



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:21 am BST

PDB ID : 2AXT
Title : Crystal Structure of Photosystem II from *Thermosynechococcus elongatus*
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.
Deposited on : 2005-09-06
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

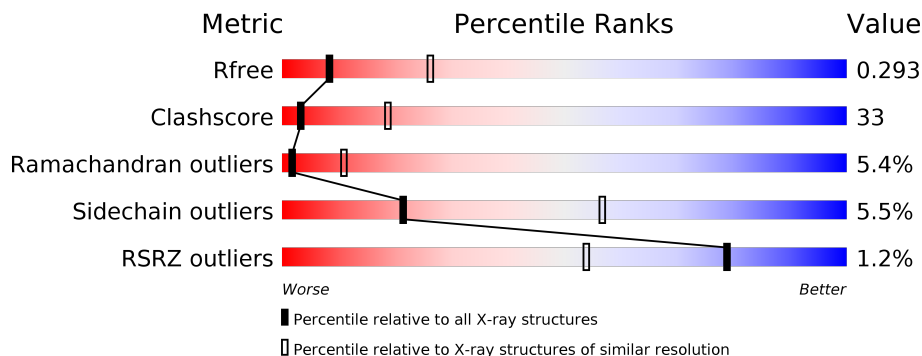
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.





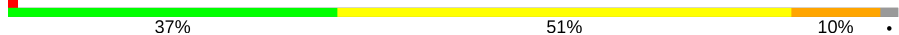

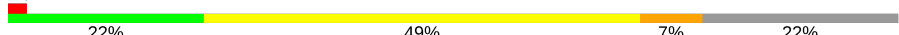

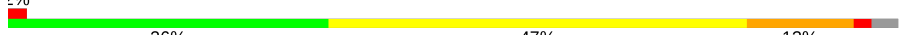




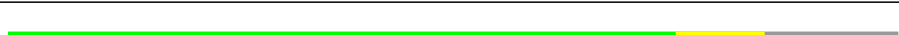


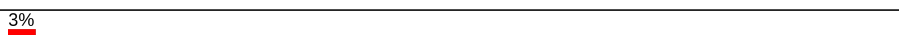
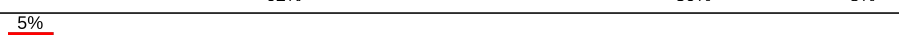

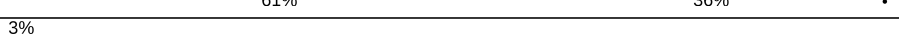
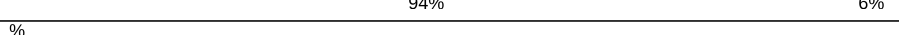






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	
1	a	344	
2	B	510	
2	b	510	
3	C	473	
3	c	473	

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	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
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	X
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-
20	CLA	C	498	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	499	X	-	-	-
20	CLA	C	500	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	D	354	X	-	-	-
20	CLA	D	355	X	-	-	-
20	CLA	a	5558	X	-	-	-
20	CLA	a	5559	X	-	-	-
20	CLA	a	5560	X	-	-	-
20	CLA	a	5563	X	-	-	-
20	CLA	b	5511	X	-	-	-
20	CLA	b	5512	X	-	-	-
20	CLA	b	5513	X	-	-	-
20	CLA	b	5514	X	-	-	-
20	CLA	b	5515	X	-	-	-
20	CLA	b	5516	X	-	-	-
20	CLA	b	5517	X	-	-	-
20	CLA	b	5518	X	-	-	-
20	CLA	b	5519	X	-	-	-
20	CLA	b	5520	X	-	-	-
20	CLA	b	5521	X	-	-	-
20	CLA	b	5522	X	-	-	-
20	CLA	b	5523	X	-	-	-
20	CLA	b	5524	X	-	-	-
20	CLA	b	5525	X	-	-	-
20	CLA	b	5526	X	-	-	-
20	CLA	c	5491	X	-	-	-
20	CLA	c	5492	X	-	-	-
20	CLA	c	5493	X	-	-	-
20	CLA	c	5494	X	-	-	-
20	CLA	c	5495	X	-	-	-
20	CLA	c	5496	X	-	-	-
20	CLA	c	5497	X	-	-	-
20	CLA	c	5498	X	-	-	-
20	CLA	c	5499	X	-	-	-
20	CLA	c	5500	X	-	-	-
20	CLA	c	5501	X	-	-	-
20	CLA	c	5502	X	-	-	-
20	CLA	c	5503	X	-	-	-
20	CLA	d	5354	X	-	-	-
20	CLA	d	5355	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	x	5130	-	-	-	X
27	LMT	A	569	-	-	-	X
27	LMT	t	5217	-	-	-	X
29	UNK	C	489	-	-	-	X
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 48254 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	Total 2623	C 1718	N 432	O 458	S 15	0	0	0
1	a	335	Total 2623	C 1718	N 432	O 458	S 15	0	0	0

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	488	Total 3800	C 2498	N 632	O 657	S 13	0	0	0
2	b	488	Total 3800	C 2498	N 632	O 657	S 13	0	0	0

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	447	Total 3421	C 2244	N 571	O 593	S 13	0	0	0
3	c	447	Total 3421	C 2244	N 571	O 593	S 13	0	0	0

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	340	Total 2696	C 1789	N 436	O 459	S 12	0	0	0
4	d	340	Total 2696	C 1789	N 436	O 459	S 12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	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
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

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

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

- Molecule 17 is a protein called Unassigned subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

