



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 02:51 AM EDT

PDB ID : 11YO / pdb_000011yo
Title : Single-conformation model re-refinement of 2F/S3-rich PSII intermediate structure at 2.09 Angstrom resolution
Authors : Wang, J.; Armstrong, W.H.; Batista, V.S.
Deposited on : 2026-03-18
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
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

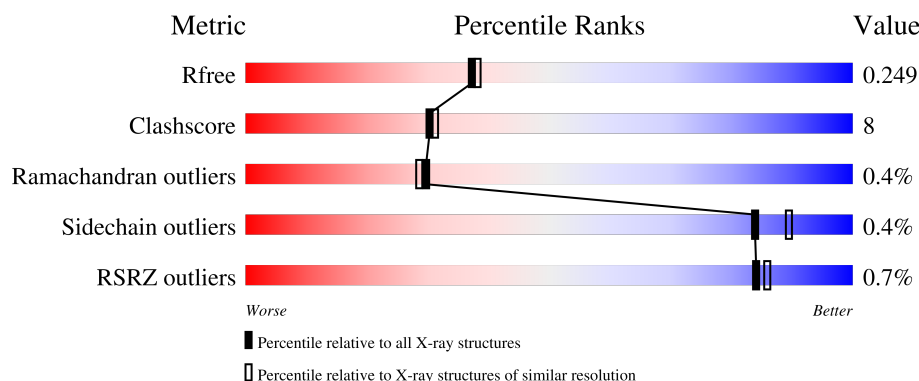
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



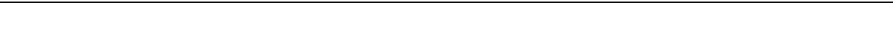
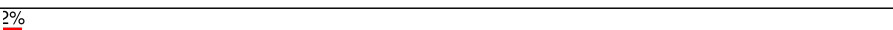
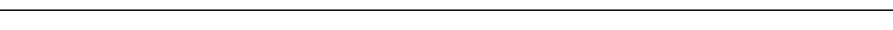
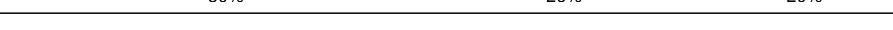
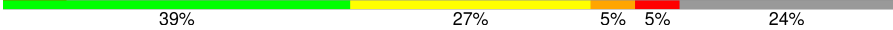
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	344	 83% 13% ..
1	a	344	 83% 13% ..
2	B	510	 84% 14% .
2	b	510	 83% 15% ..
3	C	461	 87% 8% .

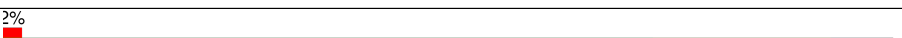
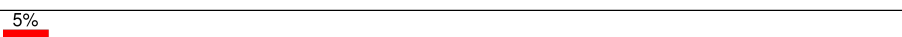
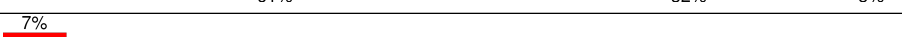
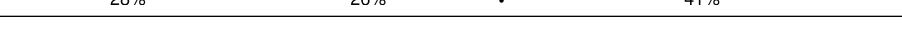
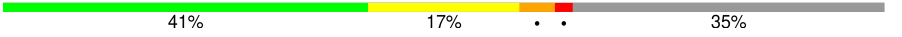
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Mol	Chain	Length	Quality of chain
3	c	461	 89% 8% ..
4	D	352	 82% 14% ..
4	d	352	 80% 16% .
5	E	84	 71% 26% .
5	e	84	 61% 33% ...
6	F	45	 51% 24% 24%
6	f	45	 60% 16% 24%
7	H	66	 82% 11% 5% ..
7	h	66	 74% 15% 5% . 5%
8	I	38	 87% 5% . 5%
8	i	38	 87% 8% 5%
9	J	40	 58% 32% 10%
9	j	40	 60% 30% 10%
10	K	46	 50% 26% . 20%
10	k	46	 54% 22% .. 20%
11	L	37	 92% 8%
11	l	37	 84% 11% ..
12	M	36	 78% 14% 8%
12	m	36	 61% 22% . . 11%
13	O	272	 71% 17% . 10%
13	o	272	 74% 12% . 10%
14	R	41	 44% 37% . 17%
14	r	41	 39% 27% 5% 5% 24%
15	T	32	 75% 16% . 6%
15	t	32	 84% 6% . 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	HEC	F	101	X	-	-	-
34	HEC	V	201	X	-	-	-
34	HEC	f	101	X	-	-	-
34	HEC	v	201	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 52261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	64	0
			2619	1714	431	459	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3426	2249	571	593	13			
3	c	451	Total	C	N	O	S	0	12	0
			3500	2290	587	610	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	3	0
			2723	1804	444	463	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	36	Total	C	N	O		0	0	0
			296	197	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
14	r	31	Total	C	N	O	0	0	0
			240	162	42	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
15	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
16	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
18	x	39	Total	C	N	O	0	0	0
			286	191	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
19	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

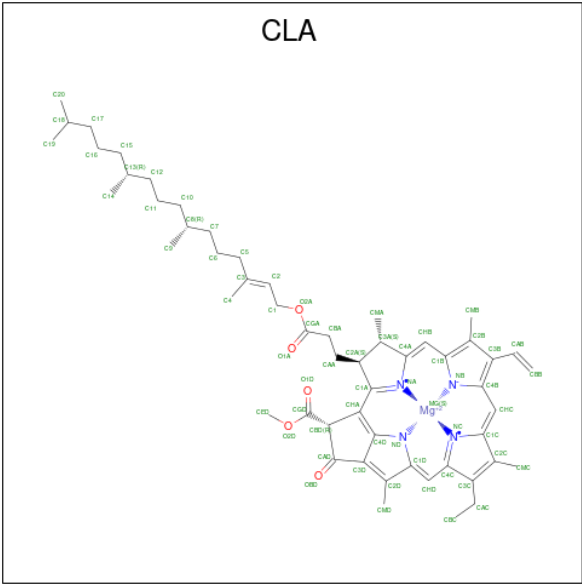
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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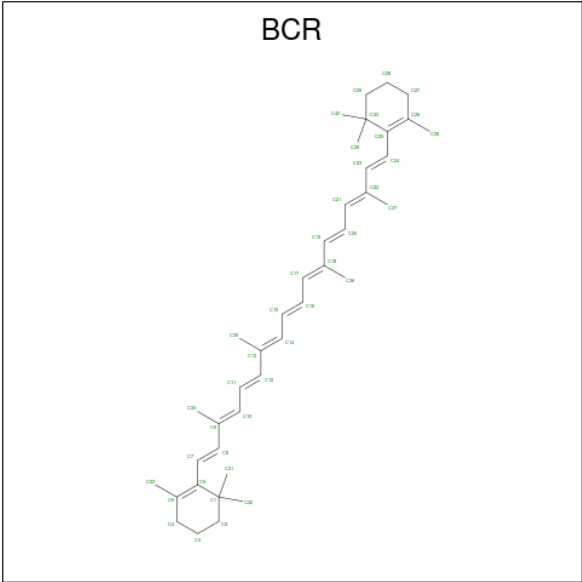
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	C	1	Total C 40 40	0	0
23	C	1	Total C 40 40	0	0
23	C	1	Total C 40 40	0	0
23	D	1	Total C 40 40	0	0
23	H	1	Total C 40 40	0	0
23	T	1	Total C 40 40	0	0
23	Y	1	Total C 40 40	0	0
23	a	1	Total C 40 40	0	0
23	b	1	Total C 40 40	0	0
23	b	1	Total C 40 40	0	0

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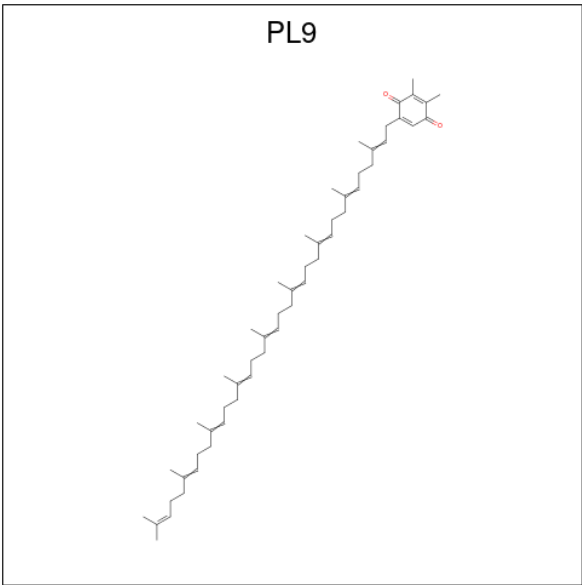
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C 40 40	0	0
23	c	1	Total C 40 40	0	0
23	c	1	Total C 40 40	0	0
23	d	1	Total C 40 40	0	0
23	h	1	Total C 40 40	0	0
23	k	1	Total C 40 40	0	0
23	k	1	Total C 40 40	0	0
23	t	1	Total C 40 40	0	0

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

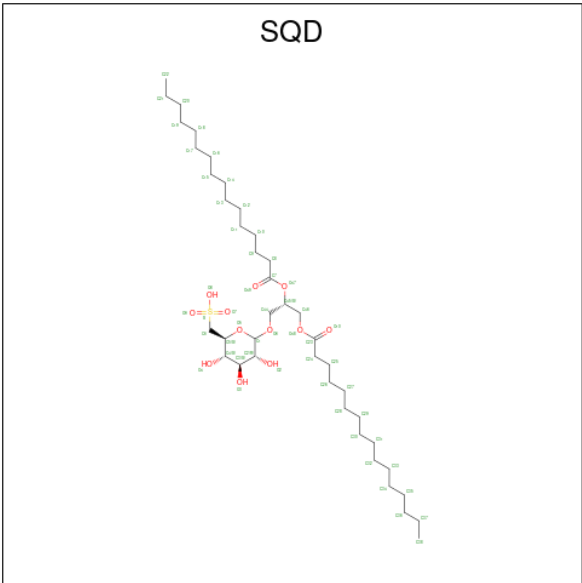
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

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



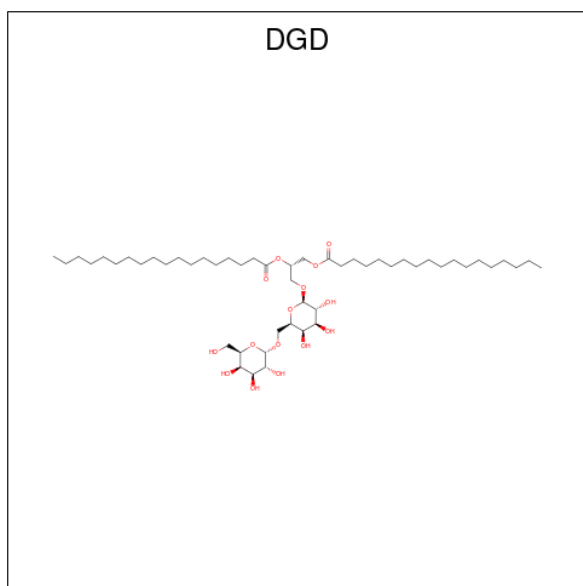
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 52 39 12 1	0	0
26	A	1	Total C O 39 35 4	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 36 25 10 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O 36 31 5	0	0
26	f	1	Total C O S 41 28 12 1	0	0
26	l	1	Total C O S 49 36 12 1	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



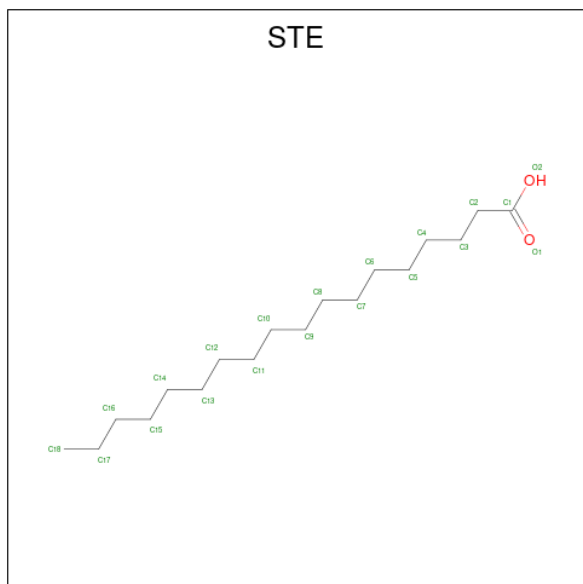
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 66 51 15	0	0
27	C	1	Total C O 62 47 15	0	0
27	C	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 62 47 15	0	0
27	H	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	h	1	Total C O 62 47 15	0	0

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 5 5	0	0
28	B	1	Total C O 12 10 2	0	0
28	B	1	Total C O 17 15 2	0	0
28	B	1	Total C O 12 10 2	0	0
28	B	1	Total C O 18 16 2	0	0

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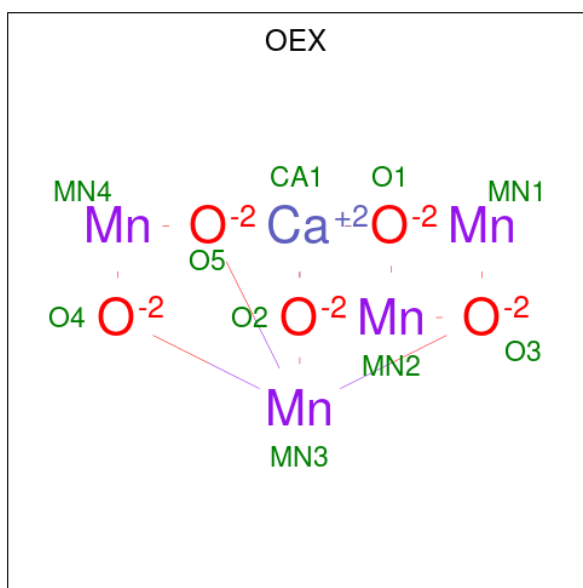
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C 16 16	0	0
28	C	1	Total C O 12 10 2	0	0
28	C	1	Total C 16 16	0	0
28	C	1	Total C O 12 10 2	0	0
28	E	1	Total C O 12 10 2	0	0
28	E	1	Total C 7 7	0	0
28	H	1	Total C 18 18	0	0
28	H	1	Total C 8 8	0	0
28	I	1	Total C 15 15	0	0
28	J	1	Total C O 12 10 2	0	0
28	M	1	Total C O 15 13 2	0	0
28	M	1	Total C 10 10	0	0
28	T	1	Total C 15 15	0	0
28	X	1	Total C O 20 18 2	0	0
28	Z	1	Total C 8 8	0	0
28	a	1	Total C 10 10	0	0
28	a	1	Total C O 12 10 2	0	0
28	a	1	Total C 15 15	0	0
28	b	1	Total C 16 16	0	0
28	b	1	Total C O 20 18 2	0	0
28	b	1	Total C O 16 14 2	0	0

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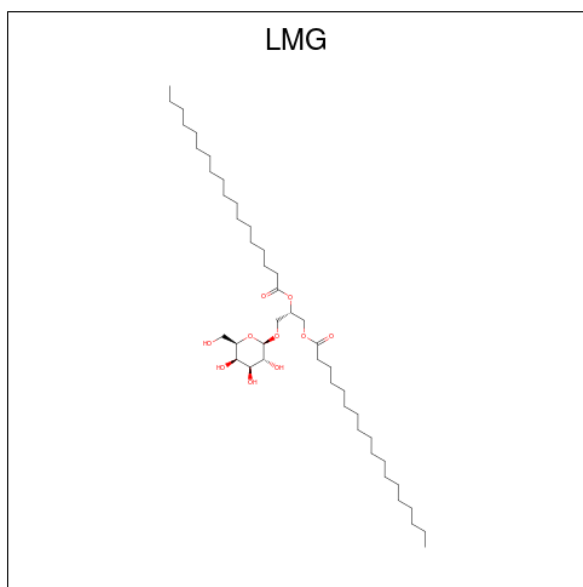
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b	1	Total C O 20 18 2	0	0
28	b	1	Total C 10 10	0	0
28	c	1	Total C O 12 10 2	0	0
28	c	1	Total C O 20 18 2	0	0
28	d	1	Total C O 20 18 2	0	0
28	d	1	Total C O 17 15 2	0	0
28	h	1	Total C 14 14	0	0
28	j	1	Total C O 12 10 2	0	0
28	m	1	Total C 18 18	0	0
28	m	1	Total C O 12 10 2	0	0
28	t	1	Total C O 14 12 2	0	0
28	x	1	Total C O 20 18 2	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



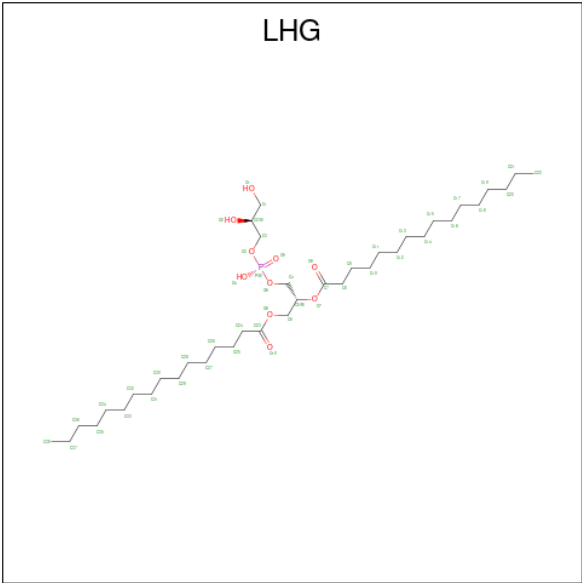
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			28	24	4		
30	C	1	Total	C	O	0	0
			48	38	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	D	1	Total	C	O	0	0
			32	27	5		
30	M	1	Total	C	O	0	0
			51	41	10		
30	a	1	Total	C	O	0	0
			55	45	10		
30	b	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			55	45	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	c	1	Total	C	O	0	0
			37	27	10		
30	c	1	Total	C	O	0	0
			48	38	10		
30	c	1	Total	C	O	0	0
			49	39	10		
30	d	1	Total	C	O	0	0
			44	34	10		

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



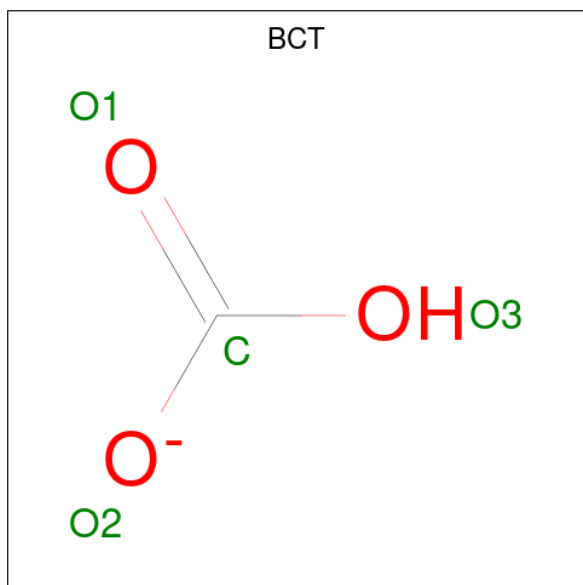
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	E	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		

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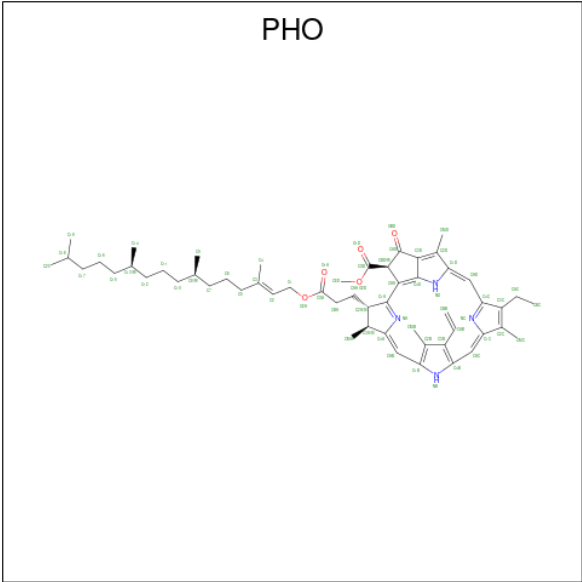
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			39	28	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



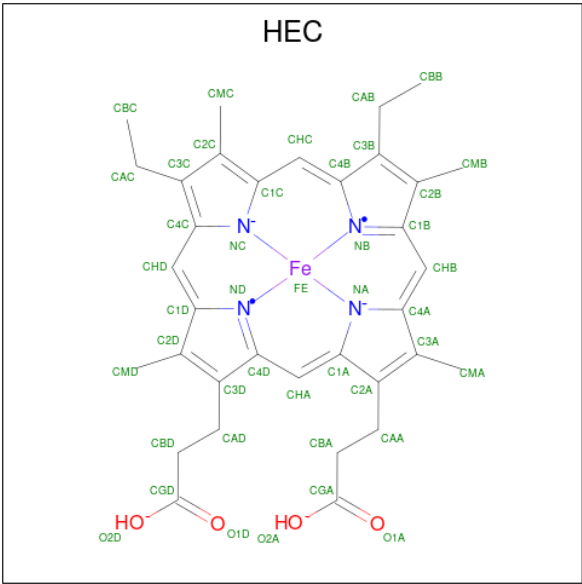
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 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
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	a	1	Total	C	N	O	0	0
			64	55	4	5		
33	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	137	Total 137	O 137	0	4
35	B	234	Total 234	O 234	0	0
35	C	167	Total 167	O 167	0	0
35	D	116	Total 116	O 116	0	0
35	E	37	Total 37	O 37	0	0
35	F	10	Total 10	O 10	0	0
35	H	34	Total 34	O 34	0	0
35	I	20	Total 20	O 20	0	0
35	J	14	Total 14	O 14	0	0
35	K	3	Total 3	O 3	0	0
35	L	10	Total 10	O 10	0	0
35	M	8	Total 8	O 8	0	0
35	O	105	Total 105	O 105	0	0
35	R	3	Total 3	O 3	0	0
35	T	9	Total 9	O 9	0	0
35	U	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	V	64	Total O 64 64	0	0
35	X	17	Total O 17 17	0	0
35	Y	3	Total O 3 3	0	0
35	a	121	Total O 121 121	0	4
35	b	194	Total O 194 194	0	0
35	c	169	Total O 169 169	0	0
35	d	108	Total O 108 108	0	0
35	e	22	Total O 22 22	0	0
35	f	5	Total O 5 5	0	0
35	h	22	Total O 22 22	0	0
35	i	17	Total O 17 17	0	0
35	j	7	Total O 7 7	0	0
35	k	4	Total O 4 4	0	0
35	l	11	Total O 11 11	0	0
35	m	6	Total O 6 6	0	0
35	o	98	Total O 98 98	0	0
35	r	8	Total O 8 8	0	0
35	t	7	Total O 7 7	0	0
35	u	64	Total O 64 64	0	0
35	v	63	Total O 63 63	0	0
35	x	7	Total O 7 7	0	0

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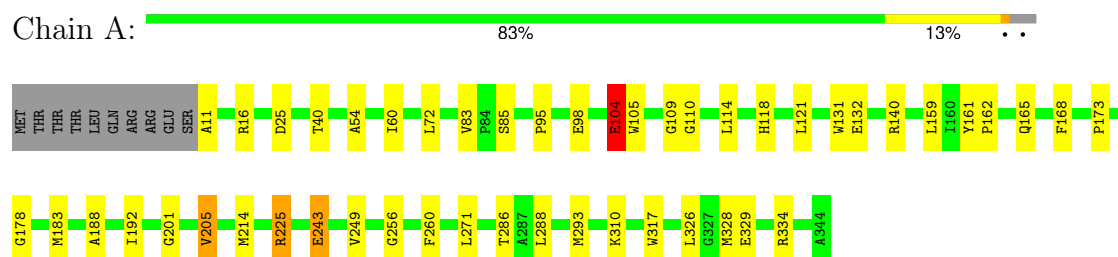
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	y	9	Total	O	0	0
			9	9		
35	z	9	Total	O	0	0
			9	9		

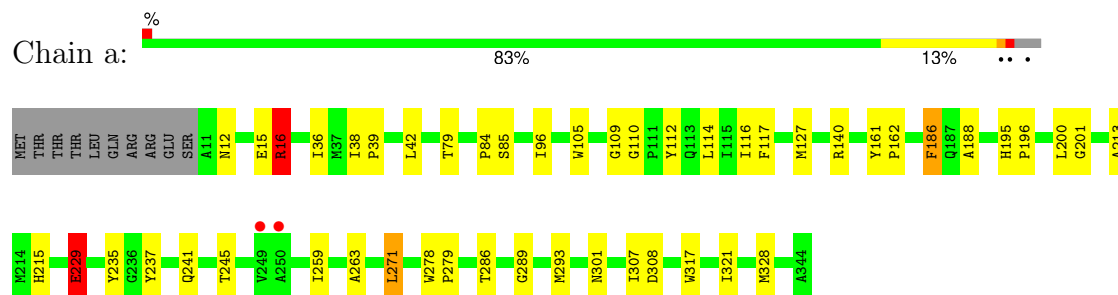
3 Residue-property plots [i](#)

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

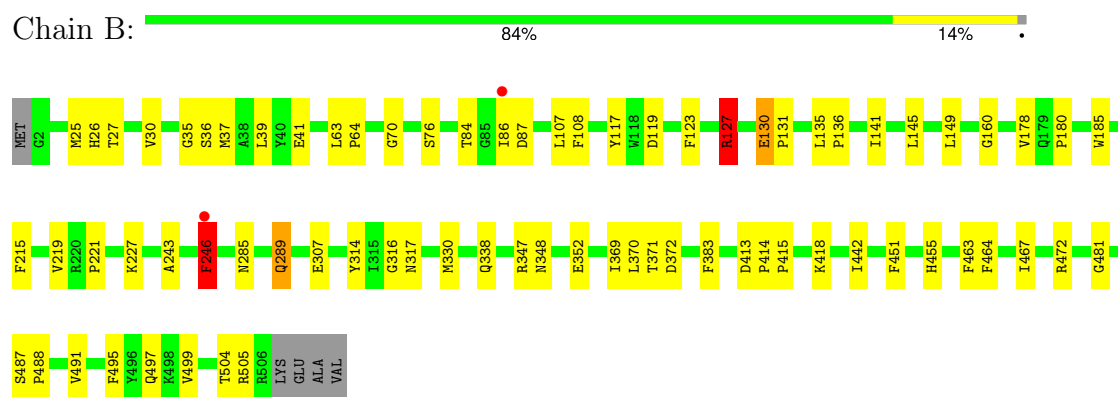
- Molecule 1: Photosystem II protein D1 1



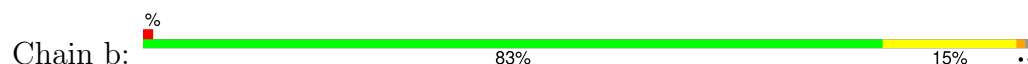
- Molecule 1: Photosystem II protein D1 1

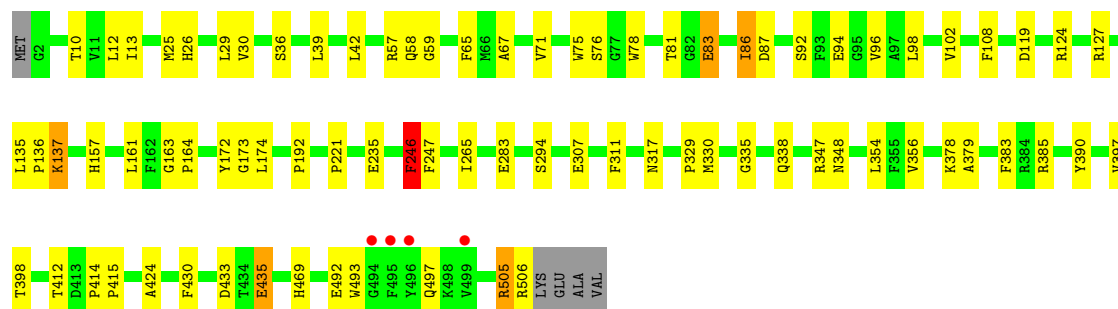


- Molecule 2: Photosystem II CP47 reaction center protein



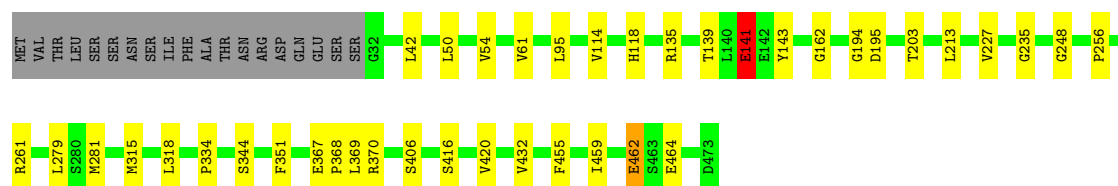
- Molecule 2: Photosystem II CP47 reaction center protein





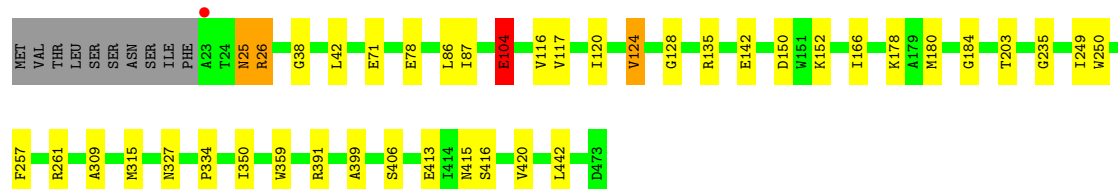
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



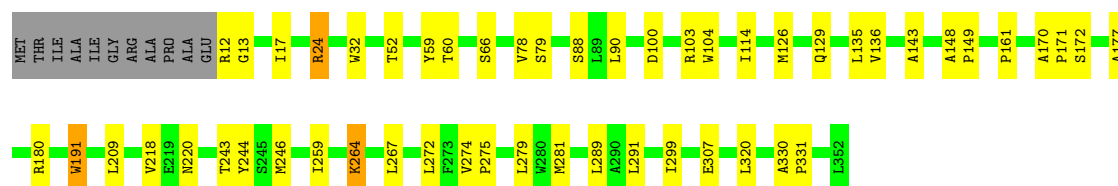
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 8% ..



- Molecule 4: Photosystem II D2 protein

Chain D: 82% 14% ..



- Molecule 4: Photosystem II D2 protein

Chain d: 80% 16% .





- Molecule 5: Cytochrome b559 subunit alpha



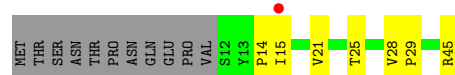
- Molecule 5: Cytochrome b559 subunit alpha



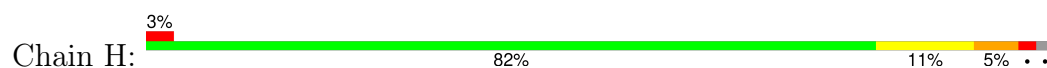
- Molecule 6: Cytochrome b559 subunit beta



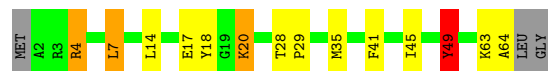
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  87% 5% • 5%



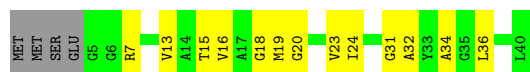
- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



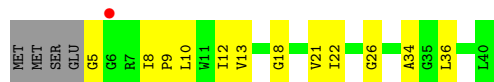
- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 32% 10%



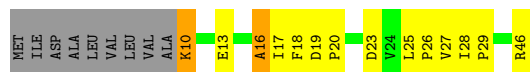
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 60% 30% 10%



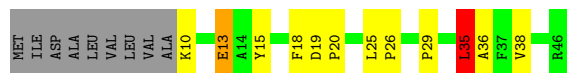
- Molecule 10: Photosystem II reaction center protein K

Chain K:  50% 26% • 20%

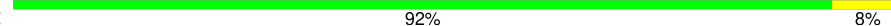


- Molecule 10: Photosystem II reaction center protein K

Chain k:  54% 22% • • 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 8%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 



- Molecule 12: Photosystem II reaction center protein M

Chain M: 



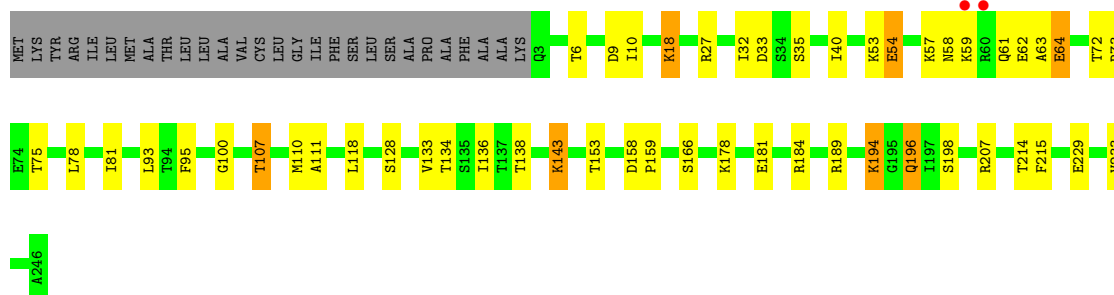
- Molecule 12: Photosystem II reaction center protein M

Chain m: 



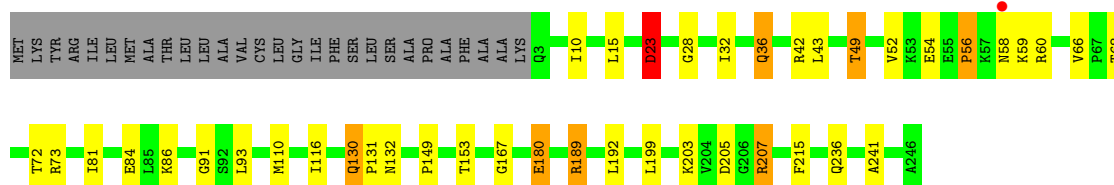
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 

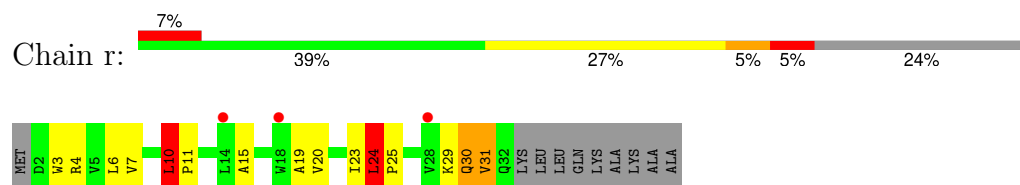


- Molecule 14: Photosystem II protein Y

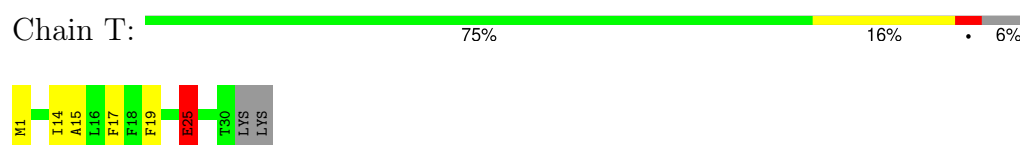
Chain R: 



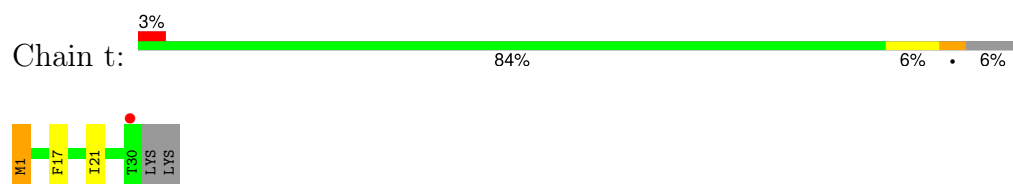
- Molecule 14: Photosystem II protein Y



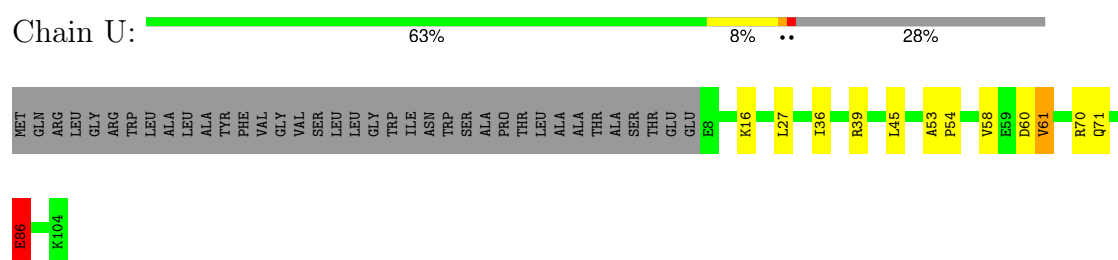
- Molecule 15: Photosystem II reaction center protein T



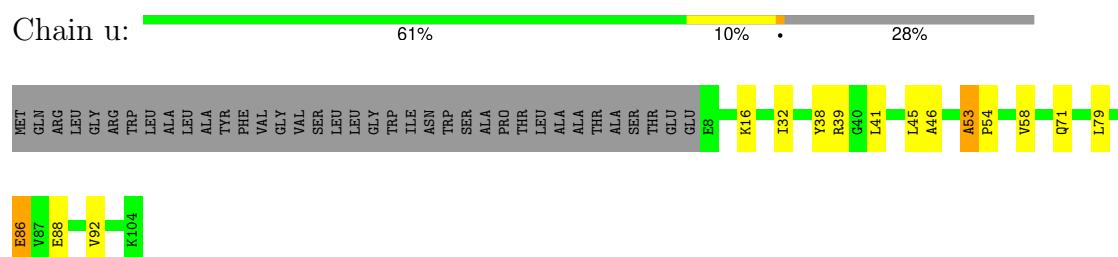
- Molecule 15: Photosystem II reaction center protein T



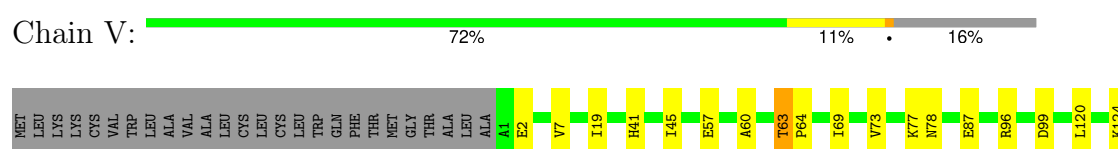
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



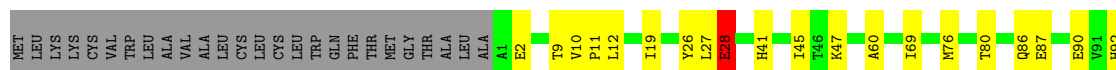
- Molecule 17: Cytochrome c-550





- Molecule 17: Cytochrome c-550

Chain v: 64% 19% 16%



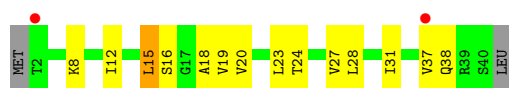
- Molecule 18: Photosystem II reaction center X protein

Chain X: 2% 73% 20% 7%



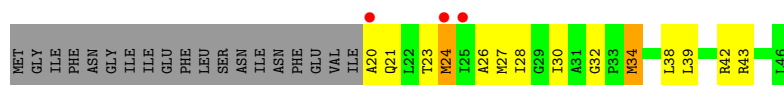
- Molecule 18: Photosystem II reaction center X protein

Chain x: 5% 61% 32% 5%



- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 7% 28% 26% 41%



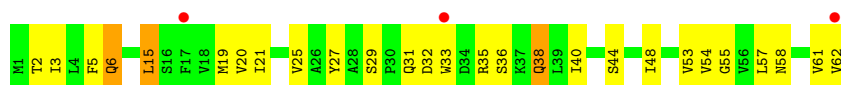
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 41% 17% 35%

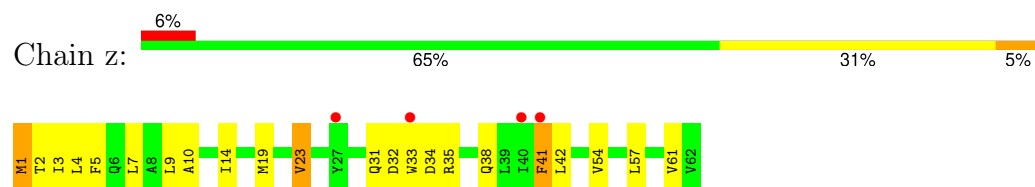


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 5% 56% 39% 5%



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.65-2.09) 99.8 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.183 , 0.243 0.195 , 0.249	Depositor DCC
R_{free} test set	4162 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52261	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: LHG, PHO, PL9, BCR, LMG, SQD, FME, CLA, OEX, DGD, HEC, FE2, CL, BCT, STE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/2707	0.87	8/3692 (0.2%)
1	a	0.81	3/2704 (0.1%)	1.00	14/3688 (0.4%)
2	B	0.81	7/4155 (0.2%)	1.03	19/5661 (0.3%)
2	b	0.78	3/4118 (0.1%)	0.88	15/5611 (0.3%)
3	C	0.78	4/3539 (0.1%)	0.85	6/4819 (0.1%)
3	c	0.69	4/3619 (0.1%)	0.88	6/4926 (0.1%)
4	D	0.78	2/2812 (0.1%)	0.84	3/3832 (0.1%)
4	d	0.76	2/2821 (0.1%)	0.97	16/3844 (0.4%)
5	E	0.56	0/688	0.74	1/940 (0.1%)
5	e	0.63	1/683 (0.1%)	1.04	6/932 (0.6%)
6	F	0.55	0/284	0.62	0/387
6	f	0.58	0/284	0.77	0/387
7	H	0.94	2/523 (0.4%)	1.11	6/713 (0.8%)
7	h	0.77	1/511 (0.2%)	1.07	3/697 (0.4%)
8	I	0.77	0/293	1.06	3/396 (0.8%)
8	i	0.70	0/293	0.75	0/396
9	J	0.61	0/263	0.90	0/356
9	j	0.56	0/263	0.76	0/356
10	K	0.81	1/303 (0.3%)	0.81	1/416 (0.2%)
10	k	0.85	2/303 (0.7%)	1.16	4/416 (1.0%)
11	L	0.76	0/311	0.83	0/422
11	l	0.83	0/303	0.90	1/412 (0.2%)
12	M	0.71	0/249	0.78	0/341
12	m	0.84	0/244	1.13	2/334 (0.6%)
13	O	0.81	3/1904 (0.2%)	1.09	17/2585 (0.7%)
13	o	0.72	0/1905	0.95	8/2583 (0.3%)
14	R	0.74	1/277 (0.4%)	1.25	2/380 (0.5%)
14	r	0.70	0/246	1.19	6/339 (1.8%)
15	T	0.79	0/257	1.11	3/349 (0.9%)
15	t	0.72	0/255	0.76	0/346
16	U	0.60	0/785	0.85	2/1064 (0.2%)
16	u	0.71	0/785	0.96	4/1064 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.67	0/1085	0.84	1/1473 (0.1%)
17	v	0.71	1/1085 (0.1%)	1.05	5/1473 (0.3%)
18	X	0.54	0/284	0.76	0/384
18	x	0.59	1/289 (0.3%)	1.09	3/391 (0.8%)
19	Y	0.80	0/197	1.17	2/264 (0.8%)
19	y	0.54	0/219	0.91	3/294 (1.0%)
20	Z	0.65	0/490	1.11	4/669 (0.6%)
20	z	0.72	3/488 (0.6%)	1.17	5/666 (0.8%)
All	All	0.75	41/42824 (0.1%)	0.94	179/58298 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	3
2	B	0	3
2	b	0	2
3	C	0	1
3	c	0	1
4	d	0	3
5	e	0	1
7	H	0	3
7	h	0	1
8	I	0	1
10	k	0	1
12	m	0	1
13	O	0	3
13	o	0	3
15	T	0	1
16	U	0	1
16	u	0	1
17	V	0	1
17	v	0	1
19	y	0	1
20	Z	0	1
20	z	0	1
All	All	0	37

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	435	GLU	CD-OE2	-15.11	0.96	1.25
3	C	462	GLU	CB-CG	-12.05	1.16	1.52
4	d	16	ASP	CG-OD1	10.70	1.45	1.25
7	H	3	ARG	CZ-NH1	10.54	1.47	1.32
2	b	435	GLU	CG-CD	10.05	1.77	1.52
1	a	229	GLU	CB-CG	10.05	1.82	1.52
3	C	462	GLU	CG-CD	-9.95	1.27	1.52
2	B	127	ARG	CB-CG	9.63	1.81	1.52
2	B	127	ARG	NE-CZ	9.60	1.43	1.33
2	B	127	ARG	CD-NE	9.56	1.59	1.46
13	O	194	LYS	CB-CG	8.89	1.79	1.52
4	D	281	MET	SD-CE	-8.67	1.57	1.79
17	v	28	GLU	CB-CG	8.30	1.77	1.52
10	K	10	LYS	CD-CE	8.25	1.77	1.52
3	c	104	GLU	CB-CG	7.94	1.76	1.52
2	b	435	GLU	CD-OE1	7.92	1.40	1.25
2	B	127	ARG	CG-CD	7.78	1.75	1.52
3	C	462	GLU	CD-OE1	-7.68	1.10	1.25
3	c	104	GLU	CD-OE1	7.65	1.39	1.25
13	O	194	LYS	CG-CD	7.64	1.75	1.52
3	C	462	GLU	CA-CB	-7.22	1.41	1.53
7	h	20	LYS	CD-CE	7.17	1.74	1.52
20	z	1	MET	CA-CB	-6.66	1.40	1.53
7	H	3	ARG	CZ-NH2	6.57	1.42	1.33
5	e	73	LYS	CD-CE	6.48	1.71	1.52
20	z	1	MET	CG-SD	6.38	1.96	1.80
4	D	264	LYS	CD-CE	6.34	1.71	1.52
1	a	229	GLU	CG-CD	6.30	1.67	1.52
14	R	24	LEU	CG-CD1	6.13	1.72	1.52
13	O	196	GLN	CG-CD	6.11	1.67	1.52
3	c	104	GLU	CG-CD	5.90	1.66	1.52
1	a	110	GLY	CA-C	-5.89	1.47	1.51
18	x	15	LEU	CG-CD2	5.69	1.71	1.52
20	z	23	VAL	CA-CB	5.63	1.57	1.54
3	c	315	MET	CG-SD	-5.56	1.66	1.80
10	k	35	LEU	CB-CG	5.54	1.64	1.53
2	B	127	ARG	CA-C	5.49	1.59	1.52
2	B	130	GLU	CD-OE2	5.42	1.35	1.25
2	B	127	ARG	CZ-NH1	5.34	1.40	1.32
4	d	16	ASP	CG-OD2	5.16	1.35	1.25
10	k	35	LEU	CG-CD2	5.02	1.69	1.52

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	GLU	CA-CB-CG	19.99	154.08	114.10
2	B	246	PHE	CB-CG-CD2	-15.71	93.99	120.70
4	d	16	ASP	N-CA-CB	-14.96	88.02	110.16
3	c	104	GLU	CG-CD-OE2	-14.84	84.28	118.40
7	h	20	LYS	CB-CG-CD	14.07	143.66	111.30
2	B	130	GLU	CG-CD-OE2	-13.99	86.22	118.40
4	D	264	LYS	CB-CG-CD	13.04	141.28	111.30
2	B	246	PHE	CB-CG-CD1	13.01	142.82	120.70
2	B	127	ARG	CA-CB-CG	-12.93	88.24	114.10
13	O	143	LYS	CA-CB-CG	12.57	139.24	114.10
1	a	229	GLU	CG-CD-OE2	-12.35	89.99	118.40
3	C	462	GLU	CB-CG-CD	-12.29	91.71	112.60
13	O	194	LYS	CB-CG-CD	-12.00	83.70	111.30
17	v	28	GLU	CG-CD-OE2	-11.79	91.27	118.40
1	a	16	ARG	NE-CZ-NH1	-11.67	109.83	121.50
2	B	127	ARG	CG-CD-NE	-11.63	86.42	112.00
18	x	15	LEU	CB-CG-CD1	11.58	145.43	110.70
17	v	28	GLU	N-CA-CB	11.46	126.63	110.01
1	a	186[A]	PHE	CB-CG-CD2	-11.46	101.22	120.70
14	R	24	LEU	CB-CG-CD2	11.43	145.00	110.70
2	B	246	PHE	CD1-CG-CD2	-10.73	102.50	118.60
4	d	16	ASP	OD1-CG-OD2	-10.72	97.17	122.90
20	z	1	MET	CA-CB-CG	10.71	135.53	114.10
17	v	28	GLU	CB-CA-C	-10.70	94.09	110.88
20	z	41	PHE	CB-CG-CD2	-10.50	102.84	120.70
7	H	3	ARG	NE-CZ-NH1	-10.45	111.05	121.50
13	O	196	GLN	CG-CD-NE2	-10.43	100.75	116.40
16	U	86	GLU	CA-CB-CG	10.35	134.80	114.10
4	d	242	GLU	CG-CD-OE2	-10.26	94.81	118.40
13	O	194	LYS	CD-CE-NZ	10.17	144.46	111.90
1	a	110	GLY	O-C-N	-10.11	117.43	121.07
7	H	20	LYS	CB-CG-CD	10.00	134.29	111.30
1	a	229	GLU	N-CA-CB	-9.96	93.39	110.32
5	e	81	GLU	CG-CD-OE2	-9.95	95.52	118.40
2	B	227	LYS	CG-CD-CE	9.88	134.03	111.30
2	B	127	ARG	NE-CZ-NH1	-9.70	111.80	121.50
5	e	8	ARG	NE-CZ-NH1	9.68	131.18	121.50
3	c	104	GLU	CA-CB-CG	-9.45	95.21	114.10
20	Z	38	GLN	CG-CD-NE2	-9.44	102.24	116.40
17	v	28	GLU	CG-CD-OE1	9.39	139.99	118.40
10	k	35	LEU	CD1-CG-CD2	-9.22	90.52	110.80
4	d	242	GLU	OE1-CD-OE2	-9.21	100.79	122.90
15	T	25	GLU	CG-CD-OE2	-9.20	97.25	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	2	GLU	CG-CD-OE2	-9.08	97.52	118.40
5	e	8	ARG	NE-CZ-NH2	-9.06	111.05	119.20
20	z	41	PHE	CB-CA-C	8.82	126.84	110.70
14	R	24	LEU	CB-CA-C	-8.79	92.85	110.17
2	b	83	GLU	CB-CA-C	-8.76	96.24	109.90
13	O	64	GLU	CA-CB-CG	8.75	131.60	114.10
3	c	104	GLU	OE1-CD-OE2	-8.59	102.29	122.90
10	k	35	LEU	CB-CA-C	8.47	124.37	110.81
12	m	2	GLU	CG-CD-OE2	-8.46	98.93	118.40
2	b	246	PHE	N-CA-CB	-8.32	97.80	110.20
2	B	246	PHE	N-CA-CB	-8.30	97.52	110.30
2	b	246	PHE	CB-CG-CD2	-8.29	106.61	120.70
2	B	227	LYS	CA-CB-CG	-8.28	97.53	114.10
20	Z	38	GLN	CB-CA-C	-8.27	96.90	110.79
18	x	15	LEU	CB-CA-C	-8.27	97.78	110.92
2	B	472	ARG	CG-CD-NE	-8.26	93.82	112.00
16	u	86	GLU	CG-CD-OE2	-8.25	99.42	118.40
16	u	16	LYS	CD-CE-NZ	-8.20	85.68	111.90
1	a	229	GLU	CG-CD-OE1	8.19	137.24	118.40
5	e	81	GLU	CA-CB-CG	-8.18	97.75	114.10
1	a	186[A]	PHE	CB-CG-CD1	7.79	133.94	120.70
19	Y	24	MET	CA-CB-CG	-7.79	98.52	114.10
19	Y	34	MET	CB-CA-C	-7.73	97.71	110.85
4	d	233	ARG	CG-CD-NE	7.73	129.00	112.00
2	B	130	GLU	OE1-CD-OE2	-7.72	104.37	122.90
3	c	104	GLU	CB-CA-C	7.49	122.46	109.65
4	d	233	ARG	CB-CG-CD	-7.38	94.33	111.30
7	H	49	TYR	CB-CA-C	7.32	124.17	110.63
1	a	271	LEU	CB-CA-C	-7.30	99.42	110.88
3	C	462	GLU	CG-CD-OE1	-7.29	101.63	118.40
1	a	271	LEU	CB-CG-CD2	7.23	132.40	110.70
13	O	54	GLU	CG-CD-OE2	-7.04	102.20	118.40
3	C	462	GLU	CA-CB-CG	-7.00	100.09	114.10
2	b	435	GLU	CA-CB-CG	6.99	128.08	114.10
4	d	233	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	b	505	ARG	CB-CG-CD	6.92	127.20	111.30
12	m	13	LEU	CB-CG-CD2	6.91	131.44	110.70
2	b	83	GLU	CG-CD-OE1	-6.87	102.61	118.40
7	h	49	TYR	CB-CA-C	6.86	123.85	110.67
4	d	16	ASP	CB-CG-OD2	-6.82	102.70	118.40
15	T	25	GLU	CG-CD-OE1	6.79	134.03	118.40
4	d	233	ARG	NE-CZ-NH1	-6.74	114.76	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	73	LYS	CB-CG-CD	-6.74	95.80	111.30
13	o	130	GLN	N-CA-CB	6.70	122.30	110.37
2	B	127	ARG	N-CA-C	-6.63	103.31	111.40
7	H	49	TYR	CB-CG-CD2	-6.61	110.88	120.80
13	o	180	GLU	CA-CB-CG	6.58	127.25	114.10
10	K	10	LYS	CB-CG-CD	-6.54	96.26	111.30
2	b	505	ARG	CG-CD-NE	6.54	126.38	112.00
1	a	186[A]	PHE	CD1-CG-CD2	-6.53	108.80	118.60
14	r	24	LEU	CB-CA-C	-6.52	98.22	112.38
16	U	86	GLU	CG-CD-OE2	-6.50	103.46	118.40
1	a	186[A]	PHE	CB-CA-C	6.49	123.12	110.67
2	B	246	PHE	N-CA-C	-6.48	104.07	112.23
3	C	370	ARG	CG-CD-NE	-6.45	97.82	112.00
15	T	25	GLU	CA-CB-CG	-6.42	101.25	114.10
8	I	2	GLU	CA-CB-CG	-6.42	101.26	114.10
2	B	227	LYS	N-CA-C	-6.40	103.82	111.69
2	b	246	PHE	CB-CG-CD1	6.37	131.52	120.70
13	o	189	ARG	CA-CB-CG	-6.34	101.43	114.10
1	a	16	ARG	N-CA-CB	-6.33	100.77	110.20
4	d	291	LEU	CD1-CG-CD2	-6.29	96.97	110.80
20	z	41	PHE	CB-CG-CD1	6.27	131.37	120.70
13	O	54	GLU	N-CA-C	-6.24	101.22	110.46
13	o	36	GLN	CB-CA-C	6.20	120.87	109.46
16	u	86	GLU	CA-CB-CG	-6.19	101.72	114.10
1	A	183[A]	MET	CA-CB-CG	6.18	126.47	114.10
19	y	17	GLU	CB-CA-C	-6.17	98.37	110.10
2	b	83	GLU	CG-CD-OE2	6.15	132.54	118.40
1	A	225	ARG	N-CA-CB	6.12	119.44	109.95
17	V	63	THR	C-N-CD	-6.10	99.97	125.00
5	E	32	ILE	CA-CB-CG1	5.97	120.55	110.40
3	C	141	GLU	CG-CD-OE2	-5.92	104.78	118.40
13	O	64	GLU	CG-CD-OE2	-5.91	104.81	118.40
13	O	54	GLU	CB-CA-C	-5.89	100.26	110.45
3	C	462	GLU	CG-CD-OE2	5.83	131.81	118.40
2	B	127	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
2	b	86	ILE	CA-CB-CG1	-5.81	100.53	110.40
16	u	86	GLU	CB-CG-CD	5.80	122.46	112.60
13	O	143	LYS	CD-CE-NZ	5.79	130.44	111.90
13	o	130	GLN	CG-CD-NE2	-5.77	107.74	116.40
13	o	207	ARG	CG-CD-NE	5.75	124.66	112.00
18	x	15	LEU	CA-CB-CG	-5.73	96.25	116.30
10	k	35	LEU	CB-CG-CD2	-5.72	93.55	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	r	30	GLN	CA-C-N	5.72	131.99	121.70
14	r	30	GLN	C-N-CA	5.72	131.99	121.70
1	A	104	GLU	CG-CD-OE2	-5.69	105.32	118.40
19	y	17	GLU	CG-CD-OE2	-5.65	105.41	118.40
20	z	41	PHE	CD1-CG-CD2	-5.63	110.16	118.60
13	O	214	THR	OG1-CB-CG2	5.62	120.54	109.30
14	r	10	LEU	CB-CG-CD2	5.60	127.50	110.70
4	d	291	LEU	CB-CG-CD2	-5.59	93.94	110.70
13	O	18	LYS	CA-CB-CG	-5.58	102.93	114.10
13	O	78	LEU	CD1-CG-CD2	-5.57	98.56	110.80
2	B	289	GLN	CB-CG-CD	-5.49	103.27	112.60
2	b	246	PHE	CB-CA-C	5.48	120.73	110.70
13	O	54	GLU	CB-CG-CD	5.47	121.90	112.60
7	H	49	TYR	CD1-CG-CD2	-5.47	109.90	118.10
4	d	290	ALA	CA-C-N	5.44	131.35	122.65
4	d	290	ALA	C-N-CA	5.44	131.35	122.65
4	D	191	TRP	CA-CB-CG	5.41	123.88	113.60
4	d	259	ILE	CA-CB-CG1	-5.41	101.20	110.40
13	O	10	ILE	CG1-CB-CG2	5.40	126.89	110.70
4	D	24	ARG	CB-CA-C	5.39	118.43	109.53
19	y	17	GLU	OE1-CD-OE2	-5.37	110.01	122.90
7	H	20	LYS	CA-CB-CG	-5.37	103.36	114.10
1	A	225	ARG	N-CA-C	-5.37	101.22	109.76
13	o	23	ASP	CA-CB-CG	5.36	117.96	112.60
14	r	10	LEU	CB-CA-C	-5.34	99.64	110.17
2	B	472	ARG	CB-CA-C	5.34	120.92	110.67
3	c	124	VAL	CG1-CB-CG2	-5.33	99.08	110.80
14	r	24	LEU	CB-CG-CD2	5.31	126.62	110.70
1	a	16	ARG	CA-CB-CG	-5.30	103.50	114.10
10	k	13	GLU	CB-CG-CD	5.28	121.58	112.60
4	d	242	GLU	CG-CD-OE1	5.27	130.52	118.40
5	e	81	GLU	CG-CD-OE1	5.24	130.46	118.40
2	b	83	GLU	CA-CB-CG	5.22	124.55	114.10
13	O	64	GLU	N-CA-CB	-5.21	103.24	111.05
1	A	205	VAL	N-CA-CB	-5.18	103.06	110.52
4	d	16	ASP	N-CA-C	-5.17	105.73	111.36
17	v	107	LEU	CB-CG-CD2	5.16	126.19	110.70
1	a	16	ARG	N-CA-C	-5.14	105.36	111.69
20	Z	54	VAL	N-CA-C	-5.13	101.68	109.78
2	b	385	ARG	NE-CZ-NH2	-5.12	114.59	119.20
7	h	4	ARG	CG-CD-NE	5.12	123.26	112.00
1	A	104	GLU	CB-CA-C	-5.10	102.85	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	30	LEU	CB-CG-CD2	5.09	125.98	110.70
8	I	2	GLU	CG-CD-OE1	5.08	130.09	118.40
3	c	26	ARG	CA-CB-CG	-5.08	103.95	114.10
2	b	137	LYS	CD-CE-NZ	-5.08	95.66	111.90
20	Z	6	GLN	CB-CG-CD	-5.06	104.00	112.60
1	A	104	GLU	OE1-CD-OE2	-5.05	110.77	122.90
1	A	243	GLU	CA-CB-CG	5.05	124.20	114.10
13	O	78	LEU	N-CA-CB	-5.04	102.06	110.23
2	b	246	PHE	CD1-CG-CD2	-5.03	111.05	118.60
13	o	207	ARG	CD-NE-CZ	5.01	131.41	124.40

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLU	Sidechain
1	A	243	GLU	Sidechain
2	B	127	ARG	Sidechain
2	B	130	GLU	Sidechain
2	B	246	PHE	Sidechain
3	C	141	GLU	Sidechain
7	H	3	ARG	Sidechain
7	H	4	ARG	Sidechain
7	H	49	TYR	Sidechain
8	I	2	GLU	Sidechain
13	O	196	GLN	Sidechain
13	O	54	GLU	Sidechain
13	O	64	GLU	Sidechain
15	T	25	GLU	Sidechain
16	U	86	GLU	Sidechain
17	V	63	THR	Peptide
20	Z	38	GLN	Sidechain
1	a	16	ARG	Sidechain
1	a	186[A]	PHE	Sidechain
1	a	229	GLU	Sidechain
2	b	246	PHE	Sidechain
2	b	87	ASP	Sidechain
3	c	104	GLU	Sidechain
4	d	16	ASP	Sidechain
4	d	242	GLU	Sidechain
4	d	294	ARG	Peptide
5	e	81	GLU	Sidechain

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Mol	Chain	Res	Type	Group
7	h	49	TYR	Sidechain
10	k	13	GLU	Sidechain
12	m	2	GLU	Sidechain
13	o	180	GLU	Sidechain
13	o	23	ASP	Sidechain
13	o	36	GLN	Sidechain
16	u	86	GLU	Sidechain
17	v	28	GLU	Sidechain
19	y	17	GLU	Sidechain
20	z	41	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2517	36	0
1	a	2619	0	2508	41	0
2	B	4005	0	3871	65	0
2	b	3978	0	3836	71	0
3	C	3426	0	3351	28	3
3	c	3500	0	3424	39	0
4	D	2717	0	2621	46	0
4	d	2723	0	2627	47	0
5	E	666	0	651	19	0
5	e	664	0	648	33	0
6	F	275	0	282	9	0
6	f	275	0	282	6	0
7	H	510	0	532	8	3
7	h	498	0	518	17	0
8	I	296	0	311	2	0
8	i	296	0	311	1	0
9	J	257	0	268	15	0
9	j	257	0	268	15	0
10	K	293	0	305	15	0
10	k	293	0	305	15	0
11	L	304	0	316	5	0
11	l	296	0	304	9	0
12	M	256	0	269	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	m	251	0	267	7	0
13	O	1870	0	1830	43	0
13	o	1874	0	1846	27	0
14	R	271	0	298	20	0
14	r	240	0	250	17	0
15	T	258	0	261	4	0
15	t	256	0	256	3	0
16	U	774	0	773	13	0
16	u	774	0	773	9	0
17	V	1064	0	1073	13	0
17	v	1064	0	1073	30	0
18	X	281	0	312	6	0
18	x	286	0	314	16	0
19	Y	196	0	217	13	0
19	y	218	0	241	10	0
20	Z	479	0	516	28	0
20	z	477	0	509	18	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	0	192	3	0
22	B	1035	0	1139	15	0
22	C	839	0	922	23	0
22	D	195	0	216	8	0
22	a	195	0	216	2	0
22	b	970	0	1067	21	0
22	c	839	0	919	12	0
22	d	195	0	216	5	0
22	h	65	0	72	6	0
23	A	40	0	56	2	0
23	B	120	0	168	13	0
23	C	120	0	168	3	0
23	D	40	0	56	3	0
23	H	40	0	56	2	0
23	T	40	0	56	4	0
23	Y	40	0	56	4	0
23	a	40	0	56	2	0
23	b	120	0	168	3	0
23	c	80	0	112	3	0
23	d	40	0	56	2	0
23	h	40	0	56	1	0
23	k	80	0	112	5	0
23	t	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	0	80	3	0
25	D	55	0	80	2	0
25	a	55	0	80	5	0
25	d	55	0	80	0	0
26	A	91	0	135	0	0
26	B	54	0	77	0	0
26	D	36	0	45	0	0
26	a	90	0	132	2	0
26	f	41	0	46	0	0
26	l	49	0	64	8	0
27	A	66	0	96	4	0
27	C	186	0	245	1	0
27	H	62	0	81	1	0
27	c	186	0	243	1	0
27	h	62	0	80	0	0
28	A	5	0	6	0	0
28	B	75	0	117	1	0
28	C	40	0	63	1	0
28	E	19	0	26	0	0
28	H	26	0	47	0	0
28	I	15	0	26	2	0
28	J	12	0	16	0	0
28	M	25	0	38	0	0
28	T	15	0	29	0	0
28	X	20	0	35	1	0
28	Z	8	0	12	0	0
28	a	37	0	58	1	0
28	b	82	0	141	2	0
28	c	32	0	51	1	0
28	d	37	0	61	2	0
28	h	14	0	27	1	0
28	j	12	0	16	1	0
28	m	30	0	51	0	0
28	t	14	0	20	0	0
28	x	20	0	35	2	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	B	28	0	40	0	0
30	C	96	0	132	2	0
30	D	83	0	117	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	51	0	72	0	0
30	a	55	0	86	5	0
30	b	106	0	158	2	0
30	c	134	0	181	2	0
30	d	44	0	58	0	0
31	B	49	0	74	2	0
31	D	96	0	140	1	0
31	E	49	0	74	1	0
31	L	49	0	74	0	0
31	a	91	0	131	4	0
31	d	88	0	125	6	0
31	l	49	0	74	1	0
32	D	4	0	1	0	0
32	a	4	0	1	0	0
33	D	128	0	148	5	0
33	a	64	0	74	0	0
33	d	64	0	74	2	0
34	F	43	0	32	6	0
34	V	43	0	30	2	0
34	f	43	0	32	9	0
34	v	43	0	30	0	0
35	A	137	0	0	5	0
35	B	234	0	0	2	1
35	C	167	0	0	0	1
35	D	116	0	0	1	0
35	E	37	0	0	2	0
35	F	10	0	0	0	0
35	H	34	0	0	1	0
35	I	20	0	0	0	0
35	J	14	0	0	6	0
35	K	3	0	0	2	0
35	L	10	0	0	0	0
35	M	8	0	0	0	0
35	O	105	0	0	6	0
35	R	3	0	0	0	0
35	T	9	0	0	1	0
35	U	52	0	0	5	0
35	V	64	0	0	3	0
35	X	17	0	0	0	0
35	Y	3	0	0	0	0
35	a	121	0	0	2	0
35	b	194	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	169	0	0	7	0
35	d	108	0	0	2	0
35	e	22	0	0	2	0
35	f	5	0	0	1	0
35	h	22	0	0	0	0
35	i	17	0	0	0	0
35	j	7	0	0	3	0
35	k	4	0	0	1	0
35	l	11	0	0	0	0
35	m	6	0	0	2	0
35	o	98	0	0	2	0
35	r	8	0	0	1	0
35	t	7	0	0	0	0
35	u	64	0	0	1	0
35	v	63	0	0	3	0
35	x	7	0	0	0	0
35	y	9	0	0	1	0
35	z	9	0	0	0	0
All	All	52261	0	51722	859	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (859) 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:O:194:LYS:CD	13:O:194:LYS:CG	1.75	1.64
2:B:127:ARG:CD	2:B:127:ARG:CG	1.75	1.61
3:c:104:GLU:CB	3:c:104:GLU:CG	1.76	1.60
2:B:127:ARG:CG	2:B:127:ARG:CB	1.81	1.57
10:K:10:LYS:CE	10:K:10:LYS:CD	1.77	1.57
1:a:229:GLU:CG	1:a:229:GLU:CB	1.82	1.56
13:O:194:LYS:CG	13:O:194:LYS:CB	1.79	1.55
17:v:28:GLU:CG	17:v:28:GLU:CB	1.77	1.55
2:b:435:GLU:CD	2:b:435:GLU:CG	1.77	1.54
17:v:110:LYS:NZ	35:v:301:HOH:O	1.71	1.22
18:x:15:LEU:O	18:x:15:LEU:HD23	1.39	1.21
13:o:189:ARG:NH2	35:o:301:HOH:O	1.74	1.18
14:R:24:LEU:HD13	14:R:24:LEU:C	1.78	1.08
18:x:15:LEU:HD23	18:x:15:LEU:C	1.80	1.05
5:e:74:GLN:OE1	35:e:201:HOH:O	1.74	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:307:GLU:OE1	35:d:501:HOH:O	1.75	1.04
13:O:194:LYS:CD	13:O:194:LYS:CB	2.36	1.03
14:R:24:LEU:HD13	14:R:24:LEU:O	1.57	1.03
2:B:127:ARG:CG	2:B:127:ARG:CA	2.38	1.01
4:D:246:MET:HE3	4:D:264:LYS:HD2	1.45	0.98
16:U:86:GLU:OE2	35:U:201:HOH:O	1.80	0.98
13:O:27:ARG:NH1	35:O:302:HOH:O	1.96	0.98
2:B:127:ARG:CG	2:B:127:ARG:NE	2.29	0.94
4:d:103:ARG:HG3	5:e:73:LYS:HE2	1.50	0.94
2:b:81:THR:OG1	2:b:83:GLU:OE2	1.87	0.92
16:u:53:ALA:HB1	16:u:54:PRO:HD2	1.52	0.91
13:O:53:LYS:O	35:O:301:HOH:O	1.89	0.90
3:c:104:GLU:CG	3:c:104:GLU:CA	2.48	0.90
16:U:60:ASP:OD2	35:U:202:HOH:O	1.90	0.90
9:J:19:MET:N	35:J:201:HOH:O	1.90	0.89
14:R:16:ALA:O	14:R:20:VAL:HG23	1.74	0.88
14:r:10:LEU:HB3	14:r:11:PRO:HD3	1.53	0.88
20:z:1:MET:HG3	20:z:4:LEU:HD23	1.55	0.87
5:E:81:GLU:OE2	35:E:201:HOH:O	1.93	0.86
14:R:24:LEU:HB3	14:R:25:PRO:CD	2.05	0.86
14:R:24:LEU:C	14:R:24:LEU:CD1	2.49	0.86
18:x:15:LEU:HD21	18:x:19:VAL:HG23	1.58	0.85
18:x:15:LEU:C	18:x:15:LEU:CD2	2.50	0.84
7:H:3:ARG:HG3	7:H:3:ARG:HH21	1.43	0.84
2:B:243:ALA:O	2:B:246:PHE:HD1	1.59	0.84
3:c:327[A]:ASN:ND2	35:c:601:HOH:O	2.11	0.82
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.60	0.82
2:B:246:PHE:CE1	22:B:708:CLA:HBC2	2.14	0.82
14:r:10:LEU:HB3	14:r:11:PRO:CD	2.08	0.81
2:B:246:PHE:HE1	22:B:708:CLA:HBC2	1.45	0.81
23:T:701:BCR:HC8	23:T:701:BCR:H311	1.63	0.80
11:l:7:ARG:NH2	26:l:101:SQD:O9	2.15	0.80
18:x:15:LEU:HD21	18:x:19:VAL:CG2	2.12	0.80
5:e:70:PHE:O	35:e:201:HOH:O	1.98	0.80
19:Y:34:MET:SD	19:Y:38:LEU:HD11	2.22	0.80
31:a:411:LHG:O4	4:d:141:TYR:OH	2.00	0.80
23:D:405:BCR:H23C	23:D:405:BCR:H392	1.63	0.79
10:k:35:LEU:HD12	10:k:35:LEU:C	2.08	0.79
13:o:28:GLY:O	35:o:302:HOH:O	2.01	0.78
17:v:104:MET:HA	17:v:107:LEU:HD22	1.64	0.78
2:B:243:ALA:O	2:B:246:PHE:CD1	2.38	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:56:ASP:OD2	18:X:2:THR:N	2.18	0.77
10:K:10:LYS:CE	10:K:10:LYS:CG	2.64	0.76
14:R:24:LEU:HB3	14:R:25:PRO:HD3	1.65	0.75
17:v:28:GLU:CG	17:v:28:GLU:CA	2.64	0.74
20:z:1:MET:SD	20:z:57:LEU:HD22	2.26	0.74
2:B:127:ARG:CG	2:B:127:ARG:HA	2.16	0.74
6:f:15:ILE:HD12	35:f:201:HOH:O	1.87	0.74
16:U:58:VAL:O	16:U:61:VAL:HG22	1.89	0.73
33:d:407:PHO:HBC2	33:d:407:PHO:HHD	1.71	0.73
10:k:35:LEU:HD12	10:k:35:LEU:O	1.89	0.72
3:c:391[A]:ARG:NE	35:c:603:HOH:O	2.22	0.72
16:U:39:ARG:NH2	17:V:60:ALA:O	2.22	0.72
10:k:10:LYS:HD2	10:k:10:LYS:N	2.05	0.71
2:B:467:ILE:HD12	4:D:126:MET:HE2	1.70	0.71
9:J:36:LEU:O	35:J:202:HOH:O	2.07	0.71
10:K:46:ARG:NH2	35:K:201:HOH:O	2.23	0.71
1:A:25:ASP:OD1	35:A:501:HOH:O	2.07	0.71
20:Z:32:ASP:CG	20:Z:35:ARG:HG2	2.16	0.71
9:j:34:ALA:O	35:j:201:HOH:O	2.10	0.70
6:F:15:ILE:HD13	14:R:23:ILE:HD11	1.74	0.70
12:m:5:GLN:O	35:m:201:HOH:O	2.09	0.70
28:a:416:STE:O2	35:a:501:HOH:O	2.10	0.69
5:e:26:THR:HB	34:f:101:HEC:HBB2	1.74	0.69
23:d:405:BCR:H331	23:d:405:BCR:C8	2.21	0.69
7:h:41:PHE:CE1	22:h:701:CLA:HMC1	2.27	0.69
1:a:229:GLU:CG	1:a:229:GLU:CA	2.71	0.69
16:U:70:ARG:NH2	35:U:204:HOH:O	2.25	0.68
2:b:492:GLU:OE1	35:b:701:HOH:O	2.11	0.68
23:B:719:BCR:H383	23:B:719:BCR:H23C	1.74	0.68
9:j:18:GLY:O	9:j:21:VAL:HG12	1.93	0.68
2:b:65:PHE:HE2	22:b:604:CLA:HED2	1.59	0.68
2:b:307:GLU:OE1	35:b:702:HOH:O	2.12	0.68
13:o:130:GLN:HB3	13:o:131:PRO:CD	2.24	0.68
7:h:41:PHE:HE1	22:h:701:CLA:HHC	1.60	0.67
18:x:15:LEU:O	18:x:15:LEU:CD2	2.30	0.67
9:j:9:PRO:HG2	9:j:12:ILE:HD12	1.75	0.67
22:B:707:CLA:H193	31:B:722:LHG:H142	1.75	0.67
13:O:194:LYS:HA	13:O:194:LYS:HD3	1.74	0.67
5:E:8:ARG:HD3	5:E:13:ILE:HG12	1.77	0.67
5:e:78:THR:O	5:e:82:GLN:HG3	1.95	0.67
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:195:HIS:CD2	1:a:293:MET:HE2	2.30	0.66
30:a:418:LMG:H312	35:a:617:HOH:O	1.95	0.66
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.77	0.66
2:b:86:ILE:HG13	2:b:86:ILE:O	1.96	0.66
30:b:620:LMG:O10	12:m:4:ASN:ND2	2.29	0.66
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.78	0.66
19:Y:34:MET:CE	20:Z:21:ILE:HG21	2.27	0.65
2:B:246:PHE:CE2	2:B:463:PHE:HA	2.31	0.65
2:b:81:THR:CB	2:b:83:GLU:OE2	2.43	0.65
10:k:19:ASP:OD2	35:k:201:HOH:O	2.14	0.65
14:r:30:GLN:O	35:r:101:HOH:O	2.14	0.65
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.79	0.65
22:b:602:CLA:H43	7:h:45:ILE:HG22	1.79	0.65
15:T:25:GLU:OE2	35:T:801:HOH:O	2.15	0.64
9:j:36:LEU:O	35:j:201:HOH:O	2.15	0.64
9:j:18:GLY:O	9:j:22:ILE:HD12	1.96	0.64
2:B:127:ARG:CD	2:B:127:ARG:CB	2.76	0.64
23:t:701:BCR:HC8	23:t:701:BCR:H321	1.79	0.64
34:F:101:HEC:HBC3	34:F:101:HEC:HHD	1.78	0.64
13:o:130:GLN:HB3	13:o:131:PRO:HD2	1.81	0.63
25:D:406:PL9:H412	11:L:29:LEU:HD23	1.81	0.63
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.62	0.63
3:C:50:LEU:O	3:C:54:VAL:HG23	1.98	0.63
20:Z:32:ASP:OD1	20:Z:35:ARG:HG2	1.98	0.63
17:v:76:MET:HE1	17:v:115:ILE:HB	1.80	0.63
4:d:236:ASN:O	4:d:239:GLN:HG2	1.98	0.63
23:Y:101:BCR:H321	23:Y:101:BCR:HC8	1.81	0.62
4:D:59:TYR:O	5:E:65:LEU:HD12	1.98	0.62
19:Y:20:ALA:N	19:Y:23:THR:HG1	1.97	0.62
3:C:135:ARG:NH1	20:Z:33:TRP:HB2	2.15	0.62
5:E:68:ASP:O	5:E:72:ALA:HB2	1.98	0.62
4:D:24:ARG:HD2	18:X:37:VAL:HG12	1.82	0.62
5:e:36:LEU:O	5:e:40:THR:HG23	2.00	0.62
22:B:727:CLA:O1D	22:B:727:CLA:H2A	1.99	0.62
4:d:170:ALA:HB1	4:d:171:PRO:HD2	1.81	0.61
3:C:42:LEU:HD21	22:C:512:CLA:H2A	1.82	0.61
19:Y:34:MET:SD	19:Y:38:LEU:CD1	2.88	0.61
22:D:403:CLA:HBB1	22:D:403:CLA:HMB3	1.82	0.61
16:u:53:ALA:HB1	16:u:54:PRO:CD	2.29	0.61
2:b:246:PHE:HD1	2:b:247:PHE:N	1.99	0.61
23:b:619:BCR:H331	23:b:619:BCR:C8	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:207:ARG:HG3	13:O:207:ARG:HH11	1.65	0.61
16:U:16:LYS:NZ	35:U:207:HOH:O	2.32	0.61
7:H:17:GLU:OE2	7:H:20:LYS:HE2	2.01	0.61
3:c:391[A]:ARG:NH1	35:c:606:HOH:O	2.33	0.60
5:e:30:LEU:HD11	34:f:101:HEC:HBB3	1.83	0.60
5:E:8:ARG:HD3	5:E:13:ILE:CG1	2.31	0.60
23:B:718:BCR:H331	23:B:718:BCR:C8	2.32	0.60
2:b:127:ARG:NH1	7:h:18:TYR:O	2.34	0.60
10:k:18:PHE:CE1	20:z:9:LEU:HD23	2.36	0.60
14:r:30:GLN:HA	14:r:31:VAL:CB	2.31	0.60
9:J:20:GLY:O	9:J:24:ILE:HD12	2.02	0.60
2:B:246:PHE:HE2	2:B:463:PHE:HA	1.66	0.60
10:K:17:ILE:HG23	10:K:18:PHE:CD1	2.36	0.60
20:Z:15:LEU:HD22	20:Z:19:MET:HG3	1.84	0.60
17:v:28:GLU:CB	17:v:28:GLU:CD	2.72	0.60
4:d:267:LEU:C	4:d:267:LEU:HD23	2.27	0.59
16:u:39:ARG:NH1	17:v:60:ALA:O	2.35	0.59
2:b:102:VAL:HG21	22:b:606:CLA:C14	2.32	0.59
3:c:87:ILE:HD12	22:c:503:CLA:HMA3	1.83	0.59
4:d:246:MET:HE3	4:d:264:LYS:CG	2.32	0.59
13:O:189:ARG:NE	35:O:305:HOH:O	2.35	0.59
3:c:166:ILE:HG21	22:c:513:CLA:H192	1.83	0.59
20:z:32:ASP:HB2	20:z:35:ARG:HB2	1.85	0.59
1:A:85:SER:HA	1:A:109:GLY:HA3	1.85	0.59
19:Y:24:MET:SD	19:Y:27:MET:SD	3.01	0.59
19:y:39:LEU:HB3	19:y:46:LEU:HD21	1.85	0.59
23:H:101:BCR:H331	23:H:101:BCR:C8	2.32	0.59
14:R:18:TRP:O	14:R:22:ASN:HB2	2.03	0.59
10:k:35:LEU:C	10:k:35:LEU:CD1	2.75	0.59
17:v:104:MET:HA	17:v:107:LEU:CD2	2.33	0.59
17:v:10:VAL:HG23	17:v:69:ILE:HD11	1.84	0.58
20:Z:36:SER:O	20:Z:40:ILE:HG12	2.03	0.58
16:u:79:LEU:O	35:u:201:HOH:O	2.17	0.58
2:b:497:GLN:HE21	4:d:24:ARG:NH1	2.02	0.58
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	1.86	0.58
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.86	0.58
20:z:31:GLN:HG3	20:z:32:ASP:OD1	2.02	0.58
3:c:391[B]:ARG:NH2	35:c:603:HOH:O	2.35	0.58
2:B:117:TYR:HA	11:L:1:MET:HE1	1.86	0.58
23:C:524:BCR:H331	23:C:524:BCR:C8	2.32	0.58
2:b:39:LEU:HD22	28:b:624:STE:H72	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:149:PRO:HA	13:o:192:LEU:HD12	1.85	0.58
17:v:122:GLU:N	17:v:123:PRO:HD2	2.19	0.58
2:b:174:LEU:O	35:b:703:HOH:O	2.17	0.57
4:d:272:LEU:C	4:d:272:LEU:HD23	2.29	0.57
2:B:285:ASN:O	2:B:289:GLN:HG2	2.04	0.57
12:M:20:VAL:HG13	12:m:20:VAL:HG13	1.87	0.57
14:R:24:LEU:CB	14:R:25:PRO:CD	2.82	0.57
22:C:513:CLA:C12	22:C:513:CLA:H91	2.34	0.57
30:a:418:LMG:O10	30:a:418:LMG:O9	2.22	0.57
22:C:510:CLA:H141	22:C:510:CLA:H171	1.86	0.57
20:Z:3:ILE:HA	20:Z:6:GLN:OE1	2.03	0.57
5:E:65:LEU:O	5:E:67:THR:HG23	2.05	0.57
2:b:435:GLU:CD	2:b:435:GLU:CB	2.74	0.57
22:c:502:CLA:H202	22:c:508:CLA:HBB1	1.85	0.57
5:E:8:ARG:HG3	6:F:13:TYR:CD2	2.40	0.56
9:j:5:GLY:N	35:j:202:HOH:O	2.38	0.56
2:B:185:TRP:HB3	22:B:727:CLA:HMA3	1.86	0.56
13:O:27:ARG:O	13:O:27:ARG:HG2	2.04	0.56
3:c:87:ILE:HD12	22:c:503:CLA:CMA	2.36	0.56
5:e:23:HIS:HA	5:e:26:THR:OG1	2.06	0.56
2:b:29:LEU:HD23	26:l:101:SQD:H222	1.88	0.56
20:z:31:GLN:CG	20:z:32:ASP:OD1	2.54	0.56
23:B:719:BCR:H331	23:B:719:BCR:C8	2.36	0.56
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.41	0.56
30:D:409:LMG:H402	6:F:26:LEU:HB3	1.87	0.56
20:Z:53:VAL:HG12	20:Z:57:LEU:HD12	1.88	0.56
35:A:600:HOH:O	13:O:107:THR:HG21	2.06	0.56
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.09	0.56
4:d:39:PRO:O	4:d:43:LEU:HG	2.05	0.56
19:Y:34:MET:HE1	20:Z:21:ILE:HG21	1.88	0.55
20:Z:2:THR:HG22	20:Z:6:GLN:OE1	2.07	0.55
2:b:398:THR:HG22	2:b:412:THR:HG22	1.87	0.55
9:J:19:MET:O	9:J:23:VAL:HG23	2.05	0.55
2:b:246:PHE:CD1	2:b:246:PHE:C	2.84	0.55
7:H:12:ARG:HB3	7:H:13:PRO:CD	2.36	0.55
23:H:101:BCR:H331	23:H:101:BCR:HC8	1.88	0.55
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.42	0.55
22:C:506:CLA:HBC3	22:C:506:CLA:HMC1	1.89	0.55
2:b:246:PHE:HD1	2:b:246:PHE:C	2.15	0.55
3:c:406:SER:HA	3:c:420:VAL:HG23	1.88	0.55
19:y:20:ALA:O	19:y:23:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.41	0.55
7:h:17:GLU:OE2	7:h:20:LYS:HE2	2.07	0.55
13:O:58:ASN:C	13:O:58:ASN:OD1	2.49	0.54
5:e:18:ARG:NH1	14:r:23:ILE:HD11	2.22	0.54
20:Z:55:GLY:HA2	20:Z:58:ASN:HB3	1.89	0.54
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.89	0.54
3:C:406:SER:HA	3:C:420:VAL:HG23	1.89	0.54
1:A:11:ALA:O	1:A:16:ARG:NH2	2.40	0.54
1:A:310:LYS:NZ	35:A:507:HOH:O	2.39	0.54
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.42	0.54
2:b:36:SER:OG	23:b:618:BCR:H362	2.07	0.54
4:d:16:ASP:OD1	28:d:402:STE:H183	2.06	0.54
20:Z:20:VAL:HG12	20:Z:21:ILE:HD13	1.89	0.54
5:e:68:ASP:O	5:e:72:ALA:HB2	2.08	0.54
9:J:19:MET:HB2	35:J:201:HOH:O	2.07	0.54
3:c:25:ASN:O	3:c:26:ARG:HB2	2.05	0.54
19:y:39:LEU:HB3	19:y:46:LEU:CD2	2.37	0.54
27:A:411:DGD:HD5	2:b:75:TRP:HB3	1.89	0.54
4:D:218:VAL:HG22	4:D:244:TYR:CE1	2.43	0.54
35:b:701:HOH:O	5:e:3:GLY:N	2.41	0.54
3:C:315:MET:HE3	3:C:351:PHE:HZ	1.74	0.53
22:B:711:CLA:H193	22:B:713:CLA:H8	1.89	0.53
5:E:26:THR:O	5:E:30:LEU:HG	2.07	0.53
20:z:10:ALA:O	20:z:14:ILE:HG12	2.07	0.53
13:O:33:ASP:OD2	13:O:35:SER:OG	2.27	0.53
7:h:41:PHE:CZ	22:h:701:CLA:CBB	2.91	0.53
13:o:199:LEU:HD23	13:o:215:PHE:HB3	1.91	0.53
22:C:513:CLA:H91	22:C:513:CLA:H122	1.89	0.53
2:b:65:PHE:CE2	22:b:604:CLA:HED2	2.41	0.53
3:c:135:ARG:NH1	20:z:33:TRP:CE2	2.77	0.53
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.91	0.53
17:V:99:ASP:N	17:V:99:ASP:OD1	2.41	0.53
12:m:32:GLN:C	35:m:202:HOH:O	2.50	0.53
1:a:127:MET:HE3	3:c:442:LEU:HD11	1.90	0.53
4:d:79:SER:HA	4:d:172:SER:HB3	1.90	0.53
17:v:11:PRO:O	17:v:69:ILE:HD12	2.08	0.53
18:x:12:ILE:HG21	28:x:101:STE:H141	1.91	0.53
20:z:19:MET:O	20:z:23:VAL:HG23	2.08	0.53
2:B:487:SER:OG	2:B:488:PRO:HD2	2.09	0.53
19:Y:34:MET:HE3	20:Z:21:ILE:HG21	1.89	0.53
14:r:20:VAL:O	14:r:24:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:120:LEU:O	35:V:301:HOH:O	2.19	0.53
2:b:102:VAL:HG21	22:b:606:CLA:H141	1.91	0.53
2:B:246:PHE:CE1	22:B:708:CLA:CBC	2.91	0.52
13:O:63:ALA:N	35:O:309:HOH:O	2.41	0.52
23:D:405:BCR:H331	23:D:405:BCR:C8	2.38	0.52
2:b:246:PHE:CD1	2:b:247:PHE:N	2.77	0.52
3:c:350:ILE:HG21	3:c:359[A]:TRP:HB2	1.90	0.52
2:B:84:THR:HG21	13:o:66:VAL:HG11	1.91	0.52
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.41	0.52
17:v:110:LYS:HD2	17:v:110:LYS:C	2.35	0.52
1:A:104:GLU:CD	13:O:73:ARG:HG2	2.35	0.52
19:Y:39:LEU:HD21	20:Z:25:VAL:HA	1.90	0.52
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.92	0.52
1:a:289:GLY:O	1:a:293:MET:HE3	2.09	0.52
2:b:67:ALA:HA	2:b:71:VAL:O	2.10	0.52
3:c:413[A]:GLU:OE2	17:v:47:LYS:NZ	2.32	0.52
5:e:26:THR:HG22	14:r:15:ALA:HB1	1.92	0.52
11:l:7:ARG:NH2	26:l:101:SQD:H62	2.25	0.52
3:C:279:LEU:HD12	22:C:510:CLA:HED2	1.92	0.52
20:Z:31:GLN:NE2	20:Z:32:ASP:HB3	2.25	0.52
2:b:76:SER:HG	2:b:78:TRP:CD1	2.28	0.52
3:c:203:THR:O	3:c:235:GLY:HA3	2.09	0.52
34:f:101:HEC:HMC1	34:f:101:HEC:HBC2	1.92	0.52
20:Z:32:ASP:OD2	20:Z:35:ARG:CG	2.58	0.52
2:b:119:ASP:OD1	2:b:124:ARG:NH2	2.34	0.52
3:C:95:LEU:HD21	22:C:502:CLA:OBD	2.10	0.52
13:O:58:ASN:HB3	35:b:702:HOH:O	2.10	0.52
14:R:6:LEU:CD2	14:R:10:LEU:HD12	2.40	0.52
2:b:378:LYS:NZ	35:b:705:HOH:O	2.42	0.52
14:r:30:GLN:CA	14:r:31:VAL:CB	2.88	0.52
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.91	0.52
9:j:9:PRO:CG	9:j:12:ILE:HD12	2.40	0.52
2:B:499:VAL:HG12	4:D:135:LEU:HB3	1.92	0.51
22:D:402:CLA:HBC3	22:D:402:CLA:HHD	1.92	0.51
7:h:63:LYS:O	7:h:64:ALA:HB2	2.08	0.51
2:b:192:PRO:HG3	7:h:49:TYR:CD1	2.45	0.51
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.46	0.51
10:k:35:LEU:O	10:k:35:LEU:CD1	2.57	0.51
2:b:137:LYS:HD2	7:h:14:LEU:O	2.09	0.51
4:d:218:VAL:HG22	4:d:244:TYR:CE1	2.46	0.51
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:92:SER:O	2:b:96:VAL:HG23	2.09	0.51
2:b:378:LYS:HE3	35:b:705:HOH:O	2.11	0.51
5:e:27:ILE:HD11	34:f:101:HEC:HBC3	1.92	0.51
11:l:7:ARG:NH2	26:l:101:SQD:S	2.83	0.51
10:K:26:PRO:O	10:K:29:PRO:HD2	2.11	0.51
3:c:178:LYS:NZ	3:c:184:GLY:O	2.40	0.51
6:f:28:VAL:CG2	6:f:29:PRO:HD3	2.38	0.51
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.10	0.51
9:j:26:GLY:HA2	28:j:101:STE:H62	1.93	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.92	0.51
2:b:26:HIS:O	2:b:30:VAL:HG23	2.11	0.51
7:h:41:PHE:HE1	22:h:701:CLA:HMC1	1.75	0.51
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.93	0.51
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.28	0.51
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.93	0.51
23:B:719:BCR:H23C	23:B:719:BCR:C38	2.42	0.50
20:Z:32:ASP:OD2	20:Z:35:ARG:HG2	2.11	0.50
3:c:38:GLY:HA3	22:c:512:CLA:HMD2	1.92	0.50
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.94	0.50
22:d:401:CLA:H151	31:d:408:LHG:H222	1.93	0.50
28:B:724:STE:C1	35:B:806:HOH:O	2.58	0.50
16:U:27:LEU:HD13	16:U:61:VAL:HG13	1.92	0.50
2:B:76:SER:HB2	30:a:418:LMG:HC4	1.92	0.50
17:V:124:LYS:NZ	35:V:304:HOH:O	2.44	0.50
1:a:114:LEU:C	1:a:114:LEU:HD23	2.36	0.50
12:m:9:ILE:HG13	12:m:13:LEU:HD22	1.93	0.50
18:x:16:SER:HB3	28:x:101:STE:H71	1.91	0.50
23:c:516:BCR:H382	23:c:516:BCR:H23C	1.92	0.50
23:h:702:BCR:H331	23:h:702:BCR:C8	2.41	0.50
14:r:3:TRP:HA	14:r:6:LEU:HD21	1.93	0.50
31:a:411:LHG:H212	22:b:613:CLA:H172	1.92	0.50
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.46	0.50
22:C:509:CLA:CBB	22:C:510:CLA:HED1	2.41	0.50
22:c:504:CLA:H193	22:c:511:CLA:HAB	1.92	0.50
18:x:16:SER:O	18:x:20:VAL:HG23	2.11	0.50
4:D:79:SER:HA	4:D:172:SER:HB3	1.94	0.50
34:V:201:HEC:HMC1	34:V:201:HEC:HBC3	1.93	0.50
22:b:606:CLA:HMB1	22:b:606:CLA:HBB1	1.93	0.50
18:x:27:VAL:O	18:x:31:ILE:HG13	2.11	0.50
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.42	0.50
1:A:329[A]:GLU:HG3	35:A:620:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:124:VAL:HG11	23:c:515:BCR:H16C	1.93	0.50
5:e:14:ILE:HD11	9:j:10:LEU:HD21	1.93	0.50
10:k:35:LEU:O	10:k:36:ALA:C	2.54	0.50
13:o:205:ASP:OD1	13:o:207:ARG:HB2	2.11	0.50
19:y:39:LEU:O	19:y:44:GLY:N	2.45	0.50
3:c:128:GLY:HA3	22:c:514:CLA:C3C	2.42	0.50
14:r:19:ALA:O	14:r:23:ILE:HG22	2.12	0.50
2:B:383:PHE:O	13:O:166:SER:HA	2.12	0.49
22:B:706:CLA:H72	23:B:719:BCR:H311	1.93	0.49
4:D:209:LEU:HD23	4:D:209:LEU:C	2.37	0.49
23:b:618:BCR:H331	23:b:618:BCR:C8	2.42	0.49
5:e:18:ARG:O	5:e:22:ILE:HG13	2.12	0.49
13:O:194:LYS:HD3	13:O:194:LYS:CA	2.42	0.49
16:U:86:GLU:OE1	35:U:203:HOH:O	2.20	0.49
4:d:103:ARG:NH2	35:d:504:HOH:O	2.43	0.49
22:d:403:CLA:HBC3	22:d:403:CLA:HHD	1.94	0.49
31:d:408:LHG:H281	15:t:17:PHE:CD1	2.47	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.93	0.49
7:H:44:ILE:HG22	7:H:48:ILE:HD12	1.93	0.49
9:j:10:LEU:HD23	9:j:13:VAL:HG21	1.94	0.49
2:b:505:ARG:HG2	2:b:506:ARG:H	1.77	0.49
4:d:52:THR:O	4:d:66:SER:HA	2.12	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.49
2:B:495:PHE:HD2	2:B:505:ARG:NH1	2.10	0.49
13:O:57:LYS:HE2	2:b:338:GLN:HA	1.94	0.49
2:b:506:ARG:NH2	35:b:710:HOH:O	2.45	0.49
17:v:12:LEU:HB2	17:v:19:ILE:HG22	1.94	0.49
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.94	0.49
2:B:371:THR:HG23	2:B:372:ASP:O	2.13	0.49
4:D:272:LEU:C	4:D:272:LEU:HD23	2.37	0.49
3:c:78:GLU:OE2	35:c:602:HOH:O	2.20	0.49
2:b:235:GLU:OE1	2:b:469:HIS:ND1	2.35	0.49
10:k:19:ASP:N	10:k:20:PRO:HD2	2.27	0.49
20:z:9:LEU:HD13	20:z:54:VAL:HG11	1.93	0.49
28:b:621:STE:H142	28:b:621:STE:H183	1.95	0.49
7:h:28:THR:HB	7:h:29:PRO:HD3	1.94	0.49
4:D:104:TRP:HZ2	22:D:404:CLA:HED2	1.77	0.49
18:X:8:LYS:O	18:X:12:ILE:HG12	2.13	0.49
1:a:196:PRO:O	1:a:200:LEU:HD22	2.13	0.49
5:e:13:ILE:O	5:e:19:TYR:CB	2.61	0.49
27:A:411:DGD:HB61	28:I:101:STE:C5	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ILE:C	2:B:370:LEU:HD12	2.38	0.49
27:C:518:DGD:O1A	27:C:518:DGD:HA41	2.12	0.49
13:O:194:LYS:CB	13:O:194:LYS:HD2	2.37	0.49
2:b:81:THR:HB	2:b:83:GLU:OE2	2.12	0.49
2:b:102:VAL:HG11	22:b:606:CLA:H142	1.94	0.49
2:b:164:PRO:HG3	22:b:606:CLA:O1D	2.13	0.49
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.13	0.48
4:D:279:LEU:HD22	33:D:408:PHO:HBC3	1.94	0.48
23:a:406:BCR:H392	30:a:418:LMG:H341	1.95	0.48
30:c:523:LMG:C30	30:c:523:LMG:HC91	2.43	0.48
2:B:84:THR:HG21	13:o:66:VAL:CG1	2.42	0.48
5:E:36:LEU:O	5:E:40:THR:HG23	2.13	0.48
16:U:45:LEU:HD21	16:U:71:GLN:HG2	1.94	0.48
17:V:2:GLU:HB2	35:V:353:HOH:O	2.13	0.48
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.95	0.48
14:r:24:LEU:HD22	14:r:24:LEU:O	2.13	0.48
5:e:13:ILE:HG22	5:e:19:TYR:CD1	2.48	0.48
19:y:41:VAL:C	19:y:43:ARG:H	2.21	0.48
1:A:256:GLY:O	1:A:260:PHE:CA	2.61	0.48
18:X:10:PHE:CE2	18:X:14:LEU:HD22	2.48	0.48
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.95	0.48
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.95	0.48
20:z:3:ILE:O	20:z:7:LEU:HD23	2.14	0.48
2:B:370:LEU:HD12	2:B:370:LEU:N	2.29	0.48
4:D:274:VAL:HG22	25:D:406:PL9:H222	1.95	0.48
33:D:408:PHO:HBC2	33:D:408:PHO:HHD	1.94	0.48
19:y:20:ALA:O	19:y:24:MET:HG2	2.14	0.48
25:A:408:PL9:H361	6:F:25:THR:HG21	1.95	0.48
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.43	0.48
22:B:704:CLA:HBD	22:B:705:CLA:H43	1.96	0.48
1:a:42:LEU:HD13	26:a:414:SQD:H301	1.96	0.48
1:a:308:ASP:OD1	1:a:308:ASP:C	2.57	0.48
14:r:10:LEU:CB	14:r:11:PRO:CD	2.85	0.48
2:B:36:SER:OG	23:B:718:BCR:H362	2.14	0.48
2:B:413:ASP:OD1	35:B:801:HOH:O	2.20	0.48
34:f:101:HEC:HBB3	34:f:101:HEC:HHC	1.95	0.48
22:C:509:CLA:HBC3	22:C:511:CLA:H92	1.96	0.48
11:l:7:ARG:NH2	26:l:101:SQD:C6	2.76	0.48
3:C:344:SER:O	13:O:75:THR:HG22	2.14	0.48
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.43	0.48
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:25:LEU:N	10:k:26:PRO:CD	2.77	0.48
17:v:41:HIS:HA	17:v:45:ILE:O	2.14	0.48
23:k:102:BCR:C8	23:k:102:BCR:H331	2.43	0.48
3:C:139:THR:HB	3:C:141:GLU:OE1	2.13	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.47
20:Z:31:GLN:CG	20:Z:32:ASP:H	2.26	0.47
4:d:13:GLY:O	4:d:16:ASP:HB2	2.14	0.47
7:h:41:PHE:CD1	22:h:701:CLA:HMC1	2.48	0.47
11:l:2:GLU:O	11:l:2:GLU:HG2	2.14	0.47
4:D:246:MET:HE3	4:D:264:LYS:CD	2.31	0.47
13:O:194:LYS:CD	13:O:194:LYS:HB3	2.38	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47
13:o:60:ARG:O	13:o:60:ARG:HG3	2.14	0.47
16:u:88:GLU:O	16:u:92:VAL:HG22	2.13	0.47
20:z:34:ASP:O	20:z:38:GLN:OE1	2.32	0.47
1:A:54[A]:ALA:HA	1:A:72:LEU:HD12	1.95	0.47
20:Z:44:SER:O	20:Z:48:ILE:HG13	2.15	0.47
2:B:414:PRO:N	2:B:415:PRO:HD2	2.30	0.47
10:K:13:GLU:O	10:K:16:ALA:HB2	2.12	0.47
1:a:36:ILE:HG23	22:a:405:CLA:HBB1	1.96	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.47
23:A:405:BCR:H363	28:I:101:STE:H121	1.96	0.47
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.15	0.47
17:v:108:THR:O	17:v:111:ASP:HB2	2.14	0.47
1:a:15:GLU:HA	1:a:15:GLU:OE1	2.14	0.47
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.61	0.47
2:B:497:GLN:O	4:D:24:ARG:HG2	2.15	0.47
10:K:23:ASP:OD2	19:Y:21:GLN:NE2	2.46	0.47
10:K:25:LEU:N	10:K:26:PRO:HD2	2.29	0.47
1:a:201:GLY:HA3	1:a:286:THR:HB	1.96	0.47
2:b:135:LEU:N	2:b:136:PRO:CD	2.78	0.47
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.50	0.47
14:R:24:LEU:HD13	14:R:25:PRO:N	2.25	0.47
16:U:27:LEU:HD13	16:U:61:VAL:CG1	2.44	0.47
33:d:407:PHO:HBC2	33:d:407:PHO:CHD	2.38	0.47
1:A:256:GLY:O	1:A:260:PHE:HA	2.15	0.47
1:a:12:ASN:C	1:a:12:ASN:OD1	2.57	0.47
2:b:12:LEU:HB2	22:b:612:CLA:HMC2	1.96	0.47
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.96	0.47
14:r:29:LYS:C	14:r:31:VAL:CB	2.88	0.47
14:R:23:ILE:O	14:R:24:LEU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:38:GLN:HA	18:X:38:GLN:OE1	2.14	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.50	0.47
14:r:24:LEU:N	14:r:25:PRO:HD2	2.30	0.47
19:y:17:GLU:O	19:y:20:ALA:HB3	2.15	0.47
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.97	0.46
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.95	0.46
14:R:6:LEU:O	14:R:9:LEU:N	2.48	0.46
2:b:221:PRO:HB3	22:b:609:CLA:O1D	2.16	0.46
2:B:497:GLN:HB2	2:B:504:THR:HB	1.97	0.46
3:C:227:VAL:HG13	3:C:227:VAL:O	2.16	0.46
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.96	0.46
7:h:35:MET:HB3	7:h:35:MET:HE2	1.63	0.46
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.97	0.46
1:a:215:HIS:ND1	25:a:410:PL9:O1	2.37	0.46
25:a:410:PL9:H48	4:d:39:PRO:HG3	1.98	0.46
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.97	0.46
4:d:157:PHE:CE2	4:d:171:PRO:HG2	2.51	0.46
14:r:29:LYS:O	14:r:31:VAL:CB	2.63	0.46
5:E:26:THR:HB	34:F:101:HEC:CAB	2.45	0.46
17:V:77:LYS:O	17:V:96:ARG:HB2	2.16	0.46
4:d:194:ASN:HA	4:d:295:SER:OG	2.16	0.46
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.81	0.46
5:e:61:ARG:NH1	17:v:125:ILE:O	2.43	0.46
34:F:101:HEC:HBC3	34:F:101:HEC:CHD	2.45	0.46
3:c:104:GLU:CB	3:c:104:GLU:CD	2.82	0.46
3:c:391[A]:ARG:CZ	35:c:603:HOH:O	2.63	0.46
17:v:90:GLU:HB2	35:v:312:HOH:O	2.16	0.46
7:H:66:GLY:N	35:H:204:HOH:O	2.49	0.46
20:Z:53:VAL:CG1	20:Z:57:LEU:HD12	2.45	0.46
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.51	0.46
3:c:415:ASN:OD1	27:c:519:DGD:O4D	2.34	0.46
17:v:87:GLU:CD	17:v:96:ARG:HH12	2.24	0.46
3:C:61:VAL:HG12	3:C:118:HIS:O	2.16	0.46
13:O:207:ARG:HG3	13:O:207:ARG:NH1	2.30	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.46
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.51	0.46
2:b:102:VAL:HG21	22:b:606:CLA:H142	1.97	0.46
2:b:356:VAL:HG21	2:b:424:ALA:HB3	1.98	0.46
4:d:261:PHE:CZ	31:d:408:LHG:HC81	2.50	0.46
3:C:213:LEU:HG	22:C:507:CLA:H203	1.98	0.45
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:GLY:O	4:D:17:ILE:HG12	2.16	0.45
13:O:32:ILE:HD11	13:O:136:ILE:HG13	1.96	0.45
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.51	0.45
23:B:719:BCR:C38	23:B:719:BCR:C23	2.94	0.45
4:D:52:THR:O	4:D:66:SER:HA	2.16	0.45
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.48	0.45
13:o:52:VAL:HG23	13:o:68:THR:HG21	1.99	0.45
17:v:9:THR:O	17:v:124:LYS:NZ	2.50	0.45
1:a:195:HIS:CG	1:a:293:MET:HE2	2.51	0.45
1:A:60[A]:ILE:HB	1:A:83:VAL:CG1	2.47	0.45
2:B:149[B]:LEU:HG	22:B:704:CLA:H18	1.98	0.45
22:C:503:CLA:H51	22:C:504:CLA:C4C	2.47	0.45
5:E:14:ILE:HD12	9:J:13:VAL:HG11	1.97	0.45
17:v:69:ILE:HD12	17:v:69:ILE:H	1.81	0.45
9:J:19:MET:CB	35:J:201:HOH:O	2.65	0.45
12:M:31:SER:O	12:m:32:GLN:HB3	2.16	0.45
4:d:49:LEU:HD13	23:d:405:BCR:C15	2.47	0.45
3:C:455:PHE:HD2	8:I:33:LYS:HG3	1.81	0.45
4:D:136:VAL:O	4:D:136:VAL:CG1	2.64	0.45
2:b:493:TRP:HD1	5:e:5:THR:CG2	2.29	0.45
19:y:46:LEU:O	35:y:101:HOH:O	2.21	0.45
35:A:528:HOH:O	4:D:243:THR:HG22	2.16	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.97	0.45
22:b:616:CLA:HAA2	22:b:616:CLA:HBD	1.98	0.45
22:d:401:CLA:HBA1	22:d:401:CLA:C4A	2.47	0.45
10:K:10:LYS:CD	10:K:10:LYS:NZ	2.73	0.45
13:O:194:LYS:CD	13:O:194:LYS:CA	2.94	0.45
2:b:59:GLY:O	22:b:607:CLA:HED2	2.17	0.45
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.97	0.45
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.98	0.45
1:A:271:LEU:HD21	25:A:408:PL9:C4	2.46	0.45
17:V:69:ILE:O	17:V:73:VAL:HG23	2.17	0.45
1:a:245:THR:HB	4:d:265:ARG:HE	1.82	0.45
22:a:405:CLA:HBC2	22:a:405:CLA:HHD	1.99	0.45
5:e:13:ILE:O	5:e:19:TYR:HB2	2.17	0.45
1:A:114:LEU:C	1:A:114:LEU:HD23	2.41	0.45
14:R:13:LEU:HD12	14:R:13:LEU:HA	1.80	0.45
23:t:701:BCR:H311	23:t:701:BCR:C8	2.47	0.45
22:A:402:CLA:H191	31:D:411:LHG:H182	1.99	0.44
3:C:114:VAL:HG22	28:C:522:STE:H102	1.99	0.44
13:O:143:LYS:HD2	13:O:198:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:85:SER:HA	1:a:109:GLY:HA3	1.99	0.44
2:b:505:ARG:HG2	2:b:506:ARG:N	2.32	0.44
1:A:161[A]:TYR:CZ	1:A:165[A]:GLN:HG3	2.52	0.44
22:A:402:CLA:HBB1	22:A:402:CLA:HMB3	1.98	0.44
2:B:26:HIS:O	2:B:30:VAL:HG23	2.16	0.44
2:B:215:PHE:CE1	2:B:219:VAL:HG21	2.51	0.44
22:D:404:CLA:H18	18:X:15:LEU:HD11	2.00	0.44
20:Z:27:TYR:HE2	20:Z:33:TRP:CH2	2.36	0.44
22:b:615:CLA:H61	22:b:615:CLA:H92	1.84	0.44
22:C:513:CLA:H41	22:C:513:CLA:H72	1.99	0.44
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.47	0.44
1:a:16:ARG:HG2	1:a:16:ARG:HH11	1.82	0.44
22:b:615:CLA:H161	7:h:7:LEU:HD11	1.98	0.44
3:c:25:ASN:O	3:c:26:ARG:CB	2.65	0.44
4:d:16:ASP:OD2	4:d:16:ASP:N	2.50	0.44
4:d:225:ASP:HB2	4:d:234:ALA:HB1	1.99	0.44
23:B:719:BCR:H20C	23:B:719:BCR:H361	1.78	0.44
13:O:18:LYS:NZ	35:O:311:HOH:O	2.50	0.44
14:R:10:LEU:N	14:R:11:PRO:CD	2.81	0.44
16:U:45:LEU:HD21	16:U:71:GLN:CG	2.48	0.44
23:a:406:BCR:H331	23:a:406:BCR:C8	2.47	0.44
1:A:161[A]:TYR:HB3	1:A:162[A]:PRO:HD3	1.99	0.44
2:B:119:ASP:H	11:L:1:MET:CE	2.30	0.44
4:D:330:ALA:HB3	4:D:331:PRO:HD3	2.00	0.44
22:D:403:CLA:HBA1	22:D:403:CLA:C4A	2.47	0.44
17:V:41:HIS:HA	17:V:45:ILE:O	2.18	0.44
3:c:142:GLU:OE1	3:c:142:GLU:N	2.48	0.44
25:A:408:PL9:H253	31:E:101:LHG:H211	2.00	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
17:V:87:GLU:CD	17:V:96:ARG:HH12	2.25	0.44
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.99	0.44
1:a:263:ALA:HA	31:a:413:LHG:H291	1.98	0.44
3:c:257:PHE:O	3:c:261:ARG:HG3	2.18	0.44
1:A:40:THR:O	1:A:118:HIS:HB3	2.17	0.44
14:R:6:LEU:O	14:R:7:VAL:C	2.59	0.44
2:b:348:ASN:HB3	2:b:354:LEU:HD11	2.00	0.44
20:z:1:MET:CG	20:z:4:LEU:HB3	2.48	0.44
1:A:201:GLY:HA3	1:A:286:THR:HB	1.99	0.44
2:B:347:ARG:HA	2:B:352:GLU:O	2.18	0.44
2:B:467:ILE:HD12	4:D:126:MET:CE	2.42	0.44
10:K:28:ILE:N	10:K:29:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.00	0.44
1:a:301:ASN:C	1:a:301:ASN:OD1	2.61	0.44
1:A:288:LEU:HD13	3:C:432:VAL:HG13	1.99	0.44
22:B:715:CLA:H2	22:B:716:CLA:HBB2	1.99	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.47	0.44
4:D:274:VAL:N	4:D:275:PRO:HD2	2.33	0.44
4:D:307:GLU:HG3	35:D:590:HOH:O	2.18	0.44
10:K:10:LYS:N	35:K:202:HOH:O	2.50	0.44
3:c:413[A]:GLU:HG2	35:c:614:HOH:O	2.17	0.44
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.00	0.44
23:B:717:BCR:H24C	23:B:717:BCR:H371	1.81	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.43
23:D:405:BCR:H15C	23:D:405:BCR:H351	1.84	0.43
9:J:15:THR:HG22	9:J:19:MET:CE	2.48	0.43
9:J:18:GLY:HA3	23:Y:101:BCR:H371	1.99	0.43
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.00	0.43
22:b:605:CLA:HMA1	22:b:606:CLA:H3A	2.00	0.43
1:A:173[A]:PRO:HB2	1:A:178[A]:GLY:HA3	2.00	0.43
5:E:3:GLY:N	35:E:203:HOH:O	2.51	0.43
3:c:350:ILE:CG2	3:c:359[A]:TRP:HB2	2.48	0.43
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.44	0.43
22:A:402:CLA:H193	22:A:402:CLA:H162	1.89	0.43
4:D:100:ASP:OD1	4:D:100:ASP:C	2.61	0.43
9:J:34:ALA:O	35:J:202:HOH:O	2.21	0.43
13:O:184:ARG:NH2	13:O:229[A]:GLU:OE2	2.45	0.43
14:R:24:LEU:CD1	14:R:25:PRO:N	2.82	0.43
15:T:15:ALA:HB2	23:T:701:BCR:H14C	1.99	0.43
23:T:701:BCR:H311	23:T:701:BCR:C8	2.41	0.43
20:z:38:GLN:O	20:z:42:LEU:HD13	2.18	0.43
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.07	0.43
15:T:15:ALA:O	15:T:19:PHE:HD1	2.02	0.43
5:e:30:LEU:HD11	34:f:101:HEC:CBB	2.48	0.43
6:f:21:VAL:O	6:f:25:THR:HG23	2.18	0.43
10:k:26:PRO:O	10:k:29:PRO:HD2	2.18	0.43
18:x:24:THR:HG22	18:x:28:LEU:CD1	2.49	0.43
2:B:317:ASN:HA	2:B:330:MET:HE1	1.99	0.43
3:C:143:TYR:CE2	22:C:514:CLA:HED3	2.53	0.43
22:C:512:CLA:HAA1	22:C:512:CLA:HBD	2.00	0.43
22:D:403:CLA:H202	22:D:403:CLA:H162	1.89	0.43
1:a:278:TRP:CD1	1:a:278:TRP:C	2.97	0.43
2:b:57:ARG:NH1	2:b:335:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:515:BCR:H24C	23:c:515:BCR:H371	1.80	0.43
2:B:141:ILE:O	2:B:145:LEU:HG	2.19	0.43
23:B:718:BCR:H24C	23:B:718:BCR:H371	1.77	0.43
22:C:511:CLA:H203	22:C:511:CLA:HBC3	2.00	0.43
6:F:27:ALA:HB1	34:F:101:HEC:HAC	2.01	0.43
13:O:72:THR:O	13:O:73:ARG:HB2	2.18	0.43
2:b:10:THR:HB	2:b:13:ILE:HD12	2.01	0.43
3:c:116:VAL:O	3:c:120:ILE:HG12	2.18	0.43
13:o:10:ILE:HG23	13:o:15:LEU:HB2	2.01	0.43
17:v:2:GLU:HB2	35:v:320:HOH:O	2.18	0.43
18:x:37:VAL:CG1	18:x:38:GLN:N	2.81	0.43
2:B:123:PHE:O	2:B:131:PRO:HA	2.19	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.00	0.43
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.43
10:K:19:ASP:N	10:K:20:PRO:HD2	2.34	0.43
20:Z:5:PHE:HB2	20:Z:57:LEU:HB3	2.00	0.43
2:b:414:PRO:N	2:b:415:PRO:CD	2.81	0.43
23:k:102:BCR:H24C	23:k:102:BCR:H371	1.74	0.43
1:a:42:LEU:HD12	26:a:414:SQD:H321	2.00	0.43
2:b:378:LYS:CE	35:b:705:HOH:O	2.66	0.43
22:d:404:CLA:H92	18:x:18:ALA:HB2	2.01	0.43
5:e:81:GLU:O	5:e:83:LEU:N	2.48	0.43
7:h:41:PHE:CE1	22:h:701:CLA:CMC	2.98	0.43
10:k:19:ASP:N	10:k:20:PRO:CD	2.82	0.43
1:A:11:ALA:O	1:A:16:ARG:CZ	2.67	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.43
4:D:267:LEU:C	4:D:267:LEU:HD23	2.44	0.43
22:D:404:CLA:HBC2	28:X:101:STE:H102	2.00	0.43
3:c:42:LEU:HD21	22:c:512:CLA:H2A	2.01	0.43
4:d:178:ILE:O	4:d:182:LEU:HG	2.18	0.43
5:e:26:THR:CB	34:f:101:HEC:HBB2	2.47	0.43
9:j:18:GLY:O	9:j:22:ILE:CD1	2.65	0.43
6:F:33:PHE:O	6:F:37:ILE:HG13	2.19	0.43
10:K:17:ILE:HG23	10:K:18:PHE:CE1	2.54	0.43
13:O:118:LEU:HD13	13:O:233:VAL:HG11	1.99	0.43
1:a:263:ALA:O	25:a:410:PL9:H152	2.19	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.43
23:t:701:BCR:HC7	23:t:701:BCR:H331	1.83	0.43
1:A:326:LEU:HD22	17:V:134:LYS:HB2	2.01	0.42
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.07	0.42
4:D:291:LEU:HD21	27:H:102:DGD:CGB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.01	0.42
11:l:16:SER:OG	31:l:102:LHG:HC62	2.19	0.42
13:o:84:GLU:OE1	13:o:86:LYS:HG2	2.19	0.42
1:A:214:MET:HE3	1:A:214:MET:HB3	1.85	0.42
2:B:338:GLN:HB3	13:o:58:ASN:ND2	2.34	0.42
2:B:442:ILE:HD12	4:D:299:ILE:HG12	2.02	0.42
33:D:407:PHO:ND	33:D:407:PHO:NC	2.66	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.52	0.42
13:O:178:LYS:HG3	13:O:181:GLU:OE1	2.18	0.42
23:T:701:BCR:H11C	23:T:701:BCR:H341	1.91	0.42
17:V:57:GLU:CD	17:V:57:GLU:H	2.28	0.42
2:b:433:ASP:OD1	2:b:433:ASP:C	2.62	0.42
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.00	0.42
17:v:108:THR:O	17:v:111:ASP:N	2.52	0.42
2:B:414:PRO:O	2:B:418:LYS:HG3	2.18	0.42
19:Y:32:GLY:HA3	23:Y:101:BCR:C15	2.49	0.42
25:a:410:PL9:C30	4:d:45:LEU:HD22	2.50	0.42
11:l:7:ARG:HH22	26:l:101:SQD:H62	1.84	0.42
3:C:367:GLU:N	3:C:368:PRO:CD	2.82	0.42
22:C:502:CLA:HHC	22:C:502:CLA:HBB1	2.02	0.42
13:O:194:LYS:HD2	13:O:194:LYS:HB3	1.99	0.42
5:e:18:ARG:NH1	34:f:101:HEC:CGA	2.83	0.42
34:f:101:HEC:HBC2	34:f:101:HEC:CMC	2.49	0.42
17:v:80:THR:HA	17:v:86:GLN:O	2.19	0.42
18:x:23:LEU:O	18:x:24:THR:C	2.63	0.42
27:A:411:DGD:HA42	2:b:98:LEU:HD11	2.02	0.42
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.01	0.42
33:D:407:PHO:HBC2	33:D:407:PHO:HHO	2.00	0.42
13:O:110:MET:HE2	13:O:110:MET:HB3	1.95	0.42
20:Z:55:GLY:CA	20:Z:58:ASN:HB3	2.50	0.42
1:a:116:ILE:HG13	1:a:117:PHE:N	2.35	0.42
2:b:42:LEU:HD13	2:b:94:GLU:HG3	2.02	0.42
13:o:54:GLU:O	13:o:56:PRO:HD3	2.20	0.42
2:B:119:ASP:H	11:L:1:MET:HE3	1.84	0.42
30:C:520:LMG:H201	10:K:27:VAL:HG11	2.01	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.42
6:F:30:THR:O	6:F:34:LEU:HG	2.20	0.42
9:J:16:VAL:C	35:J:201:HOH:O	2.62	0.42
1:a:321:ILE:HD11	4:d:179:PHE:HB2	2.01	0.42
3:c:104:GLU:CG	3:c:104:GLU:C	2.92	0.42
4:d:261:PHE:CE1	31:d:408:LHG:HC81	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:7:ARG:CZ	26:l:101:SQD:O9	2.68	0.42
17:v:26:TYR:HD2	17:v:27:LEU:HD23	1.84	0.42
22:C:503:CLA:H62	22:C:513:CLA:H42	2.01	0.42
23:C:515:BCR:H24C	23:C:515:BCR:H371	1.91	0.42
5:E:17:VAL:HG23	9:J:7:ARG:CB	2.48	0.42
10:K:28:ILE:HD11	19:Y:28:ILE:HD13	2.02	0.42
34:V:201:HEC:HBC3	34:V:201:HEC:CMC	2.50	0.42
20:Z:29:SER:HB3	20:Z:31:GLN:HG3	2.01	0.42
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.01	0.42
25:a:410:PL9:H301	4:d:45:LEU:HD22	2.02	0.42
5:E:27:ILE:HD11	34:F:101:HEC:HBC2	2.01	0.42
14:R:6:LEU:HD12	14:R:6:LEU:HA	1.79	0.42
20:Z:61:VAL:O	20:Z:62:VAL:O	2.38	0.42
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.54	0.42
22:c:510:CLA:HBA1	22:c:510:CLA:H3A	1.84	0.42
19:y:17:GLU:HB3	19:y:18:VAL:H	1.36	0.42
3:C:256:PRO:O	3:C:261:ARG:NH1	2.53	0.42
22:D:402:CLA:HBC3	22:D:402:CLA:CHD	2.49	0.42
20:Z:55:GLY:HA2	20:Z:58:ASN:CB	2.50	0.42
2:b:247:PHE:CE2	22:b:602:CLA:H102	2.55	0.42
22:d:403:CLA:HBC3	22:d:403:CLA:CHD	2.50	0.42
16:u:38:TYR:HB2	16:u:41:LEU:HD12	2.02	0.42
17:v:10:VAL:CG2	17:v:69:ILE:HD11	2.49	0.42
17:v:26:TYR:CD2	17:v:27:LEU:HD23	2.54	0.42
4:D:12:ARG:HG3	4:D:17:ILE:HD11	2.02	0.41
20:Z:31:GLN:CD	20:Z:32:ASP:H	2.28	0.41
1:a:307:ILE:HG13	6:f:45:ARG:CD	2.49	0.41
30:a:418:LMG:O10	30:a:418:LMG:C10	2.68	0.41
10:k:38:VAL:HG21	23:k:101:BCR:H19C	2.02	0.41
13:o:23:ASP:O	13:o:203:LYS:HD2	2.20	0.41
16:u:45:LEU:HD21	16:u:71:GLN:HB3	2.01	0.41
22:B:714:CLA:O1D	22:B:714:CLA:H2A	2.20	0.41
4:d:126:MET:HA	4:d:129:GLN:OE1	2.19	0.41
31:d:408:LHG:H321	15:t:21:ILE:HD11	2.01	0.41
20:z:32:ASP:OD1	20:z:32:ASP:N	2.52	0.41
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.55	0.41
1:A:162[A]:PRO:HB3	1:A:168[A]:PHE:HA	2.03	0.41
6:F:20:TRP:HE1	34:F:101:HEC:C1A	2.33	0.41
14:R:19:ALA:O	14:R:23:ILE:HG22	2.20	0.41
3:c:249:ILE:O	3:c:250:TRP:C	2.63	0.41
13:o:72:THR:O	13:o:73:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:8:LYS:HA	18:x:8:LYS:HD2	1.88	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
22:B:714:CLA:H141	22:B:714:CLA:H161	1.81	0.41
13:O:133:VAL:C	13:O:134:THR:HG23	2.46	0.41
1:a:229:GLU:CB	1:a:229:GLU:CD	2.86	0.41
3:C:194:GLY:O	3:C:195:ASP:HB2	2.20	0.41
4:D:32:TRP:CD2	30:D:413:LMG:H161	2.54	0.41
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.51	0.41
16:U:53:ALA:HB1	16:U:54:PRO:HA	2.02	0.41
19:Y:26:ALA:O	19:Y:30:ILE:HG22	2.21	0.41
31:a:411:LHG:H221	22:b:613:CLA:H202	2.03	0.41
30:b:622:LMG:C28	30:b:622:LMG:O9	2.68	0.41
22:c:509:CLA:HED3	22:c:509:CLA:H2A	2.02	0.41
22:c:510:CLA:H142	22:c:510:CLA:H111	1.96	0.41
20:z:31:GLN:HG3	20:z:32:ASP:N	2.35	0.41
23:A:405:BCR:H371	23:A:405:BCR:H24C	1.83	0.41
22:C:502:CLA:HAA1	22:C:502:CLA:HBD	2.02	0.41
4:D:259:ILE:O	4:D:259:ILE:HG13	2.21	0.41
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.41
2:b:497:GLN:NE2	4:d:24:ARG:NH1	2.68	0.41
22:b:614:CLA:HBA2	22:b:614:CLA:C4A	2.50	0.41
9:j:10:LEU:HD23	9:j:13:VAL:CG2	2.51	0.41
12:m:8:LEU:HD22	15:t:1:FME:HE3	2.03	0.41
20:z:1:MET:O	20:z:2:THR:C	2.60	0.41
2:B:221:PRO:HA	22:B:709:CLA:HED3	2.02	0.41
23:B:719:BCR:H24C	23:B:719:BCR:H371	1.93	0.41
9:J:7:ARG:HH21	9:J:7:ARG:HD3	1.63	0.41
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.92	0.41
2:b:157:HIS:CD2	2:b:157:HIS:C	2.98	0.41
3:c:150:ASP:OD2	3:c:152:LYS:HB2	2.20	0.41
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.55	0.41
4:d:232:PHE:CE1	31:d:409:LHG:HC42	2.56	0.41
7:h:4:ARG:CB	7:h:4:ARG:HH11	2.33	0.41
16:u:32:ILE:HG13	16:u:46:ALA:HB1	2.02	0.41
18:x:15:LEU:HD21	18:x:19:VAL:HG21	1.98	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.87	0.41
4:D:103:ARG:O	4:D:104:TRP:C	2.64	0.41
11:L:14:ARG:HH22	26:l:101:SQD:H3	1.86	0.41
13:O:189:ARG:NH2	35:O:305:HOH:O	2.52	0.41
13:O:215:PHE:CD1	13:O:215:PHE:C	2.98	0.41
23:Y:101:BCR:H361	23:Y:101:BCR:H20C	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:347:ARG:O	2:b:397:VAL:HA	2.21	0.41
28:d:402:STE:H61	28:h:704:STE:H71	2.03	0.41
23:B:718:BCR:H15C	23:B:718:BCR:H351	1.82	0.41
3:C:279:LEU:CD1	22:C:510:CLA:HED2	2.50	0.41
3:C:315:MET:HE1	3:C:369:LEU:CD1	2.50	0.41
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.90	0.41
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.03	0.41
13:O:111:ALA:HA	2:b:76:SER:O	2.21	0.41
16:U:36:ILE:O	16:U:36:ILE:HG22	2.20	0.41
19:Y:42:ARG:HH12	20:Z:31:GLN:NE2	2.19	0.41
2:b:161:LEU:HD23	2:b:161:LEU:HA	1.82	0.41
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.55	0.41
4:d:239:GLN:HB2	4:d:241:GLU:OE1	2.21	0.41
2:B:37:MET:O	2:B:41:GLU:HG3	2.20	0.41
2:B:348:ASN:OD1	2:B:348:ASN:C	2.64	0.41
2:B:464:PHE:CZ	31:B:722:LHG:H252	2.56	0.41
22:B:704:CLA:H42	22:B:705:CLA:H42	2.03	0.41
17:V:19:ILE:HD13	17:V:19:ILE:HG21	1.82	0.41
3:c:117:VAL:HG11	28:c:521:STE:H132	2.03	0.41
22:c:506:CLA:HHC	22:c:506:CLA:HBB1	2.02	0.41
14:r:4:ARG:HA	14:r:7:VAL:HG22	2.03	0.41
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.56	0.40
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.02	0.40
23:B:719:BCR:H11C	23:B:719:BCR:H341	1.95	0.40
22:C:506:CLA:HBD	22:C:506:CLA:HAA1	2.03	0.40
4:D:60:THR:O	5:E:65:LEU:HD11	2.21	0.40
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.03	0.40
7:H:44:ILE:HG22	7:H:48:ILE:CD1	2.50	0.40
13:O:93:LEU:O	13:O:128:SER:HA	2.21	0.40
2:b:317:ASN:HA	2:b:330:MET:CE	2.51	0.40
2:b:398:THR:CG2	2:b:412:THR:HG22	2.51	0.40
5:e:22:ILE:HG23	14:r:19:ALA:CB	2.51	0.40
10:k:38:VAL:CG2	23:k:101:BCR:H19C	2.51	0.40
17:v:92:HIS:ND1	17:v:93:PRO:HD2	2.37	0.40
2:B:135:LEU:N	2:B:136:PRO:CD	2.84	0.40
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.51	0.40
14:R:34:LEU:O	14:R:35:LEU:O	2.39	0.40
4:d:85:MET:HE1	5:e:72:ALA:HB2	2.02	0.40
5:e:25:ILE:HD12	5:e:25:ILE:N	2.36	0.40
17:v:122:GLU:N	17:v:123:PRO:CD	2.84	0.40
19:y:41:VAL:HG12	19:y:42:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:SD	33:D:408:PHO:HED3	2.60	0.40
27:A:411:DGD:HBN1	8:I:7:THR:HG21	2.04	0.40
3:C:281:MET:HG3	30:C:516:LMG:H391	2.03	0.40
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.03	0.40
9:j:10:LEU:HA	9:j:13:VAL:HG22	2.03	0.40
2:B:35:GLY:O	2:B:39:LEU:HG	2.20	0.40
22:C:514:CLA:C4B	23:C:524:BCR:H383	2.51	0.40
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.03	0.40
15:T:14:ILE:O	15:T:17:PHE:HB2	2.21	0.40
2:b:157:HIS:HA	2:b:163:GLY:HA3	2.04	0.40
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.56	0.40
4:d:330:ALA:HB3	4:d:331:PRO:HD3	2.03	0.40
7:h:63:LYS:O	7:h:64:ALA:CB	2.69	0.40
2:B:86:ILE:CG1	2:B:87:ASP:N	2.84	0.40
2:B:451:PHE:CD1	2:B:451:PHE:C	2.99	0.40
22:C:513:CLA:O2A	22:C:513:CLA:H43	2.21	0.40
22:C:514:CLA:H92	22:C:514:CLA:C4	2.51	0.40
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.22	0.40
30:D:409:LMG:O3	9:J:32:ALA:HA	2.21	0.40
1:a:161[A]:TYR:HB3	1:a:162[A]:PRO:HD3	2.03	0.40
3:c:180:MET:HE1	30:c:522:LMG:HC72	2.03	0.40
6:f:14:PRO:O	6:f:15:ILE:HD13	2.21	0.40
23:k:102:BCR:H20C	23:k:102:BCR:H361	1.94	0.40
13:o:84:GLU:OE1	13:o:86:LYS:NZ	2.42	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:462:GLU:OE1	7:H:3:ARG:NH2[4_557]	2.07	0.13
35:B:1027:HOH:O	35:C:762:HOH:O[1_455]	2.14	0.06
3:C:462:GLU:OE1	7:H:3:ARG:CZ[4_557]	2.17	0.03
3:C:462:GLU:OE1	7:H:3:ARG:NH1[4_557]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	36
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	490 (97%)	12 (2%)	1 (0%)	43	44
3	C	441/461 (96%)	428 (97%)	12 (3%)	1 (0%)	43	44
3	c	451/461 (98%)	433 (96%)	16 (4%)	2 (0%)	30	28
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	4
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	7
13	o	242/272 (89%)	227 (94%)	13 (5%)	2 (1%)	16	12
14	R	32/41 (78%)	25 (78%)	6 (19%)	1 (3%)	3	1
14	r	29/41 (71%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/32 (88%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	8
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	15
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	1 (4%)	2 (7%)	1	0
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
All	All	5238/5700 (92%)	5054 (96%)	164 (3%)	20 (0%)	30	28

