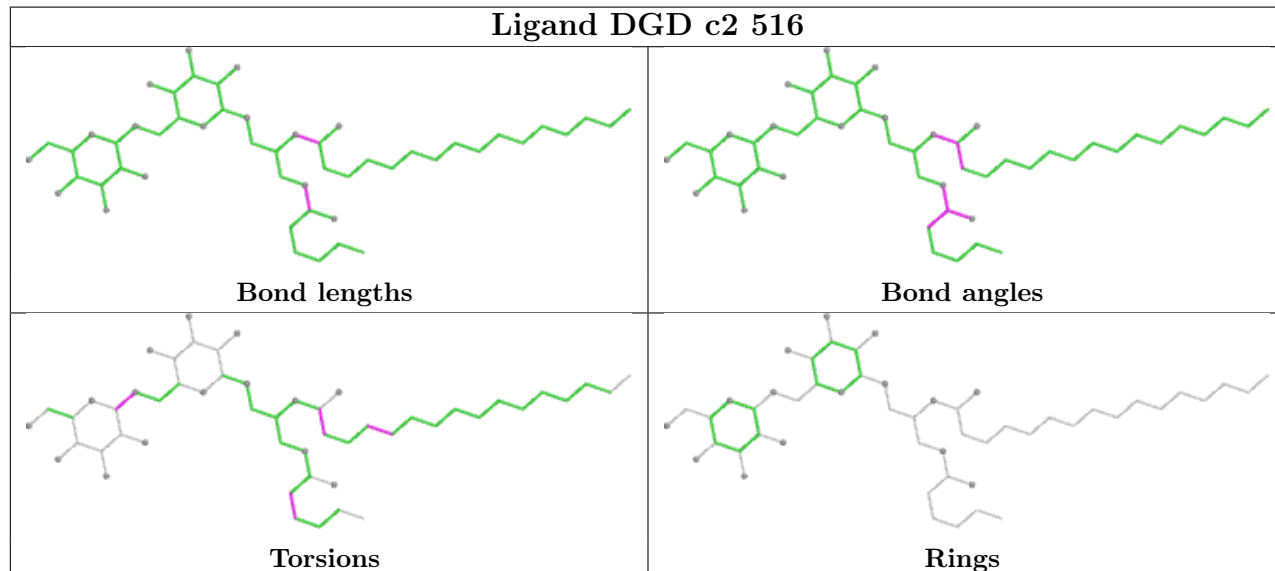
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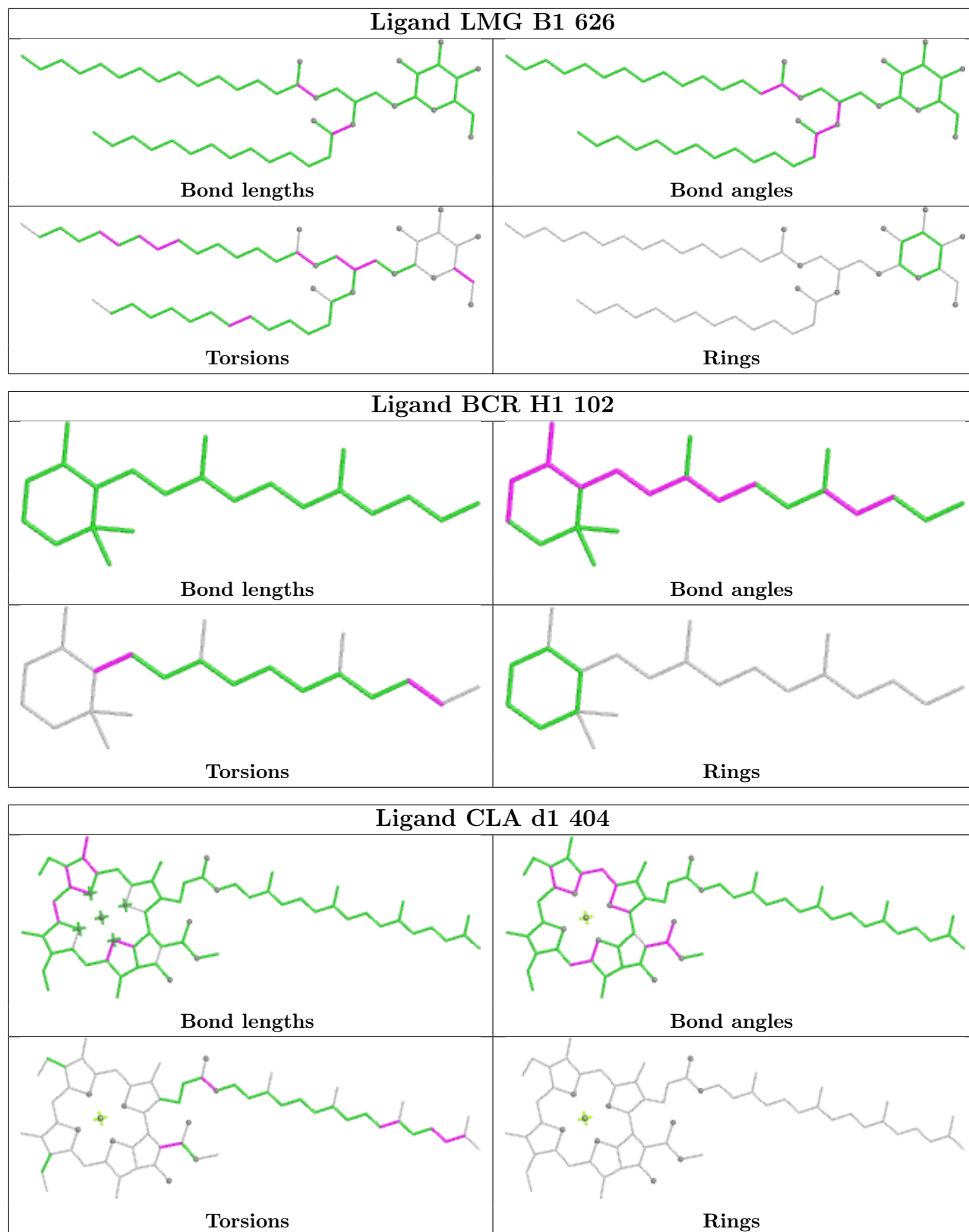


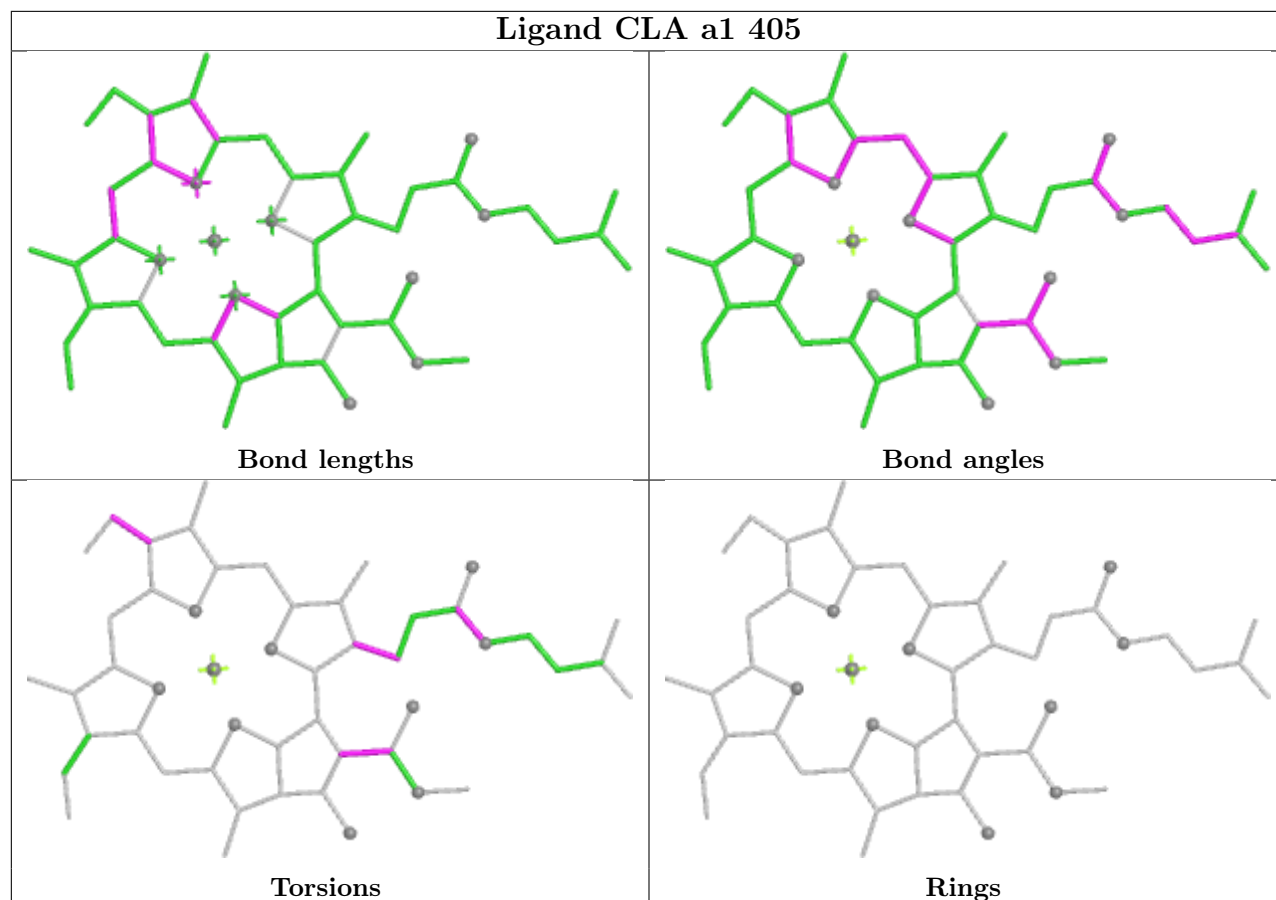
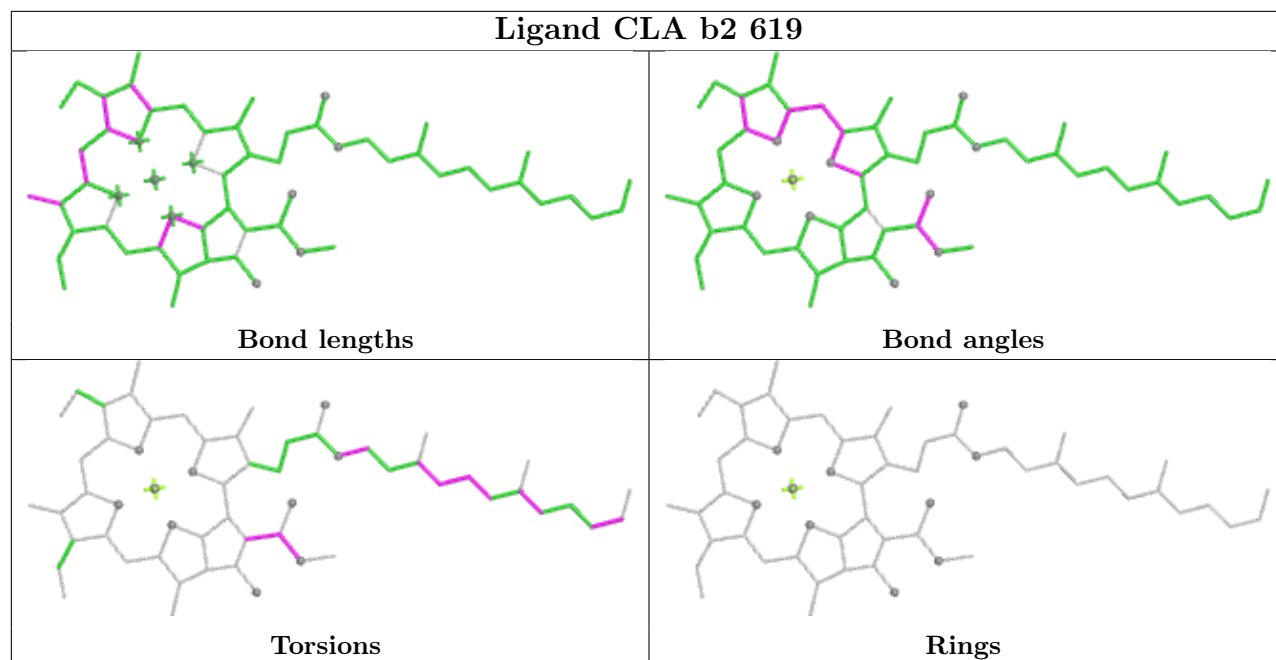
Ligand CLA c2 504

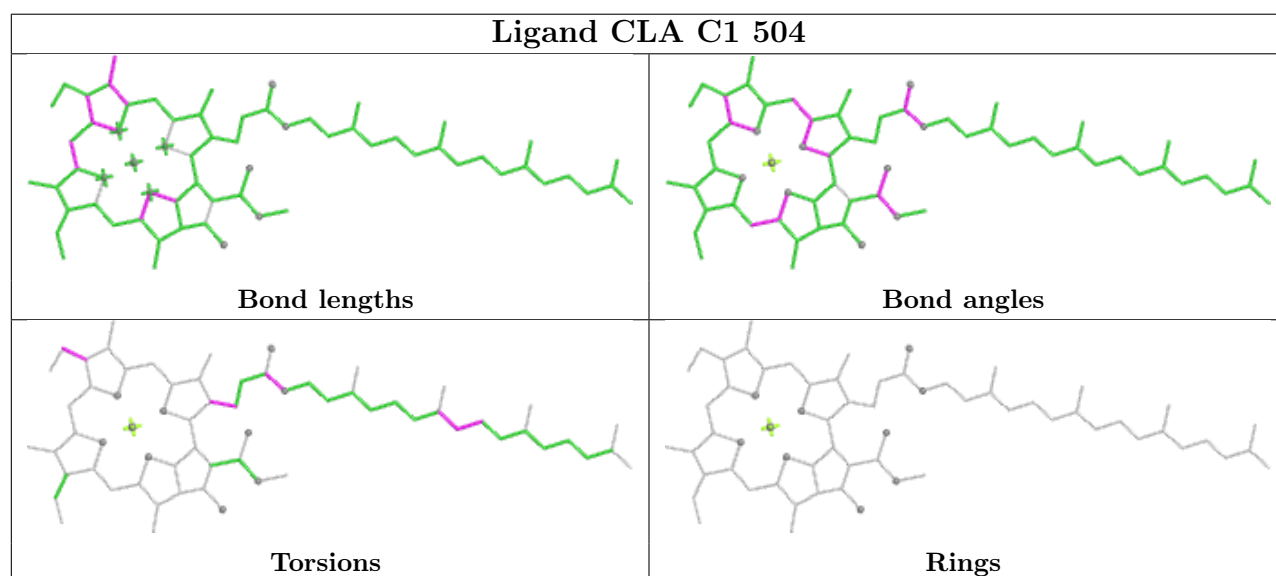
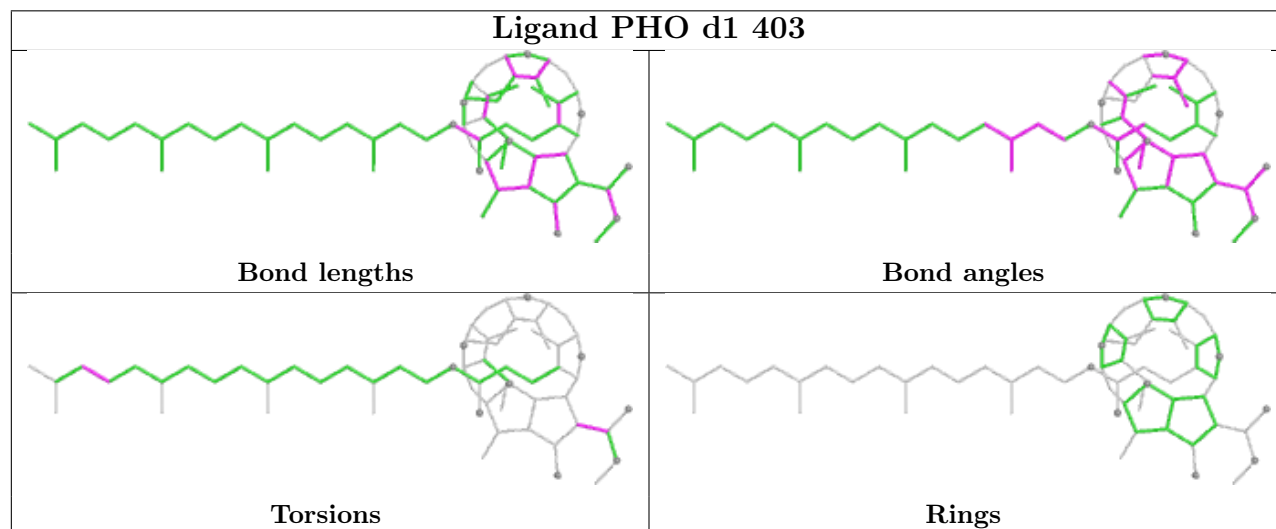
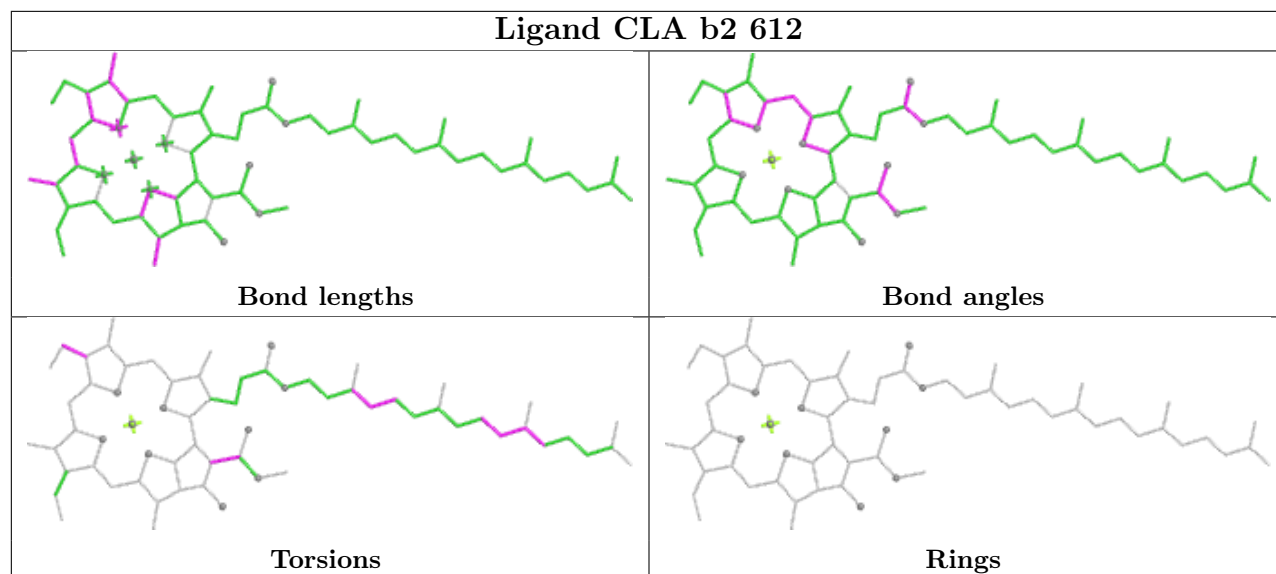


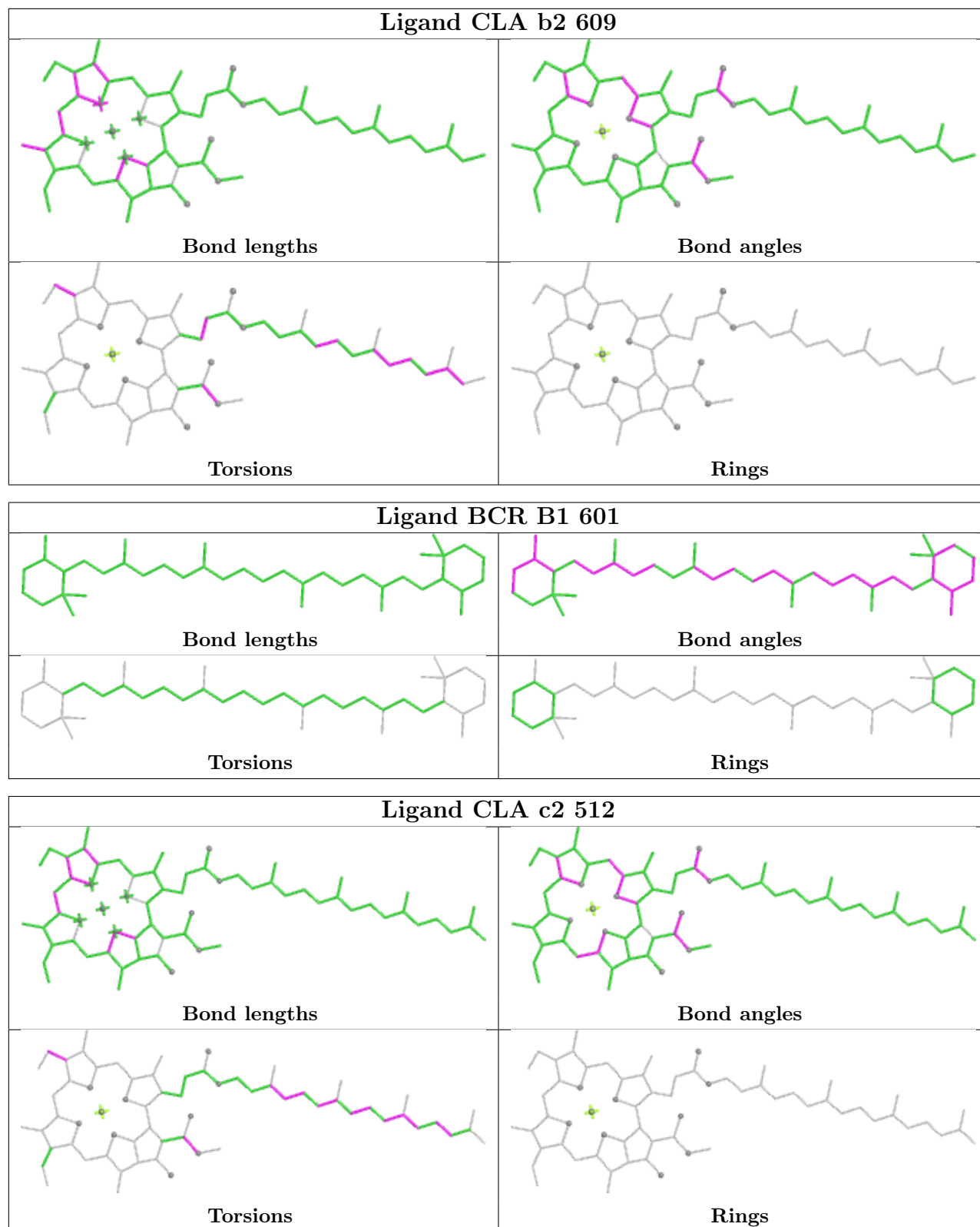
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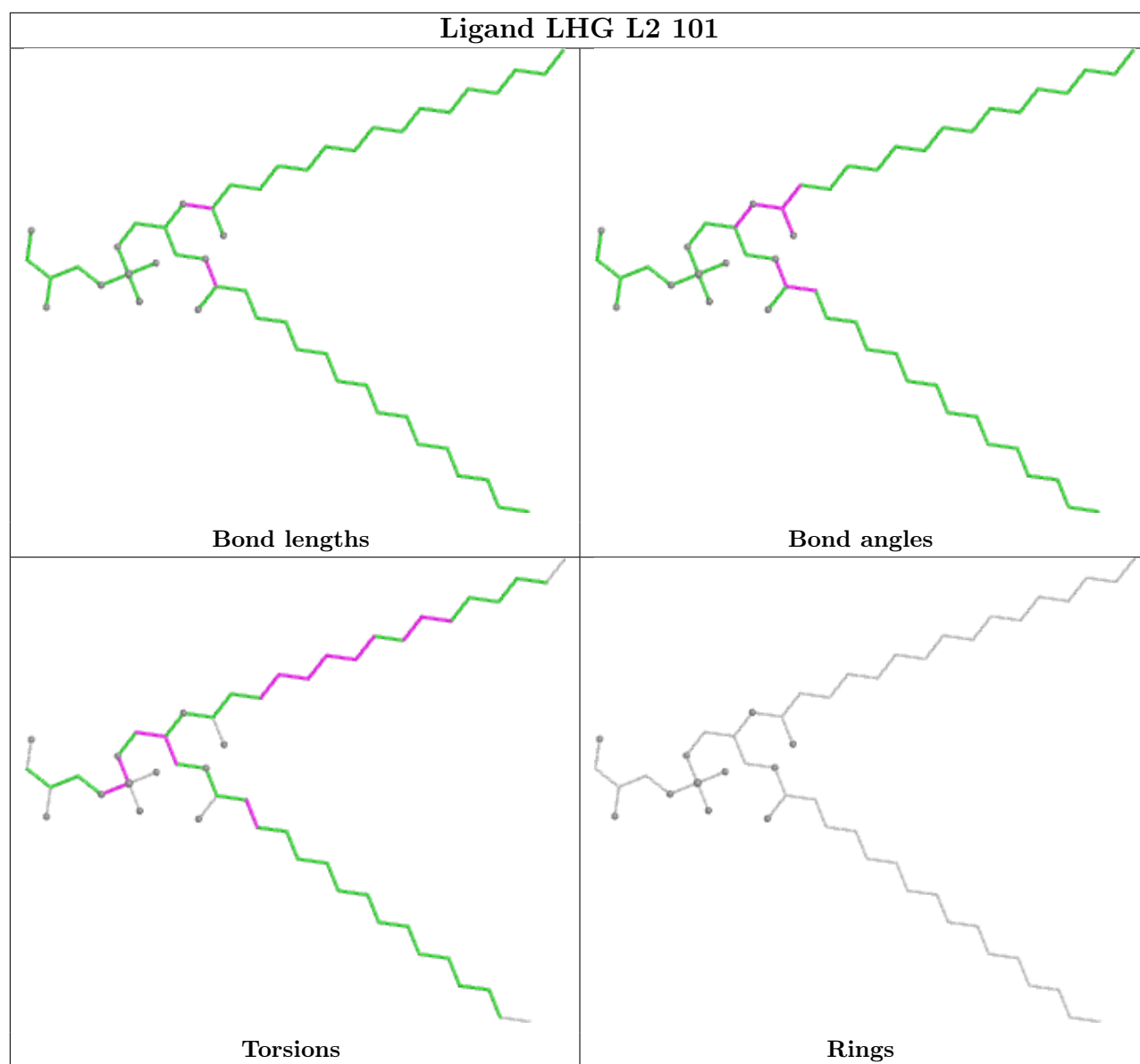




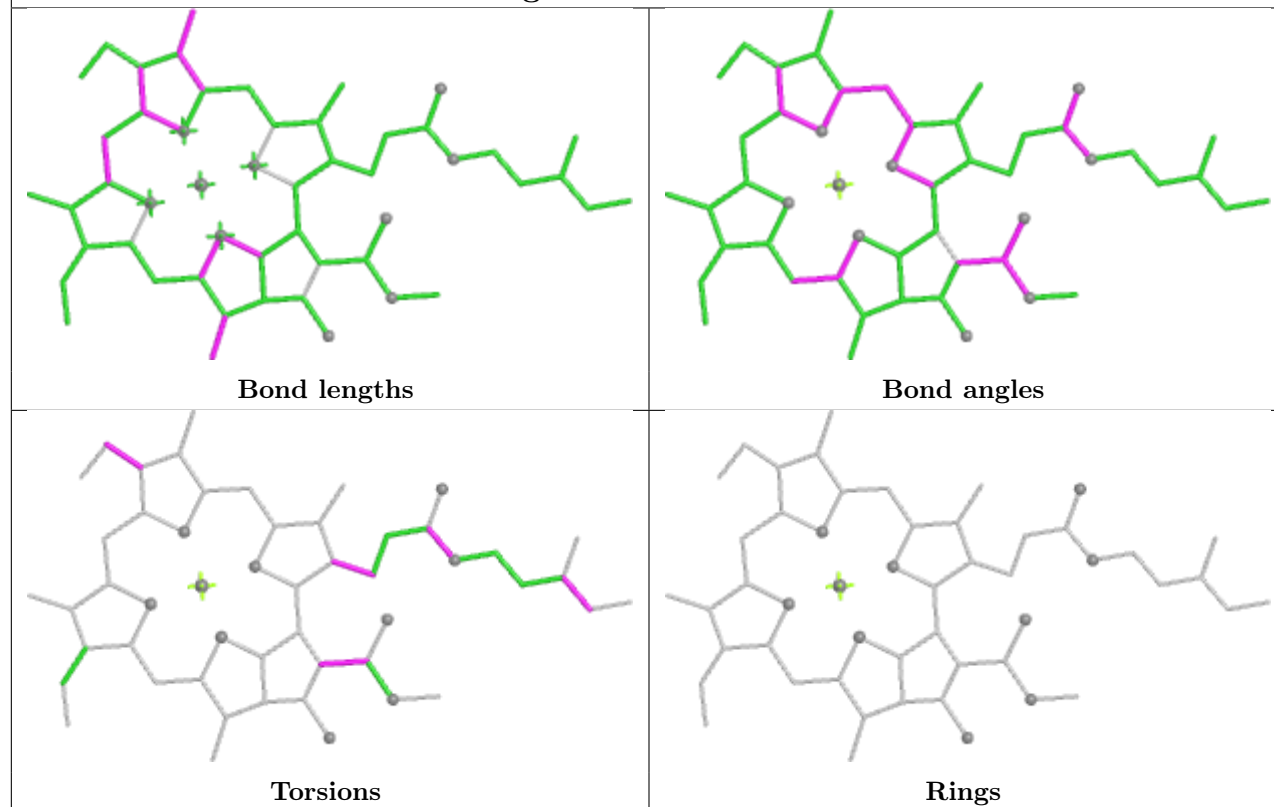




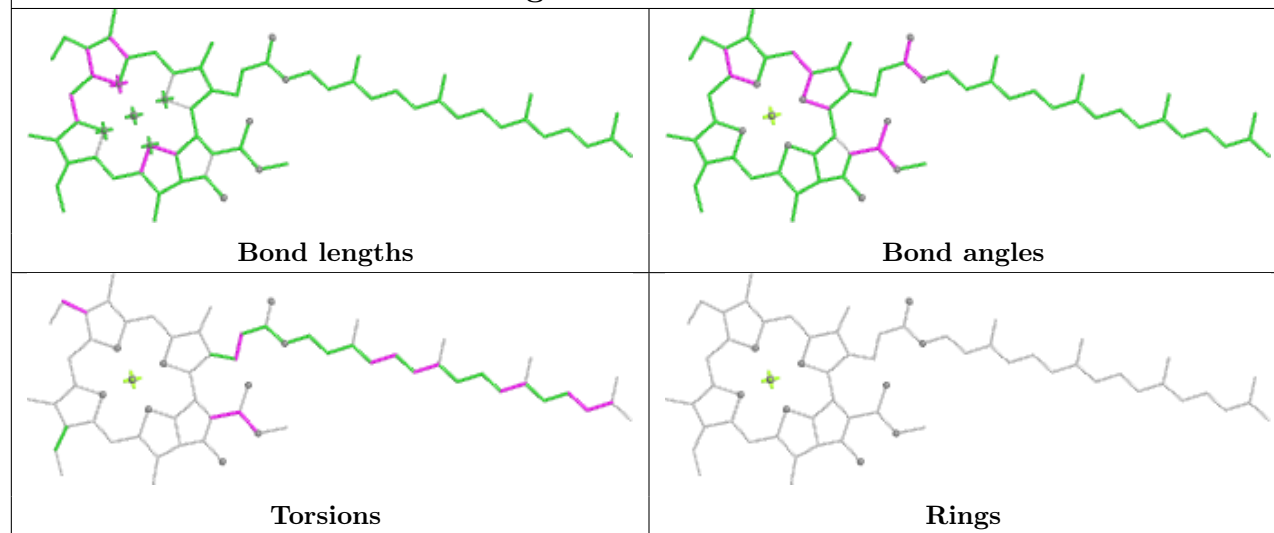


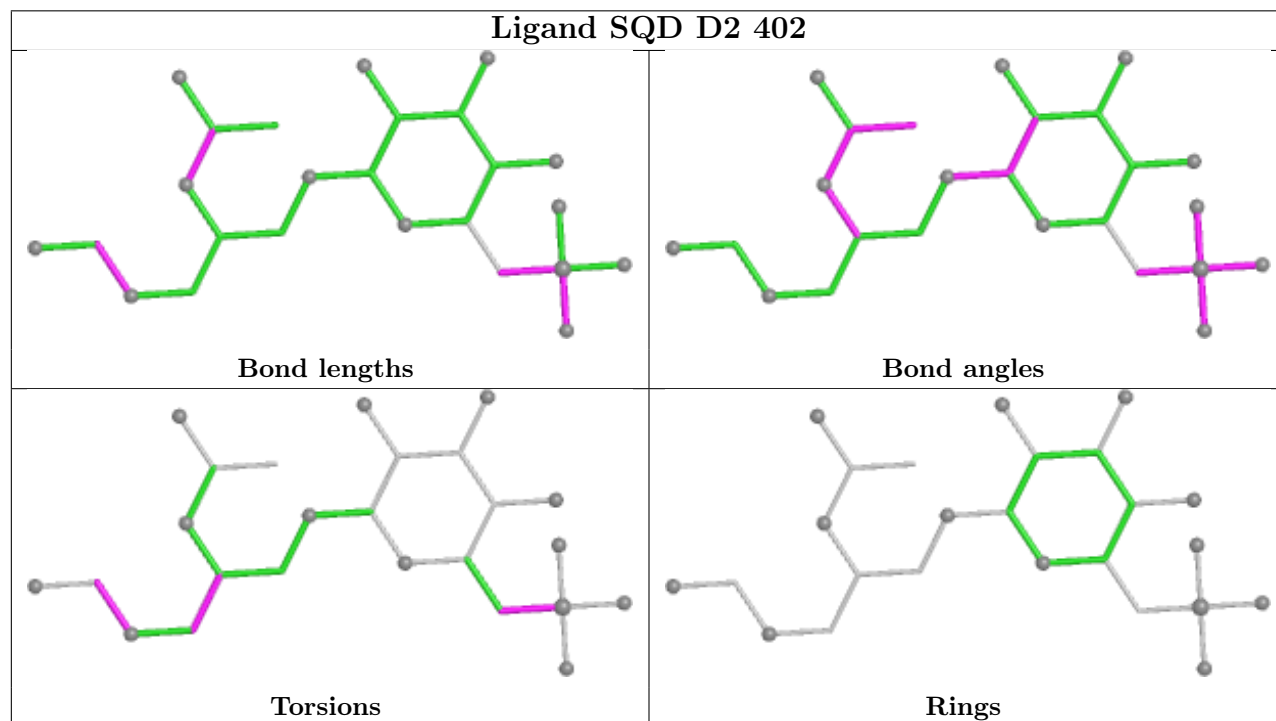
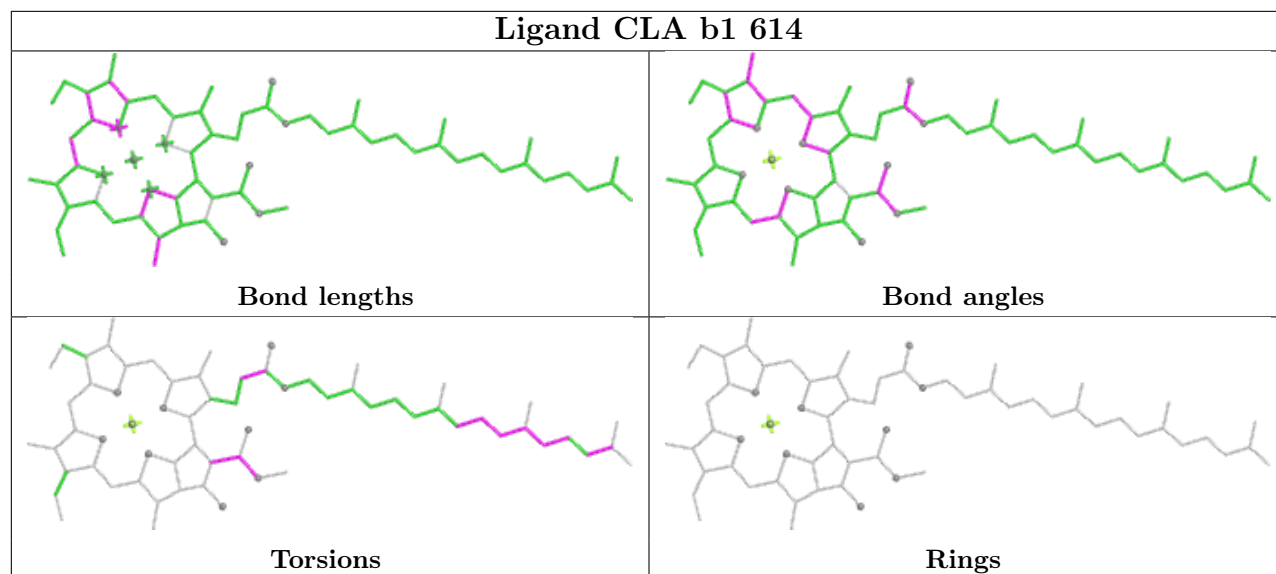


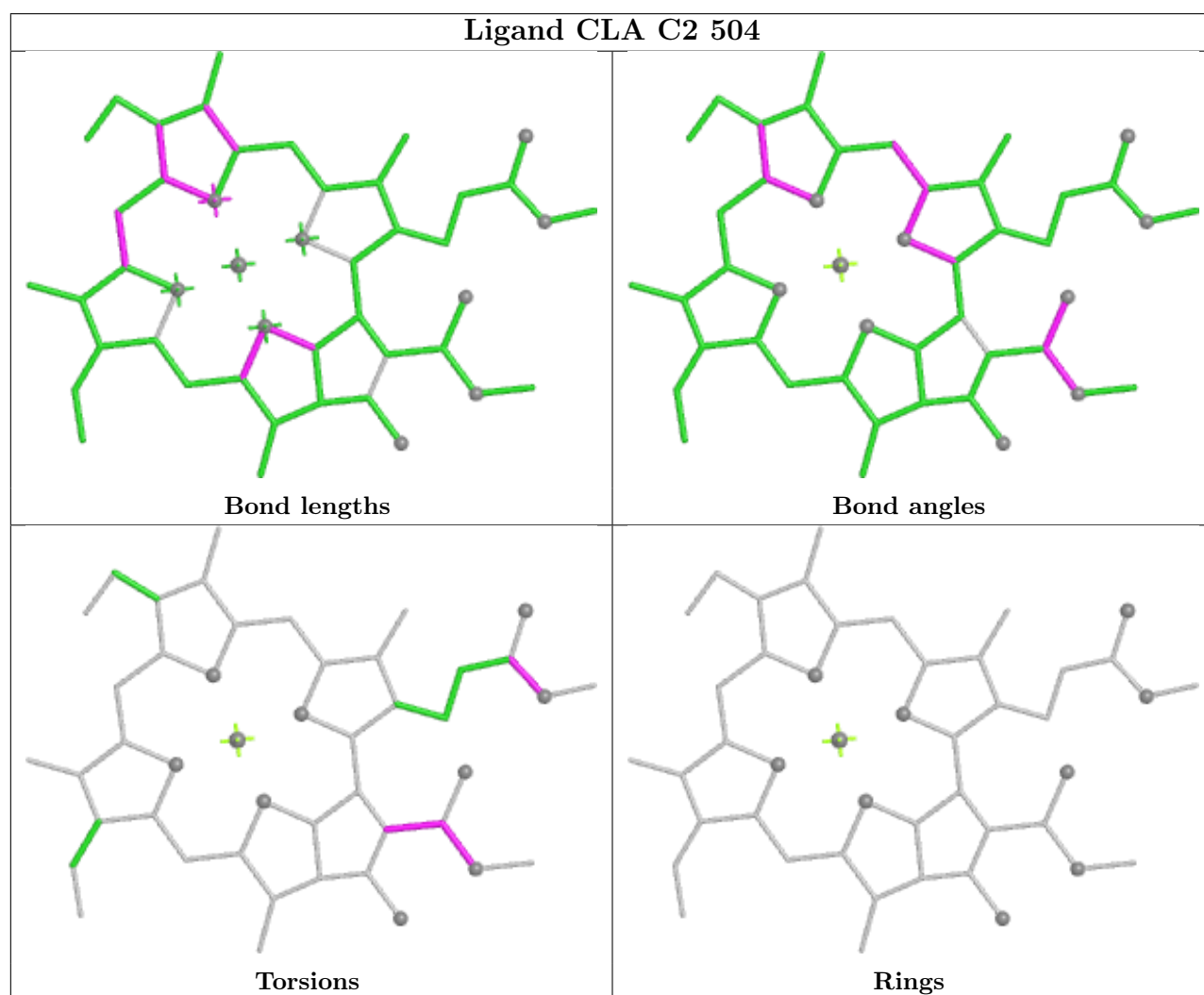
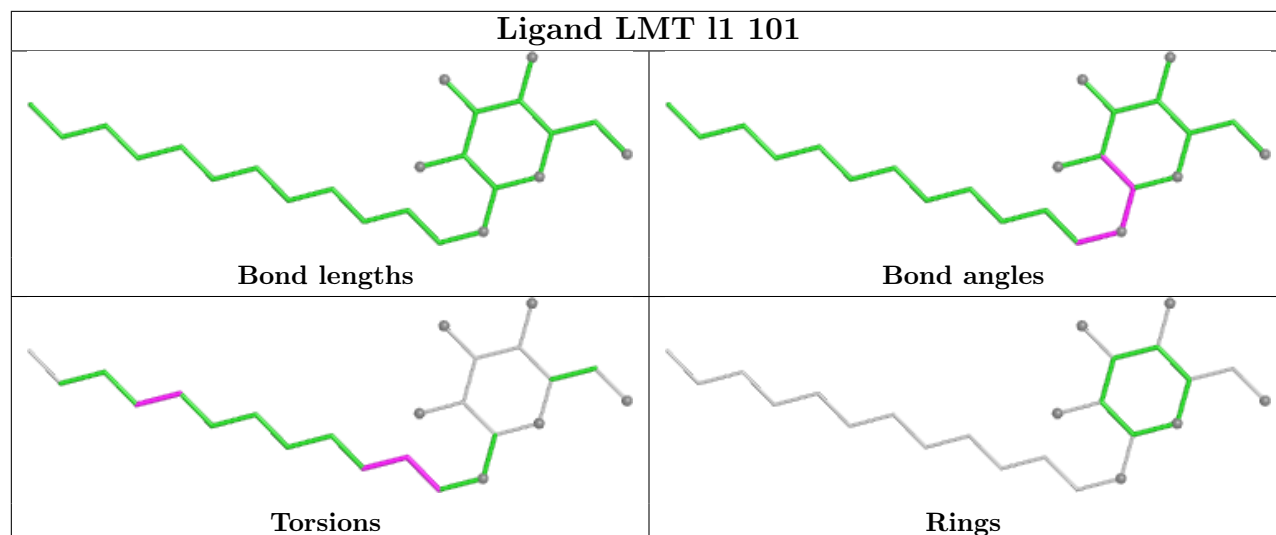
Ligand CLA A2 404

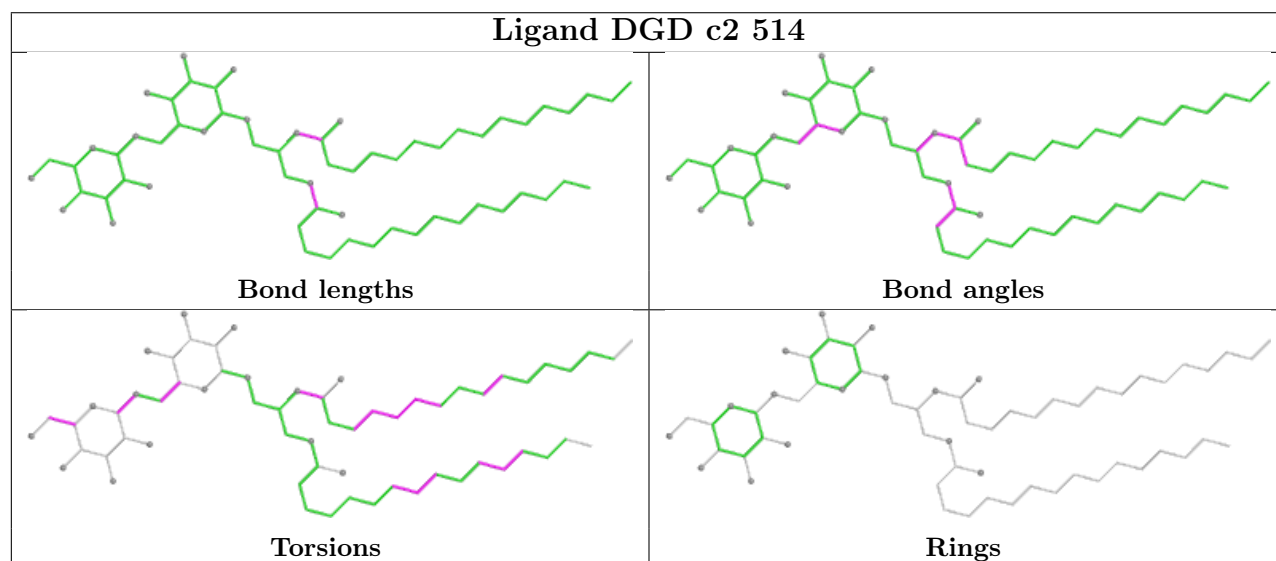
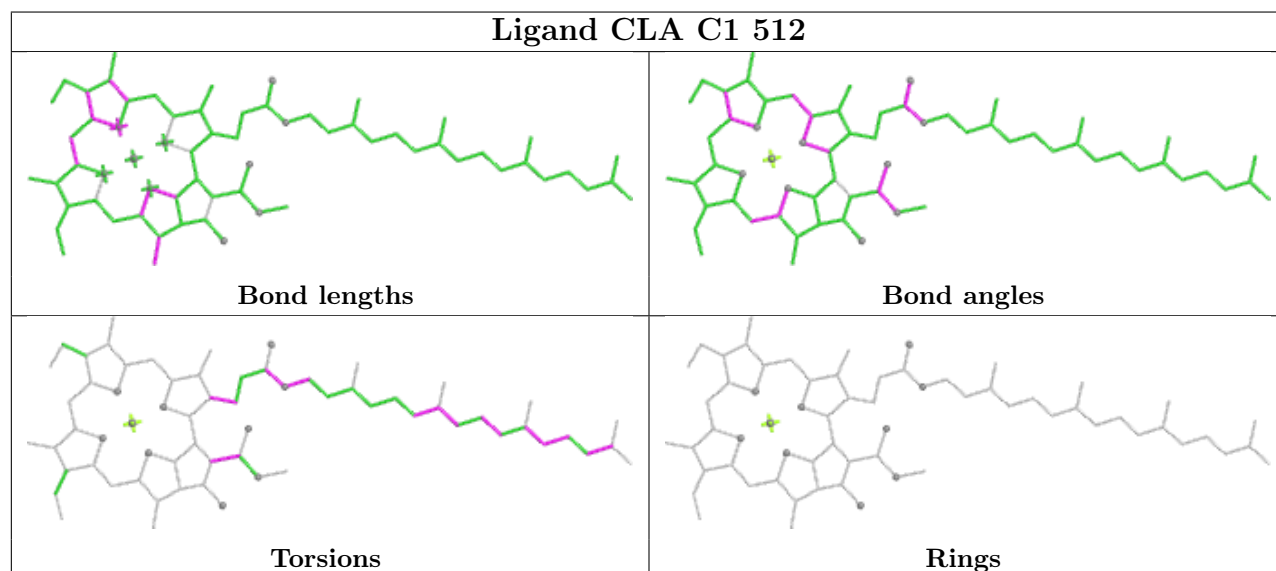
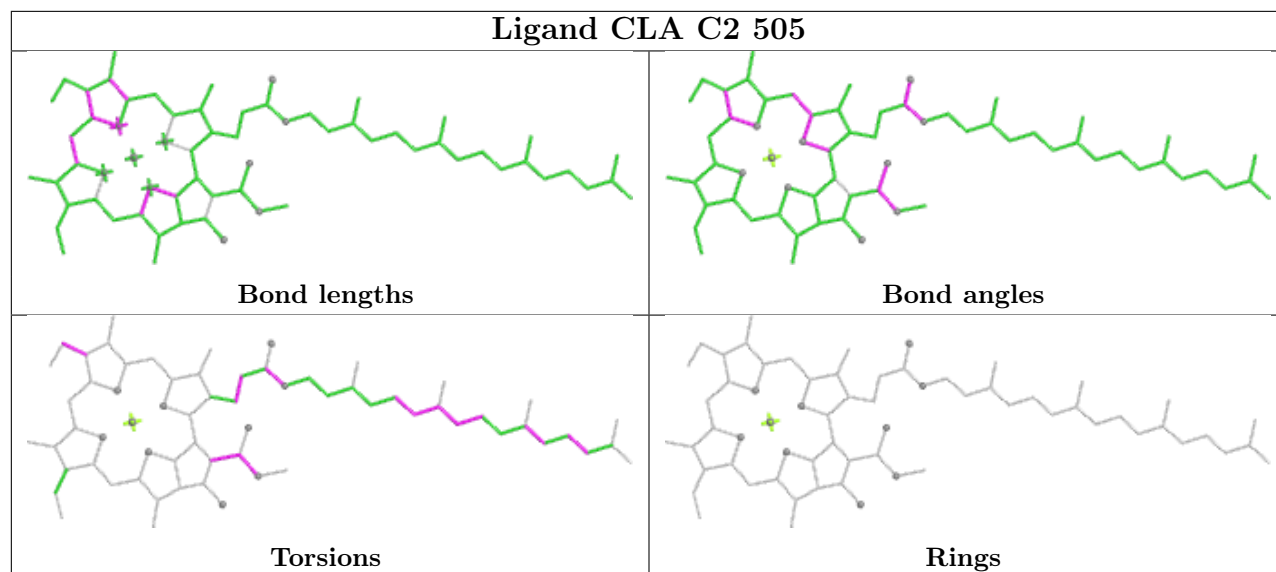


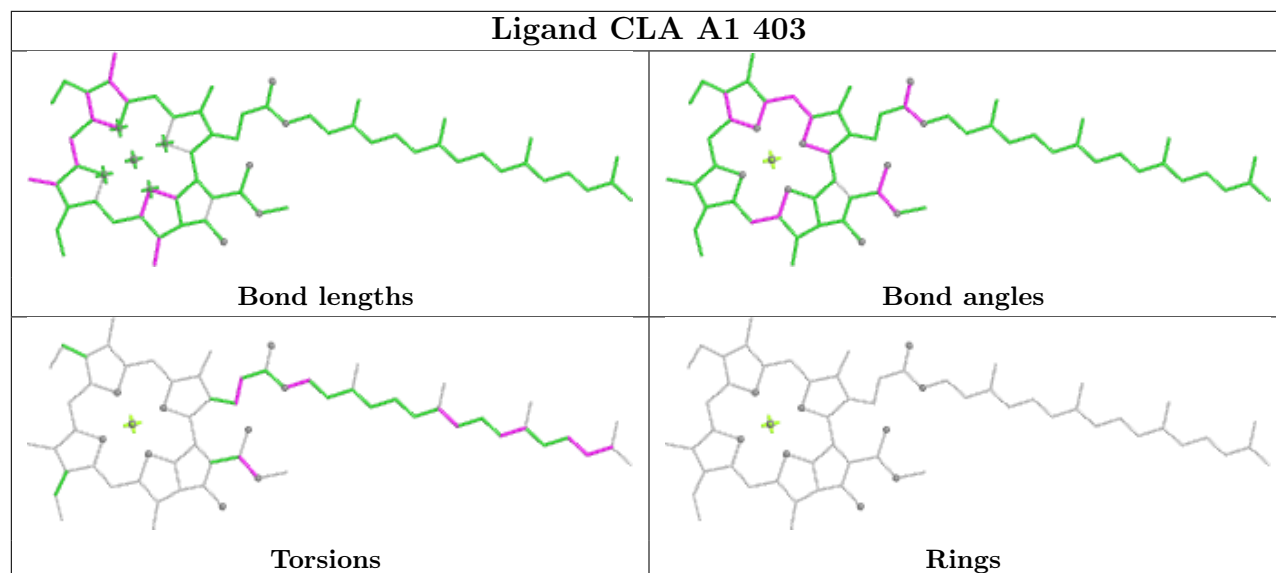
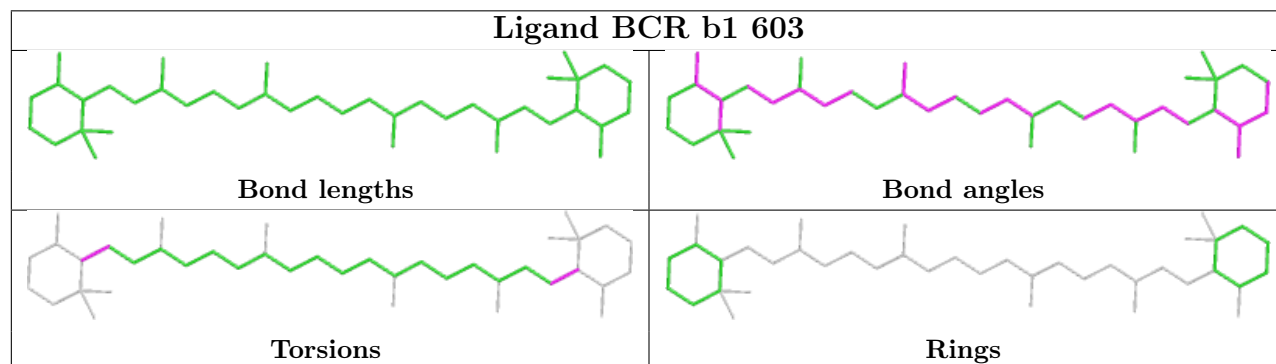
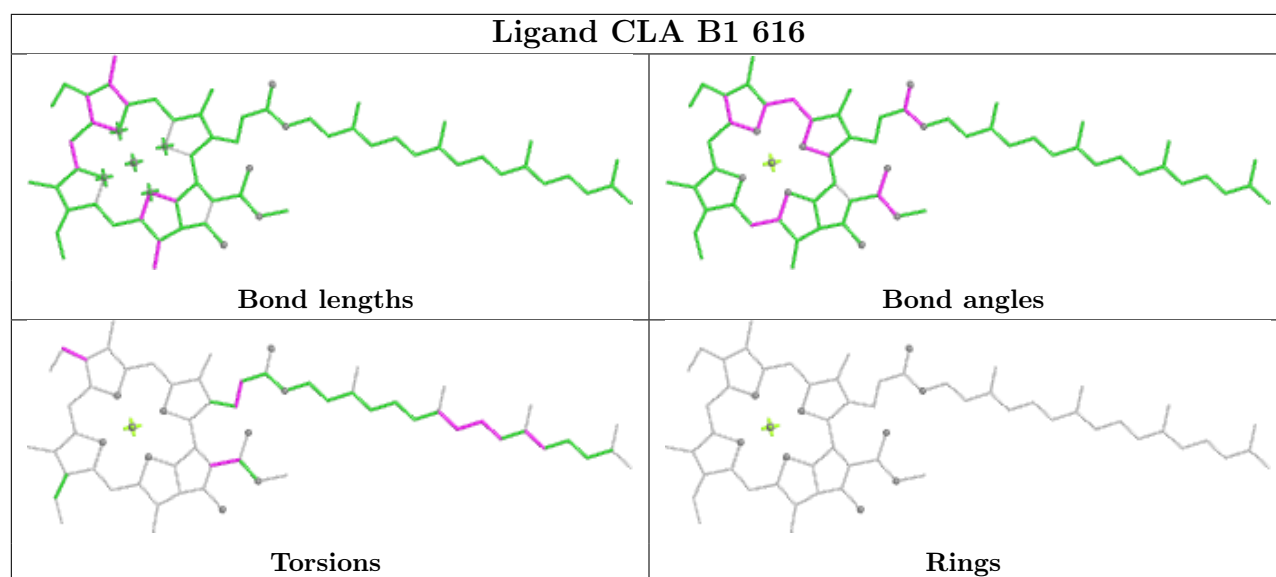
Ligand CLA b1 609

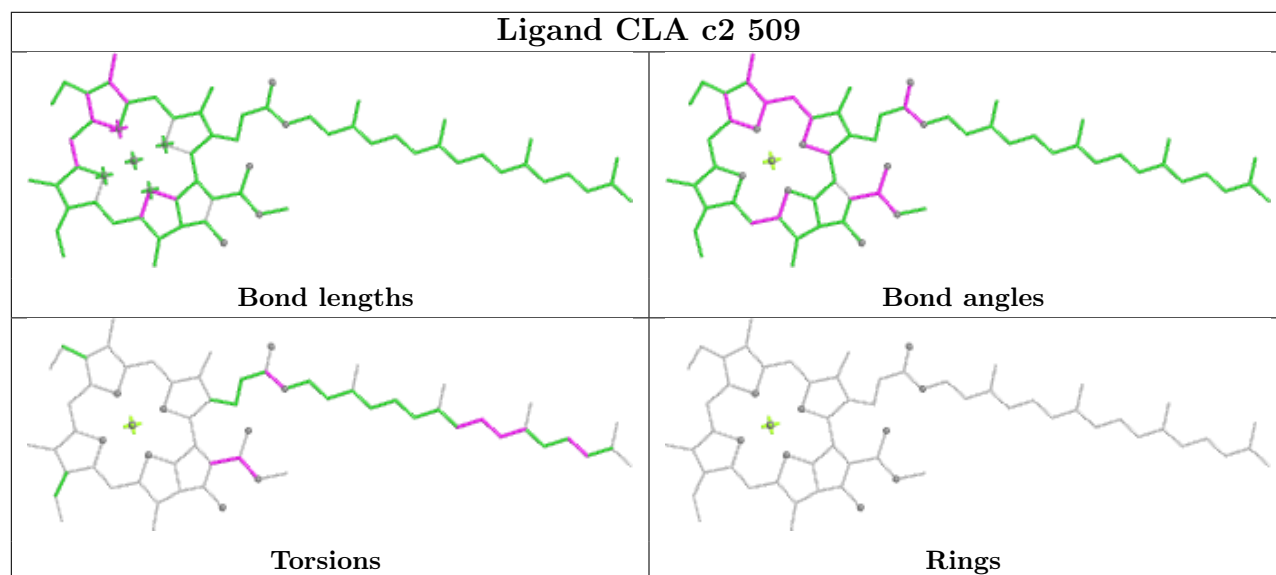
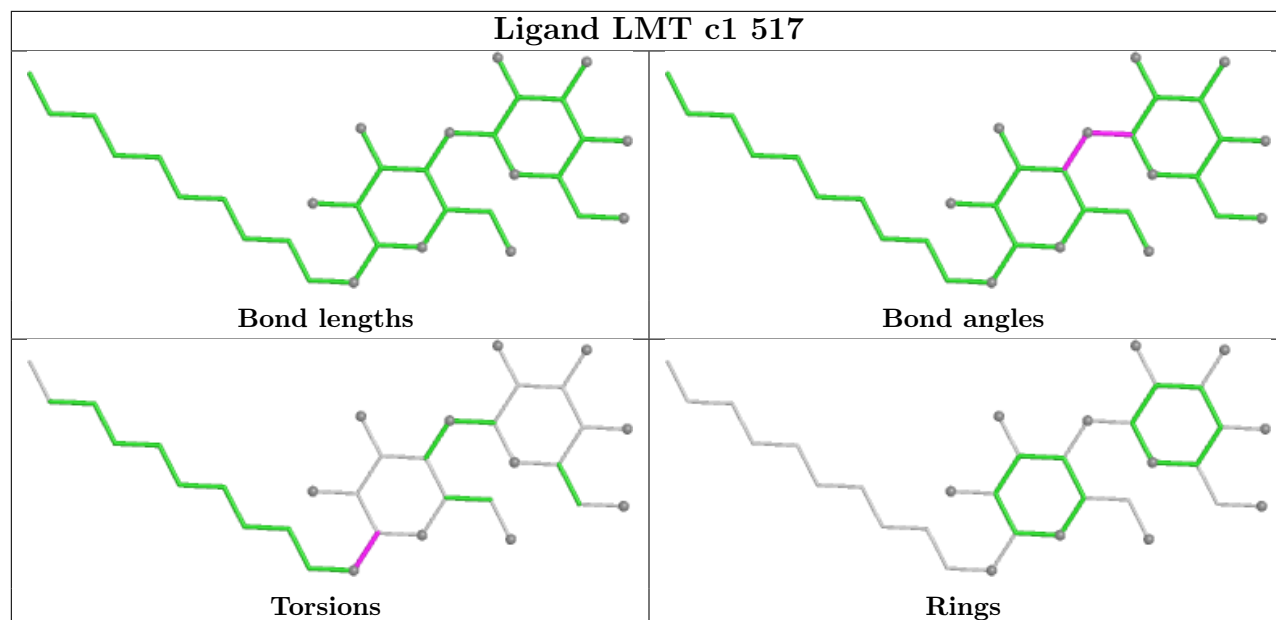




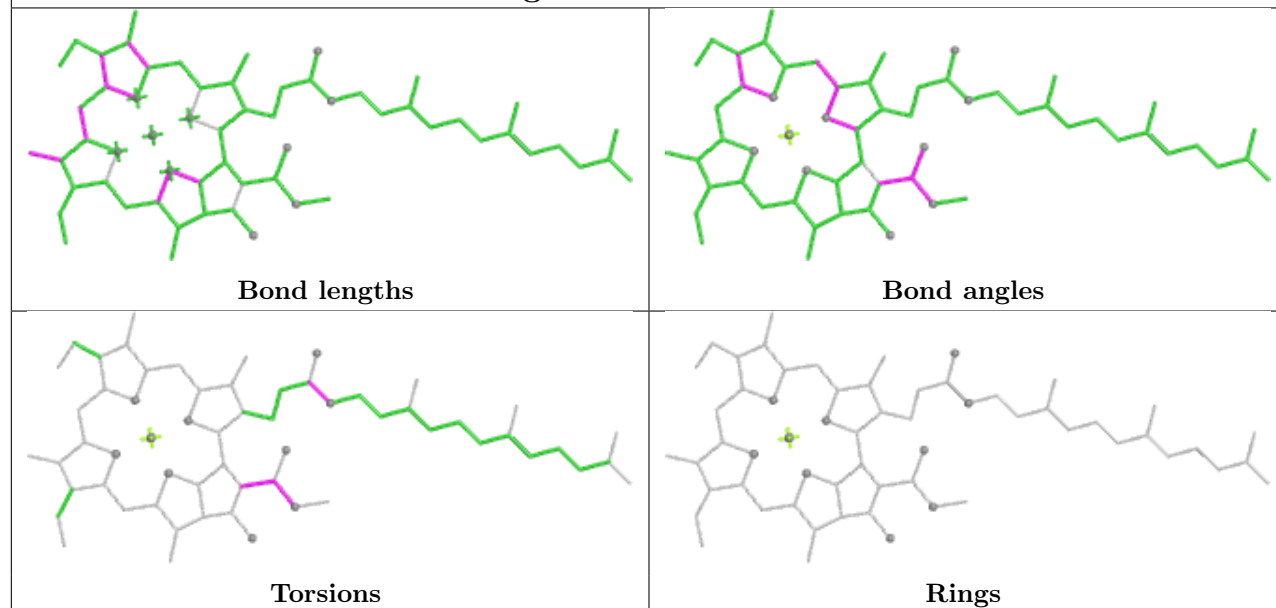




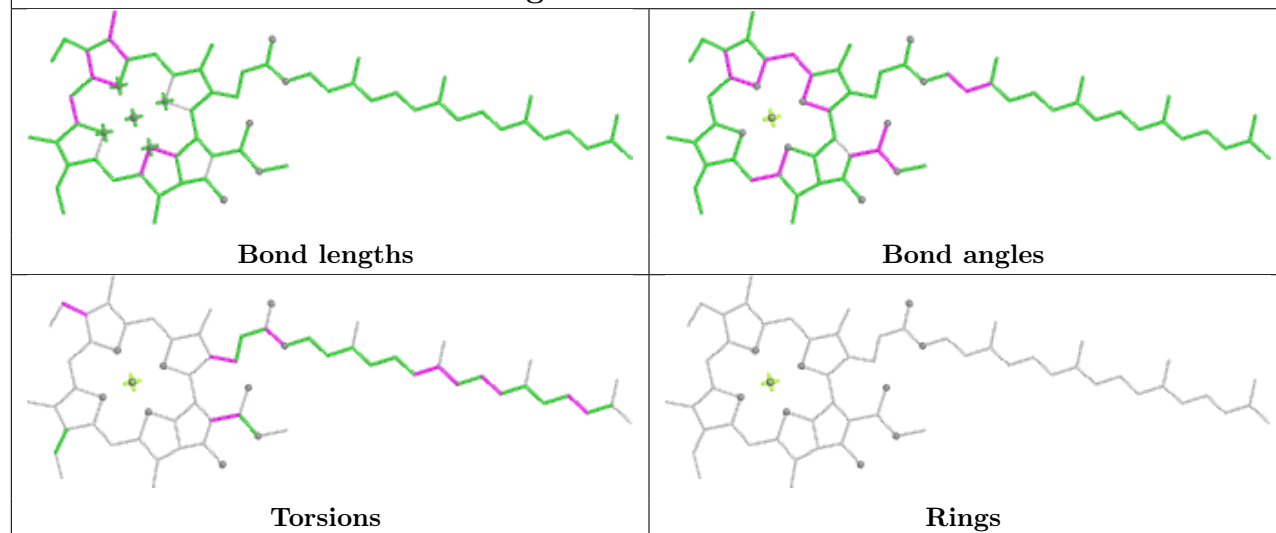


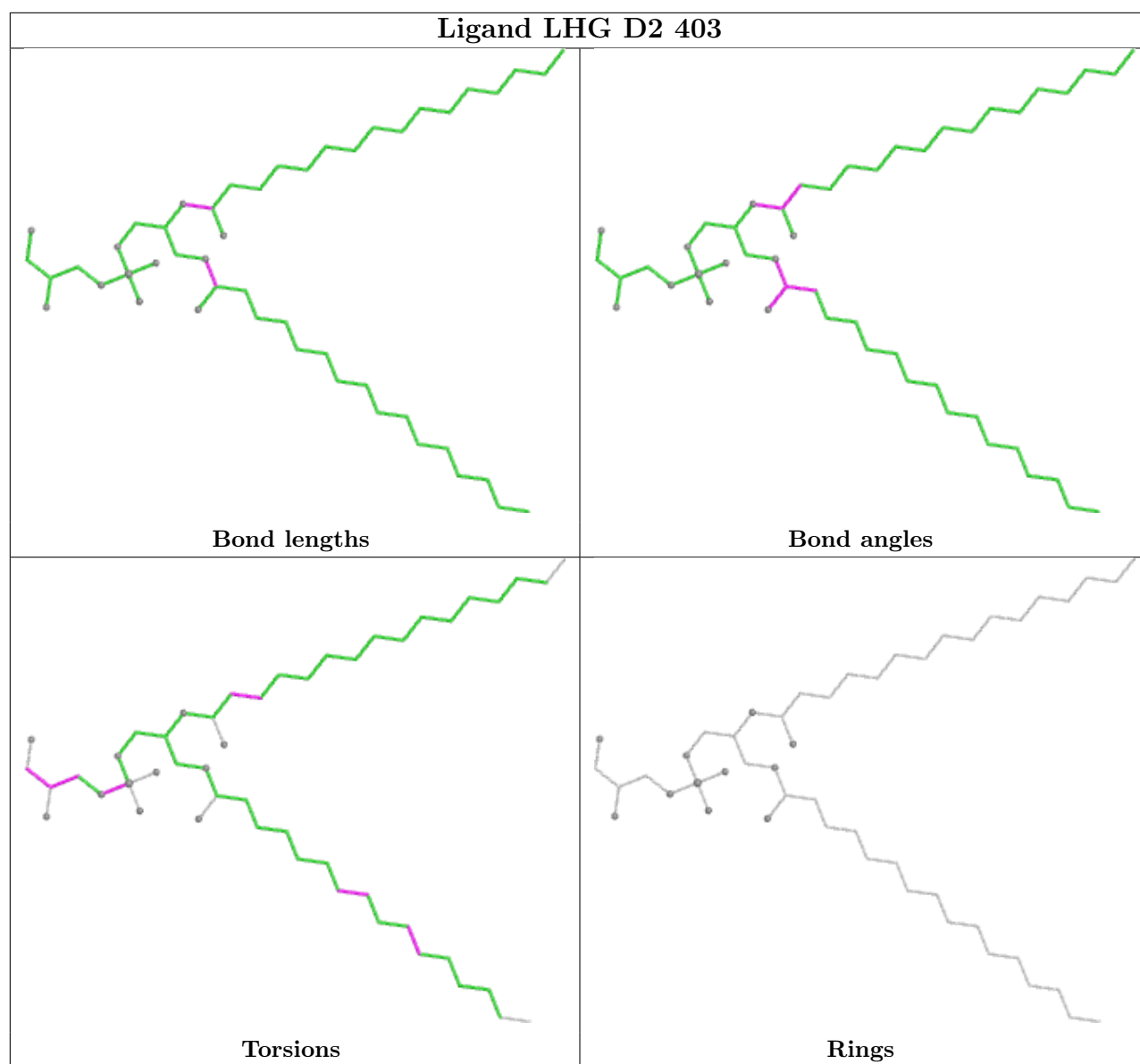


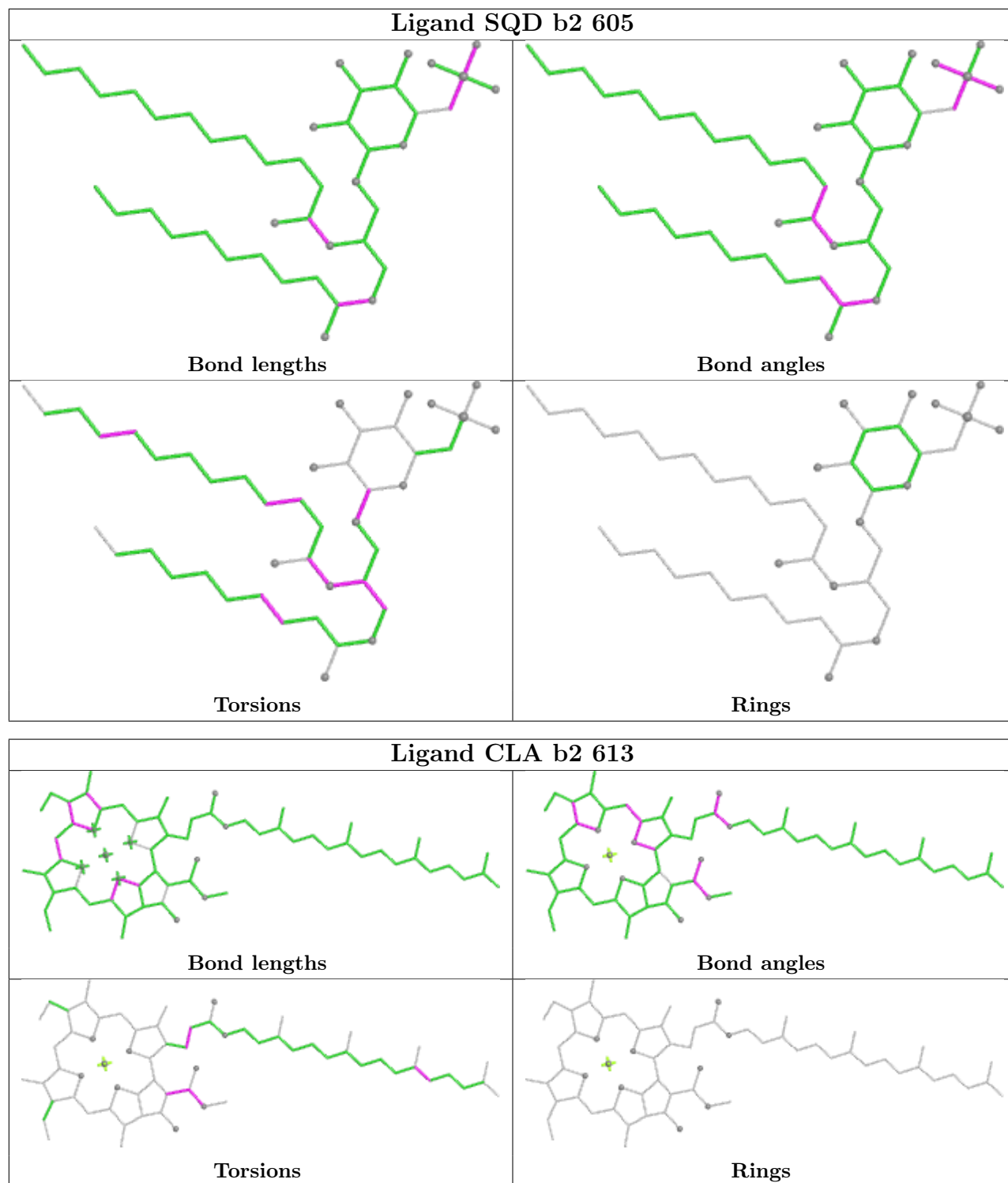
Ligand CLA B2 618

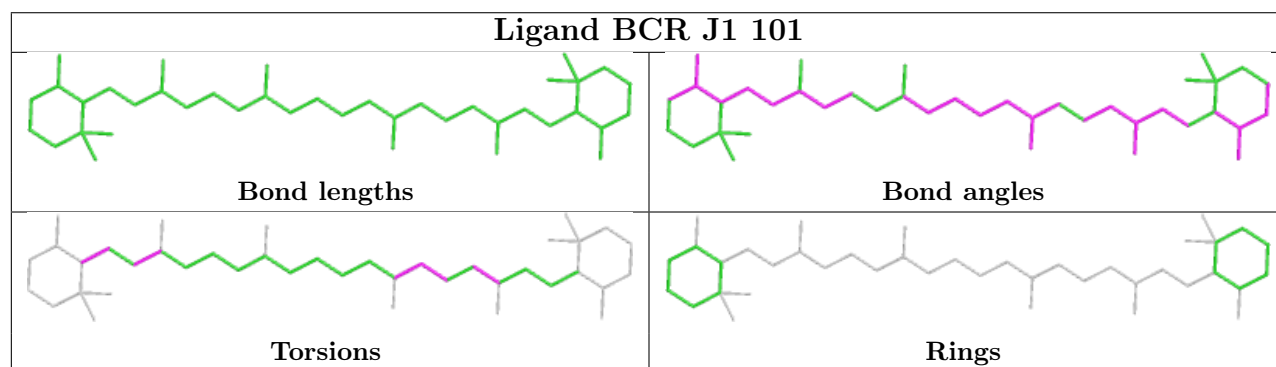
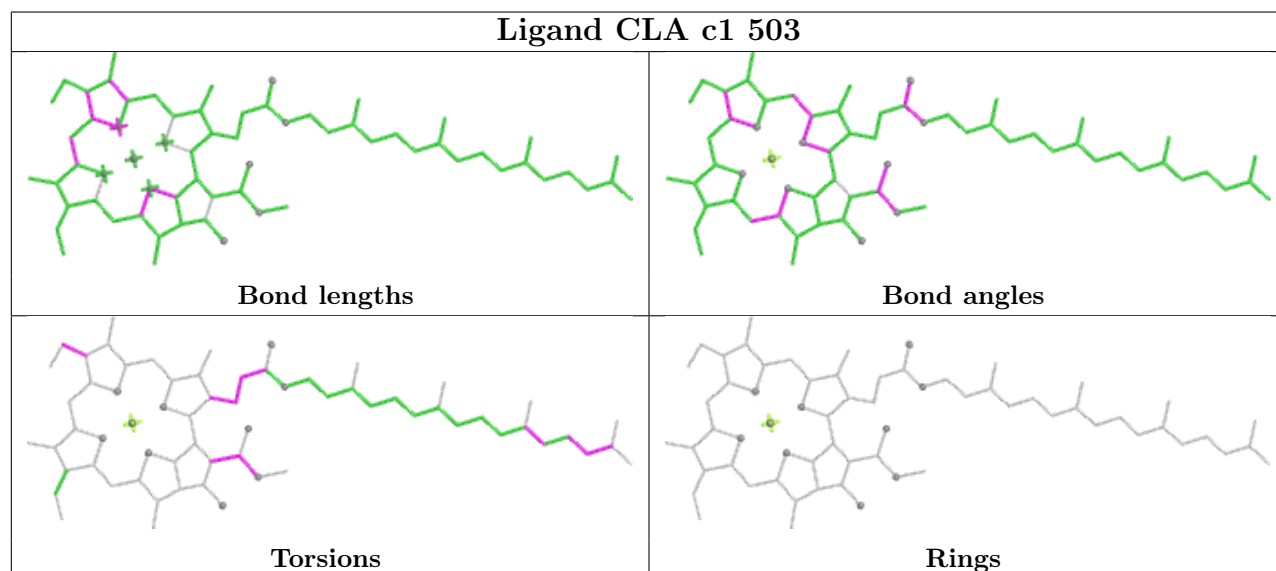
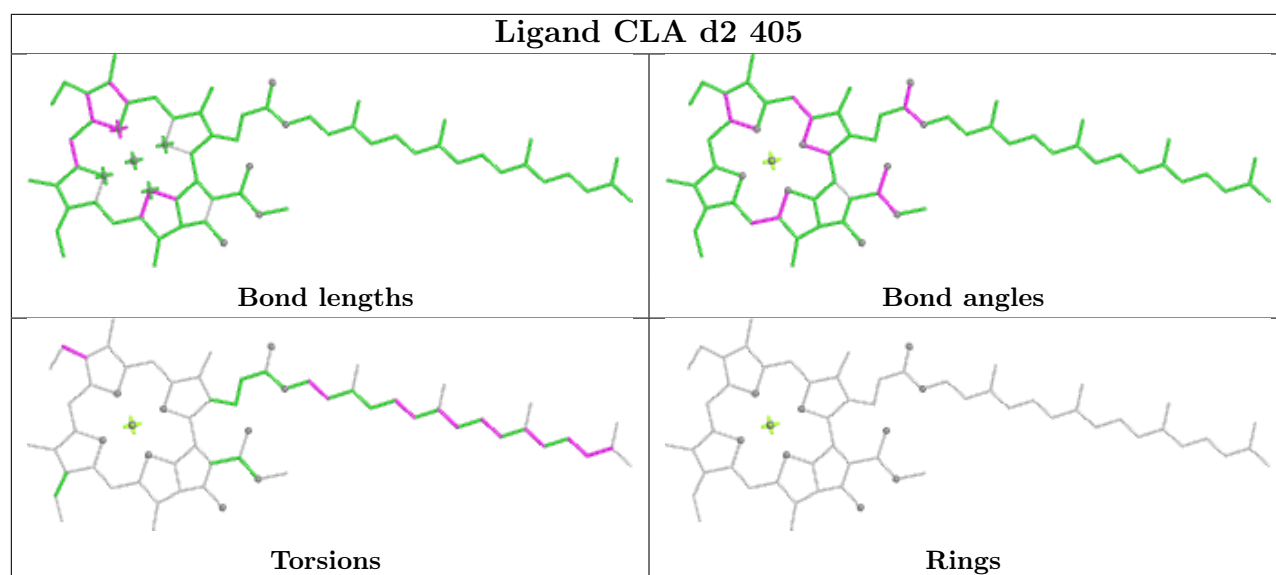


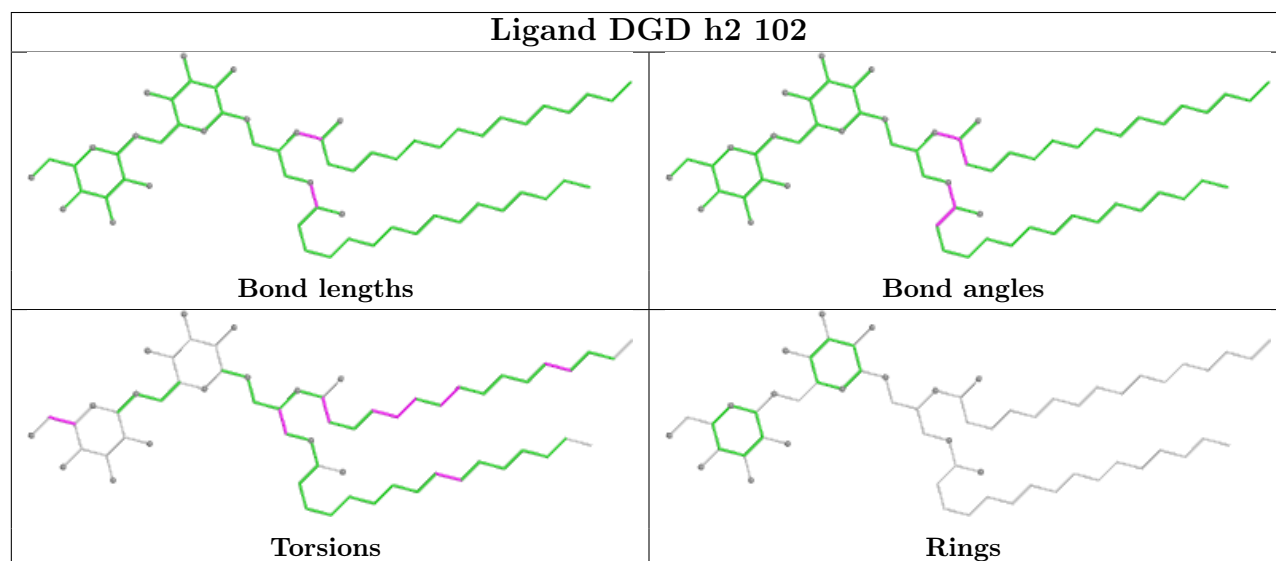
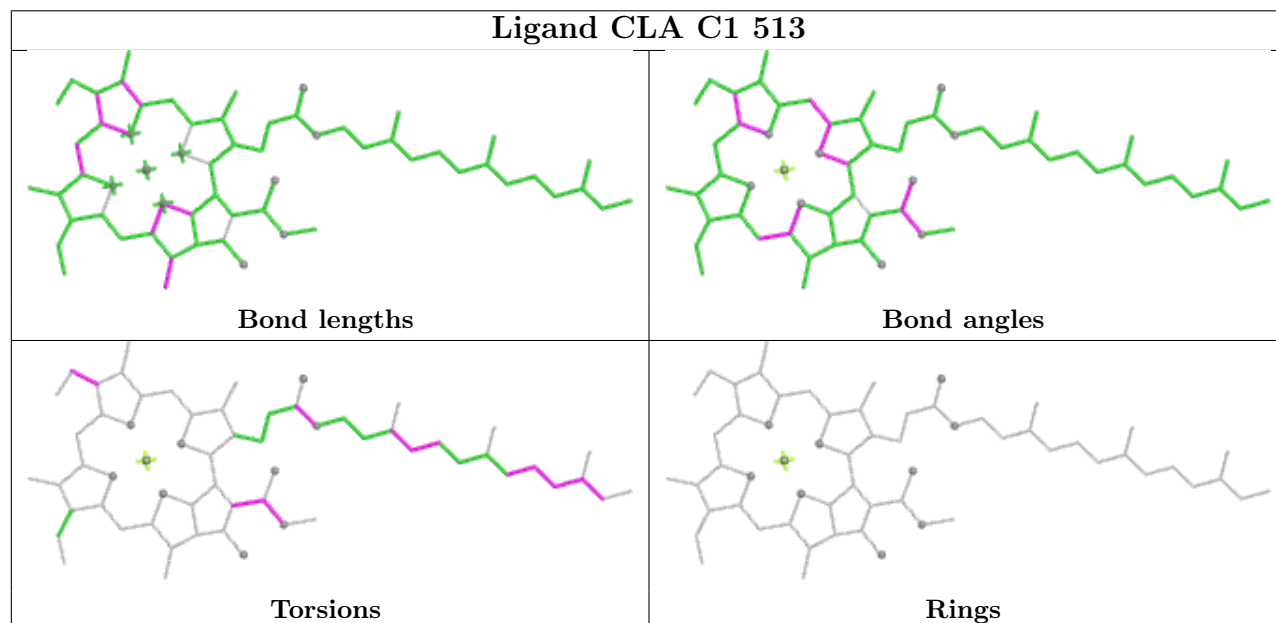
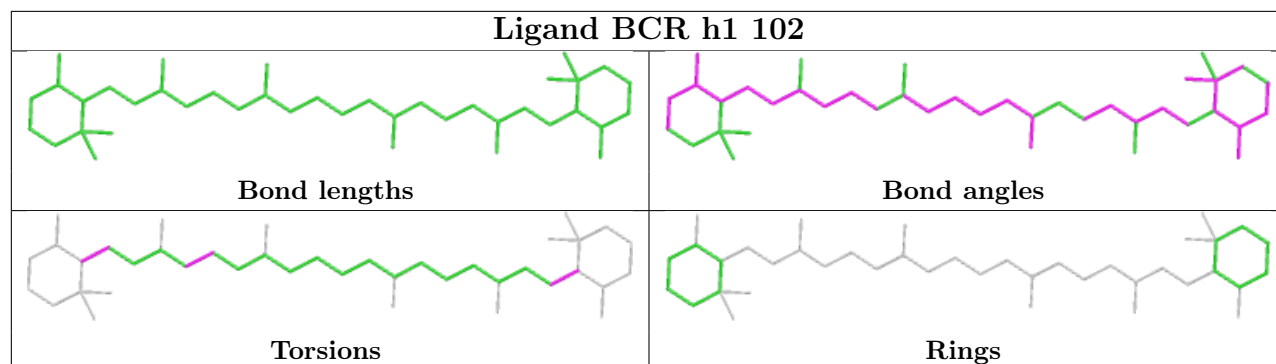
Ligand CLA d2 402