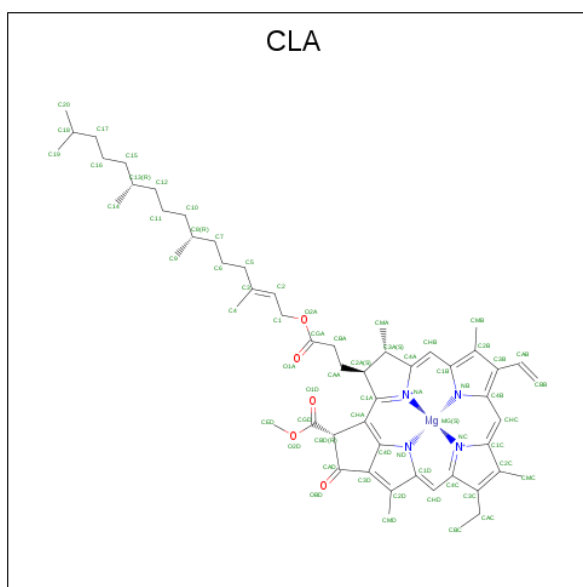
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

- Molecule 19 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	55	45	1	4	5	0	0
20	B	1	41	33	1	4	3	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0
20	B	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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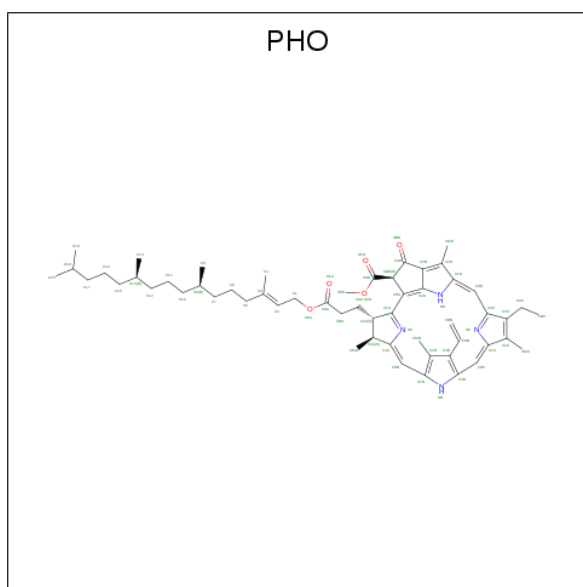
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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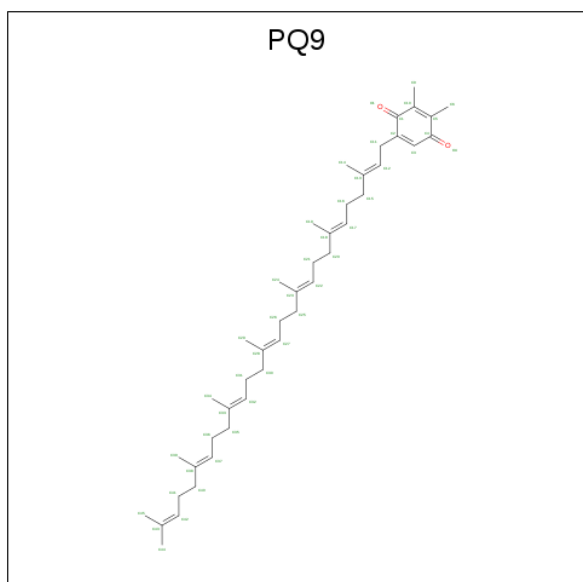
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	c	1	60	50	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	46	36	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	47	37	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	65	55	1	4	5	0	0
20	c	1	51	41	1	4	5	0	0
20	c	1	50	40	1	4	5	0	0
20	d	1	65	55	1	4	5	0	0
20	d	1	50	40	1	4	5	0	0

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



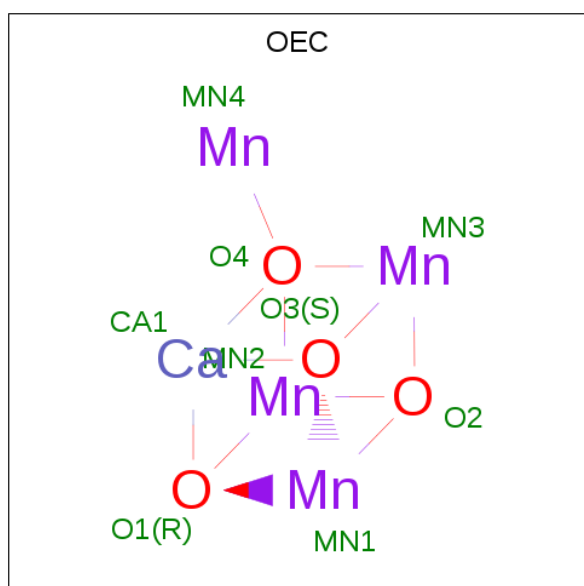
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
21	A	1	64	55	4	5	0	0
21	A	1	64	55	4	5	0	0
21	a	1	64	55	4	5	0	0
21	a	1	64	55	4	5	0	0

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACO SA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: C₄₃H₆₄O₂).