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
14	r	31	VAL
16	u	53	ALA
2	b	294	SER
3	c	416	SER
19	Y	43	ARG
13	o	23	ASP
19	y	41	VAL
13	O	138	THR
3	c	25	ASN
7	H	12	ARG
19	y	42	ARG
13	o	56	PRO
14	R	24	LEU
1	a	259	ILE
20	z	61	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	89
1	a	269/280 (96%)	268 (100%)	1 (0%)	84	89
2	B	407/407 (100%)	407 (100%)	0	100	100
2	b	402/407 (99%)	401 (100%)	1 (0%)	87	93
3	C	345/362 (95%)	345 (100%)	0	100	100
3	c	354/362 (98%)	354 (100%)	0	100	100
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	277/283 (98%)	277 (100%)	0	100	100
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	43
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	58
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	37
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	42
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	205 (100%)	1 (0%)	81	88
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	28/33 (85%)	28 (100%)	0	100	100
14	r	23/33 (70%)	21 (91%)	2 (9%)	9	7
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	83 (99%)	1 (1%)	63	72
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	116 (99%)	1 (1%)	70	78
17	v	117/138 (85%)	116 (99%)	1 (1%)	70	78
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	22 (100%)	0	100	100
20	Z	52/52 (100%)	51 (98%)	1 (2%)	50	58
20	z	51/52 (98%)	51 (100%)	0	100	100
All	All	4326/4654 (93%)	4308 (100%)	18 (0%)	84	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
13	O	107	THR
16	U	61	VAL
17	V	7	VAL
20	Z	15	LEU
1	a	271	LEU
2	b	246	PHE
7	h	7	LEU
10	k	35	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
14	r	10	LEU
14	r	24	LEU
17	v	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	165[A]	GLN
1	A	315	ASN
2	B	14	ASN
2	B	26	HIS
3	C	53	HIS
3	C	56	HIS
3	C	385	GLN
3	C	415	ASN
4	D	186	GLN
4	D	350	ASN
5	E	82	GLN
12	M	32	GLN
13	O	155	ASN
1	a	165[A]	GLN
2	b	157	HIS
2	b	274	GLN
2	b	338	GLN
2	b	497	GLN
3	c	53	HIS
3	c	56	HIS
3	c	311	GLN
3	c	378	ASN
3	c	418	ASN
4	d	250	ASN
7	h	59	ASN
13	o	80	GLN
13	o	124	ASN
14	r	30	GLN
16	u	78	ASN
17	v	25	GLN
17	v	118	HIS
18	x	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.01	1 (12%)	8,9,11	1.94	3 (37%)
15	FME	t	1	15	8,9,10	1.53	1 (12%)	8,9,11	1.03	1 (12%)
15	FME	T	1	15	8,9,10	1.19	1 (12%)	8,9,11	1.50	2 (25%)
8	FME	I	1	8	8,9,10	0.81	0	8,9,11	1.07	0
12	FME	m	1	12	8,9,10	0.96	0	8,9,11	1.56	2 (25%)
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	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
8	FME	i	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
15	FME	T	1	15	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.04	1.42	1.46
15	T	1	FME	CB-CA	2.45	1.58	1.53
8	i	1	FME	CA-N	-2.08	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.90	116.83	122.82
15	T	1	FME	C-CA-N	3.15	115.58	109.50
15	t	1	FME	CB-CA-N	2.63	115.30	110.52
12	m	1	FME	CA-N-CN	-2.39	119.14	122.82
12	m	1	FME	C-CA-N	-2.38	104.90	109.50
8	i	1	FME	C-CA-N	2.24	113.82	109.50
8	i	1	FME	O1-CN-N	-2.21	119.61	125.32
15	T	1	FME	O1-CN-N	-2.17	119.71	125.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 192 ligands modelled in this entry, 6 are monoatomic - leaving 186 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
32	BCT	a	409	21	3,3,3	0.93	0	2,3,3	3.97	2 (100%)
33	PHO	D	408	-	58,69,69	1.95	13 (22%)	55,99,99	1.80	12 (21%)
31	LHG	E	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.26	6 (11%)
28	STE	t	702	-	13,13,19	0.57	0	13,13,19	1.33	2 (15%)
22	CLA	b	605	2	69,73,73	1.20	7 (10%)	82,113,113	1.51	13 (15%)
22	CLA	b	606	2	69,73,73	1.26	7 (10%)	82,113,113	1.61	15 (18%)
34	HEC	V	201	17	50,50,50	1.54	5 (10%)	68,82,82	1.38	8 (11%)
22	CLA	c	511	3	69,73,73	1.16	6 (8%)	82,113,113	1.53	12 (14%)
28	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.35	2 (12%)
22	CLA	h	701	35	69,73,73	1.39	9 (13%)	82,113,113	1.41	8 (9%)
27	DGD	H	102	-	63,63,67	1.52	11 (17%)	77,77,81	1.54	16 (20%)
23	BCR	d	405	-	41,41,41	1.30	5 (12%)	56,56,56	1.40	12 (21%)
28	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.53	0
28	STE	B	724	-	11,11,19	0.80	0	11,11,19	1.19	2 (18%)
28	STE	X	101	-	19,19,19	0.56	0	19,19,19	1.26	3 (15%)
28	STE	m	102	-	11,11,19	0.78	0	11,11,19	1.56	2 (18%)
22	CLA	b	604	2	69,73,73	1.31	9 (13%)	82,113,113	1.68	10 (12%)
22	CLA	C	503	3	69,73,73	1.18	8 (11%)	82,113,113	1.24	8 (9%)
22	CLA	b	612	2	69,73,73	1.11	5 (7%)	82,113,113	1.45	9 (10%)
22	CLA	c	505	35	64,68,73	1.33	10 (15%)	76,107,113	1.50	13 (17%)
23	BCR	B	718	-	41,41,41	1.37	5 (12%)	56,56,56	1.61	11 (19%)
26	SQD	D	410	-	34,36,54	1.09	3 (8%)	42,45,65	1.96	11 (26%)
28	STE	B	725	-	17,17,19	0.75	0	17,17,19	0.85	0
28	STE	A	412	-	4,4,19	0.52	0	3,3,19	0.41	0
27	DGD	A	411	-	67,67,67	1.47	9 (13%)	81,81,81	1.69	18 (22%)
33	PHO	a	404	-	58,69,69	2.08	10 (17%)	55,99,99	1.74	14 (25%)
22	CLA	c	509	3	68,72,73	1.26	9 (13%)	80,111,113	1.74	17 (21%)
28	STE	M	103	-	9,9,19	0.51	0	8,8,19	0.55	0
28	STE	a	416	-	11,11,19	0.90	1 (9%)	11,11,19	0.88	0
28	STE	J	101	-	11,11,19	0.66	0	11,11,19	1.54	2 (18%)
22	CLA	B	705	2	69,73,73	1.36	9 (13%)	82,113,113	1.62	12 (14%)
26	SQD	a	414	-	35,35,54	1.18	2 (5%)	37,37,65	1.40	5 (13%)
28	STE	C	523	-	11,11,19	0.81	0	11,11,19	1.03	1 (9%)
22	CLA	b	611	2	69,73,73	1.21	11 (15%)	82,113,113	1.52	13 (15%)
23	BCR	k	102	-	41,41,41	1.25	6 (14%)	56,56,56	1.18	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	C	521	-	11,11,19	0.91	0	11,11,19	1.46	3 (27%)
22	CLA	B	713	2	69,73,73	1.15	7 (10%)	82,113,113	1.48	12 (14%)
22	CLA	B	710	35	69,73,73	1.36	10 (14%)	82,113,113	1.51	12 (14%)
22	CLA	a	405	1	69,73,73	1.43	12 (17%)	82,113,113	1.34	7 (8%)
22	CLA	b	614	2	69,73,73	1.30	11 (15%)	82,113,113	1.53	8 (9%)
25	PL9	A	408	-	55,55,55	1.16	2 (3%)	68,69,69	1.64	15 (22%)
28	STE	Z	101	-	7,7,19	0.38	0	6,6,19	0.47	0
26	SQD	A	409	-	50,52,54	1.05	5 (10%)	60,63,65	2.09	16 (26%)
29	OEX	a	419[A]	3,35,1	0,14,14	-	-	-	-	-
22	CLA	B	708	2	69,73,73	1.31	10 (14%)	82,113,113	1.72	15 (18%)
25	PL9	D	406	-	55,55,55	1.49	8 (14%)	68,69,69	1.71	15 (22%)
34	HEC	v	201	17	50,50,50	1.83	6 (12%)	68,82,82	1.38	5 (7%)
22	CLA	c	503	3	69,73,73	1.20	9 (13%)	82,113,113	1.43	8 (9%)
22	CLA	B	714	2	69,73,73	1.19	12 (17%)	82,113,113	1.28	11 (13%)
23	BCR	C	501	-	41,41,41	1.28	5 (12%)	56,56,56	1.15	3 (5%)
22	CLA	C	511	-	69,73,73	1.25	9 (13%)	82,113,113	1.17	6 (7%)
31	LHG	l	102	-	48,48,48	0.86	2 (4%)	51,54,54	1.16	6 (11%)
23	BCR	H	101	-	41,41,41	1.29	6 (14%)	56,56,56	1.40	10 (17%)
22	CLA	b	615	2	69,73,73	1.25	9 (13%)	82,113,113	1.35	10 (12%)
25	PL9	d	406	-	55,55,55	1.61	8 (14%)	68,69,69	1.74	16 (23%)
28	STE	M	102	-	14,14,19	0.75	0	14,14,19	1.02	0
30	LMG	D	409	-	51,51,55	1.29	5 (9%)	59,59,63	1.37	7 (11%)
28	STE	B	720	-	16,16,19	0.66	0	16,16,19	1.39	2 (12%)
22	CLA	D	403	35	69,73,73	1.30	8 (11%)	82,113,113	1.34	8 (9%)
30	LMG	C	516	-	48,48,55	1.26	7 (14%)	56,56,63	1.45	5 (8%)
28	STE	I	101	-	14,14,19	0.66	0	13,13,19	0.35	0
22	CLA	c	510	3	69,73,73	1.22	6 (8%)	82,113,113	1.80	8 (9%)
26	SQD	a	412	-	52,54,54	1.01	5 (9%)	62,65,65	1.95	13 (20%)
28	STE	b	601	-	15,15,19	0.49	0	14,14,19	0.67	0
28	STE	c	521	-	19,19,19	0.71	0	19,19,19	0.94	1 (5%)
28	STE	d	402	-	19,19,19	0.53	0	19,19,19	1.14	1 (5%)
22	CLA	C	507	3	69,73,73	1.20	9 (13%)	82,113,113	1.36	11 (13%)
27	DGD	C	517	-	63,63,67	1.34	7 (11%)	77,77,81	1.36	11 (14%)
22	CLA	B	709	2	69,73,73	1.22	7 (10%)	82,113,113	1.36	7 (8%)
28	STE	E	103	-	6,6,19	0.43	0	5,5,19	0.52	0
29	OEX	A	413[A]	3,35,1	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEC	F	101	6,5	50,50,50	1.69	7 (14%)	68,82,82	1.48	9 (13%)
23	BCR	B	719	-	41,41,41	1.45	8 (19%)	56,56,56	1.55	11 (19%)
22	CLA	A	403	35	69,73,73	1.28	6 (8%)	82,113,113	1.50	16 (19%)
23	BCR	Y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	5 (8%)
30	LMG	M	101	-	51,51,55	1.11	3 (5%)	59,59,63	1.50	11 (18%)
22	CLA	d	401	35	69,73,73	1.27	7 (10%)	82,113,113	1.53	14 (17%)
28	STE	h	704	-	13,13,19	0.45	0	12,12,19	0.62	0
25	PL9	a	410	-	55,55,55	0.93	3 (5%)	68,69,69	1.70	15 (22%)
28	STE	a	417	-	14,14,19	0.45	0	13,13,19	0.71	0
31	LHG	L	101	-	48,48,48	0.98	4 (8%)	51,54,54	1.35	6 (11%)
22	CLA	A	402	1	69,73,73	1.31	10 (14%)	82,113,113	1.32	9 (10%)
28	STE	H	104	-	7,7,19	0.43	0	6,6,19	0.55	0
28	STE	c	501	-	11,11,19	0.80	0	11,11,19	1.06	1 (9%)
28	STE	b	624	-	19,19,19	0.79	0	19,19,19	0.96	1 (5%)
30	LMG	d	410	-	44,44,55	1.43	6 (13%)	52,52,63	1.56	8 (15%)
31	LHG	D	412	-	46,46,48	1.30	6 (13%)	49,52,54	1.35	4 (8%)
22	CLA	c	513	3	69,73,73	1.22	11 (15%)	82,113,113	1.52	11 (13%)
22	CLA	a	403	35	69,73,73	1.31	9 (13%)	82,113,113	1.60	11 (13%)
23	BCR	C	524	-	41,41,41	1.34	4 (9%)	56,56,56	1.58	15 (26%)
23	BCR	c	515	-	41,41,41	1.43	5 (12%)	56,56,56	1.31	8 (14%)
33	PHO	D	407	-	58,69,69	1.73	10 (17%)	55,99,99	1.65	12 (21%)
27	DGD	c	517	-	63,63,67	1.36	10 (15%)	77,77,81	1.45	10 (12%)
26	SQD	l	101	-	47,49,54	1.10	3 (6%)	57,60,65	2.39	15 (26%)
22	CLA	C	502	3	69,73,73	1.19	8 (11%)	82,113,113	1.48	10 (12%)
27	DGD	c	519	-	63,63,67	1.32	8 (12%)	77,77,81	1.57	16 (20%)
22	CLA	C	514	3	69,73,73	1.27	8 (11%)	82,113,113	1.57	10 (12%)
34	HEC	f	101	6,5	50,50,50	1.76	7 (14%)	68,82,82	1.63	12 (17%)
23	BCR	B	717	-	41,41,41	1.38	4 (9%)	56,56,56	1.32	5 (8%)
22	CLA	A	404	1	58,62,73	1.36	6 (10%)	68,99,113	1.66	11 (16%)
28	STE	a	415	-	9,9,19	0.57	0	8,8,19	0.38	0
22	CLA	b	610	35	69,73,73	1.31	10 (14%)	82,113,113	1.48	12 (14%)
22	CLA	C	510	3	69,73,73	1.33	12 (17%)	82,113,113	1.57	17 (20%)
31	LHG	D	411	-	48,48,48	1.05	3 (6%)	51,54,54	1.27	6 (11%)
28	STE	x	101	-	19,19,19	0.79	0	19,19,19	0.77	1 (5%)
31	LHG	B	722	-	48,48,48	1.13	3 (6%)	51,54,54	1.45	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	b	623	-	15,15,19	0.88	1 (6%)	15,15,19	0.91	1 (6%)
27	DGD	h	703	-	63,63,67	1.30	9 (14%)	77,77,81	1.69	17 (22%)
22	CLA	B	727	35	69,73,73	1.43	13 (18%)	82,113,113	1.38	10 (12%)
33	PHO	d	407	-	58,69,69	2.09	12 (20%)	55,99,99	1.71	11 (20%)
22	CLA	D	404	4	69,73,73	1.35	14 (20%)	82,113,113	1.61	10 (12%)
22	CLA	B	706	2	69,73,73	1.15	8 (11%)	82,113,113	1.51	7 (8%)
22	CLA	B	712	2	69,73,73	1.18	8 (11%)	82,113,113	1.54	11 (13%)
22	CLA	C	504	3	69,73,73	1.30	10 (14%)	82,113,113	1.47	16 (19%)
30	LMG	c	522	-	48,48,55	1.51	6 (12%)	56,56,63	1.31	11 (19%)
22	CLA	b	609	-	69,73,73	1.19	7 (10%)	82,113,113	1.53	13 (15%)
23	BCR	a	406	-	41,41,41	1.35	4 (9%)	56,56,56	1.57	13 (23%)
22	CLA	C	512	3	69,73,73	1.27	9 (13%)	82,113,113	1.08	4 (4%)
22	CLA	C	505	35	63,67,73	1.29	7 (11%)	74,105,113	1.30	7 (9%)
28	STE	C	522	-	15,15,19	0.47	0	14,14,19	0.78	0
22	CLA	b	608	2	69,73,73	1.28	11 (15%)	82,113,113	1.61	12 (14%)
23	BCR	k	101	-	41,41,41	1.26	4 (9%)	56,56,56	1.17	6 (10%)
22	CLA	B	707	35	69,73,73	1.41	13 (18%)	82,113,113	1.34	7 (8%)
28	STE	E	102	-	11,11,19	0.94	0	11,11,19	0.77	0
23	BCR	A	405	-	41,41,41	1.37	3 (7%)	56,56,56	1.55	13 (23%)
22	CLA	B	716	2	64,68,73	1.27	8 (12%)	76,107,113	1.35	11 (14%)
26	SQD	f	102	-	39,41,54	1.19	4 (10%)	49,52,65	1.74	11 (22%)
30	LMG	b	620	-	51,51,55	1.19	5 (9%)	59,59,63	1.58	11 (18%)
22	CLA	C	508	35	69,73,73	1.24	12 (17%)	82,113,113	1.54	10 (12%)
22	CLA	c	502	3	69,73,73	1.18	9 (13%)	82,113,113	1.56	10 (12%)
30	LMG	B	721	-	26,26,55	0.84	2 (7%)	26,26,63	1.35	2 (7%)
22	CLA	c	514	3	69,73,73	1.15	9 (13%)	82,113,113	1.53	10 (12%)
28	STE	B	701	-	11,11,19	1.04	0	11,11,19	0.97	1 (9%)
23	BCR	T	701	-	41,41,41	1.27	6 (14%)	56,56,56	1.39	8 (14%)
22	CLA	c	508	35	69,73,73	1.21	8 (11%)	82,113,113	1.50	10 (12%)
31	LHG	a	413	-	41,41,48	0.86	1 (2%)	44,47,54	1.27	3 (6%)
26	SQD	B	723	-	52,54,54	1.00	3 (5%)	62,65,65	1.88	12 (19%)
30	LMG	a	418	-	55,55,55	1.50	8 (14%)	63,63,63	1.29	4 (6%)
27	DGD	C	519	-	63,63,67	1.07	4 (6%)	77,77,81	1.44	10 (12%)
22	CLA	B	704	2	69,73,73	1.18	7 (10%)	82,113,113	1.58	15 (18%)
22	CLA	C	506	3	69,73,73	1.18	9 (13%)	82,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	b	621	-	19,19,19	0.61	0	19,19,19	0.86	1 (5%)
22	CLA	c	507	3	69,73,73	1.22	10 (14%)	82,113,113	1.53	10 (12%)
31	LHG	a	411	-	48,48,48	0.91	1 (2%)	51,54,54	1.47	6 (11%)
22	CLA	B	702	2	69,73,73	1.39	10 (14%)	82,113,113	1.48	15 (18%)
23	BCR	b	618	-	41,41,41	1.42	4 (9%)	56,56,56	1.34	8 (14%)
30	LMG	c	523	-	49,49,55	1.16	5 (10%)	57,57,63	1.34	9 (15%)
22	CLA	d	403	4	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
22	CLA	c	504	3	69,73,73	1.13	6 (8%)	82,113,113	1.69	10 (12%)
28	STE	m	101	-	17,17,19	0.50	0	16,16,19	0.63	0
22	CLA	B	715	2	69,73,73	1.37	10 (14%)	82,113,113	1.40	12 (14%)
30	LMG	C	520	-	48,48,55	1.27	6 (12%)	56,56,63	1.47	10 (17%)
27	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.51	14 (18%)
30	LMG	D	413	-	31,31,55	1.69	4 (12%)	33,33,63	1.09	1 (3%)
22	CLA	B	703	2	69,73,73	1.16	7 (10%)	82,113,113	1.55	9 (10%)
27	DGD	C	518	-	63,63,67	1.50	11 (17%)	77,77,81	1.61	14 (18%)
22	CLA	a	402	1	69,73,73	1.28	9 (13%)	82,113,113	1.53	17 (20%)
22	CLA	c	512	3	69,73,73	1.35	11 (15%)	82,113,113	1.33	7 (8%)
31	LHG	d	409	-	38,38,48	1.07	3 (7%)	41,44,54	1.14	2 (4%)
23	BCR	b	619	-	41,41,41	1.33	4 (9%)	56,56,56	1.41	10 (17%)
23	BCR	t	701	-	41,41,41	1.23	4 (9%)	56,56,56	1.43	8 (14%)
22	CLA	b	616	2	64,68,73	1.23	9 (14%)	76,107,113	1.41	9 (11%)
23	BCR	D	405	-	41,41,41	1.32	5 (12%)	56,56,56	1.31	5 (8%)
23	BCR	h	702	-	41,41,41	1.24	4 (9%)	56,56,56	1.28	7 (12%)
22	CLA	C	513	3	69,73,73	1.26	11 (15%)	82,113,113	1.49	14 (17%)
31	LHG	d	408	-	48,48,48	0.78	0	51,54,54	1.17	5 (9%)
26	SQD	A	410	-	38,38,54	1.03	3 (7%)	40,40,65	1.28	4 (10%)
22	CLA	B	711	2	69,73,73	1.28	8 (11%)	82,113,113	1.33	12 (14%)
22	CLA	D	402	4	69,73,73	1.27	9 (13%)	82,113,113	1.39	11 (13%)
22	CLA	b	602	2	69,73,73	1.19	7 (10%)	82,113,113	1.71	16 (19%)
28	STE	B	726	-	15,15,19	0.48	0	14,14,19	0.58	0
32	BCT	D	401	21	3,3,3	0.81	0	2,3,3	5.42	2 (100%)
23	BCR	c	516	-	41,41,41	1.46	4 (9%)	56,56,56	1.59	14 (25%)
22	CLA	d	404	4	69,73,73	1.29	10 (14%)	82,113,113	1.34	9 (10%)
30	LMG	b	622	-	55,55,55	1.43	8 (14%)	63,63,63	1.55	12 (19%)
22	CLA	c	506	3	69,73,73	1.17	9 (13%)	82,113,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	b	617	-	41,41,41	1.39	4 (9%)	56,56,56	1.61	14 (25%)
22	CLA	C	509	3	69,73,73	1.24	9 (13%)	82,113,113	1.36	9 (10%)
30	LMG	c	520	-	37,37,55	1.45	6 (16%)	45,45,63	1.45	6 (13%)
23	BCR	C	515	-	41,41,41	1.48	8 (19%)	56,56,56	1.34	6 (10%)
28	STE	T	702	-	14,14,19	0.48	0	13,13,19	0.53	0
22	CLA	b	603	2	69,73,73	1.27	9 (13%)	82,113,113	1.56	15 (18%)
28	STE	b	625	-	9,9,19	0.59	0	8,8,19	0.33	0
22	CLA	b	607	35	69,73,73	1.27	10 (14%)	82,113,113	1.44	13 (15%)
22	CLA	b	613	2	69,73,73	1.31	12 (17%)	82,113,113	1.56	14 (17%)
28	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.60	3 (27%)

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
33	PHO	D	408	-	-	2/37/103/103	0/5/6/6
31	LHG	E	101	-	-	27/53/53/53	-
28	STE	t	702	-	-	4/11/11/17	-
22	CLA	b	605	2	-	13/39/115/115	-
22	CLA	b	606	2	-	8/39/115/115	-
34	HEC	V	201	17	1/1/3/7	6/14/54/54	-
22	CLA	c	511	3	-	9/39/115/115	-
28	STE	d	411	-	-	4/14/14/17	-
22	CLA	h	701	35	-	11/39/115/115	-
27	DGD	H	102	-	-	18/51/91/95	0/2/2/2
23	BCR	d	405	-	-	10/29/63/63	0/2/2/2
28	STE	H	103	-	-	6/15/15/17	-
28	STE	B	724	-	-	4/9/9/17	-
28	STE	X	101	-	-	9/17/17/17	-
28	STE	m	102	-	-	2/9/9/17	-
22	CLA	b	604	2	-	8/39/115/115	-
22	CLA	C	503	3	-	9/39/115/115	-
22	CLA	b	612	2	-	4/39/115/115	-
22	CLA	c	505	35	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B	718	-	-	7/29/63/63	0/2/2/2
26	SQD	D	410	-	-	7/28/48/69	0/1/1/1
28	STE	B	725	-	-	6/15/15/17	-
28	STE	A	412	-	-	1/2/2/17	-
27	DGD	A	411	-	-	25/55/95/95	0/2/2/2
33	PHO	a	404	-	-	5/37/103/103	0/5/6/6
22	CLA	c	509	3	-	5/38/114/115	-
28	STE	M	103	-	-	4/7/7/17	-
28	STE	a	416	-	-	4/9/9/17	-
28	STE	J	101	-	-	3/9/9/17	-
22	CLA	B	705	2	-	8/39/115/115	-
26	SQD	a	414	-	-	19/37/37/69	-
28	STE	C	523	-	-	6/9/9/17	-
22	CLA	b	611	2	-	7/39/115/115	-
23	BCR	k	102	-	-	4/29/63/63	0/2/2/2
28	STE	C	521	-	-	2/9/9/17	-
22	CLA	B	713	2	-	13/39/115/115	-
22	CLA	B	710	35	-	5/39/115/115	-
22	CLA	a	405	1	-	11/39/115/115	-
22	CLA	b	614	2	-	13/39/115/115	-
25	PL9	A	408	-	-	25/53/73/73	0/1/1/1
28	STE	Z	101	-	-	3/5/5/17	-
26	SQD	A	409	-	-	22/47/67/69	0/1/1/1
34	HEC	v	201	17	1/1/3/7	4/14/54/54	-
22	CLA	B	708	2	-	2/39/115/115	-
25	PL9	D	406	-	-	12/53/73/73	0/1/1/1
22	CLA	c	503	3	-	4/39/115/115	-
22	CLA	B	714	2	-	10/39/115/115	-
23	BCR	C	501	-	-	13/29/63/63	0/2/2/2
22	CLA	C	511	-	-	10/39/115/115	-
31	LHG	l	102	-	-	24/53/53/53	-
23	BCR	H	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	615	2	-	10/39/115/115	-
25	PL9	d	406	-	-	18/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	M	102	-	-	5/12/12/17	-
30	LMG	D	409	-	-	16/46/66/70	0/1/1/1
28	STE	B	720	-	-	9/14/14/17	-
22	CLA	D	403	35	-	6/39/115/115	-
30	LMG	C	516	-	-	18/43/63/70	0/1/1/1
28	STE	I	101	-	-	4/12/12/17	-
22	CLA	c	510	3	-	10/39/115/115	-
26	SQD	a	412	-	-	24/49/69/69	0/1/1/1
28	STE	b	601	-	-	8/13/13/17	-
28	STE	c	521	-	-	7/17/17/17	-
28	STE	d	402	-	-	9/17/17/17	-
22	CLA	C	507	3	-	8/39/115/115	-
27	DGD	C	517	-	-	21/51/91/95	0/2/2/2
34	HEC	F	101	6,5	1/1/3/7	6/14/54/54	-
22	CLA	B	709	2	-	3/39/115/115	-
28	STE	E	103	-	-	1/4/4/17	-
23	BCR	B	719	-	-	1/29/63/63	0/2/2/2
22	CLA	A	403	35	-	10/39/115/115	-
23	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
30	LMG	M	101	-	-	24/46/66/70	0/1/1/1
22	CLA	d	401	35	-	5/39/115/115	-
28	STE	h	704	-	-	6/11/11/17	-
25	PL9	a	410	-	-	20/53/73/73	0/1/1/1
28	STE	a	417	-	-	4/12/12/17	-
31	LHG	L	101	-	-	20/53/53/53	-
22	CLA	A	402	1	-	7/39/115/115	-
28	STE	H	104	-	-	3/5/5/17	-
28	STE	c	501	-	-	2/9/9/17	-
28	STE	b	624	-	-	8/17/17/17	-
30	LMG	d	410	-	-	12/39/59/70	0/1/1/1
31	LHG	D	412	-	-	24/51/51/53	-
22	CLA	c	513	3	-	21/39/115/115	-
22	CLA	a	403	35	-	1/39/115/115	-
23	BCR	C	524	-	-	8/29/63/63	0/2/2/2
23	BCR	c	515	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PHO	D	407	-	-	6/37/103/103	0/5/6/6
27	DGD	c	517	-	-	21/51/91/95	0/2/2/2
26	SQD	l	101	-	-	21/44/64/69	0/1/1/1
22	CLA	C	502	3	-	3/39/115/115	-
27	DGD	c	519	-	-	19/51/91/95	0/2/2/2
34	HEC	f	101	6,5	1/1/3/7	5/14/54/54	-
22	CLA	C	514	3	-	15/39/115/115	-
23	BCR	B	717	-	-	7/29/63/63	0/2/2/2
22	CLA	A	404	1	-	4/26/102/115	-
28	STE	a	415	-	-	4/7/7/17	-
22	CLA	b	610	35	-	4/39/115/115	-
22	CLA	C	510	3	-	13/39/115/115	-
31	LHG	D	411	-	-	17/53/53/53	-
28	STE	x	101	-	-	11/17/17/17	-
31	LHG	B	722	-	-	18/53/53/53	-
28	STE	b	623	-	-	11/13/13/17	-
27	DGD	h	703	-	-	15/51/91/95	0/2/2/2
22	CLA	B	727	35	-	13/39/115/115	-
33	PHO	d	407	-	-	5/37/103/103	0/5/6/6
22	CLA	D	404	4	-	7/39/115/115	-
22	CLA	B	706	2	-	6/39/115/115	-
22	CLA	B	712	2	-	9/39/115/115	-
22	CLA	C	504	3	-	8/39/115/115	-
30	LMG	c	522	-	-	25/43/63/70	0/1/1/1
22	CLA	b	609	-	-	7/39/115/115	-
23	BCR	a	406	-	-	3/29/63/63	0/2/2/2
22	CLA	C	512	3	-	3/39/115/115	-
22	CLA	C	505	35	-	4/32/108/115	-
28	STE	C	522	-	-	2/13/13/17	-
22	CLA	b	608	2	-	7/39/115/115	-
23	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	B	707	35	-	4/39/115/115	-
28	STE	E	102	-	-	5/9/9/17	-
23	BCR	A	405	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	716	2	-	10/33/109/115	-
26	SQD	f	102	-	-	14/36/56/69	0/1/1/1
30	LMG	b	620	-	-	15/46/66/70	0/1/1/1
22	CLA	C	508	35	-	9/39/115/115	-
22	CLA	c	502	3	-	3/39/115/115	-
30	LMG	B	721	-	-	12/22/22/70	-
22	CLA	c	514	3	-	8/39/115/115	-
28	STE	B	701	-	-	3/9/9/17	-
23	BCR	T	701	-	-	3/29/63/63	0/2/2/2
22	CLA	c	508	35	-	3/39/115/115	-
31	LHG	a	413	-	-	19/46/46/53	-
26	SQD	B	723	-	-	29/49/69/69	0/1/1/1
30	LMG	a	418	-	-	25/50/70/70	0/1/1/1
27	DGD	C	519	-	-	17/51/91/95	0/2/2/2
22	CLA	B	704	2	-	11/39/115/115	-
22	CLA	C	506	3	-	12/39/115/115	-
28	STE	b	621	-	-	10/17/17/17	-
22	CLA	c	507	3	-	13/39/115/115	-
31	LHG	a	411	-	-	25/53/53/53	-
22	CLA	B	702	2	-	8/39/115/115	-
23	BCR	b	618	-	-	1/29/63/63	0/2/2/2
30	LMG	c	523	-	-	20/44/64/70	0/1/1/1
22	CLA	d	403	4	-	10/39/115/115	-
22	CLA	c	504	3	-	8/39/115/115	-
28	STE	m	101	-	-	5/15/15/17	-
22	CLA	B	715	2	-	7/39/115/115	-
30	LMG	C	520	-	-	19/43/63/70	0/1/1/1
27	DGD	c	518	-	-	23/51/91/95	0/2/2/2
30	LMG	D	413	-	-	14/33/33/70	-
22	CLA	B	703	2	-	11/39/115/115	-
27	DGD	C	518	-	-	14/51/91/95	0/2/2/2
22	CLA	a	402	1	-	8/39/115/115	-
22	CLA	c	512	3	-	12/39/115/115	-
31	LHG	d	409	-	-	10/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	BCR	t	701	-	-	7/29/63/63	0/2/2/2
22	CLA	b	616	2	-	11/33/109/115	-
23	BCR	D	405	-	-	9/29/63/63	0/2/2/2
23	BCR	h	702	-	-	5/29/63/63	0/2/2/2
22	CLA	C	513	3	-	14/39/115/115	-
31	LHG	d	408	-	-	14/53/53/53	-
26	SQD	A	410	-	-	15/39/39/69	-
22	CLA	B	711	2	-	8/39/115/115	-
22	CLA	D	402	4	-	7/39/115/115	-
22	CLA	b	602	2	-	8/39/115/115	-
28	STE	B	726	-	-	5/13/13/17	-
23	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	CLA	d	404	4	-	9/39/115/115	-
30	LMG	b	622	-	-	22/50/70/70	0/1/1/1
22	CLA	c	506	3	-	11/39/115/115	-
23	BCR	b	617	-	-	10/29/63/63	0/2/2/2
22	CLA	C	509	3	-	5/39/115/115	-
30	LMG	c	520	-	-	12/31/51/70	0/1/1/1
23	BCR	C	515	-	-	7/29/63/63	0/2/2/2
28	STE	T	702	-	-	8/12/12/17	-
22	CLA	b	603	2	-	8/39/115/115	-
28	STE	b	625	-	-	4/7/7/17	-
22	CLA	b	607	35	-	16/39/115/115	-
22	CLA	b	613	2	-	5/39/115/115	-
28	STE	j	101	-	-	2/9/9/17	-

All (1032) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	407	PHO	C1B-C2B	9.97	1.50	1.39
33	a	404	PHO	C1B-C2B	8.14	1.48	1.39
33	D	408	PHO	C1B-C2B	8.14	1.48	1.39
34	f	101	HEC	C3D-C2D	7.19	1.52	1.36
33	D	408	PHO	C3B-C4B	7.18	1.48	1.41
34	v	201	HEC	C3D-C2D	7.14	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	407	PHO	C1B-C2B	7.09	1.47	1.39
34	F	101	HEC	C3D-C2D	6.94	1.51	1.36
30	D	413	LMG	C7-C8	6.86	1.67	1.51
33	d	407	PHO	C3B-C4B	6.86	1.48	1.41
27	A	411	DGD	O5D-C6D	-6.74	1.32	1.43
33	a	404	PHO	C3B-C4B	6.39	1.48	1.41
33	a	404	PHO	C1D-C2D	6.18	1.46	1.39
34	v	201	HEC	FE-NA	6.16	2.15	1.95
34	f	101	HEC	FE-NA	5.54	2.13	1.95
33	D	407	PHO	C3B-C4B	5.50	1.47	1.41
34	V	201	HEC	C3D-C2D	5.49	1.48	1.36
23	C	515	BCR	C1-C6	-5.42	1.46	1.53
23	c	515	BCR	C1-C6	-5.33	1.47	1.53
30	a	418	LMG	C4-C3	5.11	1.65	1.52
30	b	622	LMG	O1-C7	-5.09	1.34	1.43
22	A	403	CLA	C1D-ND	4.92	1.44	1.37
22	b	606	CLA	C1D-ND	4.84	1.44	1.37
25	d	406	PL9	C3-C4	-4.82	1.42	1.49
22	a	403	CLA	C1D-ND	4.82	1.44	1.37
27	c	519	DGD	C6D-C5D	4.74	1.65	1.51
30	d	410	LMG	O1-C7	-4.69	1.35	1.43
34	V	201	HEC	FE-ND	4.68	2.09	1.94
30	c	522	LMG	O1-C7	-4.65	1.35	1.43
25	d	406	PL9	C6-C1	-4.64	1.40	1.48
30	c	522	LMG	O1-C1	4.64	1.47	1.40
27	H	102	DGD	O5D-C1E	4.63	1.47	1.40
22	h	701	CLA	C1D-ND	4.61	1.43	1.37
22	B	702	CLA	C4B-NB	4.47	1.43	1.37
27	C	517	DGD	O5D-C6D	-4.47	1.36	1.43
27	C	518	DGD	C4D-C3D	4.46	1.63	1.52
23	A	405	BCR	C1-C6	-4.46	1.48	1.53
23	B	719	BCR	C1-C6	-4.37	1.48	1.53
23	b	618	BCR	C1-C6	-4.32	1.48	1.53
22	A	404	CLA	C1D-ND	4.32	1.43	1.37
22	D	403	CLA	MG-NB	-4.31	1.97	2.05
33	D	408	PHO	C4D-ND	-4.31	1.32	1.38
30	c	520	LMG	C7-C8	4.29	1.64	1.50
27	C	518	DGD	O5D-C6D	-4.29	1.36	1.43
23	b	618	BCR	C30-C25	-4.27	1.48	1.53
22	B	705	CLA	C1B-C2B	4.21	1.53	1.43
22	d	404	CLA	MG-NB	-4.20	1.97	2.05
22	a	405	CLA	C1C-NC	-4.19	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	523	LMG	C4-C5	4.19	1.62	1.53
23	C	524	BCR	C30-C25	-4.18	1.48	1.53
30	a	418	LMG	C4-C5	4.18	1.61	1.53
23	c	516	BCR	C30-C25	-4.15	1.48	1.53
25	d	406	PL9	C46-C44	-4.13	1.42	1.51
33	a	404	PHO	C3D-C4D	4.12	1.46	1.41
22	C	505	CLA	C1B-NB	-4.10	1.32	1.37
30	b	620	LMG	O7-C8	-4.10	1.37	1.46
22	c	510	CLA	C1D-ND	4.09	1.43	1.37
23	c	516	BCR	C1-C6	-4.08	1.48	1.53
22	B	705	CLA	C3B-C4B	4.06	1.54	1.42
22	B	707	CLA	MG-NB	-4.05	1.97	2.05
25	D	406	PL9	C52-C5	-4.05	1.42	1.50
22	D	404	CLA	MG-NB	-4.04	1.97	2.05
22	C	514	CLA	C1D-ND	4.03	1.43	1.37
22	B	727	CLA	C1B-C2B	4.01	1.52	1.43
23	B	717	BCR	C33-C5	-4.01	1.44	1.50
22	B	715	CLA	C4B-NB	4.00	1.43	1.37
33	d	407	PHO	CAC-C3C	-4.00	1.44	1.51
22	d	403	CLA	C1D-ND	4.00	1.43	1.37
27	c	517	DGD	C6D-C5D	3.99	1.63	1.51
22	B	710	CLA	C4B-NB	3.99	1.43	1.37
31	B	722	LHG	O7-C5	-3.97	1.37	1.46
22	b	614	CLA	C4B-NB	3.96	1.43	1.37
26	a	414	SQD	O47-C7	3.96	1.45	1.34
27	A	411	DGD	C3E-C2E	3.96	1.62	1.52
30	D	409	LMG	O1-C1	3.94	1.46	1.40
23	b	617	BCR	C1-C6	-3.92	1.48	1.53
22	C	504	CLA	C1D-ND	3.92	1.43	1.37
23	B	718	BCR	C30-C25	-3.91	1.48	1.53
23	H	101	BCR	C30-C25	-3.90	1.48	1.53
22	c	512	CLA	C4B-NB	3.90	1.43	1.37
22	A	404	CLA	MG-ND	-3.89	1.98	2.05
25	D	406	PL9	C6-C1	-3.89	1.42	1.48
31	D	411	LHG	P-O3	3.87	1.74	1.59
23	b	619	BCR	C30-C25	-3.84	1.48	1.53
22	c	510	CLA	C1B-C2B	3.84	1.52	1.43
23	b	617	BCR	C33-C5	-3.81	1.44	1.50
27	H	102	DGD	O5D-C6D	-3.80	1.37	1.43
22	h	701	CLA	C1B-C2B	3.80	1.52	1.43
22	C	502	CLA	C1B-NB	-3.79	1.32	1.37
22	C	510	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	MG-ND	-3.78	1.98	2.05
26	l	101	SQD	O48-C23	3.77	1.44	1.33
22	b	604	CLA	C1D-ND	3.77	1.42	1.37
27	C	517	DGD	O2E-C2E	-3.76	1.33	1.43
33	d	407	PHO	C1D-C2D	3.75	1.43	1.39
26	B	723	SQD	O47-C7	3.74	1.44	1.34
22	b	613	CLA	MG-NB	-3.73	1.98	2.05
22	B	708	CLA	C1D-ND	3.71	1.42	1.37
27	c	518	DGD	C6D-C5D	3.70	1.62	1.51
22	b	610	CLA	MG-NB	-3.68	1.98	2.05
22	a	402	CLA	C1B-NB	-3.67	1.33	1.37
30	d	410	LMG	C4-C5	3.66	1.60	1.53
23	k	101	BCR	C1-C6	-3.66	1.49	1.53
23	c	516	BCR	C33-C5	-3.65	1.45	1.50
25	A	408	PL9	C21-C19	3.65	1.58	1.51
22	a	405	CLA	C1B-C2B	3.64	1.51	1.43
22	B	711	CLA	C1B-NB	-3.64	1.33	1.37
34	F	101	HEC	FE-NB	3.64	2.06	1.94
22	a	405	CLA	MG-ND	-3.62	1.98	2.05
30	D	409	LMG	C4-C5	3.61	1.60	1.53
22	B	711	CLA	C1D-ND	3.60	1.42	1.37
22	d	401	CLA	C1B-C2B	3.60	1.51	1.43
22	B	708	CLA	C1D-C2D	3.59	1.52	1.45
22	b	616	CLA	C1D-ND	3.59	1.42	1.37
23	A	405	BCR	C33-C5	-3.59	1.45	1.50
22	b	612	CLA	MG-ND	-3.57	1.98	2.05
23	b	619	BCR	C1-C6	-3.56	1.49	1.53
22	B	707	CLA	C1D-ND	3.56	1.42	1.37
31	D	412	LHG	P-O6	3.55	1.73	1.59
26	f	102	SQD	O48-C23	3.55	1.43	1.33
27	c	519	DGD	C4E-C5E	-3.55	1.45	1.53
22	h	701	CLA	C4B-NB	3.54	1.42	1.37
27	C	518	DGD	C4E-C5E	3.53	1.60	1.53
27	h	703	DGD	O2D-C2D	-3.53	1.34	1.43
23	h	702	BCR	C1-C6	-3.53	1.49	1.53
22	C	511	CLA	C1D-ND	3.51	1.42	1.37
23	D	405	BCR	C1-C6	-3.50	1.49	1.53
25	D	406	PL9	C21-C19	-3.50	1.44	1.51
22	b	603	CLA	C1D-ND	3.48	1.42	1.37
33	a	404	PHO	CBD-CGD	-3.47	1.48	1.52
22	B	709	CLA	C1D-ND	3.47	1.42	1.37
30	C	520	LMG	O7-C8	-3.47	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	717	BCR	C1-C6	-3.46	1.49	1.53
22	c	512	CLA	CHC-C1C	3.46	1.45	1.38
26	l	101	SQD	O47-C7	3.46	1.44	1.34
22	c	512	CLA	C1D-ND	3.46	1.42	1.37
33	D	407	PHO	C4D-ND	-3.46	1.33	1.38
22	B	702	CLA	C1B-C2B	3.46	1.51	1.43
22	B	702	CLA	C1D-ND	3.45	1.42	1.37
30	b	622	LMG	C1-C2	3.45	1.62	1.52
22	b	614	CLA	CMC-C2C	-3.43	1.43	1.50
22	B	708	CLA	CMD-C2D	-3.43	1.43	1.50
30	C	516	LMG	O1-C7	-3.43	1.37	1.43
22	b	608	CLA	CMB-C2B	-3.42	1.43	1.50
31	B	722	LHG	C24-C23	3.42	1.60	1.50
22	B	727	CLA	CMC-C2C	-3.40	1.43	1.50
31	d	409	LHG	C6-C5	3.40	1.61	1.50
23	b	617	BCR	C30-C25	-3.38	1.49	1.53
22	B	716	CLA	MG-NB	-3.38	1.99	2.05
22	b	616	CLA	O2D-CED	-3.38	1.37	1.45
26	A	410	SQD	O48-C23	3.38	1.43	1.33
22	b	604	CLA	C4B-NB	3.37	1.42	1.37
26	D	410	SQD	O48-C23	3.37	1.43	1.33
30	C	520	LMG	O1-C7	-3.37	1.37	1.43
22	b	609	CLA	C1D-ND	3.37	1.42	1.37
33	a	404	PHO	C4D-CHA	3.37	1.44	1.39
31	a	411	LHG	O7-C5	-3.37	1.38	1.46
22	C	510	CLA	MG-NB	-3.37	1.99	2.05
23	d	405	BCR	C33-C5	-3.36	1.45	1.50
22	b	615	CLA	CMB-C2B	-3.36	1.43	1.50
22	c	508	CLA	MG-NB	-3.34	1.99	2.05
30	d	410	LMG	C7-C8	3.34	1.61	1.50
22	D	402	CLA	MG-ND	-3.34	1.99	2.05
26	a	412	SQD	O2-C2	-3.33	1.34	1.43
23	B	718	BCR	C33-C5	-3.33	1.45	1.50
23	t	701	BCR	C30-C25	-3.33	1.49	1.53
30	M	101	LMG	C7-C8	3.33	1.61	1.50
22	C	505	CLA	C4B-NB	3.32	1.42	1.37
25	d	406	PL9	C7-C3	3.31	1.55	1.51
27	c	519	DGD	O5D-C6D	-3.31	1.38	1.43
30	b	620	LMG	O1-C1	3.31	1.45	1.40
22	B	715	CLA	CMB-C2B	-3.30	1.44	1.50
22	B	709	CLA	C1B-C2B	3.30	1.50	1.43
26	A	409	SQD	O2-C2	-3.29	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	520	LMG	C4-C5	3.28	1.60	1.53
27	A	411	DGD	C4E-C5E	3.28	1.60	1.53
22	C	512	CLA	C1B-C2B	3.27	1.50	1.43
22	B	705	CLA	O2D-CED	-3.27	1.38	1.45
26	A	410	SQD	O47-C7	3.27	1.43	1.34
22	c	505	CLA	C1B-NB	-3.27	1.33	1.37
23	T	701	BCR	C1-C6	-3.27	1.49	1.53
23	a	406	BCR	C1-C6	-3.26	1.49	1.53
23	d	405	BCR	C30-C25	-3.25	1.49	1.53
27	C	519	DGD	O5D-C6D	-3.25	1.38	1.43
22	B	710	CLA	C1B-C2B	3.25	1.50	1.43
26	D	410	SQD	O2-C2	-3.24	1.34	1.43
22	B	706	CLA	C4B-NB	3.24	1.42	1.37
30	b	622	LMG	O7-C8	-3.23	1.39	1.46
22	B	711	CLA	CHC-C1C	3.23	1.44	1.38
27	C	518	DGD	C4D-C5D	3.23	1.59	1.53
31	d	409	LHG	P-O6	3.23	1.72	1.59
27	h	703	DGD	O5D-C6D	-3.22	1.38	1.43
22	b	610	CLA	C1D-ND	3.22	1.42	1.37
27	C	518	DGD	O3G-C3G	-3.22	1.38	1.43
22	B	703	CLA	C3B-C4B	3.21	1.52	1.42
23	c	515	BCR	C30-C25	-3.21	1.49	1.53
22	c	508	CLA	C1B-C2B	3.20	1.50	1.43
22	B	712	CLA	C1D-ND	3.20	1.42	1.37
22	C	512	CLA	CMB-C2B	-3.19	1.44	1.50
22	C	513	CLA	MG-ND	-3.19	1.99	2.05
22	D	402	CLA	CMD-C2D	-3.19	1.44	1.50
22	B	710	CLA	C3B-C4B	3.19	1.52	1.42
22	B	707	CLA	C3B-C4B	3.18	1.52	1.42
22	d	401	CLA	C1D-ND	3.18	1.42	1.37
23	C	501	BCR	C30-C25	-3.18	1.49	1.53
23	Y	101	BCR	C30-C25	-3.17	1.49	1.53
25	a	410	PL9	C53-C6	-3.16	1.44	1.50
26	l	101	SQD	O2-C2	-3.15	1.35	1.43
22	d	404	CLA	MG-ND	-3.15	1.99	2.05
30	D	409	LMG	C7-C8	3.15	1.60	1.50
30	C	516	LMG	C7-C8	3.15	1.60	1.50
22	D	404	CLA	C1D-ND	3.14	1.42	1.37
22	c	509	CLA	C1D-ND	3.14	1.42	1.37
22	B	715	CLA	C1D-ND	3.14	1.42	1.37
27	C	519	DGD	C6D-C5D	3.14	1.61	1.51
22	c	509	CLA	O2D-CED	-3.13	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C1B-C2B	3.13	1.50	1.43
22	B	705	CLA	C1C-NC	-3.13	1.33	1.37
26	f	102	SQD	O47-C7	3.13	1.43	1.34
30	a	418	LMG	C3-C2	3.13	1.60	1.52
22	b	611	CLA	C1B-C2B	3.13	1.50	1.43
27	c	517	DGD	O5D-C1E	3.12	1.45	1.40
22	b	609	CLA	CMB-C2B	-3.12	1.44	1.50
23	b	618	BCR	C33-C5	-3.11	1.46	1.50
27	c	518	DGD	O2E-C2E	-3.11	1.35	1.43
22	a	405	CLA	CMC-C2C	-3.10	1.44	1.50
33	D	408	PHO	C3A-C2A	-3.10	1.52	1.54
22	c	503	CLA	C1D-ND	3.10	1.41	1.37
27	h	703	DGD	O4D-C4D	-3.10	1.35	1.43
23	B	718	BCR	C37-C22	-3.09	1.44	1.50
22	A	402	CLA	C1B-C2B	3.09	1.50	1.43
22	B	710	CLA	MG-NB	-3.09	1.99	2.05
22	C	505	CLA	C1D-ND	3.08	1.41	1.37
22	C	506	CLA	C1B-C2B	3.08	1.50	1.43
22	D	402	CLA	C1B-C2B	3.08	1.50	1.43
30	c	522	LMG	C7-C8	3.08	1.60	1.50
30	b	622	LMG	C7-C8	3.08	1.60	1.50
30	d	410	LMG	O7-C8	-3.08	1.39	1.46
22	B	714	CLA	C4B-NB	3.08	1.41	1.37
23	T	701	BCR	C30-C25	-3.08	1.49	1.53
25	D	406	PL9	C37-C38	-3.07	1.41	1.50
22	b	608	CLA	CHC-C1C	3.07	1.44	1.38
22	a	402	CLA	C1D-ND	3.07	1.41	1.37
23	k	101	BCR	C30-C25	-3.07	1.49	1.53
22	b	603	CLA	MG-NB	-3.07	1.99	2.05
22	C	513	CLA	CHC-C1C	3.06	1.44	1.38
33	d	407	PHO	CMC-C2C	-3.06	1.45	1.50
27	C	519	DGD	O6D-C5D	-3.06	1.36	1.44
22	b	614	CLA	C1D-ND	3.06	1.41	1.37
22	b	615	CLA	C4B-NB	3.05	1.41	1.37
22	c	508	CLA	C1D-ND	3.05	1.41	1.37
22	B	716	CLA	C1D-ND	3.04	1.41	1.37
22	C	513	CLA	C4B-NB	3.04	1.41	1.37
22	b	605	CLA	C3B-C4B	3.04	1.51	1.42
22	b	603	CLA	C1B-NB	-3.04	1.33	1.37
23	B	719	BCR	C33-C5	-3.04	1.46	1.50
22	c	511	CLA	O2D-CED	-3.03	1.38	1.45
33	D	407	PHO	CBD-CGD	-3.03	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	524	BCR	C1-C6	-3.02	1.49	1.53
22	C	504	CLA	C4B-NB	3.02	1.41	1.37
22	C	514	CLA	C4B-NB	3.02	1.41	1.37
31	D	412	LHG	O8-C6	-3.02	1.38	1.45
22	c	509	CLA	C4B-NB	3.01	1.41	1.37
23	C	515	BCR	C33-C5	-3.01	1.46	1.50
22	B	715	CLA	C1B-C2B	3.01	1.50	1.43
22	b	613	CLA	CMB-C2B	-3.01	1.44	1.50
26	f	102	SQD	O2-C2	-3.01	1.35	1.43
22	c	513	CLA	C4B-NB	3.00	1.41	1.37
31	L	101	LHG	O7-C5	-3.00	1.39	1.46
22	b	608	CLA	C1D-C2D	3.00	1.51	1.45
22	B	703	CLA	MG-NB	-2.99	1.99	2.05
23	k	102	BCR	C1-C6	-2.99	1.50	1.53
22	C	508	CLA	C1B-C2B	2.99	1.50	1.43
30	C	520	LMG	O1-C1	2.98	1.45	1.40
23	h	702	BCR	C30-C25	-2.98	1.50	1.53
22	C	508	CLA	C1B-NB	-2.98	1.33	1.37
22	b	608	CLA	C1D-ND	2.98	1.41	1.37
33	D	407	PHO	CMC-C2C	-2.98	1.46	1.50
22	D	403	CLA	CHC-C1C	2.98	1.44	1.38
22	B	727	CLA	C1D-ND	2.98	1.41	1.37
22	C	507	CLA	C1B-NB	-2.98	1.34	1.37
22	C	512	CLA	C3B-C4B	2.97	1.51	1.42
30	a	418	LMG	C1-C2	2.97	1.61	1.52
27	c	519	DGD	O6D-C5D	-2.97	1.37	1.44
22	b	608	CLA	C4B-NB	2.97	1.41	1.37
22	c	509	CLA	C1B-C2B	2.97	1.50	1.43
22	D	403	CLA	C1D-ND	2.96	1.41	1.37
30	c	520	LMG	C1-C2	2.96	1.61	1.52
27	H	102	DGD	C1E-C2E	2.96	1.61	1.52
23	C	501	BCR	C1-C6	-2.95	1.50	1.53
23	D	405	BCR	C30-C25	-2.95	1.50	1.53
22	B	712	CLA	C3B-C4B	2.95	1.51	1.42
22	B	710	CLA	CMB-C2B	-2.95	1.44	1.50
22	B	708	CLA	C1B-NB	-2.95	1.34	1.37
22	b	610	CLA	C1B-C2B	2.95	1.50	1.43
22	c	512	CLA	C1B-C2B	2.95	1.50	1.43
27	A	411	DGD	C1E-C2E	2.94	1.61	1.52
22	b	615	CLA	C1D-ND	2.94	1.41	1.37
23	a	406	BCR	C35-C13	-2.94	1.44	1.50
22	C	514	CLA	C1B-C2B	2.94	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	O2D-CED	-2.94	1.38	1.45
22	C	508	CLA	O2D-CED	-2.94	1.38	1.45
22	B	711	CLA	CMD-C2D	-2.94	1.44	1.50
33	D	408	PHO	C1D-C2D	2.93	1.42	1.39
27	C	517	DGD	C3E-C2E	2.93	1.59	1.52
31	D	412	LHG	O7-C5	-2.93	1.39	1.46
22	B	707	CLA	CMD-C2D	-2.93	1.44	1.50
23	b	619	BCR	C33-C5	-2.93	1.46	1.50
30	c	523	LMG	O1-C7	-2.93	1.38	1.43
22	b	611	CLA	CMD-C2D	-2.93	1.44	1.50
22	B	716	CLA	O2D-CED	-2.92	1.38	1.45
22	C	506	CLA	CHC-C1C	2.92	1.44	1.38
22	B	713	CLA	MG-NB	-2.92	2.00	2.05
31	E	101	LHG	P-O6	2.91	1.70	1.59
22	C	510	CLA	C1B-C2B	2.91	1.50	1.43
26	B	723	SQD	O2-C2	-2.91	1.35	1.43
23	c	515	BCR	C33-C5	-2.91	1.46	1.50
22	d	401	CLA	C4B-NB	2.91	1.41	1.37
23	t	701	BCR	C27-C26	-2.91	1.45	1.51
22	b	606	CLA	O2D-CED	-2.90	1.38	1.45
22	B	708	CLA	C3D-C4D	2.90	1.50	1.44
22	d	403	CLA	C1B-NB	-2.90	1.34	1.37
22	C	511	CLA	C1B-C2B	2.90	1.49	1.43
22	C	512	CLA	C4B-NB	2.90	1.41	1.37
22	B	702	CLA	C3B-C4B	2.89	1.51	1.42
27	H	102	DGD	O2D-C2D	-2.89	1.35	1.43
22	a	405	CLA	CHC-C4B	-2.89	1.32	1.39
22	B	707	CLA	CMC-C2C	-2.89	1.44	1.50
33	D	408	PHO	CAC-C3C	-2.89	1.46	1.51
27	c	519	DGD	O2D-C2D	-2.88	1.35	1.43
26	a	414	SQD	O48-C23	2.88	1.41	1.33
22	a	405	CLA	CMD-C2D	-2.88	1.44	1.50
23	C	501	BCR	C33-C5	-2.88	1.46	1.50
22	B	709	CLA	MG-NB	-2.88	2.00	2.05
30	c	520	LMG	C3-C2	2.88	1.59	1.52
22	b	605	CLA	C1B-C2B	2.88	1.49	1.43
31	l	102	LHG	C24-C23	-2.88	1.42	1.50
22	a	402	CLA	CMB-C2B	-2.87	1.44	1.50
25	D	406	PL9	C11-C9	-2.87	1.45	1.51
22	B	716	CLA	CMB-C2B	-2.87	1.44	1.50
22	D	402	CLA	O2D-CED	-2.86	1.38	1.45
31	D	412	LHG	O3-C3	-2.86	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	520	LMG	O1-C1	2.86	1.45	1.40
22	c	506	CLA	C1D-ND	2.86	1.41	1.37
22	B	713	CLA	MG-ND	-2.85	2.00	2.05
22	C	509	CLA	C3B-C4B	2.85	1.51	1.42
30	c	523	LMG	C7-C8	2.85	1.59	1.50
23	B	719	BCR	C37-C22	-2.85	1.45	1.50
22	c	505	CLA	CMD-C2D	-2.85	1.44	1.50
22	B	711	CLA	CMB-C2B	-2.84	1.44	1.50
22	C	514	CLA	CMC-C2C	-2.84	1.44	1.50
22	B	727	CLA	CHC-C1C	2.84	1.44	1.38
22	C	508	CLA	C3B-C4B	2.84	1.51	1.42
22	B	702	CLA	CMB-C2B	-2.84	1.45	1.50
25	d	406	PL9	C37-C38	-2.83	1.41	1.50
26	a	412	SQD	O48-C23	2.83	1.41	1.33
23	Y	101	BCR	C1-C6	-2.82	1.50	1.53
22	d	404	CLA	C1D-ND	2.82	1.41	1.37
30	b	622	LMG	C4-C5	2.82	1.59	1.53
34	F	101	HEC	FE-NA	2.81	2.04	1.95
22	c	511	CLA	CMB-C2B	-2.81	1.45	1.50
22	C	509	CLA	C1D-ND	2.81	1.41	1.37
23	a	406	BCR	C33-C5	-2.81	1.46	1.50
30	C	520	LMG	C7-C8	2.81	1.59	1.50
27	c	517	DGD	O1G-C1A	2.80	1.41	1.33
22	c	505	CLA	C4B-NB	2.80	1.41	1.37
22	B	712	CLA	CHC-C1C	2.80	1.44	1.38
22	c	510	CLA	C4B-NB	2.80	1.41	1.37
22	b	604	CLA	C1B-NB	-2.80	1.34	1.37
22	c	502	CLA	C1D-ND	2.79	1.41	1.37
22	C	511	CLA	MG-NB	-2.79	2.00	2.05
22	b	603	CLA	CMB-C2B	-2.79	1.45	1.50
22	C	504	CLA	C1B-C2B	2.79	1.49	1.43
22	b	613	CLA	MG-NA	2.79	2.12	2.06
22	B	727	CLA	MG-ND	-2.79	2.00	2.05
22	B	727	CLA	MG-NA	2.79	2.12	2.06
30	c	520	LMG	O7-C10	2.79	1.41	1.35
22	c	504	CLA	CMC-C2C	-2.79	1.45	1.50
22	C	513	CLA	C3B-C4B	2.78	1.50	1.42
22	D	404	CLA	CMB-C2B	-2.78	1.45	1.50
27	H	102	DGD	C4E-C3E	2.77	1.59	1.52
22	C	509	CLA	C1B-C2B	2.77	1.49	1.43
22	d	403	CLA	CMB-C2B	-2.77	1.45	1.50
22	d	404	CLA	O2D-CGD	2.77	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	709	CLA	CMD-C2D	-2.77	1.45	1.50
27	H	102	DGD	C4E-C5E	2.77	1.58	1.53
22	C	509	CLA	C4B-NB	2.77	1.41	1.37
22	b	616	CLA	MG-NB	-2.76	2.00	2.05
22	c	506	CLA	C1B-C2B	2.76	1.49	1.43
25	d	406	PL9	C41-C39	-2.76	1.45	1.51
22	C	509	CLA	CHC-C1C	2.76	1.44	1.38
23	T	701	BCR	C38-C26	-2.76	1.46	1.50
33	d	407	PHO	CMD-C2D	-2.76	1.46	1.51
27	H	102	DGD	C4D-C5D	2.76	1.58	1.53
22	D	404	CLA	CMC-C2C	-2.76	1.45	1.50
22	b	604	CLA	C1B-C2B	2.76	1.49	1.43
22	C	507	CLA	C3B-C4B	2.76	1.50	1.42
22	d	401	CLA	MG-NA	2.75	2.12	2.06
22	b	605	CLA	MG-NB	-2.75	2.00	2.05
26	A	409	SQD	O47-C7	2.75	1.42	1.34
30	D	413	LMG	O8-C28	2.75	1.41	1.33
22	C	513	CLA	C1D-ND	2.75	1.41	1.37
22	c	502	CLA	C1B-C2B	2.74	1.49	1.43
33	D	408	PHO	CMC-C2C	-2.74	1.46	1.50
33	d	407	PHO	CBD-CGD	-2.74	1.49	1.52
34	F	101	HEC	FE-NC	2.74	2.04	1.95
30	a	418	LMG	O7-C10	2.74	1.42	1.34
22	B	727	CLA	CMB-C2B	-2.74	1.45	1.50
22	B	707	CLA	CMB-C2B	-2.74	1.45	1.50
22	A	402	CLA	C3B-C4B	2.73	1.50	1.42
22	c	507	CLA	CHC-C4B	-2.73	1.33	1.39
34	V	201	HEC	CMC-C2C	2.73	1.56	1.50
22	C	507	CLA	MG-ND	-2.73	2.00	2.05
27	h	703	DGD	C4D-C3D	2.73	1.59	1.52
22	b	607	CLA	C1B-NB	-2.72	1.34	1.37
23	d	405	BCR	C1-C6	-2.72	1.50	1.53
23	H	101	BCR	C33-C5	-2.72	1.46	1.50
22	c	506	CLA	C3B-C4B	2.72	1.50	1.42
22	C	510	CLA	C4B-NB	2.72	1.41	1.37
22	b	613	CLA	C1D-ND	2.71	1.41	1.37
22	C	512	CLA	MG-NB	-2.71	2.00	2.05
22	a	403	CLA	C1B-NB	-2.71	1.34	1.37
34	v	201	HEC	C1C-NC	-2.71	1.34	1.39
22	B	727	CLA	C1B-NB	-2.70	1.34	1.37
22	c	514	CLA	C1B-C2B	2.70	1.49	1.43
22	a	405	CLA	MG-NB	-2.70	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	710	CLA	C1D-ND	2.70	1.41	1.37
22	B	710	CLA	CHC-C1C	2.70	1.43	1.38
22	C	513	CLA	C1D-C2D	2.69	1.50	1.45
22	C	503	CLA	C3B-C4B	2.69	1.50	1.42
23	T	701	BCR	C33-C5	-2.69	1.46	1.50
31	D	411	LHG	O7-C5	-2.69	1.40	1.46
22	b	610	CLA	CMD-C2D	-2.69	1.45	1.50
22	B	704	CLA	MG-NC	2.68	2.12	2.06
30	C	516	LMG	C4-C5	2.68	1.58	1.53
23	C	515	BCR	C36-C18	-2.68	1.45	1.50
22	c	511	CLA	C1D-ND	2.68	1.41	1.37
22	B	705	CLA	CMC-C2C	-2.68	1.45	1.50
22	d	401	CLA	O2D-CED	-2.68	1.39	1.45
22	c	514	CLA	CMB-C2B	-2.68	1.45	1.50
22	C	505	CLA	CHC-C1C	2.67	1.43	1.38
22	b	607	CLA	CMD-C2D	-2.67	1.45	1.50
22	b	609	CLA	C4B-NB	2.67	1.41	1.37
22	C	508	CLA	C1D-ND	2.67	1.41	1.37
27	H	102	DGD	O6E-C1E	2.67	1.48	1.41
22	C	503	CLA	C1B-C2B	2.67	1.49	1.43
22	b	613	CLA	C1B-C2B	2.67	1.49	1.43
27	A	411	DGD	C6E-C5E	2.66	1.60	1.51
23	B	718	BCR	C1-C6	-2.66	1.50	1.53
22	B	715	CLA	CHC-C1C	2.66	1.43	1.38
22	b	606	CLA	CHC-C1C	2.65	1.43	1.38
33	d	407	PHO	C4D-CHA	2.65	1.43	1.39
22	B	714	CLA	C1A-CHA	-2.65	1.32	1.43
22	b	604	CLA	CHC-C1C	2.65	1.43	1.38
22	b	602	CLA	CAC-C3C	-2.64	1.44	1.51
22	b	604	CLA	C3B-C4B	2.64	1.50	1.42
22	a	403	CLA	CHC-C1C	2.64	1.43	1.38
27	c	517	DGD	O6D-C1D	2.64	1.48	1.41
33	a	404	PHO	O2D-CGD	2.64	1.39	1.33
23	T	701	BCR	C27-C26	-2.63	1.46	1.51
22	a	402	CLA	C4B-NB	2.63	1.41	1.37
22	B	727	CLA	C4B-NB	2.63	1.41	1.37
33	D	408	PHO	C3B-C2B	-2.63	1.36	1.40
27	c	517	DGD	C1D-C2D	2.63	1.60	1.52
22	c	514	CLA	C4B-NB	2.63	1.41	1.37
22	b	615	CLA	CMD-C2D	-2.62	1.45	1.50
23	k	101	BCR	C33-C5	-2.62	1.46	1.50
22	b	614	CLA	O2D-CGD	2.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	704	CLA	C3B-C4B	2.61	1.50	1.42
30	C	516	LMG	O6-C5	-2.61	1.38	1.44
22	a	402	CLA	MG-ND	-2.60	2.00	2.05
22	c	509	CLA	CHC-C1C	2.60	1.43	1.38
22	b	615	CLA	O2D-CED	-2.60	1.39	1.45
22	c	506	CLA	MG-NB	-2.60	2.00	2.05
22	B	707	CLA	C1B-C2B	2.60	1.49	1.43
22	B	702	CLA	C3D-C4D	2.60	1.50	1.44
22	b	605	CLA	C1B-NB	-2.60	1.34	1.37
23	Y	101	BCR	C33-C5	-2.60	1.46	1.50
22	c	505	CLA	CHC-C1C	2.60	1.43	1.38
22	C	512	CLA	MG-ND	-2.60	2.00	2.05
31	D	412	LHG	C8-C7	-2.59	1.43	1.50
22	b	611	CLA	C3B-C4B	2.59	1.50	1.42
26	f	102	SQD	O3-C3	-2.59	1.36	1.43
22	b	607	CLA	O2D-CED	-2.59	1.39	1.45
23	C	524	BCR	C33-C5	-2.59	1.46	1.50
26	A	409	SQD	O48-C23	2.59	1.40	1.33
22	c	502	CLA	C4B-NB	2.59	1.41	1.37
22	c	514	CLA	C3B-C4B	2.58	1.50	1.42
30	a	418	LMG	C12-C11	2.58	1.61	1.52
22	d	404	CLA	O1D-CGD	2.58	1.27	1.21
25	D	406	PL9	C51-C49	2.58	1.57	1.50
22	a	405	CLA	CMB-C2B	-2.58	1.45	1.50
22	c	505	CLA	MG-NB	-2.58	2.00	2.05
31	E	101	LHG	O7-C5	-2.57	1.40	1.46
22	C	504	CLA	MG-NA	2.57	2.12	2.06
22	B	727	CLA	C1C-NC	-2.57	1.33	1.37
22	c	502	CLA	C1B-NB	-2.57	1.34	1.37
30	c	522	LMG	C1-C2	2.57	1.60	1.52
22	B	703	CLA	CMC-C2C	-2.57	1.45	1.50
22	B	714	CLA	C1D-ND	2.56	1.41	1.37
27	c	518	DGD	C4D-C3D	2.56	1.59	1.52
22	C	510	CLA	CMD-C2D	-2.56	1.45	1.50
27	h	703	DGD	C1E-C2E	2.56	1.60	1.52
22	b	602	CLA	C1D-ND	2.56	1.41	1.37
22	b	604	CLA	CMD-C2D	-2.56	1.45	1.50
22	A	402	CLA	C5-C3	-2.56	1.46	1.51
23	D	405	BCR	C33-C5	-2.56	1.46	1.50
30	b	622	LMG	C3-C2	2.56	1.59	1.52
23	k	102	BCR	C30-C25	-2.55	1.50	1.53
22	C	514	CLA	C3B-C4B	2.55	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	711	CLA	O2D-CED	-2.55	1.39	1.45
22	b	610	CLA	C3D-C4D	2.55	1.49	1.44
22	c	504	CLA	C1B-C2B	2.55	1.49	1.43
22	b	614	CLA	C1B-NB	-2.55	1.34	1.37
22	b	611	CLA	MG-NA	2.55	2.12	2.06
23	B	717	BCR	C30-C25	-2.55	1.50	1.53
22	B	709	CLA	O2D-CGD	2.55	1.39	1.33
22	C	511	CLA	O2D-CED	-2.55	1.39	1.45
30	M	101	LMG	O6-C5	-2.54	1.38	1.44
22	C	508	CLA	CMB-C2B	-2.54	1.45	1.50
22	C	506	CLA	O2D-CED	-2.54	1.39	1.45
22	C	511	CLA	CMC-C2C	-2.54	1.45	1.50
27	c	519	DGD	O4D-C4D	-2.54	1.36	1.43
22	B	716	CLA	MG-NA	2.54	2.12	2.06
22	c	509	CLA	C3B-C4B	2.53	1.50	1.42
22	c	513	CLA	CMC-C2C	-2.53	1.45	1.50
22	D	402	CLA	C1D-ND	2.53	1.41	1.37
31	L	101	LHG	O8-C23	2.53	1.40	1.33
22	A	404	CLA	C1B-NB	-2.53	1.34	1.37
22	C	508	CLA	CMD-C2D	-2.53	1.45	1.50
22	D	403	CLA	C1B-C2B	2.53	1.49	1.43
22	C	511	CLA	CHC-C1C	2.53	1.43	1.38
31	d	409	LHG	O8-C23	2.53	1.40	1.33
22	c	510	CLA	O2D-CED	-2.53	1.39	1.45
22	c	504	CLA	C1D-ND	2.53	1.41	1.37
22	a	405	CLA	C1D-ND	2.52	1.41	1.37
30	D	413	LMG	C9-C8	2.52	1.58	1.50
27	H	102	DGD	C3E-C2E	2.52	1.58	1.52
22	c	505	CLA	CMC-C2C	-2.52	1.45	1.50
33	D	408	PHO	CMB-C2B	-2.52	1.46	1.51
22	B	714	CLA	MG-ND	-2.52	2.00	2.05
22	b	610	CLA	C1B-NB	-2.51	1.34	1.37
22	C	503	CLA	O2D-CED	-2.51	1.39	1.45
22	a	403	CLA	OBD-CAD	-2.51	1.18	1.22
22	a	403	CLA	CMB-C2B	-2.51	1.45	1.50
22	c	507	CLA	CAC-C3C	-2.51	1.44	1.51
22	c	514	CLA	O2D-CED	-2.50	1.39	1.45
27	c	517	DGD	O5D-C6D	-2.50	1.39	1.43
22	B	704	CLA	C1B-C2B	2.50	1.49	1.43
22	h	701	CLA	C3B-C4B	2.49	1.50	1.42
22	b	615	CLA	MG-ND	-2.49	2.00	2.05
22	c	514	CLA	C1D-ND	2.49	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	620	LMG	C4-C5	2.49	1.58	1.53
22	A	403	CLA	C1B-C2B	2.49	1.49	1.43
26	A	410	SQD	O47-C45	-2.49	1.42	1.47
22	b	608	CLA	C3B-C4B	2.49	1.50	1.42
22	B	711	CLA	C1B-C2B	2.49	1.49	1.43
27	C	518	DGD	C4E-C3E	2.49	1.58	1.52
23	b	618	BCR	C36-C18	-2.48	1.45	1.50
22	b	614	CLA	O2D-CED	-2.48	1.39	1.45
22	b	607	CLA	C1D-ND	2.48	1.41	1.37
30	c	522	LMG	C3-C2	2.48	1.58	1.52
22	c	513	CLA	C1B-NB	-2.48	1.34	1.37
22	C	510	CLA	CMB-C2B	-2.48	1.45	1.50
22	c	503	CLA	CMD-C2D	-2.47	1.45	1.50
22	c	507	CLA	C1B-NB	-2.47	1.34	1.37
22	D	403	CLA	O2D-CED	-2.47	1.39	1.45
22	c	513	CLA	C1D-ND	2.47	1.41	1.37
22	b	602	CLA	C4B-NB	2.47	1.41	1.37
33	D	407	PHO	CAC-C3C	-2.47	1.47	1.51
22	b	606	CLA	MG-NA	2.46	2.12	2.06
34	f	101	HEC	FE-NB	2.46	2.02	1.94
22	b	609	CLA	MG-NB	-2.46	2.00	2.05
22	b	605	CLA	CMB-C2B	-2.46	1.45	1.50
23	H	101	BCR	C4-C5	-2.45	1.46	1.51
22	h	701	CLA	CHC-C1C	2.45	1.43	1.38
22	b	610	CLA	CMC-C2C	-2.45	1.45	1.50
22	c	505	CLA	C3B-C4B	2.45	1.49	1.42
22	B	714	CLA	C1B-NB	-2.45	1.34	1.37
22	C	509	CLA	MG-NA	2.44	2.12	2.06
22	c	507	CLA	MG-ND	-2.44	2.00	2.05
26	B	723	SQD	O48-C23	2.44	1.40	1.33
31	D	412	LHG	O2-C2	-2.44	1.36	1.43
22	d	401	CLA	CMB-C2B	-2.44	1.45	1.50
27	c	517	DGD	C4E-C3E	2.44	1.58	1.52
22	B	709	CLA	CHC-C4B	-2.44	1.34	1.39
22	D	402	CLA	CHC-C4B	-2.44	1.34	1.39
22	a	403	CLA	CMC-C2C	-2.44	1.45	1.50
22	c	508	CLA	C4B-NB	2.44	1.41	1.37
22	A	404	CLA	CMD-C2D	-2.44	1.45	1.50
22	b	613	CLA	CMC-C2C	-2.43	1.45	1.50
22	c	507	CLA	CHC-C1C	2.43	1.43	1.38
22	c	506	CLA	CHC-C1C	2.43	1.43	1.38
22	A	402	CLA	O2D-CED	-2.43	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	102	DGD	O3E-C3E	-2.43	1.36	1.43
27	C	517	DGD	C6D-C5D	2.42	1.58	1.51
27	C	518	DGD	C2B-C1B	-2.42	1.43	1.50
22	b	608	CLA	MG-NB	-2.42	2.01	2.05
22	B	708	CLA	CAC-C3C	-2.42	1.44	1.51
22	D	404	CLA	C3B-C4B	2.42	1.49	1.42
22	C	511	CLA	MG-NA	2.42	2.12	2.06
22	h	701	CLA	O2D-CED	-2.42	1.39	1.45
22	C	505	CLA	C3B-C4B	2.42	1.49	1.42
27	C	519	DGD	O4E-C4E	-2.42	1.37	1.43
22	B	705	CLA	C1B-NB	-2.41	1.34	1.37
22	c	507	CLA	C1D-ND	2.41	1.41	1.37
22	A	402	CLA	CHC-C1C	2.41	1.43	1.38
22	c	503	CLA	CHC-C1C	2.41	1.43	1.38
23	C	501	BCR	C27-C26	-2.41	1.46	1.51
22	D	404	CLA	CHC-C4B	-2.41	1.34	1.39
22	B	708	CLA	MG-NA	2.40	2.12	2.06
22	a	403	CLA	C4B-NB	2.40	1.41	1.37
25	D	406	PL9	C3-C4	-2.40	1.45	1.49
22	B	704	CLA	CHC-C1C	2.40	1.43	1.38
22	B	727	CLA	O2D-CED	-2.40	1.39	1.45
33	D	407	PHO	CMB-C2B	-2.40	1.46	1.51
34	F	101	HEC	CMC-C2C	2.40	1.55	1.50
26	D	410	SQD	O3-C3	-2.40	1.37	1.43
22	D	404	CLA	CMD-C2D	-2.39	1.45	1.50
22	C	507	CLA	C1D-ND	2.39	1.41	1.37
22	B	714	CLA	CMB-C2B	-2.39	1.45	1.50
22	B	712	CLA	C1C-NC	-2.39	1.34	1.37
22	D	404	CLA	C3D-C4D	2.39	1.49	1.44
23	B	719	BCR	C35-C13	-2.39	1.46	1.50
33	d	407	PHO	C4D-ND	-2.39	1.35	1.38
30	D	413	LMG	O8-C9	2.39	1.50	1.45
22	b	608	CLA	O2D-CED	-2.39	1.40	1.45
22	B	713	CLA	O2D-CED	-2.39	1.40	1.45
22	D	404	CLA	C1B-C2B	2.39	1.48	1.43
27	c	518	DGD	C1E-C2E	2.39	1.59	1.52
22	a	402	CLA	CHC-C1C	2.39	1.43	1.38
22	C	506	CLA	C3B-C4B	2.39	1.49	1.42
34	v	201	HEC	FE-NC	2.39	2.03	1.95
22	C	513	CLA	CMB-C2B	-2.39	1.45	1.50
22	b	613	CLA	C1B-NB	-2.38	1.34	1.37
26	a	412	SQD	O47-C7	2.38	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMC-C2C	-2.38	1.45	1.50
33	a	404	PHO	C4D-ND	-2.38	1.35	1.38
22	A	403	CLA	O2D-CED	-2.38	1.40	1.45
22	b	616	CLA	C4B-NB	2.38	1.41	1.37
22	a	402	CLA	C1B-C2B	2.38	1.48	1.43
22	B	707	CLA	MG-NA	2.38	2.11	2.06
27	c	517	DGD	O6E-C5E	-2.38	1.38	1.44
22	C	513	CLA	O2D-CED	-2.38	1.40	1.45
22	h	701	CLA	CMC-C2C	-2.38	1.45	1.50
22	b	614	CLA	CAC-C3C	-2.37	1.45	1.51
22	C	502	CLA	C4B-NB	2.37	1.41	1.37
22	B	710	CLA	C1A-CHA	-2.37	1.33	1.43
27	C	517	DGD	C4E-C3E	2.37	1.58	1.52
34	f	101	HEC	FE-ND	2.37	2.02	1.94
22	b	614	CLA	CMB-C2B	-2.37	1.45	1.50
22	D	404	CLA	C1B-NB	-2.37	1.34	1.37
22	c	505	CLA	MG-ND	-2.36	2.01	2.05
22	C	510	CLA	C3B-C4B	2.36	1.49	1.42
22	A	404	CLA	C4B-NB	2.36	1.41	1.37
23	B	717	BCR	C4-C5	-2.36	1.46	1.51
27	c	517	DGD	C1E-C2E	2.36	1.59	1.52
22	C	504	CLA	O2D-CED	-2.36	1.40	1.45
33	a	404	PHO	C3B-C2B	-2.35	1.37	1.40
22	c	507	CLA	CMA-C3A	-2.35	1.48	1.53
27	h	703	DGD	O2G-C2G	-2.35	1.41	1.46
22	d	404	CLA	O2D-CED	-2.35	1.40	1.45
22	c	506	CLA	CMC-C2C	-2.35	1.46	1.50
22	c	513	CLA	C3B-C4B	2.35	1.49	1.42
23	h	702	BCR	C33-C5	-2.35	1.47	1.50
22	B	706	CLA	CMA-C3A	-2.35	1.48	1.53
22	B	702	CLA	C1D-C2D	2.35	1.50	1.45
22	C	507	CLA	C4B-NB	2.34	1.40	1.37
22	A	404	CLA	MG-NB	-2.34	2.01	2.05
31	l	102	LHG	P-O6	2.34	1.68	1.59
22	b	612	CLA	CMC-C2C	-2.33	1.46	1.50
22	b	609	CLA	MG-ND	-2.33	2.01	2.05
22	B	704	CLA	C1D-ND	2.33	1.40	1.37
22	C	513	CLA	C1B-C2B	2.33	1.48	1.43
22	A	403	CLA	CMB-C2B	-2.33	1.46	1.50
22	A	402	CLA	C1B-NB	-2.33	1.34	1.37
23	D	405	BCR	C27-C26	-2.33	1.46	1.51
22	b	602	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C1B-NB	-2.33	1.34	1.37
27	c	518	DGD	C6E-C5E	2.32	1.59	1.51
22	a	405	CLA	O1D-CGD	2.32	1.27	1.21
22	D	404	CLA	MG-ND	-2.32	2.01	2.05
22	C	504	CLA	CHC-C1C	2.32	1.43	1.38
22	C	506	CLA	O2D-CGD	2.32	1.38	1.33
22	c	506	CLA	C4B-NB	2.32	1.40	1.37
22	C	509	CLA	C1D-C2D	2.32	1.49	1.45
22	B	703	CLA	O2D-CED	-2.32	1.40	1.45
22	b	609	CLA	C3B-C4B	2.32	1.49	1.42
30	a	418	LMG	O8-C9	-2.32	1.40	1.45
33	D	408	PHO	CHA-CBD	-2.32	1.49	1.51
22	c	513	CLA	CHC-C1C	2.31	1.43	1.38
27	A	411	DGD	C4D-C3D	2.31	1.58	1.52
22	b	608	CLA	C3D-C4D	2.31	1.49	1.44
22	B	714	CLA	O2D-CED	-2.31	1.40	1.45
27	c	518	DGD	C4E-C3E	2.31	1.58	1.52
27	c	517	DGD	O2G-C2G	-2.31	1.41	1.46
22	a	405	CLA	C4B-NB	2.31	1.40	1.37
23	C	515	BCR	C30-C25	-2.31	1.50	1.53
34	F	101	HEC	CMA-C3A	2.31	1.55	1.50
33	D	407	PHO	C1A-C2A	2.31	1.54	1.51
27	H	102	DGD	C6D-C5D	2.31	1.58	1.51
22	C	506	CLA	OBD-CAD	2.30	1.26	1.22
22	a	402	CLA	CMC-C2C	-2.30	1.46	1.50
22	h	701	CLA	O2A-CGA	2.30	1.40	1.33
22	b	613	CLA	C3C-C2C	2.30	1.41	1.36
22	C	514	CLA	CMB-C2B	-2.30	1.46	1.50
22	b	615	CLA	C1B-C2B	2.30	1.48	1.43
22	C	507	CLA	CHC-C1C	2.30	1.43	1.38
22	C	506	CLA	CMC-C2C	-2.30	1.46	1.50
22	C	503	CLA	CAC-C3C	-2.30	1.45	1.51
31	a	413	LHG	P-O6	2.30	1.68	1.59
22	b	615	CLA	C3B-C4B	2.30	1.49	1.42
23	B	718	BCR	C36-C18	-2.30	1.46	1.50
23	B	719	BCR	C30-C25	-2.30	1.50	1.53
22	B	713	CLA	C1B-NB	-2.30	1.34	1.37
22	B	727	CLA	C3B-C4B	2.29	1.49	1.42
22	b	611	CLA	CHC-C4B	-2.29	1.34	1.39
33	d	407	PHO	C3B-C2B	-2.29	1.37	1.40
27	C	518	DGD	C1E-C2E	2.29	1.59	1.52
22	c	507	CLA	O2D-CED	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	407	PHO	CHA-CBD	-2.28	1.49	1.51
23	T	701	BCR	C4-C5	-2.28	1.46	1.51
27	C	517	DGD	C2A-C1A	-2.28	1.44	1.50
22	D	403	CLA	C1D-C2D	2.28	1.49	1.45
22	b	610	CLA	C4C-C3C	2.28	1.48	1.45
22	C	502	CLA	MG-NB	-2.28	2.01	2.05
27	A	411	DGD	C4E-C3E	2.28	1.58	1.52
22	C	511	CLA	C3D-C4D	2.28	1.49	1.44
22	c	506	CLA	C3D-C4D	2.28	1.49	1.44
22	b	610	CLA	CMB-C2B	-2.28	1.46	1.50
22	C	510	CLA	O2D-CED	-2.27	1.40	1.45
22	b	602	CLA	C1B-C2B	2.27	1.48	1.43
30	a	418	LMG	C7-C8	2.27	1.57	1.50
23	a	406	BCR	C30-C25	-2.27	1.50	1.53
27	C	518	DGD	O6E-C1E	2.27	1.47	1.41
22	d	404	CLA	CMC-C2C	-2.27	1.46	1.50
30	C	516	LMG	C3-C2	2.27	1.58	1.52
23	k	102	BCR	C4-C5	-2.27	1.46	1.51
22	b	616	CLA	CMC-C2C	-2.27	1.46	1.50
22	b	612	CLA	CMB-C2B	-2.27	1.46	1.50
22	c	508	CLA	CMB-C2B	-2.27	1.46	1.50
22	c	504	CLA	C4B-NB	2.27	1.40	1.37
26	A	409	SQD	O47-C45	-2.27	1.41	1.46
22	C	510	CLA	O2A-CGA	2.27	1.40	1.33
22	b	616	CLA	C3B-C4B	2.27	1.49	1.42
22	A	402	CLA	MG-ND	-2.27	2.01	2.05
22	C	502	CLA	C1D-C2D	2.27	1.49	1.45
22	b	607	CLA	CMB-C2B	-2.26	1.46	1.50
22	b	616	CLA	CMB-C2B	-2.26	1.46	1.50
22	c	502	CLA	MG-NB	-2.26	2.01	2.05
22	B	706	CLA	C1D-ND	2.26	1.40	1.37
22	B	706	CLA	C3B-C2B	-2.26	1.33	1.41
31	D	411	LHG	O8-C6	-2.26	1.40	1.45
33	a	404	PHO	CMC-C2C	-2.26	1.47	1.50
34	F	101	HEC	CMD-C2D	2.26	1.55	1.50
22	C	503	CLA	CHC-C1C	2.26	1.43	1.38
34	V	201	HEC	FE-NC	2.26	2.02	1.95
22	c	512	CLA	O2D-CED	-2.26	1.40	1.45
22	C	511	CLA	C3B-C4B	2.26	1.49	1.42
22	C	502	CLA	CMC-C2C	-2.26	1.46	1.50
22	c	511	CLA	MG-NB	-2.26	2.01	2.05
22	b	603	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	CMB-C2B	-2.26	1.46	1.50
22	C	507	CLA	C1B-C2B	2.25	1.48	1.43
22	d	401	CLA	C3D-C4D	2.25	1.49	1.44
22	A	402	CLA	C1C-NC	-2.25	1.34	1.37
22	B	702	CLA	CMC-C2C	-2.25	1.46	1.50
22	C	504	CLA	MG-NB	-2.25	2.01	2.05
30	d	410	LMG	O8-C9	-2.25	1.40	1.45
23	d	405	BCR	C37-C22	-2.25	1.46	1.50
34	f	101	HEC	C2A-C3A	-2.25	1.31	1.36
22	c	514	CLA	MG-NB	-2.24	2.01	2.05
33	D	408	PHO	C5-C3	-2.24	1.46	1.51
22	B	712	CLA	C1B-C2B	2.24	1.48	1.43
23	A	405	BCR	C37-C22	-2.24	1.46	1.50
22	c	503	CLA	MG-NB	-2.24	2.01	2.05
22	B	706	CLA	MG-NA	2.24	2.11	2.06
22	B	702	CLA	O2D-CED	-2.24	1.40	1.45
30	C	516	LMG	O7-C8	-2.24	1.41	1.46
22	B	715	CLA	MG-NA	2.24	2.11	2.06
28	a	416	STE	O1-C1	2.24	1.29	1.22
22	b	605	CLA	C4B-NB	2.24	1.40	1.37
33	d	407	PHO	CAA-C2A	-2.23	1.49	1.54
22	b	602	CLA	CHC-C1C	2.23	1.43	1.38
22	c	503	CLA	CMC-C2C	-2.23	1.46	1.50
31	L	101	LHG	O2-C2	2.23	1.49	1.43
22	c	509	CLA	CMA-C3A	-2.23	1.48	1.53
22	c	512	CLA	C1C-C2C	2.23	1.49	1.44
22	b	603	CLA	CHC-C4B	-2.23	1.34	1.39
22	B	716	CLA	CMC-C2C	-2.23	1.46	1.50
27	C	517	DGD	C4D-C3D	2.23	1.58	1.52
22	h	701	CLA	MG-NB	-2.22	2.01	2.05
33	d	407	PHO	C3D-CAD	-2.22	1.43	1.47
22	c	508	CLA	CHC-C4B	-2.22	1.34	1.39
22	B	714	CLA	C3C-C2C	2.22	1.41	1.36
22	b	614	CLA	C1B-C2B	2.22	1.48	1.43
22	B	712	CLA	C1D-C2D	2.22	1.49	1.45
22	B	708	CLA	C1B-C2B	2.22	1.48	1.43
23	b	619	BCR	C37-C22	-2.22	1.46	1.50
23	C	515	BCR	C31-C1	-2.22	1.49	1.53
22	C	505	CLA	O2D-CED	-2.21	1.40	1.45
22	C	507	CLA	O2D-CED	-2.21	1.40	1.45
22	B	707	CLA	C3D-C4D	2.21	1.49	1.44
22	c	502	CLA	CMC-C2C	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	O2D-CED	-2.21	1.40	1.45
22	b	613	CLA	CAC-C3C	-2.21	1.45	1.51
22	b	604	CLA	CMB-C2B	-2.21	1.46	1.50
22	B	716	CLA	CMD-C2D	-2.20	1.46	1.50
23	C	515	BCR	C4-C5	-2.20	1.46	1.51
30	b	622	LMG	O6-C1	2.20	1.47	1.41
23	k	102	BCR	C33-C5	-2.20	1.47	1.50
22	B	706	CLA	C1B-C2B	2.20	1.48	1.43
22	C	512	CLA	MG-NA	2.19	2.11	2.06
22	B	711	CLA	C3B-C4B	2.19	1.49	1.42
22	B	705	CLA	CMB-C2B	-2.19	1.46	1.50
23	k	102	BCR	C39-C30	-2.19	1.49	1.53
22	B	707	CLA	CMA-C3A	-2.19	1.48	1.53
22	B	715	CLA	CAC-C3C	-2.19	1.45	1.51
30	D	409	LMG	C4-C3	2.19	1.58	1.52
22	C	505	CLA	C1B-C2B	2.19	1.48	1.43
22	b	608	CLA	C1B-C2B	2.19	1.48	1.43
22	B	715	CLA	O2D-CED	-2.19	1.40	1.45
22	A	402	CLA	MG-NB	-2.19	2.01	2.05
30	C	516	LMG	C4-C3	2.19	1.58	1.52
22	C	509	CLA	CMD-C2D	-2.18	1.46	1.50
22	D	402	CLA	C1A-CHA	-2.18	1.34	1.43
22	B	713	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	514	CLA	CHC-C1C	2.18	1.42	1.38
33	D	408	PHO	CMD-C2D	-2.18	1.47	1.51
22	D	404	CLA	MG-NA	2.18	2.11	2.06
22	D	402	CLA	CMB-C2B	-2.18	1.46	1.50
34	V	201	HEC	C2A-C3A	-2.18	1.32	1.36
23	c	516	BCR	C35-C13	-2.18	1.46	1.50
22	A	402	CLA	C1D-ND	2.18	1.40	1.37
22	C	510	CLA	O2D-CGD	2.17	1.38	1.33
22	a	403	CLA	C1B-C2B	2.17	1.48	1.43
27	C	518	DGD	C6D-C5D	2.17	1.58	1.51
22	c	512	CLA	C3B-C4B	2.17	1.49	1.42
28	b	623	STE	C2-C1	2.17	1.55	1.50
22	C	509	CLA	CAC-C3C	-2.17	1.45	1.51
22	B	710	CLA	C3B-C2B	-2.17	1.33	1.41
22	B	703	CLA	C1A-CHA	-2.17	1.34	1.43
22	C	502	CLA	C1D-ND	2.17	1.40	1.37
22	d	404	CLA	CMB-C2B	-2.17	1.46	1.50
30	c	522	LMG	C9-C8	2.17	1.57	1.50
30	B	721	LMG	C14-C13	2.16	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	721	LMG	O7-C10	2.16	1.38	1.30
22	c	505	CLA	O1D-CGD	2.16	1.26	1.21
22	C	504	CLA	C3D-C4D	2.16	1.49	1.44
22	b	606	CLA	CMD-C2D	-2.16	1.46	1.50
25	d	406	PL9	C53-C6	-2.16	1.46	1.50
30	c	520	LMG	O1-C7	-2.16	1.40	1.43
22	C	508	CLA	CHC-C1C	2.16	1.42	1.38
25	a	410	PL9	C40-C39	-2.16	1.45	1.50
22	c	503	CLA	O2D-CED	-2.16	1.40	1.45
22	a	403	CLA	MG-NB	-2.16	2.01	2.05
22	c	503	CLA	CHC-C4B	-2.16	1.34	1.39
22	b	610	CLA	C3B-C4B	2.15	1.49	1.42
22	d	403	CLA	C1B-C2B	2.15	1.48	1.43
22	b	607	CLA	MG-NB	-2.15	2.01	2.05
22	c	512	CLA	CMB-C2B	-2.15	1.46	1.50
22	D	403	CLA	MG-NA	2.15	2.11	2.06
22	B	705	CLA	C1D-ND	2.15	1.40	1.37
22	b	605	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	710	CLA	O2D-CED	-2.15	1.40	1.45
22	b	616	CLA	C1B-C2B	2.15	1.48	1.43
34	v	201	HEC	CMD-C2D	2.15	1.55	1.50
22	b	609	CLA	C3D-C4D	2.15	1.49	1.44
22	B	708	CLA	CMA-C3A	-2.14	1.48	1.53
22	b	613	CLA	CAA-C2A	-2.14	1.50	1.54
22	C	514	CLA	C1D-C2D	2.14	1.49	1.45
22	c	511	CLA	CMD-C2D	-2.14	1.46	1.50
25	D	406	PL9	C7-C8	-2.14	1.47	1.50
30	C	520	LMG	C1-C2	2.14	1.58	1.52
22	C	503	CLA	MG-NA	2.14	2.11	2.06
22	B	707	CLA	CAC-C3C	-2.14	1.45	1.51
22	B	712	CLA	MG-ND	-2.14	2.01	2.05
22	C	506	CLA	C1D-ND	2.13	1.40	1.37
22	B	713	CLA	C1C-NC	-2.13	1.34	1.37
22	b	607	CLA	C1A-CHA	-2.13	1.34	1.43
22	B	712	CLA	C3D-C4D	2.13	1.49	1.44
30	d	410	LMG	O6-C5	-2.13	1.39	1.44
22	A	403	CLA	CMD-C2D	-2.13	1.46	1.50
27	h	703	DGD	O2E-C2E	-2.13	1.37	1.43
23	C	515	BCR	C35-C13	-2.13	1.46	1.50
33	D	407	PHO	CMD-C2D	-2.13	1.47	1.51
22	C	502	CLA	MG-ND	-2.13	2.01	2.05
27	c	519	DGD	O4E-C4E	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	C3D-C4D	2.13	1.49	1.44
22	C	502	CLA	C1C-NC	-2.12	1.34	1.37
22	B	715	CLA	MG-ND	-2.12	2.01	2.05
30	c	523	LMG	C1-C2	2.12	1.58	1.52
22	C	507	CLA	CMB-C2B	-2.12	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.12	1.46	1.50
22	B	706	CLA	CMB-C2B	-2.12	1.46	1.50
23	t	701	BCR	C32-C1	-2.12	1.49	1.53
31	L	101	LHG	C1-C2	2.12	1.59	1.51
23	k	101	BCR	C4-C5	-2.12	1.47	1.51
31	B	722	LHG	P-O6	2.12	1.67	1.59
22	B	714	CLA	CHC-C1C	2.12	1.42	1.38
22	d	403	CLA	C3B-C4B	2.12	1.48	1.42
22	C	514	CLA	O2D-CED	-2.12	1.40	1.45
27	h	703	DGD	C4E-C5E	2.12	1.57	1.53
22	C	513	CLA	CMD-C2D	-2.12	1.46	1.50
22	D	402	CLA	CAC-C3C	-2.12	1.45	1.51
23	t	701	BCR	C1-C6	-2.12	1.51	1.53
25	a	410	PL9	C46-C44	-2.12	1.46	1.51
22	c	504	CLA	O2D-CGD	2.11	1.38	1.33
27	A	411	DGD	O5D-C1E	2.11	1.43	1.40
22	C	508	CLA	MG-NA	2.11	2.11	2.06
22	b	607	CLA	CMA-C3A	-2.11	1.48	1.53
22	b	611	CLA	C1D-ND	2.11	1.40	1.37
22	c	502	CLA	CHC-C4B	-2.11	1.34	1.39
22	d	404	CLA	C4B-NB	2.11	1.40	1.37
25	d	406	PL9	C45-C44	2.11	1.55	1.50
22	b	607	CLA	MG-NA	2.11	2.11	2.06
22	c	513	CLA	C1D-C2D	2.10	1.49	1.45
27	c	519	DGD	C2A-C1A	-2.10	1.44	1.50
22	c	507	CLA	C1B-C2B	2.10	1.48	1.43
22	b	611	CLA	CHC-C1C	2.10	1.42	1.38
22	C	503	CLA	CMB-C2B	-2.10	1.46	1.50
22	c	502	CLA	C3C-C2C	2.10	1.41	1.36
22	c	513	CLA	CMD-C2D	-2.10	1.46	1.50
26	a	412	SQD	O3-C3	-2.10	1.37	1.43
22	C	512	CLA	O1D-CGD	2.10	1.26	1.21
22	B	709	CLA	CAB-C3B	-2.09	1.41	1.47
22	b	603	CLA	CMC-C2C	-2.09	1.46	1.50
30	b	622	LMG	C19-C18	2.09	1.62	1.51
22	a	405	CLA	C3B-C4B	2.09	1.48	1.42
26	A	409	SQD	O3-C3	-2.09	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	514	CLA	CMC-C2C	-2.09	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.09	1.46	1.50
23	B	719	BCR	C5-C6	-2.09	1.31	1.34
22	B	708	CLA	MG-NB	-2.09	2.01	2.05
23	C	524	BCR	C35-C13	-2.09	1.46	1.50
22	A	403	CLA	MG-NB	-2.08	2.01	2.05
23	C	515	BCR	C34-C9	-2.08	1.46	1.50
27	h	703	DGD	O3E-C3E	-2.08	1.37	1.43
34	f	101	HEC	CMC-C2C	2.08	1.55	1.50
22	b	611	CLA	O2D-CED	-2.08	1.40	1.45
25	A	408	PL9	C21-C22	2.08	1.60	1.53
23	c	515	BCR	C4-C5	-2.08	1.47	1.51
22	B	703	CLA	O2D-CGD	2.08	1.38	1.33
30	c	523	LMG	O6-C5	-2.08	1.39	1.44
23	B	719	BCR	C31-C1	-2.08	1.49	1.53
22	b	602	CLA	C1D-C2D	2.08	1.49	1.45
22	b	606	CLA	MG-NB	-2.07	2.01	2.05
23	h	702	BCR	C27-C26	-2.07	1.47	1.51
22	c	507	CLA	CMD-C2D	-2.07	1.46	1.50
30	D	409	LMG	O1-C7	-2.07	1.40	1.43
22	b	613	CLA	O2D-CED	-2.07	1.40	1.45
22	C	506	CLA	C4B-NB	2.07	1.40	1.37
30	b	620	LMG	C1-C2	2.07	1.58	1.52
31	E	101	LHG	C24-C23	2.07	1.56	1.50
23	k	102	BCR	C35-C13	-2.07	1.46	1.50
22	B	706	CLA	CAB-C3B	-2.07	1.41	1.47
23	d	405	BCR	C35-C13	-2.07	1.46	1.50
22	C	508	CLA	C4B-NB	2.06	1.40	1.37
22	c	513	CLA	MG-ND	-2.06	2.01	2.05
22	b	603	CLA	O2D-CGD	2.06	1.38	1.33
22	c	509	CLA	CMC-C2C	-2.06	1.46	1.50
23	b	617	BCR	C36-C18	-2.06	1.46	1.50
23	C	501	BCR	C39-C30	-2.06	1.49	1.53
22	c	508	CLA	CAB-C3B	-2.06	1.41	1.47
22	C	504	CLA	C3B-C4B	2.06	1.48	1.42
22	c	509	CLA	CMB-C2B	-2.05	1.46	1.50
22	d	403	CLA	CHC-C1C	2.05	1.42	1.38
23	D	405	BCR	C37-C22	-2.05	1.46	1.50
22	b	606	CLA	CMB-C2B	-2.05	1.46	1.50
23	H	101	BCR	C35-C13	-2.05	1.46	1.50
22	b	608	CLA	O2A-CGA	2.05	1.39	1.33
27	c	518	DGD	O1G-C1G	2.05	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C32-C1	-2.05	1.49	1.53
22	c	503	CLA	C4B-NB	2.05	1.40	1.37
22	B	713	CLA	C5-C3	-2.05	1.47	1.51
23	c	515	BCR	C27-C26	-2.05	1.47	1.51
22	B	703	CLA	OBD-CAD	2.05	1.26	1.22
27	c	518	DGD	C3E-C2E	2.05	1.57	1.52
22	C	510	CLA	CMC-C2C	-2.05	1.46	1.50
26	a	412	SQD	O47-C45	-2.04	1.41	1.46
22	B	714	CLA	CAB-C3B	-2.04	1.41	1.47
22	c	512	CLA	C5-C3	-2.04	1.47	1.51
22	B	704	CLA	MG-NA	2.04	2.11	2.06
22	b	611	CLA	C4B-NB	2.04	1.40	1.37
22	b	613	CLA	MG-ND	-2.04	2.01	2.05
22	B	707	CLA	CHC-C1C	2.04	1.42	1.38
22	B	716	CLA	CAB-C3B	-2.04	1.42	1.47
22	b	611	CLA	C3C-C2C	2.04	1.41	1.36
22	b	612	CLA	CMD-C2D	-2.04	1.46	1.50
22	d	403	CLA	O1D-CGD	2.04	1.26	1.21
22	C	508	CLA	C4D-CHA	2.04	1.45	1.38
22	c	510	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	510	CLA	C1D-C2D	2.03	1.49	1.45
22	B	714	CLA	MG-NB	-2.03	2.01	2.05
22	B	704	CLA	CMD-C2D	-2.03	1.46	1.50
27	C	518	DGD	C1D-C2D	2.03	1.58	1.52
33	D	408	PHO	C3D-CAD	-2.03	1.43	1.47
22	D	403	CLA	C3D-C4D	2.03	1.48	1.44
22	b	614	CLA	CHC-C1C	2.02	1.42	1.38
23	B	719	BCR	C4-C5	-2.02	1.47	1.51
22	B	702	CLA	CHC-C1C	2.02	1.42	1.38
22	D	404	CLA	C1C-NC	-2.02	1.34	1.37
22	C	503	CLA	CMC-C2C	-2.02	1.46	1.50
22	c	505	CLA	C1D-ND	2.02	1.40	1.37
22	b	616	CLA	CAC-C3C	-2.02	1.45	1.51
22	B	727	CLA	CMD-C2D	-2.02	1.46	1.50
27	A	411	DGD	O1G-C1A	2.02	1.39	1.33
22	d	404	CLA	C1B-C2B	2.02	1.47	1.43
22	C	508	CLA	MG-NB	-2.02	2.01	2.05
22	c	511	CLA	C5-C3	-2.02	1.47	1.51
22	B	707	CLA	O2D-CED	-2.02	1.40	1.45
34	v	201	HEC	C3B-C2B	-2.02	1.32	1.36
22	C	512	CLA	CHC-C4B	-2.02	1.34	1.39
22	c	510	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	101	LMG	O4-C4	-2.02	1.38	1.43
34	f	101	HEC	CHA-C4D	-2.02	1.34	1.39
22	C	513	CLA	C1A-CHA	-2.01	1.34	1.43
22	c	513	CLA	CMB-C2B	-2.01	1.46	1.50
23	H	101	BCR	C1-C6	-2.01	1.51	1.53
22	b	611	CLA	C1D-C2D	2.01	1.49	1.45
22	c	503	CLA	C1B-C2B	2.01	1.47	1.43
22	c	508	CLA	C1B-NB	-2.01	1.35	1.37
22	B	705	CLA	CHC-C1C	2.01	1.42	1.38
22	a	402	CLA	C3B-C4B	2.01	1.48	1.42
22	b	614	CLA	MG-ND	-2.01	2.01	2.05
22	c	512	CLA	C3D-C4D	2.01	1.48	1.44
22	c	504	CLA	O2D-CED	-2.01	1.40	1.45
30	b	620	LMG	O6-C1	2.01	1.47	1.41
22	B	714	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	715	CLA	C3B-C4B	2.00	1.48	1.42
22	b	615	CLA	MG-NA	2.00	2.11	2.06
27	c	518	DGD	O3G-C1D	-2.00	1.36	1.40