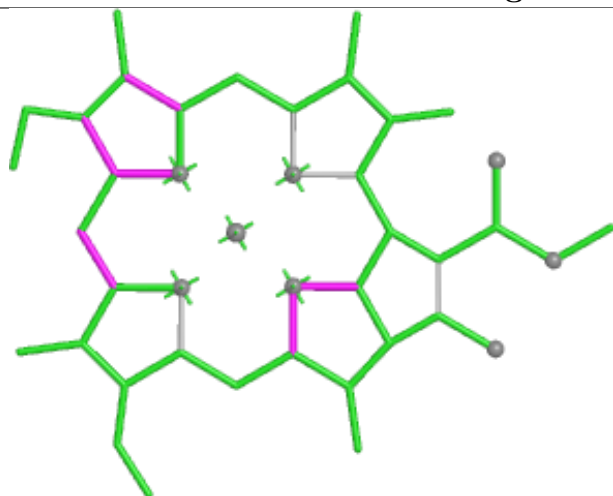




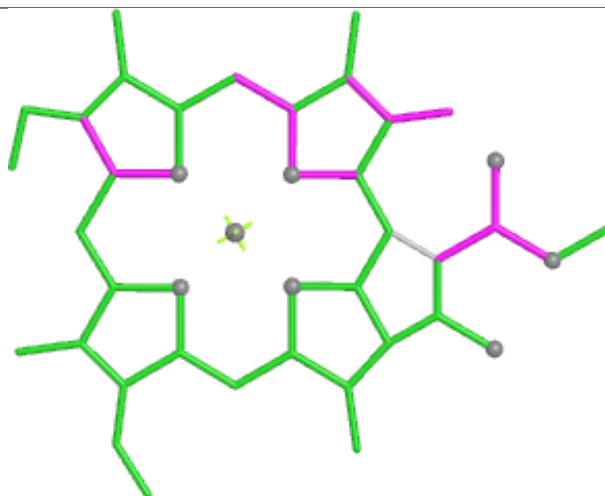




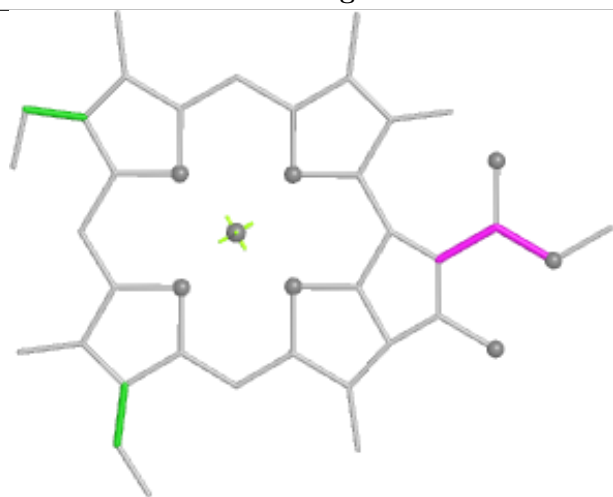
Ligand CLA C2 518



Bond lengths



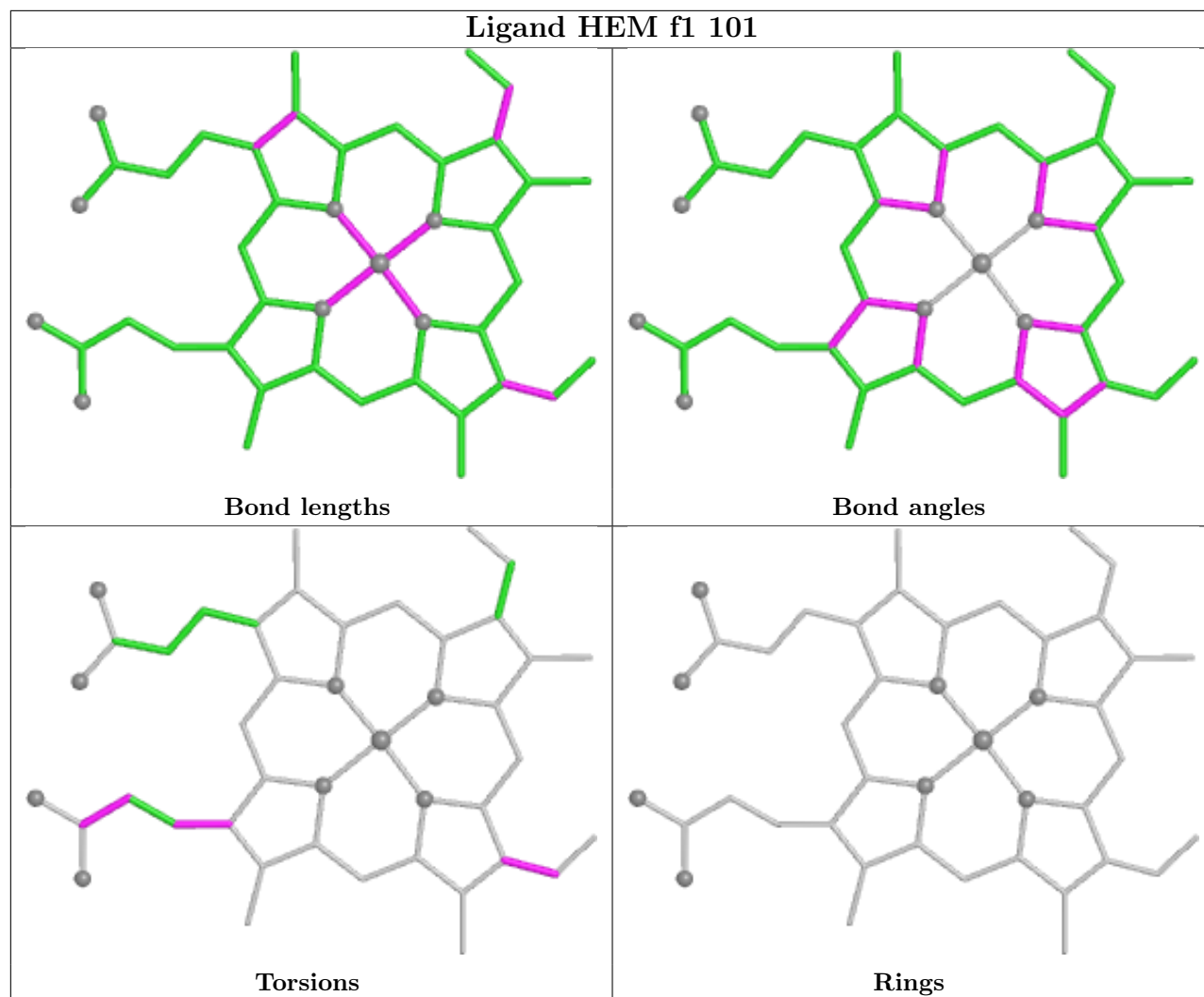
Bond angles

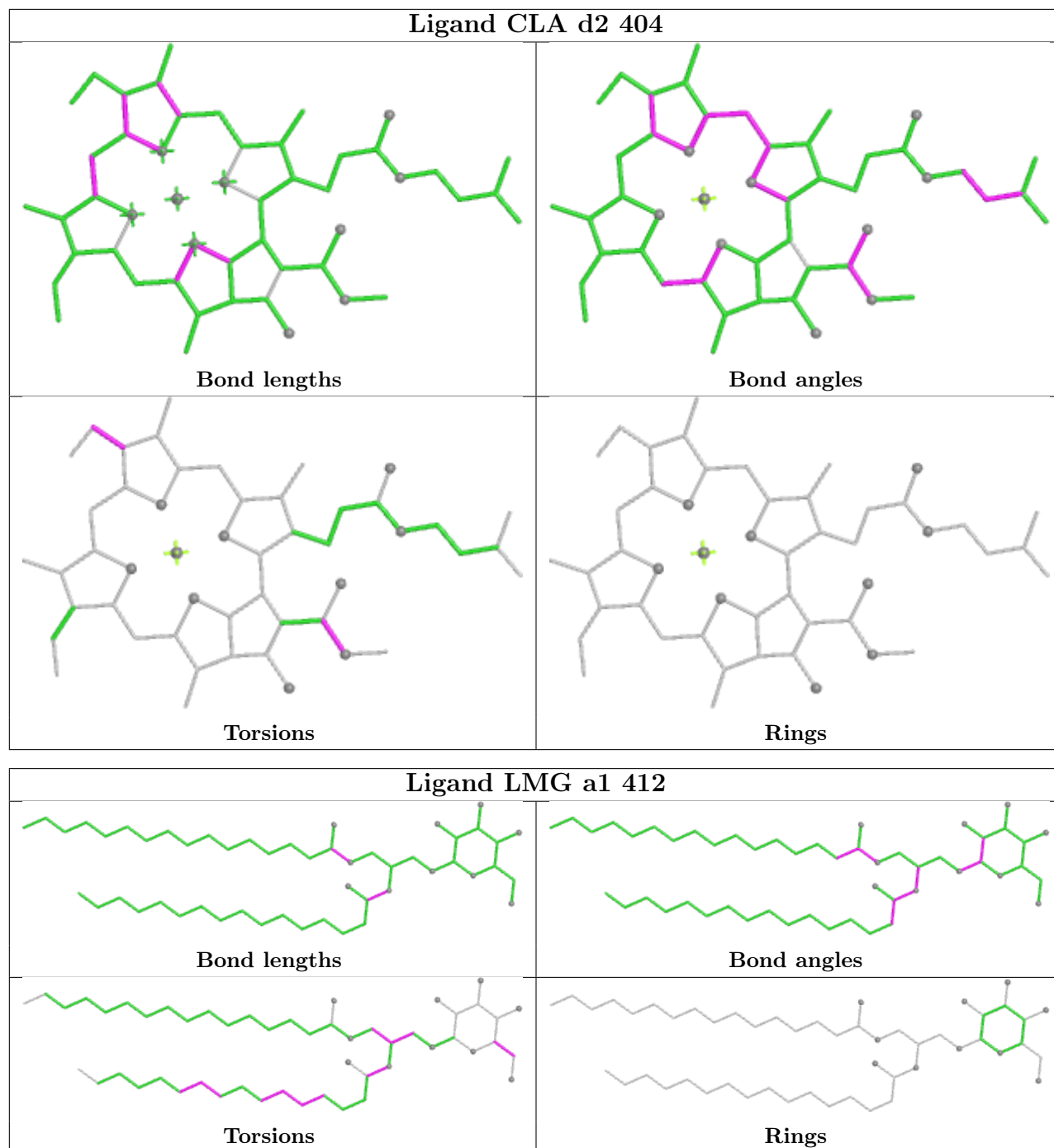


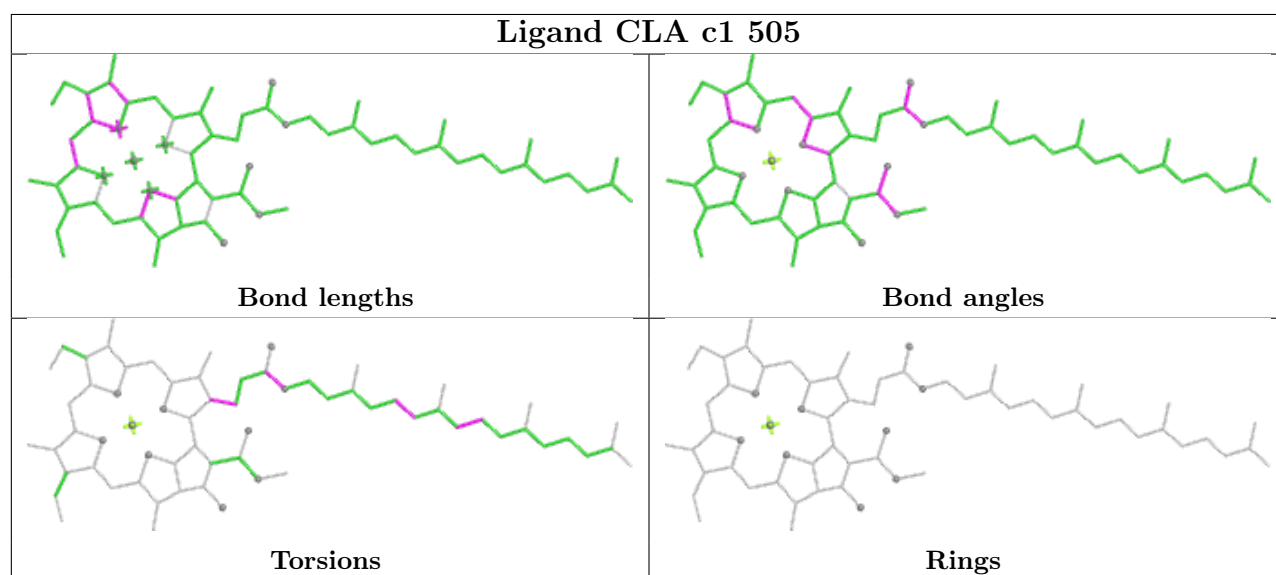
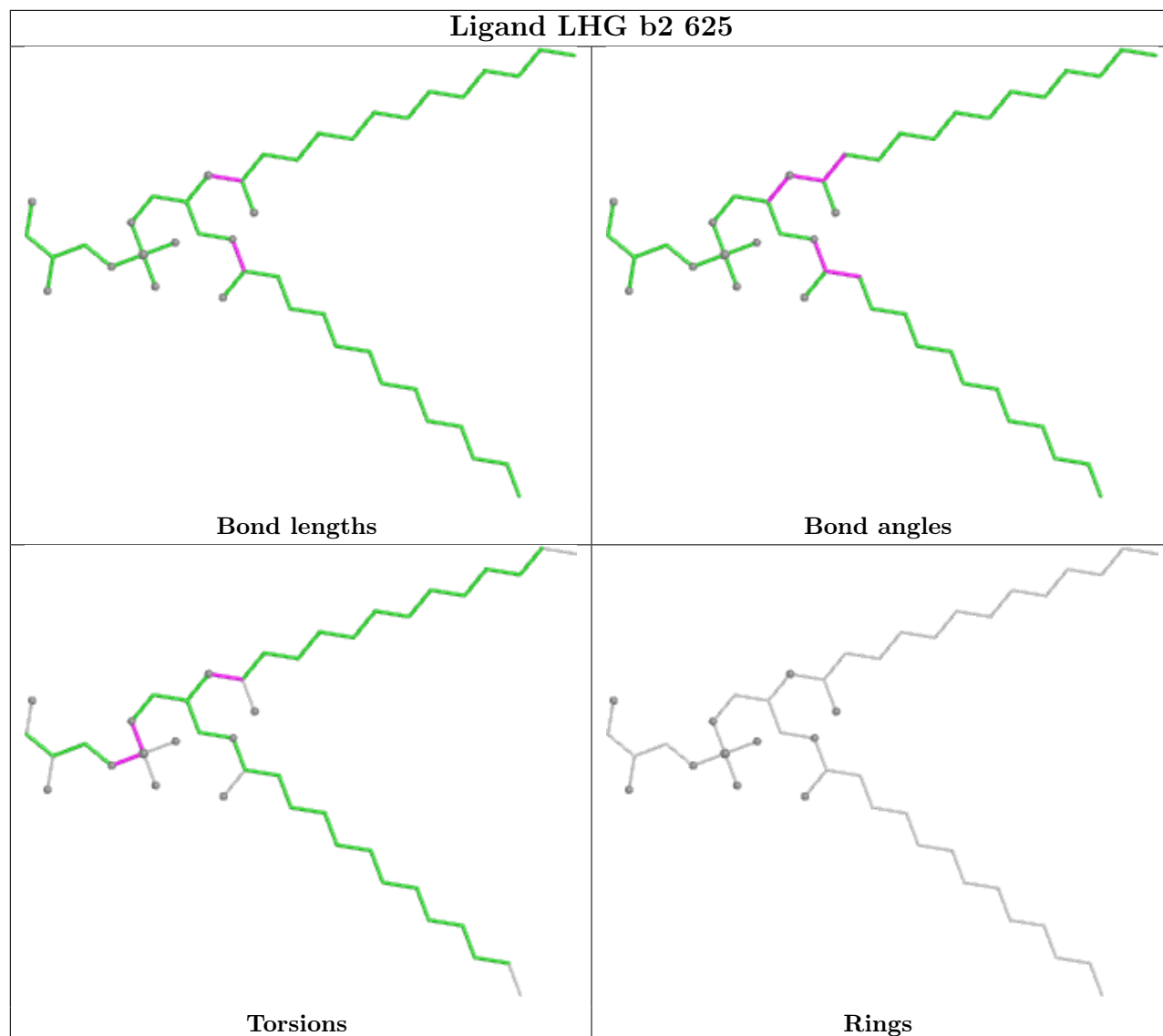
Torsions

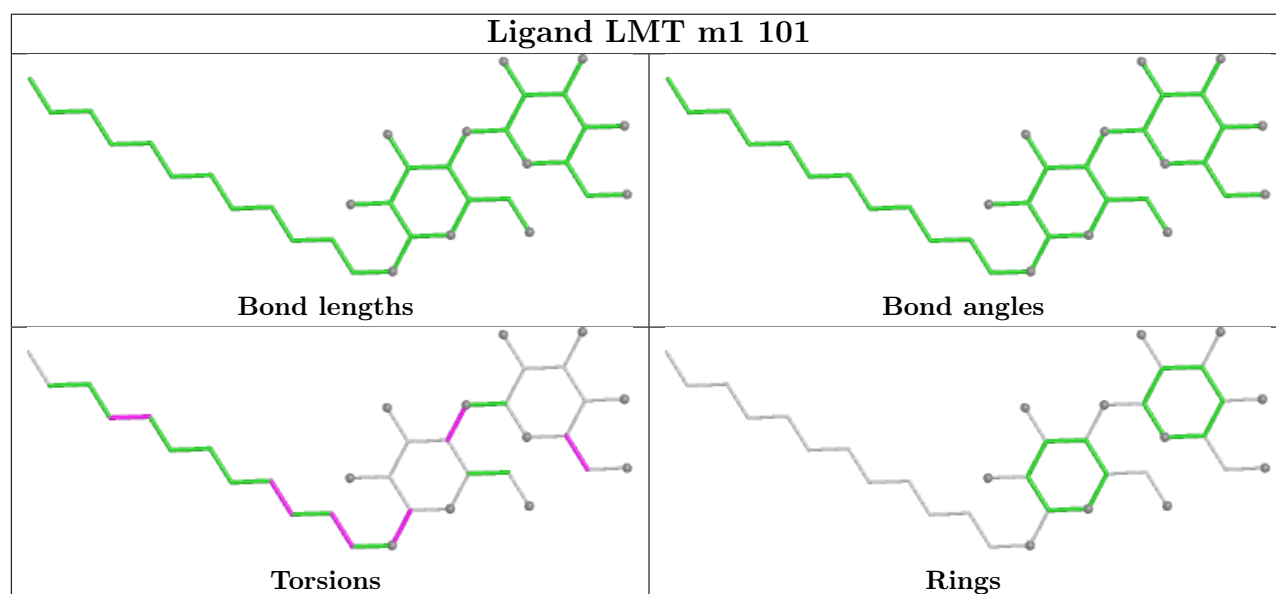
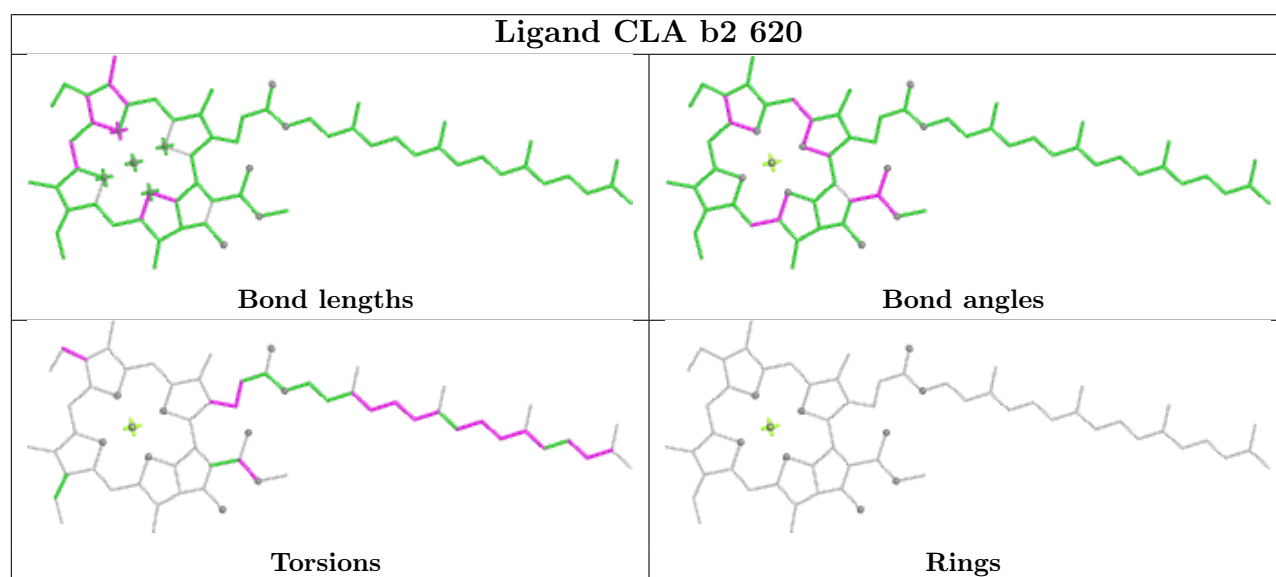
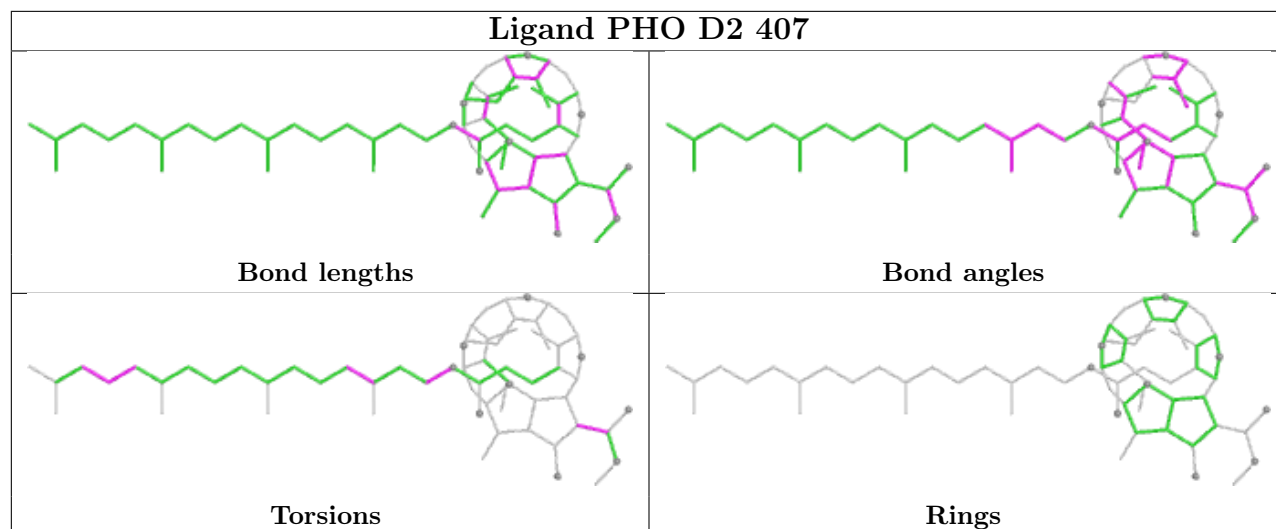


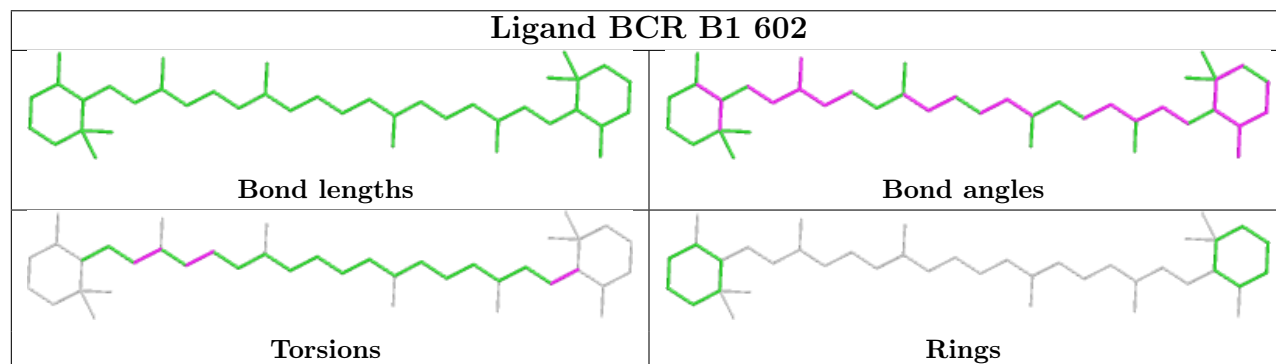
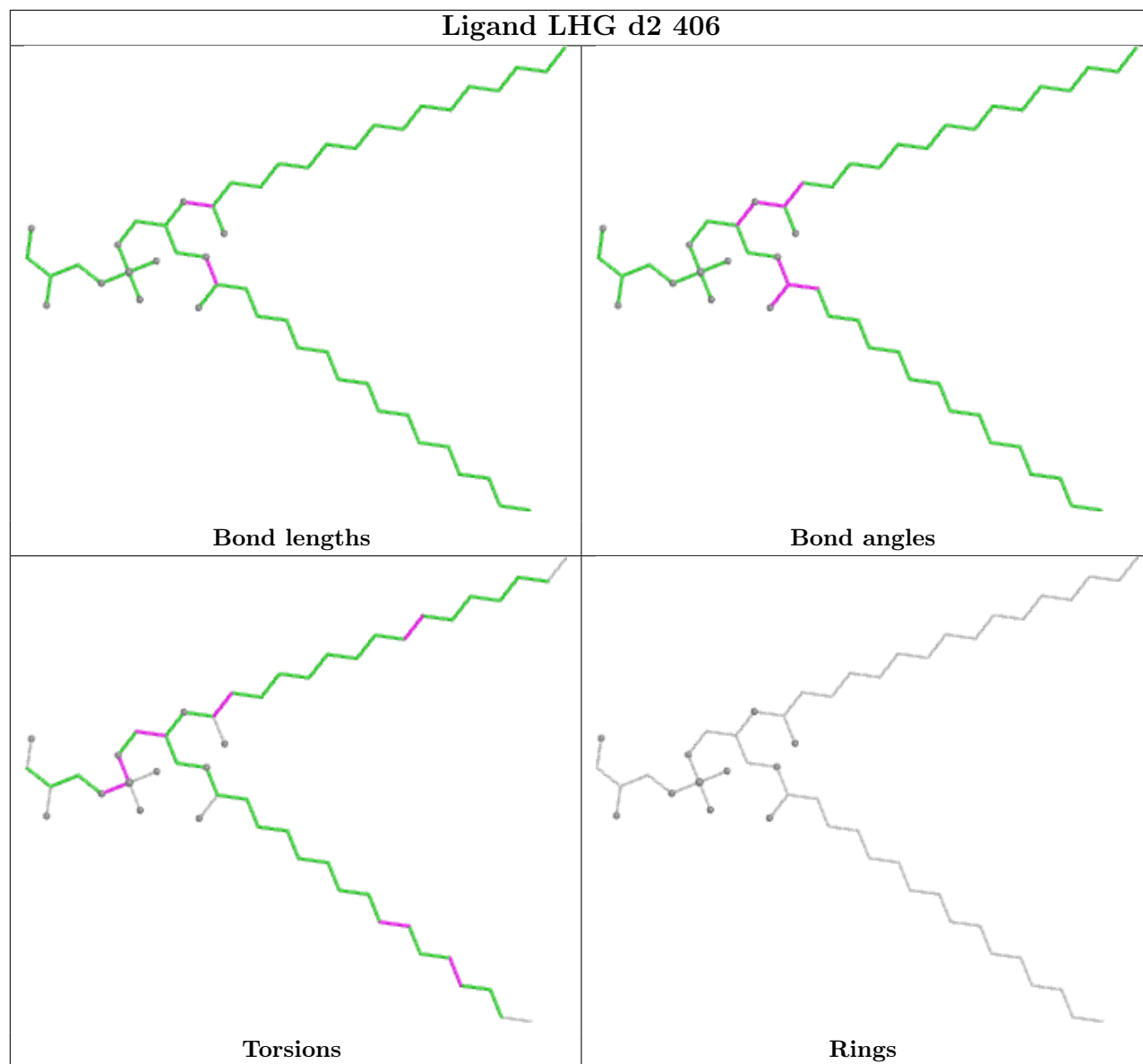
Rings

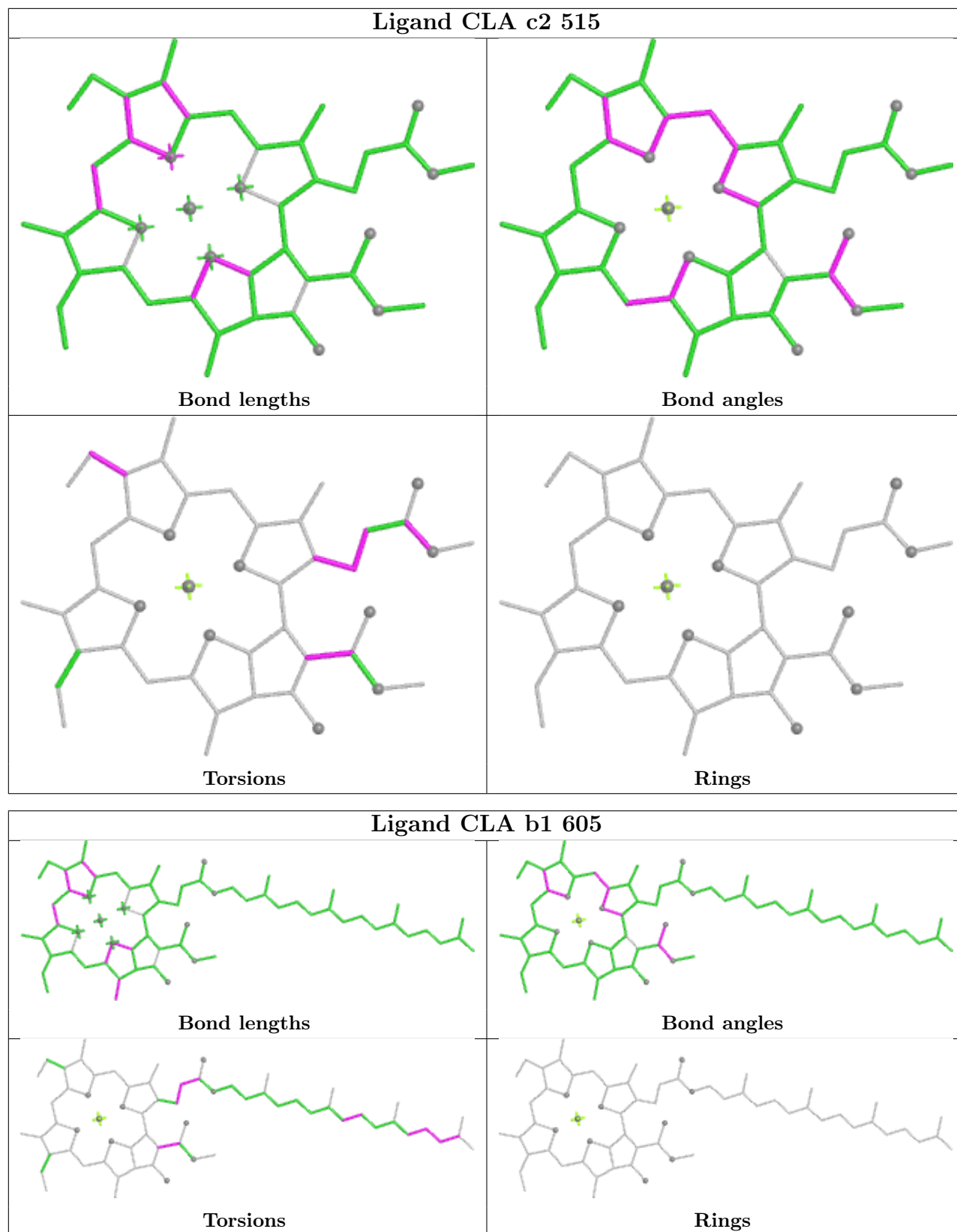


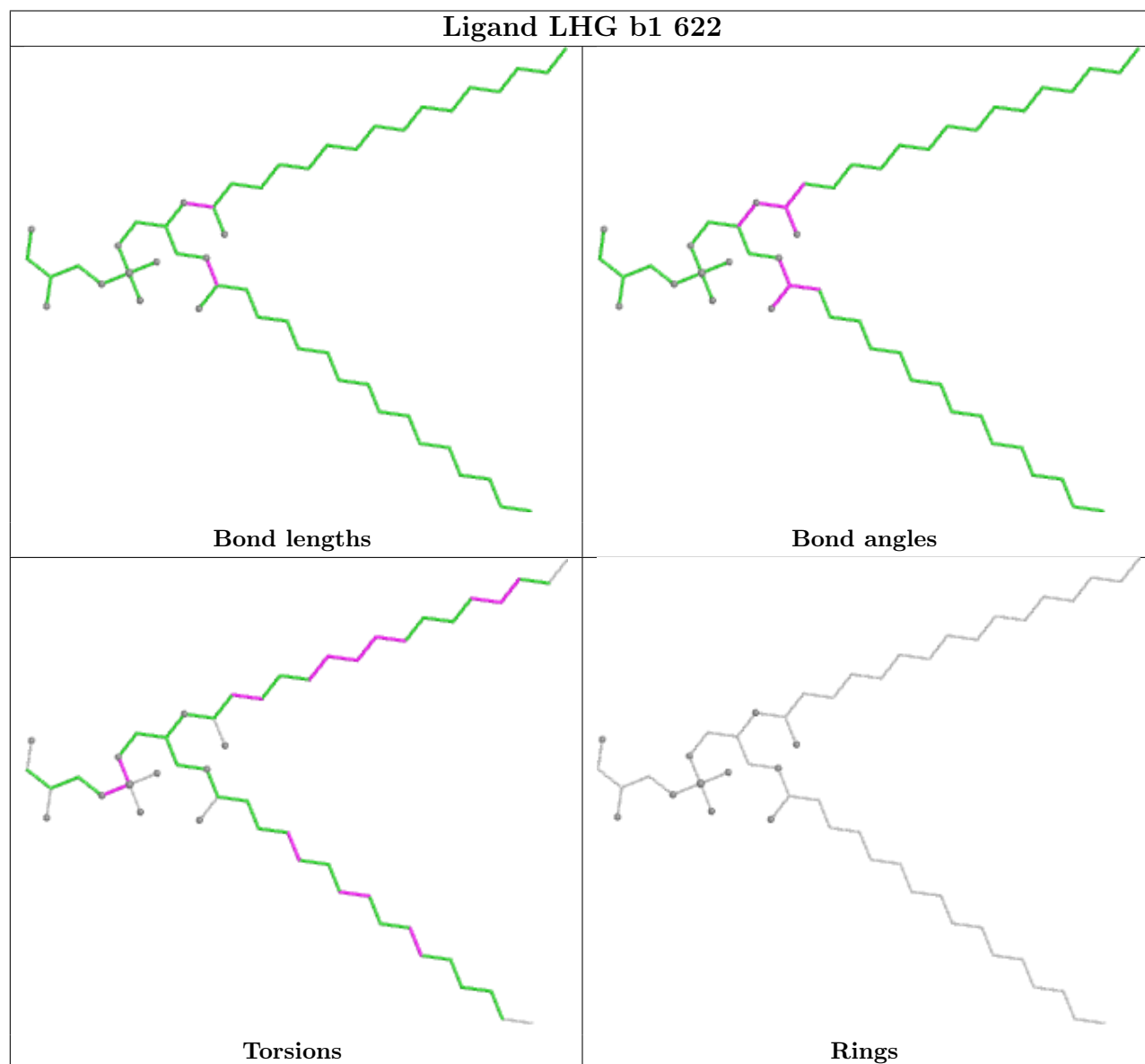
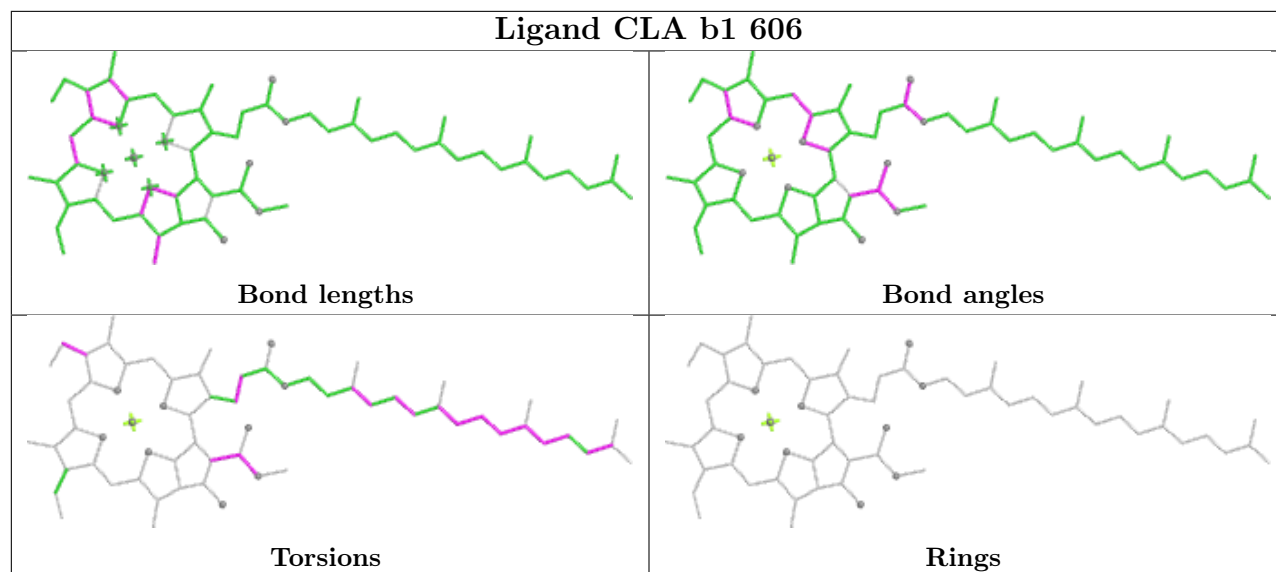


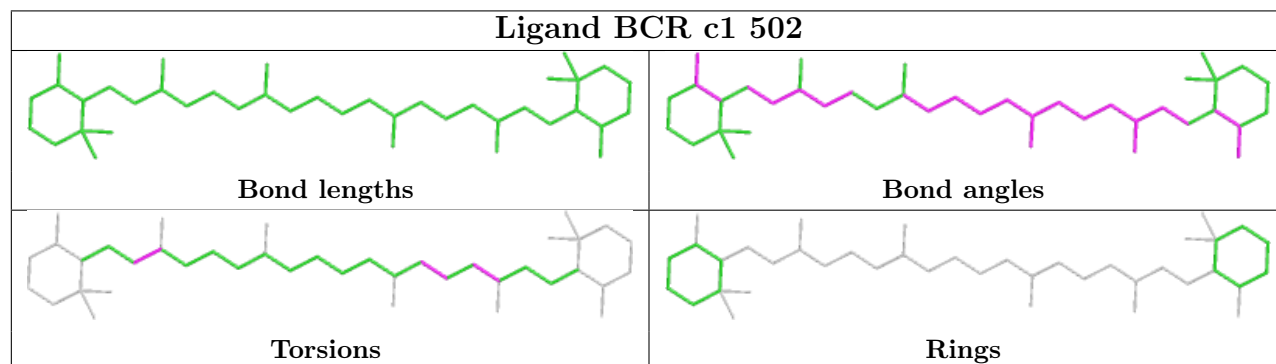
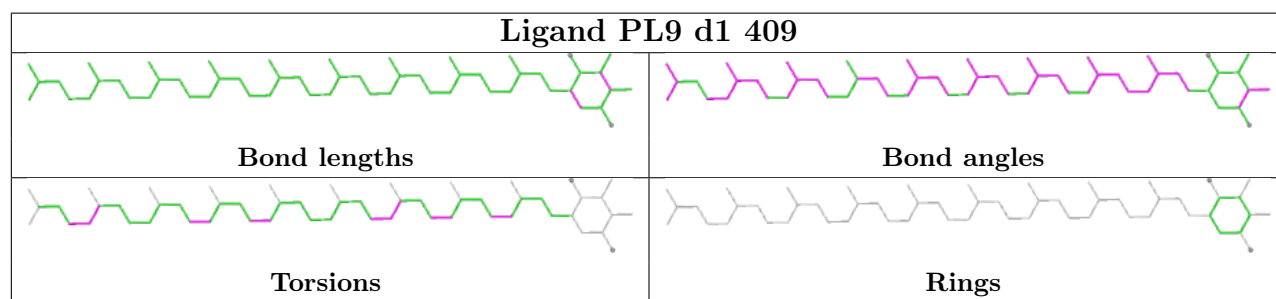
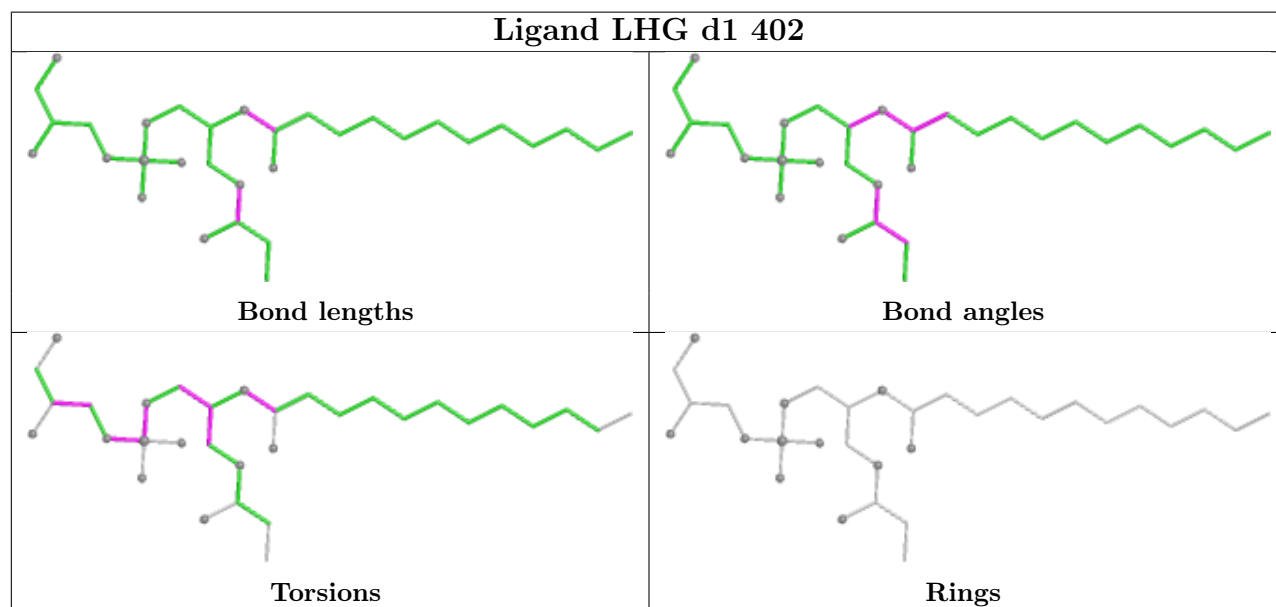
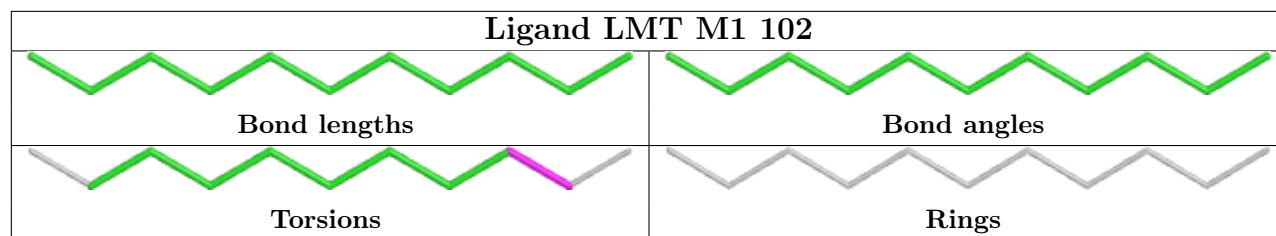


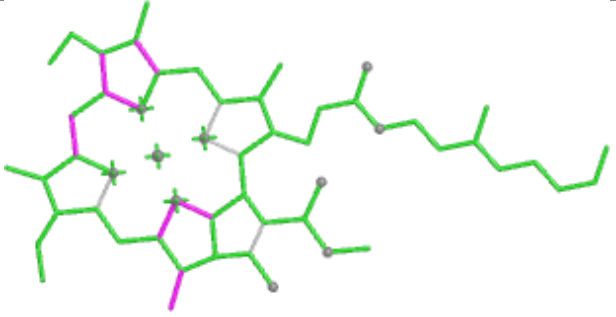
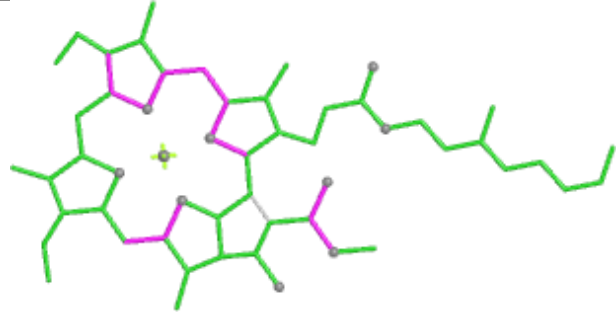
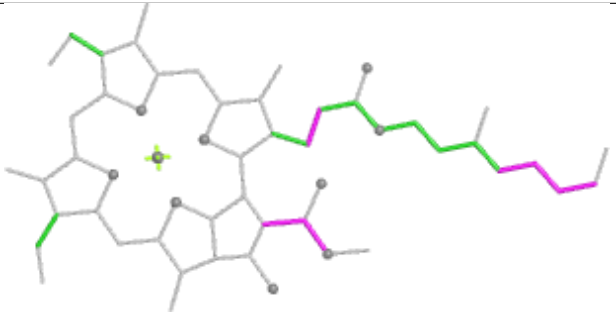
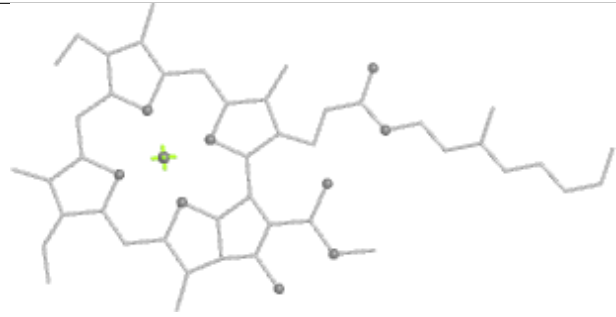


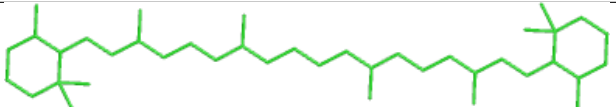
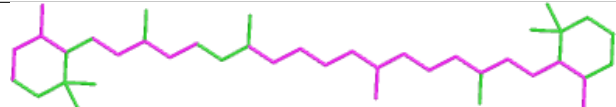
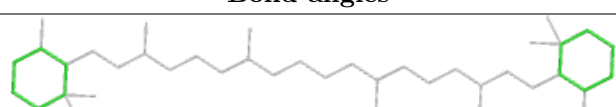


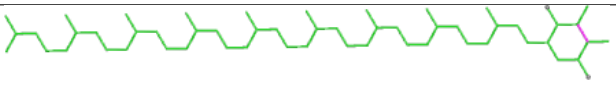
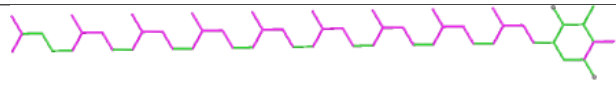
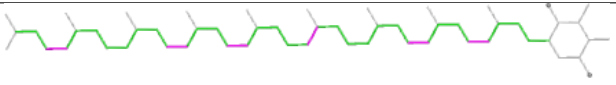
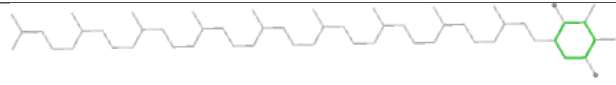


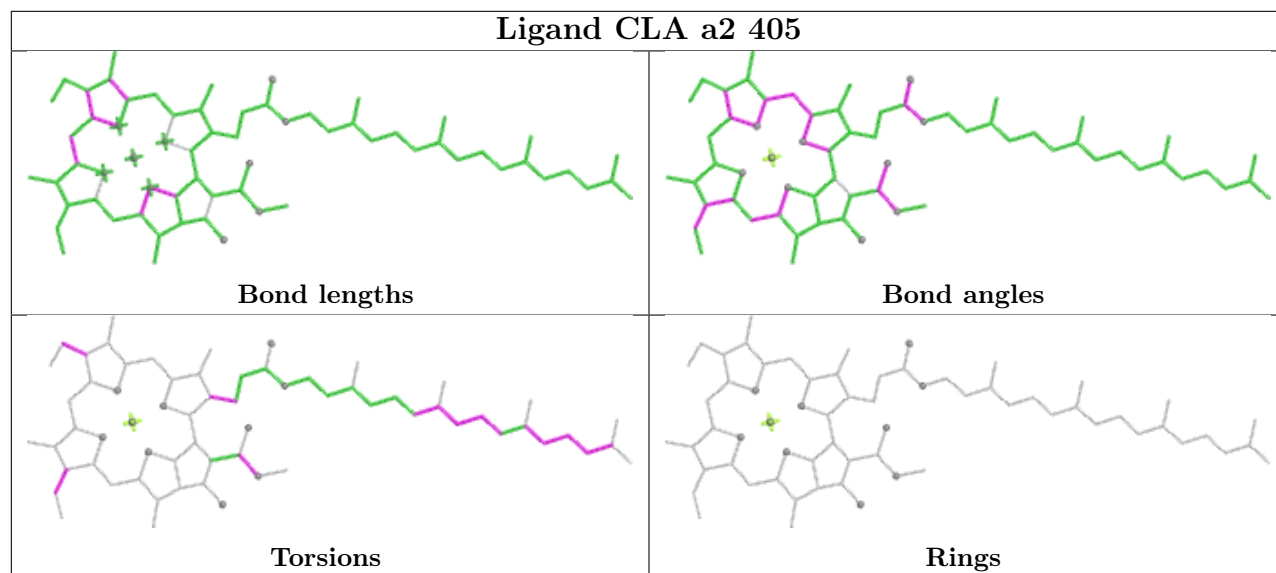
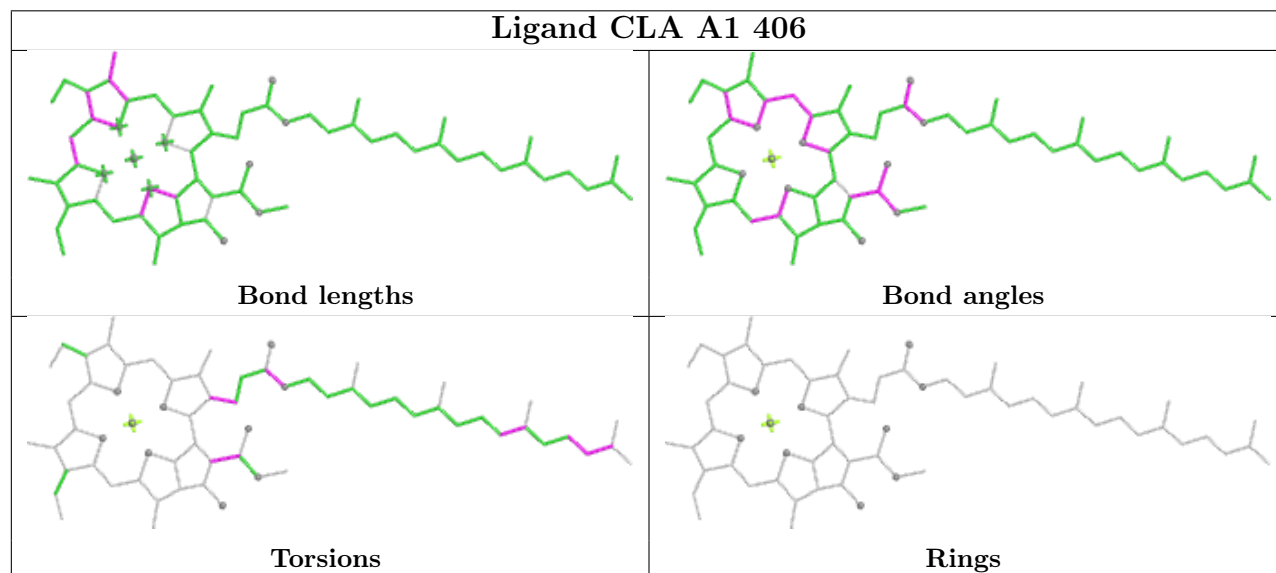
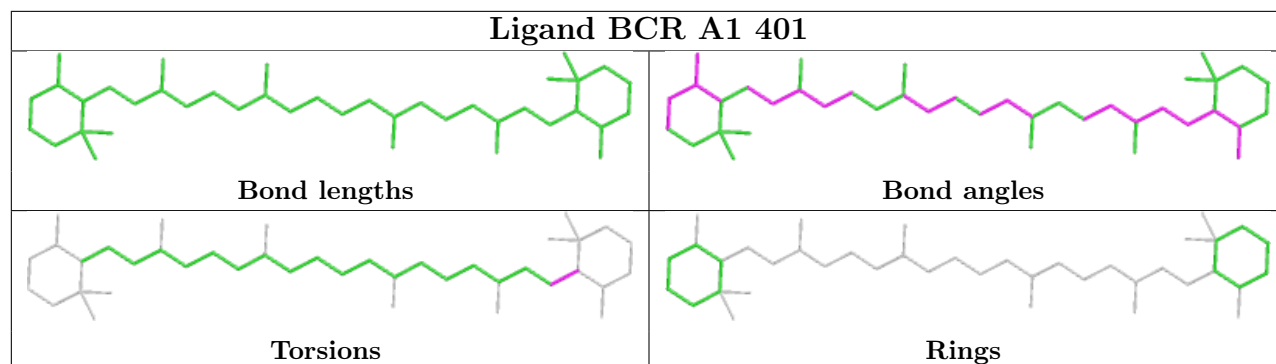


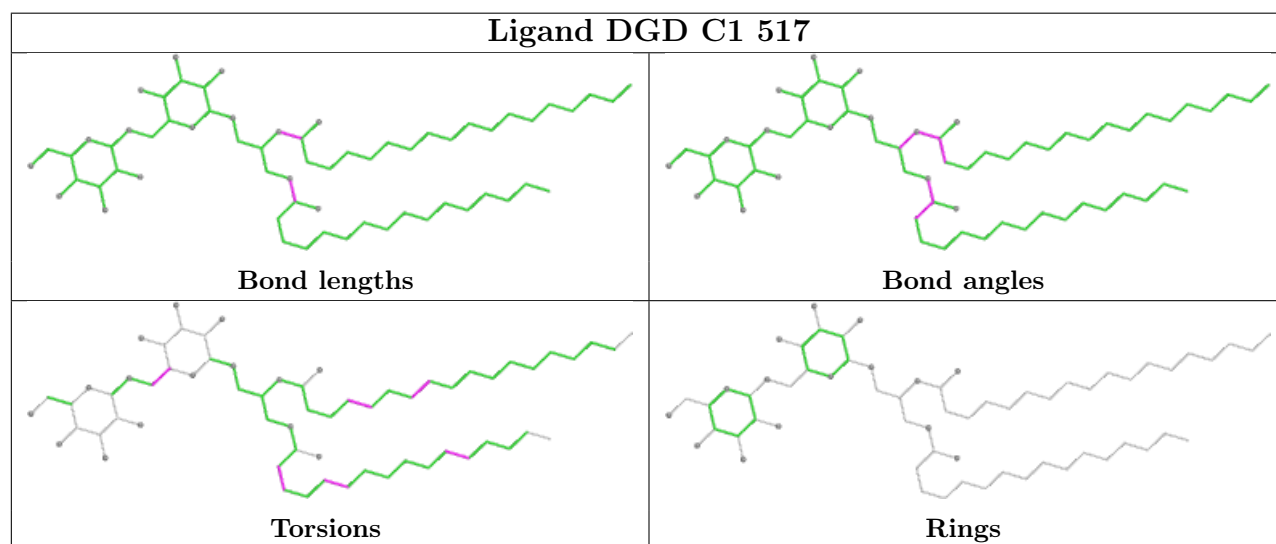
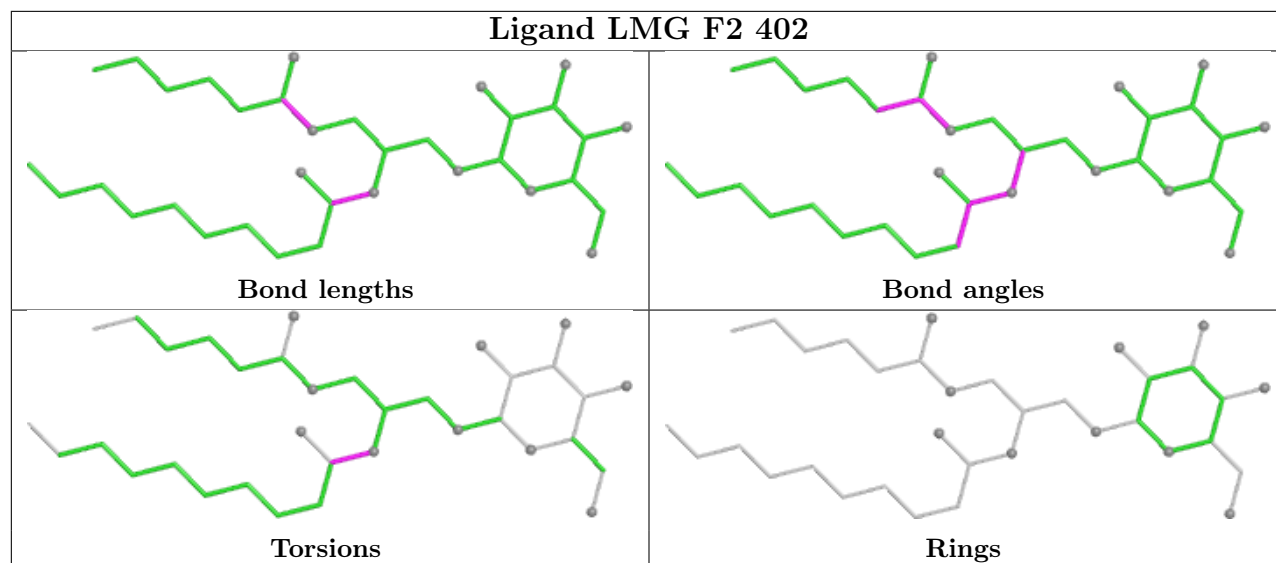


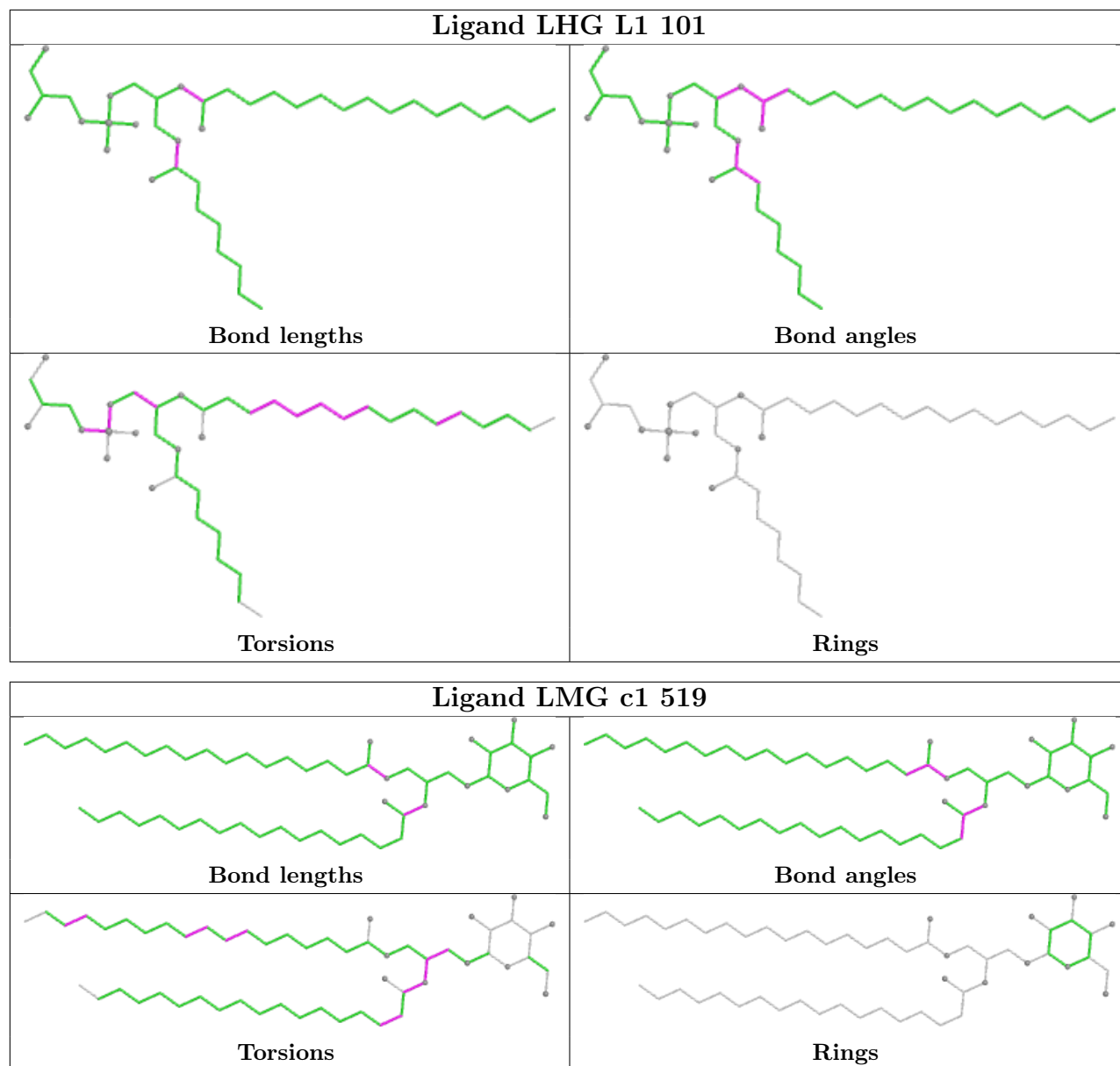
Ligand CLA c2 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

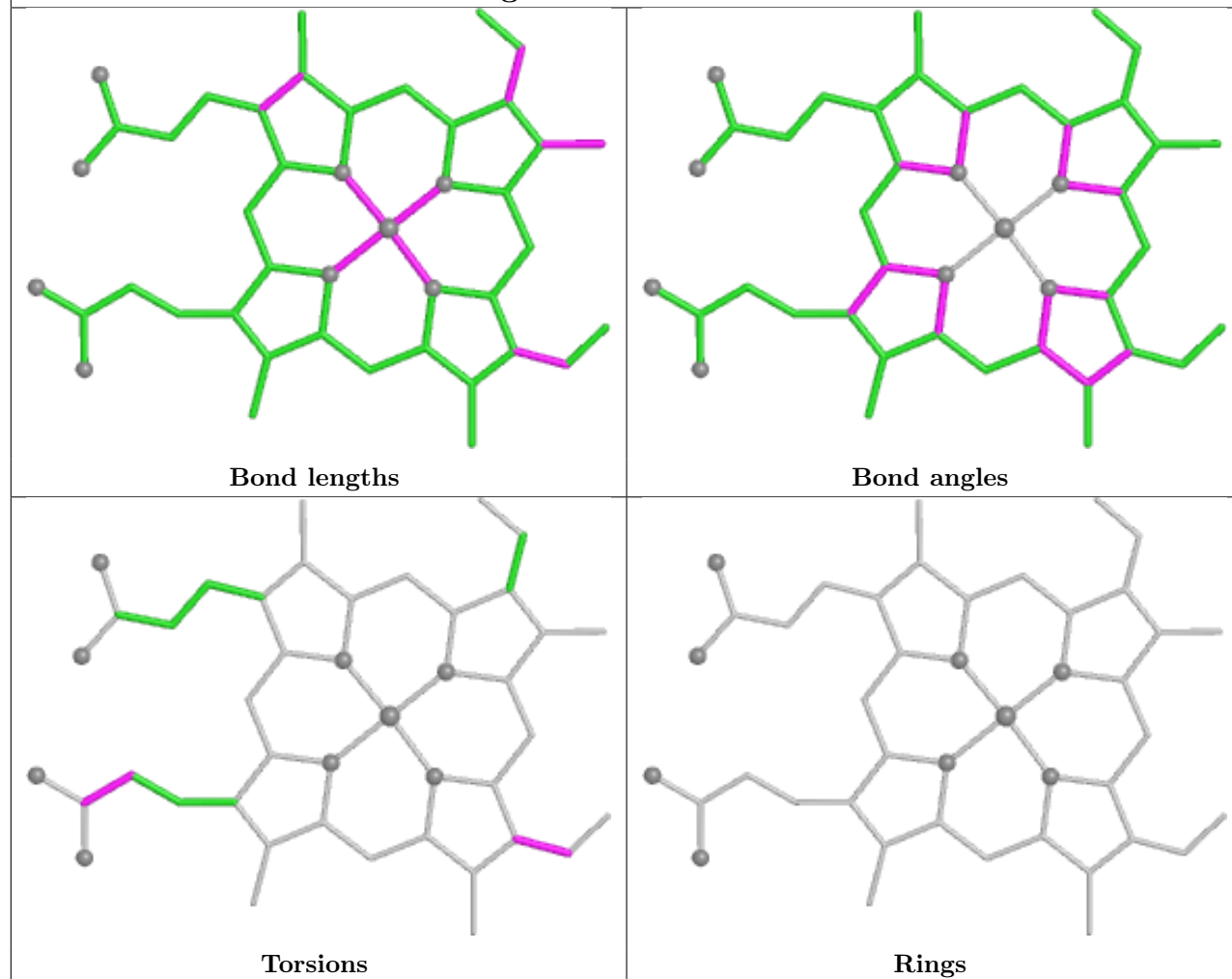
Ligand PL9 D2 408	
	
Bond lengths	Bond angles
	
Torsions	Rings



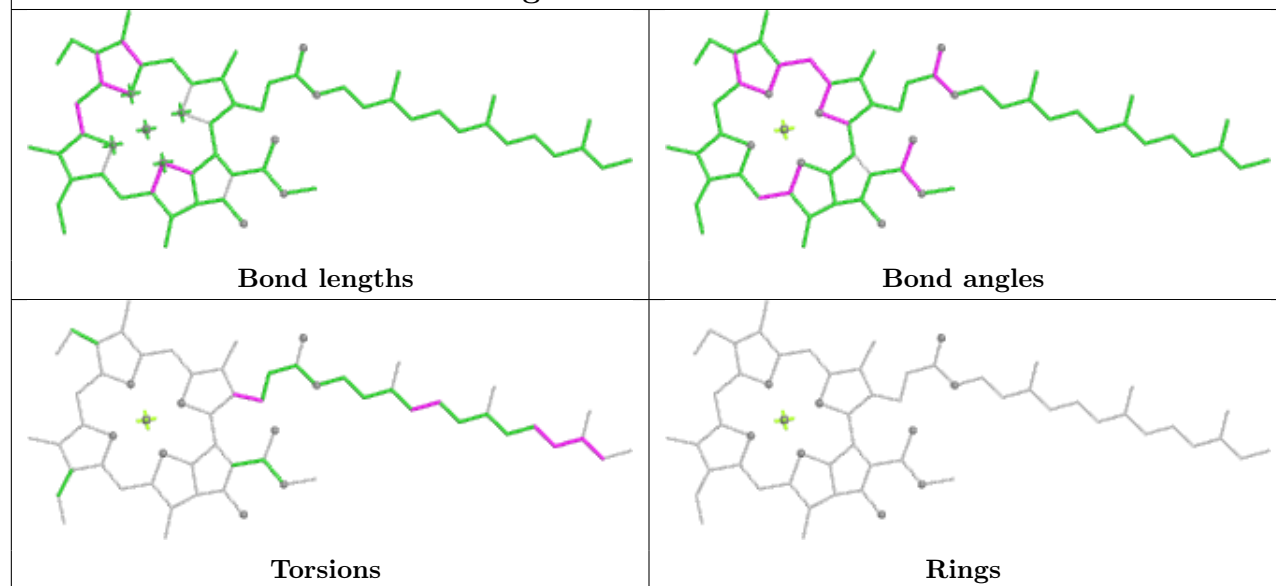


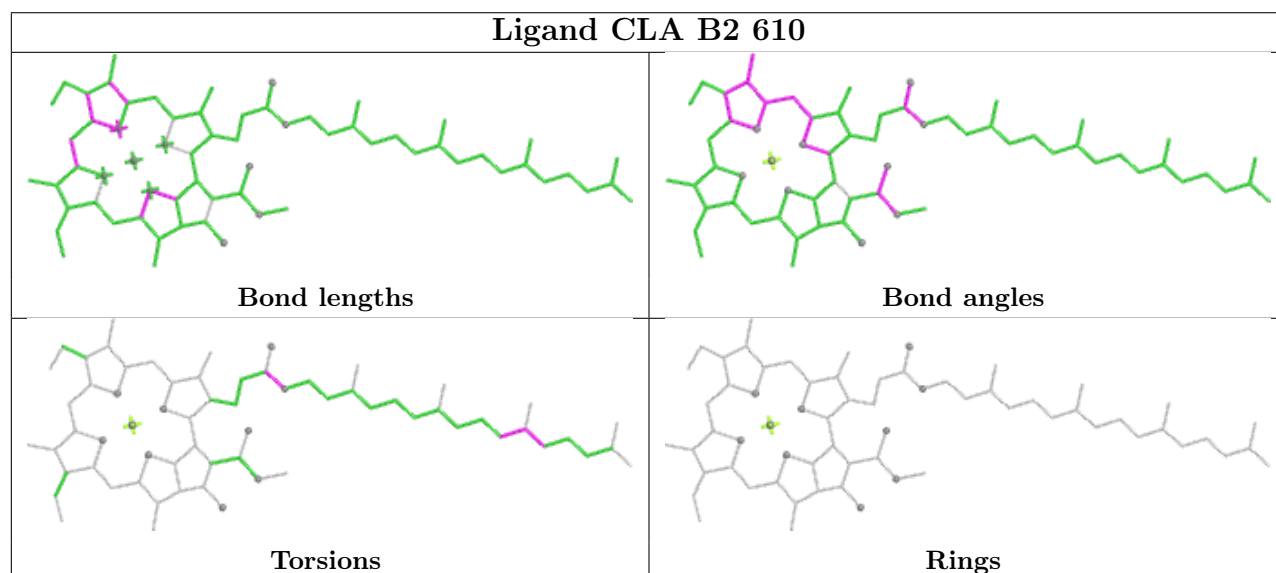
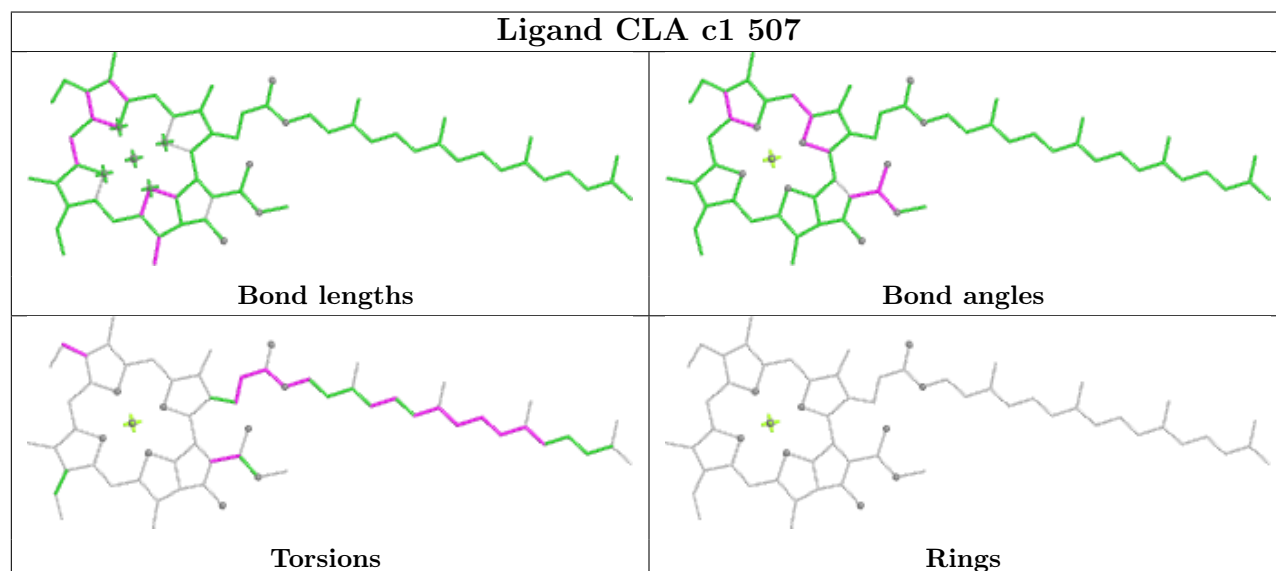
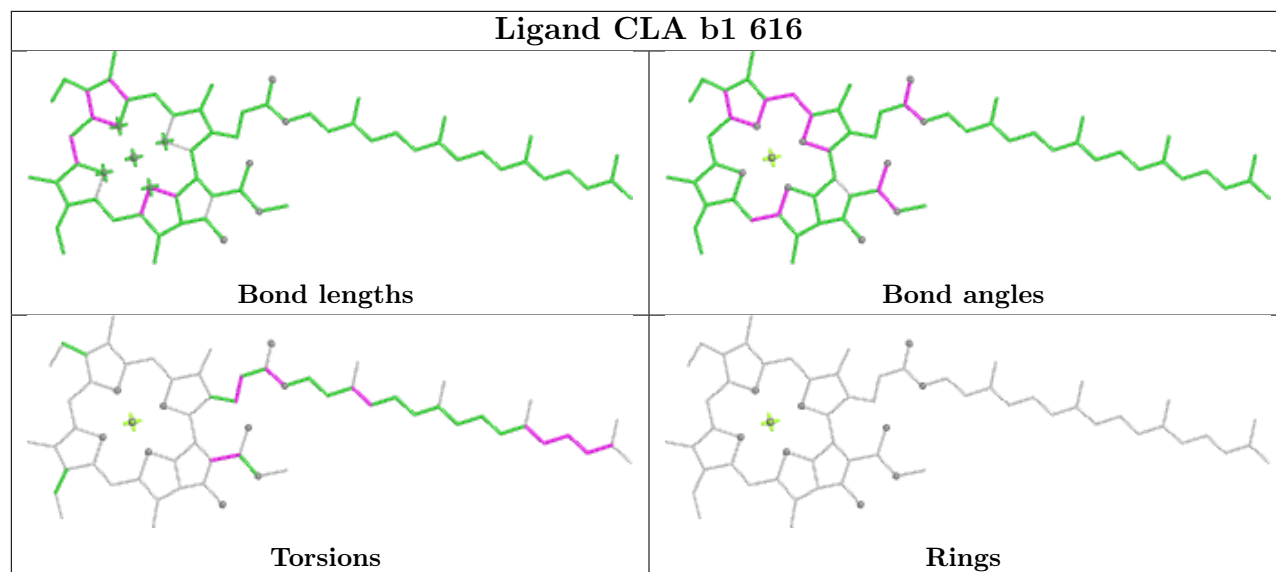


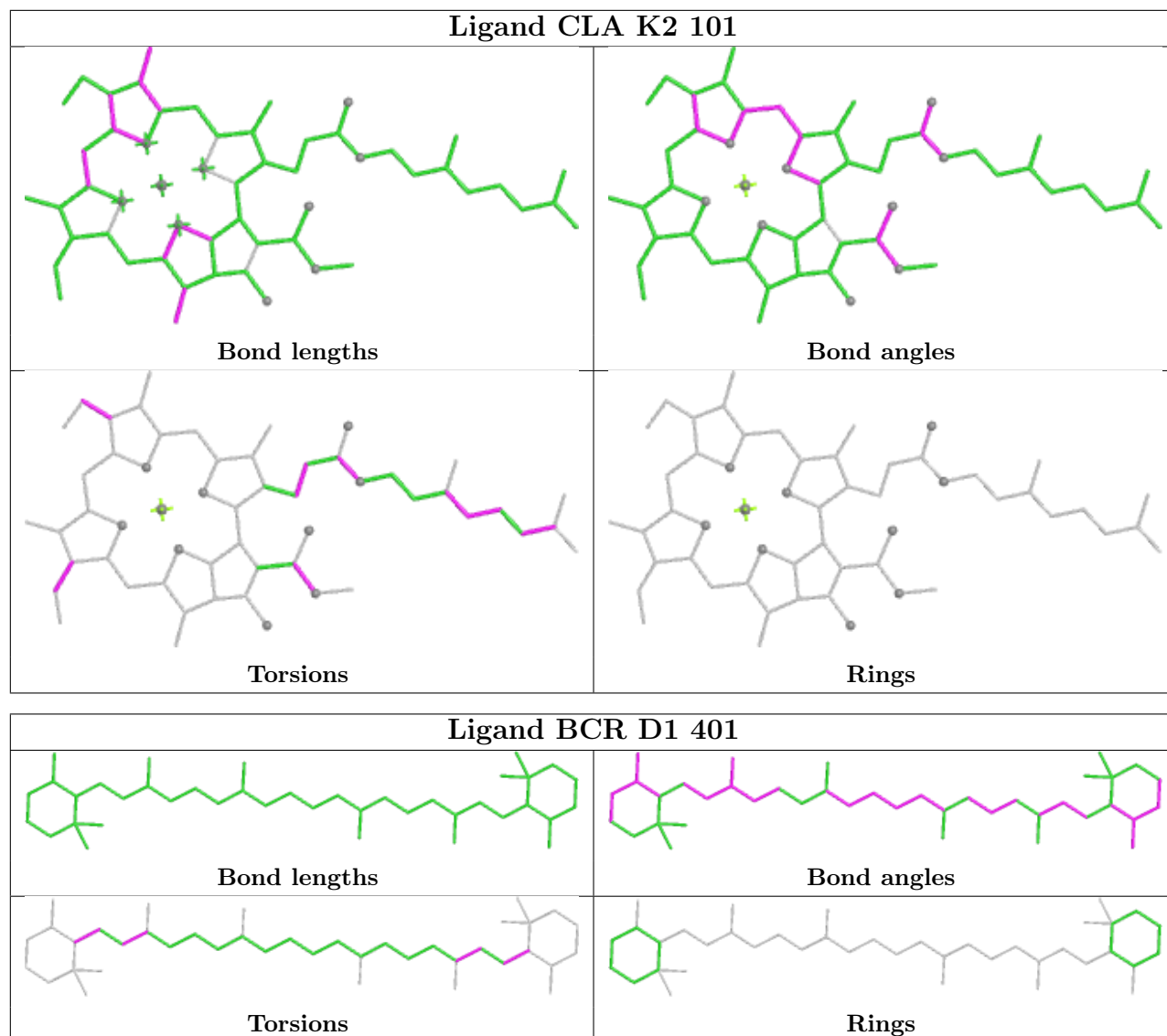
Ligand HEM E1 101

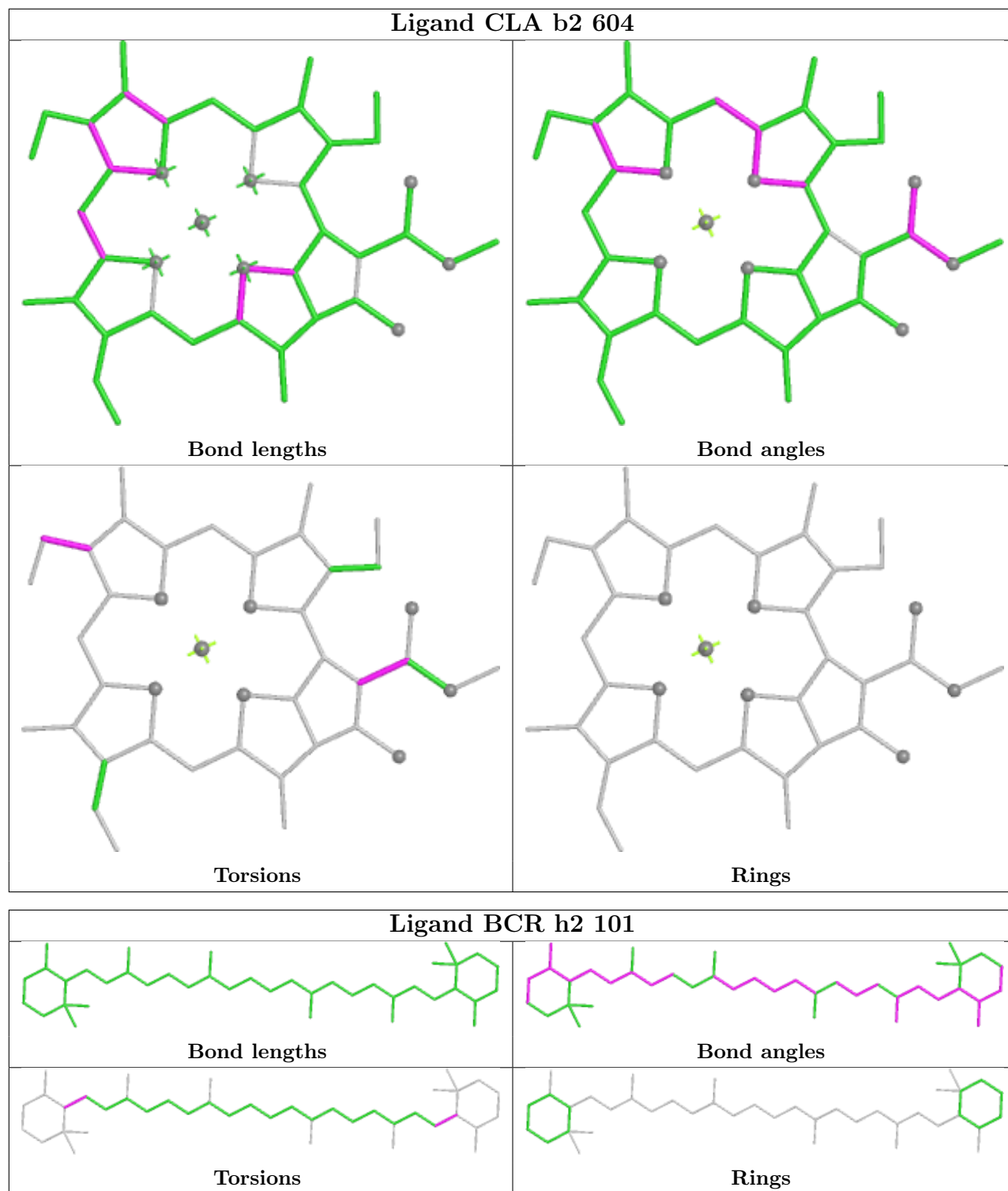


Ligand CLA A2 403

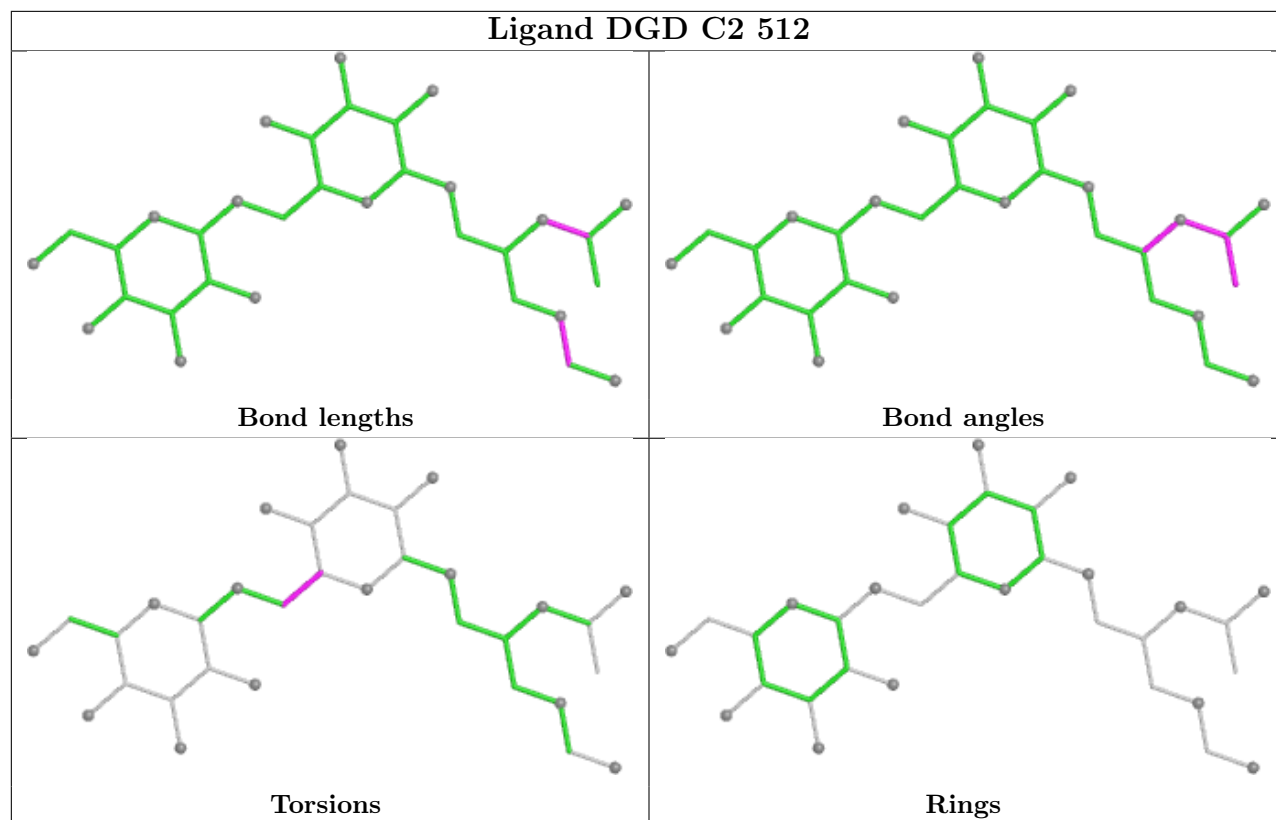




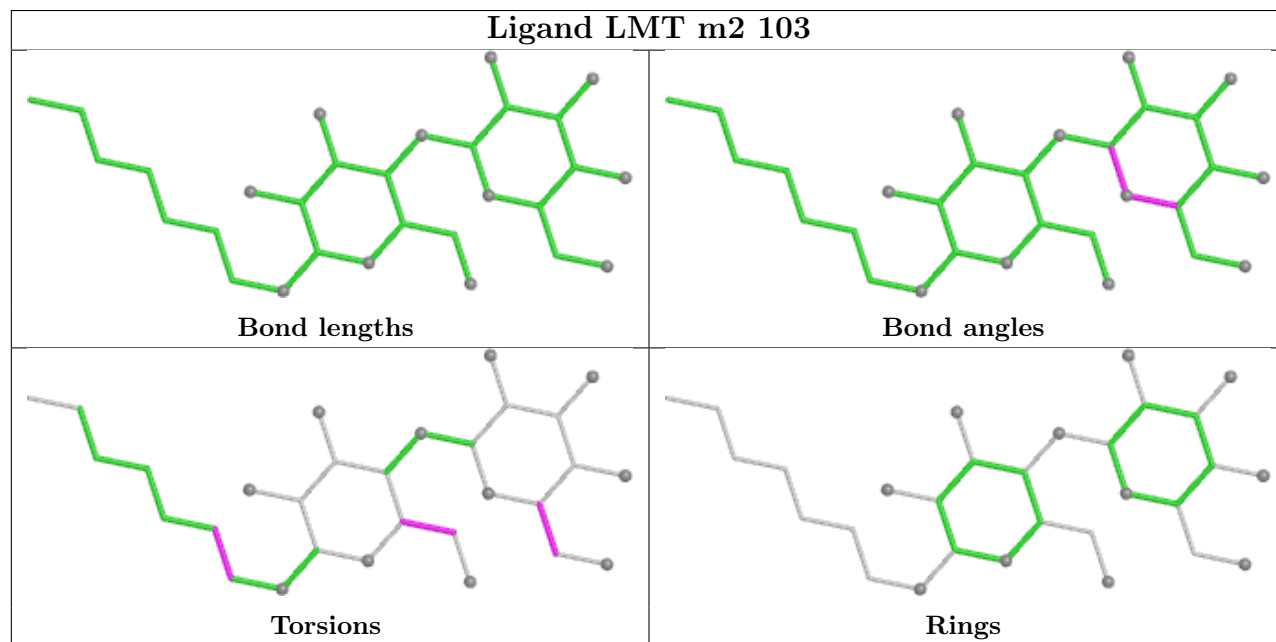


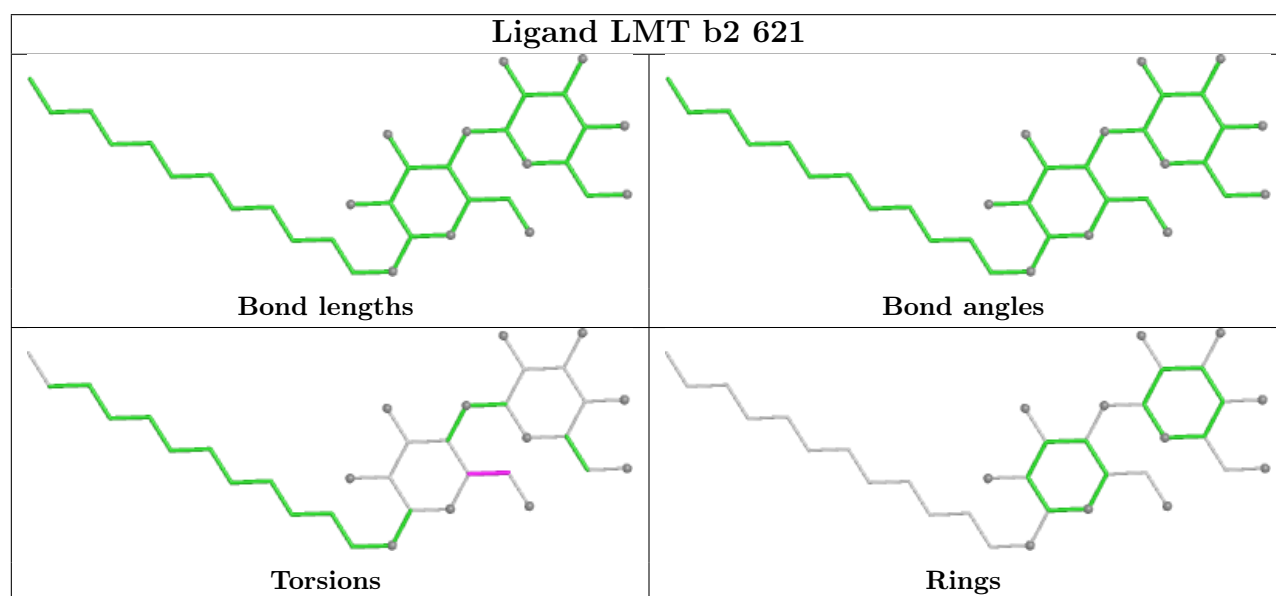
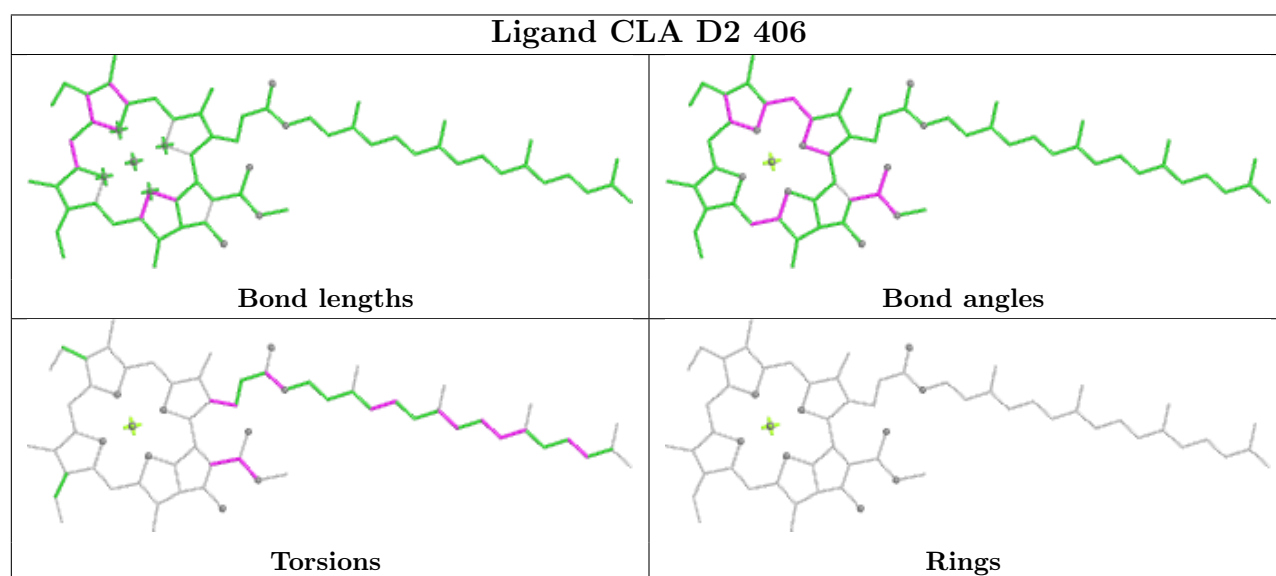
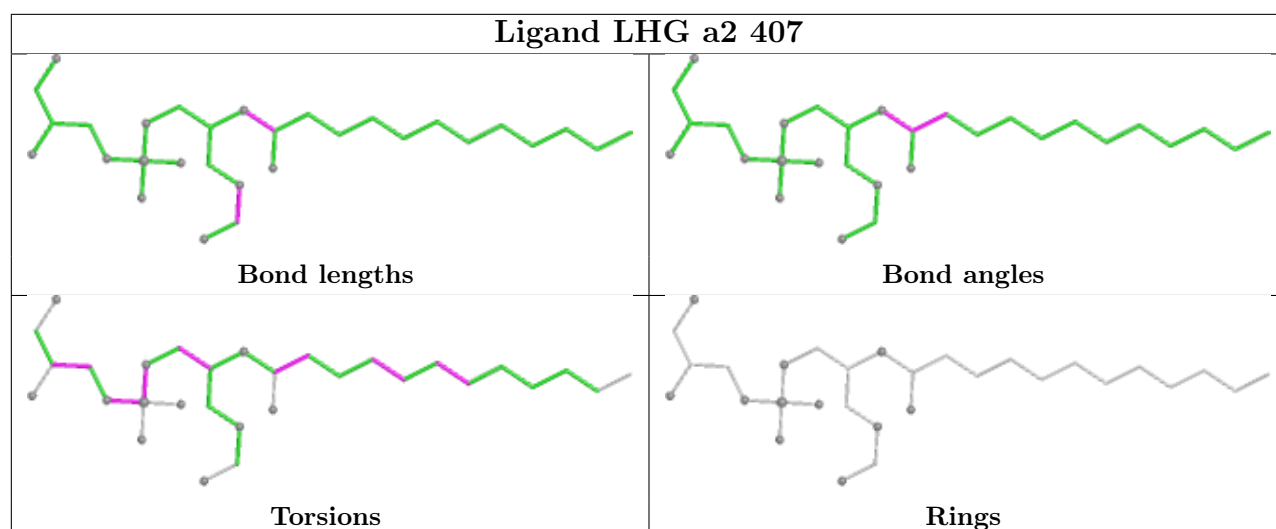