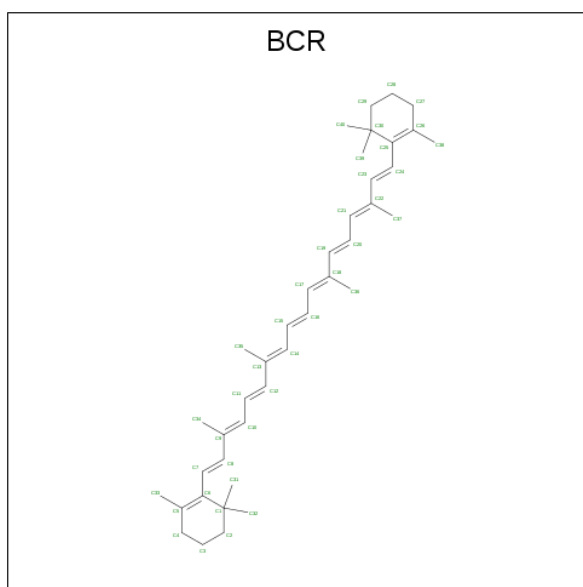
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Ca	Mn	0	0
			5	1	4		
23	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



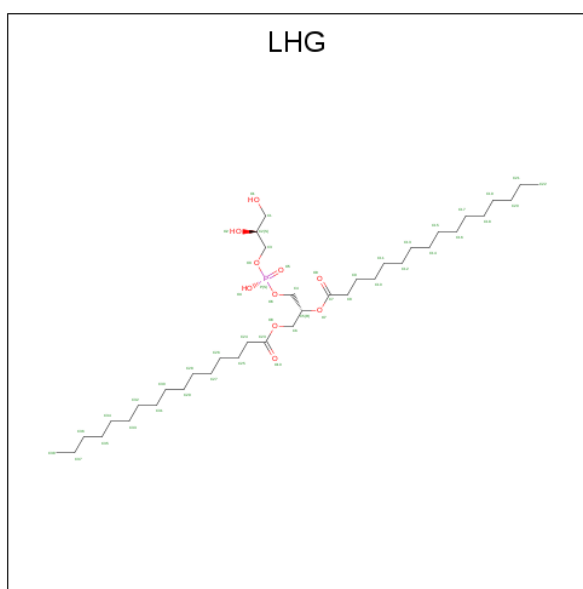
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total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

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

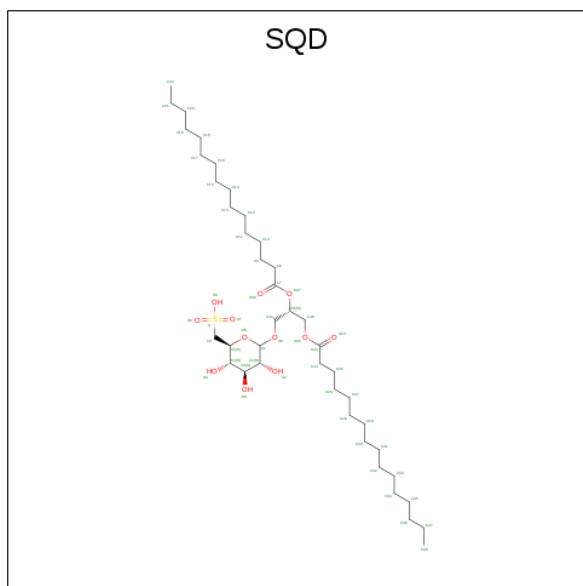
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 39 28 10 1	0	0
25	a	1	Total C O P 39 28 10 1	0	0

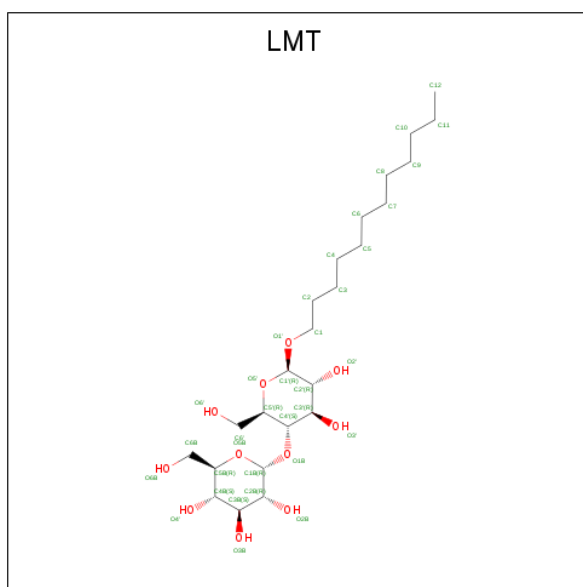
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



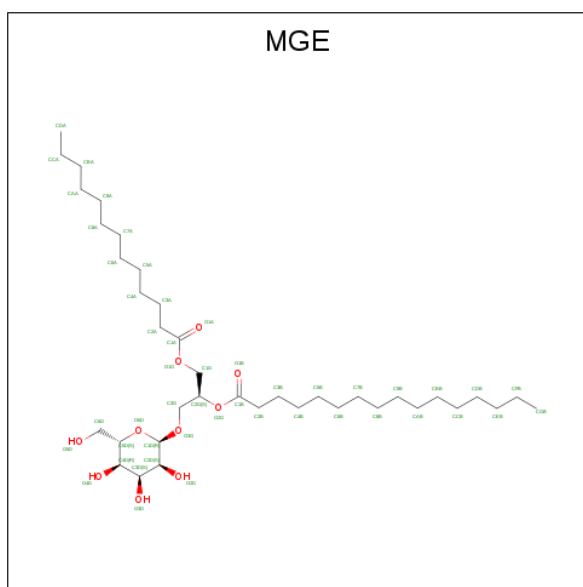
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	T	1	Total	C	O	0	0
			35	24	11		
27	a	1	Total	C	O	0	0
			35	24	11		
27	m	1	Total	C	O	0	0
			35	24	11		
27	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).