All (1497) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C4A-NA-C1A	12.08	112.19	106.68
26	l	101	SQD	O6-C1-C2	10.85	124.75	108.27
22	c	504	CLA	C4A-NA-C1A	9.62	111.07	106.68
26	a	412	SQD	O6-C1-C2	9.29	122.37	108.27
22	c	509	CLA	C4A-NA-C1A	8.78	110.68	106.68
22	b	604	CLA	C4A-NA-C1A	8.75	110.67	106.68
22	b	602	CLA	C4A-NA-C1A	8.61	110.61	106.68
22	C	508	CLA	C4A-NA-C1A	8.51	110.56	106.68
22	c	514	CLA	C4A-NA-C1A	8.36	110.49	106.68
22	b	614	CLA	C4A-NA-C1A	8.34	110.48	106.68
22	c	502	CLA	C4A-NA-C1A	7.97	110.32	106.68
22	h	701	CLA	C4A-NA-C1A	7.89	110.28	106.68
22	D	404	CLA	C4A-NA-C1A	7.78	110.23	106.68
22	C	514	CLA	C4A-NA-C1A	7.74	110.21	106.68
22	a	403	CLA	C4A-NA-C1A	7.72	110.20	106.68
22	B	704	CLA	C4A-NA-C1A	7.60	110.15	106.68
26	A	409	SQD	O6-C1-C2	7.57	119.76	108.27
22	C	510	CLA	C4A-NA-C1A	7.43	110.07	106.68
22	A	404	CLA	C4A-NA-C1A	7.25	109.99	106.68
22	B	706	CLA	C4A-NA-C1A	7.17	109.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	C4A-NA-C1A	7.08	109.91	106.68
22	b	612	CLA	C4A-NA-C1A	7.06	109.90	106.68
22	c	507	CLA	C4A-NA-C1A	7.05	109.90	106.68
26	B	723	SQD	O6-C1-C2	6.88	118.72	108.27
27	A	411	DGD	C4E-C3E-C2E	-6.86	98.78	110.83
22	C	506	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	c	508	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	a	410	PL9	C7-C3-C4	6.64	122.38	116.91
22	B	703	CLA	C3B-C4B-NB	-6.60	104.64	110.53
22	B	709	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	C	502	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	c	503	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	c	505	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	B	707	CLA	C4A-NA-C1A	6.13	109.48	106.68
22	B	712	CLA	C4A-NA-C1A	6.10	109.46	106.68
22	d	401	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	a	405	CLA	C4A-NA-C1A	6.02	109.43	106.68
25	D	406	PL9	C7-C3-C4	5.95	121.81	116.91
22	c	511	CLA	C4A-NA-C1A	5.95	109.39	106.68
26	l	101	SQD	O7-S-C6	5.92	115.60	106.76
22	c	512	CLA	C4A-NA-C1A	5.89	109.36	106.68
32	D	401	BCT	O2-C-O1	5.81	134.55	119.68
22	B	708	CLA	O2D-CGD-CBD	5.78	121.33	111.23
25	A	408	PL9	C7-C3-C4	5.69	121.60	116.91
22	D	404	CLA	O2D-CGD-O1D	-5.69	112.78	123.85
22	b	608	CLA	C4A-NA-C1A	5.67	109.27	106.68
22	c	506	CLA	C4A-NA-C1A	5.65	109.26	106.68
22	b	608	CLA	C3B-C4B-NB	-5.62	105.51	110.53
22	D	403	CLA	C3B-C4B-NB	-5.60	105.53	110.53
22	b	609	CLA	C4A-NA-C1A	5.40	109.14	106.68
22	b	613	CLA	C1-C2-C3	-5.39	117.36	126.20
22	B	702	CLA	C4A-NA-C1A	5.33	109.11	106.68
22	b	605	CLA	C4A-NA-C1A	5.26	109.08	106.68
34	f	101	HEC	CAB-C3B-C4B	5.24	131.60	124.79
22	B	708	CLA	O2D-CGD-O1D	-5.22	113.69	123.85
32	a	409	BCT	O2-C-O1	5.18	132.93	119.68
33	d	407	PHO	C2B-C1B-NB	-5.18	105.69	109.43
22	c	513	CLA	C1-C2-C3	-5.15	117.75	126.20
22	a	402	CLA	C4A-NA-C1A	5.11	109.01	106.68
25	d	406	PL9	C40-C39-C41	5.07	124.03	115.23
22	b	604	CLA	C1-C2-C3	-5.05	117.93	126.20
22	C	509	CLA	C4A-NA-C1A	5.02	108.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	408	PHO	C2B-C1B-NB	-4.99	105.82	109.43
30	d	410	LMG	O1-C1-C2	-4.99	100.70	108.27
32	D	401	BCT	O3-C-O1	-4.99	106.91	119.68
22	B	703	CLA	C4A-NA-C1A	4.99	108.95	106.68
22	B	714	CLA	C3B-C4B-NB	-4.96	106.10	110.53
26	D	410	SQD	O6-C1-C2	4.95	115.79	108.27
22	c	504	CLA	C11-C12-C13	-4.95	99.53	115.97
30	b	622	LMG	C1-O6-C5	-4.92	104.10	113.72
22	C	507	CLA	C4A-NA-C1A	4.91	108.92	106.68
26	A	409	SQD	O8-S-C6	4.90	115.43	105.97
33	d	407	PHO	C4D-CHA-CBD	-4.78	106.16	108.45
22	b	606	CLA	O2D-CGD-O1D	-4.75	114.61	123.85
23	B	718	BCR	C29-C30-C25	4.74	117.32	110.44
22	C	513	CLA	C4A-NA-C1A	4.72	108.83	106.68
22	b	610	CLA	CAC-C3C-C4C	4.71	130.92	124.79
22	B	715	CLA	C4A-NA-C1A	4.71	108.83	106.68
31	L	101	LHG	O4-P-O5	4.71	134.34	112.44
22	B	713	CLA	C1-C2-C3	-4.70	118.50	126.20
22	B	706	CLA	C3B-C4B-NB	-4.69	106.34	110.53
26	D	410	SQD	O8-S-C6	4.69	115.03	105.97
34	v	201	HEC	C1D-ND-C4D	4.68	110.75	105.21
22	c	509	CLA	O2D-CGD-O1D	-4.68	114.74	123.85
22	D	402	CLA	C4A-NA-C1A	4.67	108.81	106.68
33	a	404	PHO	C2B-C1B-NB	-4.66	106.06	109.43
22	c	502	CLA	O2D-CGD-O1D	-4.65	114.79	123.85
22	B	705	CLA	O1D-CGD-CBD	4.65	133.70	124.52
22	B	713	CLA	C3B-C4B-NB	-4.65	106.38	110.53
23	B	718	BCR	C15-C14-C13	-4.65	120.75	127.28
22	c	511	CLA	O2D-CGD-O1D	-4.65	114.80	123.85
25	a	410	PL9	C7-C3-C2	-4.65	117.91	123.39
22	B	705	CLA	O2D-CGD-O1D	-4.64	114.82	123.85
27	H	102	DGD	O3G-C3G-C2G	-4.64	99.54	110.82
30	b	620	LMG	O1-C1-C2	-4.62	101.26	108.27
22	b	606	CLA	C4A-NA-C1A	4.61	108.78	106.68
22	B	702	CLA	O2D-CGD-CBD	4.60	119.28	111.23
22	b	613	CLA	C4A-NA-C1A	4.59	108.77	106.68
34	F	101	HEC	CAB-C3B-C4B	-4.55	118.87	124.79
26	A	409	SQD	O9-S-O7	-4.54	99.04	113.82
22	B	705	CLA	C4A-NA-C1A	4.53	108.75	106.68
22	b	606	CLA	O2D-CGD-CBD	4.53	119.15	111.23
34	V	201	HEC	CHB-C4A-NA	4.52	129.38	124.45
31	E	101	LHG	O4-P-O5	4.52	133.47	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	703	DGD	C4E-C3E-C2E	-4.49	102.95	110.83
26	f	102	SQD	O9-S-O7	-4.48	99.26	113.82
31	a	413	LHG	O4-P-O5	4.48	133.27	112.44
22	b	611	CLA	C4A-NA-C1A	4.47	108.72	106.68
25	D	406	PL9	C30-C29-C31	-4.47	107.47	115.23
22	C	511	CLA	C4A-NA-C1A	4.44	108.70	106.68
22	b	616	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
27	C	517	DGD	O3G-C3G-C2G	-4.41	100.10	110.82
22	B	710	CLA	C4A-NA-C1A	4.40	108.69	106.68
26	A	409	SQD	O7-S-C6	4.40	113.33	106.76
26	B	723	SQD	O7-S-C6	4.38	113.30	106.76
25	d	406	PL9	C7-C3-C4	4.38	120.52	116.91
23	b	617	BCR	C2-C1-C6	4.37	116.78	110.44
34	f	101	HEC	CBD-CAD-C3D	-4.36	100.47	112.53
26	A	409	SQD	C3-C4-C5	4.35	118.12	110.23
33	D	408	PHO	O1D-CGD-CBD	4.34	131.31	124.72
27	C	518	DGD	O2D-C2D-C1D	-4.32	99.79	110.08
26	l	101	SQD	O9-S-C6	4.31	113.19	106.76
22	B	708	CLA	C4A-NA-C1A	4.31	108.65	106.68
34	v	201	HEC	CHB-C1B-NB	4.31	129.06	124.42
22	d	403	CLA	C4A-NA-C1A	4.29	108.64	106.68
22	B	705	CLA	C7-C6-C5	-4.28	101.85	113.26
22	b	611	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
26	B	723	SQD	O47-C7-C8	4.26	120.70	111.48
31	d	409	LHG	O4-P-O5	4.25	132.23	112.44
22	c	506	CLA	C3B-C4B-NB	-4.24	106.75	110.53
22	B	710	CLA	O2D-CGD-O1D	-4.23	115.62	123.85
33	D	408	PHO	C4D-CHA-CBD	-4.22	106.43	108.45
22	b	612	CLA	CHB-C4A-NA	4.22	130.49	124.40
34	F	101	HEC	C1D-ND-C4D	4.20	110.18	105.21
31	D	412	LHG	O4-P-O5	4.19	131.94	112.44
22	d	404	CLA	C3B-C4B-NB	-4.19	106.79	110.53
23	B	719	BCR	C2-C1-C6	4.19	116.52	110.44
22	a	402	CLA	CMB-C2B-C1B	-4.17	119.07	125.42
22	A	402	CLA	C4A-NA-C1A	4.16	108.58	106.68
27	C	518	DGD	O3G-C3G-C2G	-4.15	100.73	110.82
22	b	609	CLA	CMB-C2B-C1B	-4.14	119.11	125.42
31	a	411	LHG	O4-P-O5	4.13	131.65	112.44
22	B	710	CLA	CAA-C2A-C3A	-4.12	101.86	113.00
22	A	403	CLA	C4A-NA-C1A	4.12	108.56	106.68
22	A	403	CLA	CED-O2D-CGD	-4.12	106.57	115.92
26	a	414	SQD	O48-C23-O10	-4.11	113.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O7-S-C6	4.11	112.90	106.76
26	D	410	SQD	O9-S-C6	4.11	112.89	106.76
26	D	410	SQD	C3-C4-C5	4.11	117.68	110.23
22	B	716	CLA	C3B-C4B-NB	-4.10	106.87	110.53
22	b	607	CLA	C3B-C4B-NB	-4.09	106.88	110.53
26	a	412	SQD	C3-C4-C5	4.09	117.65	110.23
22	B	727	CLA	CAA-C2A-C3A	-4.09	101.95	113.00
31	a	411	LHG	O8-C23-O10	-4.07	113.44	123.63
26	f	102	SQD	O6-C1-C2	4.07	114.45	108.27
23	B	717	BCR	C2-C1-C6	4.06	116.33	110.44
22	b	610	CLA	C4A-NA-C1A	4.06	108.53	106.68
22	b	605	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
31	D	411	LHG	O4-P-O5	4.05	131.27	112.44
23	B	719	BCR	C29-C30-C25	4.04	116.31	110.44
22	C	514	CLA	C3A-C2A-C1A	4.04	107.38	101.34
22	C	507	CLA	C3B-C4B-NB	-4.00	106.96	110.53
25	A	408	PL9	C7-C3-C2	-3.98	118.69	123.39
22	B	708	CLA	C3B-C4B-NB	-3.98	106.98	110.53
22	b	605	CLA	O1D-CGD-CBD	3.97	132.35	124.52
33	d	407	PHO	O1D-CGD-CBD	3.97	130.74	124.72
26	D	410	SQD	C1-C2-C3	-3.96	101.67	110.01
22	C	503	CLA	C3B-C4B-NB	-3.96	106.99	110.53
27	C	518	DGD	O5D-C6D-C5D	-3.95	100.52	109.42
26	A	410	SQD	C45-O47-C7	3.94	123.47	117.78
31	a	411	LHG	O8-C23-C24	3.94	123.84	111.83
27	C	519	DGD	O3G-C3G-C2G	-3.92	101.28	110.82
22	b	613	CLA	O2D-CGD-CBD	3.92	118.08	111.23
22	b	603	CLA	C4A-NA-C1A	3.91	108.47	106.68
22	c	507	CLA	C1-O2A-CGA	3.91	126.12	116.65
22	b	615	CLA	CMB-C2B-C1B	-3.91	119.47	125.42
22	D	402	CLA	C1-C2-C3	-3.90	119.81	126.20
22	b	611	CLA	O2D-CGD-CBD	3.89	118.04	111.23
33	D	407	PHO	C1A-C2A-C3A	-3.89	99.14	102.84
23	c	516	BCR	C27-C26-C25	3.89	127.95	122.70
31	d	408	LHG	O4-P-O5	3.87	130.45	112.44
26	A	409	SQD	C1-C2-C3	-3.87	101.87	110.01
22	b	603	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
22	B	727	CLA	C4A-NA-C1A	3.83	108.43	106.68
22	B	710	CLA	O2D-CGD-CBD	3.83	117.92	111.23
26	a	412	SQD	O8-S-C6	3.83	113.36	105.97
22	b	606	CLA	C3B-C4B-NB	-3.82	107.12	110.53
27	h	703	DGD	O3G-C3G-C2G	-3.82	101.53	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	j	101	STE	O2-C1-C2	3.82	126.06	114.00
27	H	102	DGD	C1E-O6E-C5E	3.80	121.13	113.72
23	C	524	BCR	C11-C10-C9	-3.79	121.96	127.28
33	d	407	PHO	C1-C2-C3	-3.78	120.00	126.20
27	H	102	DGD	C3E-C4E-C5E	-3.78	103.38	110.23
22	B	713	CLA	C4A-NA-C1A	3.78	108.40	106.68
33	D	407	PHO	CBC-CAC-C3C	-3.78	107.47	112.87
22	C	513	CLA	C1-C2-C3	-3.75	120.05	126.20
30	C	516	LMG	O6-C1-O1	-3.75	101.17	110.04
22	C	504	CLA	C4D-CHA-C1A	3.75	125.72	121.24
26	B	723	SQD	O48-C23-O10	-3.75	114.25	123.63
22	C	504	CLA	C7-C6-C5	-3.74	103.30	113.26
26	l	101	SQD	O48-C23-C24	3.74	123.23	111.83
31	l	102	LHG	O4-P-O5	3.73	129.78	112.44
22	C	506	CLA	C3B-C4B-NB	-3.73	107.20	110.53
26	l	101	SQD	O47-C7-C8	3.73	119.54	111.48
26	B	723	SQD	O5-C5-C4	3.72	116.41	109.70
34	V	201	HEC	CBD-CAD-C3D	-3.72	102.25	112.53
22	b	609	CLA	C3B-C4B-NB	-3.72	107.21	110.53
28	m	102	STE	O2-C1-O1	-3.71	113.79	123.33
22	C	505	CLA	O2A-CGA-O1A	-3.70	114.37	123.63
23	b	618	BCR	C36-C18-C17	-3.69	116.83	122.82
34	F	101	HEC	CAB-C3B-C2B	3.69	134.34	127.56
31	B	722	LHG	O8-C23-C24	3.69	123.08	111.83
22	b	615	CLA	C4A-NA-C1A	3.69	108.36	106.68
30	a	418	LMG	C1-C2-C3	-3.68	102.26	110.01
22	B	716	CLA	C4A-NA-C1A	3.68	108.36	106.68
22	B	727	CLA	CAA-CBA-CGA	-3.68	102.76	113.21
33	a	404	PHO	C3B-C4B-NB	-3.68	105.07	107.46
22	B	715	CLA	O2D-CGD-CBD	3.68	117.66	111.23
22	b	602	CLA	CHB-C4A-NA	3.67	129.70	124.40
27	c	519	DGD	O5D-C1E-C2E	3.65	113.82	108.27
25	d	406	PL9	C42-C43-C44	-3.64	119.29	127.62
26	a	414	SQD	O47-C7-C8	3.64	119.36	111.48
25	D	406	PL9	C7-C3-C2	-3.64	119.10	123.39
26	A	409	SQD	O47-C7-C8	3.63	119.33	111.48
22	D	404	CLA	O2D-CGD-CBD	3.61	117.55	111.23
23	T	701	BCR	C27-C26-C25	3.61	127.59	122.70
30	d	410	LMG	O2-C2-C1	-3.61	101.47	110.08
22	C	502	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
22	C	509	CLA	C3B-C4B-NB	-3.60	107.31	110.53
30	C	520	LMG	O1-C1-C2	-3.60	102.80	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	C4A-NA-C1A	3.60	108.32	106.68
30	C	520	LMG	O2-C2-C1	-3.60	101.50	110.08
22	C	513	CLA	C3B-C4B-NB	-3.60	107.32	110.53
34	F	101	HEC	CBD-CAD-C3D	-3.60	102.58	112.53
22	C	505	CLA	C4A-NA-C1A	3.60	108.32	106.68
25	a	410	PL9	C22-C23-C24	-3.59	119.40	127.62
22	C	512	CLA	C4A-NA-C1A	3.59	108.32	106.68
26	a	412	SQD	O9-S-O7	-3.59	102.15	113.82
30	d	410	LMG	C7-O1-C1	-3.59	106.11	113.80
31	B	722	LHG	O4-P-O5	3.58	129.11	112.44
27	c	517	DGD	O3G-C3G-C2G	-3.58	102.11	110.82
22	c	513	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
22	B	712	CLA	C16-C15-C13	-3.57	104.11	115.97
27	c	519	DGD	O3G-C3G-C2G	-3.56	102.15	110.82
22	a	402	CLA	C3B-C4B-NB	-3.56	107.35	110.53
30	c	520	LMG	C9-C8-C7	-3.56	103.48	111.78
27	c	518	DGD	O3G-C3G-C2G	-3.56	102.16	110.82
28	d	411	STE	O2-C1-C2	3.56	125.24	114.00
22	B	712	CLA	C11-C12-C13	-3.56	104.15	115.97
22	b	603	CLA	C3B-C4B-NB	-3.55	107.36	110.53
26	B	723	SQD	O9-S-O7	-3.52	102.37	113.82
23	b	617	BCR	C29-C30-C25	3.52	115.55	110.44
22	c	505	CLA	C3B-C4B-NB	-3.50	107.40	110.53
22	b	607	CLA	C4A-NA-C1A	3.50	108.28	106.68
27	C	518	DGD	O4D-C4D-C3D	3.50	118.62	110.38
22	C	514	CLA	O2A-CGA-O1A	-3.50	114.88	123.63
22	a	403	CLA	O2D-CGD-CBD	3.49	117.33	111.23
27	A	411	DGD	O3G-C3G-C2G	-3.48	102.34	110.82
23	a	406	BCR	C34-C9-C10	-3.48	117.17	122.82
26	a	412	SQD	C1-C2-C3	-3.48	102.69	110.01
22	b	610	CLA	C1-C2-C3	-3.48	120.50	126.20
33	D	407	PHO	C2B-C1B-NB	-3.48	106.92	109.43
22	C	503	CLA	C4A-NA-C1A	3.47	108.26	106.68
22	b	610	CLA	CAA-CBA-CGA	-3.47	103.35	113.21
22	c	504	CLA	C3B-C4B-NB	-3.47	107.43	110.53
22	b	604	CLA	CHB-C4A-NA	3.47	129.41	124.40
22	h	701	CLA	CHB-C4A-NA	3.47	129.40	124.40
22	c	505	CLA	CMB-C2B-C1B	-3.47	120.14	125.42
26	l	101	SQD	O5-C5-C4	3.46	115.94	109.70
22	B	715	CLA	C5-C3-C2	-3.46	113.39	121.17
22	d	403	CLA	CED-O2D-CGD	-3.45	108.08	115.92
26	l	101	SQD	O9-S-O7	-3.45	102.61	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	CED-O2D-CGD	-3.44	108.10	115.92
27	h	703	DGD	C4D-C3D-C2D	-3.44	104.78	110.83
23	A	405	BCR	C27-C26-C25	3.43	127.34	122.70
22	c	507	CLA	CBC-CAC-C3C	-3.43	103.11	112.42
30	D	409	LMG	C3-C4-C5	-3.43	104.02	110.23
22	C	513	CLA	O2A-CGA-O1A	-3.42	115.07	123.63
22	a	405	CLA	O2A-CGA-O1A	-3.41	115.09	123.63
26	l	101	SQD	C3-C4-C5	3.41	116.42	110.23
22	b	603	CLA	CHB-C1B-NB	3.40	129.15	124.05
22	B	705	CLA	C3B-C4B-NB	-3.39	107.50	110.53
33	d	407	PHO	O2D-CGD-O1D	-3.39	117.25	123.85
33	D	408	PHO	C3B-C4B-NB	-3.38	105.26	107.46
27	A	411	DGD	O6E-C1E-O5D	-3.38	102.06	110.04
26	B	723	SQD	O8-S-C6	3.38	112.50	105.97
30	M	101	LMG	C9-C8-C7	-3.38	103.91	111.78
33	D	408	PHO	O2D-CGD-O1D	-3.37	117.28	123.85
26	A	409	SQD	O47-C7-O49	-3.37	115.83	123.70
22	b	602	CLA	O2D-CGD-CBD	3.36	117.11	111.23
25	D	406	PL9	C22-C23-C24	-3.36	119.94	127.62
22	b	603	CLA	CMB-C2B-C1B	-3.36	120.31	125.42
22	h	701	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
22	c	503	CLA	O1D-CGD-CBD	3.35	131.13	124.52
22	b	605	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
22	b	605	CLA	C3B-C4B-NB	-3.35	107.54	110.53
22	c	510	CLA	O2A-CGA-O1A	-3.34	115.27	123.63
34	f	101	HEC	CAB-C3B-C2B	-3.34	121.42	127.56
27	h	703	DGD	O2D-C2D-C1D	-3.34	102.11	110.08
25	d	406	PL9	C36-C34-C33	-3.33	113.68	121.17
34	f	101	HEC	CHB-C1B-NB	3.33	128.01	124.42
26	B	723	SQD	C3-C4-C5	3.32	116.26	110.23
22	C	513	CLA	CHB-C4A-NA	3.32	129.19	124.40
33	a	404	PHO	OBD-CAD-CBD	-3.32	120.95	125.82
22	B	711	CLA	C3B-C4B-NB	-3.31	107.57	110.53
34	f	101	HEC	CBA-CAA-C2A	-3.31	103.37	112.53
22	B	708	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
22	A	404	CLA	CHB-C4A-NA	3.31	129.17	124.40
30	D	409	LMG	O3-C3-C2	-3.30	102.59	110.38
23	D	405	BCR	C3-C4-C5	-3.30	108.17	114.06
22	a	403	CLA	CHB-C4A-NA	3.29	129.16	124.40
22	b	615	CLA	C3B-C4B-NB	-3.29	107.59	110.53
23	B	717	BCR	C29-C30-C25	3.29	115.22	110.44
22	B	702	CLA	O2D-CGD-O1D	-3.29	117.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	518	DGD	O5D-C1E-C2E	3.29	113.27	108.27
26	f	102	SQD	O5-C5-C4	3.28	115.62	109.70
22	C	511	CLA	C3B-C4B-NB	-3.28	107.60	110.53
33	a	404	PHO	CBC-CAC-C3C	-3.28	108.18	112.87
28	m	102	STE	O2-C1-C2	3.27	124.35	114.00
22	B	714	CLA	CHC-C4B-NB	3.27	128.95	124.05
22	c	508	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
22	C	514	CLA	C4-C3-C5	3.27	120.90	115.23
22	c	510	CLA	CHB-C4A-NA	3.27	129.11	124.40
22	B	708	CLA	CHC-C4B-NB	3.26	128.94	124.05
23	H	101	BCR	C2-C1-C6	3.26	115.18	110.44
22	B	704	CLA	C3B-C4B-NB	-3.25	107.62	110.53
22	B	712	CLA	CMB-C2B-C3B	3.25	134.19	126.55
22	b	614	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
27	h	703	DGD	O6D-C1D-C2D	-3.24	103.71	110.37
22	C	505	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
23	h	702	BCR	C27-C26-C25	3.24	127.08	122.70
22	b	608	CLA	CHB-C1B-NB	3.24	128.91	124.05
26	l	101	SQD	O2-C2-C1	3.24	117.79	110.08
33	D	407	PHO	CMB-C2B-C3B	3.24	131.15	124.68
22	C	504	CLA	C4A-NA-C1A	3.24	108.16	106.68
27	C	518	DGD	C3D-C4D-C5D	-3.23	104.38	110.23
22	C	508	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
22	B	704	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
23	C	515	BCR	C36-C18-C17	-3.21	117.61	122.82
22	c	503	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
22	B	712	CLA	C3B-C4B-NB	-3.21	107.66	110.53
27	c	518	DGD	O6D-C1D-O3G	-3.21	102.46	110.04
22	b	616	CLA	CMB-C2B-C1B	-3.21	120.54	125.42
23	a	406	BCR	C40-C30-C25	3.21	115.27	110.24
23	b	617	BCR	C27-C26-C25	3.21	127.03	122.70
22	b	607	CLA	C1-O2A-CGA	3.20	124.41	116.65
22	c	502	CLA	O2D-CGD-CBD	3.20	116.82	111.23
22	d	401	CLA	CMC-C2C-C1C	3.19	130.02	125.03
22	c	514	CLA	C3B-C4B-NB	-3.18	107.69	110.53
33	a	404	PHO	C1-C2-C3	-3.18	120.98	126.20
30	M	101	LMG	C38-C37-C36	-3.18	98.28	114.37
23	B	719	BCR	C3-C4-C5	-3.18	108.38	114.06
22	c	512	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
23	d	405	BCR	C27-C26-C25	3.17	126.99	122.70
26	a	414	SQD	O48-C23-C24	3.17	121.50	111.83
22	B	704	CLA	CHB-C4A-NA	3.17	128.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	k	102	BCR	C2-C1-C6	3.17	115.04	110.44
22	B	703	CLA	O2A-CGA-O1A	-3.17	115.71	123.63
23	b	617	BCR	C15-C14-C13	-3.16	122.85	127.28
22	a	402	CLA	CMB-C2B-C3B	3.16	133.97	126.55
22	B	705	CLA	OBD-CAD-C3D	3.15	135.78	128.42
22	b	608	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
26	A	410	SQD	O47-C45-C44	3.15	115.01	107.96
34	v	201	HEC	CHD-C1D-ND	3.15	128.26	124.37
22	B	712	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
22	c	503	CLA	C3B-C4B-NB	-3.15	107.72	110.53
22	c	507	CLA	O1D-CGD-CBD	3.15	130.72	124.52
26	a	412	SQD	O47-C7-O49	-3.14	116.36	123.70
23	c	516	BCR	C2-C1-C6	3.14	115.00	110.44
33	D	408	PHO	C1-C2-C3	-3.14	121.06	126.20
22	A	404	CLA	O2D-CGD-CBD	3.13	116.70	111.23
22	c	512	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	D	406	PL9	C42-C43-C44	-3.12	120.47	127.62
33	a	404	PHO	CMA-C3A-C4A	-3.12	107.88	114.61
22	c	509	CLA	O2D-CGD-CBD	3.12	116.68	111.23
33	D	408	PHO	CMB-C2B-C3B	3.12	130.91	124.68
22	b	614	CLA	CHD-C1D-ND	-3.11	120.42	124.80
22	C	502	CLA	C3B-C4B-NB	-3.11	107.75	110.53
22	b	606	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
30	c	520	LMG	O6-C1-O1	-3.11	102.70	110.04
23	B	718	BCR	C35-C13-C14	-3.11	117.78	122.82
22	B	707	CLA	C3B-C4B-NB	-3.11	107.76	110.53
22	c	509	CLA	CHB-C4A-NA	3.10	128.87	124.40
23	c	515	BCR	C33-C5-C6	-3.10	121.11	124.48
27	c	517	DGD	O3G-C1D-C2D	-3.09	103.58	108.27
22	b	607	CLA	C6-C7-C8	-3.09	105.69	115.97
22	d	403	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
22	b	616	CLA	CMB-C2B-C3B	3.09	133.81	126.55
22	b	616	CLA	C4A-NA-C1A	3.09	108.09	106.68
22	c	508	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
28	J	101	STE	C3-C2-C1	-3.08	106.48	114.51
22	c	513	CLA	CHB-C4A-NA	3.08	128.84	124.40
23	a	406	BCR	C29-C30-C25	3.08	114.91	110.44
22	A	404	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
22	a	403	CLA	C4D-C3D-CAD	-3.06	104.78	108.11
22	c	504	CLA	CHB-C4A-NA	3.06	128.82	124.40
28	C	521	STE	C3-C2-C1	-3.06	106.52	114.51
27	H	102	DGD	C3G-C2G-C1G	-3.06	104.65	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	716	CLA	CED-O2D-CGD	-3.06	108.98	115.92
22	C	509	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
23	c	516	BCR	C8-C9-C10	3.05	123.81	119.01
22	B	706	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
22	c	511	CLA	C3B-C4B-NB	-3.05	107.81	110.53
22	b	602	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
27	c	519	DGD	O6E-C1E-C2E	-3.05	104.10	110.37
22	B	713	CLA	CAC-C3C-C4C	3.05	128.76	124.79
22	B	712	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
27	A	411	DGD	C3G-C2G-C1G	-3.05	104.68	111.78
23	b	617	BCR	C36-C18-C17	-3.05	117.88	122.82
22	c	505	CLA	O2A-CGA-O1A	-3.04	116.02	123.63
22	d	403	CLA	CMB-C2B-C3B	3.04	133.70	126.55
23	a	406	BCR	C39-C30-C25	-3.04	105.47	110.24
26	B	723	SQD	O48-C23-C24	3.03	121.09	111.83
25	D	406	PL9	C7-C8-C9	-3.03	121.61	126.83
23	C	524	BCR	C2-C1-C6	3.03	114.84	110.44
22	B	716	CLA	CAA-CBA-CGA	-3.03	104.60	113.21
26	A	409	SQD	O48-C23-O10	-3.03	116.05	123.63
22	B	710	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	A	402	CLA	CMB-C2B-C3B	3.03	133.67	126.55
23	k	102	BCR	C27-C26-C25	3.03	126.80	122.70
22	b	616	CLA	C3B-C4B-NB	-3.03	107.83	110.53
33	D	408	PHO	C1A-C2A-C3A	-3.02	99.96	102.84
26	A	409	SQD	O4-C4-C3	-3.02	103.26	110.38
22	b	609	CLA	C4D-CHA-C1A	3.02	124.84	121.24
22	c	512	CLA	O2D-CGD-CBD	3.02	116.50	111.23
22	b	615	CLA	CHB-C1B-NB	3.01	128.57	124.05
22	A	403	CLA	C3A-C2A-C1A	3.01	105.85	101.34
22	c	514	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
28	x	101	STE	C3-C2-C1	-3.00	106.68	114.51
23	c	515	BCR	C2-C1-C6	3.00	114.79	110.44
22	c	502	CLA	CED-O2D-CGD	-2.99	109.12	115.92
22	B	727	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
33	a	404	PHO	C4D-CHA-CBD	-2.99	107.02	108.45
27	C	519	DGD	C4D-C3D-C2D	-2.99	105.58	110.83
26	D	410	SQD	O48-C23-O10	-2.99	116.15	123.63
22	C	510	CLA	CED-O2D-CGD	2.99	122.70	115.92
22	C	502	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
22	D	403	CLA	CHC-C4B-NB	2.98	128.52	124.05
27	H	102	DGD	O2D-C2D-C1D	-2.98	102.97	110.08
26	f	102	SQD	C45-O47-C7	2.98	124.93	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CMB-C2B-C3B	2.98	133.56	126.55
23	b	619	BCR	C37-C22-C21	-2.98	117.99	122.82
27	h	703	DGD	C6D-C5D-C4D	2.98	118.31	112.07
31	B	722	LHG	O8-C23-O10	-2.97	116.19	123.63
27	A	411	DGD	O3G-C1D-C2D	-2.97	103.76	108.27
26	l	101	SQD	O5-C1-C2	-2.97	104.27	110.37
23	C	524	BCR	C34-C9-C10	-2.97	118.01	122.82
27	c	518	DGD	C4D-C3D-C2D	2.96	116.03	110.83
30	c	523	LMG	O6-C1-O1	-2.96	103.06	110.04
27	c	517	DGD	C4E-C3E-C2E	-2.96	105.64	110.83
22	a	405	CLA	CAC-C3C-C4C	2.96	128.64	124.79
23	b	619	BCR	C12-C13-C14	-2.95	114.36	119.01
30	C	516	LMG	C9-C8-C7	-2.95	104.90	111.78
25	d	406	PL9	O1-C4-C3	-2.95	117.62	120.73
23	t	701	BCR	C27-C26-C25	2.95	126.69	122.70
22	B	710	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
22	c	509	CLA	CHD-C1D-ND	-2.94	120.66	124.80
22	b	611	CLA	CMC-C2C-C1C	-2.94	120.43	125.03
26	f	102	SQD	O47-C7-O49	-2.94	116.83	123.70
26	D	410	SQD	O48-C23-C24	2.94	120.80	111.83
30	b	620	LMG	O3-C3-C2	-2.94	103.44	110.38
22	b	613	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
22	C	507	CLA	O1D-CGD-CBD	2.94	130.31	124.52
25	A	408	PL9	C20-C19-C21	2.93	120.32	115.23
22	C	504	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	a	403	CLA	CAC-C3C-C4C	2.92	128.59	124.79
22	B	710	CLA	CMD-C2D-C3D	2.92	134.39	127.69
30	b	620	LMG	C9-C8-C7	-2.92	104.98	111.78
22	c	507	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	h	701	CLA	O1D-CGD-CBD	2.92	130.27	124.52
22	d	404	CLA	O2A-CGA-O1A	-2.92	116.34	123.63
23	H	101	BCR	C27-C26-C25	2.91	126.64	122.70
22	A	402	CLA	CMB-C2B-C1B	-2.91	120.98	125.42
25	d	406	PL9	C22-C23-C24	-2.91	120.96	127.62
33	a	404	PHO	C3D-C4D-ND	2.91	111.44	107.71
23	d	405	BCR	C33-C5-C6	-2.91	121.31	124.48
22	b	612	CLA	C11-C12-C13	-2.90	106.31	115.97
22	b	610	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
27	c	517	DGD	CDB-CCB-CBB	-2.90	99.71	114.37
30	D	409	LMG	O1-C1-C2	-2.90	103.87	108.27
23	c	516	BCR	C1-C6-C5	-2.89	118.68	122.64
22	C	514	CLA	O2D-CGD-O1D	-2.89	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	710	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	a	414	SQD	O49-C7-C8	-2.89	112.50	123.78
22	B	714	CLA	O1D-CGD-CBD	2.88	130.21	124.52
28	d	411	STE	O2-C1-O1	-2.88	115.92	123.33
27	c	519	DGD	C8B-C7B-C6B	-2.88	99.81	114.37
33	d	407	PHO	C3B-C4B-NB	-2.88	105.59	107.46
23	D	405	BCR	C2-C1-C6	2.88	114.62	110.44
22	b	614	CLA	O2D-CGD-CBD	2.88	116.26	111.23
27	c	518	DGD	O2E-C2E-C1E	-2.88	103.22	110.08
22	C	504	CLA	CMB-C2B-C1B	-2.88	121.04	125.42
25	A	408	PL9	C36-C34-C33	-2.87	114.72	121.17
30	b	622	LMG	O6-C5-C6	2.86	113.53	106.44
22	B	709	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
25	d	406	PL9	C37-C38-C39	-2.86	121.08	127.62
23	b	619	BCR	C2-C1-C6	2.86	114.59	110.44
22	b	606	CLA	CED-O2D-CGD	-2.86	109.43	115.92
22	d	404	CLA	CGD-CBD-CAD	-2.86	101.59	110.85
26	D	410	SQD	C46-C45-C44	-2.86	104.43	113.67
27	h	703	DGD	O3E-C3E-C2E	-2.85	103.65	110.38
22	d	401	CLA	C1-O2A-CGA	2.85	123.55	116.65
22	b	613	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	C	504	CLA	CMA-C3A-C4A	2.85	119.42	111.77
27	h	703	DGD	CDB-CCB-CBB	-2.85	99.98	114.37
22	b	614	CLA	CHB-C4A-NA	2.84	128.50	124.40
22	B	702	CLA	CHD-C1D-ND	-2.84	120.81	124.80
26	a	412	SQD	O9-S-C6	2.84	111.00	106.76
22	B	711	CLA	C4A-NA-C1A	2.83	107.97	106.68
23	c	516	BCR	C35-C13-C14	-2.83	118.23	122.82
30	b	622	LMG	O8-C28-O10	-2.83	116.55	123.63
22	A	403	CLA	C1-O2A-CGA	2.83	123.50	116.65
34	v	201	HEC	CHA-C4D-ND	2.83	127.47	124.42
30	M	101	LMG	C1-O6-C5	-2.83	108.20	113.72
25	A	408	PL9	O1-C4-C3	-2.82	117.75	120.73
25	a	410	PL9	C36-C34-C33	-2.82	114.83	121.17
22	C	502	CLA	O2D-CGD-CBD	2.82	116.16	111.23
23	t	701	BCR	C1-C6-C5	-2.82	118.78	122.64
22	C	507	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
23	a	406	BCR	C2-C1-C6	2.81	114.53	110.44
22	d	401	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	H	101	BCR	C29-C30-C25	2.81	114.52	110.44
23	k	101	BCR	C27-C26-C25	2.80	126.49	122.70
23	A	405	BCR	C38-C26-C25	-2.80	121.43	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	BCR	C27-C26-C25	2.80	126.49	122.70
22	B	706	CLA	C6-C5-C3	-2.80	106.65	113.47
22	c	504	CLA	CHC-C4B-NB	2.80	128.25	124.05
34	f	101	HEC	C1D-ND-C4D	2.80	108.52	105.21
22	B	702	CLA	CMB-C2B-C1B	-2.79	121.16	125.42
22	B	713	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
25	d	406	PL9	C17-C18-C19	-2.79	121.23	127.62
22	c	508	CLA	O1D-CGD-CBD	2.79	130.02	124.52
22	b	612	CLA	O1D-CGD-CBD	2.79	130.02	124.52
23	T	701	BCR	C7-C8-C9	-2.79	122.11	126.23
26	f	102	SQD	O8-S-C6	2.78	111.35	105.97
23	b	618	BCR	C15-C14-C13	-2.78	123.37	127.28
28	B	720	STE	C3-C2-C1	-2.78	107.25	114.51
22	d	404	CLA	C4A-NA-C1A	2.78	107.95	106.68
22	C	507	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	Y	101	BCR	C27-C26-C25	2.78	126.46	122.70
22	d	401	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
23	B	719	BCR	C30-C25-C26	-2.78	118.84	122.64
25	a	410	PL9	C35-C34-C36	2.78	120.05	115.23
30	C	516	LMG	C36-C35-C34	-2.77	100.34	114.37
22	B	708	CLA	CHD-C1D-ND	-2.77	120.90	124.80
25	A	408	PL9	C25-C24-C26	2.77	120.04	115.23
30	b	620	LMG	O7-C10-O9	-2.77	117.24	123.70
22	d	404	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
23	d	405	BCR	C2-C1-C6	2.76	114.45	110.44
25	a	410	PL9	C37-C38-C39	-2.76	121.30	127.62
30	d	410	LMG	C3-C4-C5	-2.76	105.23	110.23
22	c	511	CLA	C7-C6-C5	-2.76	105.91	113.26
22	B	706	CLA	CHD-C1D-ND	-2.76	120.92	124.80
22	a	403	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
22	b	602	CLA	C1-C2-C3	-2.75	121.68	126.20
27	C	518	DGD	C1D-O6D-C5D	-2.75	108.35	113.72
22	B	711	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
23	d	405	BCR	C16-C15-C14	-2.75	117.89	123.52
30	c	523	LMG	C9-C8-C7	-2.75	105.38	111.78
22	B	708	CLA	C6-C7-C8	-2.75	106.83	115.97
26	a	412	SQD	O48-C23-C24	2.74	120.20	111.83
22	D	403	CLA	CAA-C2A-C1A	-2.74	102.98	111.97
22	A	404	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
34	V	201	HEC	C1D-C2D-C3D	-2.74	104.09	106.98
31	E	101	LHG	O8-C23-O10	-2.74	116.77	123.63
22	C	510	CLA	CMC-C2C-C1C	-2.74	120.75	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	718	BCR	C39-C30-C25	-2.74	105.95	110.24
27	C	518	DGD	O6E-C1E-O5D	-2.74	103.58	110.04
23	A	405	BCR	C33-C5-C6	-2.74	121.50	124.48
23	A	405	BCR	C16-C15-C14	-2.73	117.93	123.52
26	f	102	SQD	C1-C2-C3	-2.73	104.27	110.01
27	h	703	DGD	O3E-C3E-C4E	2.73	116.81	110.38
22	D	402	CLA	CHB-C4A-NA	2.73	128.34	124.40
22	d	401	CLA	CMD-C2D-C3D	2.72	133.94	127.69
22	b	604	CLA	C3B-C4B-NB	-2.72	108.10	110.53
22	A	403	CLA	C4-C3-C5	-2.72	110.51	115.23
30	b	622	LMG	O1-C7-C8	-2.72	104.21	110.82
22	C	510	CLA	C6-C5-C3	-2.72	106.85	113.47
26	l	101	SQD	C1-C2-C3	-2.71	104.30	110.01
22	c	505	CLA	CMA-C3A-C4A	2.71	119.06	111.77
22	B	727	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
27	C	519	DGD	O6D-C1D-O3G	-2.71	103.64	110.04
22	A	402	CLA	C3B-C4B-NB	-2.71	108.11	110.53
30	a	418	LMG	C1-O6-C5	-2.70	108.44	113.72
22	c	505	CLA	CMB-C2B-C3B	2.70	132.90	126.55
34	F	101	HEC	CHC-C4B-NB	2.70	127.71	124.37
22	C	514	CLA	C6-C5-C3	2.70	120.04	113.47
22	b	608	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
23	H	101	BCR	C11-C10-C9	-2.70	123.49	127.28
30	c	522	LMG	O7-C10-O9	-2.70	117.40	123.70
22	b	605	CLA	C16-C15-C13	-2.70	107.00	115.97
27	h	703	DGD	O5D-C6D-C5D	-2.70	103.34	109.42
22	b	603	CLA	CHD-C1D-ND	-2.69	121.01	124.80
22	C	511	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
22	c	514	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
26	a	412	SQD	C1-O5-C5	-2.69	108.46	113.72
30	c	522	LMG	O2-C2-C1	-2.69	103.66	110.08
30	b	622	LMG	C3-C4-C5	-2.69	105.35	110.23
22	B	727	CLA	C1-C2-C3	-2.69	121.79	126.20
30	c	522	LMG	C3-C4-C5	-2.69	105.36	110.23
23	b	618	BCR	C8-C7-C6	-2.69	119.82	127.00
22	B	713	CLA	C7-C6-C5	-2.68	106.11	113.26
23	b	618	BCR	C27-C26-C25	2.68	126.33	122.70
31	D	411	LHG	C18-C17-C16	-2.68	100.81	114.37
22	c	509	CLA	C1-C2-C3	-2.68	121.80	126.20
22	b	609	CLA	CMB-C2B-C3B	2.68	132.85	126.55
27	C	519	DGD	C3G-C2G-C1G	-2.68	105.54	111.78
34	f	101	HEC	CHD-C4C-NC	2.68	128.71	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
22	b	602	CLA	CMB-C2B-C3B	2.68	132.84	126.55
34	F	101	HEC	CBB-CAB-C3B	2.67	119.67	112.42
25	D	406	PL9	C20-C19-C21	2.67	119.87	115.23
22	C	509	CLA	CHD-C1D-ND	-2.67	121.04	124.80
23	C	515	BCR	C15-C16-C17	-2.67	118.05	123.52
22	b	612	CLA	C1-C2-C3	-2.67	121.82	126.20
23	b	618	BCR	C30-C25-C26	-2.67	118.98	122.64
23	C	524	BCR	C8-C9-C10	2.67	123.20	119.01
33	D	407	PHO	C1-C2-C3	-2.67	121.83	126.20
23	k	102	BCR	C24-C23-C22	-2.67	122.29	126.23
28	b	624	STE	C3-C2-C1	-2.66	107.56	114.51
22	A	402	CLA	C11-C12-C13	-2.66	107.13	115.97
27	C	518	DGD	C6D-O5D-C1E	2.66	119.50	113.80
22	C	514	CLA	CMA-C3A-C4A	2.66	118.92	111.77
25	A	408	PL9	C32-C33-C34	-2.66	121.54	127.62
25	D	406	PL9	C40-C39-C38	-2.66	116.81	123.63
23	c	516	BCR	C15-C16-C17	-2.66	118.08	123.52
25	a	410	PL9	O2-C1-C2	-2.65	115.79	121.83
23	b	617	BCR	C38-C26-C25	-2.65	121.59	124.48
22	C	507	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
22	b	602	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
23	C	501	BCR	C27-C26-C25	2.65	126.28	122.70
22	C	513	CLA	C6-C5-C3	-2.65	107.02	113.47
22	B	714	CLA	C1-C2-C3	-2.65	121.86	126.20
22	A	403	CLA	C3B-C4B-NB	-2.65	108.17	110.53
25	D	406	PL9	C32-C33-C34	-2.65	121.57	127.62
25	A	408	PL9	O2-C1-C2	-2.64	115.81	121.83
22	d	401	CLA	O2D-CGD-CBD	2.64	115.85	111.23
23	B	718	BCR	C3-C4-C5	-2.64	109.34	114.06
22	C	505	CLA	C6-C5-C3	2.64	119.89	113.47
25	D	406	PL9	C36-C34-C33	-2.64	115.25	121.17
30	D	409	LMG	O4-C4-C5	2.64	115.82	109.32
22	C	504	CLA	CHB-C1B-NB	2.64	128.01	124.05
22	b	616	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	c	506	CLA	C4D-C3D-CAD	-2.64	105.24	108.11
22	c	513	CLA	C3C-C4C-NC	-2.64	107.05	110.43
22	b	604	CLA	C11-C12-C13	-2.63	107.21	115.97
22	b	611	CLA	CHD-C1D-ND	-2.63	121.10	124.80
23	C	515	BCR	C27-C26-C25	2.63	126.26	122.70
22	B	711	CLA	CHD-C4C-NC	2.63	128.31	124.23
22	b	607	CLA	C6-C5-C3	2.63	119.86	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	519	DGD	O6D-C1D-O3G	-2.63	103.84	110.04
30	c	520	LMG	O6-C1-C2	-2.62	104.98	110.37
23	b	619	BCR	C29-C30-C25	2.62	114.25	110.44
26	A	409	SQD	O5-C1-O6	2.62	116.24	110.04
26	D	410	SQD	O9-S-O7	-2.62	105.30	113.82
27	h	703	DGD	O5E-C6E-C5E	-2.62	102.41	111.33
26	B	723	SQD	C25-C24-C23	-2.62	104.11	113.69
26	l	101	SQD	O10-C23-C24	-2.61	113.56	123.78
22	A	404	CLA	CHD-C1D-ND	-2.61	121.13	124.80
23	h	702	BCR	C7-C8-C9	-2.61	122.37	126.23
30	C	520	LMG	C9-C8-C7	-2.61	105.70	111.78
22	B	702	CLA	C3B-C4B-NB	-2.61	108.20	110.53
31	B	722	LHG	C20-C19-C18	-2.61	101.18	114.37
22	B	704	CLA	O1D-CGD-CBD	2.61	129.66	124.52
22	C	508	CLA	CHB-C4A-NA	2.61	128.16	124.40
23	a	406	BCR	C27-C26-C25	2.61	126.22	122.70
22	D	404	CLA	O1D-CGD-CBD	2.60	129.65	124.52
22	c	511	CLA	O1D-CGD-CBD	2.60	129.65	124.52
23	H	101	BCR	C16-C15-C14	-2.60	118.19	123.52
33	D	407	PHO	C6-C5-C3	2.60	119.81	113.47
30	D	409	LMG	O2-C2-C1	-2.60	103.87	110.08
30	M	101	LMG	C1-C2-C3	-2.60	104.54	110.01
23	H	101	BCR	C38-C26-C25	-2.60	121.64	124.48
25	a	410	PL9	C27-C28-C29	-2.60	121.67	127.62
22	B	704	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
30	b	622	LMG	O5-C6-C5	-2.60	102.48	111.33
22	b	605	CLA	CMB-C2B-C3B	2.60	132.67	126.55
22	C	504	CLA	C6-C5-C3	2.60	119.80	113.47
23	B	718	BCR	C37-C22-C23	-2.60	114.12	118.09
30	C	520	LMG	C1-O6-C5	-2.60	108.64	113.72
27	c	519	DGD	C4D-C3D-C2D	-2.60	106.27	110.83
22	c	514	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	d	401	CLA	C2B-C1B-NB	-2.60	107.63	110.33
22	b	613	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	B	704	CLA	C11-C10-C8	-2.60	107.34	115.97
33	D	407	PHO	C3B-C4B-NB	-2.59	105.77	107.46
22	A	403	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
22	b	613	CLA	C7-C6-C5	-2.59	106.36	113.26
22	D	404	CLA	CHB-C4A-NA	2.59	128.13	124.40
22	b	606	CLA	CHB-C1B-NB	2.59	127.93	124.05
22	B	709	CLA	CAA-CBA-CGA	-2.59	105.87	113.21
22	A	403	CLA	CHC-C4B-NB	2.58	127.92	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	CHD-C1D-ND	-2.58	121.17	124.80
22	B	715	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
23	d	405	BCR	C24-C23-C22	-2.58	122.42	126.23
33	D	407	PHO	CMA-C3A-C2A	-2.58	104.16	114.13
22	B	713	CLA	C4-C3-C5	2.58	119.71	115.23
22	c	514	CLA	C3A-C2A-C1A	2.58	105.20	101.34
28	C	521	STE	O2-C1-C2	2.57	122.14	114.00
23	A	405	BCR	C7-C8-C9	-2.57	122.43	126.23
22	c	514	CLA	O2D-CGD-CBD	2.57	115.72	111.23
27	A	411	DGD	O5D-C6D-C5D	-2.57	103.63	109.42
22	C	502	CLA	CHB-C1B-NB	2.57	127.90	124.05
22	C	510	CLA	CHD-C1D-ND	-2.57	121.19	124.80
33	D	408	PHO	C4B-NB-C1B	2.57	112.56	108.82
22	B	711	CLA	C7-C6-C5	-2.57	106.42	113.26
28	t	702	STE	C3-C2-C1	-2.57	107.81	114.51
22	C	511	CLA	O2D-CGD-CBD	2.56	115.71	111.23
22	C	502	CLA	CED-O2D-CGD	-2.56	110.10	115.92
22	B	716	CLA	CHC-C4B-NB	2.56	127.88	124.05
27	H	102	DGD	C1G-O1G-C1A	2.55	126.44	117.12
22	b	606	CLA	C1-C2-C3	-2.55	122.02	126.20
23	d	405	BCR	C38-C26-C25	-2.55	121.70	124.48
23	B	719	BCR	C15-C16-C17	-2.54	118.31	123.52
27	C	519	DGD	O3E-C3E-C2E	-2.54	104.38	110.38
22	C	509	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
27	C	517	DGD	C6B-C5B-C4B	-2.54	101.52	114.37
22	B	716	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
33	a	404	PHO	C1A-C2A-C3A	-2.54	100.42	102.84
27	c	518	DGD	C3G-C2G-C1G	-2.54	105.87	111.78
22	C	510	CLA	CAC-C3C-C2C	2.54	132.22	127.56
30	M	101	LMG	O7-C10-O9	-2.53	117.78	123.70
22	B	705	CLA	C4D-CHA-C1A	2.53	124.27	121.24
23	T	701	BCR	C2-C1-C6	2.53	114.11	110.44
26	A	409	SQD	O48-C23-C24	2.53	119.54	111.83
26	B	723	SQD	C1-C2-C3	-2.53	104.70	110.01
27	C	517	DGD	O1G-C1A-C2A	-2.52	104.14	111.83
22	c	503	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	C	515	BCR	C2-C1-C6	2.52	114.11	110.44
22	B	707	CLA	C4D-CHA-C1A	2.52	124.25	121.24
22	a	405	CLA	C1-O2A-CGA	-2.52	110.54	116.65
23	c	515	BCR	C27-C26-C25	2.52	126.11	122.70
25	A	408	PL9	C35-C34-C33	-2.52	117.15	123.63
30	c	523	LMG	O8-C28-O10	-2.52	117.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	BCR	C37-C22-C21	-2.52	118.74	122.82
23	A	405	BCR	C19-C18-C17	-2.52	115.05	119.01
23	b	619	BCR	C11-C10-C9	-2.52	123.75	127.28
30	b	622	LMG	O7-C10-O9	-2.52	117.82	123.70
34	F	101	HEC	CBC-CAC-C3C	-2.52	105.60	112.42
22	D	402	CLA	C1D-ND-C4D	2.52	108.08	106.31
22	C	513	CLA	CHD-C1D-ND	-2.51	121.27	124.80
30	a	418	LMG	C9-C8-C7	-2.51	105.93	111.78
22	b	610	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
22	c	511	CLA	CHB-C4A-NA	2.51	128.02	124.40
34	V	201	HEC	O1D-CGD-CBD	-2.51	115.13	123.09
33	d	407	PHO	O2A-CGA-O1A	-2.51	117.35	123.63
23	C	524	BCR	C39-C30-C25	-2.51	106.31	110.24
22	B	708	CLA	CED-O2D-CGD	-2.51	110.22	115.92
22	C	503	CLA	C16-C15-C13	-2.51	107.63	115.97
22	b	602	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
25	d	406	PL9	C27-C28-C29	-2.51	121.89	127.62
26	a	412	SQD	O48-C23-O10	-2.50	117.36	123.63
22	B	705	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
27	c	518	DGD	C3E-C4E-C5E	-2.50	105.69	110.23
25	D	406	PL9	C37-C38-C39	-2.50	121.90	127.62
27	h	703	DGD	O6E-C5E-C4E	2.50	114.21	109.70
22	B	702	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	C	516	LMG	C40-C39-C38	-2.50	101.73	114.37
22	c	510	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	B	707	CLA	CHB-C1B-NB	2.50	127.80	124.05
27	C	517	DGD	O2G-C1B-C2B	-2.50	106.07	111.48
25	d	406	PL9	C50-C49-C48	-2.50	115.16	122.66
33	D	407	PHO	C5-C3-C2	2.50	126.77	121.17
23	b	617	BCR	C11-C10-C9	-2.50	123.78	127.28
22	c	510	CLA	O1D-CGD-CBD	2.50	129.44	124.52
25	d	406	PL9	C12-C13-C14	-2.49	121.91	127.62
31	L	101	LHG	C6-C5-C4	-2.49	105.97	111.78
27	c	517	DGD	C8B-C7B-C6B	-2.49	101.76	114.37
22	B	702	CLA	CMB-C2B-C3B	2.49	132.41	126.55
22	C	510	CLA	C9-C8-C10	-2.49	102.39	111.27
22	B	708	CLA	C1-O2A-CGA	2.49	122.68	116.65
30	D	413	LMG	O7-C10-O9	-2.49	117.88	123.70
22	b	603	CLA	CHB-C1B-C2B	-2.49	120.20	127.43
22	a	402	CLA	O1D-CGD-CBD	2.49	129.43	124.52
34	f	101	HEC	C3C-C4C-NC	-2.49	107.39	110.15
23	b	617	BCR	C3-C4-C5	-2.49	109.62	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	t	701	BCR	C34-C9-C10	-2.48	118.79	122.82
22	B	703	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	B	708	CLA	CHB-C1B-NB	2.48	127.77	124.05
23	T	701	BCR	C3-C4-C5	-2.48	109.64	114.06
22	c	508	CLA	C7-C6-C5	-2.48	106.66	113.26
22	c	509	CLA	C3A-C2A-C1A	2.47	105.05	101.34
27	A	411	DGD	O2D-C2D-C1D	-2.47	104.19	110.08
22	c	505	CLA	CMC-C2C-C1C	2.47	128.89	125.03
23	C	501	BCR	C2-C1-C6	2.47	114.03	110.44
33	D	407	PHO	OBD-CAD-CBD	-2.47	122.20	125.82
22	A	404	CLA	CMB-C2B-C3B	2.47	132.35	126.55
22	B	709	CLA	C3B-C2B-C1B	-2.47	104.26	107.17
22	b	611	CLA	CMC-C2C-C3C	2.47	132.82	126.15
30	c	522	LMG	C9-C8-C7	-2.47	106.03	111.78
22	C	514	CLA	CHB-C4A-NA	2.47	127.96	124.40
23	C	524	BCR	C29-C30-C25	2.47	114.02	110.44
22	b	609	CLA	O1D-CGD-CBD	2.47	129.38	124.52
22	B	716	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
27	c	519	DGD	O2G-C1B-C2B	-2.46	106.16	111.48
22	B	713	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	c	511	CLA	O2D-CGD-CBD	2.46	115.53	111.23
22	B	714	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	a	406	BCR	C37-C22-C21	-2.46	118.83	122.82
30	b	622	LMG	C40-C39-C38	-2.46	101.94	114.37
22	C	510	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	C	524	BCR	C35-C13-C14	-2.46	118.83	122.82
23	c	516	BCR	C33-C5-C6	-2.46	121.80	124.48
23	C	524	BCR	C15-C16-C17	-2.46	118.49	123.52
31	D	412	LHG	C3-C2-C1	-2.46	103.50	111.77
22	h	701	CLA	C1-O2A-CGA	2.45	122.59	116.65
23	a	406	BCR	C38-C26-C27	-2.45	108.36	113.60
22	C	509	CLA	CMB-C2B-C3B	2.45	132.32	126.55
27	h	703	DGD	C4B-C3B-C2B	-2.45	104.11	113.13
23	c	515	BCR	C24-C23-C22	-2.45	122.61	126.23
22	B	709	CLA	CHC-C4B-NB	2.45	127.72	124.05
23	T	701	BCR	C38-C26-C27	-2.45	108.38	113.60
23	B	718	BCR	C38-C26-C25	-2.45	121.81	124.48
30	d	410	LMG	O3-C3-C2	-2.45	104.61	110.38
22	d	404	CLA	CMB-C2B-C3B	2.45	132.30	126.55
28	B	724	STE	C3-C2-C1	-2.45	108.13	114.51
22	c	514	CLA	C1-C2-C3	-2.44	122.19	126.20
22	b	611	CLA	CGD-CBD-CAD	-2.44	102.93	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	622	LMG	O1-C1-C2	-2.44	104.56	108.27
22	b	615	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
30	C	520	LMG	O3-C3-C2	-2.44	104.62	110.38
22	a	402	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	a	410	PL9	C26-C24-C23	-2.44	115.69	121.17
22	B	708	CLA	C3C-C4C-NC	-2.44	107.30	110.43
25	A	408	PL9	O2-C1-C6	2.44	124.36	120.48
27	A	411	DGD	C8B-C7B-C6B	-2.44	102.03	114.37
22	D	402	CLA	CMC-C2C-C1C	2.44	128.85	125.03
23	b	617	BCR	C33-C5-C6	-2.44	121.82	124.48
27	H	102	DGD	O3G-C1D-C2D	-2.44	104.57	108.27
23	C	524	BCR	C33-C5-C6	-2.44	121.83	124.48
22	b	616	CLA	O1D-CGD-CBD	2.44	129.32	124.52
22	C	510	CLA	C2A-C3A-C4A	2.44	105.80	101.87
22	c	511	CLA	C6-C5-C3	-2.44	107.54	113.47
26	D	410	SQD	O8-S-O9	-2.43	105.31	111.40
22	C	503	CLA	C16-C17-C18	-2.43	105.08	115.94
30	d	410	LMG	C31-C30-C29	-2.43	104.20	113.13
26	D	410	SQD	O4-C4-C3	-2.43	104.65	110.38
25	A	408	PL9	C27-C28-C29	-2.43	122.07	127.62
22	b	614	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
22	B	727	CLA	CED-O2D-CGD	-2.43	110.41	115.92
28	t	702	STE	O2-C1-C2	2.42	121.66	114.00
22	b	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
22	b	610	CLA	CAC-C3C-C2C	-2.42	123.11	127.56
22	b	608	CLA	C11-C10-C8	-2.42	107.92	115.97
22	b	614	CLA	CAC-C3C-C4C	2.42	127.94	124.79
23	T	701	BCR	C4-C5-C6	2.42	125.97	122.70
26	l	101	SQD	O47-C45-C46	2.42	117.02	108.34
22	B	703	CLA	C4B-C3B-C2B	2.42	110.31	107.30
23	t	701	BCR	C31-C1-C6	2.42	114.03	110.24
22	B	715	CLA	CHB-C4A-NA	2.41	127.89	124.40
26	A	410	SQD	O47-C7-C8	2.41	116.70	111.48
22	a	403	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
23	c	516	BCR	C34-C9-C10	-2.41	118.91	122.82
27	h	703	DGD	C1D-O6D-C5D	-2.41	109.01	113.72
22	b	616	CLA	O2D-CGD-CBD	2.41	115.44	111.23
30	a	418	LMG	O6-C1-C2	-2.41	105.42	110.37
28	B	701	STE	O2-C1-O1	-2.41	117.14	123.33
22	a	405	CLA	C2D-C1D-ND	-2.41	107.74	110.13
22	c	504	CLA	C5-C3-C2	-2.41	115.76	121.17
23	b	619	BCR	C27-C26-C25	2.41	125.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	O1D-CGD-CBD	2.41	129.27	124.52
22	B	710	CLA	C1-C2-C3	-2.41	122.25	126.20
22	B	702	CLA	C16-C15-C13	-2.41	107.97	115.97
22	c	504	CLA	C4-C3-C5	2.40	119.40	115.23
22	b	610	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	A	404	CLA	CHD-C4C-NC	2.40	127.96	124.23
28	C	523	STE	C3-C2-C1	-2.40	108.24	114.51
22	c	513	CLA	O1D-CGD-CBD	2.40	129.26	124.52
22	C	506	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	b	614	CLA	C1-C2-C3	-2.40	122.26	126.20
23	D	405	BCR	C15-C14-C13	-2.40	123.91	127.28
23	k	101	BCR	C4-C5-C6	2.40	125.95	122.70
22	b	613	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	k	101	BCR	C33-C5-C6	-2.40	121.86	124.48
33	a	404	PHO	CMB-C2B-C3B	2.40	129.48	124.68
22	h	701	CLA	C3B-C4B-NB	-2.40	108.39	110.53
22	C	506	CLA	C3D-C4D-ND	2.40	113.89	109.99
30	c	522	LMG	O8-C28-O10	-2.40	117.63	123.63
22	c	509	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
34	f	101	HEC	CHD-C1D-ND	2.40	127.33	124.37
23	b	619	BCR	C38-C26-C25	-2.39	121.87	124.48
27	C	519	DGD	O2D-C2D-C1D	-2.39	104.37	110.08
22	b	607	CLA	C2D-C1D-ND	-2.39	107.76	110.13
22	B	714	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	d	406	PL9	C47-C48-C49	-2.39	119.67	127.64
22	B	712	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	b	615	CLA	CMB-C2B-C3B	2.39	132.17	126.55
22	D	402	CLA	O2D-CGD-CBD	2.39	115.41	111.23
22	B	714	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
23	C	524	BCR	C27-C26-C25	2.38	125.93	122.70
22	c	509	CLA	CHD-C4C-NC	2.38	127.93	124.23
22	C	510	CLA	C3B-C4B-NB	-2.38	108.40	110.53
27	C	518	DGD	O6D-C1D-O3G	-2.38	104.41	110.04
27	C	517	DGD	C4E-C3E-C2E	-2.38	106.65	110.83
22	A	403	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	C	503	CLA	CMD-C2D-C3D	2.38	133.15	127.69
22	D	402	CLA	C2D-C1D-ND	-2.38	107.77	110.13
22	b	604	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
23	D	405	BCR	C7-C8-C9	-2.38	122.71	126.23
22	A	403	CLA	C2A-C1A-CHA	2.38	128.00	123.87
22	A	404	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
23	A	405	BCR	C4-C5-C6	2.38	125.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	CHB-C1B-NB	2.38	127.62	124.05
30	D	409	LMG	C38-C37-C36	-2.38	102.35	114.37
22	B	711	CLA	C9-C8-C10	-2.38	102.80	111.27
31	a	411	LHG	O8-C6-C5	-2.38	101.54	108.40
22	b	609	CLA	CHA-C1A-NA	-2.38	121.01	126.39
30	b	620	LMG	C12-C11-C10	-2.37	104.99	113.69
22	C	504	CLA	O2A-C1-C2	-2.37	98.97	108.11
27	A	411	DGD	C1D-C2D-C3D	-2.37	105.02	110.01
22	c	502	CLA	CHD-C1D-ND	-2.37	121.46	124.80
22	c	511	CLA	C2A-C3A-C4A	2.37	105.70	101.87
22	b	608	CLA	O2D-CGD-CBD	2.37	115.38	111.23
22	c	503	CLA	C1-C2-C3	-2.37	122.31	126.20
27	A	411	DGD	C3G-O3G-C1D	2.37	118.88	113.80
27	h	703	DGD	C3D-C4D-C5D	-2.37	105.93	110.23
22	B	704	CLA	C6-C7-C8	-2.37	108.09	115.97
22	B	710	CLA	C3A-C2A-C1A	2.37	104.89	101.34
22	b	606	CLA	CHD-C4C-NC	2.37	127.90	124.23
28	C	521	STE	O2-C1-O1	-2.37	117.24	123.33
27	c	518	DGD	C8B-C7B-C6B	-2.37	102.41	114.37
22	c	506	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
22	B	704	CLA	C2D-C1D-ND	-2.36	107.79	110.13
23	Y	101	BCR	C15-C16-C17	-2.36	118.68	123.52
22	b	606	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
30	b	622	LMG	C6-C5-C4	-2.36	107.23	113.02
22	B	716	CLA	CMB-C2B-C3B	2.36	132.10	126.55
26	f	102	SQD	O5-C1-O6	2.36	115.61	110.04
22	C	509	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
34	V	201	HEC	C1D-ND-C4D	2.36	108.00	105.21
22	B	713	CLA	CHA-C1A-NA	-2.35	121.06	126.39
27	c	518	DGD	O4D-C4D-C3D	2.35	115.92	110.38
22	C	508	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
23	b	617	BCR	C15-C16-C17	-2.35	118.71	123.52
23	d	405	BCR	C30-C25-C26	-2.35	119.42	122.64
22	a	402	CLA	CHA-C4D-ND	2.35	137.40	132.55
22	b	604	CLA	C11-C10-C8	-2.35	108.16	115.97
27	A	411	DGD	CDB-CCB-CBB	-2.35	102.50	114.37
22	b	608	CLA	CHD-C1D-ND	-2.35	121.50	124.80
23	c	516	BCR	C4-C5-C6	2.34	125.87	122.70
22	C	513	CLA	O2D-CGD-CBD	2.34	115.33	111.23
27	c	519	DGD	O1G-C1A-O1A	-2.34	117.77	123.63
22	b	607	CLA	CHB-C1B-NB	2.34	127.56	124.05
22	b	611	CLA	CHB-C4A-NA	2.34	127.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CHD-C1D-C2D	2.34	130.35	125.49
22	c	509	CLA	C7-C6-C5	-2.34	107.03	113.26
34	v	201	HEC	CAD-CBD-CGD	-2.34	107.46	113.67
23	h	702	BCR	C36-C18-C17	-2.34	119.03	122.82
22	C	508	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
27	A	411	DGD	CBB-CAB-C9B	-2.34	102.55	114.37
27	c	519	DGD	O1G-C1A-C2A	-2.34	104.71	111.83
23	B	719	BCR	C40-C30-C29	-2.34	99.98	108.95
22	A	402	CLA	C7-C6-C5	-2.33	107.05	113.26
23	H	101	BCR	C16-C17-C18	-2.33	124.01	127.28
22	b	603	CLA	O2D-CGD-CBD	2.33	115.30	111.23
30	b	620	LMG	O6-C1-O1	-2.33	104.54	110.04
22	C	504	CLA	CMB-C2B-C3B	2.33	132.02	126.55
22	C	513	CLA	CHB-C1B-NB	2.33	127.54	124.05
22	b	603	CLA	OBD-CAD-C3D	2.32	133.84	128.42
22	B	704	CLA	CMB-C2B-C3B	2.32	132.01	126.55
22	B	715	CLA	C2D-C1D-ND	-2.32	107.83	110.13
31	a	413	LHG	O8-C23-C24	2.32	118.91	111.83
22	C	507	CLA	C1-C2-C3	-2.32	122.40	126.20
30	c	523	LMG	C32-C31-C30	-2.32	102.64	114.37
23	B	717	BCR	C3-C4-C5	-2.32	109.92	114.06
22	b	602	CLA	C3C-C4C-NC	-2.32	107.46	110.43
22	D	404	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
22	b	605	CLA	C4-C3-C5	2.32	119.25	115.23
22	B	708	CLA	CHD-C4C-NC	2.32	127.82	124.23
28	j	101	STE	O1-C1-C2	-2.31	115.75	123.09
23	H	101	BCR	C37-C22-C21	-2.31	119.07	122.82
22	d	401	CLA	C3A-C2A-C1A	2.31	104.81	101.34
22	b	608	CLA	CMB-C2B-C3B	2.31	131.99	126.55
22	c	507	CLA	CGD-CBD-CAD	-2.31	103.36	110.85
25	A	408	PL9	C12-C13-C14	-2.31	122.33	127.62
23	B	718	BCR	C27-C26-C25	2.31	125.83	122.70
23	c	516	BCR	C7-C8-C9	-2.31	122.82	126.23
22	C	513	CLA	CBA-CAA-C2A	-2.31	106.92	113.79
31	a	411	LHG	C11-C10-C9	-2.31	102.69	114.37
22	A	402	CLA	CAA-CBA-CGA	-2.31	106.65	113.21
30	b	620	LMG	O1-C7-C8	-2.31	105.20	110.82
22	b	602	CLA	C14-C13-C15	-2.31	103.05	111.27
30	b	622	LMG	C4-C3-C2	-2.31	106.78	110.83
33	a	404	PHO	C4B-NB-C1B	2.31	112.18	108.82
23	d	405	BCR	C40-C30-C25	2.31	113.86	110.24
30	C	520	LMG	O1-C7-C8	-2.31	105.21	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	523	LMG	C38-C37-C36	-2.31	102.71	114.37
30	c	522	LMG	O3-C3-C2	-2.31	104.94	110.38
22	C	504	CLA	CHA-C1A-NA	-2.31	121.17	126.39
22	a	402	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
22	b	607	CLA	O1D-CGD-CBD	2.30	129.06	124.52
22	c	506	CLA	C11-C10-C8	-2.30	108.32	115.97
23	C	524	BCR	C38-C26-C25	-2.30	121.97	124.48
27	H	102	DGD	CAB-C9B-C8B	-2.30	102.74	114.37
22	B	706	CLA	CGD-CBD-CAD	-2.30	103.40	110.85
27	H	102	DGD	C1D-C2D-C3D	-2.30	105.17	110.01
23	t	701	BCR	C15-C16-C17	-2.30	118.81	123.52
22	C	510	CLA	CMD-C2D-C1D	2.30	128.77	124.73
27	C	519	DGD	CBB-CAB-C9B	-2.29	102.77	114.37
22	a	405	CLA	CHB-C4A-NA	2.29	127.71	124.40
27	A	411	DGD	C5B-C4B-C3B	-2.29	102.77	114.37
22	C	505	CLA	C4-C3-C5	2.29	119.21	115.23
22	b	611	CLA	C7-C6-C5	-2.29	107.15	113.26
22	C	511	CLA	CHB-C4A-NA	2.29	127.71	124.40
30	c	522	LMG	C1-O6-C5	-2.29	109.25	113.72
22	C	512	CLA	CHA-C1A-NA	-2.29	121.20	126.39
22	D	402	CLA	CBA-CAA-C2A	-2.29	106.98	113.79
22	h	701	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
22	C	513	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	c	502	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
28	J	101	STE	O2-C1-C2	2.29	121.23	114.00
27	c	519	DGD	C5B-C4B-C3B	-2.29	102.81	114.37
26	l	101	SQD	O48-C23-O10	-2.28	117.91	123.63
31	D	412	LHG	C11-C10-C9	-2.28	102.83	114.37
30	c	522	LMG	C42-C41-C40	-2.28	102.83	114.37
34	V	201	HEC	CBB-CAB-C3B	-2.28	106.23	112.42
27	c	517	DGD	C4A-C3A-C2A	-2.28	104.74	113.13
22	A	404	CLA	CED-O2D-CGD	-2.28	110.74	115.92
22	B	702	CLA	CGD-CBD-CAD	-2.28	103.47	110.85
22	B	702	CLA	CHD-C1D-C2D	2.28	130.23	125.49
22	d	401	CLA	CMD-C2D-C1D	-2.28	120.72	124.73
22	B	707	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
27	c	517	DGD	C5B-C4B-C3B	-2.28	102.86	114.37
23	C	524	BCR	C24-C23-C22	-2.28	122.87	126.23
23	k	101	BCR	C29-C30-C25	2.28	113.75	110.44
22	b	605	CLA	CHB-C1B-NB	2.28	127.46	124.05
23	b	617	BCR	C37-C22-C21	-2.28	119.13	122.82
23	b	619	BCR	C39-C30-C25	-2.28	106.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	622	LMG	O6-C1-O1	-2.27	104.67	110.04
22	d	401	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
22	B	703	CLA	C5-C3-C2	-2.27	116.06	121.17
27	A	411	DGD	C9B-C8B-C7B	-2.27	102.88	114.37
27	A	411	DGD	C2G-O2G-C1B	2.27	123.23	117.80
22	c	504	CLA	C7-C6-C5	-2.27	107.21	113.26
22	b	604	CLA	C6-C7-C8	-2.27	108.42	115.97
27	c	517	DGD	O6D-C1D-O3G	-2.27	104.68	110.04
22	C	503	CLA	O1D-CGD-CBD	2.27	129.00	124.52
22	c	510	CLA	C11-C10-C8	-2.27	108.43	115.97
22	b	616	CLA	CHC-C4B-NB	2.27	127.45	124.05
33	a	404	PHO	C2D-C1D-ND	2.27	111.07	109.43
28	b	623	STE	O2-C1-C2	2.27	121.16	114.00
23	C	524	BCR	C7-C8-C9	-2.27	122.88	126.23
27	c	518	DGD	C1D-C2D-C3D	-2.27	105.24	110.01
30	b	620	LMG	C40-C39-C38	-2.26	102.92	114.37
27	C	518	DGD	CDB-CCB-CBB	-2.26	102.93	114.37
30	C	520	LMG	O6-C5-C6	2.26	112.05	106.44
27	c	519	DGD	C6B-C5B-C4B	-2.26	102.93	114.37
23	c	516	BCR	C38-C26-C25	-2.26	122.02	124.48
22	b	613	CLA	CHB-C1B-NB	2.26	127.44	124.05
31	d	408	LHG	C18-C17-C16	-2.26	102.94	114.37
22	c	512	CLA	O1A-CGA-CBA	2.26	132.62	123.78
22	B	710	CLA	CED-O2D-CGD	-2.26	110.80	115.92
25	a	410	PL9	C12-C13-C14	-2.26	122.46	127.62
22	B	727	CLA	C4-C3-C5	2.26	119.14	115.23
22	C	504	CLA	CHD-C1D-ND	-2.26	121.63	124.80
22	b	602	CLA	CHC-C1C-NC	2.25	127.71	124.31
33	d	407	PHO	C4B-NB-C1B	2.25	112.10	108.82
23	a	406	BCR	C24-C23-C22	-2.25	122.90	126.23
27	c	517	DGD	C2G-O2G-C1B	2.25	123.19	117.80
31	E	101	LHG	C11-C10-C9	-2.25	102.98	114.37
28	X	101	STE	C15-C14-C13	-2.25	102.98	114.37
27	H	102	DGD	C3D-C4D-C5D	-2.25	106.15	110.23
31	d	408	LHG	C11-C10-C9	-2.25	102.98	114.37
31	l	102	LHG	C27-C26-C25	-2.25	103.00	114.37
22	B	709	CLA	C4D-C3D-CAD	-2.25	105.66	108.11
22	b	603	CLA	C11-C12-C13	-2.25	108.49	115.97
23	a	406	BCR	C30-C25-C26	-2.25	119.56	122.64
27	c	519	DGD	O1G-C1G-C2G	-2.25	101.92	108.40
34	f	101	HEC	CAC-C3C-C4C	-2.25	121.82	124.91
27	c	519	DGD	CDB-CCB-CBB	-2.25	103.01	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	C3B-C4B-NB	-2.25	108.53	110.53
22	C	513	CLA	CHD-C1D-C2D	2.25	130.16	125.49
22	c	505	CLA	CHB-C1B-NB	2.24	127.42	124.05
23	Y	101	BCR	C4-C5-C6	2.24	125.74	122.70
22	b	603	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
27	C	519	DGD	CDB-CCB-CBB	-2.24	103.03	114.37
22	c	507	CLA	C16-C15-C13	2.24	123.42	115.97
22	C	513	CLA	C7-C6-C5	-2.24	107.29	113.26
23	A	405	BCR	C31-C1-C6	-2.24	106.73	110.24
23	T	701	BCR	C31-C1-C6	2.24	113.76	110.24
22	b	607	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
25	d	406	PL9	C41-C39-C38	-2.24	116.14	121.17
22	c	513	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	c	501	STE	O2-C1-C2	2.24	121.07	114.00
22	B	702	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
22	b	615	CLA	CHC-C1C-NC	2.24	127.68	124.31
22	c	508	CLA	C2C-C1C-NC	2.24	112.33	109.98
22	c	512	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
27	h	703	DGD	O2E-C2E-C3E	-2.24	105.11	110.38
27	c	518	DGD	O3D-C3D-C2D	-2.23	105.11	110.38
22	a	402	CLA	C11-C10-C8	-2.23	108.54	115.97
22	B	712	CLA	C11-C10-C8	-2.23	108.54	115.97
23	Y	101	BCR	C39-C30-C25	-2.23	106.74	110.24
23	h	702	BCR	C15-C16-C17	-2.23	118.95	123.52
23	t	701	BCR	C36-C18-C19	2.23	121.50	118.09
22	D	402	CLA	CHD-C4C-NC	2.23	127.69	124.23
22	B	705	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	b	603	CLA	CMA-C3A-C4A	2.23	117.76	111.77
22	b	611	CLA	C6-C5-C3	2.23	118.89	113.47
22	b	613	CLA	C14-C13-C12	2.23	119.21	111.27
22	B	710	CLA	CMD-C2D-C1D	-2.23	120.81	124.73
27	C	517	DGD	O2D-C2D-C1D	-2.22	104.77	110.08
22	b	613	CLA	CHA-C4D-ND	2.22	137.14	132.55
31	B	722	LHG	C18-C17-C16	-2.22	103.13	114.37
25	d	406	PL9	C11-C9-C8	-2.22	116.18	121.17
30	M	101	LMG	C6-C5-C4	-2.22	107.57	113.02
22	A	403	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
22	B	713	CLA	CMB-C2B-C3B	2.22	131.77	126.55
22	C	511	CLA	CMB-C2B-C3B	2.22	131.77	126.55
22	c	508	CLA	CMC-C2C-C3C	2.22	132.14	126.15
23	t	701	BCR	C4-C5-C6	2.22	125.70	122.70
23	c	515	BCR	C16-C17-C18	-2.22	124.17	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	C2D-C1D-ND	-2.21	107.93	110.13
27	C	517	DGD	CDB-CCB-CBB	-2.21	103.17	114.37
22	B	715	CLA	CHA-C4D-ND	2.21	137.12	132.55
22	D	404	CLA	CMB-C2B-C3B	2.21	131.76	126.55
23	B	719	BCR	C1-C6-C5	-2.21	119.61	122.64
22	b	609	CLA	C1-C2-C3	-2.21	122.57	126.20
23	d	405	BCR	C7-C8-C9	-2.21	122.96	126.23
23	A	405	BCR	C2-C1-C6	2.21	113.65	110.44
22	B	715	CLA	CHC-C4B-NB	2.21	127.37	124.05
22	B	704	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
30	c	523	LMG	O2-C2-C1	-2.21	104.81	110.08
30	c	523	LMG	C1-O6-C5	-2.21	109.41	113.72
22	b	602	CLA	C3B-C4B-NB	-2.21	108.56	110.53
22	b	613	CLA	C2B-C1B-NB	-2.21	108.04	110.33
33	d	407	PHO	C3D-C4D-ND	2.21	110.54	107.71
22	c	510	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
22	B	705	CLA	CMB-C2B-C1B	2.21	128.78	125.42
28	d	402	STE	O2-C1-C2	2.20	120.96	114.00
26	l	101	SQD	C45-O47-C7	2.20	123.07	117.80
30	c	520	LMG	C40-C39-C38	-2.20	103.23	114.37
22	d	403	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
22	B	703	CLA	O1A-CGA-CBA	2.20	132.40	123.78
31	L	101	LHG	O10-C23-C24	-2.20	115.18	123.78
22	C	510	CLA	CMC-C2C-C3C	2.20	132.10	126.15
27	H	102	DGD	C6D-C5D-C4D	2.20	116.68	112.07
22	c	511	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
25	a	410	PL9	C7-C8-C9	-2.20	123.05	126.83
26	A	409	SQD	O47-C45-C46	2.20	116.22	108.34
30	C	520	LMG	C6-C5-C4	-2.19	107.63	113.02
22	C	505	CLA	C3B-C4B-NB	-2.19	108.57	110.53
22	c	506	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
23	b	618	BCR	C35-C13-C14	-2.19	119.26	122.82
22	a	402	CLA	C1D-ND-C4D	2.19	107.85	106.31
22	b	603	CLA	CHD-C1D-C2D	2.19	130.05	125.49
22	c	504	CLA	C9-C8-C10	-2.19	103.47	111.27
23	b	619	BCR	C36-C18-C17	-2.19	119.27	122.82
22	b	609	CLA	C7-C6-C5	-2.19	107.43	113.26
33	D	408	PHO	C1-O2A-CGA	2.19	121.95	116.65
22	b	615	CLA	CHA-C1A-NA	-2.19	121.44	126.39
23	H	101	BCR	C1-C6-C5	-2.19	119.64	122.64
23	C	501	BCR	C15-C16-C17	-2.19	119.04	123.52
22	b	610	CLA	CHA-C1A-NA	-2.19	121.44	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CMD-C2D-C1D	2.19	128.58	124.73
22	b	607	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
22	C	504	CLA	C5-C3-C2	-2.18	116.27	121.17
27	C	518	DGD	C5B-C4B-C3B	-2.18	103.34	114.37
33	D	407	PHO	O2D-CGD-CBD	2.18	113.34	110.95
23	c	516	BCR	C36-C18-C17	-2.18	119.28	122.82
27	C	517	DGD	CBB-CAB-C9B	-2.18	103.34	114.37
27	c	518	DGD	O5D-C1E-C2E	2.18	111.58	108.27
22	a	402	CLA	C9-C8-C10	-2.18	103.50	111.27
22	C	507	CLA	C4-C3-C5	2.18	119.01	115.23
22	b	609	CLA	CHC-C4B-NB	2.18	127.32	124.05
22	A	403	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
31	l	102	LHG	O8-C23-O10	-2.18	118.18	123.63
22	C	502	CLA	C2D-C1D-ND	-2.18	107.97	110.13
22	c	508	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
22	C	502	CLA	CHD-C1D-C2D	2.18	130.01	125.49
22	B	702	CLA	CHC-C1C-NC	2.18	127.59	124.31
22	c	503	CLA	CHD-C1D-ND	-2.17	121.74	124.80
22	b	609	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
22	b	605	CLA	C1-O2A-CGA	-2.17	111.39	116.65
22	D	404	CLA	C1-C2-C3	-2.17	122.64	126.20
22	c	514	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
31	d	409	LHG	C26-C25-C24	2.17	121.10	113.13
22	b	610	CLA	CED-O2D-CGD	-2.17	110.99	115.92
23	C	524	BCR	C31-C1-C6	2.17	113.64	110.24
31	B	722	LHG	O2-C2-C3	-2.17	102.20	109.70
22	B	715	CLA	C1D-ND-C4D	2.17	107.83	106.31
23	B	717	BCR	C15-C16-C17	-2.17	119.08	123.52
22	b	609	CLA	C1C-C2C-C3C	-2.17	104.70	106.98
22	C	507	CLA	CMB-C2B-C3B	2.17	131.65	126.55
27	c	519	DGD	O2D-C2D-C3D	-2.17	105.27	110.38
22	B	706	CLA	CHB-C4A-NA	2.16	127.52	124.40
30	D	409	LMG	O8-C28-O10	-2.16	118.21	123.63
27	C	519	DGD	O3G-C1D-C2D	-2.16	104.99	108.27
23	k	101	BCR	C30-C25-C26	-2.16	119.68	122.64
22	d	403	CLA	C3B-C4B-NB	-2.16	108.60	110.53
22	b	606	CLA	CAC-C3C-C4C	-2.16	121.97	124.79
22	b	607	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
30	B	721	LMG	O7-C10-O9	-2.16	117.77	123.33
26	A	409	SQD	C1-O5-C5	-2.16	109.50	113.72
33	d	407	PHO	CBA-CAA-C2A	-2.16	107.41	113.78
22	C	514	CLA	C5-C3-C2	-2.16	116.32	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	711	CLA	C1-C2-C3	-2.16	122.66	126.20
27	C	519	DGD	C7B-C6B-C5B	-2.16	103.45	114.37
22	B	715	CLA	C3B-C4B-NB	-2.16	108.60	110.53
22	b	602	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
22	a	402	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	C	504	CLA	C6-C7-C8	-2.16	108.79	115.97
22	C	504	CLA	C4D-C3D-CAD	-2.16	105.76	108.11
22	b	607	CLA	CHB-C4A-NA	2.16	127.51	124.40
22	B	715	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
22	C	503	CLA	CHA-C1A-NA	-2.16	121.51	126.39
22	D	403	CLA	C2B-C1B-NB	-2.16	108.09	110.33
28	B	720	STE	C4-C3-C2	-2.16	105.20	113.13
22	d	403	CLA	C1-C2-C3	-2.16	122.67	126.20
23	k	102	BCR	C15-C16-C17	-2.15	119.11	123.52
22	a	403	CLA	CHC-C4B-NB	2.15	127.28	124.05
23	a	406	BCR	C7-C8-C9	-2.15	123.05	126.23
22	B	703	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
22	c	505	CLA	O1D-CGD-CBD	2.15	128.76	124.52
30	M	101	LMG	C35-C34-C33	-2.15	103.49	114.37
22	B	714	CLA	C4-C3-C5	2.15	118.96	115.23
30	B	721	LMG	C30-C29-C28	-2.15	108.90	114.51
22	D	403	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	c	505	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
33	a	404	PHO	C4D-ND-C1D	-2.15	106.30	108.87
22	d	401	CLA	O2A-CGA-CBA	2.15	118.39	111.83
23	c	515	BCR	C37-C22-C21	-2.15	119.33	122.82
22	C	508	CLA	CMB-C2B-C3B	2.15	131.60	126.55
22	B	727	CLA	CHA-C4D-ND	2.15	136.98	132.55
30	M	101	LMG	O7-C10-C11	2.15	116.13	111.48
23	B	718	BCR	C2-C1-C6	2.15	113.56	110.44
32	a	409	BCT	O3-C-O1	-2.15	114.18	119.68
22	c	511	CLA	CHC-C4B-NB	2.15	127.27	124.05
22	B	702	CLA	C4D-CHA-C1A	2.15	123.80	121.24
23	d	405	BCR	C39-C30-C25	-2.15	106.88	110.24
22	d	404	CLA	C1-C2-C3	-2.14	122.68	126.20
22	A	403	CLA	CMB-C2B-C3B	2.14	131.59	126.55
22	B	712	CLA	CBC-CAC-C3C	2.14	118.23	112.42
23	h	702	BCR	C34-C9-C10	-2.14	119.34	122.82
22	D	404	CLA	C3B-C4B-NB	-2.14	108.62	110.53
22	a	402	CLA	C17-C16-C15	-2.14	103.68	113.28
22	B	703	CLA	CHD-C4C-NC	2.14	127.55	124.23
22	b	608	CLA	CHD-C4C-NC	2.14	127.55	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	C	524	BCR	C15-C14-C13	-2.14	124.28	127.28
22	d	401	CLA	C2A-C1A-CHA	2.14	127.58	123.87
23	b	618	BCR	C2-C1-C6	2.14	113.55	110.44
22	B	714	CLA	C2B-C1B-NB	-2.14	108.11	110.33
34	f	101	HEC	O2D-CGD-CBD	2.14	120.75	114.00
31	l	102	LHG	C6-C5-C4	-2.14	106.80	111.78
22	A	402	CLA	CHB-C4A-NA	2.14	127.48	124.40
22	B	705	CLA	C3D-C4D-ND	2.14	113.46	109.99
31	L	101	LHG	C36-C35-C34	-2.14	103.57	114.37
31	D	412	LHG	O8-C6-C5	-2.14	102.24	108.40
22	b	609	CLA	CHB-C1B-NB	2.14	127.25	124.05
27	H	102	DGD	CDB-CCB-CBB	-2.13	103.58	114.37
22	C	507	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
22	b	605	CLA	C1-C2-C3	-2.13	122.70	126.20
31	L	101	LHG	C17-C16-C15	-2.13	103.58	114.37
25	D	406	PL9	C12-C13-C14	-2.13	122.74	127.62
22	b	612	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
22	c	502	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
22	c	510	CLA	CHD-C4C-NC	2.13	127.54	124.23
23	d	405	BCR	C3-C4-C5	-2.13	110.25	114.06
31	d	408	LHG	C20-C19-C18	-2.13	103.59	114.37
22	C	513	CLA	OBD-CAD-C3D	2.13	133.40	128.42
23	a	406	BCR	C8-C7-C6	-2.13	121.31	127.00
27	C	517	DGD	C7B-C6B-C5B	-2.13	103.60	114.37
22	c	507	CLA	C4-C3-C2	-2.13	118.16	123.63
27	c	518	DGD	O6E-C1E-O5D	-2.13	105.02	110.04
23	A	405	BCR	C15-C14-C13	-2.13	124.30	127.28
28	B	724	STE	O2-C1-O1	-2.13	117.86	123.33
30	M	101	LMG	C22-C21-C20	-2.13	103.62	114.37
26	f	102	SQD	O5-C1-C2	-2.13	106.00	110.37
27	H	102	DGD	O2G-C1B-O1B	-2.13	118.74	123.70
25	a	410	PL9	C40-C39-C41	2.13	118.92	115.23
22	b	606	CLA	CBA-CAA-C2A	2.13	120.12	113.79
22	b	606	CLA	CHC-C4B-NB	2.12	127.24	124.05
23	B	719	BCR	C40-C30-C25	2.12	113.57	110.24
22	A	403	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
31	B	722	LHG	C11-C10-C9	-2.12	103.63	114.37
30	c	522	LMG	O2-C2-C3	-2.12	105.37	110.38
22	b	606	CLA	CHB-C4A-NA	2.12	127.46	124.40
22	C	510	CLA	CAC-C3C-C4C	-2.12	122.03	124.79
22	D	404	CLA	CMD-C2D-C1D	-2.12	121.00	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	719	BCR	C39-C30-C25	-2.12	106.92	110.24
22	a	403	CLA	C1D-ND-C4D	2.12	107.80	106.31
23	C	515	BCR	C11-C10-C9	-2.12	124.31	127.28
34	V	201	HEC	CHC-C1C-NC	2.12	127.70	123.86
26	a	414	SQD	C45-O47-C7	2.12	122.87	117.80
23	h	702	BCR	C15-C14-C13	-2.11	124.31	127.28
23	a	406	BCR	C11-C10-C9	-2.11	124.31	127.28
22	C	506	CLA	C1D-ND-C4D	-2.11	104.83	106.31
22	C	507	CLA	CMC-C2C-C1C	2.11	128.33	125.03
23	B	717	BCR	C33-C5-C6	-2.11	122.18	124.48
25	A	408	PL9	C22-C23-C24	-2.11	122.79	127.62
22	B	704	CLA	C2C-C1C-NC	2.11	112.20	109.98
31	l	102	LHG	C11-C10-C9	-2.11	103.71	114.37
22	a	402	CLA	C4-C3-C5	2.11	118.89	115.23
22	b	608	CLA	CHB-C4A-NA	2.11	127.44	124.40
22	b	611	CLA	CHA-C1A-NA	-2.11	121.62	126.39
28	X	101	STE	C13-C12-C11	-2.11	103.71	114.37
25	D	406	PL9	O2-C1-C6	2.11	123.83	120.48
31	d	408	LHG	C27-C26-C25	-2.11	103.72	114.37
22	b	604	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
27	h	703	DGD	C1E-O6E-C5E	2.11	117.83	113.72
27	H	102	DGD	CCB-CBB-CAB	-2.11	103.72	114.37
22	A	403	CLA	C1C-C2C-C3C	-2.11	104.77	106.98
22	B	704	CLA	CMC-C2C-C3C	2.10	131.84	126.15
31	D	411	LHG	C27-C26-C25	-2.10	103.73	114.37
22	b	612	CLA	C1-O2A-CGA	2.10	121.74	116.65
22	B	711	CLA	O2D-CGD-CBD	2.10	114.91	111.23
22	c	509	CLA	CHD-C1D-C2D	2.10	129.86	125.49
22	B	707	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	b	602	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
30	c	520	LMG	C32-C31-C30	-2.10	103.74	114.37
22	b	607	CLA	CHA-C1A-NA	-2.10	121.63	126.39
22	b	610	CLA	C4D-CHA-C1A	2.10	123.75	121.24
23	b	618	BCR	C12-C13-C14	2.10	122.31	119.01
23	B	719	BCR	C8-C7-C6	-2.10	121.39	127.00
30	d	410	LMG	C6-C5-C4	-2.10	107.86	113.02
22	b	612	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	C	510	CLA	C9-C8-C7	2.10	118.76	111.27
22	C	509	CLA	C4-C3-C5	2.10	118.87	115.23
28	b	621	STE	O2-C1-C2	2.10	120.63	114.00
27	C	518	DGD	C8B-C7B-C6B	-2.10	103.76	114.37
25	A	408	PL9	C26-C24-C23	-2.10	116.46	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	518	DGD	C7B-C6B-C5B	-2.10	103.77	114.37
27	A	411	DGD	O6D-C5D-C6D	-2.10	102.54	106.69
22	d	403	CLA	C4-C3-C5	2.10	118.86	115.23
22	c	513	CLA	C3A-C2A-C1A	2.09	104.47	101.34
27	C	517	DGD	O2D-C2D-C3D	-2.09	105.44	110.38
23	B	718	BCR	C30-C25-C26	-2.09	119.78	122.64
22	C	506	CLA	CAC-C3C-C2C	2.09	131.40	127.56
22	b	615	CLA	C5-C3-C2	-2.09	116.47	121.17
22	C	508	CLA	C4D-C3D-CAD	-2.09	105.83	108.11
22	c	504	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	C	508	CLA	C1-O2A-CGA	2.09	121.71	116.65
22	c	503	CLA	CHB-C1B-NB	2.09	127.18	124.05
23	b	617	BCR	C30-C25-C26	-2.09	119.78	122.64
22	c	509	CLA	CHC-C1C-NC	2.09	127.46	124.31
31	a	413	LHG	C11-C10-C9	-2.09	103.81	114.37
31	l	102	LHG	O10-C23-C24	-2.09	115.61	123.78
30	c	520	LMG	O1-C1-C2	2.09	111.44	108.27
30	b	620	LMG	C22-C21-C20	-2.09	103.81	114.37
22	b	615	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
22	c	509	CLA	C3C-C4C-NC	-2.09	107.76	110.43
26	A	410	SQD	C17-C16-C15	-2.09	103.82	114.37
26	A	409	SQD	O49-C7-C8	-2.09	115.62	123.78
27	A	411	DGD	O6D-C5D-C4D	2.08	113.45	109.70
22	c	514	CLA	CAC-C3C-C4C	2.08	127.50	124.79
22	C	503	CLA	C4D-C3D-CAD	-2.08	105.84	108.11
23	b	617	BCR	C8-C7-C6	-2.08	121.43	127.00
22	C	505	CLA	CHD-C1D-ND	-2.08	121.87	124.80
23	c	515	BCR	C15-C14-C13	-2.08	124.36	127.28
22	B	707	CLA	CMB-C2B-C3B	2.08	131.44	126.55
22	b	613	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	b	603	CLA	CHC-C4B-NB	2.08	127.17	124.05
22	B	712	CLA	CAC-C3C-C2C	2.08	131.38	127.56
34	F	101	HEC	CBA-CAA-C2A	-2.08	106.78	112.53
27	C	517	DGD	O2G-C1B-O1B	-2.08	118.84	123.70
30	b	620	LMG	O7-C10-C11	2.08	115.98	111.48
22	C	514	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
22	d	401	CLA	C11-C10-C8	-2.08	109.06	115.97
25	a	410	PL9	C25-C24-C26	-2.08	111.62	115.23
22	C	509	CLA	C1-O2A-CGA	-2.08	111.62	116.65
23	H	101	BCR	C30-C25-C26	-2.08	119.80	122.64
27	A	411	DGD	C1E-O6E-C5E	2.07	117.77	113.72
22	c	502	CLA	C3A-C2A-C1A	2.07	104.45	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	X	101	STE	C12-C11-C10	-2.07	103.89	114.37
25	a	410	PL9	O1-C4-C3	-2.07	118.55	120.73
23	h	702	BCR	C11-C10-C9	-2.07	124.37	127.28
22	A	403	CLA	CHD-C1D-C2D	2.07	129.79	125.49
26	f	102	SQD	O48-C23-C24	2.07	118.15	111.83
22	c	513	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
30	d	410	LMG	O7-C10-O9	-2.07	118.87	123.70
33	D	408	PHO	OBD-CAD-CBD	-2.07	122.79	125.82
27	H	102	DGD	C8B-C7B-C6B	-2.07	103.92	114.37
22	a	403	CLA	CMB-C2B-C3B	2.07	131.41	126.55
22	C	510	CLA	C1-O2A-CGA	2.07	121.65	116.65
30	M	101	LMG	O8-C28-O10	-2.07	118.46	123.63
30	c	523	LMG	C12-C11-C10	-2.07	106.13	113.69
22	a	403	CLA	CED-O2D-CGD	-2.07	111.23	115.92
22	c	509	CLA	C2A-C1A-CHA	2.07	127.45	123.87
27	c	517	DGD	O3E-C3E-C2E	-2.06	105.51	110.38
23	c	516	BCR	C40-C30-C25	2.06	113.48	110.24
27	H	102	DGD	CBB-CAB-C9B	-2.06	103.94	114.37
22	B	716	CLA	CHB-C1B-NB	2.06	127.14	124.05
22	B	716	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	c	518	DGD	CDB-CCB-CBB	-2.06	103.95	114.37
22	C	510	CLA	CHD-C1D-C2D	2.06	129.77	125.49
23	C	515	BCR	C29-C30-C25	2.06	113.43	110.44
30	c	522	LMG	C40-C39-C38	-2.06	103.96	114.37
22	c	508	CLA	C3B-C4B-NB	-2.06	108.69	110.53
22	C	508	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
22	d	403	CLA	CHA-C4D-ND	2.06	136.79	132.55
22	D	402	CLA	CHA-C4D-ND	2.06	136.79	132.55
23	b	619	BCR	C7-C8-C9	-2.06	123.19	126.23
22	a	402	CLA	CBC-CAC-C3C	2.06	118.00	112.42
22	B	711	CLA	CGD-CBD-CAD	-2.06	104.19	110.85
33	D	407	PHO	OBD-CAD-C3D	2.06	131.10	127.89
22	B	715	CLA	CAC-C3C-C4C	2.05	127.46	124.79
22	B	711	CLA	CHD-C1D-ND	-2.05	121.91	124.80
22	b	602	CLA	C4-C3-C5	2.05	118.79	115.23
30	C	520	LMG	C31-C30-C29	-2.05	105.58	113.13
22	a	402	CLA	C9-C8-C7	2.05	118.59	111.27
22	B	727	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	D	406	PL9	C50-C49-C48	-2.05	116.50	122.66
22	c	511	CLA	C1-C2-C3	-2.05	122.84	126.20
28	c	521	STE	C15-C14-C13	-2.05	104.01	114.37
33	d	407	PHO	CAA-CBA-CGA	-2.05	107.39	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	CMA-C3A-C2A	-2.05	106.06	113.98
22	c	509	CLA	C3B-C4B-NB	-2.05	108.70	110.53
22	B	711	CLA	CHB-C1B-NB	2.05	127.12	124.05
25	A	408	PL9	C11-C9-C8	-2.05	116.57	121.17
22	c	513	CLA	CHC-C1C-NC	2.05	127.39	124.31
22	b	605	CLA	CHD-C1D-C2D	2.05	129.74	125.49
22	B	714	CLA	CAC-C3C-C4C	2.04	127.45	124.79
22	B	713	CLA	CMD-C2D-C3D	2.04	132.38	127.69
22	B	714	CLA	CHB-C1B-NB	2.04	127.12	124.05
22	C	510	CLA	C1-C2-C3	-2.04	122.85	126.20
22	c	505	CLA	C5-C3-C2	-2.04	116.58	121.17
23	A	405	BCR	C8-C9-C10	2.04	122.22	119.01
22	C	504	CLA	C3A-C2A-C1A	2.04	104.40	101.34
23	d	405	BCR	C8-C7-C6	-2.04	121.54	127.00
26	B	723	SQD	O4-C4-C5	-2.04	104.30	109.32
30	c	523	LMG	C30-C29-C28	-2.04	106.22	113.69
31	D	411	LHG	C15-C14-C13	-2.04	104.06	114.37
22	a	402	CLA	C2A-C1A-CHA	2.04	127.41	123.87
30	c	522	LMG	C1-C2-C3	2.04	114.30	110.01
26	a	412	SQD	O47-C7-C8	2.04	115.89	111.48
22	A	404	CLA	C1C-C2C-C3C	-2.04	104.84	106.98
22	D	403	CLA	C1C-C2C-C3C	-2.04	104.84	106.98
23	b	617	BCR	C36-C18-C19	2.04	121.20	118.09
22	h	701	CLA	C3A-C2A-C1A	2.04	104.39	101.34
33	a	404	PHO	CBA-CAA-C2A	-2.04	107.78	113.78
22	c	513	CLA	CHD-C1D-ND	-2.04	121.94	124.80
31	D	411	LHG	C20-C19-C18	-2.04	104.08	114.37
26	A	409	SQD	C9-C8-C7	-2.03	106.24	113.69
22	B	709	CLA	CAC-C3C-C4C	2.03	127.44	124.79
22	c	507	CLA	CMB-C2B-C3B	2.03	131.33	126.55
25	d	406	PL9	C20-C19-C21	2.03	118.76	115.23
27	c	519	DGD	O4E-C4E-C5E	-2.03	104.32	109.32
23	t	701	BCR	C40-C30-C25	2.03	113.43	110.24
22	B	711	CLA	C3C-C4C-NC	-2.03	107.83	110.43
27	c	518	DGD	O3G-C1D-C2D	-2.03	105.19	108.27
30	M	101	LMG	O6-C1-O1	-2.03	105.25	110.04
31	E	101	LHG	O8-C23-C24	2.03	118.02	111.83
22	b	608	CLA	CHC-C4B-NB	2.03	127.09	124.05
23	Y	101	BCR	C10-C11-C12	-2.03	117.32	123.20
23	B	719	BCR	C27-C26-C25	2.03	125.44	122.70
27	c	519	DGD	O2D-C2D-C1D	-2.03	105.25	110.08
25	d	406	PL9	C27-C26-C24	-2.03	106.47	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	k	101	BCR	C36-C18-C19	-2.02	115.00	118.09
31	E	101	LHG	O2-C2-C3	-2.02	102.70	109.70
22	b	612	CLA	C3A-C2A-C1A	2.02	104.37	101.34
34	F	101	HEC	CHB-C1B-NB	2.02	126.60	124.42
22	c	509	CLA	O1D-CGD-CBD	2.02	128.51	124.52
22	B	708	CLA	C1-C2-C3	-2.02	122.88	126.20
22	D	403	CLA	C4B-C3B-C2B	2.02	109.82	107.30
22	c	502	CLA	C9-C8-C10	-2.02	104.07	111.27
31	E	101	LHG	C18-C17-C16	-2.02	104.15	114.37
22	B	702	CLA	C3C-C4C-NC	-2.02	107.84	110.43
31	D	411	LHG	C11-C10-C9	-2.02	104.15	114.37
22	C	502	CLA	CGD-CBD-CAD	-2.02	104.30	110.85
22	C	512	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	c	505	CLA	C3A-C2A-C1A	2.02	104.36	101.34
22	B	708	CLA	CMB-C2B-C3B	2.02	131.30	126.55
22	A	402	CLA	C6-C5-C3	2.02	118.38	113.47
22	C	512	CLA	CED-O2D-CGD	-2.02	111.34	115.92
22	c	512	CLA	C11-C12-C13	-2.02	109.26	115.97
23	A	405	BCR	C8-C7-C6	-2.02	121.61	127.00
23	T	701	BCR	C1-C6-C5	-2.02	119.88	122.64
22	B	704	CLA	C2A-C3A-C4A	2.02	105.13	101.87
22	c	502	CLA	C11-C12-C13	-2.02	109.26	115.97
26	a	412	SQD	O7-S-C6	2.02	109.77	106.76
22	b	602	CLA	CHA-C4D-ND	2.01	136.71	132.55
23	B	718	BCR	C29-C28-C27	2.01	115.71	111.28
33	D	408	PHO	C4A-C3A-C2A	2.01	104.75	102.84
22	c	508	CLA	CHA-C1A-NA	-2.01	121.83	126.39
22	B	705	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	C	506	CLA	CHD-C1D-ND	-2.01	121.97	124.80
22	B	716	CLA	CHA-C1A-NA	-2.01	121.83	126.39
26	a	412	SQD	C45-O47-C7	2.01	122.61	117.80
30	b	620	LMG	C1-O6-C5	-2.01	109.79	113.72
23	c	515	BCR	C11-C10-C9	-2.01	124.46	127.28
34	V	201	HEC	CAD-CBD-CGD	-2.01	108.33	113.67
23	c	516	BCR	C37-C22-C21	-2.01	119.56	122.82
25	D	406	PL9	O2-C1-C2	-2.01	117.27	121.83
30	C	516	LMG	O7-C10-O9	-2.01	119.01	123.70
22	B	704	CLA	C1-O2A-CGA	-2.01	111.79	116.65
34	f	101	HEC	C4D-C3D-C2D	-2.00	103.97	106.89
31	L	101	LHG	C27-C26-C25	-2.00	104.24	114.37
22	b	604	CLA	CMA-C3A-C4A	2.00	117.16	111.77
22	a	405	CLA	CHC-C1C-NC	2.00	127.33	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	PL9	O2-C1-C6	2.00	123.67	120.48
22	b	613	CLA	CMB-C2B-C3B	2.00	131.26	126.55
28	j	101	STE	O2-C1-O1	-2.00	118.18	123.33
22	b	606	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
30	C	520	LMG	O7-C10-O9	-2.00	119.03	123.70
22	B	713	CLA	C4D-CHA-C1A	2.00	123.63	121.24
31	a	411	LHG	C27-C26-C25	-2.00	104.26	114.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	F	101	HEC	NA
34	V	201	HEC	NA
34	f	101	HEC	NA
34	v	201	HEC	NA