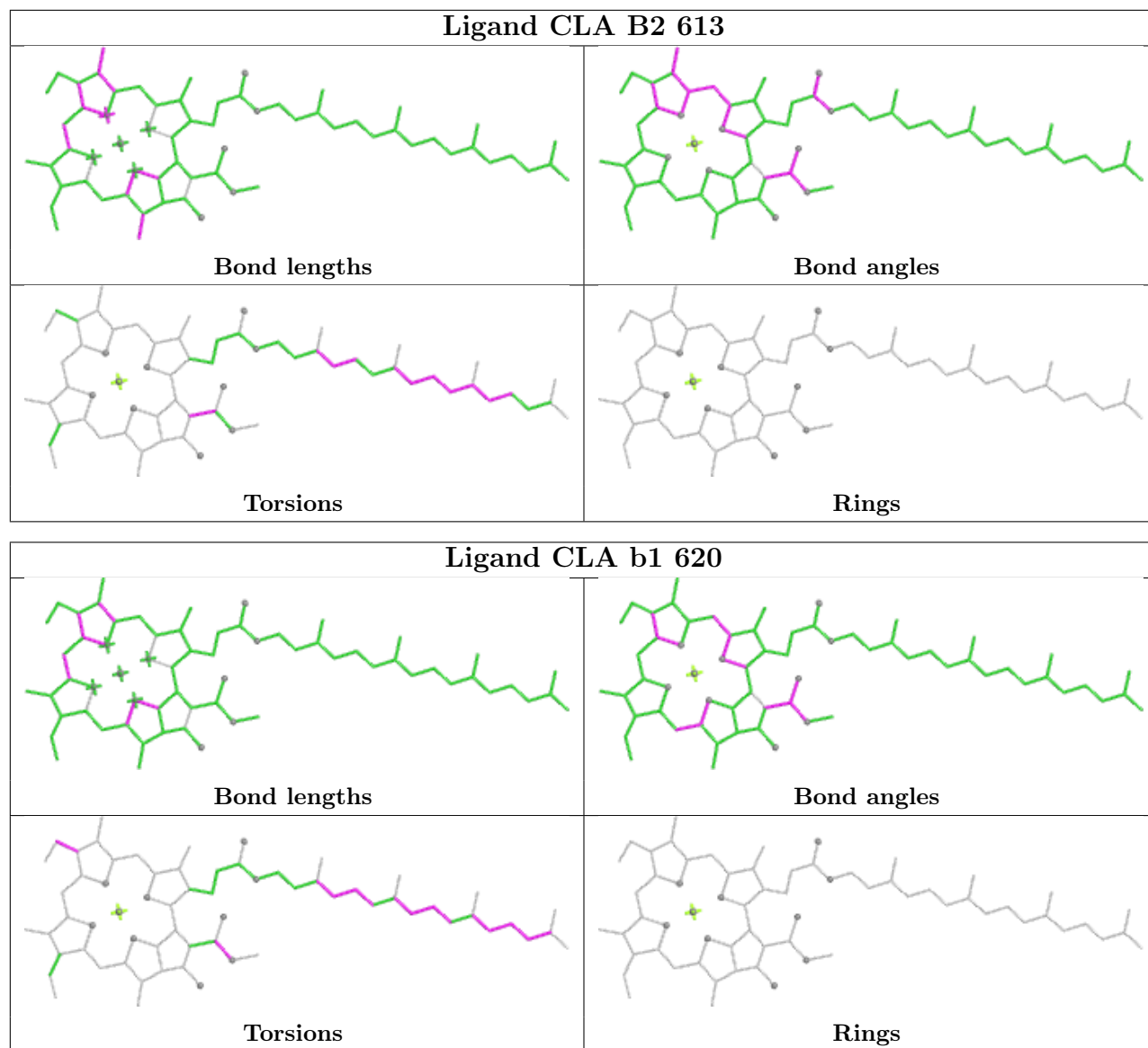
Ligand DGD C2 512



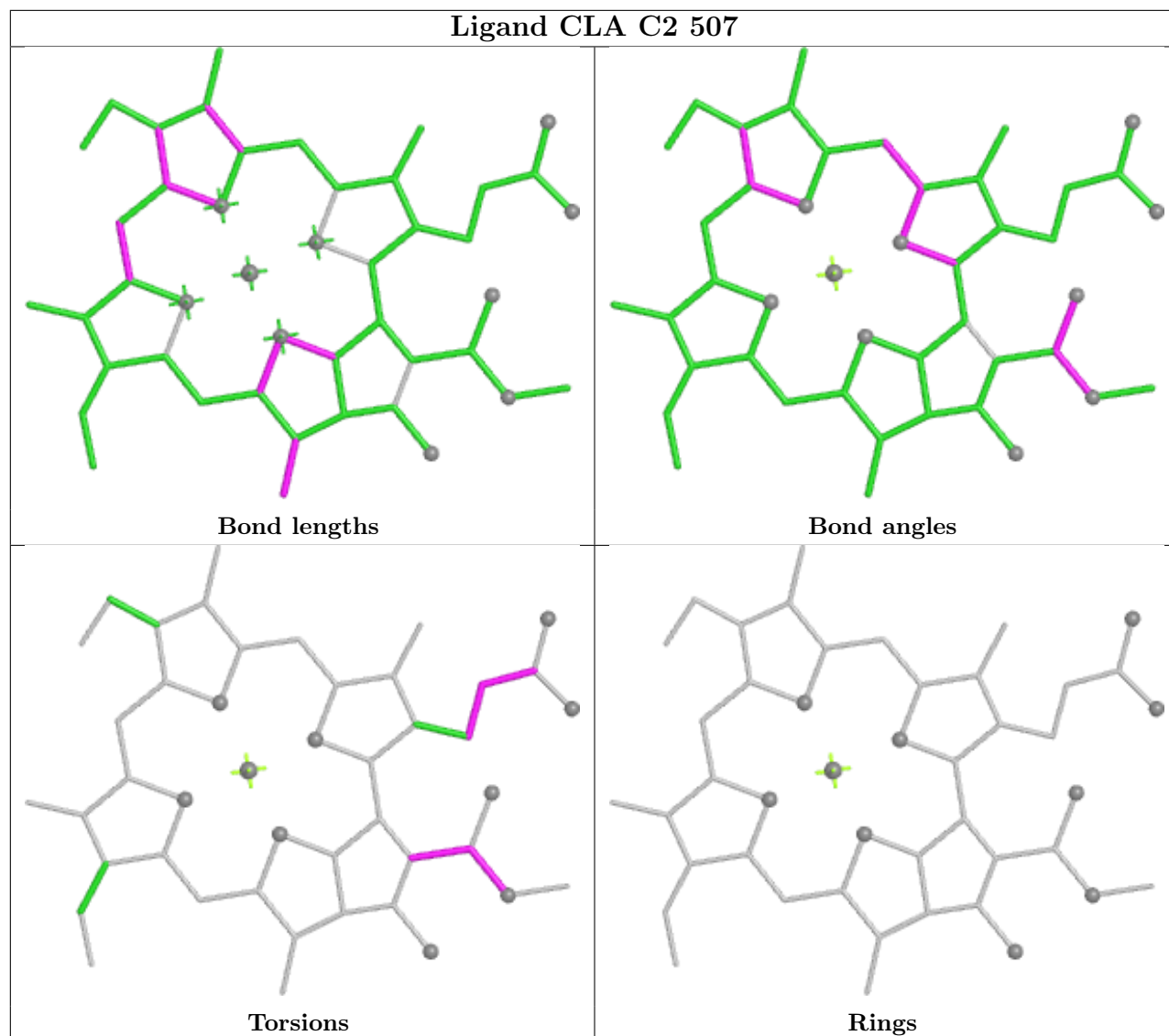
Ligand LMT m2 103



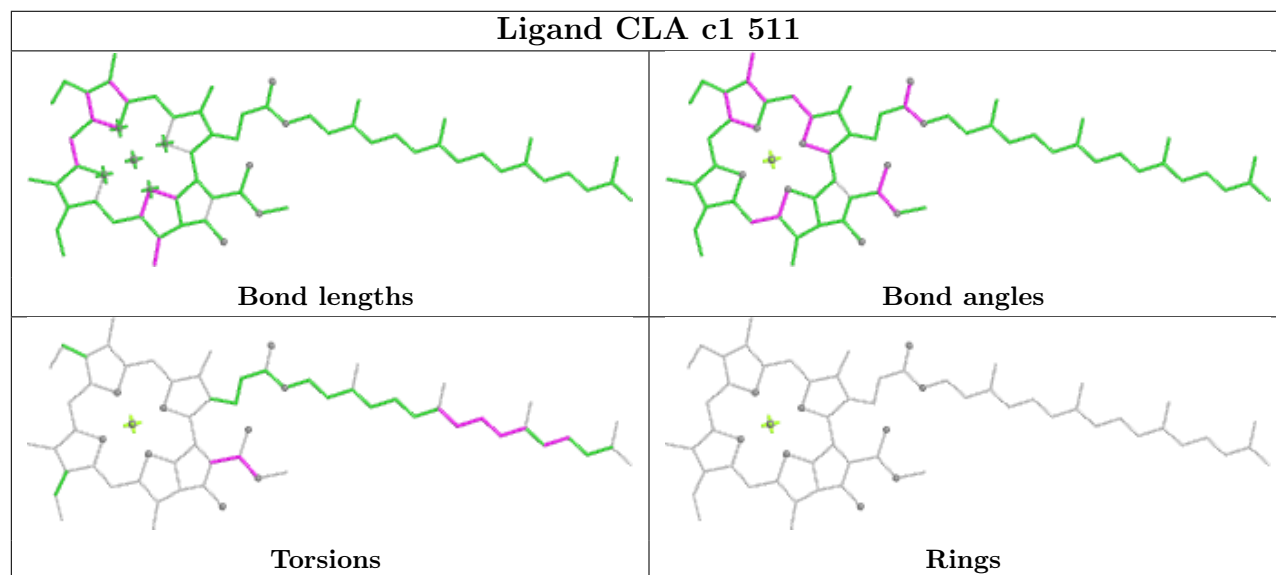


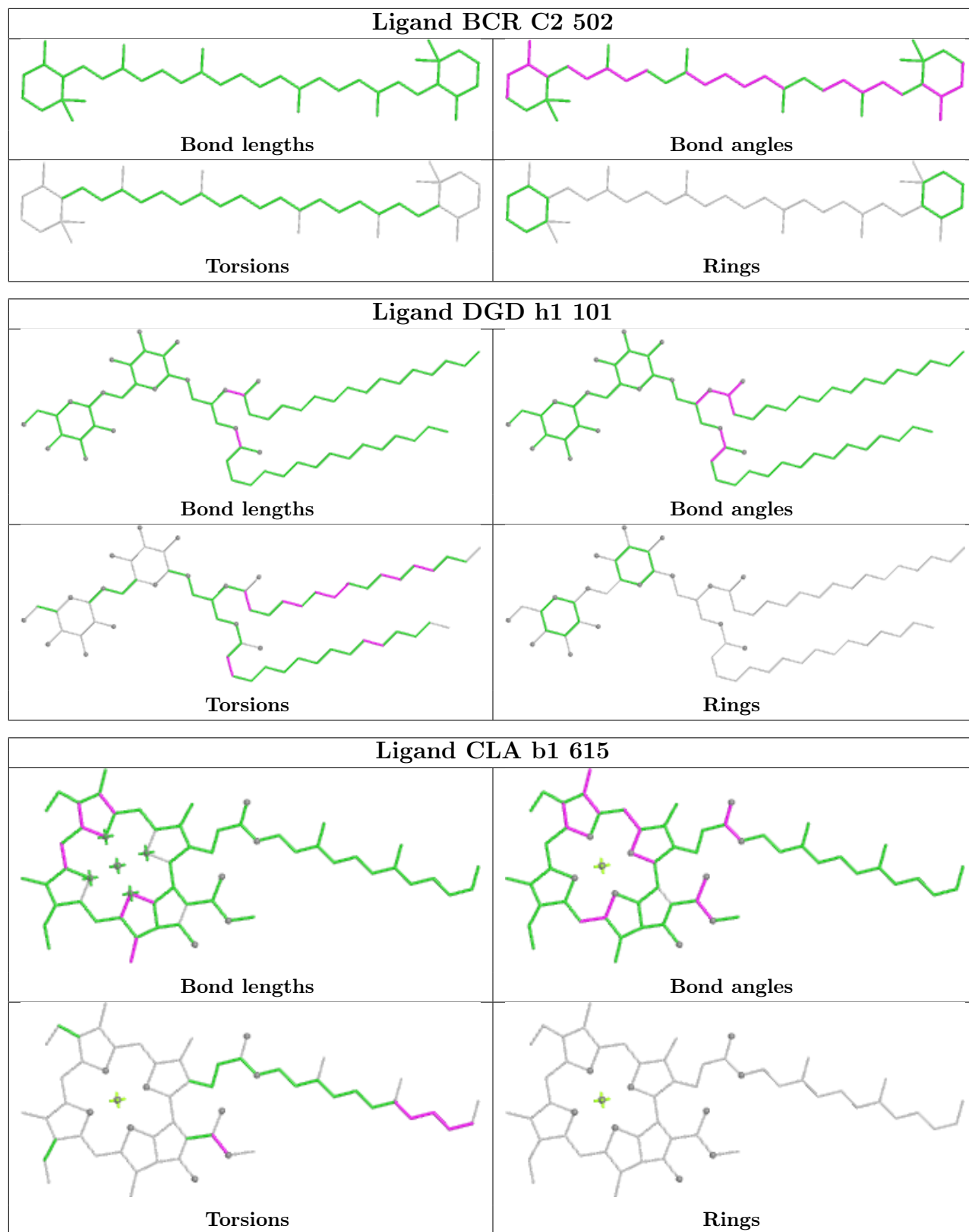


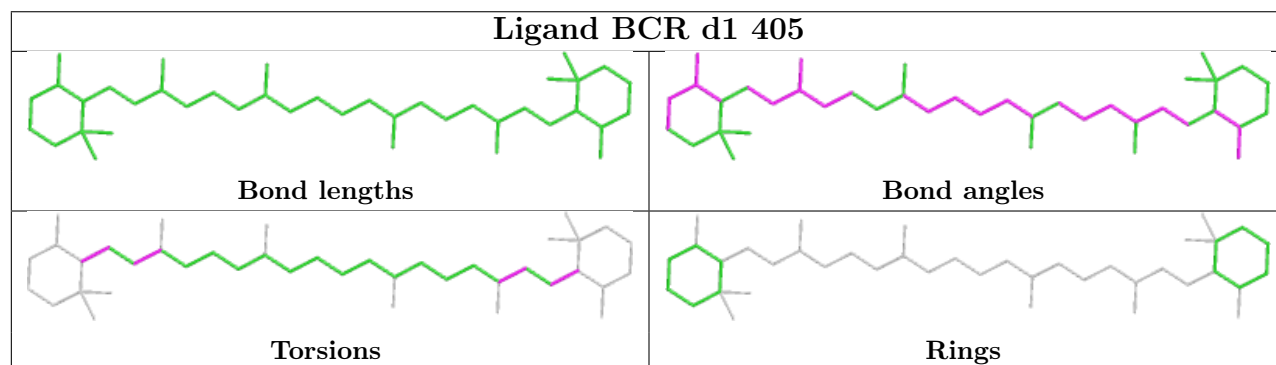
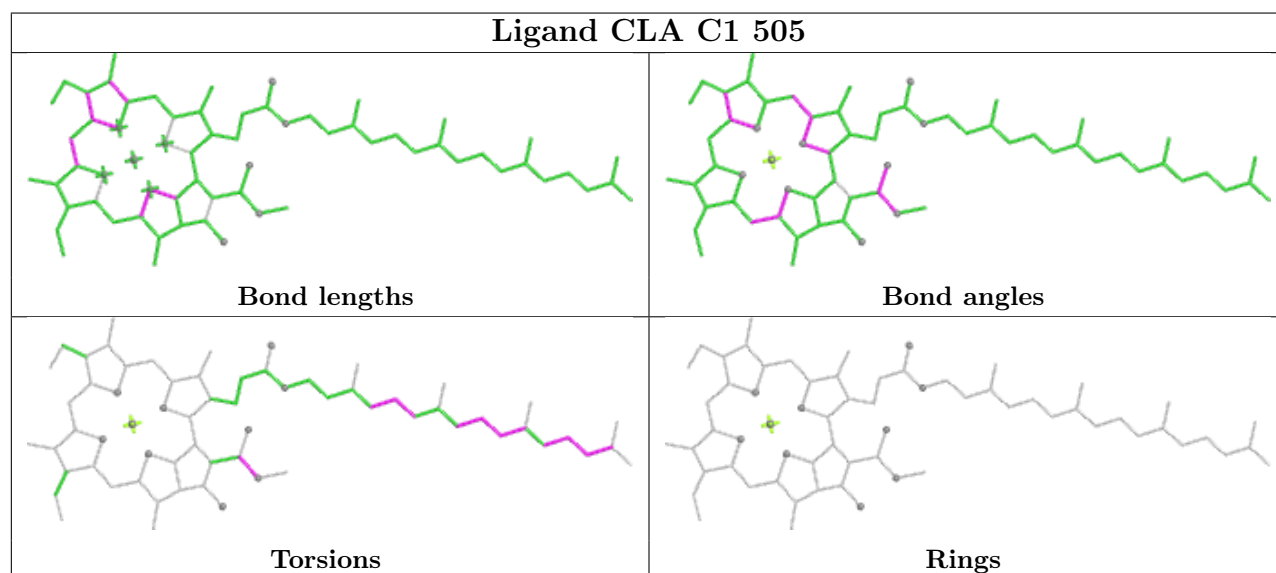
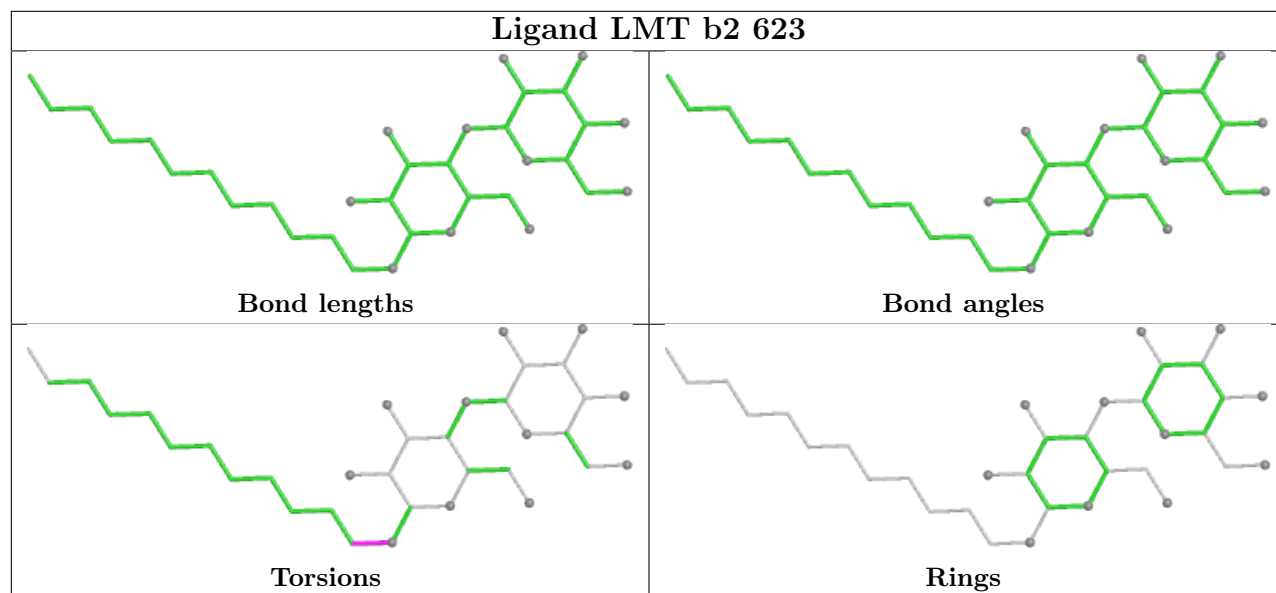
Ligand CLA C2 507



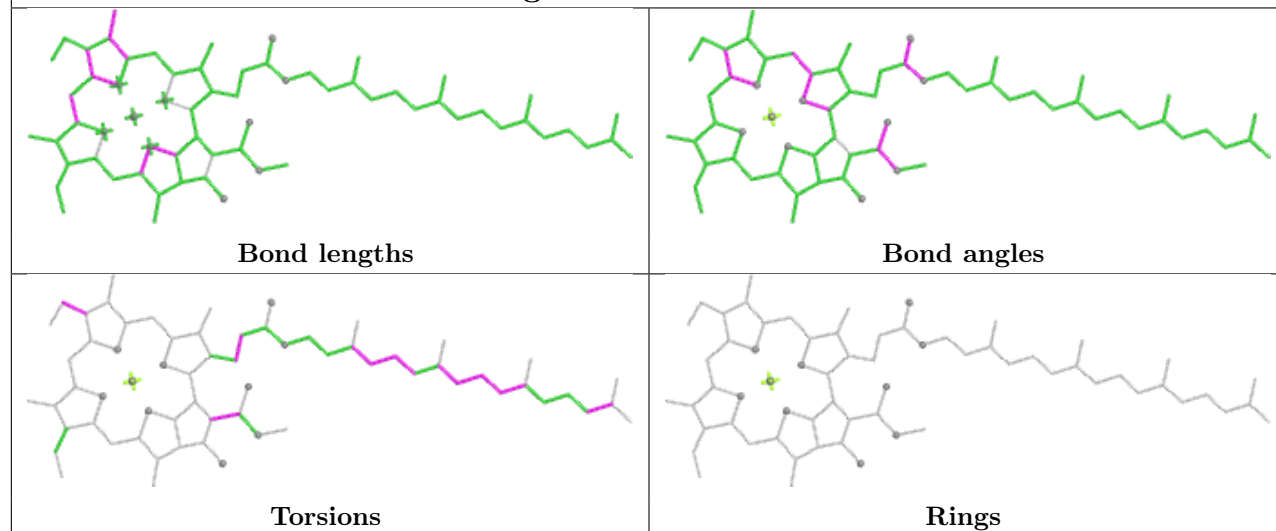
Ligand CLA c1 511



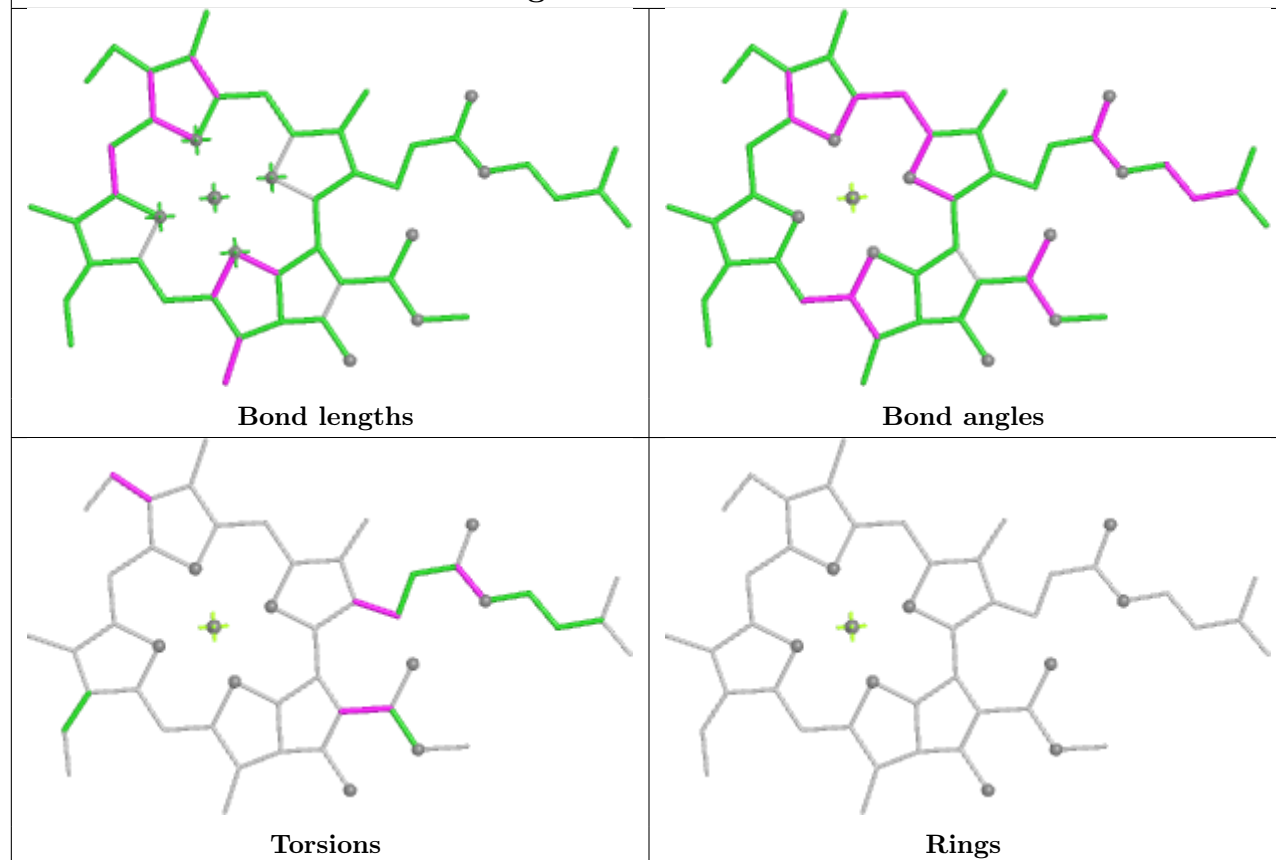


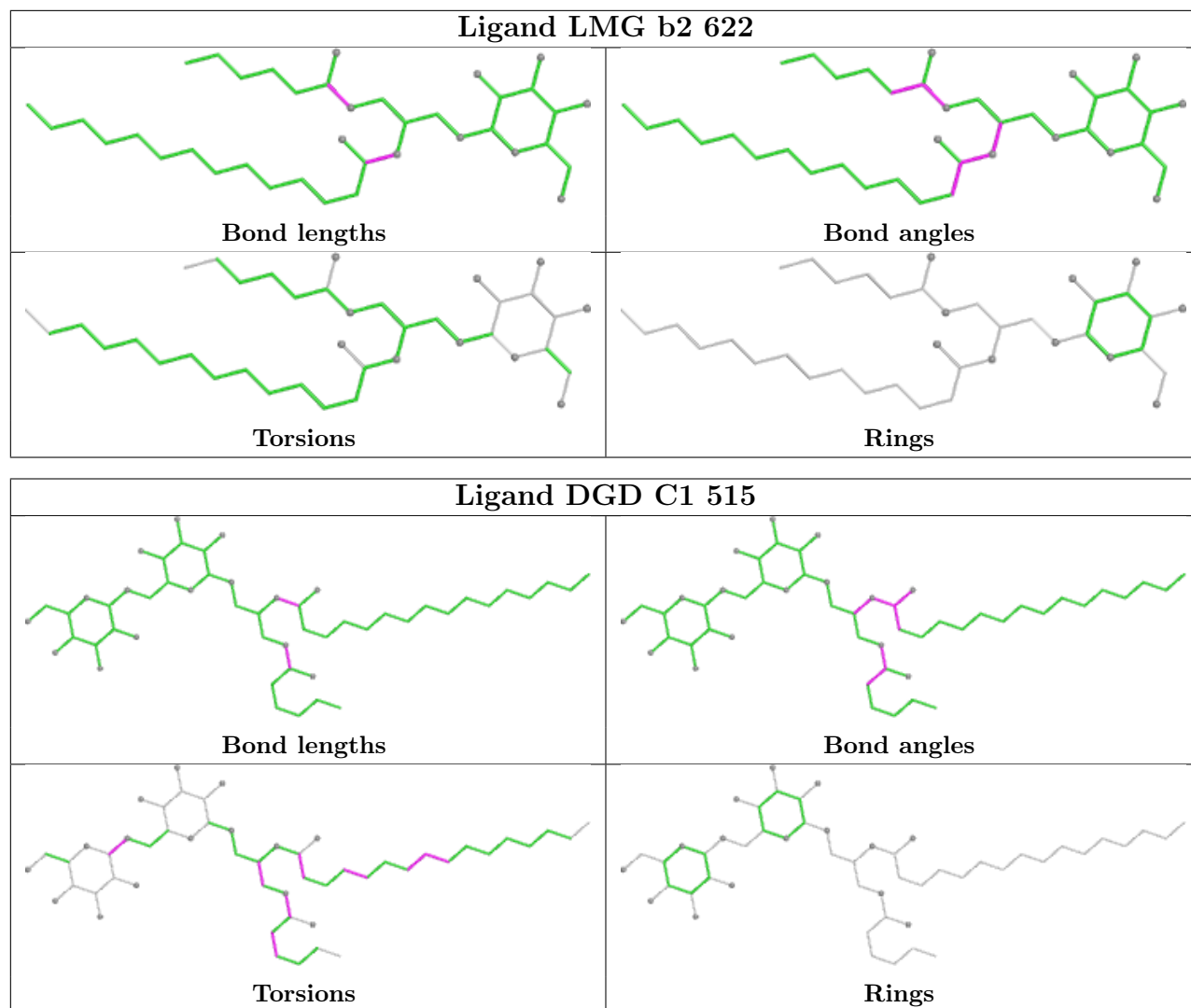


Ligand CLA C2 509

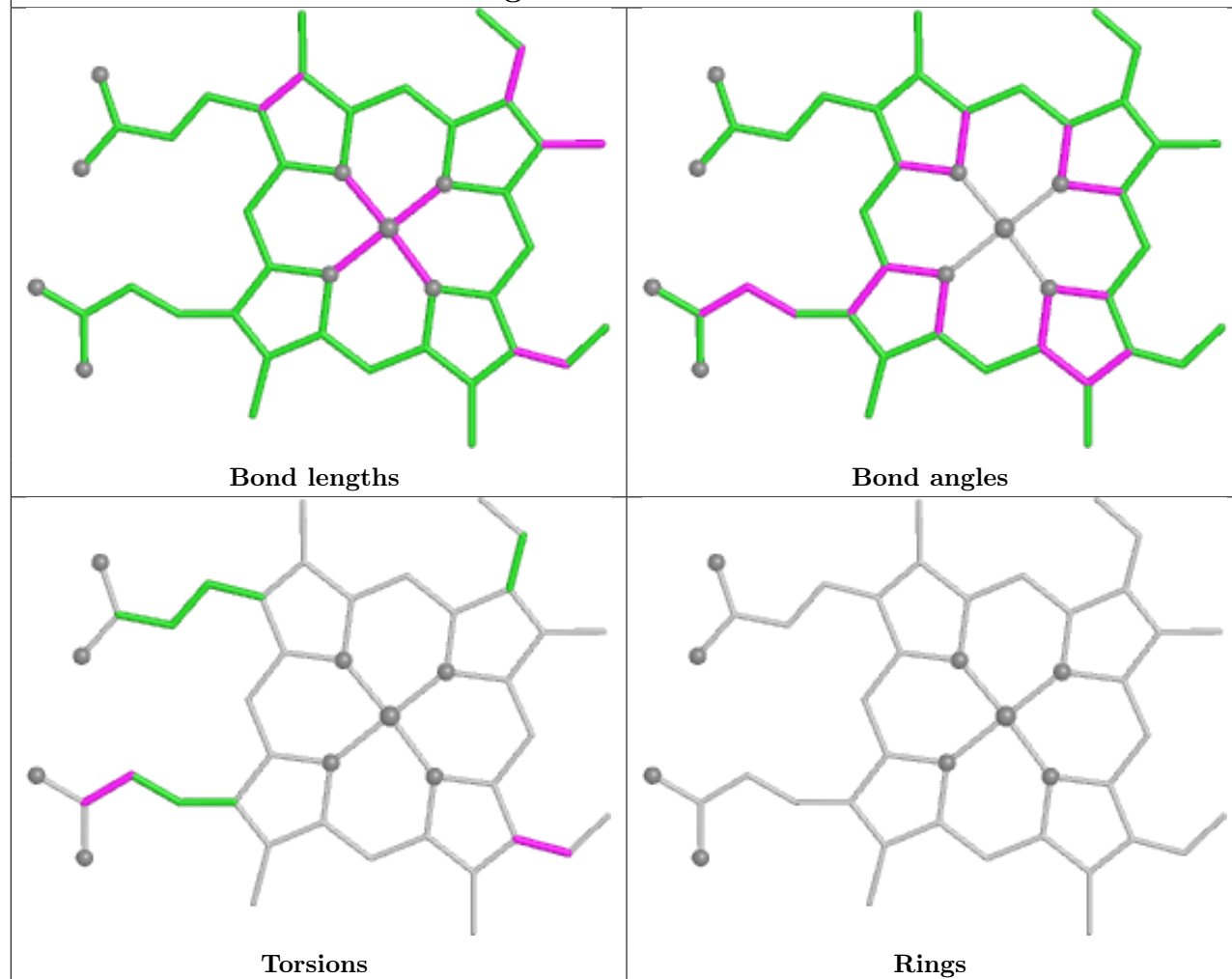


Ligand CLA a2 413

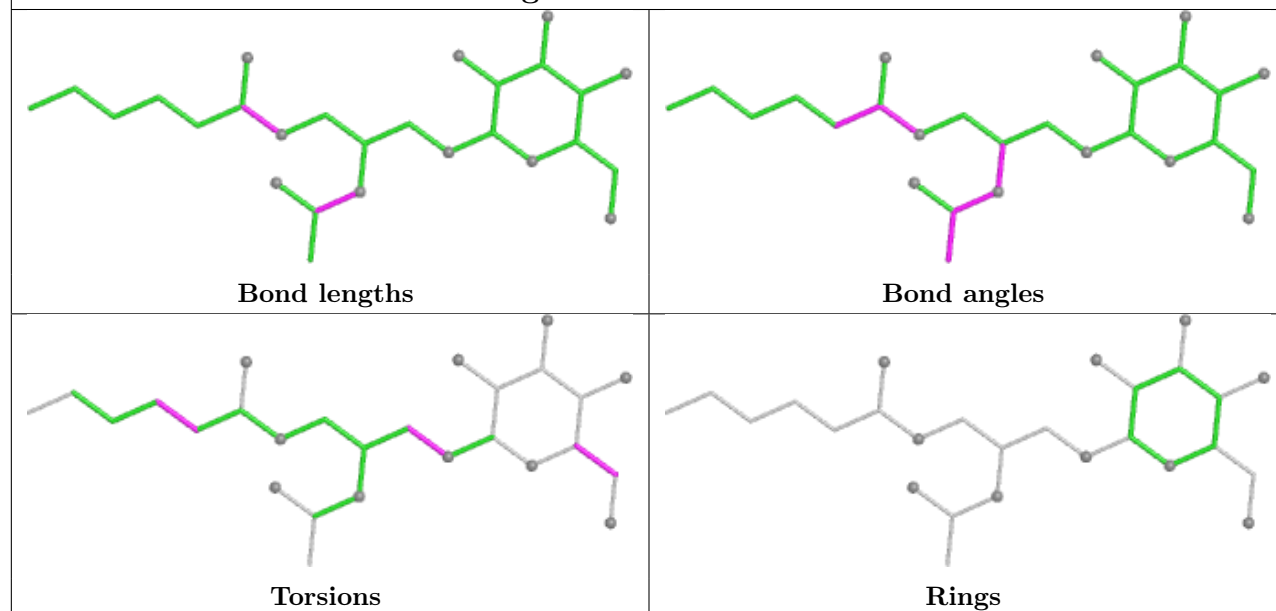




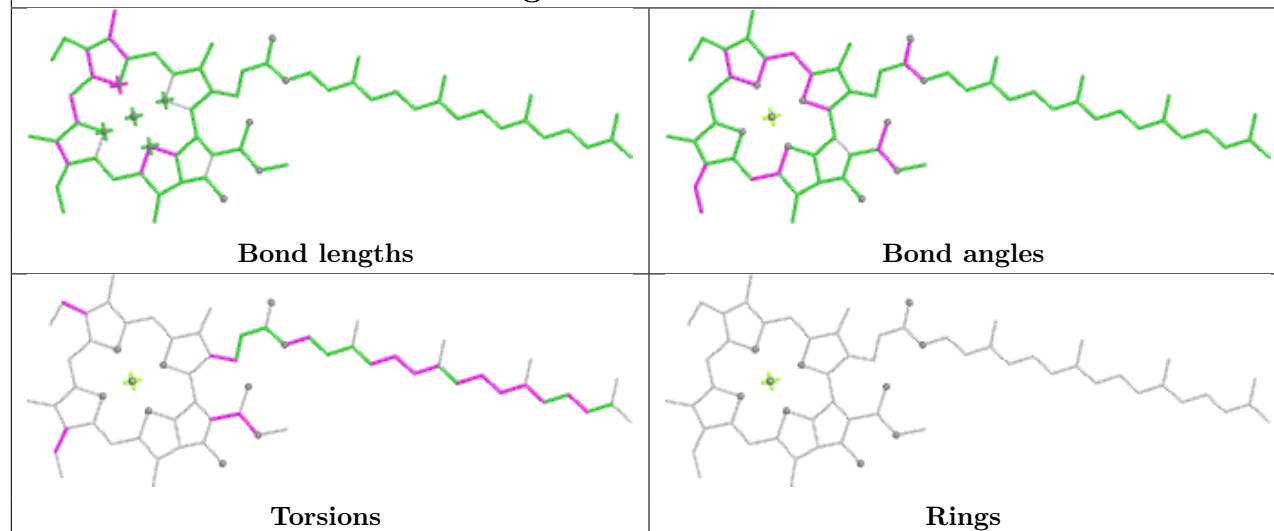
Ligand HEM e2 101



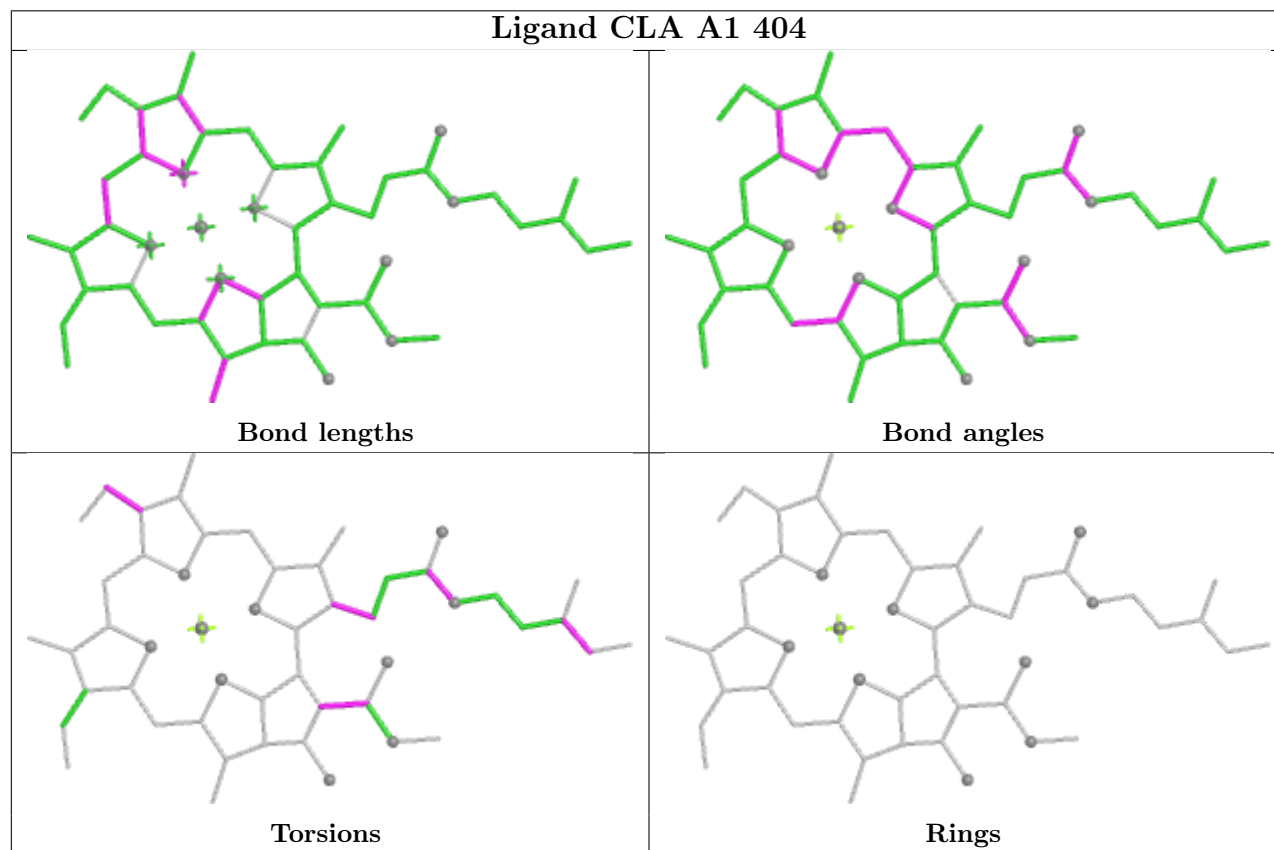
Ligand LMG d2 407

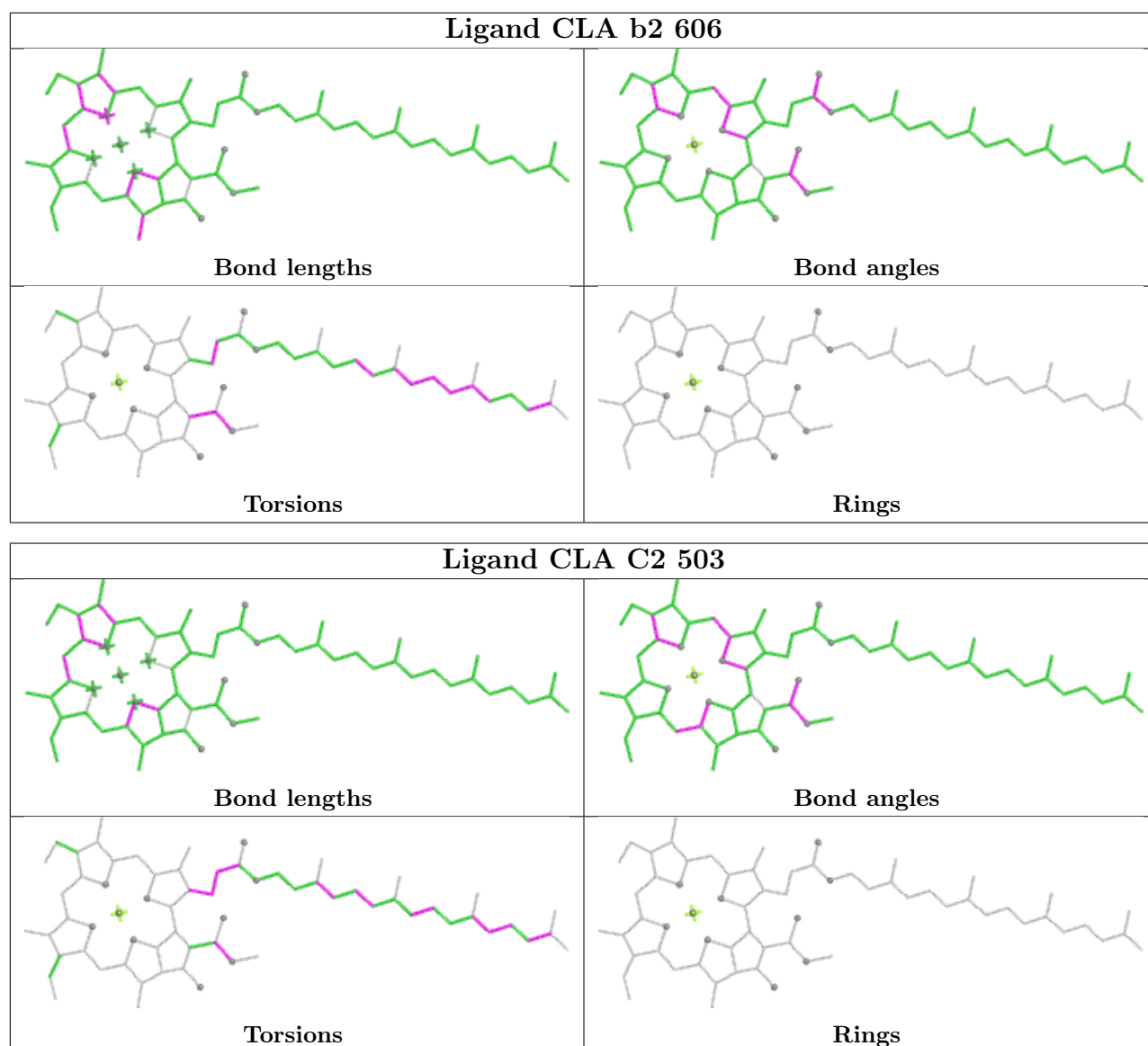


Ligand CLA C1 507



Ligand CLA A1 404





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	344/344 (100%)	-0.17	3 (0%) 81 76	31, 48, 79, 104	0
1	A2	332/344 (96%)	0.34	8 (2%) 59 52	48, 75, 91, 112	1 (0%)
1	a1	334/344 (97%)	-0.20	2 (0%) 85 81	36, 48, 68, 105	0
1	a2	334/344 (97%)	-0.21	1 (0%) 90 88	34, 50, 83, 107	0
2	B1	483/509 (94%)	0.11	6 (1%) 76 70	40, 63, 93, 108	0
2	B2	503/509 (98%)	0.14	8 (1%) 70 63	46, 65, 93, 112	0
2	b1	503/509 (98%)	-0.11	1 (0%) 91 89	36, 53, 80, 99	1 (0%)
2	b2	481/509 (94%)	0.25	14 (2%) 53 46	43, 70, 99, 115	0
3	C1	449/460 (97%)	-0.04	8 (1%) 67 60	33, 59, 78, 93	0
3	C2	444/460 (96%)	0.85	43 (9%) 13 10	73, 97, 117, 128	0
3	c1	449/460 (97%)	0.14	4 (0%) 81 76	41, 62, 84, 101	2 (0%)
3	c2	448/460 (97%)	0.13	7 (1%) 70 63	39, 70, 93, 110	0
4	D1	337/351 (96%)	-0.14	2 (0%) 85 81	36, 56, 88, 94	0
4	D2	340/351 (96%)	0.24	6 (1%) 67 60	51, 69, 85, 96	0
4	d1	339/351 (96%)	-0.30	2 (0%) 85 81	34, 45, 65, 94	0
4	d2	340/351 (96%)	-0.11	2 (0%) 85 81	36, 56, 88, 118	0
5	E1	61/84 (72%)	0.56	7 (11%) 9 7	64, 87, 141, 158	0
5	E2	63/84 (75%)	1.11	11 (17%) 4 3	77, 98, 131, 144	0
5	e1	57/84 (67%)	0.26	2 (3%) 47 40	49, 65, 87, 91	0
5	e2	60/84 (71%)	0.49	4 (6%) 24 19	59, 80, 144, 159	0
6	F1	28/43 (65%)	0.28	1 (3%) 46 39	62, 75, 123, 131	0
6	F2	31/43 (72%)	1.19	7 (22%) 2 1	81, 92, 144, 146	0
6	f1	29/43 (67%)	0.08	1 (3%) 48 41	50, 60, 95, 108	0
6	f2	29/43 (67%)	0.50	2 (6%) 23 18	64, 73, 128, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	H1	60/67 (89%)	0.46	2 (3%) 49 42	70, 84, 93, 101	0
7	H2	62/67 (92%)	0.36	0 100 100	63, 75, 92, 124	0
7	h1	62/67 (92%)	-0.10	0 100 100	47, 67, 78, 84	0
7	h2	62/67 (92%)	0.55	6 (9%) 13 10	72, 87, 98, 122	0
8	I1	34/38 (89%)	-0.06	0 100 100	53, 61, 70, 71	0
8	I2	35/38 (92%)	0.63	1 (2%) 53 46	82, 93, 105, 109	0
8	i1	34/38 (89%)	0.03	0 100 100	54, 61, 71, 76	0
8	i2	33/38 (86%)	0.15	0 100 100	60, 67, 75, 77	0
9	J1	32/39 (82%)	0.16	1 (3%) 51 44	51, 65, 89, 105	0
9	J2	35/39 (89%)	1.06	7 (20%) 3 2	75, 87, 125, 136	0
9	j1	32/39 (82%)	0.10	0 100 100	49, 63, 74, 81	0
9	j2	33/39 (84%)	0.23	1 (3%) 52 45	54, 70, 88, 110	0
10	K1	37/41 (90%)	0.15	1 (2%) 56 48	56, 66, 78, 79	0
10	K2	37/41 (90%)	1.06	6 (16%) 4 4	86, 96, 111, 117	0
10	k1	37/41 (90%)	0.23	0 100 100	56, 67, 81, 81	0
10	k2	37/41 (90%)	0.69	2 (5%) 31 26	67, 76, 89, 92	0
11	L1	37/38 (97%)	-0.26	0 100 100	39, 43, 67, 77	0
11	L2	37/38 (97%)	-0.03	0 100 100	49, 56, 61, 73	0
11	l1	37/38 (97%)	-0.16	0 100 100	36, 43, 63, 73	0
11	l2	37/38 (97%)	-0.15	0 100 100	43, 47, 73, 79	0
12	M1	40/108 (37%)	-0.11	0 100 100	32, 46, 62, 66	0
12	M2	40/108 (37%)	-0.10	0 100 100	45, 54, 67, 69	0
12	m1	40/108 (37%)	-0.05	1 (2%) 58 50	34, 44, 65, 67	0
12	m2	40/108 (37%)	-0.00	1 (2%) 58 50	44, 51, 65, 71	0
13	O1	240/329 (72%)	0.19	10 (4%) 40 34	38, 61, 96, 107	0
13	O2	205/329 (62%)	0.91	30 (14%) 6 5	54, 91, 119, 151	0
13	o1	238/329 (72%)	0.42	15 (6%) 26 21	38, 76, 121, 145	0
13	o2	245/329 (74%)	0.24	13 (5%) 32 26	41, 64, 103, 127	0
14	T1	30/32 (93%)	-0.24	1 (3%) 49 42	37, 44, 60, 68	0
14	T2	30/32 (93%)	0.10	1 (3%) 49 42	54, 63, 76, 82	0
14	t1	30/32 (93%)	-0.23	0 100 100	40, 46, 60, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	t2	29/32 (90%)	-0.31	0 100 100	38, 48, 68, 84	0
15	U1	93/155 (60%)	-0.11	0 100 100	44, 59, 75, 104	0
15	U2	90/155 (58%)	0.48	5 (5%) 30 25	74, 91, 104, 115	0
15	u1	93/155 (60%)	0.03	1 (1%) 78 72	53, 68, 88, 95	0
15	u2	93/155 (60%)	-0.17	1 (1%) 78 72	44, 58, 71, 86	0
16	V1	129/155 (83%)	0.15	1 (0%) 82 77	47, 62, 87, 93	0
16	V2	129/155 (83%)	0.89	14 (10%) 10 8	75, 96, 114, 127	0
16	v1	129/155 (83%)	0.37	5 (3%) 43 36	47, 69, 108, 124	0
16	v2	129/155 (83%)	0.08	4 (3%) 51 44	47, 63, 90, 105	0
17	Y1	27/35 (77%)	0.18	0 100 100	64, 74, 103, 118	0
17	Y2	25/35 (71%)	1.00	1 (4%) 42 36	96, 100, 107, 109	0
17	y1	27/35 (77%)	0.64	1 (3%) 45 38	64, 71, 105, 107	0
17	y2	27/35 (77%)	0.52	0 100 100	72, 79, 92, 106	0
18	X1	29/40 (72%)	1.32	5 (17%) 4 3	98, 113, 130, 135	0
18	X2	31/40 (77%)	1.42	6 (19%) 3 2	83, 101, 114, 121	0
18	x1	36/40 (90%)	0.90	6 (16%) 4 3	61, 83, 96, 102	0
18	x2	32/40 (80%)	0.96	5 (15%) 5 4	83, 104, 122, 126	0
19	S1	25/46 (54%)	0.63	1 (4%) 42 36	72, 79, 85, 98	0
19	S2	30/46 (65%)	1.39	7 (23%) 2 1	98, 114, 120, 122	0
19	s1	40/46 (86%)	0.75	2 (5%) 34 28	54, 78, 94, 95	0
19	s2	46/46 (100%)	0.95	5 (10%) 10 8	75, 90, 106, 112	0
20	W1	21/25 (84%)	0.64	1 (4%) 35 30	71, 79, 86, 90	0
20	W2	21/25 (84%)	0.52	0 100 100	66, 76, 84, 89	0
20	w1	25/25 (100%)	0.85	3 (12%) 9 7	73, 79, 96, 101	0
20	w2	20/25 (80%)	0.88	3 (15%) 5 4	91, 96, 103, 111	0
21	Q2	111/218 (50%)	1.29	24 (21%) 2 2	122, 132, 145, 151	0
21	q1	105/218 (48%)	1.08	18 (17%) 4 3	103, 125, 138, 144	0
22	Z2	59/62 (95%)	1.22	13 (22%) 2 2	108, 121, 134, 140	0
22	z2	59/62 (95%)	0.87	4 (6%) 23 18	83, 101, 116, 127	0
All	All	10516/12316 (85%)	0.21	387 (3%) 45 38	31, 66, 113, 159	4 (0%)

All (387) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C2	392	ALA	8.1
13	o2	195	GLY	7.6
13	o1	195	GLY	6.6
18	X2	17	ALA	6.2
13	O1	195	GLY	6.0
3	C2	434	GLY	5.9
13	O2	195	GLY	5.6
21	q1	147	GLY	4.9
5	E2	23	HIS	4.9
18	x1	26	THR	4.7
13	o2	200	ALA	4.7
20	w1	2	ALA	4.6
13	o1	216	VAL	4.5
3	C2	247	GLY	4.5
4	D2	324	GLY	4.4
13	o1	201	VAL	4.4
13	O2	240	TYR	4.3
1	a1	344	ALA	4.2
5	E2	22	ILE	4.2
13	o1	200	ALA	4.2
18	X2	13	SER	4.2
3	C2	232	ASP	4.1
9	J2	35	GLY	4.1
6	F2	16	PHE	4.0
19	s2	5	ALA	4.0
2	b2	408	ASN	4.0
3	C2	254	THR	4.0
13	O2	200	ALA	4.0
3	c2	194	GLY	4.0
13	o2	201	VAL	4.0
21	Q2	146	VAL	4.0
13	O1	200	ALA	3.9
13	O1	214	VAL	3.8
22	z2	42	THR	3.8
6	F2	15	ILE	3.8
15	U2	76	LYS	3.8
21	Q2	154	SER	3.8
13	O2	178(D)	ALA	3.8
13	o2	214	VAL	3.7
21	Q2	170	GLN	3.7
13	o2	213	GLY	3.7
21	Q2	214	SER	3.7
3	C2	273	SER	3.7

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Mol	Chain	Res	Type	RSRZ
5	e1	23	HIS	3.7
21	Q2	148	THR	3.6
19	S2	8	LEU	3.6
21	q1	152	VAL	3.6
13	O2	238	VAL	3.5
22	Z2	56	VAL	3.5
19	s1	7	ALA	3.5
20	w1	1	ALA	3.5
3	C2	407	VAL	3.5
20	w2	5	ALA	3.4
13	O1	216	VAL	3.4
21	q1	214	SER	3.4
3	C2	159	THR	3.4
13	O1	201	VAL	3.4
18	X2	19	VAL	3.4
4	d2	66	SER	3.3
15	U2	78	TYR	3.3
18	x1	20	LEU	3.3
2	B1	339	ALA	3.3
1	A2	170	ASP	3.3
13	O2	209	ASN	3.3
13	O2	239	PHE	3.3
3	C1	208	ILE	3.3
5	e2	20	TRP	3.3
13	O2	218	GLU	3.2
16	v1	39	SER	3.2
16	V2	98	SER	3.2
18	x1	30	ILE	3.2
4	D2	176	ALA	3.2
16	V2	127	ALA	3.2
16	V2	78	ASN	3.1
3	C2	141	GLU	3.1
2	b2	197	GLY	3.1
1	A1	12	SER	3.1
21	Q2	110	ASN	3.1
2	b2	431	GLU	3.1
3	c2	209	ILE	3.1
13	O2	241	ALA	3.1
5	E1	19	TYR	3.1
16	V2	75	TYR	3.1
10	k2	44	GLY	3.1
21	Q2	217	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
7	H1	22	ALA	3.0
16	V1	40	CYS	3.0
21	Q2	149	LEU	3.0
5	e2	19	TYR	3.0
3	C2	128	GLY	3.0
5	E1	41	GLY	3.0
21	q1	148	THR	3.0
3	C2	161	LEU	3.0
16	V2	40	CYS	3.0
3	c1	145	SER	2.9
2	B1	408	ASN	2.9
13	O1	220	LEU	2.9
13	o2	220	LEU	2.9
5	e2	77	ASP	2.9
2	B2	339	ALA	2.9
21	Q2	160	ALA	2.9
21	q1	144	LEU	2.9
22	Z2	33	TRP	2.9
1	A1	253	GLY	2.9
2	B1	201	HIS	2.9
3	C2	122	SER	2.9
22	z2	34	SER	2.9
13	O2	42	ASP	2.9
19	S2	14	ALA	2.9
18	X2	21	VAL	2.9
2	b2	186	GLY	2.8
21	q1	129	ALA	2.8
21	q1	145	ALA	2.8
16	v1	97	SER	2.8
6	F2	35	GLY	2.8
19	S1	8	LEU	2.8
4	d1	177	ALA	2.8
13	o1	178(E)	VAL	2.8
13	o2	178(E)	VAL	2.8
21	q1	141	ALA	2.8
3	C1	145	SER	2.8
19	s2	37	ALA	2.8
16	v2	98	SER	2.7
21	q1	201	LEU	2.7
21	Q2	151	SER	2.7
2	B1	431	GLU	2.7
3	C2	335	THR	2.7

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Mol	Chain	Res	Type	RSRZ
19	S2	21	ALA	2.7
3	C2	160	ILE	2.7
13	O2	85	LEU	2.7
3	C2	129	GLY	2.7
18	X1	27	GLY	2.7
13	o2	218	GLU	2.7
4	D1	177	ALA	2.7
19	s2	4	ALA	2.7
22	Z2	4	ILE	2.7
3	C2	222	GLY	2.7
21	q1	217	GLY	2.7
18	x2	32	VAL	2.7
20	W1	23	ALA	2.7
22	Z2	60	PHE	2.7
18	X1	12	TRP	2.7
18	x2	33	SER	2.7
22	Z2	16	SER	2.7
9	J2	23	THR	2.7
10	K2	36	ALA	2.7
13	O2	142	LEU	2.6
2	B1	86	SER	2.6
20	w2	6	VAL	2.6
13	O2	140	THR	2.6
22	Z2	20	ILE	2.6
13	O2	220	LEU	2.6
13	O2	198	GLU	2.6
15	U2	77	LYS	2.6
9	J2	13	VAL	2.6
18	x1	21	VAL	2.6
19	s1	17	ALA	2.6
21	q1	158	SER	2.6
3	C2	196	ILE	2.6
21	q1	182	ARG	2.6
15	u1	69	GLU	2.6
2	B1	154	GLY	2.6
13	o2	216	VAL	2.6
6	F2	32	PHE	2.6
21	Q2	191	ARG	2.6
3	C2	347	GLY	2.6
22	Z2	55	GLY	2.6
4	D1	331	ALA	2.6
13	o2	132	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
18	X2	18	ALA	2.6
19	S2	25	ALA	2.6
16	V2	39	SER	2.5
2	b2	166	ILE	2.5
3	C2	194	GLY	2.5
2	b2	144	VAL	2.5
18	X1	21	VAL	2.5
13	O2	71	MET	2.5
3	C2	378	ASN	2.5
6	f2	17	THR	2.5
16	V2	38	SER	2.5
6	F2	20	TRP	2.5
3	C2	261	ARG	2.5
3	c2	245	VAL	2.5
10	k2	43	VAL	2.5
2	b2	128	THR	2.5
5	E2	24	SER	2.5
7	h2	60	ILE	2.5
22	Z2	44	SER	2.5
3	C2	352	GLY	2.5
13	O2	144	GLY	2.5
13	O2	126	VAL	2.5
2	b2	156	PHE	2.5
13	o1	178(D)	ALA	2.5
19	s2	34	PHE	2.5
13	o1	196	ARG	2.4
21	Q2	150	ARG	2.4
3	C2	209	ILE	2.4
1	A2	97	TRP	2.4
6	f1	35	GLY	2.4
12	m2	14	GLY	2.4
13	o1	213	GLY	2.4
16	V2	17	GLY	2.4
3	C2	55	ALA	2.4
13	O2	51	LEU	2.4
16	V2	32	LEU	2.4
16	v1	98	SER	2.4
16	v2	38	SER	2.4
10	K1	44	GLY	2.4
2	B2	284	ILE	2.4
3	C1	213	LEU	2.4
13	o1	220	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
19	S2	6	LEU	2.4
1	A2	319	ASP	2.4
21	Q2	124	GLU	2.4
2	B2	403	GLY	2.4
12	m1	14	GLY	2.4
9	J2	14	VAL	2.4
13	O2	216	VAL	2.4
21	q1	200	ARG	2.4
1	a2	228	THR	2.4
4	D2	102	THR	2.4
22	z2	40	ILE	2.4
3	C2	67	MET	2.4
7	h2	26	GLY	2.4
21	q1	143	ARG	2.4
21	q1	160	ALA	2.4
15	u2	80	ASP	2.3
22	Z2	59	SER	2.3
16	v1	43	GLY	2.3
2	b2	184	ALA	2.3
16	V2	61	LEU	2.3
19	S2	15	LEU	2.3
21	Q2	141	ALA	2.3
22	Z2	39	SER	2.3
3	C2	319	VAL	2.3
6	f2	31	VAL	2.3
3	C2	49	LEU	2.3
3	C2	39	ASN	2.3
13	O2	202	ASN	2.3
4	D2	92	LEU	2.3
10	K2	18	PHE	2.3
5	E1	25	ILE	2.3
2	B2	416	THR	2.3
13	O2	77	THR	2.3
13	o1	218	GLU	2.3
21	q1	168	GLU	2.3
4	D2	172	SER	2.3
13	o1	99	ASP	2.3
20	w2	3	TRP	2.3
3	C2	233	VAL	2.3
18	X1	32	VAL	2.3
6	F2	36	ALA	2.2
8	I2	11	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
13	O2	197	ILE	2.2
17	y1	31	THR	2.2
5	E2	18	ARG	2.2
13	o2	196	ARG	2.2
13	o2	0	GLN	2.2
22	z2	38	SER	2.2
3	C1	338	GLY	2.2
3	c1	193	GLY	2.2
1	A2	105	TRP	2.2
2	b1	161	LEU	2.2
3	C2	61	VAL	2.2
10	K2	34	LEU	2.2
21	Q2	144	LEU	2.2
22	Z2	51	VAL	2.2
3	C2	208	ILE	2.2
3	C2	260	ALA	2.2
3	C2	263	ALA	2.2
18	X1	22	ILE	2.2
3	c2	141	GLU	2.2
13	O2	-2	THR	2.2
2	B2	194	ASN	2.2
9	J2	9	PRO	2.2
1	A2	256	GLY	2.2
13	o1	214	VAL	2.2
5	E2	27	ILE	2.2
16	v2	41	HIS	2.2
3	c2	159	THR	2.2
3	C2	248	GLY	2.2
5	E1	24	SER	2.2
18	x1	23	LEU	2.2
5	E2	25	ILE	2.2
20	w1	3	TRP	2.2
4	d1	176	ALA	2.2
13	O1	178(D)	ALA	2.2
10	K2	14	THR	2.2
16	V2	46	THR	2.2
5	E2	28	PRO	2.2
5	E2	59	ASN	2.2
16	v1	15	ASN	2.2
18	x2	20	LEU	2.2
5	E1	21	VAL	2.2
5	E2	21	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
13	O2	194	SER	2.2
13	O2	201	VAL	2.2
4	d2	331	ALA	2.1
19	s2	3	ALA	2.1
13	o1	-2	THR	2.1
16	V2	126	GLN	2.1
10	K2	33	LEU	2.1
3	C1	129	GLY	2.1
3	C2	126	GLY	2.1
5	e1	45	ASP	2.1
13	O2	214	VAL	2.1
18	x1	32	VAL	2.1
21	Q2	156	VAL	2.1
10	K2	32	PHE	2.1
21	Q2	189	ALA	2.1
1	A1	6	GLU	2.1
7	h2	9	GLU	2.1
18	x2	4	THR	2.1
13	O2	44	CYS	2.1
3	C1	39	ASN	2.1
3	C2	294	ASN	2.1
3	C1	96	GLY	2.1
3	c2	142	ASP	2.1
18	x2	21	VAL	2.1
2	b2	200	SER	2.1
3	C2	301	PHE	2.1
16	v2	39	SER	2.1
1	A2	54	ALA	2.1
6	F2	39	ALA	2.1
14	T1	30	ALA	2.1
21	Q2	204	ALA	2.1
21	q1	122	ARG	2.1
15	U2	44	THR	2.1
3	c2	107	ASN	2.1
21	Q2	211	ASN	2.1
2	B2	186	GLY	2.1
3	c1	65	GLY	2.1
13	O2	237	GLY	2.1
15	U2	35	TYR	2.1
1	A2	306	ILE	2.1
2	b2	181	VAL	2.1
14	T2	15	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
21	Q2	104	ILE	2.1
5	E1	78	ASP	2.1
2	b2	205	ALA	2.1
2	b2	301	ALA	2.1
3	C2	37	SER	2.1
7	h2	2	ALA	2.1
21	Q2	175	ALA	2.1
3	C2	243	THR	2.1
7	h2	40	LEU	2.1
9	J2	12	LEU	2.1
2	B2	218	ASN	2.1
4	D2	108	GLY	2.1
9	J1	17	GLY	2.1
16	V2	41	HIS	2.1
2	B2	273	TYR	2.1
5	E2	19	TYR	2.1
21	q1	172	ILE	2.1
13	O1	178(E)	VAL	2.1
1	a1	16	ARG	2.0
2	b2	300	GLU	2.0
3	C2	113	ALA	2.0
7	H1	61	SER	2.0
18	X2	6	SER	2.0
21	Q2	158	SER	2.0
13	o1	48	LYS	2.0
6	F1	20	TRP	2.0
3	C1	159	THR	2.0
1	A2	300	LEU	2.0
3	c1	222	GLY	2.0
3	C2	166	ILE	2.0
7	h2	24	GLY	2.0
9	J2	31	GLY	2.0
17	Y2	32	GLY	2.0
22	Z2	45	ILE	2.0
5	E2	46	VAL	2.0
13	O1	181	VAL	2.0
13	o2	181	VAL	2.0
13	O2	196	ARG	2.0
21	Q2	197	ARG	2.0
13	o1	205	ASP	2.0
16	V2	55	ASP	2.0
19	S2	32	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
21	Q2	198	ALA	2.0
5	e2	24	SER	2.0
3	C2	298	PRO	2.0
5	E1	23	HIS	2.0
9	j2	8	ILE	2.0
13	O1	197	ILE	2.0
22	Z2	14	VAL	2.0
3	C2	109	TYR	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
28	UNL	I2	102	17/-	0.49	0.11	80,92,102,103	0
28	UNL	k2	505	6/-	0.51	0.10	70,80,84,87	0
28	UNL	I2	103	14/-	0.55	0.10	62,93,102,104	0
32	GOL	a1	406	6/6	0.55	0.11	68,75,86,90	0
28	UNL	a2	409	18/-	0.57	0.10	61,74,86,90	0
28	UNL	C2	501	6/-	0.57	0.10	72,74,78,87	0
28	UNL	J2	101	10/-	0.57	0.12	71,82,86,88	0
28	UNL	b1	623	11/-	0.58	0.12	59,74,83,84	0
23	BCR	K1	101	31/40	0.59	0.12	64,82,93,96	0
28	UNL	D1	410	6/-	0.59	0.14	59,62,66,66	0
28	UNL	F2	403	16/-	0.59	0.15	51,76,86,89	0
28	UNL	A2	409	10/-	0.60	0.14	72,82,85,87	0
28	UNL	c2	520	15/-	0.60	0.12	86,97,106,108	0
28	UNL	B1	624	18/-	0.61	0.10	43,71,79,81	0
28	UNL	H2	102	5/-	0.62	0.14	72,81,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	UNL	K2	103	5/-	0.63	0.16	79,83,88,90	0
25	CLA	b2	604	42/65	0.63	0.13	82,109,116,127	0
25	CLA	C2	518	41/65	0.63	0.12	105,121,127,134	0
28	UNL	d2	410	13/-	0.63	0.12	74,92,108,111	0
28	UNL	C2	517	18/-	0.63	0.13	74,83,87,89	0
28	UNL	b1	629	15/-	0.63	0.10	46,59,71,83	0
28	UNL	m2	102	18/-	0.64	0.09	46,65,79,79	0
29	LMG	C2	515	24/55	0.64	0.10	82,97,104,105	0
28	UNL	k2	502	9/-	0.64	0.09	72,78,84,86	0
28	UNL	d1	410	12/-	0.65	0.13	49,72,77,79	0
28	UNL	X2	101	7/-	0.65	0.24	83,85,91,93	0
28	UNL	B2	626	15/-	0.66	0.10	79,83,92,95	0
29	LMG	I2	101	34/55	0.66	0.13	82,103,109,114	0
25	CLA	C2	510	45/65	0.66	0.14	107,116,121,126	0
33	LHG	B2	627	42/49	0.66	0.10	67,88,120,132	0
35	LMT	m2	104	29/35	0.66	0.12	49,104,119,122	0
23	BCR	K2	102	40/40	0.67	0.13	84,99,113,115	0
33	LHG	b2	625	43/49	0.68	0.10	62,87,109,126	0
32	GOL	C1	518	6/6	0.68	0.11	65,73,77,81	0
39	CA	o2	401	1/1	0.68	0.18	101,101,101,101	0
32	GOL	B1	620	6/6	0.69	0.10	63,75,81,82	0
28	UNL	t1	101	18/-	0.69	0.10	43,60,66,67	0
35	LMT	b2	621	35/35	0.69	0.11	69,110,123,123	0
28	UNL	B1	623	16/-	0.69	0.09	53,68,72,74	0
33	LHG	d1	402	32/49	0.69	0.14	45,63,76,86	0
29	LMG	j2	101	50/55	0.70	0.12	60,78,97,107	0
29	LMG	F2	402	35/55	0.70	0.11	68,81,91,92	0
28	UNL	j1	101	17/-	0.70	0.11	60,69,71,77	0
33	LHG	a2	407	30/49	0.70	0.13	55,75,94,102	0
28	UNL	a2	401	18/-	0.71	0.11	46,56,70,86	0
24	CL	A2	410	1/1	0.71	0.09	87,87,87,87	0
28	UNL	a2	410	8/-	0.71	0.10	61,68,70,76	0
28	UNL	b2	607	12/-	0.71	0.12	64,75,80,87	0
25	CLA	C2	503	65/65	0.71	0.12	94,104,112,116	0
25	CLA	D2	404	61/65	0.71	0.11	67,87,113,120	0
25	CLA	K2	101	55/65	0.71	0.10	86,98,104,109	0
28	UNL	k2	504	9/-	0.71	0.09	66,74,80,88	0
28	UNL	i2	101	14/-	0.72	0.07	62,66,73,75	0
28	UNL	M2	101	11/-	0.72	0.07	59,68,73,74	0
35	LMT	c1	517	33/35	0.72	0.12	63,100,117,119	0
25	CLA	c2	513	54/65	0.73	0.10	75,94,102,105	0
23	BCR	c2	501	40/40	0.73	0.13	66,82,89,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	UNL	b1	626	13/-	0.73	0.08	53,64,83,86	0
32	GOL	C2	514	6/6	0.73	0.09	87,93,100,101	0
35	LMT	m2	103	30/35	0.73	0.14	52,89,111,113	0
23	BCR	K2	104	29/40	0.73	0.10	92,100,109,112	0
28	UNL	b1	630	17/-	0.73	0.09	48,57,74,75	0
29	LMG	d1	411	35/55	0.74	0.11	58,76,94,99	0
23	BCR	z2	101	40/40	0.74	0.12	80,95,100,101	0
28	UNL	m2	101	18/-	0.74	0.09	44,57,79,85	0
28	UNL	B2	625	18/-	0.74	0.09	37,56,68,68	0
29	LMG	A1	412	41/55	0.74	0.11	50,75,96,100	0
29	LMG	b1	621	38/55	0.74	0.10	52,63,76,82	0
23	BCR	F2	401	40/40	0.75	0.11	67,81,107,113	0
29	LMG	B2	621	37/55	0.75	0.10	53,68,80,96	0
25	CLA	C2	505	65/65	0.75	0.12	78,100,112,118	0
28	UNL	A2	408	18/-	0.75	0.10	62,83,92,93	0
23	BCR	B1	602	40/40	0.75	0.11	49,62,74,78	0
33	LHG	A2	405	33/49	0.75	0.10	70,80,90,97	0
23	BCR	C2	502	40/40	0.75	0.13	95,106,118,120	0
28	UNL	k2	503	6/-	0.76	0.09	67,76,79,80	0
23	BCR	J1	101	40/40	0.76	0.10	50,70,86,88	0
35	LMT	i2	102	7/35	0.76	0.08	68,71,76,79	0
29	LMG	A2	412	29/55	0.76	0.10	86,94,100,102	0
32	GOL	b1	618	6/6	0.76	0.08	60,69,80,80	0
25	CLA	C2	509	65/65	0.76	0.12	90,101,106,108	0
35	LMT	C1	519	35/35	0.77	0.10	57,76,85,93	0
35	LMT	M1	103	24/35	0.77	0.10	42,68,97,101	0
35	LMT	T1	101	12/35	0.77	0.10	46,51,54,56	0
25	CLA	C2	511	50/65	0.77	0.11	85,93,100,104	0
23	BCR	k1	101	40/40	0.77	0.11	56,70,82,85	0
25	CLA	B1	604	42/65	0.77	0.11	83,98,107,113	0
28	UNL	B2	622	17/-	0.77	0.09	57,71,76,78	0
25	CLA	C1	512	65/65	0.77	0.10	63,82,102,121	0
25	CLA	c1	516	65/65	0.77	0.11	66,82,104,109	0
35	LMT	a2	406	35/35	0.78	0.11	43,80,92,94	0
28	UNL	b1	627	16/-	0.78	0.09	42,56,75,77	0
25	CLA	B1	611	62/65	0.78	0.10	58,78,87,89	0
25	CLA	c1	515	55/65	0.78	0.10	69,82,90,94	0
29	LMG	b1	624	39/55	0.78	0.12	58,73,84,87	0
37	SQD	D1	409	35/54	0.78	0.11	61,75,92,97	0
28	UNL	W2	101	9/-	0.78	0.08	64,77,83,87	0
25	CLA	C2	504	46/65	0.79	0.11	72,88,95,96	0
25	CLA	C1	513	61/65	0.79	0.10	49,68,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	UNL	a2	411	11/-	0.79	0.07	51,55,65,67	0
25	CLA	C2	507	45/65	0.79	0.11	73,93,102,113	0
23	BCR	b2	603	40/40	0.80	0.10	60,74,102,104	0
23	BCR	H2	103	24/40	0.80	0.12	65,76,82,85	0
23	BCR	j2	102	40/40	0.80	0.11	59,75,86,87	0
25	CLA	c2	515	46/65	0.80	0.11	81,100,104,109	0
29	LMG	C1	520	48/55	0.80	0.08	59,69,78,86	0
29	LMG	a1	412	51/55	0.80	0.10	54,67,77,91	0
25	CLA	C2	513	53/65	0.80	0.11	78,91,106,110	0
23	BCR	H1	102	22/40	0.80	0.12	75,88,95,100	0
23	BCR	D1	401	40/40	0.80	0.10	54,67,89,95	0
23	BCR	b2	602	40/40	0.81	0.10	51,70,78,82	0
25	CLA	C2	506	65/65	0.81	0.10	78,90,97,100	0
23	BCR	b1	602	40/40	0.81	0.10	35,57,65,73	0
25	CLA	C2	508	50/65	0.81	0.13	87,103,112,115	0
34	DGD	H2	101	62/66	0.81	0.09	51,74,83,85	0
25	CLA	C2	516	46/65	0.81	0.10	70,92,97,100	0
28	UNL	d2	411	12/-	0.81	0.08	55,67,73,79	0
39	CA	O1	401	1/1	0.81	0.06	82,82,82,82	0
29	LMG	b2	622	39/55	0.81	0.10	47,60,85,90	0
32	GOL	c2	518	6/6	0.82	0.11	50,55,59,64	0
25	CLA	d2	404	50/65	0.82	0.10	57,74,83,88	0
35	LMT	m1	101	35/35	0.82	0.11	44,80,103,112	0
25	CLA	B2	604	41/65	0.82	0.09	68,79,92,97	0
28	UNL	x1	101	15/-	0.82	0.09	55,73,79,82	0
25	CLA	c2	509	65/65	0.82	0.08	54,70,82,85	0
23	BCR	C1	521	40/40	0.82	0.10	59,68,80,84	0
34	DGD	C2	512	33/66	0.82	0.10	63,77,83,93	0
29	LMG	B1	622	31/55	0.82	0.11	66,74,81,83	0
37	SQD	B2	623	45/54	0.82	0.10	58,79,89,96	0
37	SQD	b2	605	45/54	0.82	0.08	54,83,114,124	0
29	LMG	B1	626	48/55	0.82	0.09	55,70,89,94	0
25	CLA	C1	514	45/65	0.82	0.10	73,84,92,96	0
23	BCR	B2	602	40/40	0.83	0.10	47,59,80,86	0
29	LMG	B2	620	40/55	0.83	0.09	62,74,97,98	0
25	CLA	c1	503	65/65	0.83	0.10	55,66,71,75	0
25	CLA	C1	502	65/65	0.83	0.09	51,63,68,70	0
35	LMT	b2	623	35/35	0.83	0.08	63,90,98,101	0
28	UNL	B1	625	7/-	0.83	0.08	45,52,55,63	0
25	CLA	b2	618	65/65	0.83	0.10	68,82,90,92	0
23	BCR	h2	101	40/40	0.83	0.10	71,85,107,109	0
28	UNL	b1	625	10/-	0.83	0.10	50,62,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	BCR	c1	502	40/40	0.83	0.10	57,66,72,72	0
29	LMG	b1	631	40/55	0.83	0.10	29,52,85,92	0
38	HEM	E1	101	43/43	0.83	0.13	108,134,152,155	0
29	LMG	c1	519	55/55	0.83	0.08	47,70,84,91	0
25	CLA	B2	611	65/65	0.83	0.10	51,73,81,86	0
28	UNL	a1	409	11/-	0.84	0.06	43,51,60,63	0
25	CLA	c2	512	65/65	0.84	0.09	61,76,86,93	0
23	BCR	d2	401	40/40	0.84	0.09	48,67,81,85	0
25	CLA	B2	606	65/65	0.84	0.09	53,67,75,78	0
23	BCR	k2	501	40/40	0.84	0.09	61,84,95,98	0
25	CLA	b2	610	65/65	0.84	0.09	60,82,90,92	0
25	CLA	b1	604	65/65	0.84	0.10	52,78,110,115	0
37	SQD	D2	402	25/54	0.84	0.09	85,90,96,98	0
25	CLA	c2	502	65/65	0.84	0.09	60,78,85,90	0
35	LMT	l1	101	24/35	0.84	0.08	42,55,89,90	0
38	HEM	V2	201	43/43	0.84	0.12	83,98,102,107	0
38	HEM	e2	101	43/43	0.84	0.11	126,145,163,171	0
25	CLA	A2	403	61/65	0.84	0.11	80,89,98,102	0
28	UNL	m1	102	6/-	0.84	0.08	54,55,63,66	0
29	LMG	a2	412	44/55	0.85	0.09	55,70,78,93	0
25	CLA	b2	609	61/65	0.85	0.10	77,89,95,100	0
25	CLA	A2	404	51/65	0.85	0.08	47,58,70,73	0
25	CLA	C1	509	65/65	0.85	0.09	48,59,71,80	0
28	UNL	B2	624	8/-	0.85	0.07	46,51,54,55	0
25	CLA	b2	619	59/65	0.85	0.10	71,80,106,109	0
23	BCR	c1	501	40/40	0.85	0.08	56,66,79,82	0
32	GOL	i1	101	6/6	0.85	0.12	55,57,60,64	0
25	CLA	c2	506	61/65	0.85	0.10	55,70,77,83	0
32	GOL	a2	415	6/6	0.85	0.14	47,55,59,63	0
25	CLA	c2	508	65/65	0.85	0.10	68,78,84,88	0
28	UNL	b1	628	10/-	0.85	0.08	51,57,61,67	0
25	CLA	B2	610	65/65	0.85	0.09	44,59,82,86	0
25	CLA	c1	508	50/65	0.85	0.10	57,66,77,81	0
25	CLA	c1	510	65/65	0.85	0.08	41,54,62,72	0
25	CLA	c1	513	60/65	0.85	0.07	49,59,71,72	0
34	DGD	c1	520	62/66	0.85	0.09	36,59,73,87	0
25	CLA	B1	609	65/65	0.85	0.10	54,71,81,90	0
25	CLA	C1	506	65/65	0.85	0.09	49,62,70,73	0
25	CLA	D1	403	51/65	0.85	0.09	64,74,88,90	0
34	DGD	c2	517	62/66	0.86	0.08	45,57,70,75	0
25	CLA	c1	509	65/65	0.86	0.10	51,62,68,72	0
29	LMG	A1	410	43/55	0.86	0.08	52,59,65,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	a2	405	65/65	0.86	0.09	51,60,81,87	0
25	CLA	c1	505	65/65	0.86	0.09	47,70,79,88	0
28	UNL	t1	102	9/-	0.86	0.08	45,57,68,69	0
34	DGD	C1	517	64/66	0.86	0.08	38,55,75,92	0
38	HEM	E2	101	43/43	0.86	0.13	116,132,146,152	0
25	CLA	B1	606	65/65	0.86	0.10	60,71,77,82	0
29	LMG	d2	407	27/55	0.86	0.09	49,60,64,70	0
25	CLA	c2	504	65/65	0.86	0.10	46,78,92,100	0
34	DGD	c2	516	52/66	0.86	0.10	37,63,71,75	0
23	BCR	b2	601	40/40	0.87	0.09	51,61,69,72	0
34	DGD	c1	514	51/66	0.87	0.09	46,54,62,64	0
25	CLA	b1	609	65/65	0.87	0.10	42,58,84,104	0
25	CLA	b2	624	65/65	0.87	0.08	47,60,75,82	0
25	CLA	b1	619	65/65	0.87	0.10	48,62,81,85	0
27	PHO	D2	407	64/64	0.87	0.08	58,68,81,83	0
25	CLA	b2	606	65/65	0.87	0.11	68,77,84,90	0
25	CLA	C1	511	65/65	0.87	0.10	45,56,62,68	0
35	LMT	L1	102	12/35	0.87	0.07	35,45,59,62	0
29	LMG	M1	101	31/55	0.87	0.09	41,52,63,70	0
25	CLA	c2	507	54/65	0.87	0.10	76,81,86,92	0
25	CLA	B1	618	58/65	0.87	0.10	53,64,80,86	0
29	LMG	c2	519	26/55	0.87	0.07	58,67,73,74	0
28	UNL	l1	103	12/-	0.87	0.08	35,47,53,55	0
25	CLA	b2	613	65/65	0.87	0.10	59,84,96,99	0
25	CLA	c1	507	65/65	0.88	0.09	49,62,72,80	0
23	BCR	B2	603	40/40	0.88	0.08	46,59,76,81	0
25	CLA	B2	612	65/65	0.88	0.10	58,64,71,83	0
25	CLA	c2	511	65/65	0.88	0.10	54,65,72,75	0
25	CLA	B2	619	65/65	0.88	0.07	46,55,63,71	0
25	CLA	B1	605	65/65	0.88	0.09	60,75,87,88	0
25	CLA	C1	505	65/65	0.88	0.08	43,55,64,68	0
34	DGD	C1	515	52/66	0.88	0.09	36,58,67,71	0
25	CLA	c1	512	65/65	0.88	0.10	36,50,57,60	0
36	PL9	D2	408	55/55	0.88	0.09	43,59,64,74	0
27	PHO	D1	407	63/64	0.88	0.08	40,56,63,67	0
23	BCR	C1	501	40/40	0.88	0.08	47,61,72,75	0
25	CLA	C1	507	65/65	0.88	0.09	46,67,86,105	0
25	CLA	b2	616	60/65	0.88	0.09	51,64,82,82	0
25	CLA	b1	616	65/65	0.88	0.09	39,46,57,69	0
23	BCR	A2	401	40/40	0.88	0.12	58,84,90,91	0
23	BCR	d1	405	40/40	0.88	0.09	38,51,94,99	0
25	CLA	B1	617	65/65	0.88	0.08	59,67,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B2	605	65/65	0.88	0.07	63,71,77,82	0
25	CLA	c1	506	65/65	0.88	0.08	40,54,68,73	0
25	CLA	B2	614	65/65	0.89	0.08	46,58,66,68	0
25	CLA	B2	616	54/65	0.89	0.08	43,51,57,59	0
34	DGD	c1	518	62/66	0.89	0.07	41,61,69,79	0
25	CLA	B2	617	65/65	0.89	0.08	52,63,70,74	0
25	CLA	B2	618	60/65	0.89	0.08	59,65,80,85	0
36	PL9	d1	409	55/55	0.89	0.09	28,41,50,61	0
25	CLA	b2	617	65/65	0.89	0.08	47,58,65,72	0
36	PL9	d2	409	55/55	0.89	0.09	33,44,56,57	0
25	CLA	B1	610	65/65	0.89	0.09	46,58,73,76	0
25	CLA	a1	404	60/65	0.89	0.10	49,57,82,89	0
23	BCR	B1	603	40/40	0.89	0.07	45,56,78,85	0
33	LHG	D1	404	49/49	0.89	0.09	48,60,84,90	0
25	CLA	B1	607	60/65	0.89	0.09	45,56,68,72	0
28	UNL	A1	409	14/-	0.89	0.06	44,48,57,68	0
23	BCR	B1	601	40/40	0.89	0.08	41,55,65,65	0
25	CLA	c2	505	65/65	0.89	0.08	48,61,71,80	0
25	CLA	d1	406	65/65	0.89	0.08	44,58,94,99	0
25	CLA	C1	508	65/65	0.89	0.09	47,66,76,80	0
25	CLA	c2	503	65/65	0.90	0.10	53,62,83,89	0
23	BCR	B2	601	40/40	0.90	0.07	41,56,66,68	0
29	LMG	D1	406	35/55	0.90	0.08	50,57,71,74	0
33	LHG	D2	405	49/49	0.90	0.07	52,60,66,68	0
33	LHG	L2	101	49/49	0.90	0.08	42,57,70,78	0
25	CLA	B1	616	65/65	0.90	0.08	39,49,58,66	0
23	BCR	b1	603	40/40	0.90	0.08	40,58,69,77	0
33	LHG	d2	403	49/49	0.90	0.08	42,59,69,73	0
25	CLA	b2	611	65/65	0.90	0.10	66,72,80,83	0
34	DGD	C1	516	62/66	0.90	0.07	44,53,60,61	0
31	BCT	a1	413	4/4	0.90	0.07	43,48,48,50	0
34	DGD	H1	101	62/66	0.90	0.08	50,71,84,89	0
25	CLA	b2	612	65/65	0.90	0.08	39,54,64,70	0
25	CLA	A1	405	55/65	0.90	0.08	38,46,59,65	0
25	CLA	c2	510	54/65	0.90	0.10	64,69,77,79	0
25	CLA	B2	607	65/65	0.90	0.08	49,59,73,78	0
25	CLA	B2	609	65/65	0.90	0.08	51,67,76,82	0
34	DGD	c2	514	62/66	0.90	0.07	47,59,67,69	0
25	CLA	b1	611	65/65	0.90	0.08	37,59,68,73	0
25	CLA	B1	619	65/65	0.90	0.08	32,50,57,73	0
25	CLA	A2	402	65/65	0.90	0.09	47,57,69,77	0
33	LHG	B1	621	49/49	0.90	0.08	41,57,67,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b1	617	65/65	0.90	0.07	47,56,65,68	0
25	CLA	b2	614	65/65	0.91	0.08	51,66,73,75	0
25	CLA	d1	401	65/65	0.91	0.08	30,36,44,47	0
25	CLA	B2	615	65/65	0.91	0.07	44,56,73,86	0
25	CLA	d2	405	65/65	0.91	0.08	34,44,61,77	0
25	CLA	B1	615	65/65	0.91	0.08	35,47,73,80	0
33	LHG	d2	406	49/49	0.91	0.07	36,50,59,66	0
25	CLA	c1	504	65/65	0.91	0.09	36,53,83,98	0
25	CLA	b2	620	65/65	0.91	0.09	42,56,63,72	0
25	CLA	D2	401	65/65	0.91	0.08	43,53,71,76	0
23	BCR	a1	401	40/40	0.91	0.08	47,56,64,65	0
36	PL9	D1	408	55/55	0.91	0.08	28,42,52,63	0
25	CLA	D2	406	65/65	0.91	0.07	45,57,65,67	0
24	CL	a1	402	1/1	0.91	0.05	49,49,49,49	0
23	BCR	h1	102	40/40	0.91	0.08	53,60,67,69	0
25	CLA	b1	606	65/65	0.91	0.09	44,53,61,63	0
29	LMG	d1	408	33/55	0.91	0.08	41,50,61,63	0
25	CLA	A1	404	51/65	0.91	0.07	37,48,58,70	0
25	CLA	C1	510	65/65	0.91	0.09	47,59,77,82	0
25	CLA	B1	612	65/65	0.91	0.10	52,66,71,77	0
38	HEM	f1	101	43/43	0.91	0.11	62,82,124,136	0
38	HEM	v1	201	43/43	0.91	0.10	60,66,72,75	0
34	DGD	h2	102	62/66	0.91	0.08	47,67,82,96	0
25	CLA	C1	503	60/65	0.91	0.07	38,53,67,73	0
25	CLA	C1	504	65/65	0.91	0.07	49,64,74,77	0
35	LMT	M1	102	11/35	0.91	0.08	47,52,56,58	0
25	CLA	b1	620	65/65	0.91	0.08	31,43,56,60	0
33	LHG	D2	403	49/49	0.92	0.07	45,60,68,73	0
25	CLA	b2	608	65/65	0.92	0.08	65,77,85,86	0
25	CLA	d1	404	65/65	0.92	0.07	31,43,49,51	0
27	PHO	d1	403	64/64	0.92	0.07	32,41,50,54	0
27	PHO	A2	407	64/64	0.92	0.08	53,64,72,80	0
32	GOL	c1	521	6/6	0.92	0.08	54,56,60,65	0
25	CLA	b1	615	59/65	0.92	0.08	31,43,58,64	0
27	PHO	d2	408	64/64	0.92	0.08	45,56,62,64	0
25	CLA	b1	607	65/65	0.92	0.08	33,46,69,76	0
23	BCR	a2	402	40/40	0.92	0.07	33,51,62,67	0
25	CLA	b1	610	65/65	0.92	0.07	37,47,56,63	0
25	CLA	B1	613	65/65	0.92	0.08	38,49,57,64	0
33	LHG	b1	622	49/49	0.92	0.09	36,49,57,69	0
25	CLA	B2	613	65/65	0.92	0.07	41,52,68,70	0
34	DGD	h1	101	62/66	0.92	0.07	37,48,59,65	0