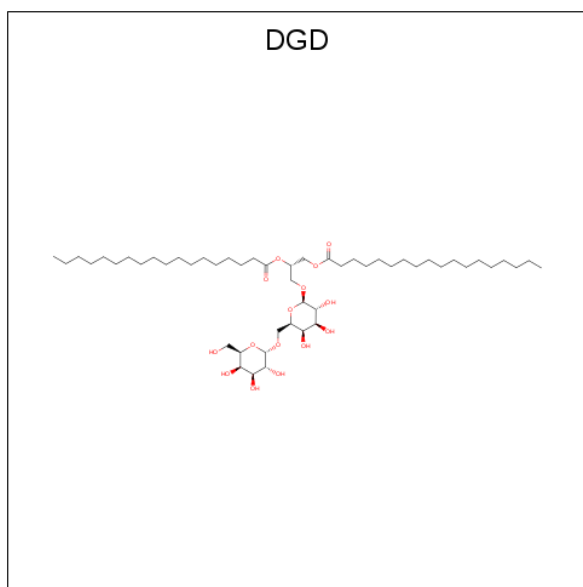


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	C	O	0	0
			47	37	10		
28	d	1	Total	C	O	0	0
			41	31	10		
28	d	1	Total	C	O	0	0
			48	38	10		
28	i	1	Total	C	O	0	0
			48	38	10		
28	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C₄H₉NO₂).

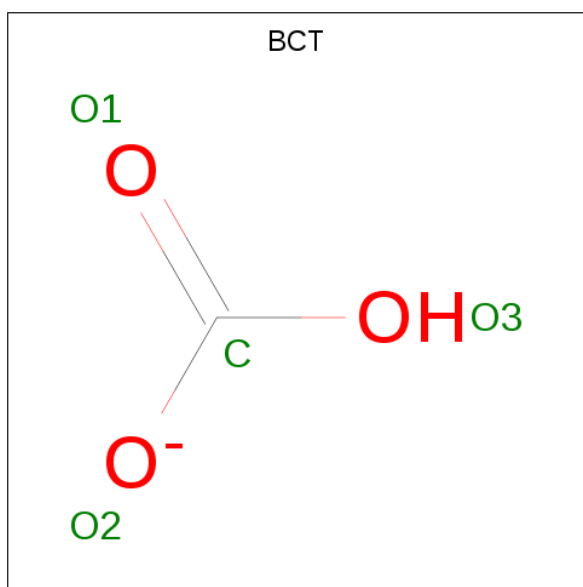
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	17	Total C 152 152	0	0
29	c	17	Total C 152 152	0	0

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



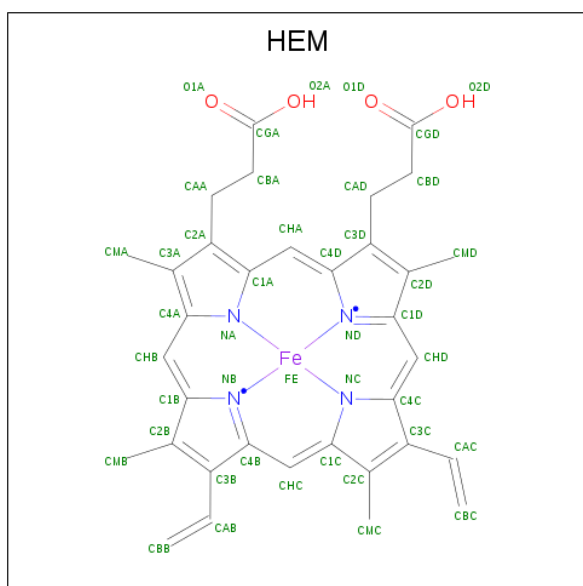
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C O 53 38 15	0	0
30	C	1	Total C O 47 32 15	0	0
30	C	1	Total C O 57 42 15	0	0
30	H	1	Total C O 54 39 15	0	0
30	c	1	Total C O 53 38 15	0	0
30	c	1	Total C O 47 32 15	0	0
30	c	1	Total C O 57 42 15	0	0
30	h	1	Total C O 54 39 15	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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



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

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

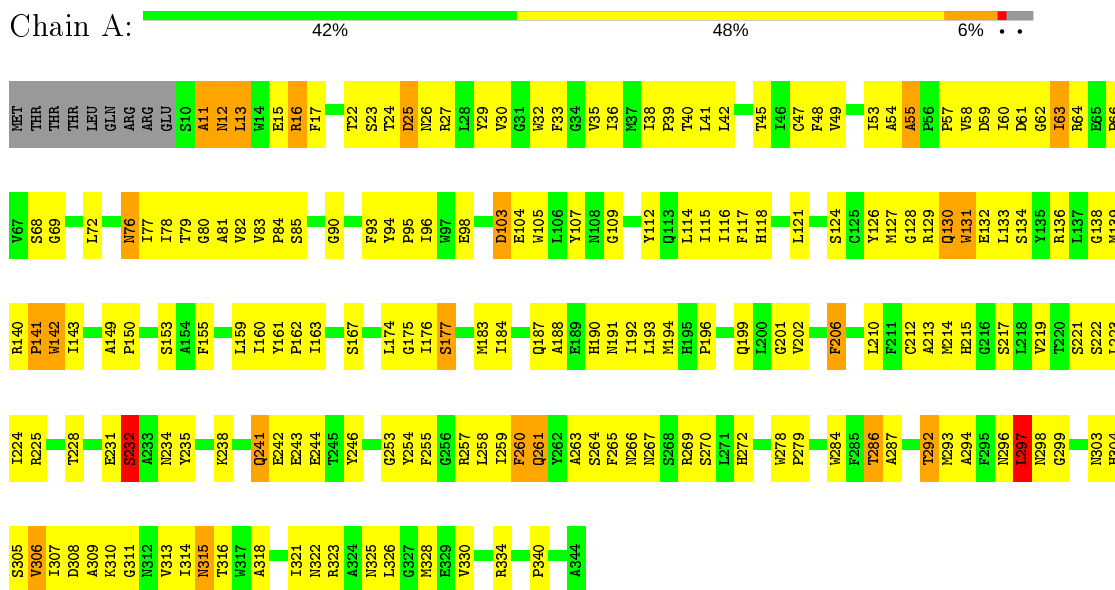
- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total	Ca	0	0
			1	1		
33	k	1	Total	Ca	0	0
			1	1		