All (1793) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	705	CLA	C11-C12-C13-C14
22	B	714	CLA	CAD-CBD-CGD-O1D
22	B	714	CLA	CAD-CBD-CGD-O2D
22	B	714	CLA	C6-C7-C8-C9
22	B	727	CLA	CAD-CBD-CGD-O1D
22	B	727	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	C6-C7-C8-C9
22	D	404	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	C2B-C3B-CAB-CBB
22	b	605	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	514	CLA	CBD-CGD-O2D-CED
22	h	701	CLA	C4B-C3B-CAB-CBB
23	B	718	BCR	C16-C17-C18-C36
23	C	501	BCR	C11-C12-C13-C35
23	C	501	BCR	C17-C18-C19-C20
23	C	501	BCR	C18-C19-C20-C21
23	C	515	BCR	C11-C10-C9-C34
23	C	515	BCR	C20-C21-C22-C37
23	C	524	BCR	C11-C10-C9-C8
23	C	524	BCR	C14-C15-C16-C17
23	D	405	BCR	C17-C18-C19-C20
23	D	405	BCR	C20-C21-C22-C37
23	D	405	BCR	C23-C24-C25-C26
23	D	405	BCR	C23-C24-C25-C30
23	H	101	BCR	C7-C8-C9-C10
23	H	101	BCR	C11-C12-C13-C35
23	T	701	BCR	C7-C8-C9-C34
23	Y	101	BCR	C1-C6-C7-C8
23	Y	101	BCR	C5-C6-C7-C8
23	Y	101	BCR	C37-C22-C23-C24
23	a	406	BCR	C11-C10-C9-C34
23	b	617	BCR	C7-C8-C9-C34
23	b	617	BCR	C35-C13-C14-C15
23	b	617	BCR	C20-C21-C22-C37
23	c	515	BCR	C18-C19-C20-C21
23	c	516	BCR	C21-C22-C23-C24
23	c	516	BCR	C37-C22-C23-C24
23	d	405	BCR	C10-C11-C12-C13
23	k	101	BCR	C7-C8-C9-C34
23	t	701	BCR	C11-C10-C9-C34
23	t	701	BCR	C11-C12-C13-C14
23	t	701	BCR	C11-C12-C13-C35
25	A	408	PL9	C12-C13-C14-C16
25	A	408	PL9	C22-C23-C24-C25
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C32-C33-C34-C35
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C37-C38-C39-C41
25	D	406	PL9	C32-C33-C34-C36
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	a	410	PL9	C22-C23-C24-C26
25	a	410	PL9	C32-C33-C34-C35
25	a	410	PL9	C32-C33-C34-C36
25	a	410	PL9	C42-C43-C44-C45
25	d	406	PL9	C32-C33-C34-C36
26	A	409	SQD	O6-C44-C45-O47
26	A	410	SQD	C46-C45-O47-C7
26	B	723	SQD	O5-C1-O6-C44
26	B	723	SQD	O6-C44-C45-O47
26	B	723	SQD	C8-C7-O47-C45
26	a	412	SQD	O47-C45-C46-O48
26	a	414	SQD	C8-C7-O47-C45
26	f	102	SQD	O5-C1-O6-C44
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
26	l	101	SQD	C8-C7-O47-C45
26	l	101	SQD	O10-C23-O48-C46
26	l	101	SQD	C24-C23-O48-C46
30	C	516	LMG	O9-C10-O7-C8
30	c	523	LMG	O6-C1-O1-C7
30	c	523	LMG	C29-C28-O8-C9
31	B	722	LHG	O1-C1-C2-O2
31	B	722	LHG	O1-C1-C2-C3
31	B	722	LHG	C1-C2-C3-O3
31	B	722	LHG	C3-O3-P-O4
31	B	722	LHG	C3-O3-P-O5
31	B	722	LHG	C3-O3-P-O6
31	D	411	LHG	O1-C1-C2-C3
31	D	411	LHG	C3-O3-P-O4
31	D	411	LHG	C3-O3-P-O5
31	D	411	LHG	C3-O3-P-O6
31	D	411	LHG	C4-O6-P-O3
31	D	411	LHG	C4-O6-P-O4
31	D	412	LHG	C3-O3-P-O6
31	E	101	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	a	411	LHG	O1-C1-C2-C3
31	a	411	LHG	C3-O3-P-O6
31	a	411	LHG	C4-O6-P-O5
31	a	413	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
31	a	413	LHG	C3-O3-P-O6
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	l	102	LHG	C3-O3-P-O4
31	l	102	LHG	C4-O6-P-O3
31	l	102	LHG	C4-O6-P-O4
31	l	102	LHG	C4-O6-P-O5
22	b	614	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C2C-C3C-CAC-CBC
22	C	510	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
30	c	523	LMG	O10-C28-O8-C9
22	C	506	CLA	C4C-C3C-CAC-CBC
25	d	406	PL9	C47-C48-C49-C50
25	d	406	PL9	C47-C48-C49-C51
34	F	101	HEC	C2B-C3B-CAB-CBB
33	d	407	PHO	CBD-CGD-O2D-CED
26	f	102	SQD	O10-C23-O48-C46
31	a	413	LHG	O10-C23-O8-C6
34	V	201	HEC	C4C-C3C-CAC-CBC
22	b	616	CLA	O1D-CGD-O2D-CED
34	f	101	HEC	C2B-C3B-CAB-CBB
22	D	404	CLA	O1D-CGD-O2D-CED
22	c	514	CLA	O1D-CGD-O2D-CED
30	M	101	LMG	O10-C28-O8-C9
30	c	522	LMG	O10-C28-O8-C9
34	F	101	HEC	C4B-C3B-CAB-CBB
26	B	723	SQD	O49-C7-O47-C45
26	a	414	SQD	O49-C7-O47-C45
26	l	101	SQD	O49-C7-O47-C45
27	A	411	DGD	O1B-C1B-O2G-C2G
30	D	413	LMG	O9-C10-O7-C8
30	b	622	LMG	O9-C10-O7-C8
22	C	510	CLA	C3-C5-C6-C7
22	C	514	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
34	V	201	HEC	C2C-C3C-CAC-CBC
26	f	102	SQD	C24-C23-O48-C46
22	c	513	CLA	CBD-CGD-O2D-CED
33	D	408	PHO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	A	411	DGD	C2B-C1B-O2G-C2G
30	C	516	LMG	C11-C10-O7-C8
30	D	413	LMG	C11-C10-O7-C8
30	c	522	LMG	C11-C10-O7-C8
22	c	509	CLA	O1D-CGD-O2D-CED
22	B	714	CLA	C4-C3-C5-C6
22	C	514	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
25	A	408	PL9	C25-C24-C26-C27
25	A	408	PL9	C40-C39-C41-C42
25	d	406	PL9	C40-C39-C41-C42
22	B	714	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
25	a	410	PL9	C33-C34-C36-C37
25	d	406	PL9	C33-C34-C36-C37
22	h	701	CLA	C3-C5-C6-C7
26	B	723	SQD	C24-C23-O48-C46
30	c	522	LMG	C29-C28-O8-C9
31	E	101	LHG	C24-C23-O8-C6
31	a	413	LHG	C24-C23-O8-C6
30	C	516	LMG	O6-C5-C6-O5
30	c	522	LMG	C4-C5-C6-O5
25	A	408	PL9	C12-C13-C14-C15
25	D	406	PL9	C37-C38-C39-C40
25	a	410	PL9	C12-C13-C14-C15
25	d	406	PL9	C42-C43-C44-C45
23	k	101	BCR	C19-C20-C21-C22
26	a	414	SQD	O10-C23-O48-C46
30	c	522	LMG	O9-C10-O7-C8
34	f	101	HEC	C4B-C3B-CAB-CBB
22	C	510	CLA	O1D-CGD-O2D-CED
25	a	410	PL9	C47-C48-C49-C51
22	b	602	CLA	C3-C5-C6-C7
22	c	511	CLA	CBD-CGD-O2D-CED
31	B	722	LHG	O2-C2-C3-O3
31	D	411	LHG	O2-C2-C3-O3
22	a	405	CLA	CBA-CGA-O2A-C1
26	D	410	SQD	C24-C23-O48-C46
30	a	418	LMG	C29-C28-O8-C9
31	l	102	LHG	C7-C8-C9-C10
27	h	703	DGD	O6E-C5E-C6E-O5E
30	C	520	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
30	C	516	LMG	C4-C5-C6-O5
22	A	404	CLA	C4-C3-C5-C6
22	b	603	CLA	C4-C3-C5-C6
25	a	410	PL9	C35-C34-C36-C37
22	A	404	CLA	C2-C3-C5-C6
22	b	603	CLA	C2-C3-C5-C6
25	A	408	PL9	C23-C24-C26-C27
25	d	406	PL9	C38-C39-C41-C42
30	c	520	LMG	O6-C5-C6-O5
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C44-C46-C47-C48
25	D	406	PL9	C34-C36-C37-C38
25	a	410	PL9	C19-C21-C22-C23
25	d	406	PL9	C34-C36-C37-C38
25	d	406	PL9	C44-C46-C47-C48
22	a	405	CLA	O1A-CGA-O2A-C1
30	b	622	LMG	O10-C28-O8-C9
31	E	101	LHG	O10-C23-O8-C6
27	C	518	DGD	O6E-C1E-O5D-C6D
30	c	522	LMG	O6-C5-C6-O5
22	C	509	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
30	c	520	LMG	C4-C5-C6-O5
22	C	503	CLA	C3-C5-C6-C7
26	a	414	SQD	C24-C23-O48-C46
30	M	101	LMG	C29-C28-O8-C9
33	a	404	PHO	CBD-CGD-O2D-CED
26	a	412	SQD	C12-C13-C14-C15
31	B	722	LHG	C28-C29-C30-C31
33	d	407	PHO	O1D-CGD-O2D-CED
22	b	607	CLA	C4-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
22	C	514	CLA	C2-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
25	A	408	PL9	C47-C48-C49-C50
22	A	403	CLA	C14-C13-C15-C16
22	B	703	CLA	C11-C12-C13-C14
22	B	707	CLA	C14-C13-C15-C16
22	B	713	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	D	402	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	611	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
22	c	512	CLA	C14-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C9
22	h	701	CLA	C14-C13-C15-C16
30	c	523	LMG	C4-C5-C6-O5
26	B	723	SQD	C2-C1-O6-C44
27	C	518	DGD	C2E-C1E-O5D-C6D
31	D	412	LHG	O2-C2-C3-O3
23	C	501	BCR	C36-C18-C19-C20
23	C	501	BCR	C37-C22-C23-C24
23	D	405	BCR	C36-C18-C19-C20
23	b	619	BCR	C11-C12-C13-C35
23	c	515	BCR	C36-C18-C19-C20
23	h	702	BCR	C11-C12-C13-C35
23	k	101	BCR	C37-C22-C23-C24
30	c	520	LMG	O9-C10-O7-C8
23	d	405	BCR	C21-C22-C23-C24
23	k	101	BCR	C17-C18-C19-C20
31	d	409	LHG	C33-C34-C35-C36
34	F	101	HEC	C2C-C3C-CAC-CBC
22	B	713	CLA	C8-C10-C11-C12
31	l	102	LHG	C23-C24-C25-C26
22	C	510	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
25	D	406	PL9	C12-C13-C14-C15
22	C	506	CLA	C10-C11-C12-C13
22	C	510	CLA	C8-C10-C11-C12
22	C	514	CLA	C15-C16-C17-C18
22	b	615	CLA	C15-C16-C17-C18
22	h	701	CLA	C13-C15-C16-C17
31	a	411	LHG	O1-C1-C2-O2
22	B	711	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	b	604	CLA	C4-C3-C5-C6
26	A	410	SQD	C23-C24-C25-C26
25	a	410	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	c	520	LMG	C11-C10-O7-C8
27	H	102	DGD	C1A-C2A-C3A-C4A
30	M	101	LMG	C28-C29-C30-C31
27	c	519	DGD	O1A-C1A-O1G-C1G
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
30	C	520	LMG	C29-C28-O8-C9
22	C	507	CLA	C15-C16-C17-C18
22	C	513	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	B	706	CLA	C2A-CAA-CBA-CGA
23	T	701	BCR	C18-C19-C20-C21
22	B	714	CLA	C13-C15-C16-C17
22	B	716	CLA	C5-C6-C7-C8
22	a	405	CLA	C5-C6-C7-C8
22	b	611	CLA	C15-C16-C17-C18
22	d	404	CLA	C5-C6-C7-C8
27	h	703	DGD	C4E-C5E-C6E-O5E
28	b	624	STE	C1-C2-C3-C4
30	D	413	LMG	C10-C11-C12-C13
30	b	622	LMG	C28-C29-C30-C31
30	c	522	LMG	C10-C11-C12-C13
31	a	413	LHG	C23-C24-C25-C26
22	B	727	CLA	C3-C5-C6-C7
22	C	502	CLA	CBD-CGD-O2D-CED
34	f	101	HEC	C4C-C3C-CAC-CBC
22	B	712	CLA	C13-C15-C16-C17
22	B	727	CLA	C15-C16-C17-C18
22	C	504	CLA	C5-C6-C7-C8
22	C	509	CLA	C15-C16-C17-C18
22	D	402	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17
22	b	613	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
22	c	510	CLA	C10-C11-C12-C13
31	E	101	LHG	O2-C2-C3-O3
31	a	411	LHG	O2-C2-C3-O3
30	a	418	LMG	O10-C28-O8-C9
28	b	623	STE	C1-C2-C3-C4
31	a	411	LHG	C23-C24-C25-C26
22	C	510	CLA	C5-C6-C7-C8
22	D	404	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	A	410	SQD	C17-C18-C19-C20
22	D	403	CLA	C15-C16-C17-C18
22	c	506	CLA	C5-C6-C7-C8
22	h	701	CLA	C8-C10-C11-C12
30	c	523	LMG	O6-C5-C6-O5
27	C	519	DGD	O1A-C1A-O1G-C1G
25	A	408	PL9	C18-C19-C21-C22
27	c	518	DGD	C1A-C2A-C3A-C4A
33	D	408	PHO	O1D-CGD-O2D-CED
22	d	404	CLA	C10-C11-C12-C13
22	B	727	CLA	CBA-CGA-O2A-C1
26	a	412	SQD	C24-C23-O48-C46
27	c	518	DGD	C1B-C2B-C3B-C4B
28	c	521	STE	C1-C2-C3-C4
30	d	410	LMG	C28-C29-C30-C31
31	a	411	LHG	C7-C8-C9-C10
31	D	411	LHG	C1-C2-C3-O3
31	E	101	LHG	C1-C2-C3-O3
31	a	411	LHG	C1-C2-C3-O3
22	b	606	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	CBA-CGA-O2A-C1
23	D	405	BCR	C14-C15-C16-C17
22	C	507	CLA	C8-C10-C11-C12
22	D	403	CLA	C13-C15-C16-C17
25	a	410	PL9	C47-C48-C49-C50
22	B	705	CLA	C8-C10-C11-C12
22	B	707	CLA	C13-C15-C16-C17
22	b	614	CLA	C8-C10-C11-C12
22	c	507	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
28	B	701	STE	C5-C6-C7-C8
22	B	706	CLA	C5-C6-C7-C8
22	B	715	CLA	C5-C6-C7-C8
22	c	509	CLA	C10-C11-C12-C13
22	c	507	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
25	A	408	PL9	C28-C29-C31-C32
25	D	406	PL9	C38-C39-C41-C42
30	b	622	LMG	C11-C10-O7-C8
22	C	514	CLA	C11-C12-C13-C14
25	d	406	PL9	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	d	406	PL9	C37-C38-C39-C40
27	c	518	DGD	C2E-C1E-O5D-C6D
22	c	512	CLA	C16-C17-C18-C19
22	d	401	CLA	C16-C17-C18-C20
23	A	405	BCR	C35-C13-C14-C15
23	A	405	BCR	C20-C21-C22-C37
23	B	717	BCR	C11-C10-C9-C34
23	B	717	BCR	C35-C13-C14-C15
23	B	717	BCR	C16-C17-C18-C36
23	B	717	BCR	C20-C21-C22-C37
23	B	718	BCR	C35-C13-C14-C15
23	B	718	BCR	C20-C21-C22-C37
23	B	719	BCR	C16-C17-C18-C36
23	C	501	BCR	C16-C17-C18-C36
23	C	501	BCR	C20-C21-C22-C37
23	C	515	BCR	C16-C17-C18-C36
23	D	405	BCR	C11-C10-C9-C34
23	H	101	BCR	C20-C21-C22-C37
23	Y	101	BCR	C11-C10-C9-C34
23	Y	101	BCR	C20-C21-C22-C37
23	a	406	BCR	C20-C21-C22-C37
23	b	619	BCR	C35-C13-C14-C15
23	c	515	BCR	C11-C10-C9-C34
23	c	515	BCR	C16-C17-C18-C36
23	d	405	BCR	C16-C17-C18-C36
23	h	702	BCR	C35-C13-C14-C15
23	k	101	BCR	C35-C13-C14-C15
23	k	101	BCR	C16-C17-C18-C36
23	k	101	BCR	C20-C21-C22-C37
23	t	701	BCR	C20-C21-C22-C37
22	C	506	CLA	C5-C6-C7-C8
22	b	615	CLA	C5-C6-C7-C8
23	C	524	BCR	C7-C8-C9-C34
23	C	524	BCR	C37-C22-C23-C24
23	b	619	BCR	C37-C22-C23-C24
23	d	405	BCR	C37-C22-C23-C24
23	k	101	BCR	C36-C18-C19-C20
23	B	717	BCR	C17-C18-C19-C20
23	k	101	BCR	C7-C8-C9-C10
22	c	507	CLA	O1A-CGA-O2A-C1
30	D	413	LMG	O10-C28-O8-C9
22	c	513	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C8-C10-C11-C12
31	d	409	LHG	O1-C1-C2-C3
26	l	101	SQD	C46-C45-O47-C7
22	b	607	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C14
22	c	507	CLA	C16-C17-C18-C19
23	B	717	BCR	C12-C13-C14-C15
23	B	717	BCR	C20-C21-C22-C23
23	C	524	BCR	C20-C21-C22-C23
23	D	405	BCR	C20-C21-C22-C23
23	T	701	BCR	C12-C13-C14-C15
23	b	617	BCR	C12-C13-C14-C15
23	c	515	BCR	C16-C17-C18-C19
23	c	515	BCR	C20-C21-C22-C23
23	d	405	BCR	C16-C17-C18-C19
23	d	405	BCR	C20-C21-C22-C23
23	h	702	BCR	C11-C10-C9-C8
23	h	702	BCR	C16-C17-C18-C19
23	t	701	BCR	C12-C13-C14-C15
27	c	518	DGD	O6E-C1E-O5D-C6D
28	C	523	STE	C7-C8-C9-C10
30	D	413	LMG	C29-C28-O8-C9
22	a	403	CLA	C13-C15-C16-C17
31	D	412	LHG	C7-C8-C9-C10
31	E	101	LHG	C23-C24-C25-C26
27	c	517	DGD	O6D-C5D-C6D-O5D
22	B	727	CLA	C2-C1-O2A-CGA
22	b	602	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C15
22	c	511	CLA	C16-C17-C18-C19
28	d	402	STE	C14-C15-C16-C17
22	c	513	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C15-C16-C17-C18
22	b	607	CLA	C10-C11-C12-C13
26	B	723	SQD	C11-C10-C9-C8
26	a	414	SQD	C11-C10-C9-C8
26	l	101	SQD	C26-C27-C28-C29
27	c	519	DGD	C3A-C4A-C5A-C6A
28	B	724	STE	C2-C3-C4-C5
28	C	521	STE	C5-C6-C7-C8
28	b	624	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	b	622	LMG	C13-C14-C15-C16
30	c	522	LMG	C13-C14-C15-C16
23	A	405	BCR	C14-C15-C16-C17
23	d	405	BCR	C14-C15-C16-C17
26	A	409	SQD	C26-C27-C28-C29
26	l	101	SQD	C24-C25-C26-C27
28	H	103	STE	C9-C10-C11-C12
28	c	521	STE	C10-C11-C12-C13
30	C	520	LMG	C31-C32-C33-C34
30	a	418	LMG	C21-C22-C23-C24
30	c	523	LMG	C12-C13-C14-C15
31	L	101	LHG	C17-C18-C19-C20
26	l	101	SQD	C23-C24-C25-C26
27	C	519	DGD	CBA-CCA-CDA-CEA
27	c	517	DGD	C4A-C5A-C6A-C7A
28	Z	101	STE	C11-C12-C13-C14
28	b	623	STE	C6-C7-C8-C9
28	c	521	STE	C11-C12-C13-C14
30	M	101	LMG	C35-C36-C37-C38
31	E	101	LHG	C17-C18-C19-C20
26	A	409	SQD	C16-C17-C18-C19
26	B	723	SQD	C11-C12-C13-C14
26	a	414	SQD	C16-C17-C18-C19
27	A	411	DGD	C2B-C3B-C4B-C5B
27	C	518	DGD	C5A-C6A-C7A-C8A
30	a	418	LMG	C33-C34-C35-C36
31	D	412	LHG	C33-C34-C35-C36
31	E	101	LHG	C11-C10-C9-C8
31	d	408	LHG	C29-C30-C31-C32
31	l	102	LHG	C12-C13-C14-C15
31	D	411	LHG	O1-C1-C2-O2
26	a	412	SQD	C29-C30-C31-C32
28	T	702	STE	C9-C10-C11-C12
30	C	520	LMG	C18-C19-C20-C21
30	M	101	LMG	C12-C13-C14-C15
31	l	102	LHG	C14-C15-C16-C17
22	B	706	CLA	C4B-C3B-CAB-CBB
22	B	715	CLA	C4B-C3B-CAB-CBB
26	B	723	SQD	C13-C14-C15-C16
30	c	520	LMG	C36-C37-C38-C39
30	c	522	LMG	C30-C31-C32-C33
31	E	101	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	B	706	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
28	I	101	STE	C10-C11-C12-C13
22	C	511	CLA	C13-C15-C16-C17
22	b	616	CLA	C5-C6-C7-C8
27	h	703	DGD	C2B-C3B-C4B-C5B
31	D	412	LHG	C10-C11-C12-C13
31	L	101	LHG	C14-C15-C16-C17
22	C	511	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C10-C8-C7
26	A	409	SQD	C12-C13-C14-C15
26	A	410	SQD	C32-C33-C34-C35
26	A	410	SQD	C12-C13-C14-C15
27	c	519	DGD	CBA-CCA-CDA-CEA
28	M	103	STE	C4-C5-C6-C7
28	x	101	STE	C7-C8-C9-C10
30	D	409	LMG	C31-C32-C33-C34
30	c	522	LMG	C11-C12-C13-C14
22	B	727	CLA	O1A-CGA-O2A-C1
26	B	723	SQD	O10-C23-O48-C46
26	D	410	SQD	O10-C23-O48-C46
22	B	703	CLA	C4-C3-C5-C6
28	B	725	STE	C9-C10-C11-C12
28	B	725	STE	C11-C12-C13-C14
28	X	101	STE	C4-C5-C6-C7
28	a	415	STE	C6-C7-C8-C9
22	b	608	CLA	C5-C6-C7-C8
30	a	418	LMG	C41-C42-C43-C44
22	B	706	CLA	C16-C17-C18-C19
22	B	710	CLA	C16-C17-C18-C19
22	C	503	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C20
22	d	401	CLA	C16-C17-C18-C19
27	A	411	DGD	CBB-CCB-CDB-CEB
28	E	102	STE	C3-C4-C5-C6
30	D	413	LMG	C14-C15-C16-C17
30	b	620	LMG	C17-C18-C19-C20
31	E	101	LHG	C30-C31-C32-C33
27	H	102	DGD	C8B-C9B-CAB-CBB
28	X	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	l	102	LHG	C9-C10-C11-C12
30	b	620	LMG	C29-C28-O8-C9
30	c	522	LMG	O1-C7-C8-C9
26	A	410	SQD	C14-C15-C16-C17
26	B	723	SQD	C18-C19-C20-C21
26	f	102	SQD	C27-C28-C29-C30
27	C	518	DGD	C6A-C7A-C8A-C9A
28	T	702	STE	C13-C14-C15-C16
28	b	623	STE	C3-C4-C5-C6
28	t	702	STE	C11-C10-C9-C8
30	C	516	LMG	C35-C36-C37-C38
30	b	622	LMG	C18-C19-C20-C21
30	b	622	LMG	C23-C24-C25-C26
30	c	522	LMG	C15-C16-C17-C18
30	c	523	LMG	C28-C29-C30-C31
33	d	407	PHO	C2C-C3C-CAC-CBC
27	c	517	DGD	C7A-C8A-C9A-CAA
27	c	519	DGD	C8B-C9B-CAB-CBB
28	I	101	STE	C2-C3-C4-C5
28	c	521	STE	C9-C10-C11-C12
30	B	721	LMG	C33-C34-C35-C36
30	C	520	LMG	C38-C39-C40-C41
31	a	411	LHG	C16-C17-C18-C19
31	d	408	LHG	C32-C33-C34-C35
27	C	517	DGD	C5B-C6B-C7B-C8B
28	B	726	STE	C11-C10-C9-C8
30	D	409	LMG	C36-C37-C38-C39
27	c	519	DGD	C7A-C8A-C9A-CAA
30	B	721	LMG	C32-C33-C34-C35
26	a	414	SQD	C10-C11-C12-C13
26	f	102	SQD	C25-C26-C27-C28
27	A	411	DGD	C9A-CAA-CBA-CCA
27	c	517	DGD	C4B-C5B-C6B-C7B
28	X	101	STE	C3-C4-C5-C6
30	a	418	LMG	C13-C14-C15-C16
31	D	412	LHG	C15-C16-C17-C18
31	L	101	LHG	C29-C30-C31-C32
22	b	615	CLA	C16-C17-C18-C19
26	f	102	SQD	C23-C24-C25-C26
22	B	715	CLA	C2B-C3B-CAB-CBB
22	c	513	CLA	C2B-C3B-CAB-CBB
22	h	701	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	501	BCR	C1-C6-C7-C8
23	C	501	BCR	C5-C6-C7-C8
23	H	101	BCR	C23-C24-C25-C26
23	b	617	BCR	C1-C6-C7-C8
23	b	617	BCR	C5-C6-C7-C8
23	k	101	BCR	C1-C6-C7-C8
23	k	101	BCR	C5-C6-C7-C8
31	L	101	LHG	C12-C13-C14-C15
31	a	413	LHG	C27-C28-C29-C30
22	B	703	CLA	C8-C10-C11-C12
27	c	518	DGD	C7A-C8A-C9A-CAA
28	b	624	STE	C14-C15-C16-C17
22	C	509	CLA	O1D-CGD-O2D-CED
31	E	101	LHG	C33-C34-C35-C36
31	L	101	LHG	C18-C19-C20-C21
22	C	511	CLA	C8-C10-C11-C12
26	l	101	SQD	C27-C28-C29-C30
27	H	102	DGD	C6A-C7A-C8A-C9A
31	D	412	LHG	C29-C30-C31-C32
26	A	409	SQD	C14-C15-C16-C17
27	c	518	DGD	C2A-C3A-C4A-C5A
28	h	704	STE	C10-C11-C12-C13
30	B	721	LMG	C14-C15-C16-C17
26	A	409	SQD	C10-C11-C12-C13
27	c	519	DGD	CCA-CDA-CEA-CFA
30	b	620	LMG	C20-C21-C22-C23
22	D	404	CLA	C13-C15-C16-C17
22	B	703	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
25	A	408	PL9	C43-C44-C46-C47
25	D	406	PL9	C33-C34-C36-C37
26	a	412	SQD	C15-C16-C17-C18
27	C	518	DGD	C8B-C9B-CAB-CBB
27	h	703	DGD	C6B-C7B-C8B-C9B
27	h	703	DGD	C9B-CAB-CBB-CCB
28	B	701	STE	C2-C3-C4-C5
28	d	411	STE	C5-C6-C7-C8
30	c	522	LMG	C33-C34-C35-C36
31	D	412	LHG	C30-C31-C32-C33
31	a	413	LHG	C17-C18-C19-C20
22	C	506	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	727	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
27	A	411	DGD	C8B-C9B-CAB-CBB
28	T	702	STE	C12-C13-C14-C15
28	x	101	STE	C2-C3-C4-C5
31	E	101	LHG	C29-C30-C31-C32
22	B	727	CLA	C10-C11-C12-C13
26	B	723	SQD	C33-C34-C35-C36
27	C	518	DGD	CCB-CDB-CEB-CFB
31	L	101	LHG	C31-C32-C33-C34
23	b	619	BCR	C14-C15-C16-C17
26	a	412	SQD	C10-C11-C12-C13
28	m	101	STE	C4-C5-C6-C7
31	E	101	LHG	C24-C25-C26-C27
26	f	102	SQD	C2-C1-O6-C44
30	c	523	LMG	C2-C1-O1-C7
22	B	705	CLA	C10-C11-C12-C13
22	b	604	CLA	C15-C16-C17-C18
28	b	601	STE	C4-C5-C6-C7
30	B	721	LMG	C31-C32-C33-C34
31	a	411	LHG	C11-C10-C9-C8
28	b	621	STE	C1-C2-C3-C4
27	H	102	DGD	C6B-C7B-C8B-C9B
26	A	409	SQD	C32-C33-C34-C35
26	a	414	SQD	C14-C15-C16-C17
28	B	701	STE	C3-C4-C5-C6
28	B	726	STE	C11-C12-C13-C14
28	M	102	STE	C9-C10-C11-C12
28	T	702	STE	C5-C6-C7-C8
28	b	621	STE	C7-C8-C9-C10
28	x	101	STE	C3-C4-C5-C6
30	b	622	LMG	C30-C31-C32-C33
31	d	409	LHG	C31-C32-C33-C34
22	c	513	CLA	C13-C15-C16-C17
22	a	402	CLA	C16-C17-C18-C19
22	c	507	CLA	C16-C17-C18-C20
26	A	409	SQD	C8-C7-O47-C45
28	B	720	STE	C1-C2-C3-C4
31	E	101	LHG	C10-C11-C12-C13
22	b	605	CLA	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
27	C	517	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
26	a	412	SQD	C24-C25-C26-C27
30	c	523	LMG	C34-C35-C36-C37
28	J	101	STE	C3-C4-C5-C6
30	D	409	LMG	C16-C17-C18-C19
22	c	513	CLA	C5-C6-C7-C8
30	M	101	LMG	C14-C15-C16-C17
25	D	406	PL9	C27-C28-C29-C30
30	b	620	LMG	C39-C40-C41-C42
22	B	716	CLA	C3-C5-C6-C7
22	a	405	CLA	C2C-C3C-CAC-CBC
23	D	405	BCR	C21-C22-C23-C24
30	a	418	LMG	C8-C7-O1-C1
26	B	723	SQD	C27-C28-C29-C30
27	c	519	DGD	C9B-CAB-CBB-CCB
28	M	103	STE	C3-C4-C5-C6
30	D	409	LMG	C17-C18-C19-C20
30	a	418	LMG	C36-C37-C38-C39
31	a	411	LHG	C17-C18-C19-C20
22	B	712	CLA	C16-C17-C18-C19
22	B	716	CLA	C11-C12-C13-C15
22	C	514	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C19
27	c	518	DGD	CAB-CBB-CCB-CDB
28	h	704	STE	C7-C8-C9-C10
30	D	409	LMG	C38-C39-C40-C41
31	B	722	LHG	C26-C27-C28-C29
31	d	408	LHG	C12-C13-C14-C15
31	d	409	LHG	C27-C28-C29-C30
22	C	506	CLA	C4-C3-C5-C6
30	b	622	LMG	C32-C33-C34-C35
31	D	412	LHG	C11-C10-C9-C8
31	D	412	LHG	C25-C26-C27-C28
22	B	711	CLA	C8-C10-C11-C12
28	T	702	STE	C11-C12-C13-C14
27	C	517	DGD	C7B-C8B-C9B-CAB
28	j	101	STE	C4-C5-C6-C7
22	c	508	CLA	C8-C10-C11-C12
27	c	517	DGD	C9B-CAB-CBB-CCB
30	M	101	LMG	C37-C38-C39-C40
28	E	102	STE	C1-C2-C3-C4
26	A	409	SQD	C30-C31-C32-C33
28	H	104	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	b	622	LMG	C12-C13-C14-C15
22	B	710	CLA	C8-C10-C11-C12
28	X	101	STE	C6-C7-C8-C9
30	C	520	LMG	C30-C31-C32-C33
30	a	418	LMG	C18-C19-C20-C21
22	C	506	CLA	O1A-CGA-O2A-C1
28	t	702	STE	C6-C7-C8-C9
30	b	622	LMG	C16-C17-C18-C19
30	c	522	LMG	C29-C30-C31-C32
30	c	522	LMG	C40-C41-C42-C43
30	d	410	LMG	O6-C5-C6-O5
26	a	412	SQD	O6-C44-C45-O47
26	l	101	SQD	C29-C30-C31-C32
27	H	102	DGD	C5A-C6A-C7A-C8A
28	d	402	STE	C9-C10-C11-C12
30	b	622	LMG	C29-C28-O8-C9
26	D	410	SQD	C26-C27-C28-C29
30	C	520	LMG	C37-C38-C39-C40
27	C	519	DGD	C3A-C4A-C5A-C6A
28	B	720	STE	C11-C12-C13-C14
30	C	520	LMG	C17-C18-C19-C20
30	b	622	LMG	C11-C12-C13-C14
26	B	723	SQD	C9-C10-C11-C12
28	d	402	STE	C6-C7-C8-C9
28	d	411	STE	C10-C11-C12-C13
30	b	620	LMG	C37-C38-C39-C40
30	c	522	LMG	C34-C35-C36-C37
30	c	523	LMG	C18-C19-C20-C21
30	d	410	LMG	C30-C31-C32-C33
31	D	412	LHG	C12-C13-C14-C15
31	l	102	LHG	C24-C25-C26-C27
30	D	409	LMG	O6-C5-C6-O5
22	B	703	CLA	C16-C17-C18-C20
22	B	716	CLA	C11-C12-C13-C14
22	B	711	CLA	C13-C15-C16-C17
26	a	414	SQD	C11-C12-C13-C14
27	C	519	DGD	C4B-C5B-C6B-C7B
28	X	101	STE	C13-C14-C15-C16
30	C	516	LMG	C16-C17-C18-C19
30	c	522	LMG	C39-C40-C41-C42
28	b	623	STE	C11-C10-C9-C8
31	D	412	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
34	V	201	HEC	C2B-C3B-CAB-CBB
26	A	410	SQD	C10-C11-C12-C13
28	a	416	STE	C4-C5-C6-C7
31	l	102	LHG	C26-C27-C28-C29
22	a	402	CLA	CBD-CGD-O2D-CED
27	C	517	DGD	O6E-C5E-C6E-O5E
26	a	412	SQD	C16-C17-C18-C19
27	C	519	DGD	C6A-C7A-C8A-C9A
30	C	520	LMG	C39-C40-C41-C42
30	c	523	LMG	C15-C16-C17-C18
30	c	523	LMG	C38-C39-C40-C41
27	c	517	DGD	C4D-C5D-C6D-O5D
26	a	412	SQD	C30-C31-C32-C33
30	M	101	LMG	C38-C39-C40-C41
30	M	101	LMG	C33-C34-C35-C36
30	c	523	LMG	C29-C30-C31-C32
31	a	411	LHG	C32-C33-C34-C35
28	H	103	STE	C5-C6-C7-C8
31	B	722	LHG	C9-C10-C11-C12
22	B	702	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C20
22	b	609	CLA	O1D-CGD-O2D-CED
31	d	409	LHG	O1-C1-C2-O2
31	a	413	LHG	C16-C17-C18-C19
30	b	620	LMG	C33-C34-C35-C36
22	B	704	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
27	c	517	DGD	C1B-C2B-C3B-C4B
27	A	411	DGD	C2A-C3A-C4A-C5A
28	c	521	STE	C11-C10-C9-C8
31	l	102	LHG	C17-C18-C19-C20
26	B	723	SQD	C16-C17-C18-C19
27	c	519	DGD	C9A-CAA-CBA-CCA
22	B	710	CLA	C15-C16-C17-C18
22	B	715	CLA	C13-C15-C16-C17
22	c	513	CLA	C15-C16-C17-C18
26	a	412	SQD	C26-C27-C28-C29
26	a	412	SQD	C34-C35-C36-C37
28	H	103	STE	C6-C7-C8-C9
22	B	705	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	b	611	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	c	512	CLA	C12-C13-C15-C16
22	d	404	CLA	C11-C12-C13-C15
27	A	411	DGD	C4B-C5B-C6B-C7B
27	C	519	DGD	C2B-C3B-C4B-C5B
26	A	410	SQD	C18-C19-C20-C21
31	L	101	LHG	C32-C33-C34-C35
33	a	404	PHO	O1D-CGD-O2D-CED
27	A	411	DGD	CCB-CDB-CEB-CFB
28	B	725	STE	C5-C6-C7-C8
22	b	614	CLA	C15-C16-C17-C18
22	c	512	CLA	C15-C16-C17-C18
22	B	704	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	C	514	CLA	C11-C10-C8-C9
22	a	405	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C12-C13-C14
27	c	519	DGD	C6B-C7B-C8B-C9B
28	B	726	STE	C4-C5-C6-C7
28	E	102	STE	C4-C5-C6-C7
30	c	523	LMG	C32-C33-C34-C35
31	E	101	LHG	C32-C33-C34-C35
30	C	516	LMG	C10-C11-C12-C13
22	C	503	CLA	C16-C17-C18-C20
27	C	518	DGD	C4A-C5A-C6A-C7A
28	H	104	STE	C6-C7-C8-C9
28	b	601	STE	C6-C7-C8-C9
31	a	411	LHG	C15-C16-C17-C18
28	B	725	STE	C2-C3-C4-C5
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	A	409	SQD	C11-C10-C9-C8
28	c	521	STE	C7-C8-C9-C10
26	B	723	SQD	O6-C44-C45-C46
26	a	412	SQD	O6-C44-C45-C46
26	a	412	SQD	C44-C45-C46-O48
27	A	411	DGD	C1G-C2G-C3G-O3G
30	a	418	LMG	O1-C7-C8-C9
30	c	522	LMG	C7-C8-C9-O8
31	E	101	LHG	C4-C5-C6-O8
27	A	411	DGD	C5B-C6B-C7B-C8B
27	c	517	DGD	O6E-C5E-C6E-O5E
31	a	411	LHG	C30-C31-C32-C33
22	d	404	CLA	C15-C16-C17-C18
22	C	514	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	C16-C17-C18-C19
22	C	514	CLA	C16-C17-C18-C19
26	a	414	SQD	C24-C25-C26-C27
28	Z	101	STE	C13-C14-C15-C16
31	B	722	LHG	C12-C13-C14-C15
26	B	723	SQD	C45-C46-O48-C23
28	b	623	STE	C5-C6-C7-C8
30	C	516	LMG	C32-C33-C34-C35
30	b	622	LMG	O6-C5-C6-O5
27	c	517	DGD	CBA-CCA-CDA-CEA
28	c	521	STE	C4-C5-C6-C7
23	b	617	BCR	C11-C10-C9-C34
23	b	619	BCR	C20-C21-C22-C37
30	c	520	LMG	C35-C36-C37-C38
33	D	407	PHO	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
25	a	410	PL9	C38-C39-C41-C42
33	D	407	PHO	C2-C3-C5-C6
30	M	101	LMG	C13-C14-C15-C16
31	a	413	LHG	C11-C12-C13-C14
22	A	402	CLA	C4C-C3C-CAC-CBC
33	D	407	PHO	C16-C17-C18-C20
27	H	102	DGD	C9A-CAA-CBA-CCA
31	D	411	LHG	C11-C10-C9-C8
22	c	504	CLA	C5-C6-C7-C8
22	c	504	CLA	C15-C16-C17-C18
27	C	519	DGD	C7B-C8B-C9B-CAB
31	d	409	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	C	516	LMG	C38-C39-C40-C41
31	d	409	LHG	C23-C24-C25-C26
22	C	513	CLA	O2A-C1-C2-C3
26	B	723	SQD	C46-C45-O47-C7
27	c	518	DGD	CAA-CBA-CCA-CDA
28	I	101	STE	C11-C10-C9-C8
28	a	415	STE	C3-C4-C5-C6
28	b	623	STE	C7-C8-C9-C10
28	m	101	STE	C7-C8-C9-C10
27	A	411	DGD	O6D-C5D-C6D-O5D
23	t	701	BCR	C10-C11-C12-C13
22	D	402	CLA	C10-C11-C12-C13
27	C	518	DGD	C3A-C4A-C5A-C6A
27	c	518	DGD	C7B-C8B-C9B-CAB
27	c	519	DGD	C4B-C5B-C6B-C7B
28	m	101	STE	C10-C11-C12-C13
31	L	101	LHG	C11-C12-C13-C14
23	h	702	BCR	C15-C16-C17-C18
30	D	409	LMG	C14-C15-C16-C17
23	C	515	BCR	C20-C21-C22-C23
23	b	618	BCR	C16-C17-C18-C19
23	t	701	BCR	C11-C10-C9-C8
31	d	409	LHG	C35-C36-C37-C38
27	A	411	DGD	C2A-C1A-O1G-C1G
28	A	412	STE	C11-C10-C9-C8
27	H	102	DGD	C4A-C5A-C6A-C7A
28	b	625	STE	C3-C4-C5-C6
28	d	411	STE	C11-C12-C13-C14
31	l	102	LHG	C10-C11-C12-C13
22	b	608	CLA	C13-C15-C16-C17
25	d	406	PL9	C13-C14-C16-C17
22	A	404	CLA	C6-C7-C8-C9
26	A	409	SQD	C17-C18-C19-C20
27	C	517	DGD	C8B-C9B-CAB-CBB
31	l	102	LHG	C33-C34-C35-C36
28	d	402	STE	C11-C12-C13-C14
28	h	704	STE	C12-C13-C14-C15
30	a	418	LMG	C32-C33-C34-C35
30	c	522	LMG	C38-C39-C40-C41
27	C	519	DGD	CDB-CEB-CFB-CGB
28	B	720	STE	C12-C13-C14-C15
27	C	518	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C11-C12-C13-C14
26	A	409	SQD	O47-C45-C46-O48
30	c	522	LMG	O1-C7-C8-O7
27	C	517	DGD	CDA-CEA-CFA-CGA
30	D	413	LMG	C33-C34-C35-C36
31	D	412	LHG	C27-C28-C29-C30
30	c	520	LMG	C34-C35-C36-C37
30	c	522	LMG	C31-C32-C33-C34
28	a	416	STE	C7-C8-C9-C10
27	c	519	DGD	C7B-C8B-C9B-CAB
28	B	720	STE	C3-C4-C5-C6
30	a	418	LMG	C23-C24-C25-C26
27	H	102	DGD	C7A-C8A-C9A-CAA
30	M	101	LMG	C40-C41-C42-C43
27	c	517	DGD	O1B-C1B-O2G-C2G
27	c	519	DGD	CDA-CEA-CFA-CGA
28	M	103	STE	C7-C8-C9-C10
22	C	514	CLA	O1A-CGA-O2A-C1
27	h	703	DGD	CAA-CBA-CCA-CDA
31	L	101	LHG	C13-C14-C15-C16
27	C	519	DGD	C2A-C1A-O1G-C1G
25	d	406	PL9	C22-C23-C24-C25
28	a	415	STE	C2-C3-C4-C5
28	b	621	STE	C12-C13-C14-C15
28	x	101	STE	C5-C6-C7-C8
31	D	411	LHG	C10-C11-C12-C13
26	l	101	SQD	C19-C20-C21-C22
22	C	508	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
22	C	511	CLA	C4-C3-C5-C6
25	d	406	PL9	C30-C29-C31-C32
28	h	704	STE	C15-C16-C17-C18
31	l	102	LHG	C32-C33-C34-C35
22	C	507	CLA	C13-C15-C16-C17
27	C	517	DGD	C6B-C7B-C8B-C9B
28	b	621	STE	C14-C15-C16-C17
28	B	725	STE	C12-C13-C14-C15
30	M	101	LMG	C17-C18-C19-C20
30	C	520	LMG	O9-C10-O7-C8
31	E	101	LHG	O1-C1-C2-O2
31	d	408	LHG	O1-C1-C2-O2
22	B	704	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	b	614	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	d	404	CLA	C11-C12-C13-C14
28	M	102	STE	C11-C10-C9-C8
22	d	403	CLA	C4B-C3B-CAB-CBB
22	A	404	CLA	C5-C6-C7-C8
26	A	409	SQD	C28-C29-C30-C31
27	A	411	DGD	CDA-CEA-CFA-CGA
28	b	625	STE	C4-C5-C6-C7
30	M	101	LMG	C15-C16-C17-C18
30	c	520	LMG	C40-C41-C42-C43
30	c	523	LMG	C20-C21-C22-C23
22	b	602	CLA	C16-C17-C18-C20
30	C	516	LMG	C36-C37-C38-C39
26	A	410	SQD	C27-C28-C29-C30
28	x	101	STE	C9-C10-C11-C12
31	D	411	LHG	C25-C26-C27-C28
31	E	101	LHG	C26-C27-C28-C29
27	c	517	DGD	CAB-CBB-CCB-CDB
30	C	520	LMG	C40-C41-C42-C43
31	L	101	LHG	C19-C20-C21-C22
22	A	403	CLA	C11-C10-C8-C7
22	B	704	CLA	C11-C12-C13-C15
22	B	704	CLA	C12-C13-C15-C16
22	B	707	CLA	C12-C13-C15-C16
22	B	713	CLA	C11-C12-C13-C15
22	B	714	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	b	602	CLA	C6-C7-C8-C10
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	b	611	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	514	CLA	C13-C15-C16-C17
27	C	517	DGD	O6D-C5D-C6D-O5D
26	D	410	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
28	a	417	STE	C10-C11-C12-C13
28	x	101	STE	C11-C10-C9-C8
28	d	402	STE	C5-C6-C7-C8
28	H	104	STE	C5-C6-C7-C8
22	c	506	CLA	C4-C3-C5-C6
25	d	406	PL9	C15-C14-C16-C17
30	a	418	LMG	O8-C28-C29-C30
22	C	511	CLA	C2-C3-C5-C6
25	a	410	PL9	C13-C14-C16-C17
25	d	406	PL9	C28-C29-C31-C32
22	B	704	CLA	C2C-C3C-CAC-CBC
26	A	410	SQD	C7-C8-C9-C10
30	c	523	LMG	C30-C31-C32-C33
31	L	101	LHG	C30-C31-C32-C33
26	l	101	SQD	O5-C1-O6-C44
30	C	520	LMG	O6-C1-O1-C7
27	c	518	DGD	CBB-CCB-CDB-CEB
28	x	101	STE	C4-C5-C6-C7
22	b	606	CLA	C8-C10-C11-C12
27	C	517	DGD	C4D-C5D-C6D-O5D
27	C	519	DGD	C6B-C7B-C8B-C9B
30	D	413	LMG	C35-C36-C37-C38
31	D	411	LHG	C17-C18-C19-C20
31	a	411	LHG	C18-C19-C20-C21
22	b	614	CLA	C5-C6-C7-C8
27	C	519	DGD	C9B-CAB-CBB-CCB
28	b	625	STE	C7-C8-C9-C10
22	A	403	CLA	C13-C15-C16-C17
26	A	409	SQD	C31-C32-C33-C34
28	E	102	STE	C5-C6-C7-C8
30	b	620	LMG	C11-C10-O7-C8
31	E	101	LHG	C35-C36-C37-C38
30	D	409	LMG	C30-C31-C32-C33
26	A	409	SQD	C44-C45-C46-O48
30	C	520	LMG	O1-C7-C8-C9
30	M	101	LMG	C7-C8-C9-O8
27	c	517	DGD	C7B-C8B-C9B-CAB
28	m	101	STE	C1-C2-C3-C4
22	C	513	CLA	C3-C5-C6-C7
27	C	518	DGD	CAA-CBA-CCA-CDA
27	h	703	DGD	CBA-CCA-CDA-CEA
28	b	601	STE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	712	CLA	C16-C17-C18-C20
22	c	504	CLA	C16-C17-C18-C20
28	C	522	STE	C6-C7-C8-C9
27	C	518	DGD	C4B-C5B-C6B-C7B
28	T	702	STE	C6-C7-C8-C9
28	X	101	STE	C11-C10-C9-C8
28	b	624	STE	C3-C4-C5-C6
26	a	412	SQD	C11-C10-C9-C8
26	a	412	SQD	C17-C18-C19-C20
27	c	518	DGD	C8B-C9B-CAB-CBB
28	m	102	STE	C5-C6-C7-C8
25	a	410	PL9	C15-C14-C16-C17
26	D	410	SQD	C30-C31-C32-C33
30	D	409	LMG	C39-C40-C41-C42
27	c	517	DGD	C3B-C4B-C5B-C6B
22	B	703	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C19
26	a	412	SQD	C28-C29-C30-C31
27	A	411	DGD	CBA-CCA-CDA-CEA
27	h	703	DGD	C3B-C4B-C5B-C6B
31	a	411	LHG	C29-C30-C31-C32
22	b	608	CLA	C4C-C3C-CAC-CBC
23	B	718	BCR	C23-C24-C25-C30
23	C	501	BCR	C23-C24-C25-C30
23	H	101	BCR	C23-C24-C25-C30
23	d	405	BCR	C23-C24-C25-C30
28	H	103	STE	C11-C10-C9-C8
30	b	622	LMG	C40-C41-C42-C43
28	b	601	STE	C3-C4-C5-C6
28	T	702	STE	C10-C11-C12-C13
31	a	413	LHG	C15-C16-C17-C18
22	B	703	CLA	C15-C16-C17-C18
27	c	519	DGD	C6A-C7A-C8A-C9A
26	B	723	SQD	C19-C20-C21-C22
27	c	518	DGD	CDA-CEA-CFA-CGA
28	C	521	STE	C3-C4-C5-C6
22	c	507	CLA	C8-C10-C11-C12
26	a	414	SQD	O47-C45-C46-O48
27	A	411	DGD	O2G-C2G-C3G-O3G
30	C	520	LMG	O1-C7-C8-O7
30	c	522	LMG	O7-C8-C9-O8
26	B	723	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	B	714	CLA	CBD-CGD-O2D-CED
26	a	412	SQD	C18-C19-C20-C21
31	B	722	LHG	C27-C28-C29-C30
23	C	515	BCR	C18-C19-C20-C21
22	C	511	CLA	C15-C16-C17-C18
22	C	513	CLA	C10-C11-C12-C13
22	c	506	CLA	C2-C3-C5-C6
27	H	102	DGD	C8A-C9A-CAA-CBA
31	l	102	LHG	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
28	B	724	STE	C3-C4-C5-C6
22	B	727	CLA	C6-C7-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C10-C8-C9
22	d	404	CLA	C14-C13-C15-C16
30	d	410	LMG	C40-C41-C42-C43
27	c	517	DGD	O6E-C1E-O5D-C6D
27	c	518	DGD	O6D-C1D-O3G-C3G
31	E	101	LHG	C27-C28-C29-C30
23	k	101	BCR	C14-C15-C16-C17
30	c	523	LMG	C37-C38-C39-C40
22	B	702	CLA	C16-C17-C18-C20
22	B	705	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	b	606	CLA	C16-C17-C18-C20
26	a	414	SQD	O6-C44-C45-O47
27	H	102	DGD	CDA-CEA-CFA-CGA
22	B	703	CLA	C10-C11-C12-C13
22	B	710	CLA	C16-C17-C18-C20
27	A	411	DGD	C4D-C5D-C6D-O5D
22	B	703	CLA	C13-C15-C16-C17
22	B	712	CLA	C10-C11-C12-C13
26	A	410	SQD	C11-C12-C13-C14
26	f	102	SQD	C24-C25-C26-C27
23	A	405	BCR	C16-C17-C18-C36
23	C	501	BCR	C11-C10-C9-C34
23	C	524	BCR	C35-C13-C14-C15
23	c	516	BCR	C16-C17-C18-C36
23	k	102	BCR	C16-C17-C18-C36
22	B	716	CLA	O1A-CGA-O2A-C1
30	D	409	LMG	O10-C28-O8-C9
27	H	102	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
31	D	412	LHG	C17-C18-C19-C20
31	E	101	LHG	O6-C4-C5-C6
27	C	518	DGD	C2B-C3B-C4B-C5B
28	b	601	STE	C12-C13-C14-C15
23	C	515	BCR	C11-C12-C13-C35
23	a	406	BCR	C11-C12-C13-C35
26	f	102	SQD	C28-C29-C30-C31
30	M	101	LMG	C32-C33-C34-C35
22	A	403	CLA	C11-C12-C13-C15
22	B	702	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C12-C13-C15
22	C	514	CLA	C6-C7-C8-C10
22	b	605	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	509	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C12-C13-C15
22	d	403	CLA	C11-C12-C13-C15
26	A	409	SQD	C27-C28-C29-C30
27	c	517	DGD	C5B-C6B-C7B-C8B
28	d	402	STE	C3-C4-C5-C6
25	d	406	PL9	C32-C33-C34-C35
31	E	101	LHG	C12-C13-C14-C15
31	a	411	LHG	C28-C29-C30-C31
31	d	408	LHG	C17-C18-C19-C20
23	C	501	BCR	C11-C12-C13-C14
23	b	617	BCR	C21-C22-C23-C24
23	d	405	BCR	C17-C18-C19-C20
22	B	716	CLA	CBA-CGA-O2A-C1
28	E	103	STE	C4-C5-C6-C7
28	a	417	STE	C11-C10-C9-C8
31	L	101	LHG	O10-C23-O8-C6
27	C	518	DGD	C2G-C3G-O3G-C1D
27	c	518	DGD	C2G-C3G-O3G-C1D
27	c	518	DGD	C5D-C6D-O5D-C1E
22	b	612	CLA	C13-C15-C16-C17
30	B	721	LMG	C29-C30-C31-C32
30	D	413	LMG	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
28	b	621	STE	C5-C6-C7-C8
22	c	513	CLA	C4-C3-C5-C6
27	H	102	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
27	H	102	DGD	CCB-CDB-CEB-CFB
28	b	623	STE	C9-C10-C11-C12
28	B	725	STE	C1-C2-C3-C4
31	D	412	LHG	C9-C10-C11-C12
31	d	408	LHG	C31-C32-C33-C34
28	B	720	STE	C9-C10-C11-C12
30	D	413	LMG	C9-C8-O7-C10
30	a	418	LMG	C9-C8-O7-C10
30	c	523	LMG	C9-C8-O7-C10
30	b	620	LMG	C15-C16-C17-C18
23	k	102	BCR	C13-C14-C15-C16
27	c	519	DGD	CCB-CDB-CEB-CFB
22	b	604	CLA	C3-C5-C6-C7
27	H	102	DGD	C3B-C4B-C5B-C6B
30	b	622	LMG	C19-C20-C21-C22
27	A	411	DGD	O6D-C1D-O3G-C3G
27	C	517	DGD	O6E-C1E-O5D-C6D
31	B	722	LHG	C18-C19-C20-C21
25	a	410	PL9	C14-C16-C17-C18
26	A	409	SQD	O6-C44-C45-C46
26	a	414	SQD	C44-C45-C46-O48
26	B	723	SQD	C10-C11-C12-C13
22	c	513	CLA	C2-C3-C5-C6
28	C	523	STE	C6-C7-C8-C9
28	b	624	STE	C7-C8-C9-C10
26	A	410	SQD	C34-C35-C36-C37
30	a	418	LMG	C30-C31-C32-C33
26	l	101	SQD	O47-C45-C46-O48
27	C	517	DGD	O1G-C1G-C2G-O2G
31	E	101	LHG	O7-C5-C6-O8
22	c	505	CLA	C8-C10-C11-C12
22	c	504	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C10-C8-C9
22	A	403	CLA	C16-C17-C18-C20
27	C	517	DGD	C8A-C9A-CAA-CBA
30	b	622	LMG	C14-C15-C16-C17
30	D	413	LMG	C15-C16-C17-C18
27	c	519	DGD	C5A-C6A-C7A-C8A
28	d	402	STE	C2-C3-C4-C5
31	B	722	LHG	C29-C30-C31-C32
22	B	707	CLA	C15-C16-C17-C18
22	c	512	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	l	101	SQD	C11-C12-C13-C14
28	d	402	STE	C4-C5-C6-C7
31	l	102	LHG	C28-C29-C30-C31
30	C	520	LMG	C32-C33-C34-C35
30	M	101	LMG	C19-C20-C21-C22
26	a	414	SQD	C30-C31-C32-C33
30	C	520	LMG	C2-C1-O1-C7
22	c	512	CLA	CBA-CGA-O2A-C1
22	b	606	CLA	C16-C17-C18-C19
27	h	703	DGD	C7B-C8B-C9B-CAB
22	b	607	CLA	O1D-CGD-O2D-CED
28	E	102	STE	C7-C8-C9-C10
27	c	518	DGD	C5A-C6A-C7A-C8A
31	D	412	LHG	C1-C2-C3-O3
22	c	506	CLA	C13-C15-C16-C17
30	d	410	LMG	C37-C38-C39-C40
22	A	402	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C19
33	D	407	PHO	C16-C17-C18-C19
22	c	510	CLA	C8-C10-C11-C12
27	C	517	DGD	C2B-C3B-C4B-C5B
26	l	101	SQD	C30-C31-C32-C33
28	X	101	STE	C12-C13-C14-C15
31	a	411	LHG	C33-C34-C35-C36
31	a	411	LHG	C14-C15-C16-C17
30	C	520	LMG	C19-C20-C21-C22
22	C	514	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C4B-C3B-CAB-CBB
22	d	401	CLA	C1A-C2A-CAA-CBA
22	B	714	CLA	O1D-CGD-O2D-CED
31	a	411	LHG	C25-C26-C27-C28
22	c	504	CLA	C16-C17-C18-C19
28	B	726	STE	C14-C15-C16-C17
26	a	414	SQD	C29-C30-C31-C32
27	A	411	DGD	CEB-CFB-CGB-CHB
26	a	412	SQD	C31-C32-C33-C34
31	B	722	LHG	C17-C18-C19-C20
22	B	713	CLA	C12-C13-C15-C16
22	B	716	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C12-C13-C15
22	c	506	CLA	C6-C7-C8-C10
22	c	513	CLA	C12-C13-C15-C16
22	c	514	CLA	C12-C13-C15-C16
22	B	704	CLA	C4C-C3C-CAC-CBC
22	c	505	CLA	C11-C12-C13-C15
22	A	402	CLA	C2C-C3C-CAC-CBC
28	T	702	STE	C15-C16-C17-C18
27	A	411	DGD	C6B-C7B-C8B-C9B
22	c	513	CLA	C3A-C2A-CAA-CBA
26	A	409	SQD	C11-C12-C13-C14
28	B	720	STE	C10-C11-C12-C13
30	c	520	LMG	C31-C32-C33-C34
30	D	409	LMG	O9-C10-O7-C8
31	E	101	LHG	O6-C4-C5-O7
26	a	412	SQD	C8-C7-O47-C45
22	A	403	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	h	701	CLA	C11-C12-C13-C14
27	C	517	DGD	C3A-C4A-C5A-C6A
23	k	101	BCR	C15-C16-C17-C18
30	D	409	LMG	C12-C13-C14-C15
30	c	520	LMG	C29-C30-C31-C32
34	v	201	HEC	C4C-C3C-CAC-CBC
30	c	520	LMG	C38-C39-C40-C41
30	d	410	LMG	C32-C33-C34-C35
22	B	705	CLA	C3-C5-C6-C7
27	c	517	DGD	O1G-C1G-C2G-O2G
30	M	101	LMG	O7-C8-C9-O8
30	a	418	LMG	O1-C7-C8-O7
31	a	413	LHG	O7-C5-C6-O8
27	c	518	DGD	C9B-CAB-CBB-CCB
27	C	519	DGD	CBB-CCB-CDB-CEB
30	B	721	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C16-C17-C18-C19
30	b	622	LMG	C7-C8-C9-O8
31	a	413	LHG	C4-C5-C6-O8
30	d	410	LMG	C36-C37-C38-C39
22	C	513	CLA	O1A-CGA-O2A-C1
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
22	B	708	CLA	O1A-CGA-O2A-C1
26	B	723	SQD	C14-C15-C16-C17
22	a	402	CLA	C2C-C3C-CAC-CBC
30	a	418	LMG	C31-C32-C33-C34
28	h	704	STE	C5-C6-C7-C8
30	D	409	LMG	C32-C33-C34-C35
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
23	B	718	BCR	C19-C20-C21-C22
31	D	411	LHG	C4-O6-P-O5
31	D	412	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O5
31	a	411	LHG	C3-O3-P-O5
31	a	413	LHG	C3-O3-P-O4
31	d	408	LHG	C4-O6-P-O5
30	d	410	LMG	C15-C16-C17-C18
22	B	712	CLA	O1A-CGA-O2A-C1
28	J	101	STE	C5-C6-C7-C8
22	B	706	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
23	A	405	BCR	C1-C6-C7-C8
27	A	411	DGD	CCA-CDA-CEA-CFA
27	H	102	DGD	C4B-C5B-C6B-C7B
22	B	705	CLA	C16-C17-C18-C20
22	c	505	CLA	C11-C12-C13-C14
22	h	701	CLA	C10-C11-C12-C13
22	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	723	SQD	C32-C33-C34-C35
22	b	603	CLA	C8-C10-C11-C12
27	h	703	DGD	CBB-CCB-CDB-CEB
22	C	504	CLA	C10-C11-C12-C13
26	a	414	SQD	C31-C32-C33-C34
27	A	411	DGD	CFA-CGA-CHA-CIA
22	B	716	CLA	C10-C11-C12-C13
22	C	513	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
22	c	506	CLA	C16-C17-C18-C19
31	l	102	LHG	O6-C4-C5-C6
27	C	519	DGD	C8A-C9A-CAA-CBA
22	C	513	CLA	CBA-CGA-O2A-C1
22	A	403	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	B	702	CLA	C11-C12-C13-C14
22	B	702	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	a	405	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	c	506	CLA	C6-C7-C8-C9
22	c	507	CLA	C14-C13-C15-C16
28	C	523	STE	C2-C3-C4-C5
22	C	514	CLA	C11-C10-C8-C7
22	b	603	CLA	C6-C7-C8-C10
22	c	510	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	d	404	CLA	C12-C13-C15-C16
30	c	522	LMG	C36-C37-C38-C39
34	v	201	HEC	C2B-C3B-CAB-CBB
22	a	405	CLA	C15-C16-C17-C18
23	b	617	BCR	C20-C21-C22-C23
27	H	102	DGD	CAB-CBB-CCB-CDB
30	a	418	LMG	C17-C18-C19-C20
22	B	715	CLA	C16-C17-C18-C20
30	C	516	LMG	C12-C13-C14-C15
22	B	712	CLA	CBA-CGA-O2A-C1
27	C	519	DGD	C1A-C2A-C3A-C4A
31	a	413	LHG	C28-C29-C30-C31
27	c	517	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
22	B	711	CLA	C15-C16-C17-C18
28	j	101	STE	C7-C8-C9-C10
22	B	709	CLA	C4-C3-C5-C6
22	c	512	CLA	O1A-CGA-O2A-C1
27	h	703	DGD	O2G-C1B-C2B-C3B
26	a	414	SQD	C17-C18-C19-C20
28	b	621	STE	C4-C5-C6-C7
30	c	520	LMG	C29-C28-O8-C9
22	B	713	CLA	C16-C17-C18-C20
25	A	408	PL9	C7-C8-C9-C11
30	a	418	LMG	O7-C8-C9-O8
30	b	622	LMG	O7-C8-C9-O8
22	b	606	CLA	C10-C11-C12-C13
30	a	418	LMG	C22-C23-C24-C25
28	a	417	STE	C1-C2-C3-C4
25	a	410	PL9	C16-C17-C18-C19
31	a	411	LHG	C27-C28-C29-C30
30	M	101	LMG	C30-C31-C32-C33
30	b	622	LMG	C34-C35-C36-C37
28	m	102	STE	C2-C3-C4-C5
22	A	402	CLA	C13-C15-C16-C17
30	M	101	LMG	O1-C7-C8-C9
22	B	711	CLA	O1D-CGD-O2D-CED
22	a	402	CLA	C4C-C3C-CAC-CBC
26	A	409	SQD	C33-C34-C35-C36
30	C	516	LMG	C15-C16-C17-C18
27	c	517	DGD	C5D-C6D-O5D-C1E
22	b	614	CLA	C13-C15-C16-C17
22	b	610	CLA	C2A-CAA-CBA-CGA
23	k	102	BCR	C15-C16-C17-C18
30	b	620	LMG	C19-C20-C21-C22
30	M	101	LMG	C36-C37-C38-C39
25	D	406	PL9	C47-C48-C49-C51
22	c	506	CLA	C15-C16-C17-C18
27	c	518	DGD	C4A-C5A-C6A-C7A
22	a	402	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	CAA-CBA-CGA-O2A
22	B	713	CLA	C6-C7-C8-C9
22	B	716	CLA	C6-C7-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	B	722	LHG	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C19
25	A	408	PL9	C12-C11-C9-C10
22	d	404	CLA	O1D-CGD-O2D-CED
31	a	411	LHG	C10-C11-C12-C13
28	c	501	STE	C7-C8-C9-C10
28	t	702	STE	C3-C4-C5-C6
31	l	102	LHG	C18-C19-C20-C21
22	A	403	CLA	C6-C7-C8-C10
22	B	704	CLA	C11-C10-C8-C7
22	C	503	CLA	C6-C7-C8-C10
22	a	402	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	h	701	CLA	C11-C12-C13-C15
28	a	416	STE	C2-C3-C4-C5
26	l	101	SQD	C10-C11-C12-C13
28	b	621	STE	C13-C14-C15-C16
27	C	517	DGD	CBB-CCB-CDB-CEB
22	A	403	CLA	C16-C17-C18-C19
22	B	713	CLA	C16-C17-C18-C19
22	b	605	CLA	C10-C11-C12-C13
28	b	623	STE	C2-C3-C4-C5
22	B	727	CLA	C3A-C2A-CAA-CBA
28	b	621	STE	C2-C3-C4-C5
26	A	409	SQD	C13-C14-C15-C16
23	Y	101	BCR	C16-C17-C18-C36
22	C	512	CLA	C13-C15-C16-C17
30	B	721	LMG	C30-C31-C32-C33
31	a	413	LHG	C14-C15-C16-C17
22	B	704	CLA	C10-C11-C12-C13
30	b	620	LMG	C22-C23-C24-C25
28	H	103	STE	C7-C8-C9-C10
28	a	416	STE	C1-C2-C3-C4
22	c	510	CLA	C13-C15-C16-C17
30	B	721	LMG	O7-C10-C11-C12
22	b	616	CLA	C8-C10-C11-C12
22	C	507	CLA	C4-C3-C5-C6
31	l	102	LHG	C31-C32-C33-C34
27	c	518	DGD	C5B-C6B-C7B-C8B
28	B	726	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	v	201	HEC	CAD-CBD-CGD-O2D
30	D	409	LMG	C21-C22-C23-C24
25	A	408	PL9	C29-C31-C32-C33
28	d	411	STE	C2-C3-C4-C5
31	l	102	LHG	C11-C12-C13-C14
27	C	517	DGD	CCA-CDA-CEA-CFA
25	a	410	PL9	C42-C43-C44-C46
28	b	623	STE	O2-C1-C2-C3
22	B	704	CLA	C11-C10-C8-C9
22	B	710	CLA	C14-C13-C15-C16
22	B	711	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C6-C7-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	a	402	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	610	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	c	513	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
31	D	411	LHG	C11-C12-C13-C14
31	E	101	LHG	C31-C32-C33-C34
31	E	101	LHG	O1-C1-C2-C3
27	h	703	DGD	C5B-C6B-C7B-C8B
31	D	412	LHG	C13-C14-C15-C16
27	c	517	DGD	C2A-C3A-C4A-C5A
34	V	201	HEC	CAD-CBD-CGD-O2D
30	M	101	LMG	C9-C8-O7-C10
30	D	413	LMG	O1-C7-C8-C9
30	C	520	LMG	C13-C14-C15-C16
28	x	101	STE	C1-C2-C3-C4
22	c	506	CLA	C16-C17-C18-C20
22	C	507	CLA	C2-C3-C5-C6
27	H	102	DGD	C5B-C6B-C7B-C8B
27	h	703	DGD	CAB-CBB-CCB-CDB
30	b	620	LMG	C32-C33-C34-C35
22	B	702	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C1A-C2A-CAA-CBA
23	c	516	BCR	C12-C13-C14-C15
23	B	718	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	c	515	BCR	C23-C24-C25-C30
23	d	405	BCR	C23-C24-C25-C26
28	b	624	STE	O1-C1-C2-C3
27	c	519	DGD	C8A-C9A-CAA-CBA
31	D	411	LHG	C13-C14-C15-C16
31	D	412	LHG	C2-C3-O3-P
27	c	519	DGD	O6D-C5D-C6D-O5D
30	C	516	LMG	C30-C31-C32-C33
31	D	411	LHG	C34-C35-C36-C37
22	b	614	CLA	C4-C3-C5-C6
25	A	408	PL9	C15-C14-C16-C17
28	I	101	STE	C12-C13-C14-C15
34	F	101	HEC	C4C-C3C-CAC-CBC
31	a	413	LHG	O6-C4-C5-C6
30	C	520	LMG	O10-C28-O8-C9
28	m	101	STE	C9-C10-C11-C12
30	a	418	LMG	C12-C13-C14-C15
22	B	702	CLA	C11-C12-C13-C15
22	B	703	CLA	C11-C12-C13-C15
22	B	713	CLA	C6-C7-C8-C10
22	D	402	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	c	513	CLA	C6-C7-C8-C10
22	d	403	CLA	C6-C7-C8-C10
22	D	404	CLA	C16-C17-C18-C19
22	B	703	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
30	d	410	LMG	C10-C11-C12-C13
28	M	102	STE	O1-C1-C2-C3
28	b	621	STE	O1-C1-C2-C3
30	B	721	LMG	O9-C10-C11-C12
34	v	201	HEC	CAD-CBD-CGD-O1D
26	a	414	SQD	C15-C16-C17-C18
25	A	408	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
28	M	102	STE	C4-C5-C6-C7
30	a	418	LMG	C35-C36-C37-C38
30	c	522	LMG	C42-C43-C44-C45
22	B	727	CLA	C4-C3-C5-C6
22	c	511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	h	701	CLA	C4-C3-C5-C6
22	B	712	CLA	C8-C10-C11-C12
22	B	727	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	D	402	CLA	O1D-CGD-O2D-CED
28	X	101	STE	C15-C16-C17-C18
28	B	724	STE	O2-C1-C2-C3
22	B	715	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
27	A	411	DGD	C7A-C8A-C9A-CAA
26	D	410	SQD	C27-C28-C29-C30
28	M	103	STE	C2-C3-C4-C5
22	B	713	CLA	C13-C15-C16-C17
27	C	519	DGD	C7A-C8A-C9A-CAA
28	M	102	STE	O2-C1-C2-C3
28	b	623	STE	O1-C1-C2-C3
23	b	617	BCR	C6-C7-C8-C9
22	a	405	CLA	C4-C3-C5-C6
25	d	406	PL9	C45-C44-C46-C47
28	b	624	STE	O2-C1-C2-C3
31	d	409	LHG	C2-C3-O3-P
22	b	609	CLA	C15-C16-C17-C18
28	a	417	STE	C5-C6-C7-C8
26	l	101	SQD	C44-C45-C46-O48
31	d	409	LHG	C26-C27-C28-C29
28	b	621	STE	O2-C1-C2-C3
30	D	413	LMG	O1-C7-C8-O7
22	c	502	CLA	C2A-CAA-CBA-CGA
27	C	517	DGD	O1G-C1A-C2A-C3A
31	a	411	LHG	C34-C35-C36-C37
27	H	102	DGD	CCA-CDA-CEA-CFA
31	B	722	LHG	C24-C25-C26-C27
31	a	413	LHG	O6-C4-C5-O7
23	C	524	BCR	C13-C14-C15-C16
30	D	413	LMG	C34-C35-C36-C37
28	b	601	STE	C7-C8-C9-C10
31	l	102	LHG	C5-C6-O8-C23
28	d	402	STE	C11-C10-C9-C8
28	x	101	STE	C10-C11-C12-C13
22	C	504	CLA	C4B-C3B-CAB-CBB
25	A	408	PL9	C47-C48-C49-C51
28	X	101	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	D	412	LHG	C14-C15-C16-C17
28	B	724	STE	O1-C1-C2-C3
22	c	503	CLA	C16-C17-C18-C20
28	H	103	STE	C11-C12-C13-C14
23	C	524	BCR	C20-C21-C22-C37
23	c	515	BCR	C35-C13-C14-C15
33	D	407	PHO	CHA-CBD-CGD-O1D
31	D	412	LHG	O10-C23-O8-C6
30	d	410	LMG	C35-C36-C37-C38
28	C	523	STE	O2-C1-C2-C3
28	h	704	STE	C11-C10-C9-C8
30	C	516	LMG	C14-C15-C16-C17
22	C	502	CLA	O1D-CGD-O2D-CED
30	M	101	LMG	O1-C7-C8-O7
22	C	510	CLA	C10-C11-C12-C13
34	V	201	HEC	CAD-CBD-CGD-O1D
22	B	709	CLA	C2-C3-C5-C6
22	b	611	CLA	C10-C11-C12-C13
31	a	411	LHG	C31-C32-C33-C34
22	B	715	CLA	C11-C12-C13-C15
22	D	403	CLA	C6-C7-C8-C10
22	a	405	CLA	C4C-C3C-CAC-CBC
30	b	622	LMG	C29-C30-C31-C32
28	C	523	STE	O1-C1-C2-C3
22	B	713	CLA	C14-C13-C15-C16
22	C	512	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	c	514	CLA	C14-C13-C15-C16
22	D	402	CLA	C4C-C3C-CAC-CBC
26	l	101	SQD	C13-C14-C15-C16
22	d	403	CLA	C2-C1-O2A-CGA
22	B	708	CLA	CBA-CGA-O2A-C1
22	B	702	CLA	C3A-C2A-CAA-CBA
22	b	612	CLA	C3A-C2A-CAA-CBA
27	c	518	DGD	C6A-C7A-C8A-C9A
30	C	516	LMG	C9-C8-O7-C10
26	l	101	SQD	C14-C15-C16-C17
23	B	718	BCR	C18-C19-C20-C21
23	b	619	BCR	C18-C19-C20-C21
27	h	703	DGD	C7A-C8A-C9A-CAA
27	c	517	DGD	O1G-C1A-C2A-C3A
28	B	720	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	c	501	STE	C2-C3-C4-C5
27	c	518	DGD	CCB-CDB-CEB-CFB
22	c	510	CLA	C15-C16-C17-C18
23	A	405	BCR	C12-C13-C14-C15
30	M	101	LMG	O6-C1-O1-C7
22	c	512	CLA	CBD-CGD-O2D-CED
27	C	518	DGD	O1A-C1A-O1G-C1G
22	b	605	CLA	C15-C16-C17-C18
30	B	721	LMG	C34-C35-C36-C37
22	B	704	CLA	O1D-CGD-O2D-CED
28	t	702	STE	C2-C3-C4-C5
22	b	610	CLA	C13-C15-C16-C17
28	B	720	STE	O1-C1-C2-C3
30	c	522	LMG	C16-C17-C18-C19
27	c	519	DGD	C3B-C4B-C5B-C6B
30	C	516	LMG	O1-C7-C8-O7
22	C	504	CLA	C14-C13-C15-C16
22	D	404	CLA	C11-C12-C13-C14
30	B	721	LMG	C16-C17-C18-C19
22	c	511	CLA	CAA-CBA-CGA-O2A
30	D	409	LMG	C10-C11-C12-C13
30	C	516	LMG	C29-C28-O8-C9
22	C	504	CLA	C11-C10-C8-C7
22	C	514	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C10-C8-C7
22	d	401	CLA	C12-C13-C15-C16
22	h	701	CLA	C12-C13-C15-C16
33	a	404	PHO	C6-C7-C8-C10
28	x	101	STE	C12-C13-C14-C15
22	C	504	CLA	C2B-C3B-CAB-CBB
22	b	604	CLA	C2B-C3B-CAB-CBB
23	A	405	BCR	C5-C6-C7-C8
23	C	501	BCR	C23-C24-C25-C26
23	c	515	BCR	C23-C24-C25-C26
26	f	102	SQD	O47-C7-C8-C9
28	b	625	STE	C1-C2-C3-C4
28	C	523	STE	C4-C5-C6-C7
30	b	620	LMG	C12-C13-C14-C15
22	c	511	CLA	C2-C1-O2A-CGA
28	C	522	STE	C11-C12-C13-C14
31	D	412	LHG	C16-C17-C18-C19
33	d	407	PHO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	D	406	PL9	C30-C29-C31-C32
26	B	723	SQD	C23-C24-C25-C26
26	a	414	SQD	O48-C23-C24-C25
26	A	410	SQD	C8-C7-O47-C45
31	E	101	LHG	C8-C7-O7-C5
30	a	418	LMG	O7-C10-C11-C12
22	C	512	CLA	C8-C10-C11-C12
22	b	615	CLA	C13-C15-C16-C17
22	b	612	CLA	CAA-CBA-CGA-O2A
30	b	620	LMG	O8-C28-C29-C30
30	c	523	LMG	O8-C28-C29-C30
31	l	102	LHG	O7-C7-C8-C9
23	Y	101	BCR	C13-C14-C15-C16
31	l	102	LHG	O6-C4-C5-O7
28	B	720	STE	C7-C8-C9-C10
25	D	406	PL9	C15-C14-C16-C17
26	B	723	SQD	O47-C7-C8-C9
26	a	412	SQD	O47-C7-C8-C9
25	D	406	PL9	C28-C29-C31-C32
28	b	623	STE	C10-C11-C12-C13
28	b	624	STE	C4-C5-C6-C7
31	L	101	LHG	C27-C28-C29-C30
22	B	714	CLA	C2A-CAA-CBA-CGA
28	J	101	STE	C6-C7-C8-C9
30	d	410	LMG	O7-C10-C11-C12
27	C	519	DGD	O1B-C1B-O2G-C2G
31	L	101	LHG	O9-C7-O7-C5
28	b	601	STE	C10-C11-C12-C13
22	B	711	CLA	C14-C13-C15-C16
22	C	513	CLA	C14-C13-C15-C16
22	d	404	CLA	C11-C10-C8-C9
22	c	511	CLA	C15-C16-C17-C18
30	a	418	LMG	C7-C8-C9-O8
26	B	723	SQD	C24-C25-C26-C27
34	f	101	HEC	CAD-CBD-CGD-O1D
34	f	101	HEC	CAD-CBD-CGD-O2D
25	A	408	PL9	C35-C34-C36-C37
30	C	516	LMG	O6-C1-O1-C7
22	B	713	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	O7-C7-C8-C9
25	D	406	PL9	C41-C42-C43-C44
34	F	101	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	A	405	BCR	C7-C8-C9-C10
23	H	101	BCR	C11-C12-C13-C14
23	k	102	BCR	C7-C8-C9-C10
26	B	723	SQD	C17-C18-C19-C20
34	F	101	HEC	CAD-CBD-CGD-O2D
31	a	413	LHG	O7-C7-C8-C9
26	a	412	SQD	C14-C15-C16-C17
30	D	409	LMG	C37-C38-C39-C40
26	a	412	SQD	C25-C26-C27-C28
27	c	518	DGD	C8A-C9A-CAA-CBA
22	b	608	CLA	C16-C17-C18-C20
22	B	713	CLA	C10-C11-C12-C13
26	f	102	SQD	C5-C6-S-O7
26	D	410	SQD	C25-C26-C27-C28
33	a	404	PHO	C4-C3-C5-C6
27	h	703	DGD	O1B-C1B-C2B-C3B
22	A	402	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	c	514	CLA	C2-C1-O2A-CGA
22	b	613	CLA	CAA-CBA-CGA-O2A
26	l	101	SQD	C25-C26-C27-C28
22	c	503	CLA	C13-C15-C16-C17
28	b	601	STE	C5-C6-C7-C8
22	d	401	CLA	C2C-C3C-CAC-CBC
26	A	410	SQD	C33-C34-C35-C36
22	B	716	CLA	O1D-CGD-O2D-CED
31	d	408	LHG	C33-C34-C35-C36
26	f	102	SQD	C30-C31-C32-C33
22	c	514	CLA	O1A-CGA-O2A-C1
28	x	101	STE	C11-C12-C13-C14
33	d	407	PHO	C3A-C2A-CAA-CBA
31	a	413	LHG	O9-C7-C8-C9
22	B	705	CLA	C13-C15-C16-C17
25	A	408	PL9	C38-C39-C41-C42
31	d	408	LHG	C7-C8-C9-C10
30	b	620	LMG	C14-C15-C16-C17
23	C	515	BCR	C11-C10-C9-C8
23	c	515	BCR	C12-C13-C14-C15
22	b	612	CLA	CAA-CBA-CGA-O1A
26	A	409	SQD	O10-C23-C24-C25
22	b	604	CLA	C8-C10-C11-C12
22	B	712	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C4C-C3C-CAC-CBC
27	c	517	DGD	O1B-C1B-C2B-C3B
22	B	711	CLA	C16-C17-C18-C19
28	a	415	STE	C1-C2-C3-C4
22	C	506	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C12-C13-C14
26	A	410	SQD	O10-C23-C24-C25
27	c	519	DGD	C4A-C5A-C6A-C7A
22	B	709	CLA	C13-C15-C16-C17
30	b	622	LMG	C21-C22-C23-C24
31	D	412	LHG	C28-C29-C30-C31
22	c	511	CLA	CAA-CBA-CGA-O1A
27	A	411	DGD	O1B-C1B-C2B-C3B
26	a	412	SQD	O10-C23-O48-C46
28	Z	101	STE	C10-C11-C12-C13
27	C	517	DGD	C5D-C6D-O5D-C1E
30	M	101	LMG	C8-C7-O1-C1
30	b	620	LMG	C8-C7-O1-C1
26	B	723	SQD	O48-C23-C24-C25
22	b	602	CLA	C2A-CAA-CBA-CGA
27	C	517	DGD	O1A-C1A-O1G-C1G
27	A	411	DGD	O1G-C1G-C2G-C3G
30	B	721	LMG	O10-C28-C29-C30
27	C	517	DGD	C5A-C6A-C7A-C8A
31	D	412	LHG	C31-C32-C33-C34
22	b	613	CLA	CAA-CBA-CGA-O1A
27	C	517	DGD	O1B-C1B-C2B-C3B
22	b	609	CLA	C13-C15-C16-C17
33	a	404	PHO	C5-C6-C7-C8
22	a	405	CLA	C2-C3-C5-C6
30	a	418	LMG	C42-C43-C44-C45
22	c	510	CLA	CAD-CBD-CGD-O2D
33	D	407	PHO	CAD-CBD-CGD-O2D
26	l	101	SQD	C16-C17-C18-C19
27	c	518	DGD	C3B-C4B-C5B-C6B
22	b	610	CLA	C10-C11-C12-C13
22	c	513	CLA	C8-C10-C11-C12
22	D	402	CLA	C2-C1-O2A-CGA
31	B	722	LHG	C32-C33-C34-C35
26	A	409	SQD	O47-C7-C8-C9
30	c	523	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	C	519	DGD	C9A-CAA-CBA-CCA
26	B	723	SQD	O49-C7-C8-C9
30	d	410	LMG	O10-C28-O8-C9
34	V	201	HEC	C4B-C3B-CAB-CBB
22	B	713	CLA	CAA-CBA-CGA-O1A
22	B	712	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

118 monomers are involved in 227 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	408	PHO	3	0
31	E	101	LHG	1	0
22	b	605	CLA	1	0
22	b	606	CLA	7	0
34	V	201	HEC	2	0
22	c	511	CLA	1	0
22	h	701	CLA	6	0
27	H	102	DGD	1	0
23	d	405	BCR	2	0
28	B	724	STE	1	0
28	X	101	STE	1	0
22	b	604	CLA	2	0
22	C	503	CLA	2	0
22	b	612	CLA	1	0
23	B	718	BCR	4	0
27	A	411	DGD	4	0
22	c	509	CLA	1	0
28	a	416	STE	1	0
22	B	705	CLA	2	0
26	a	414	SQD	2	0
23	k	102	BCR	3	0
22	B	713	CLA	1	0
22	a	405	CLA	2	0
22	b	614	CLA	1	0
25	A	408	PL9	3	0
22	B	708	CLA	3	0
25	D	406	PL9	2	0
22	c	503	CLA	2	0
22	B	714	CLA	2	0
22	C	511	CLA	2	0
31	l	102	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	H	101	BCR	2	0
22	b	615	CLA	3	0
30	D	409	LMG	2	0
22	D	403	CLA	3	0
30	C	516	LMG	1	0
28	I	101	STE	2	0
22	c	510	CLA	2	0
28	c	521	STE	1	0
28	d	402	STE	2	0
22	C	507	CLA	1	0
22	B	709	CLA	1	0
34	F	101	HEC	6	0
23	B	719	BCR	8	0
23	Y	101	BCR	4	0
22	d	401	CLA	2	0
28	h	704	STE	1	0
25	a	410	PL9	5	0
22	A	402	CLA	3	0
28	b	624	STE	1	0
22	c	513	CLA	1	0
23	C	524	BCR	2	0
23	c	515	BCR	2	0
33	D	407	PHO	2	0
26	l	101	SQD	8	0
22	C	502	CLA	3	0
27	c	519	DGD	1	0
22	C	514	CLA	3	0
34	f	101	HEC	9	0
23	B	717	BCR	1	0
22	C	510	CLA	4	0
31	D	411	LHG	1	0
28	x	101	STE	2	0
31	B	722	LHG	2	0
22	B	727	CLA	2	0
33	d	407	PHO	2	0
22	D	404	CLA	3	0
22	B	706	CLA	1	0
22	C	504	CLA	1	0
30	c	522	LMG	1	0
22	b	609	CLA	1	0
23	a	406	BCR	2	0
22	C	512	CLA	2	0

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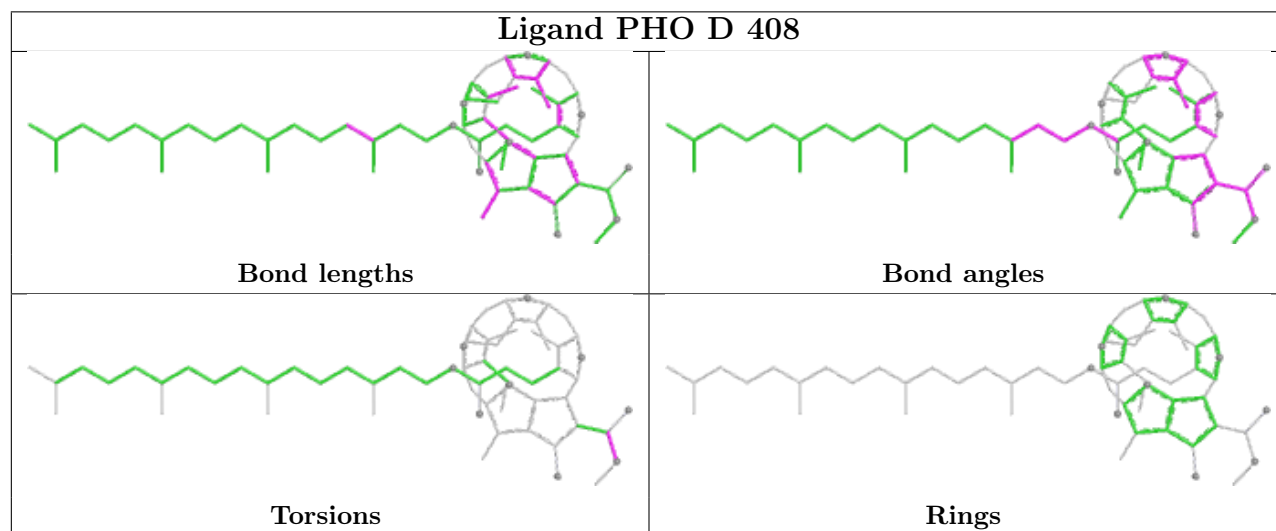
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	522	STE	1	0
23	k	101	BCR	2	0
22	B	707	CLA	1	0
23	A	405	BCR	2	0
22	B	716	CLA	1	0
30	b	620	LMG	1	0
22	c	502	CLA	1	0
22	c	514	CLA	1	0
23	T	701	BCR	4	0
22	c	508	CLA	1	0
31	a	413	LHG	1	0
30	a	418	LMG	5	0
22	B	704	CLA	3	0
22	C	506	CLA	2	0
28	b	621	STE	1	0
31	a	411	LHG	3	0
23	b	618	BCR	2	0
30	c	523	LMG	1	0
22	d	403	CLA	2	0
22	c	504	CLA	1	0
22	B	715	CLA	1	0
30	C	520	LMG	1	0
30	D	413	LMG	1	0
27	C	518	DGD	1	0
22	c	512	CLA	2	0
31	d	409	LHG	1	0
23	b	619	BCR	1	0
23	t	701	BCR	3	0
22	b	616	CLA	2	0
23	D	405	BCR	3	0
23	h	702	BCR	1	0
22	C	513	CLA	5	0
31	d	408	LHG	5	0
22	B	711	CLA	1	0
22	D	402	CLA	2	0
22	b	602	CLA	2	0
23	c	516	BCR	1	0
22	d	404	CLA	1	0
30	b	622	LMG	1	0
22	c	506	CLA	1	0
22	C	509	CLA	2	0
23	C	515	BCR	1	0

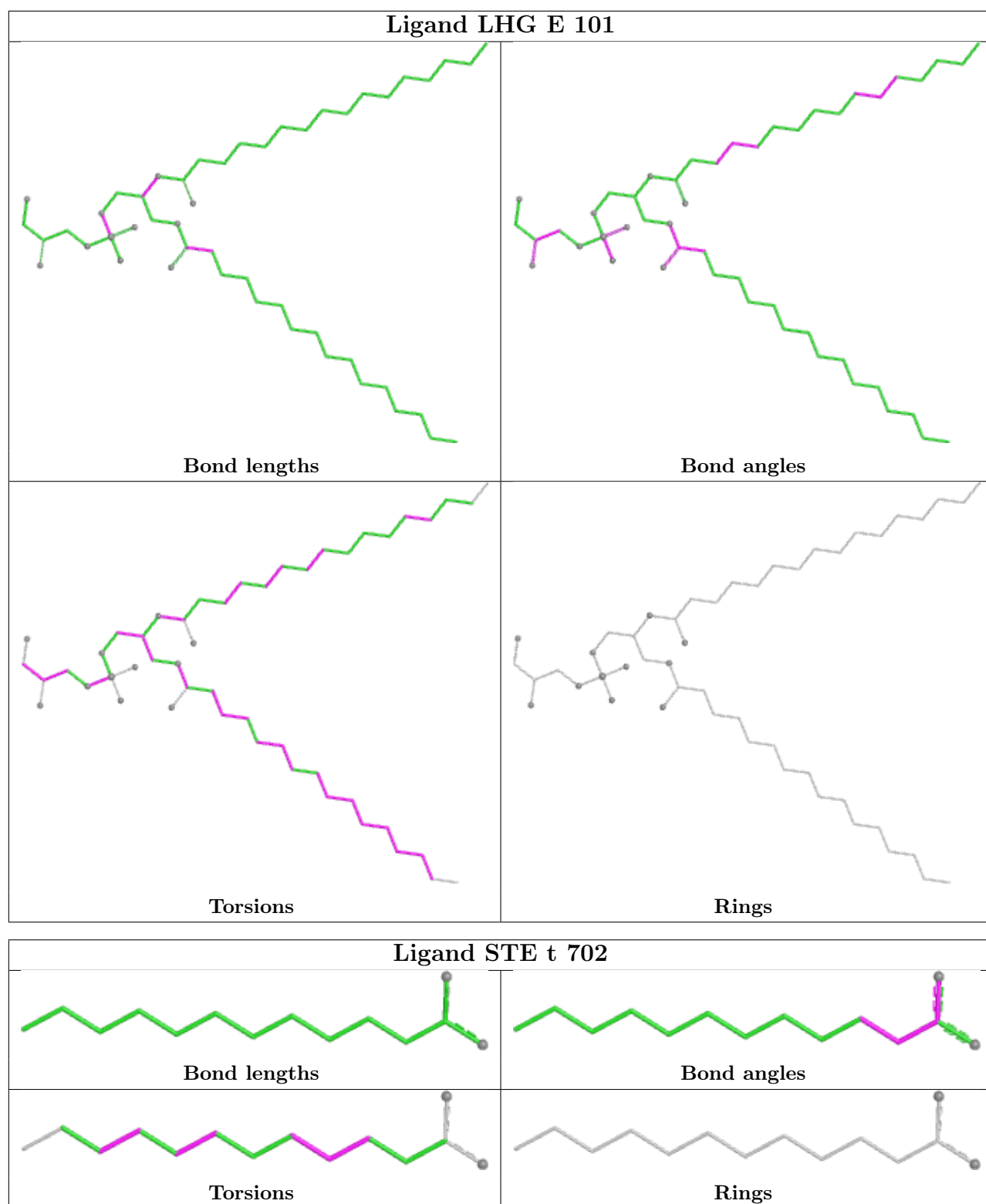
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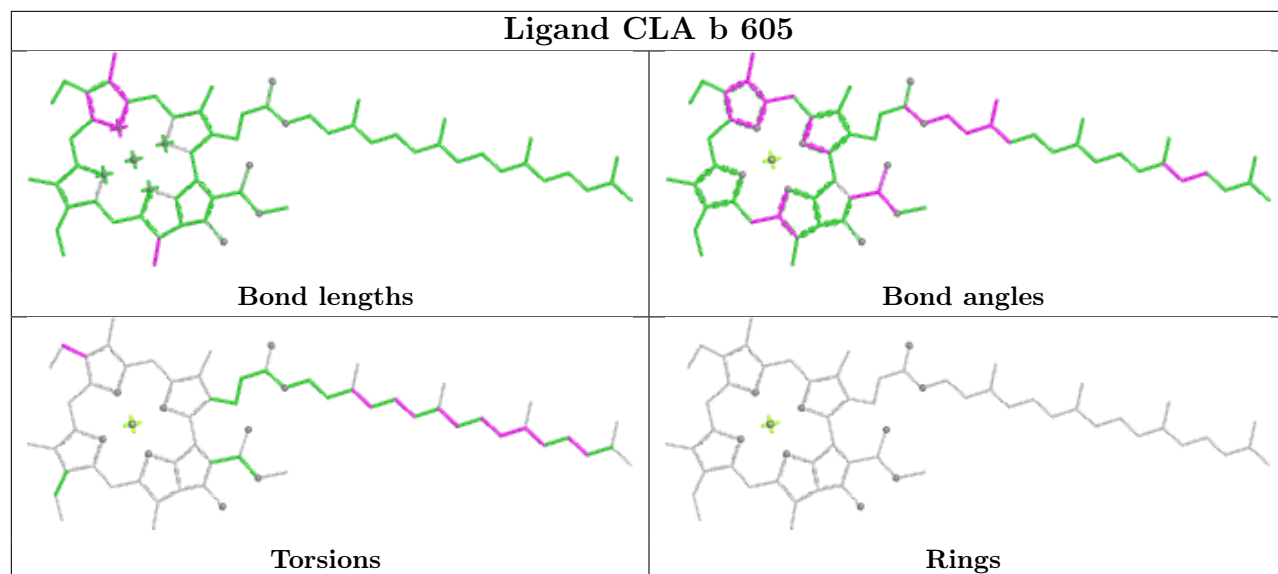
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	607	CLA	1	0
22	b	613	CLA	2	0
28	j	101	STE	1	0

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

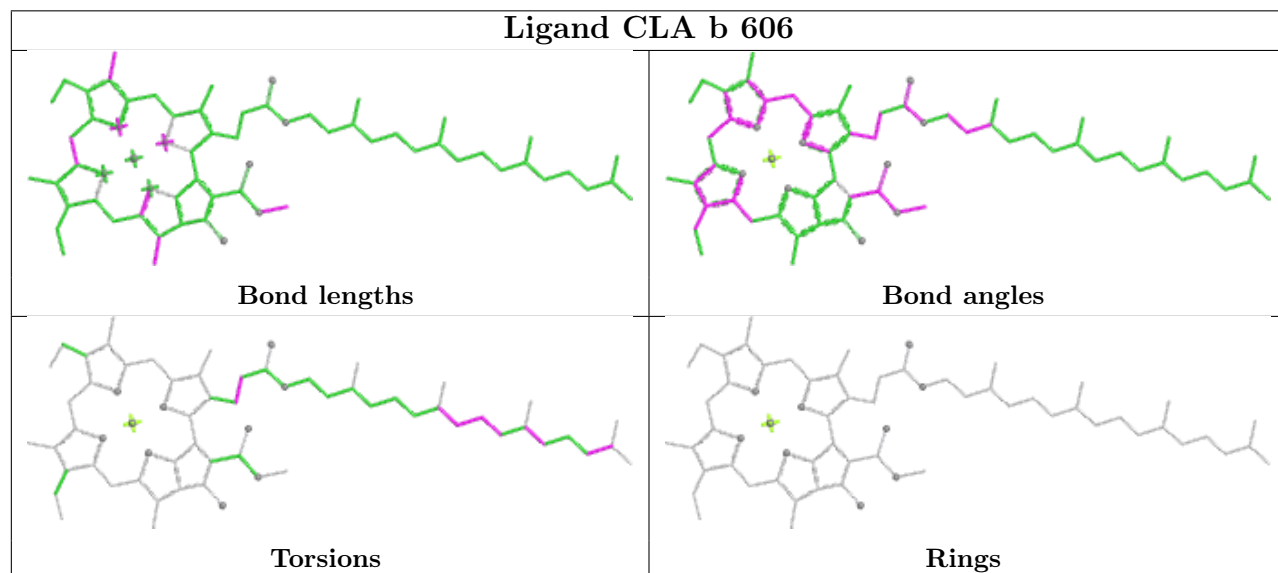




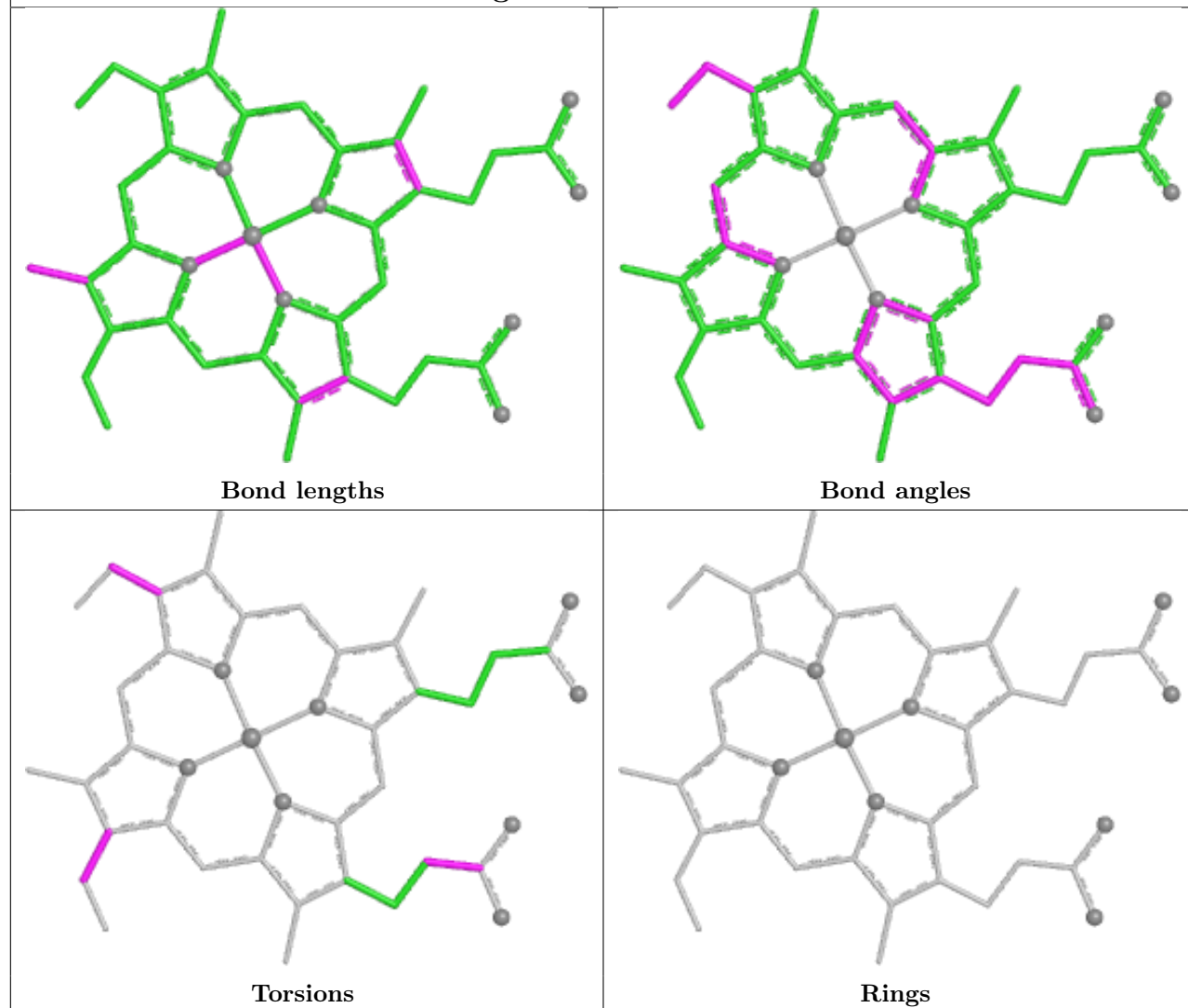
Ligand CLA b 605



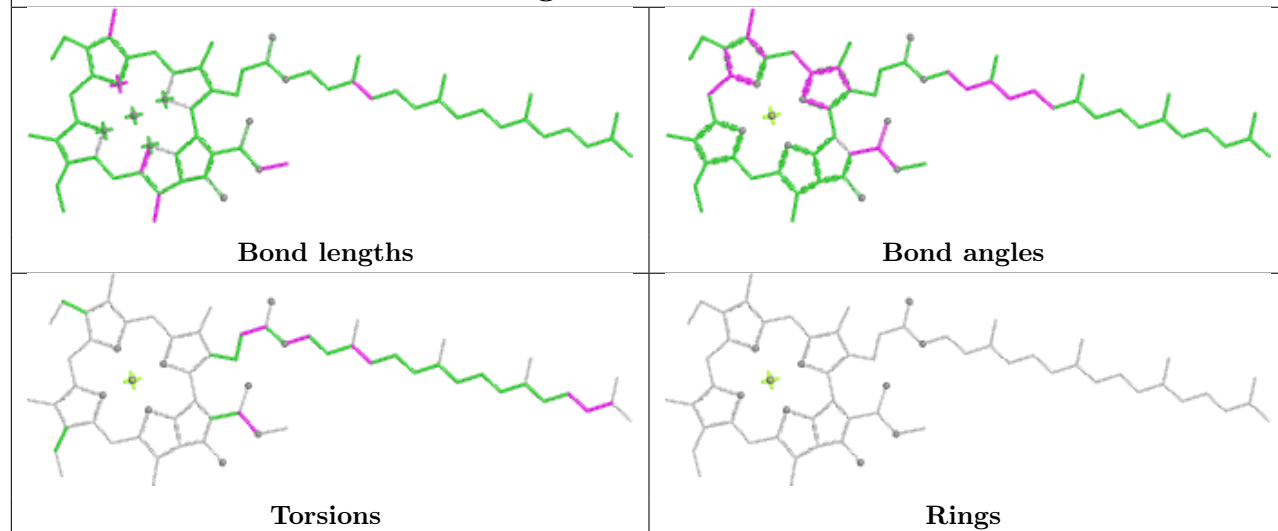
Ligand CLA b 606

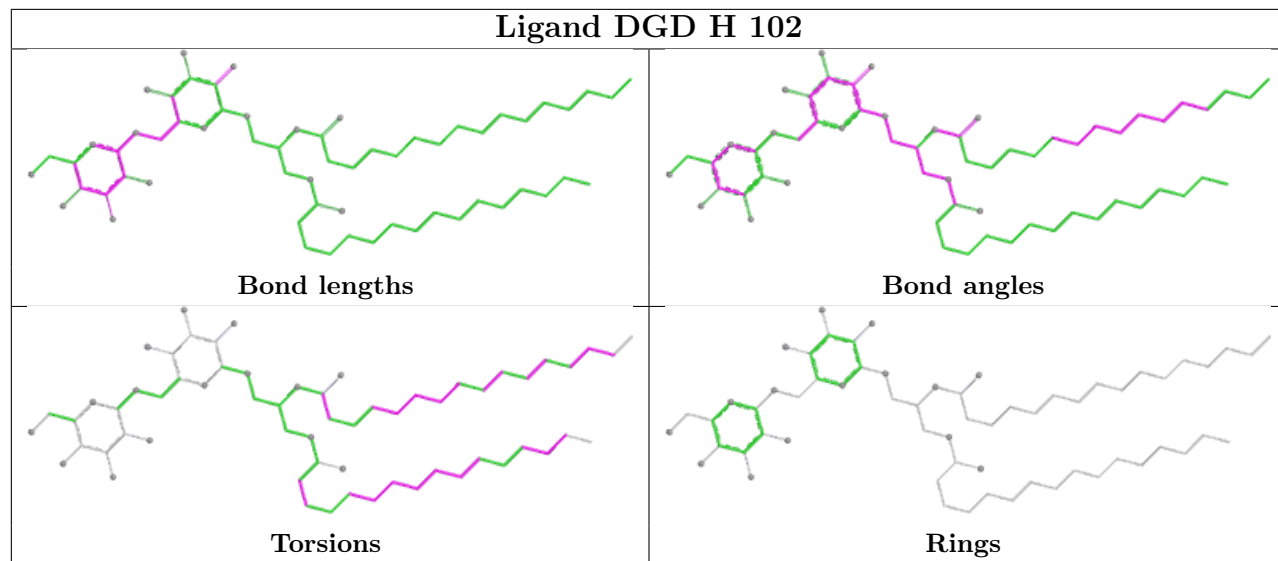
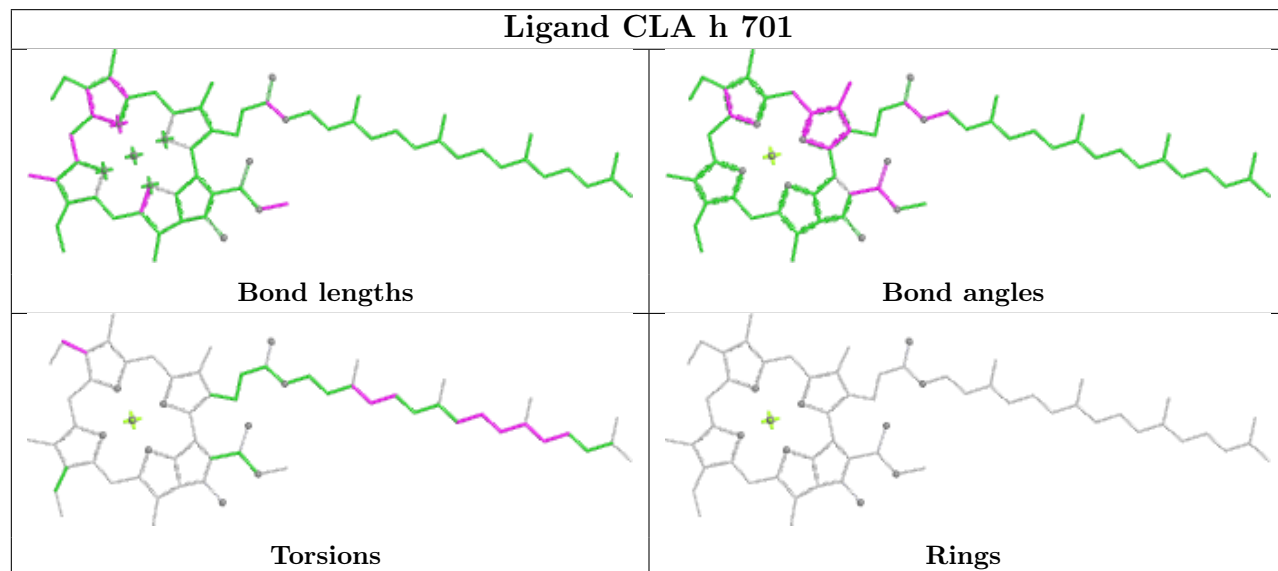
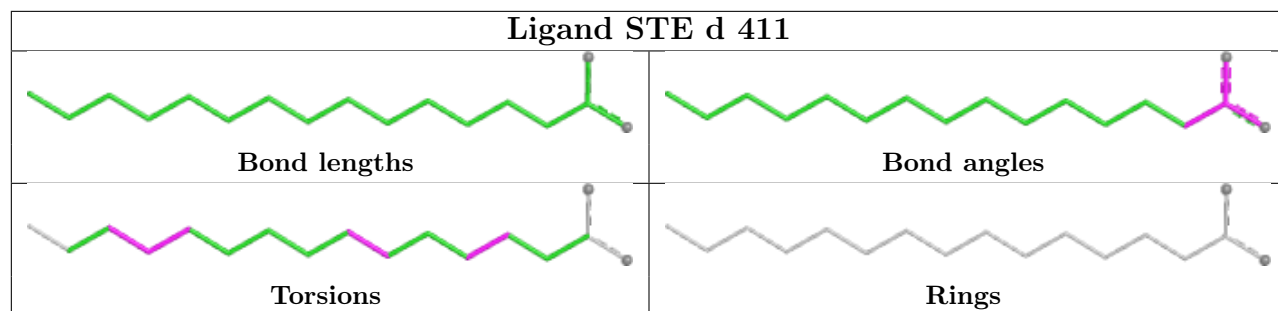


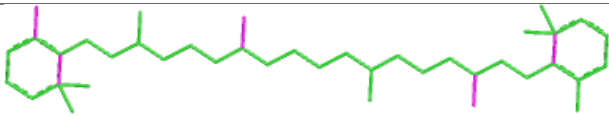
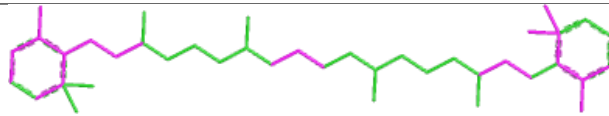
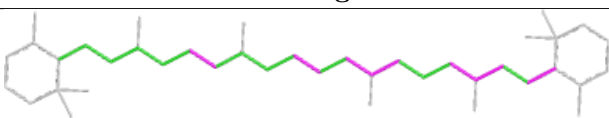
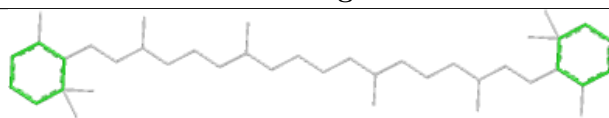
Ligand HEC V 201



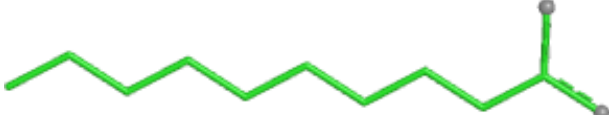
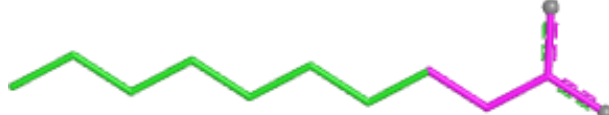
Ligand CLA c 511

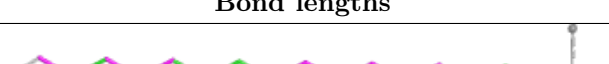
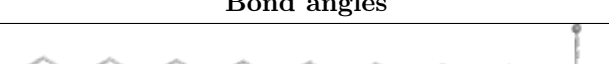


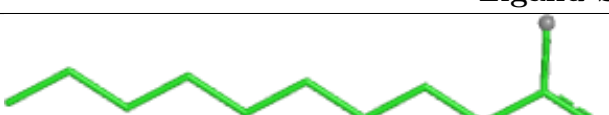
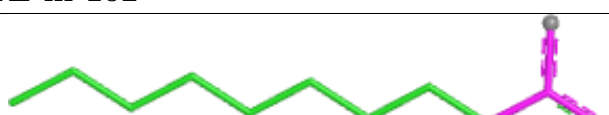
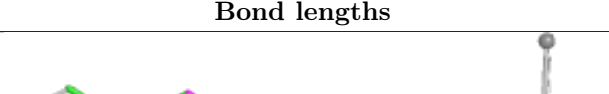
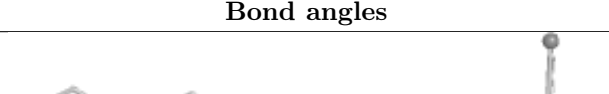


Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

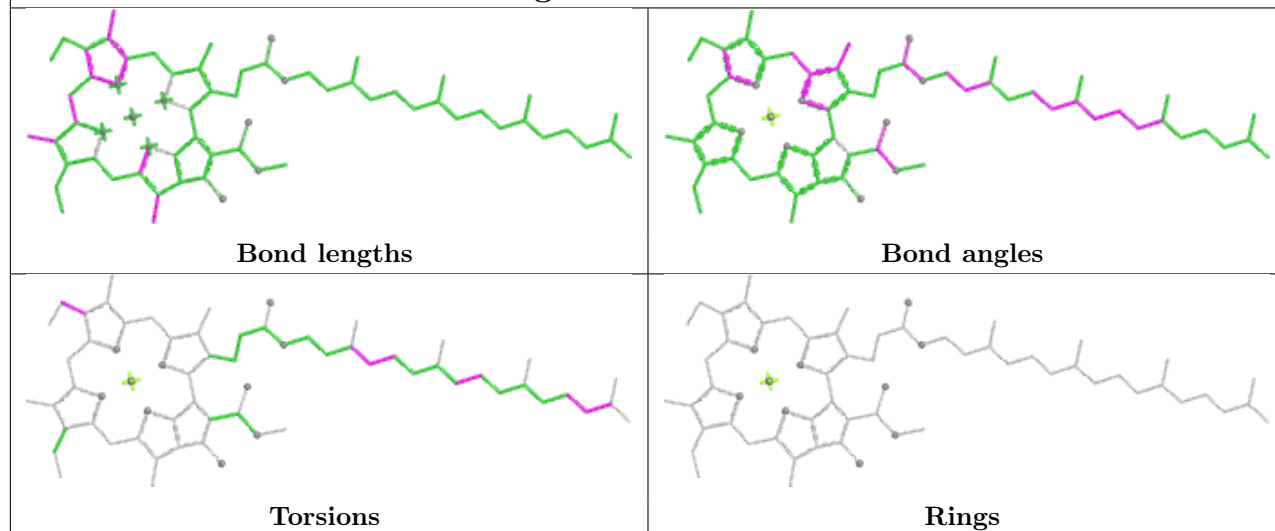
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 724	
	
Bond lengths	Bond angles
	
Torsions	Rings

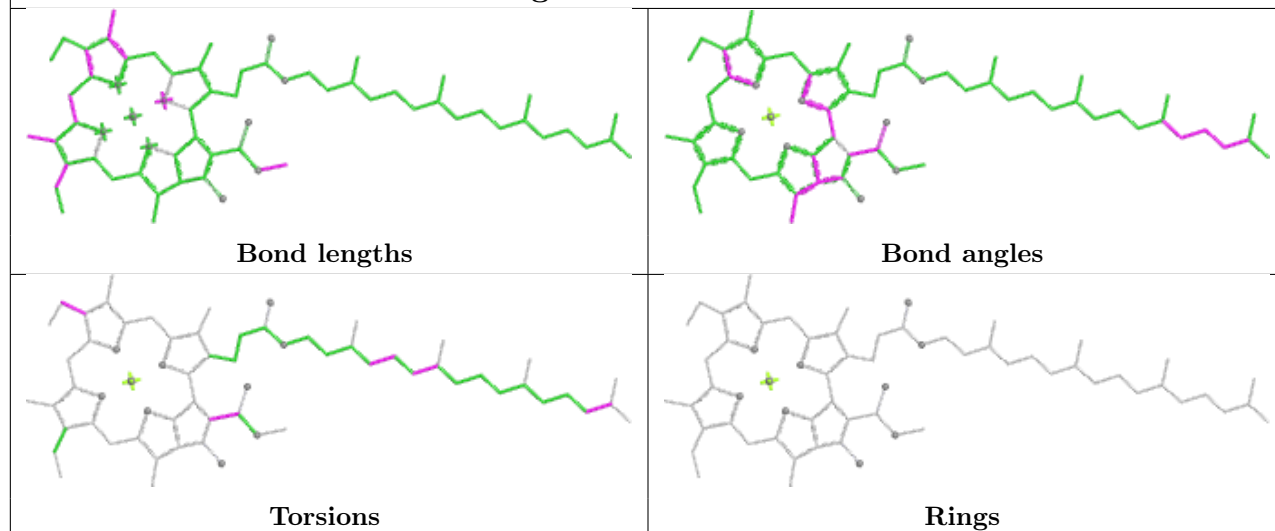
Ligand STE X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

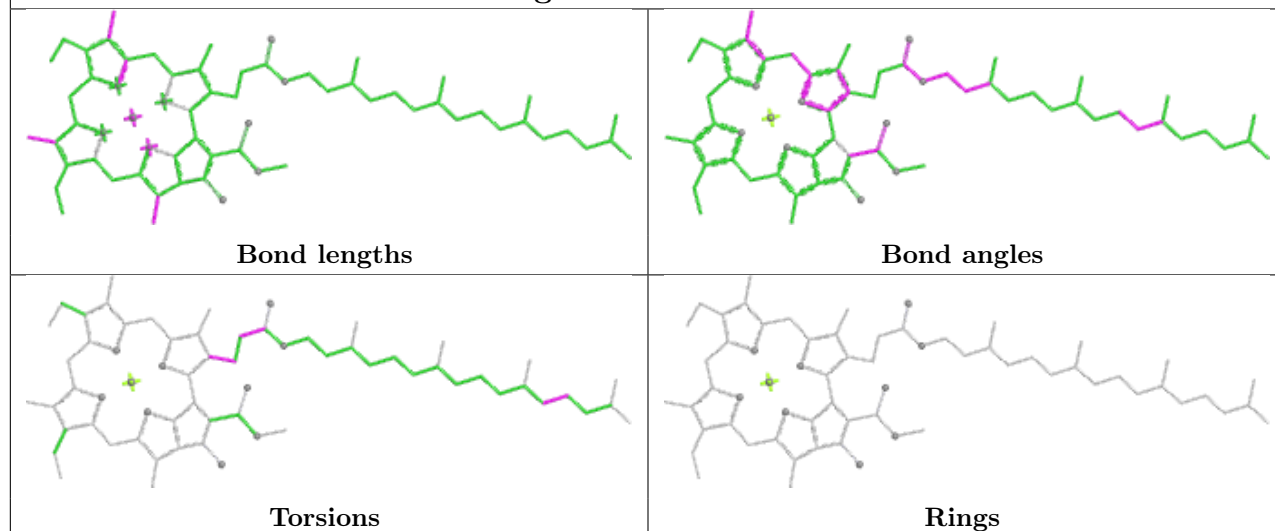
Ligand CLA b 604



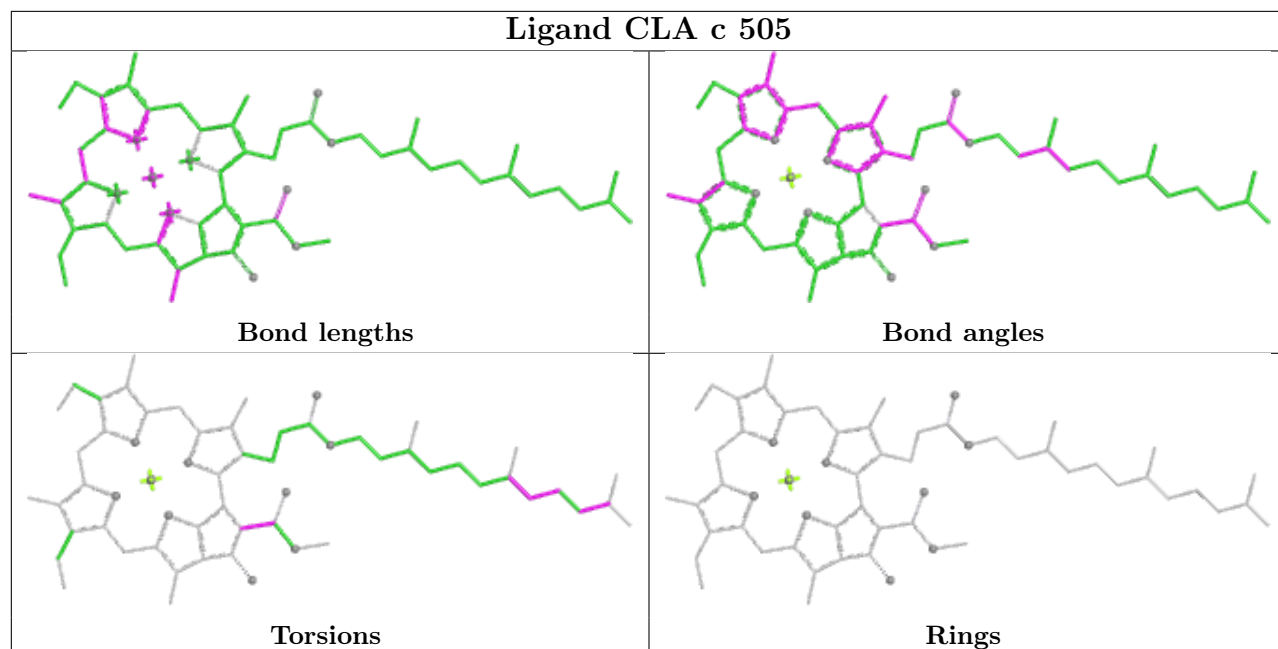
Ligand CLA C 503



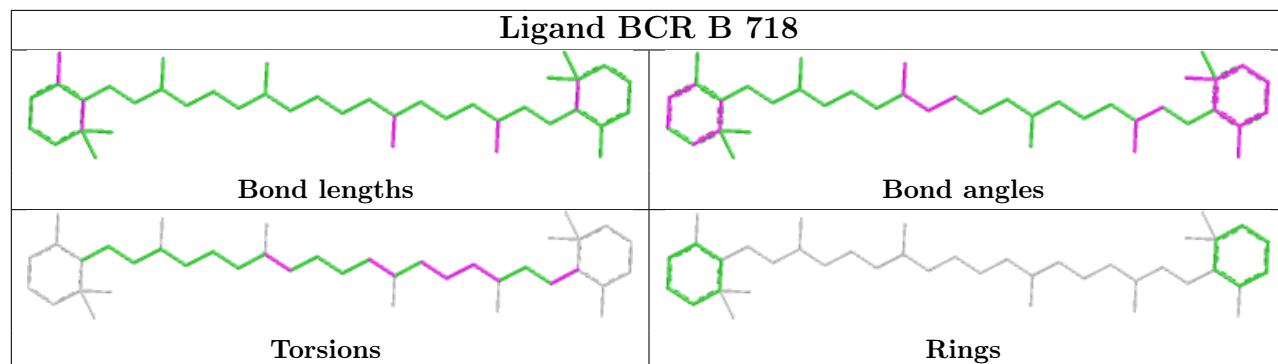
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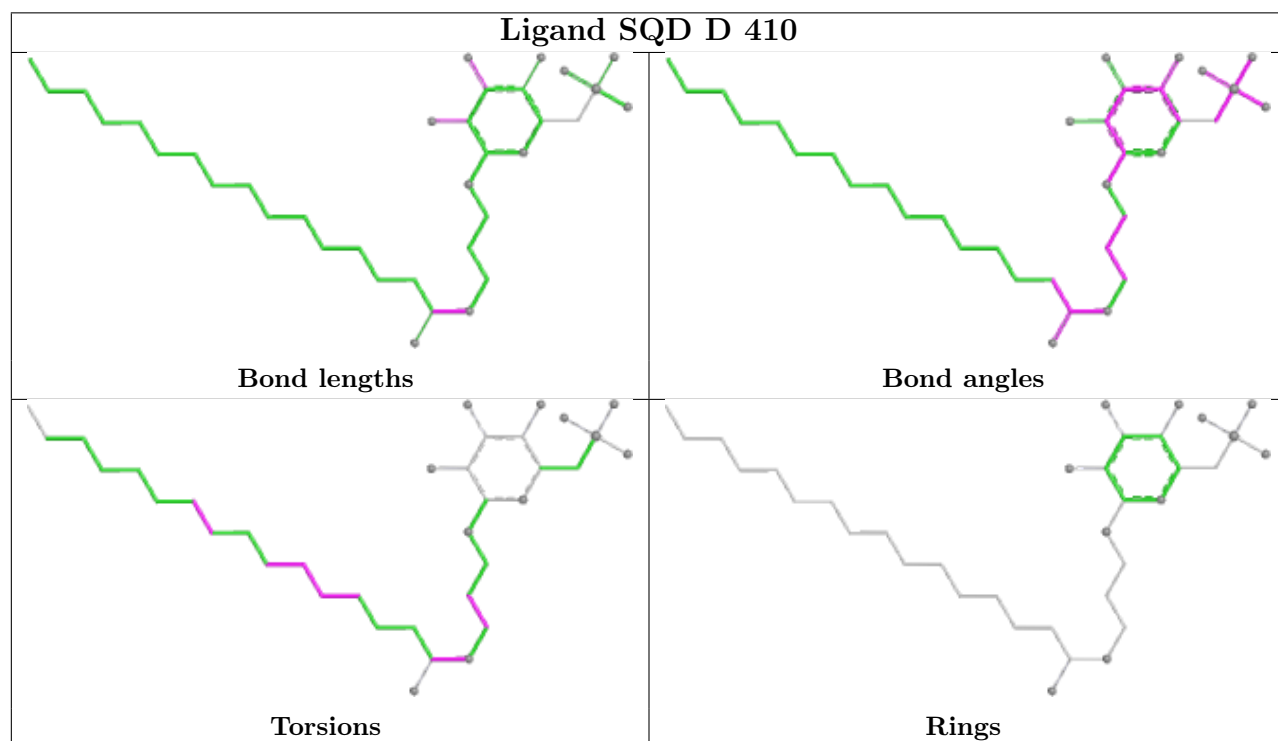
Ligand CLA c 505

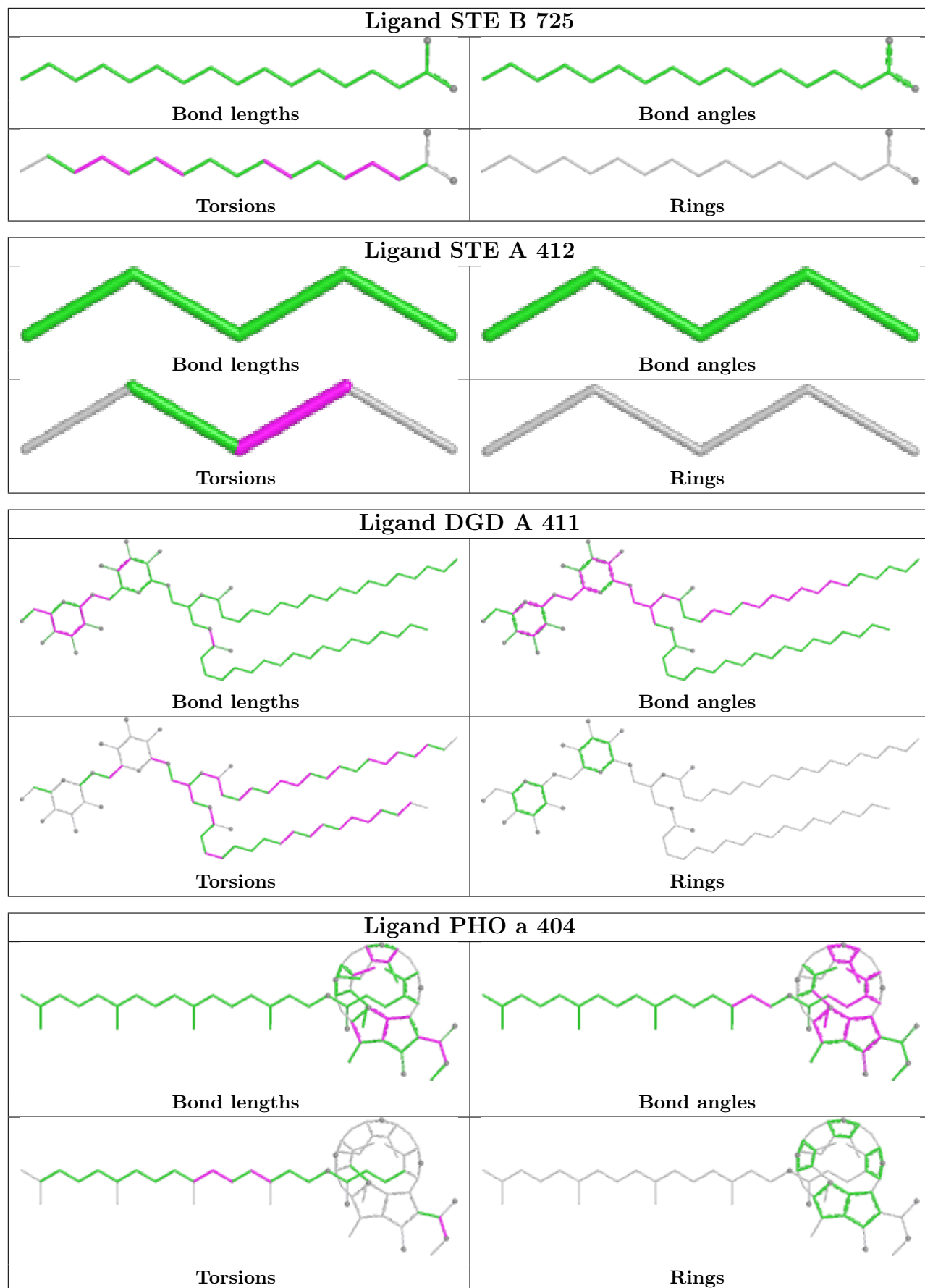


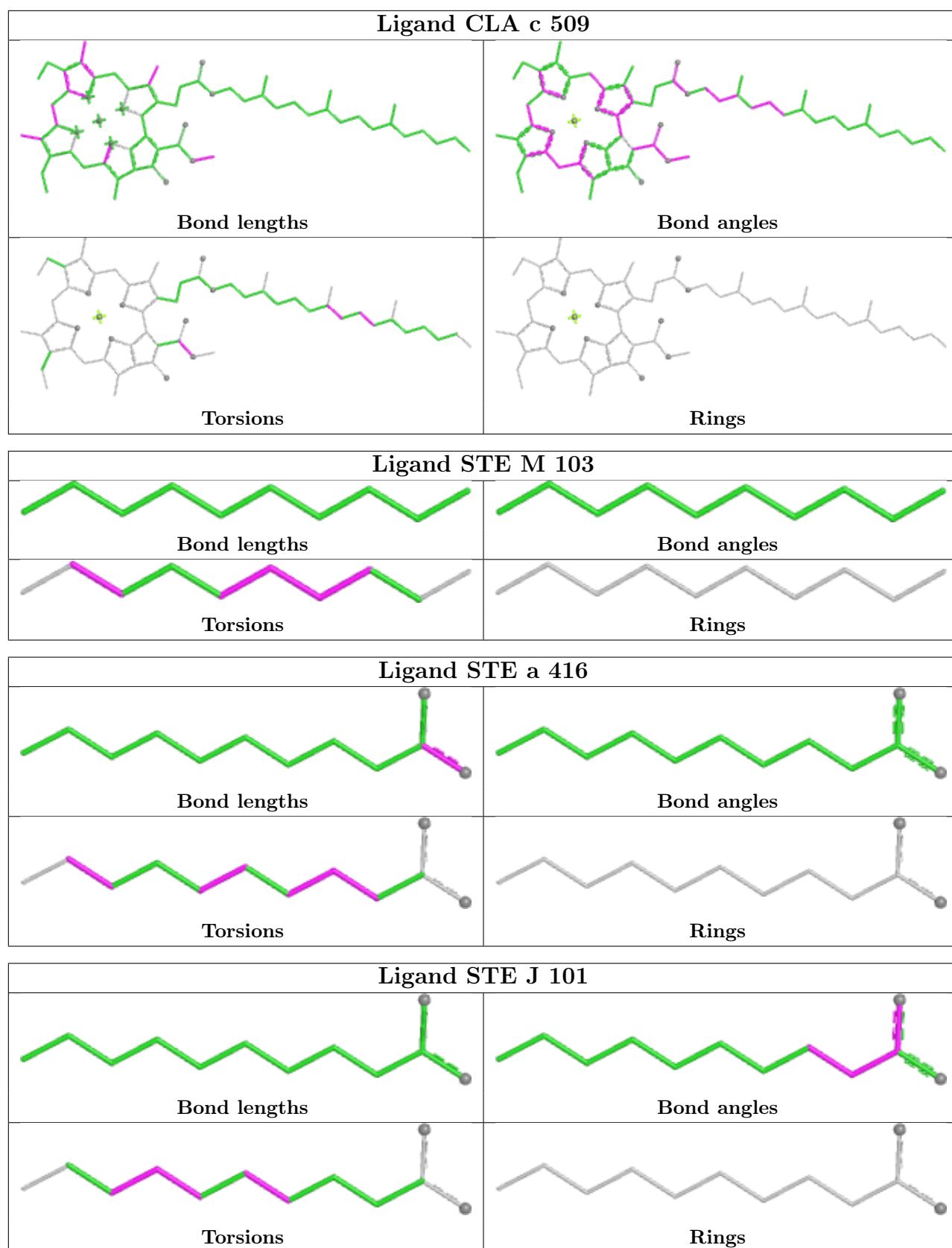
Ligand BCR B 718

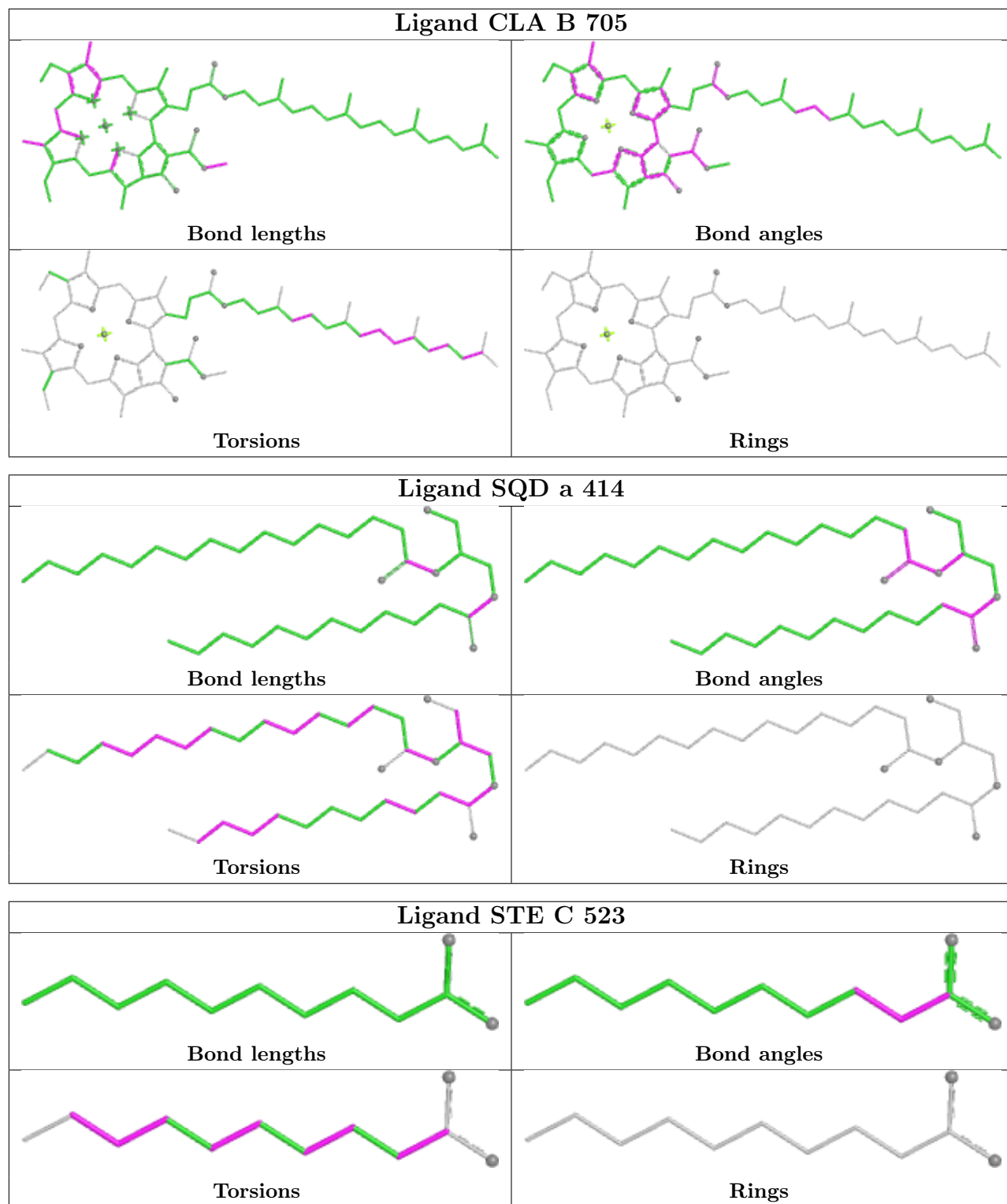


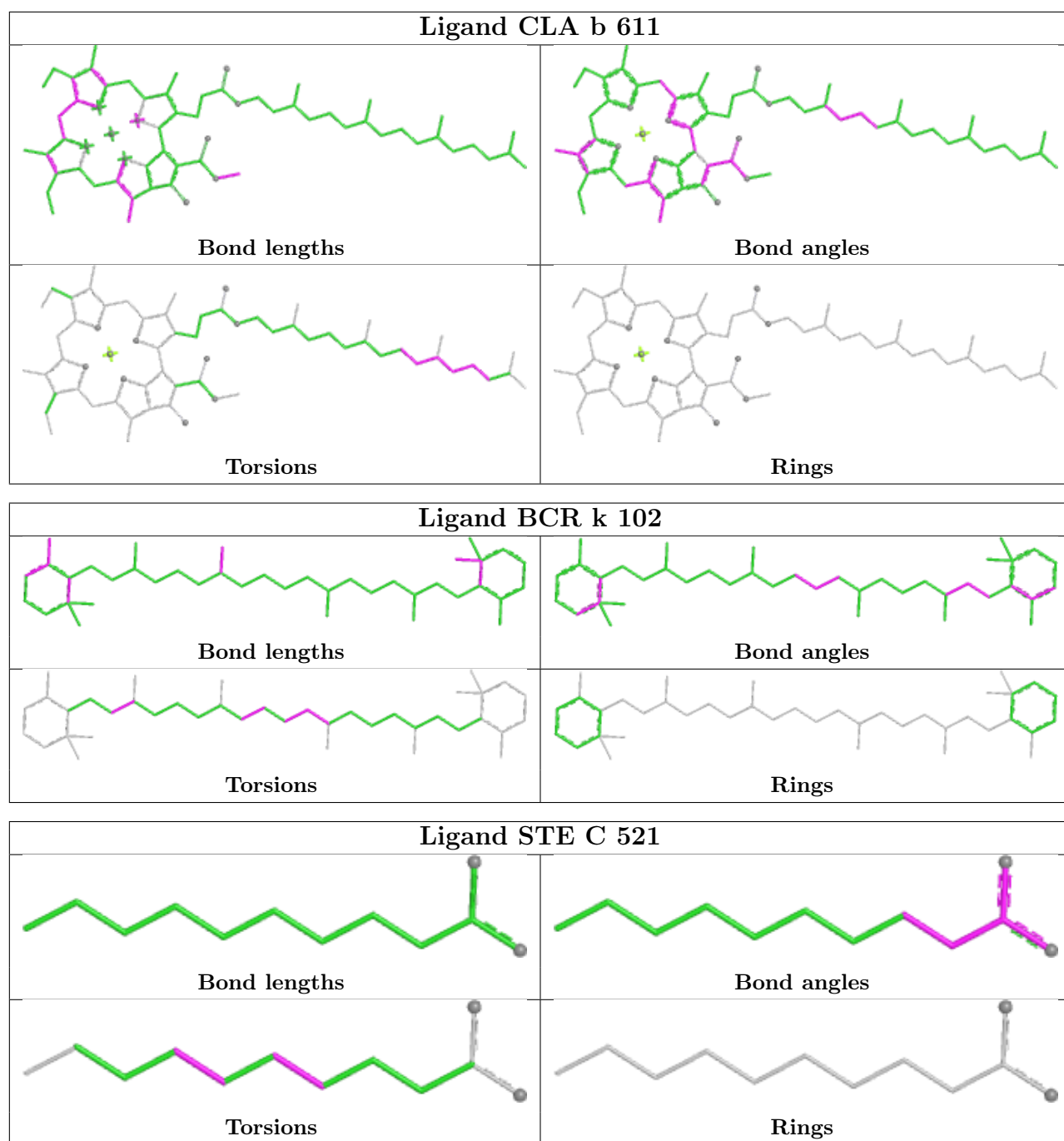
Ligand SQD D 410



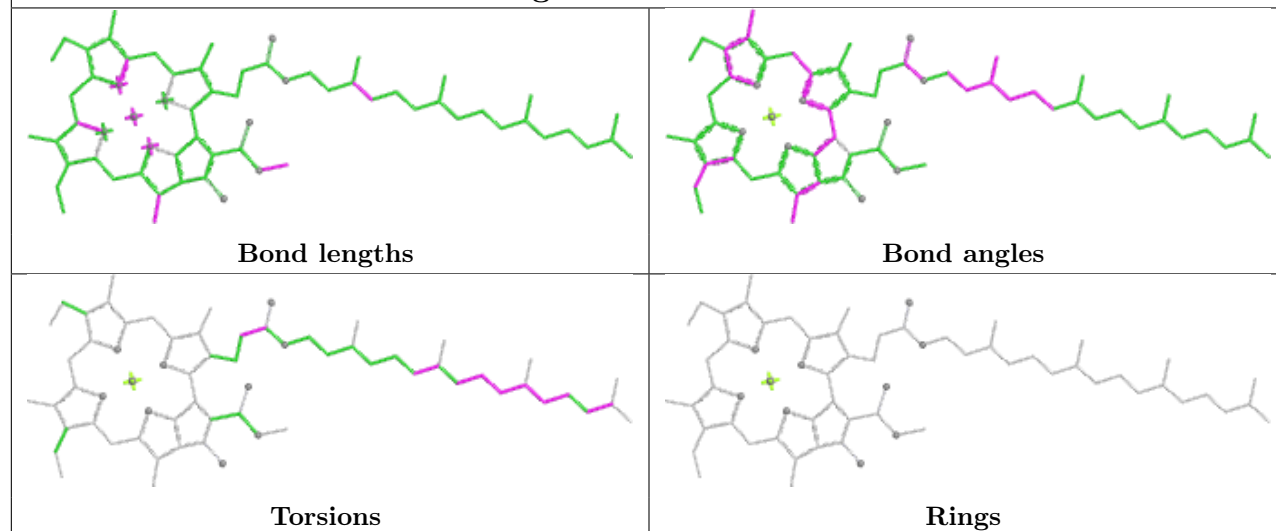




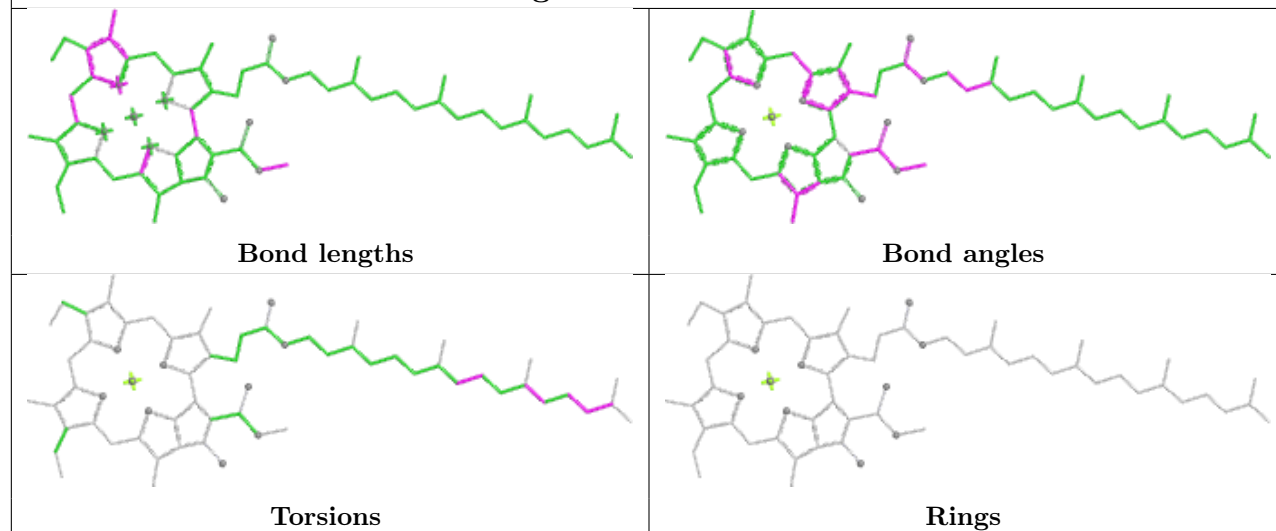




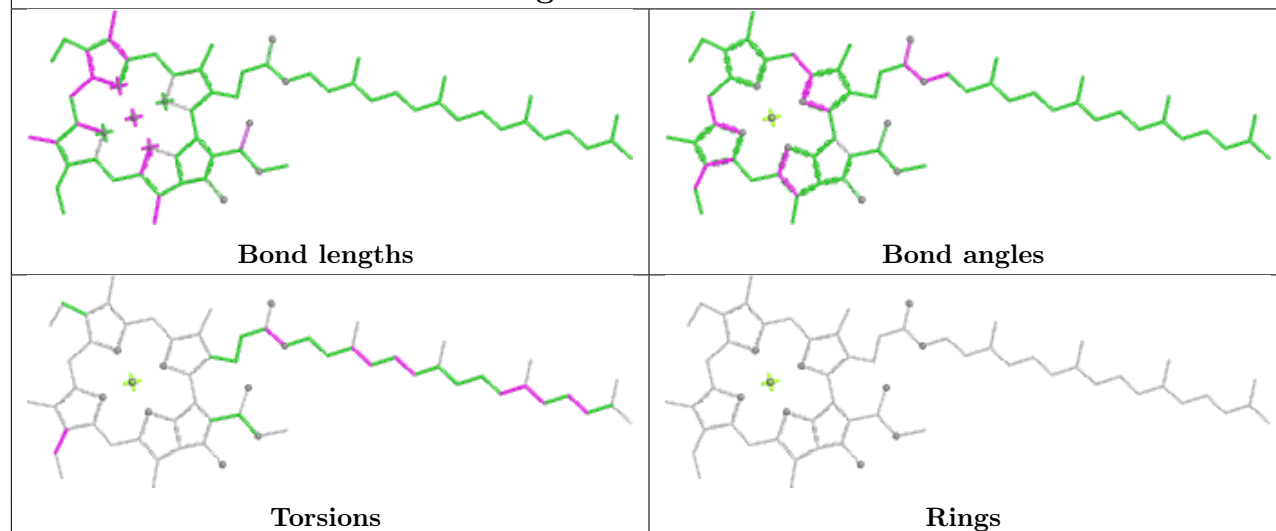
Ligand CLA B 713

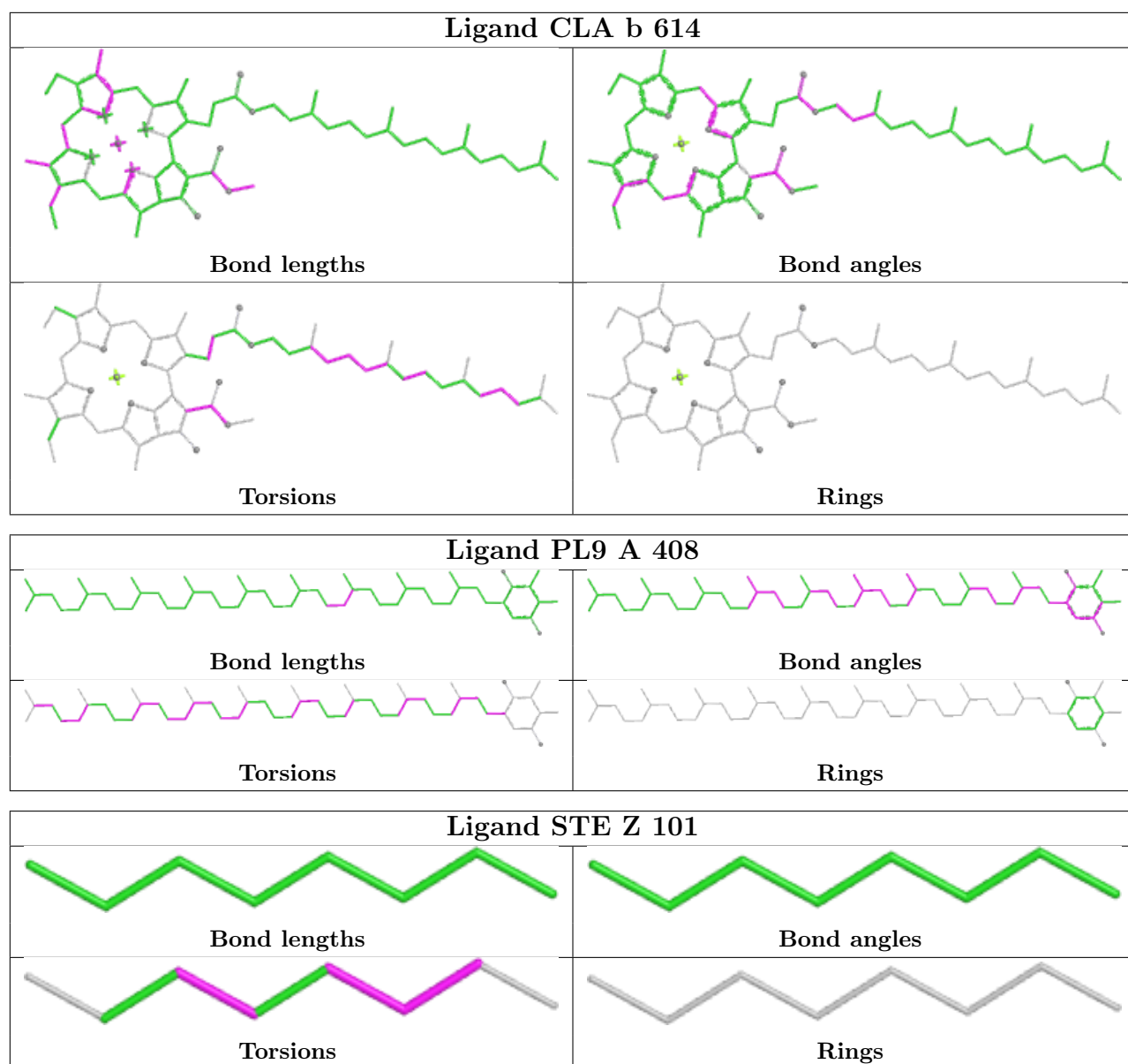


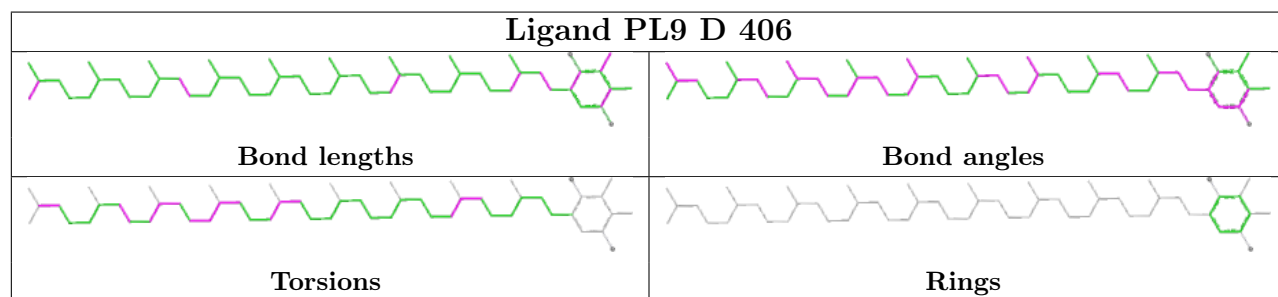
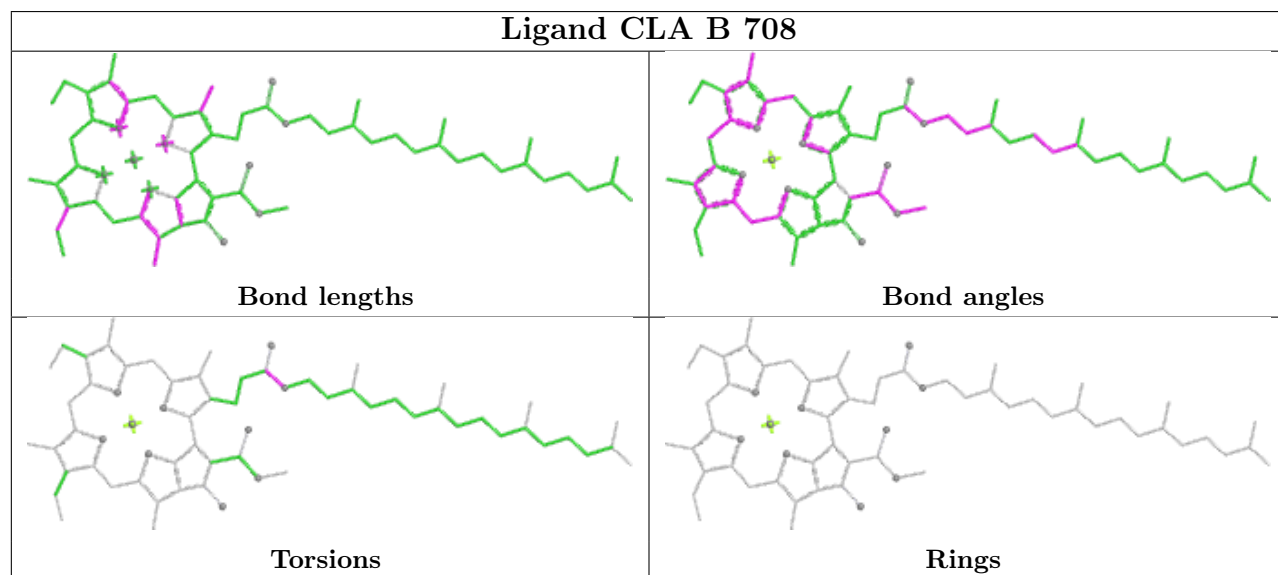
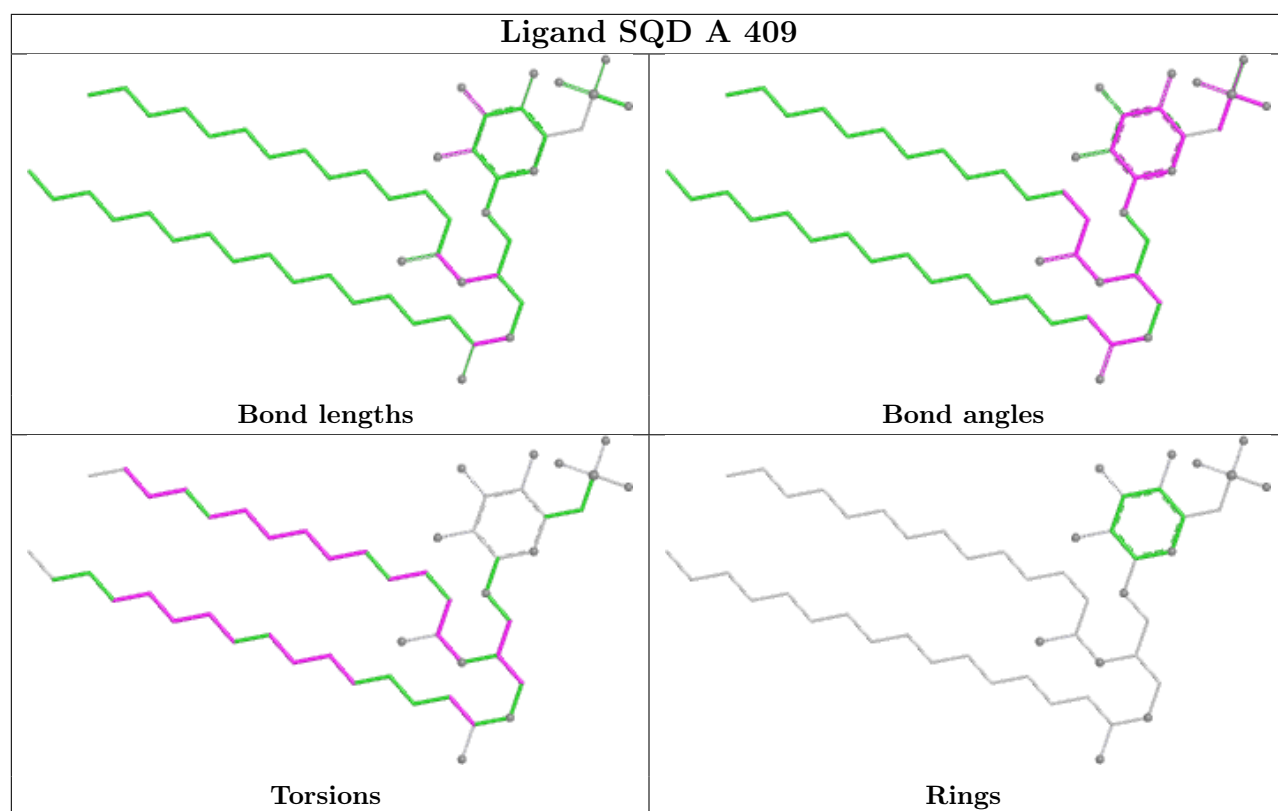
Ligand CLA B 710