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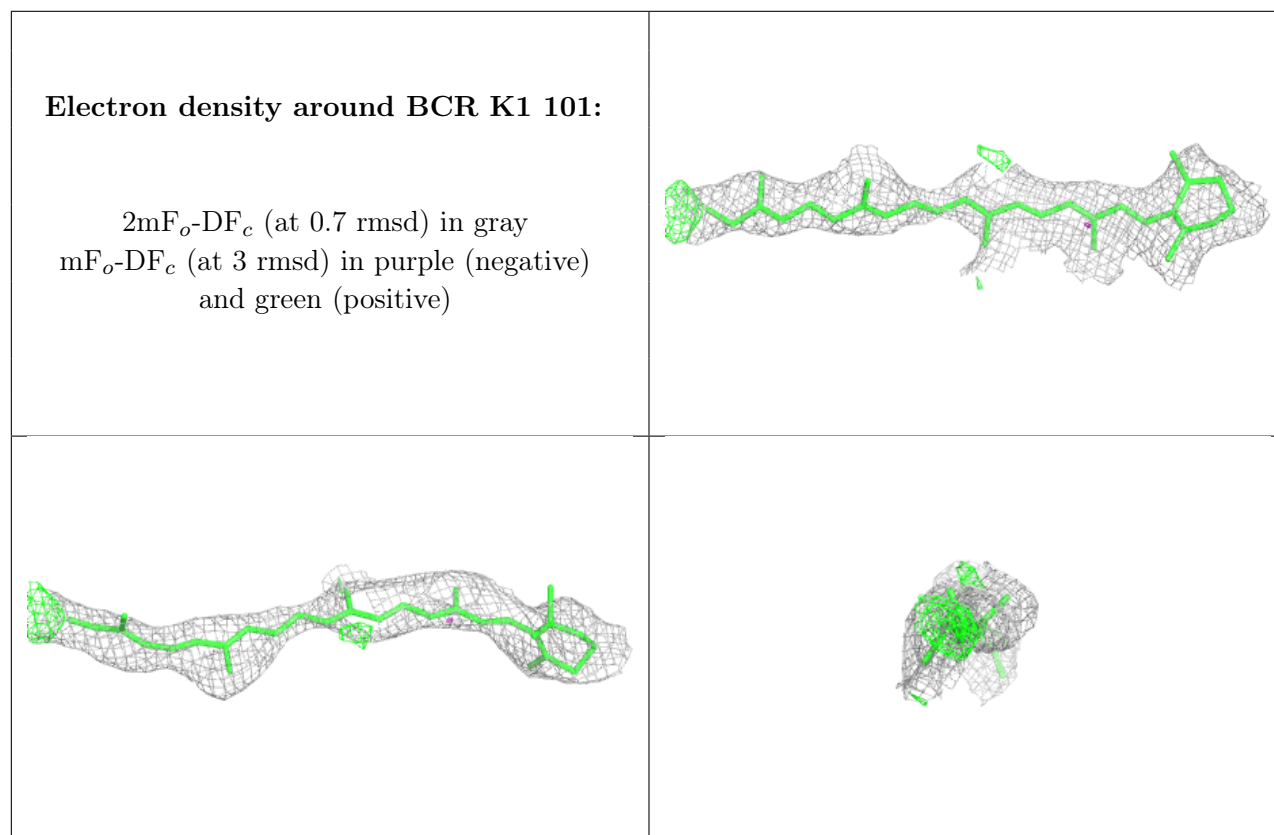
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b1	612	65/65	0.92	0.07	45,54,60,68	0
31	BCT	A2	413	4/4	0.92	0.07	65,69,71,72	0
25	CLA	c1	511	65/65	0.93	0.08	38,53,71,78	0
31	BCT	A1	413	4/4	0.93	0.06	54,60,62,63	0
33	LHG	d1	407	49/49	0.93	0.07	34,44,53,67	0
26	OEX	A2	406	10/10	0.93	0.09	68,84,93,94	0
25	CLA	a1	405	50/65	0.93	0.07	25,33,49,55	0
23	BCR	b1	601	40/40	0.93	0.07	36,47,56,57	0
25	CLA	b1	613	65/65	0.93	0.07	36,44,54,68	0
25	CLA	a2	404	65/65	0.93	0.07	30,42,52,53	0
27	PHO	a2	416	64/64	0.93	0.07	35,46,53,62	0
25	CLA	b1	605	65/65	0.93	0.07	38,52,60,66	0
25	CLA	a2	413	50/65	0.93	0.06	33,46,57,66	0
24	CL	A1	402	1/1	0.93	0.12	39,39,39,39	0
38	HEM	V1	201	43/43	0.93	0.08	35,61,66,71	0
33	LHG	l2	101	44/49	0.93	0.06	36,53,66,72	0
25	CLA	B2	608	65/65	0.93	0.07	43,53,70,76	0
25	CLA	D1	402	65/65	0.93	0.06	31,40,58,63	0
23	BCR	A1	401	40/40	0.93	0.07	36,48,54,58	0
25	CLA	B1	614	65/65	0.93	0.07	43,55,62,67	0
33	LHG	L1	101	41/49	0.93	0.06	30,46,61,85	0
33	LHG	a1	407	43/49	0.93	0.06	36,52,66,70	0
25	CLA	d2	402	65/65	0.94	0.06	24,37,48,52	0
25	CLA	b2	615	60/65	0.94	0.07	45,54,67,74	0
25	CLA	a1	403	65/65	0.94	0.07	29,37,48,51	0
25	CLA	A1	406	65/65	0.94	0.07	28,37,46,55	0
33	LHG	l1	102	49/49	0.94	0.07	25,43,67,75	0
27	PHO	A1	408	64/64	0.94	0.07	30,42,50,56	0
25	CLA	B1	608	65/65	0.94	0.07	46,58,71,81	0
27	PHO	a1	411	64/64	0.94	0.06	33,41,47,50	0
38	HEM	v2	201	43/43	0.94	0.09	47,60,66,78	0
33	LHG	D1	405	49/49	0.94	0.06	35,45,54,56	0
25	CLA	b1	614	65/65	0.94	0.08	35,45,54,56	0
25	CLA	A1	403	65/65	0.95	0.06	27,37,49,54	0
25	CLA	b1	608	65/65	0.95	0.07	37,48,58,63	0
31	BCT	a2	417	4/4	0.96	0.05	59,65,67,73	0
26	OEX	A1	407	10/10	0.97	0.08	45,49,63,68	0
30	FE	A1	411	1/1	0.97	0.02	52,52,52,52	0
30	FE	a1	410	1/1	0.98	0.07	49,49,49,49	0
30	FE	a2	414	1/1	0.98	0.03	57,57,57,57	0
26	OEX	a2	408	10/10	0.98	0.07	42,49,58,61	0
26	OEX	a1	408	10/10	0.98	0.08	39,49,62,70	0

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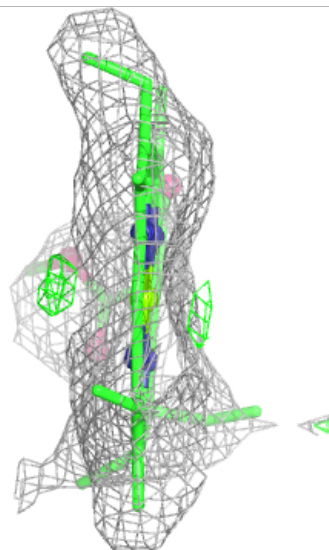
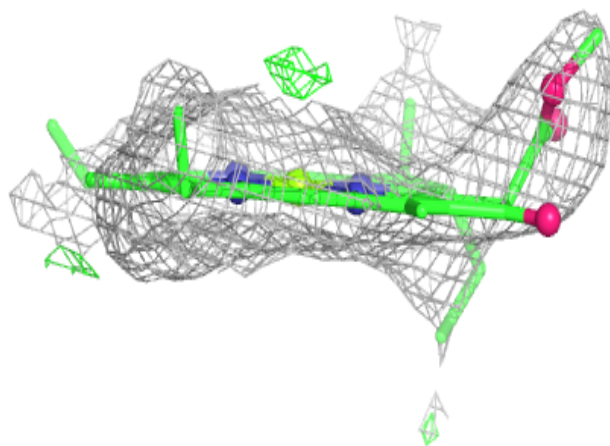
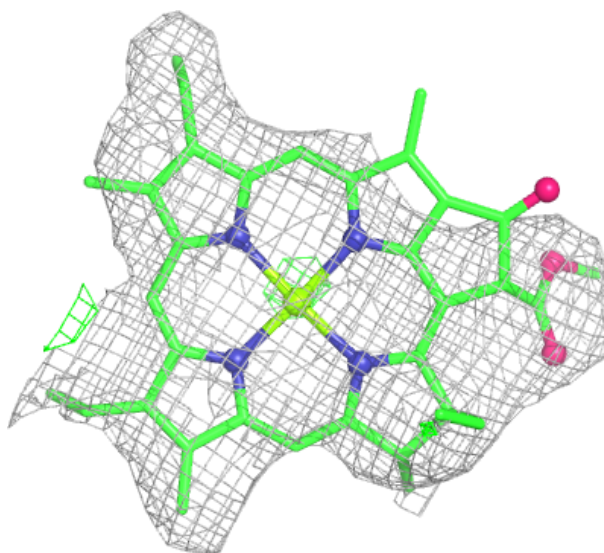
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CL	a2	403	1/1	0.98	0.03	37,37,37,37	0
30	FE	A2	411	1/1	0.99	0.04	63,63,63,63	0

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.



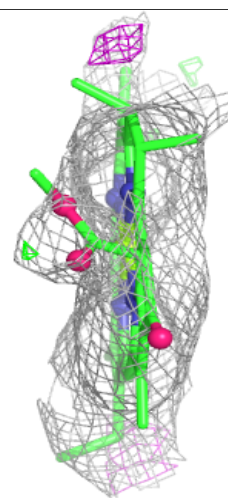
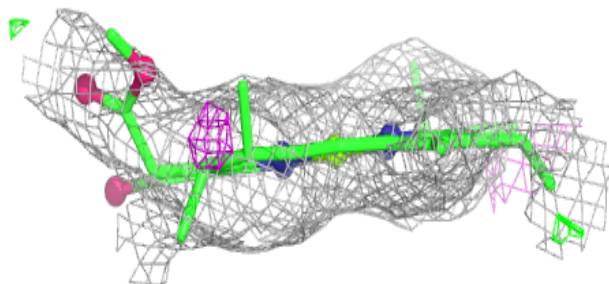
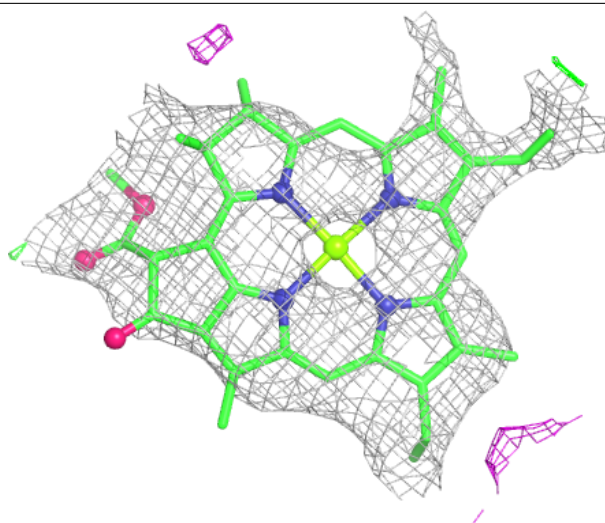
Electron density around CLA b2 604:

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



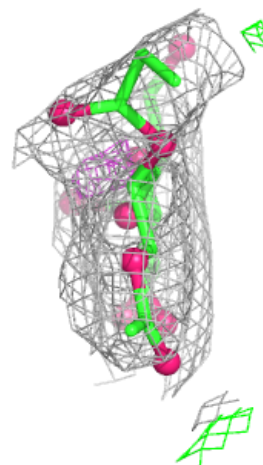
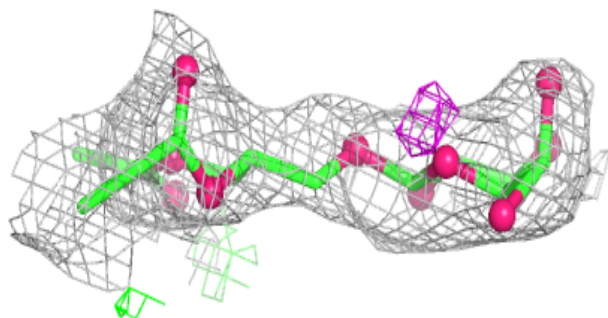
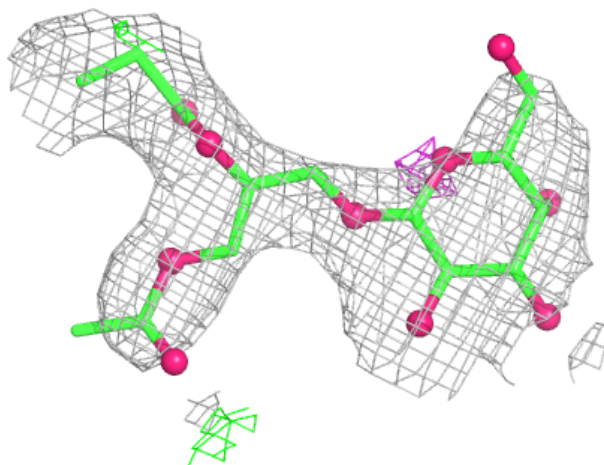
Electron density around CLA C2 518:

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



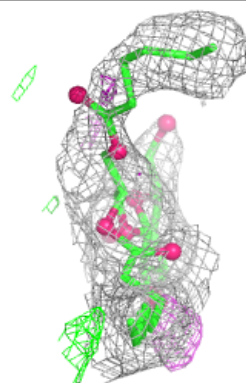
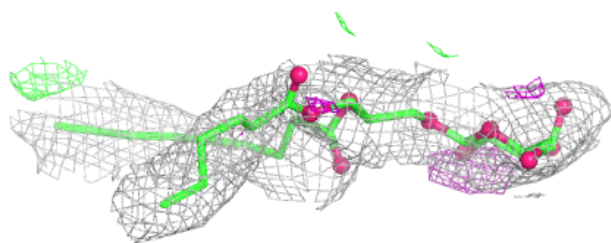
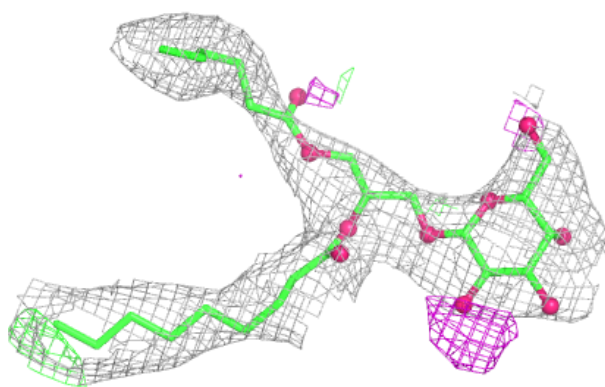
Electron density around LMG C2 515:

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



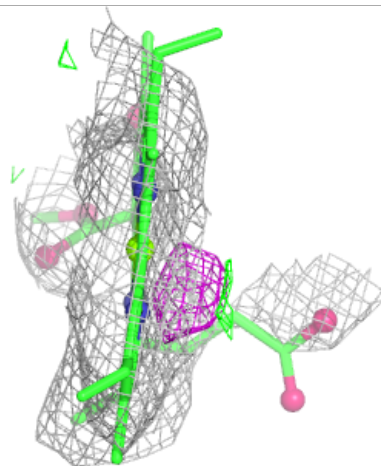
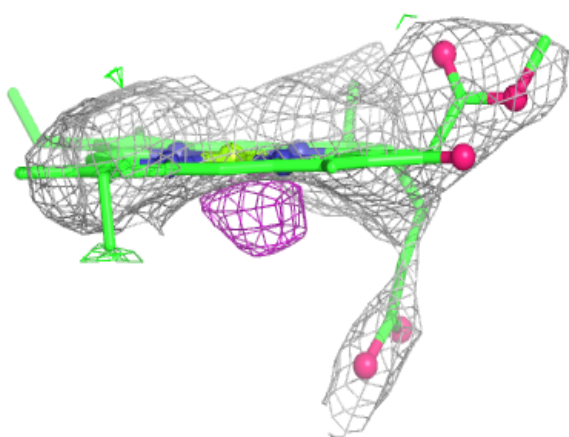
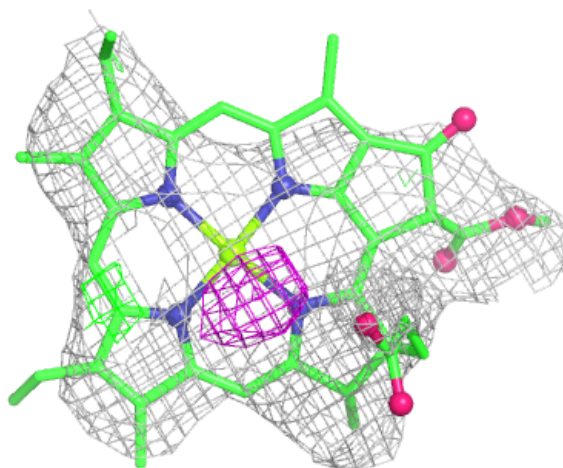
Electron density around LMG I2 101:

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



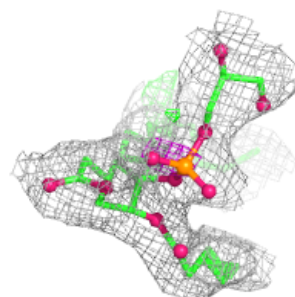
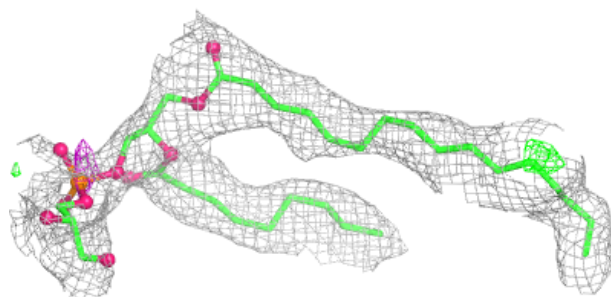
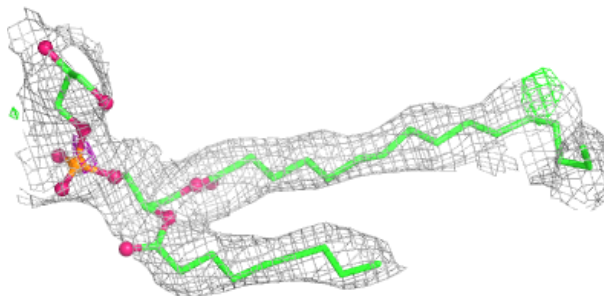
Electron density around CLA C2 510:

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

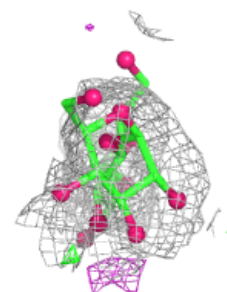
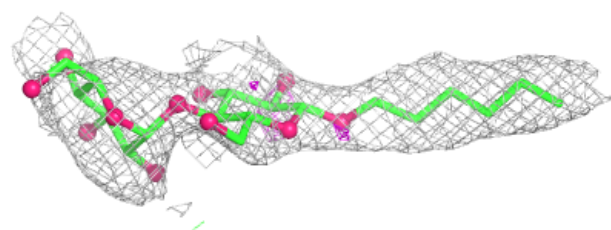
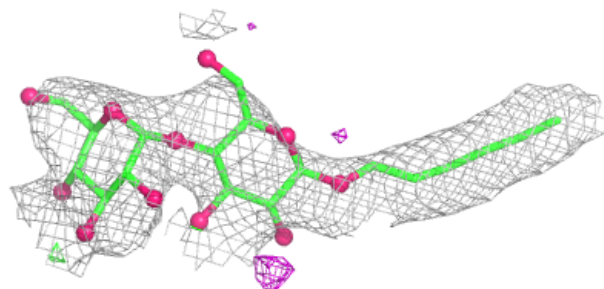


Electron density around LHG B2 627:

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

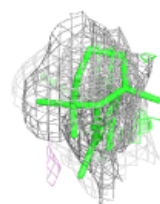
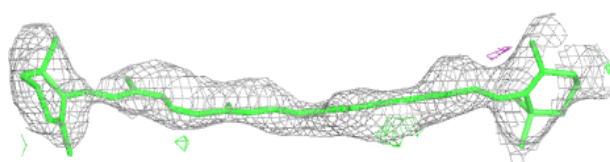
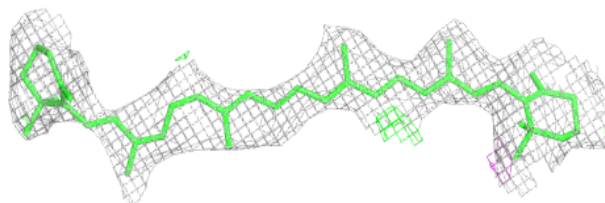
**Electron density around LMT m2 104:**

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

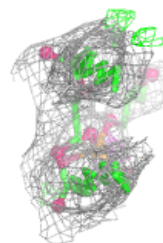
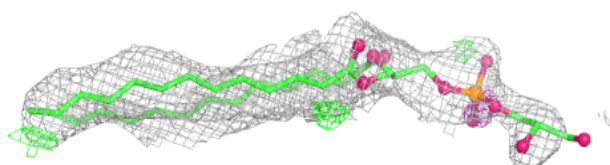
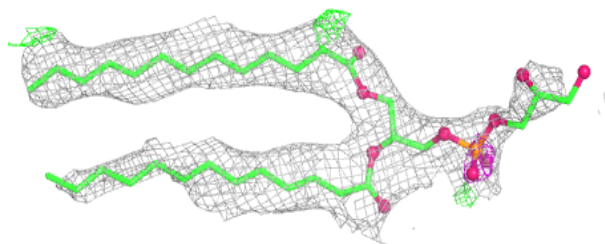


Electron density around BCR K2 102:

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

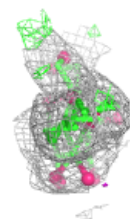
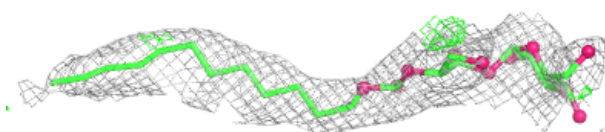
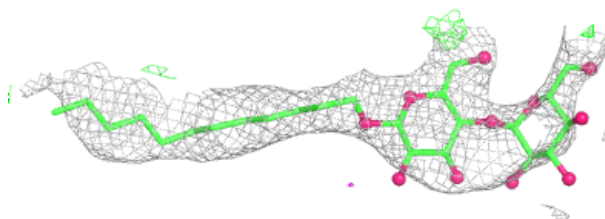
**Electron density around LHG b2 625:**

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

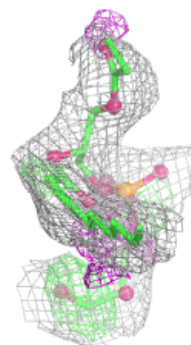
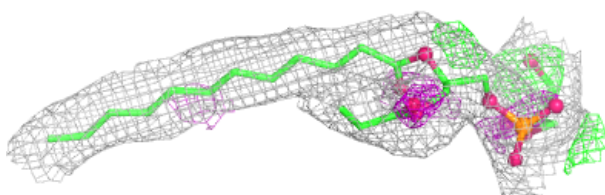
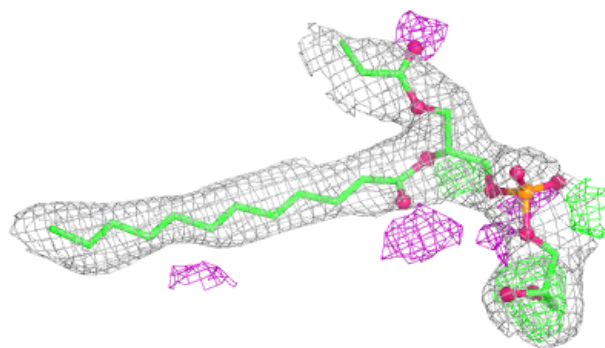


Electron density around LMT b2 621:

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

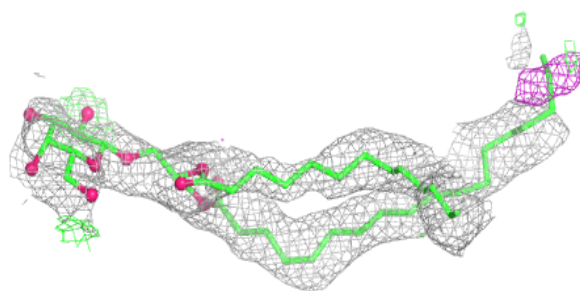
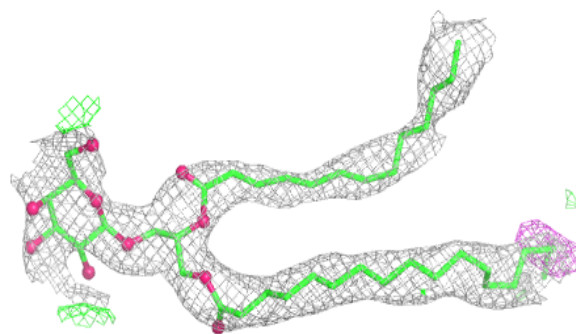
**Electron density around LHG d1 402:**

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

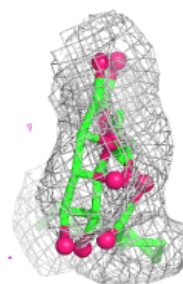
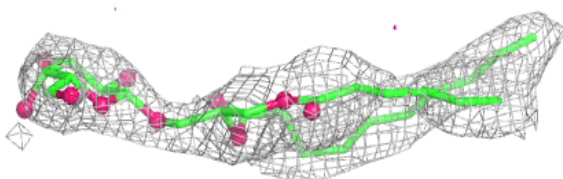
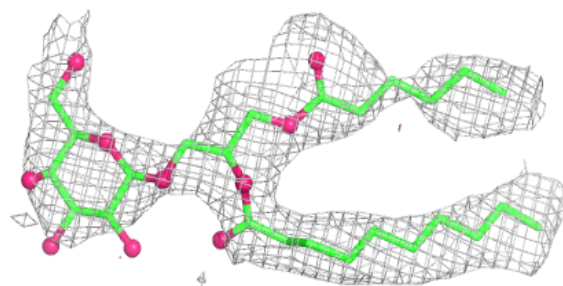


Electron density around LMG j2 101:

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

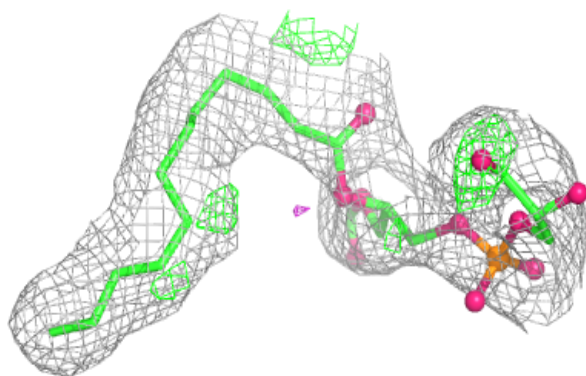
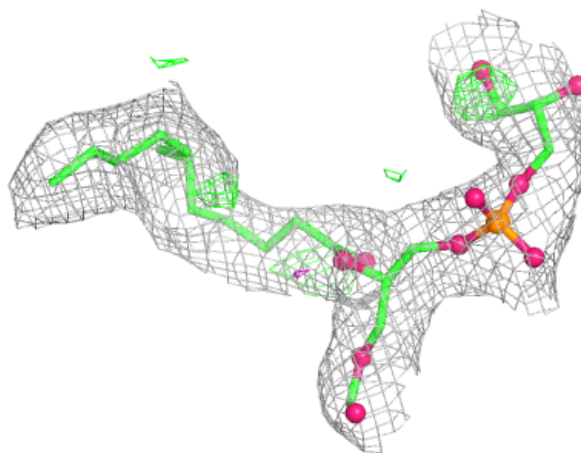
**Electron density around LMG F2 402:**

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



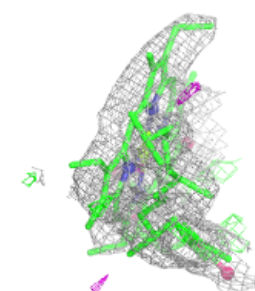
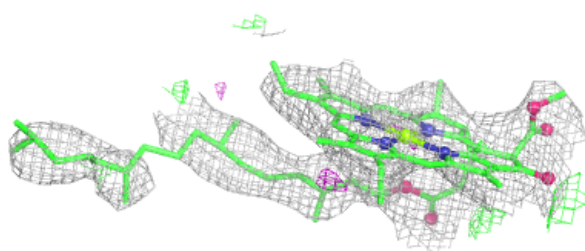
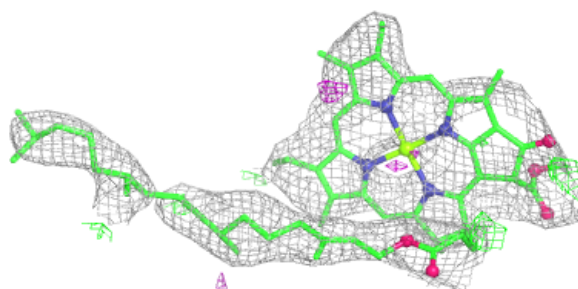
Electron density around LHG a2 407:

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

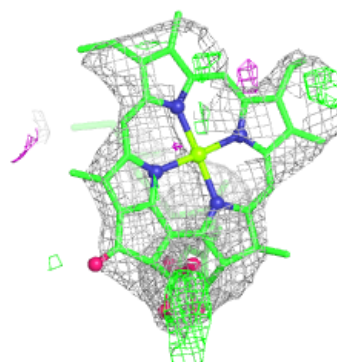
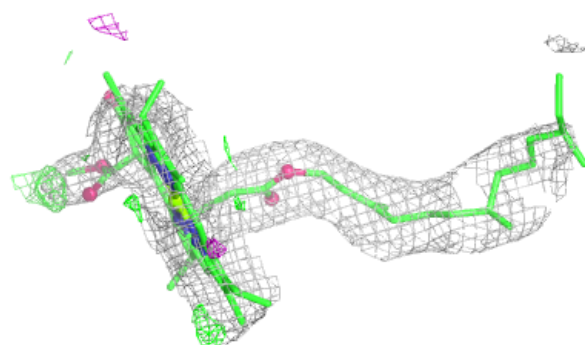
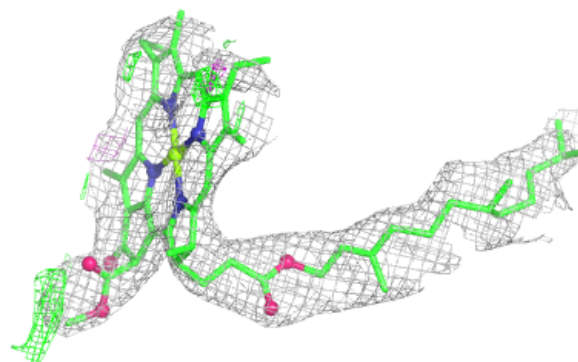


Electron density around CLA C2 503:

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

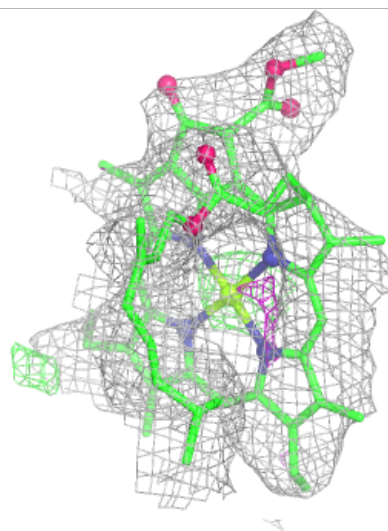
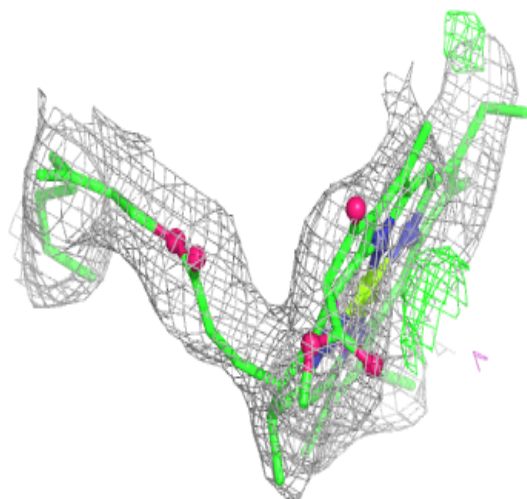
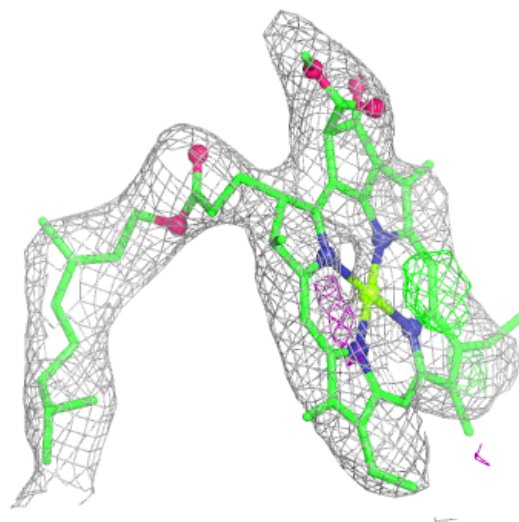
**Electron density around CLA D2 404:**

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



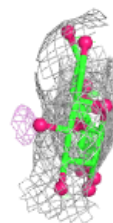
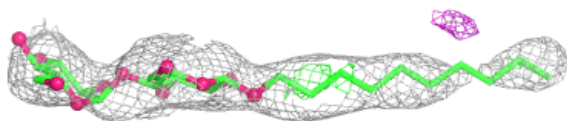
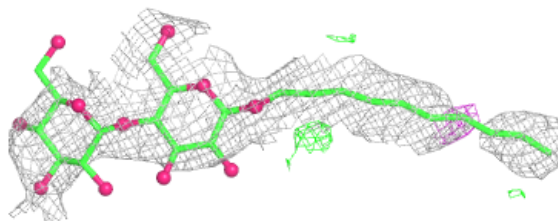
Electron density around CLA K2 101:

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



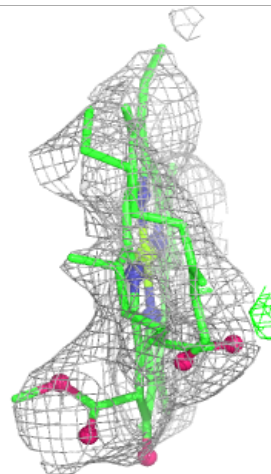
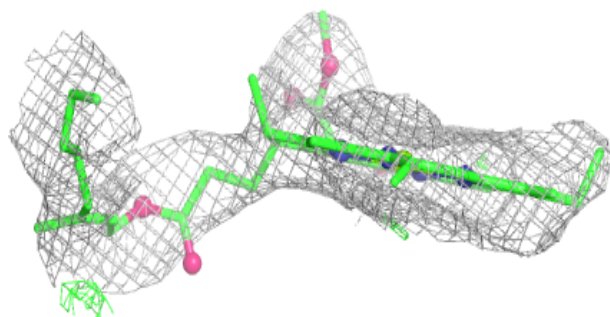
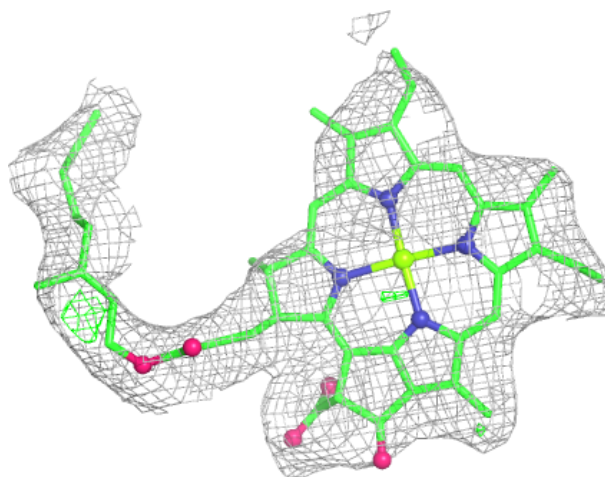
Electron density around LMT c1 517:

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



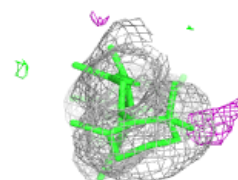
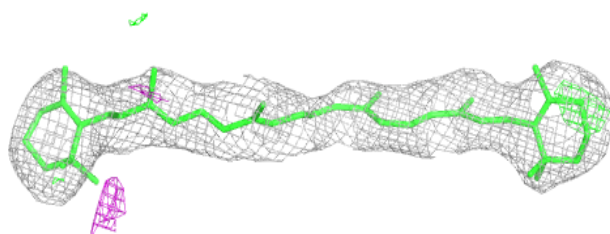
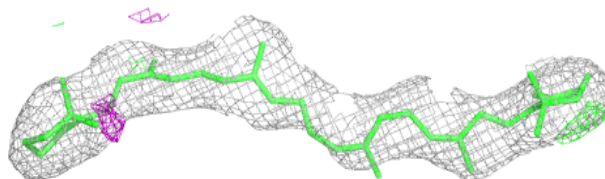
Electron density around CLA c2 513:

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

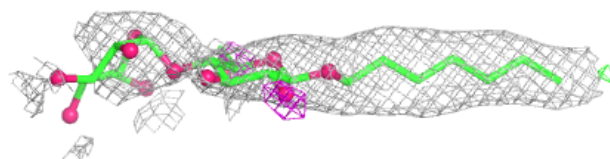
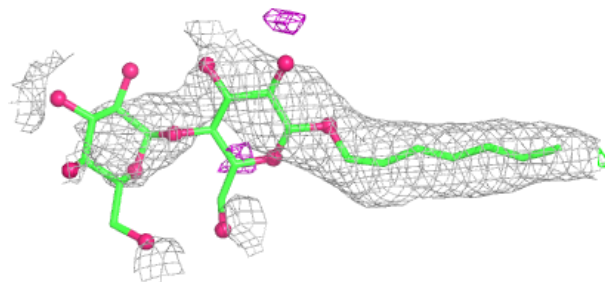


Electron density around BCR c2 501:

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

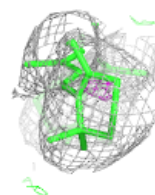
**Electron density around LMT m2 103:**

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

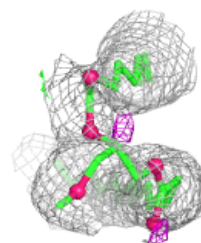
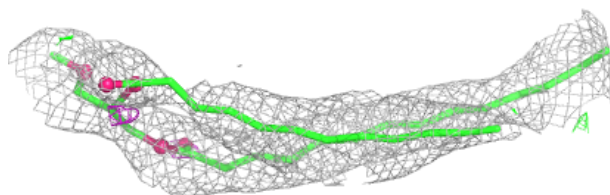
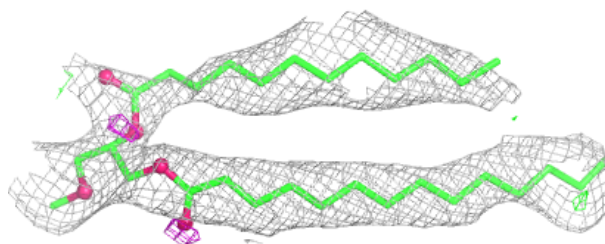


Electron density around BCR K2 104:

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

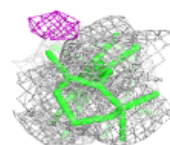
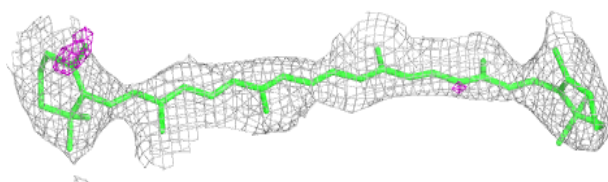
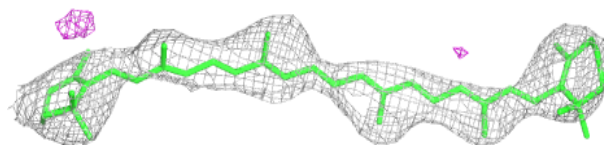
**Electron density around LMG d1 411:**

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

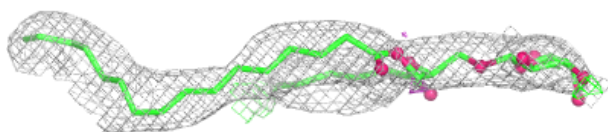
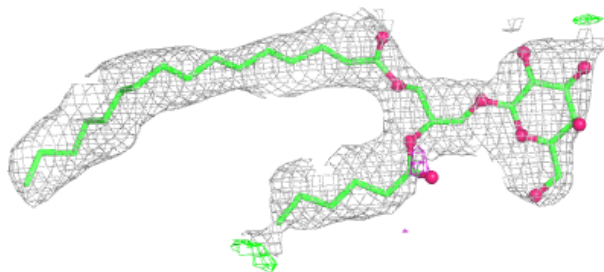


Electron density around BCR z2 101:

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

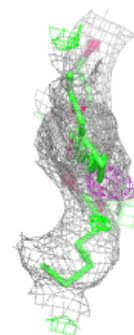
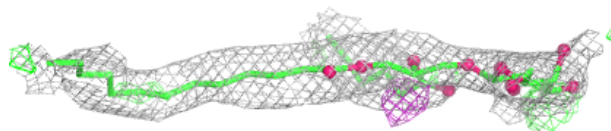
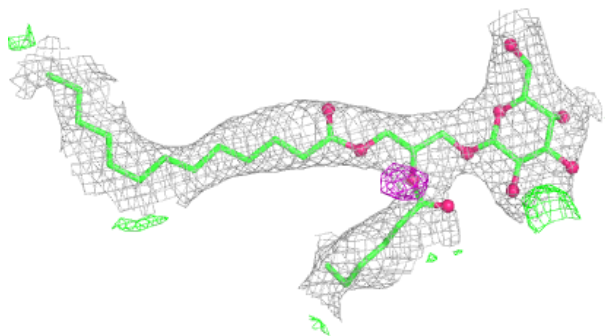
**Electron density around LMG A1 412:**

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

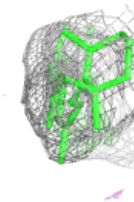
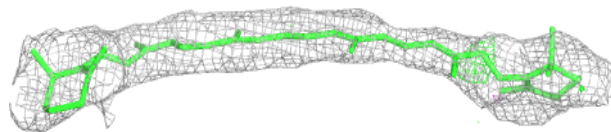
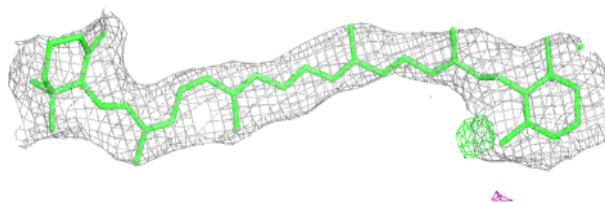


Electron density around LMG b1 621:

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

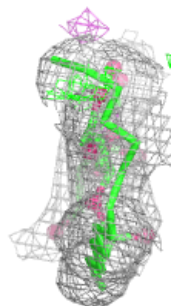
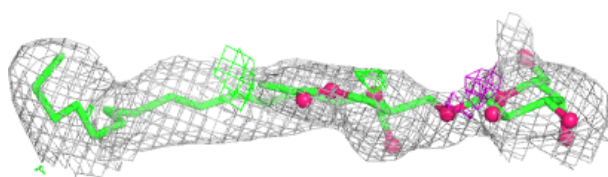
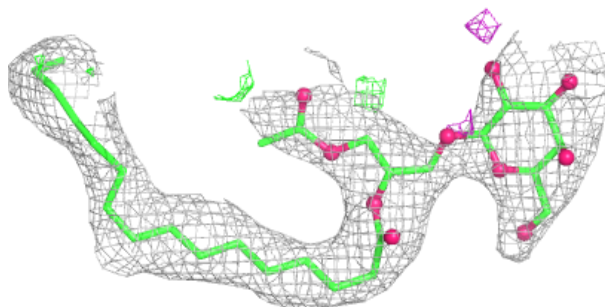
**Electron density around BCR F2 401:**

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



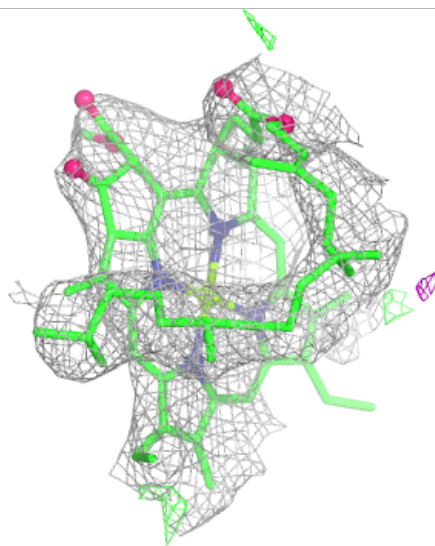
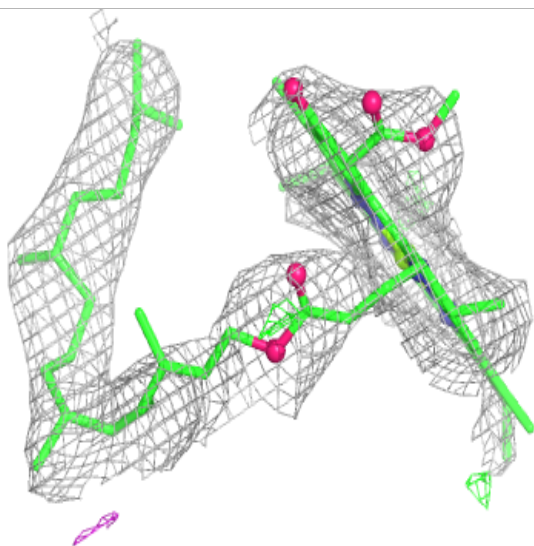
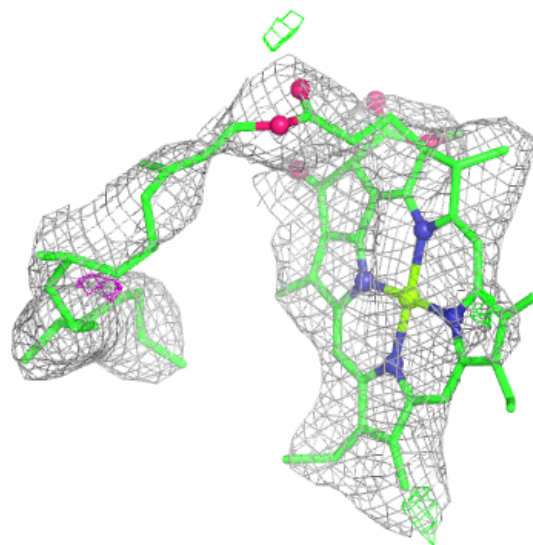
Electron density around LMG B2 621:

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



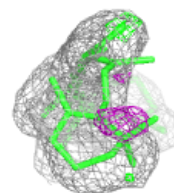
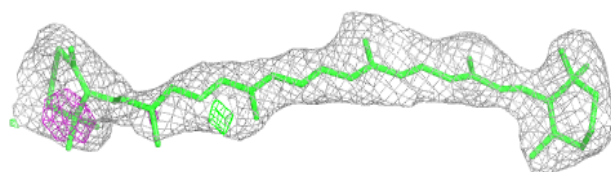
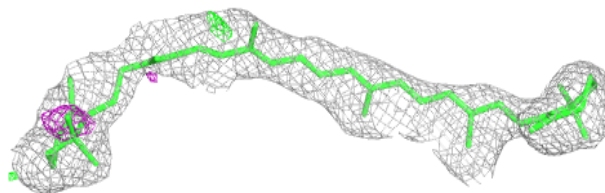
Electron density around CLA C2 505:

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



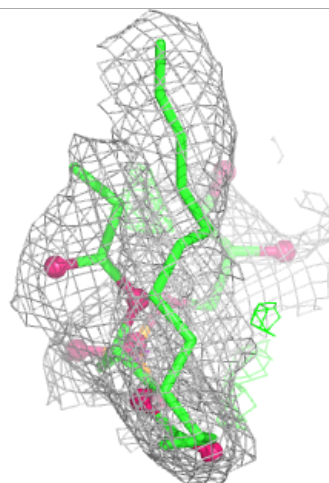
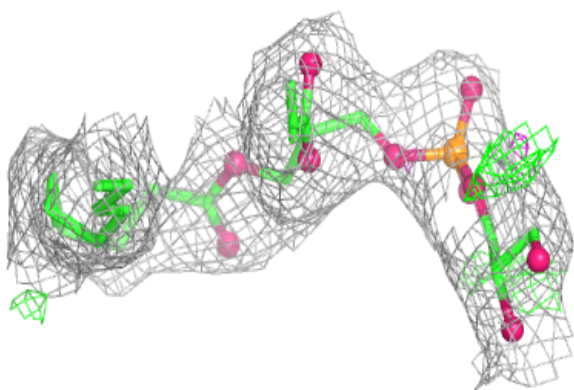
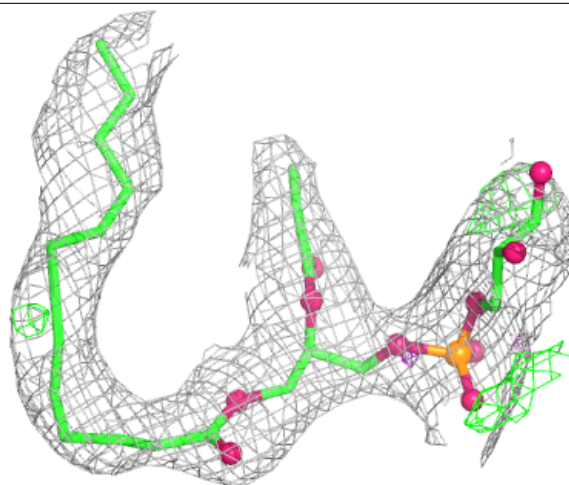
Electron density around BCR B1 602:

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



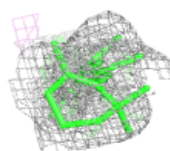
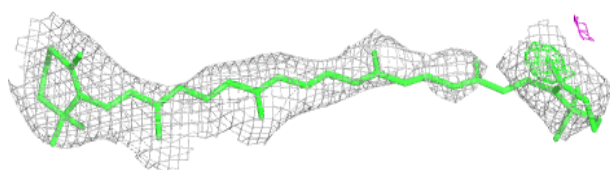
Electron density around LHG A2 405:

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

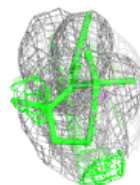
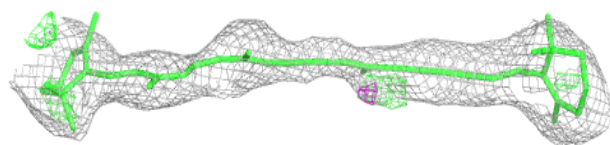
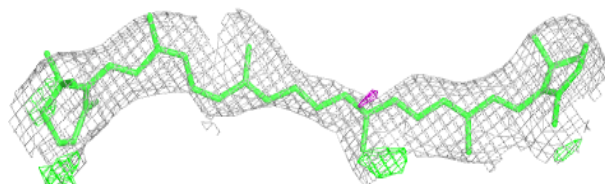


Electron density around BCR C2 502:

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

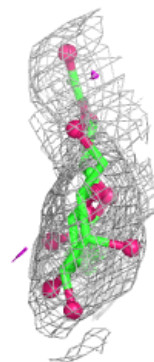
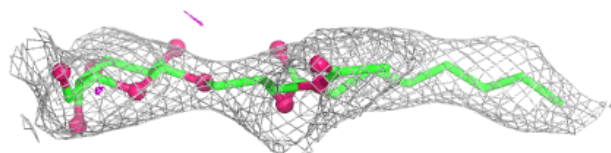
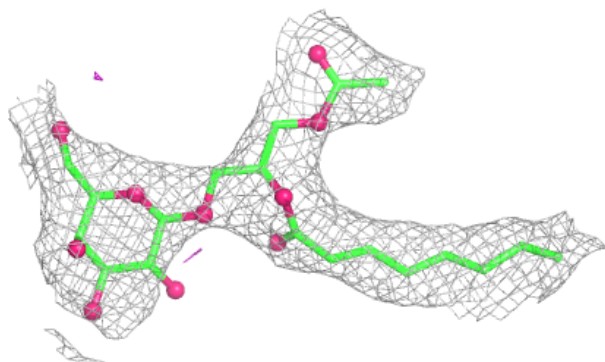
**Electron density around BCR J1 101:**

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



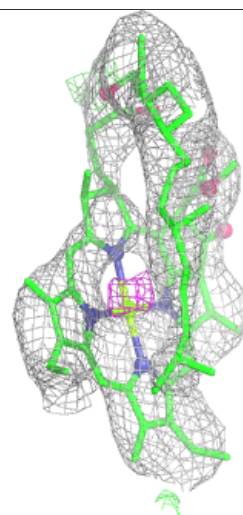
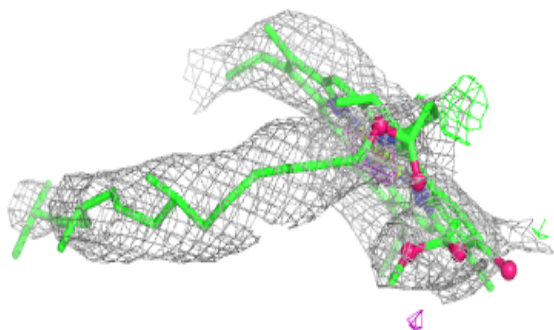
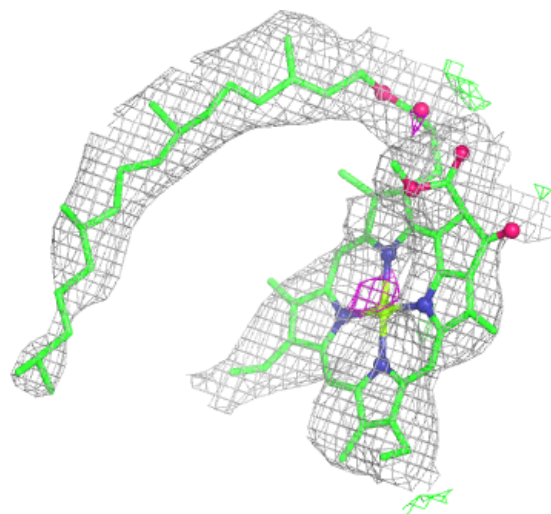
Electron density around LMG A2 412:

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



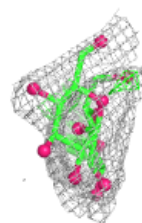
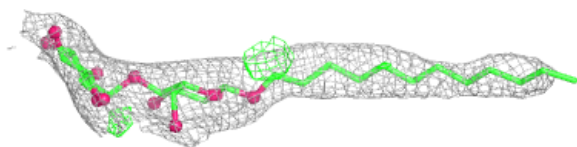
Electron density around CLA C2 509:

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

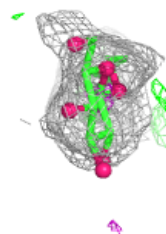
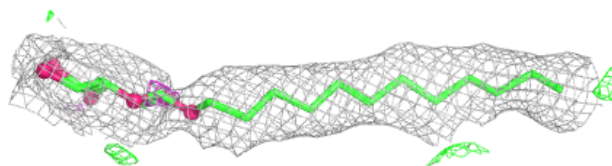
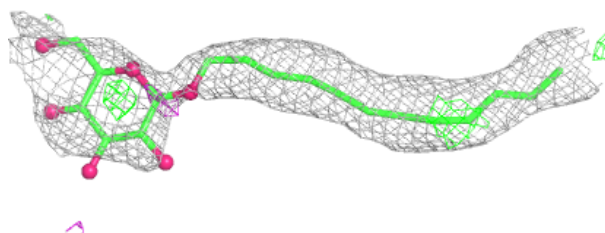


Electron density around LMT C1 519:

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

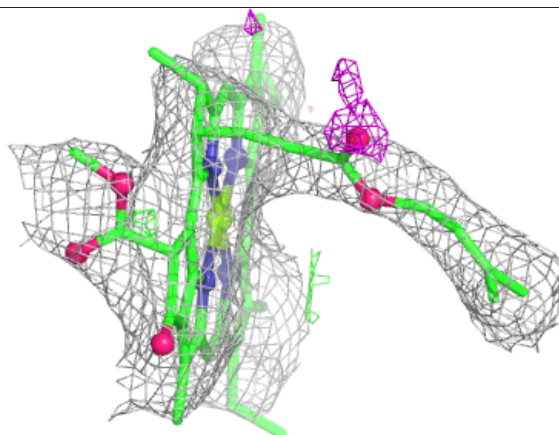
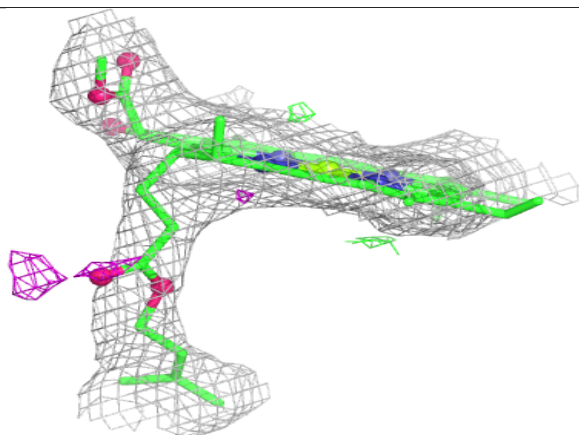
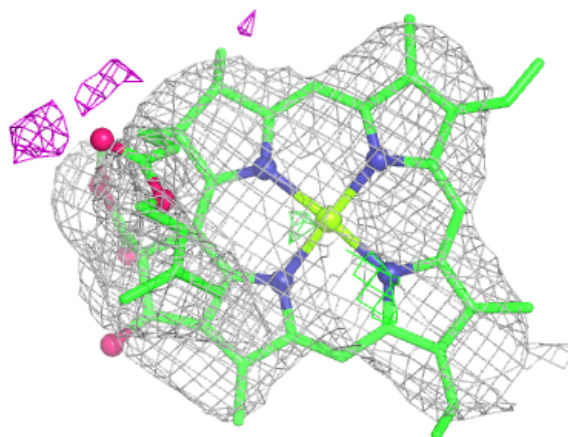
**Electron density around LMT M1 103:**

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

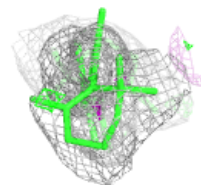
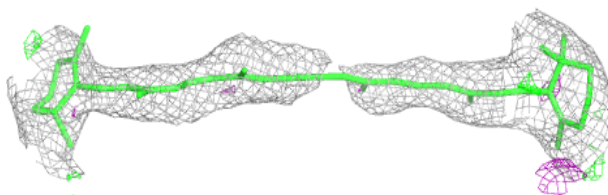
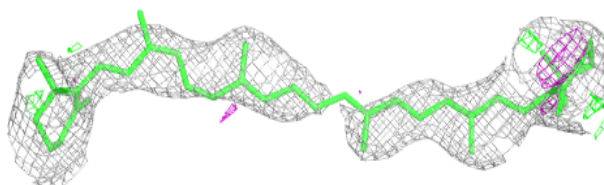


Electron density around CLA C2 511:

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

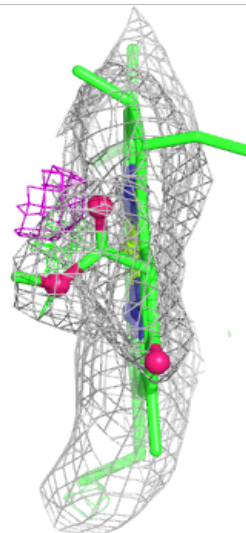
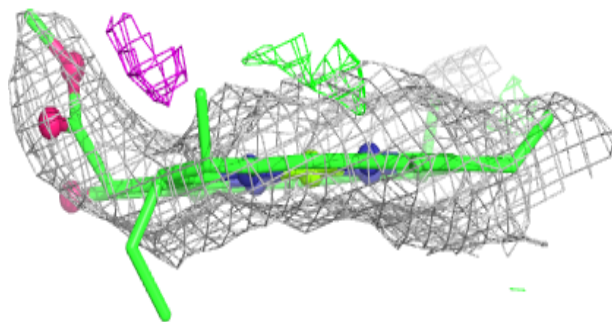
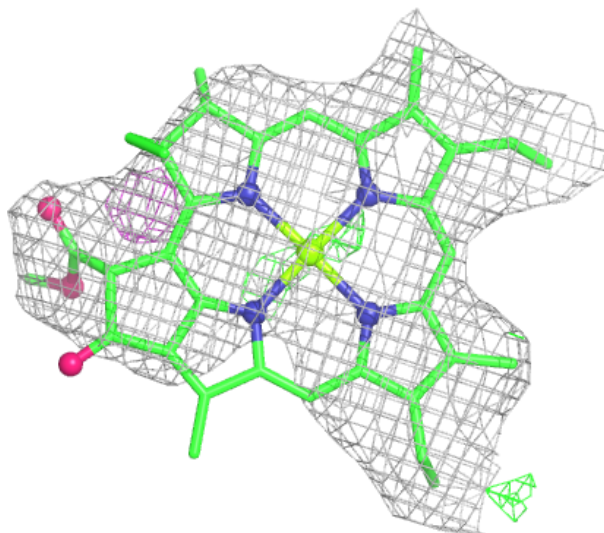
**Electron density around BCR k1 101:**

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



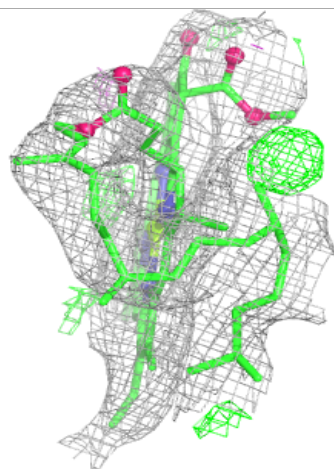
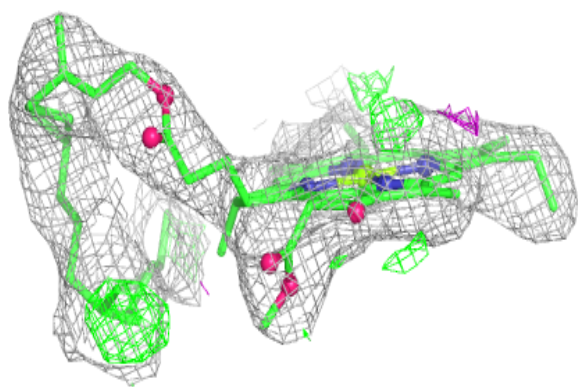
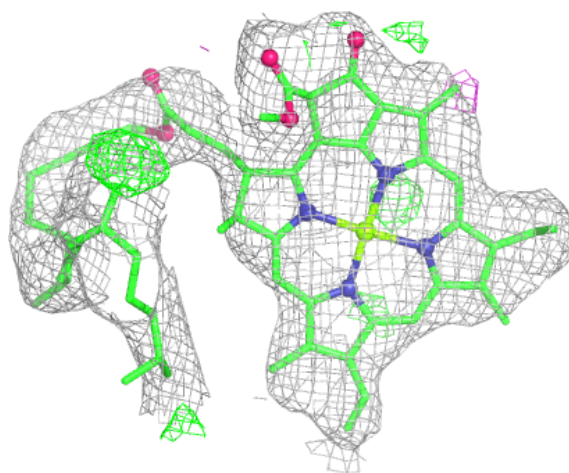
Electron density around CLA B1 604:

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



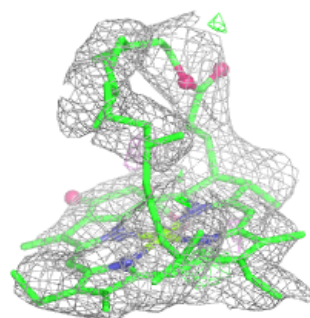
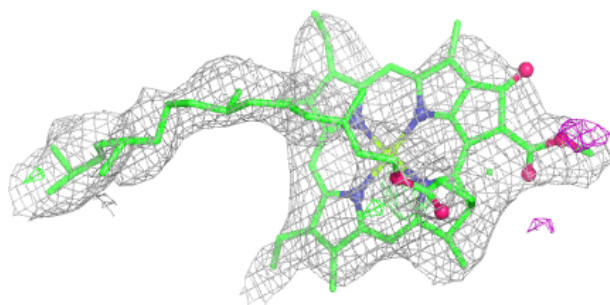
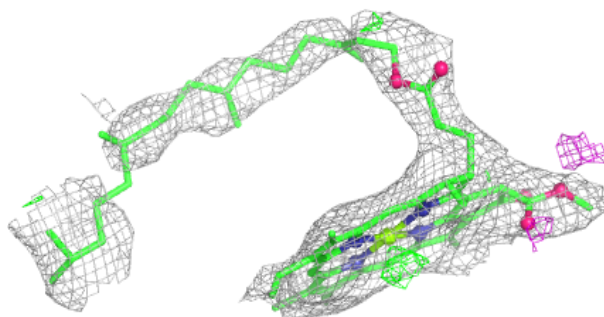
Electron density around CLA C1 512:

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

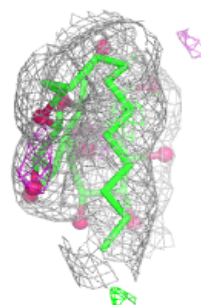
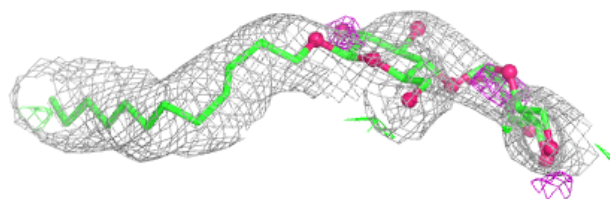
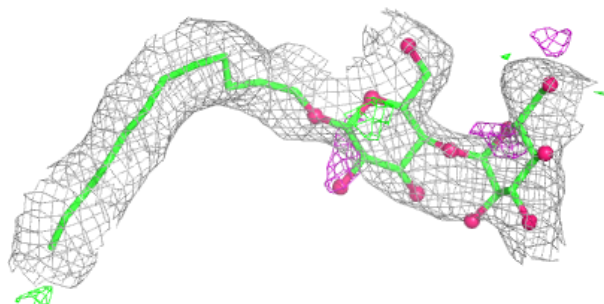


Electron density around CLA c1 516:

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

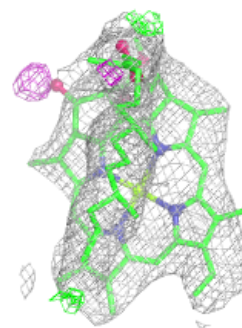
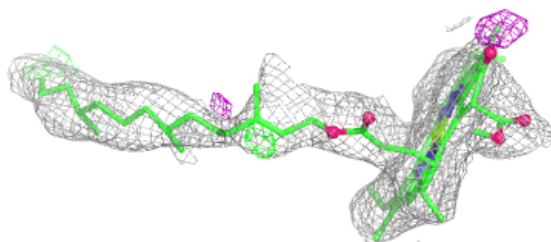
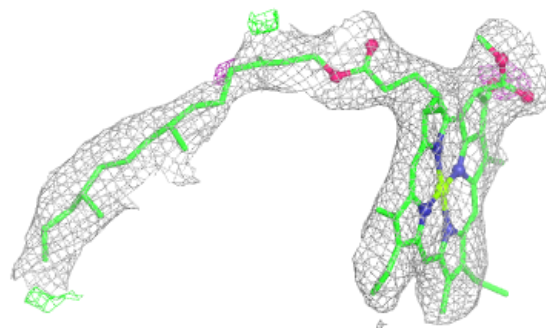
**Electron density around LMT a2 406:**

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



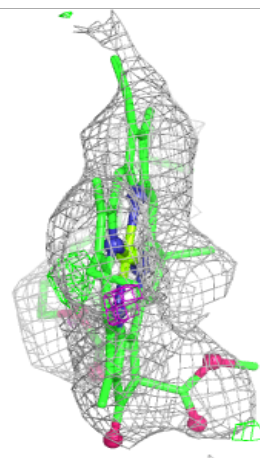
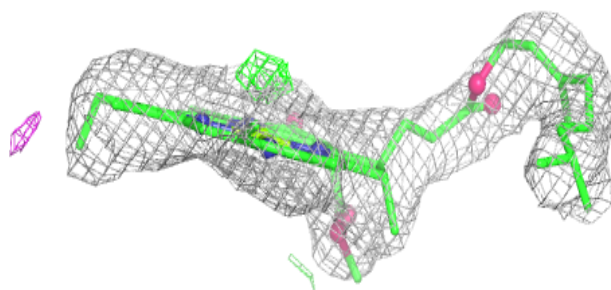
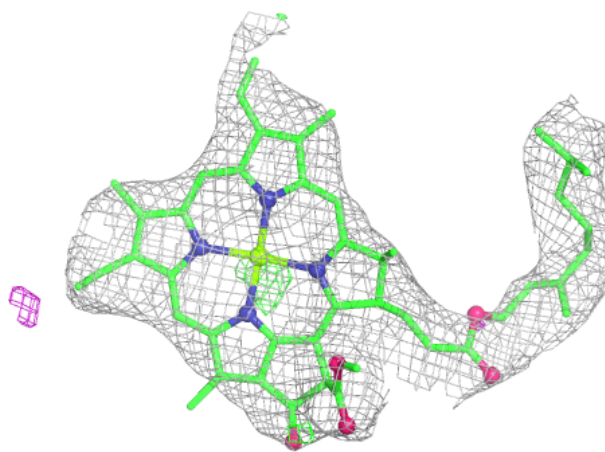
Electron density around CLA B1 611:

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



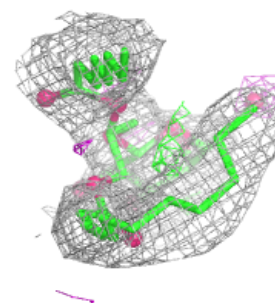
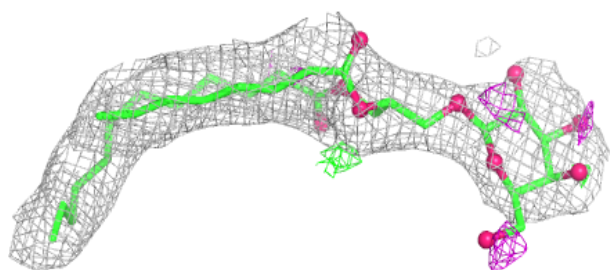
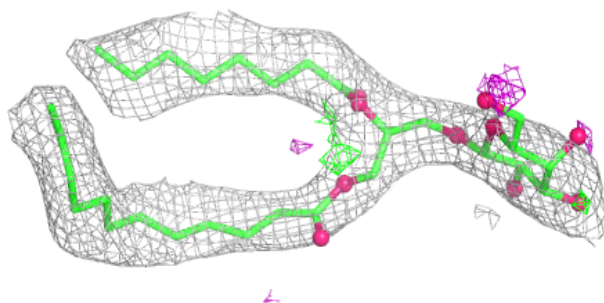
Electron density around CLA c1 515:

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

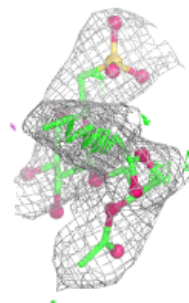
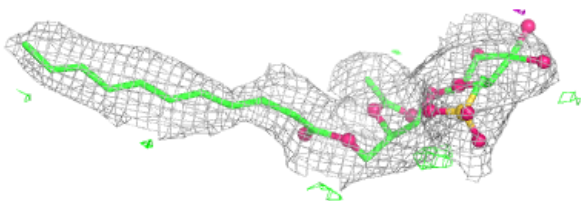
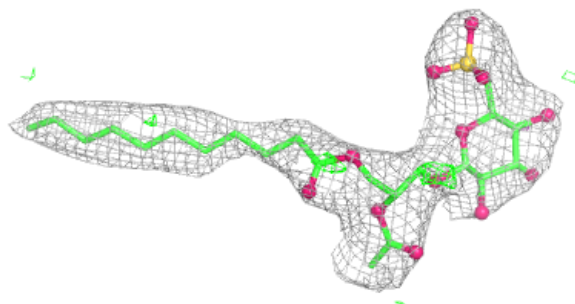


Electron density around LMG b1 624:

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

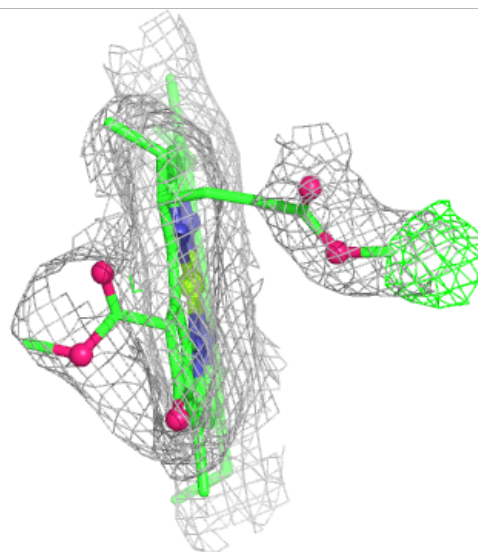
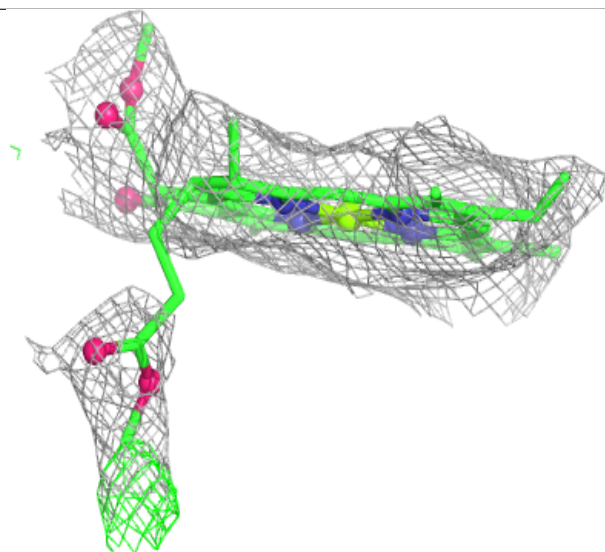
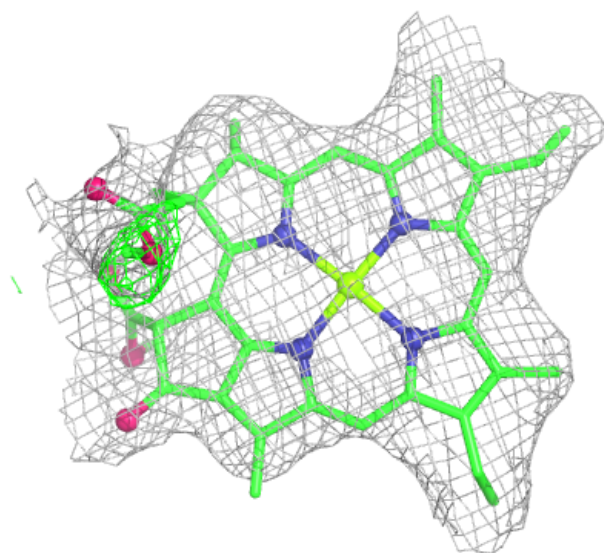
**Electron density around SQD D1 409:**