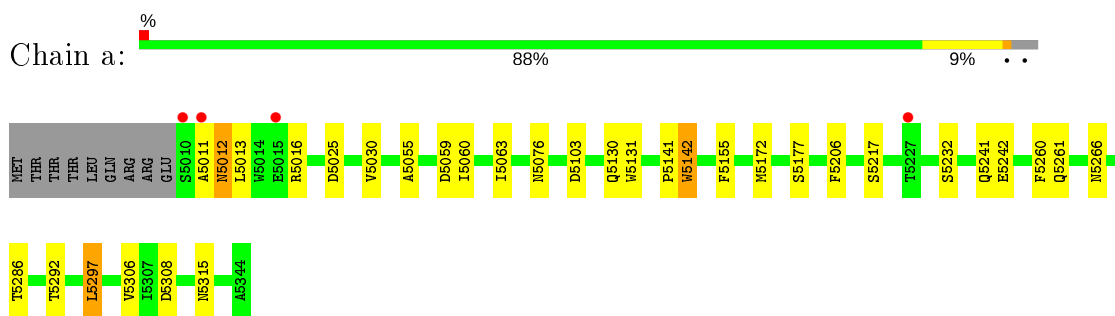
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

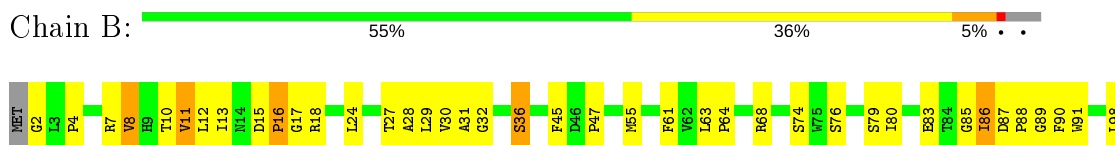
- Molecule 1: Photosystem Q(B) protein

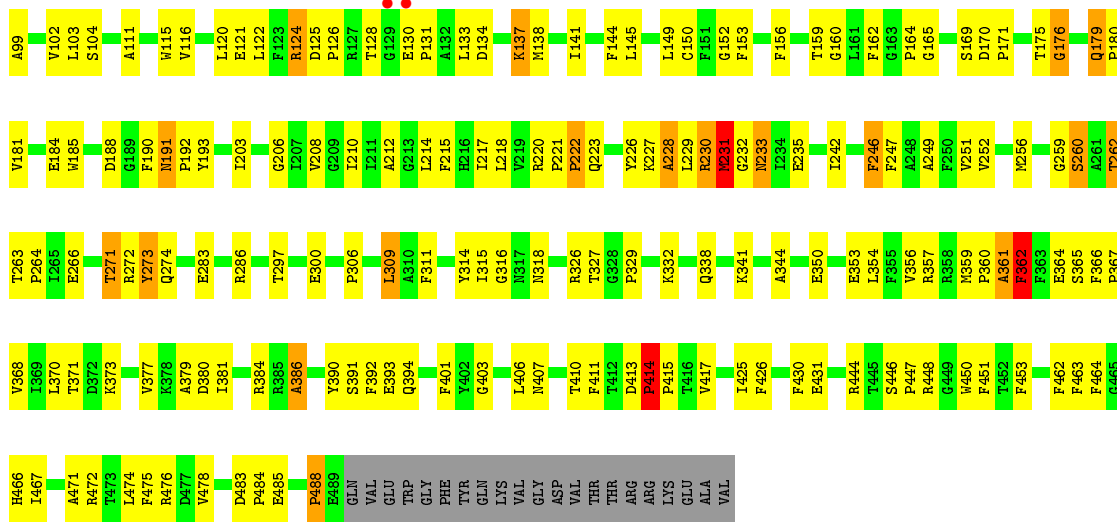


- Molecule 1: Photosystem Q(B) protein

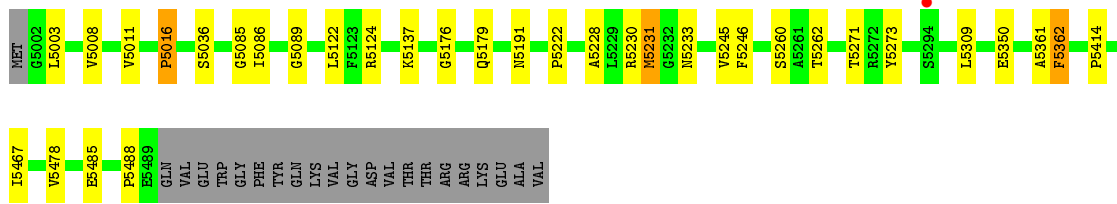
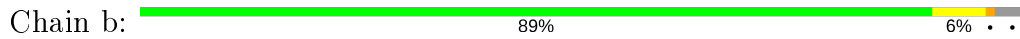