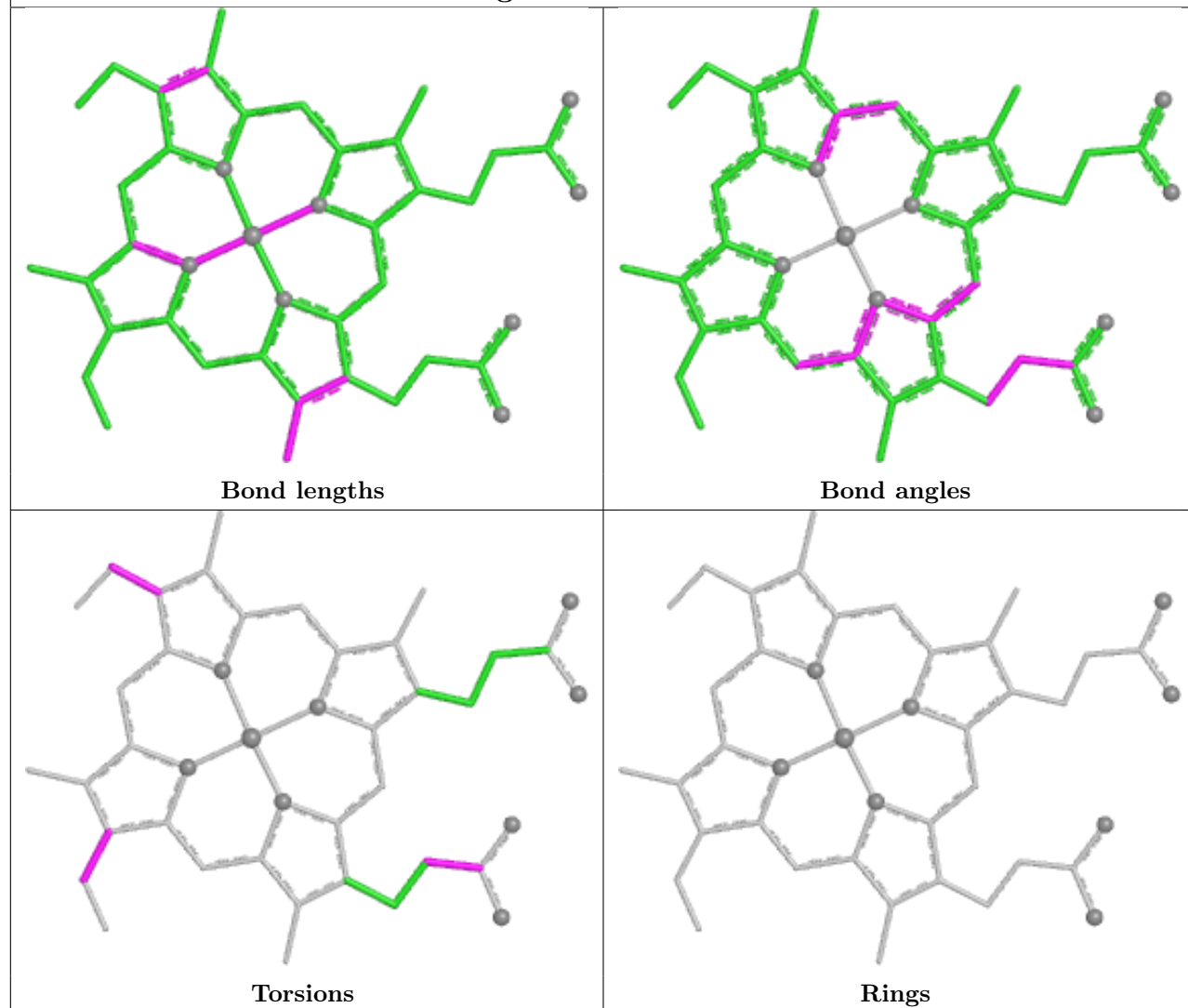
Ligand CLA a 405



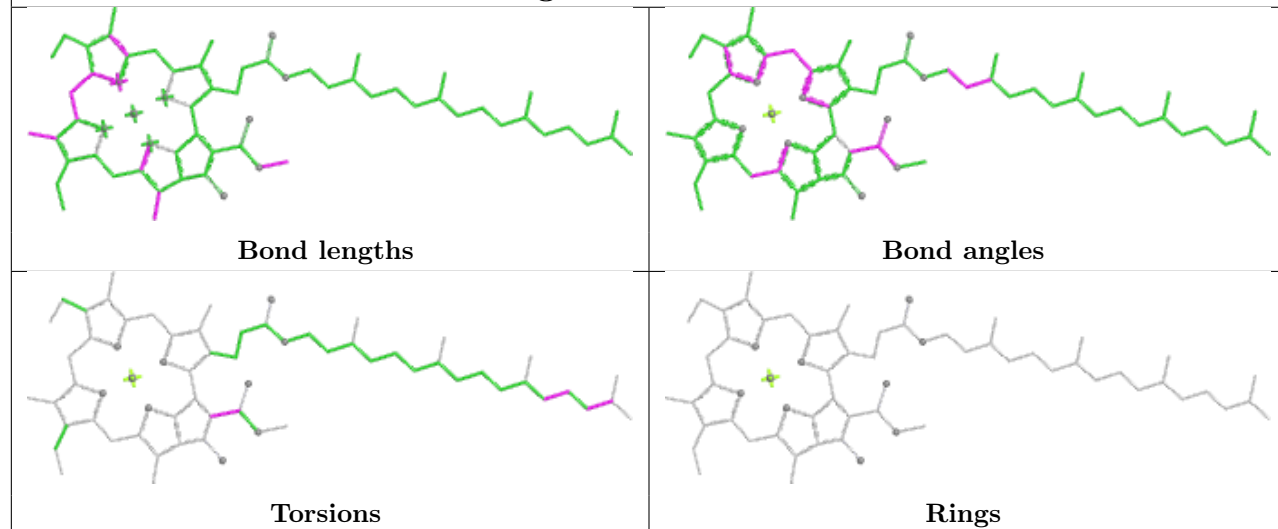


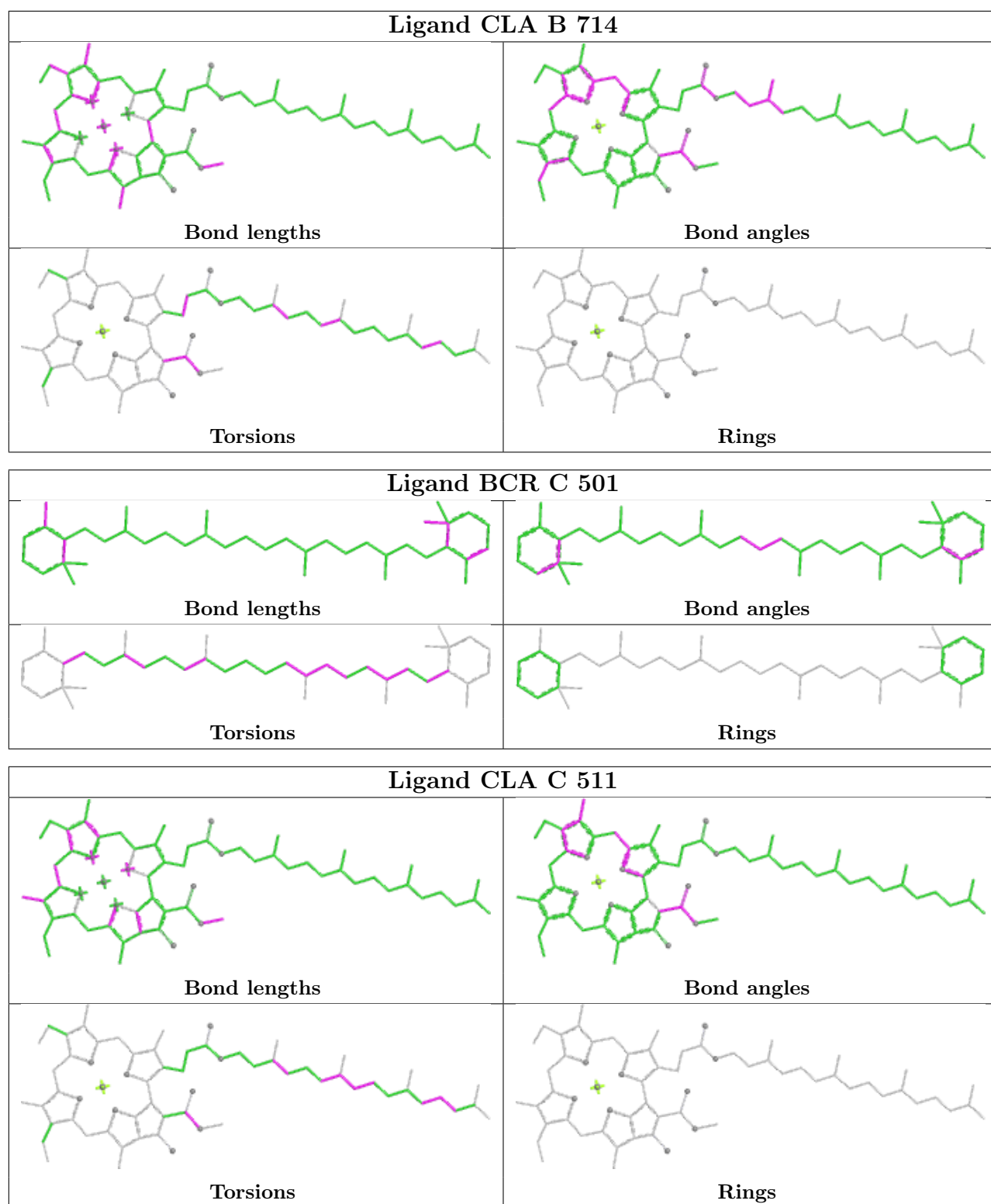


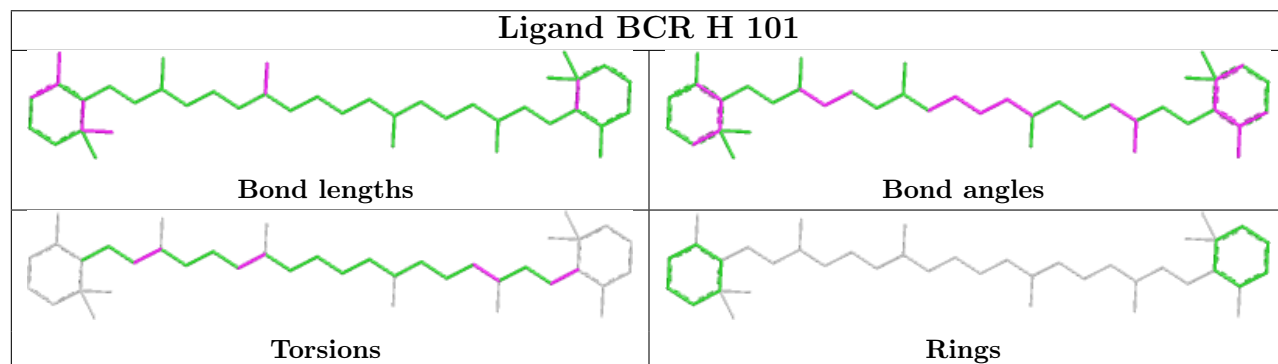
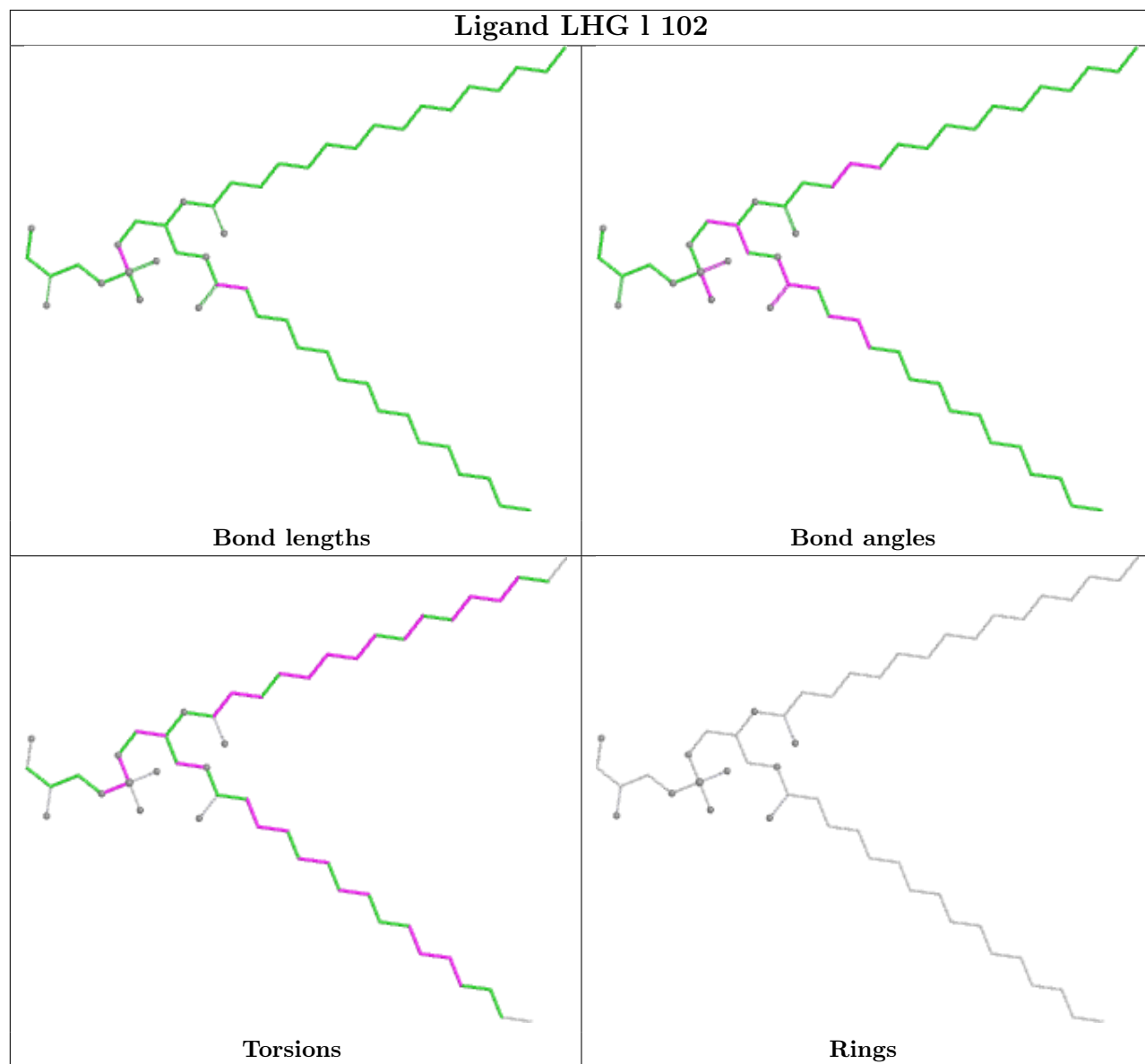
Ligand HEC v 201

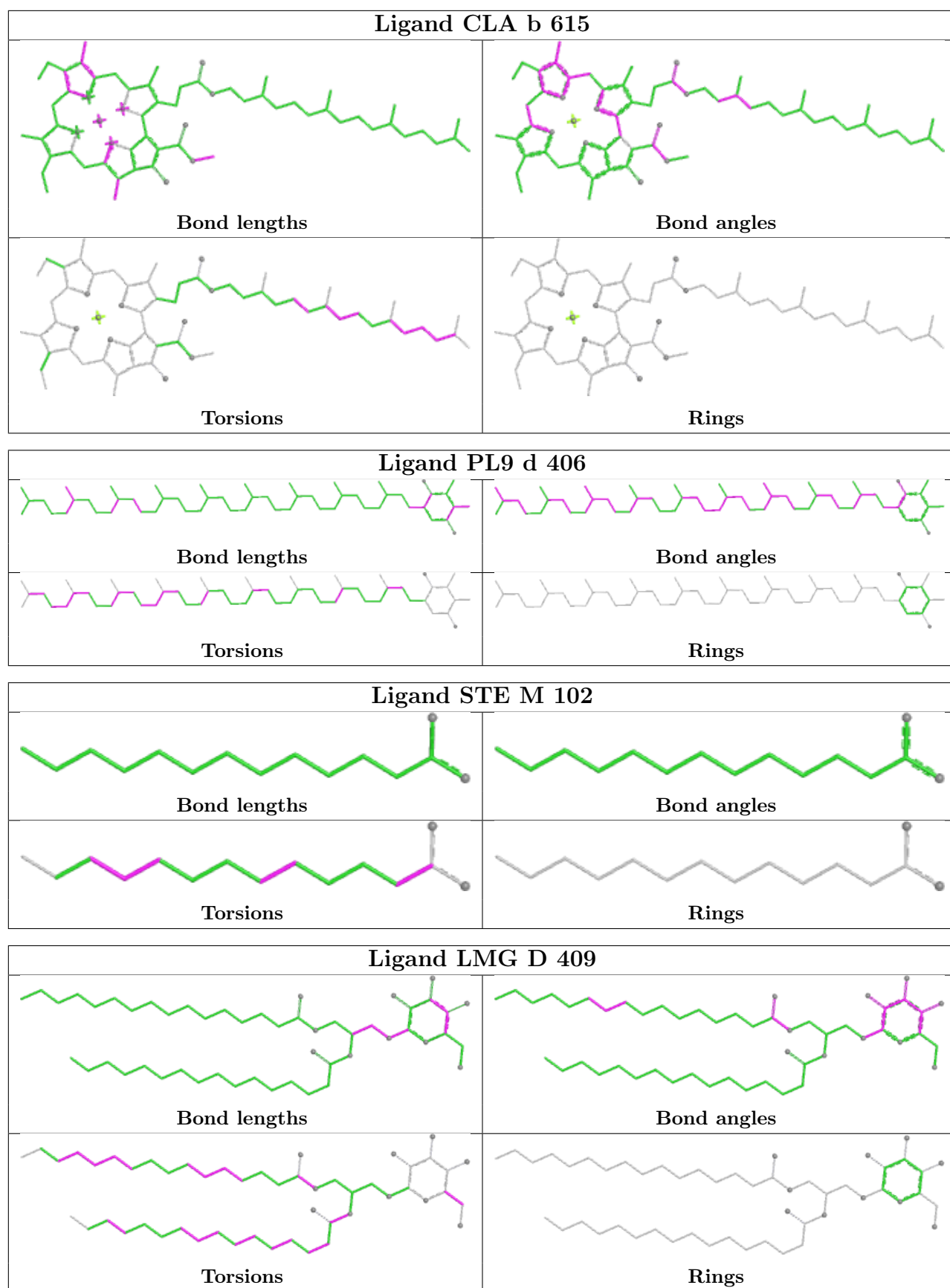


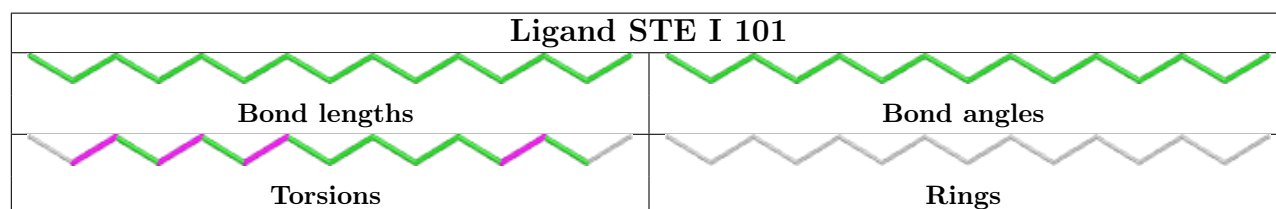
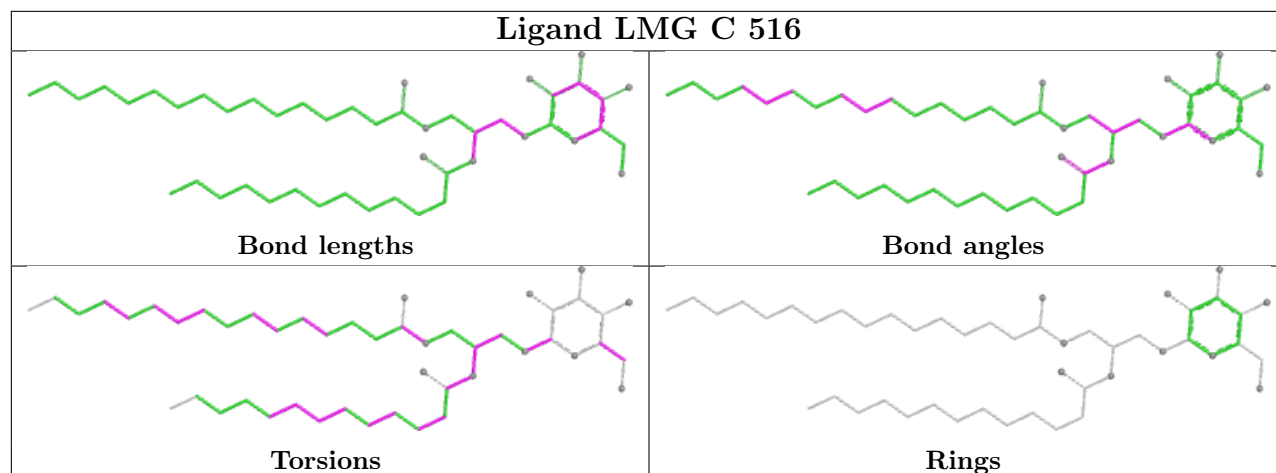
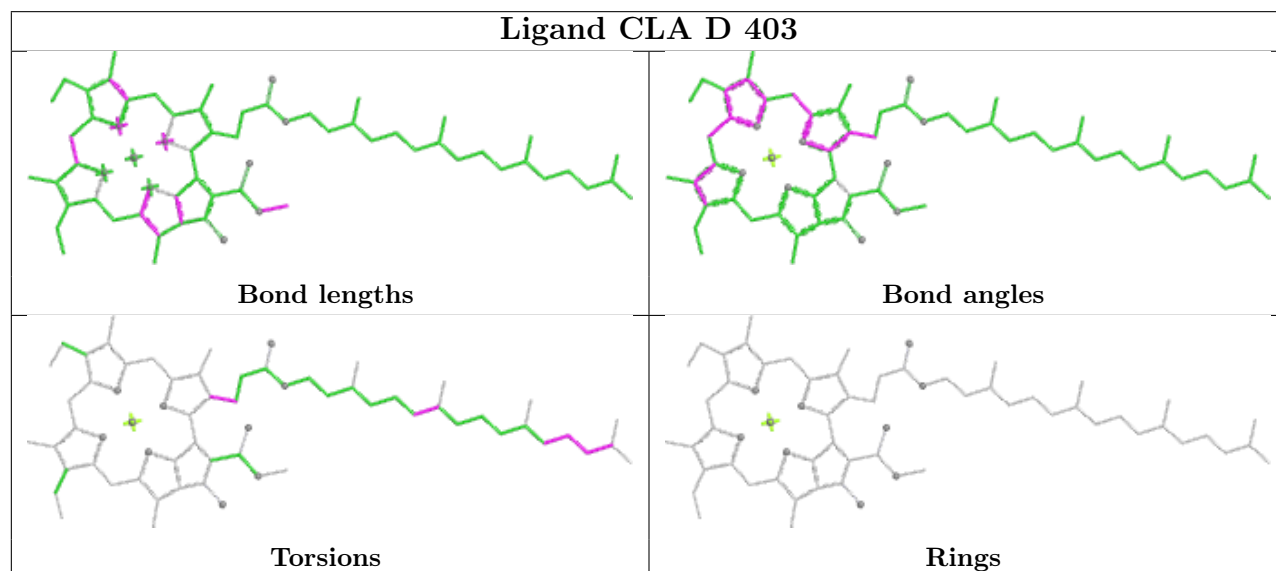
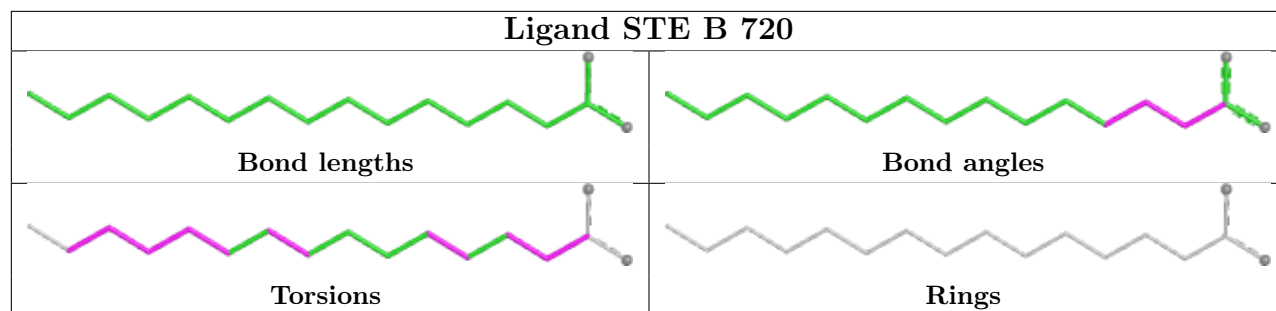
Ligand CLA c 503

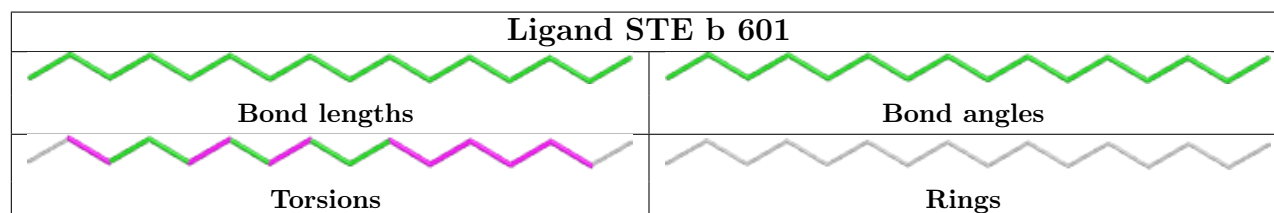
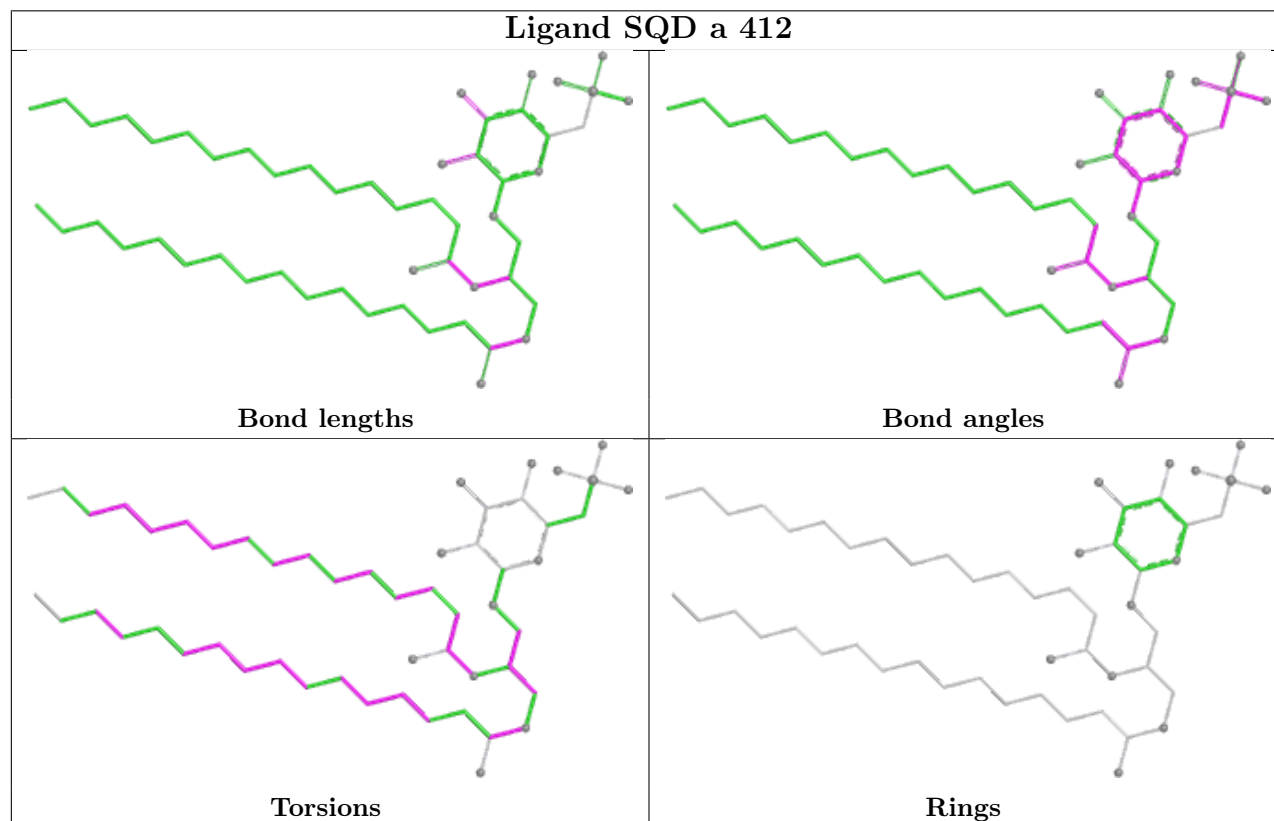
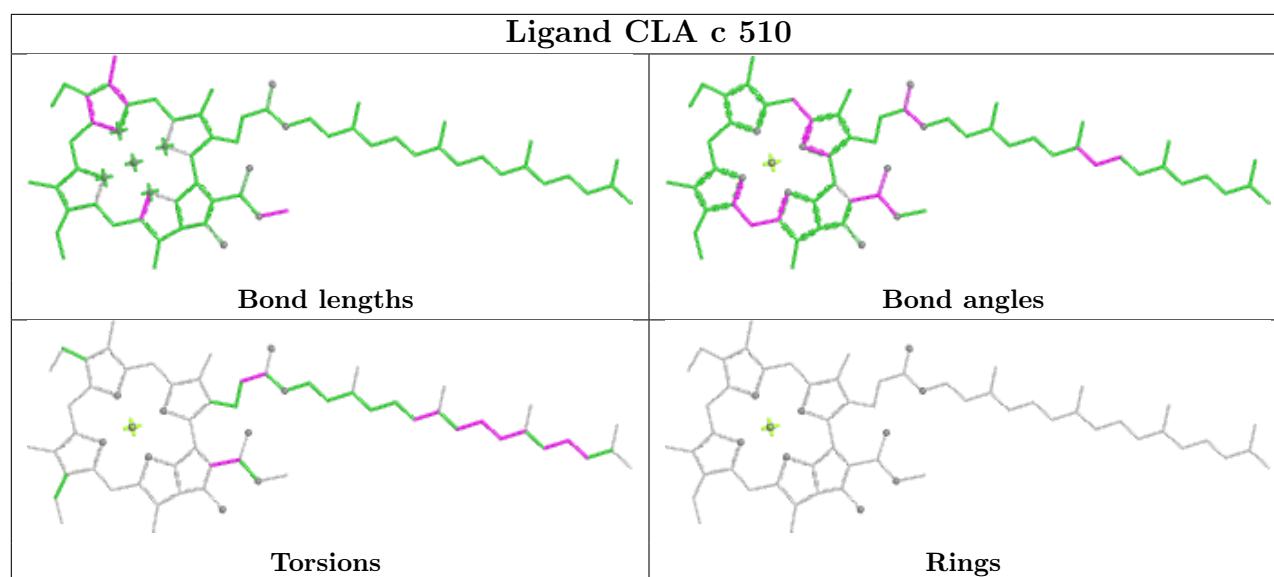


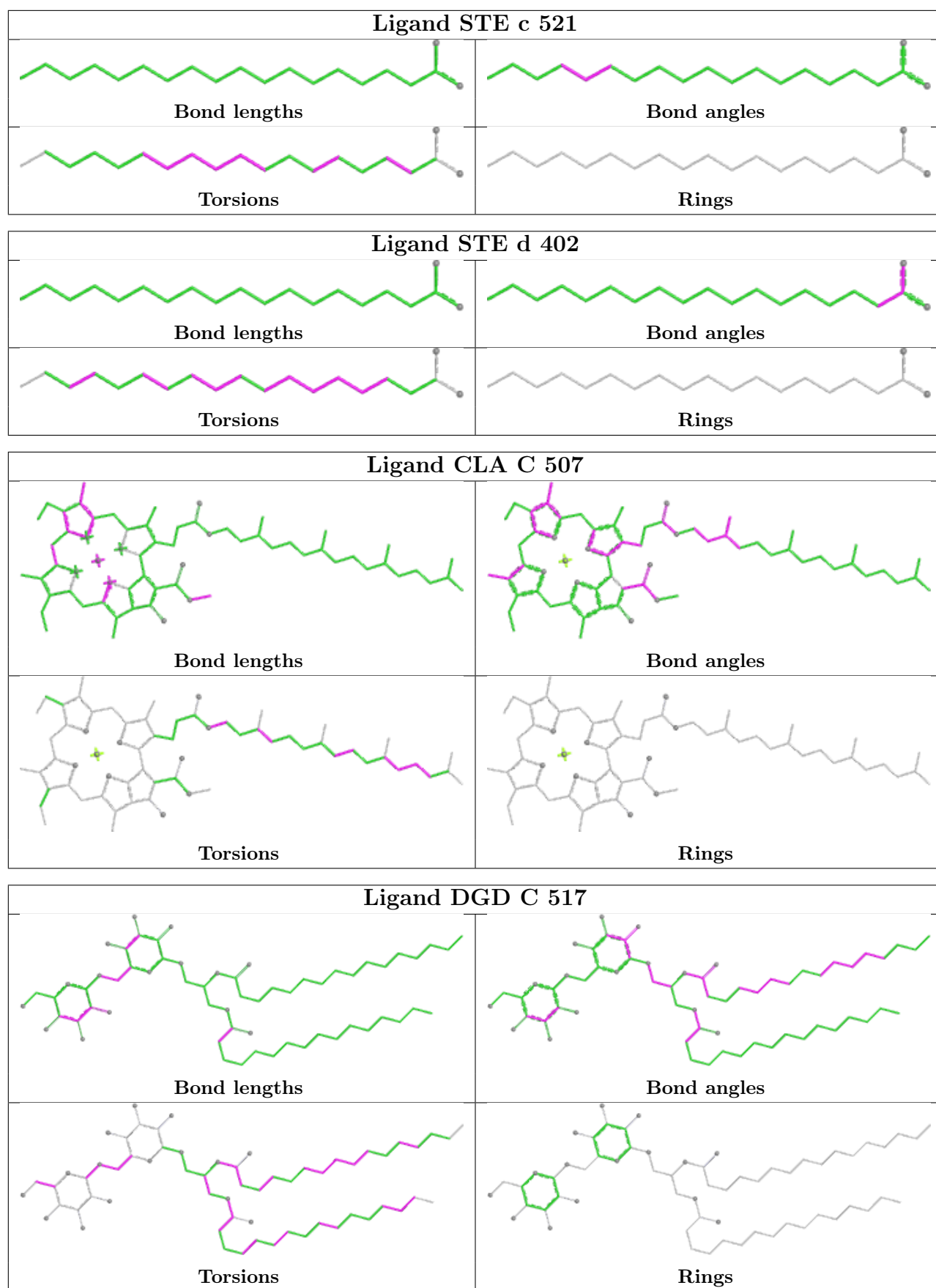


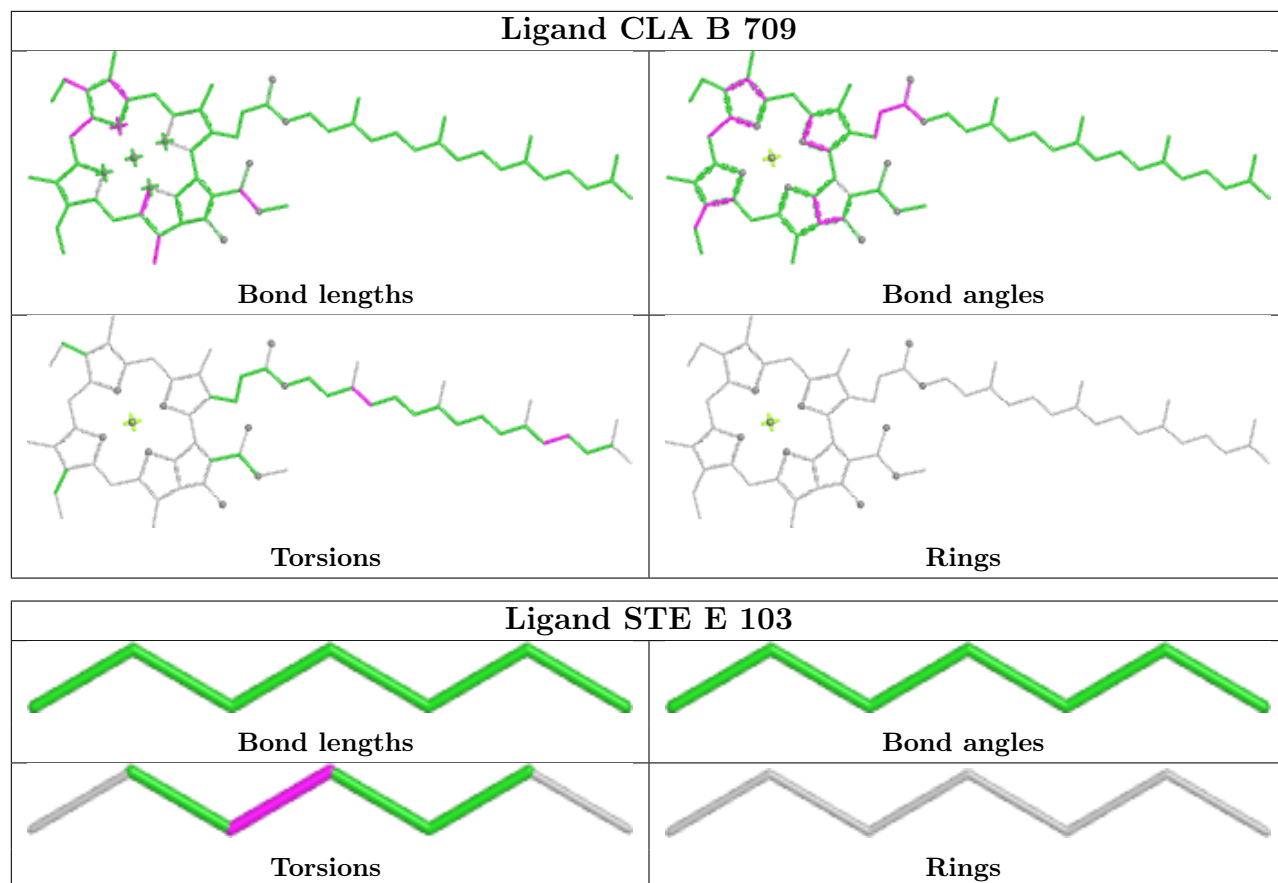




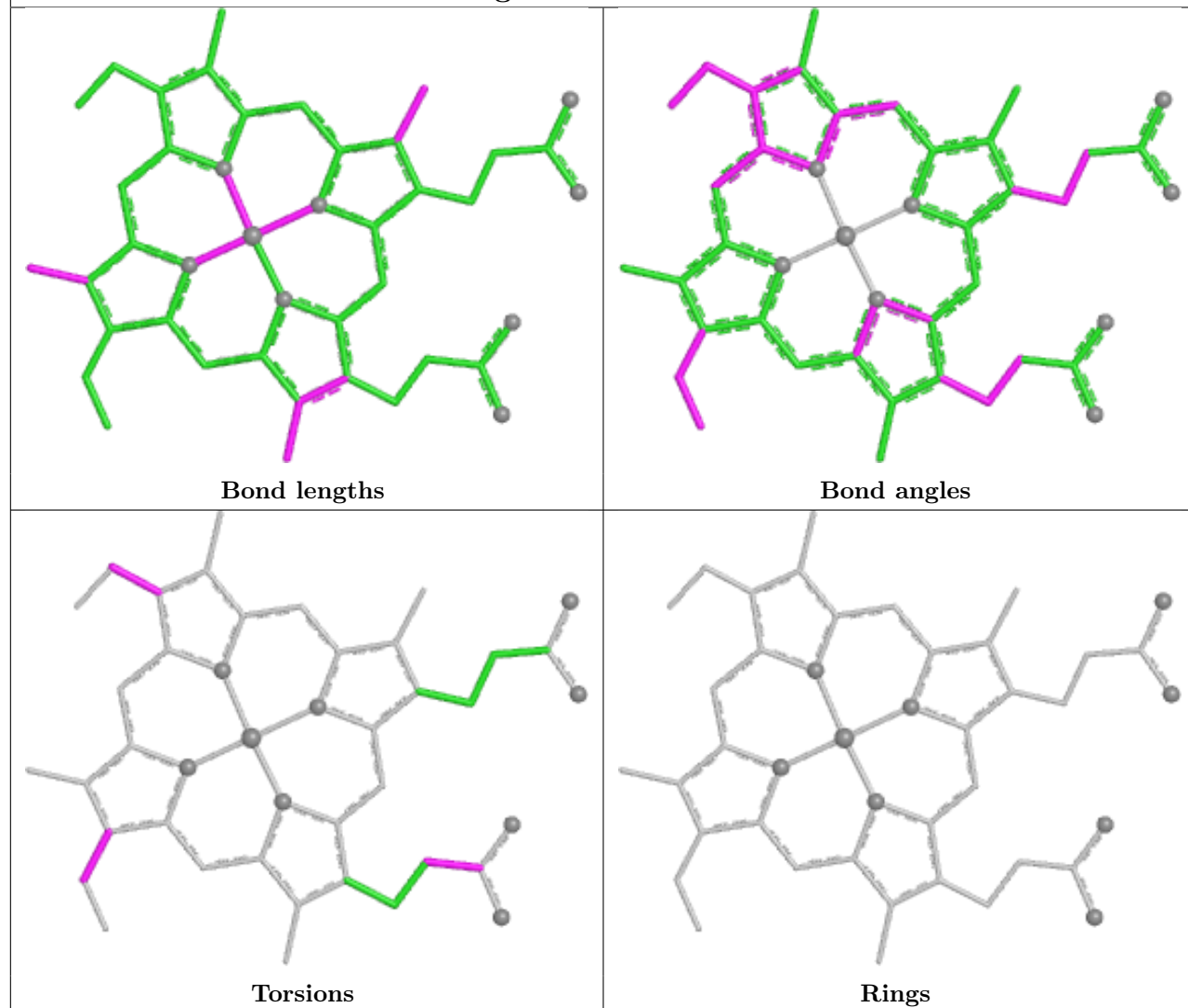




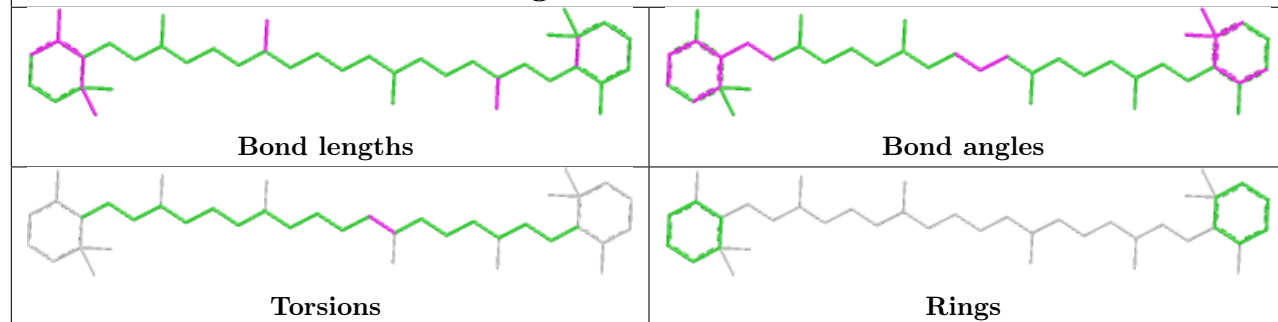


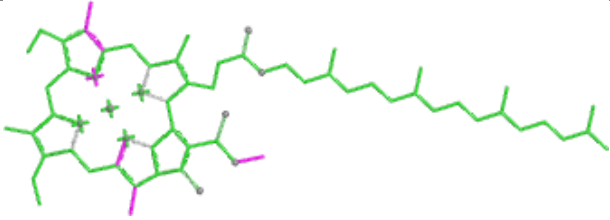
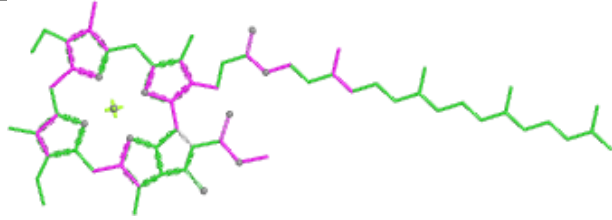
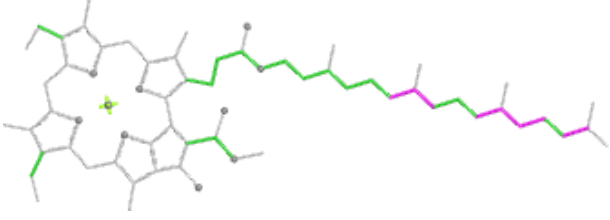
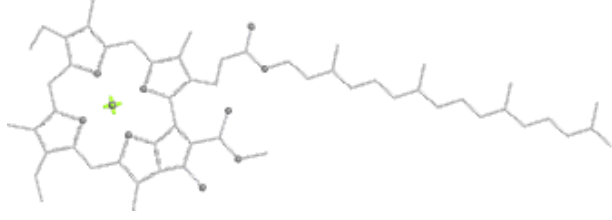
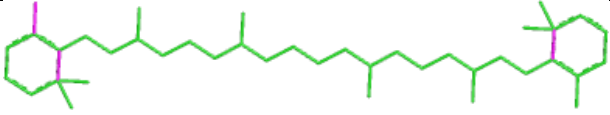
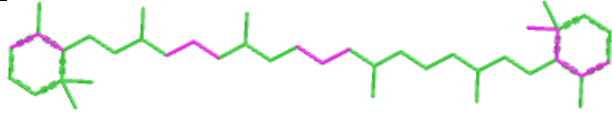
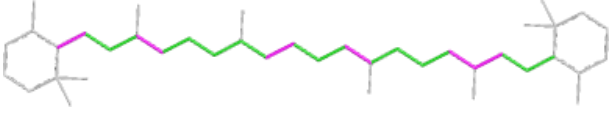
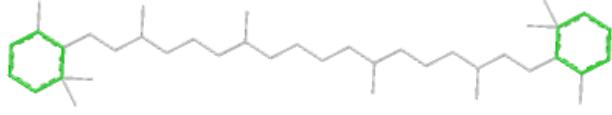
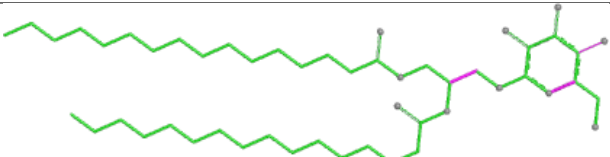
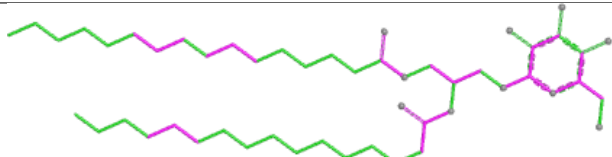
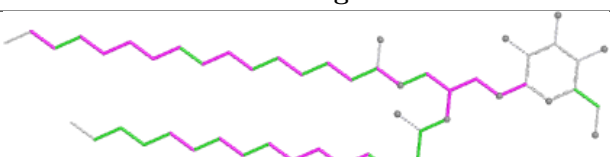
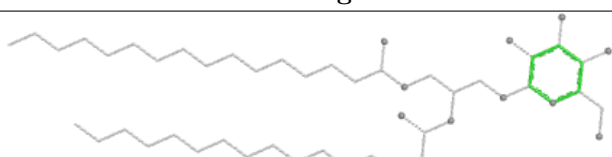


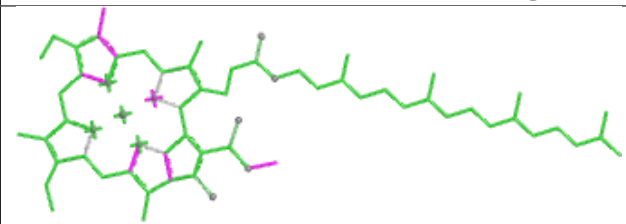
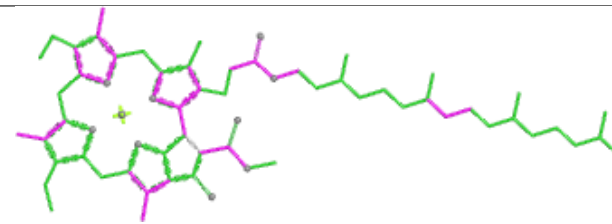
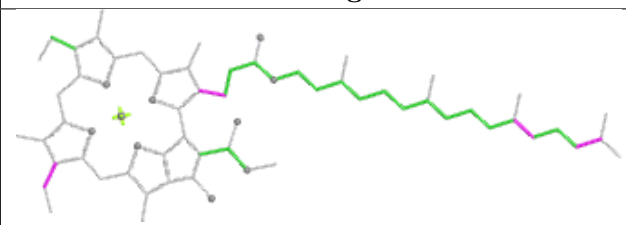
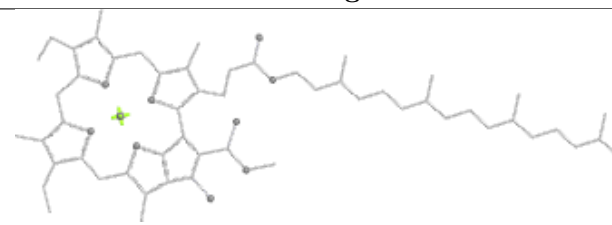
Ligand HEC F 101



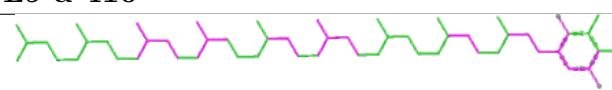
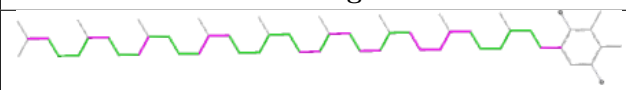
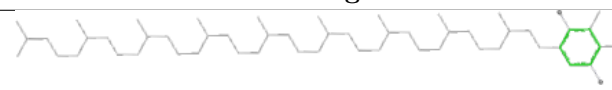
Ligand BCR B 719



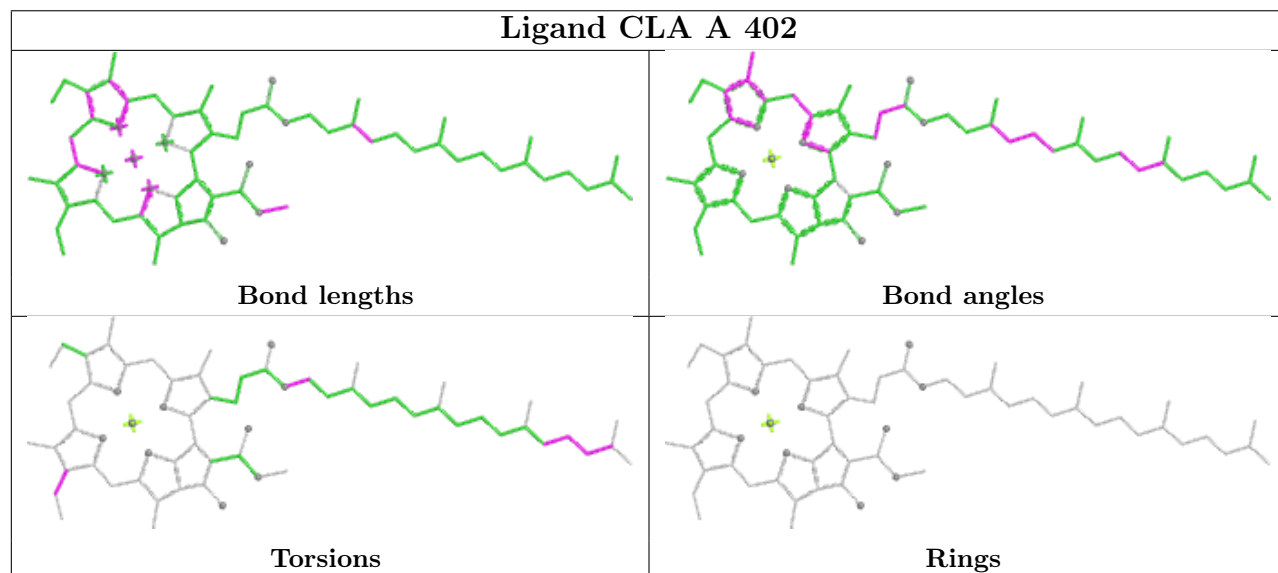
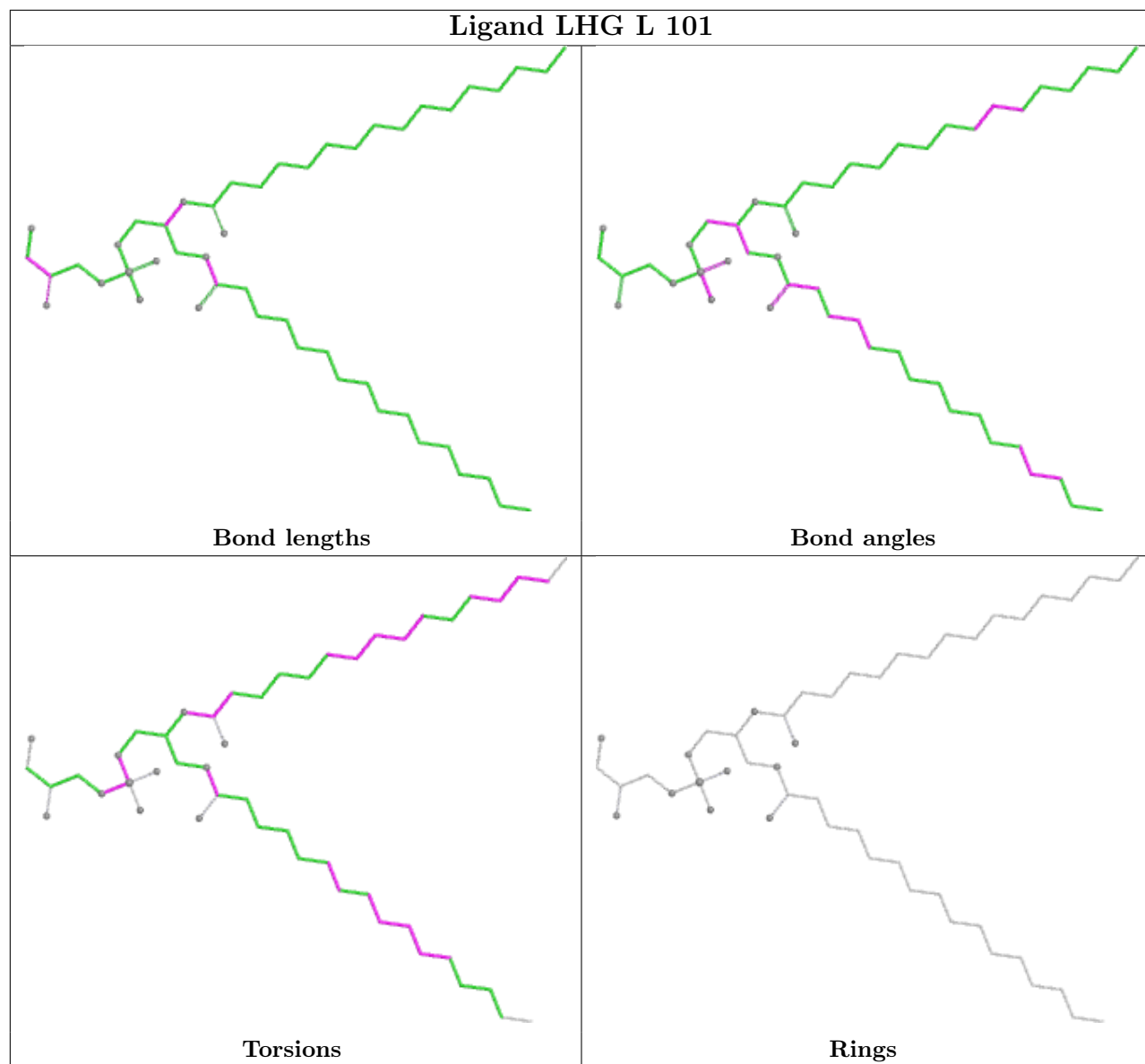
Ligand CLA A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

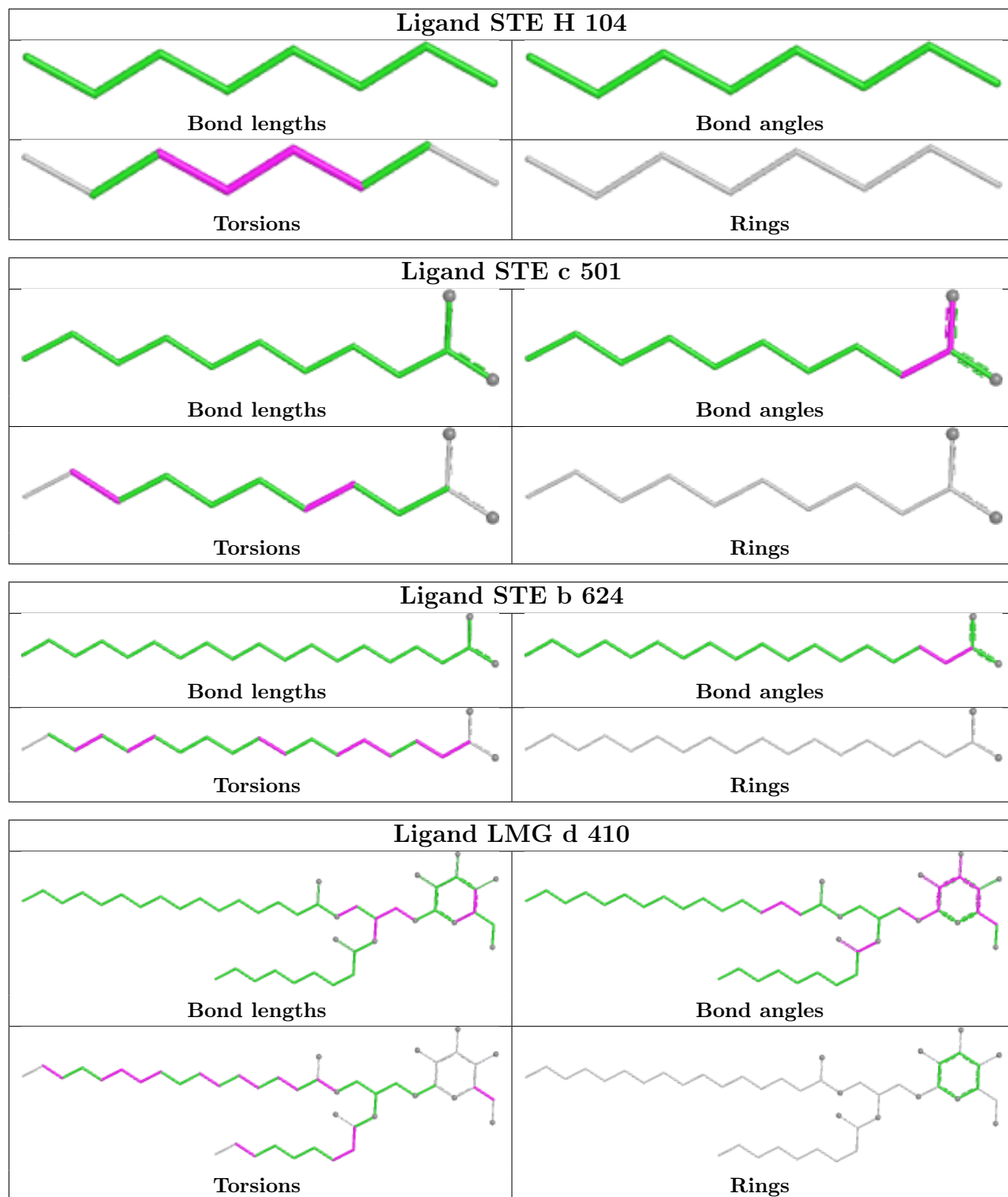
Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

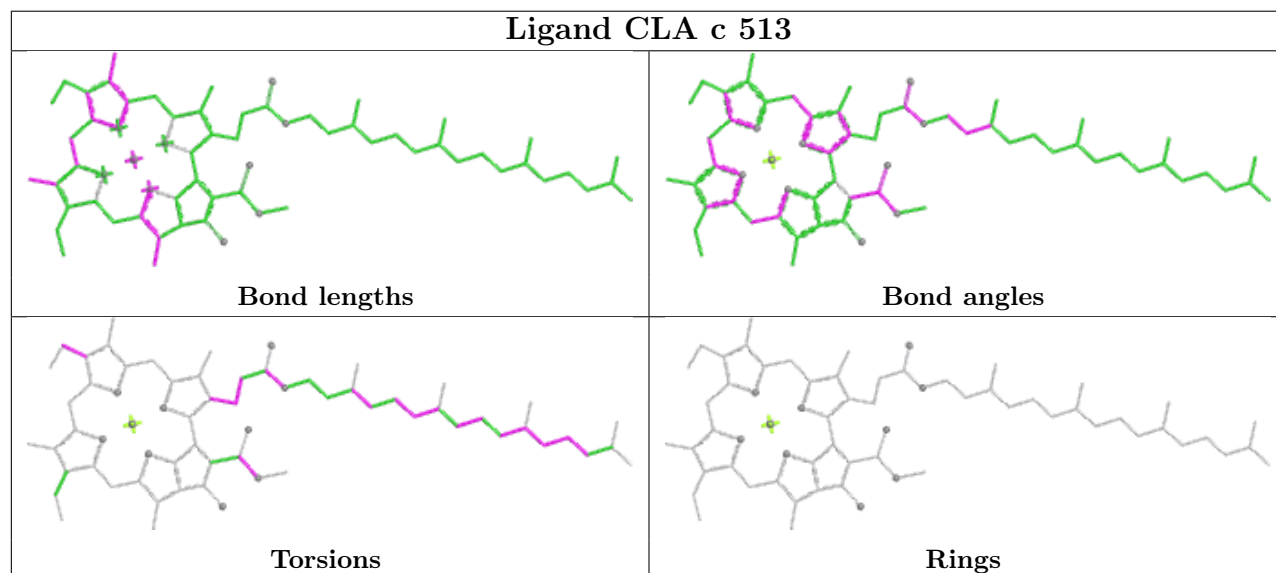
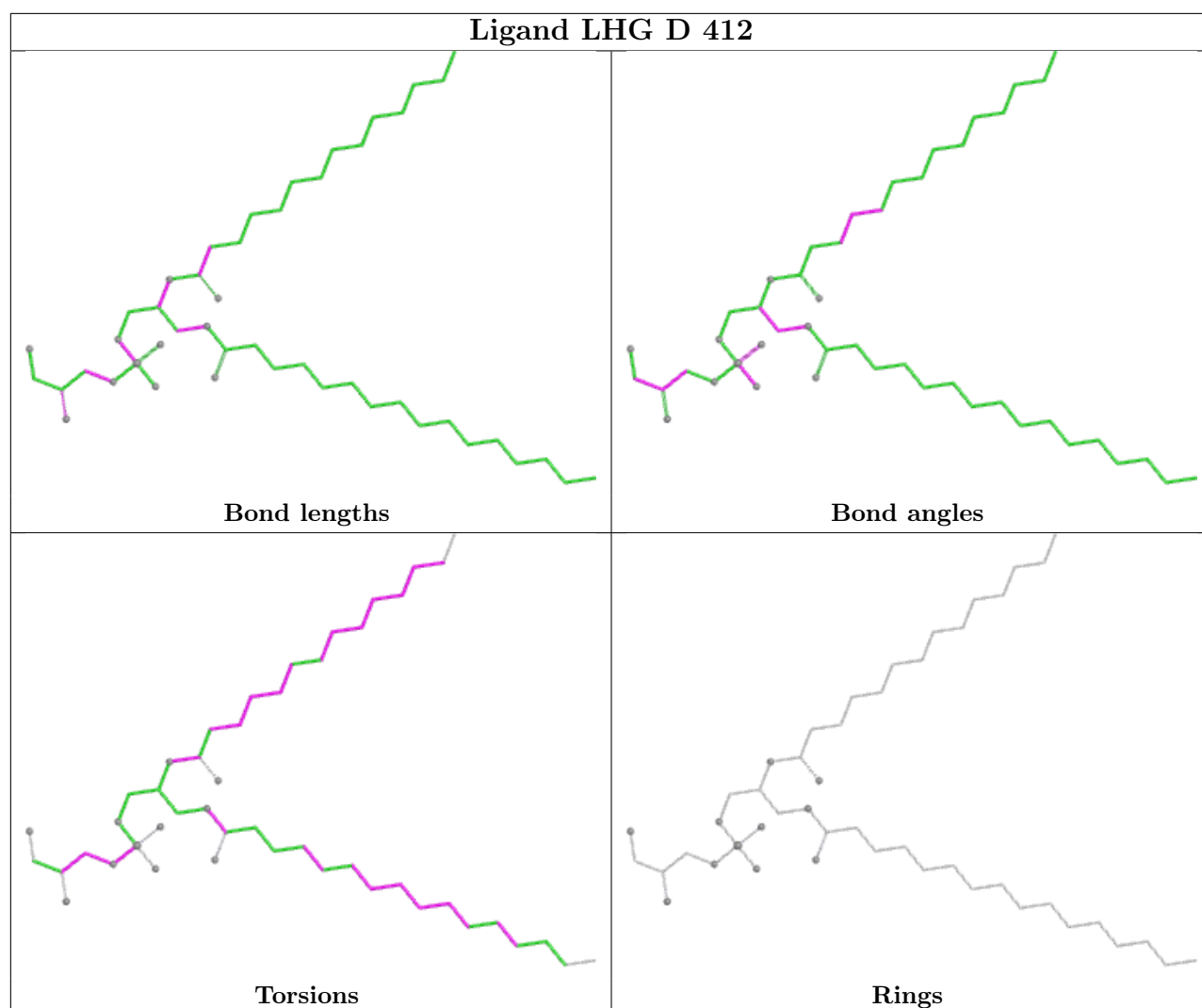
Ligand STE h 704	
	
Bond lengths	Bond angles
	
Torsions	Rings

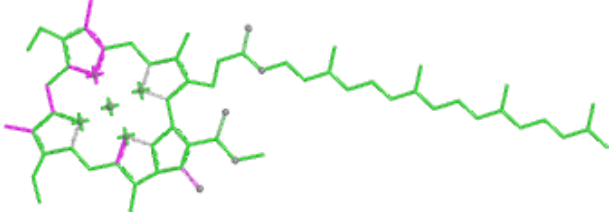
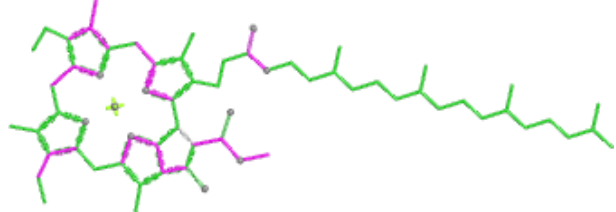
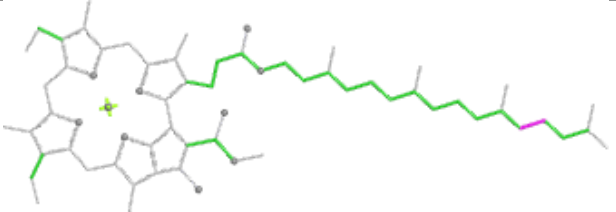
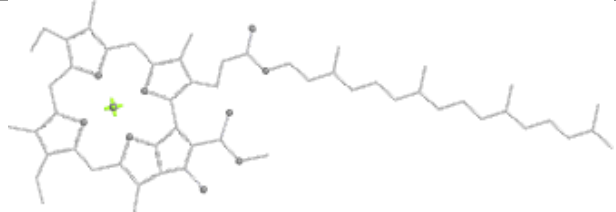
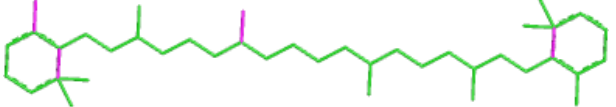
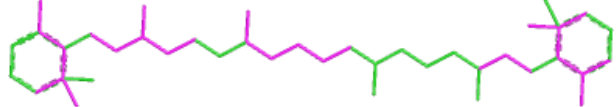
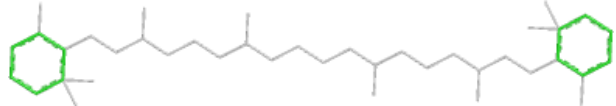
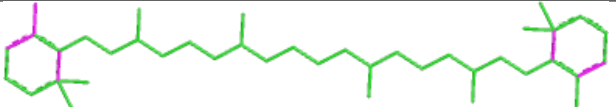
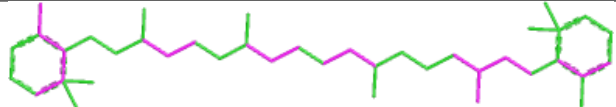
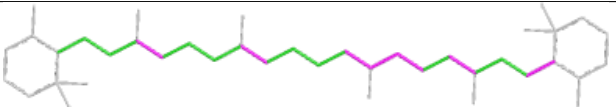
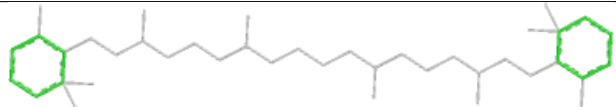
Ligand PL9 a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

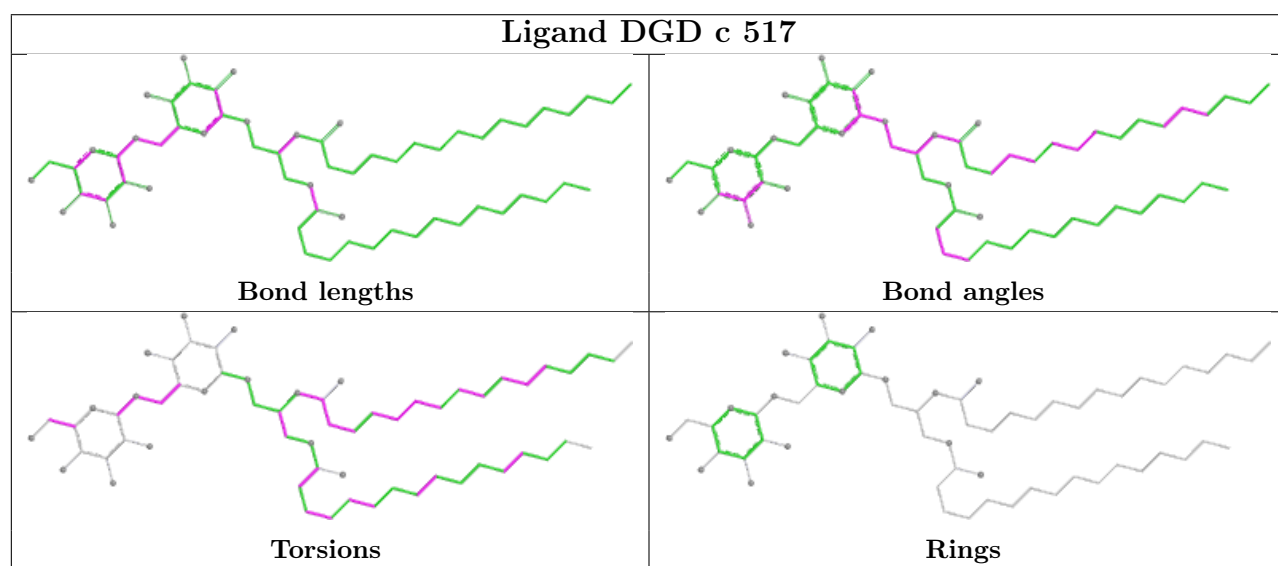
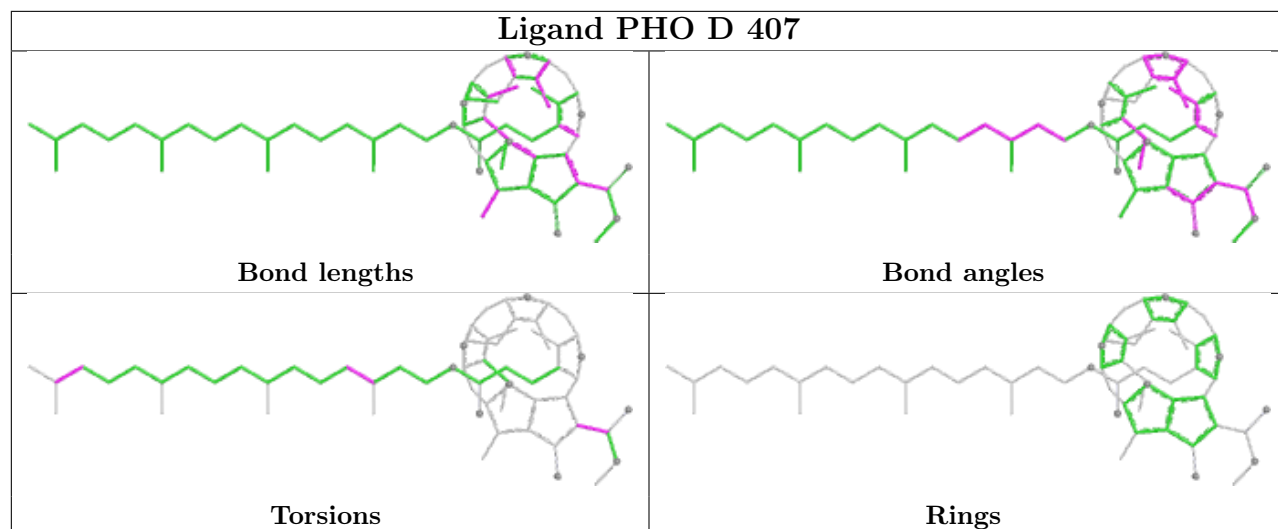
Ligand STE a 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

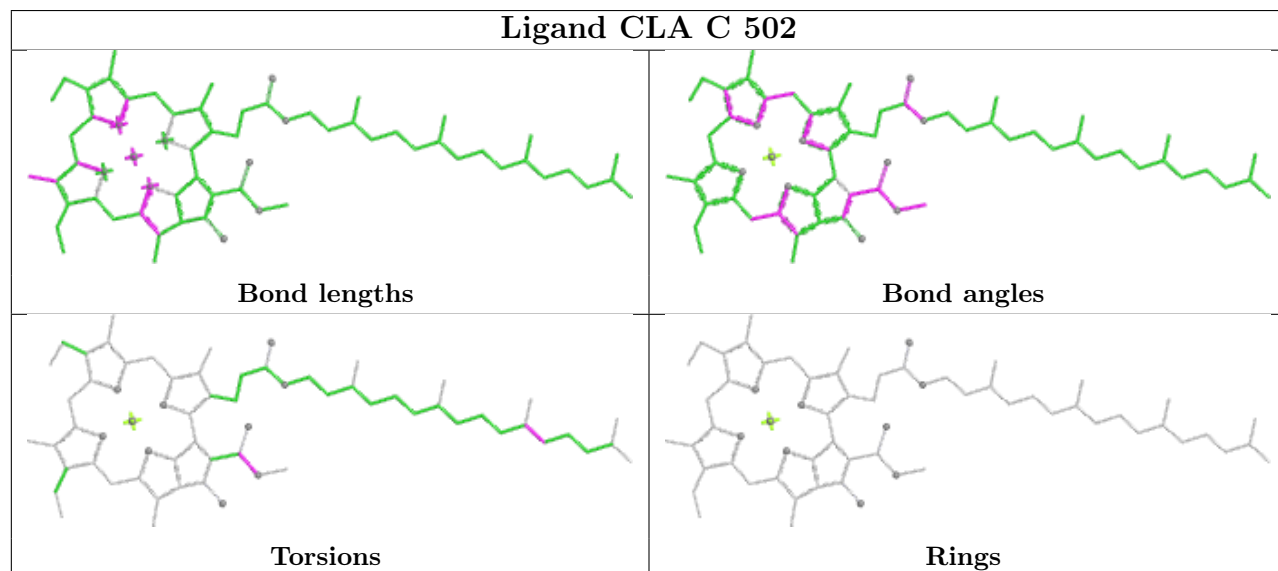
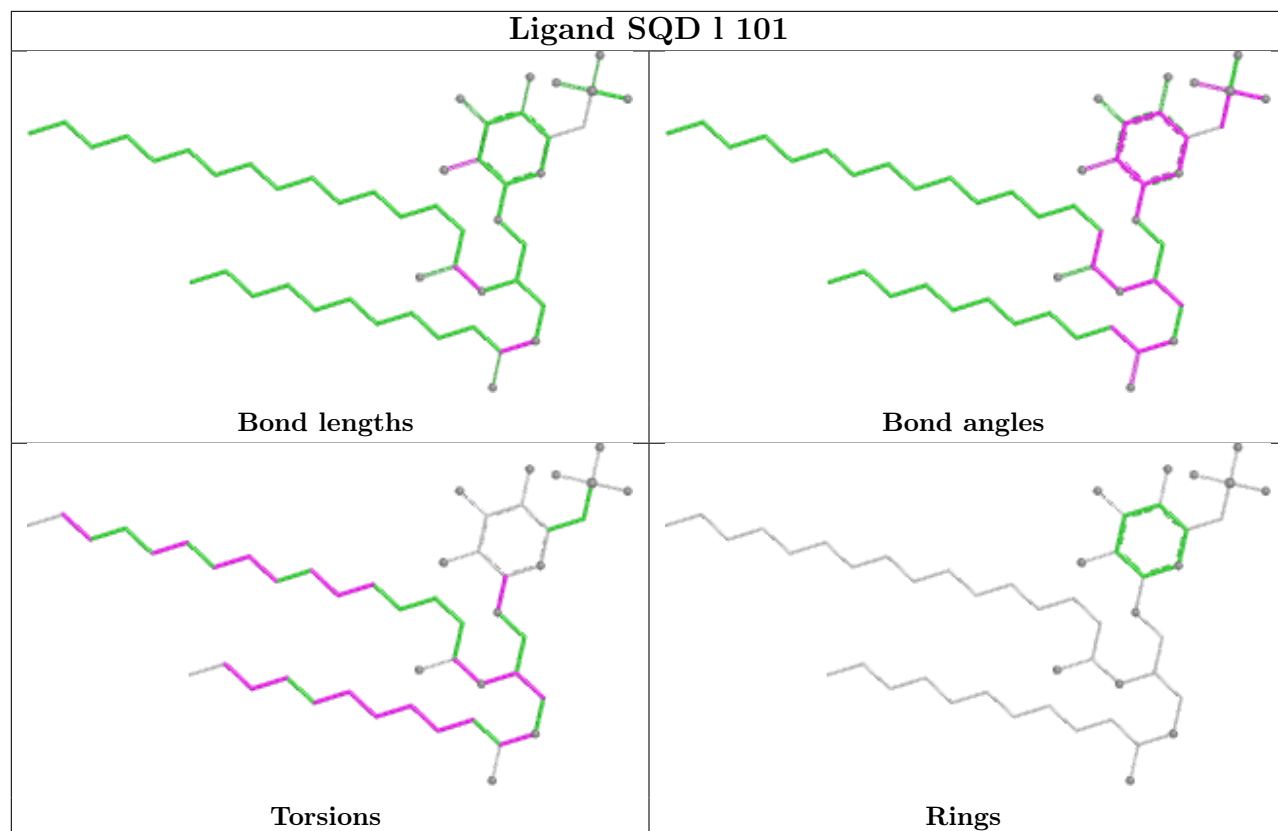


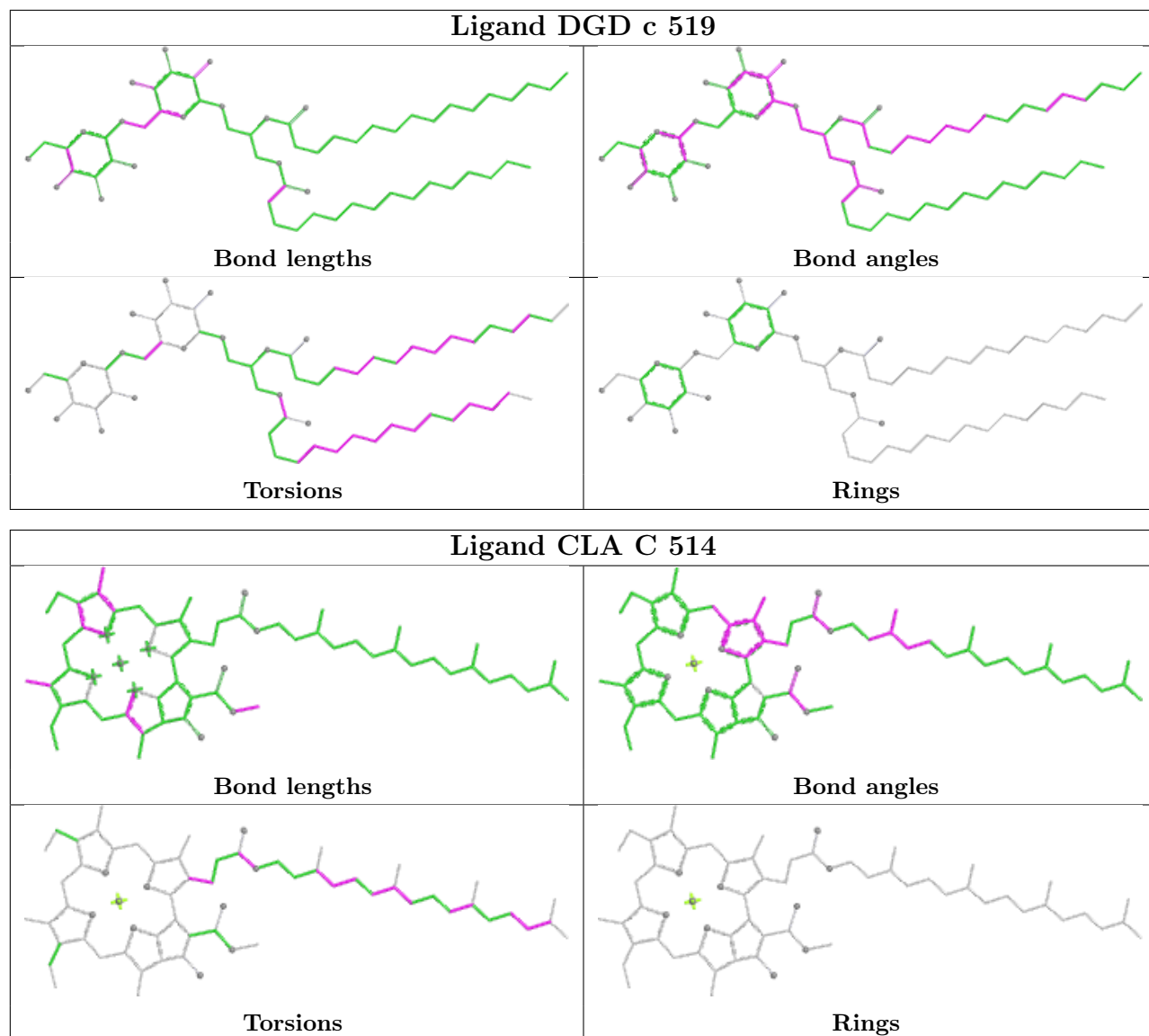




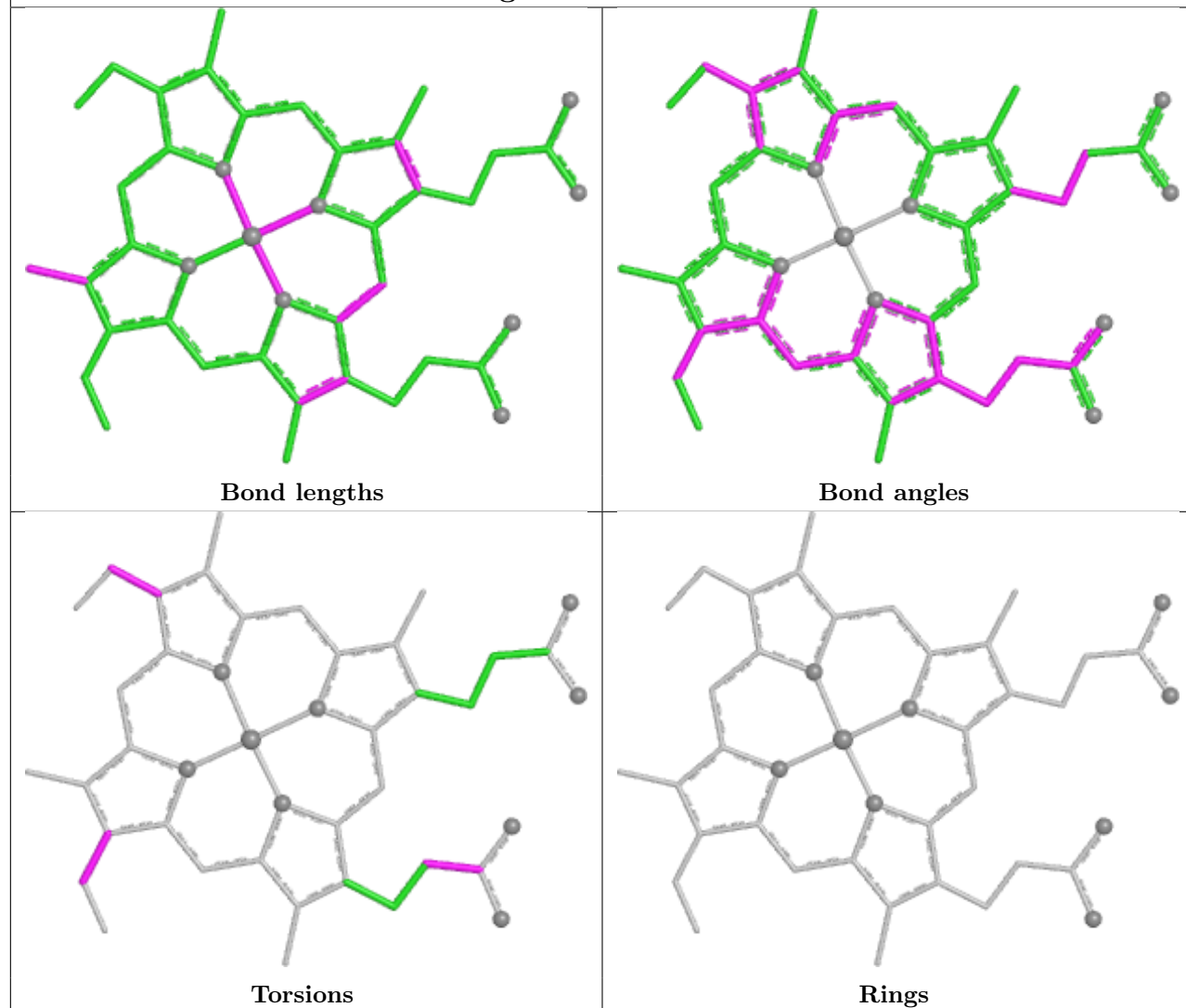
Ligand CLA a 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 524	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings



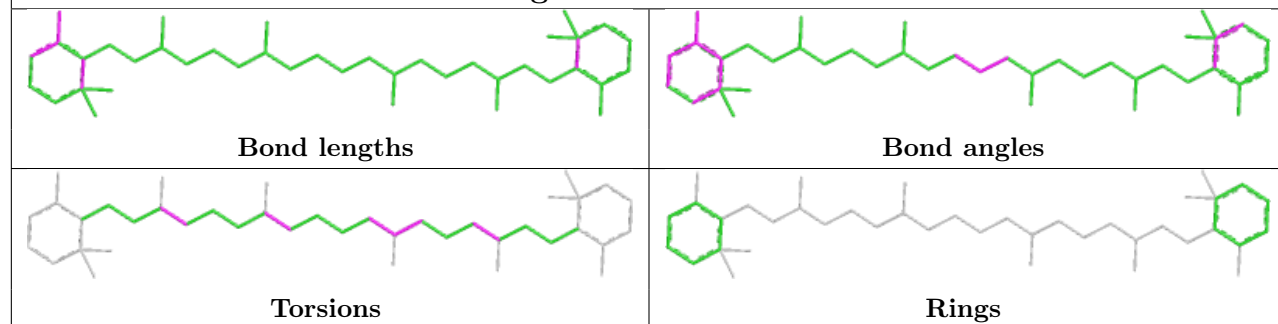


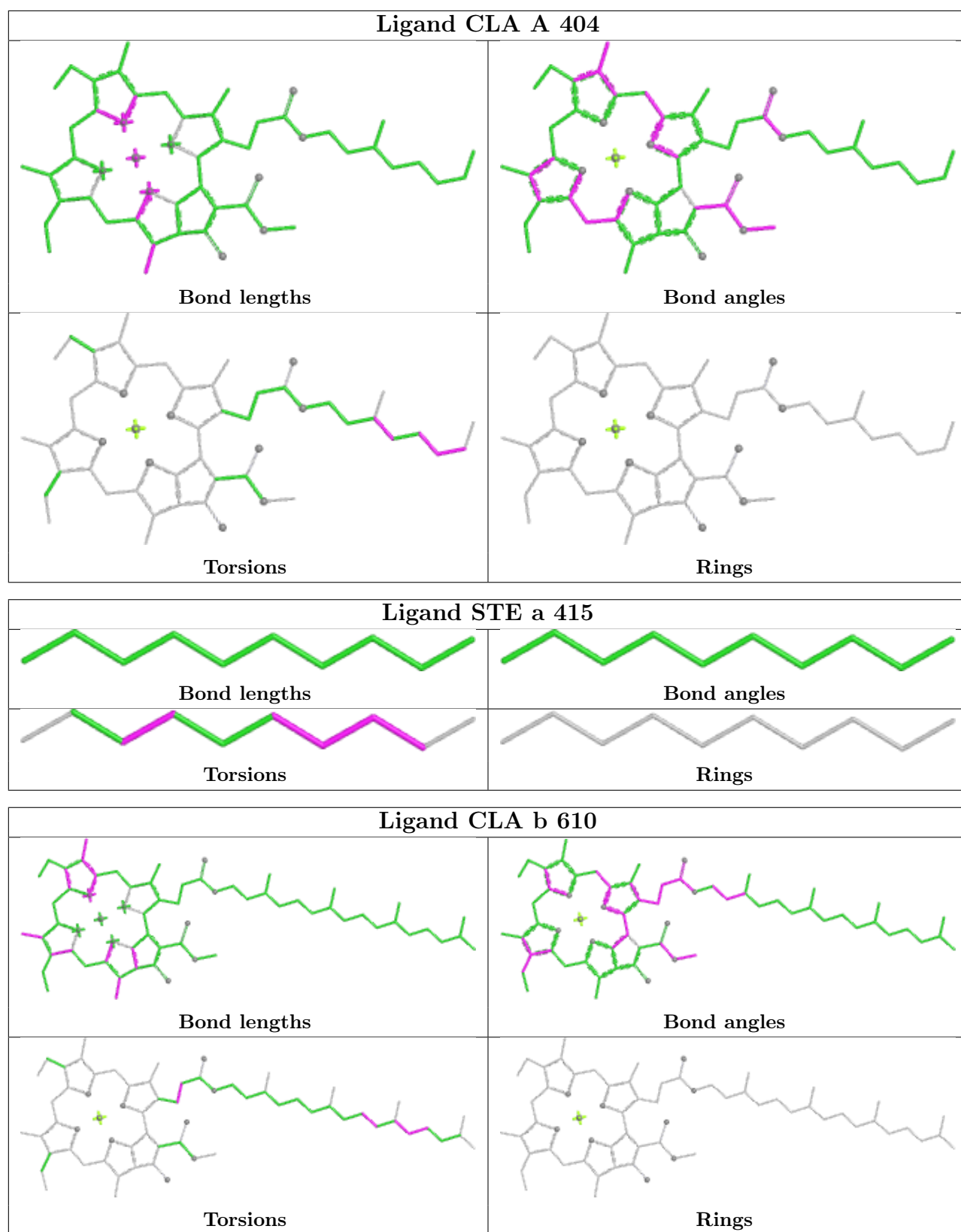


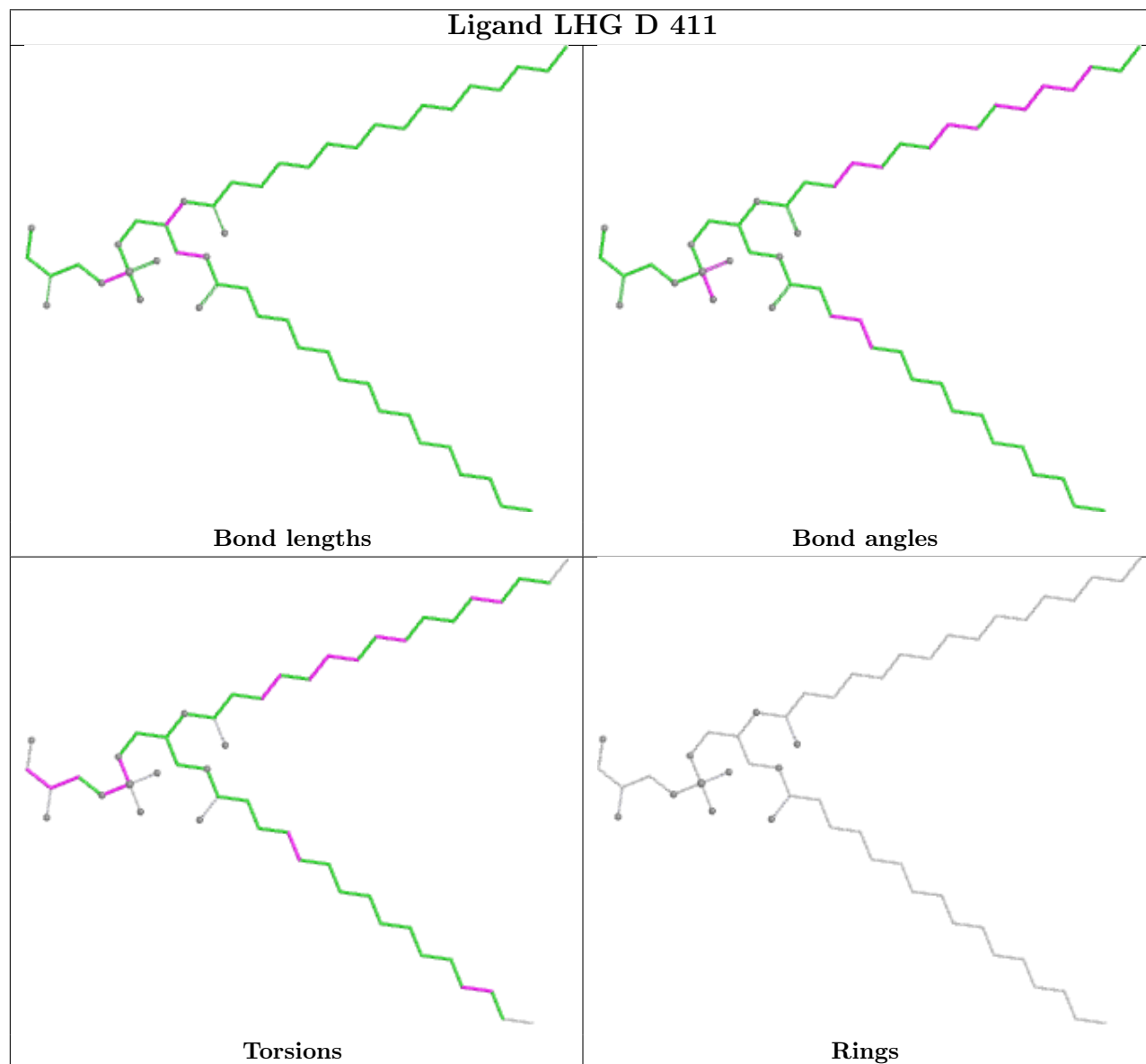
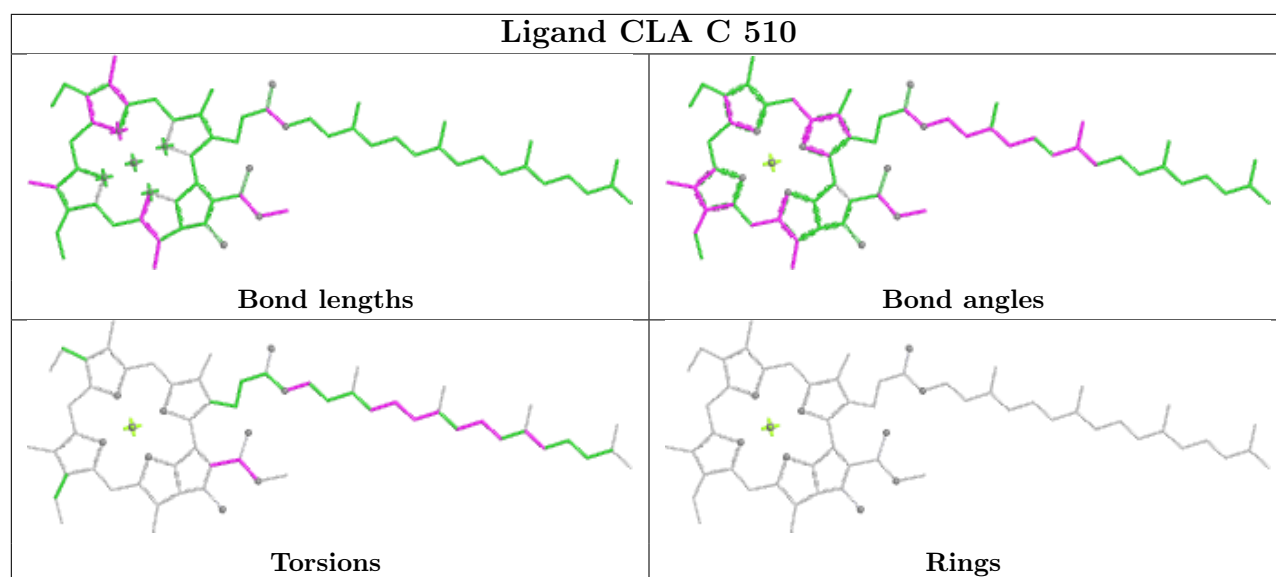
Ligand HEC f 101

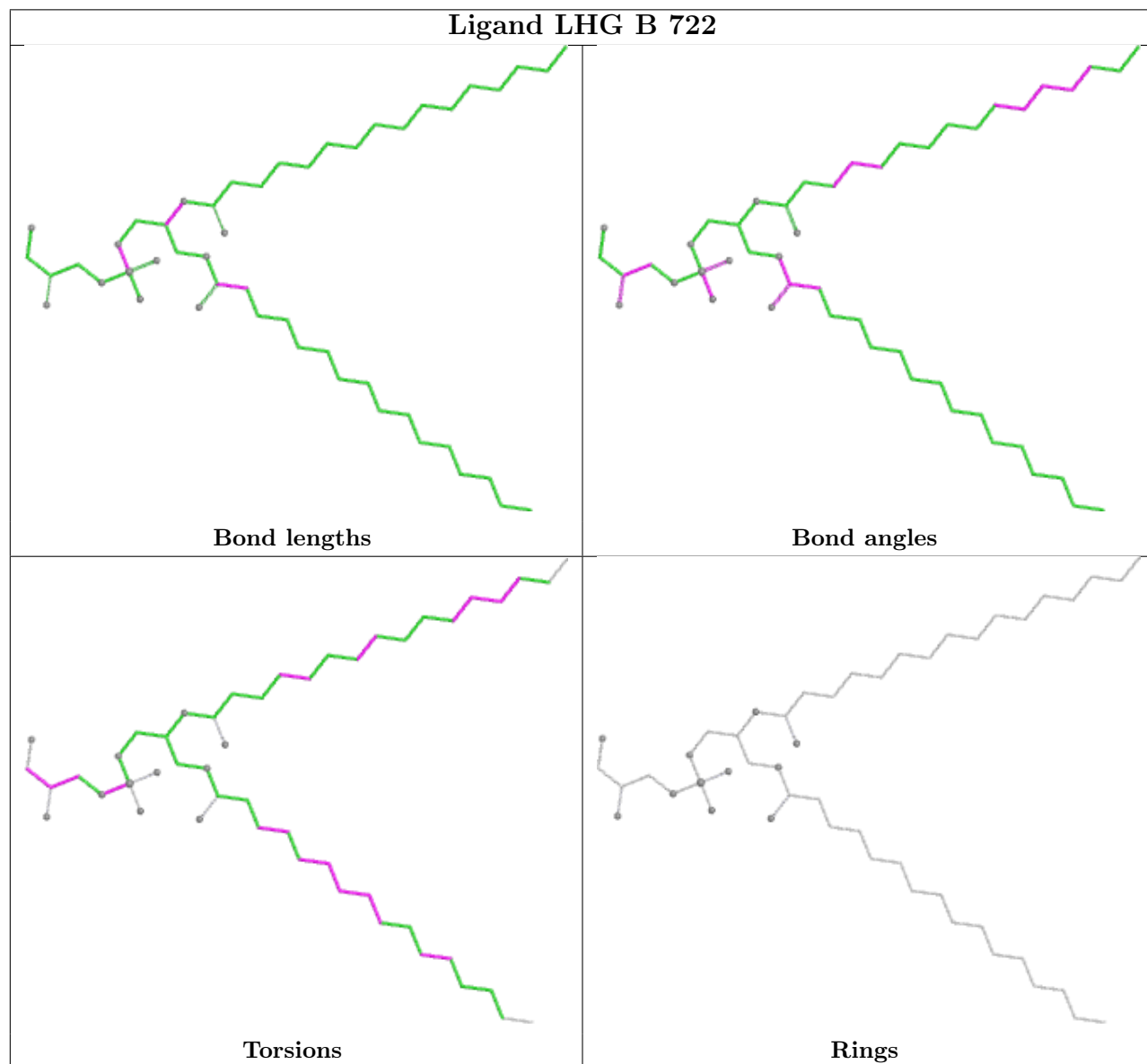
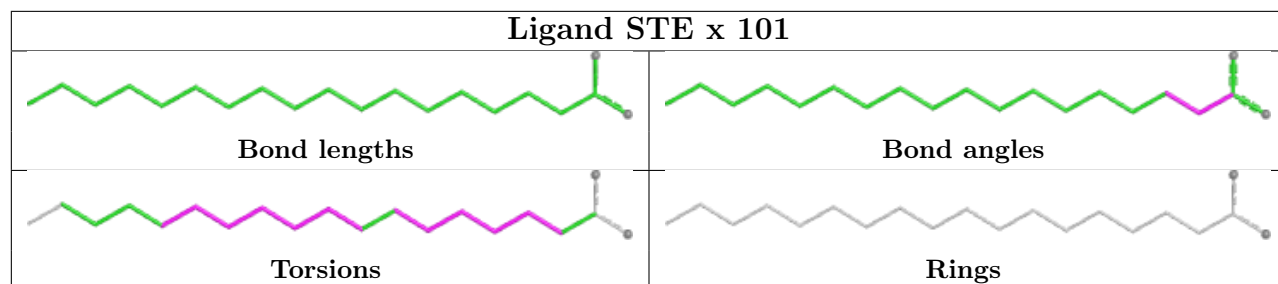


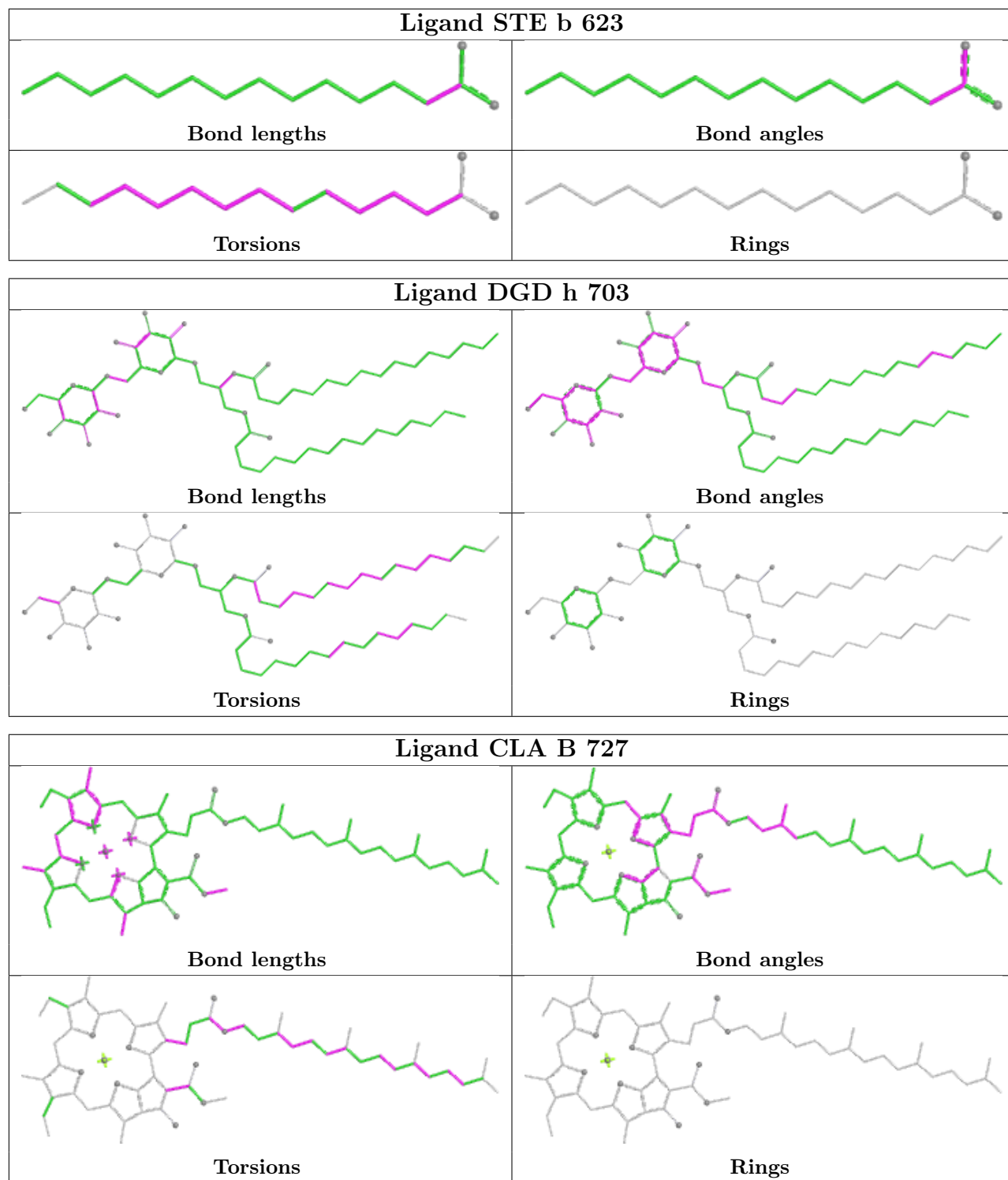
Ligand BCR B 717

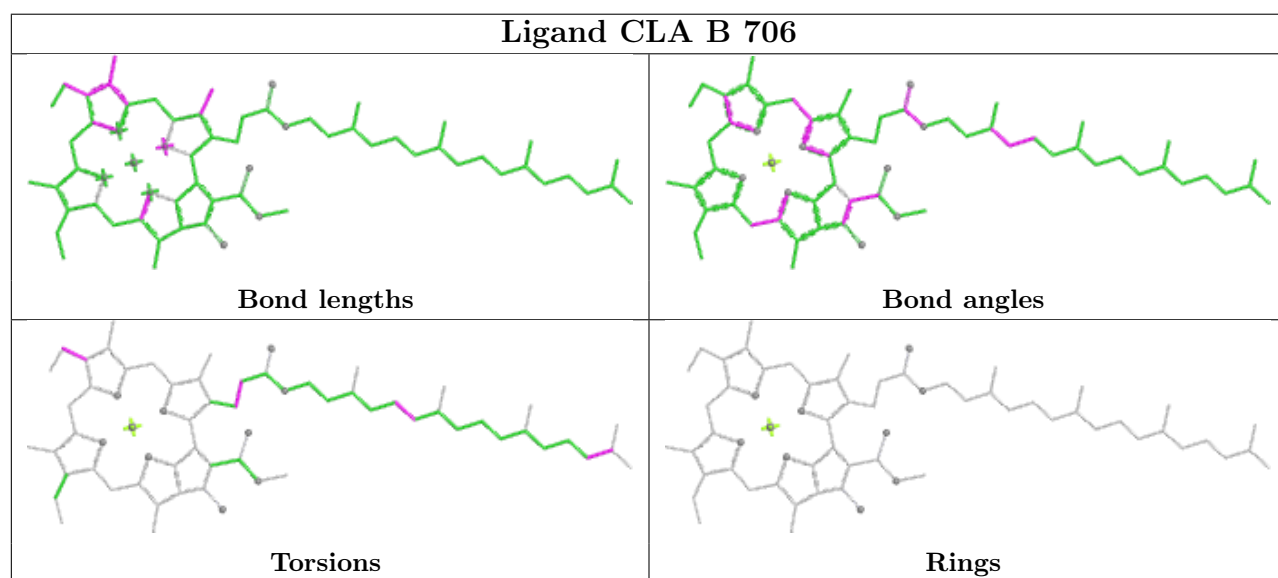
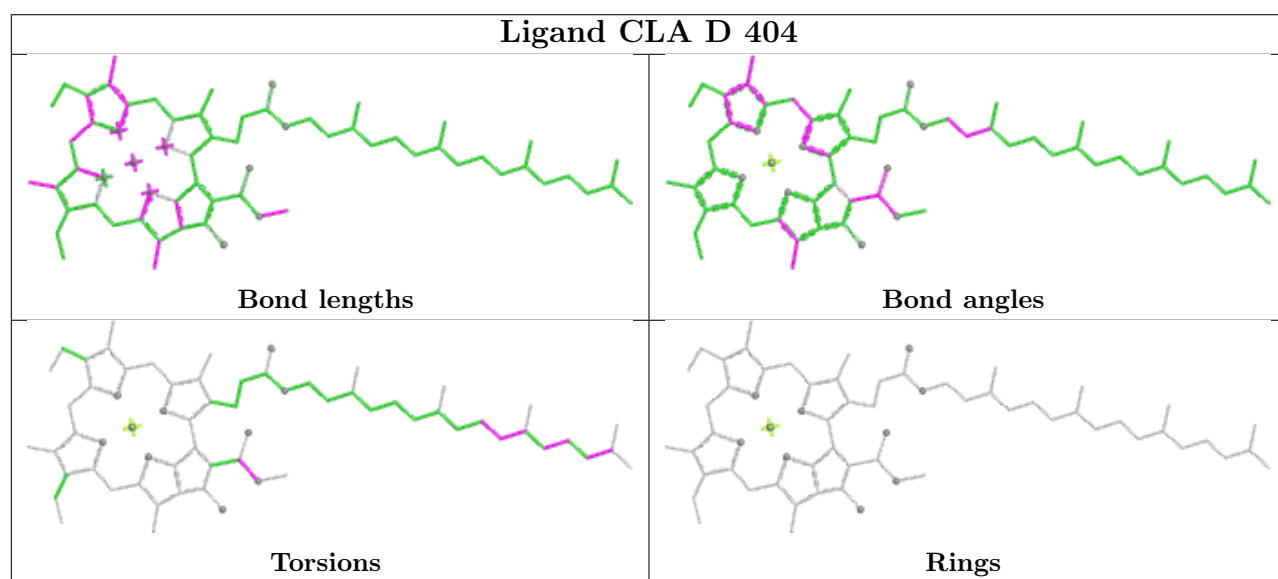
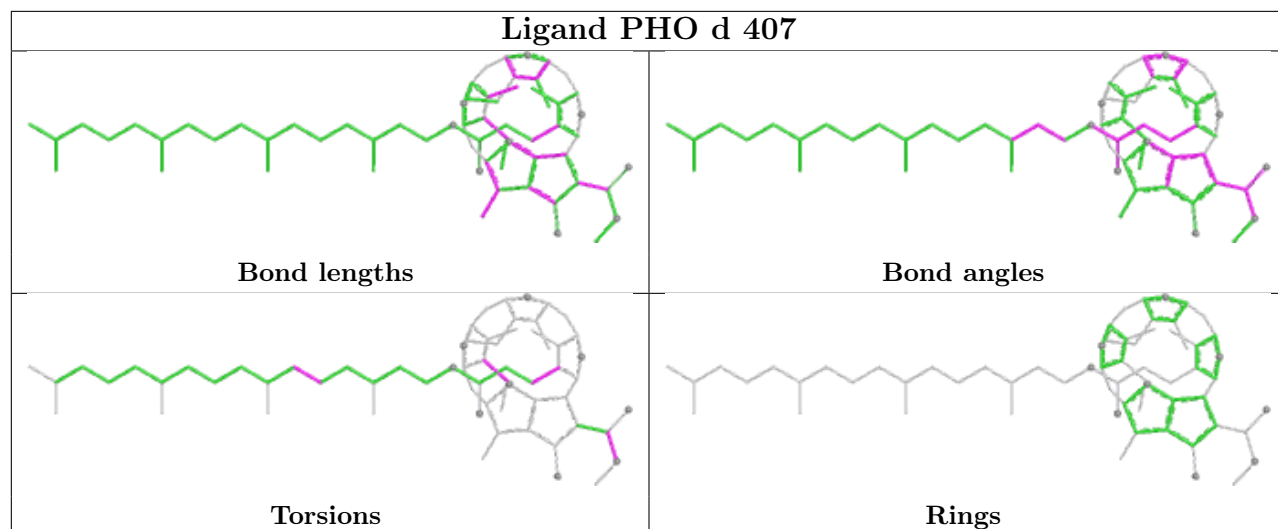


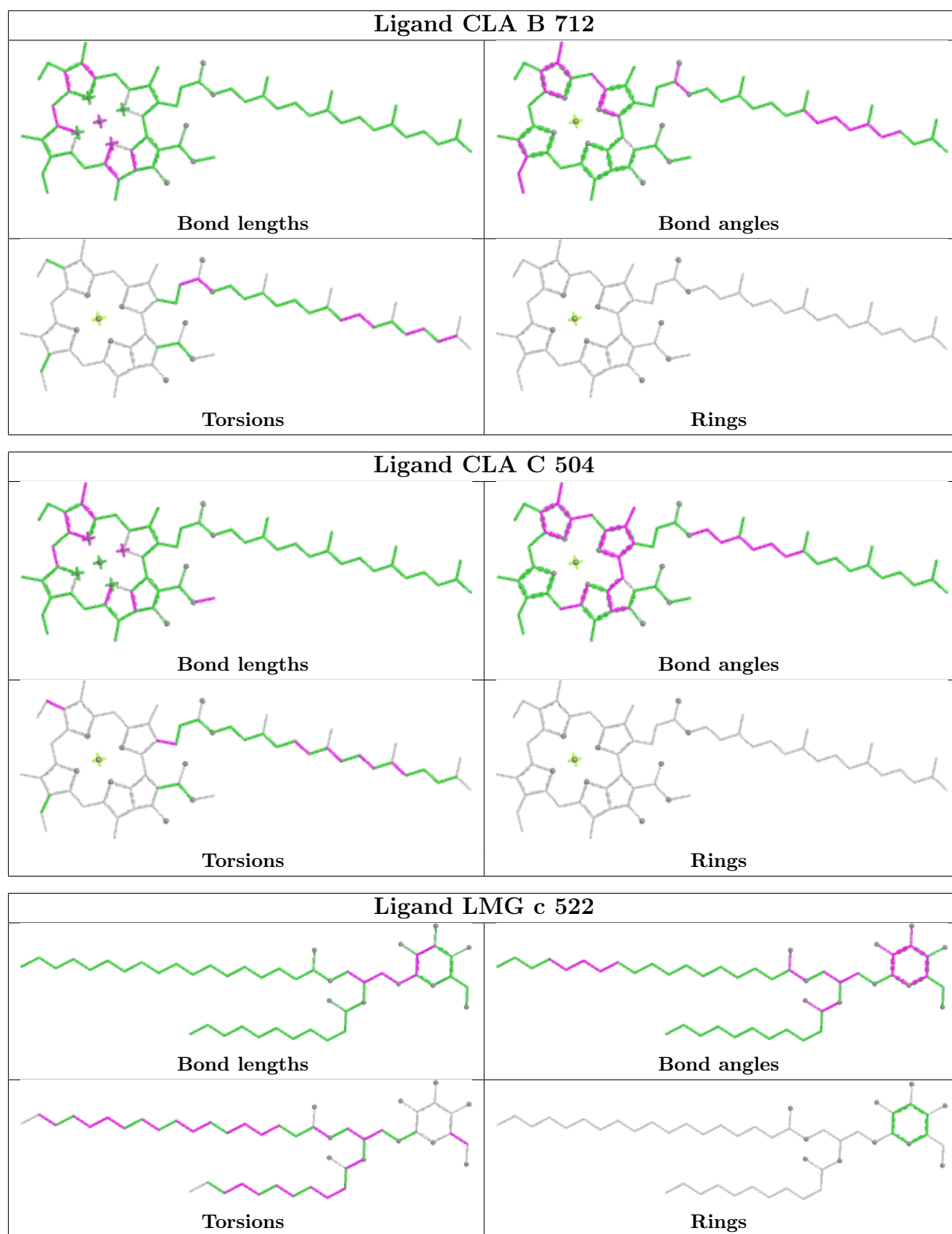


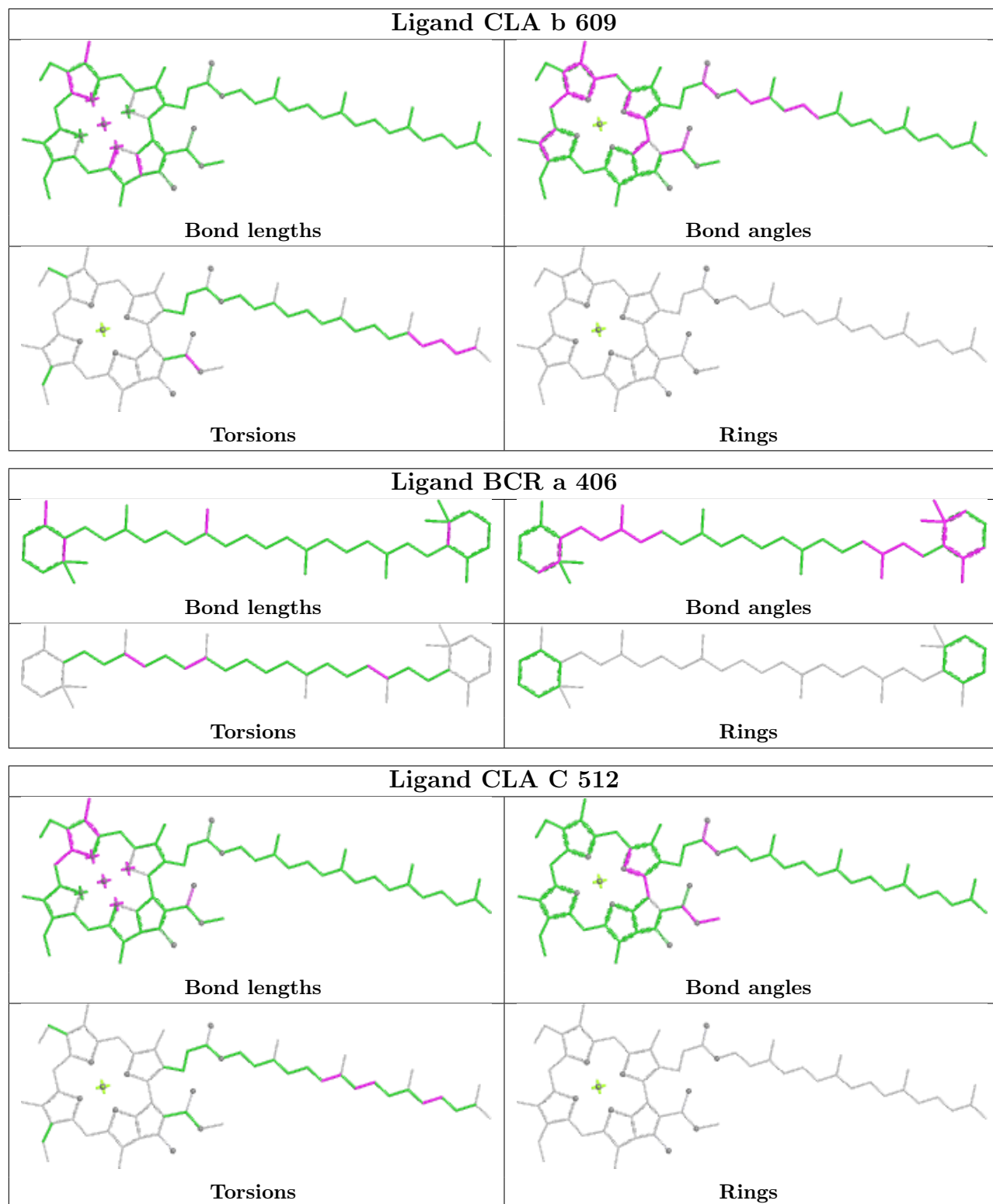


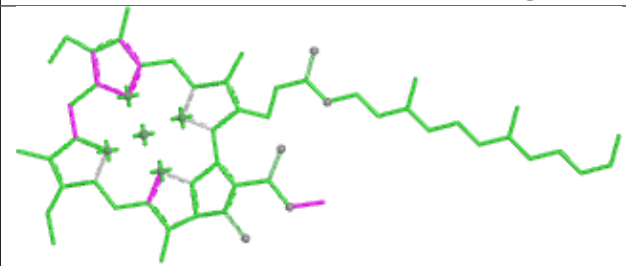
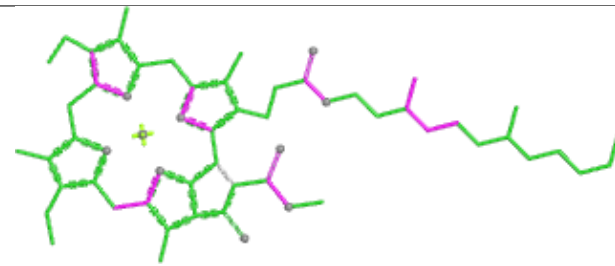
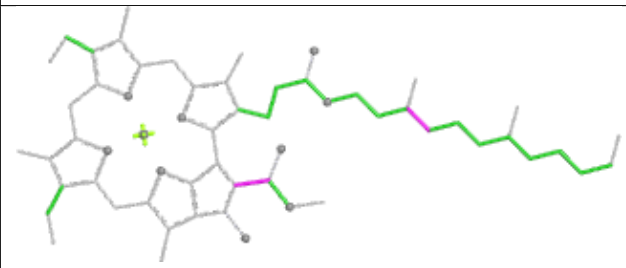
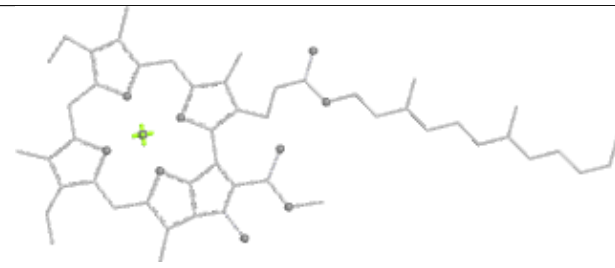


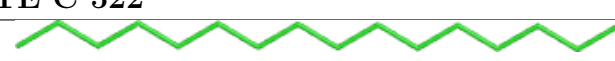
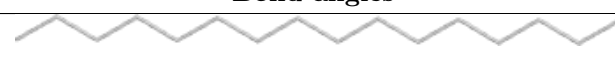


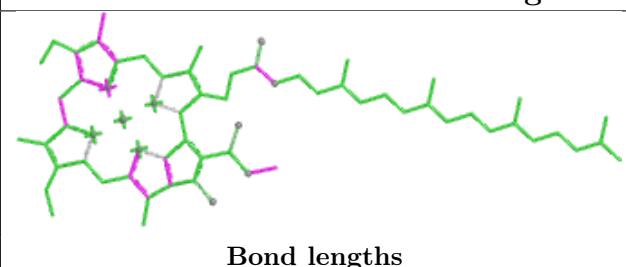
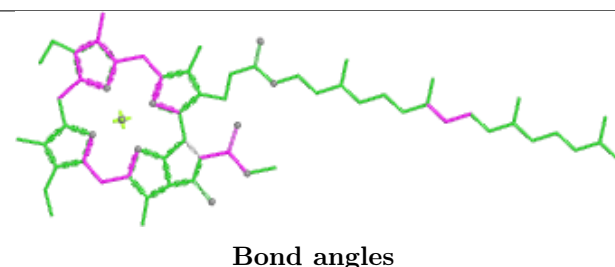
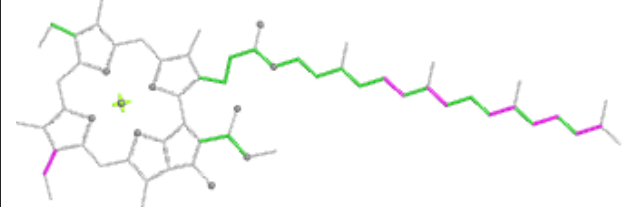
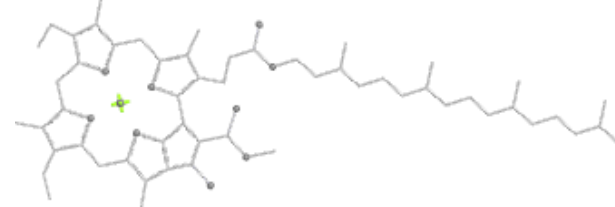