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



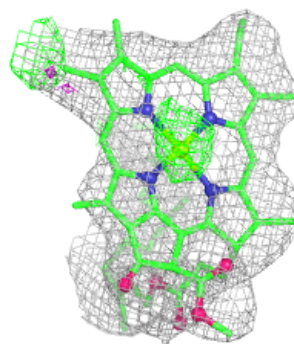
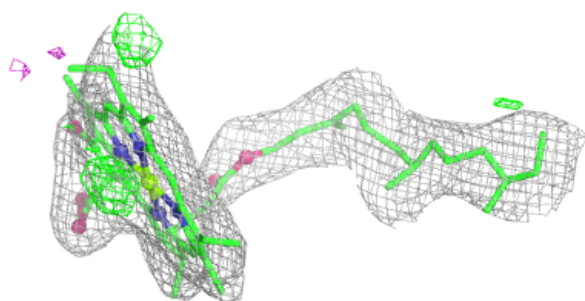
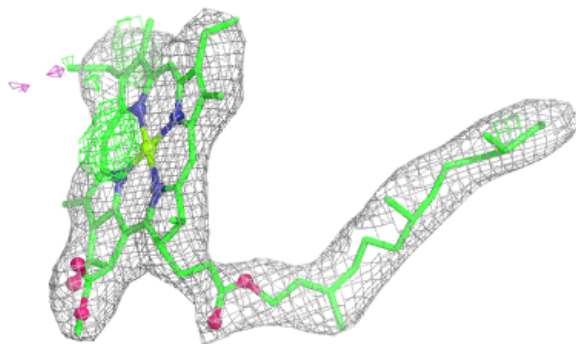
Electron density around CLA C2 504:

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



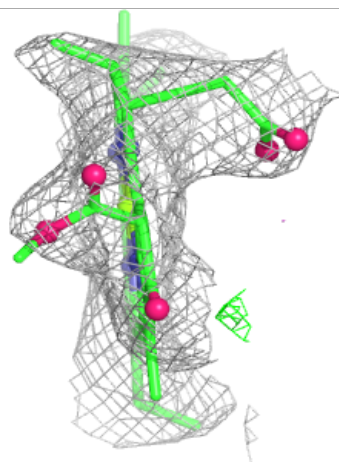
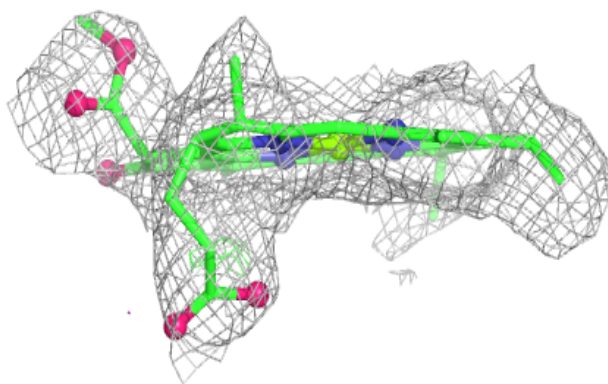
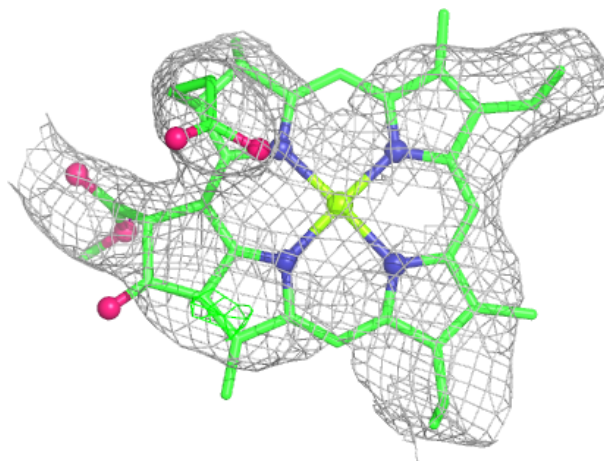
Electron density around CLA C1 513:

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



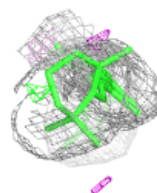
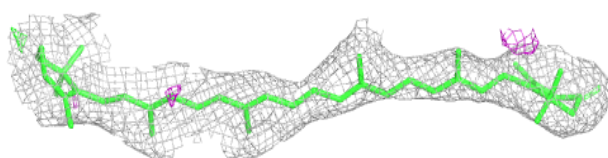
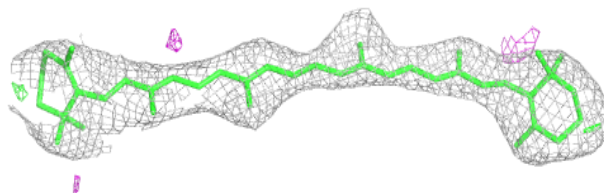
Electron density around CLA C2 507:

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

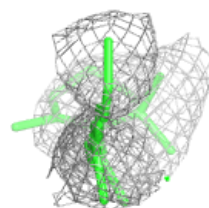
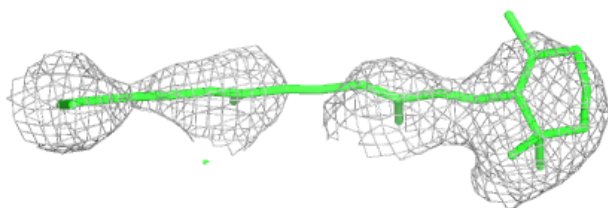
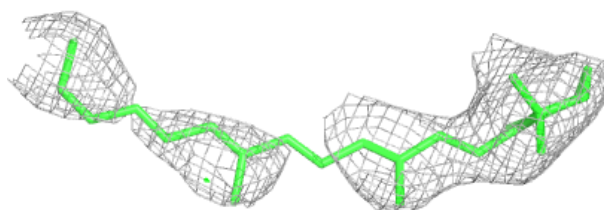


Electron density around BCR b2 603:

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

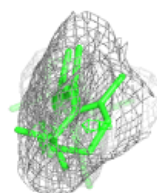
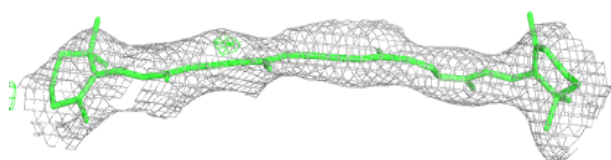
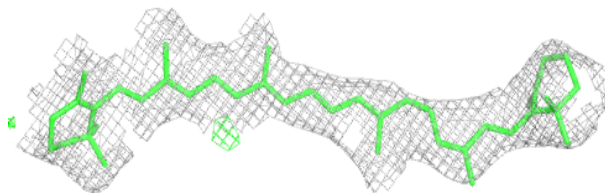
**Electron density around BCR H2 103:**

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

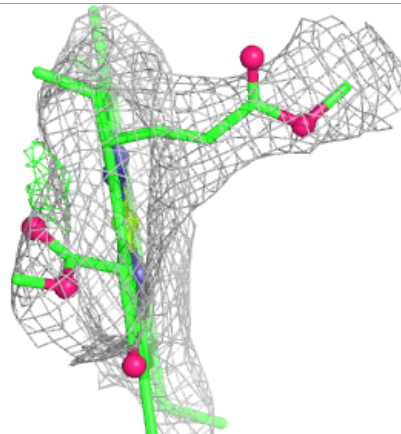
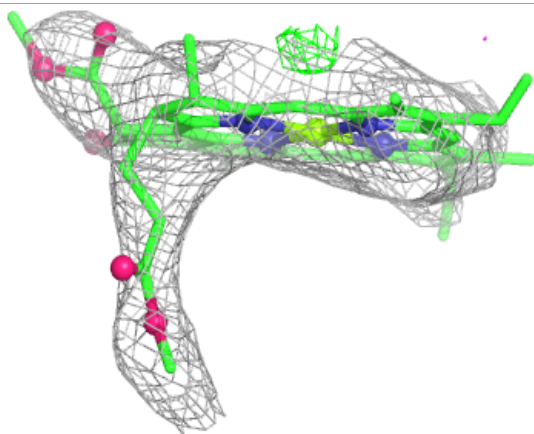
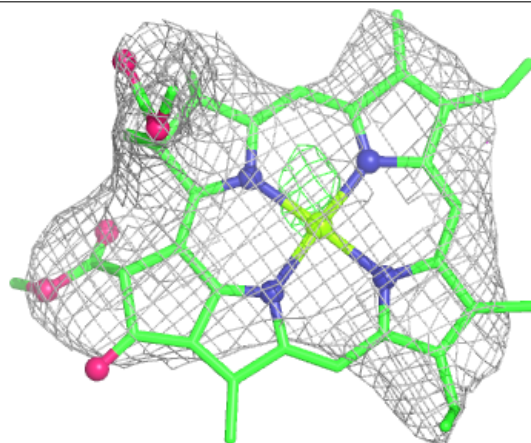


Electron density around BCR j2 102:

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

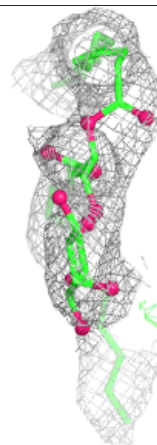
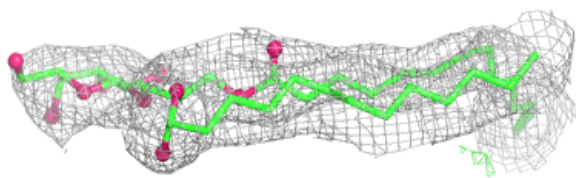
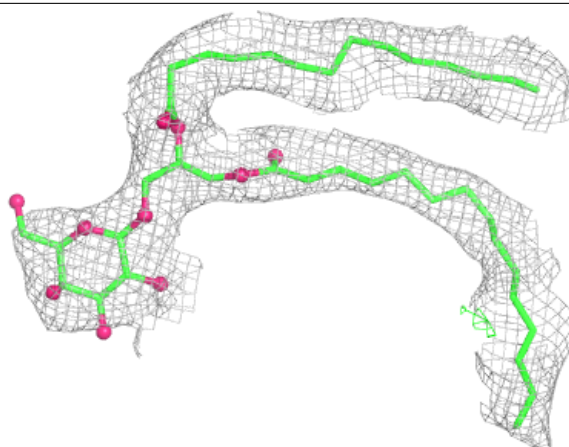
**Electron density around CLA c2 515:**

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

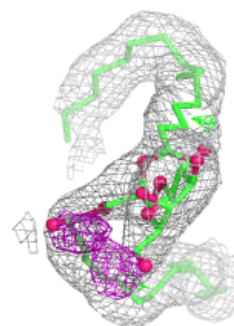
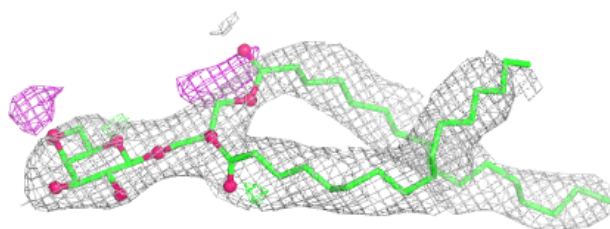
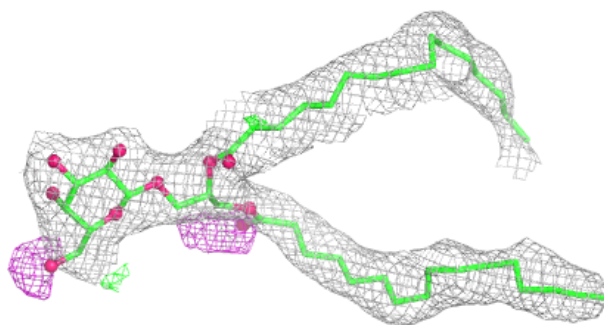


Electron density around LMG C1 520:

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

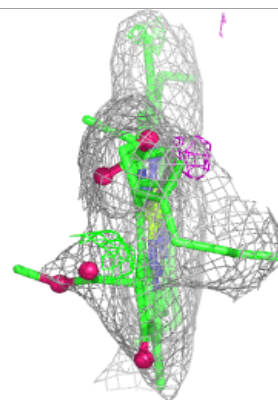
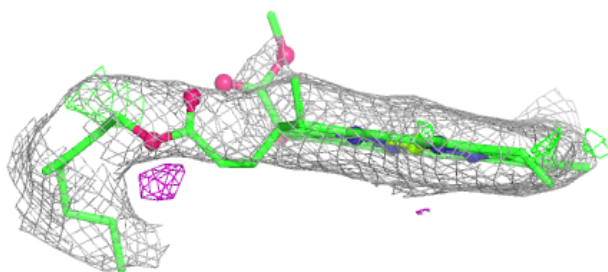
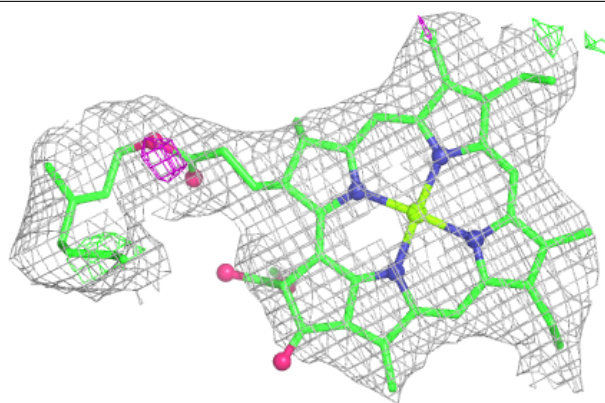
**Electron density around LMG a1 412:**

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

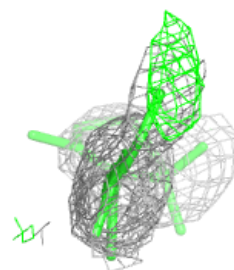
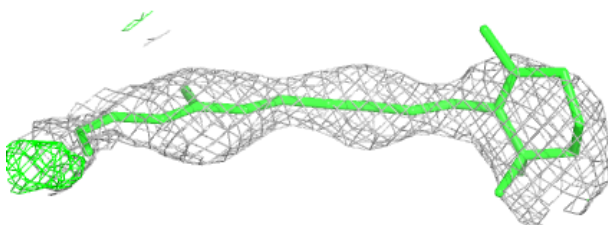
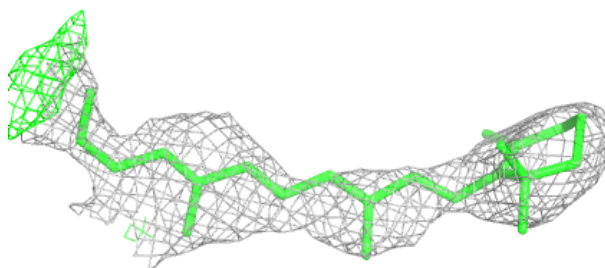


Electron density around CLA C2 513:

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

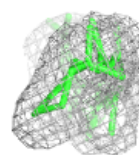
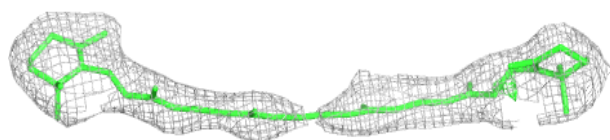
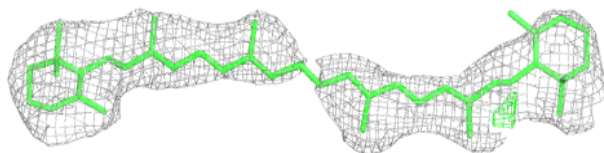
**Electron density around BCR H1 102:**

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

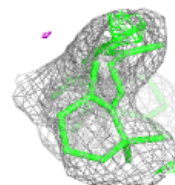
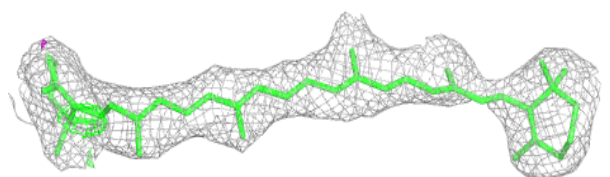
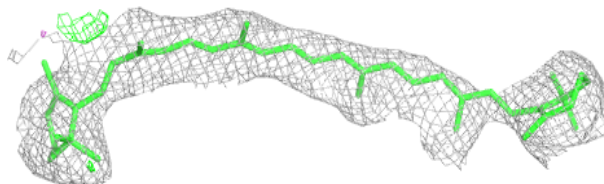


Electron density around BCR D1 401:

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

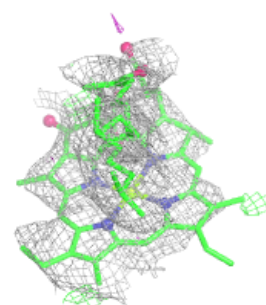
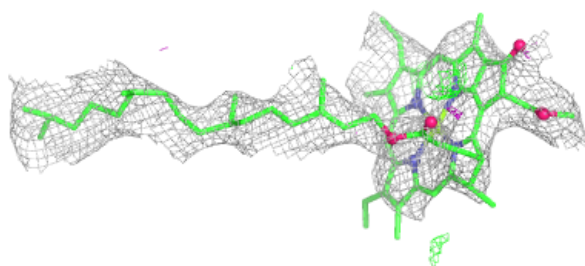
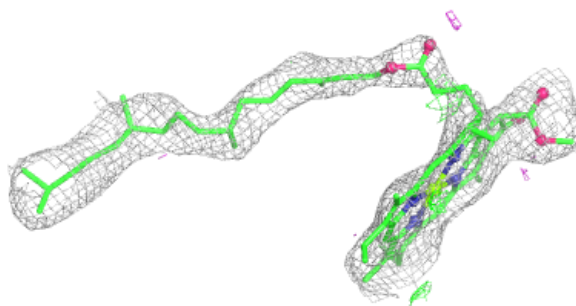
**Electron density around BCR b2 602:**

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

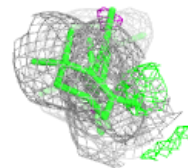
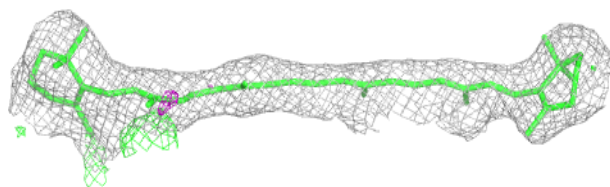
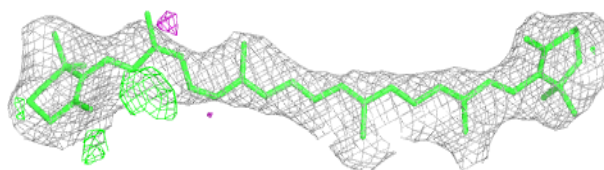


Electron density around CLA C2 506:

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

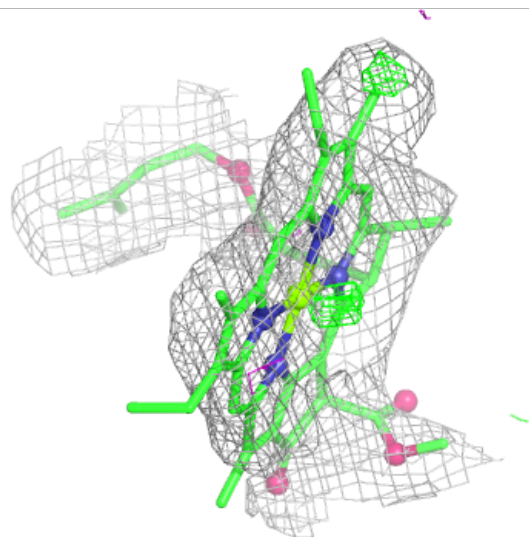
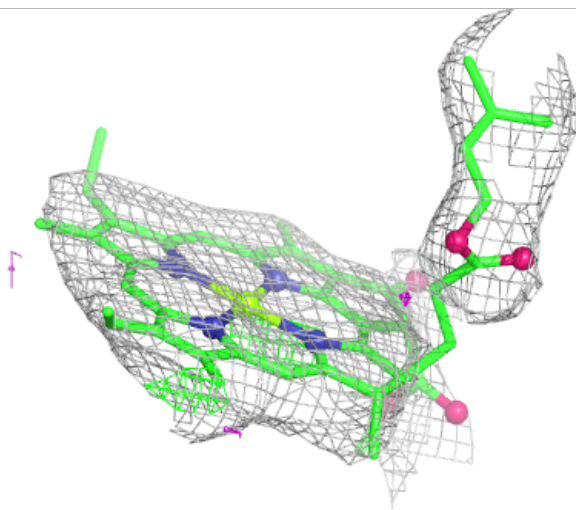
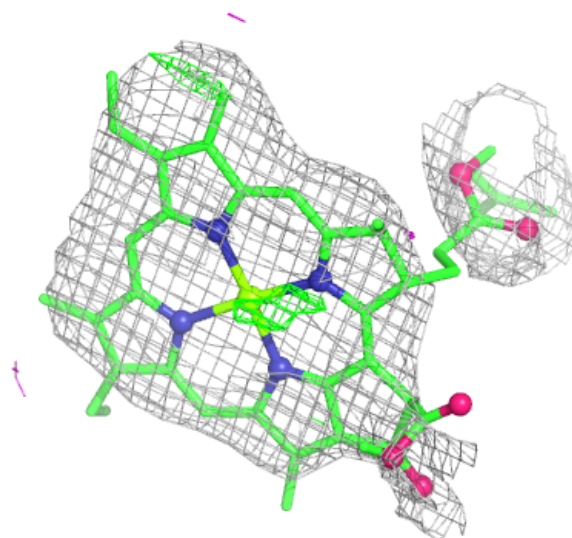
**Electron density around BCR b1 602:**

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



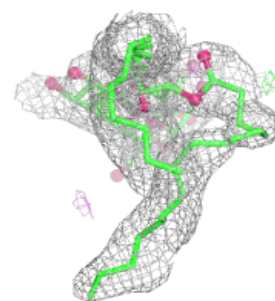
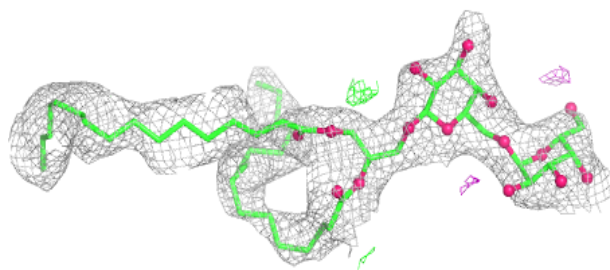
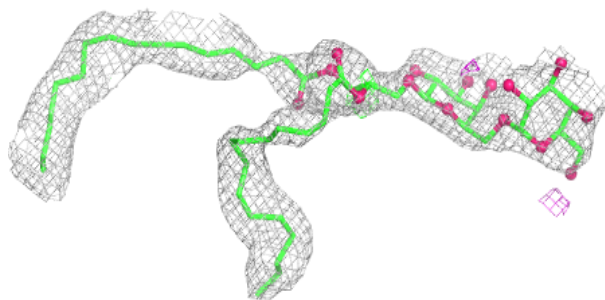
Electron density around CLA C2 508:

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



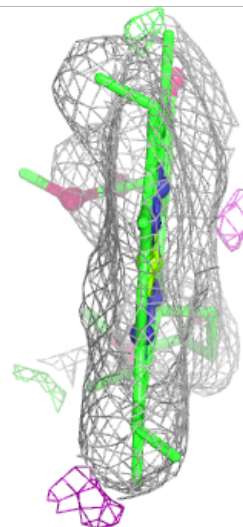
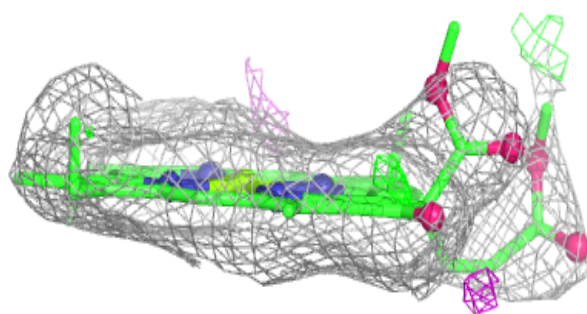
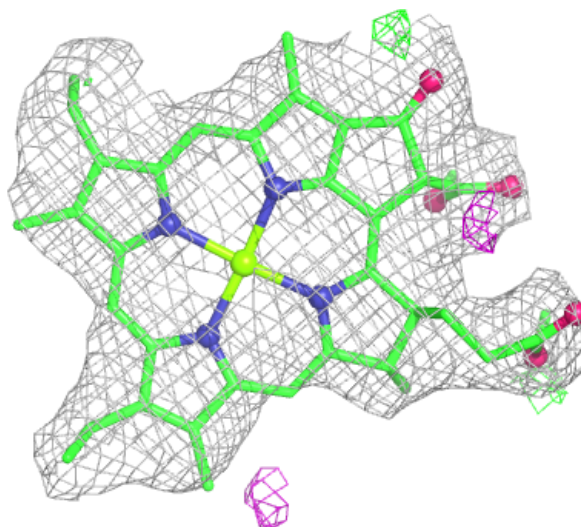
Electron density around DGD H2 101:

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



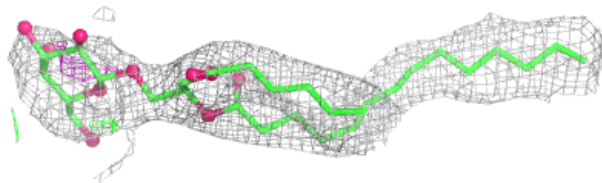
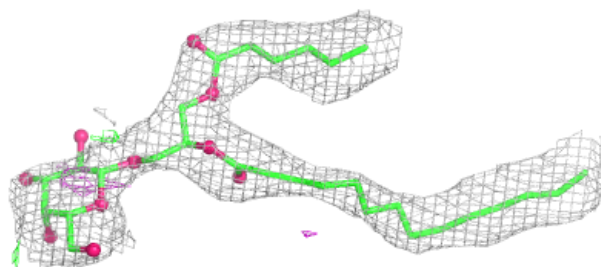
Electron density around CLA C2 516:

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



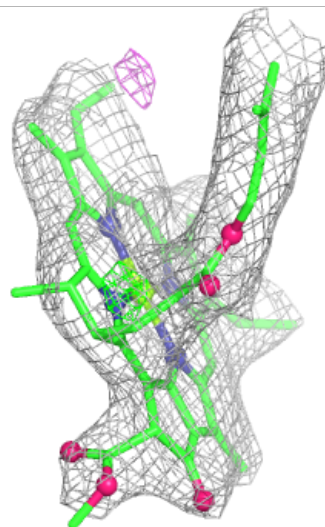
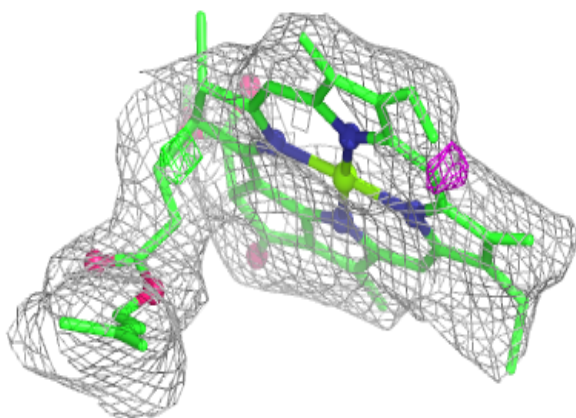
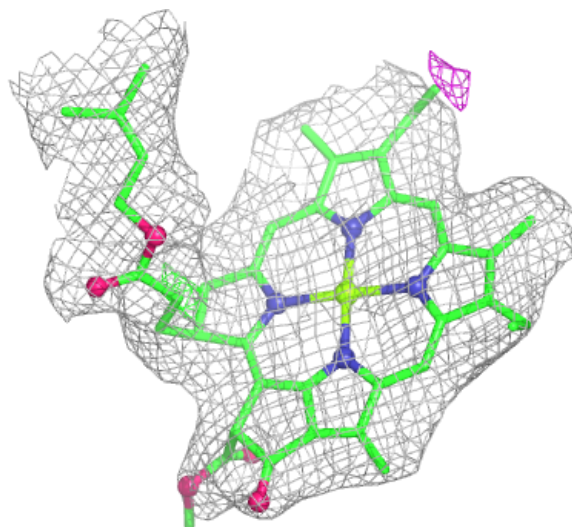
Electron density around LMG b2 622:

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



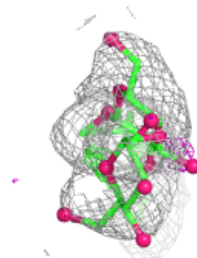
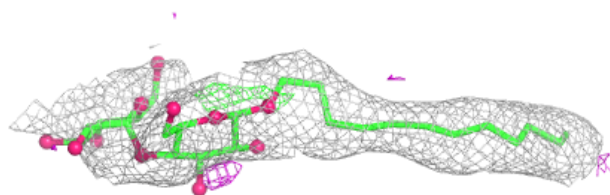
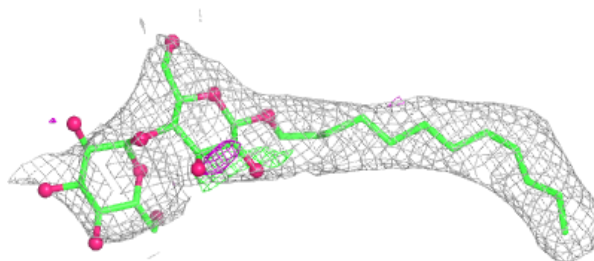
Electron density around CLA d2 404:

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



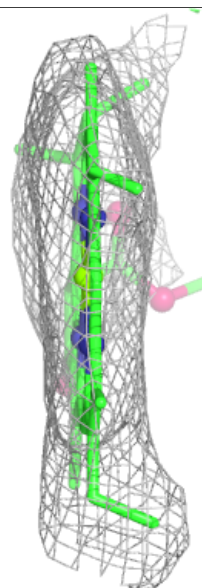
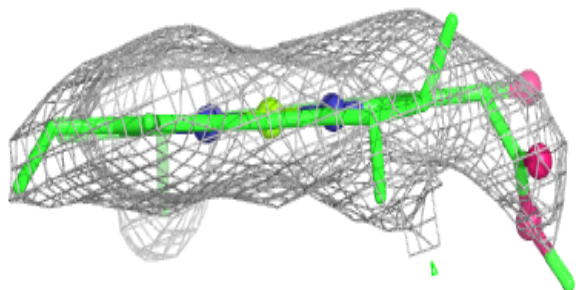
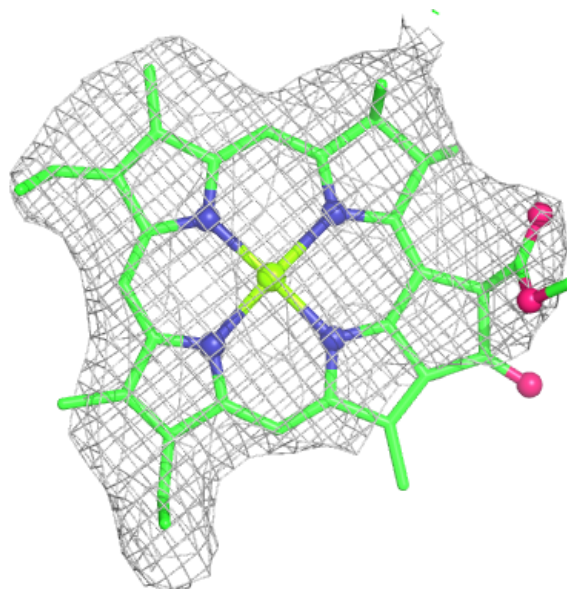
Electron density around LMT m1 101:

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



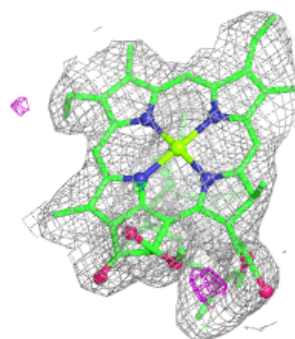
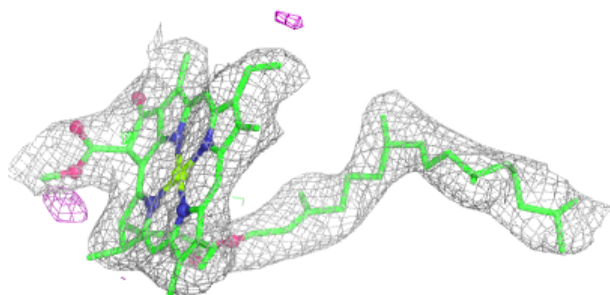
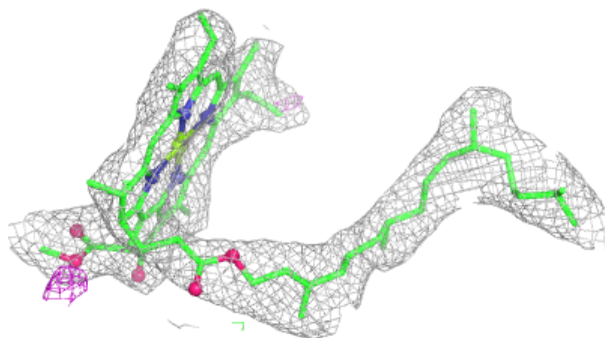
Electron density around CLA B2 604:

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

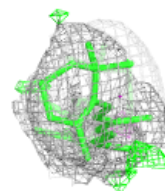
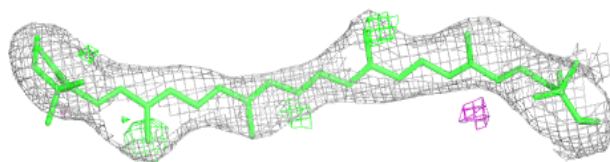
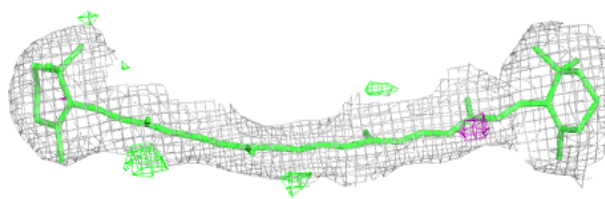


Electron density around CLA c2 509:

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

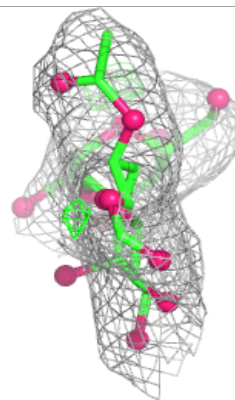
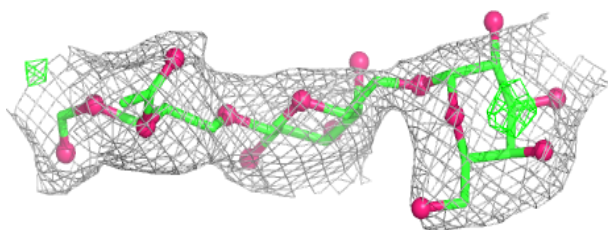
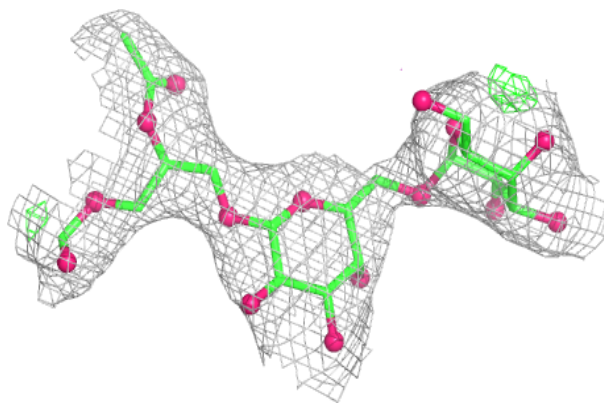
**Electron density around BCR C1 521:**

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

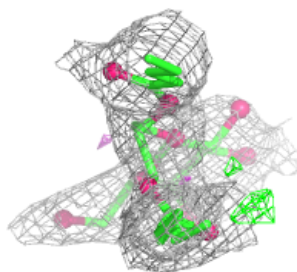
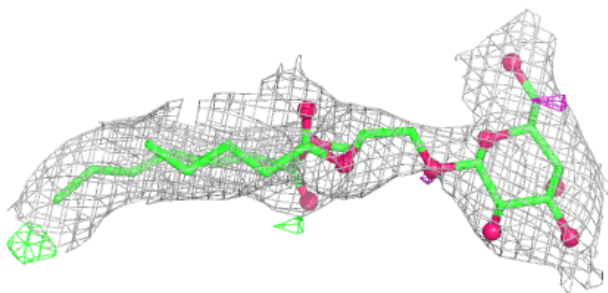
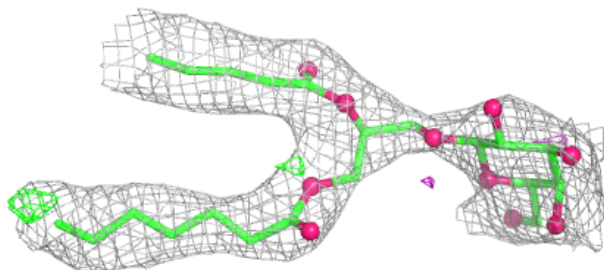


Electron density around DGD C2 512:

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

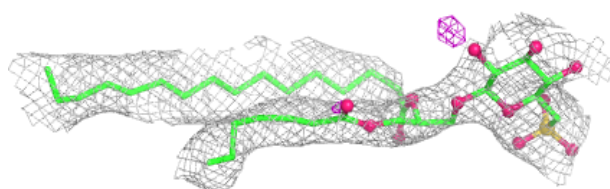
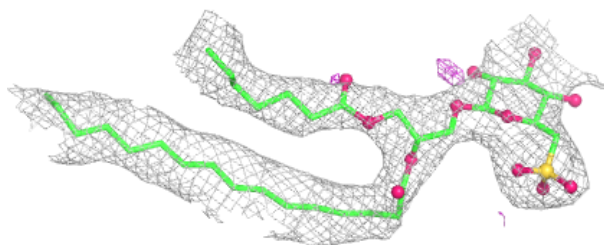
**Electron density around LMG B1 622:**

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

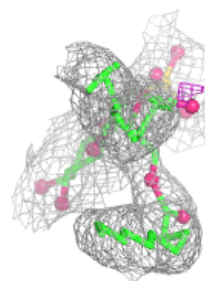
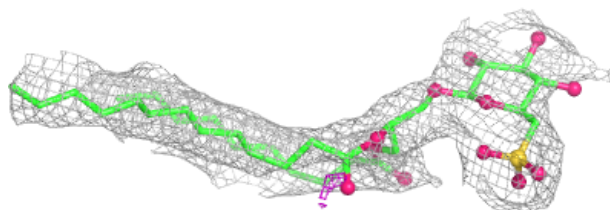
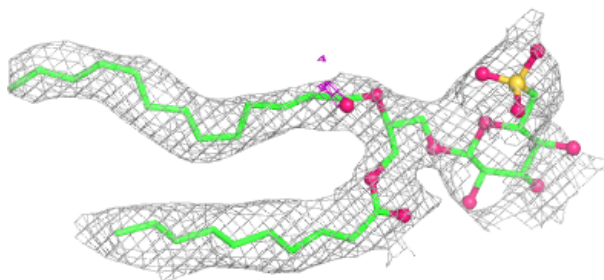


Electron density around SQD B2 623:

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

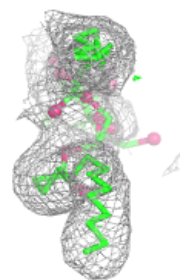
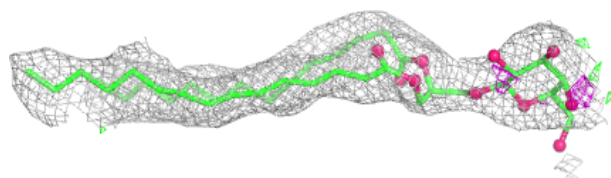
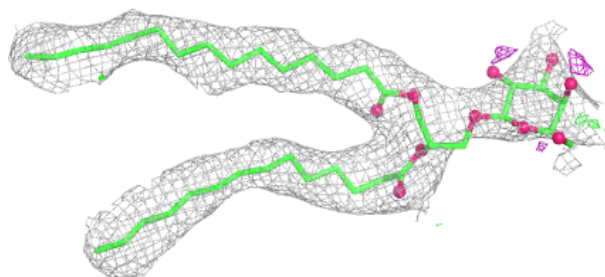
**Electron density around SQD b2 605:**

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



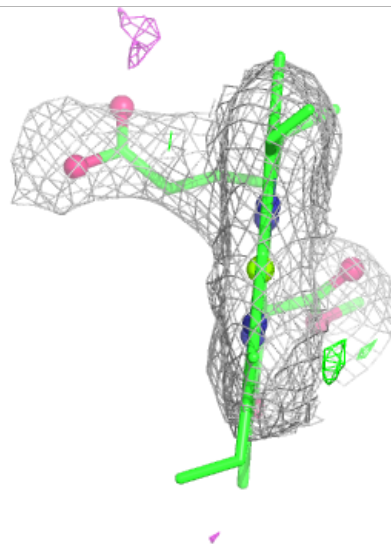
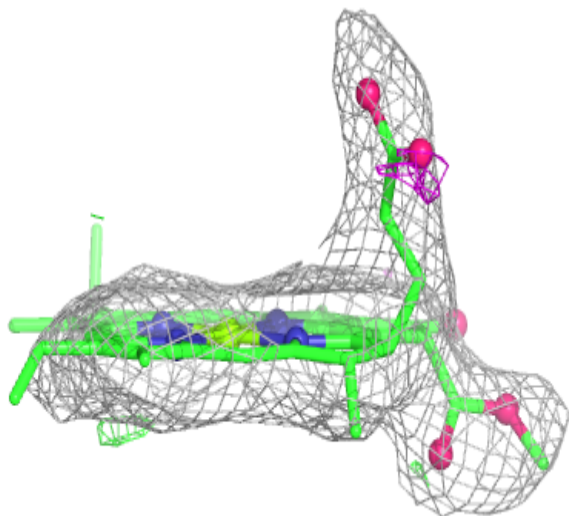
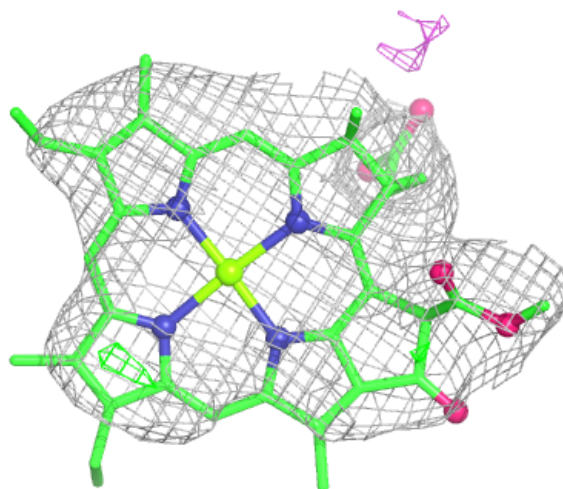
Electron density around LMG B1 626:

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



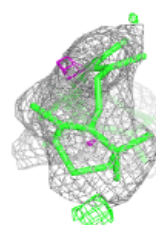
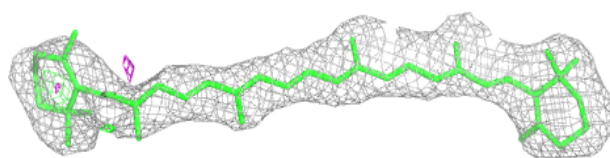
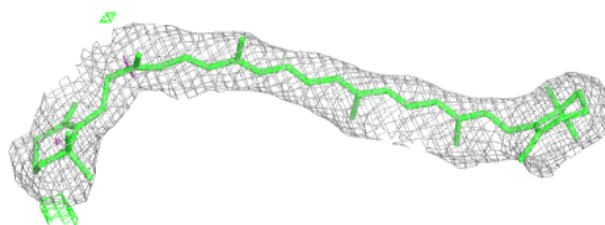
Electron density around CLA C1 514:

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

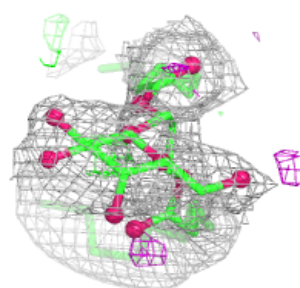
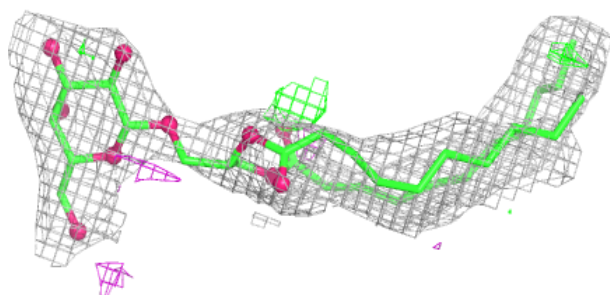
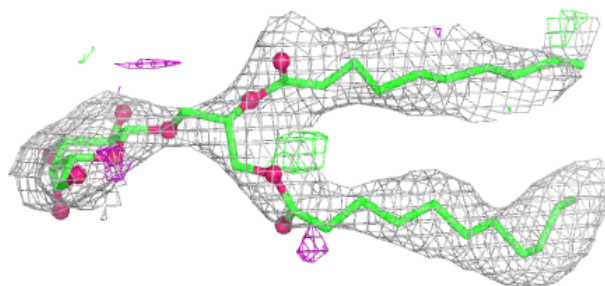


Electron density around BCR B2 602:

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

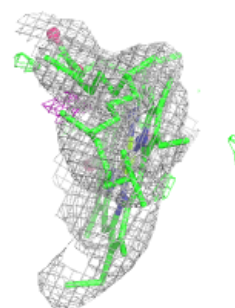
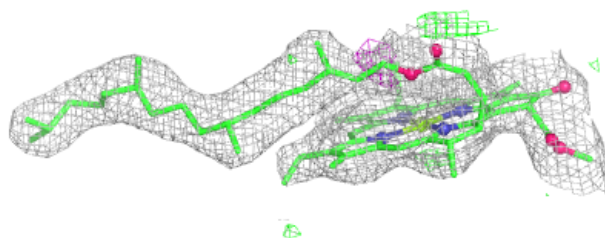
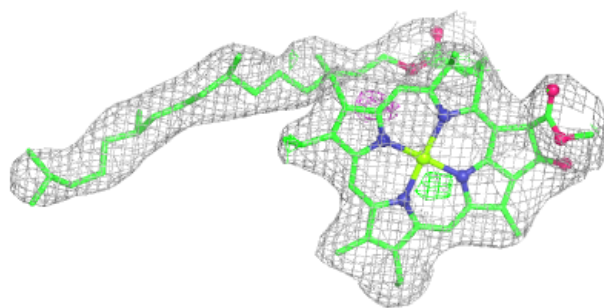
**Electron density around LMG B2 620:**

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

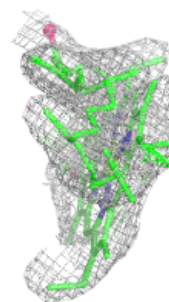
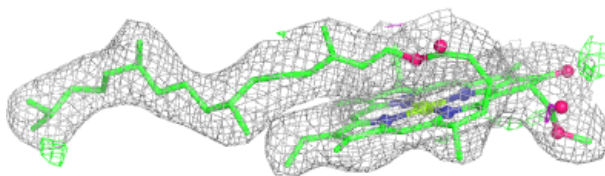
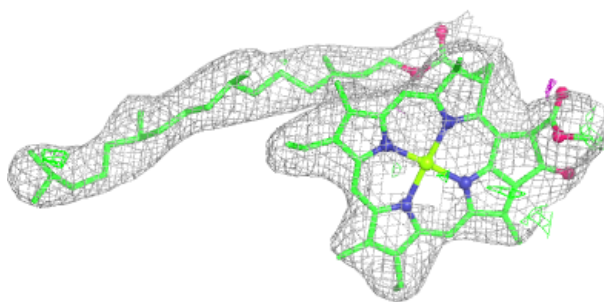


Electron density around CLA c1 503:

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

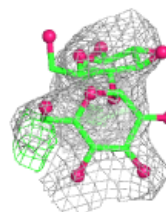
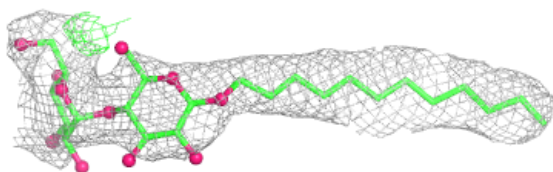
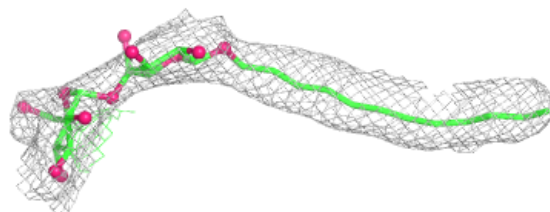
**Electron density around CLA C1 502:**

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



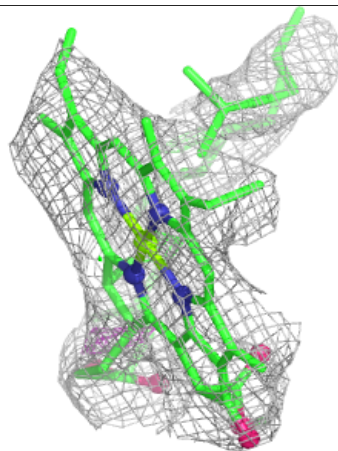
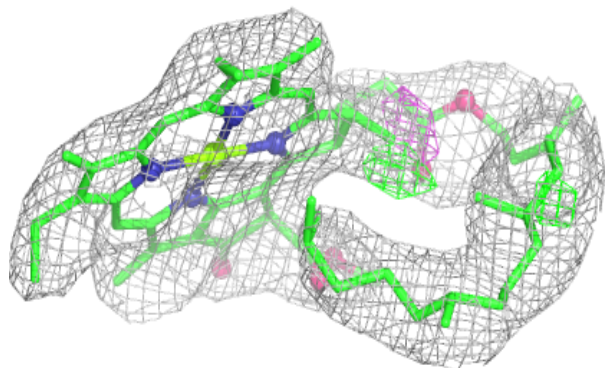
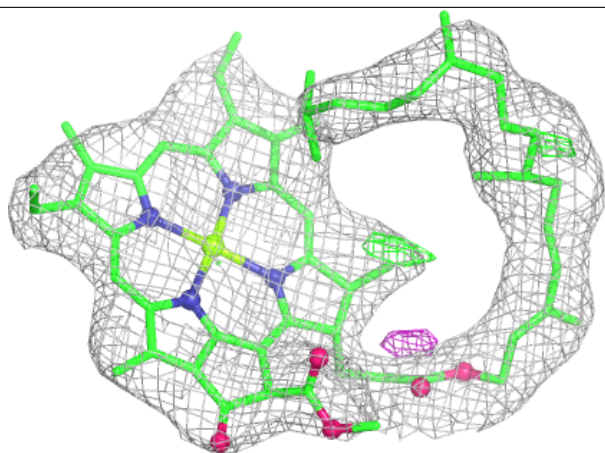
Electron density around LMT b2 623:

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

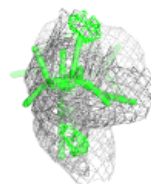
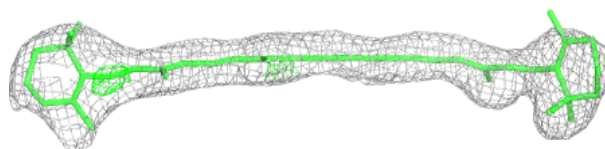
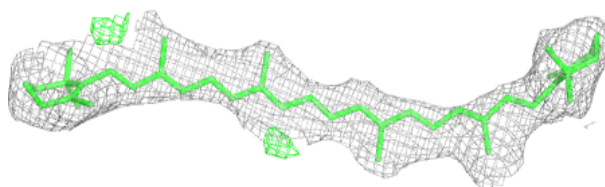


Electron density around CLA b2 618:

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

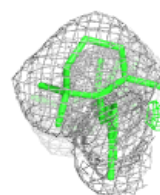
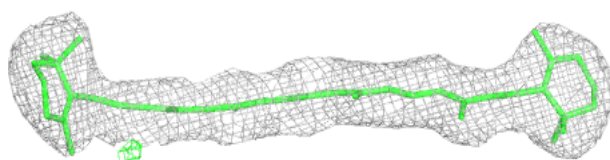
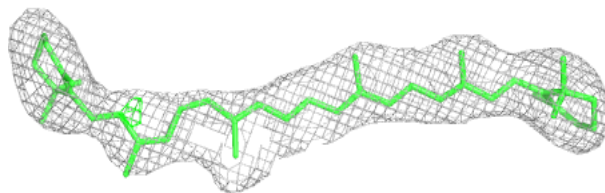
**Electron density around BCR h2 101:**

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

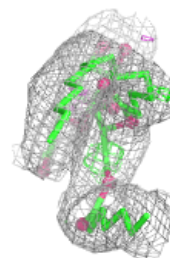
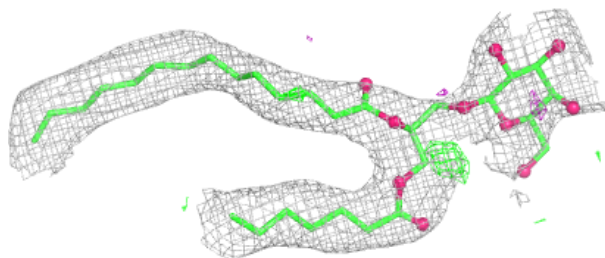


Electron density around BCR c1 502:

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

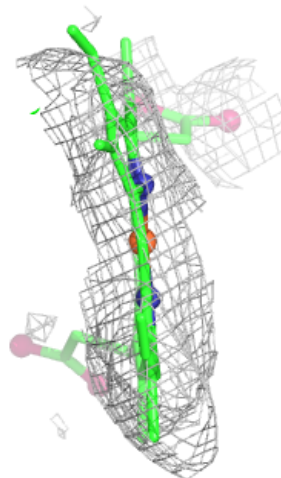
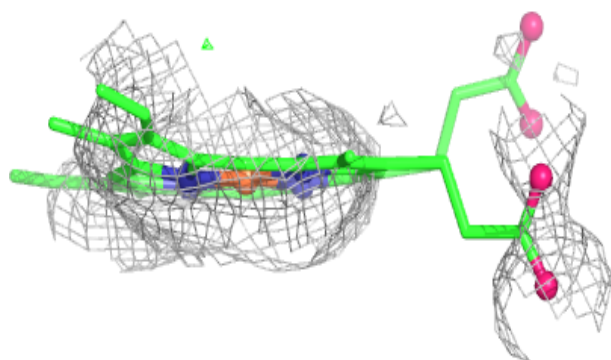
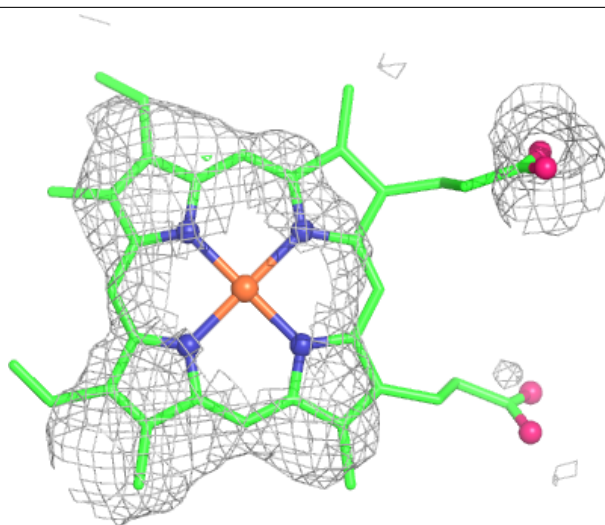
**Electron density around LMG b1 631:**

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



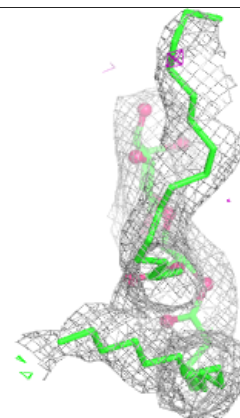
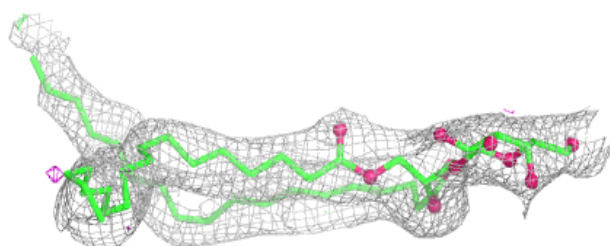
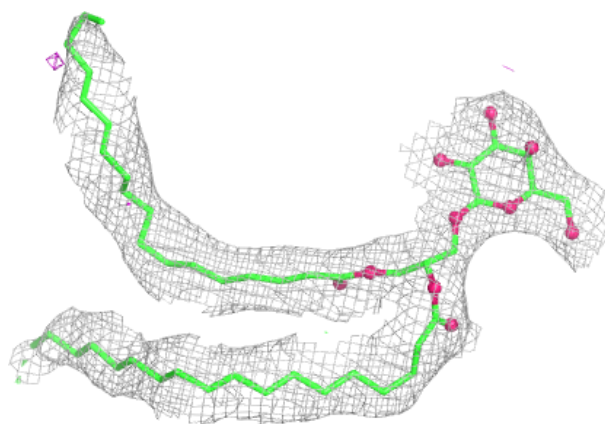
Electron density around HEM E1 101:

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

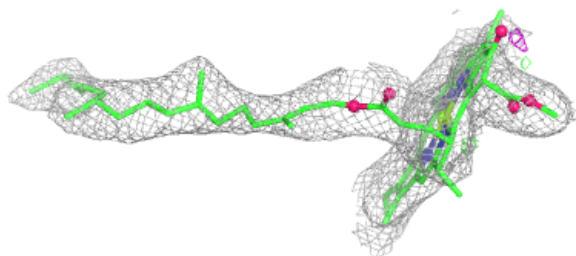
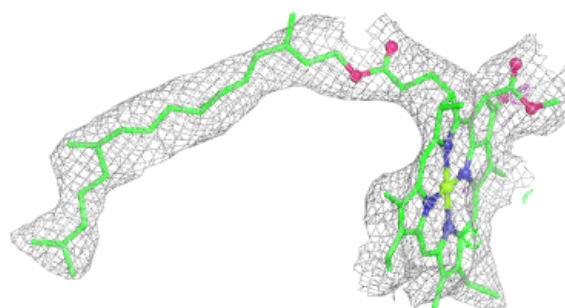


Electron density around LMG c1 519:

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

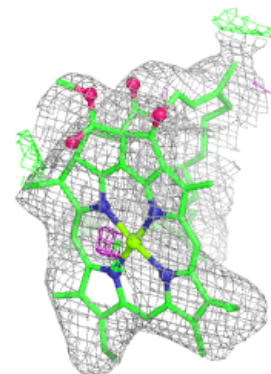
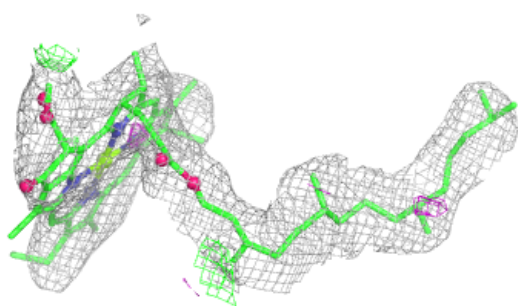
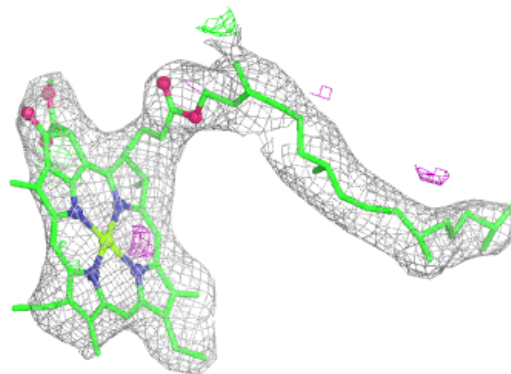
**Electron density around CLA B2 611:**

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

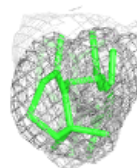
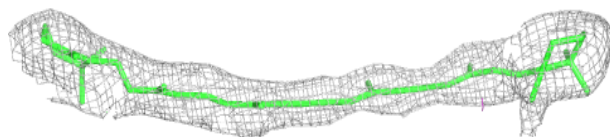
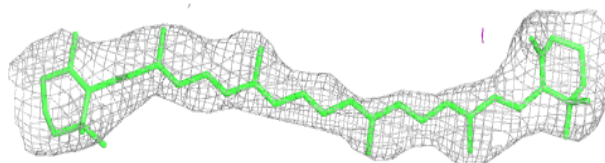


Electron density around CLA c2 512:

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

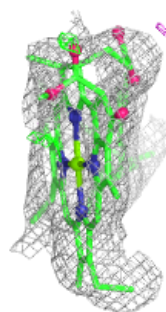
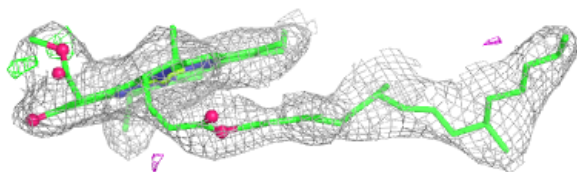
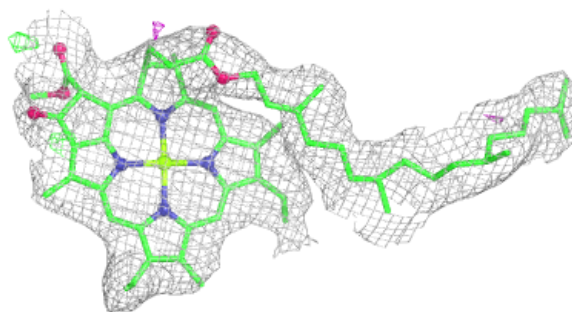
**Electron density around BCR d2 401:**

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

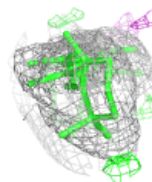
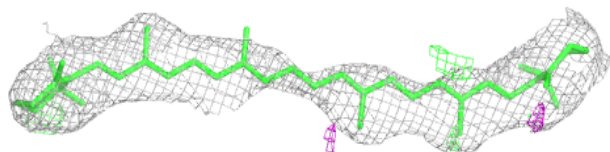
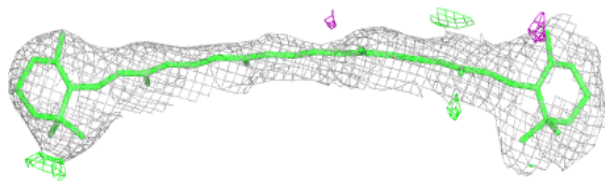


Electron density around CLA B2 606:

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

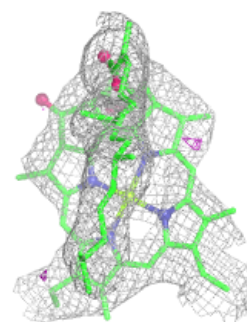
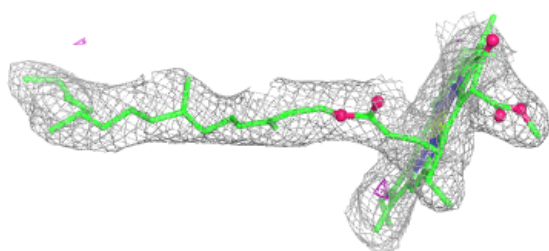
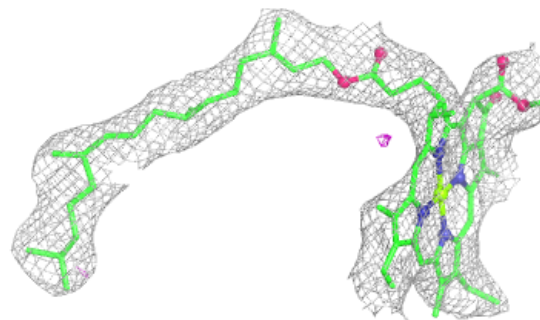
**Electron density around BCR k2 501:**

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

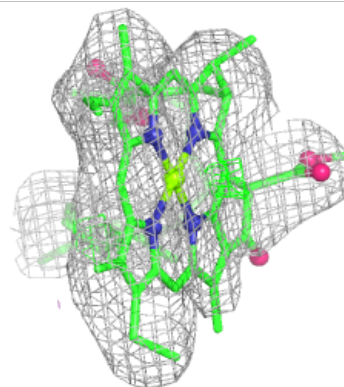
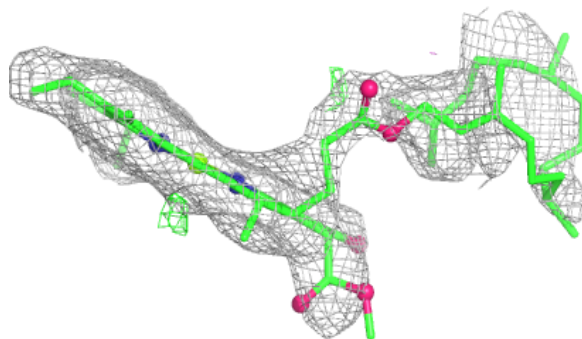
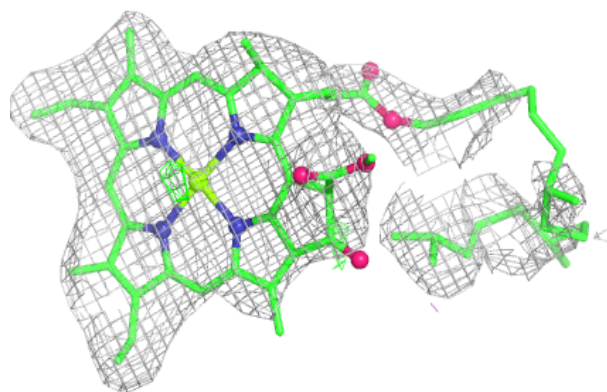


Electron density around CLA b2 610:

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

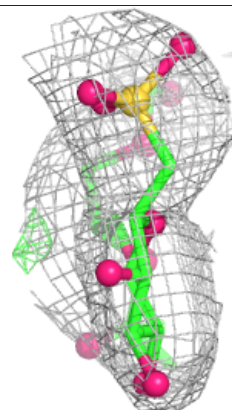
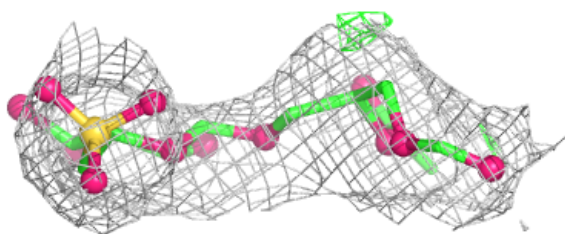
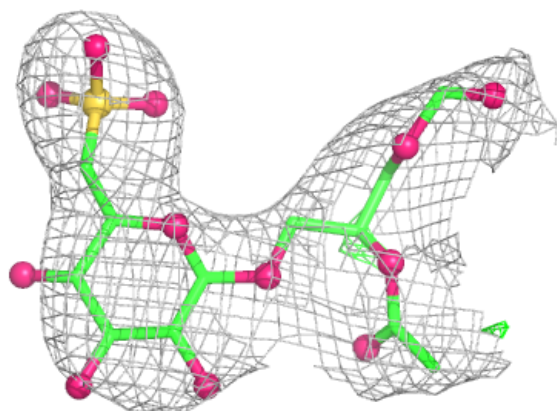
**Electron density around CLA b1 604:**

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

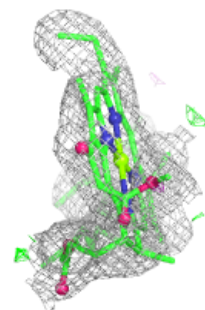
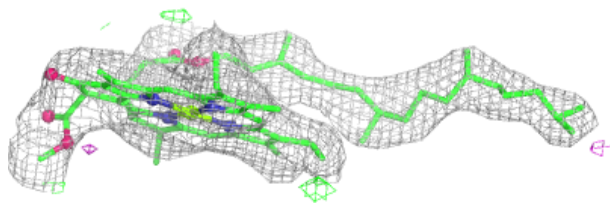
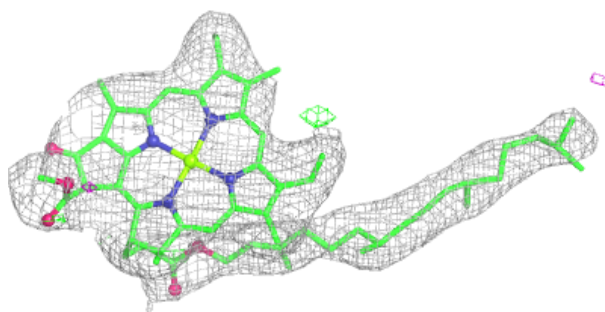


Electron density around SQD D2 402:

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

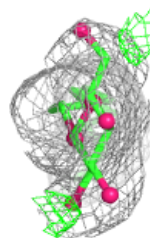
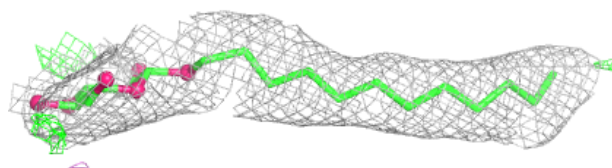
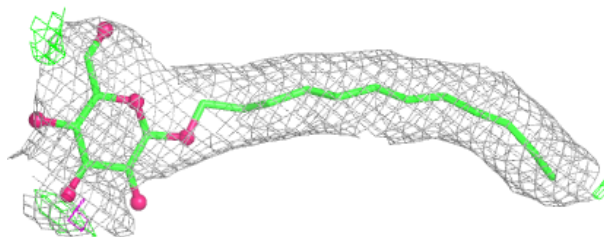
**Electron density around CLA c2 502:**

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



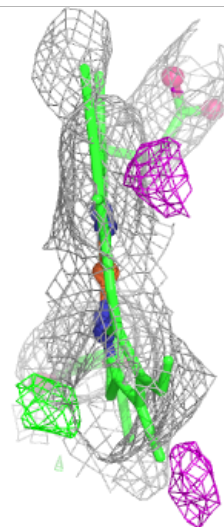
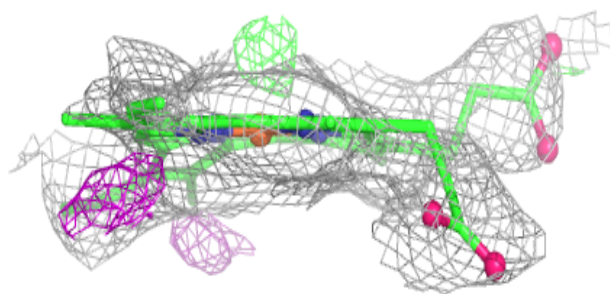
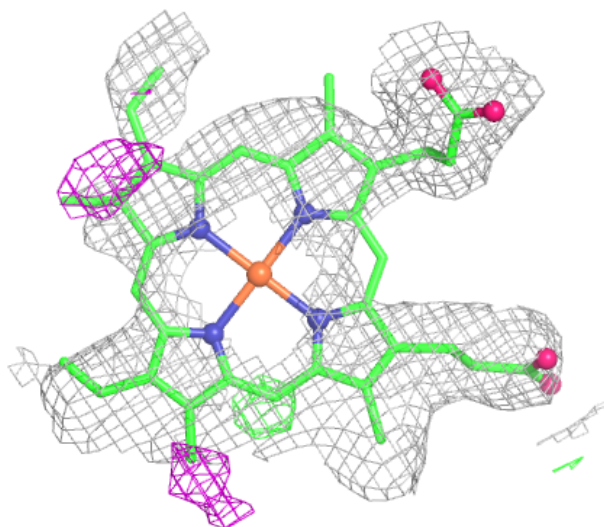
Electron density around LMT 11 101:

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



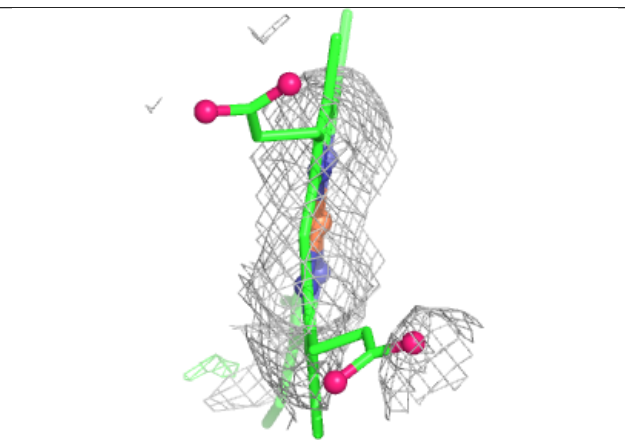
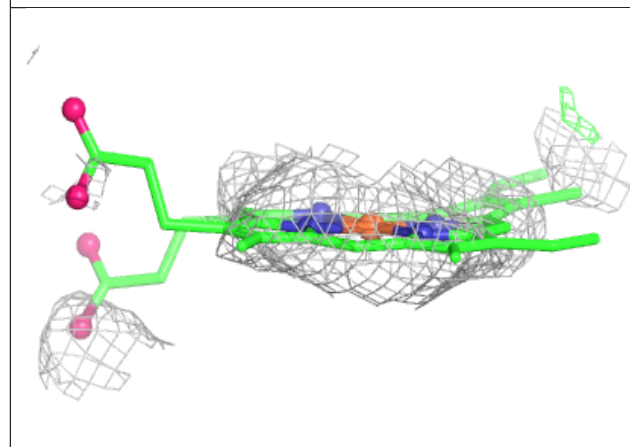
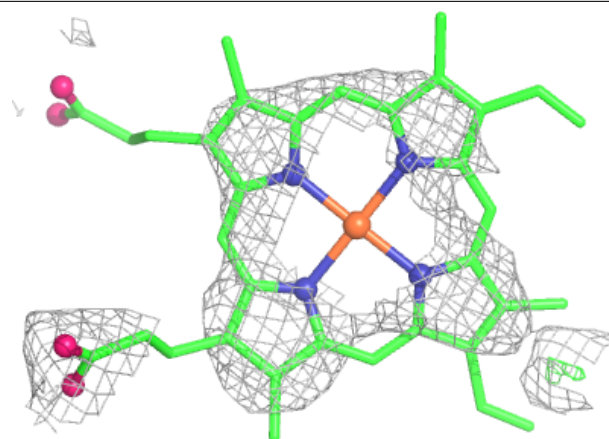
Electron density around HEM V2 201:

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



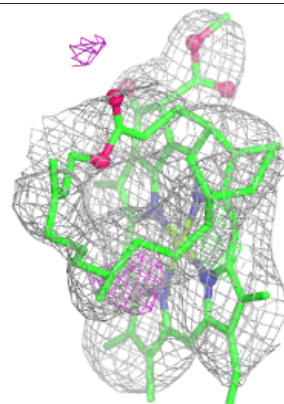
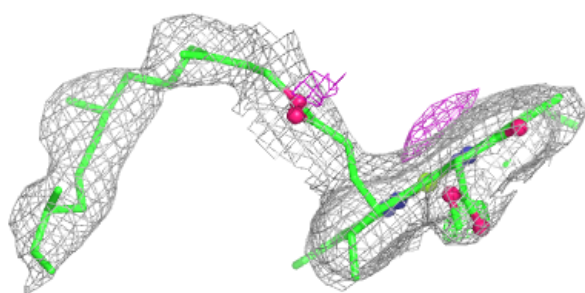
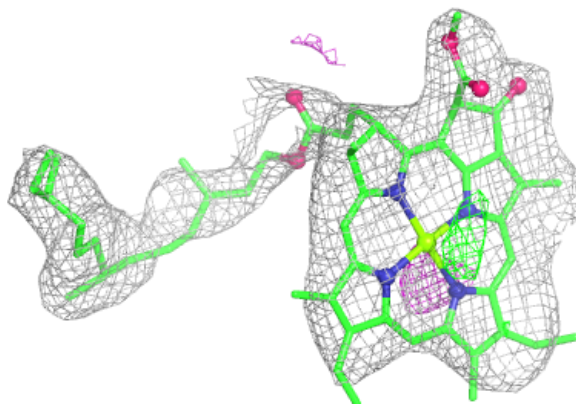
Electron density around HEM e2 101:

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

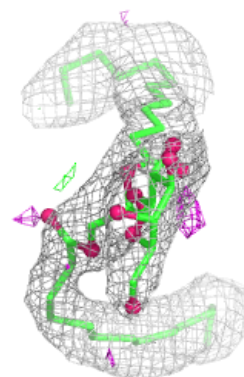
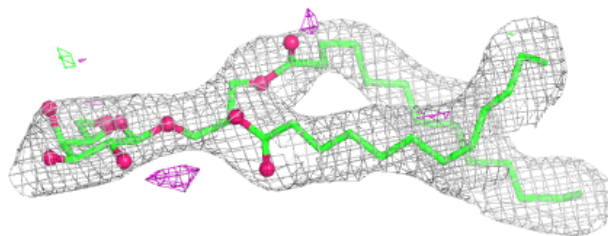
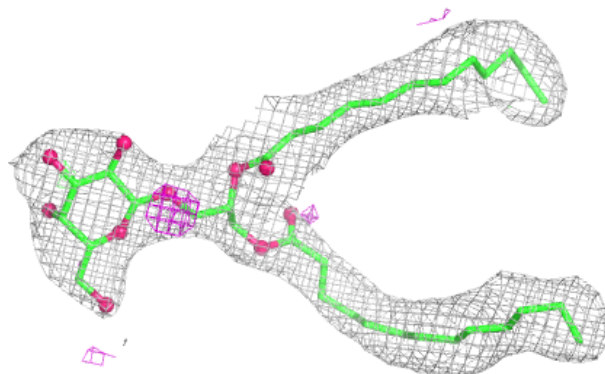


Electron density around CLA A2 403:

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

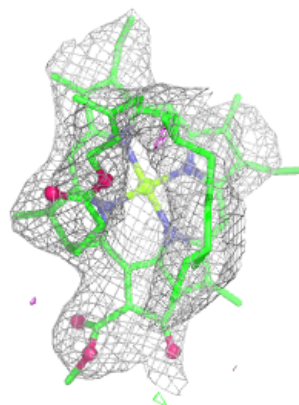
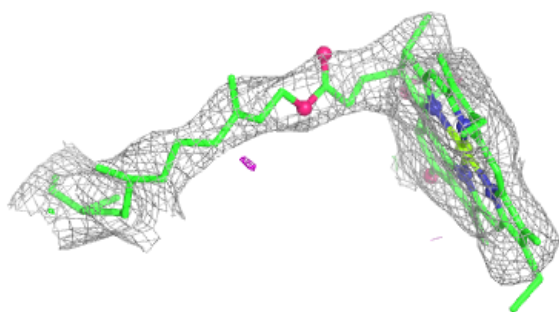
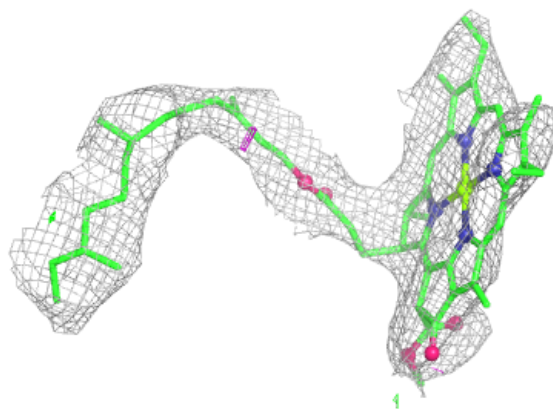
**Electron density around LMG a2 412:**

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



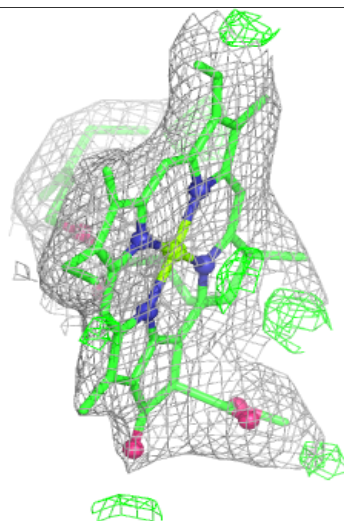
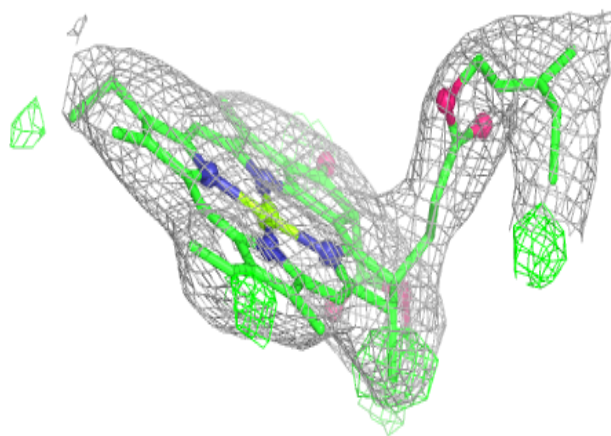
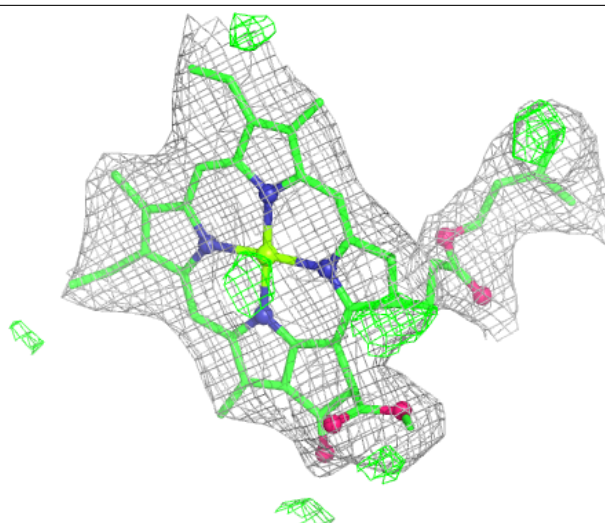
Electron density around CLA b2 609:

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



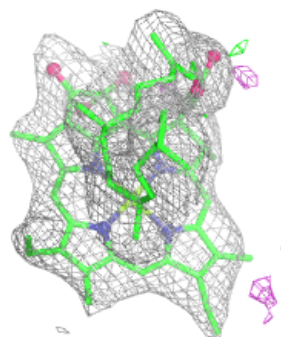
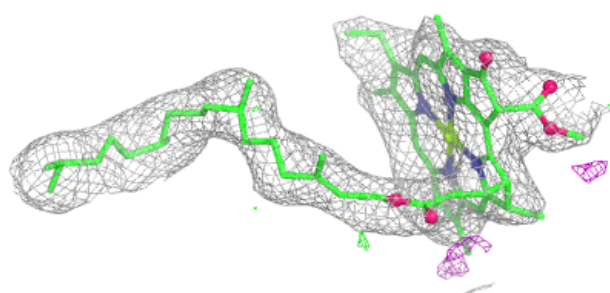
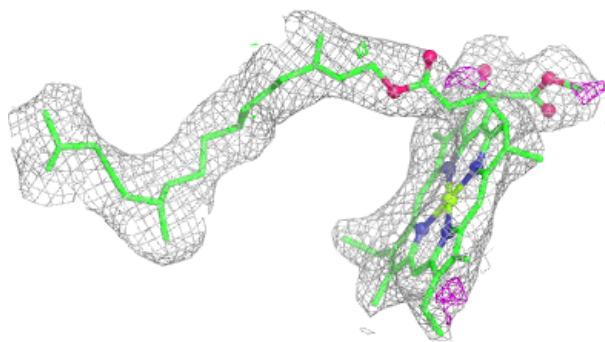
Electron density around CLA A2 404:

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

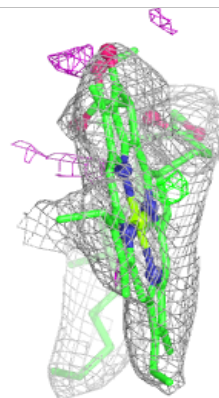
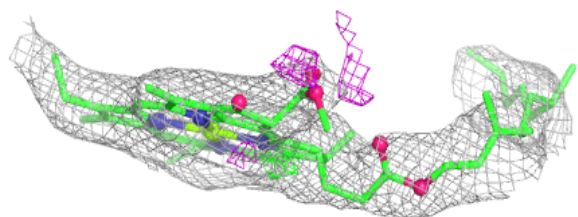
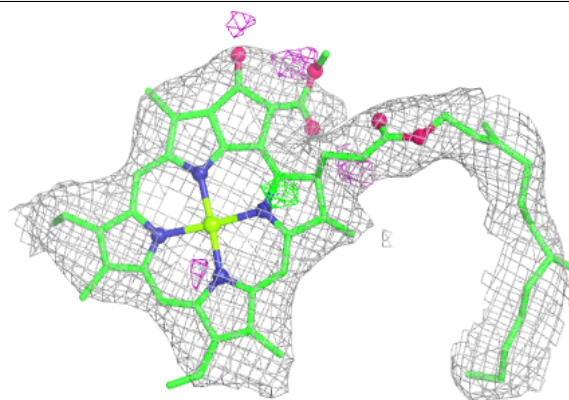


Electron density around CLA C1 509:

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

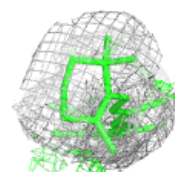
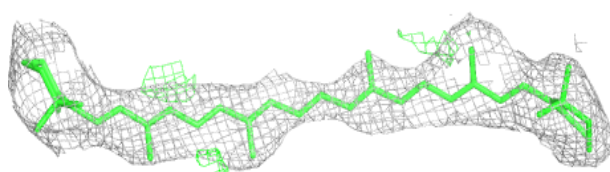
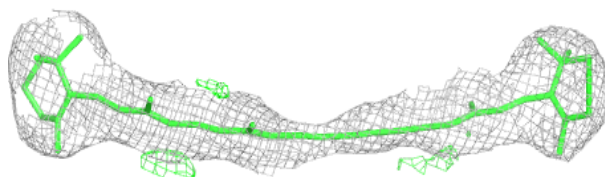
**Electron density around CLA b2 619:**