- Molecule 2: CP47 protein

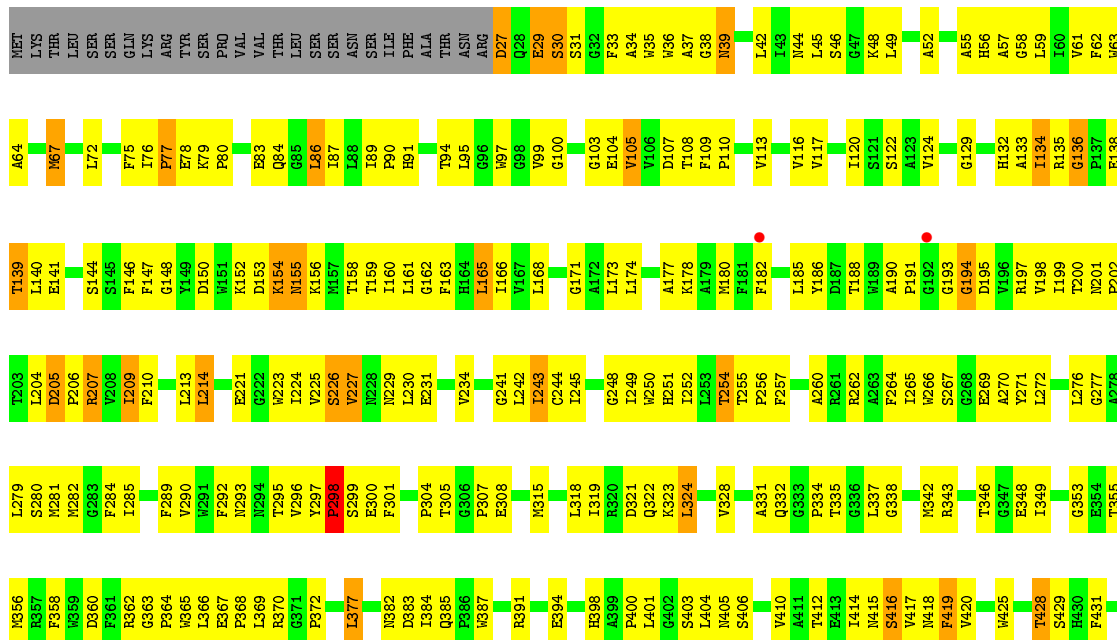


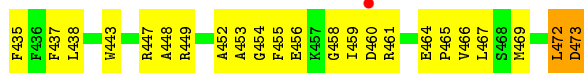


• Molecule 2: CP47 protein

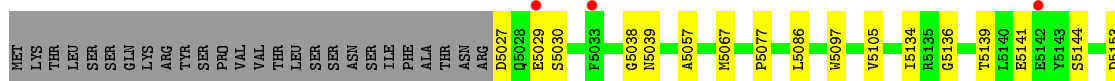
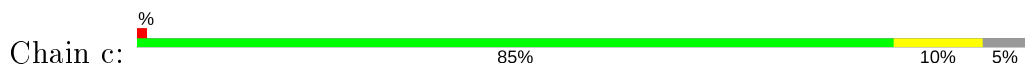


• Molecule 3: photosystem II CP43 protein

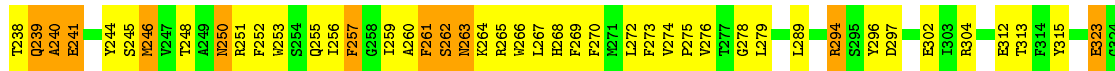
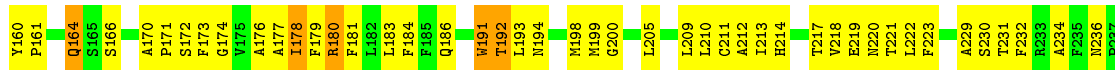




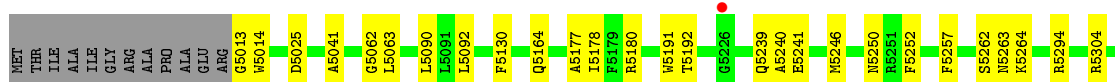
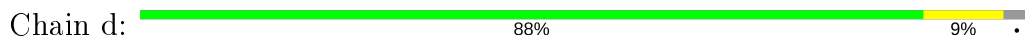
• Molecule 3: photosystem II CP43 protein



• Molecule 4: photosystem II reaction center D2 protein

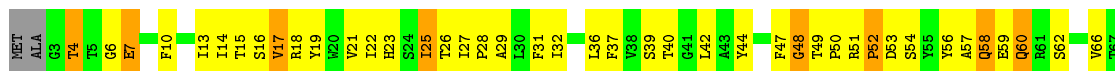


• Molecule 4: photosystem II reaction center D2 protein

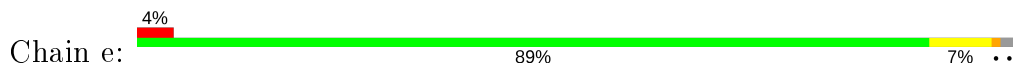


• Molecule 5: Cytochrome b559 alpha subunit





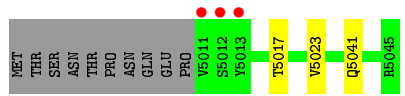
• Molecule 5: Cytochrome b559 alpha subunit



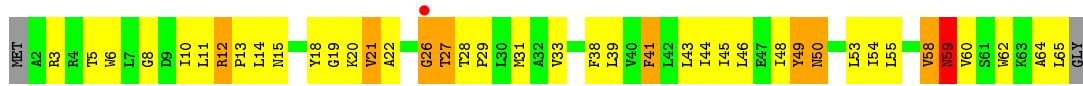
• Molecule 6: Cytochrome b559 beta subunit