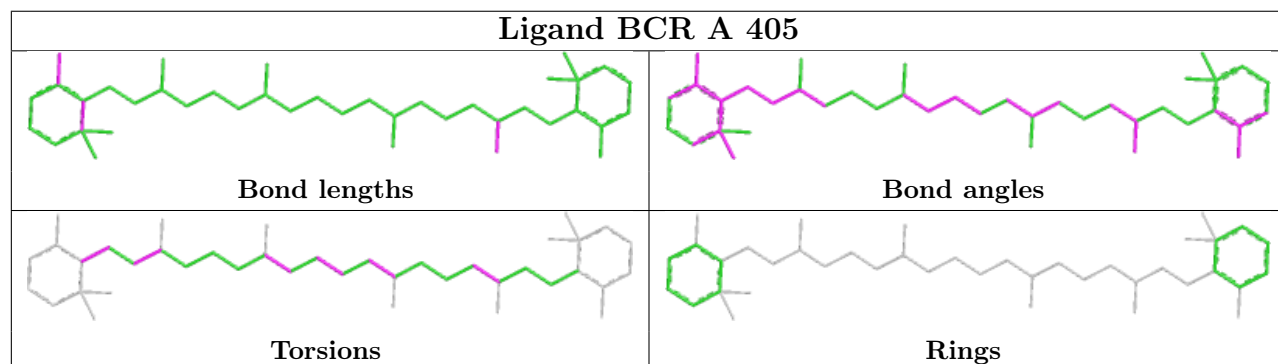
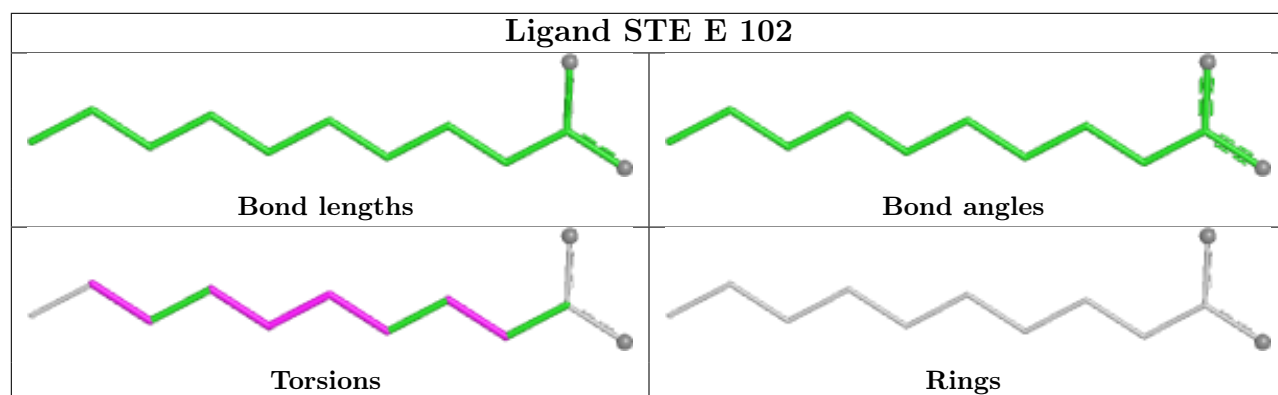
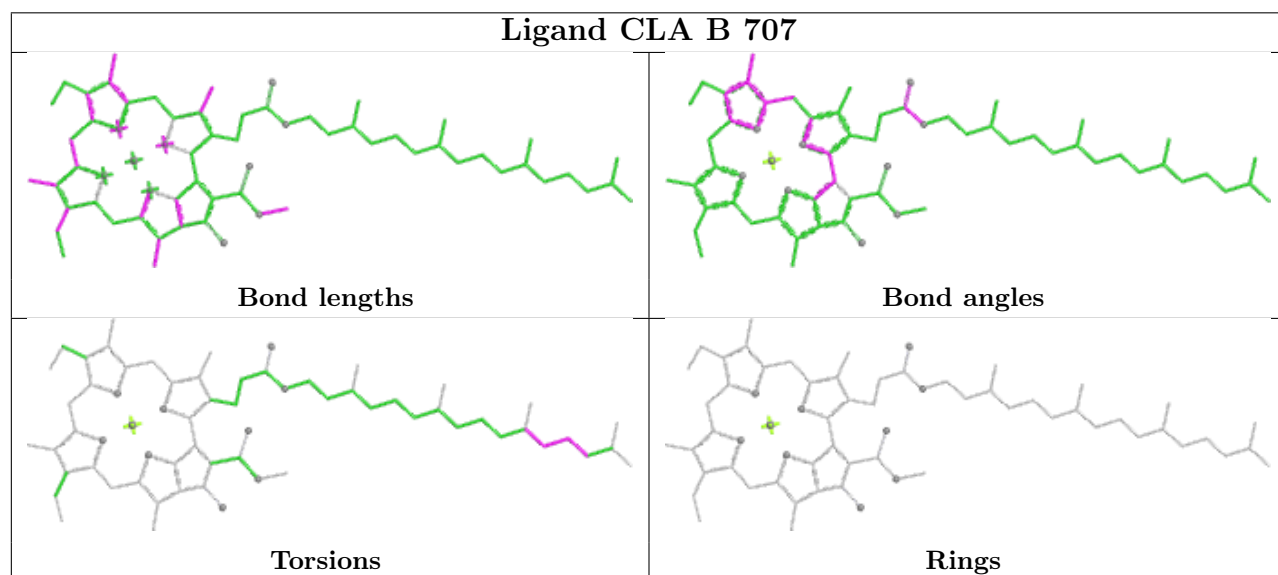
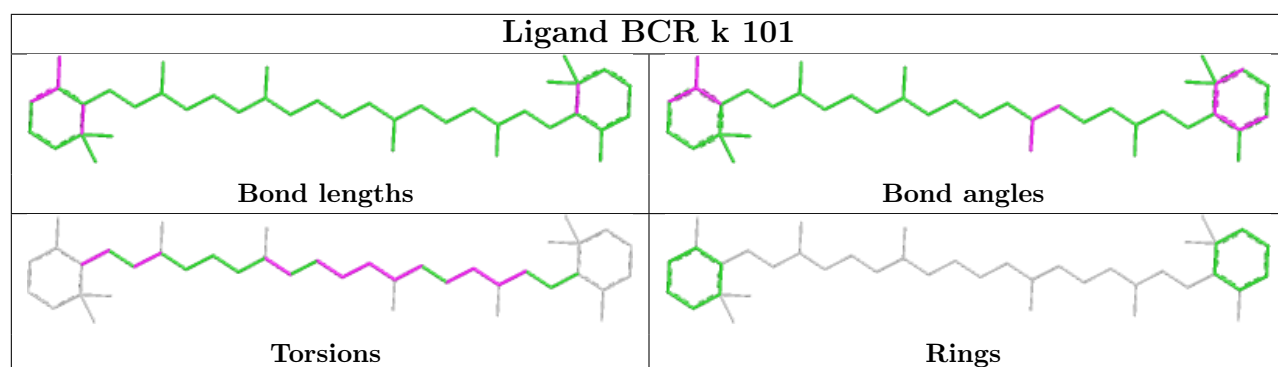


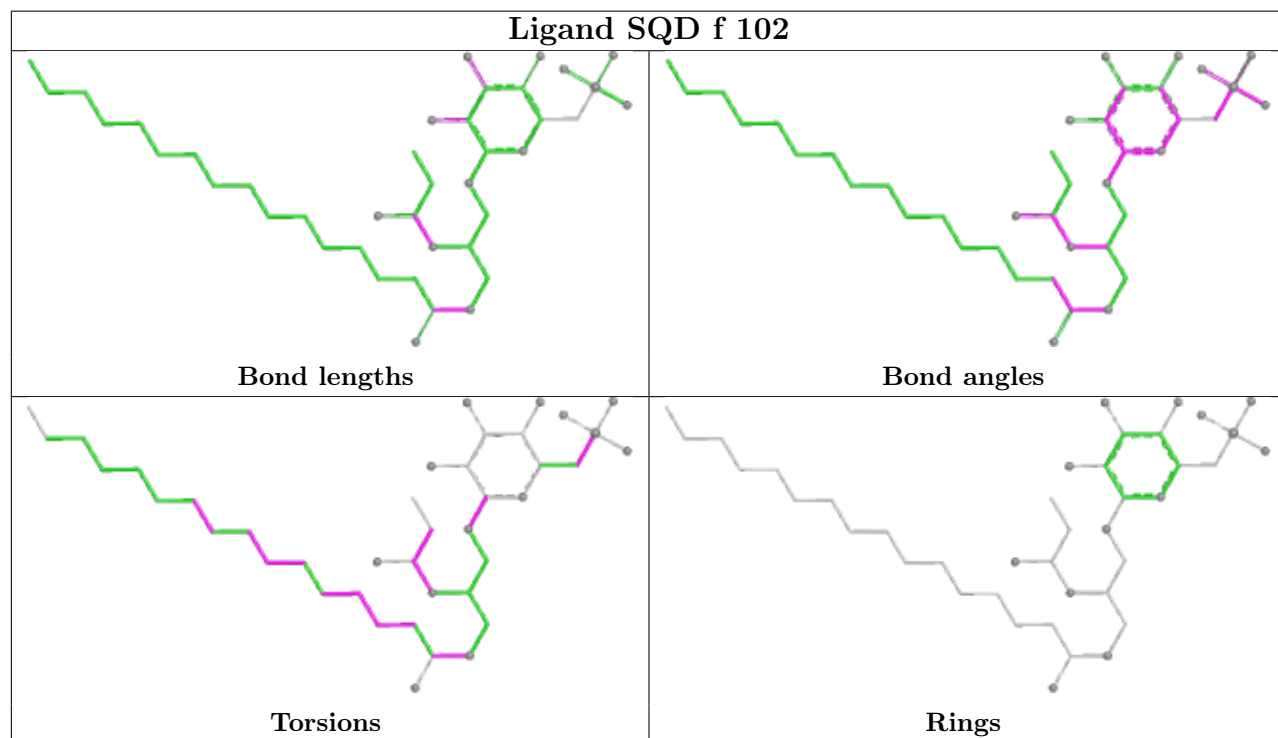
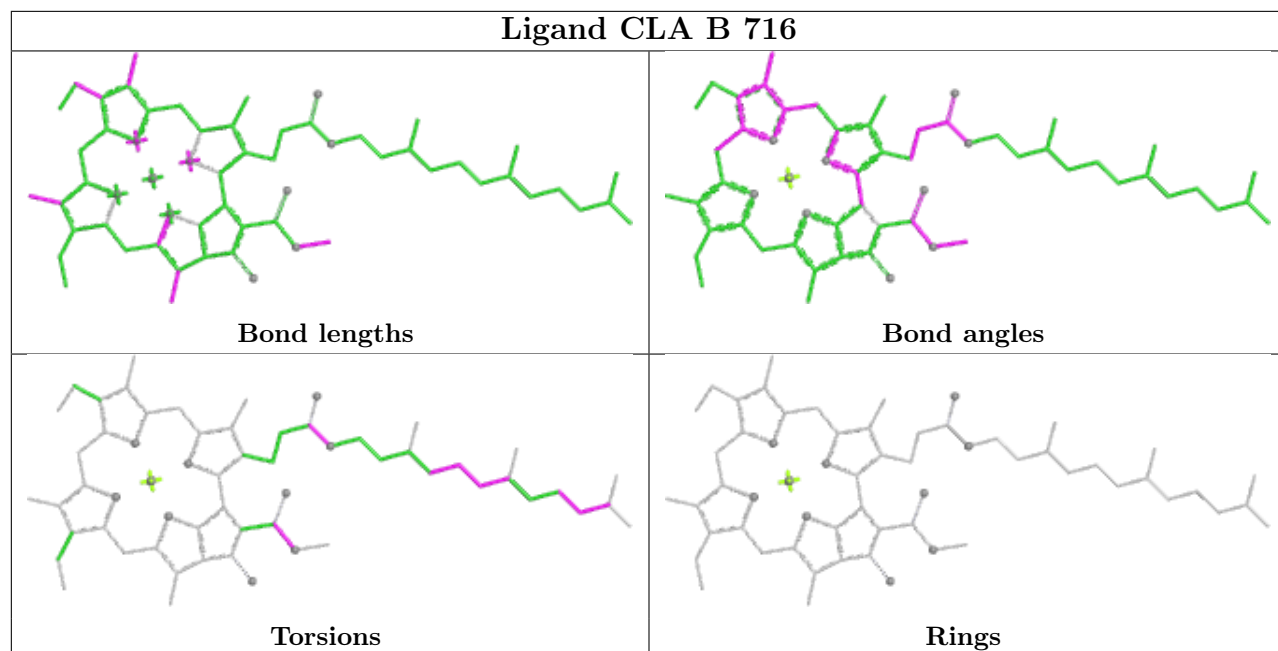


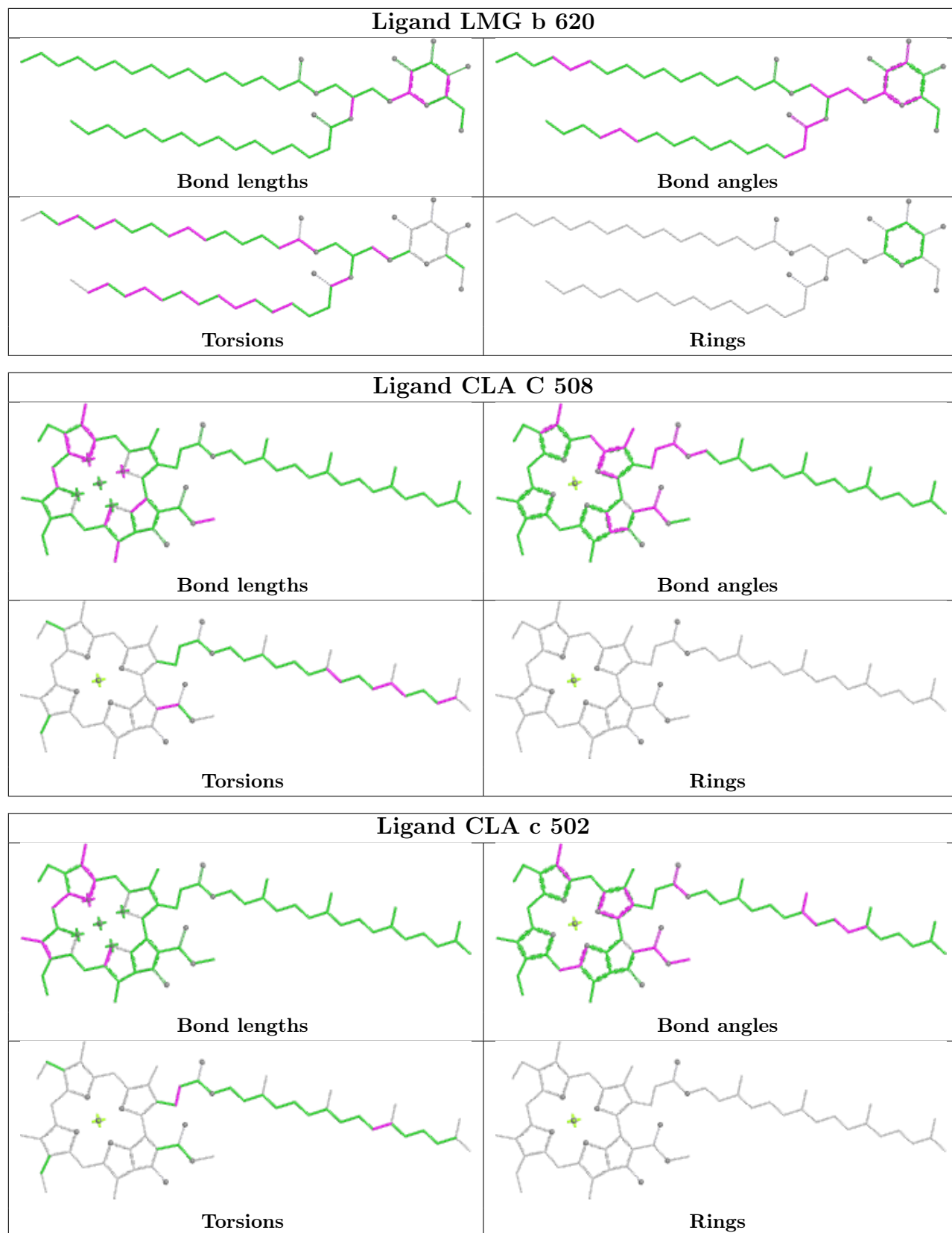
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

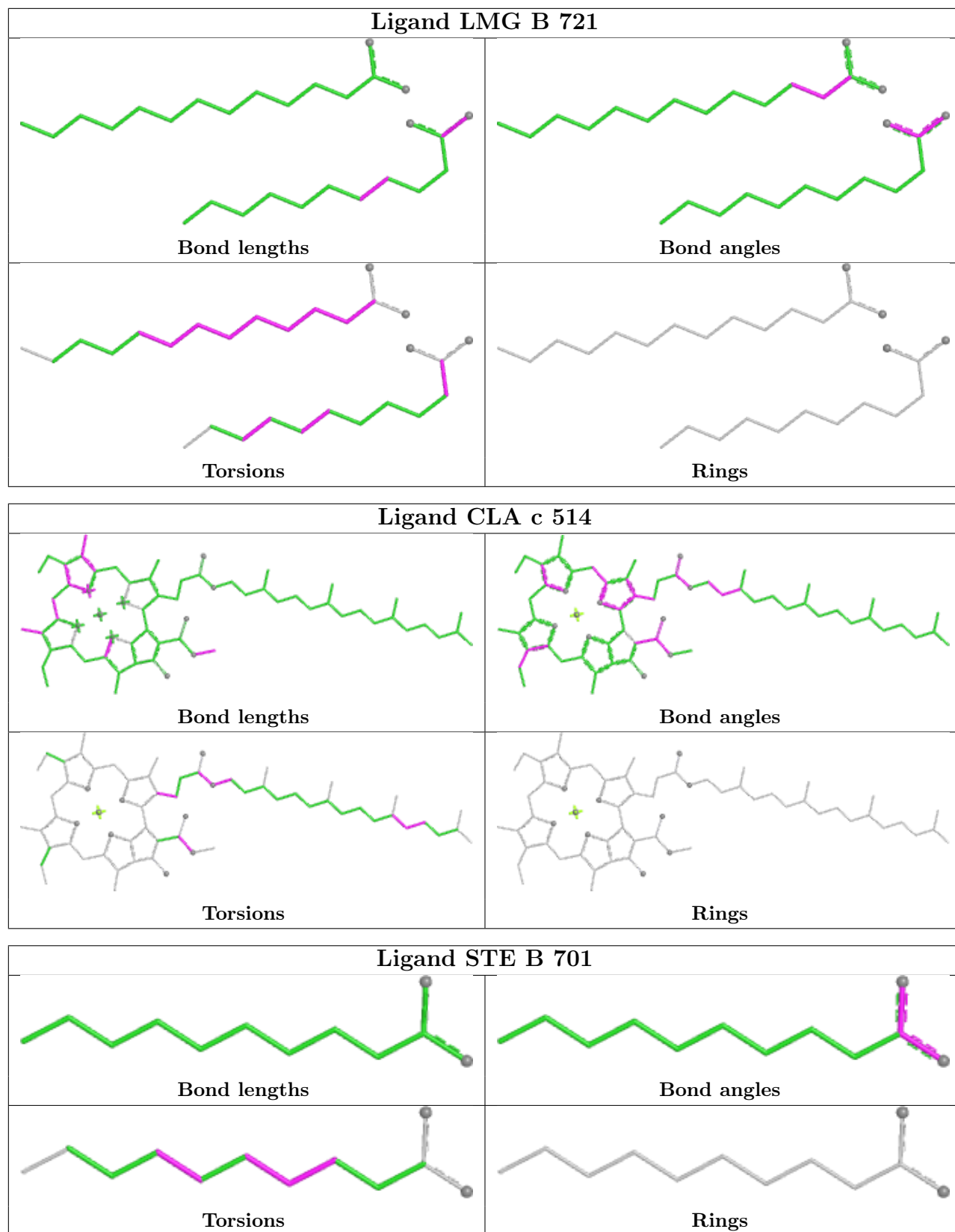
Ligand STE C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

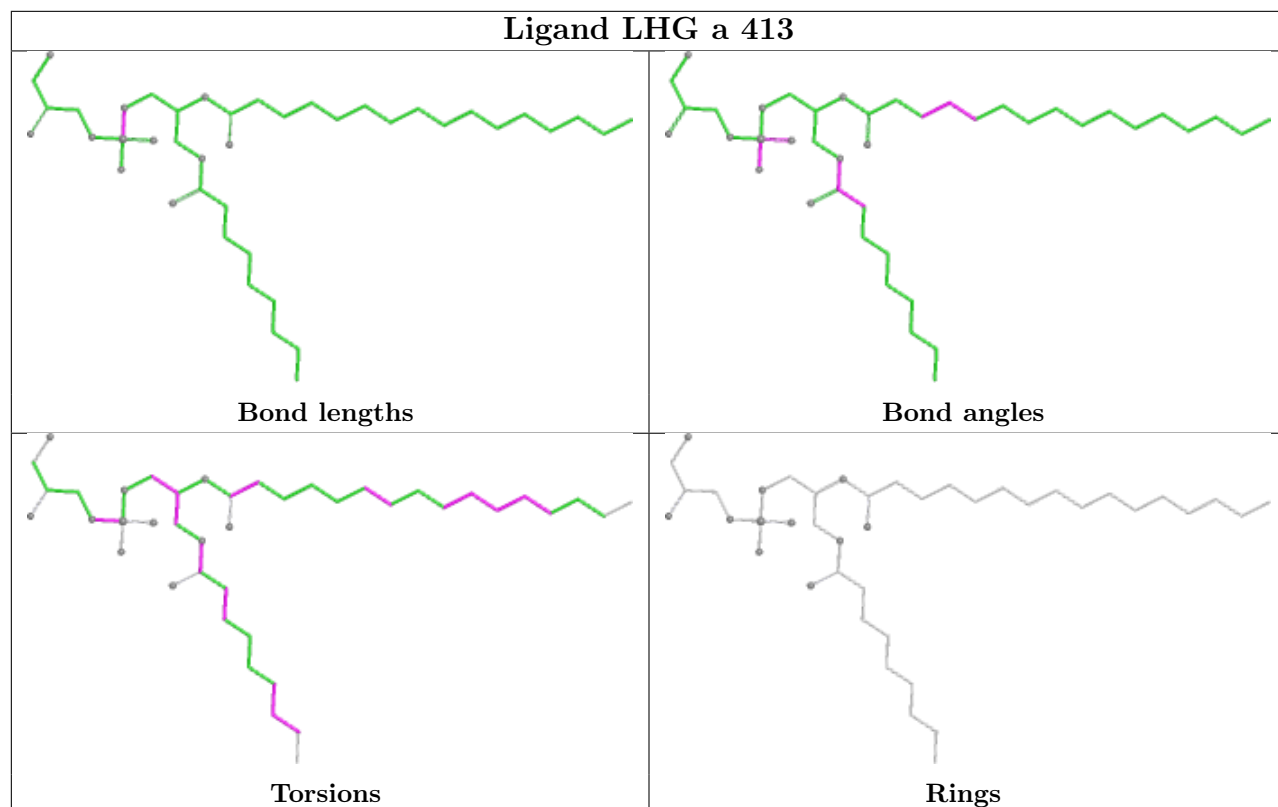
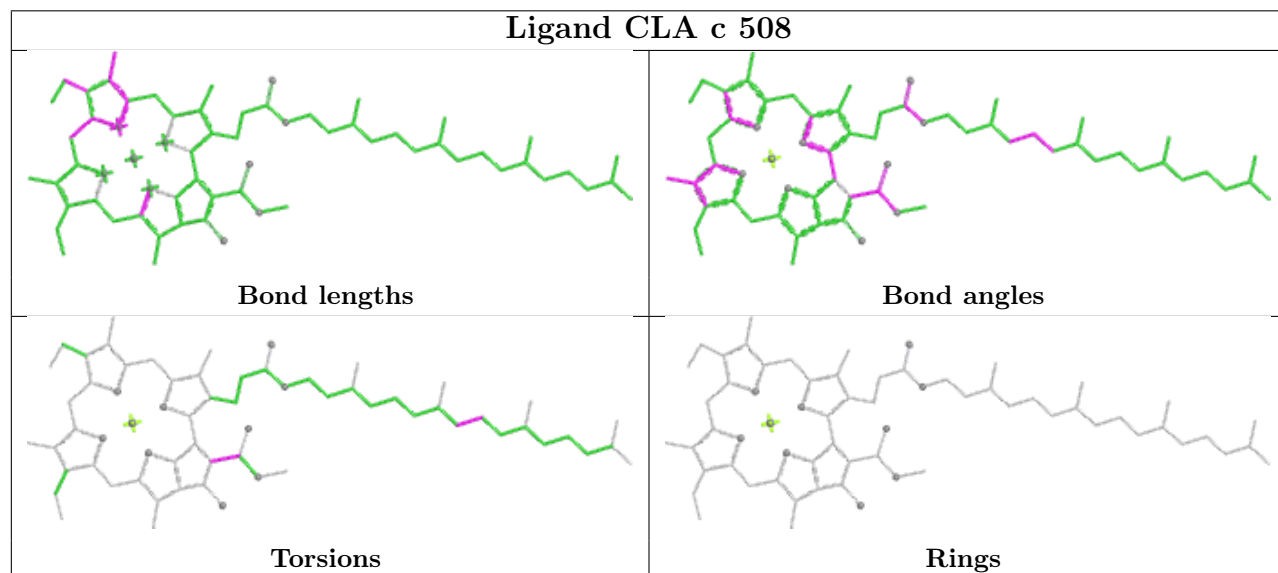
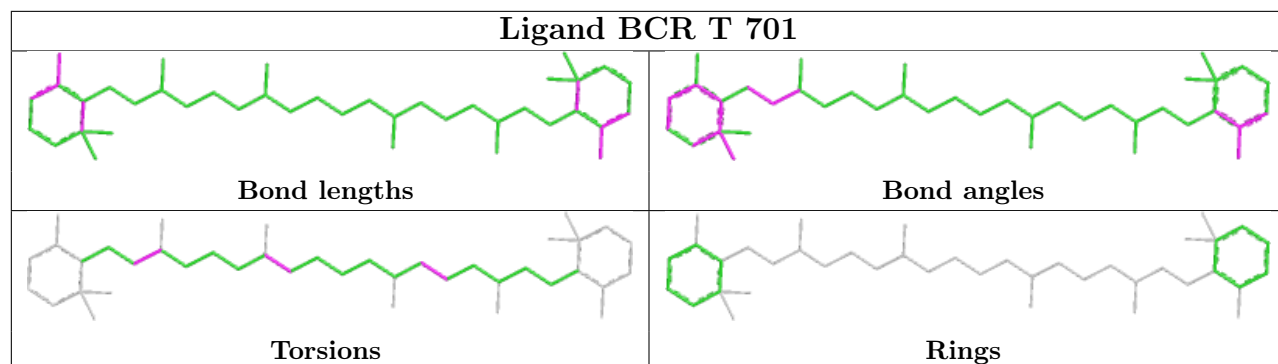
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

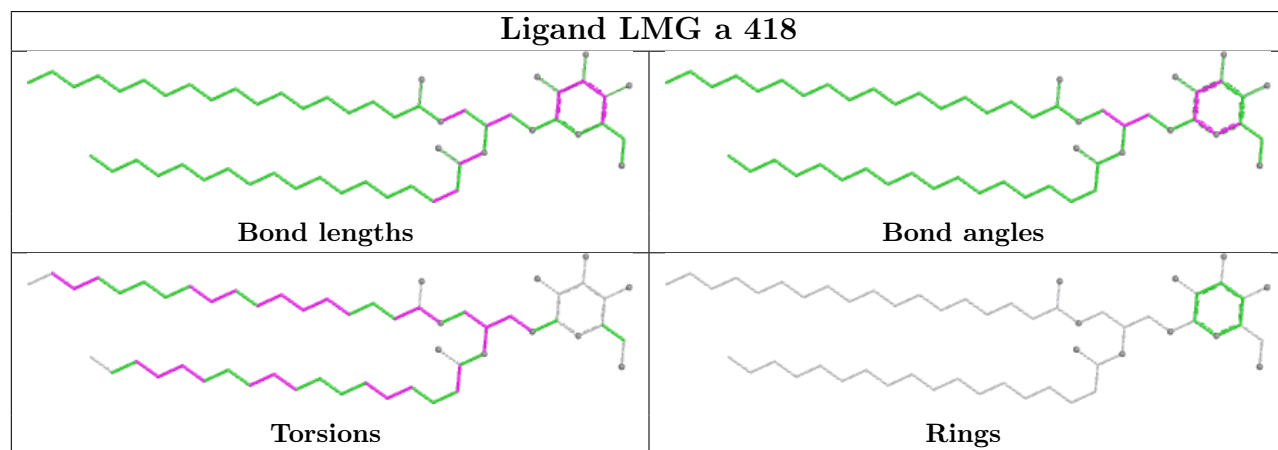
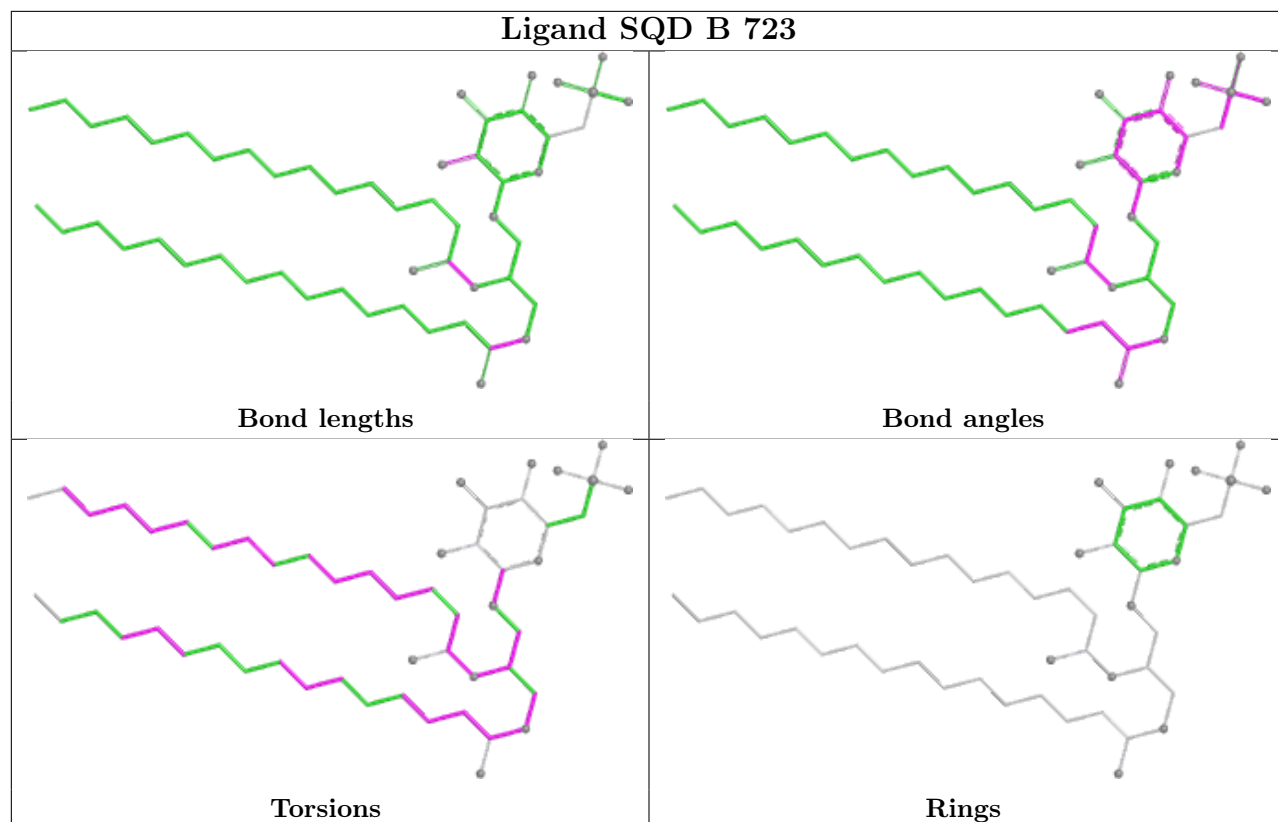


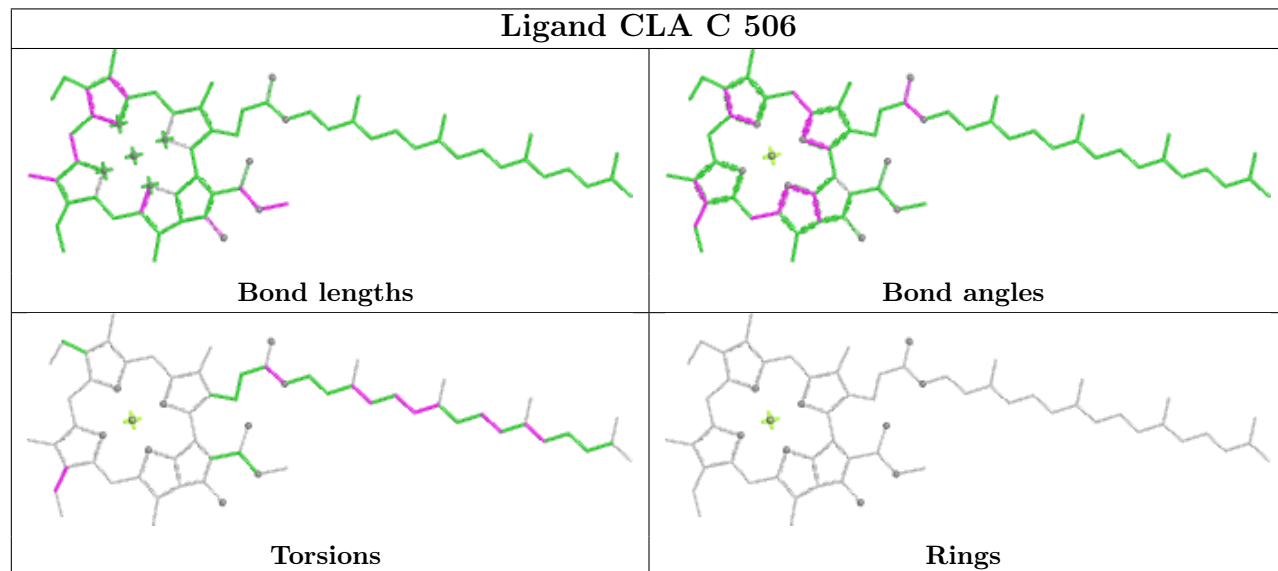
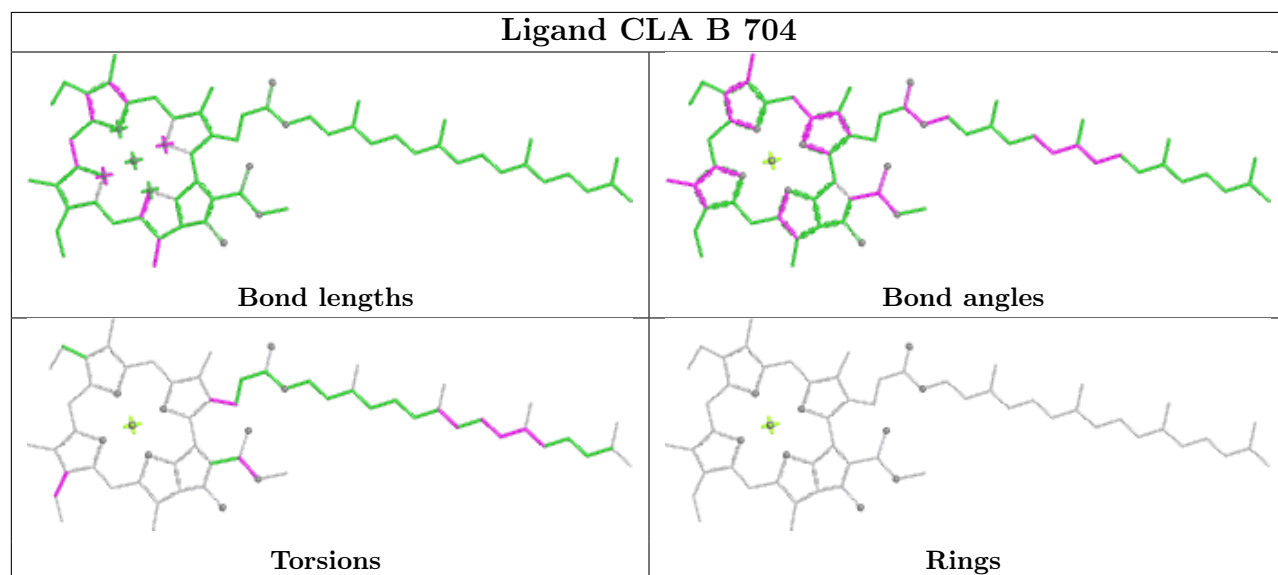
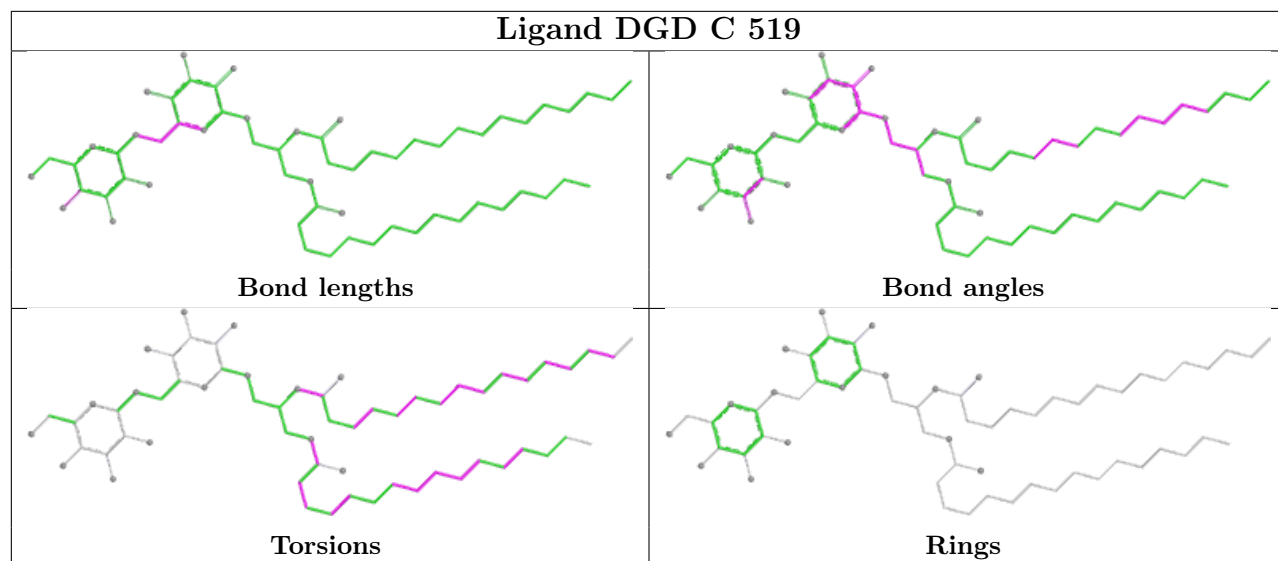


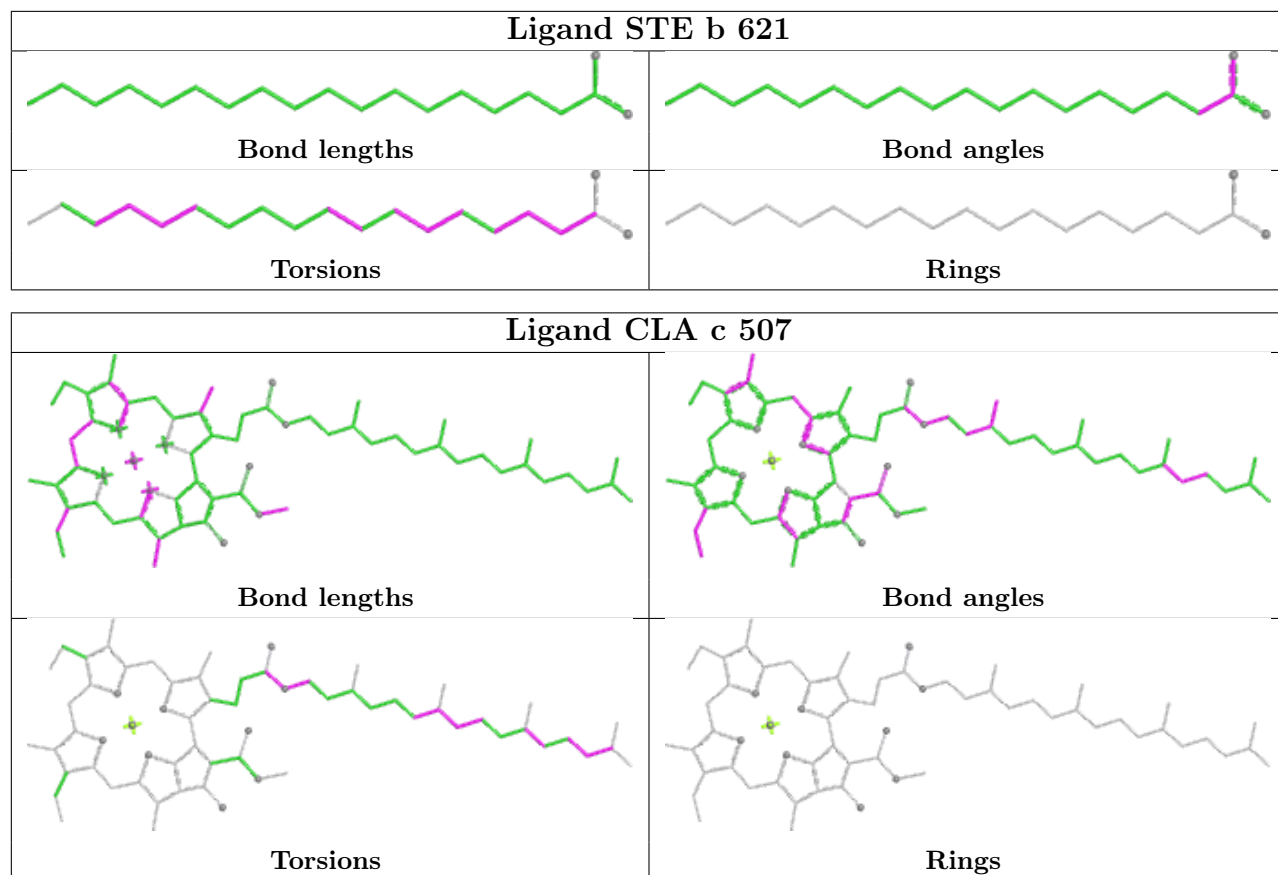


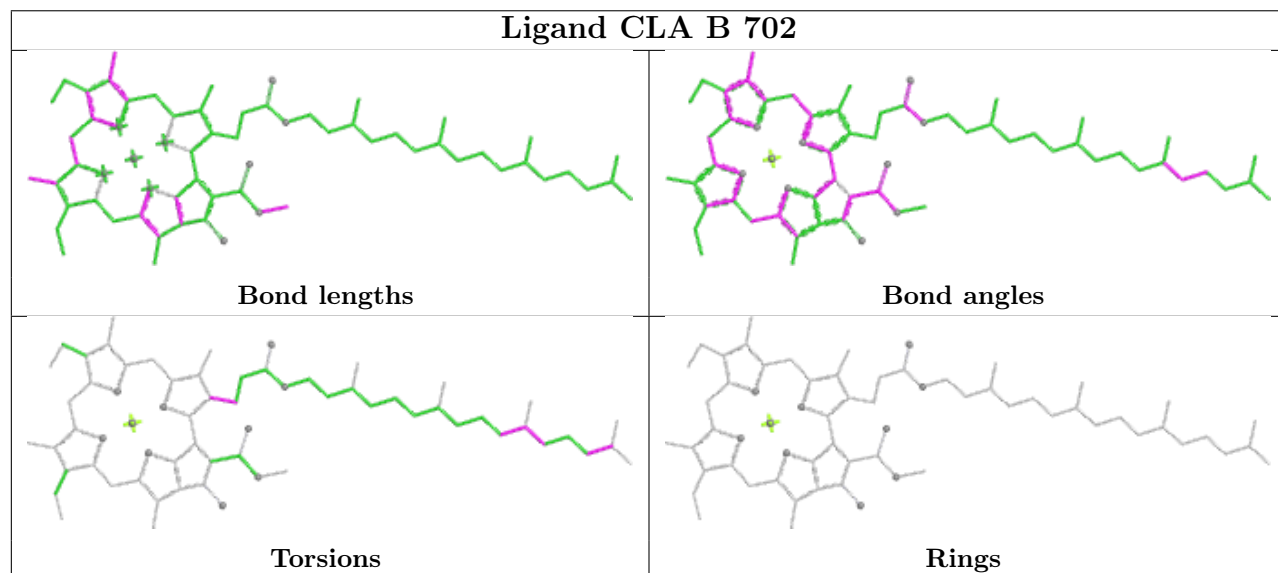
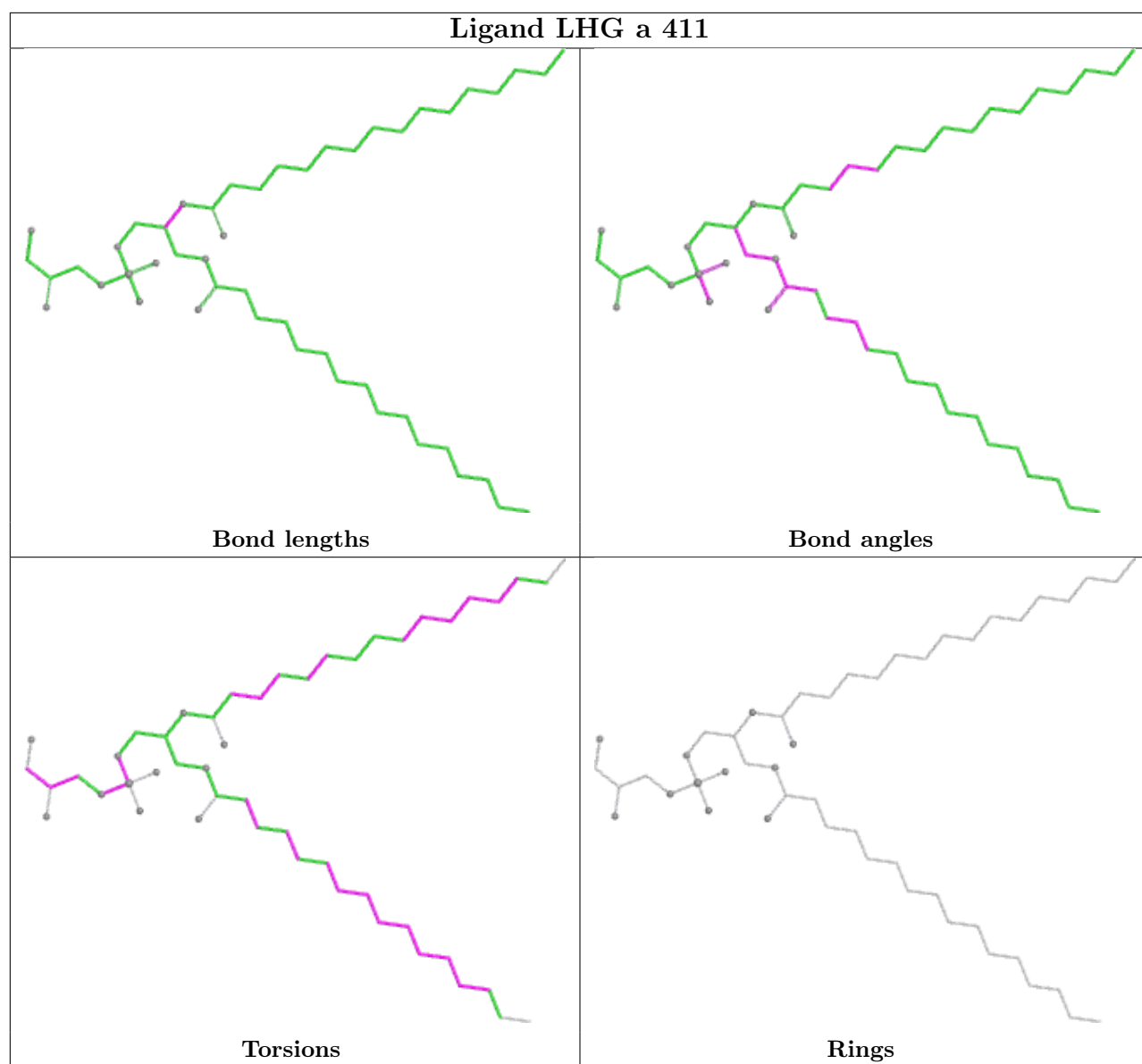


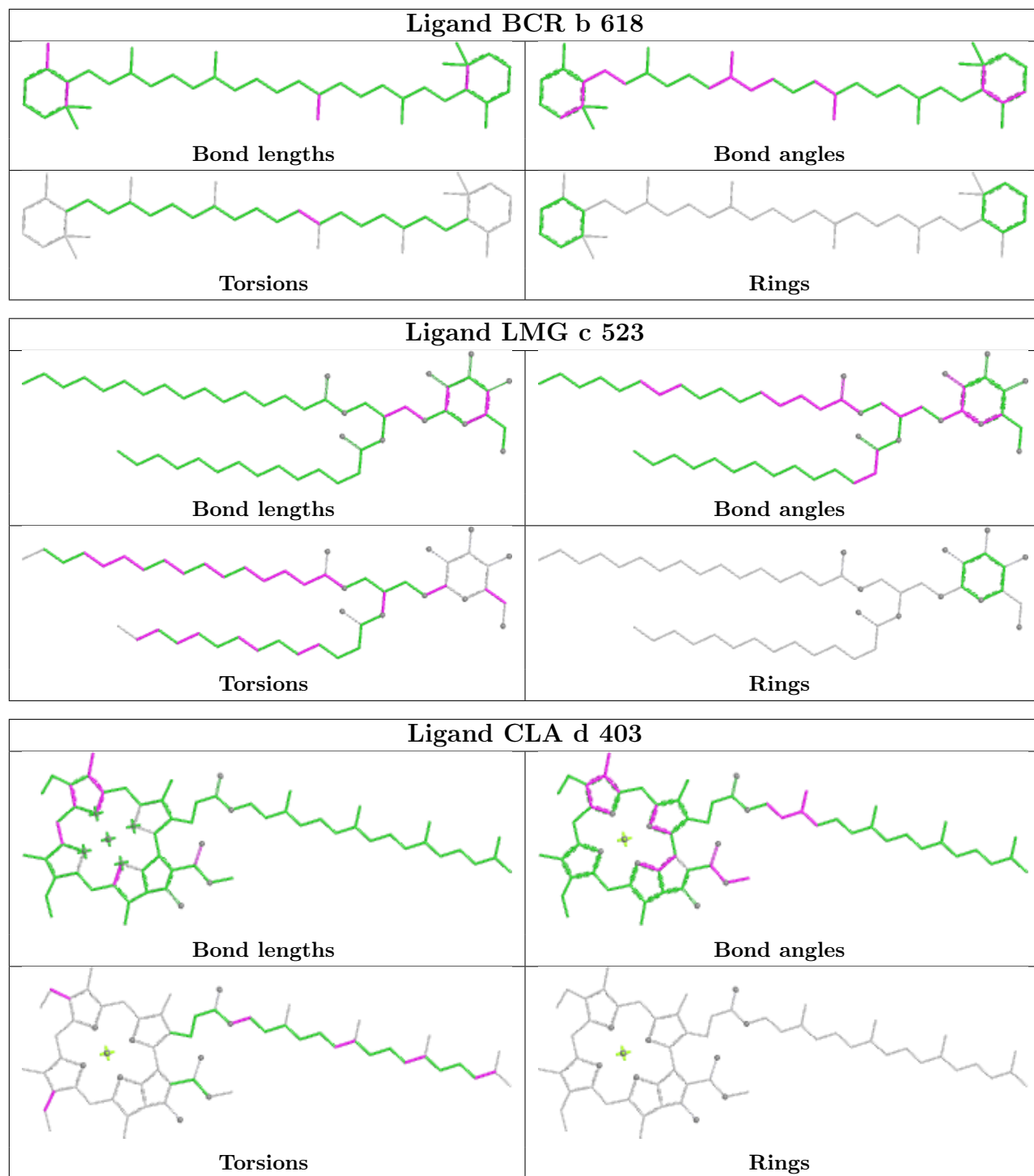


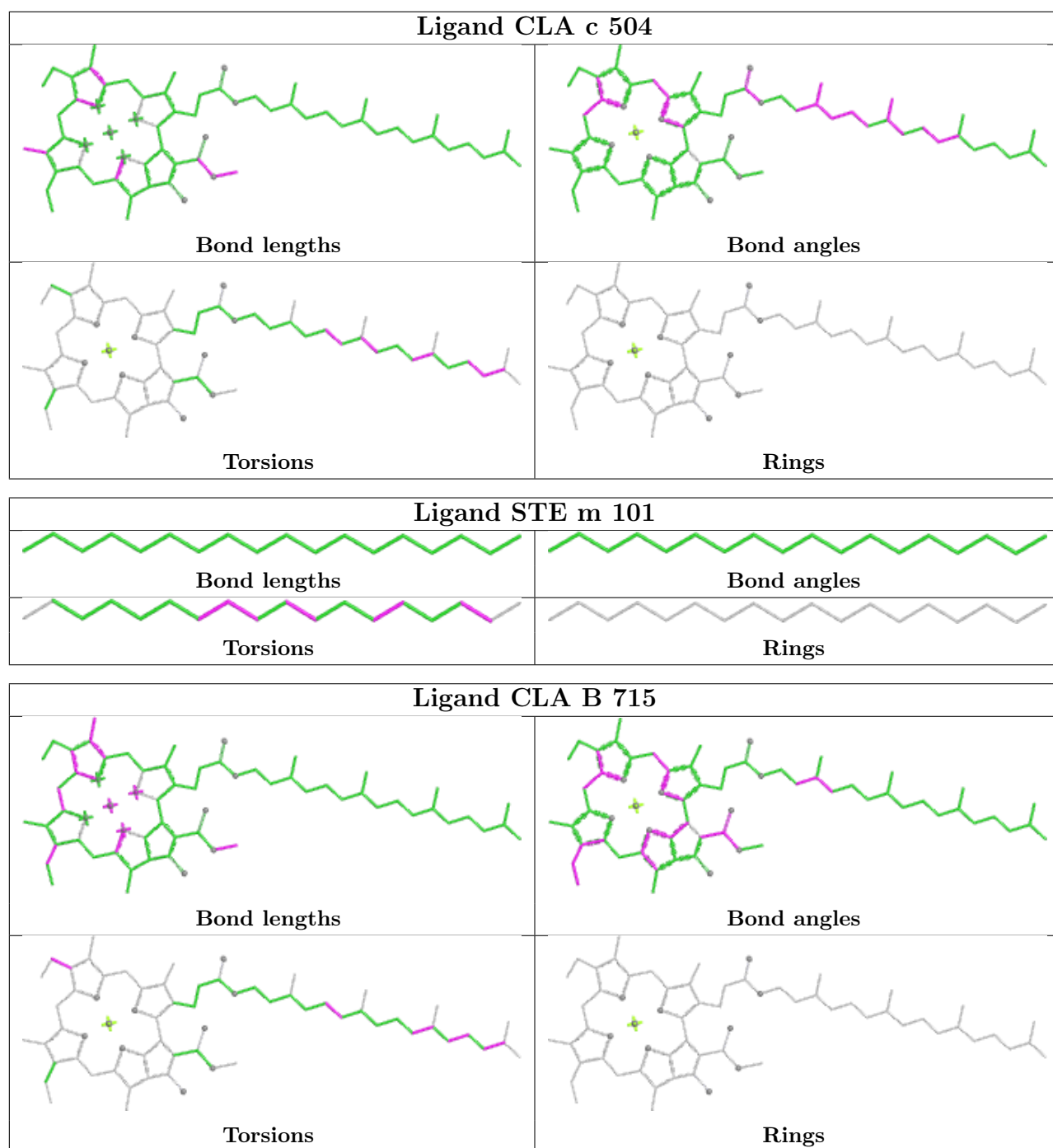


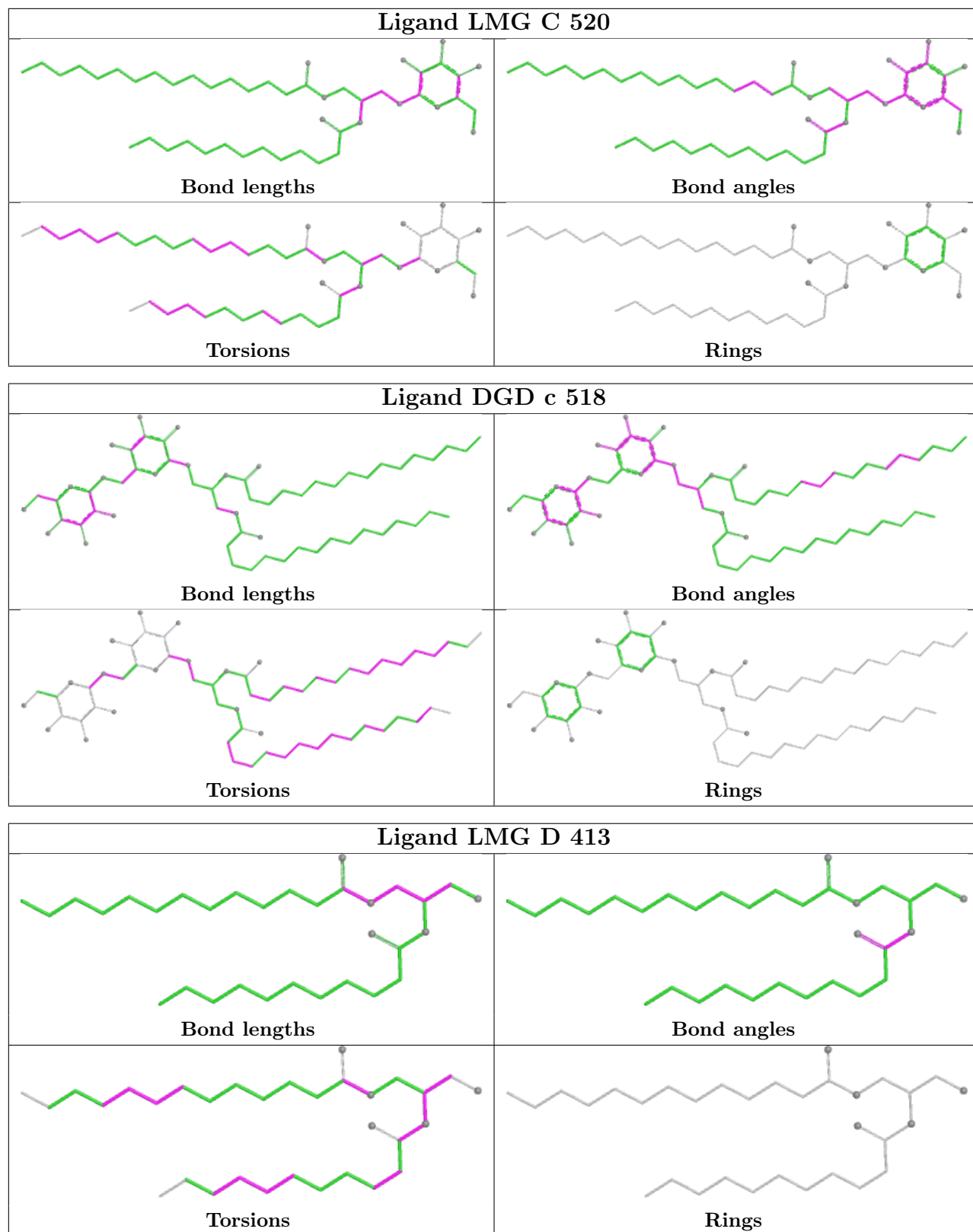


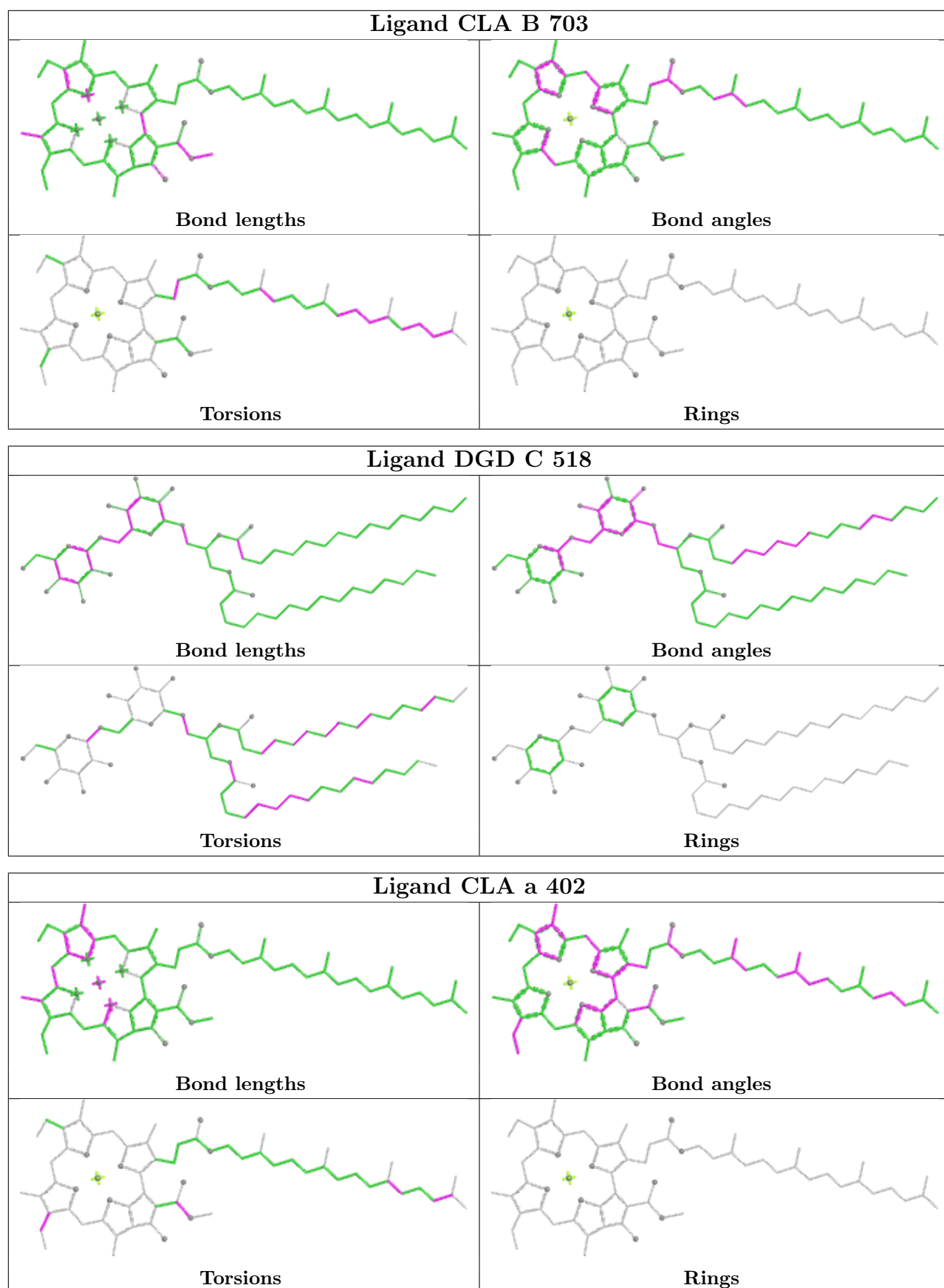




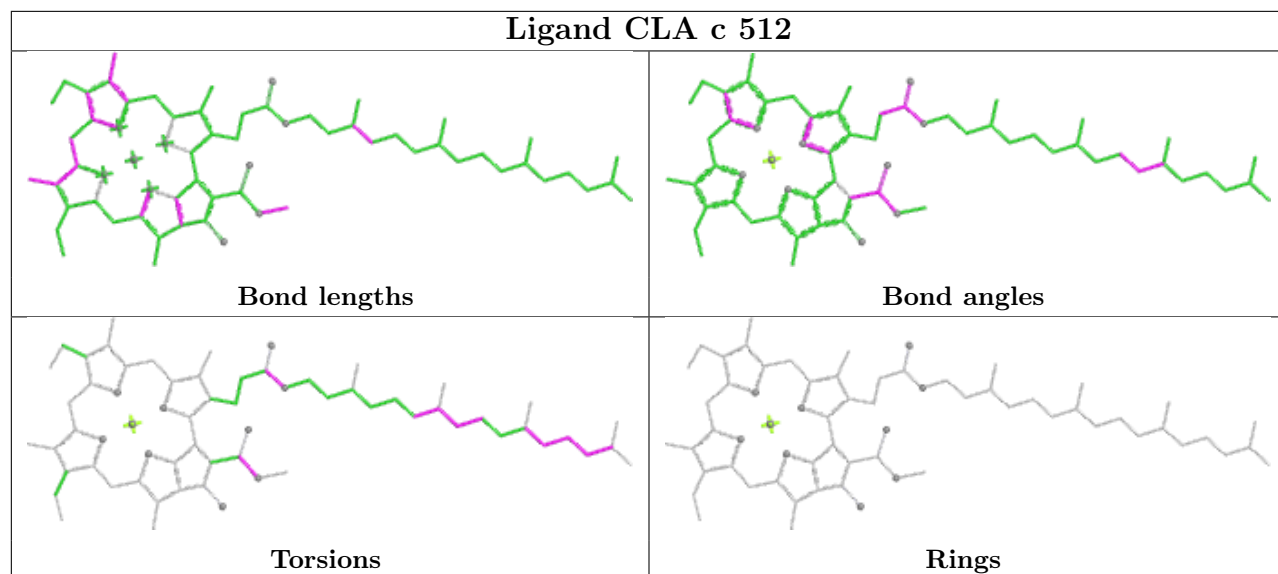




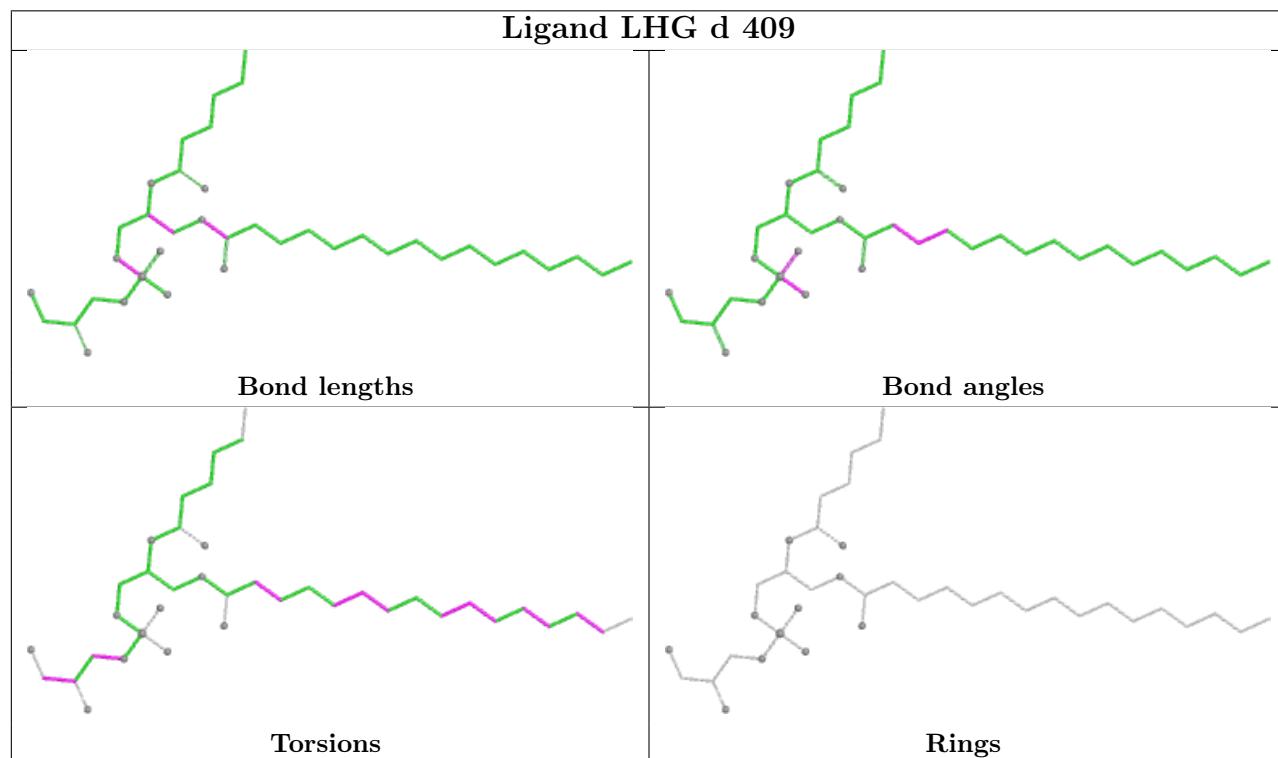




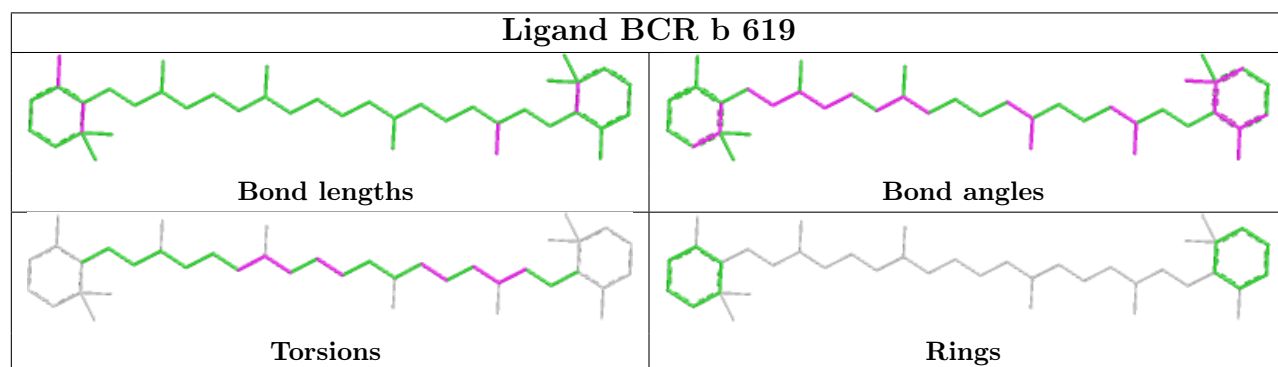
Ligand CLA c 512



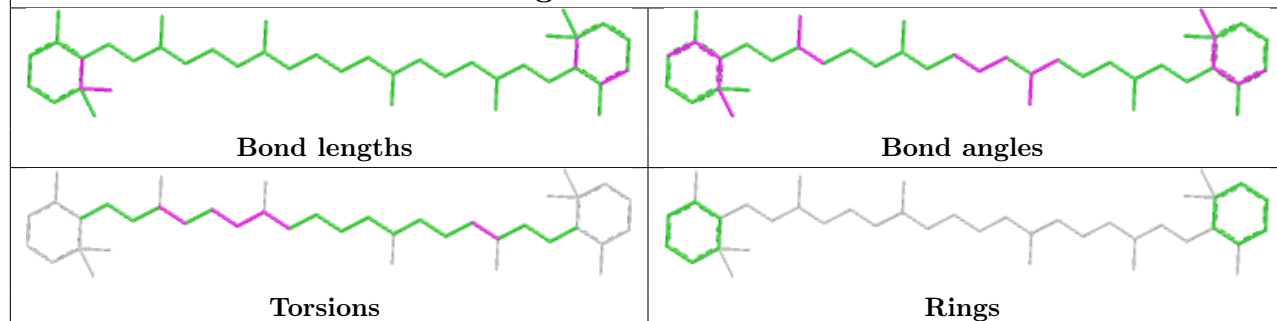
Ligand LHG d 409



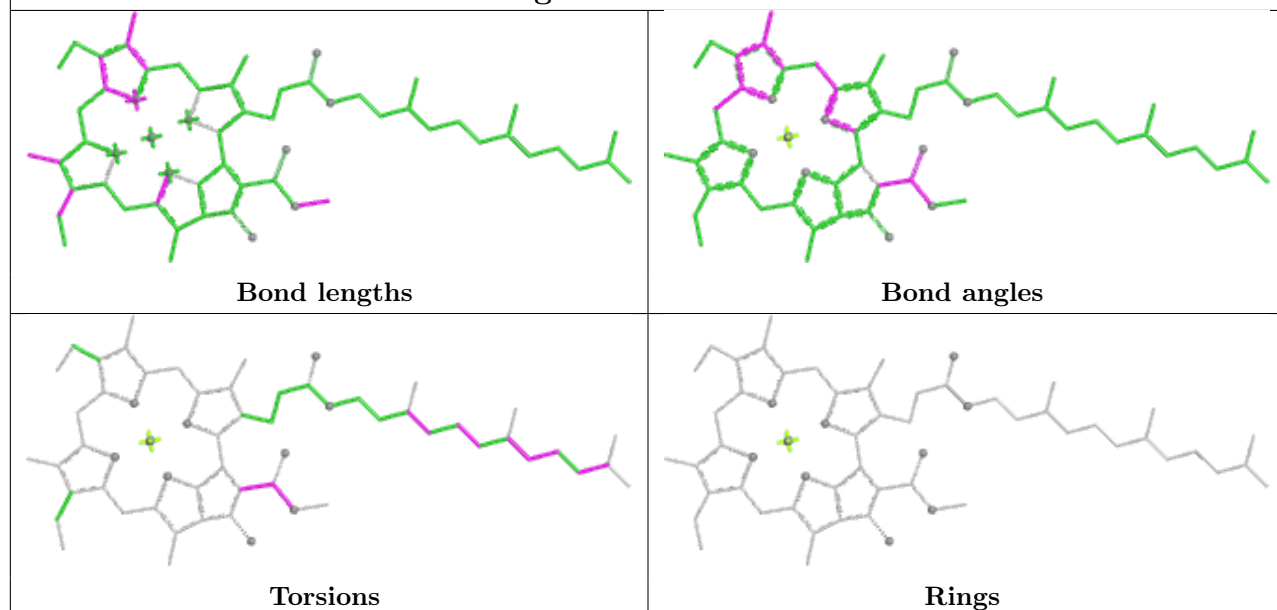
Ligand BCR b 619



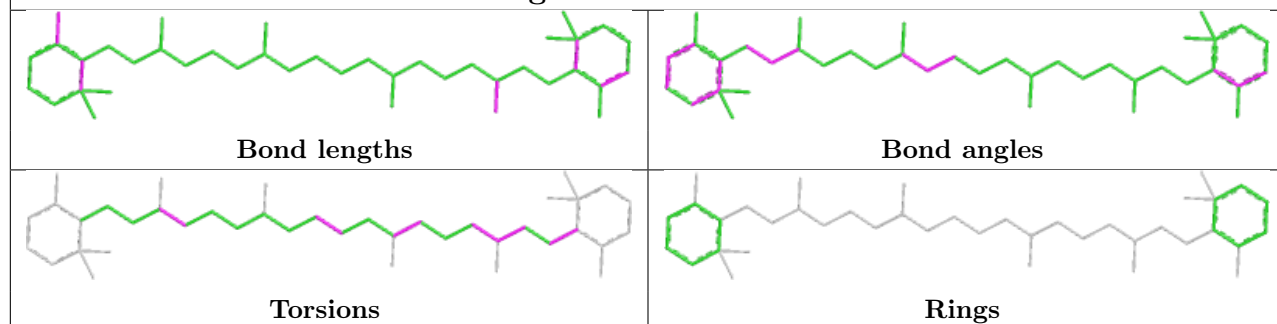
Ligand BCR t 701



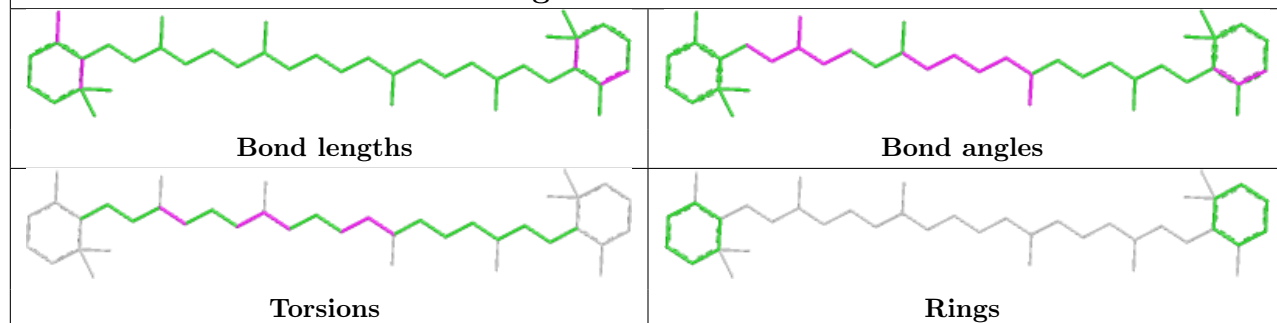
Ligand CLA b 616

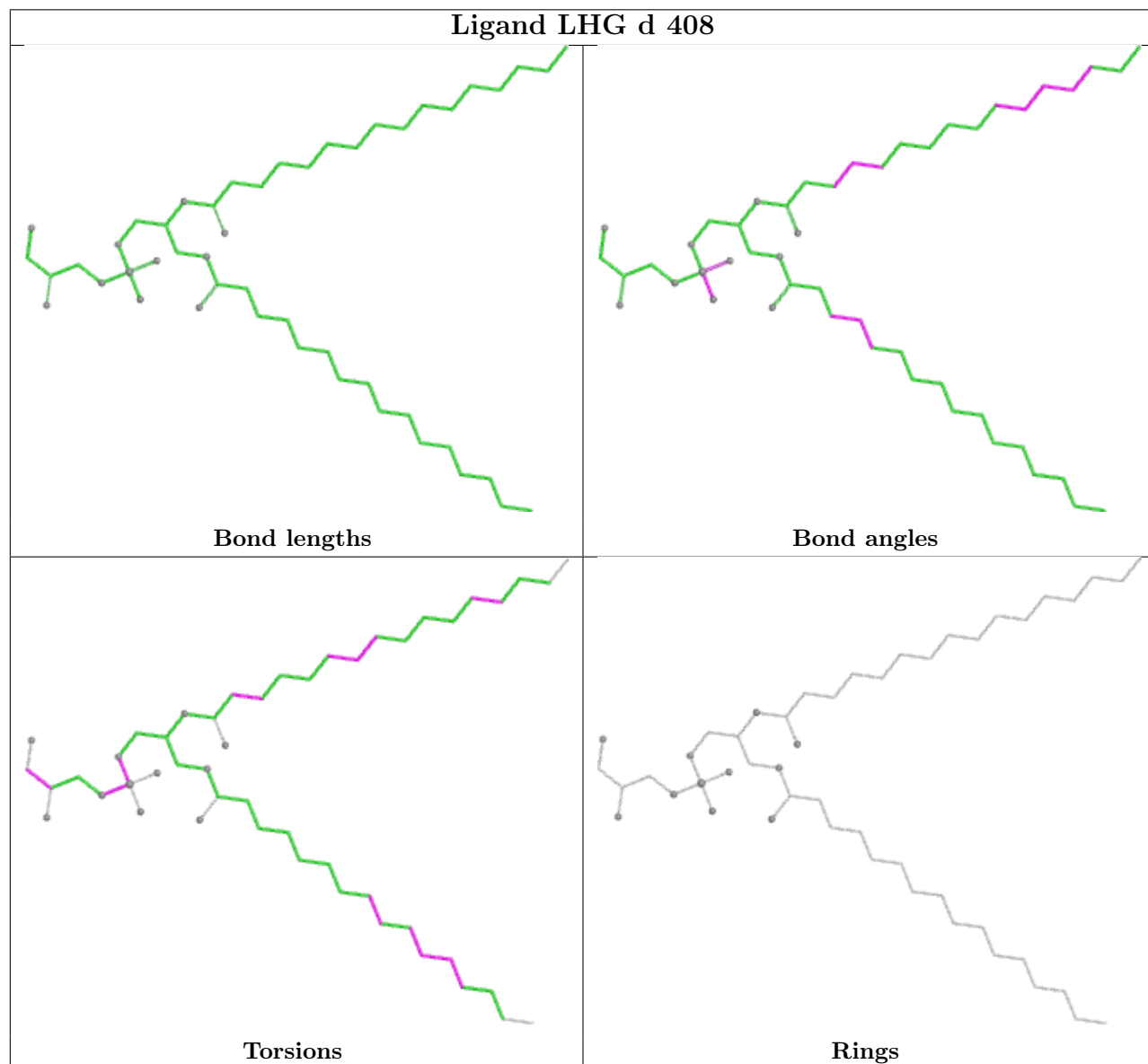
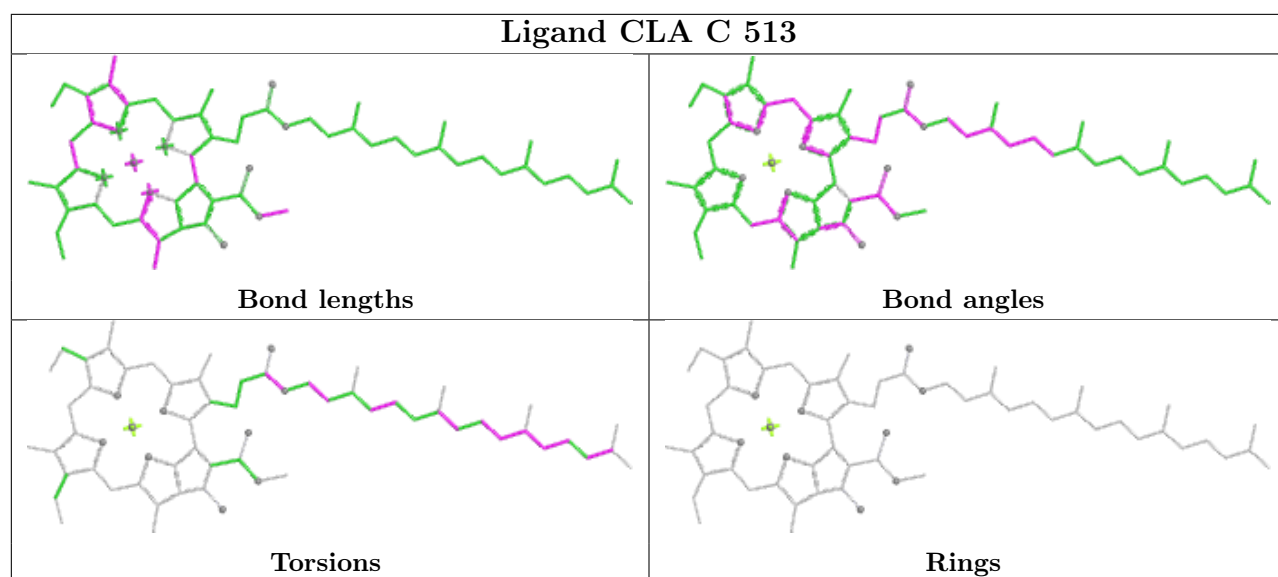


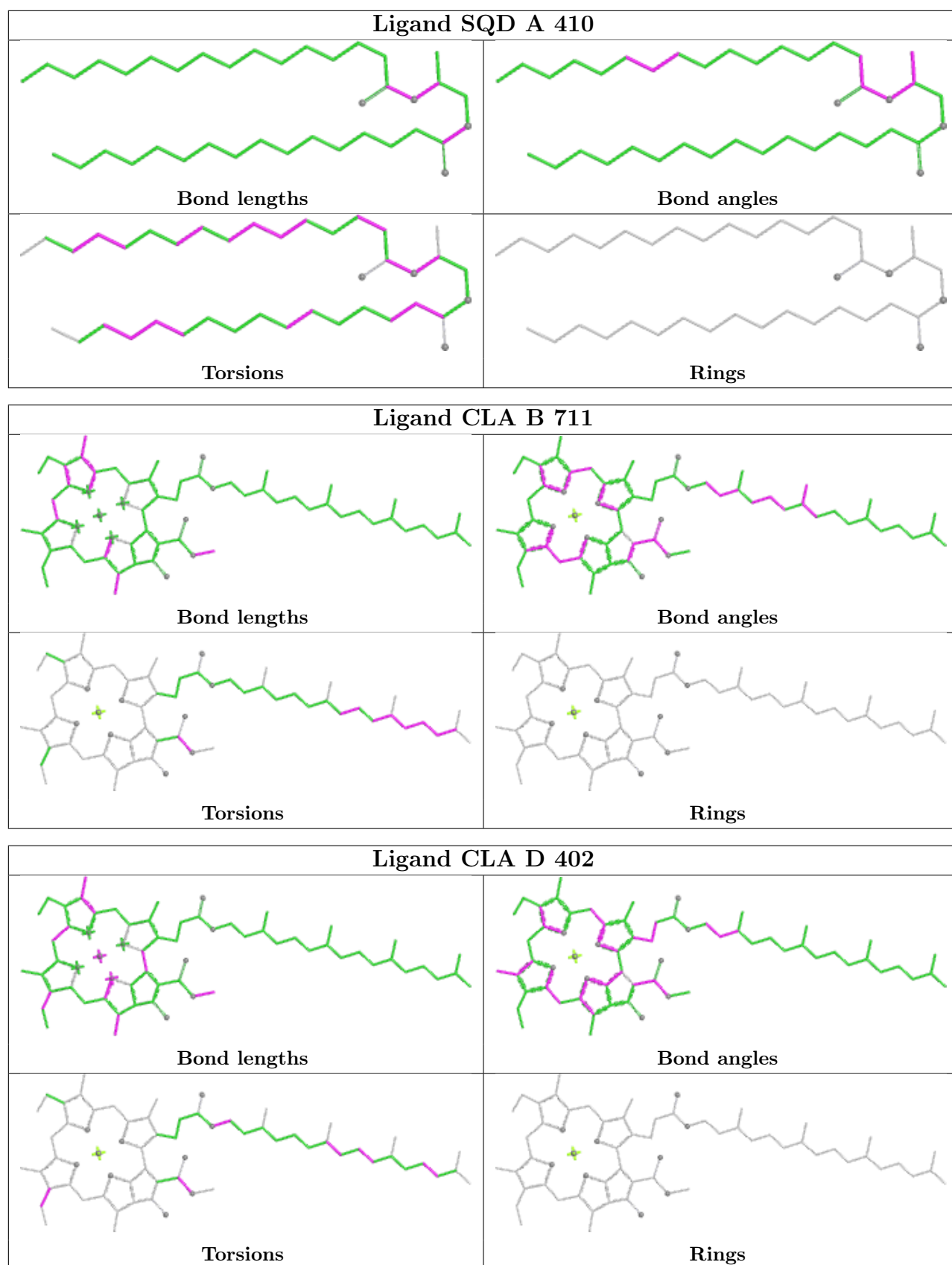
Ligand BCR D 405

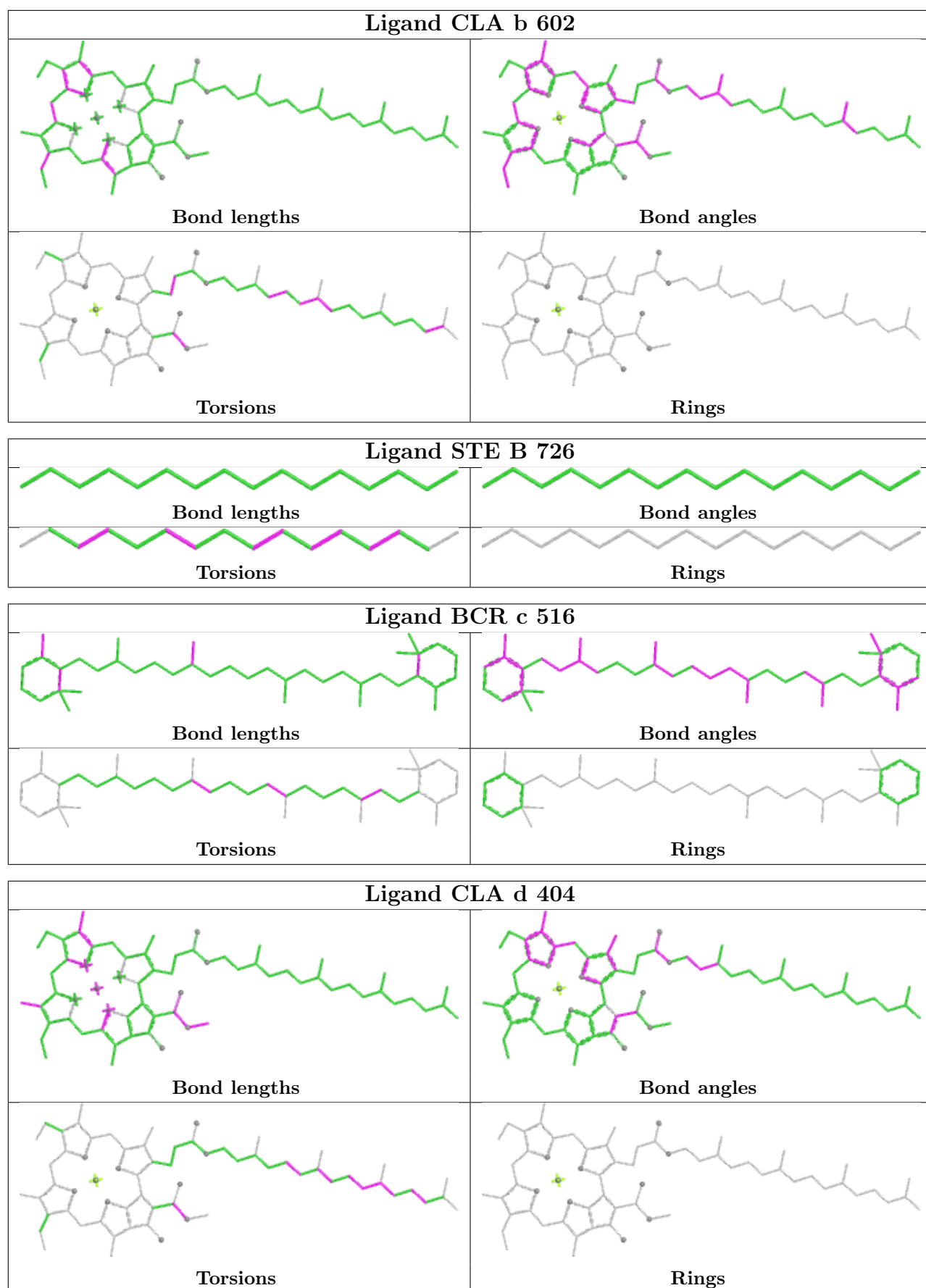


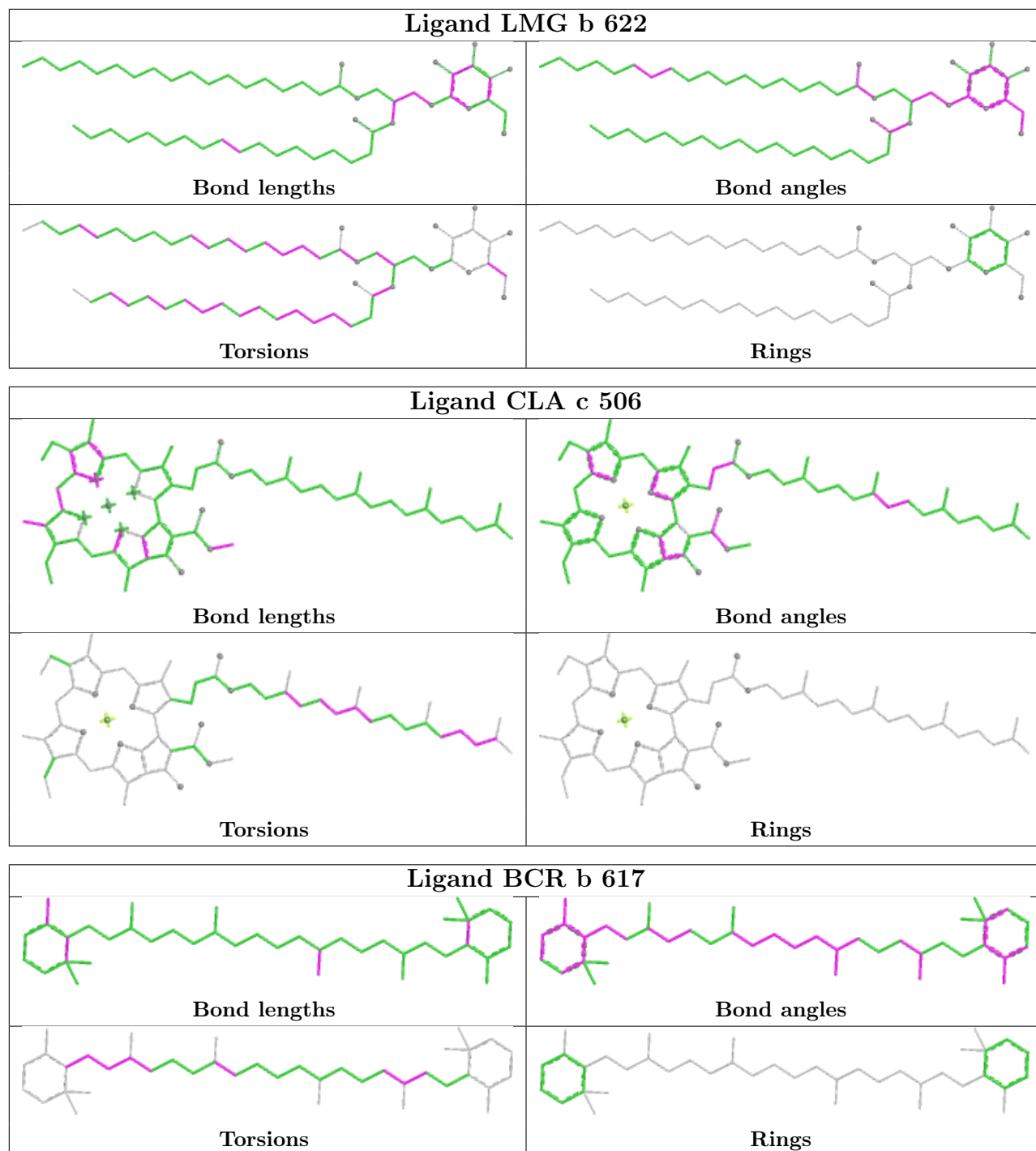
Ligand BCR h 702

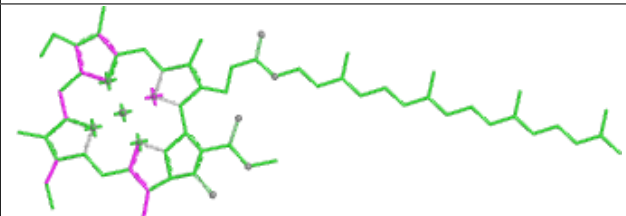
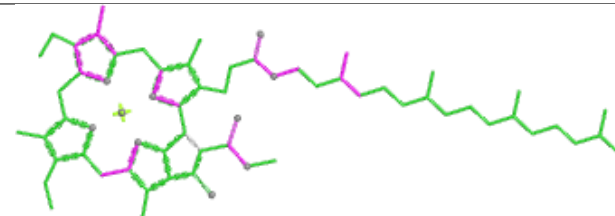
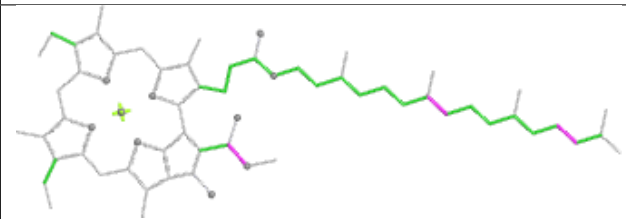
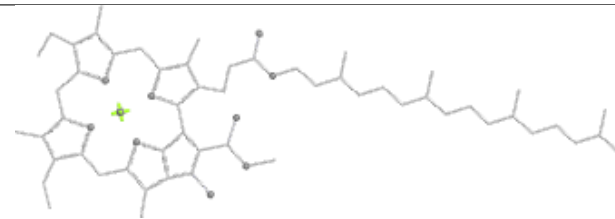


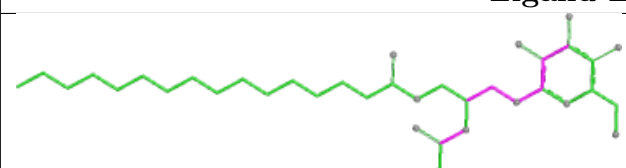
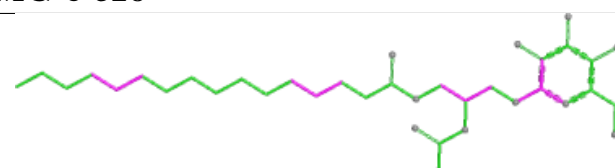
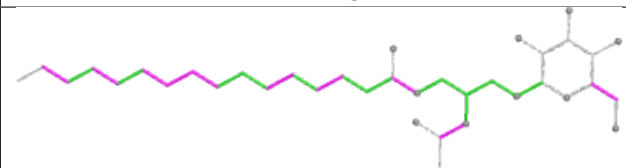
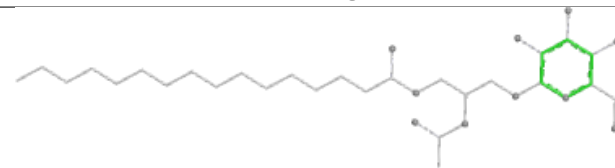


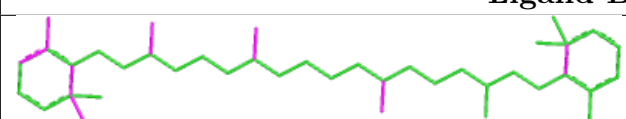
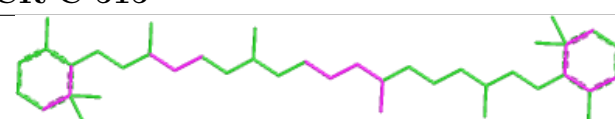
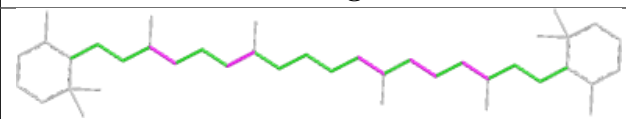
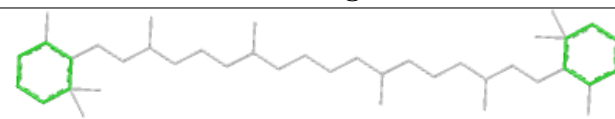


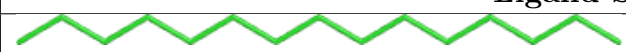
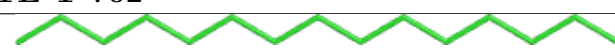


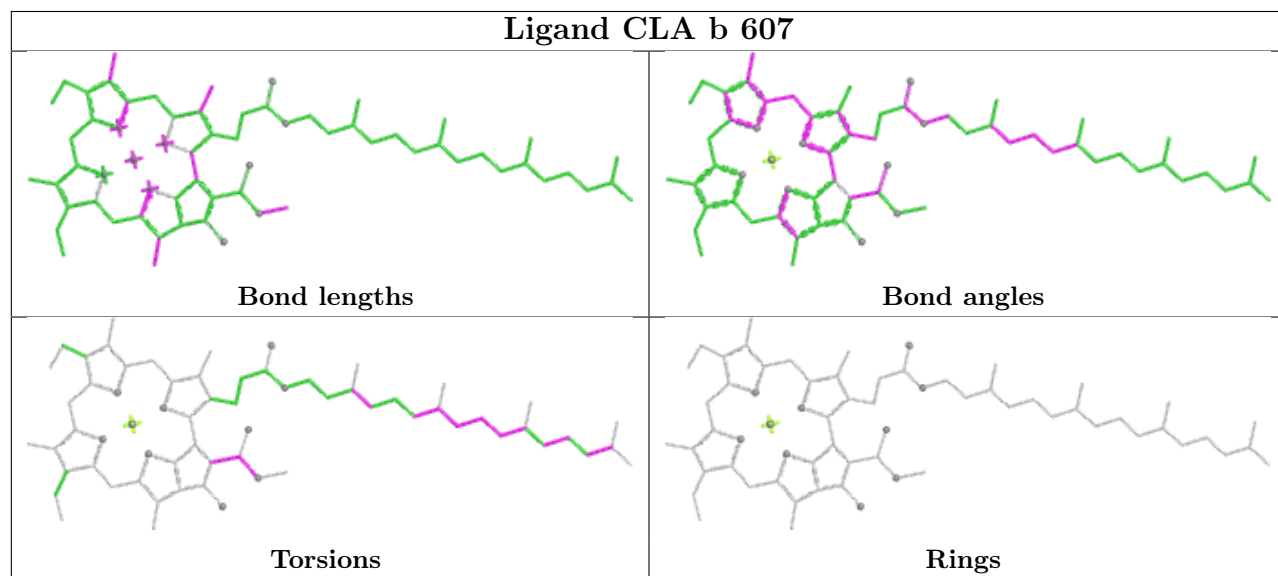
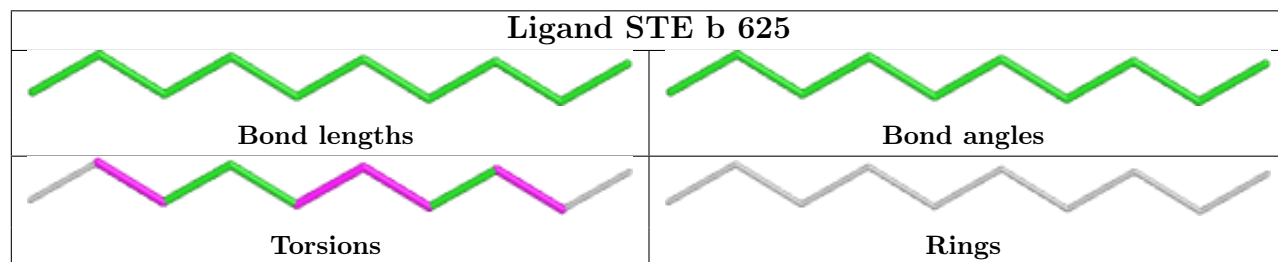
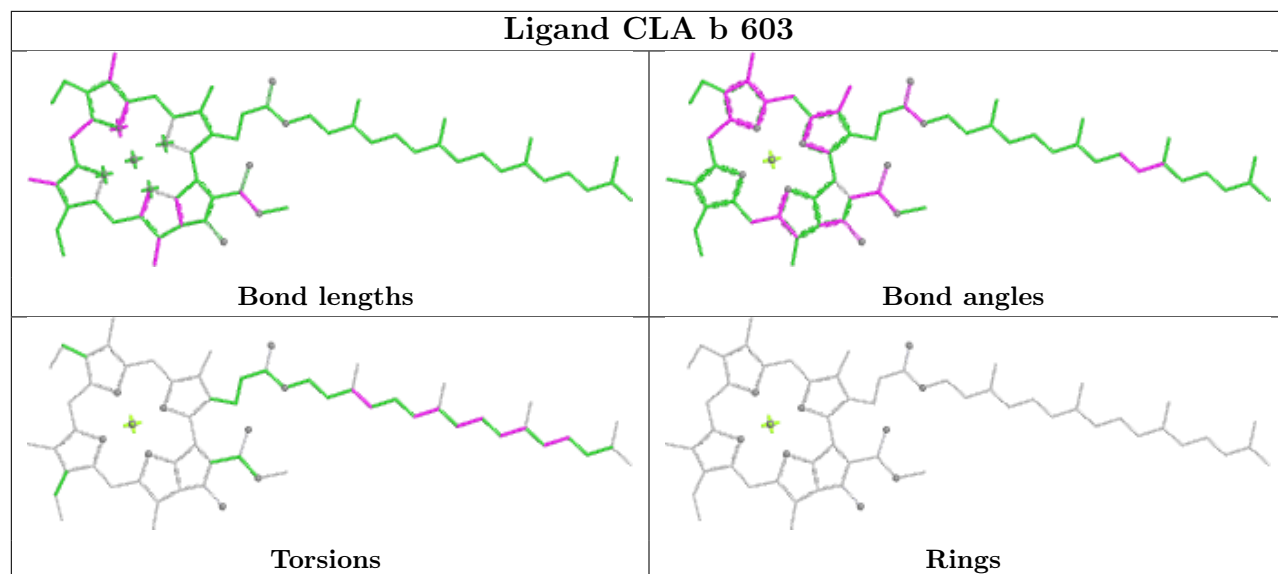


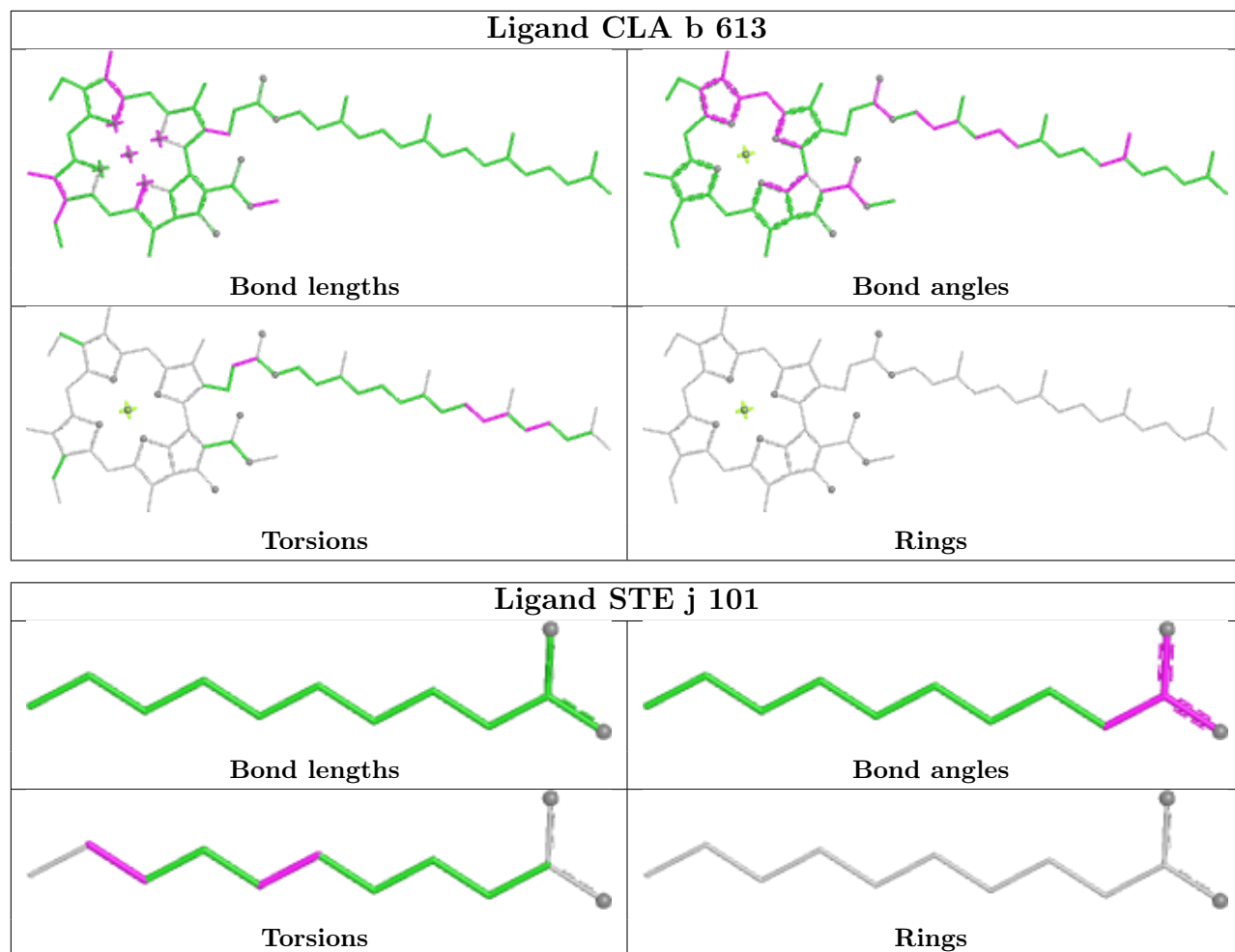
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE T 702	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.52	0 100 100	22, 30, 51, 82	0
1	a	334/344 (97%)	-0.42	2 (0%) 85 87	22, 31, 58, 86	0
2	B	505/510 (99%)	-0.36	2 (0%) 88 90	17, 33, 62, 90	4 (0%)
2	b	505/510 (99%)	-0.23	4 (0%) 82 84	23, 36, 72, 104	0
3	C	442/461 (95%)	-0.29	0 100 100	16, 37, 54, 82	1 (0%)
3	c	451/461 (97%)	-0.21	1 (0%) 91 92	21, 40, 62, 95	2 (0%)
4	D	341/352 (96%)	-0.48	0 100 100	23, 31, 49, 77	0
4	d	341/352 (96%)	-0.34	1 (0%) 90 91	25, 34, 58, 77	1 (0%)
5	E	82/84 (97%)	0.27	1 (1%) 76 78	34, 52, 70, 81	1 (1%)
5	e	82/84 (97%)	0.30	1 (1%) 76 78	37, 59, 77, 80	0
6	F	34/45 (75%)	0.01	1 (2%) 53 56	39, 44, 65, 86	0
6	f	34/45 (75%)	0.23	1 (2%) 53 56	39, 49, 78, 93	0
7	H	65/66 (98%)	-0.11	2 (3%) 51 54	33, 41, 61, 69	0
7	h	63/66 (95%)	0.10	0 100 100	40, 50, 63, 73	0
8	I	35/38 (92%)	-0.26	0 100 100	31, 38, 73, 80	0
8	i	35/38 (92%)	-0.19	0 100 100	31, 40, 71, 80	0
9	J	36/40 (90%)	0.01	0 100 100	32, 50, 77, 90	0
9	j	36/40 (90%)	0.26	1 (2%) 55 57	41, 50, 85, 94	0
10	K	37/46 (80%)	0.20	0 100 100	44, 53, 69, 85	0
10	k	37/46 (80%)	0.15	0 100 100	47, 55, 67, 83	0
11	L	37/37 (100%)	-0.50	0 100 100	26, 31, 64, 72	0
11	l	36/37 (97%)	-0.48	0 100 100	24, 31, 75, 88	0
12	M	32/36 (88%)	-0.48	0 100 100	28, 35, 65, 70	0
12	m	31/36 (86%)	-0.50	0 100 100	25, 34, 53, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.16	2 (0%) 82 84	24, 42, 83, 131	1 (0%)
13	o	244/272 (89%)	-0.19	1 (0%) 88 90	25, 41, 78, 122	0
14	R	34/41 (82%)	1.14	2 (5%) 28 30	64, 78, 93, 110	0
14	r	31/41 (75%)	1.29	3 (9%) 13 14	83, 102, 116, 126	0
15	T	29/32 (90%)	-0.56	0 100 100	26, 31, 61, 77	0
15	t	29/32 (90%)	-0.50	1 (3%) 48 50	27, 33, 82, 88	0
16	U	97/134 (72%)	-0.20	0 100 100	31, 43, 69, 89	0
16	u	97/134 (72%)	-0.26	0 100 100	31, 40, 59, 80	0
17	V	137/163 (84%)	-0.28	0 100 100	31, 40, 57, 83	0
17	v	137/163 (84%)	-0.07	0 100 100	30, 46, 69, 87	0
18	X	38/41 (92%)	0.05	1 (2%) 57 60	42, 51, 71, 82	0
18	x	39/41 (95%)	0.22	2 (5%) 33 35	47, 59, 90, 105	0
19	Y	27/46 (58%)	1.05	3 (11%) 10 10	53, 73, 89, 94	0
19	y	30/46 (65%)	0.55	0 100 100	59, 72, 86, 96	0
20	Z	62/62 (100%)	0.67	3 (4%) 35 38	53, 66, 109, 130	0
20	z	62/62 (100%)	0.66	4 (6%) 25 26	54, 70, 105, 115	0
All	All	5302/5700 (93%)	-0.21	39 (0%) 84 86	16, 38, 74, 131	10 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	R	35	LEU	4.4
13	O	60	ARG	3.4
9	j	6	GLY	3.2
3	c	23	ALA	3.1
7	H	41	PHE	3.1
13	o	58	ASN	3.1
7	H	65	LEU	3.0
14	r	14	LEU	3.0
2	B	246	PHE	2.9
20	Z	33	TRP	2.9
19	Y	25	ILE	2.9
20	z	33	TRP	2.9
1	a	250	ALA	2.8
2	b	495	PHE	2.7
20	Z	62	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	499	VAL	2.7
18	X	2	THR	2.6
5	e	79	PHE	2.6
6	F	12	SER	2.5
20	Z	17	PHE	2.5
1	a	249	VAL	2.5
5	E	79	PHE	2.4
20	z	40	ILE	2.4
20	z	27	TYR	2.4
2	B	86	ILE	2.4
2	b	494	GLY	2.3
18	x	2	THR	2.3
19	Y	20	ALA	2.2
14	r	18	TRP	2.2
13	O	59	LYS	2.2
18	x	37	VAL	2.2
14	R	34	LEU	2.2
4	d	237	PRO	2.1
6	f	15	ILE	2.1
20	z	41	PHE	2.1
2	b	496	TYR	2.0
14	r	28	VAL	2.0
19	Y	24	MET	2.0
15	t	30	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	t	1	10/11	0.92	0.09	28,34,63,66	0
12	FME	M	1	10/11	0.93	0.10	39,46,55,65	0
8	FME	I	1	10/11	0.93	0.09	37,47,57,58	0
8	FME	i	1	10/11	0.96	0.11	38,45,49,49	0
15	FME	T	1	10/11	0.96	0.08	25,36,51,65	0
12	FME	m	1	10/11	0.97	0.07	30,44,66,70	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	H	103	18/20	0.80	0.17	44,67,73,79	0
28	STE	d	402	20/20	0.80	0.17	42,66,78,82	0
28	STE	b	624	20/20	0.81	0.15	44,56,69,71	0
31	LHG	E	101	49/49	0.82	0.13	50,72,92,97	0
28	STE	A	412	5/20	0.83	0.20	39,52,56,64	0
28	STE	I	101	15/20	0.83	0.14	39,52,65,72	0
30	LMG	b	622	55/55	0.83	0.15	47,68,82,90	0
28	STE	J	101	12/20	0.83	0.14	46,57,69,70	0
28	STE	a	415	10/20	0.84	0.13	34,52,54,55	0
28	STE	m	102	12/20	0.84	0.14	44,53,61,64	0
30	LMG	a	418	55/55	0.84	0.13	33,55,90,109	0
28	STE	E	102	12/20	0.84	0.15	60,69,80,86	0
28	STE	c	501	12/20	0.84	0.11	53,60,76,82	0
31	LHG	a	413	42/49	0.84	0.14	49,78,98,103	0
28	STE	b	623	16/20	0.85	0.14	50,56,87,90	0
28	STE	x	101	20/20	0.85	0.13	46,53,63,67	0
28	STE	C	523	12/20	0.85	0.14	34,45,53,59	0
28	STE	b	625	10/20	0.85	0.13	43,52,58,63	0
30	LMG	c	522	48/55	0.85	0.13	37,71,94,102	0
25	PL9	A	408	55/55	0.85	0.15	47,61,72,82	0
28	STE	B	726	16/20	0.85	0.14	48,58,69,70	0
28	STE	B	724	12/20	0.86	0.12	40,48,56,67	0
27	DGD	A	411	66/66	0.86	0.11	40,56,71,82	0
30	LMG	D	413	32/55	0.86	0.13	36,51,68,73	0
22	CLA	h	701	65/65	0.86	0.12	46,63,79,82	0
28	STE	B	720	17/20	0.86	0.13	31,46,61,68	0
28	STE	c	521	20/20	0.86	0.11	41,50,65,74	0
28	STE	a	416	12/20	0.86	0.11	49,57,62,65	0
28	STE	h	704	14/20	0.86	0.16	42,56,74,77	0
30	LMG	C	516	48/55	0.87	0.11	40,55,71,82	0
28	STE	a	417	15/20	0.87	0.14	37,54,66,66	0
28	STE	C	522	16/20	0.87	0.12	38,48,57,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SQD	a	414	36/54	0.87	0.12	31,56,74,81	0
28	STE	j	101	12/20	0.87	0.12	46,50,59,64	0
25	PL9	a	410	55/55	0.87	0.14	40,62,77,84	0
26	SQD	B	723	54/54	0.87	0.11	37,58,81,90	0
28	STE	b	601	16/20	0.88	0.14	32,43,66,68	0
26	SQD	f	102	41/54	0.89	0.13	54,82,91,98	0
26	SQD	D	410	36/54	0.89	0.12	51,68,82,84	0
30	LMG	C	520	48/55	0.89	0.11	42,62,74,77	0
28	STE	B	725	18/20	0.89	0.11	41,48,76,79	0
26	SQD	A	410	39/54	0.89	0.12	37,55,87,89	0
28	STE	d	411	17/20	0.89	0.11	41,49,58,64	0
30	LMG	c	520	37/55	0.89	0.10	41,61,73,77	0
28	STE	b	621	20/20	0.89	0.10	35,48,65,74	0
28	STE	B	701	12/20	0.89	0.13	45,59,73,79	0
28	STE	X	101	20/20	0.89	0.11	33,43,71,82	0
28	STE	E	103	7/20	0.90	0.12	47,58,62,63	0
28	STE	C	521	12/20	0.90	0.11	40,46,54,55	0
30	LMG	b	620	51/55	0.90	0.10	33,48,69,76	0
28	STE	H	104	8/20	0.90	0.12	46,51,57,60	0
28	STE	t	702	14/20	0.90	0.11	38,49,59,61	0
23	BCR	h	702	40/40	0.90	0.11	34,53,64,75	0
23	BCR	c	515	40/40	0.90	0.10	43,53,63,69	0
23	BCR	d	405	40/40	0.90	0.11	37,48,77,91	0
30	LMG	B	721	28/55	0.91	0.12	34,47,60,68	0
28	STE	m	101	18/20	0.91	0.11	34,41,65,69	0
22	CLA	C	514	65/65	0.91	0.09	40,56,83,93	0
26	SQD	l	101	49/54	0.91	0.09	34,57,82,95	0
30	LMG	c	523	49/55	0.91	0.10	35,57,74,86	0
30	LMG	M	101	51/55	0.91	0.09	31,45,63,66	0
23	BCR	k	101	40/40	0.91	0.11	36,55,72,73	0
23	BCR	Y	101	40/40	0.92	0.09	41,49,62,66	0
22	CLA	B	727	65/65	0.92	0.09	30,50,80,96	0
27	DGD	H	102	62/66	0.92	0.09	25,41,51,56	0
26	SQD	a	412	54/54	0.92	0.10	41,58,79,87	0
23	BCR	C	524	40/40	0.92	0.10	44,52,58,66	0
23	BCR	D	405	40/40	0.92	0.10	27,40,76,83	0
28	STE	M	102	15/20	0.92	0.11	32,44,71,80	0
28	STE	T	702	15/20	0.92	0.11	39,46,66,71	0
23	BCR	k	102	40/40	0.93	0.10	39,48,54,60	0
22	CLA	c	513	65/65	0.93	0.10	40,51,79,95	0
27	DGD	h	703	62/66	0.93	0.09	31,43,53,62	0
28	STE	Z	101	8/20	0.93	0.12	49,51,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	504	65/65	0.93	0.09	30,42,48,52	0
23	BCR	H	101	40/40	0.93	0.08	35,41,51,65	0
23	BCR	B	718	40/40	0.93	0.08	23,33,46,47	0
23	BCR	b	618	40/40	0.94	0.06	26,35,45,48	0
23	BCR	b	619	40/40	0.94	0.07	32,44,55,64	0
22	CLA	C	511	65/65	0.94	0.08	30,43,54,66	0
23	BCR	c	516	40/40	0.94	0.08	29,39,48,60	0
22	CLA	c	514	65/65	0.94	0.09	43,60,91,95	0
30	LMG	D	409	51/55	0.94	0.10	34,44,69,78	0
22	CLA	C	512	65/65	0.94	0.09	28,47,57,71	0
27	DGD	C	518	62/66	0.94	0.09	32,46,80,101	0
22	CLA	C	513	65/65	0.94	0.09	33,49,82,87	0
27	DGD	c	518	62/66	0.94	0.08	30,49,74,79	0
22	CLA	B	706	65/65	0.94	0.08	22,32,62,68	0
22	CLA	c	509	64/65	0.94	0.09	33,42,73,93	0
22	CLA	c	510	65/65	0.94	0.09	34,43,53,61	0
26	SQD	A	409	52/54	0.94	0.09	29,55,73,82	0
31	LHG	B	722	49/49	0.94	0.10	30,42,61,64	0
22	CLA	c	512	65/65	0.94	0.10	37,50,58,63	0
23	BCR	b	617	40/40	0.94	0.07	29,37,45,47	0
22	CLA	b	616	60/65	0.95	0.09	28,41,80,84	0
23	BCR	A	405	40/40	0.95	0.07	22,31,41,44	0
27	DGD	C	519	62/66	0.95	0.08	30,41,61,74	0
28	STE	M	103	10/20	0.95	0.07	35,42,45,48	0
23	BCR	B	717	40/40	0.95	0.07	26,35,50,53	0
22	CLA	c	504	65/65	0.95	0.07	21,42,50,52	0
23	BCR	B	719	40/40	0.95	0.06	23,36,48,54	0
23	BCR	C	501	40/40	0.95	0.09	35,49,62,65	0
23	BCR	t	701	40/40	0.95	0.07	22,33,45,46	0
23	BCR	C	515	40/40	0.95	0.07	24,36,44,46	0
25	PL9	D	406	55/55	0.95	0.07	22,30,43,47	0
22	CLA	c	507	65/65	0.95	0.08	29,42,82,90	0
22	CLA	c	508	65/65	0.95	0.07	25,39,51,54	0
22	CLA	C	503	65/65	0.95	0.07	29,38,47,52	0
23	BCR	T	701	40/40	0.95	0.06	28,35,50,51	0
22	CLA	C	509	65/65	0.95	0.08	27,37,88,99	0
23	BCR	a	406	40/40	0.95	0.06	20,30,44,46	0
22	CLA	b	606	65/65	0.95	0.07	23,37,61,70	0
31	LHG	D	412	47/49	0.95	0.09	23,39,70,84	0
22	CLA	b	609	65/65	0.95	0.07	28,41,55,68	0
31	LHG	a	411	49/49	0.95	0.10	30,44,66,71	0
22	CLA	b	614	65/65	0.95	0.08	21,35,60,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	l	102	49/49	0.95	0.08	31,41,49,53	0
22	CLA	d	404	65/65	0.96	0.08	26,37,75,92	0
22	CLA	B	716	60/65	0.96	0.09	22,32,81,86	0
22	CLA	a	402	65/65	0.96	0.06	20,28,36,51	0
22	CLA	a	403	65/65	0.96	0.08	27,36,86,96	0
22	CLA	a	405	65/65	0.96	0.08	17,28,64,69	0
27	DGD	C	517	62/66	0.96	0.09	21,35,66,73	0
22	CLA	b	602	65/65	0.96	0.07	24,36,52,55	0
22	CLA	b	604	65/65	0.96	0.08	21,32,71,85	0
22	CLA	b	605	65/65	0.96	0.07	20,30,42,48	0
22	CLA	B	704	65/65	0.96	0.08	21,27,63,69	0
27	DGD	c	519	62/66	0.96	0.07	28,44,72,86	0
22	CLA	b	608	65/65	0.96	0.07	28,39,54,61	0
22	CLA	C	502	65/65	0.96	0.06	22,32,44,54	0
22	CLA	b	610	65/65	0.96	0.07	23,33,42,51	0
22	CLA	b	612	65/65	0.96	0.07	23,31,43,48	0
22	CLA	A	403	65/65	0.96	0.08	21,30,76,84	0
22	CLA	b	615	65/65	0.96	0.07	28,38,51,53	0
22	CLA	B	709	65/65	0.96	0.06	24,34,44,50	0
22	CLA	c	502	65/65	0.96	0.07	27,36,46,51	0
22	CLA	c	503	65/65	0.96	0.07	28,40,53,61	0
22	CLA	C	505	59/65	0.96	0.07	27,38,63,73	0
22	CLA	c	505	60/65	0.96	0.07	32,42,65,70	0
22	CLA	c	506	65/65	0.96	0.07	26,36,61,65	0
22	CLA	C	507	65/65	0.96	0.08	24,39,70,83	0
22	CLA	C	508	65/65	0.96	0.07	25,35,49,53	0
22	CLA	B	710	65/65	0.96	0.07	19,30,39,44	0
22	CLA	C	510	65/65	0.96	0.08	25,40,52,64	0
22	CLA	c	511	65/65	0.96	0.07	32,45,52,61	0
30	LMG	d	410	44/55	0.96	0.07	34,43,70,71	0
22	CLA	B	711	65/65	0.96	0.06	18,27,43,50	0
31	LHG	D	411	49/49	0.96	0.07	21,37,44,56	0
25	PL9	d	406	55/55	0.96	0.06	21,31,38,41	0
22	CLA	B	712	65/65	0.96	0.07	21,28,39,44	0
22	CLA	B	715	65/65	0.96	0.07	24,33,56,65	0
22	CLA	d	401	65/65	0.96	0.06	20,29,35,44	0
31	LHG	d	409	39/49	0.96	0.08	34,43,60,64	0
22	CLA	d	403	65/65	0.96	0.07	21,31,47,53	0
32	BCT	a	409	4/4	0.96	0.07	31,32,40,49	0
33	PHO	D	408	64/64	0.96	0.06	22,30,36,43	0
33	PHO	a	404	64/64	0.96	0.06	19,28,35,37	0
33	PHO	d	407	64/64	0.96	0.06	26,36,44,51	0