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

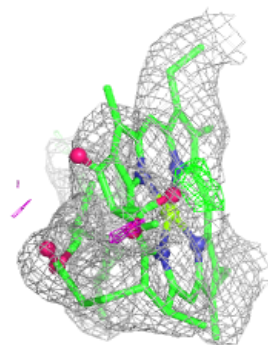
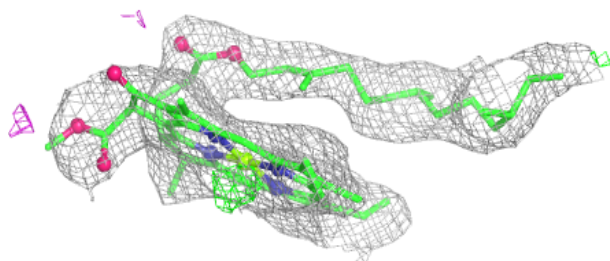
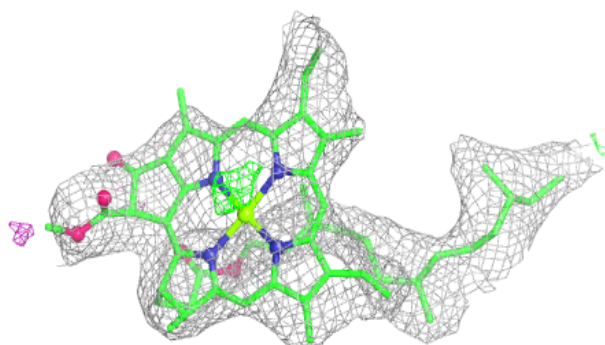


Electron density around BCR c1 501:

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

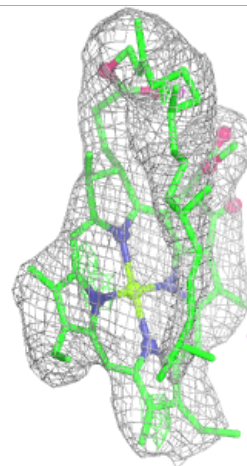
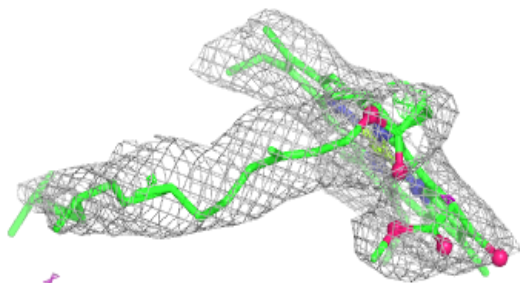
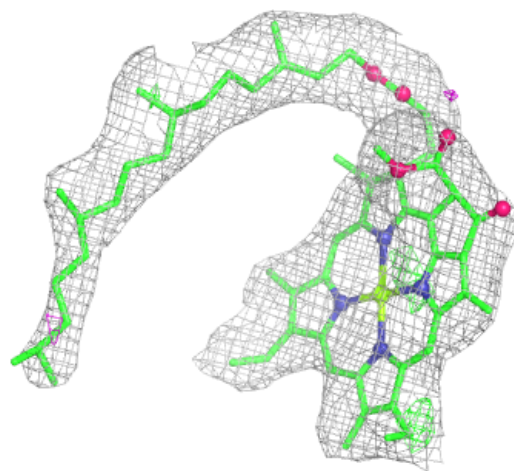
**Electron density around CLA c2 506:**

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



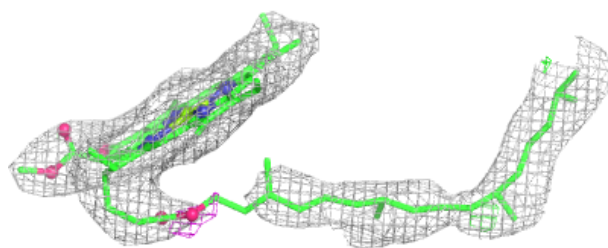
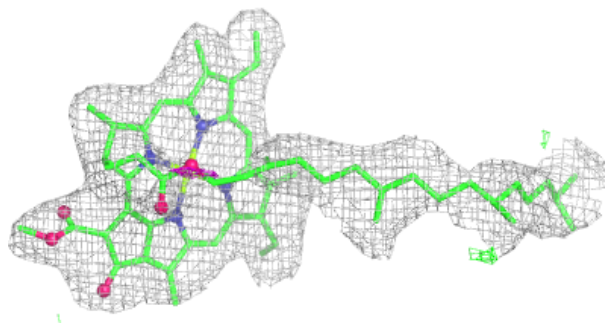
Electron density around CLA c2 508:

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



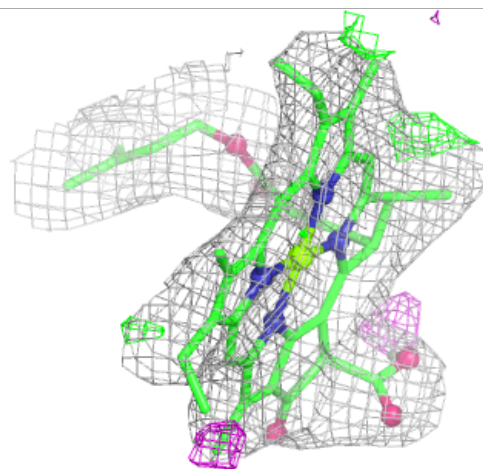
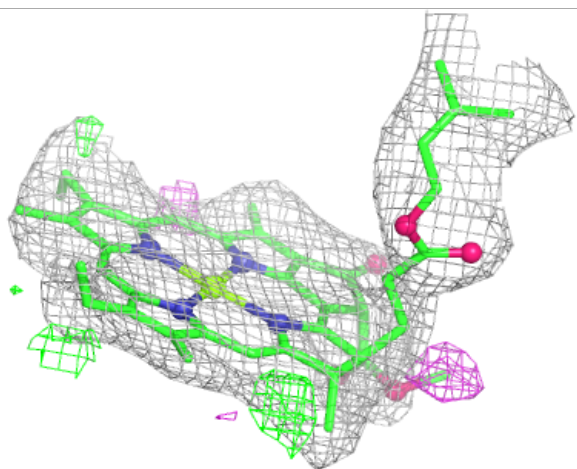
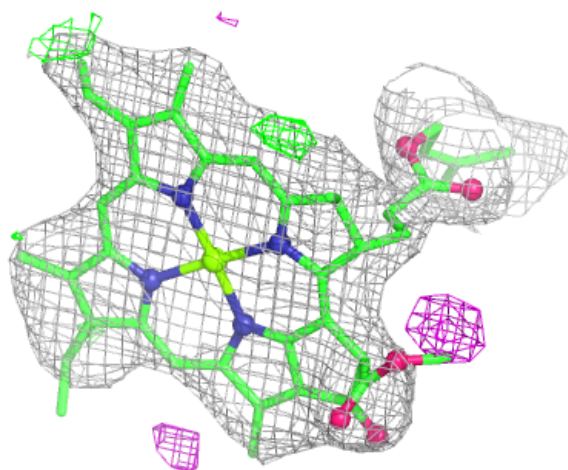
Electron density around CLA B2 610:

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



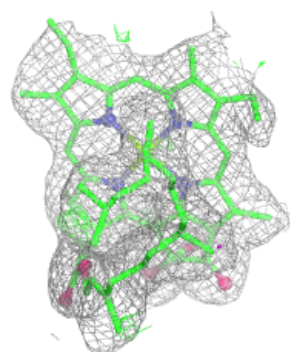
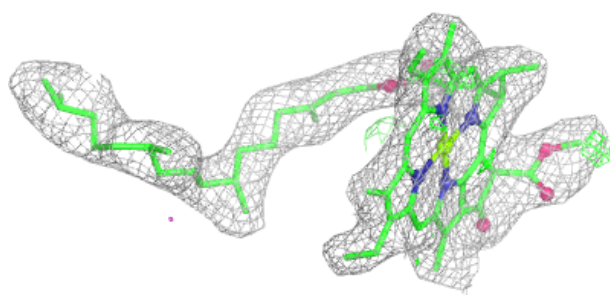
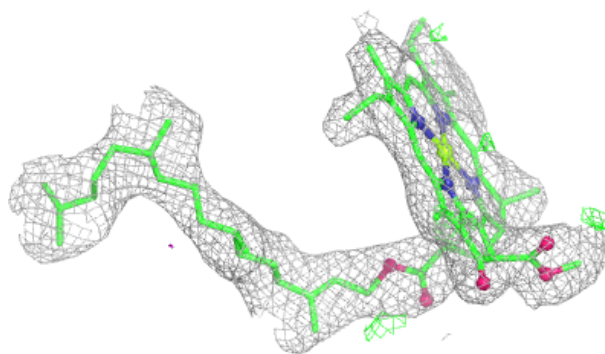
Electron density around CLA c1 508:

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

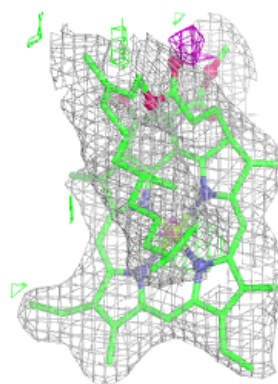
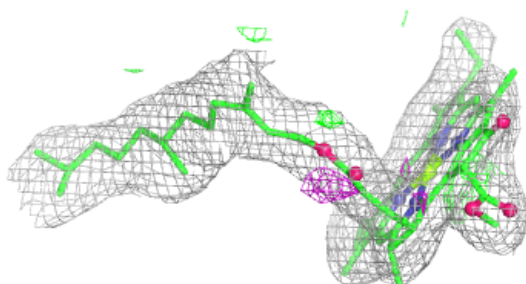
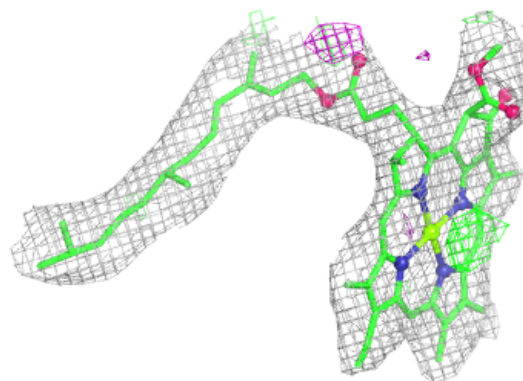


Electron density around CLA c1 510:

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

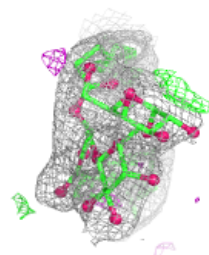
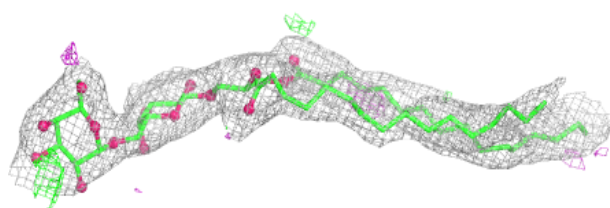
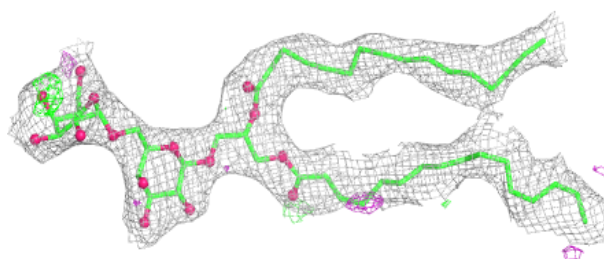
**Electron density around CLA c1 513:**

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

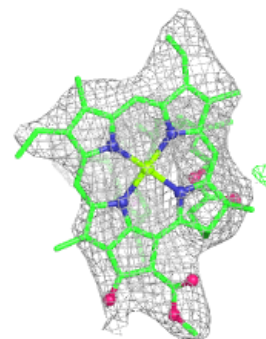
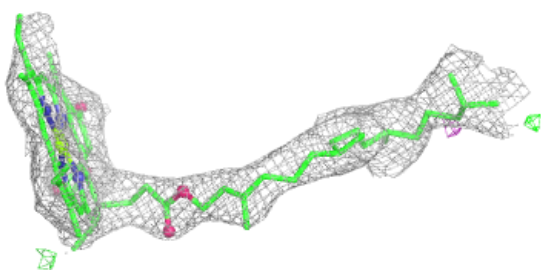
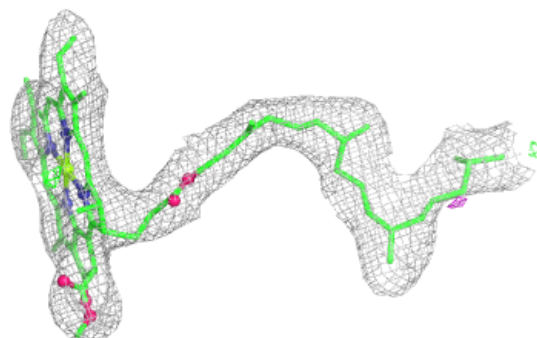


Electron density around DGD c1 520:

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

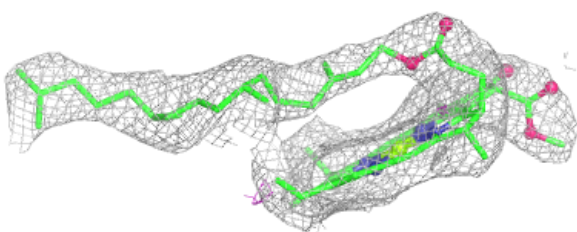
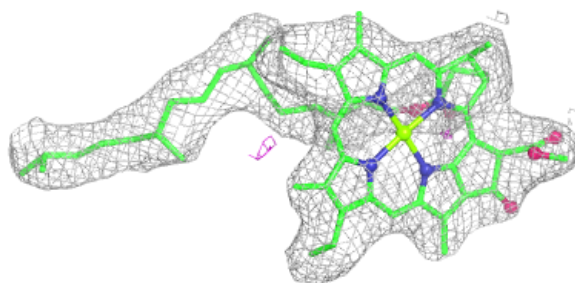
**Electron density around CLA B1 609:**

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



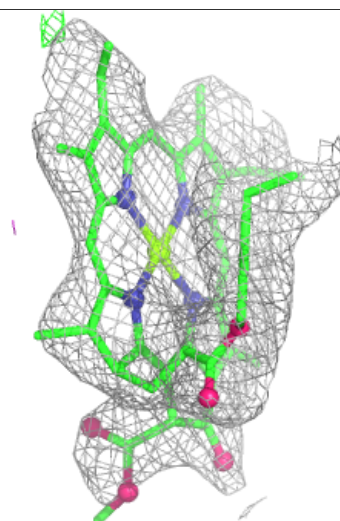
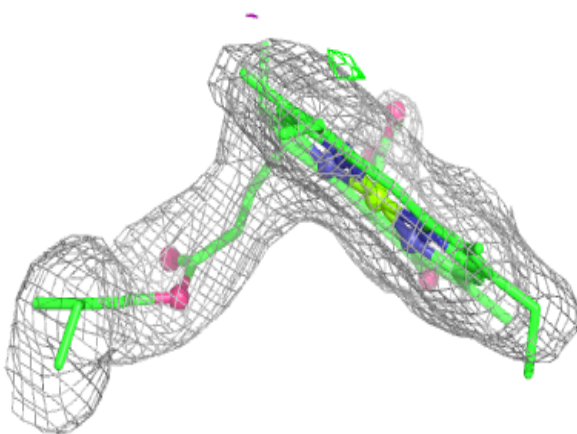
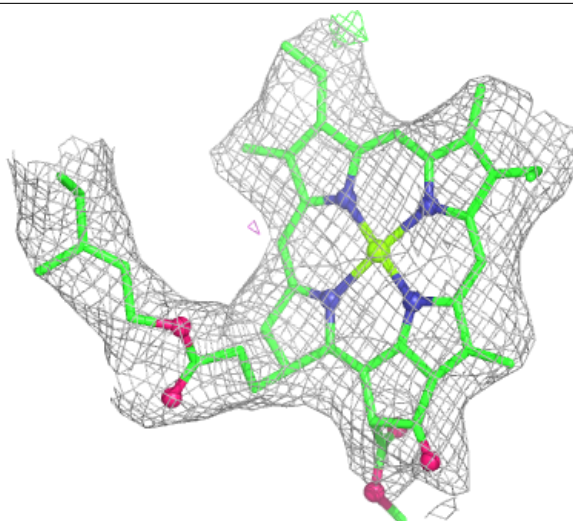
Electron density around CLA C1 506:

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



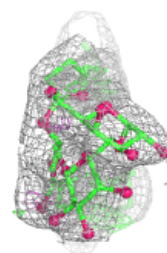
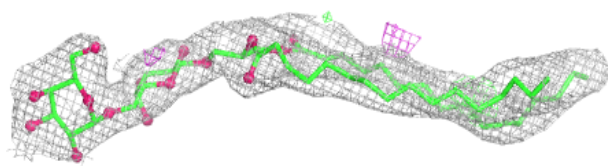
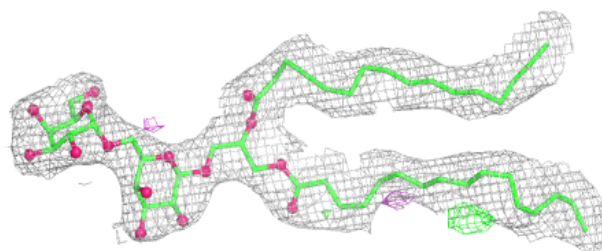
Electron density around CLA D1 403:

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



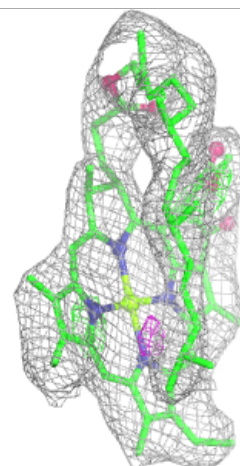
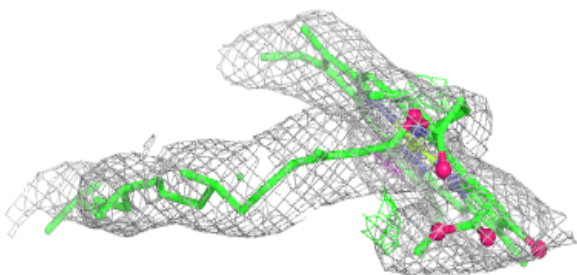
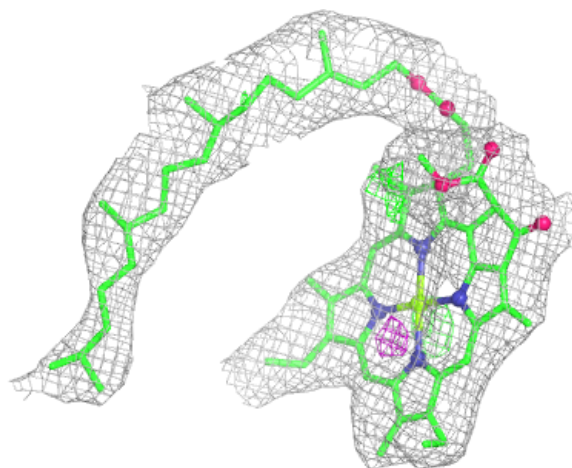
Electron density around DGD c2 517:

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



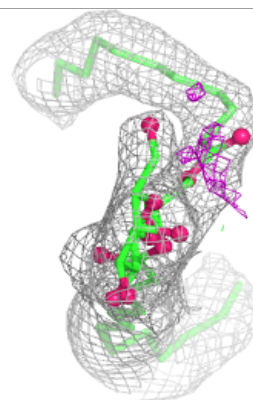
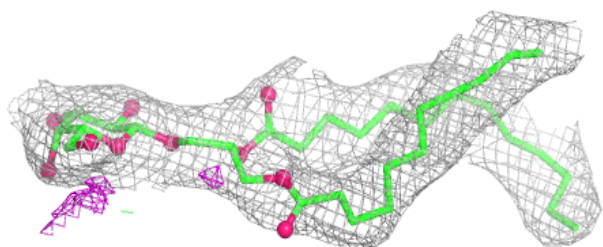
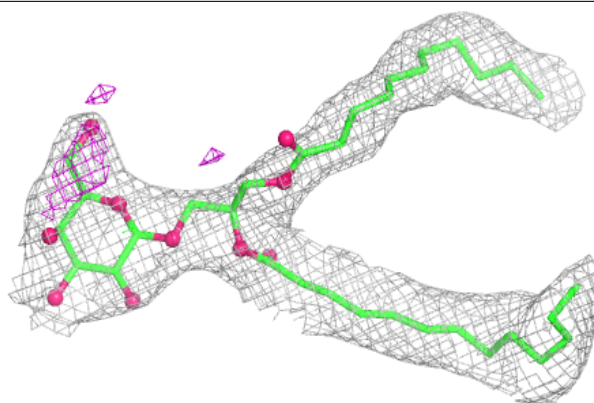
Electron density around CLA c1 509:

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

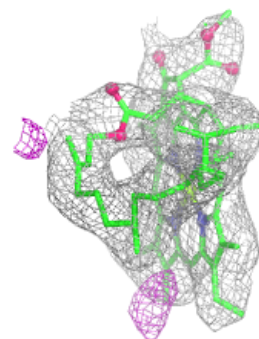
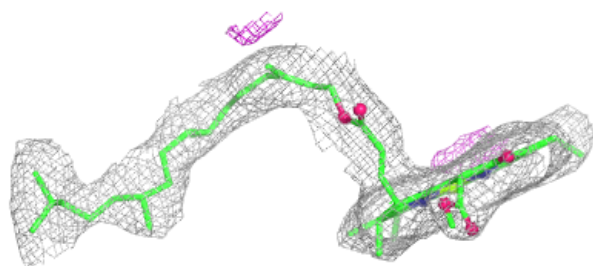
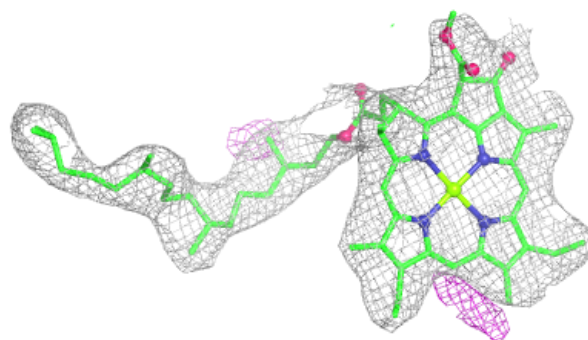


Electron density around LMG A1 410:

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

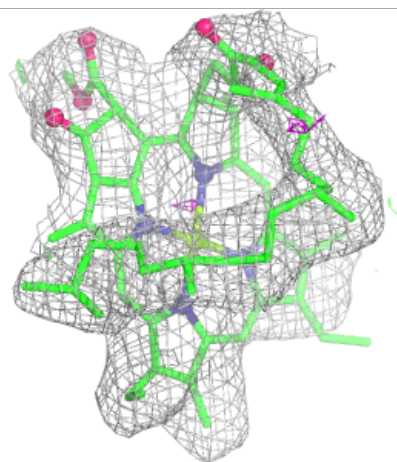
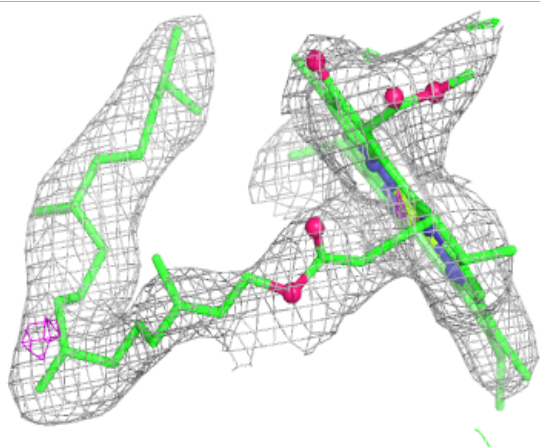
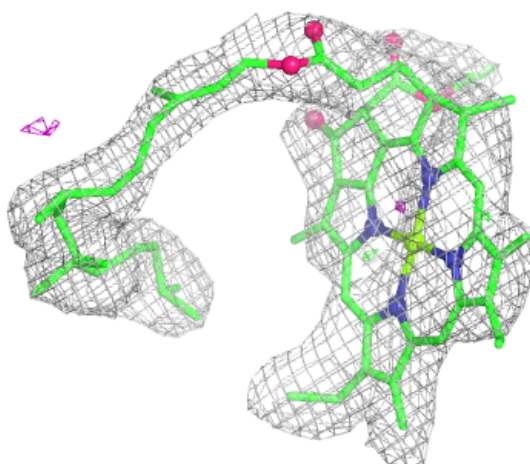
**Electron density around CLA a2 405:**

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



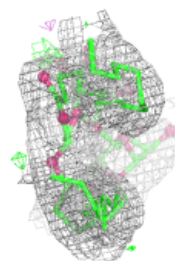
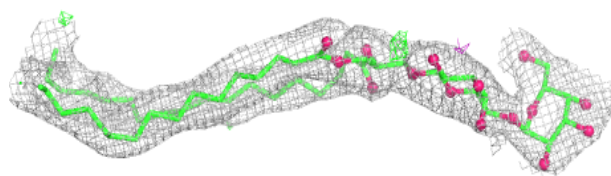
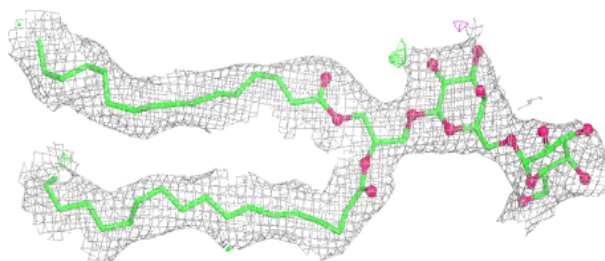
Electron density around CLA c1 505:

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



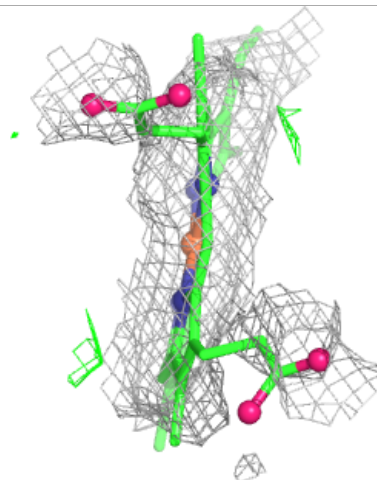
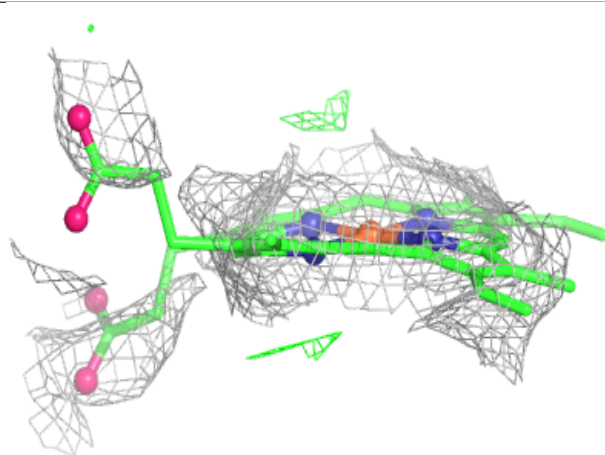
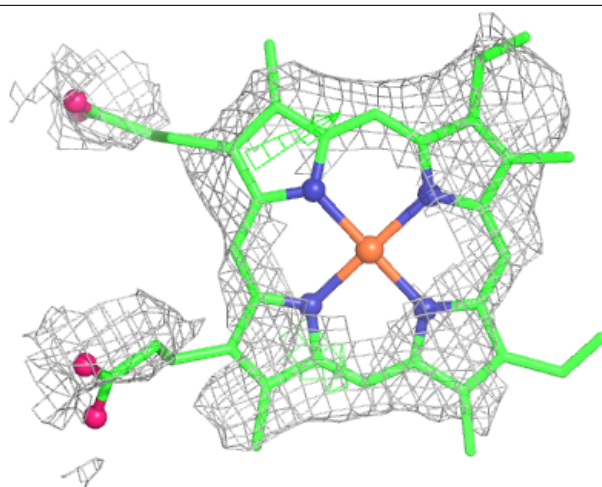
Electron density around DGD C1 517:

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



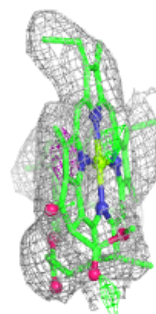
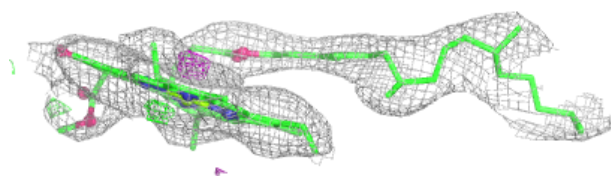
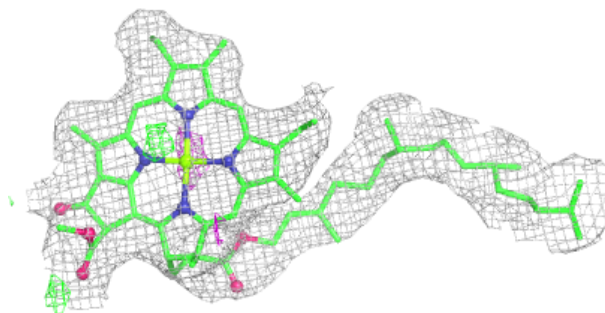
Electron density around HEM E2 101:

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

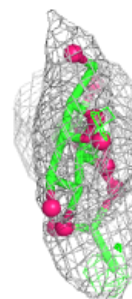
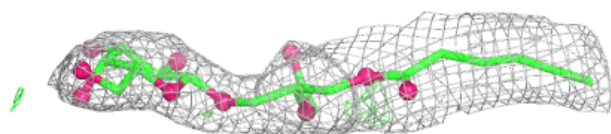
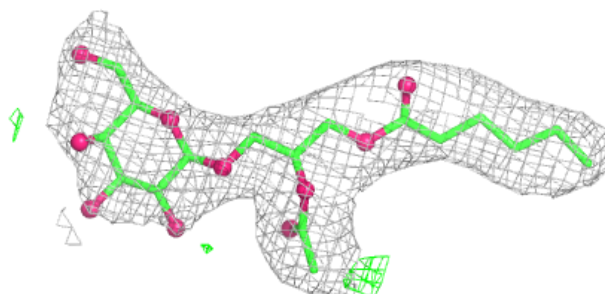


Electron density around CLA B1 606:

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

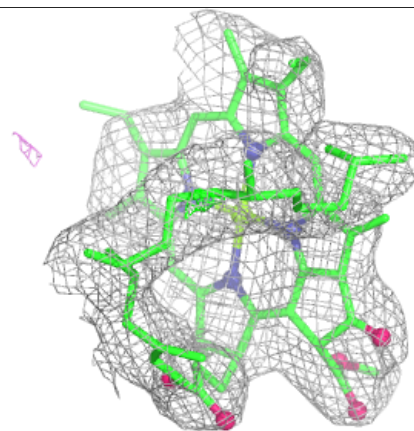
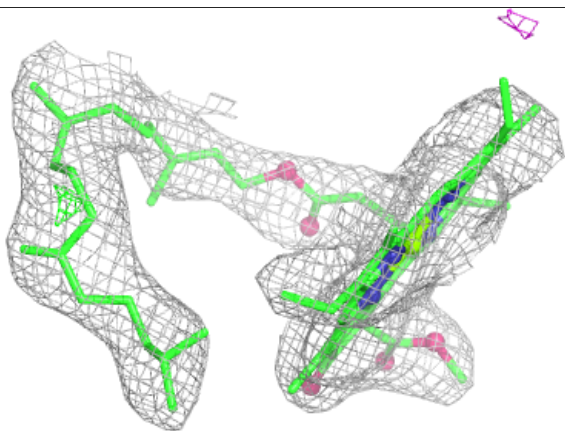
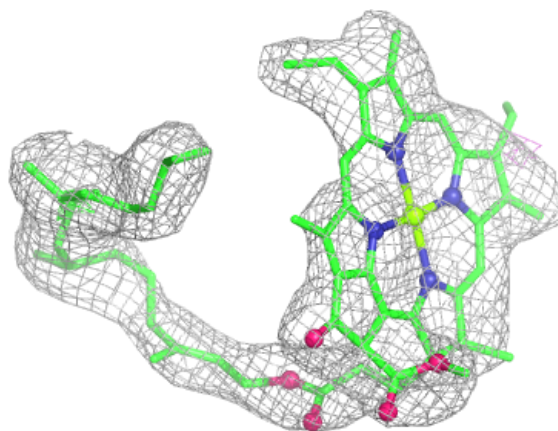
**Electron density around LMG d2 407:**

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



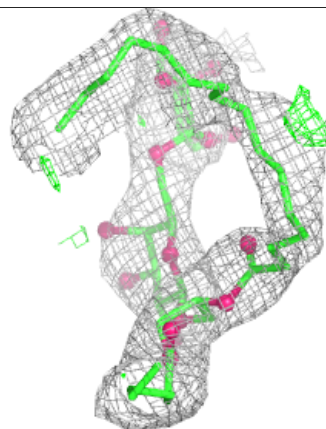
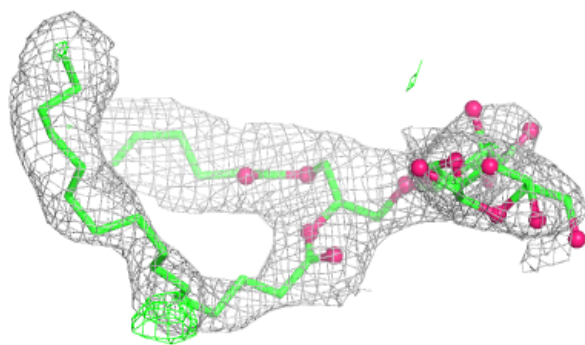
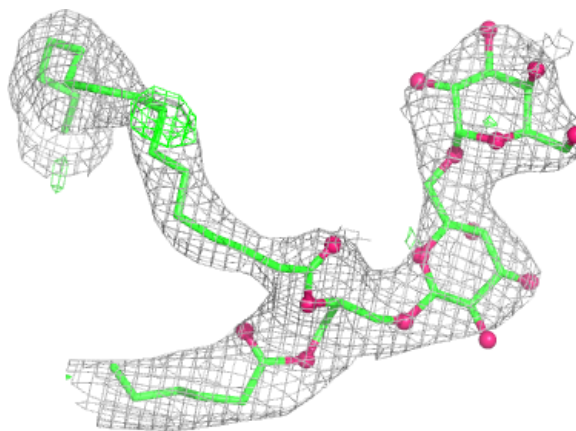
Electron density around CLA c2 504:

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

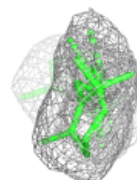
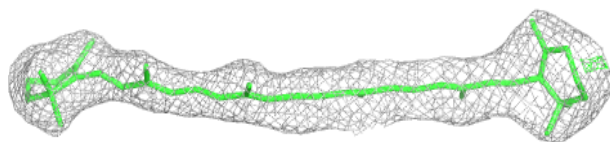
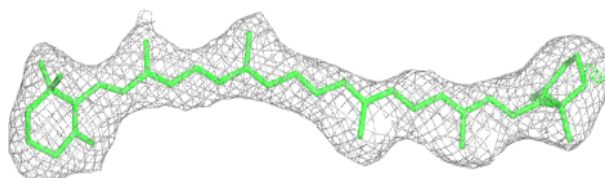


Electron density around DGD c2 516:

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

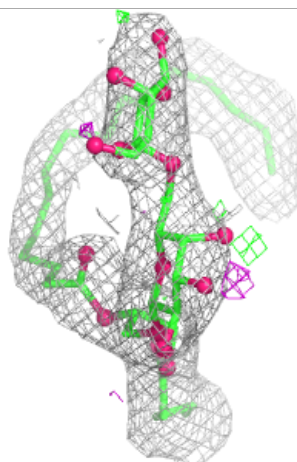
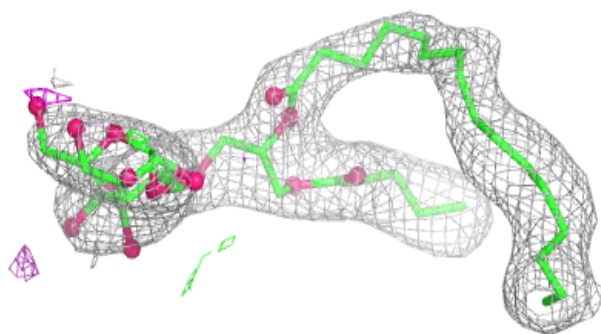
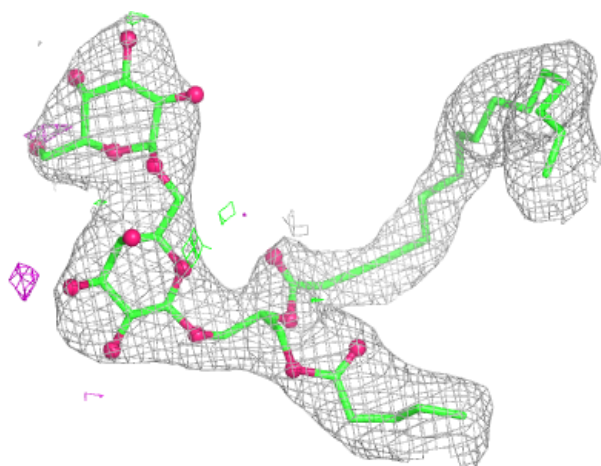
**Electron density around BCR b2 601:**

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



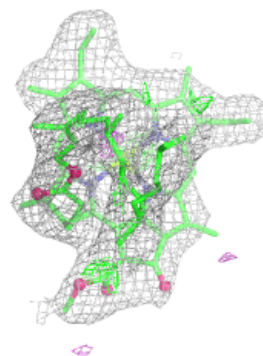
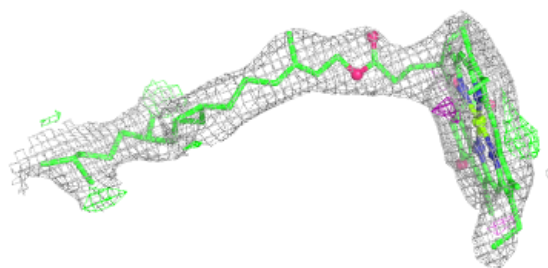
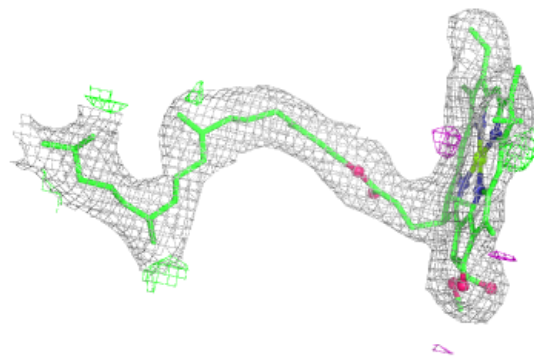
Electron density around DGD c1 514:

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

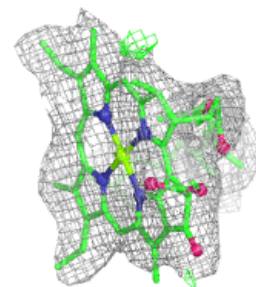
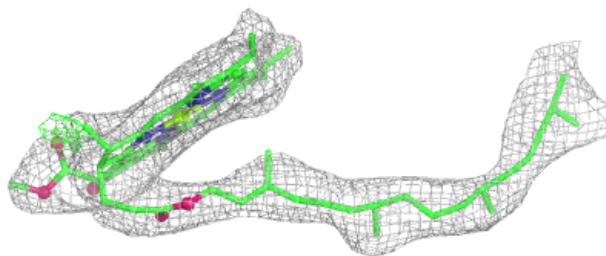
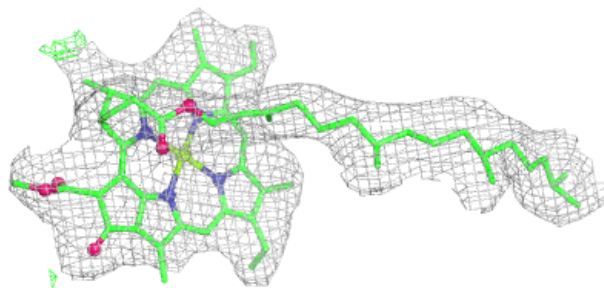


Electron density around CLA b1 609:

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

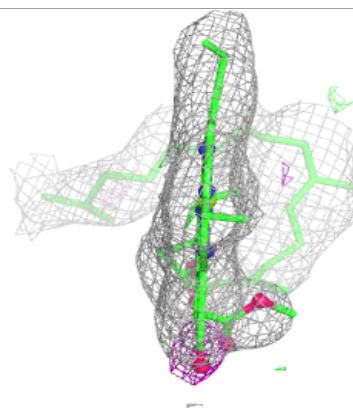
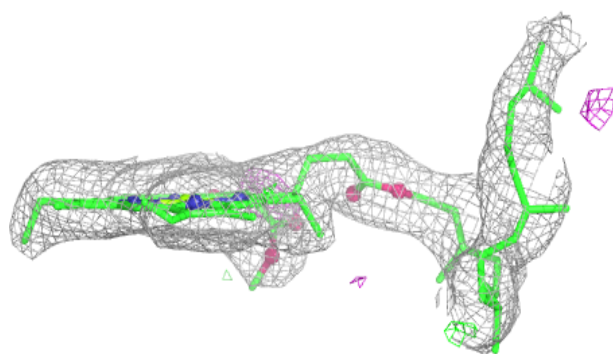
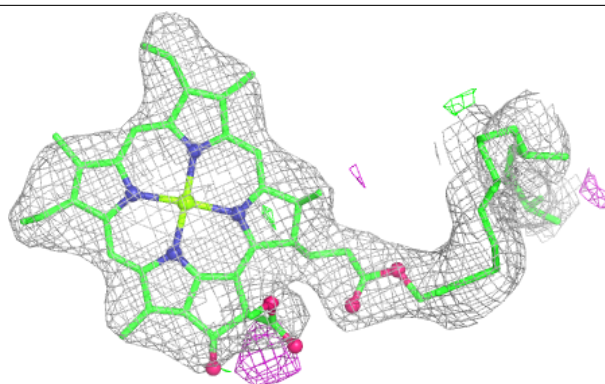
**Electron density around CLA b2 624:**

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

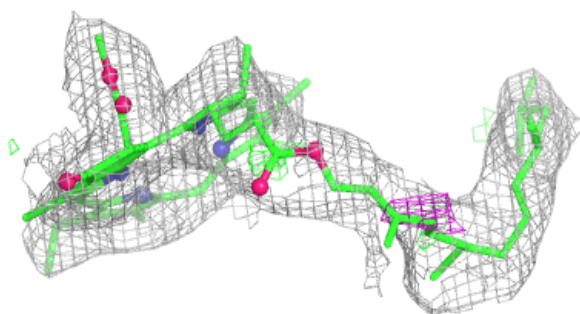
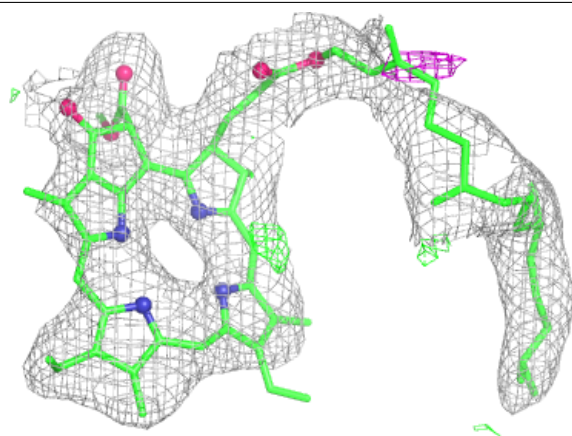


Electron density around CLA b1 619:

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

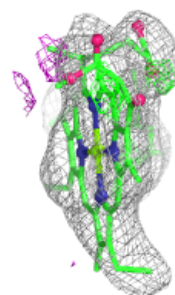
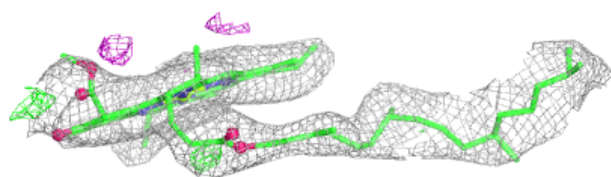
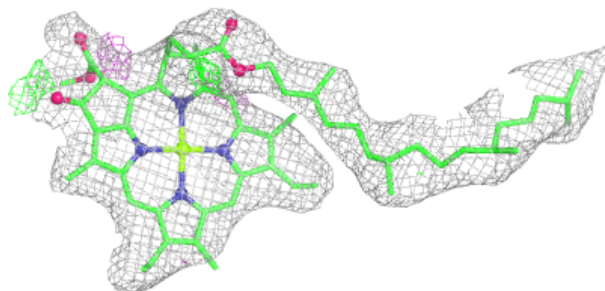
**Electron density around PHO D2 407:**

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



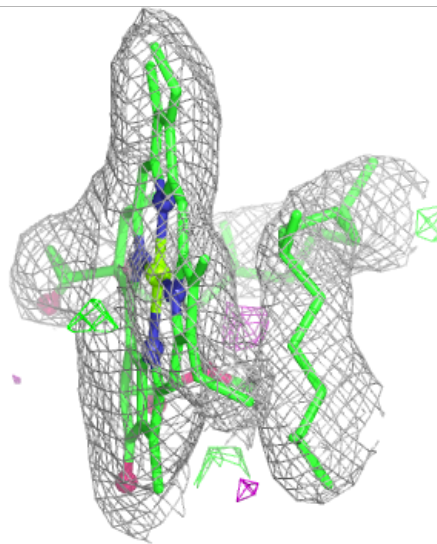
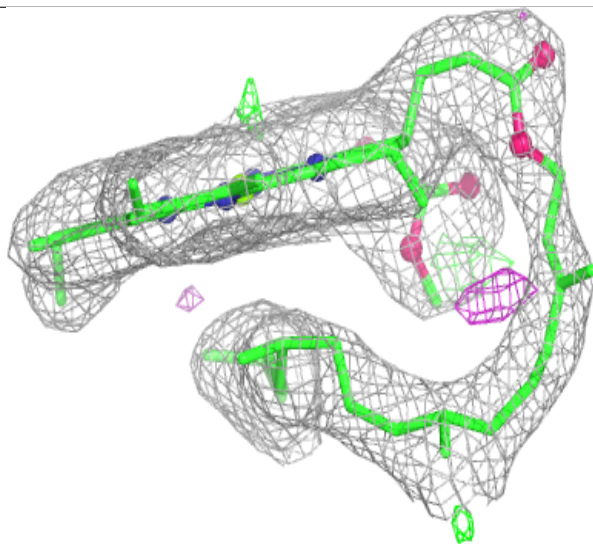
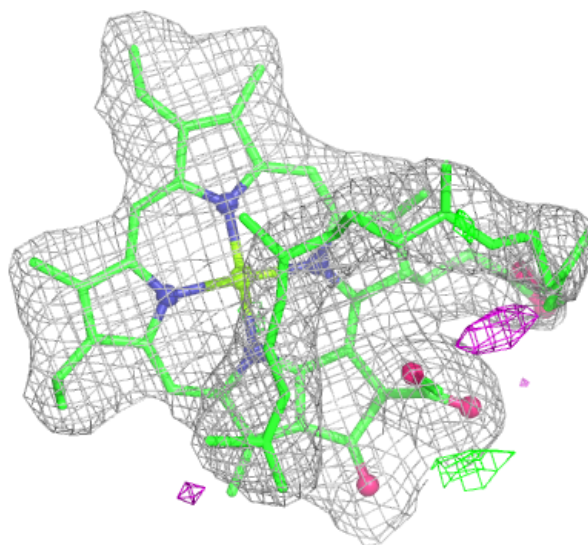
Electron density around CLA b2 606:

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



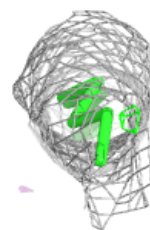
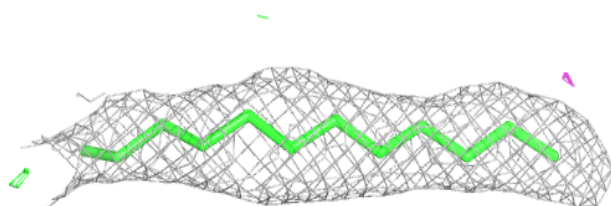
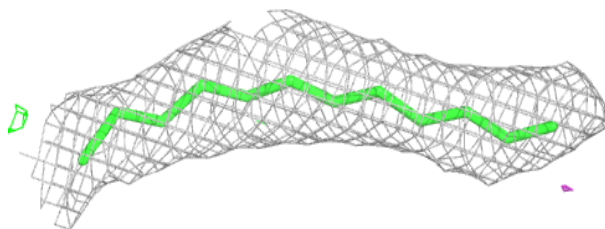
Electron density around CLA C1 511:

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

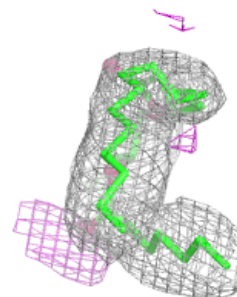
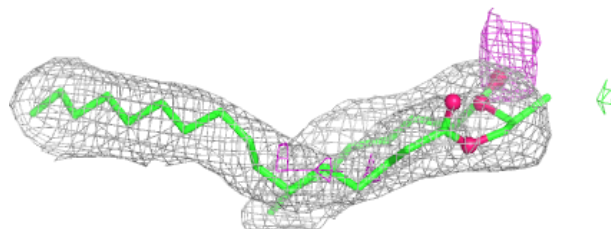
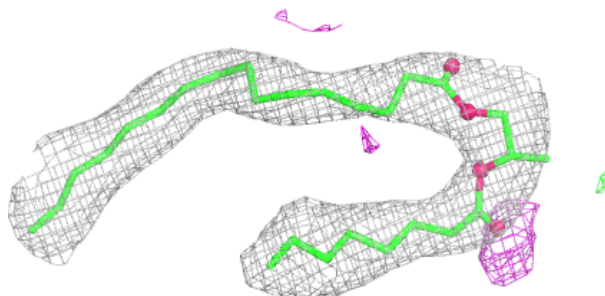


Electron density around LMT L1 102:

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

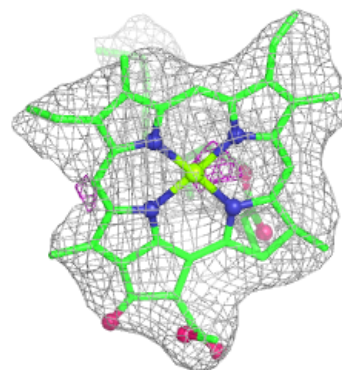
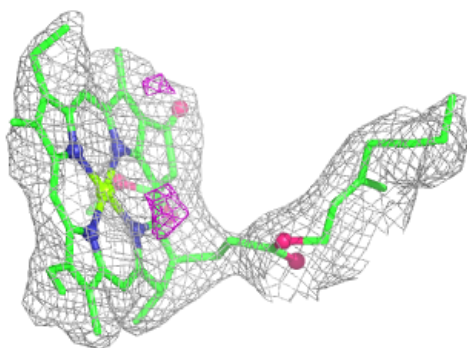
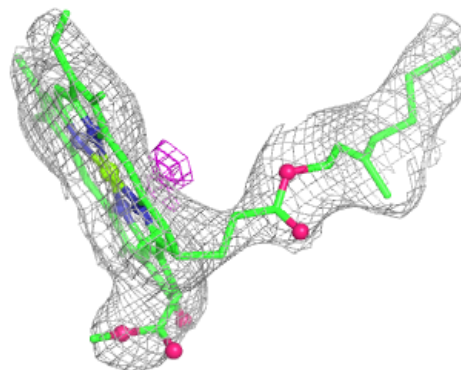
**Electron density around LMG M1 101:**

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

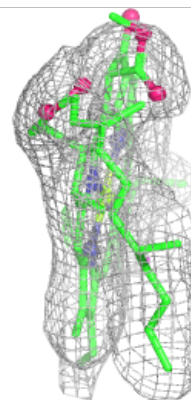
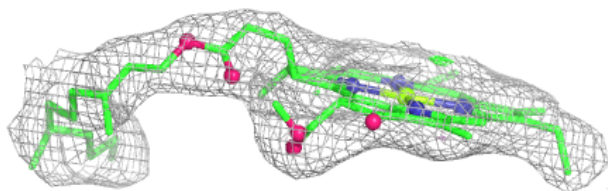
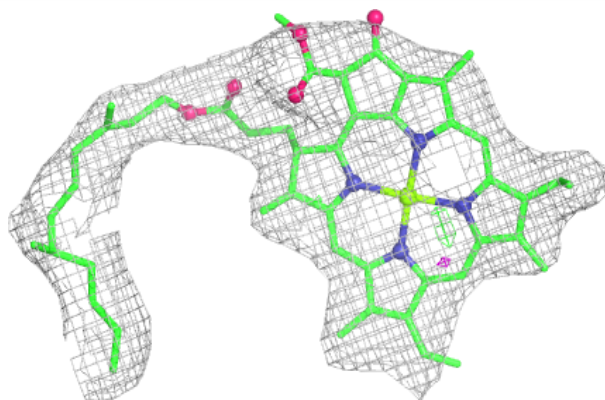


Electron density around CLA c2 507:

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

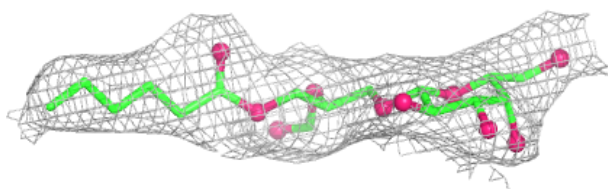
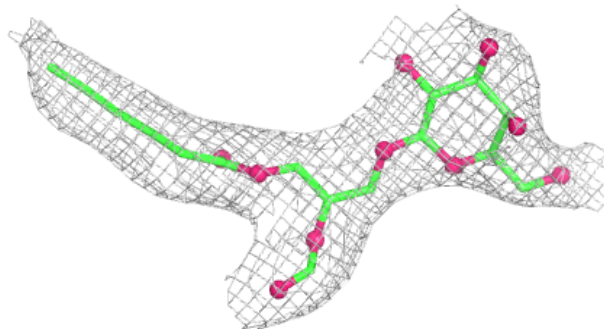
**Electron density around CLA B1 618:**

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

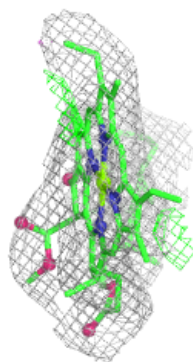
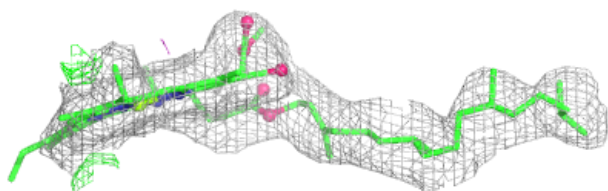
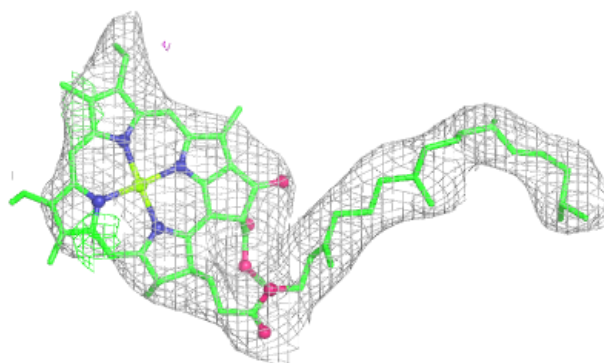


Electron density around LMG c2 519:

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

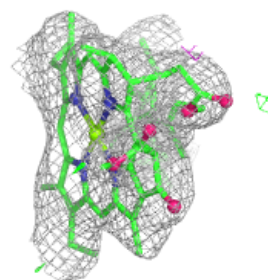
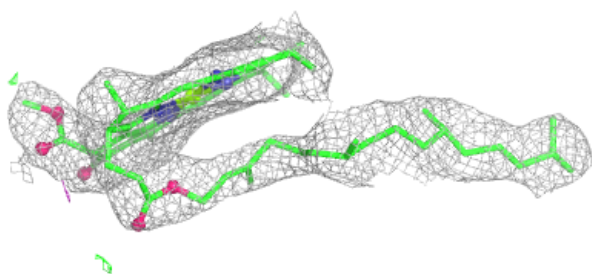
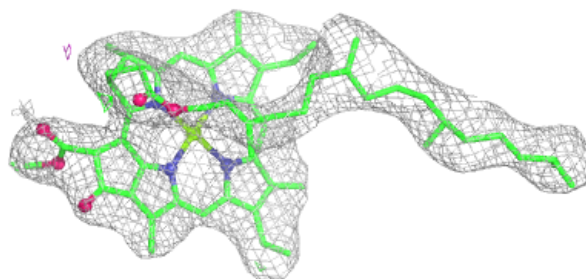
**Electron density around CLA b2 613:**

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

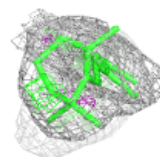
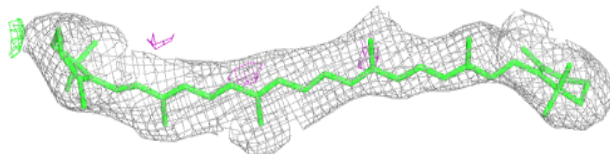
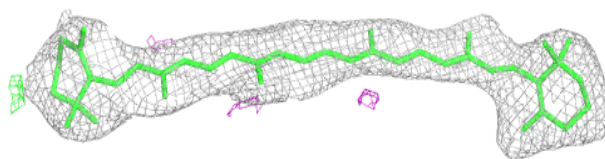


Electron density around CLA c1 507:

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

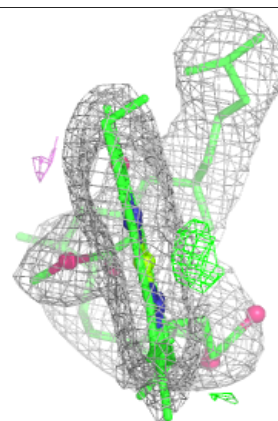
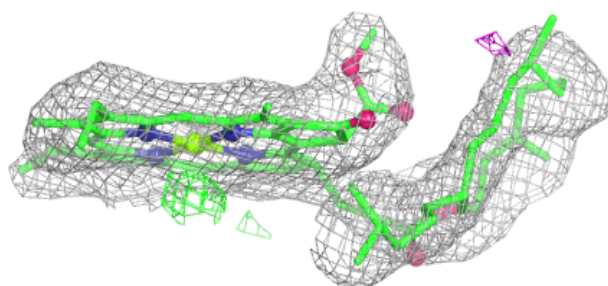
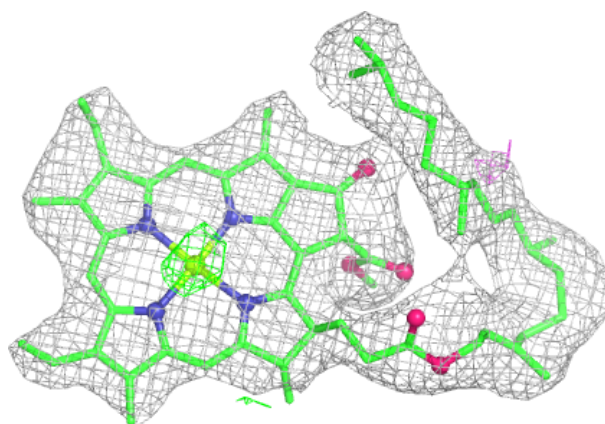
**Electron density around BCR B2 603:**

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



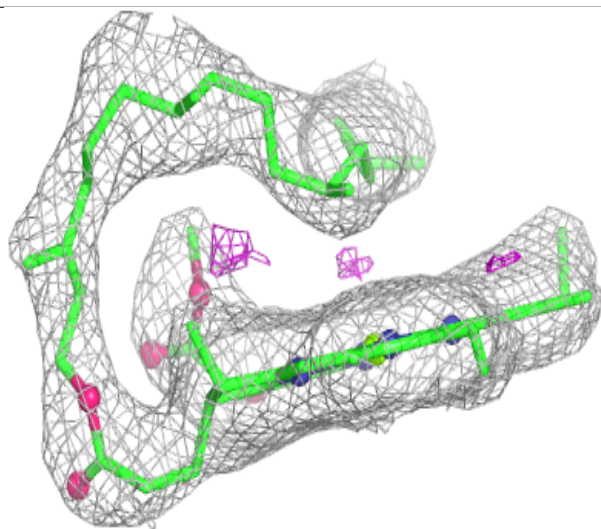
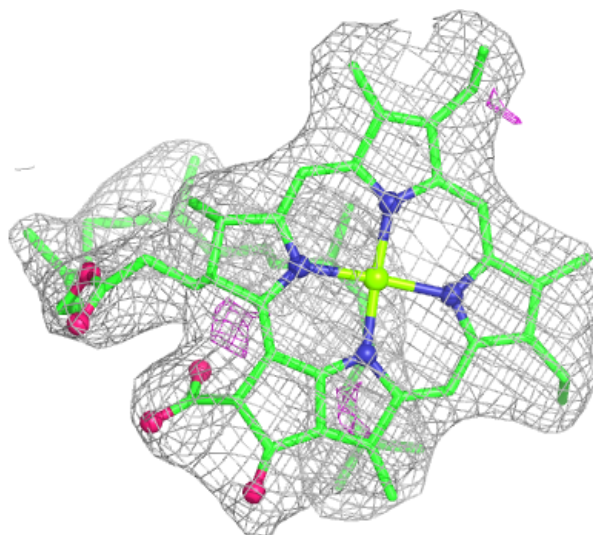
Electron density around CLA B2 612:

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



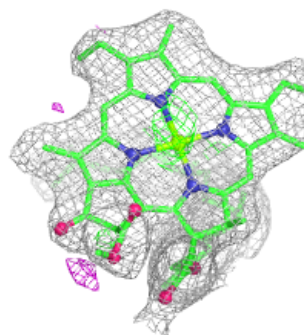
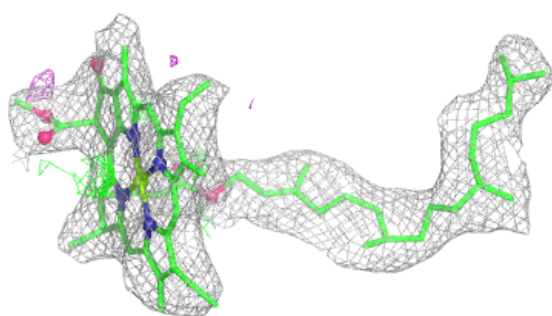
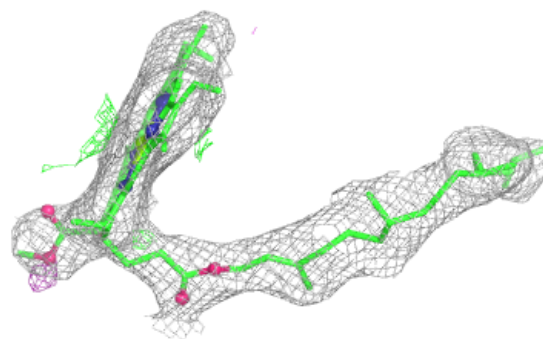
Electron density around CLA c2 511:

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

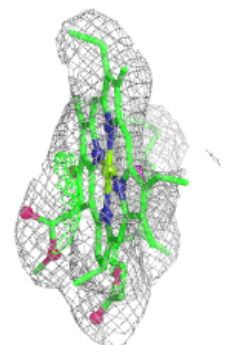
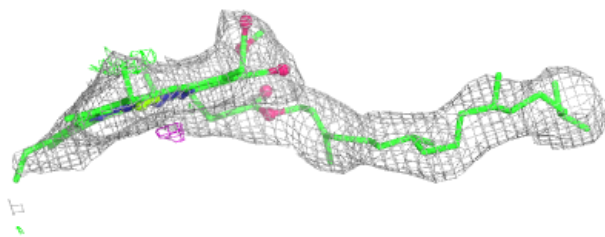
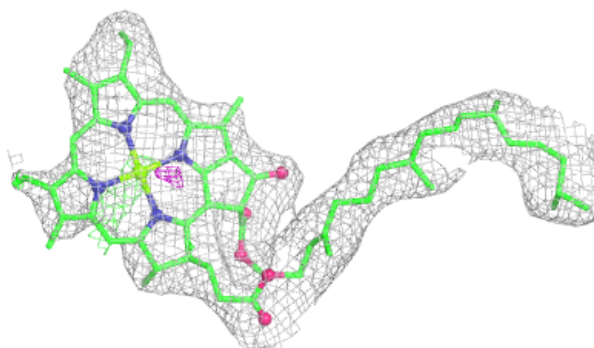


Electron density around CLA B2 619:

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

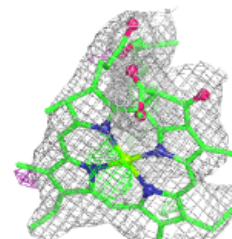
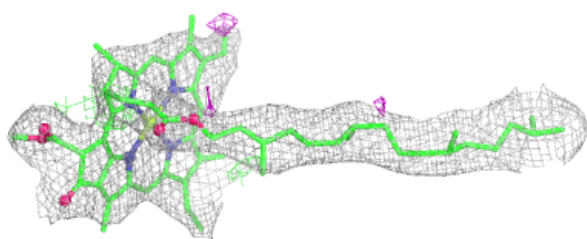
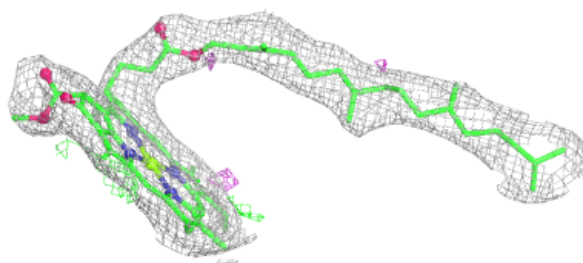
**Electron density around CLA B1 605:**

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



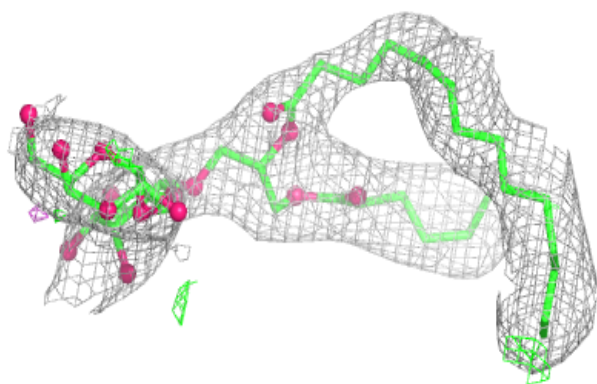
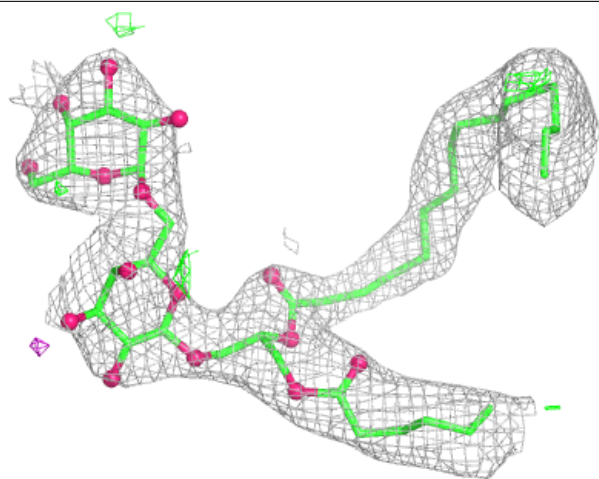
Electron density around CLA C1 505:

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



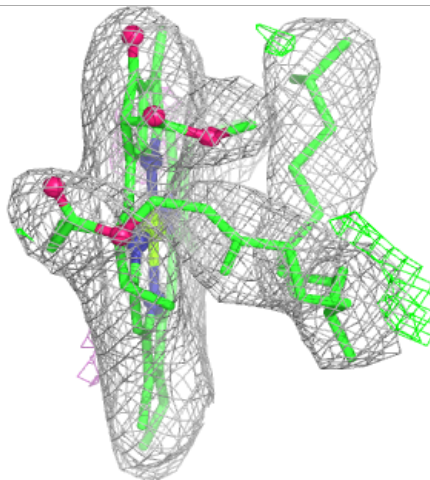
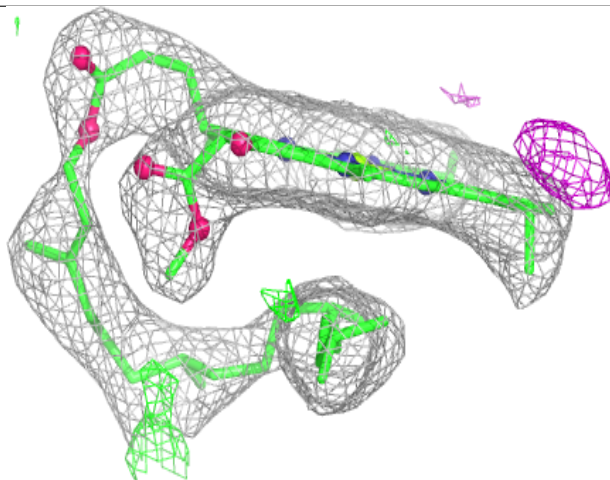
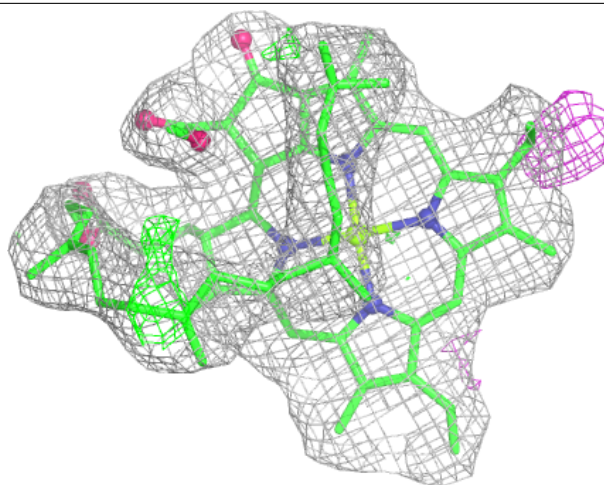
Electron density around DGD C1 515:

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



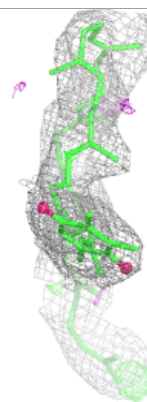
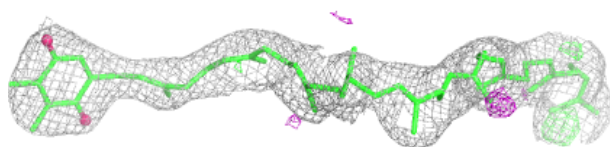
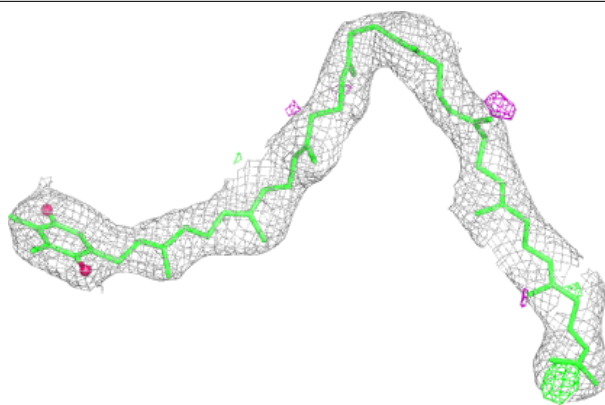
Electron density around CLA c1 512:

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

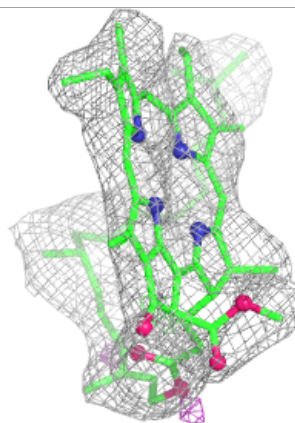
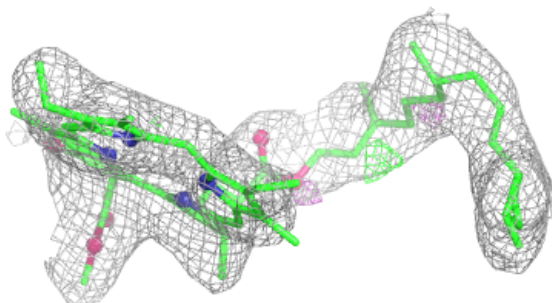
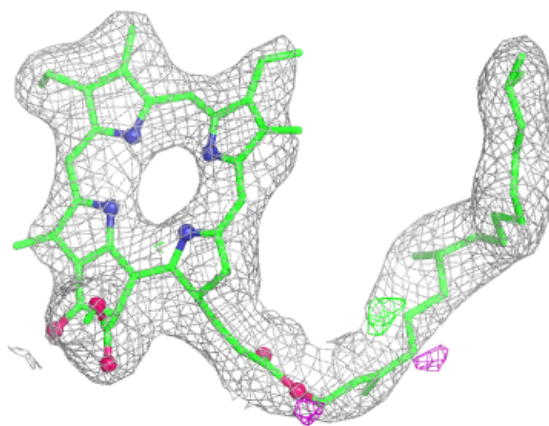


Electron density around PL9 D2 408:

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

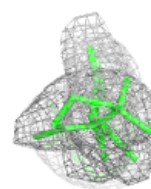
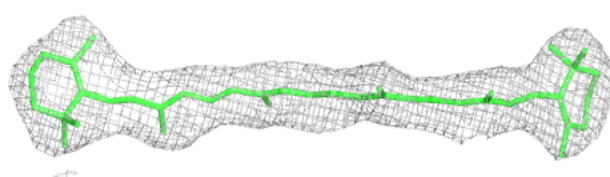
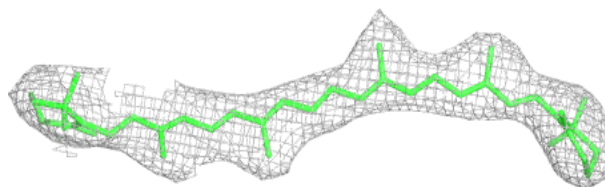
**Electron density around PHO D1 407:**

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

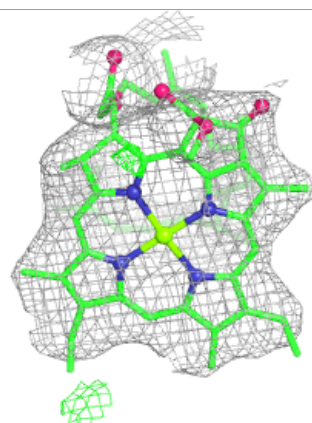
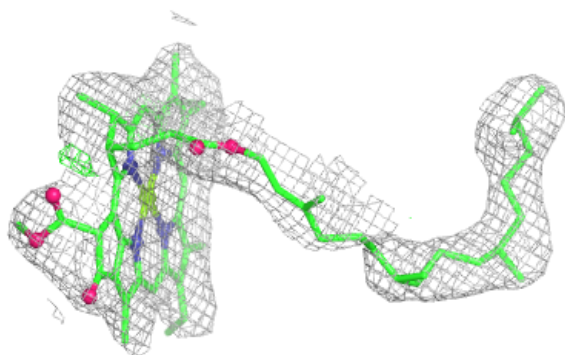
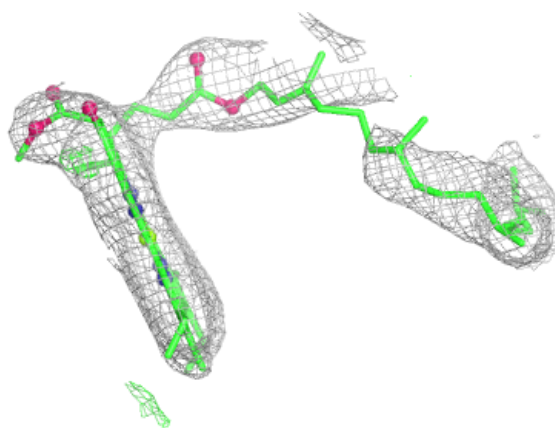


Electron density around BCR C1 501:

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

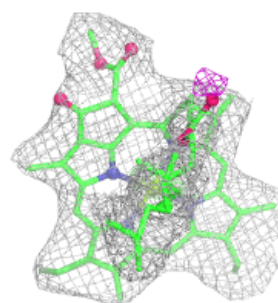
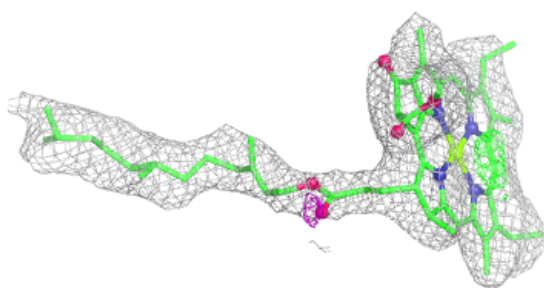
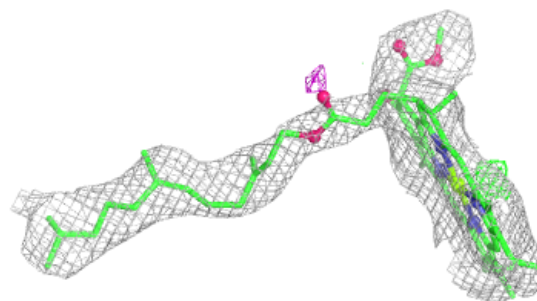
**Electron density around CLA C1 507:**

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

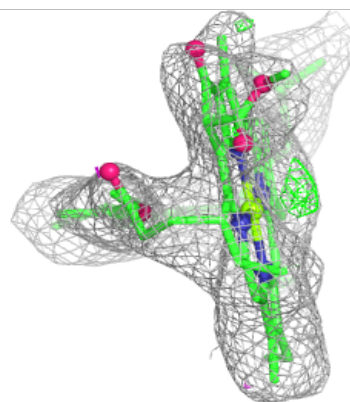
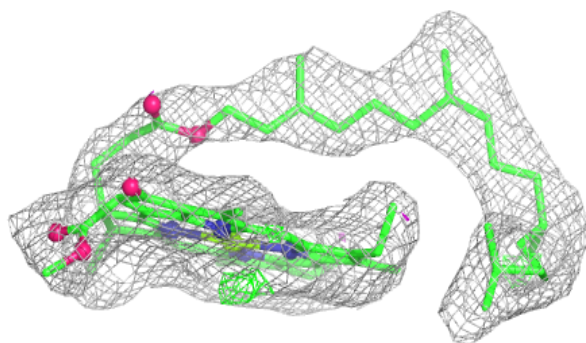
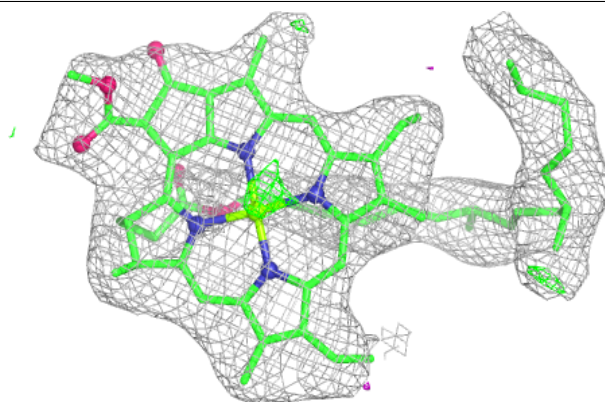


Electron density around CLA b2 616:

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

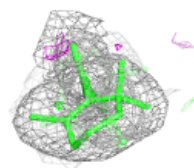
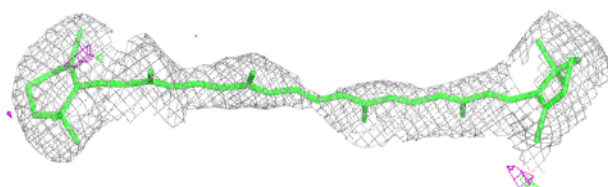
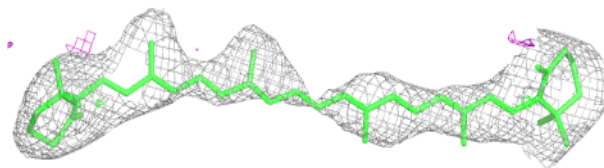
**Electron density around CLA b1 616:**

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

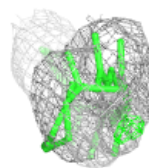
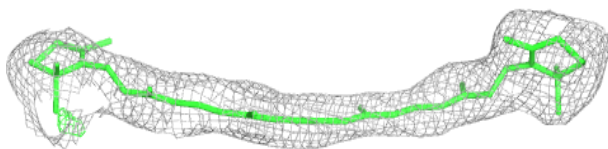
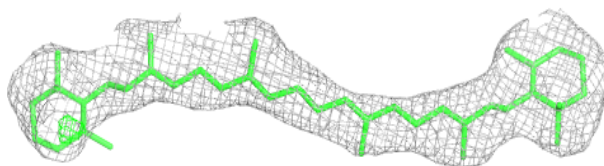


Electron density around BCR A2 401:

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

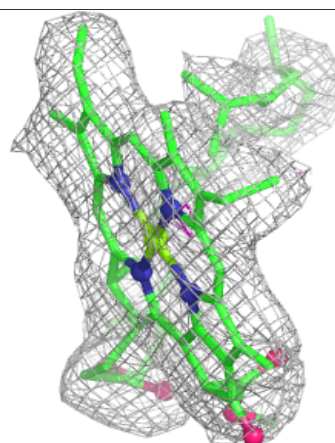
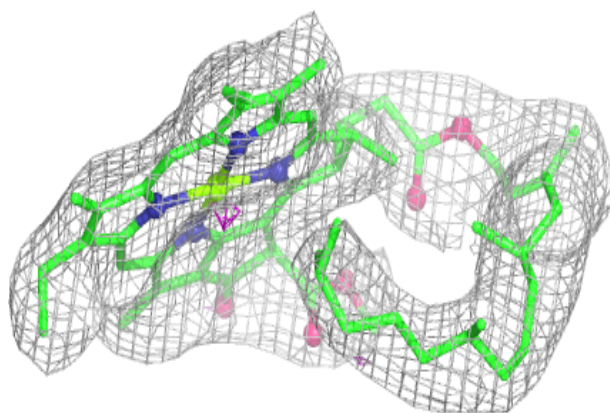
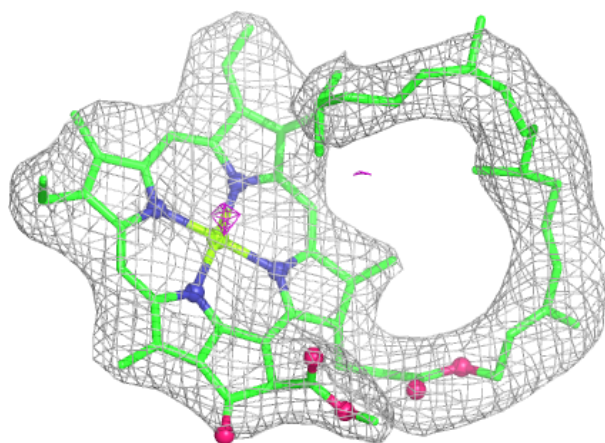
**Electron density around BCR d1 405:**

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



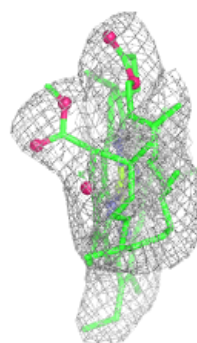
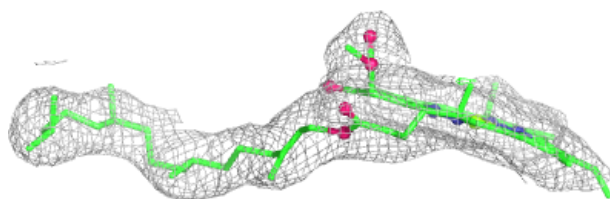
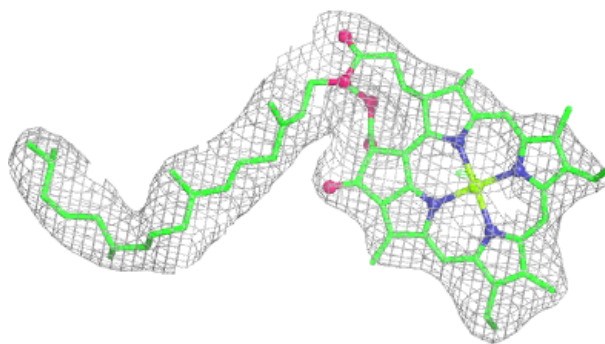
Electron density around CLA B1 617:

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

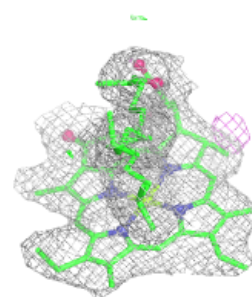
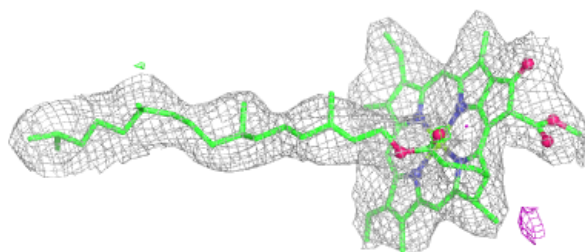
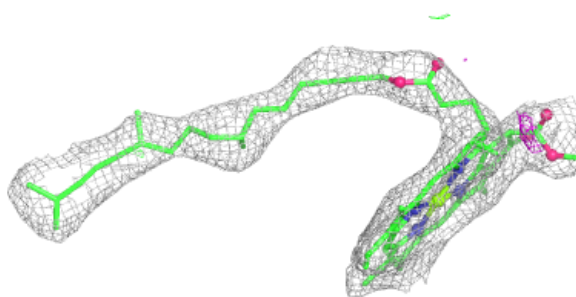


Electron density around CLA B2 605:

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

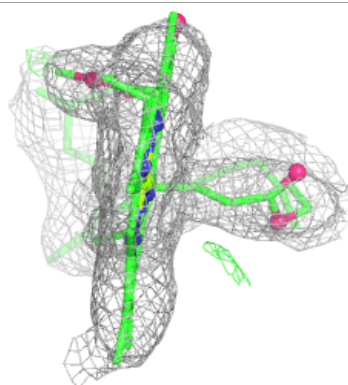
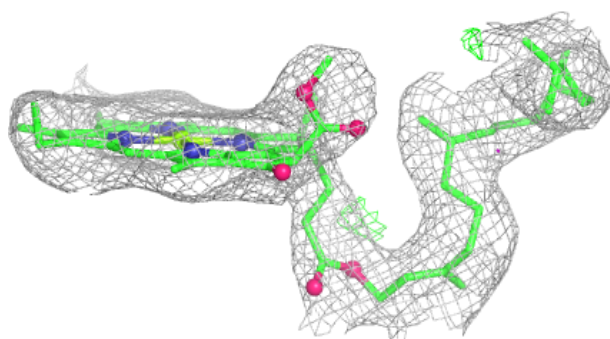
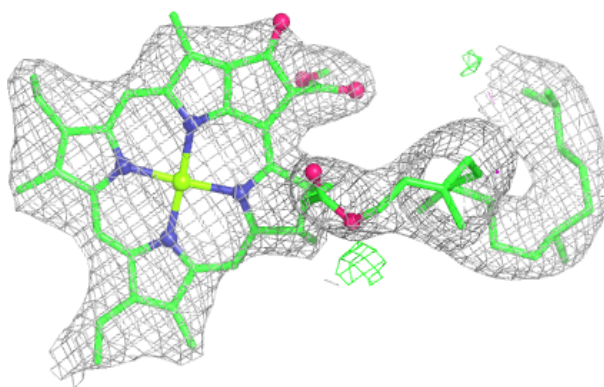
**Electron density around CLA c1 506:**

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

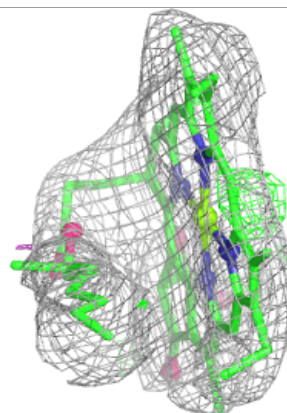
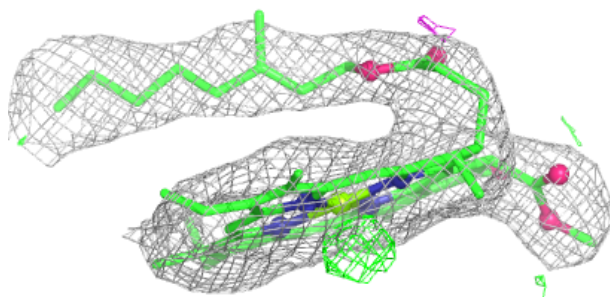
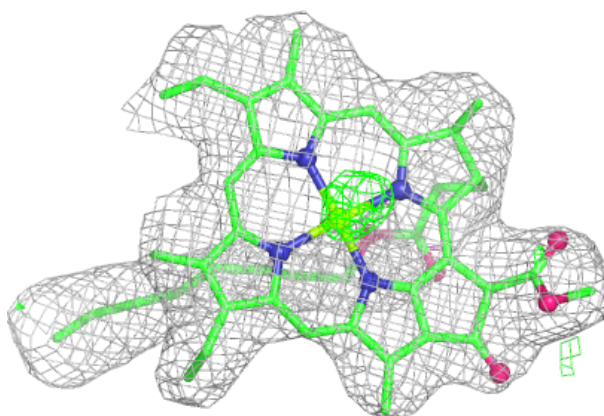


Electron density around CLA B2 614:

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

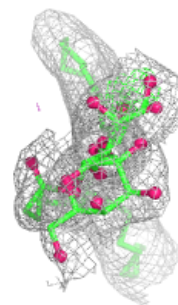
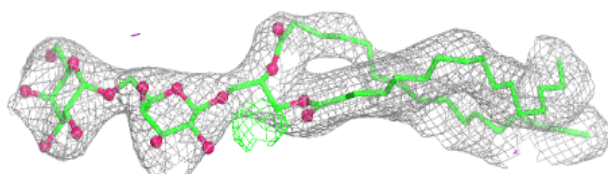
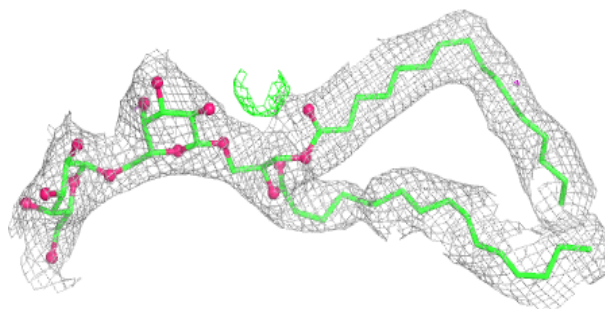
**Electron density around CLA B2 616:**

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



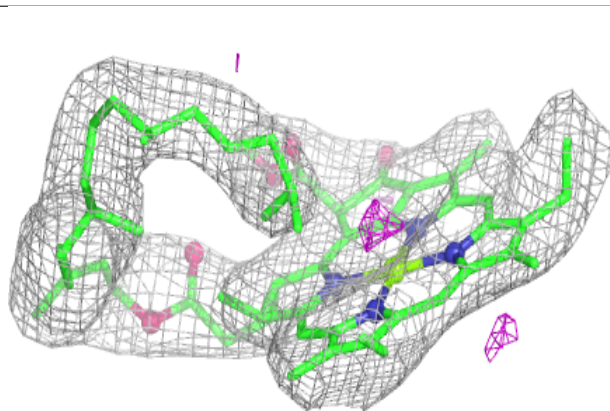
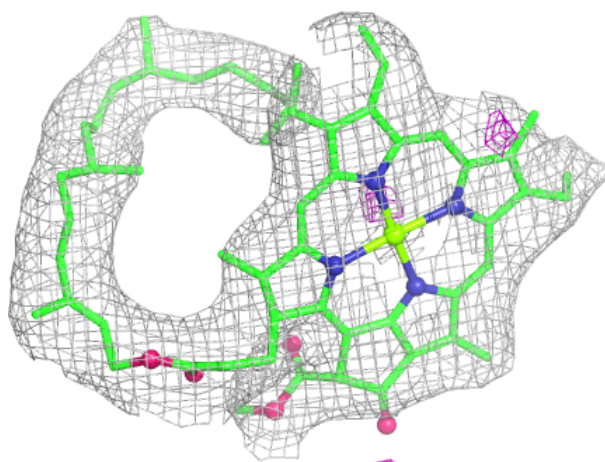
Electron density around DGD c1 518:

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



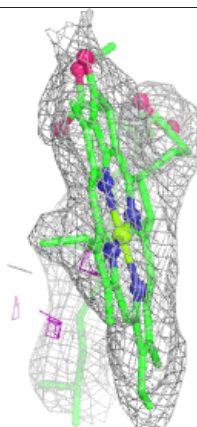
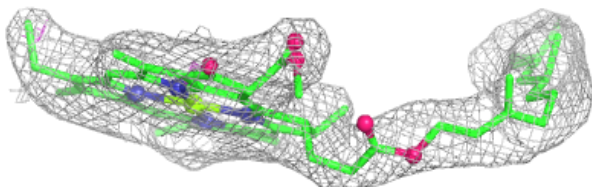
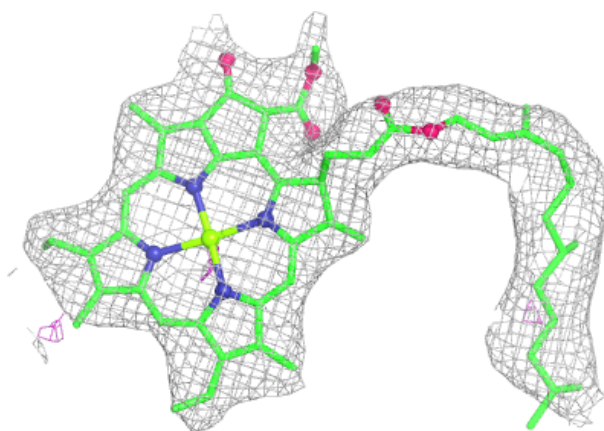
Electron density around CLA B2 617:

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

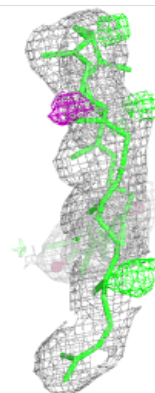
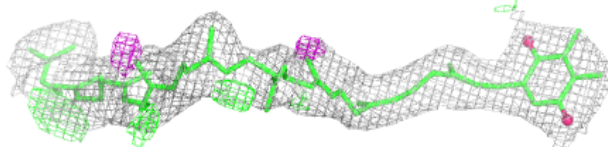
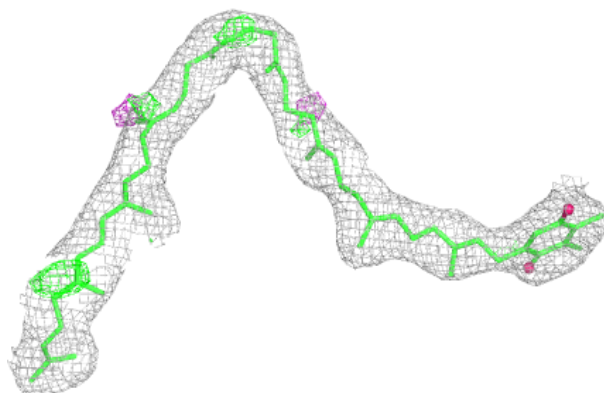


Electron density around CLA B2 618:

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

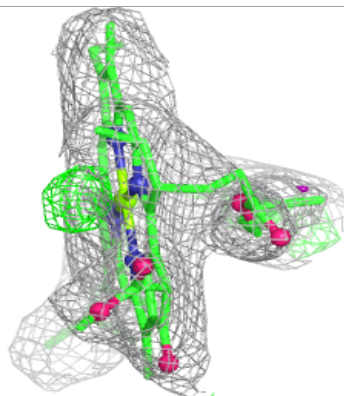
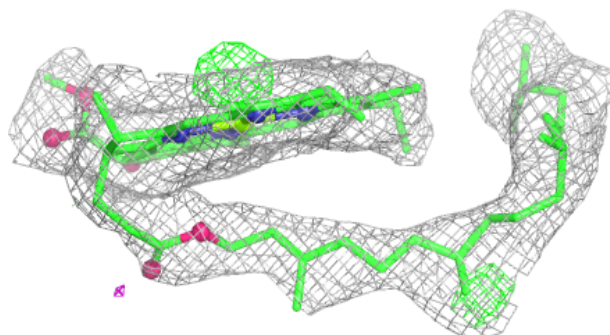
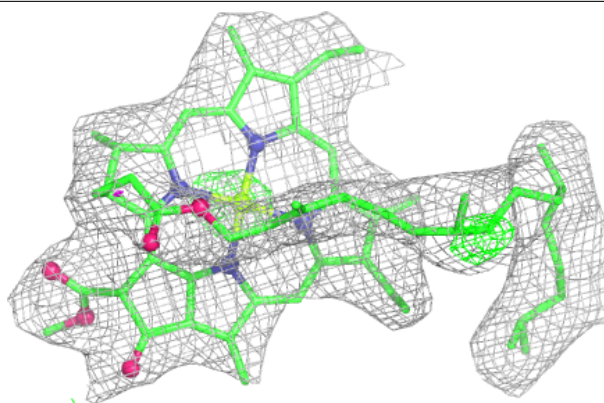
**Electron density around PL9 d1 409:**

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

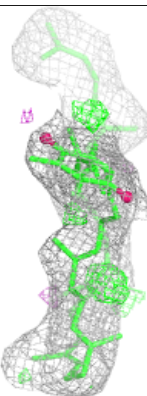
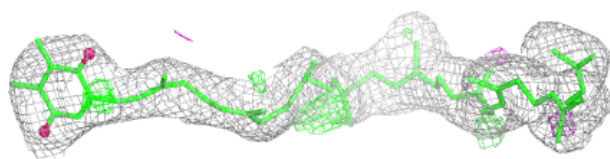
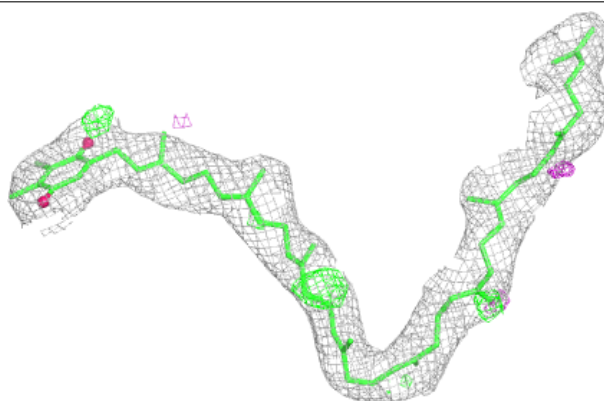


Electron density around CLA b2 617:

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

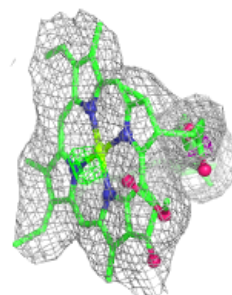
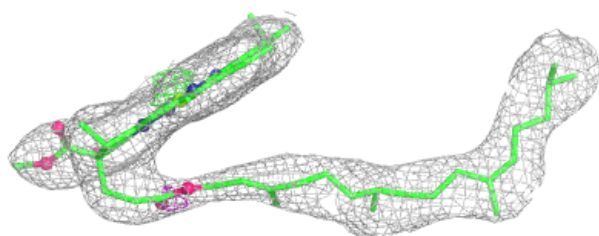
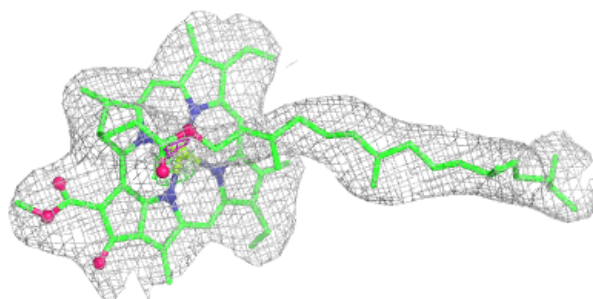
**Electron density around PL9 d2 409:**

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

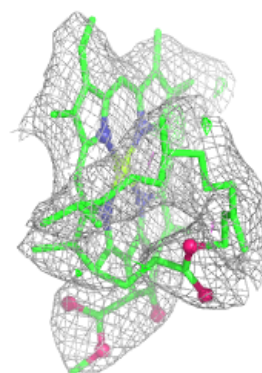
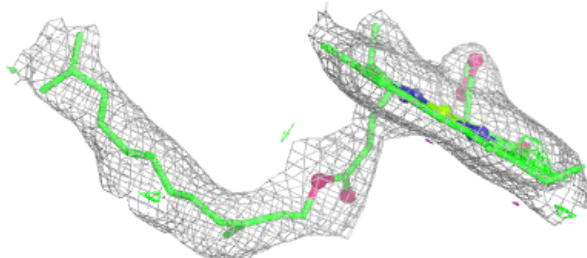
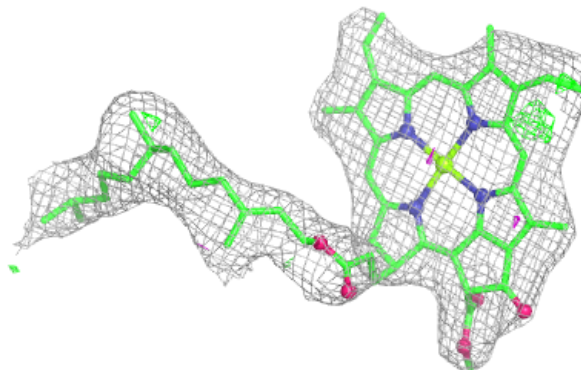


Electron density around CLA B1 610:

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

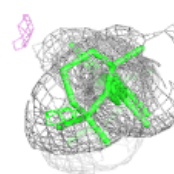
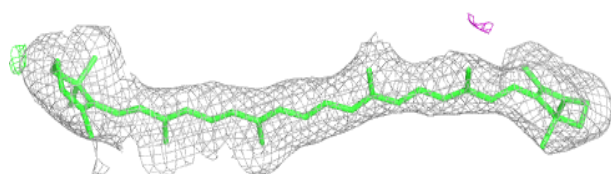
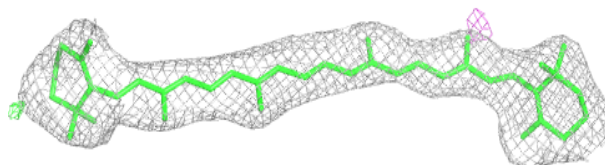
**Electron density around CLA a1 404:**

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

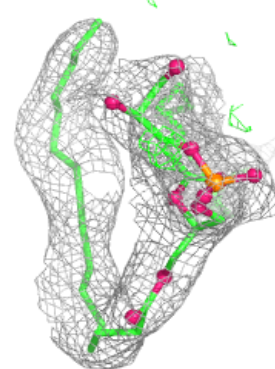
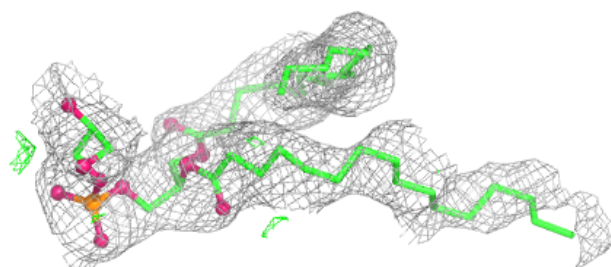
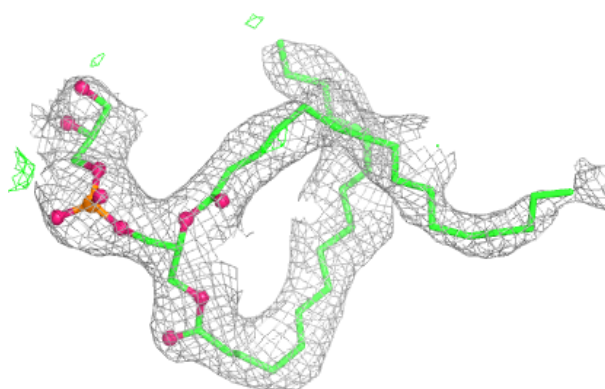


Electron density around BCR B1 603:

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

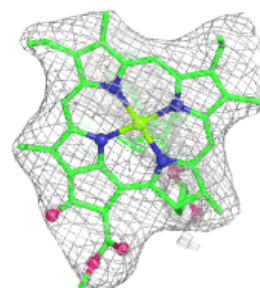
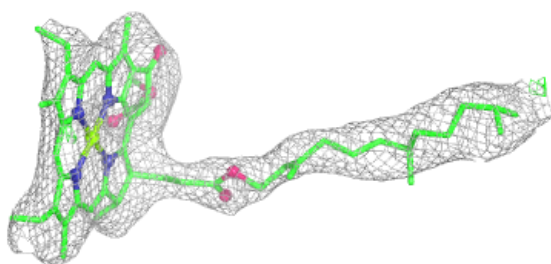
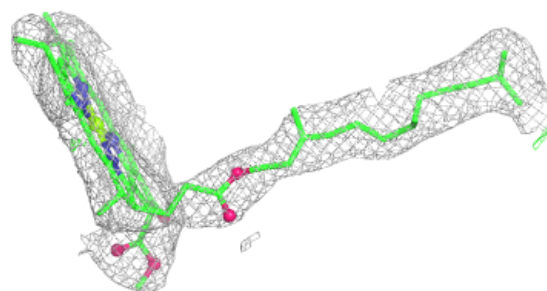
**Electron density around LHG D1 404:**

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

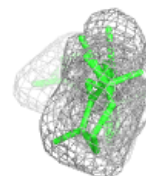
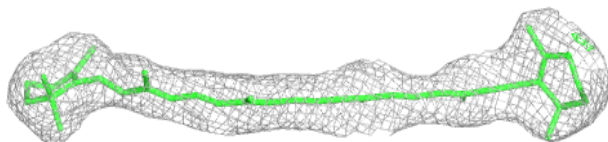
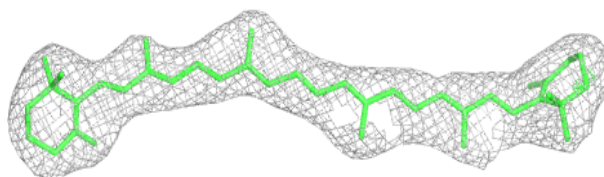


Electron density around CLA B1 607:

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

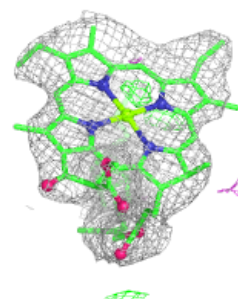
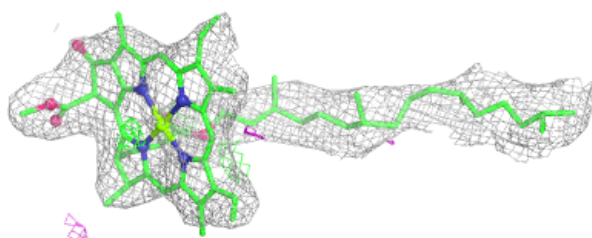
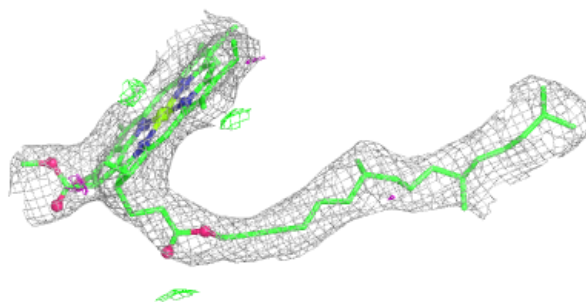
**Electron density around BCR B1 601:**

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

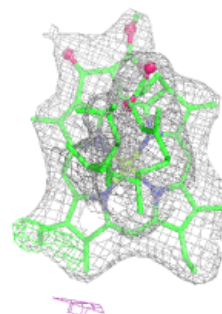
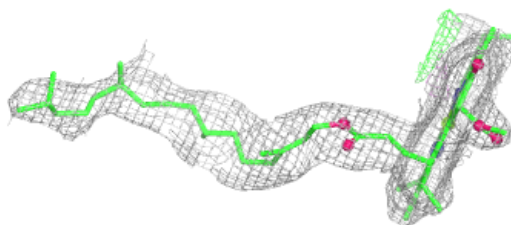
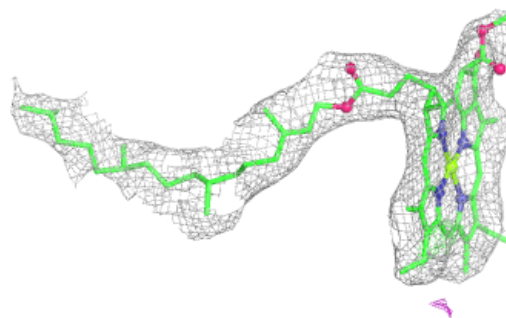


Electron density around CLA c2 505:

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

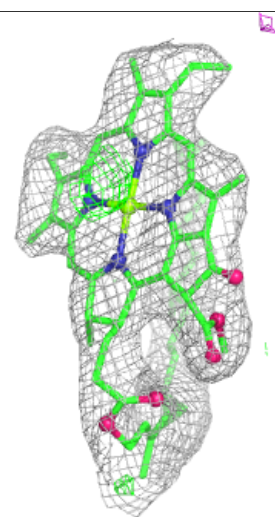
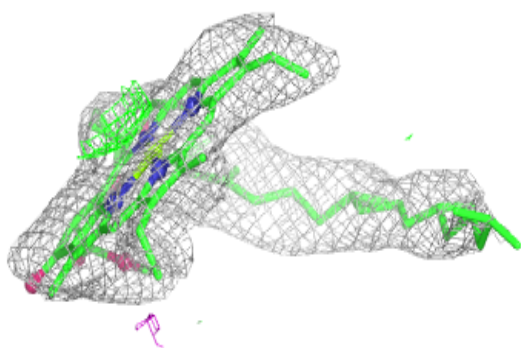
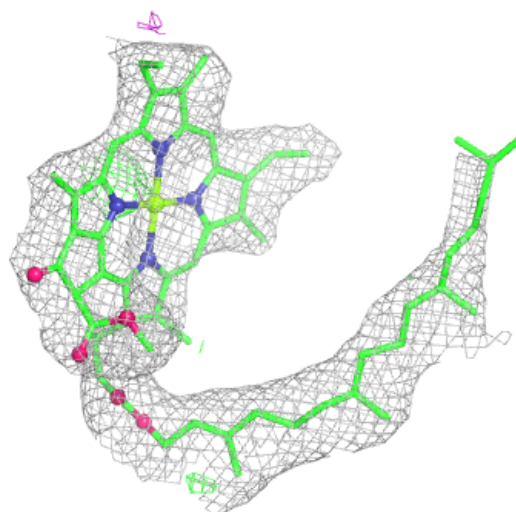
**Electron density around CLA d1 406:**

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



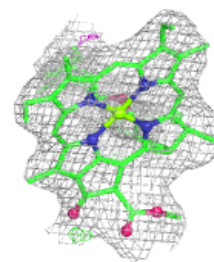
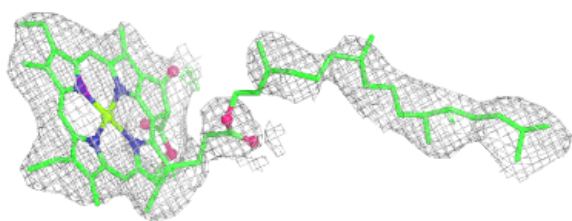
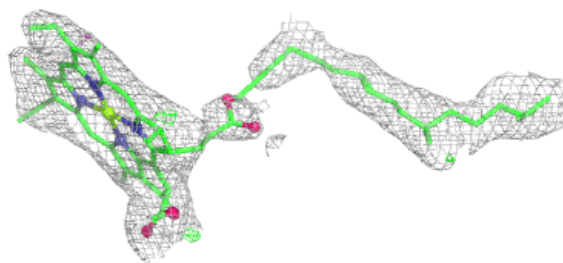
Electron density around CLA C1 508:

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

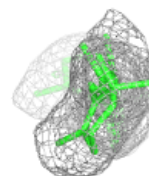
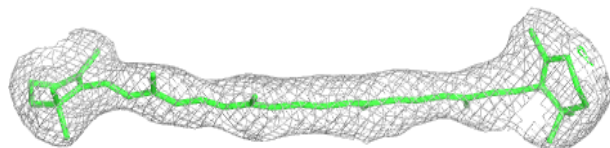
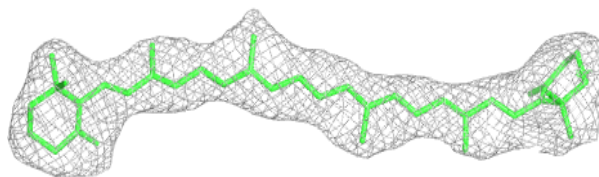


Electron density around CLA c2 503:

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

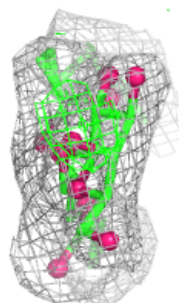
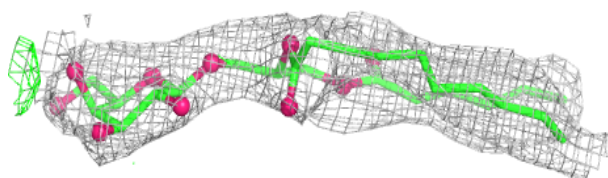
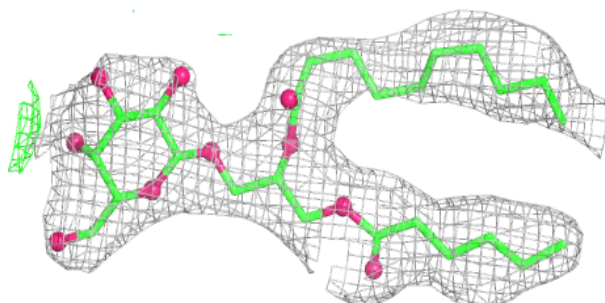
**Electron density around BCR B2 601:**

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

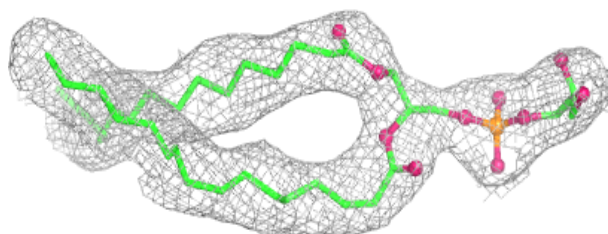
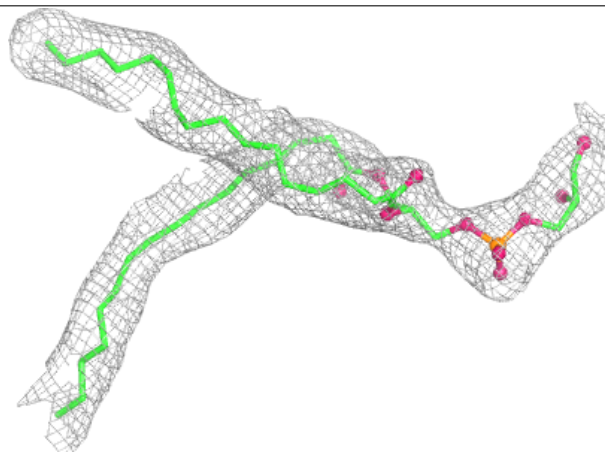


Electron density around LMG D1 406:

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

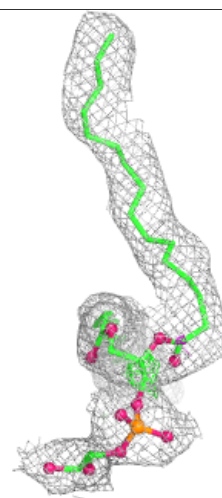
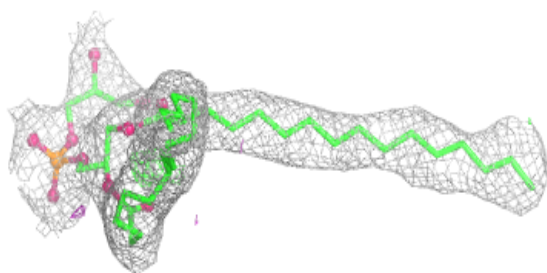
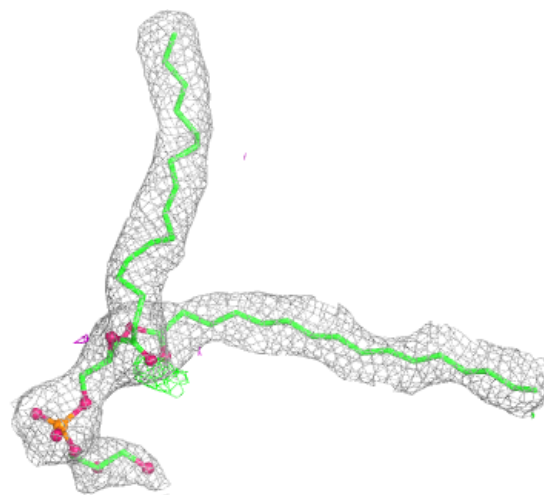
**Electron density around LHG D2 405:**

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



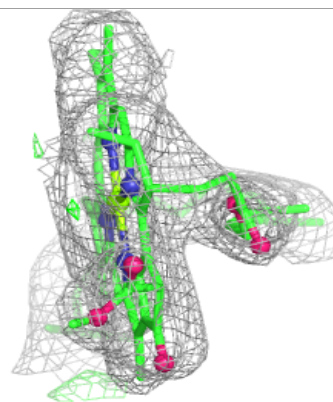
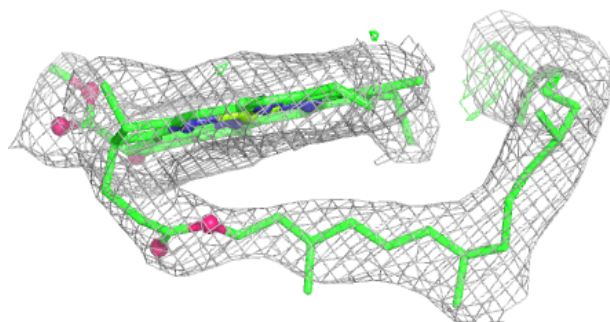
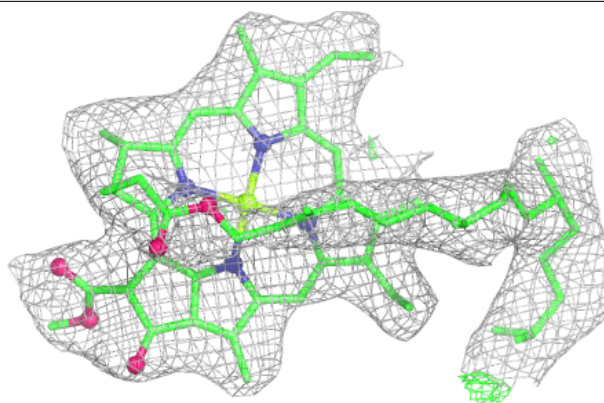
Electron density around LHG L2 101:

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

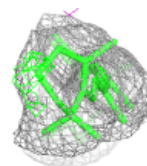
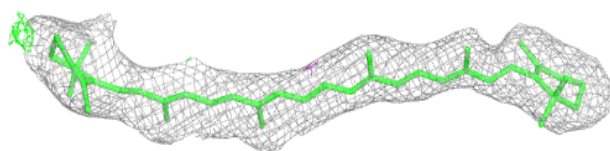
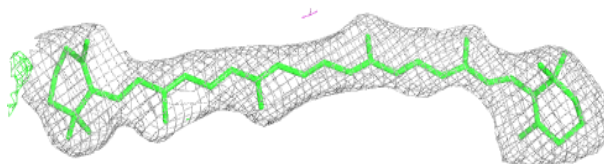


Electron density around CLA B1 616:

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

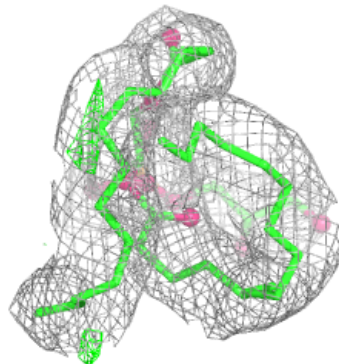
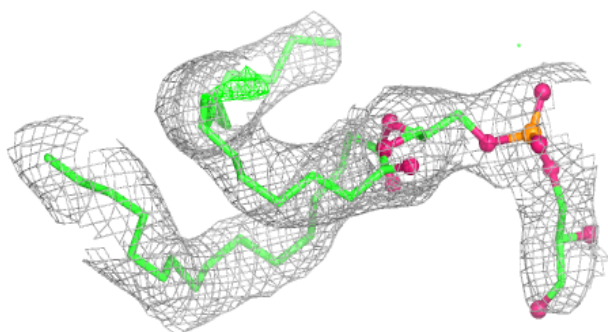
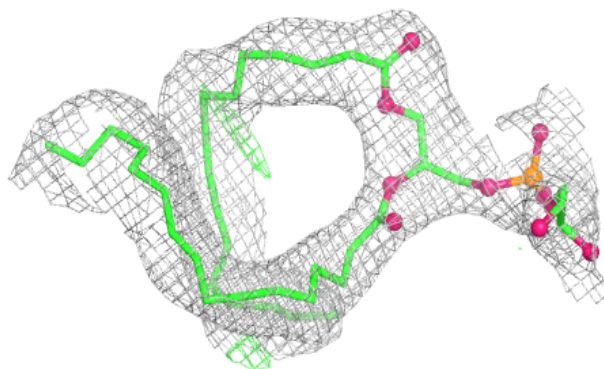
**Electron density around BCR b1 603:**

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

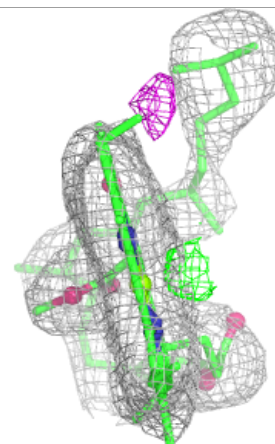
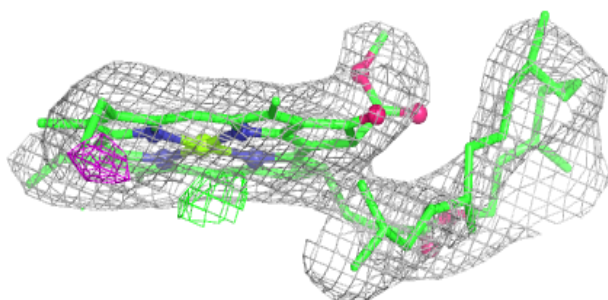
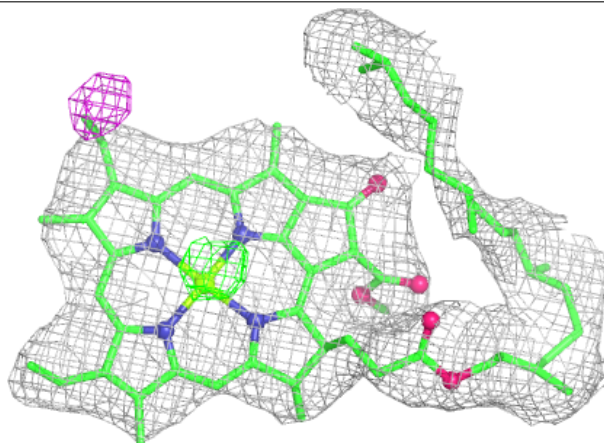


Electron density around LHG d2 403:

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

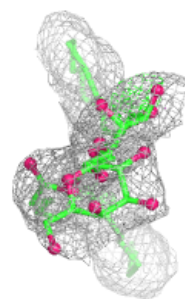
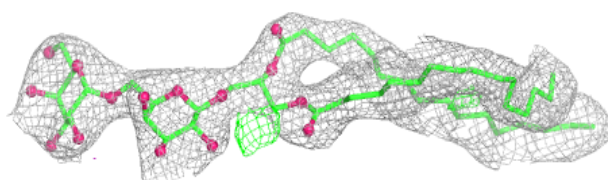
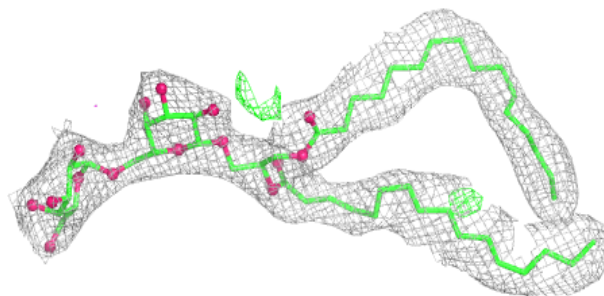
**Electron density around CLA b2 611:**

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

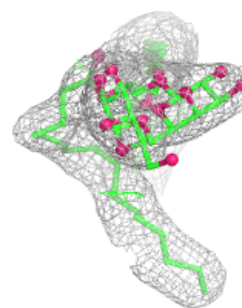
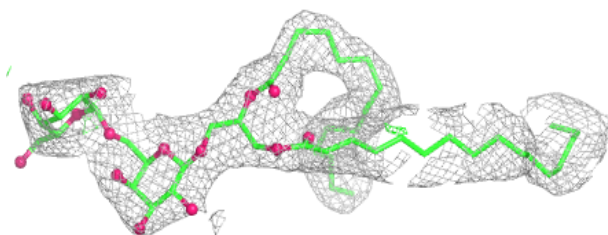
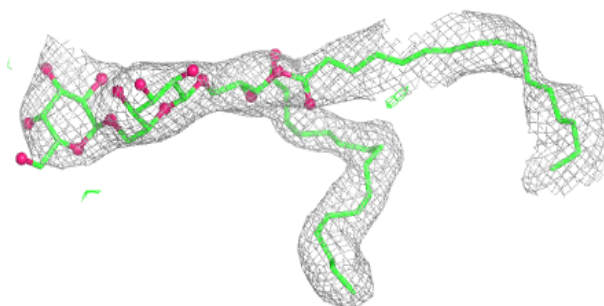


Electron density around DGD C1 516:

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

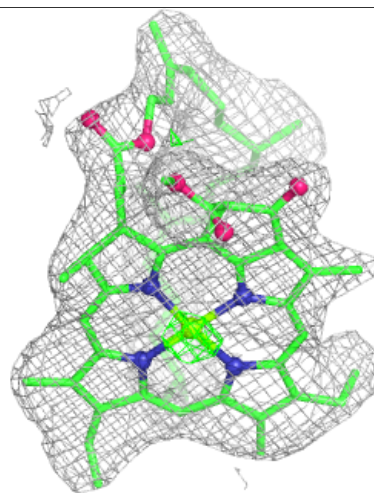
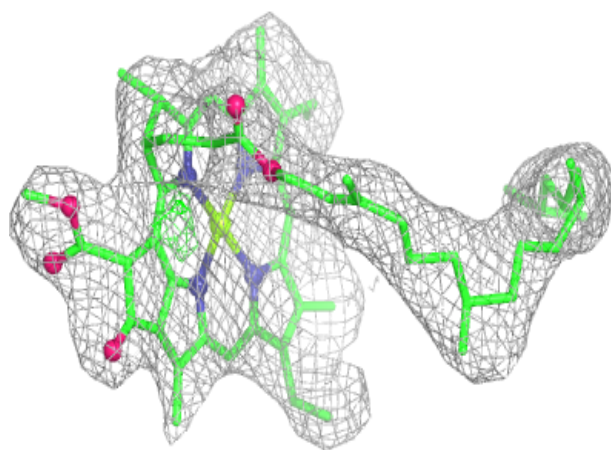
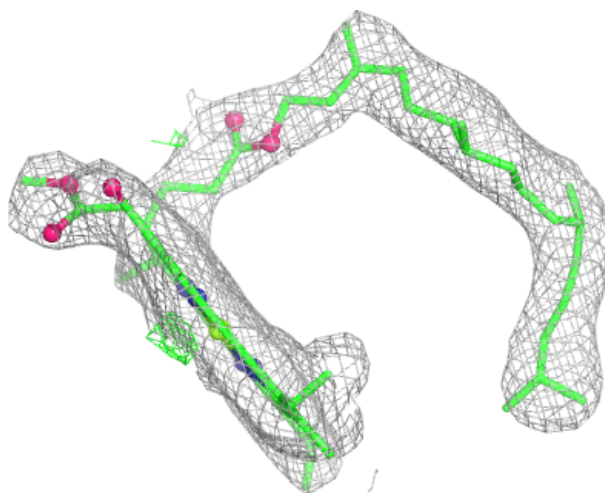
**Electron density around DGD H1 101:**

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



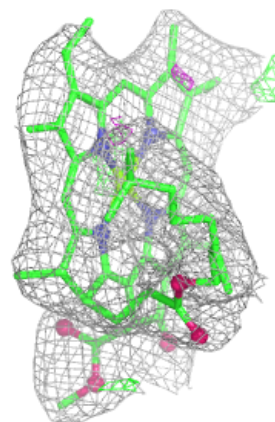
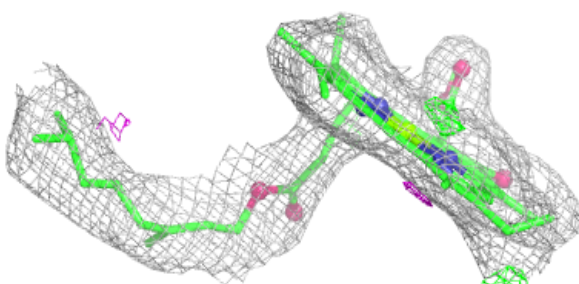
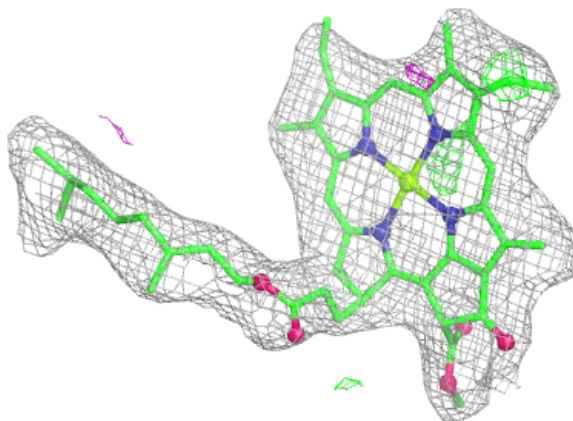
Electron density around CLA b2 612:

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

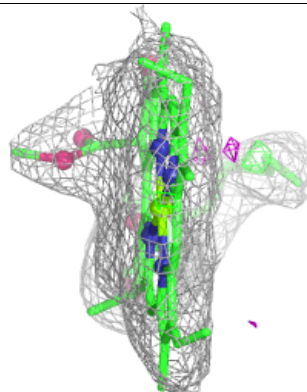
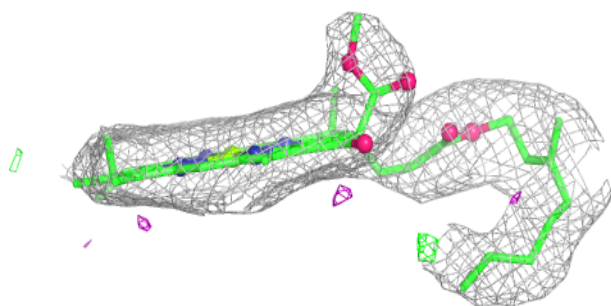
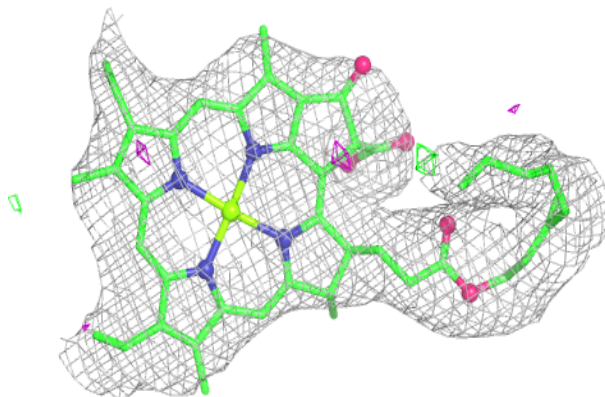


Electron density around CLA A1 405:

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

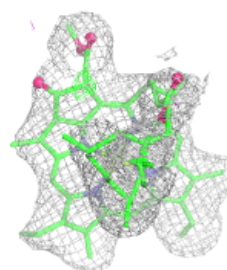
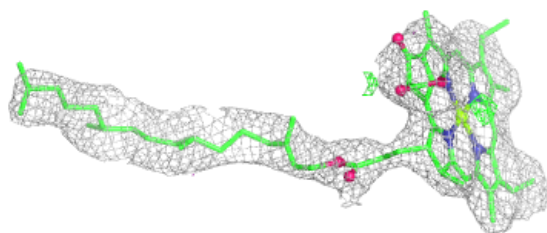
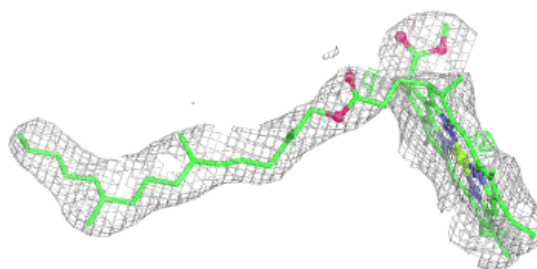
**Electron density around CLA c2 510:**

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

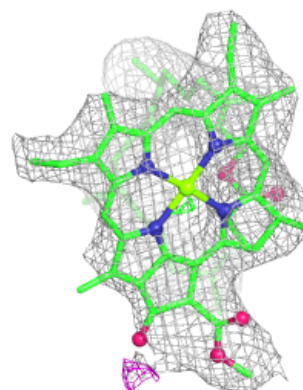
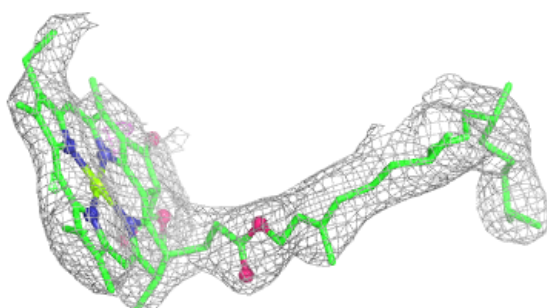
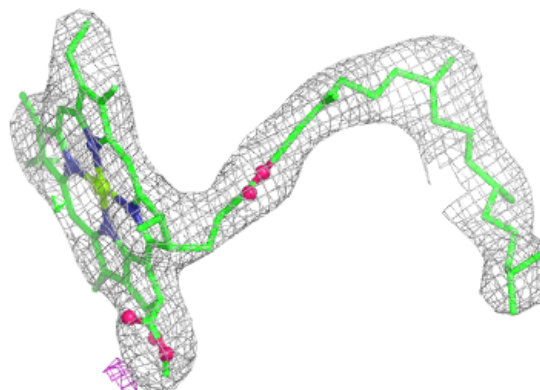


Electron density around CLA B2 607:

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

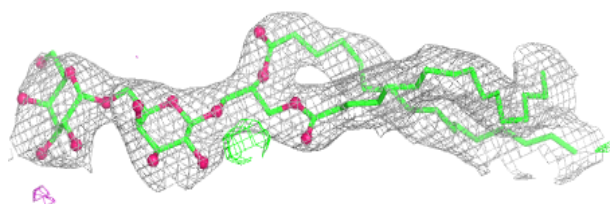
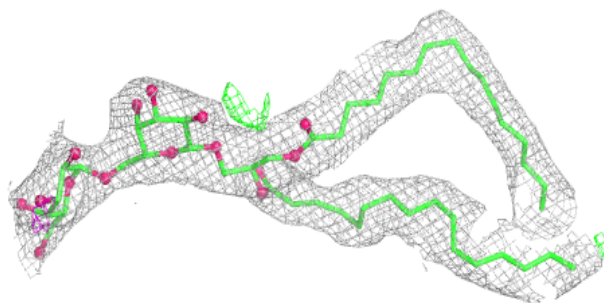
**Electron density around CLA B2 609:**

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

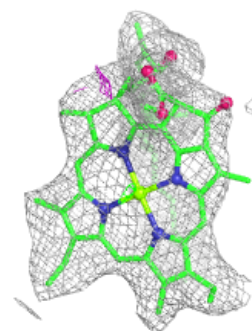
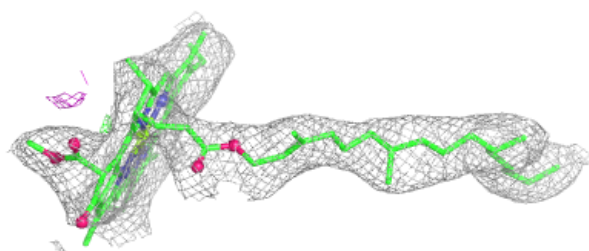
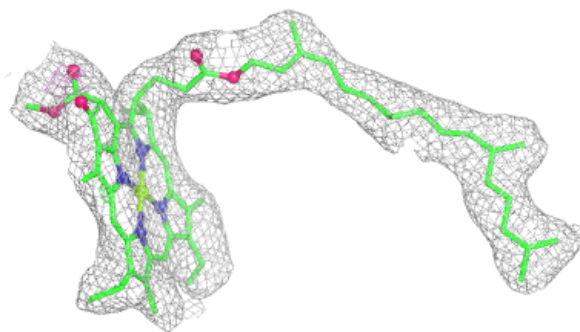


Electron density around DGD c2 514:

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

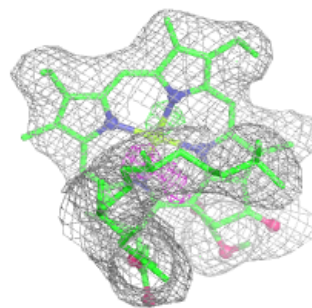
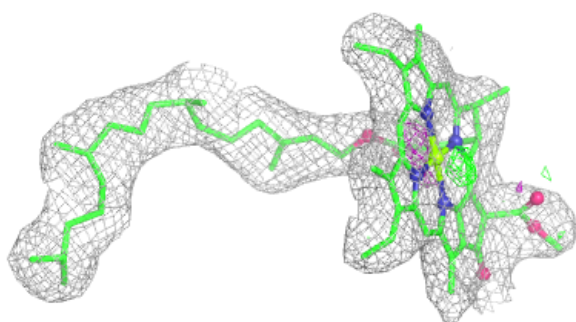
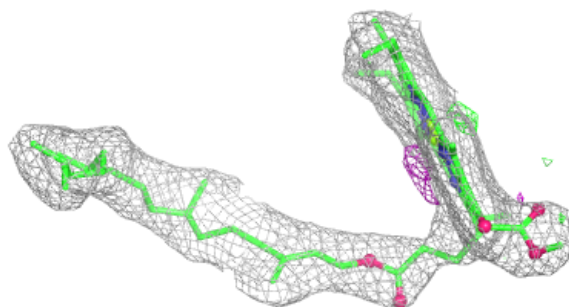
**Electron density around CLA b1 611:**

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

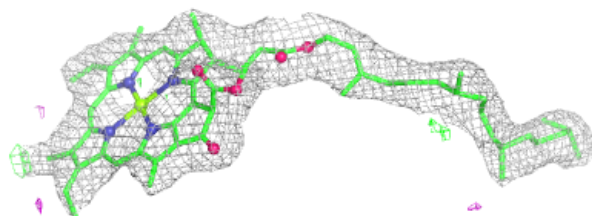
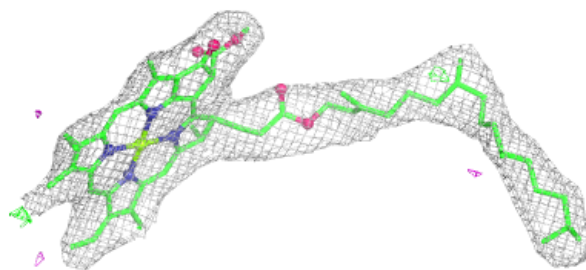


Electron density around CLA B1 619:

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

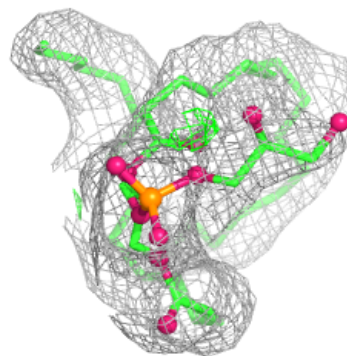
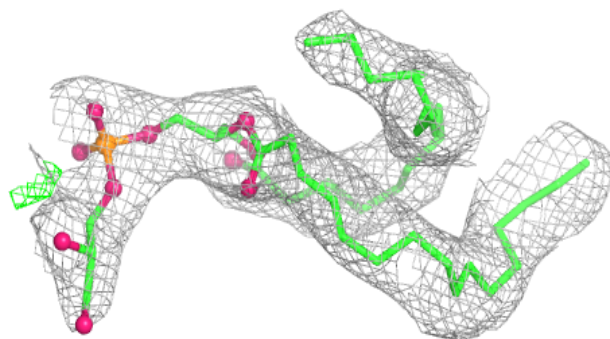
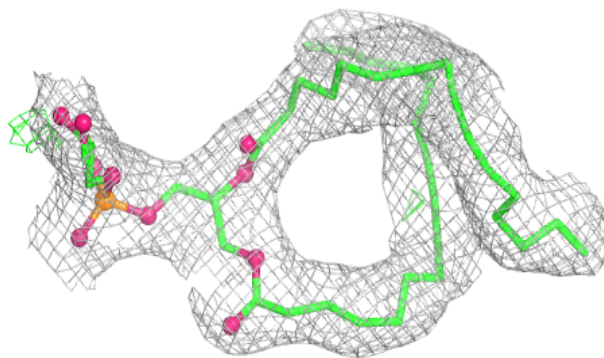
**Electron density around CLA A2 402:**

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



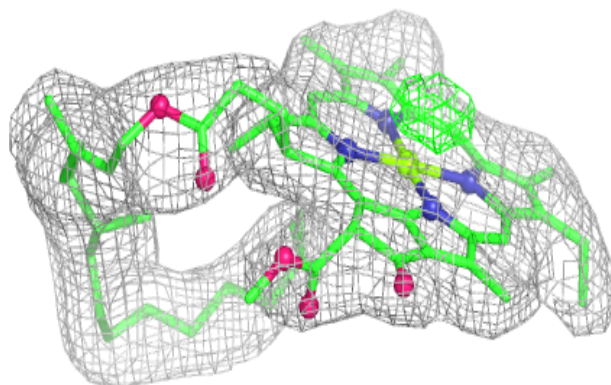
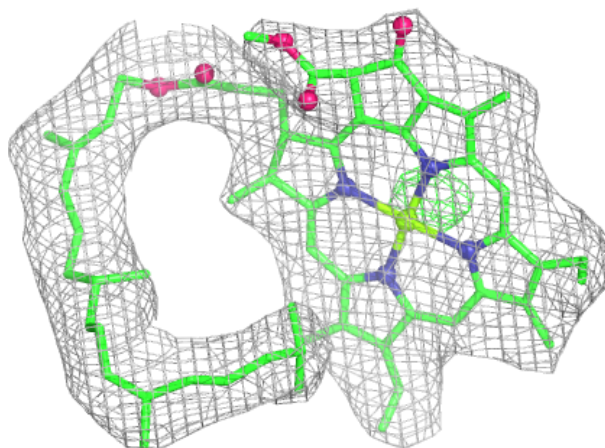
Electron density around LHG B1 621:

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



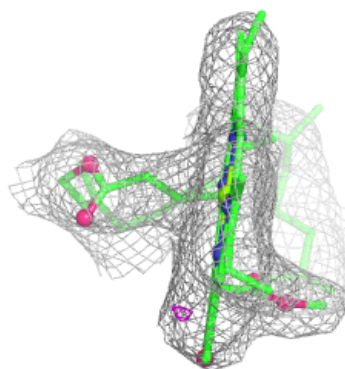
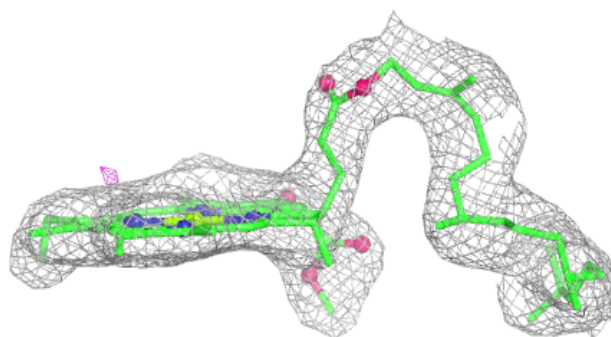
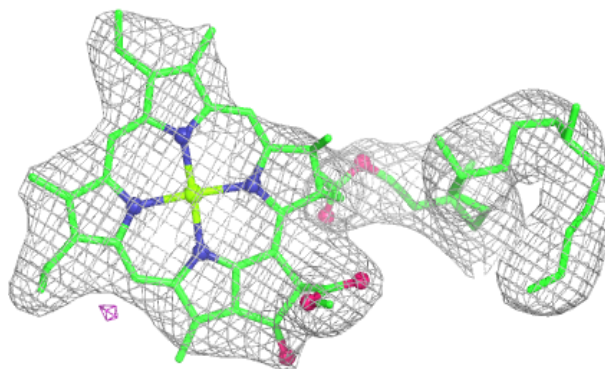
Electron density around CLA b1 617:

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

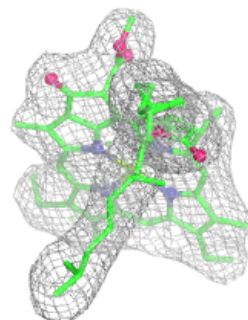
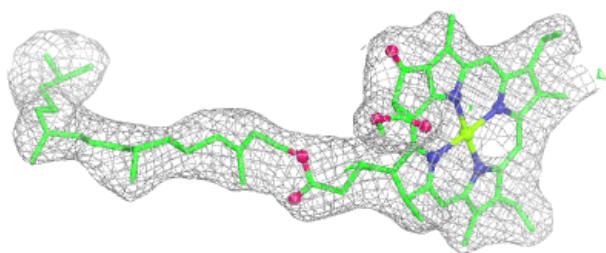
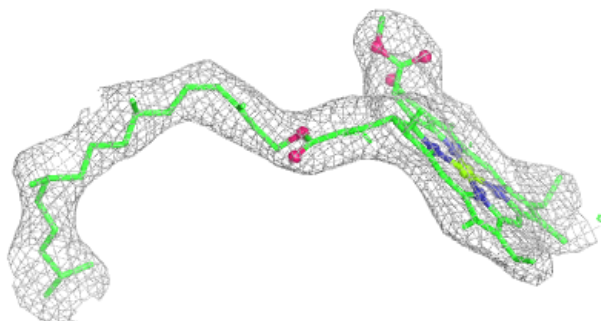


Electron density around CLA b2 614:

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

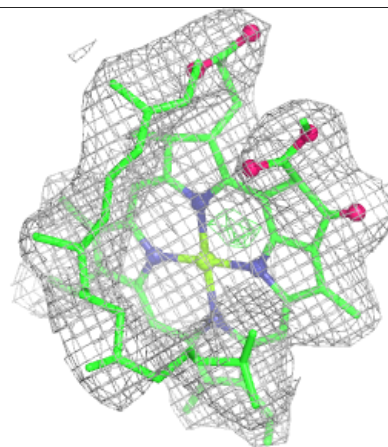
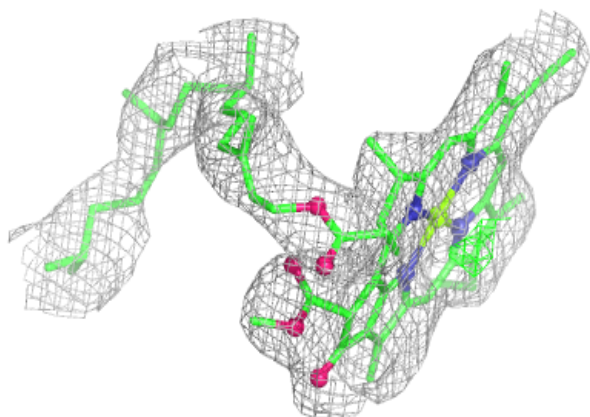
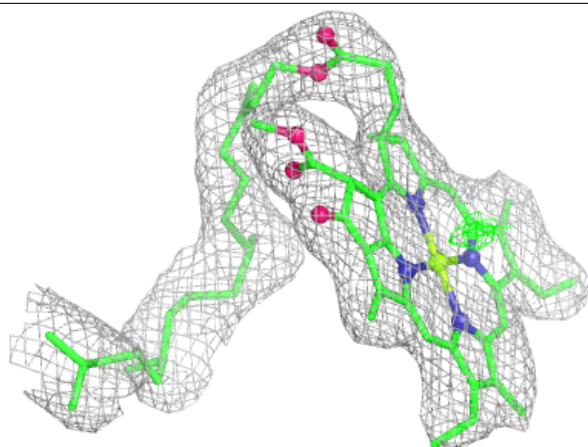
**Electron density around CLA d1 401:**

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



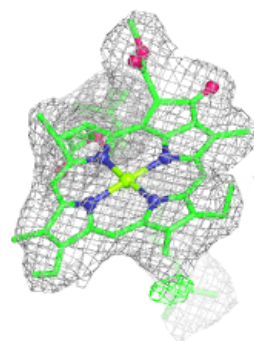
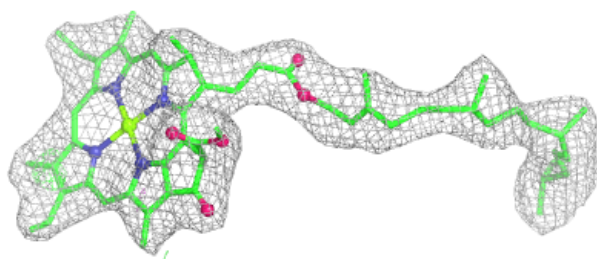
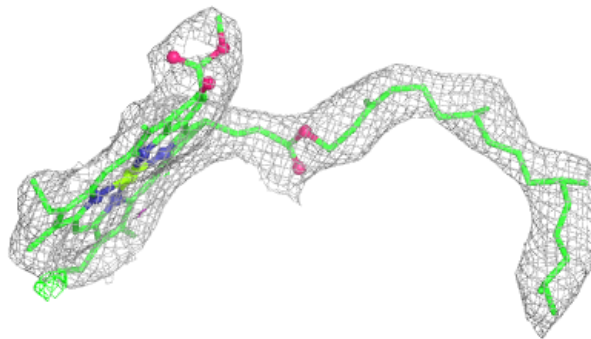
Electron density around CLA B2 615:

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



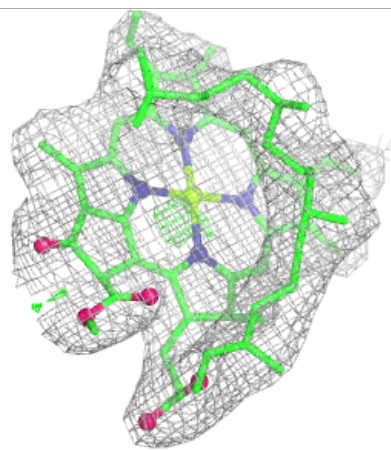
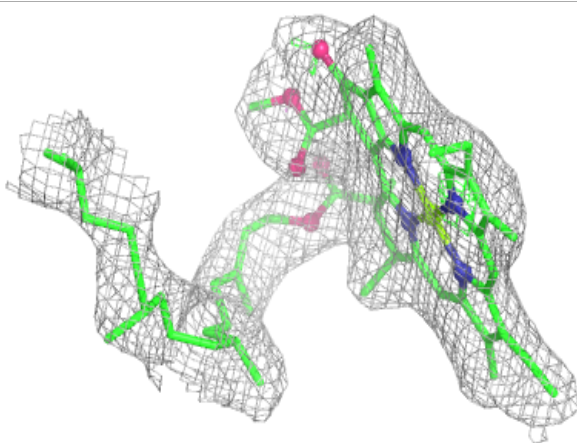
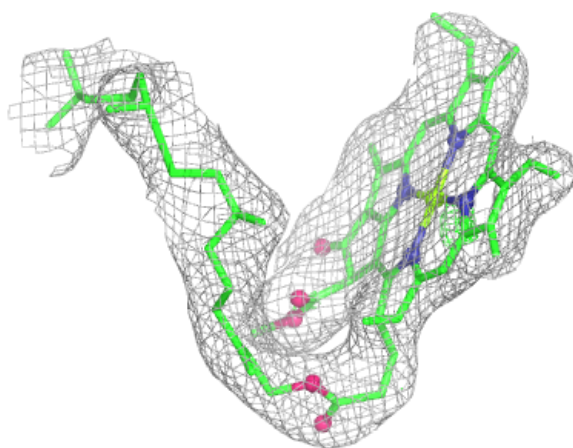
Electron density around CLA d2 405:

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



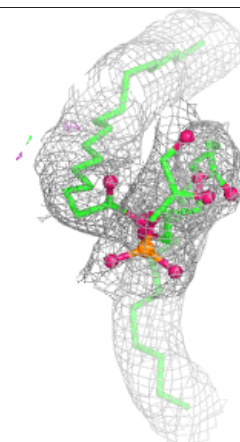
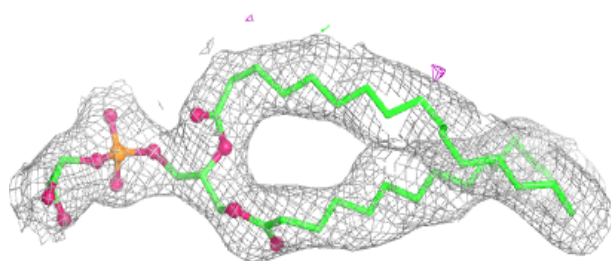
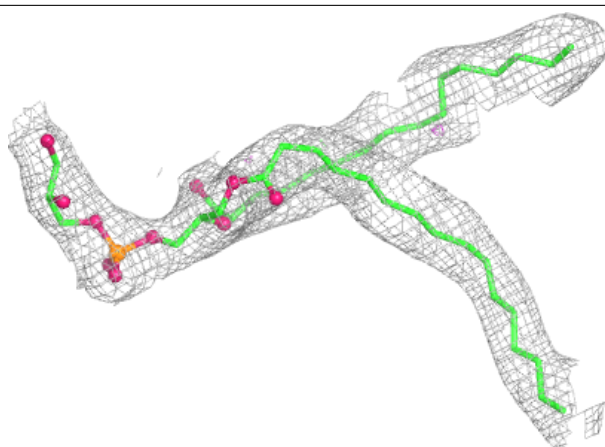
Electron density around CLA B1 615:

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



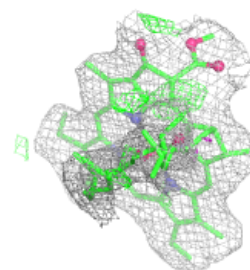
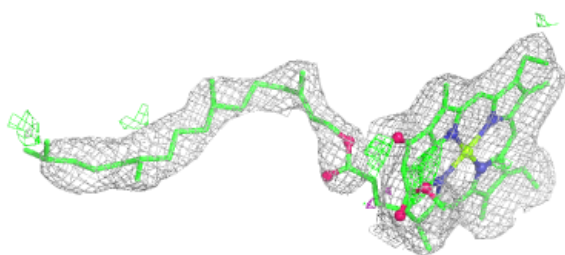
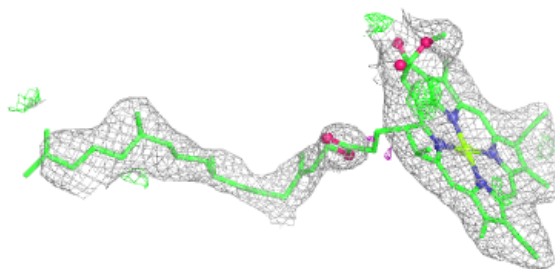
Electron density around LHG d2 406:

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

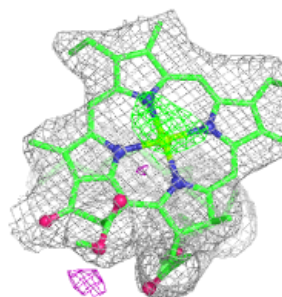
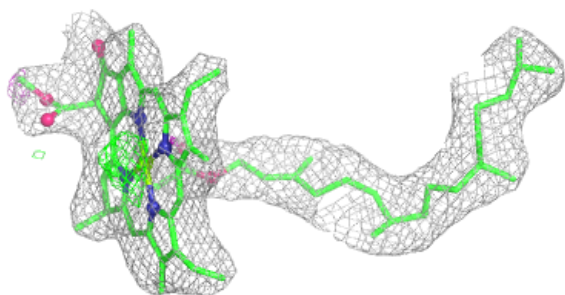
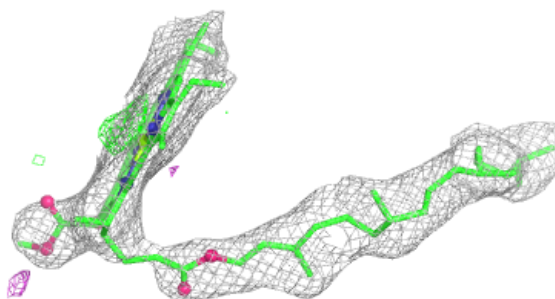


Electron density around CLA c1 504:

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

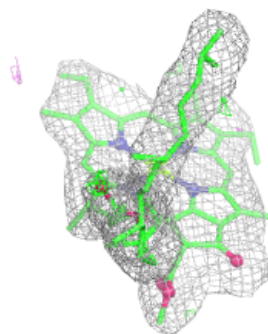
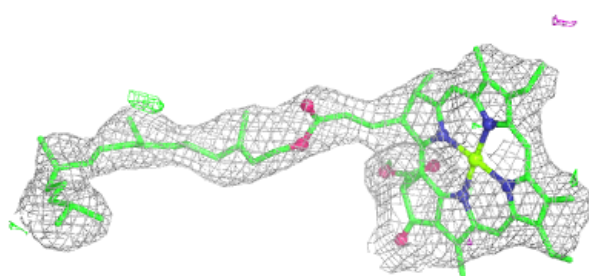
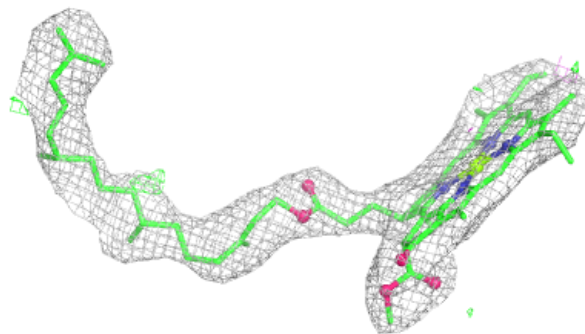
**Electron density around CLA b2 620:**

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

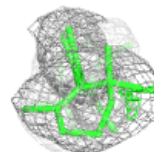
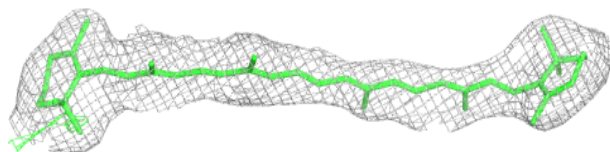
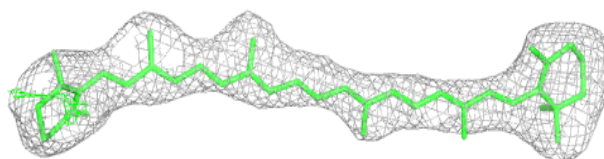


Electron density around CLA D2 401:

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

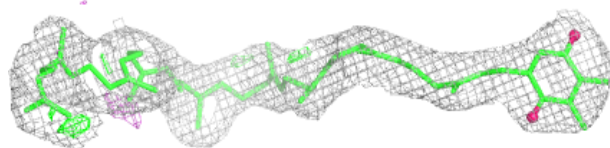
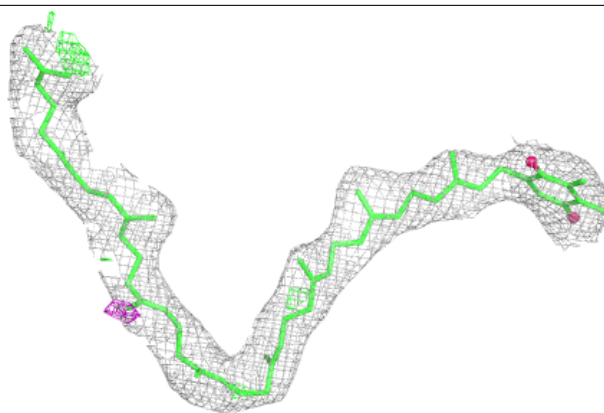
**Electron density around BCR a1 401:**

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

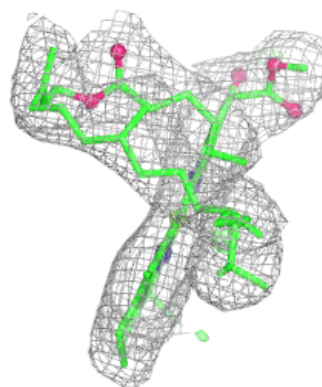
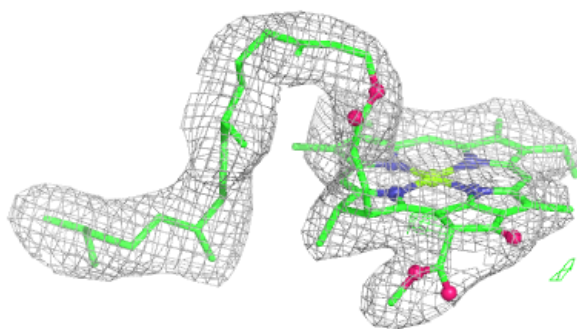
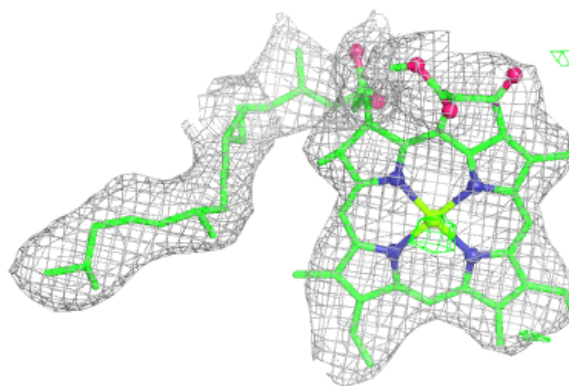


Electron density around PL9 D1 408:

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

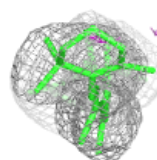
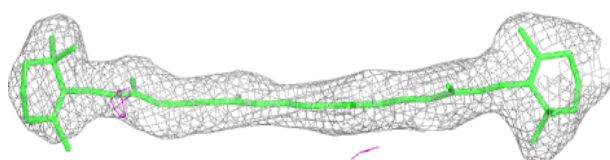
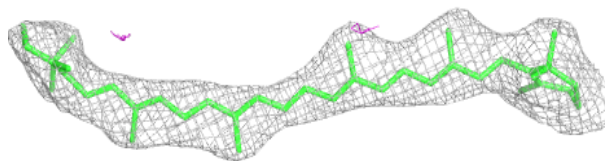
**Electron density around CLA D2 406:**

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

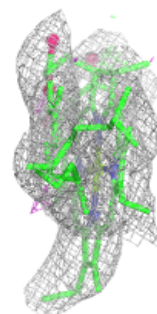
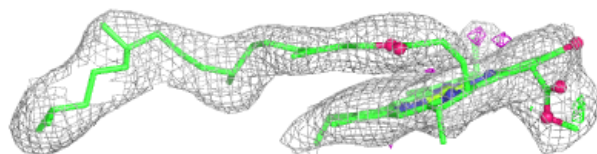
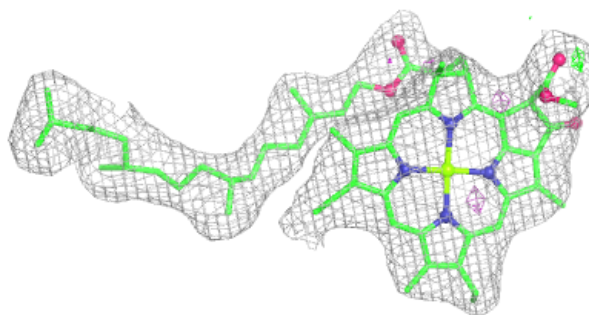


Electron density around BCR h1 102:

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

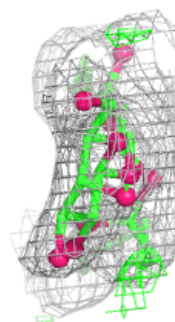
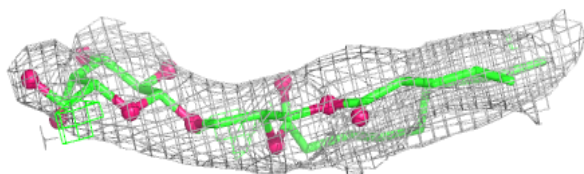
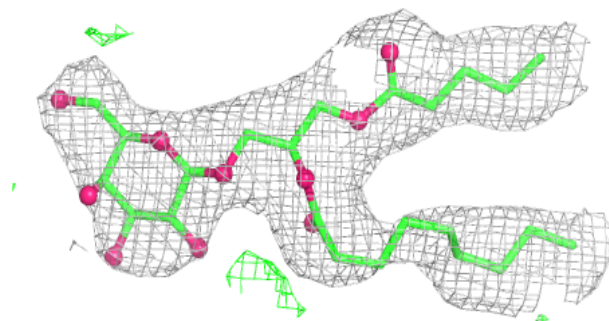
**Electron density around CLA b1 606:**

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



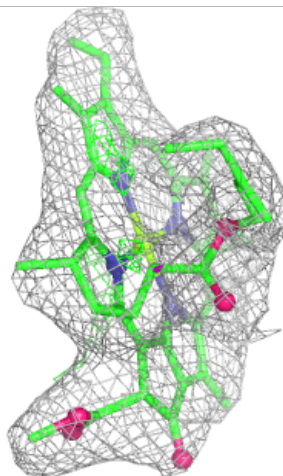
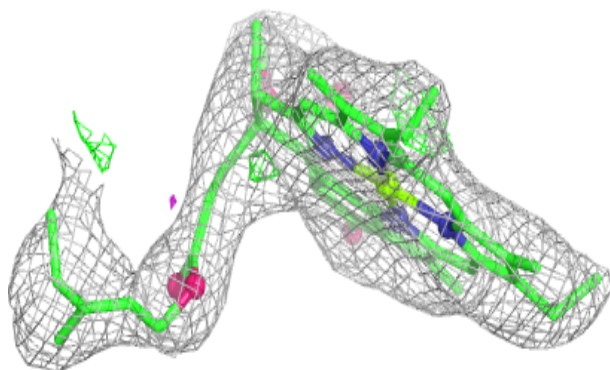
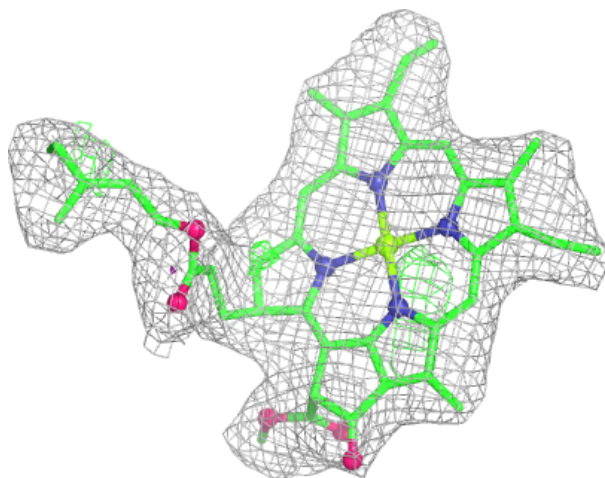
Electron density around LMG d1 408:

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



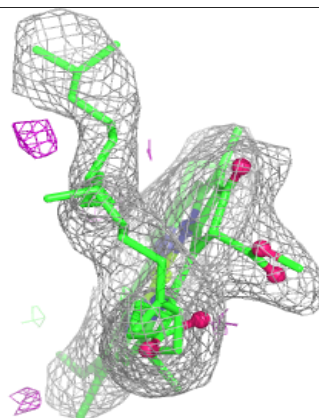
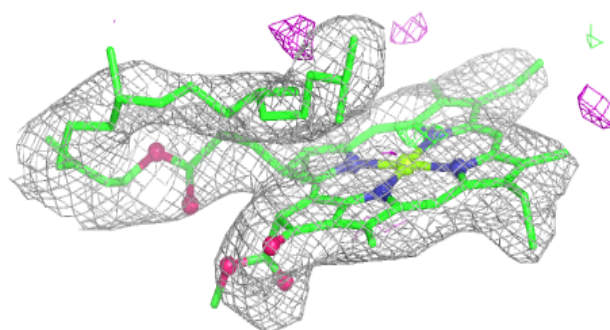
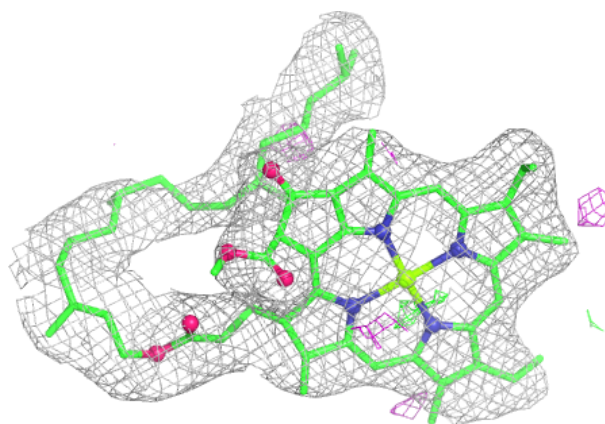
Electron density around CLA A1 404:

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



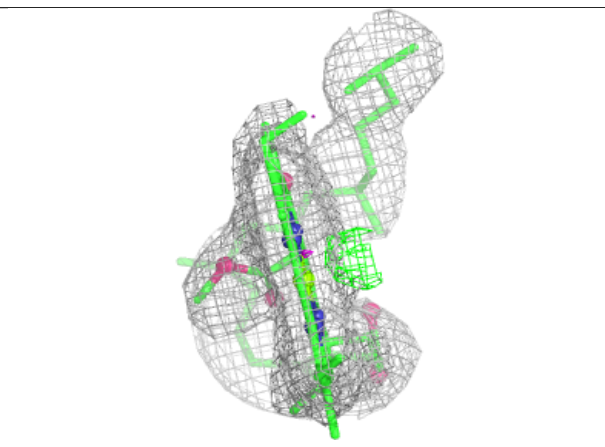
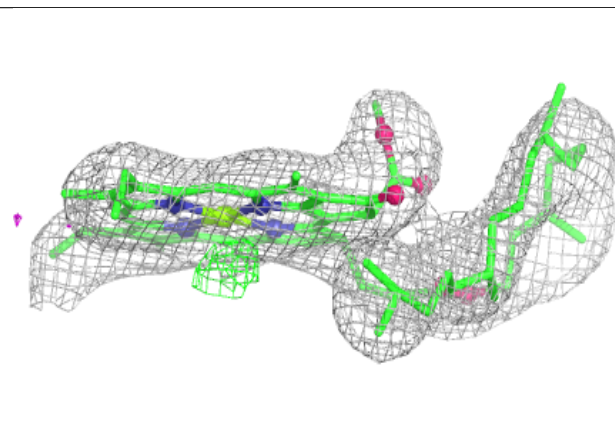
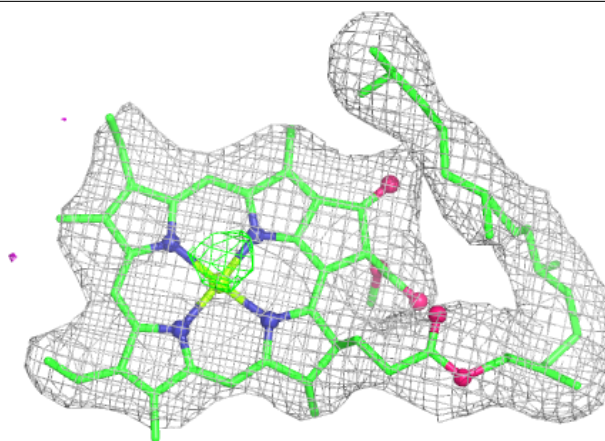
Electron density around CLA C1 510:

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



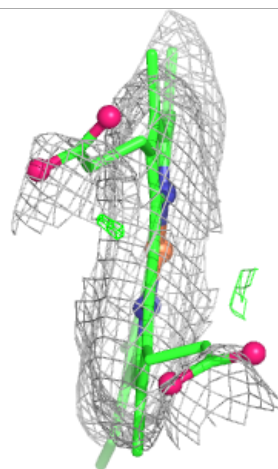
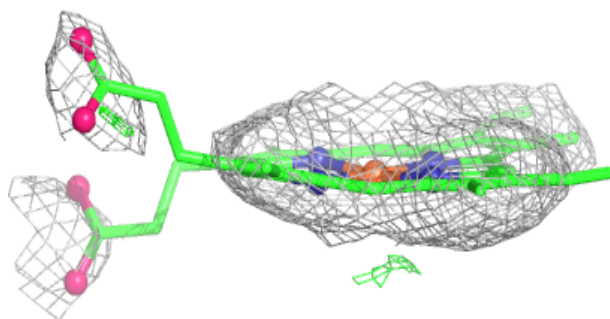
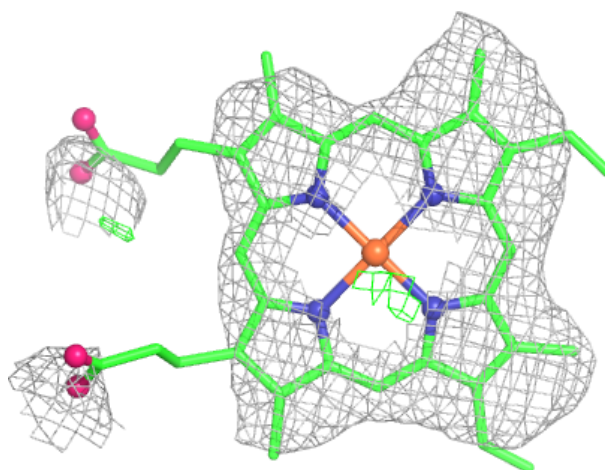
Electron density around CLA B1 612:

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



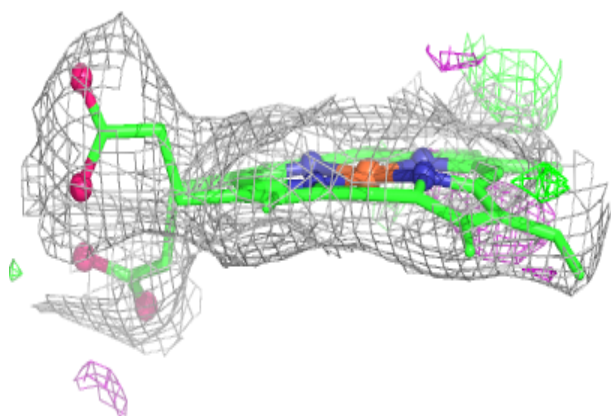
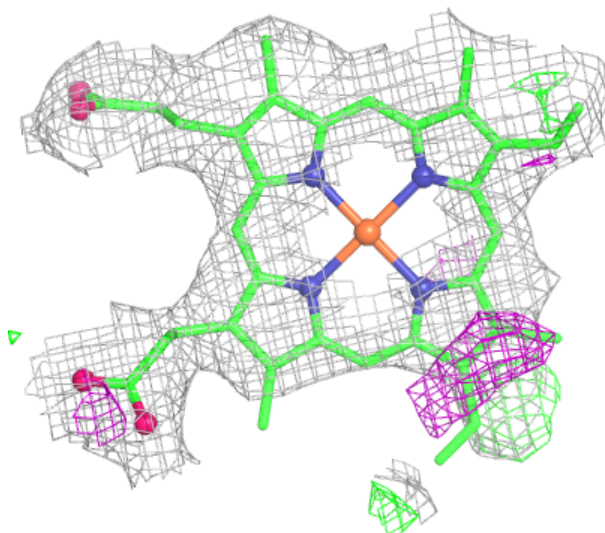
Electron density around HEM f1 101:

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



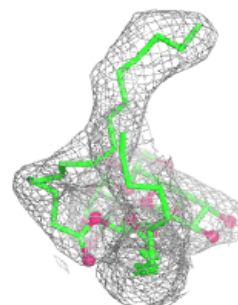
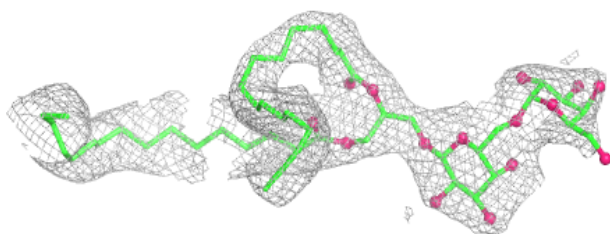
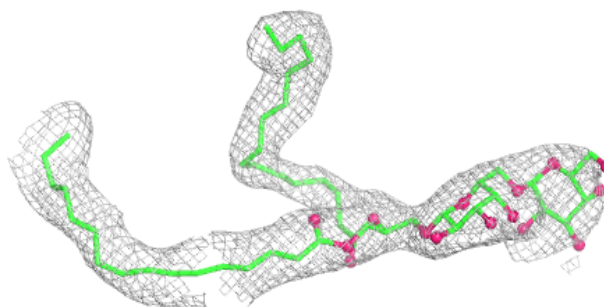
Electron density around HEM v1 201:

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

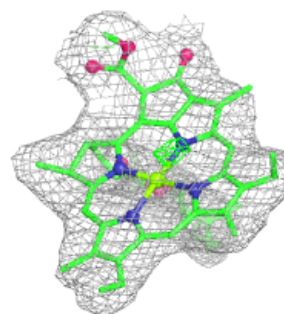
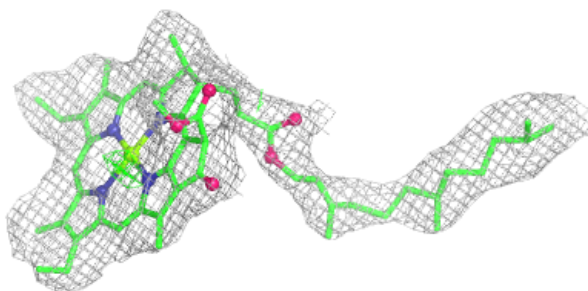
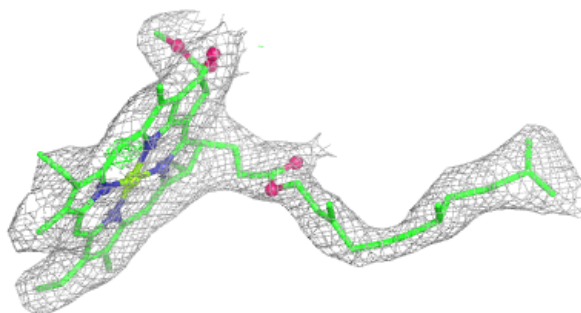


Electron density around DGD h2 102:

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

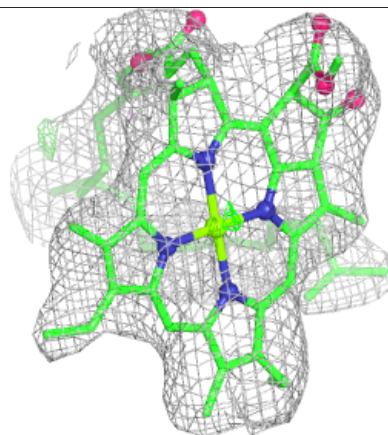
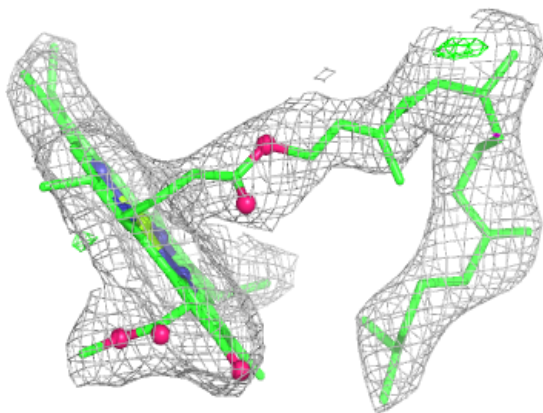
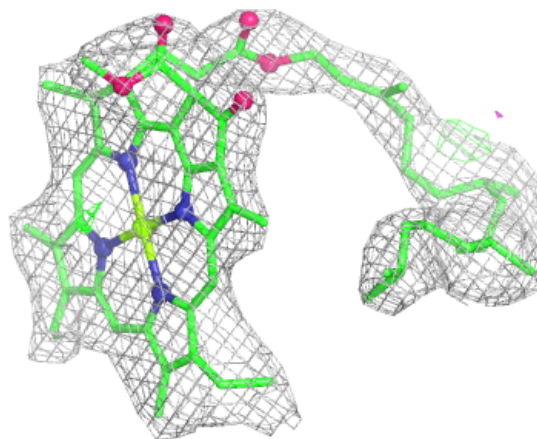
**Electron density around CLA C1 503:**

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

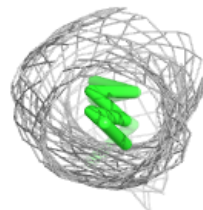
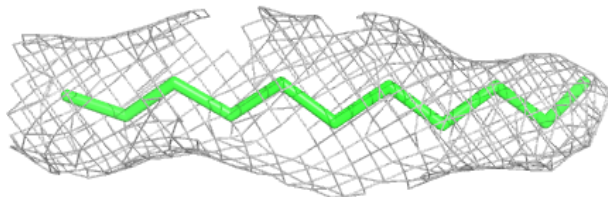
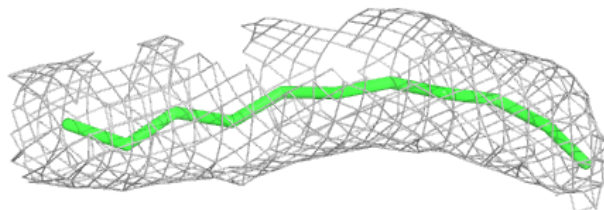


Electron density around CLA C1 504:

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

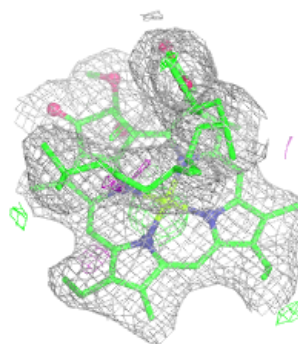
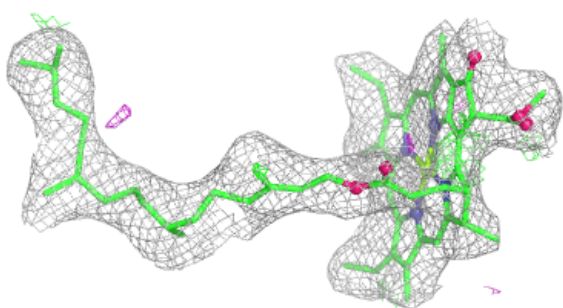
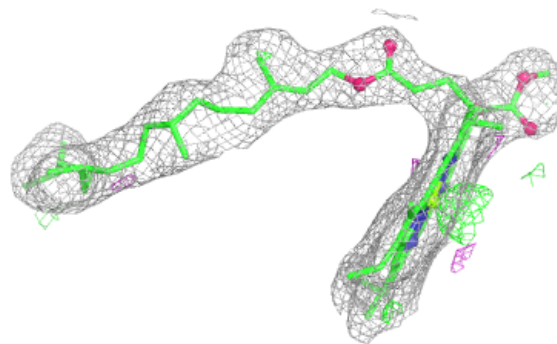
**Electron density around LMT M1 102:**

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

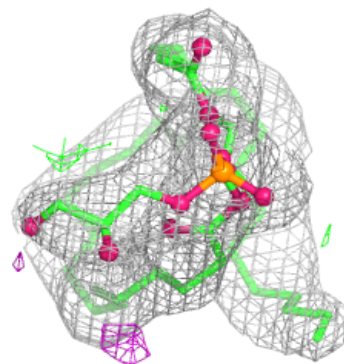
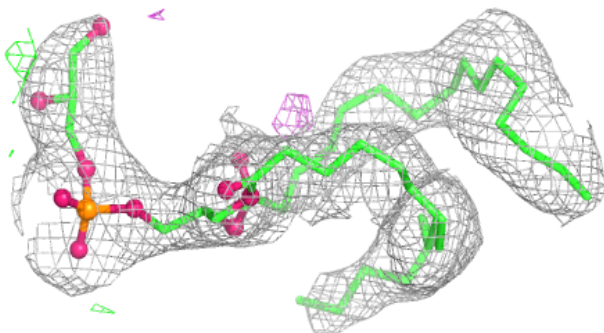
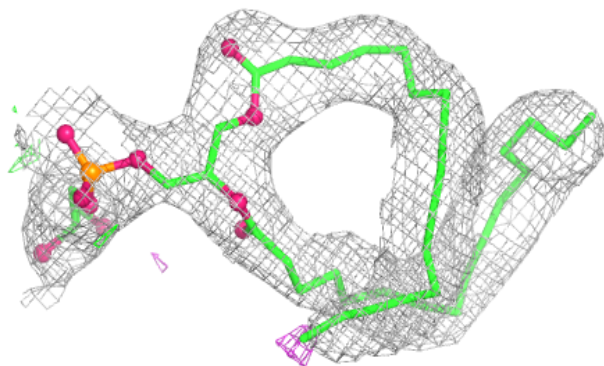


Electron density around CLA b1 620:

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

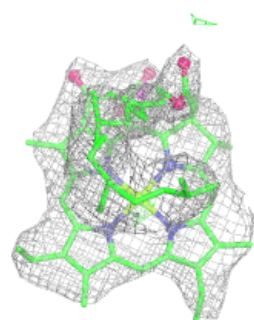
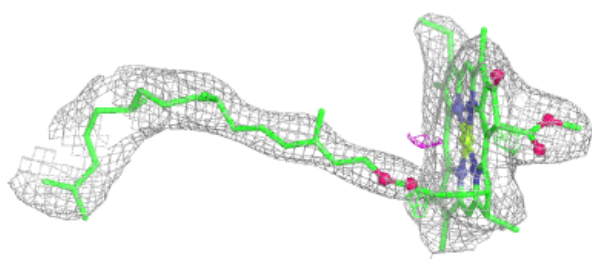
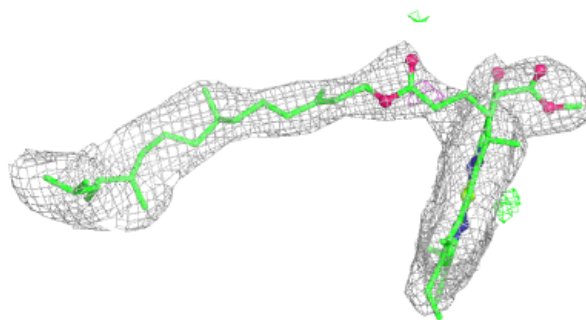
**Electron density around LHG D2 403:**

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

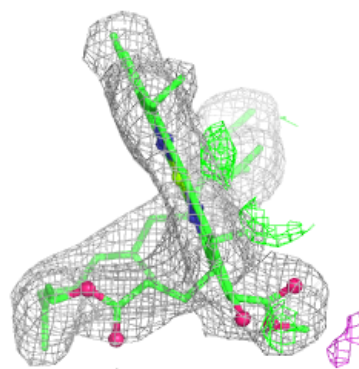
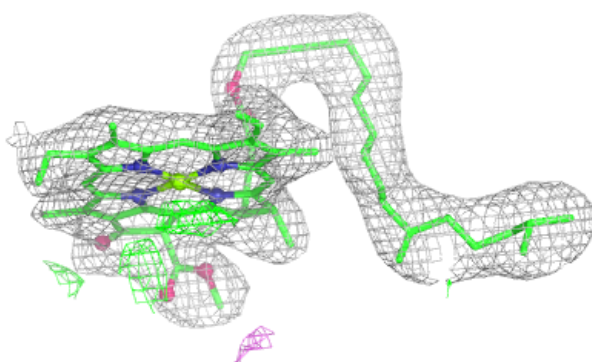
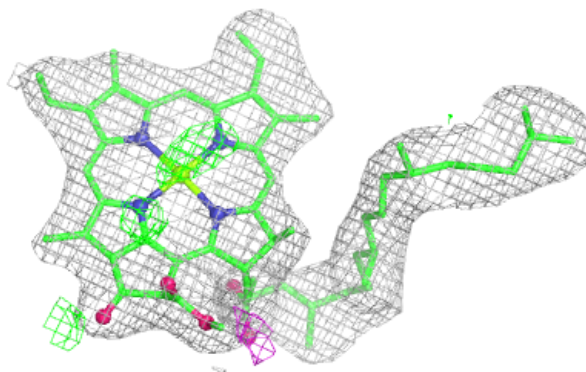


Electron density around CLA b2 608:

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

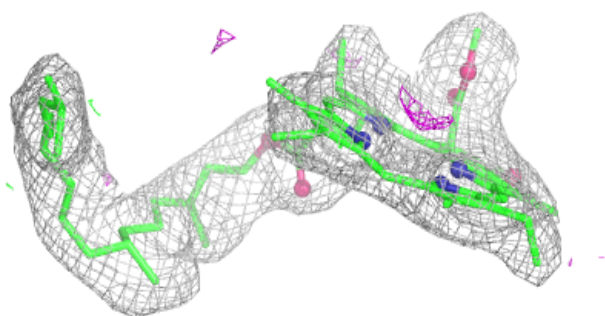
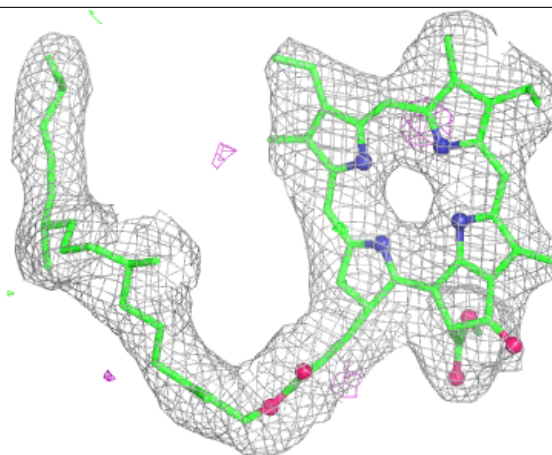
**Electron density around CLA d1 404:**

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

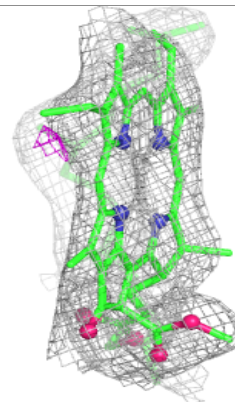
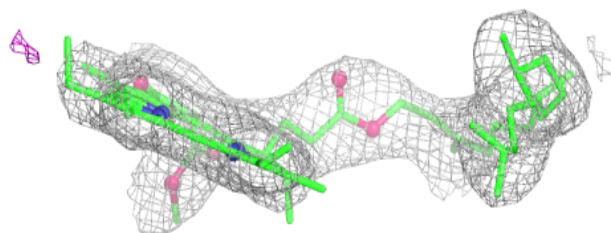
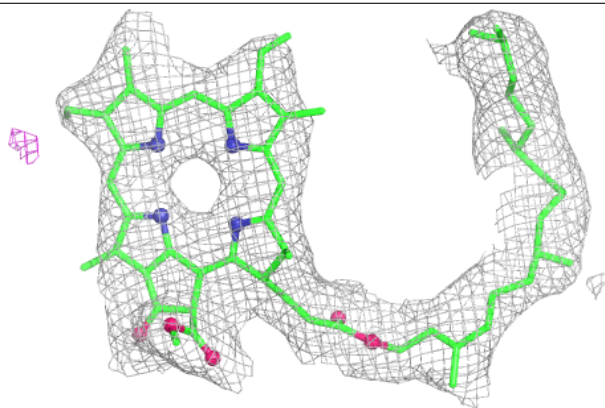


Electron density around PHO d1 403:

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

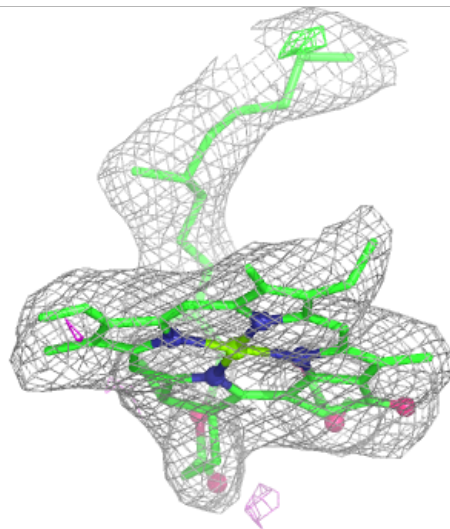
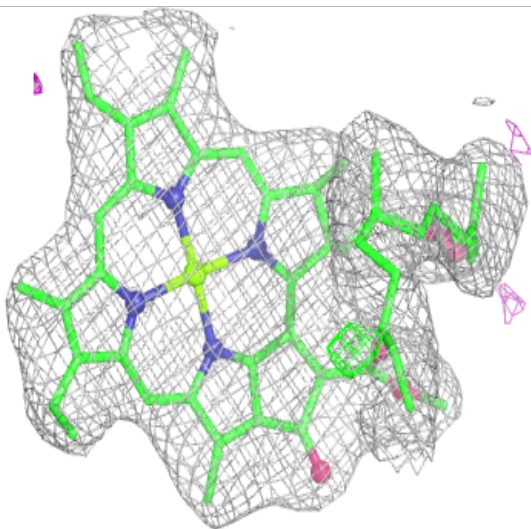
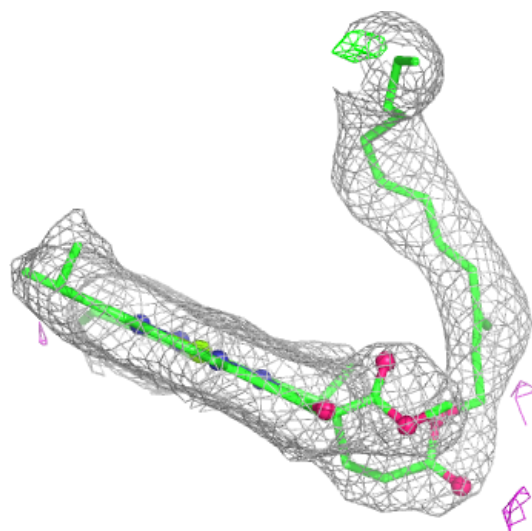
**Electron density around PHO A2 407:**

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



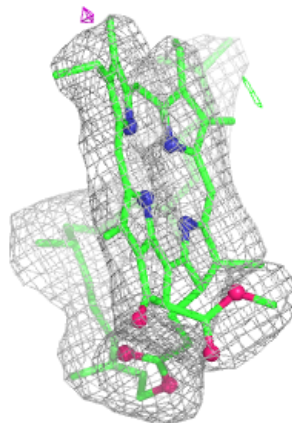
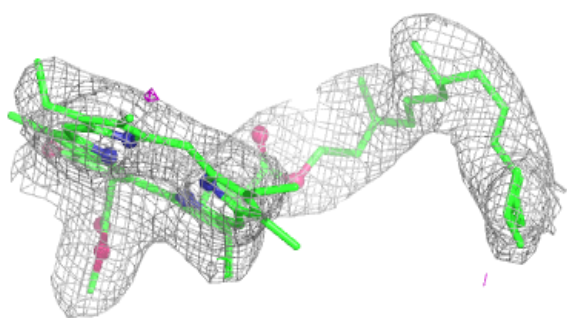
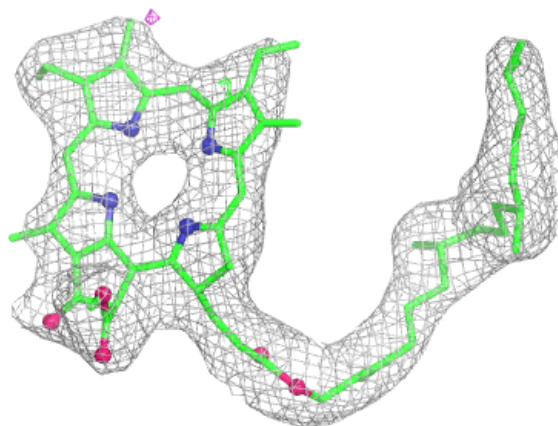
Electron density around CLA b1 615:

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



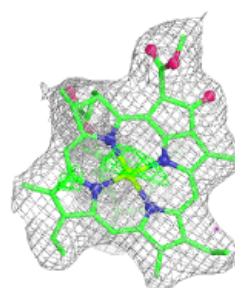
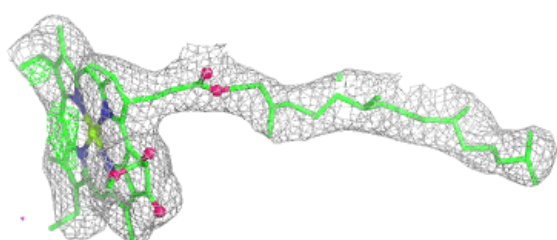
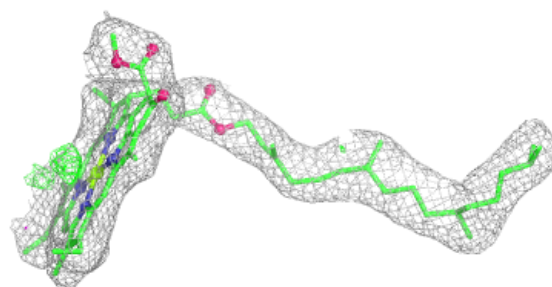
Electron density around PHO d2 408:

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

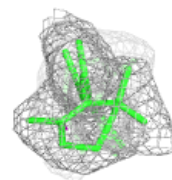
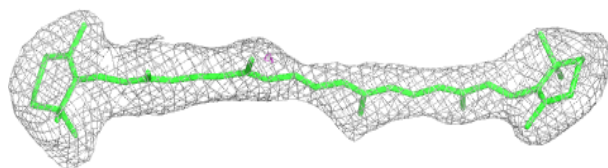
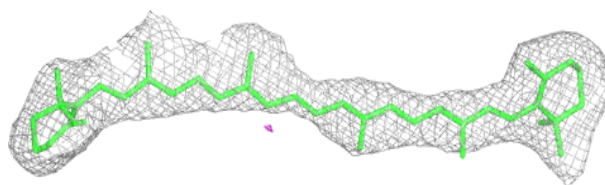


Electron density around CLA b1 607:

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

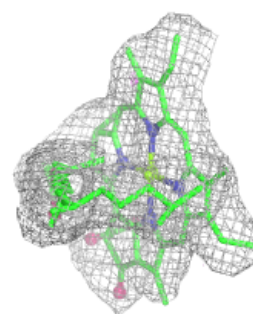
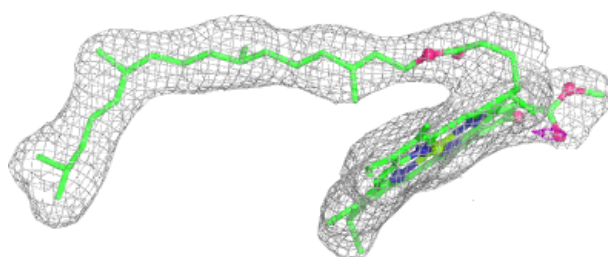
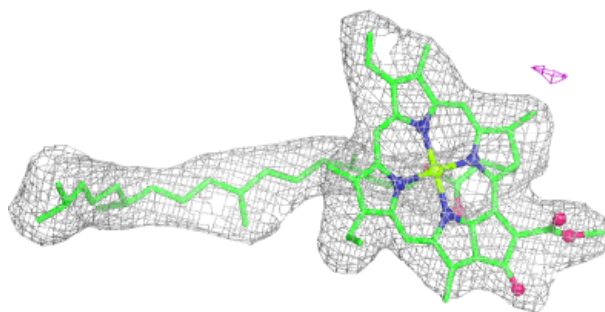
**Electron density around BCR a2 402:**

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



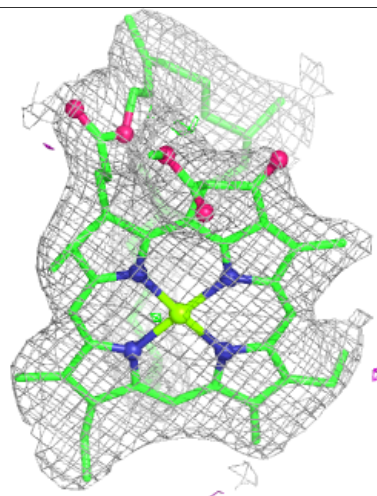
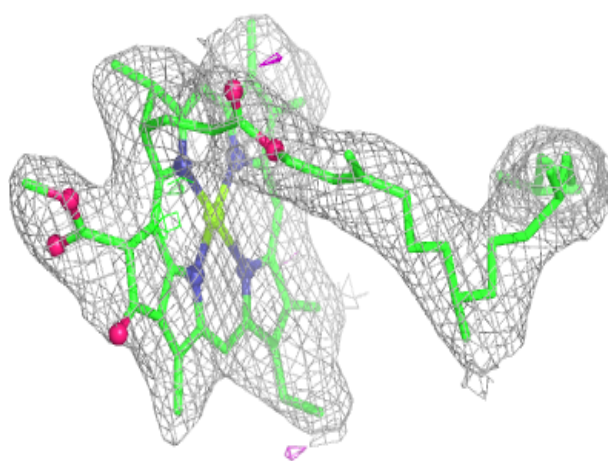
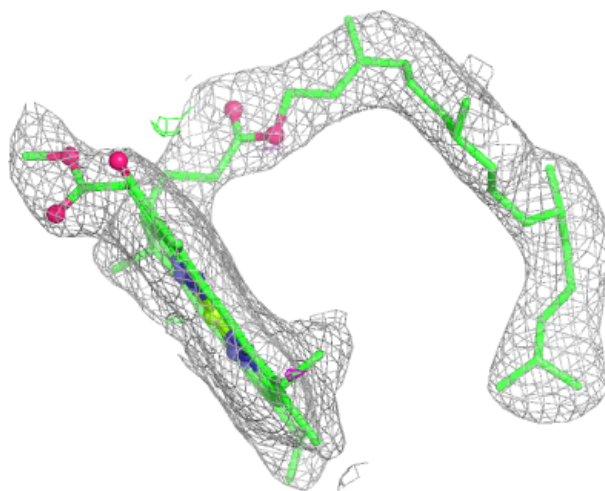
Electron density around CLA b1 610:

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



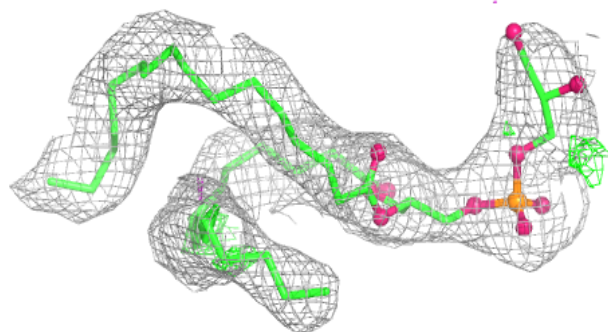
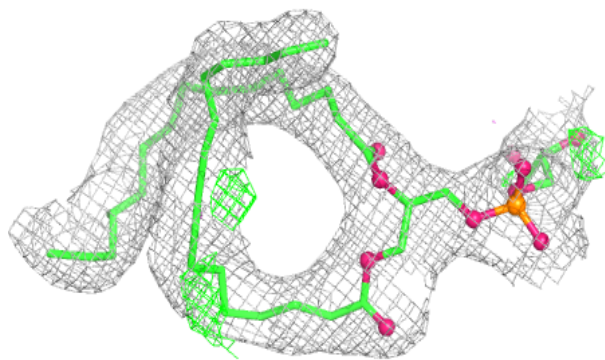
Electron density around CLA B1 613:

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



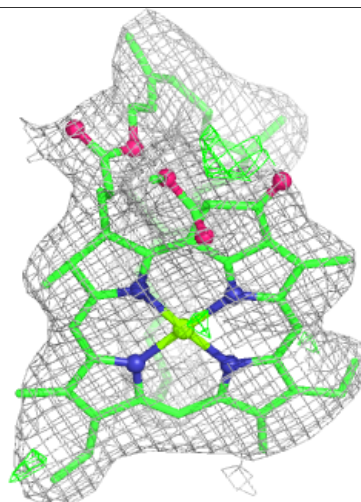
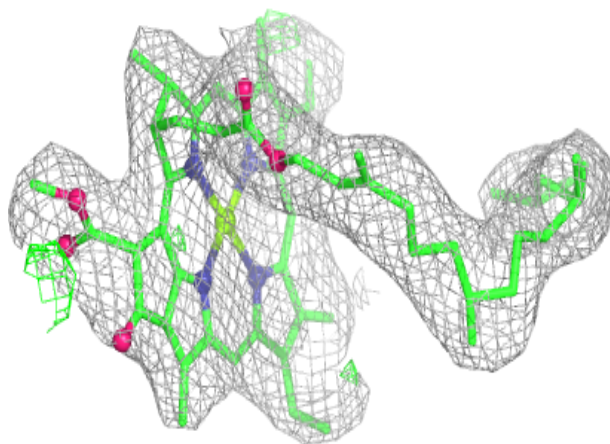
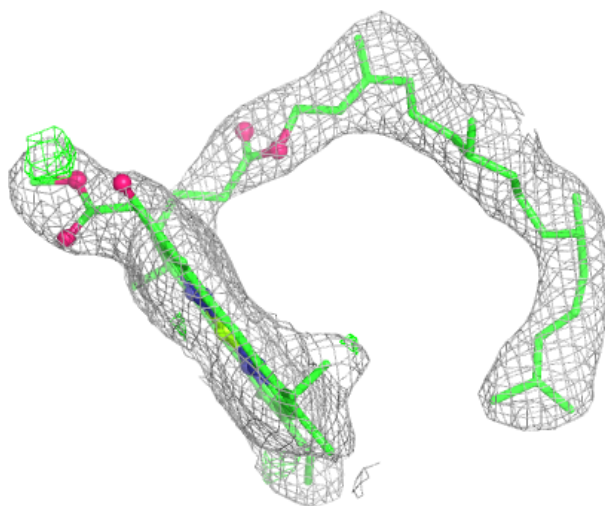
Electron density around LHG b1 622:

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



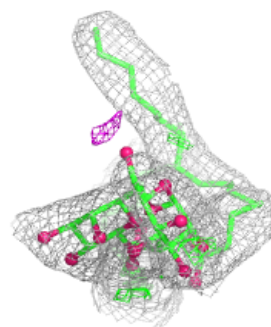
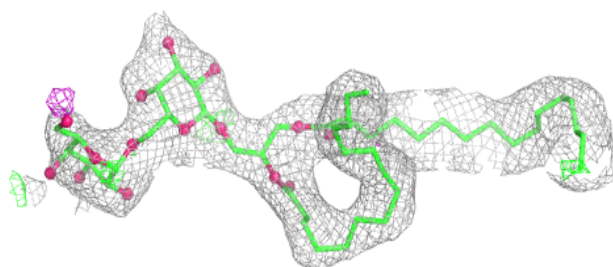
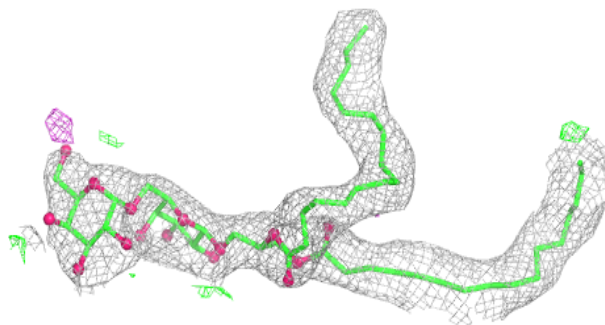
Electron density around CLA B2 613:

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



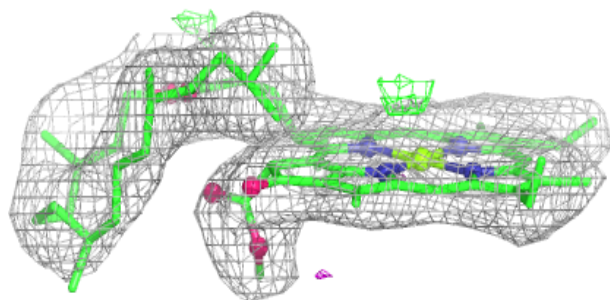
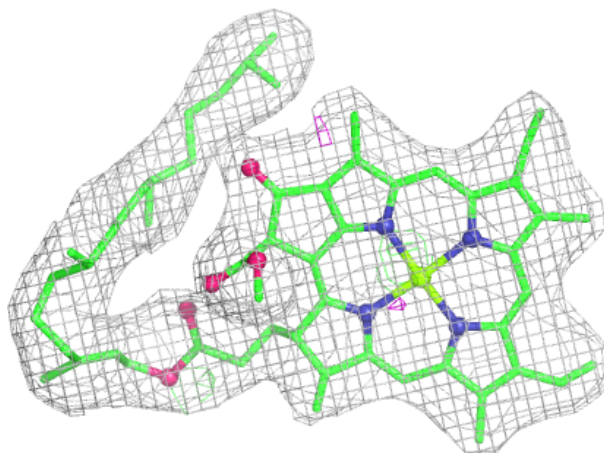
Electron density around DGD h1 101:

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



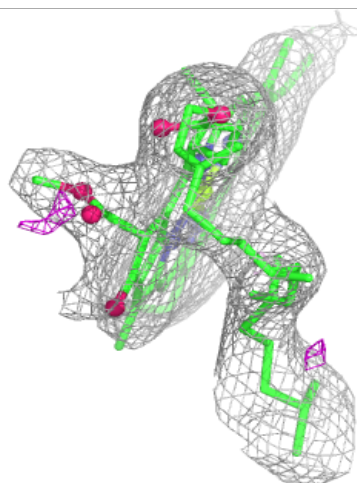
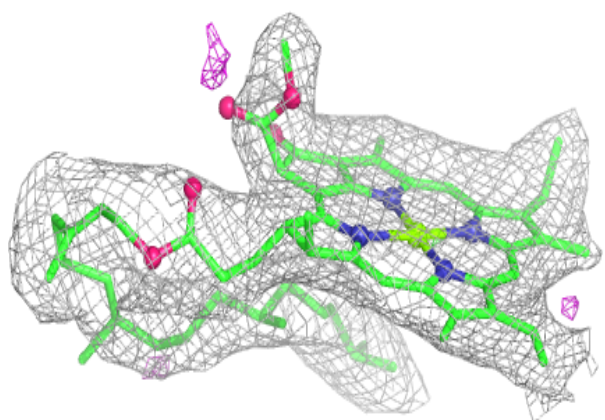
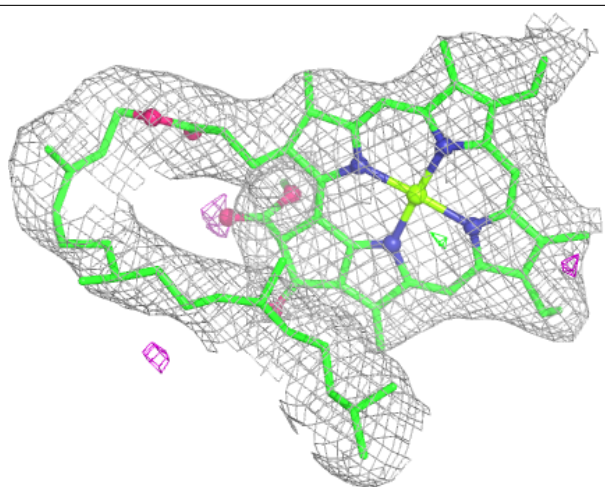
Electron density around CLA b1 612:

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



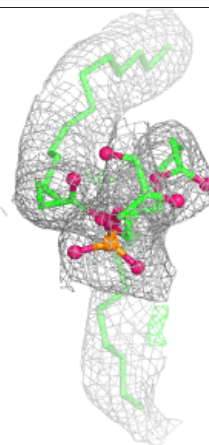
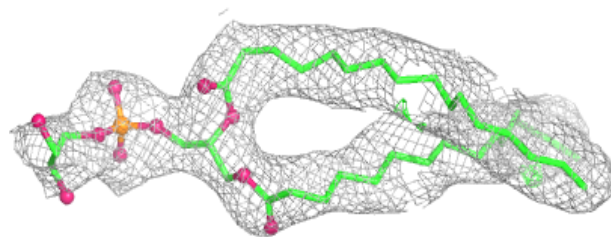
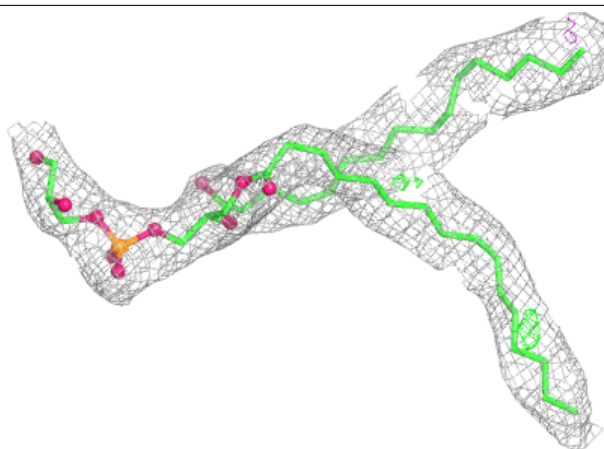
Electron density around CLA c1 511:

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



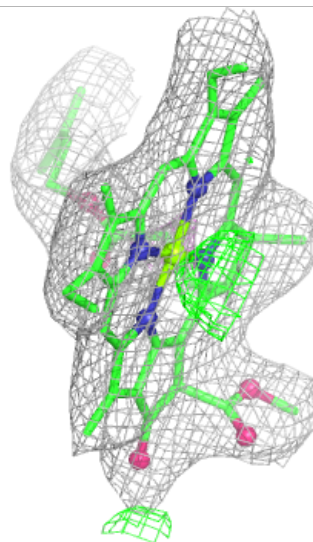
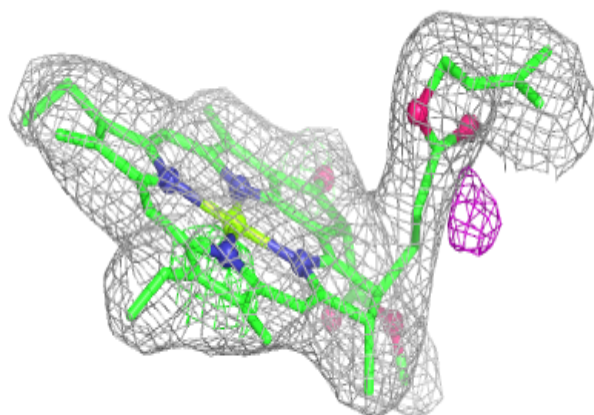
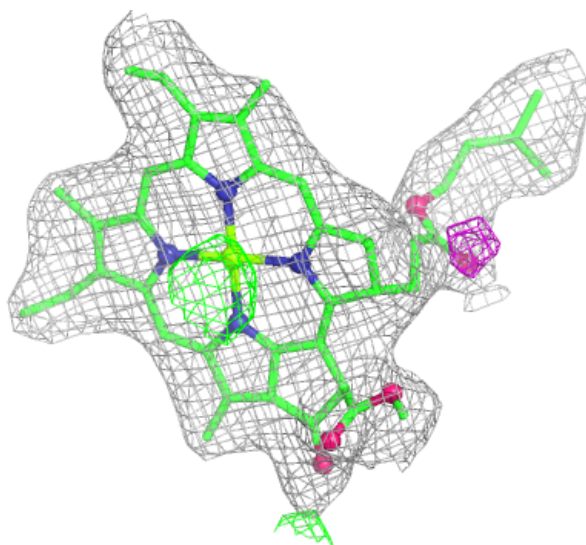
Electron density around LHG d1 407:

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



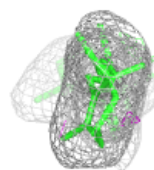
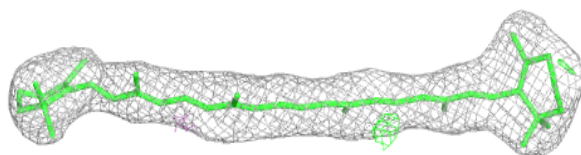
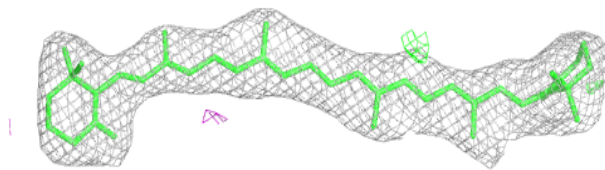
Electron density around CLA a1 405:

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



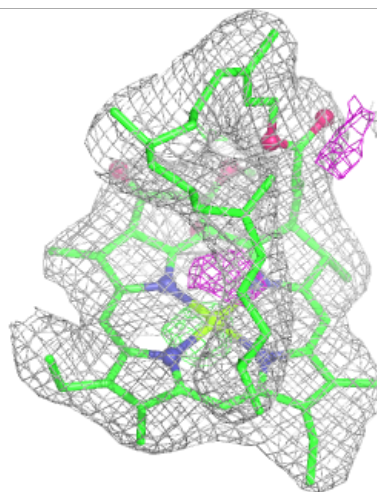
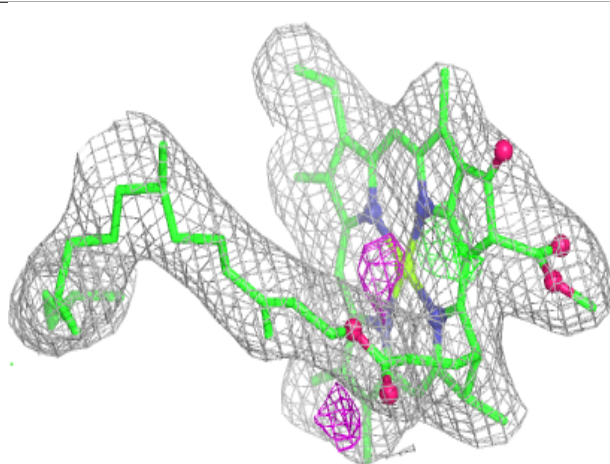
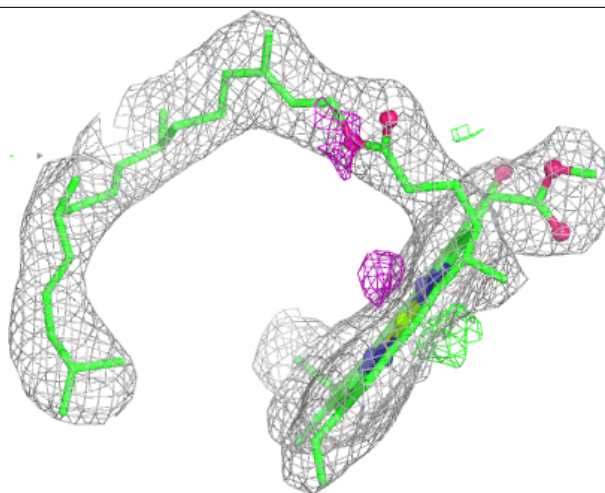
Electron density around BCR b1 601:

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



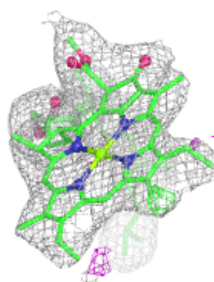
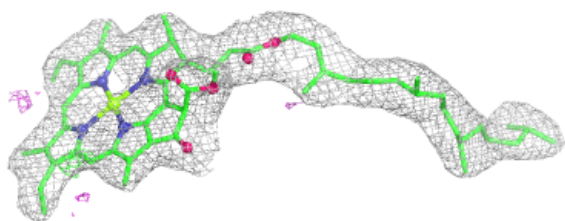
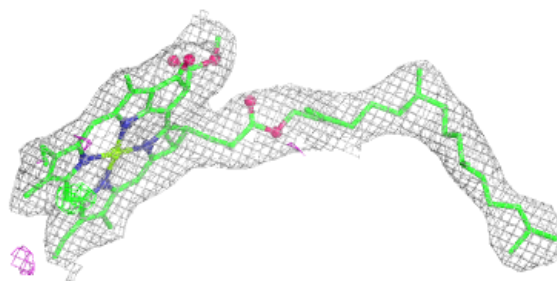
Electron density around CLA b1 613:

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



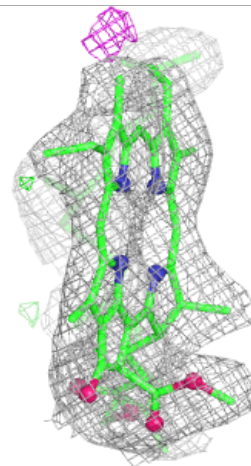
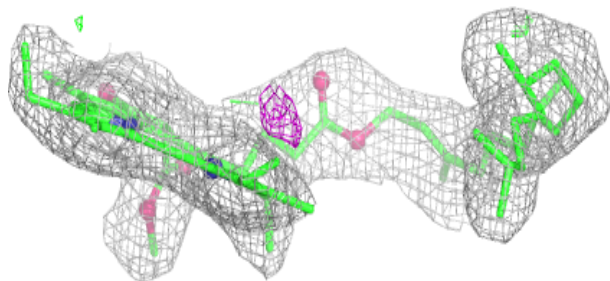
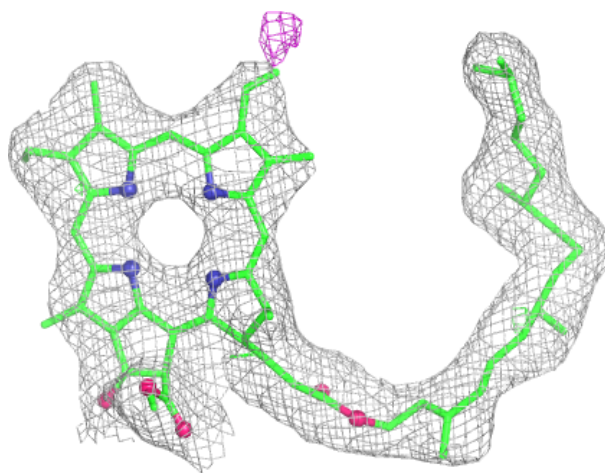
Electron density around CLA a2 404:

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



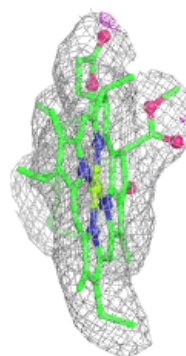
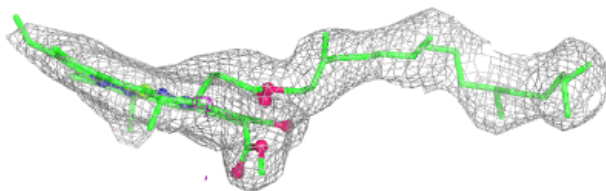
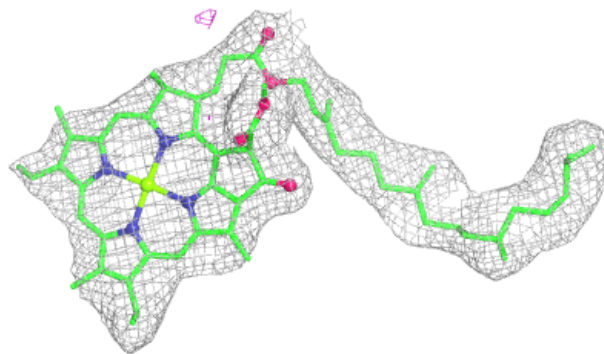
Electron density around PHO a2 416:

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



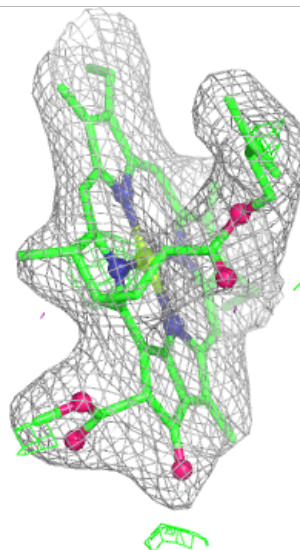
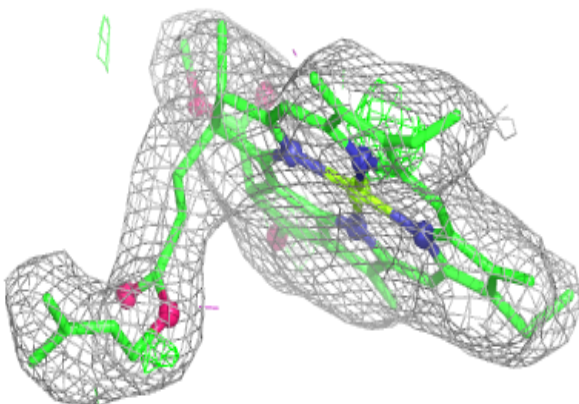
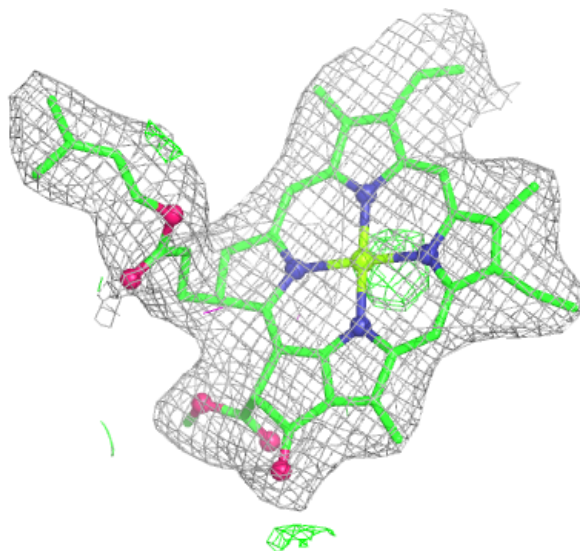
Electron density around CLA b1 605:

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



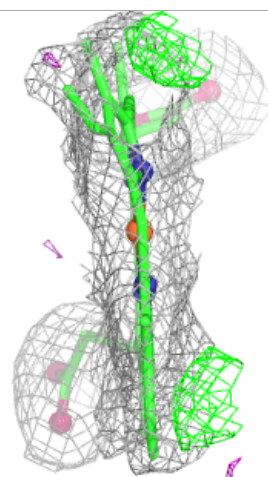
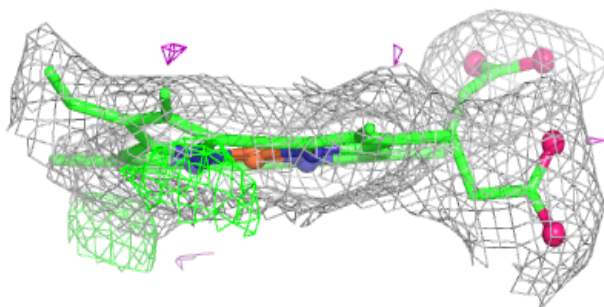
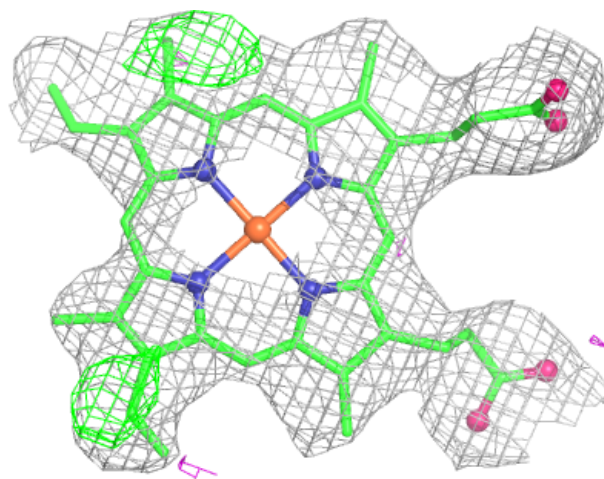
Electron density around CLA a2 413:

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



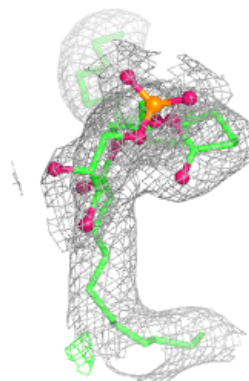
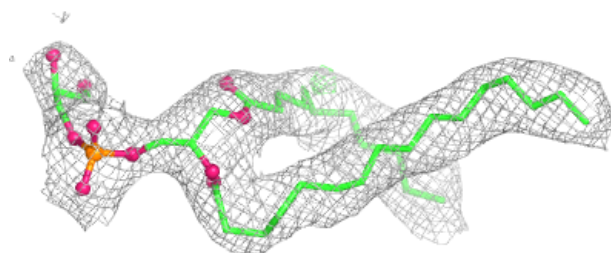
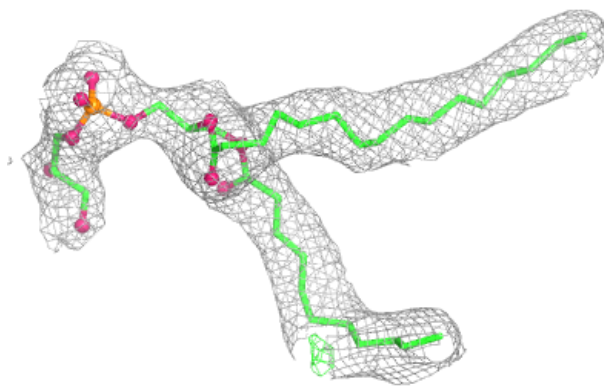
Electron density around HEM V1 201:

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

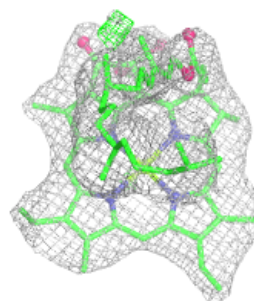
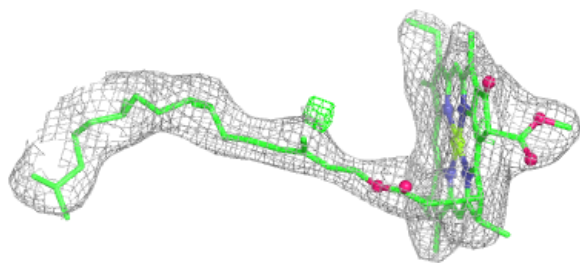
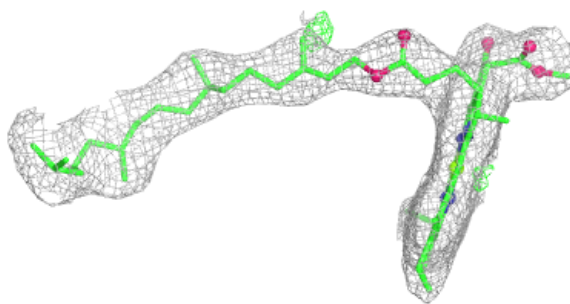


Electron density around LHG 12 101:

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

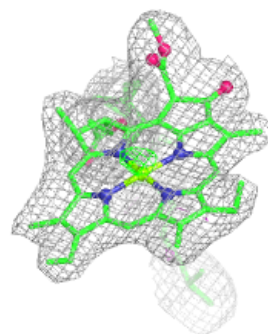
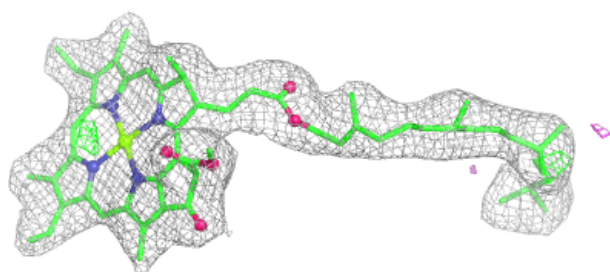
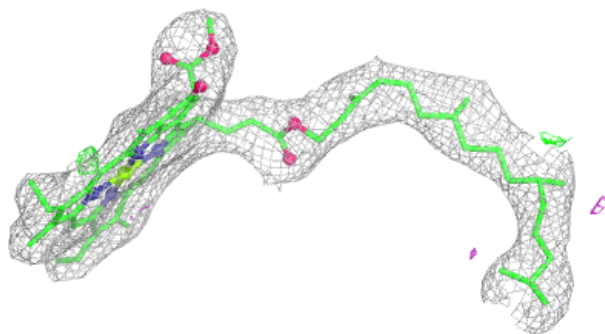
**Electron density around CLA B2 608:**

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

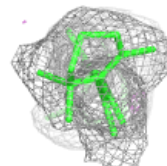
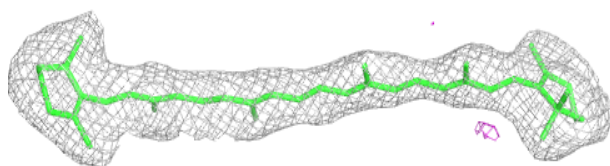
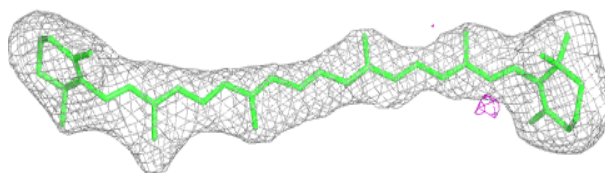


Electron density around CLA D1 402:

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

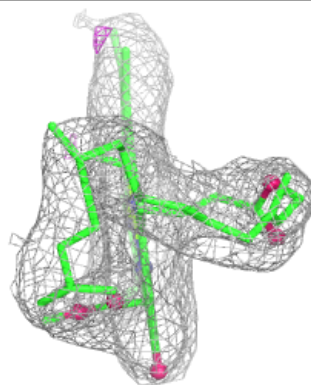
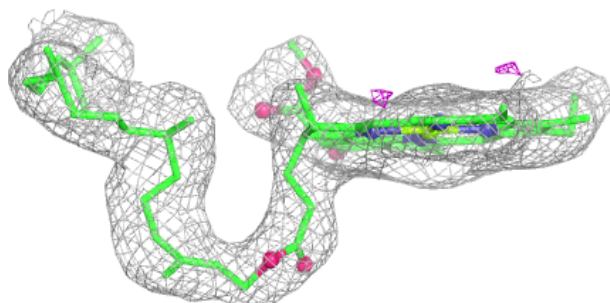
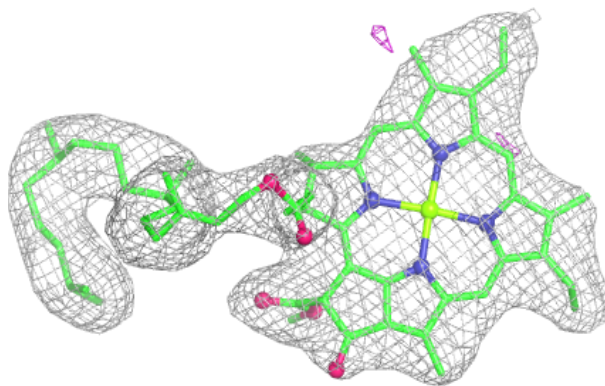
**Electron density around BCR A1 401:**

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

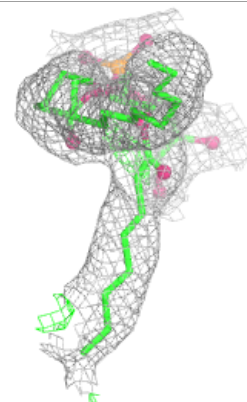
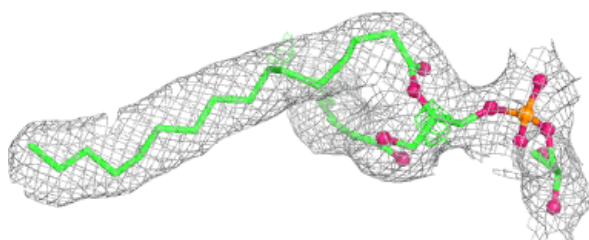
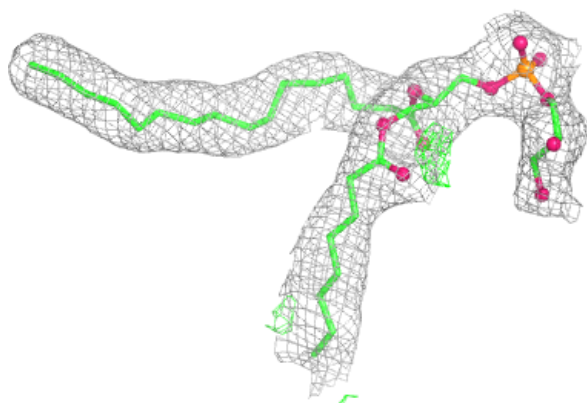


Electron density around CLA B1 614:

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

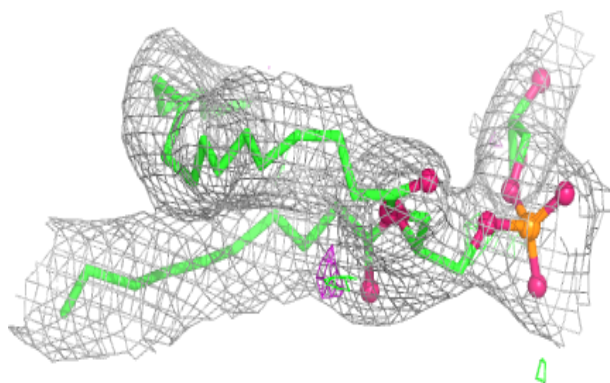
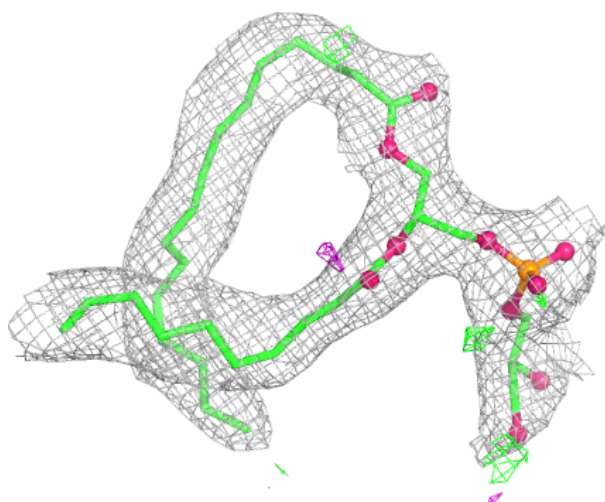
**Electron density around LHG L1 101:**

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



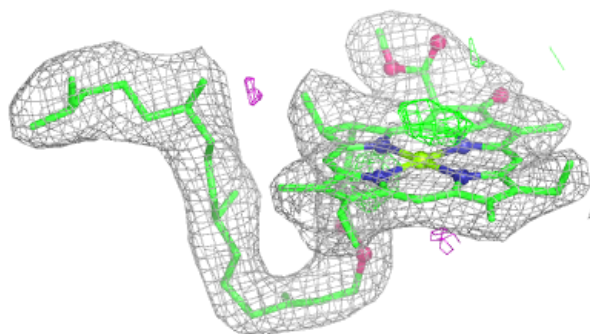
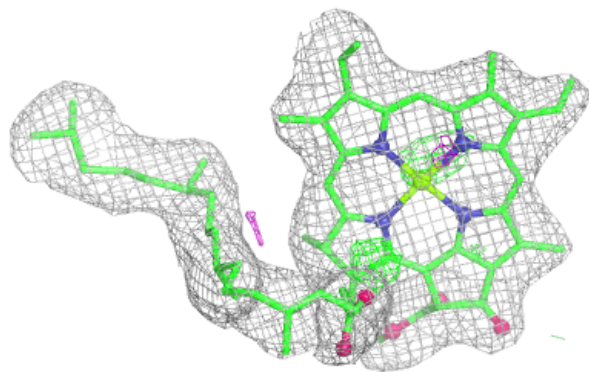
Electron density around LHG a1 407:

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



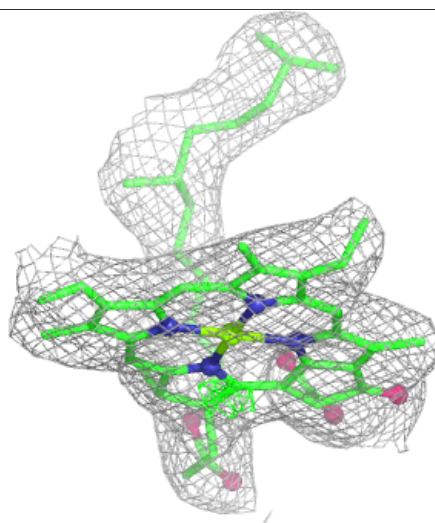
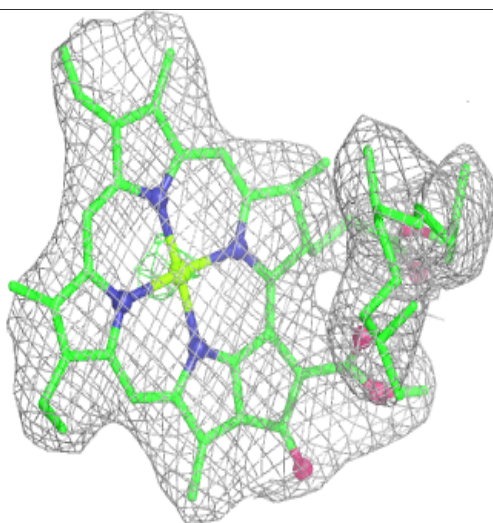
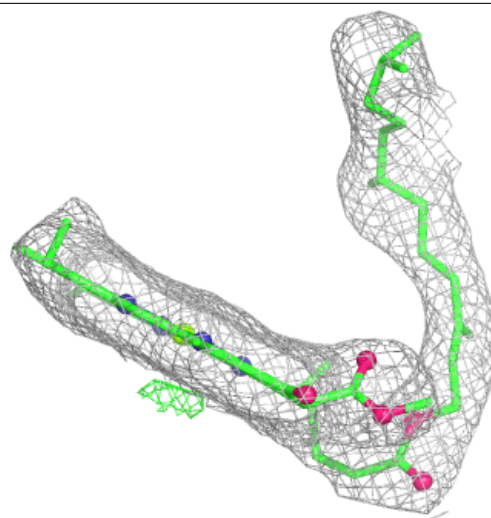
Electron density around CLA d2 402:

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



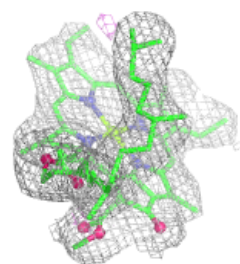
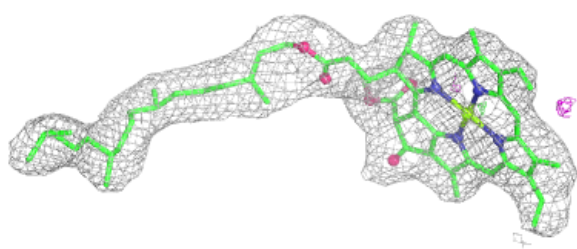
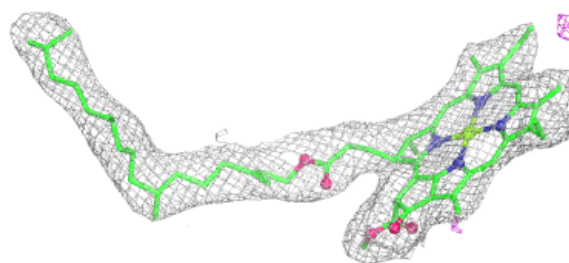
Electron density around CLA b2 615:

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

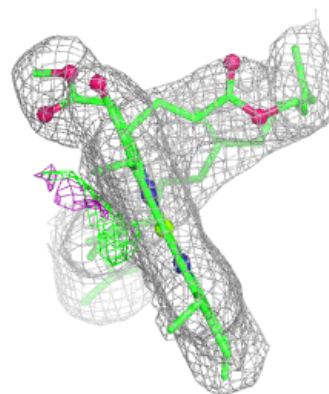
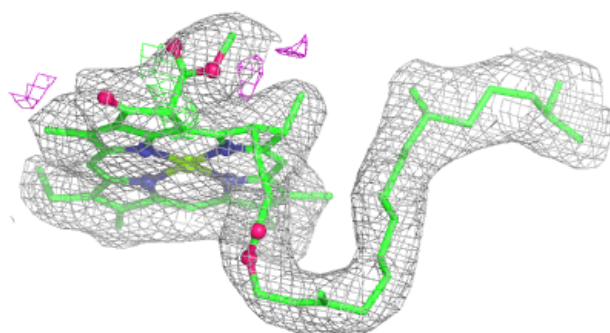
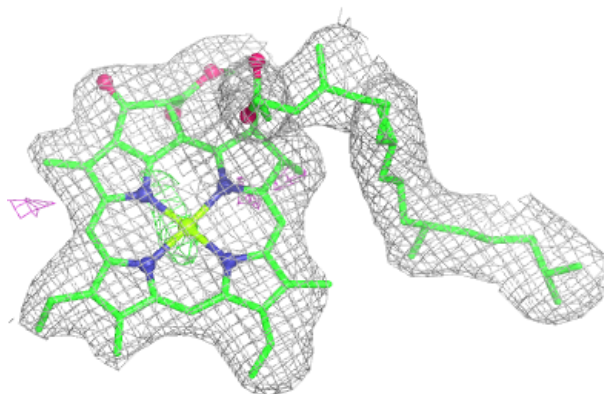


Electron density around CLA a1 403:

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

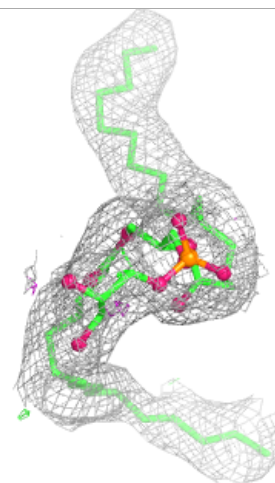
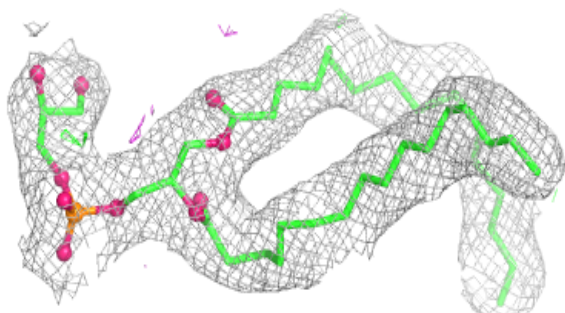
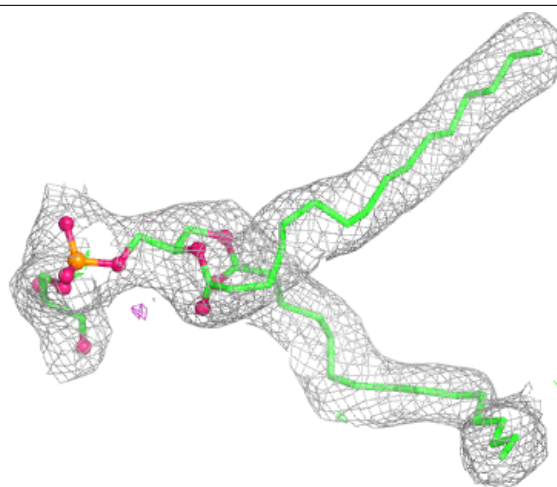
**Electron density around CLA A1 406:**

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



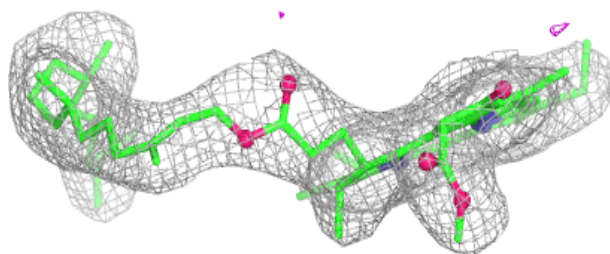
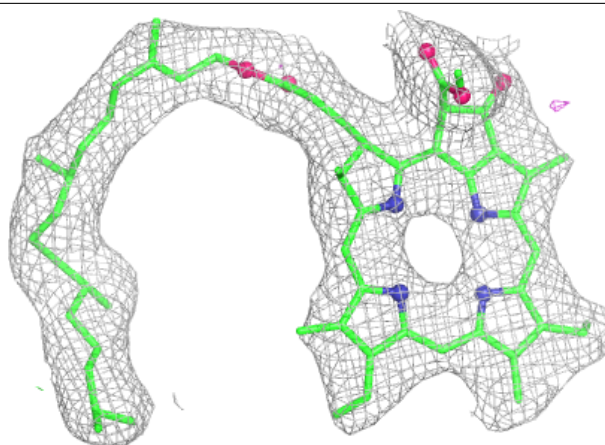
Electron density around LHG l1 102:

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



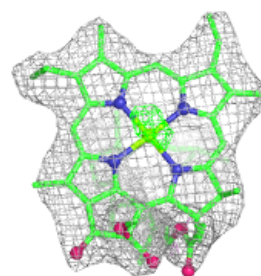
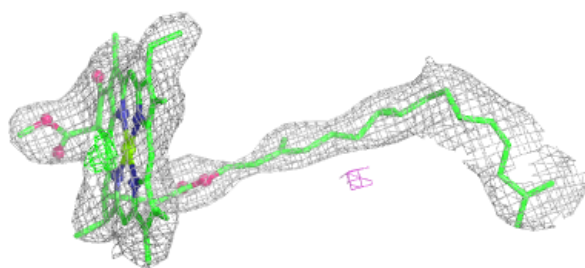
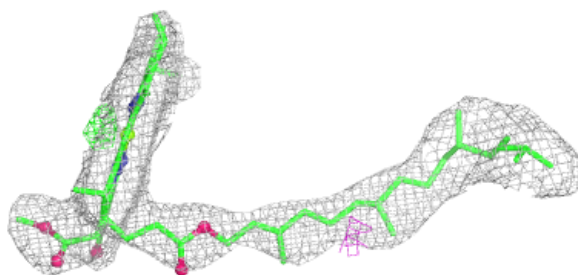
Electron density around PHO A1 408:

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



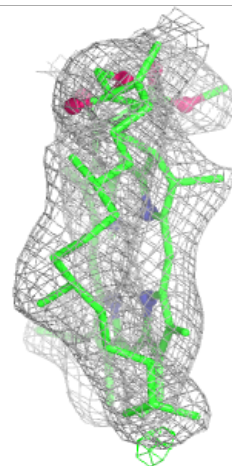
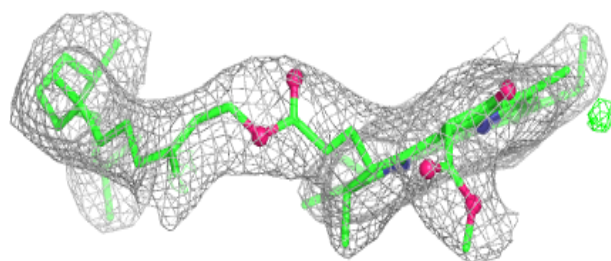
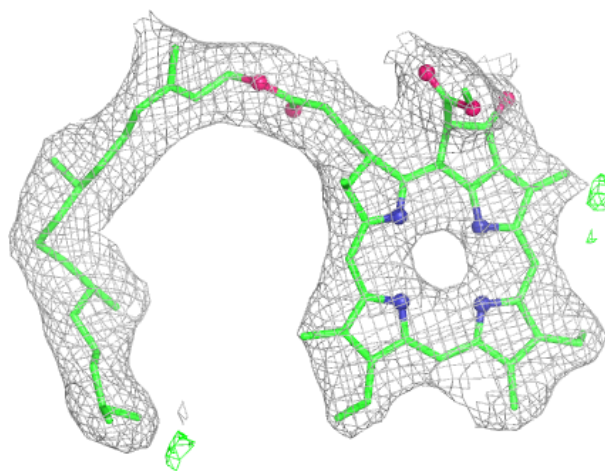
Electron density around CLA B1 608:

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



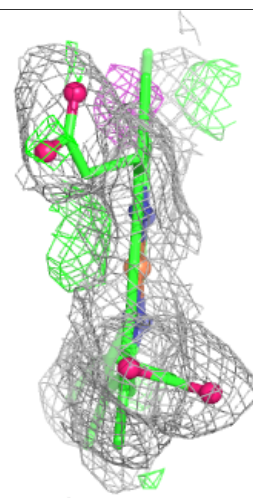
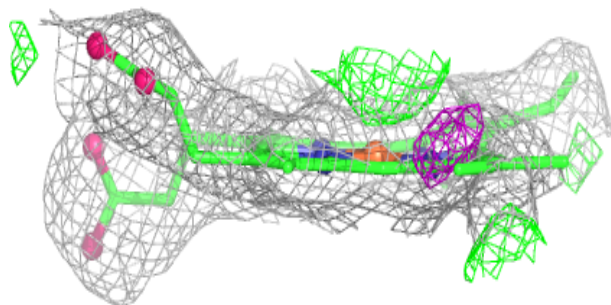
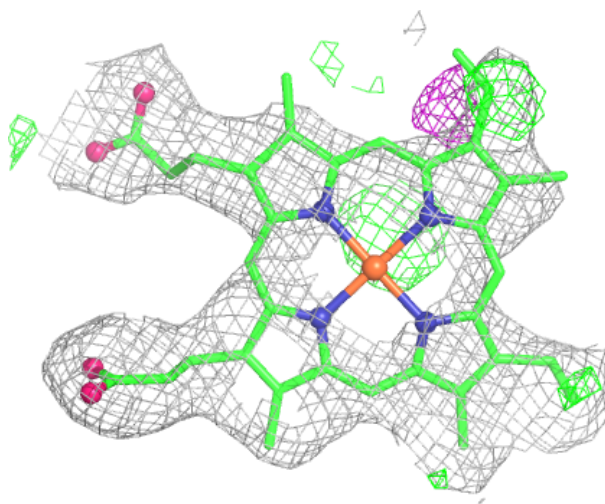
Electron density around PHO a1 411:

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



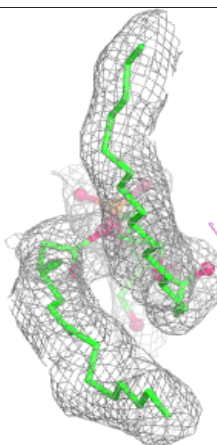
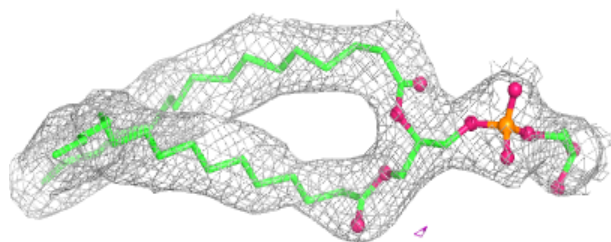
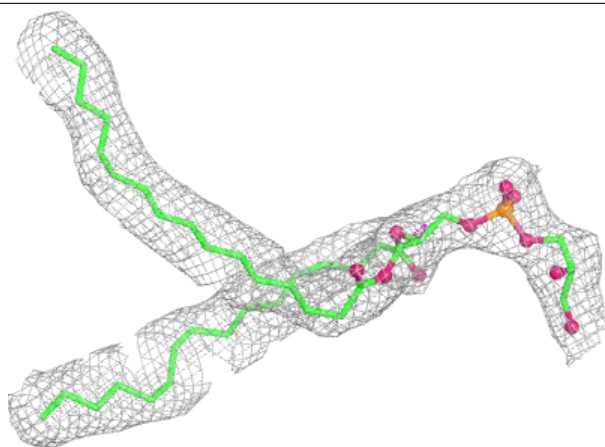
Electron density around HEM v2 201:

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

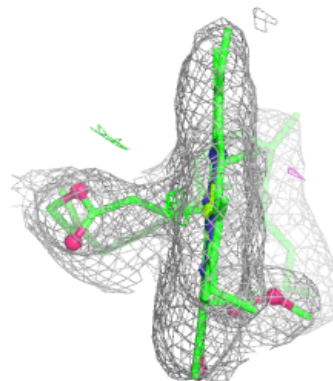
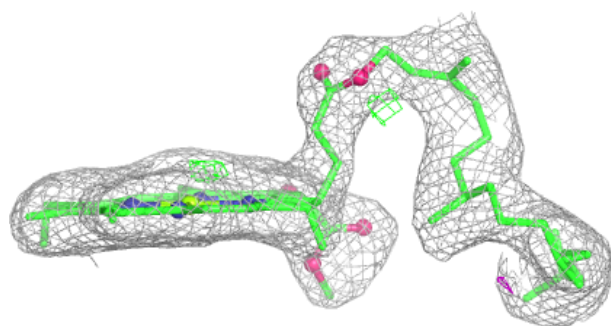
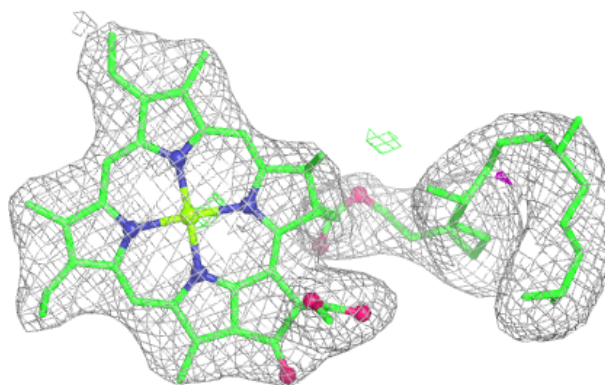


Electron density around LHG D1 405:

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

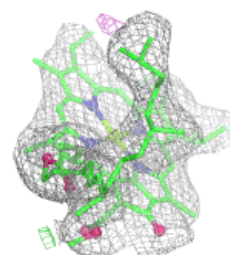
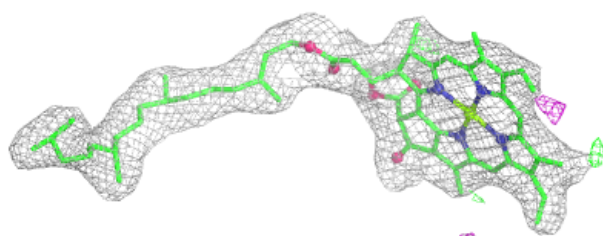
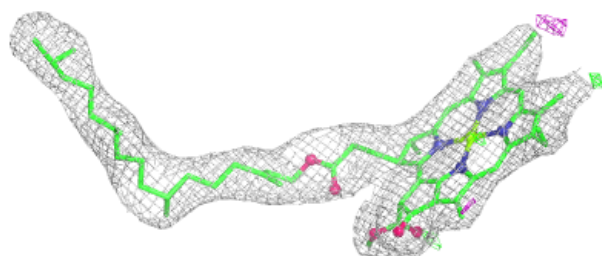
**Electron density around CLA b1 614:**

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

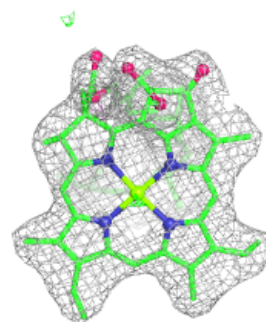
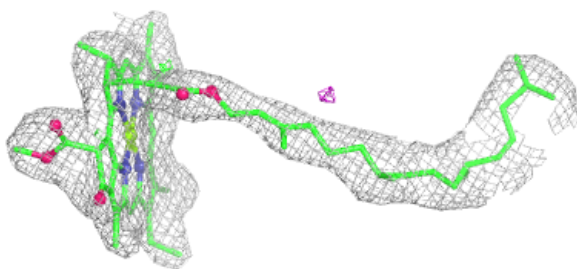
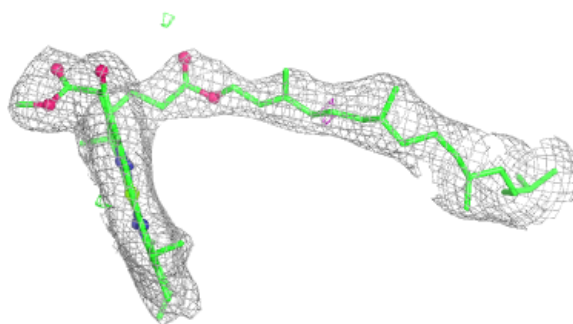


Electron density around CLA A1 403:

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

**Electron density around CLA b1 608:**

$2mF_o-DF_c$ (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.