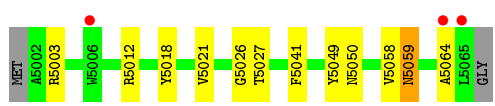
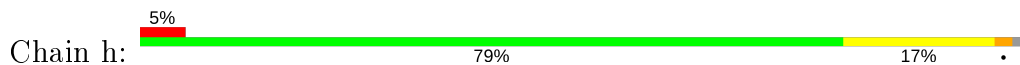
• Molecule 6: Cytochrome b559 beta subunit



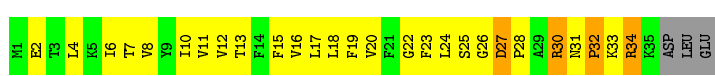
• Molecule 7: Photosystem II reaction center H protein



• Molecule 7: Photosystem II reaction center H protein

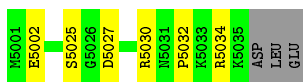


• Molecule 8: Photosystem II reaction center I protein

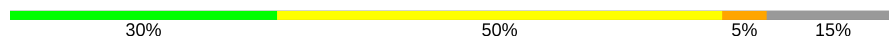


- Molecule 8: Photosystem II reaction center I protein

Chain i:  76% 16% 8%



- Molecule 9: Photosystem II reaction center J protein

Chain J:  30% 50% 5% 15%



- Molecule 9: Photosystem II reaction center J protein

Chain j:  75% 10% 15%




- Molecule 10: Photosystem II reaction center protein K

Chain K:  35% 59% 5%



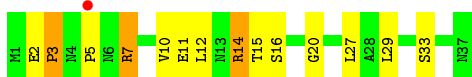
- Molecule 10: Photosystem II reaction center protein K

Chain k:  89% 11%




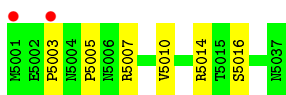
- Molecule 11: Photosystem II reaction center L protein

Chain L:  3% 62% 30% 8%

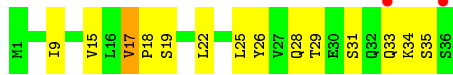


- Molecule 11: Photosystem II reaction center L protein

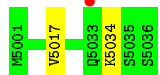
Chain l:  5% 84% 16%



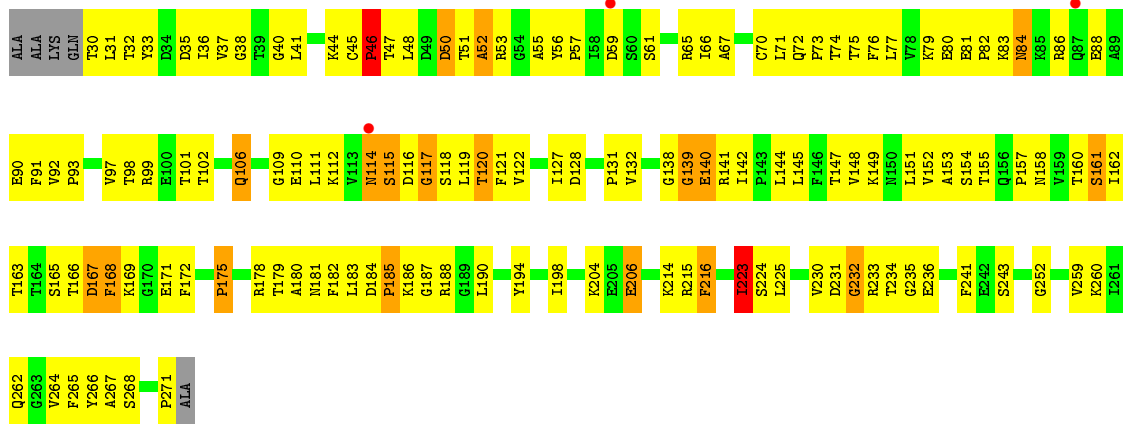
• Molecule 12: Photosystem II reaction center M protein



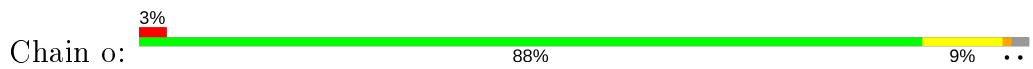
• Molecule 12: Photosystem II reaction center M protein



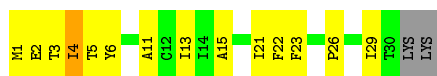
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



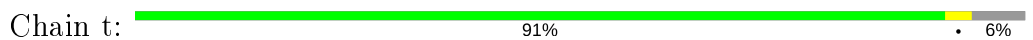
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

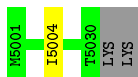


• Molecule 14: Photosystem II reaction center T protein

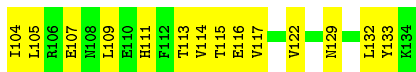


• Molecule 14: Photosystem II reaction center T protein

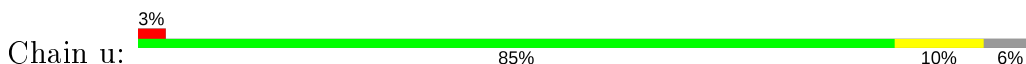




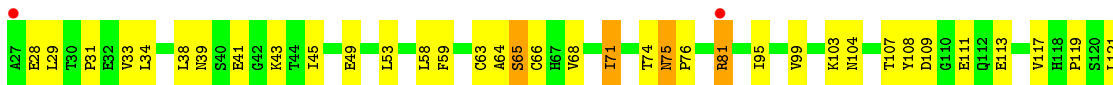
• Molecule 15: Photosystem II 12 kDa extrinsic protein