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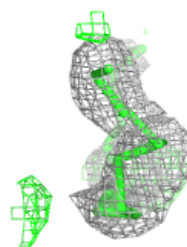
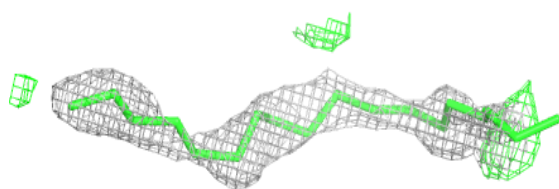
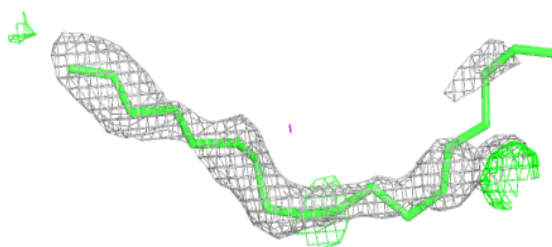
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	B	702	65/65	0.97	0.06	25,33,45,54	0
27	DGD	c	517	62/66	0.97	0.07	23,35,70,72	0
22	CLA	B	713	65/65	0.97	0.06	20,29,57,63	0
22	CLA	D	402	65/65	0.97	0.06	14,26,49,59	0
22	CLA	b	611	65/65	0.97	0.06	23,30,50,56	0
22	CLA	D	403	65/65	0.97	0.05	19,24,40,47	0
22	CLA	b	613	65/65	0.97	0.06	18,29,59,68	0
22	CLA	D	404	65/65	0.97	0.07	22,34,93,105	0
22	CLA	C	506	65/65	0.97	0.07	22,34,60,69	0
31	LHG	L	101	49/49	0.97	0.07	31,36,48,55	0
22	CLA	B	714	65/65	0.97	0.07	19,31,63,79	0
22	CLA	B	707	65/65	0.97	0.06	16,28,51,59	0
31	LHG	d	408	49/49	0.97	0.07	25,39,49,54	0
22	CLA	B	708	65/65	0.97	0.06	20,30,46,53	0
22	CLA	b	603	65/65	0.97	0.07	22,31,57,63	0
32	BCT	D	401	4/4	0.97	0.06	25,31,34,37	0
22	CLA	B	703	65/65	0.97	0.06	19,28,48,52	0
33	PHO	D	407	64/64	0.97	0.05	16,25,33,38	0
22	CLA	A	402	65/65	0.97	0.06	16,25,38,48	0
22	CLA	B	705	65/65	0.97	0.06	18,27,41,44	0
22	CLA	b	607	65/65	0.97	0.07	18,31,55,65	0
34	HEC	F	101	43/43	0.97	0.08	31,46,60,69	0
34	HEC	f	101	43/43	0.97	0.08	39,53,74,84	0
34	HEC	V	201	43/43	0.98	0.06	17,30,40,44	0
22	CLA	A	404	54/65	0.98	0.05	16,26,57,59	0
34	HEC	v	201	43/43	0.98	0.06	26,34,43,48	0
29	OEX	A	413[A]	10/10	0.99	0.04	21,28,37,37	0
29	OEX	a	419[A]	10/10	0.99	0.03	23,30,33,40	0
24	CL	a	407	1/1	0.99	0.05	29,29,29,29	0
21	FE2	a	401	1/1	0.99	0.07	44,44,44,44	0
24	CL	A	406	1/1	0.99	0.04	30,30,30,30	0
21	FE2	A	401	1/1	1.00	0.01	28,28,28,28	0
24	CL	a	408	1/1	1.00	0.06	28,28,28,28	0
24	CL	A	407	1/1	1.00	0.08	28,28,28,28	0

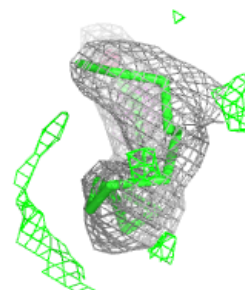
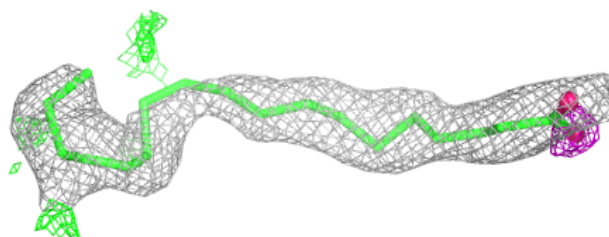
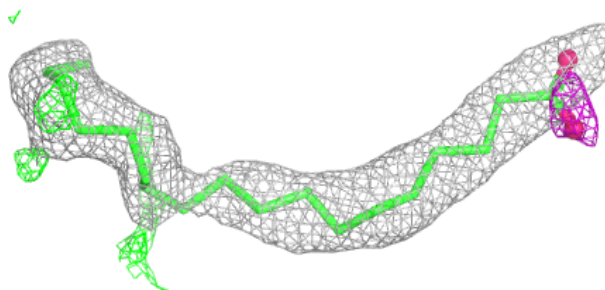
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

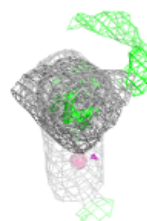
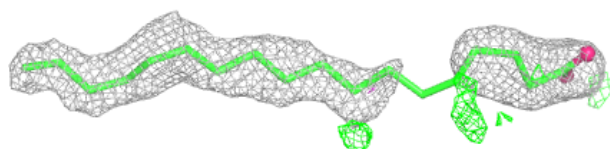
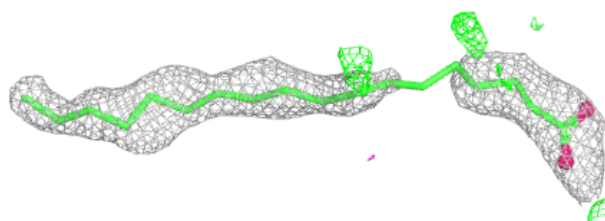
**Electron density around STE d 402:**

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



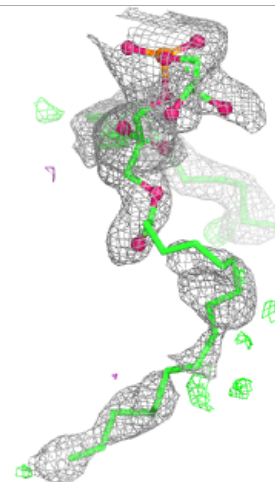
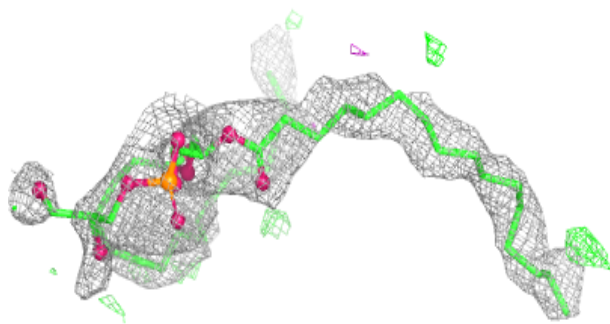
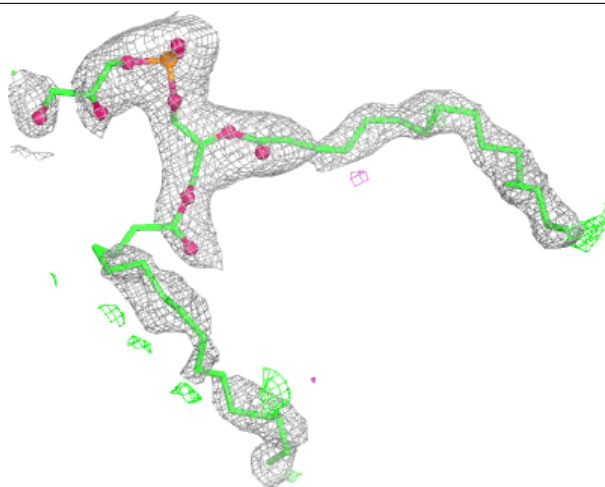
Electron density around STE b 624:

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



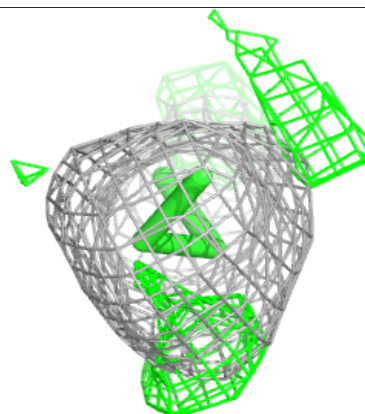
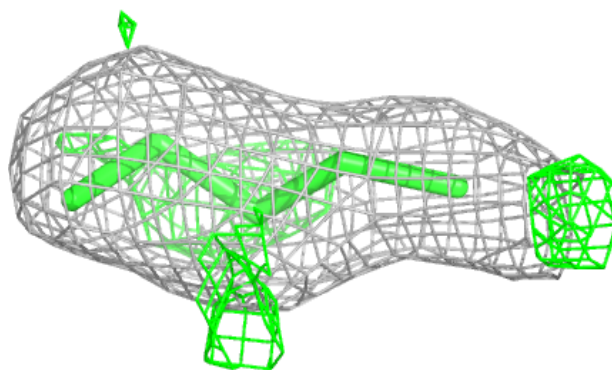
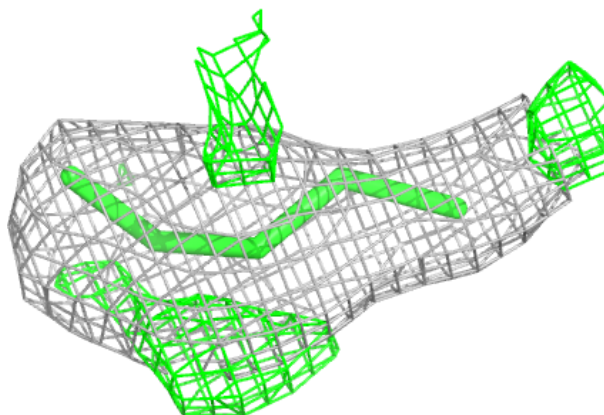
Electron density around LHG E 101:

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

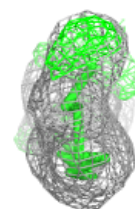
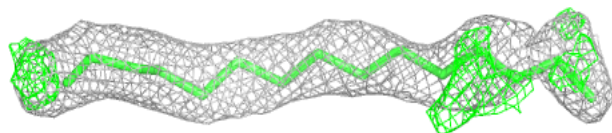
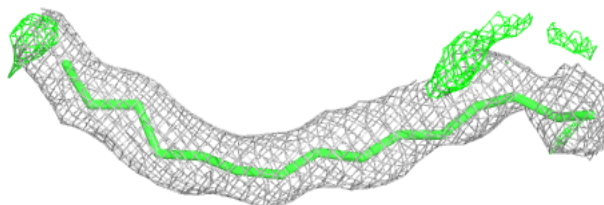


Electron density around STE A 412:

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

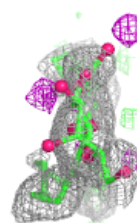
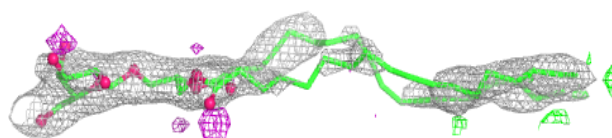
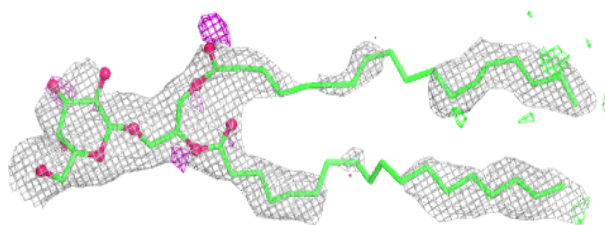
**Electron density around STE I 101:**

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

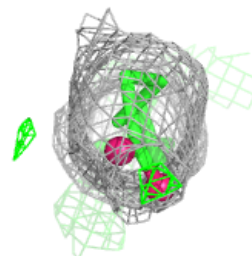
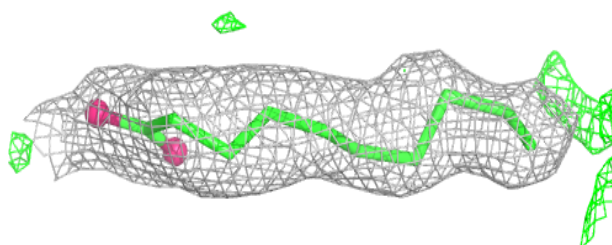
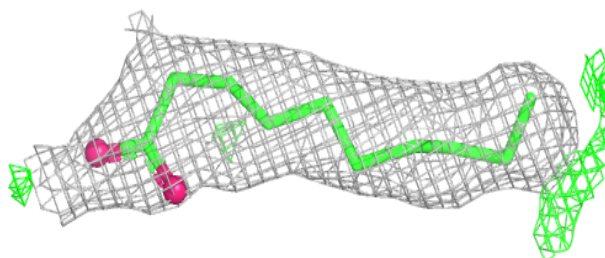


Electron density around LMG b 622:

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

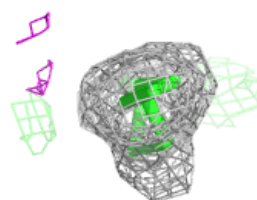
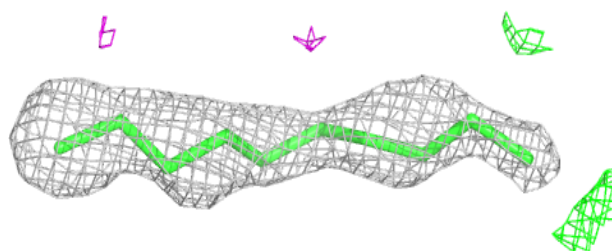
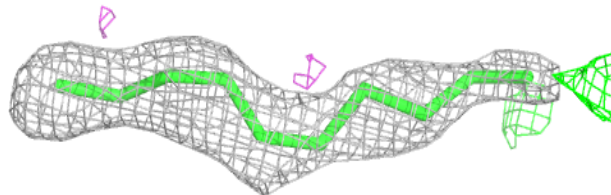
**Electron density around STE J 101:**

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

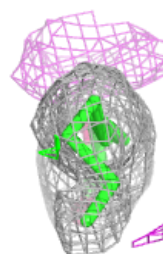
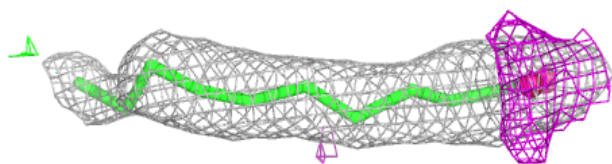
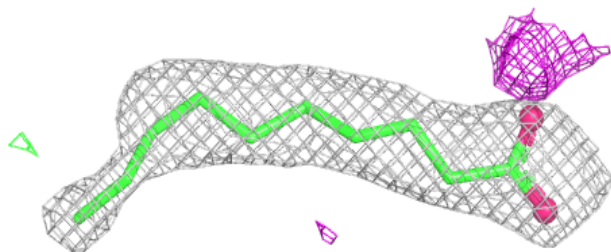


Electron density around STE a 415:

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

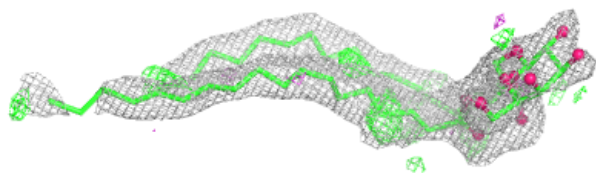
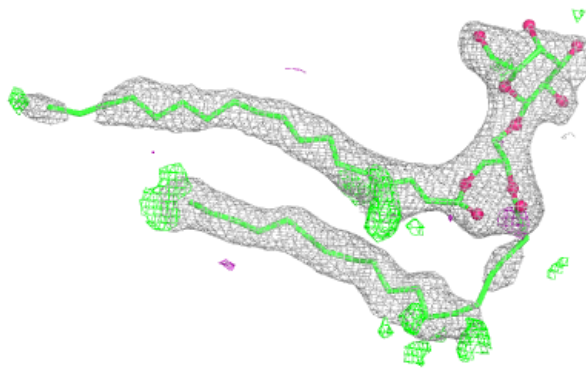
**Electron density around STE m 102:**

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

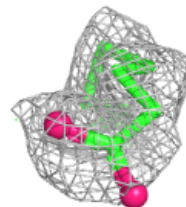
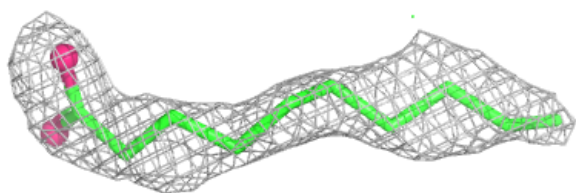
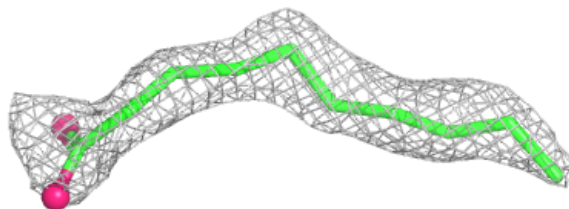


Electron density around LMG a 418:

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

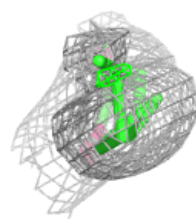
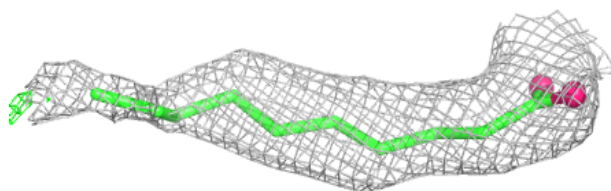
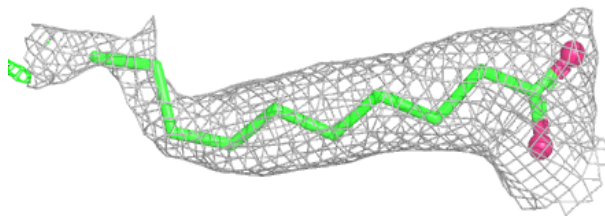
**Electron density around STE E 102:**

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

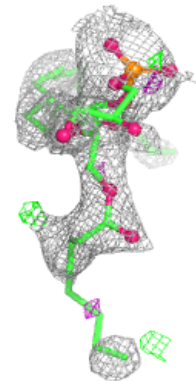
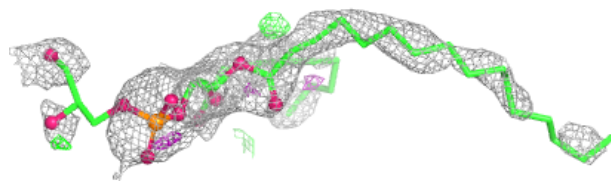
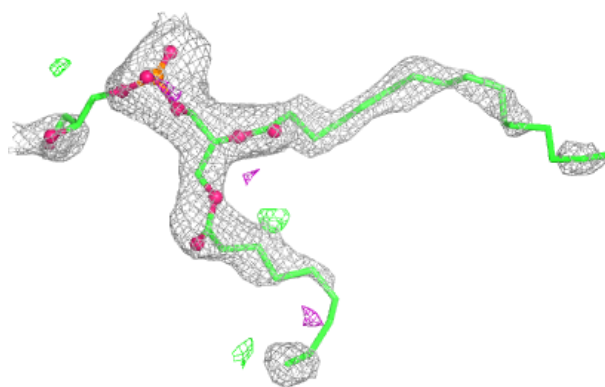


Electron density around STE c 501:

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

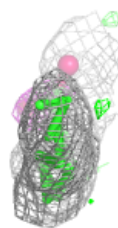
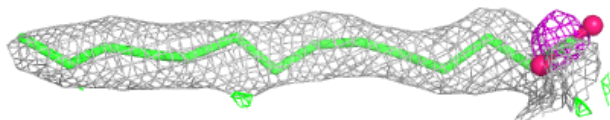
**Electron density around LHG a 413:**

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

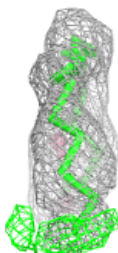
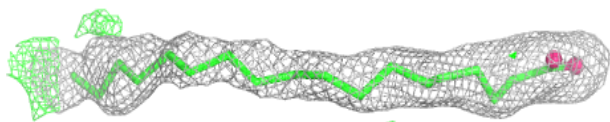
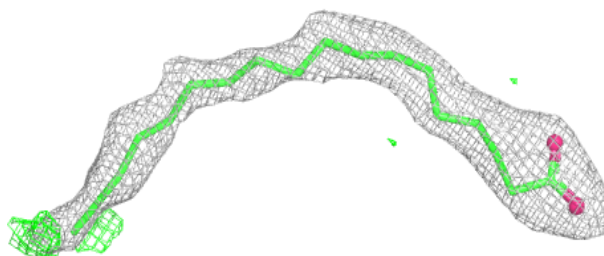


Electron density around STE b 623:

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

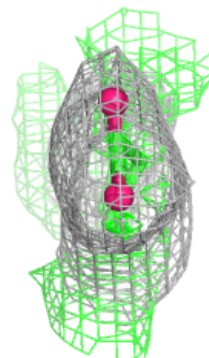
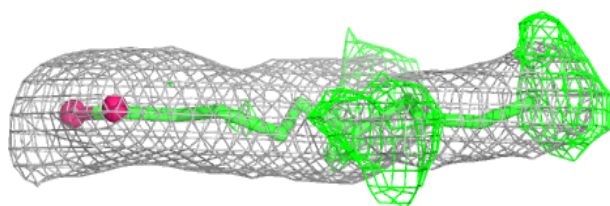
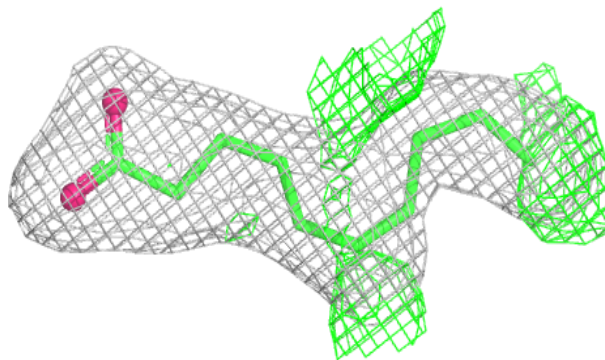
**Electron density around STE x 101:**

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

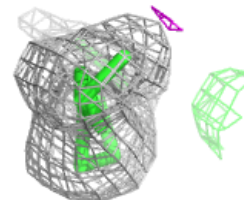
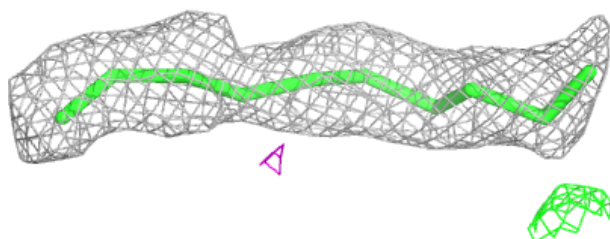
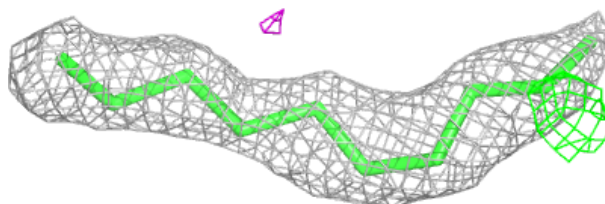


Electron density around STE C 523:

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

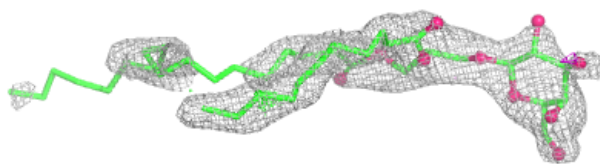
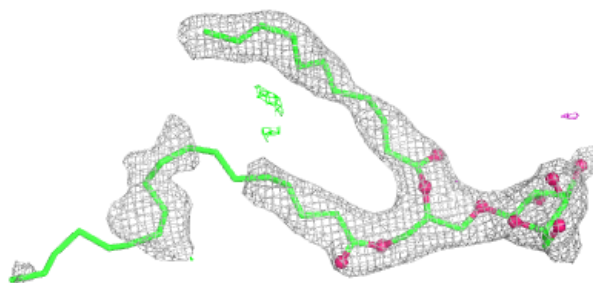
**Electron density around STE b 625:**

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

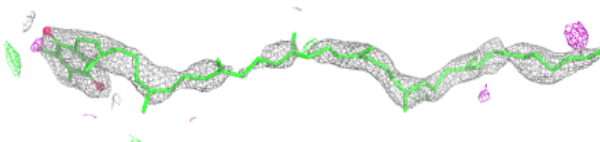
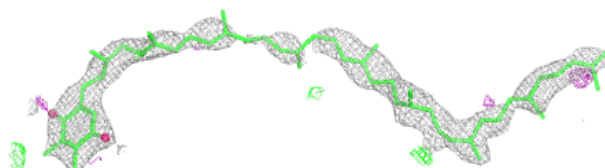


Electron density around LMG c 522:

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

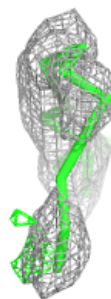
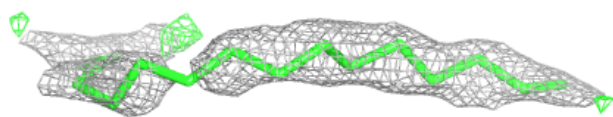
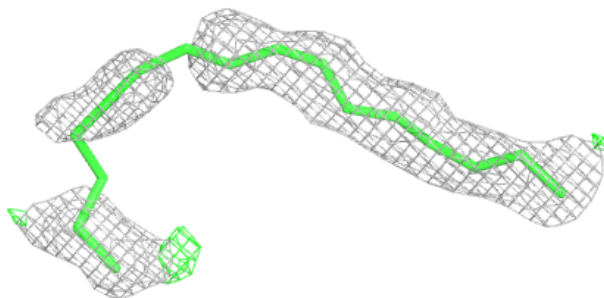
**Electron density around PL9 A 408:**

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

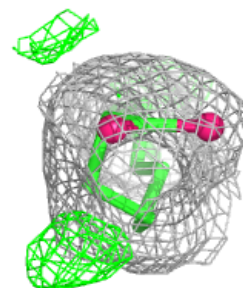
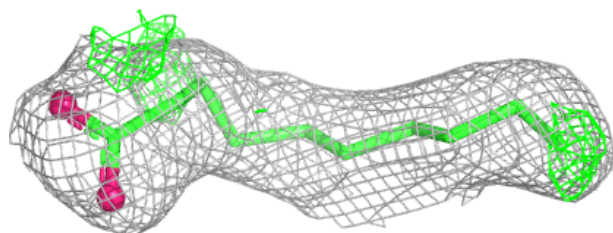
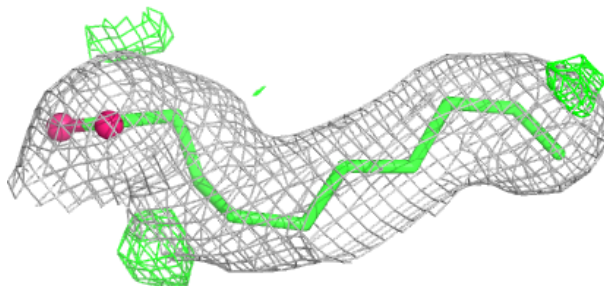


Electron density around STE B 726:

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

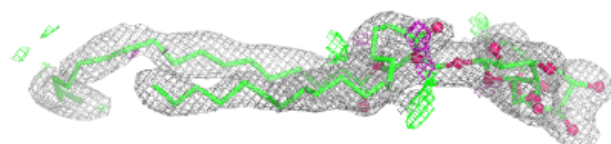
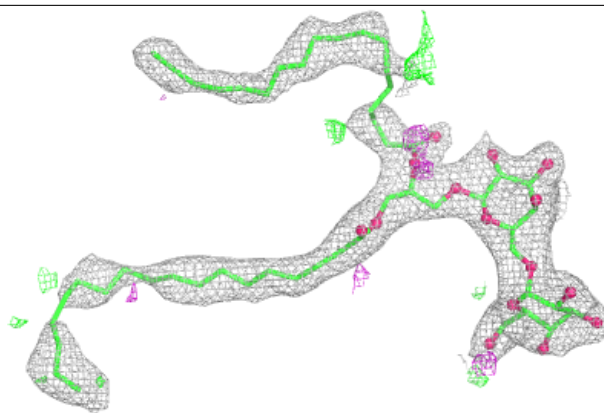
**Electron density around STE B 724:**

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

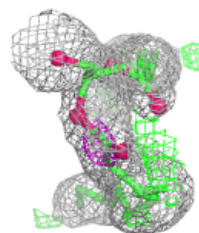
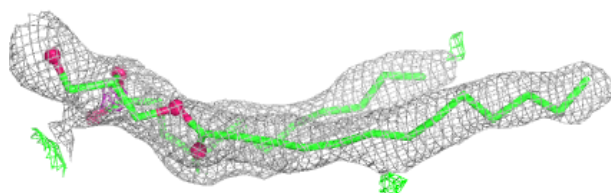
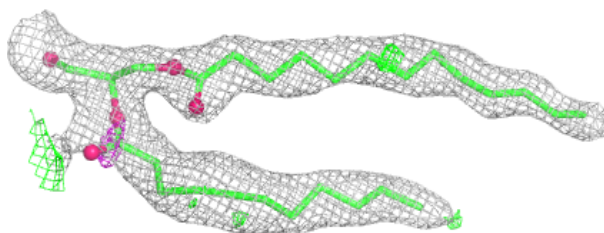


Electron density around DGD A 411:

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

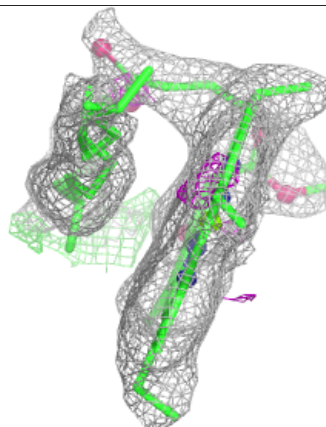
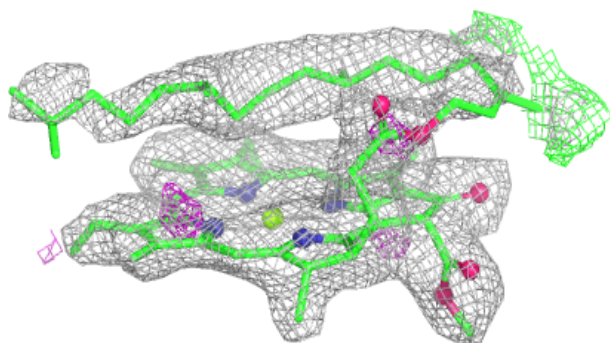
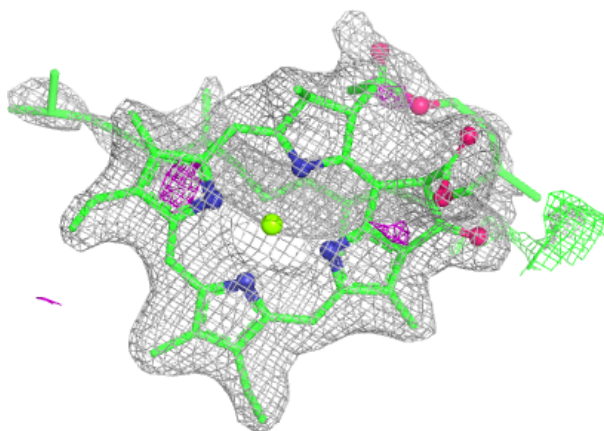
**Electron density around LMG D 413:**

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

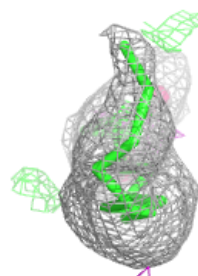
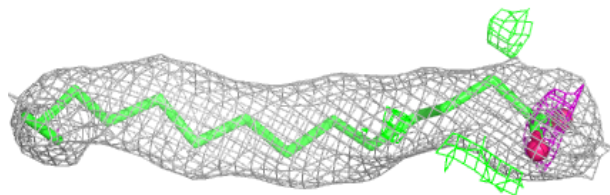
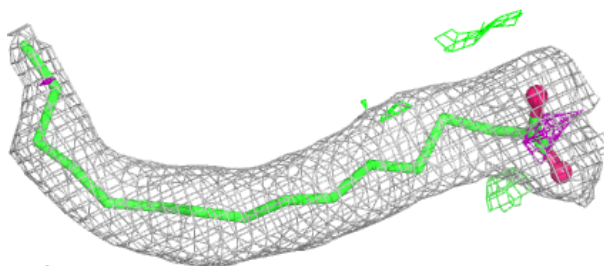


Electron density around CLA h 701:

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

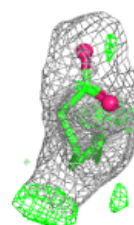
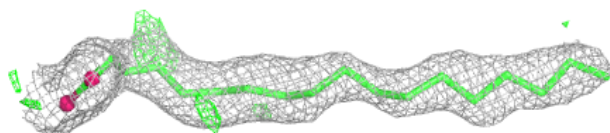
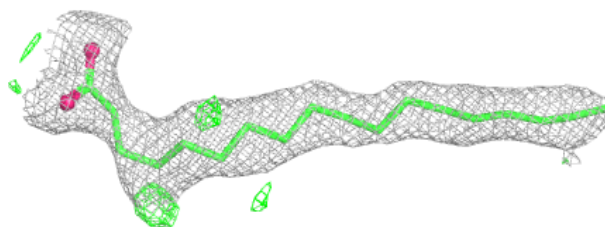
**Electron density around STE B 720:**

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

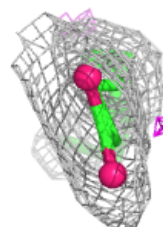
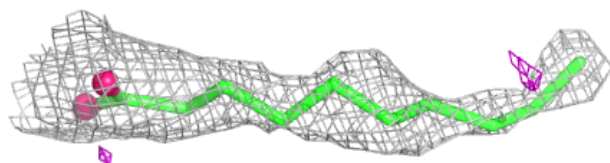
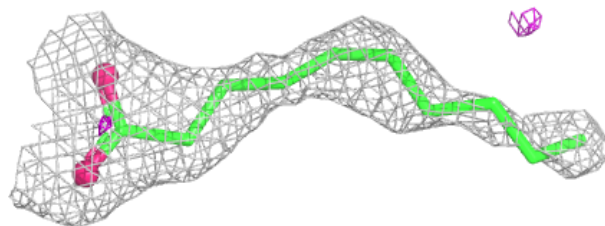


Electron density around STE c 521:

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

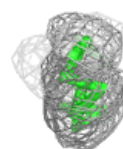
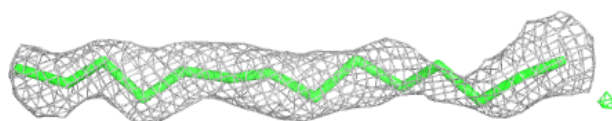
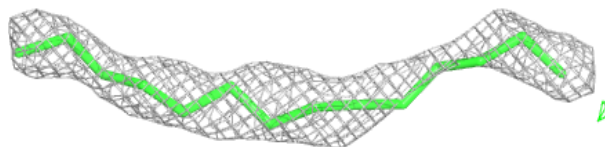
**Electron density around STE a 416:**

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

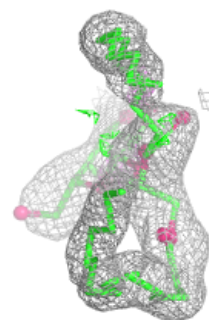
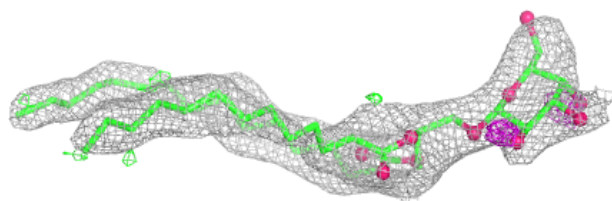
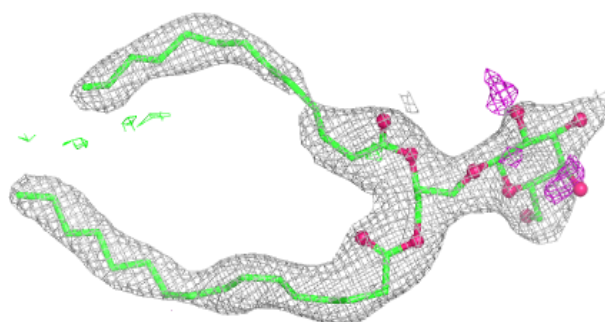


Electron density around STE h 704:

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

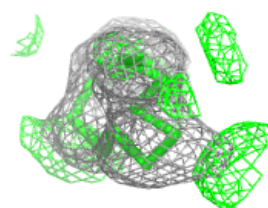
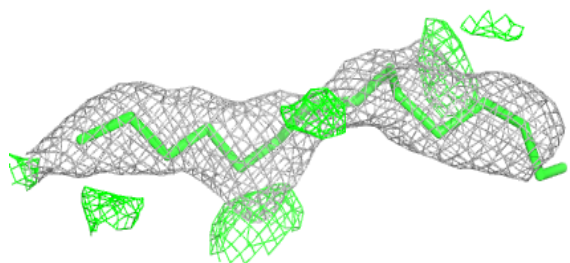
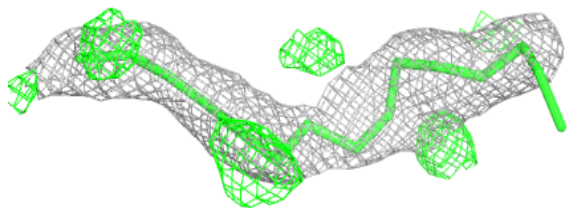
**Electron density around LMG C 516:**

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

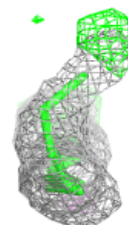
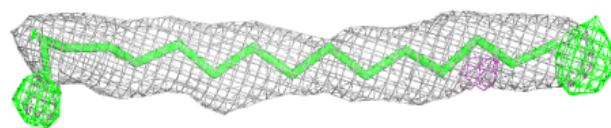
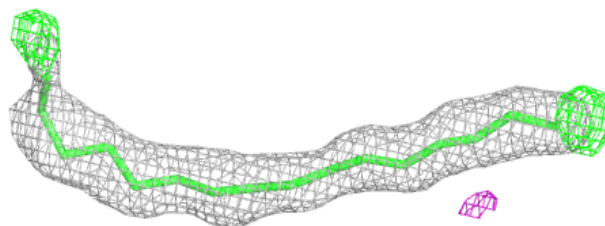


Electron density around STE a 417:

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

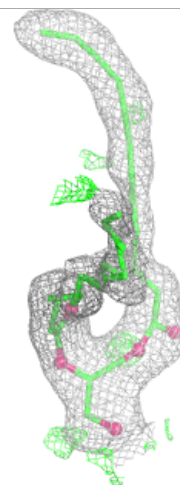
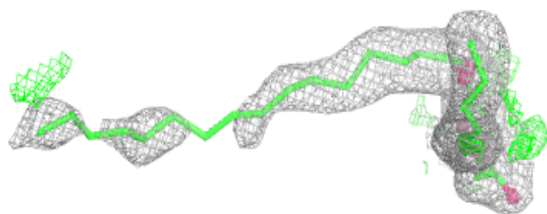
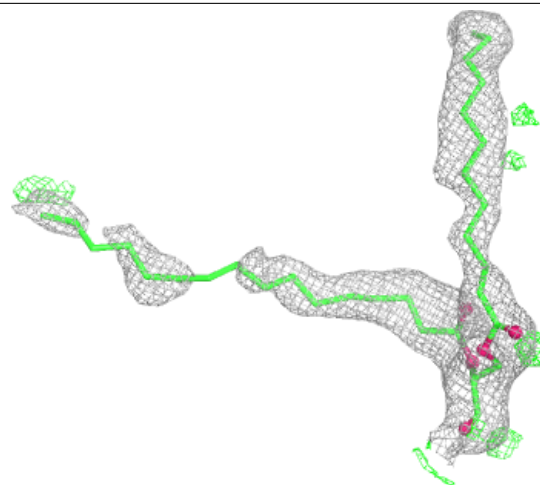
**Electron density around STE C 522:**

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



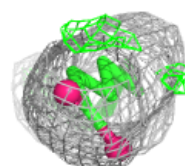
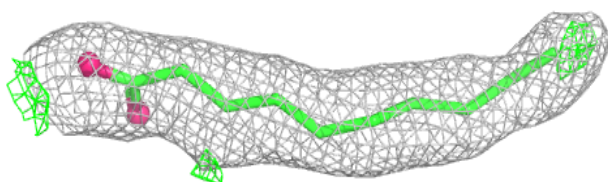
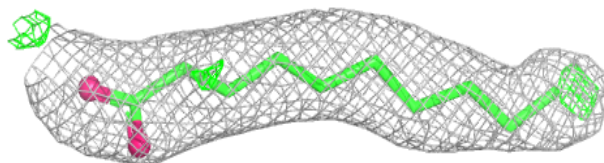
Electron density around SQD a 414:

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

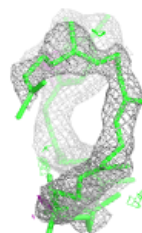
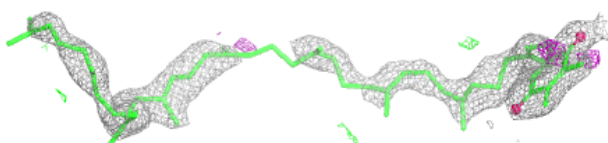
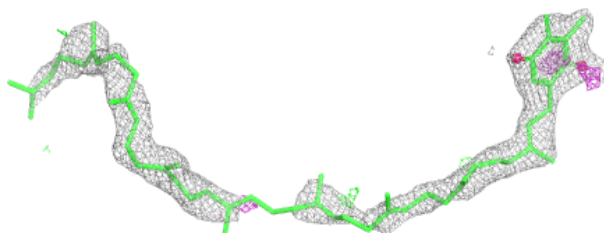


Electron density around STE j 101:

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

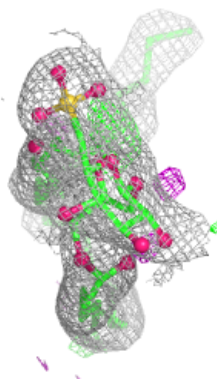
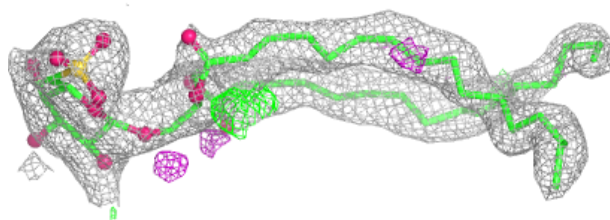
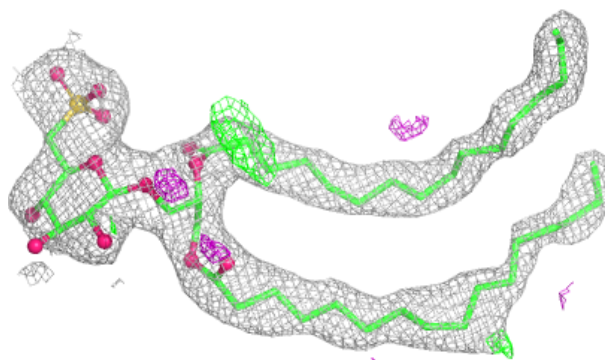
**Electron density around PL9 a 410:**

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

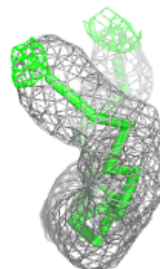
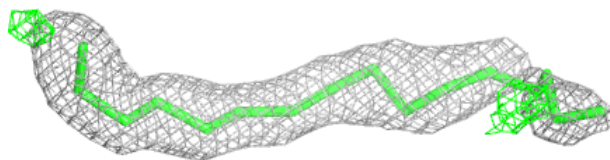
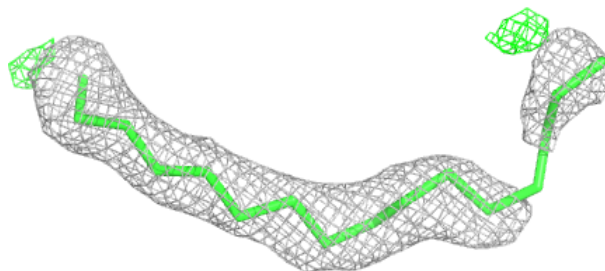


Electron density around SQD B 723:

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

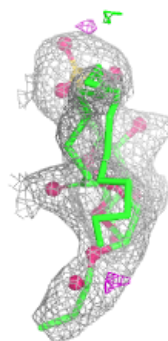
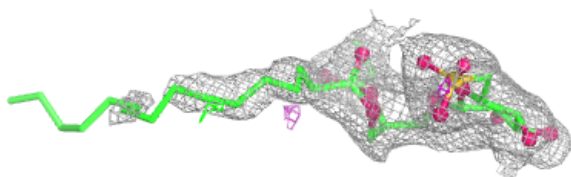
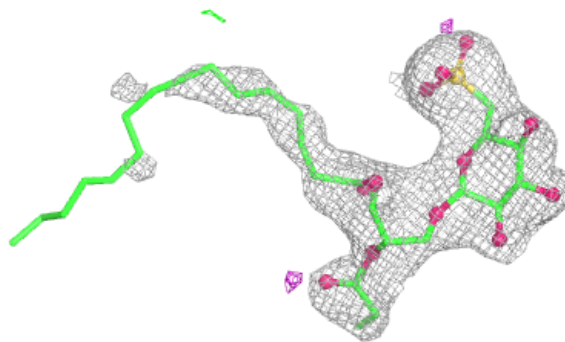
**Electron density around STE b 601:**

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

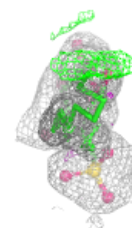
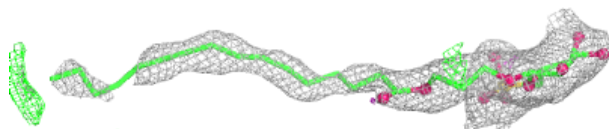
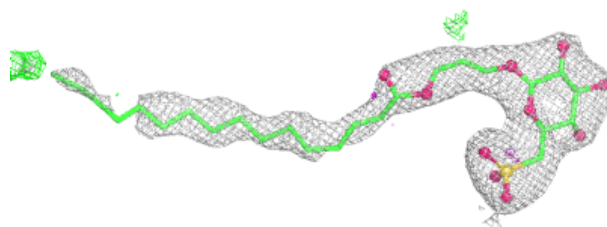


Electron density around SQD f 102:

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

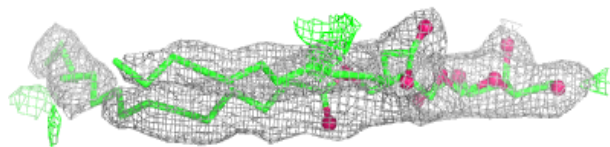
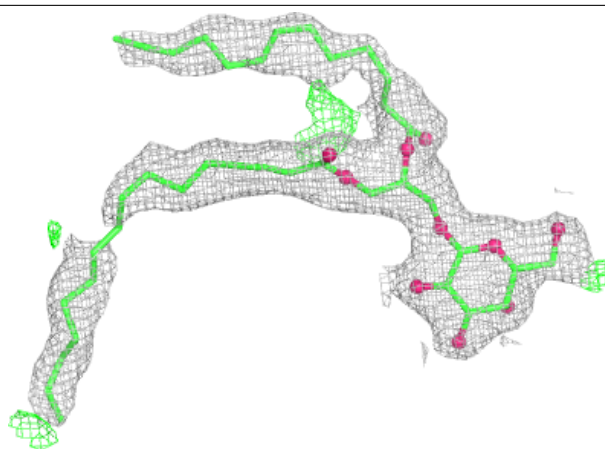
**Electron density around SQD D 410:**

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

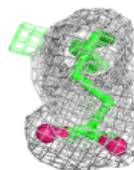
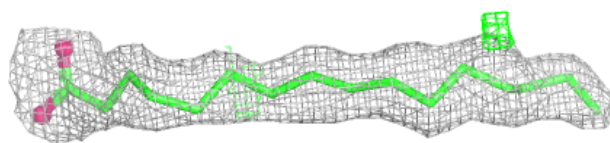
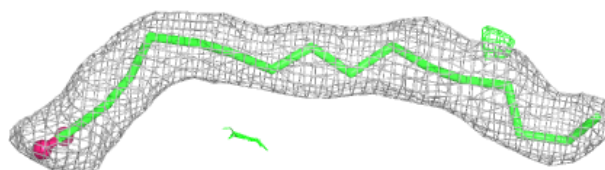


Electron density around LMG C 520:

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

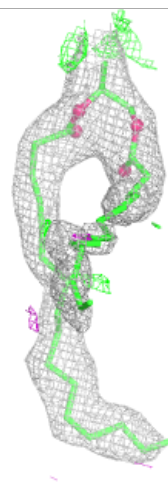
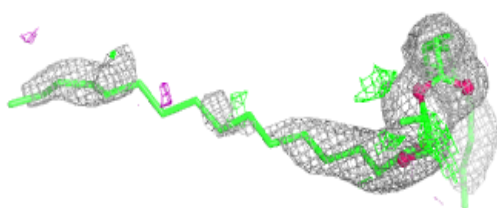
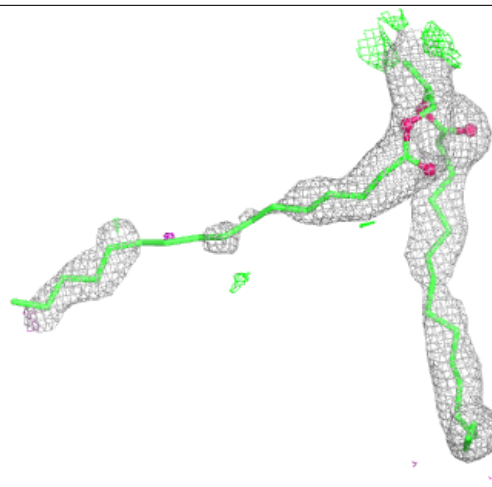
**Electron density around STE B 725:**

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



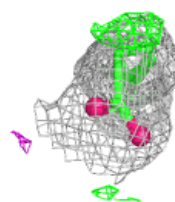
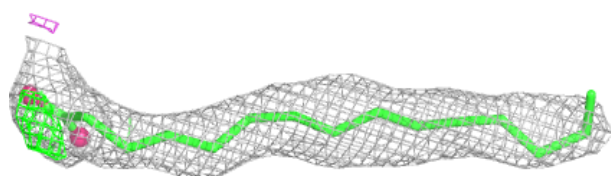
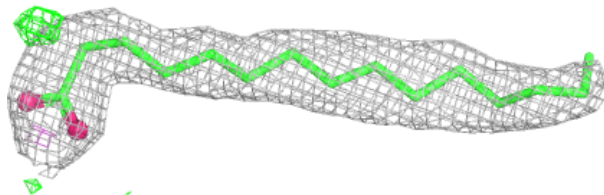
Electron density around SQD A 410:

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

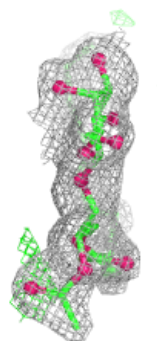
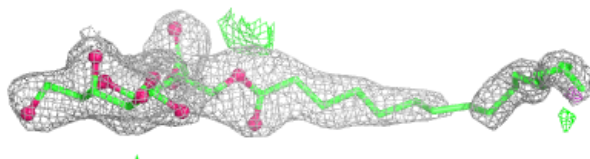


Electron density around STE d 411:

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

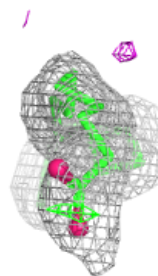
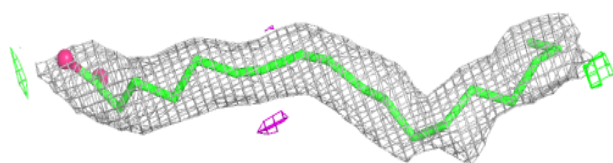
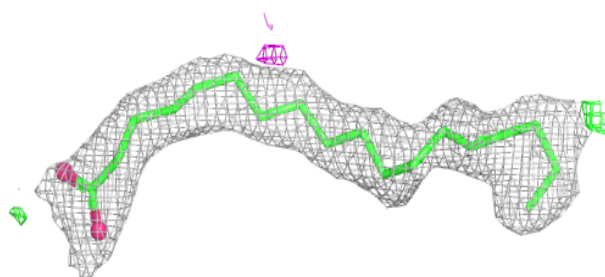
**Electron density around LMG c 520:**

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

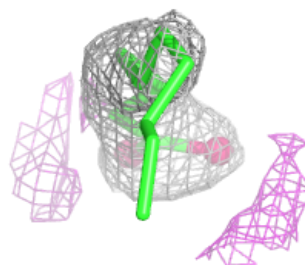
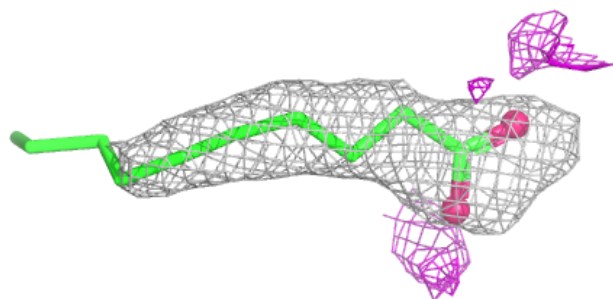
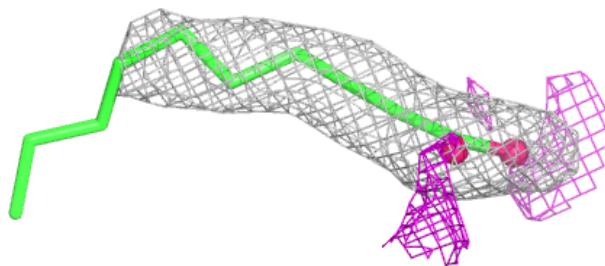


Electron density around STE b 621:

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

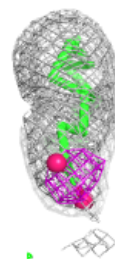
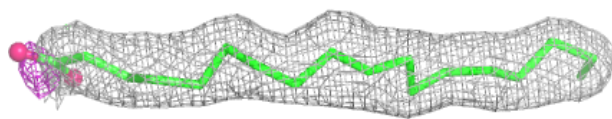
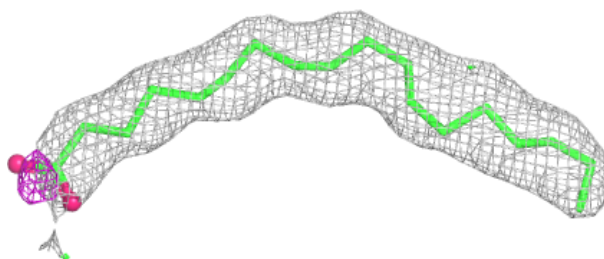
**Electron density around STE B 701:**

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

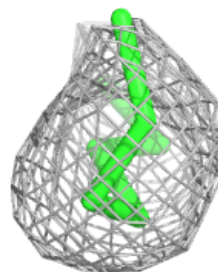
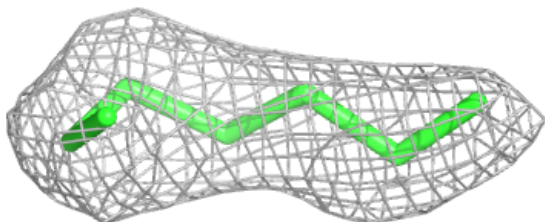
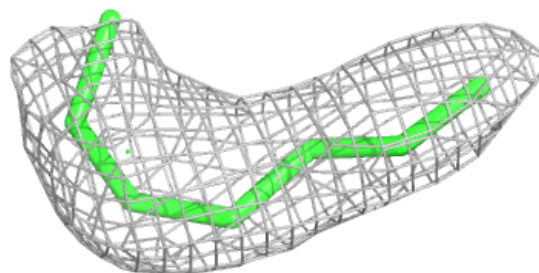


Electron density around STE X 101:

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

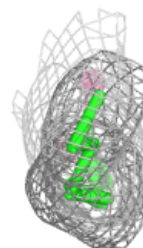
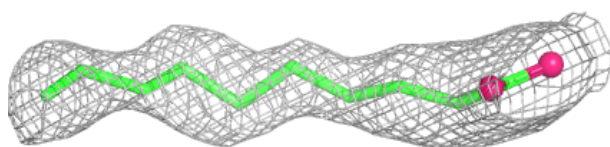
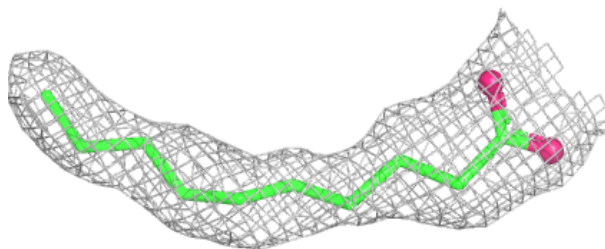
**Electron density around STE E 103:**

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

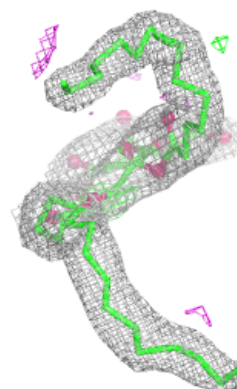
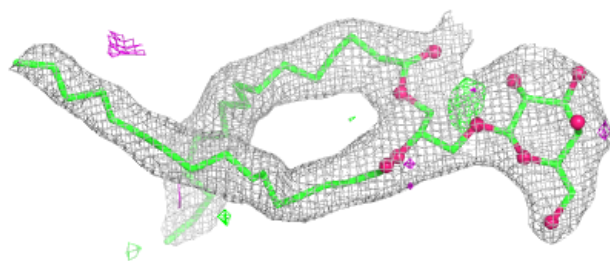
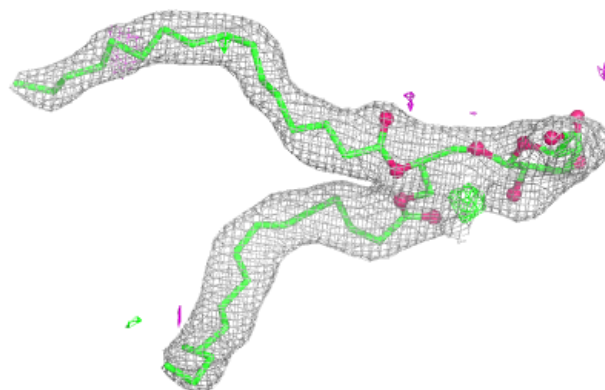


Electron density around STE C 521:

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

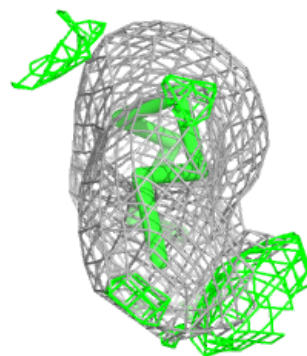
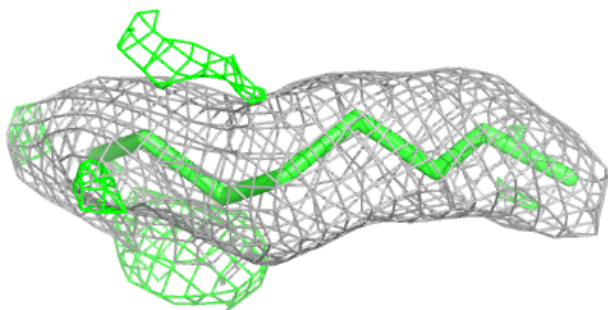
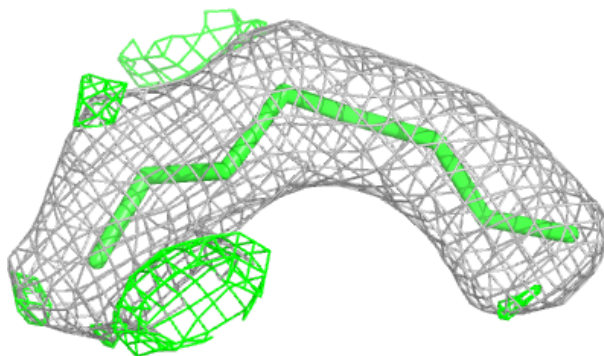
**Electron density around LMG b 620:**

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

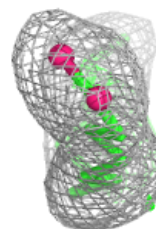
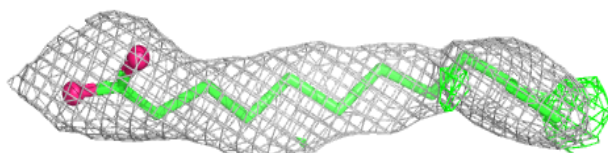
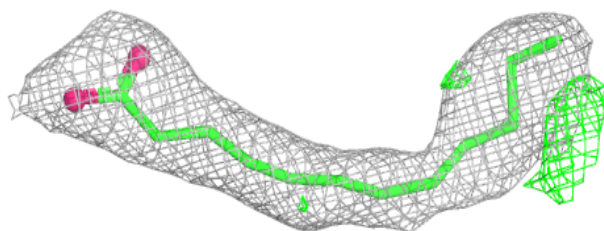


Electron density around STE H 104:

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

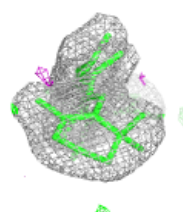
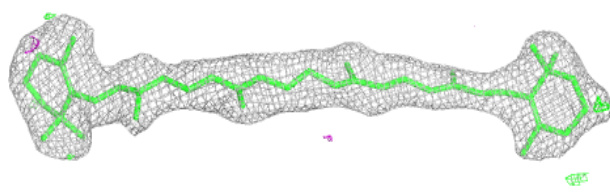
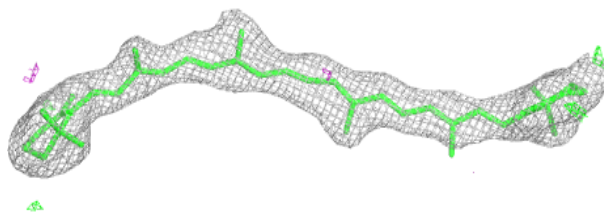
**Electron density around STE t 702:**

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

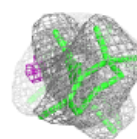
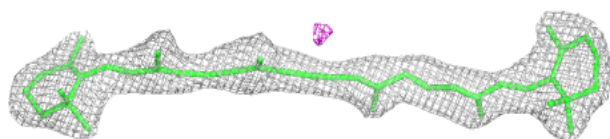
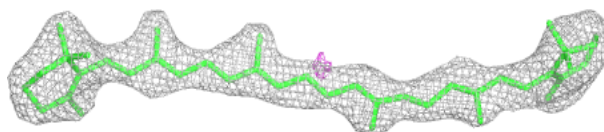


Electron density around BCR h 702:

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

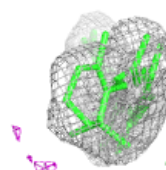
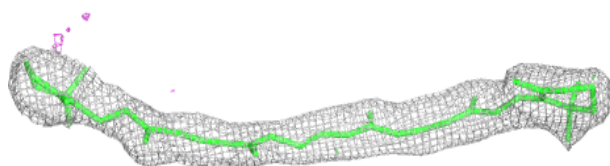
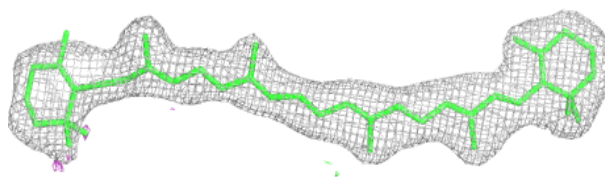
**Electron density around BCR c 515:**

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

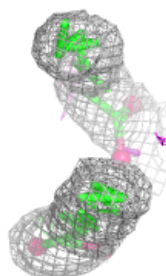
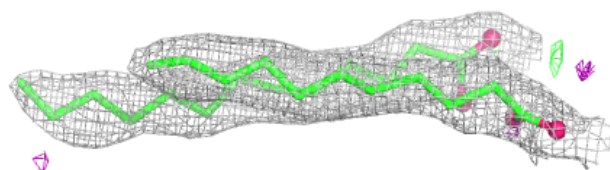
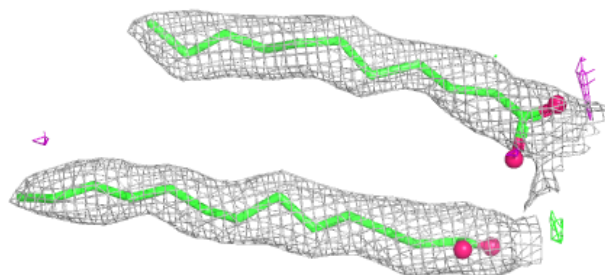


Electron density around BCR d 405:

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

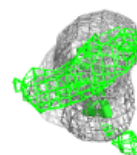
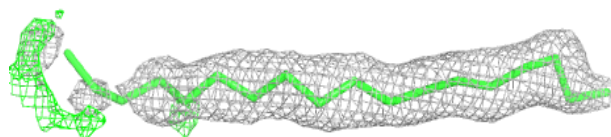
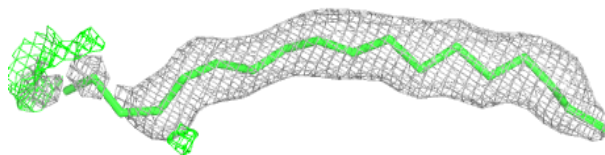
**Electron density around LMG B 721:**

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

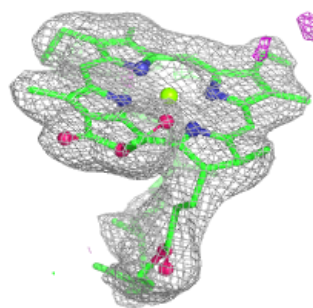
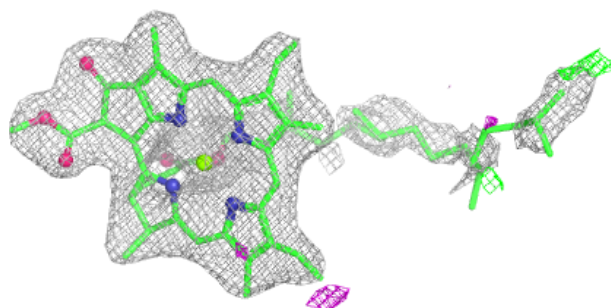
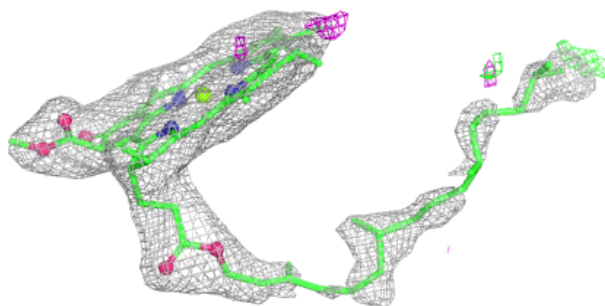


Electron density around STE m 101:

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

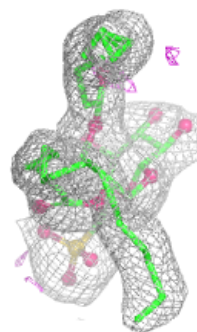
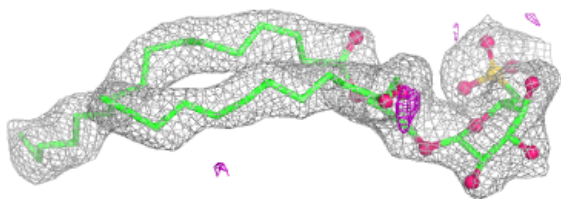
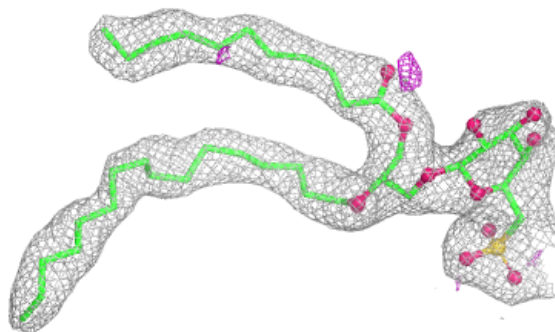
**Electron density around CLA C 514:**

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

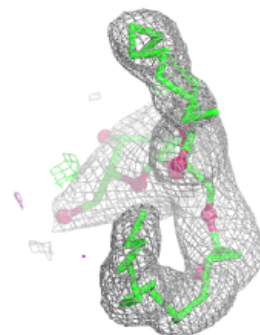
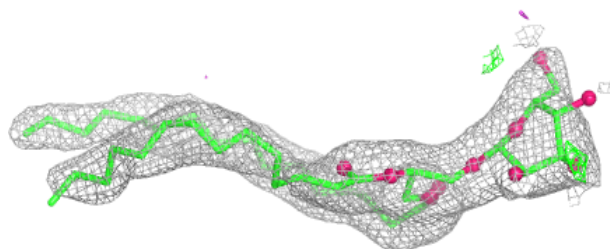
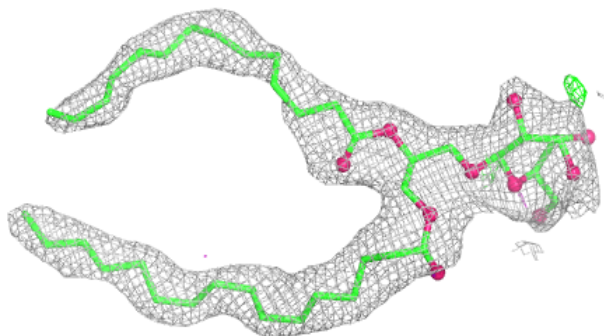


Electron density around SQD 1 101:

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

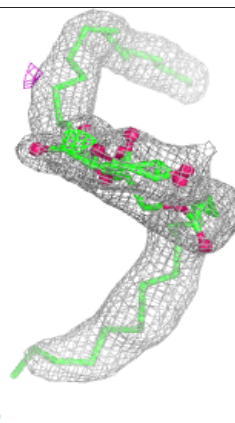
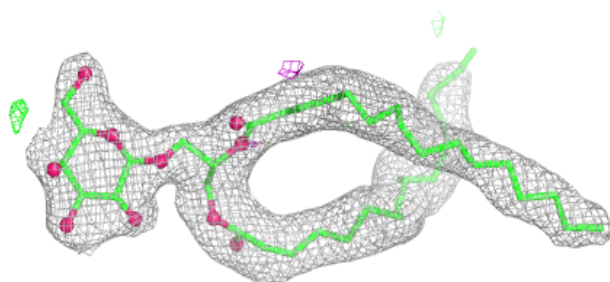
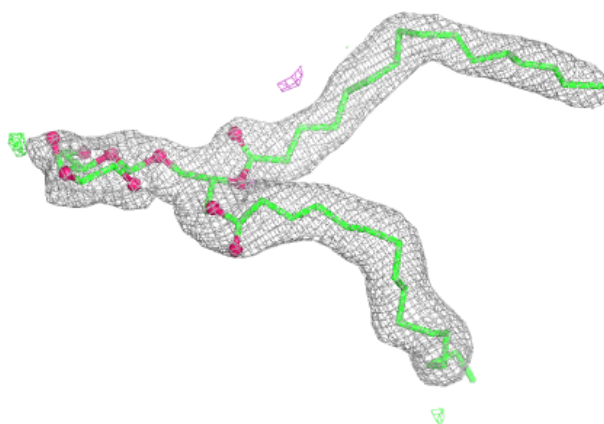
**Electron density around LMG c 523:**

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

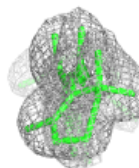
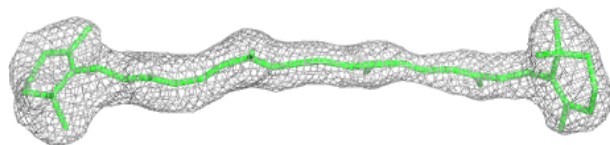
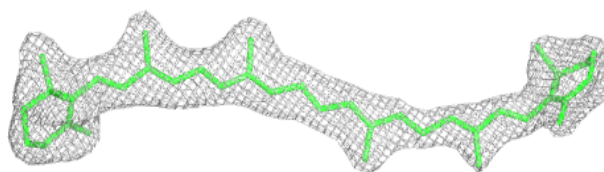


Electron density around LMG M 101:

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

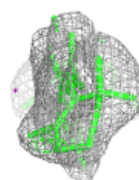
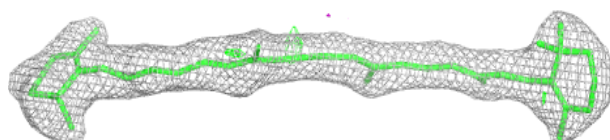
**Electron density around BCR k 101:**

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

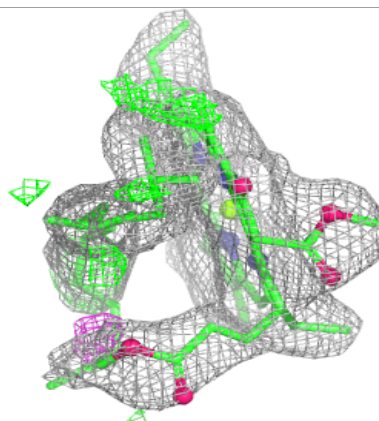
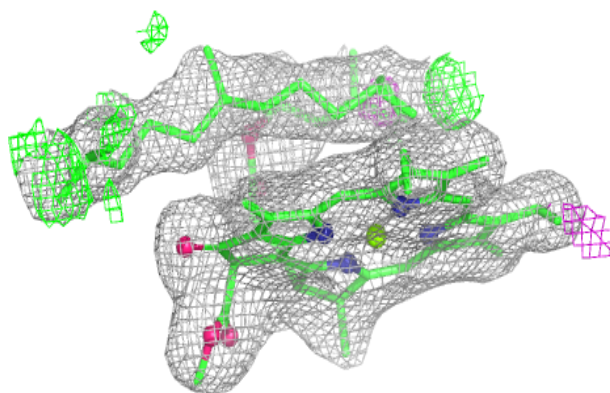
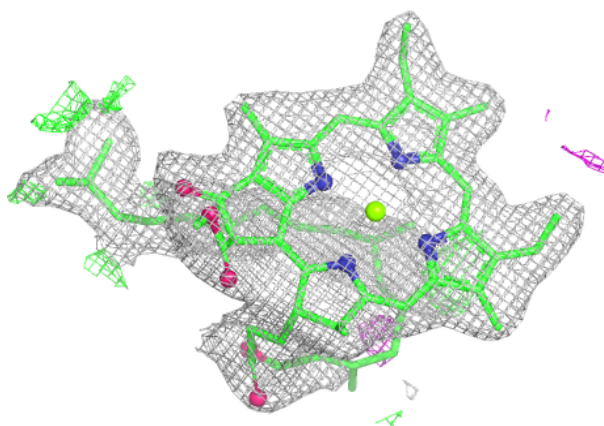


Electron density around BCR Y 101:

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

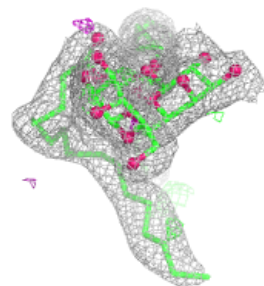
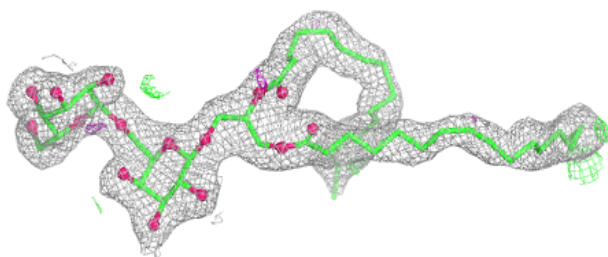
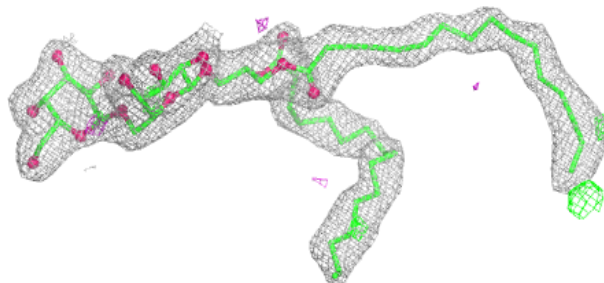
**Electron density around CLA B 727:**

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

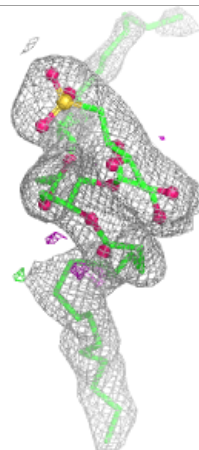
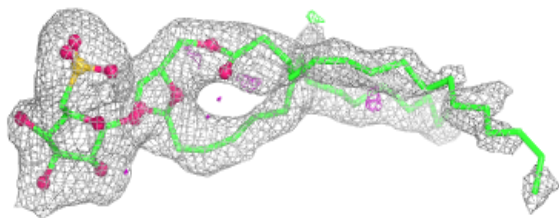
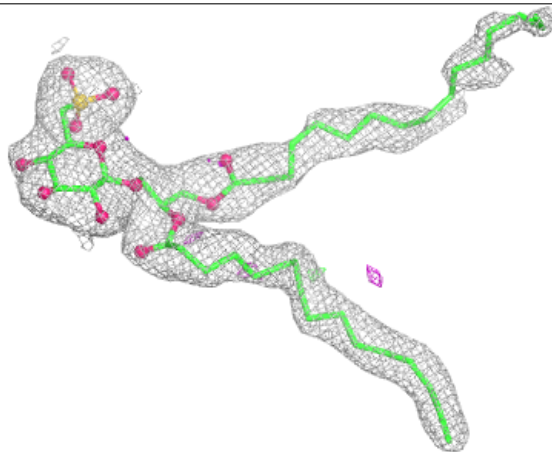


Electron density around DGD H 102:

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

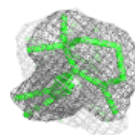
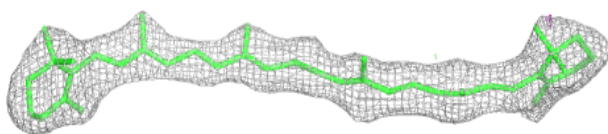
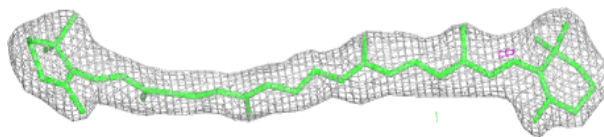
**Electron density around SQD a 412:**

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

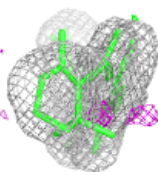
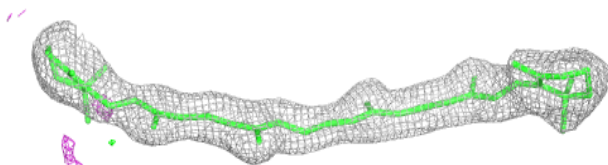
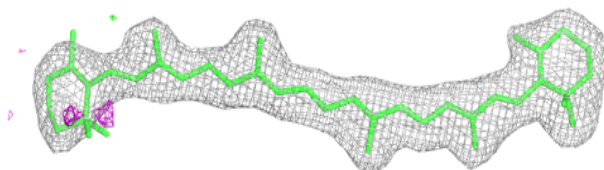


Electron density around BCR C 524:

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

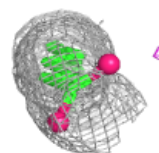
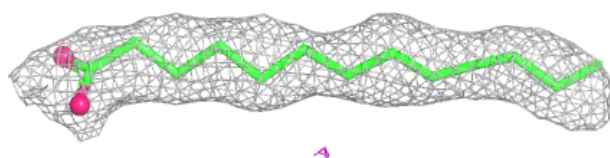
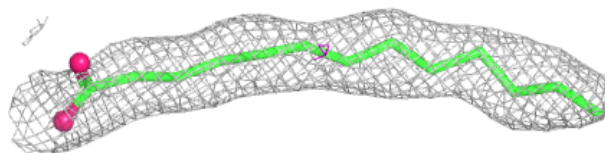
**Electron density around BCR D 405:**

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

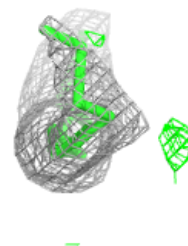
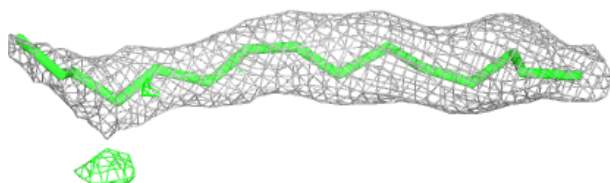
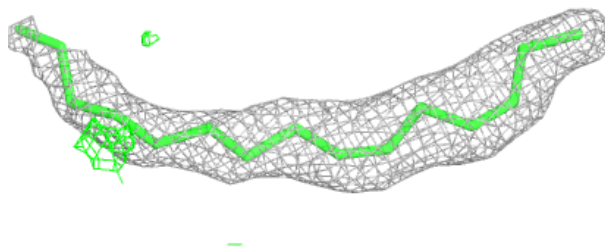


Electron density around STE M 102:

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

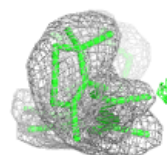
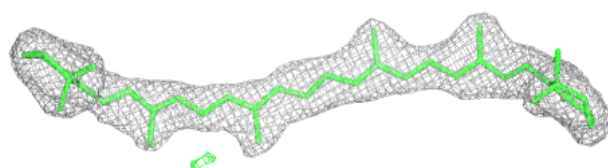
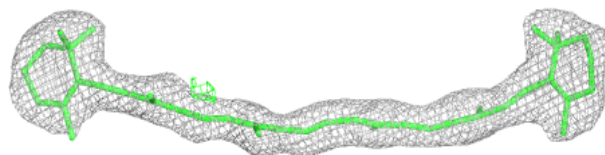
**Electron density around STE T 702:**

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



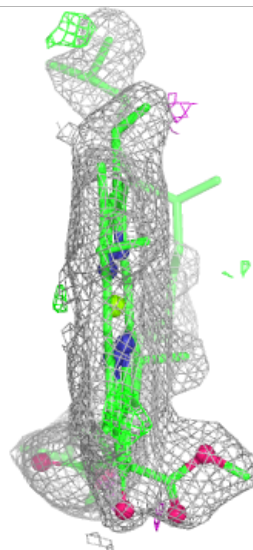
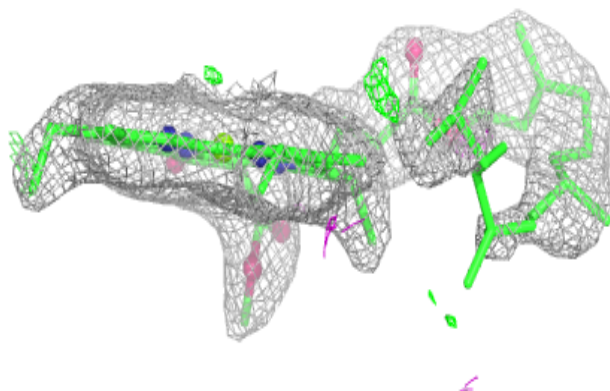
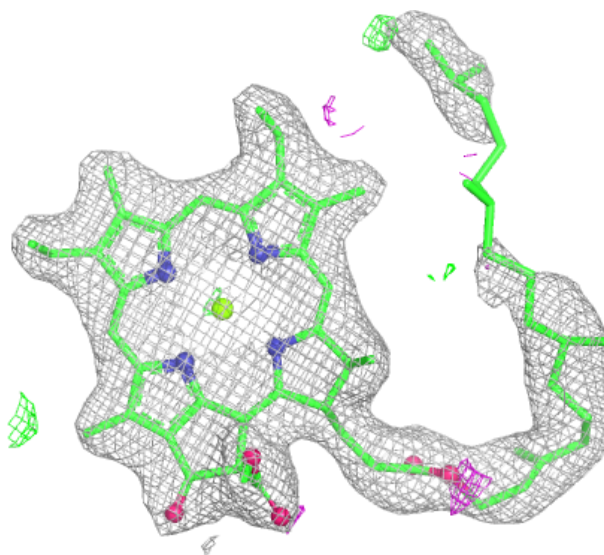
Electron density around BCR k 102:

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



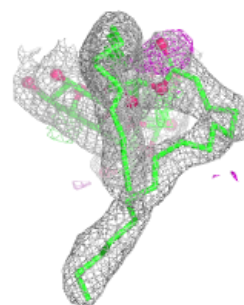
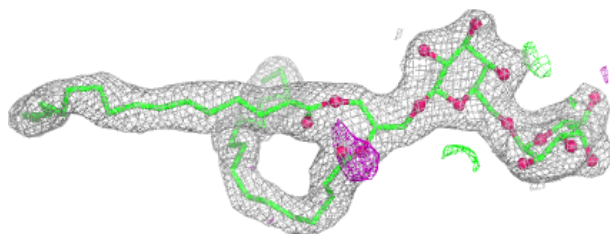
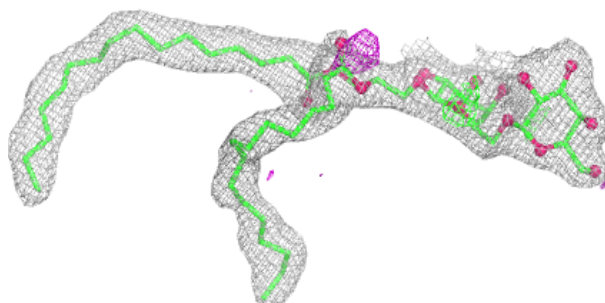
Electron density around CLA c 513:

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

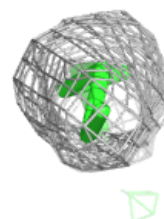
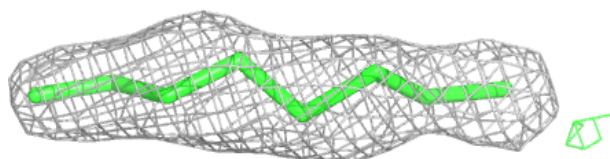
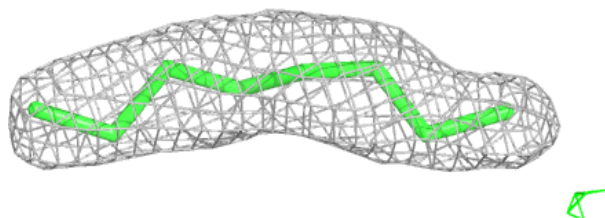


Electron density around DGD h 703:

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

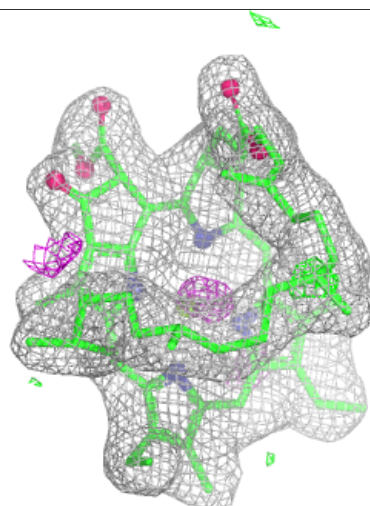
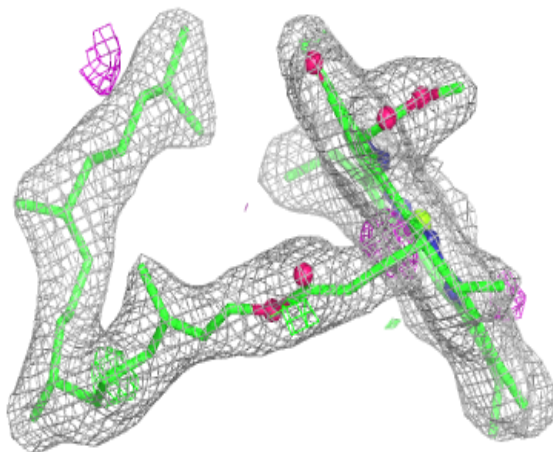
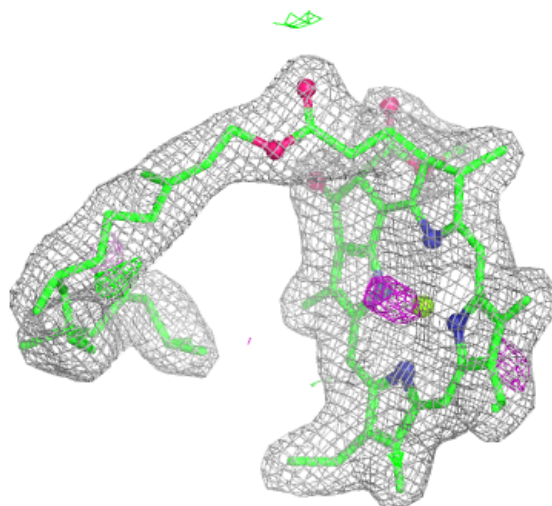
**Electron density around STE Z 101:**

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



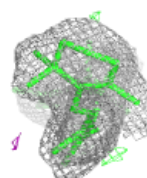
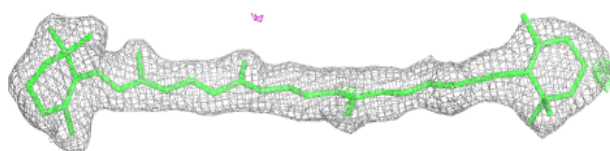
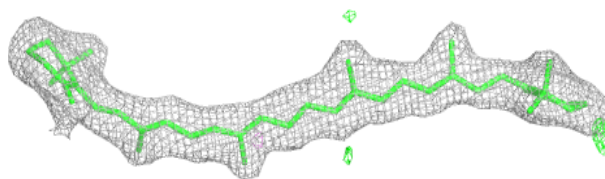
Electron density around CLA C 504:

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

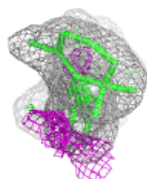
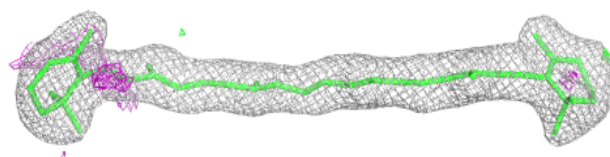
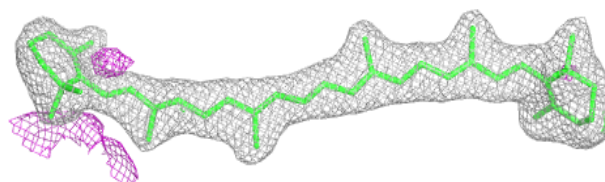


Electron density around BCR H 101:

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

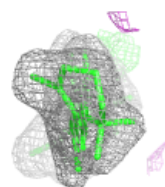
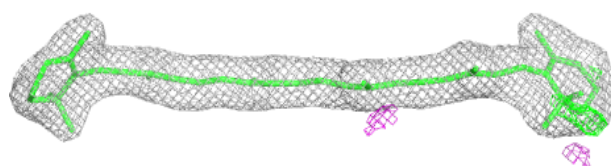
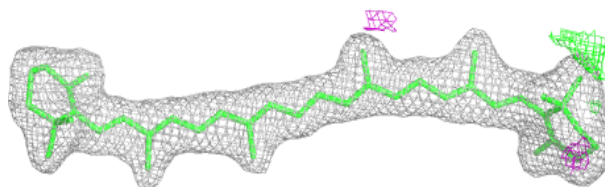
**Electron density around BCR B 718:**

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

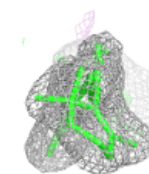
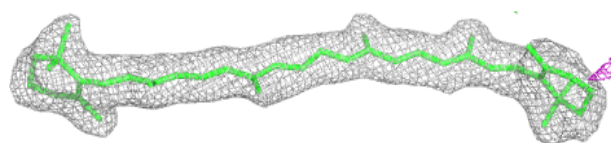
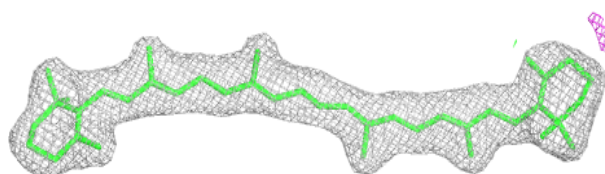


Electron density around BCR b 618:

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

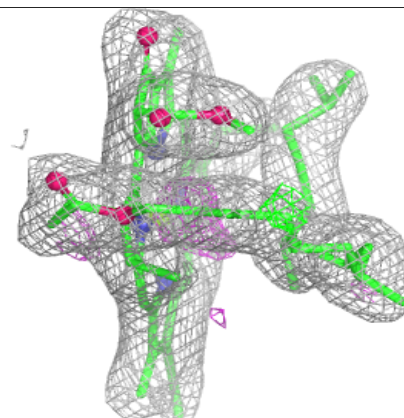
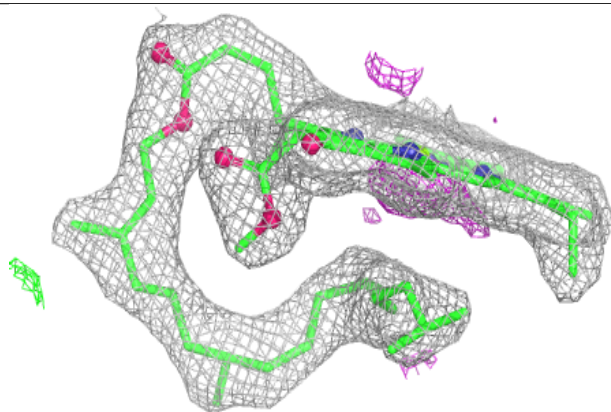
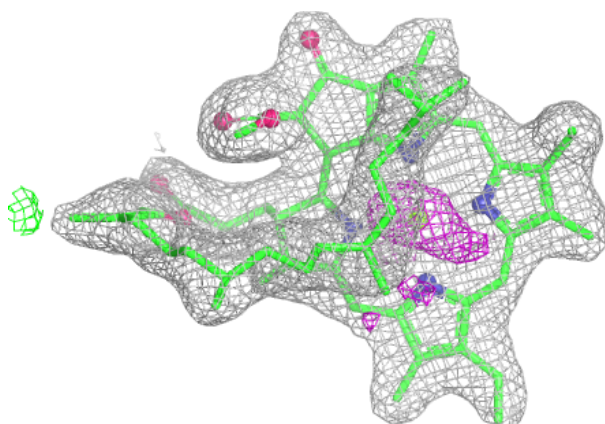
**Electron density around BCR b 619:**

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

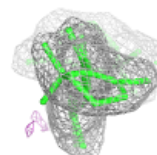
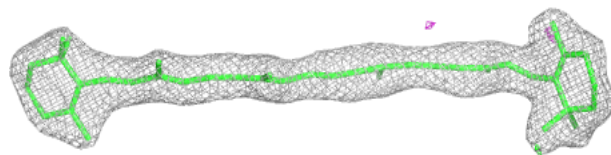
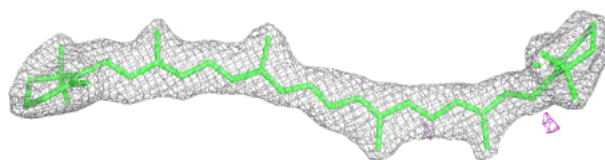


Electron density around CLA C 511:

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

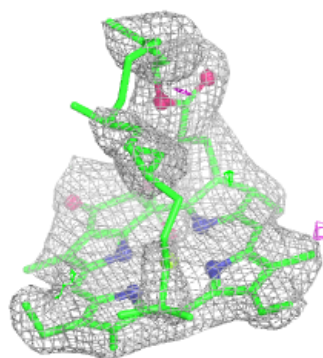
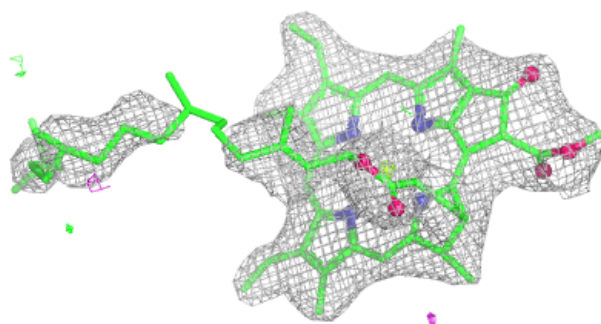
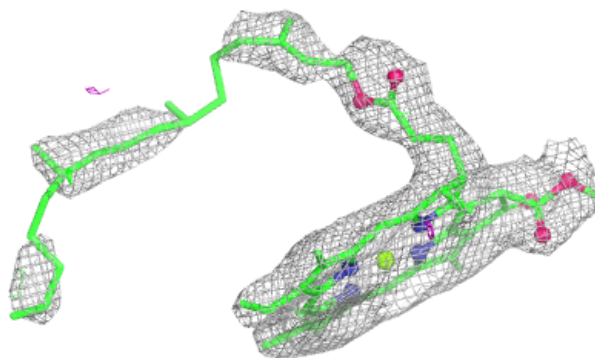
**Electron density around BCR c 516:**

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

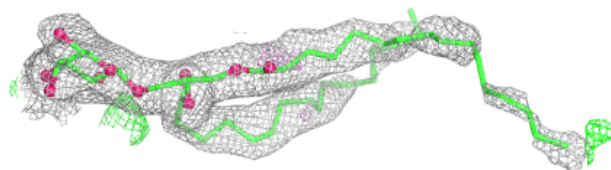


Electron density around CLA c 514:

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

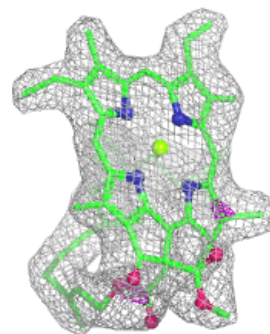
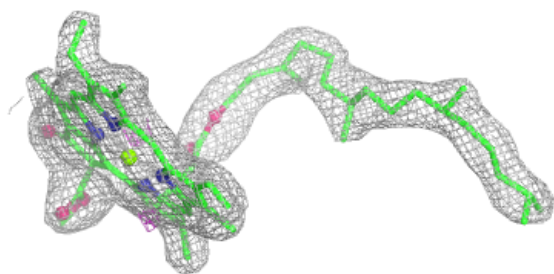
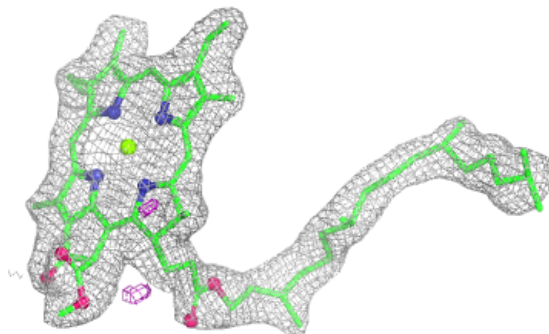
**Electron density around LMG D 409:**

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



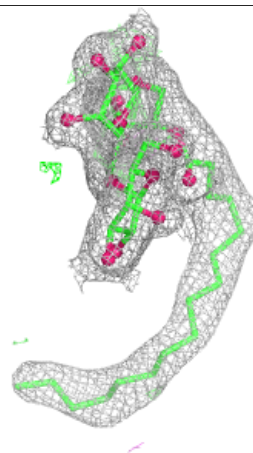
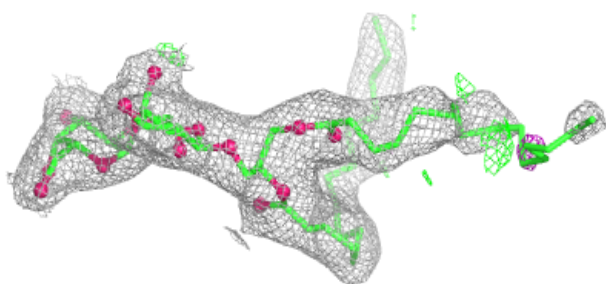
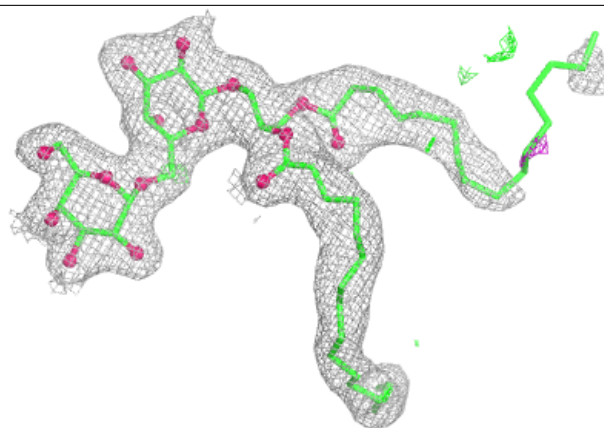
Electron density around CLA C 512:

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



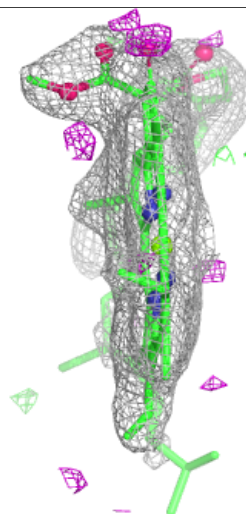
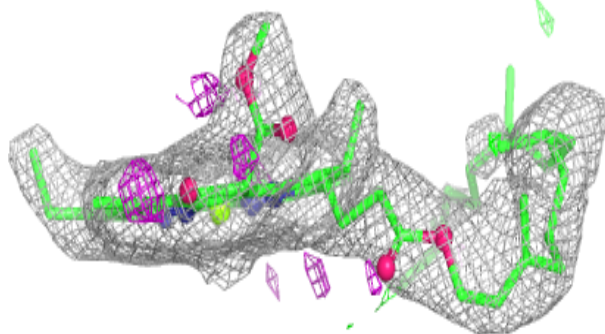
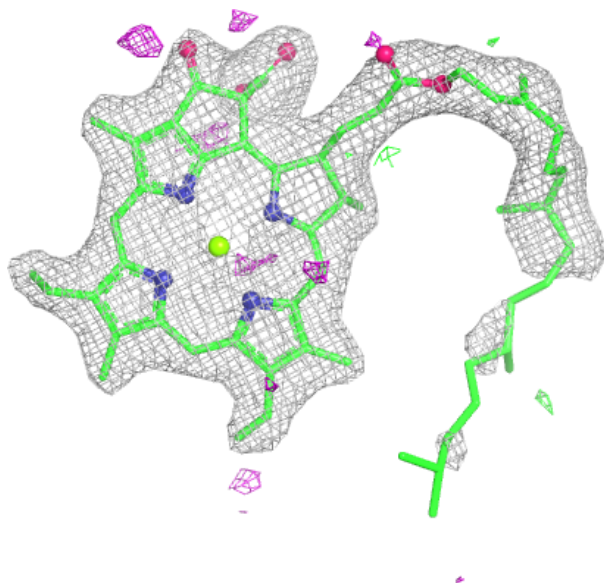
Electron density around DGD C 518:

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



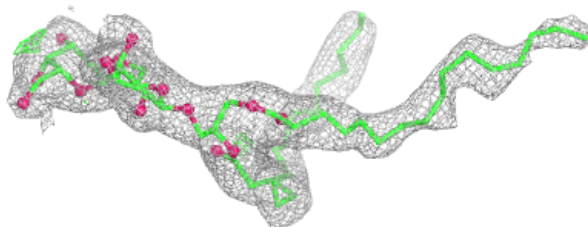
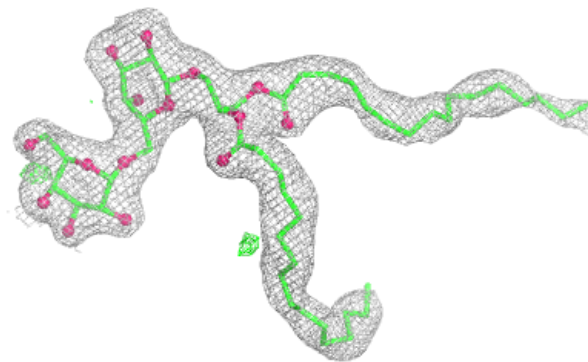
Electron density around CLA C 513:

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



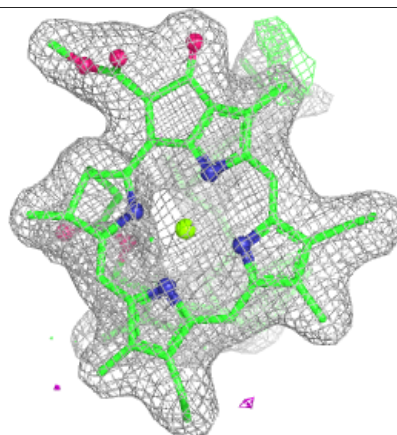
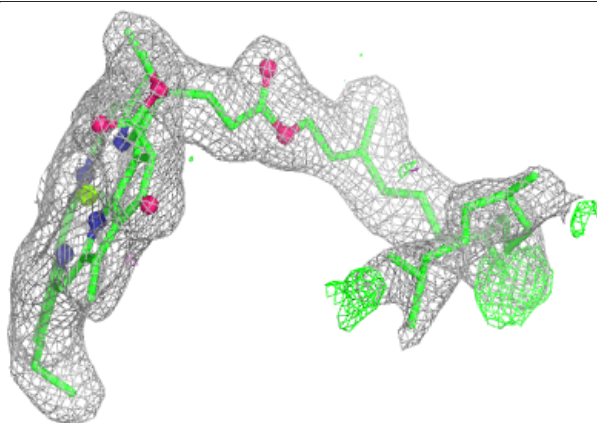
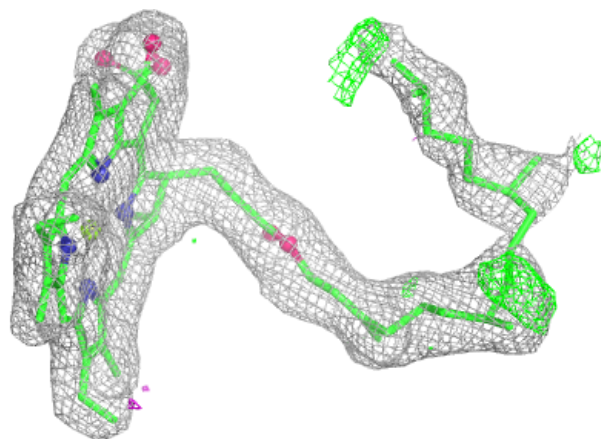
Electron density around DGD c 518:

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



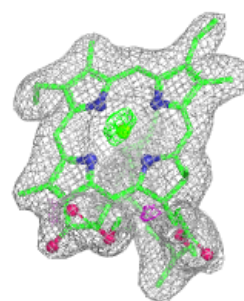
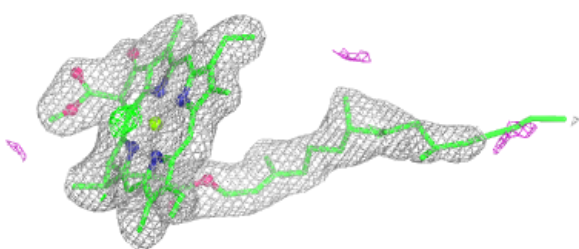
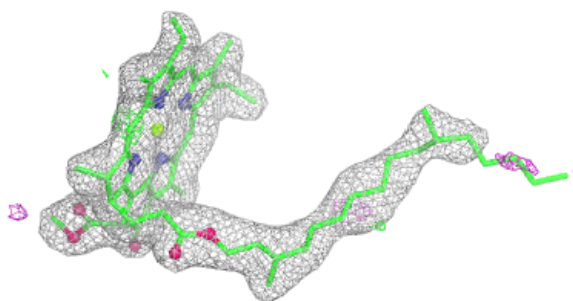
Electron density around CLA B 706:

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



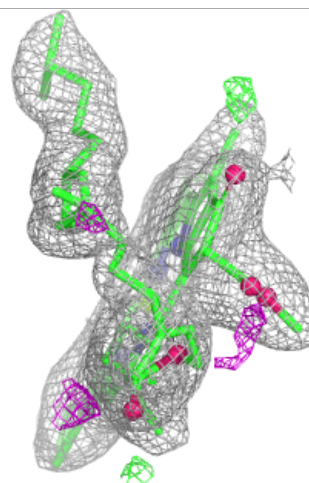
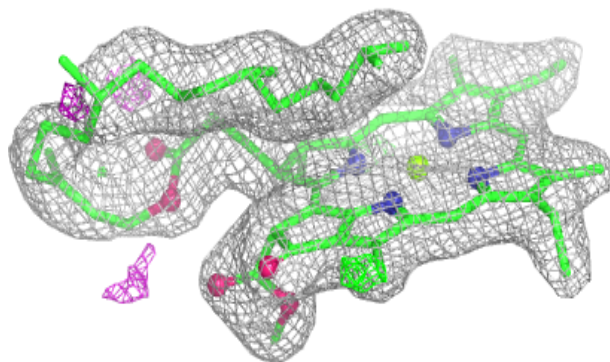
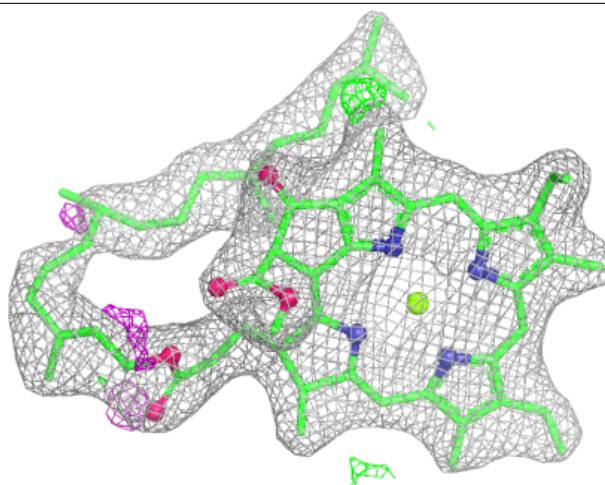
Electron density around CLA c 509:

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



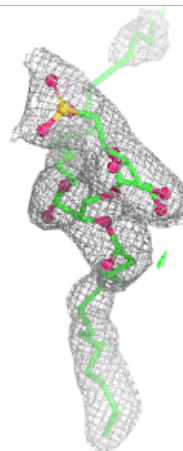
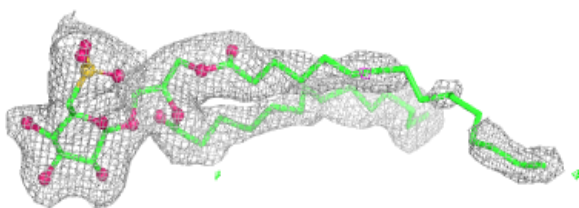
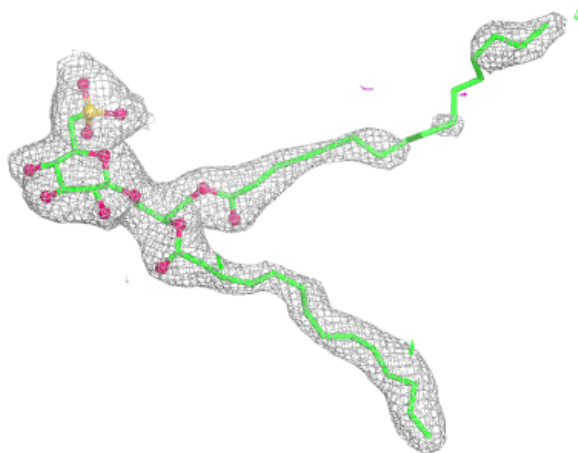
Electron density around CLA c 510:

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



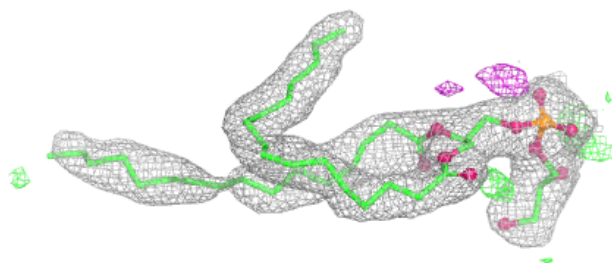
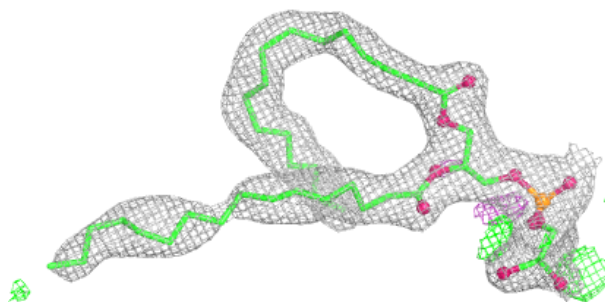
Electron density around SQD A 409:

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

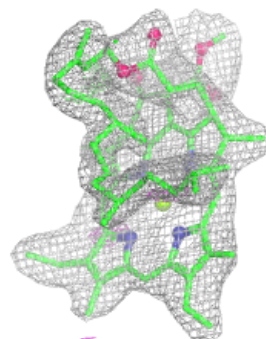
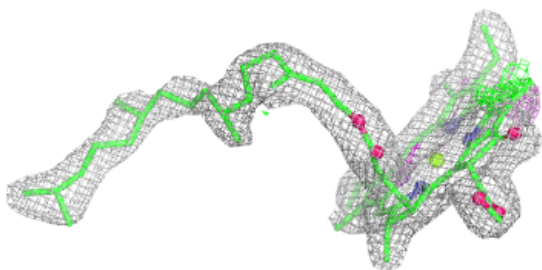
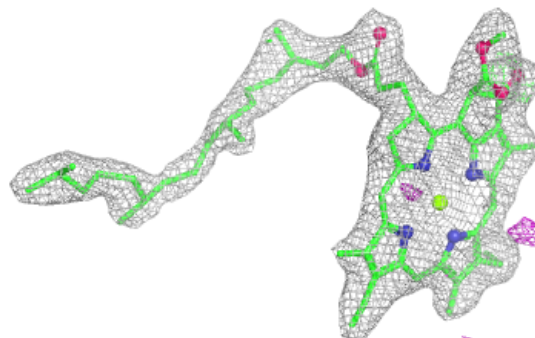


Electron density around LHG B 722:

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

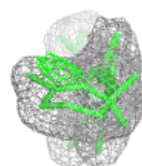
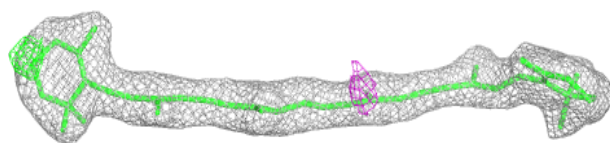
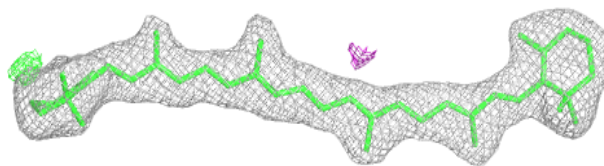
**Electron density around CLA c 512:**

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



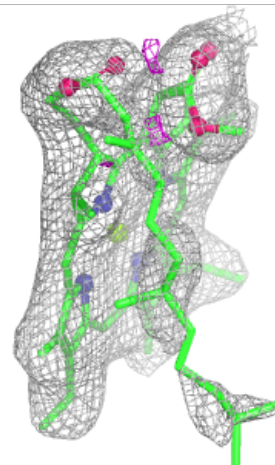
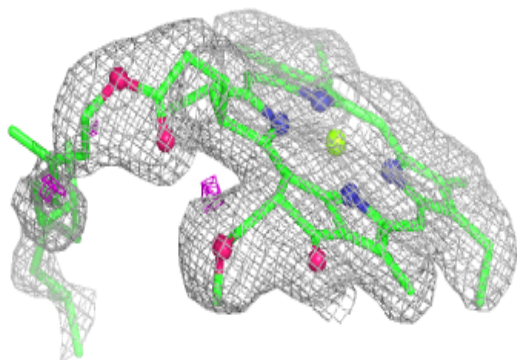
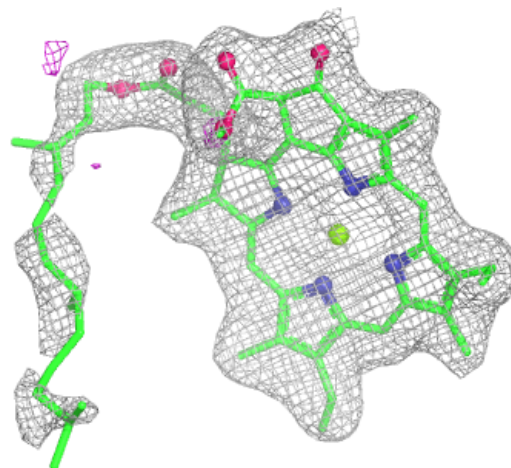
Electron density around BCR b 617:

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



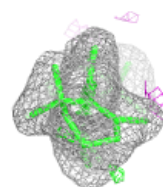
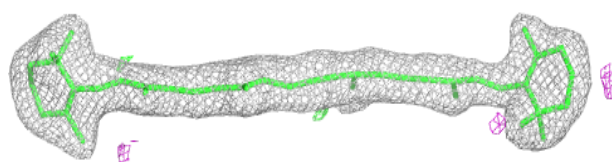
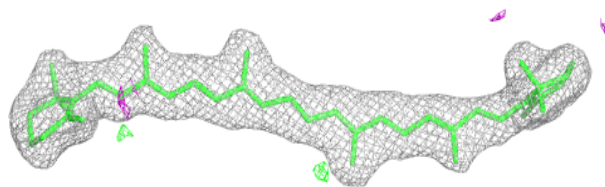
Electron density around CLA b 616:

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

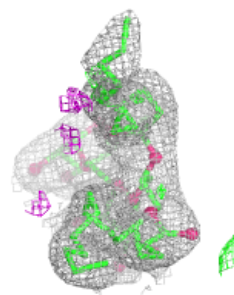
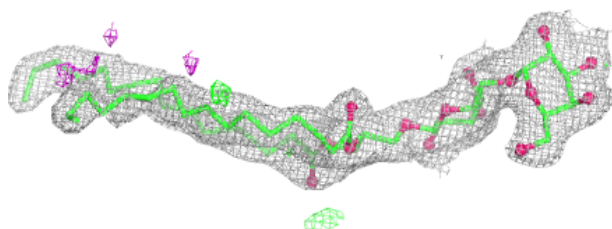
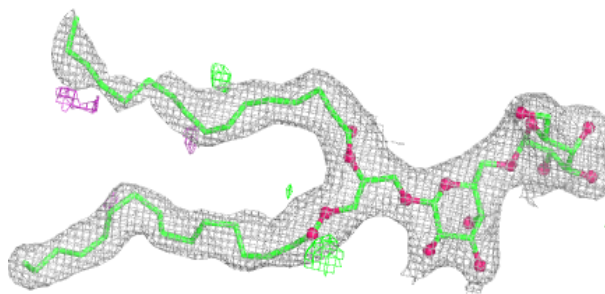


Electron density around BCR A 405:

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

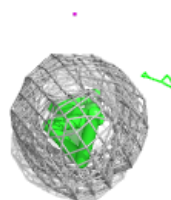
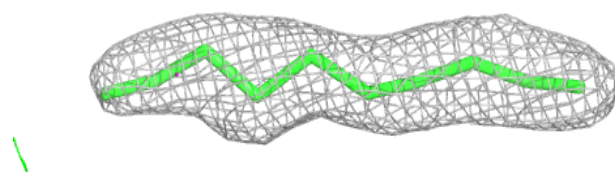
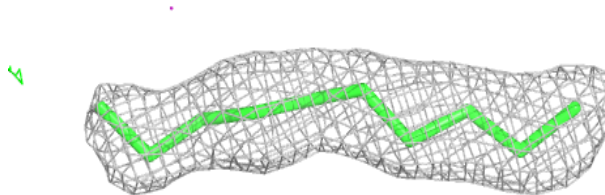
**Electron density around DGD C 519:**

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

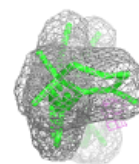
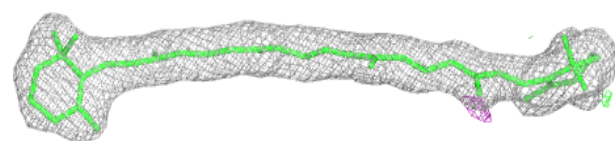
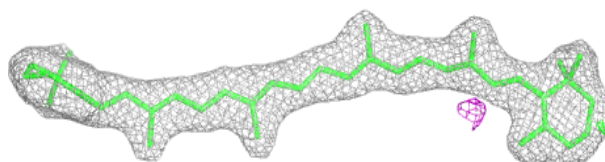


Electron density around STE M 103:

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

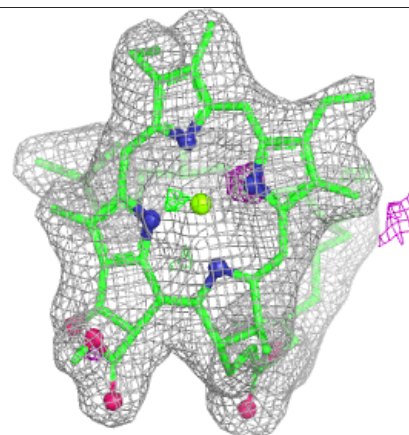
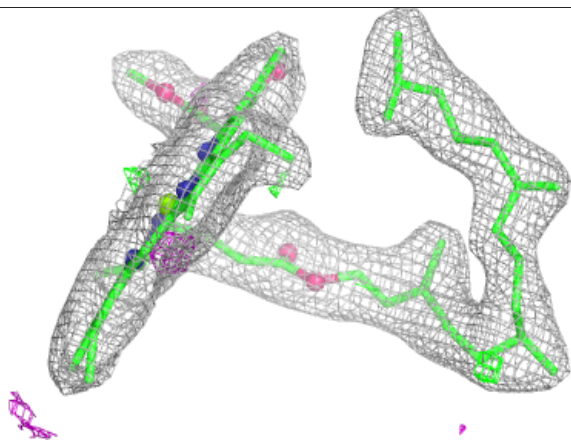
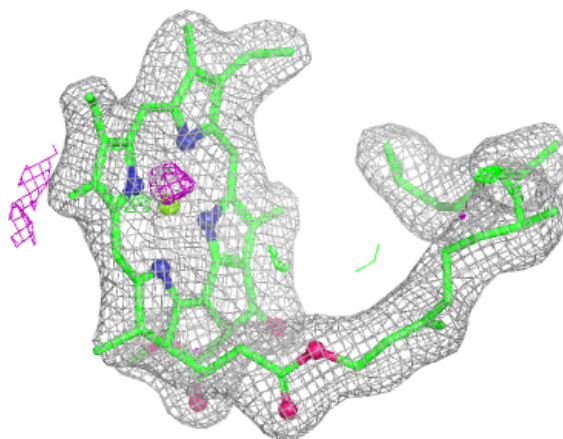
**Electron density around BCR B 717:**

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

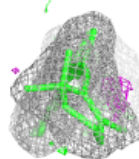
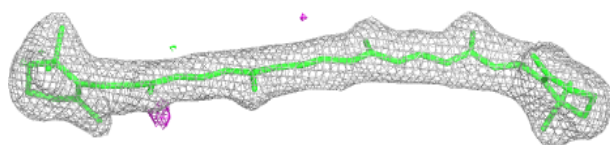
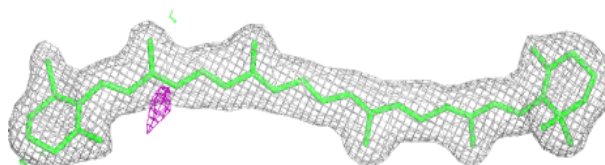


Electron density around CLA c 504:

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

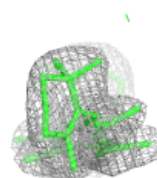
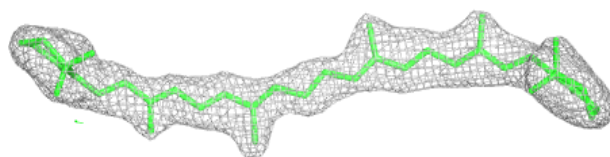
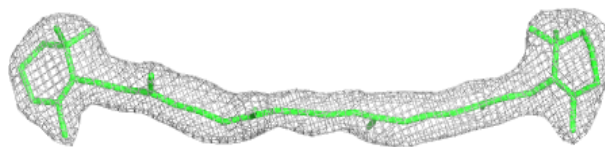
**Electron density around BCR B 719:**

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

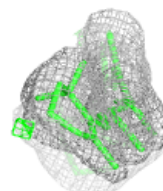
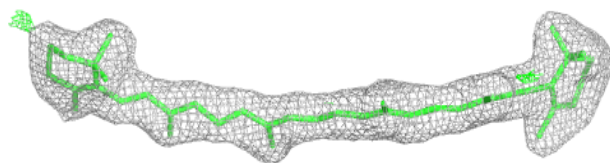
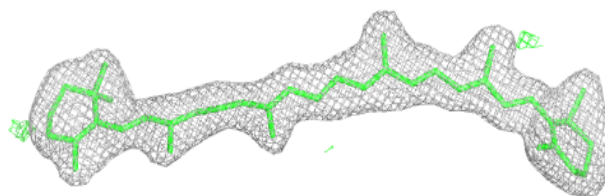


Electron density around BCR C 501:

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

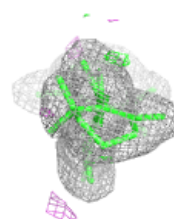
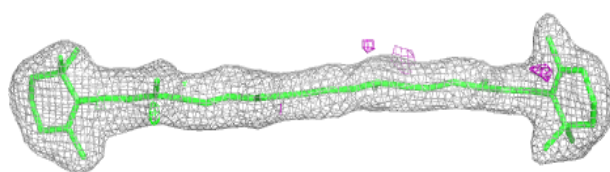
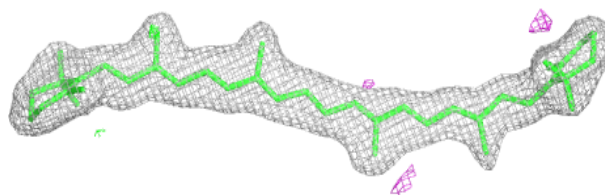
**Electron density around BCR t 701:**

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

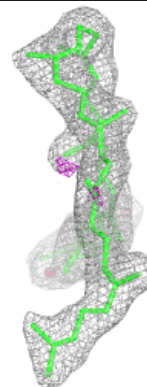
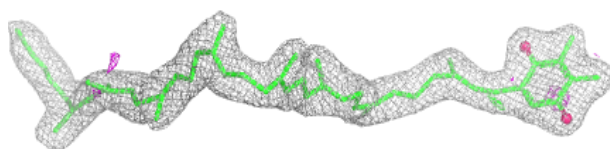
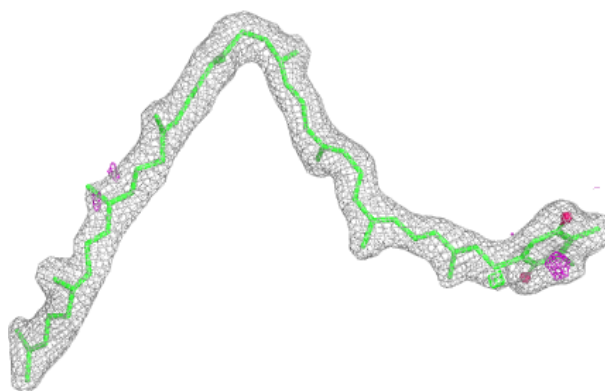


Electron density around BCR C 515:

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

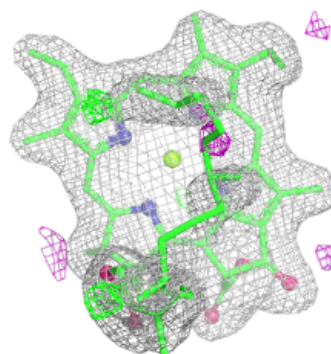
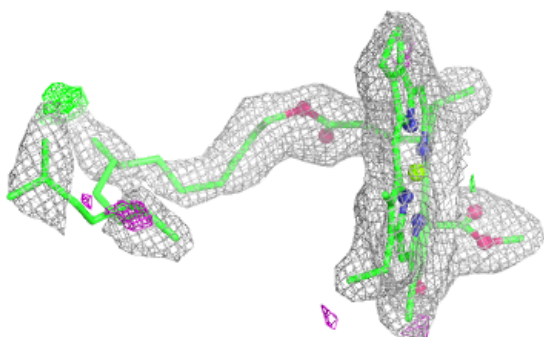
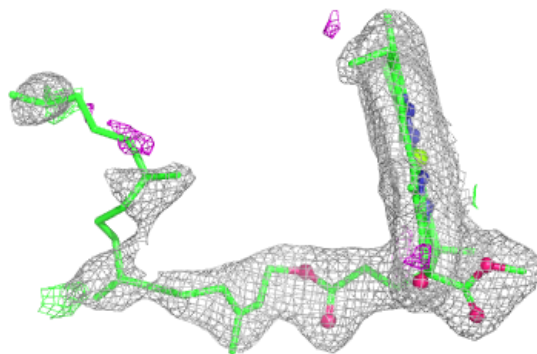
**Electron density around PL9 D 406:**

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



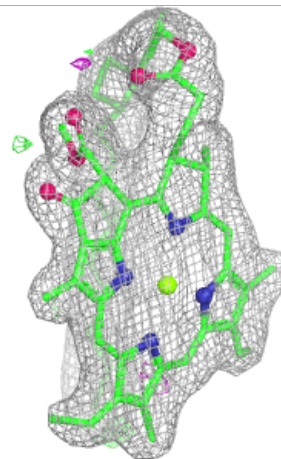
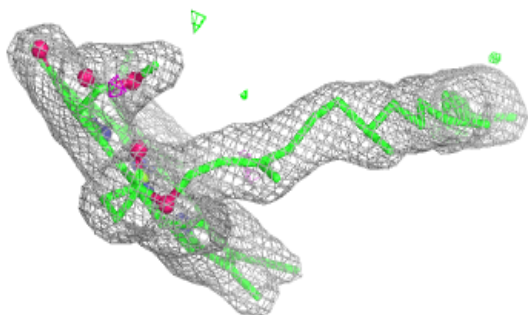
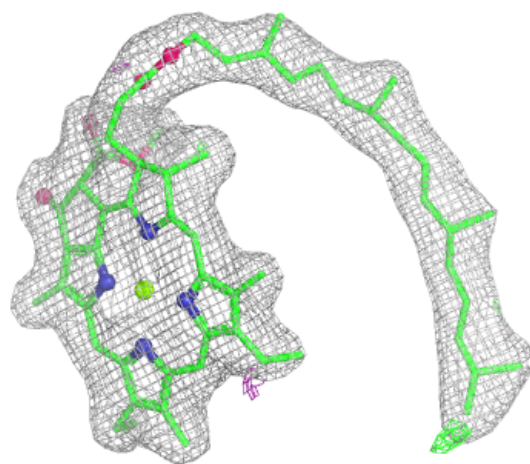
Electron density around CLA c 507:

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



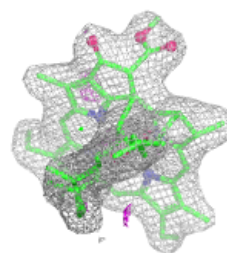
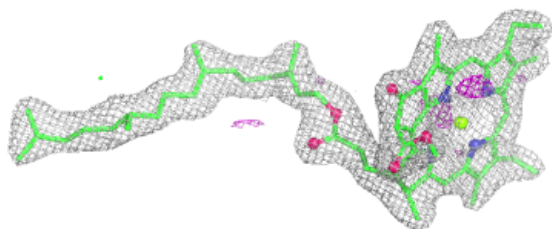
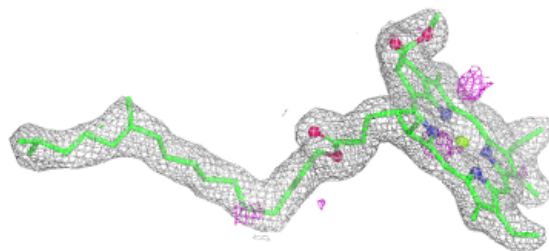
Electron density around CLA c 508:

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

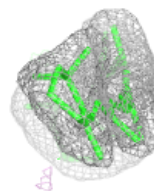
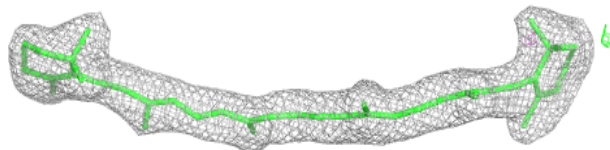
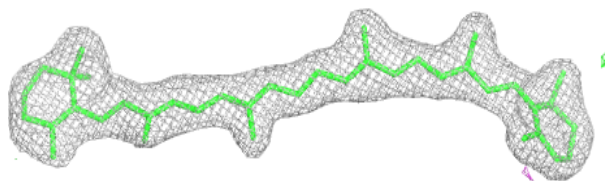


Electron density around CLA C 503:

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

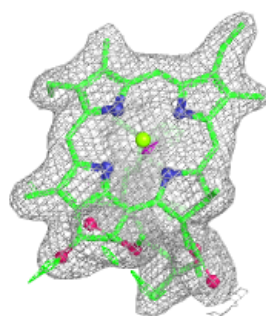
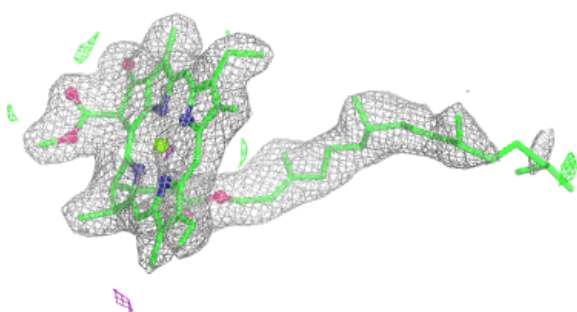
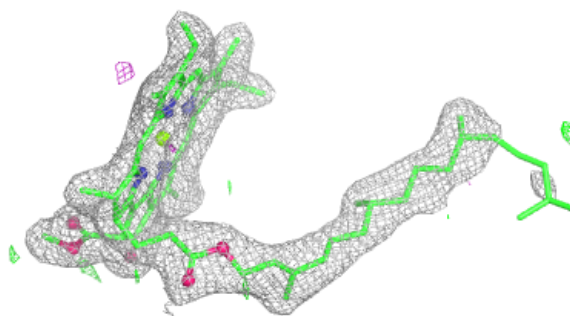
**Electron density around BCR T 701:**

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

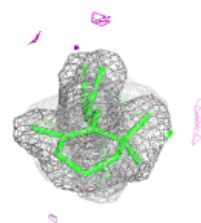
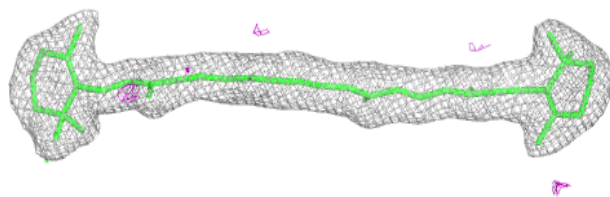
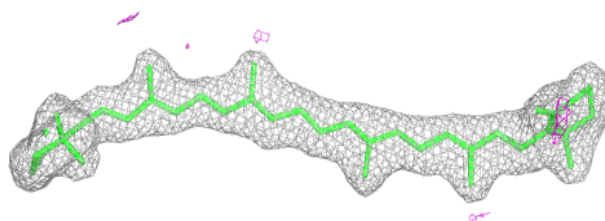


Electron density around CLA C 509:

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

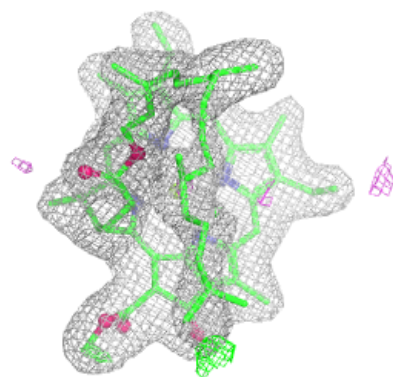
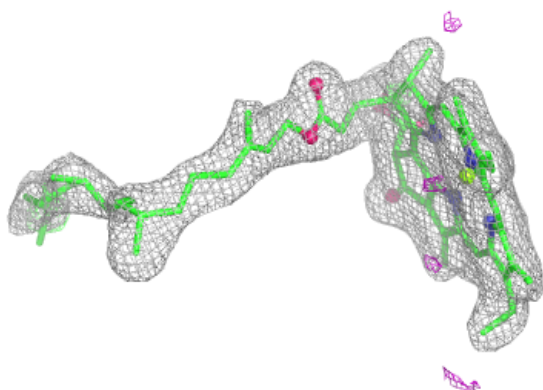
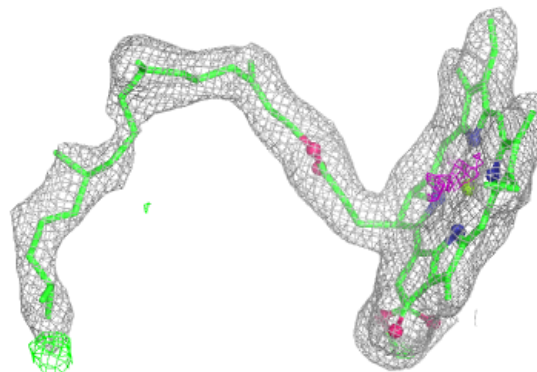
**Electron density around BCR a 406:**

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

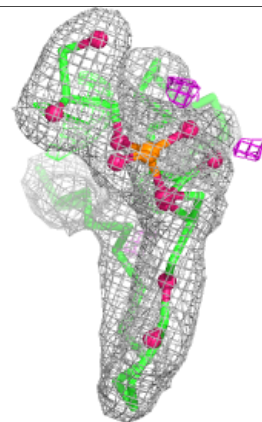
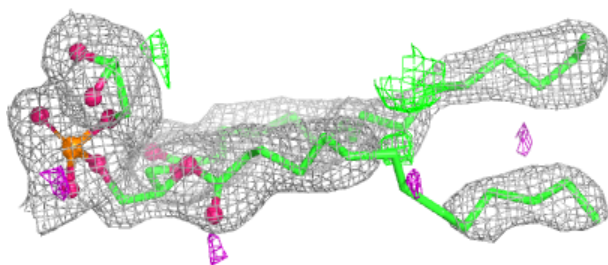
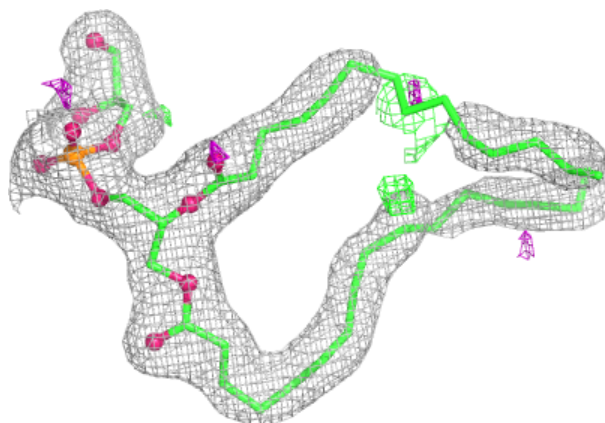


Electron density around CLA b 606:

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

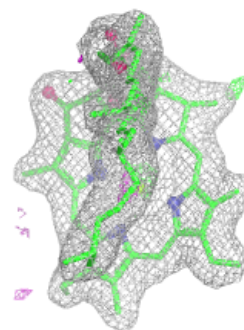
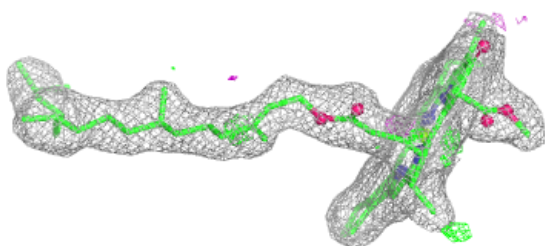
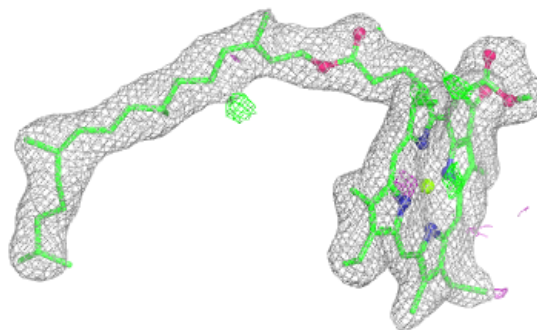
**Electron density around LHG D 412:**

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

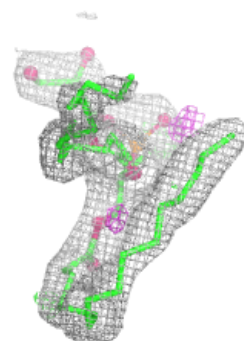
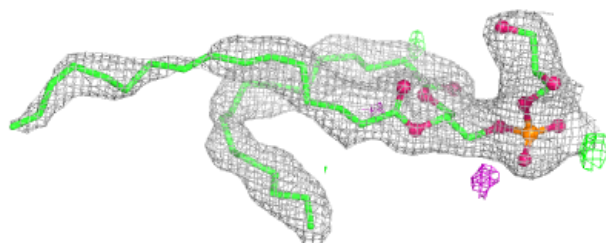
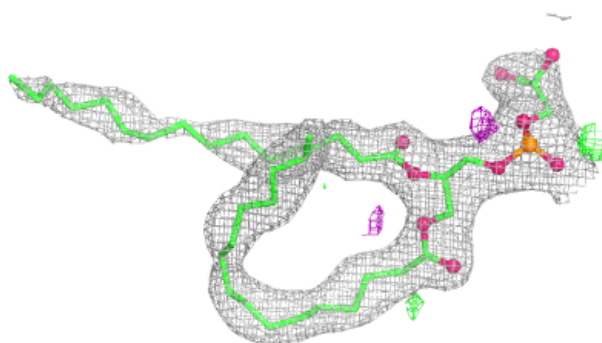


Electron density around CLA b 609:

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

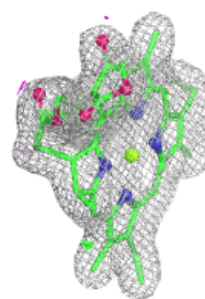
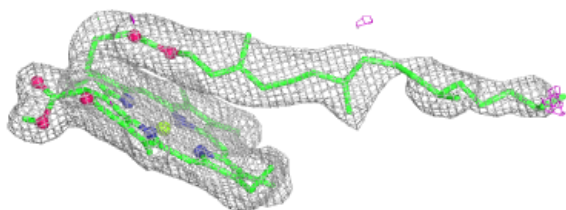
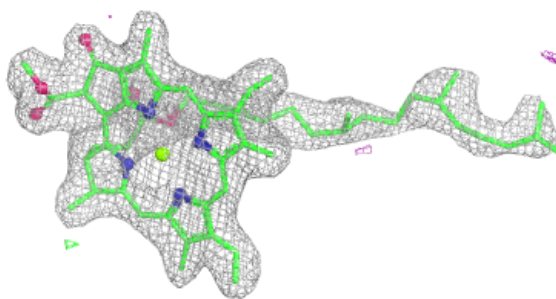
**Electron density around LHG a 411:**

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



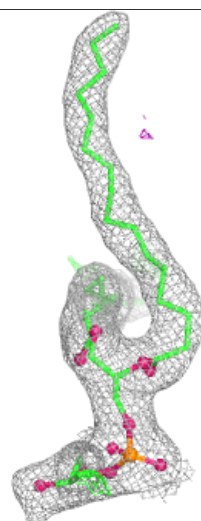
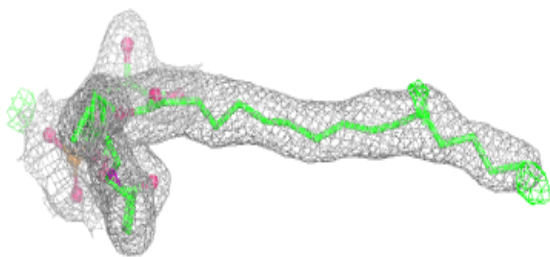
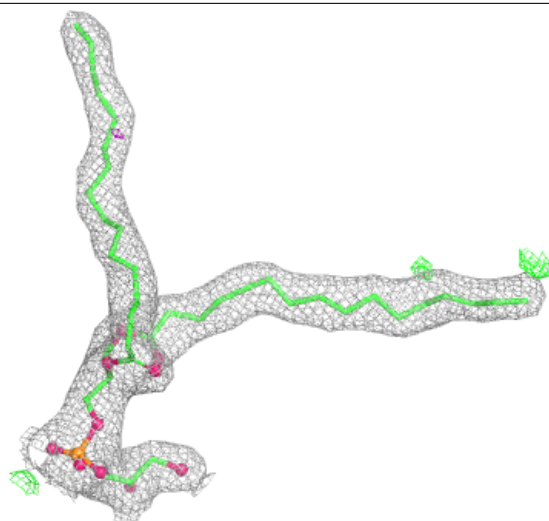
Electron density around CLA b 614:

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



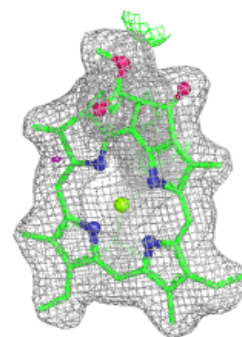
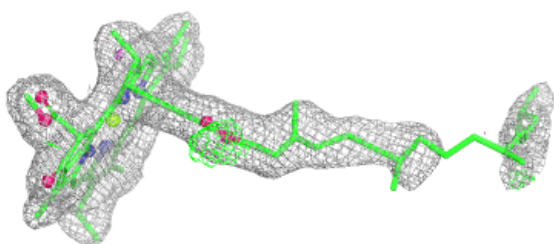
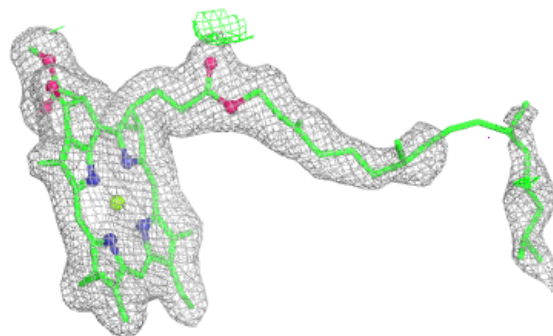
Electron density around LHG 1 102:

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



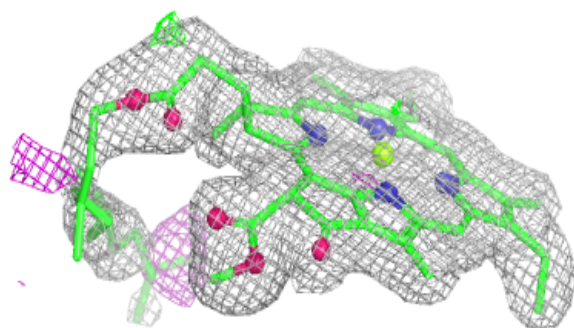
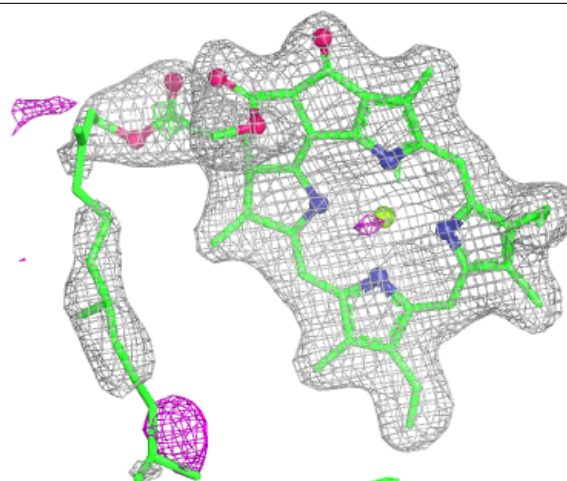
Electron density around CLA d 404:

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



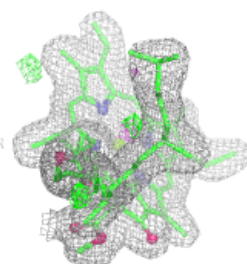
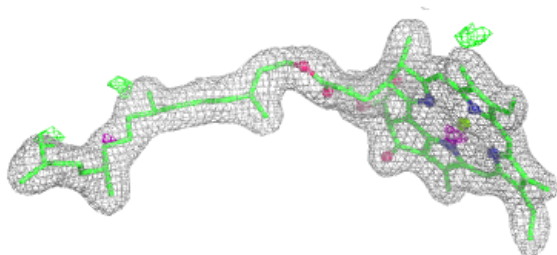
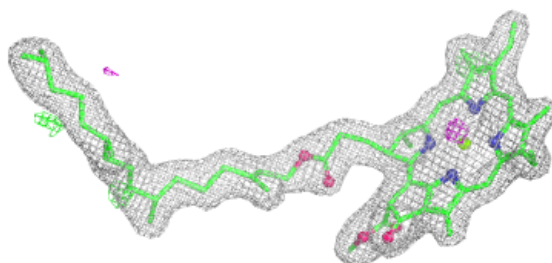
Electron density around CLA B 716:

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

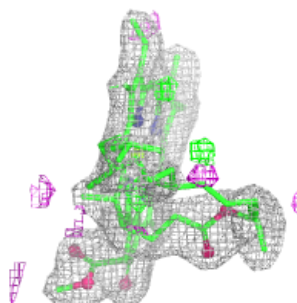
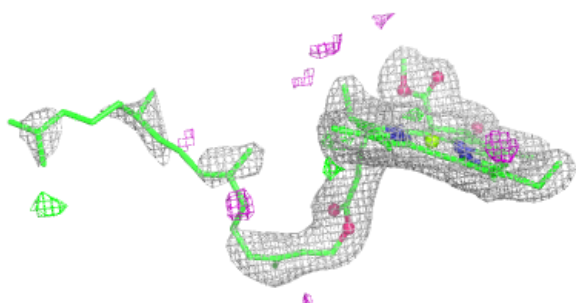
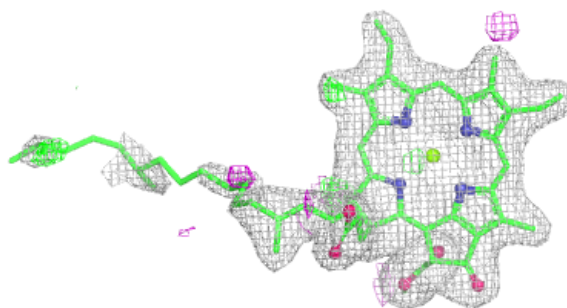


Electron density around CLA a 402:

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

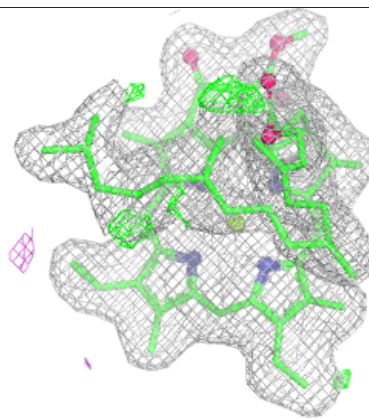
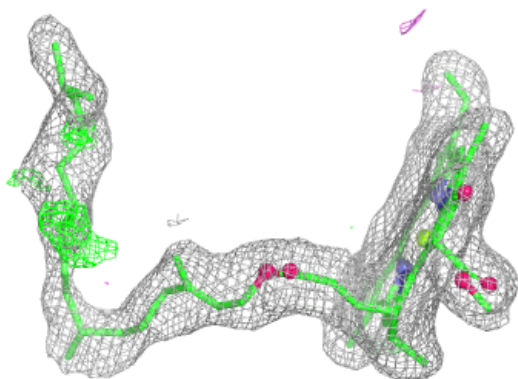
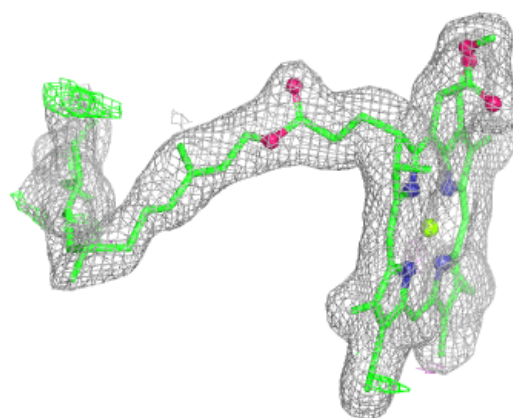
**Electron density around CLA a 403:**

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

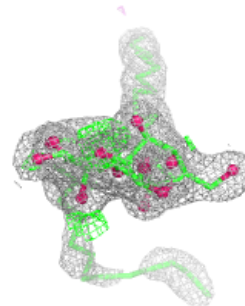
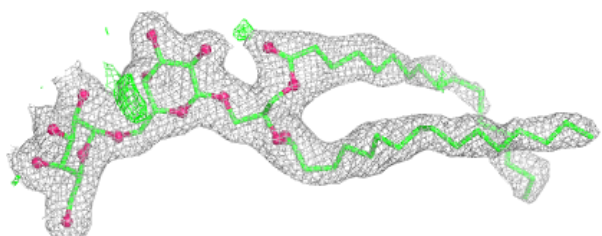
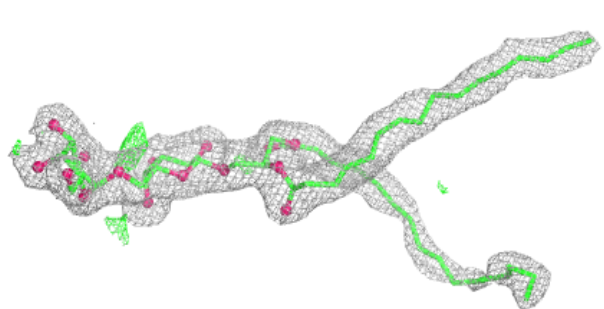


Electron density around CLA a 405:

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

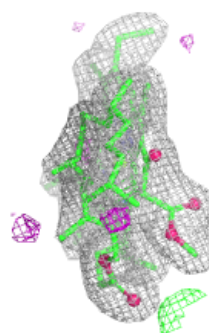
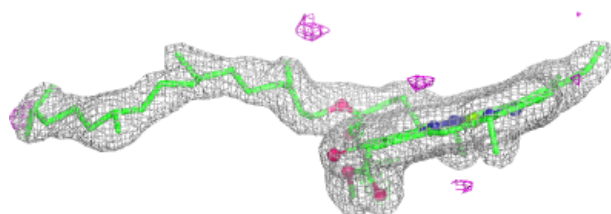
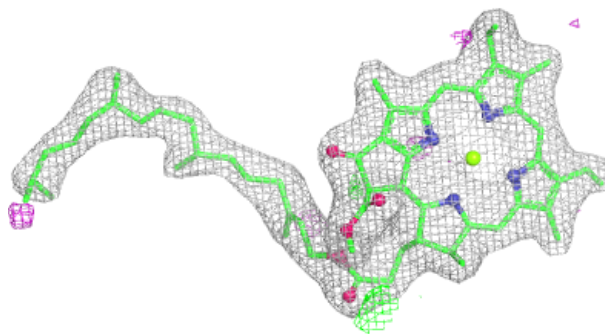
**Electron density around DGD C 517:**

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

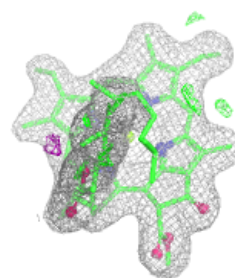
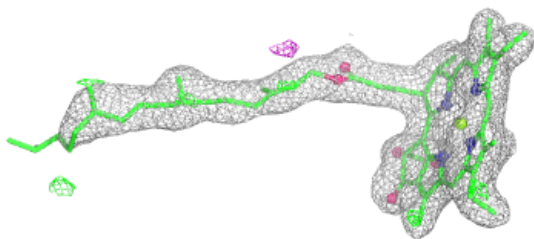
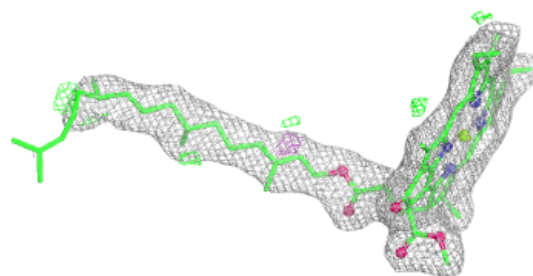


Electron density around CLA b 602:

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

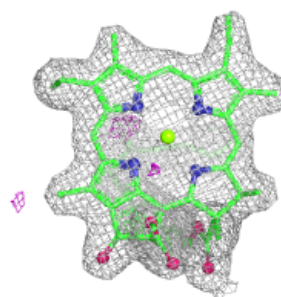
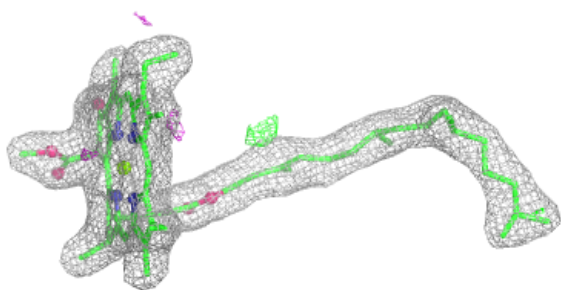
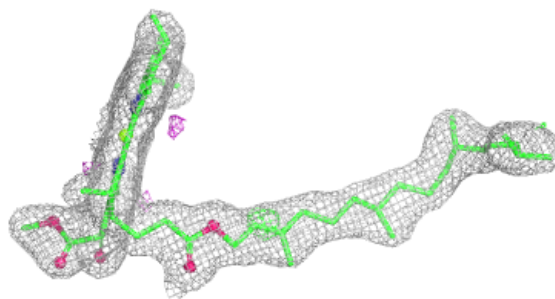
**Electron density around CLA b 604:**

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

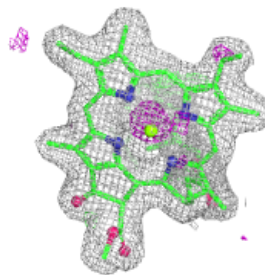
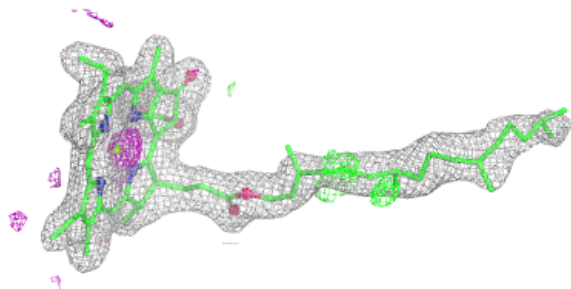
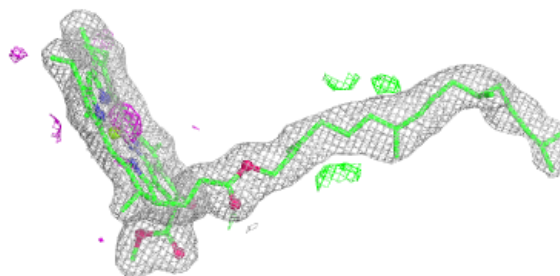


Electron density around CLA b 605:

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

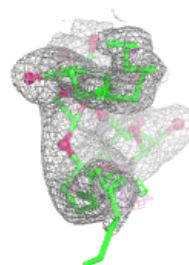
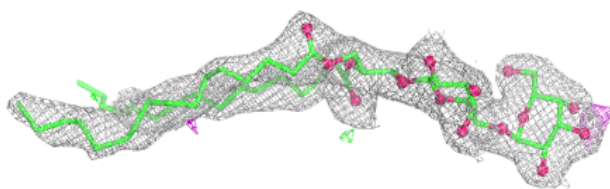
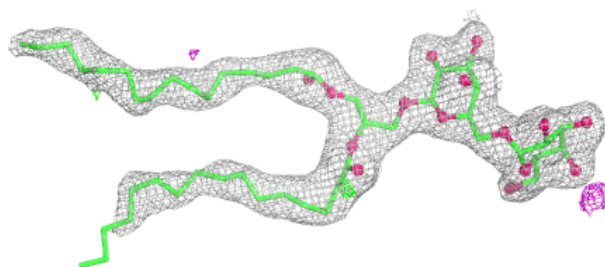
**Electron density around CLA B 704:**

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

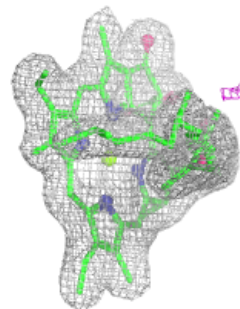
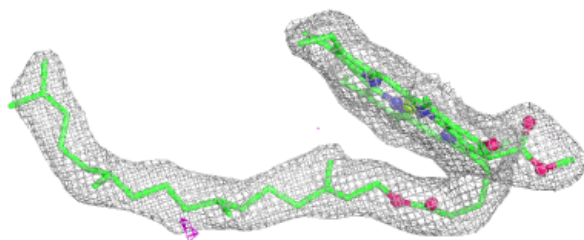
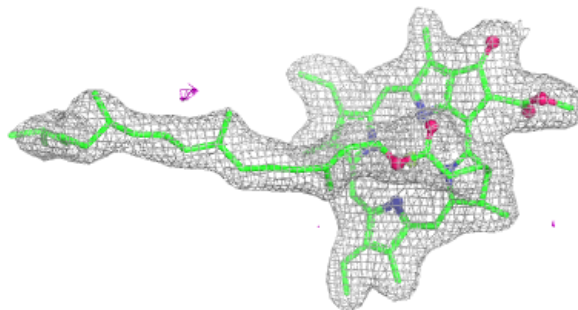


Electron density around DGD c 519:

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

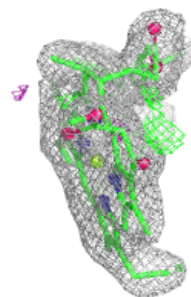
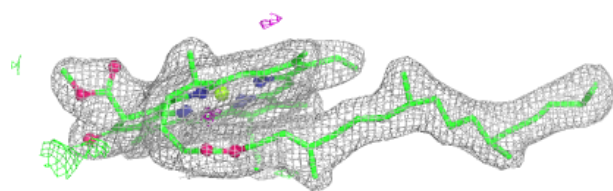
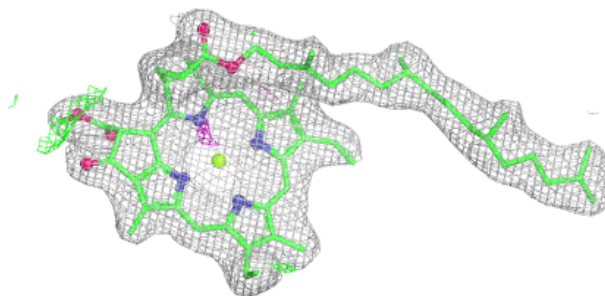
**Electron density around CLA b 608:**

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



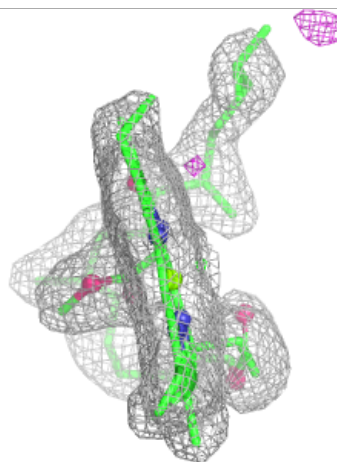
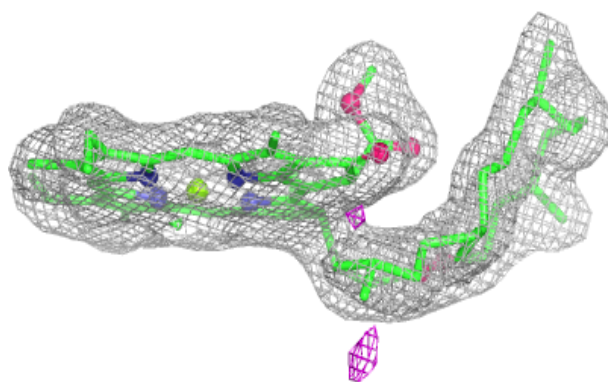
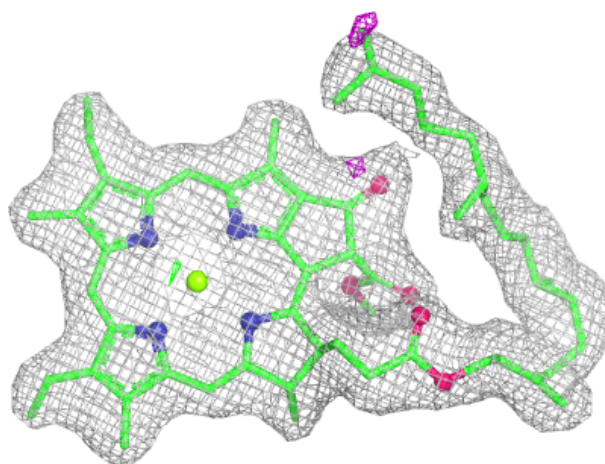
Electron density around CLA C 502:

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



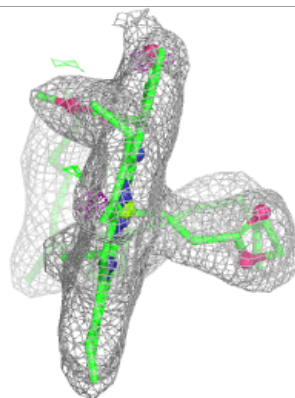
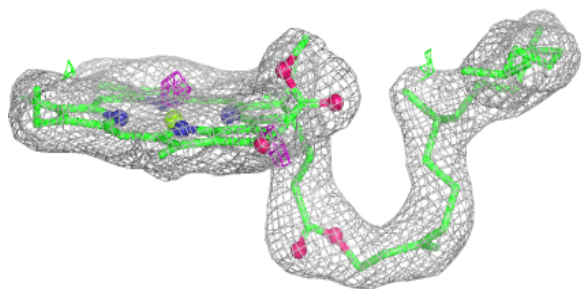
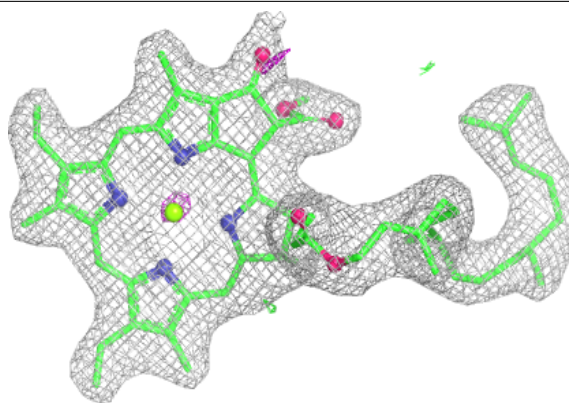
Electron density around CLA b 610:

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

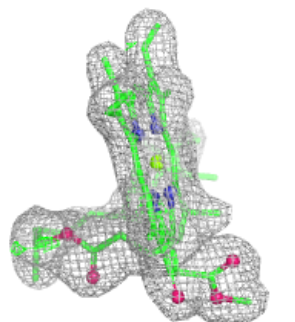
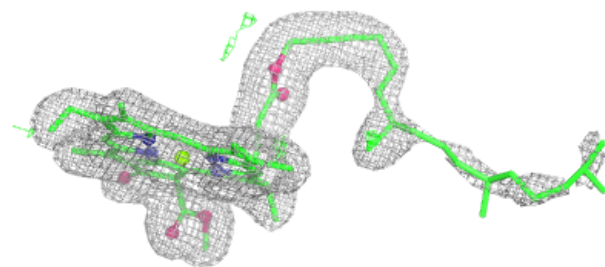
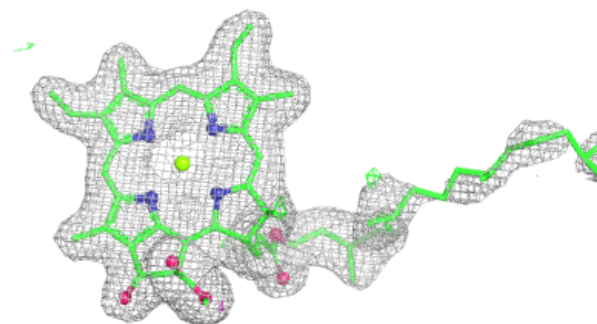


Electron density around CLA b 612:

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

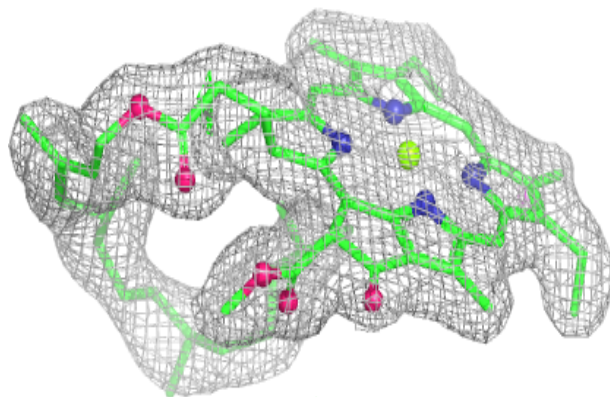
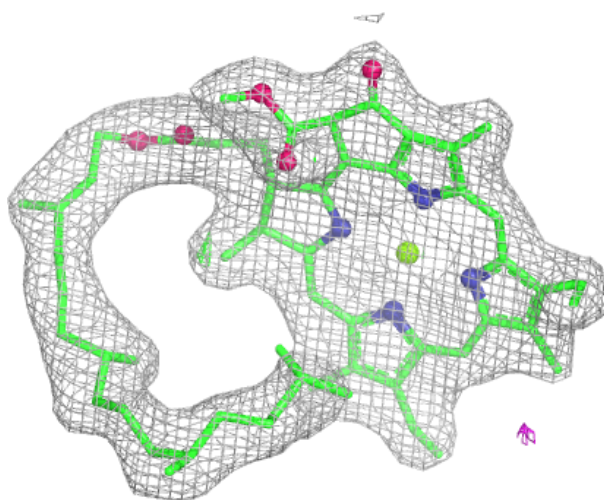
**Electron density around CLA A 403:**

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



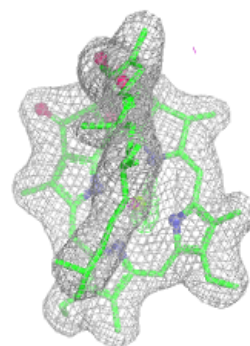
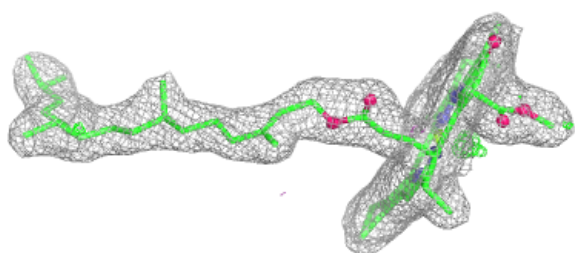
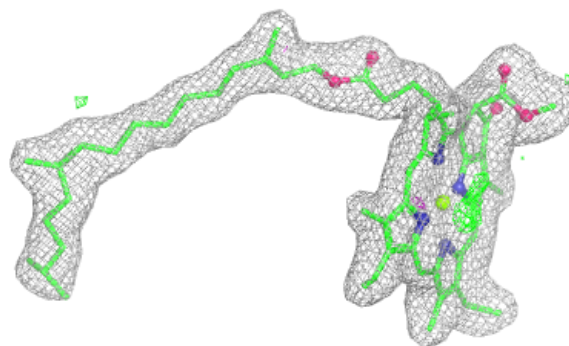
Electron density around CLA b 615:

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

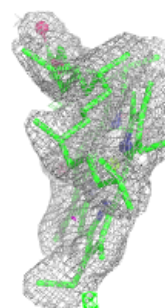
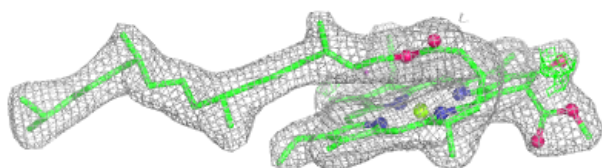
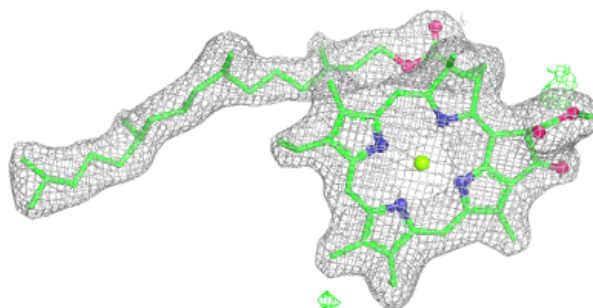


Electron density around CLA B 709:

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

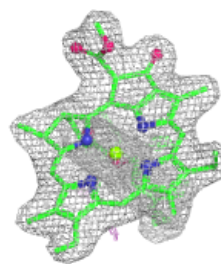
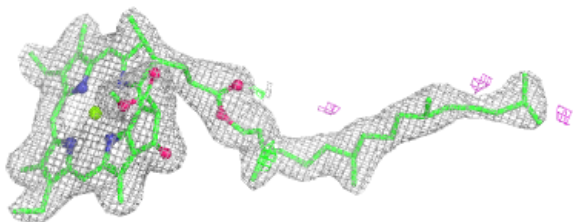
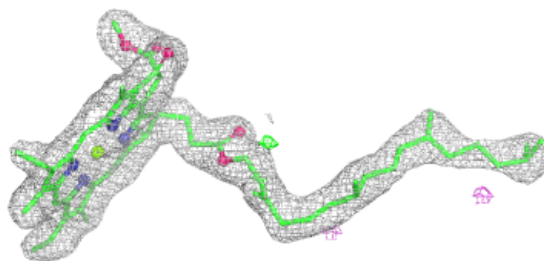
**Electron density around CLA c 502:**

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

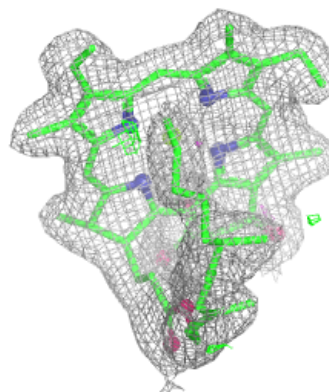
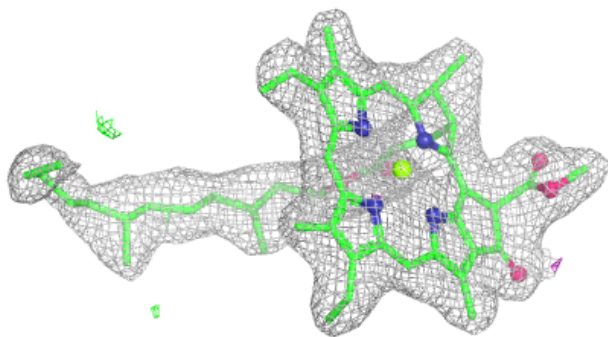
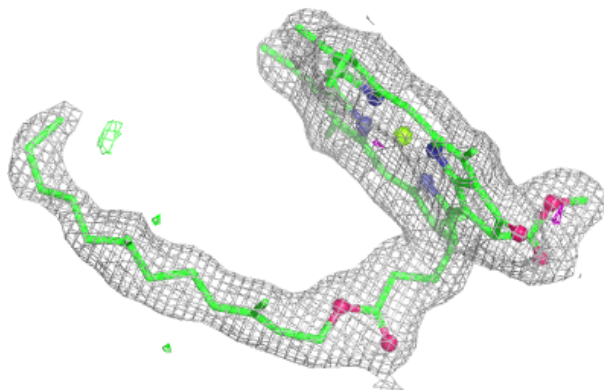


Electron density around CLA c 503:

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

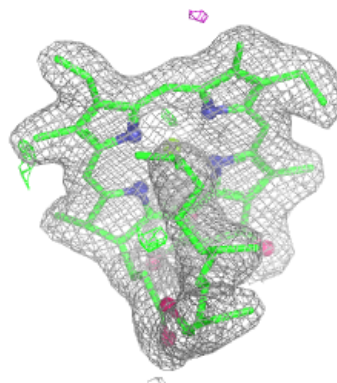
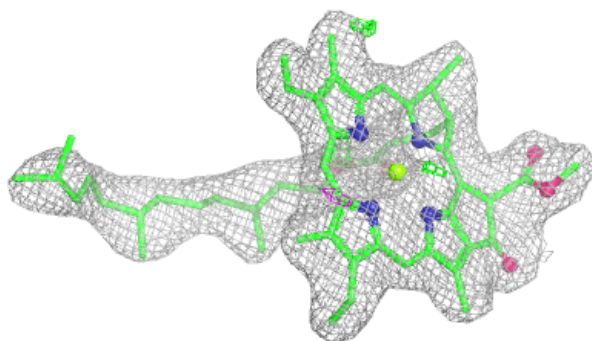
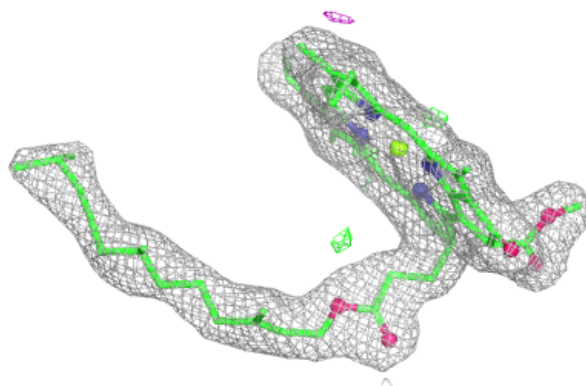
**Electron density around CLA C 505:**

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

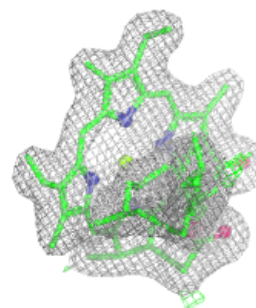
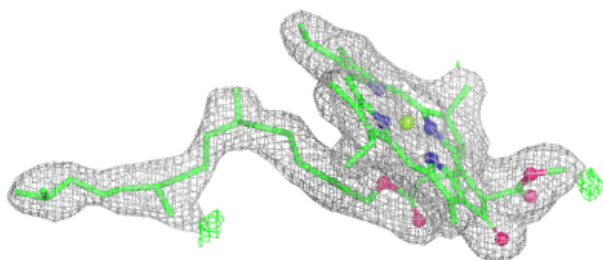
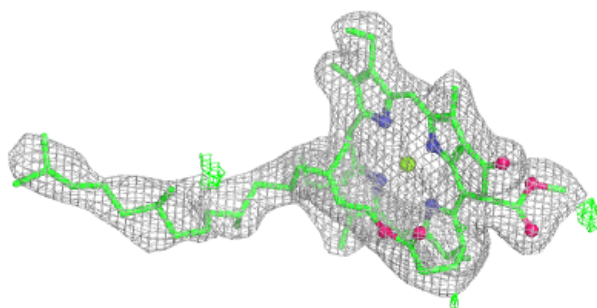


Electron density around CLA c 505:

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

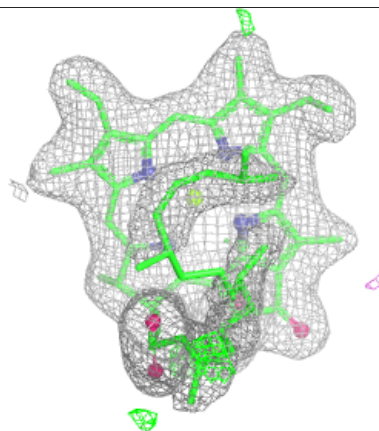
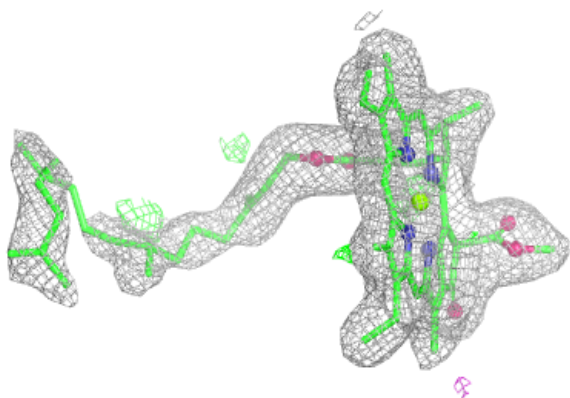
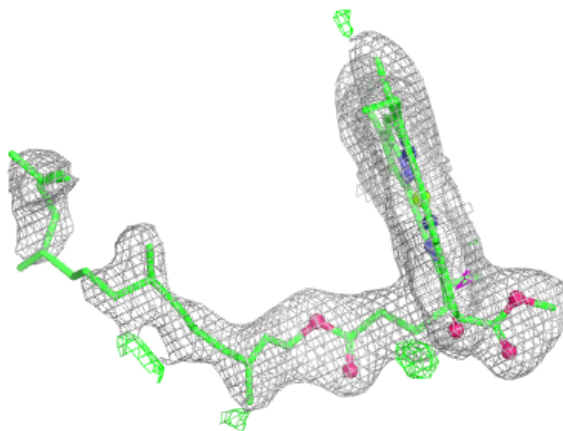
**Electron density around CLA c 506:**

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



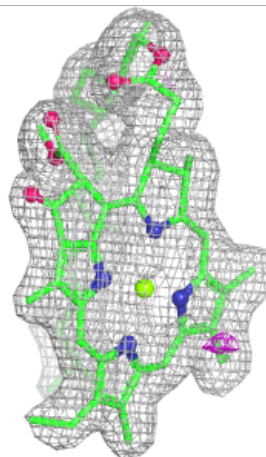
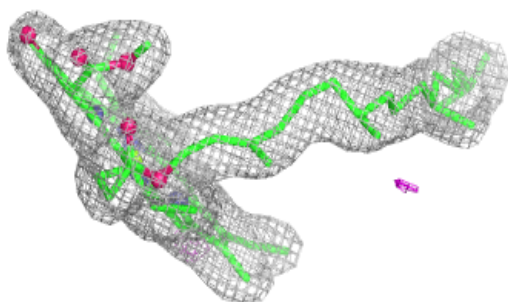
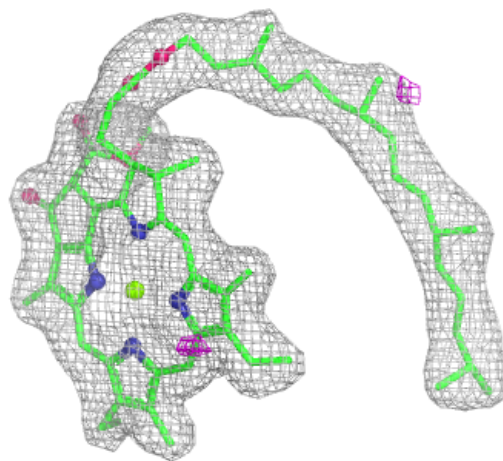
Electron density around CLA C 507:

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



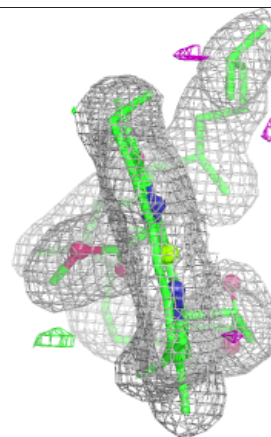
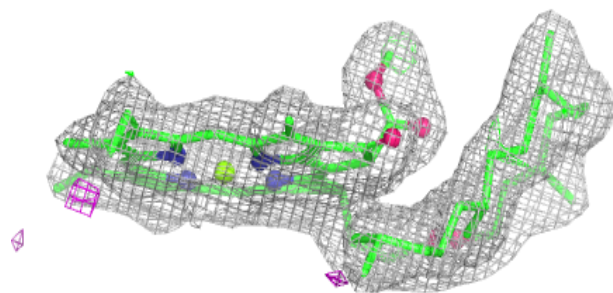
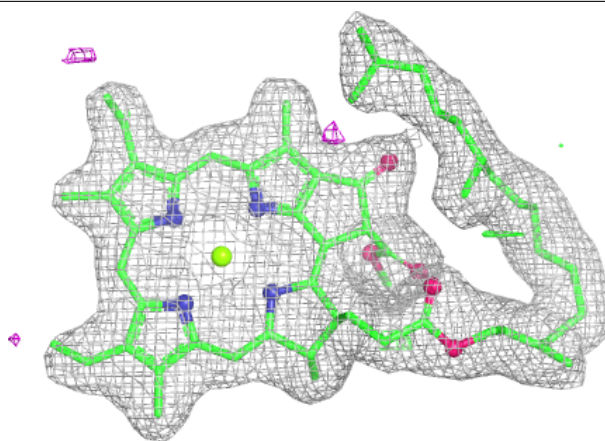
Electron density around CLA C 508:

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



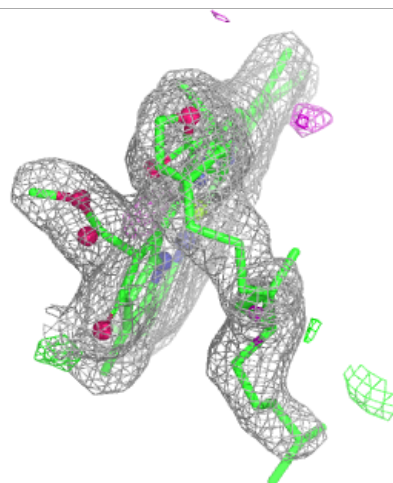
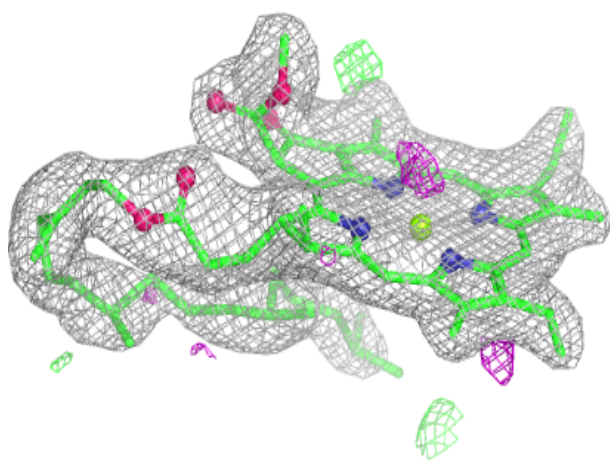
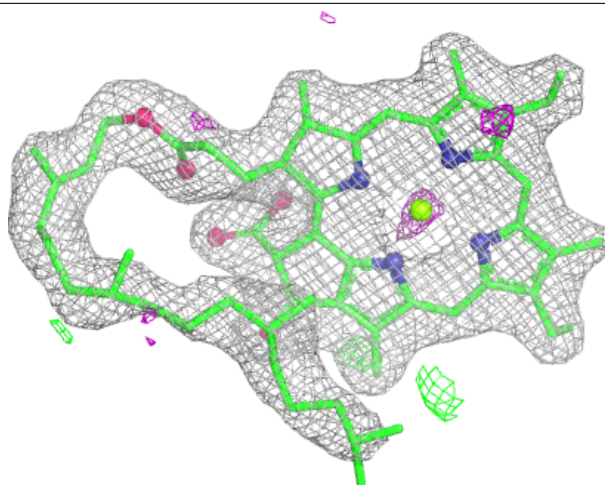
Electron density around CLA B 710:

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



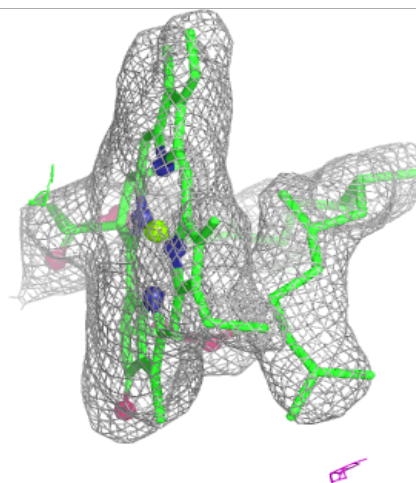
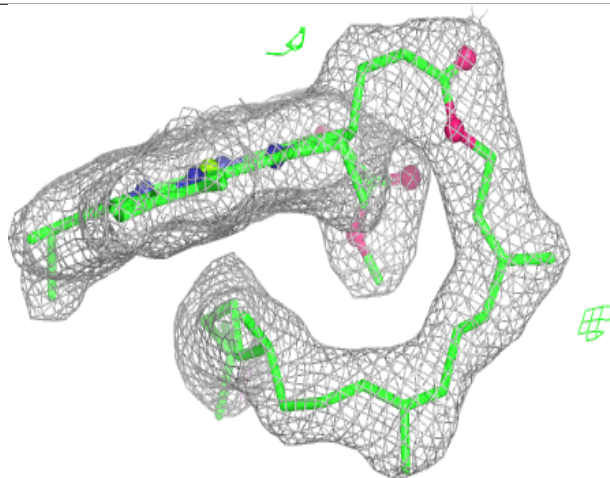
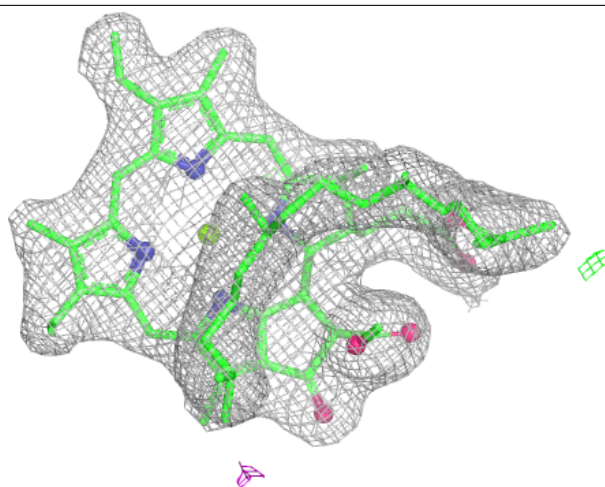
Electron density around CLA C 510:

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



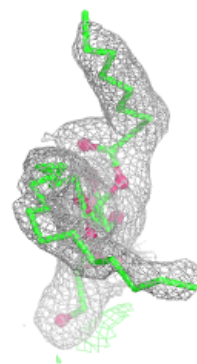
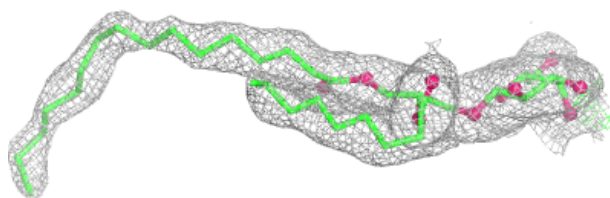
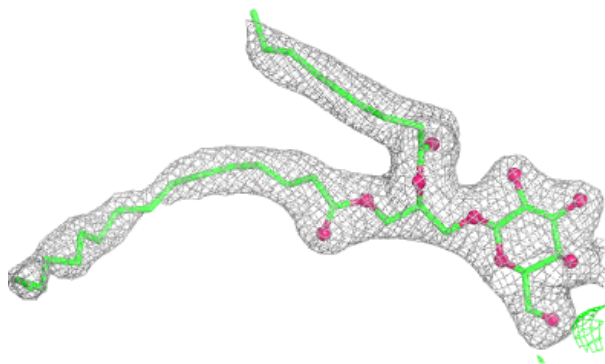
Electron density around CLA c 511:

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



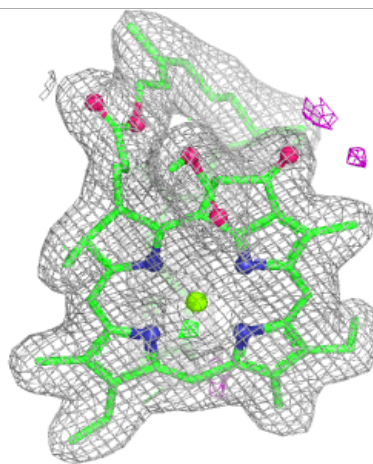
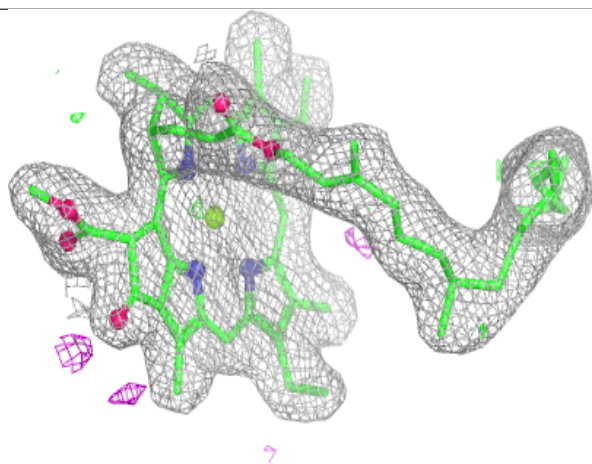
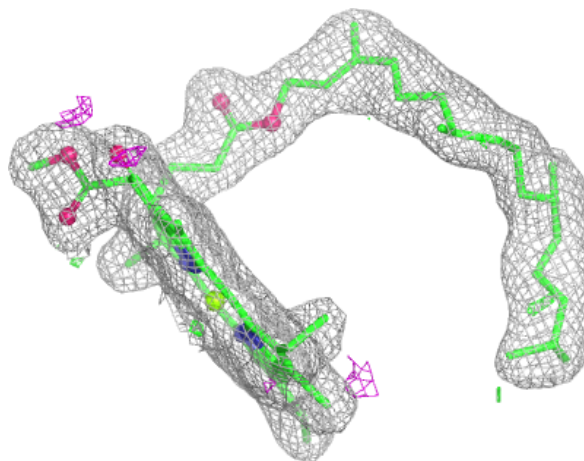
Electron density around LMG d 410:

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



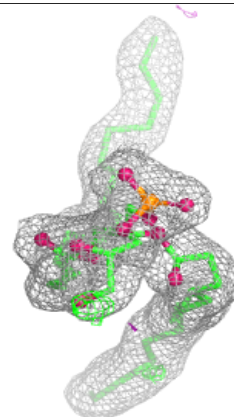
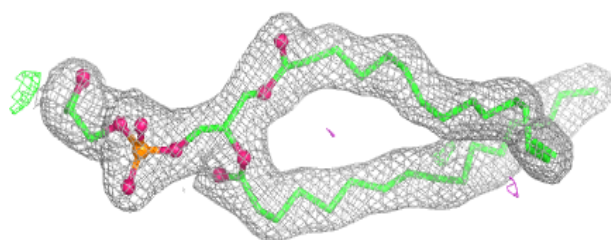
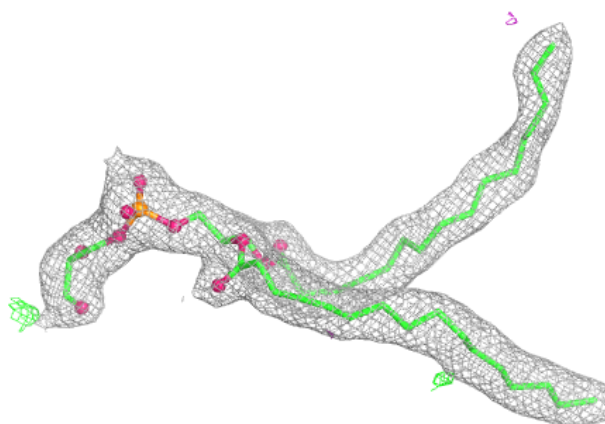
Electron density around CLA B 711:

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

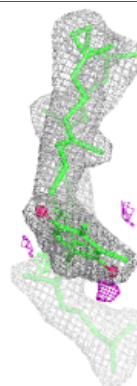
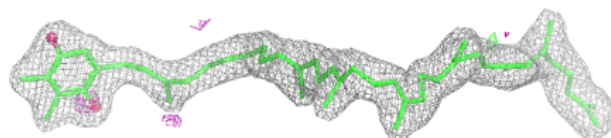
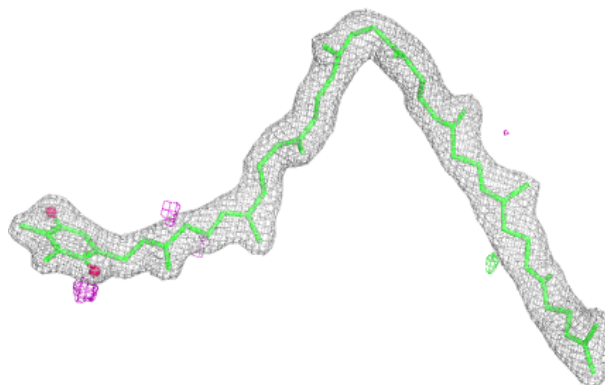


Electron density around LHG D 411:

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

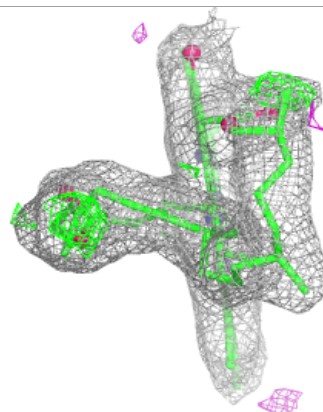
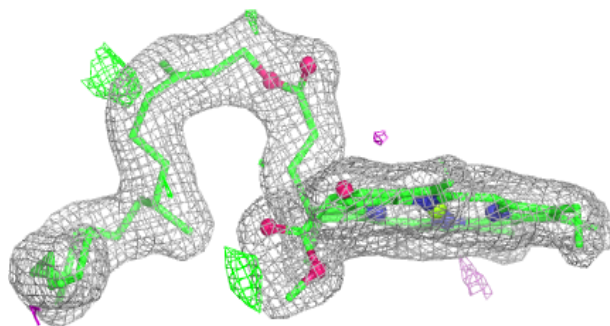
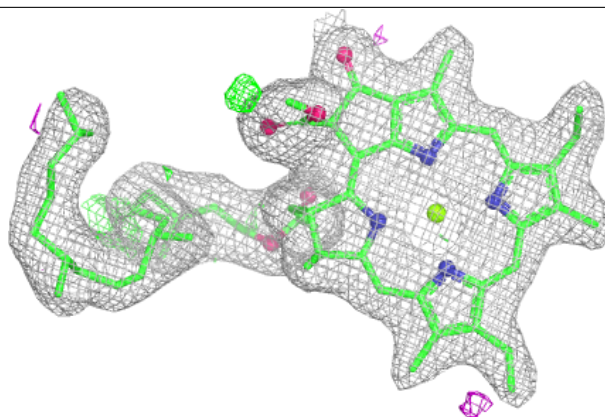
**Electron density around PL9 d 406:**

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



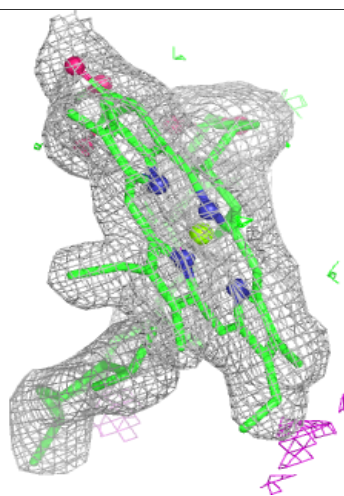
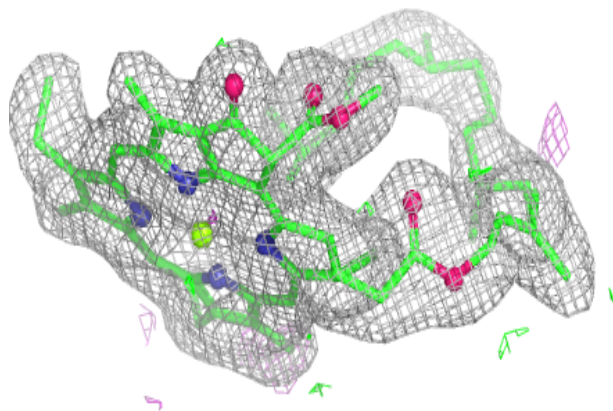
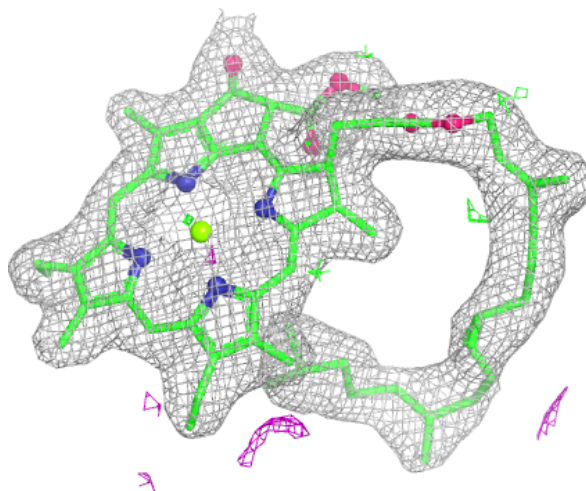
Electron density around CLA B 712:

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



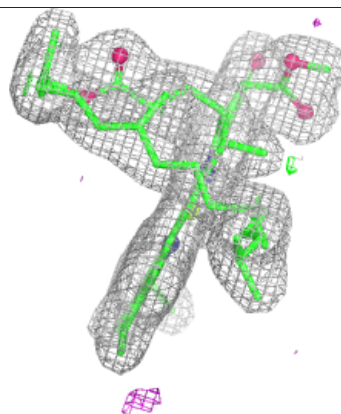
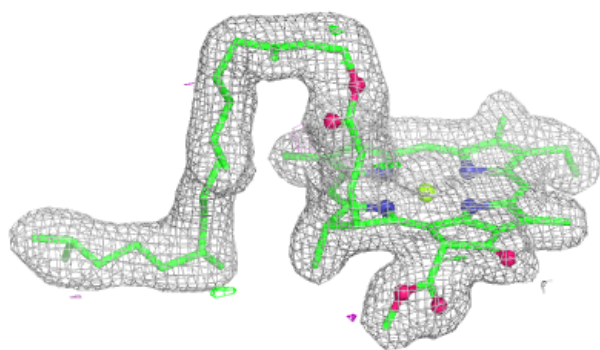
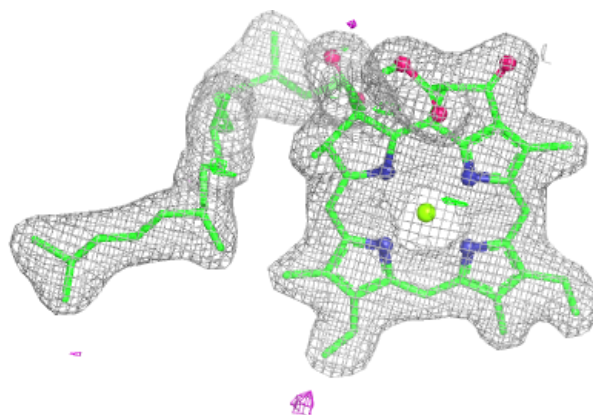
Electron density around CLA B 715:

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

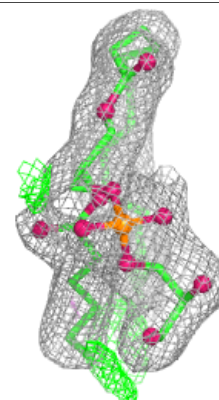
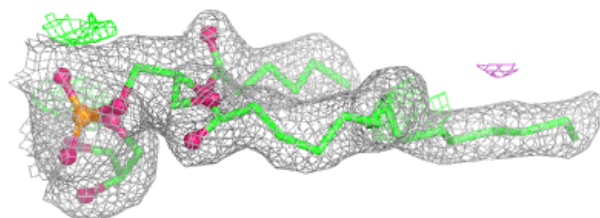
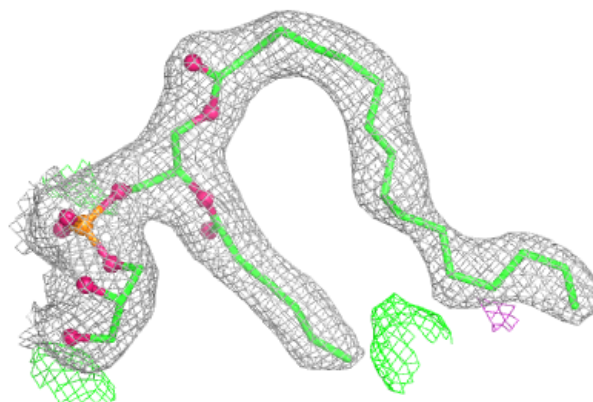


Electron density around CLA d 401:

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

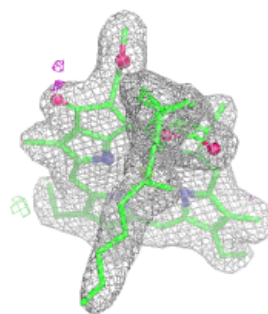
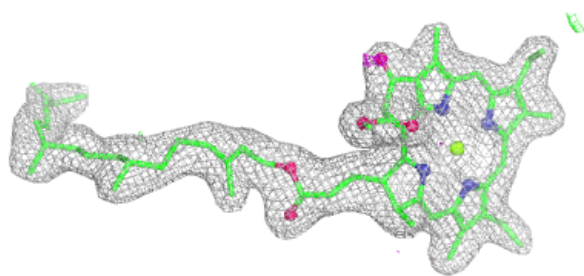
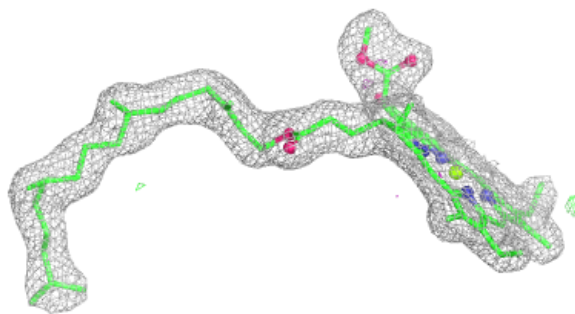
**Electron density around LHG d 409:**

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



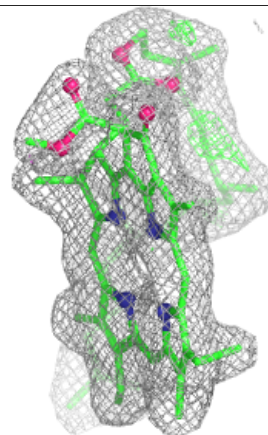
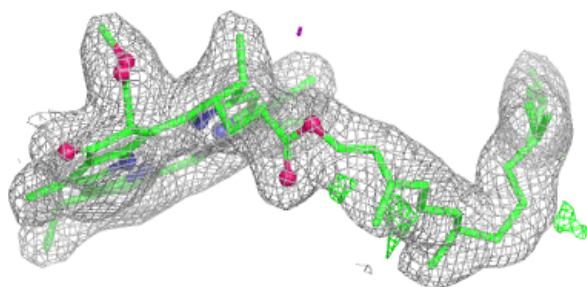
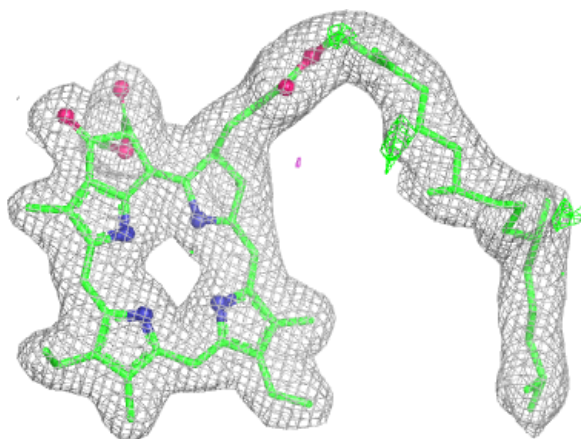
Electron density around CLA d 403:

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



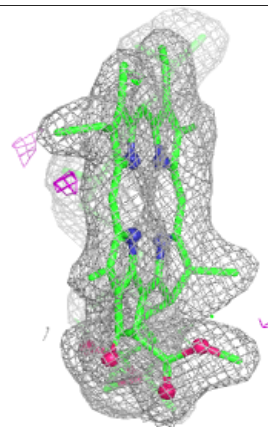
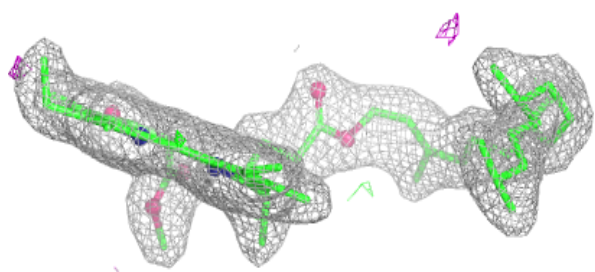
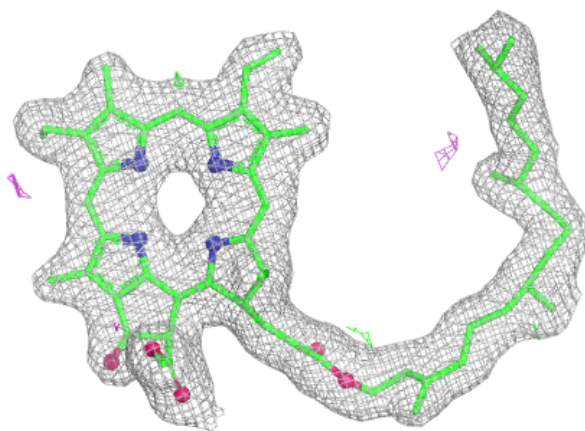
Electron density around PHO D 408:

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



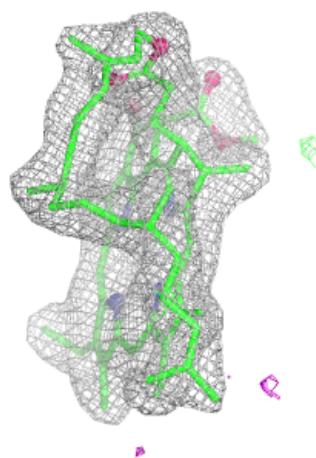
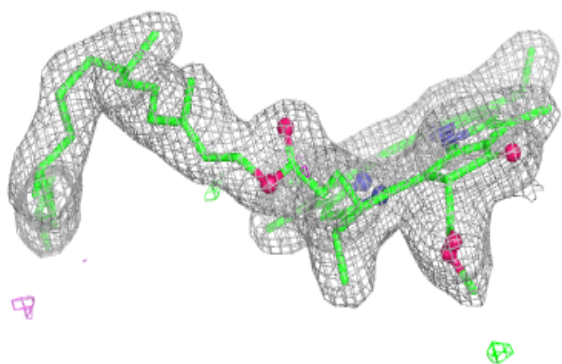
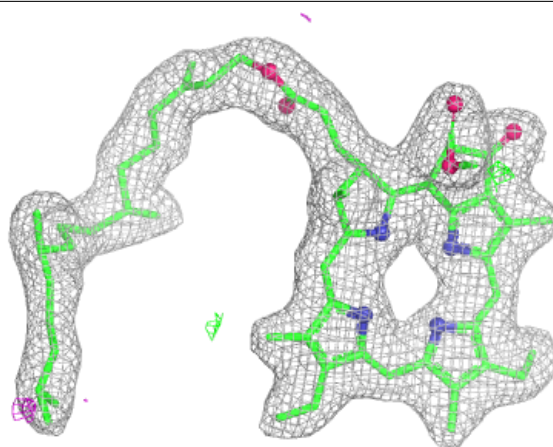
Electron density around PHO a 404:

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



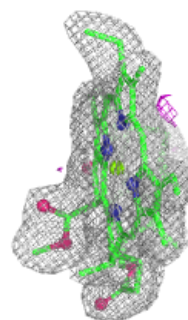
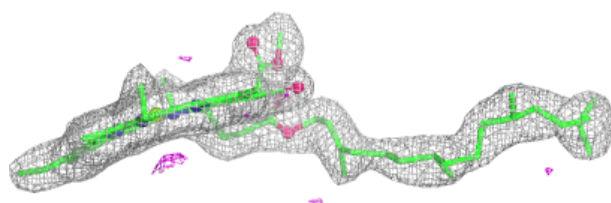
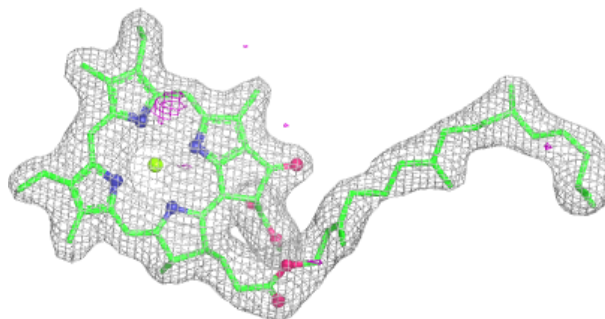
Electron density around PHO d 407:

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

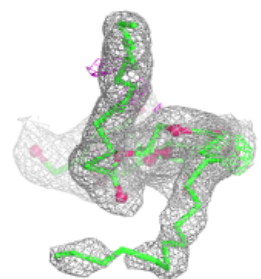
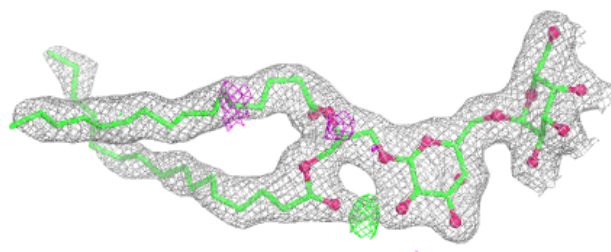
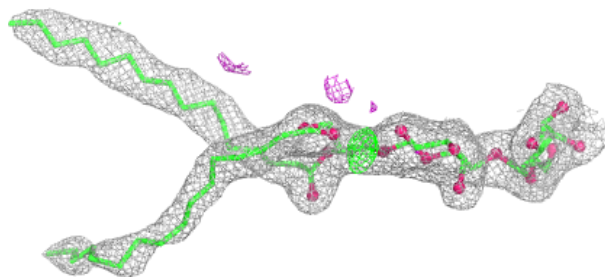


Electron density around CLA B 702:

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

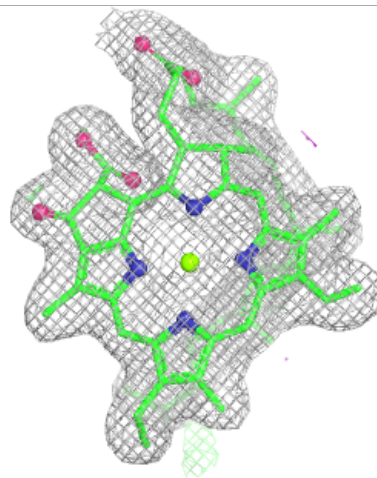
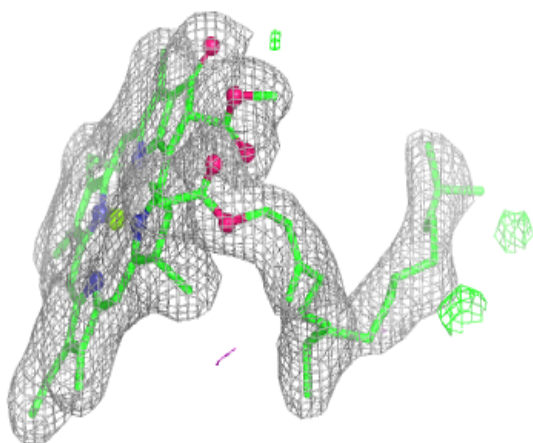
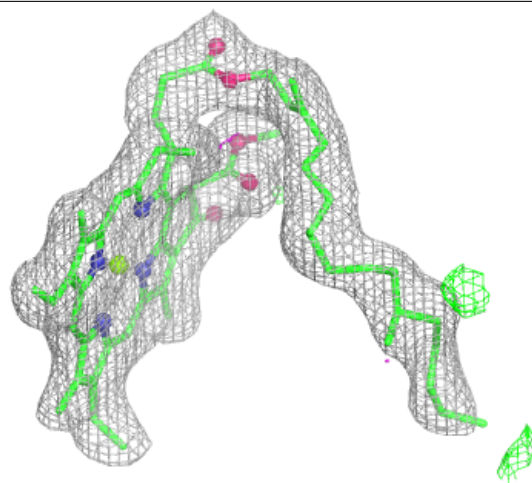
**Electron density around DGD c 517:**

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



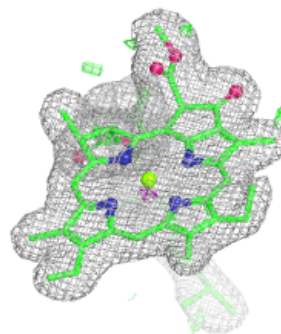
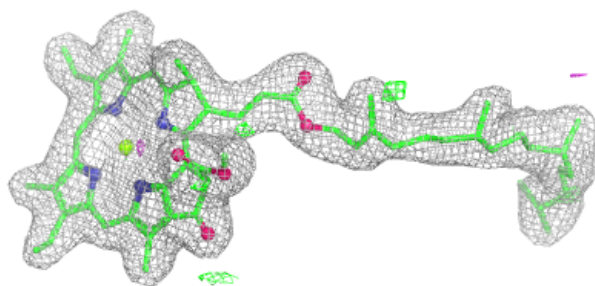
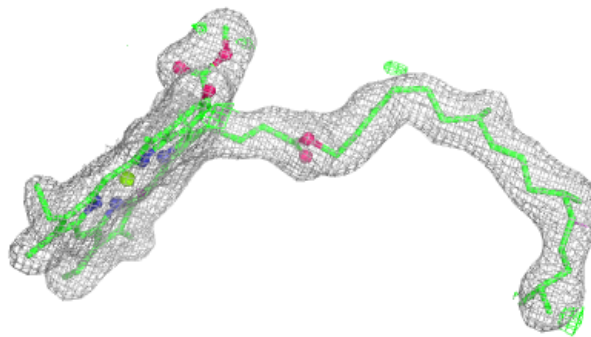
Electron density around CLA B 713:

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



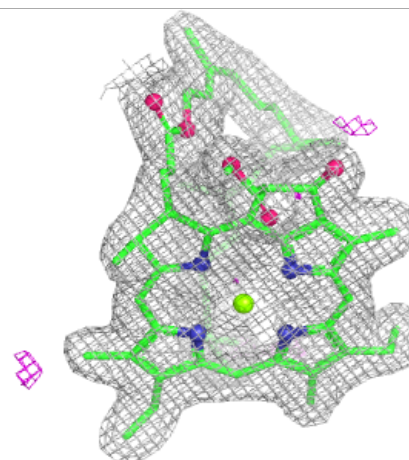
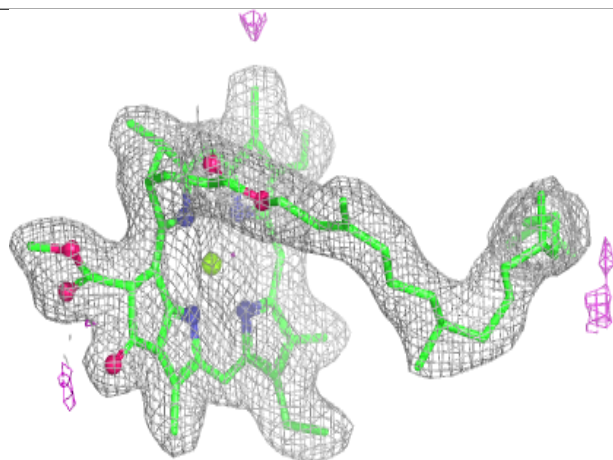
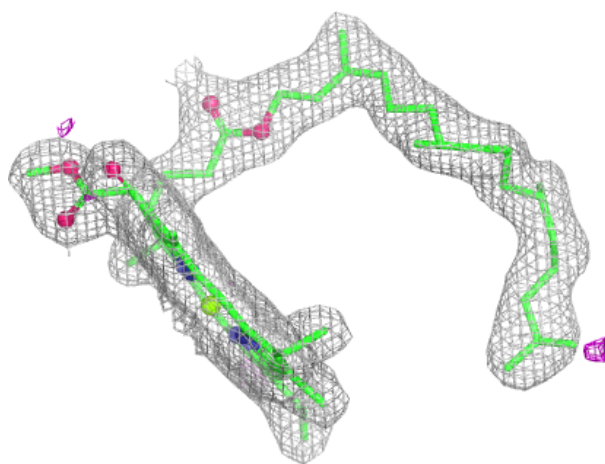
Electron density around CLA D 402:

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



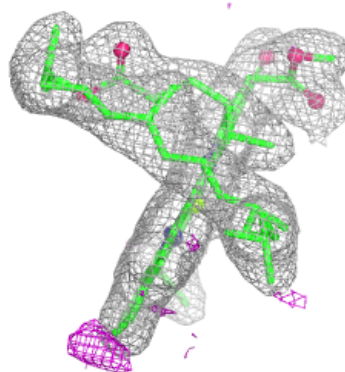
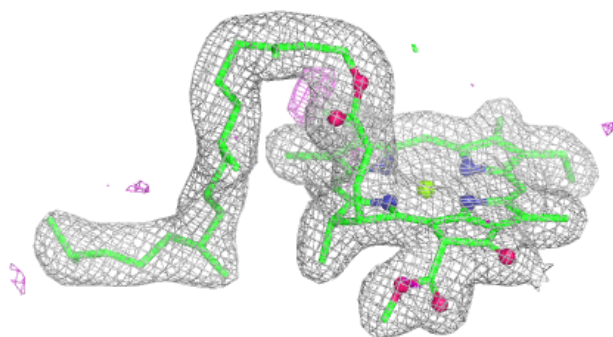
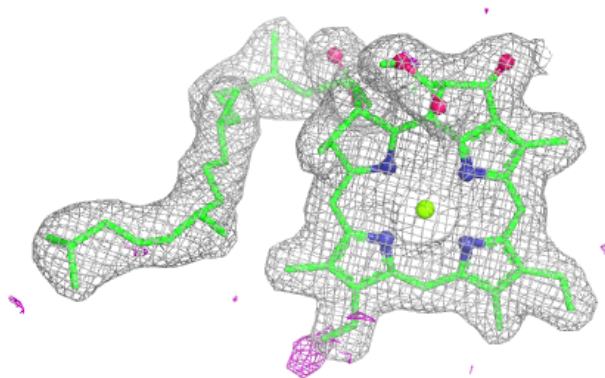
Electron density around CLA b 611:

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



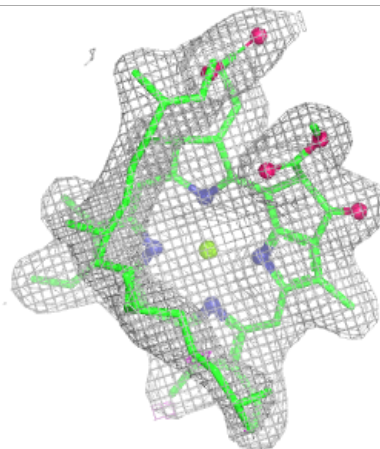
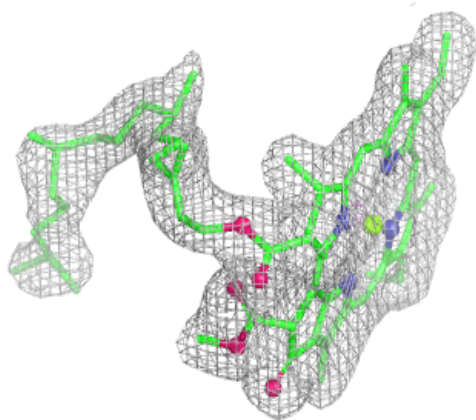
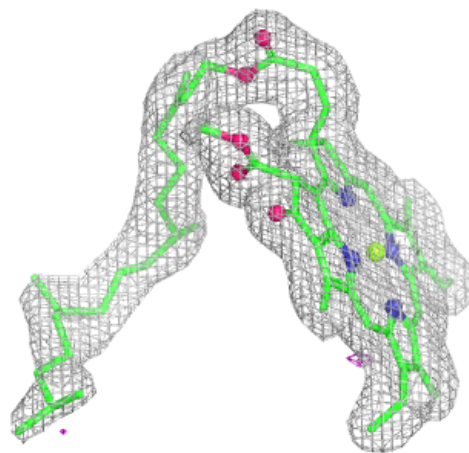
Electron density around CLA D 403:

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



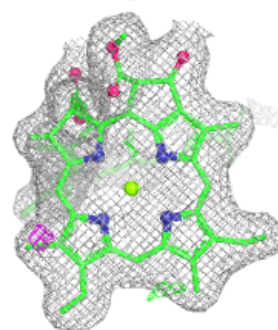
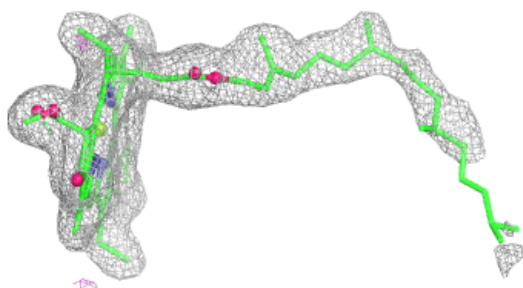
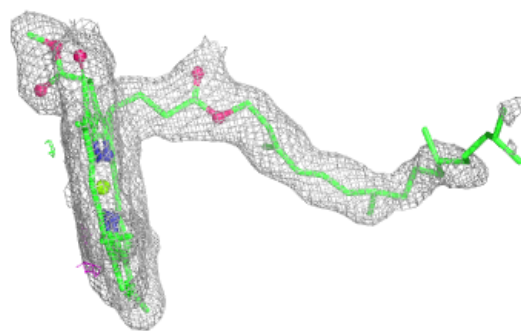
Electron density around CLA b 613:

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

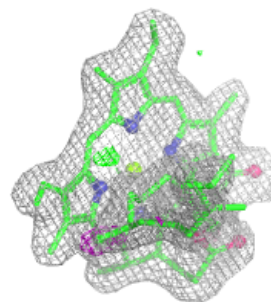
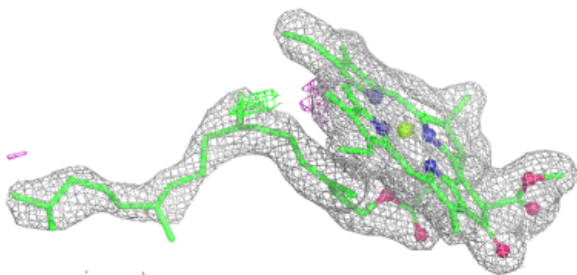
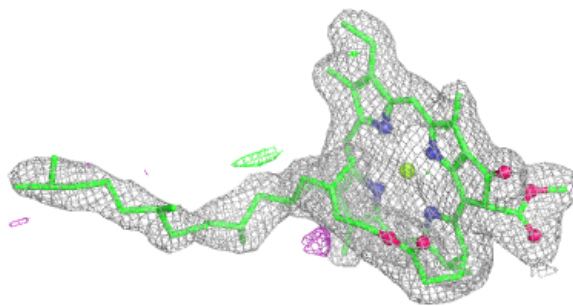


Electron density around CLA D 404:

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

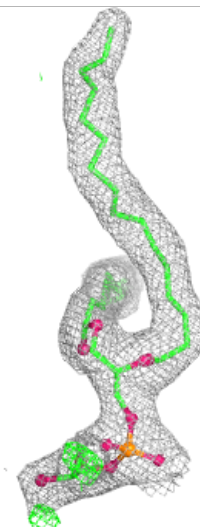
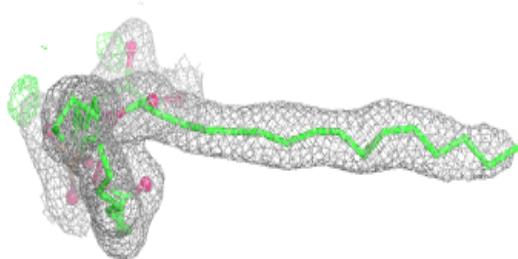
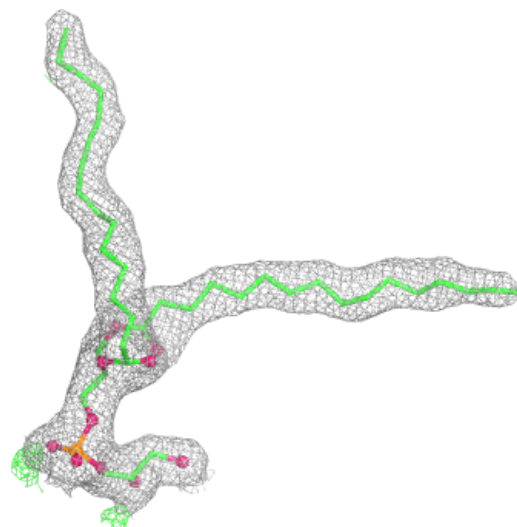
**Electron density around CLA C 506:**

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



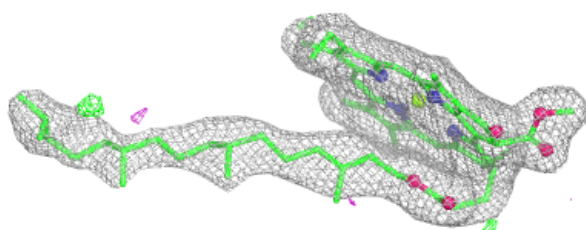
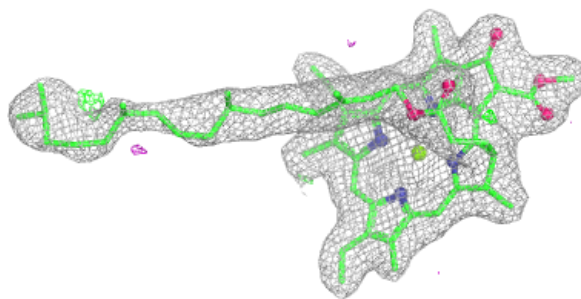
Electron density around LHG L 101:

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

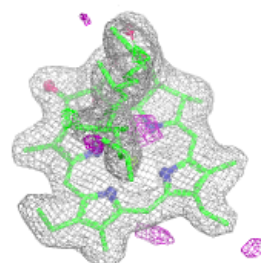
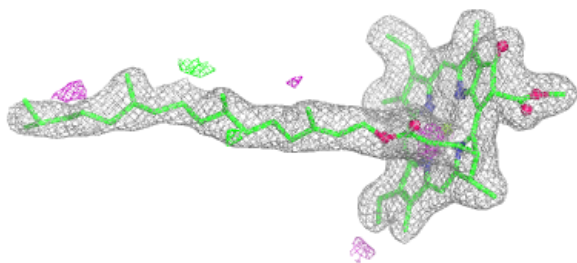
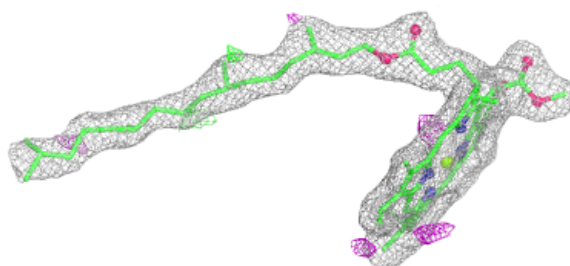


Electron density around CLA B 714:

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

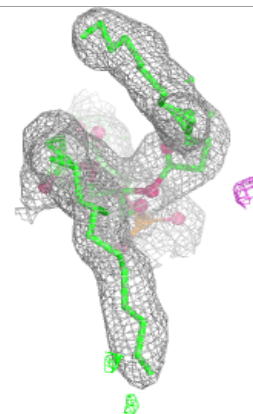
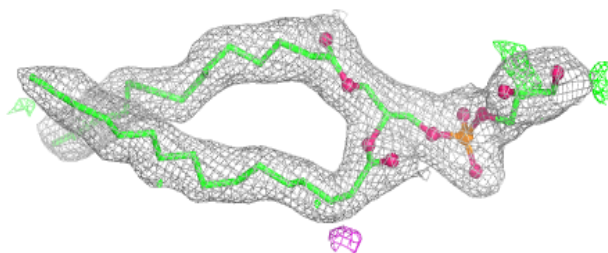
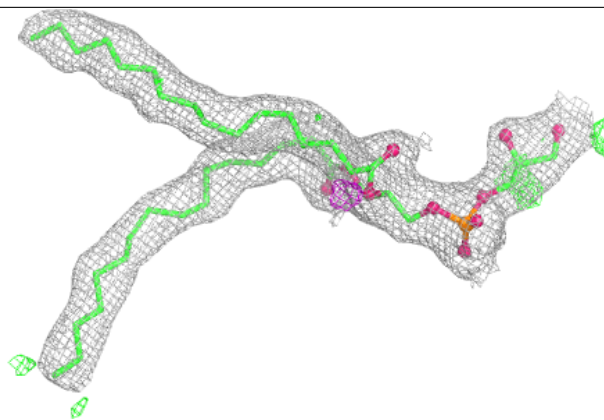
**Electron density around CLA B 707:**

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

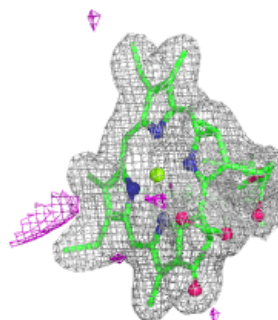
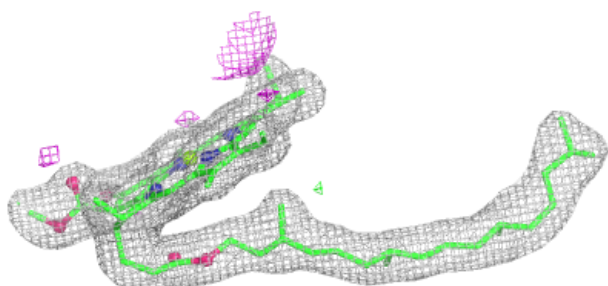
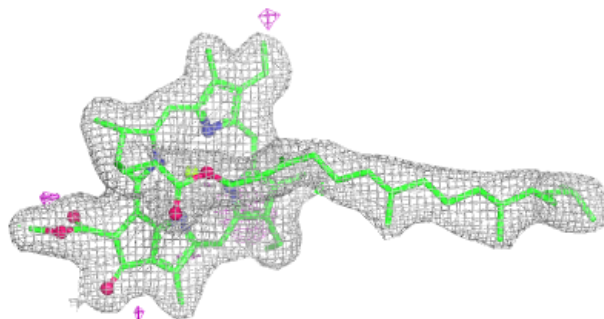


Electron density around LHG d 408:

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

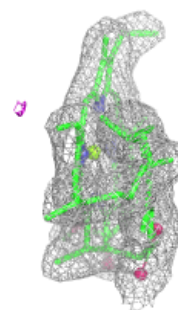
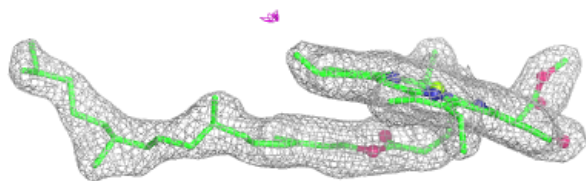
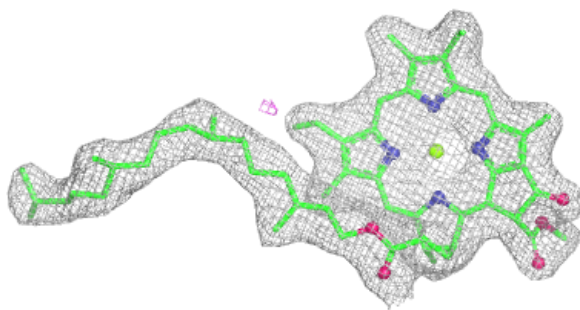
**Electron density around CLA B 708:**

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

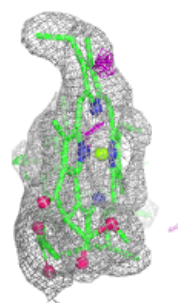
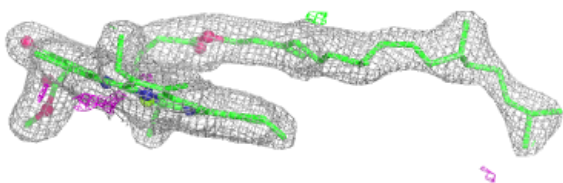
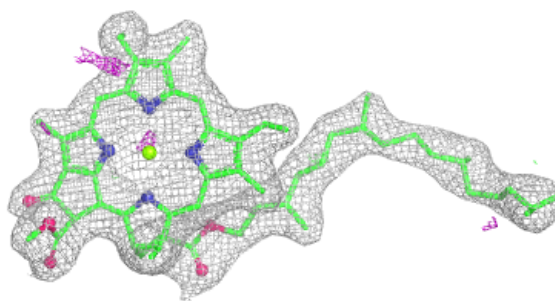


Electron density around CLA b 603:

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

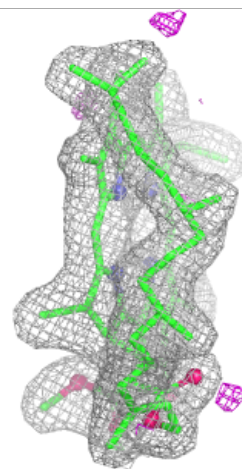
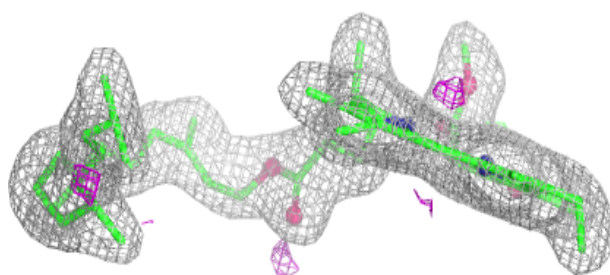
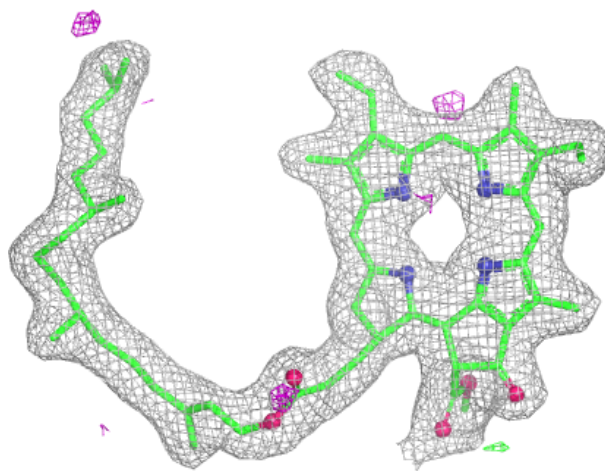
**Electron density around CLA B 703:**

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



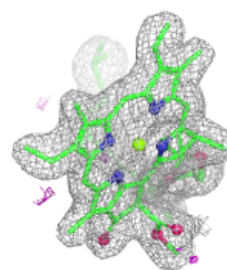
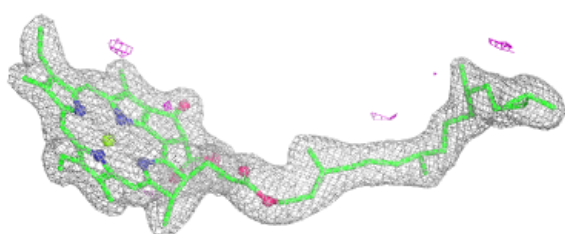
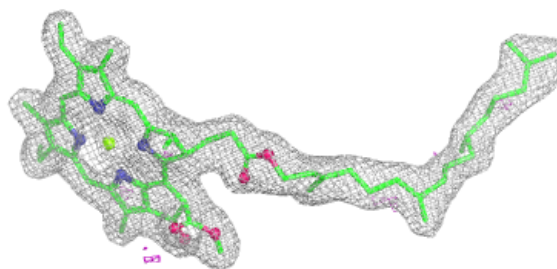
Electron density around PHO D 407:

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

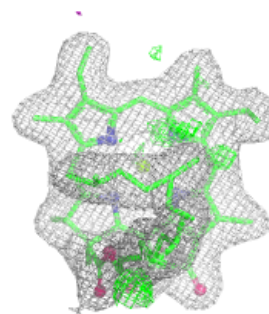
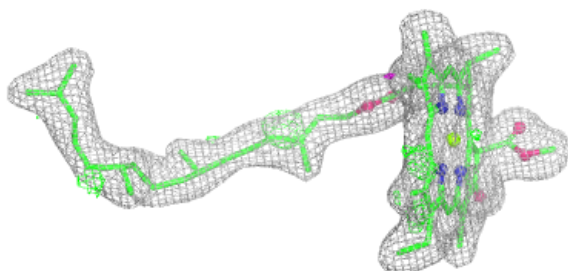
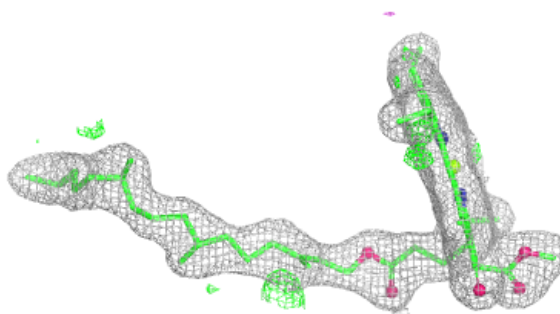


Electron density around CLA A 402:

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

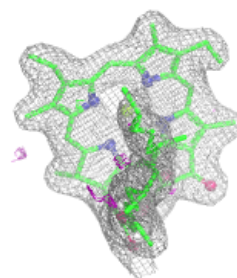
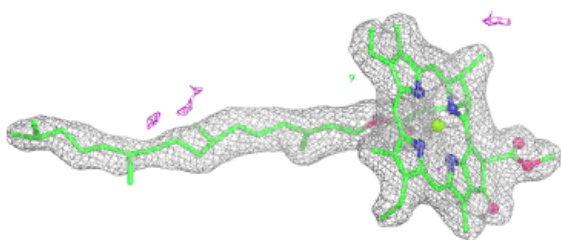
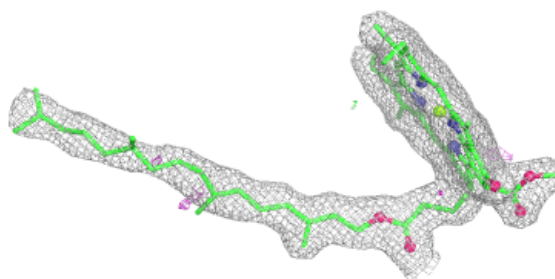
**Electron density around CLA B 705:**

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



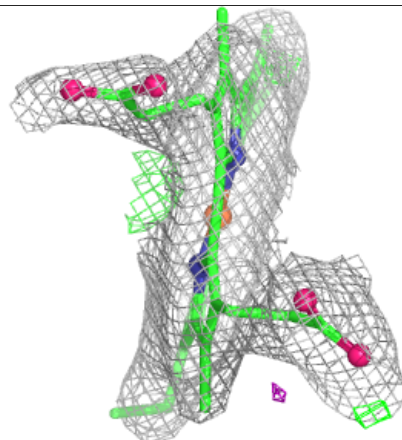
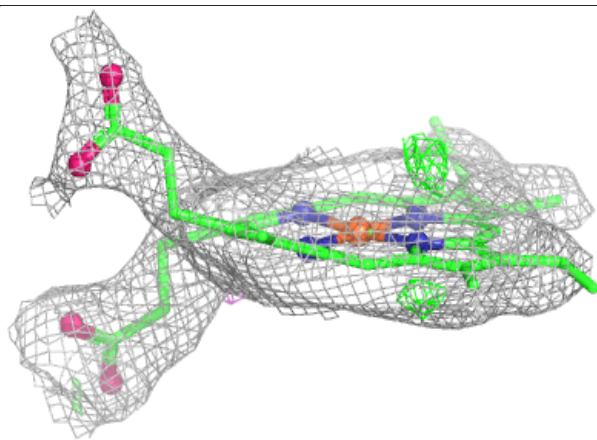
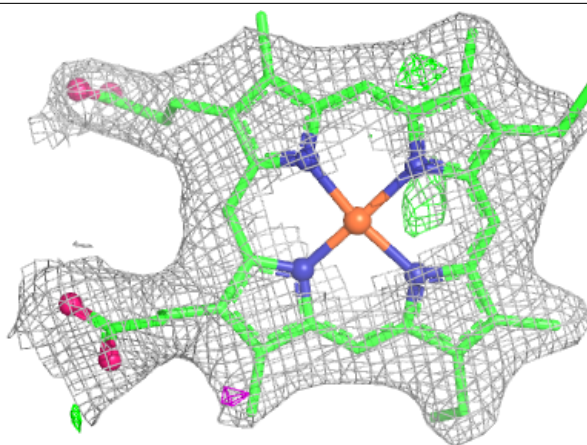
Electron density around CLA b 607:

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



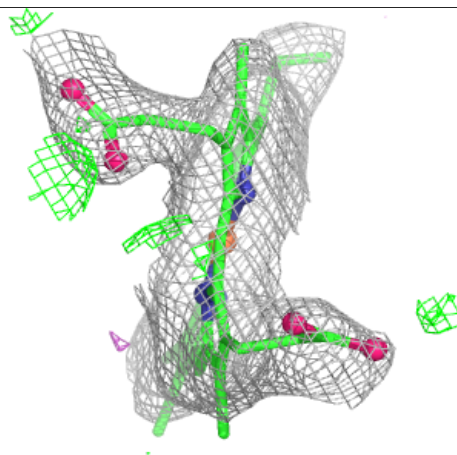
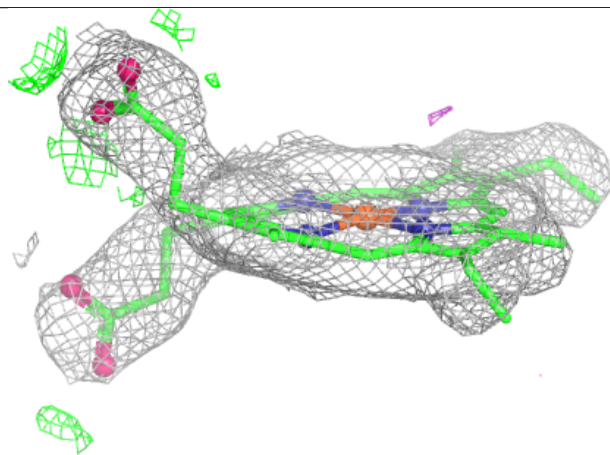
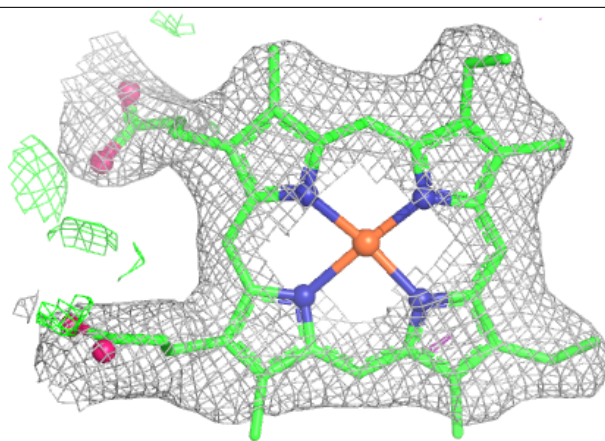
Electron density around HEC F 101:

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



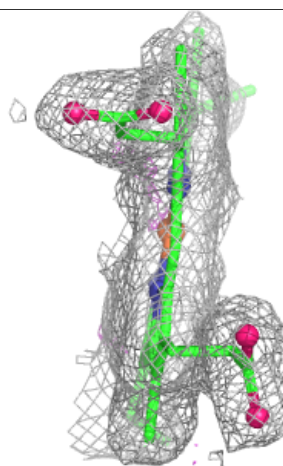
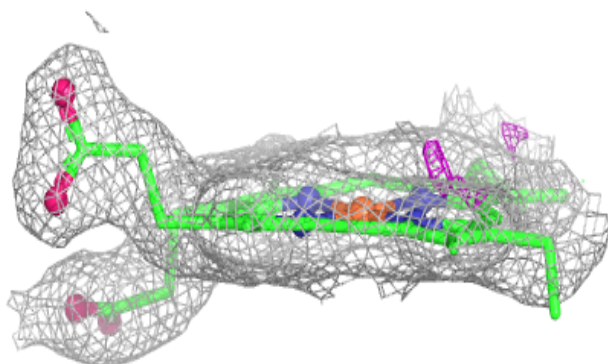
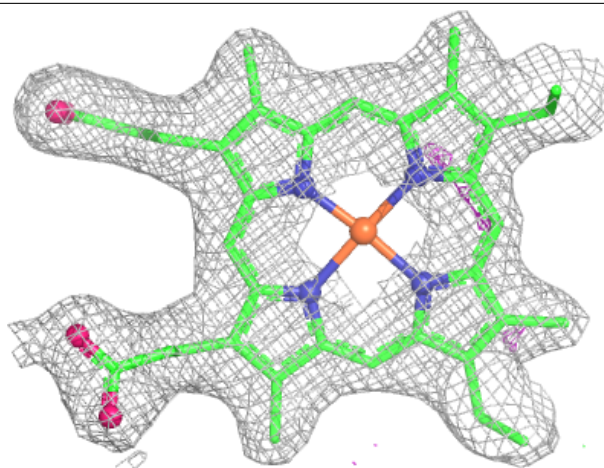
Electron density around HEC f 101:

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



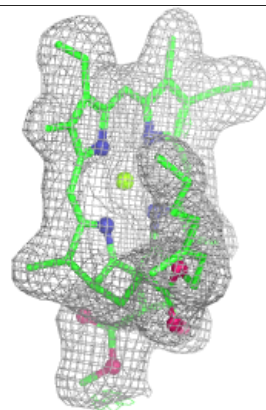
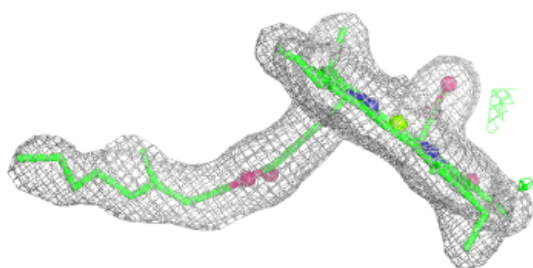
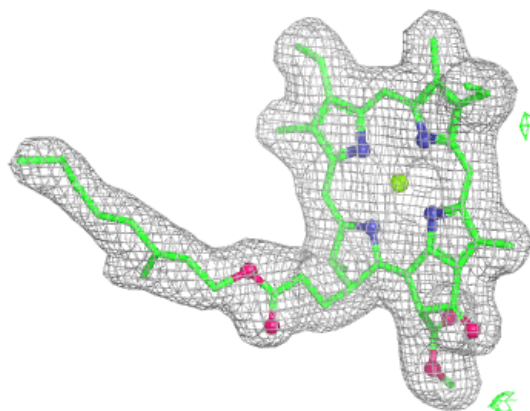
Electron density around HEC V 201:

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



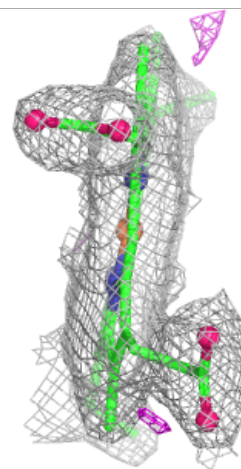
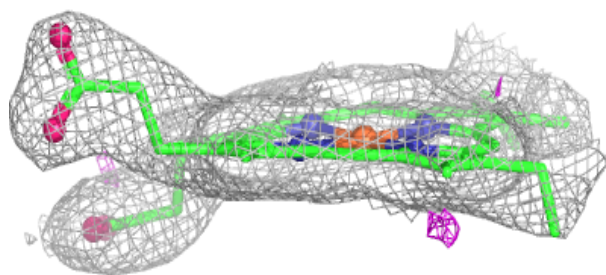
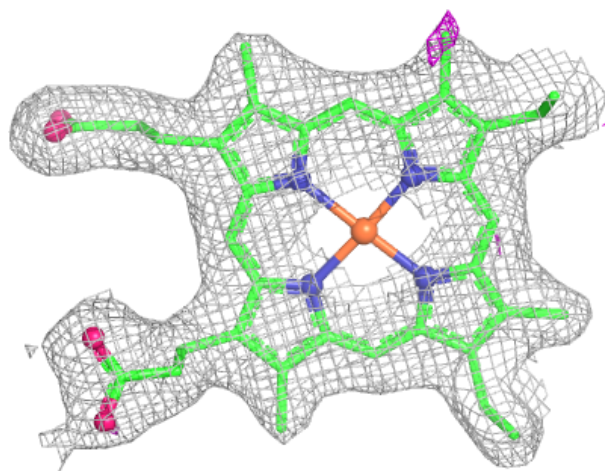
Electron density around CLA A 404:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.