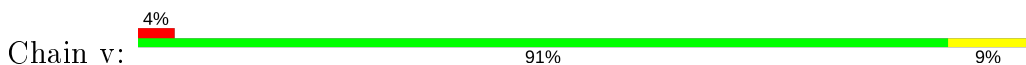
• Molecule 15: Photosystem II 12 kDa extrinsic protein



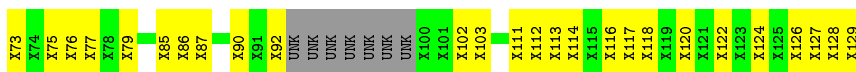
• Molecule 16: Cytochrome c-550



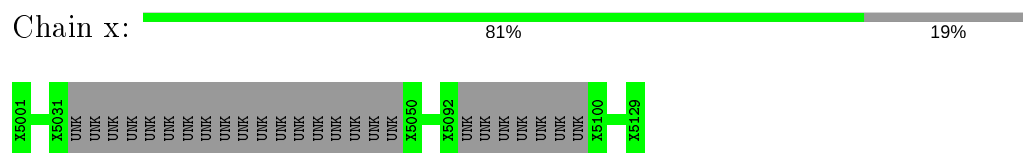
• Molecule 16: Cytochrome c-550



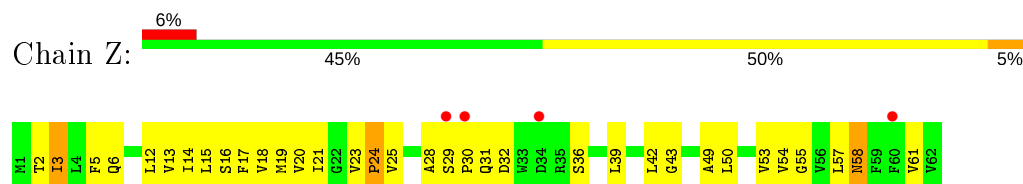
• Molecule 17: Unassigned subunits



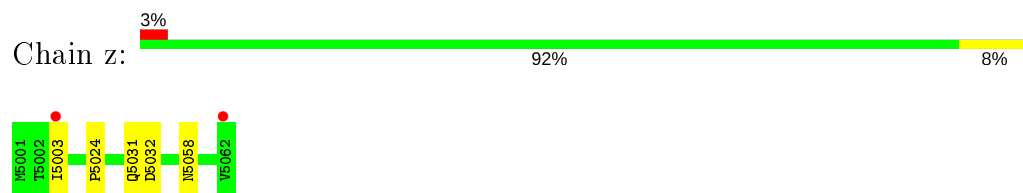
- Molecule 17: Unassigned subunits



- Molecule 18: Photosystem II reaction center Z protein



- Molecule 18: Photosystem II reaction center Z protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.98Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.241 , 0.293	Depositor DCC
R_{free} test set	1908 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtrriage
Anisotropy	0.468	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, MGE, DGD, CA, LMT, CLA, BCT, FE2, PQ9, OEC, HEM, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00
13	o	5223	ILE	CB-CA-C	-5.19	101.21	111.60
2	b	5003	LEU	N-CA-C	-5.06	97.34	111.00
13	o	5271	PRO	N-CA-C	-5.03	99.02	112.10
13	O	223	ILE	CB-CA-C	-5.03	101.55	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	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	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	57	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	1	0	0	0	0
20	A	250	0	265	15	0
20	B	1007	0	1088	74	0
20	C	774	0	783	51	0
20	D	115	0	111	8	0
20	a	250	0	265	0	0
20	b	1007	0	1088	0	0
20	c	774	0	783	0	0
20	d	115	0	111	0	0
21	A	128	0	148	12	0
21	a	128	0	148	0	0
22	A	30	0	37	2	0
22	D	30	0	37	7	0
22	a	30	0	37	0	0
22	d	30	0	37	0	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	6	0
24	C	120	0	168	20	0
24	D	40	0	56	4	0
24	H	40	0	56	3	0
24	T	40	0	56	5	0
24	X	40	0	56	9	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	t	40	0	56	0	0
24	x	40	0	56	0	0
25	A	39	0	51	4	0
25	a	39	0	51	0	0
26	A	80	0	92	0	0
26	L	47	0	60	0	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	0	0
27	A	35	0	46	0	0
27	M	35	0	46	0	0
27	T	35	0	46	3	0
27	a	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	m	35	0	46	0	0
27	t	35	0	46	0	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	0	0
28	d	136	0	194	0	0
28	i	48	0	72	0	0
28	l	48	0	72	0	0
29	C	152	0	17	2	0
29	c	152	0	17	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	0	0
32	v	43	0	30	0	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47107	1538	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1538) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:CD	17:X:26:UNK:NE2	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07
3:C:473:ASP:HB3	14:T:26:PRO:HB3	1.33	1.05
1:A:322:ASN:HD21	3:C:412:THR:HA	1.24	1.01
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.40	1.01
13:O:98:THR:HG22	13:O:99:ARG:H	1.21	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:PRO:HB3	20:B:517:CLA:HED1	1.43	1.00
16:V:38:LEU:HB2	16:V:45:ILE:HG13	1.45	0.99
2:B:68:ARG:HH22	20:B:514:CLA:HED1	1.28	0.98
2:B:263:THR:HG21	2:B:448:ARG:HH12	1.28	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.45	0.98
1:A:310:LYS:HB2	16:V:28:GLU:HB3	1.45	0.98
1:A:190:HIS:HA	1:A:298:ASN:HD22	1.26	0.97
3:C:204:LEU:HD23	3:C:204:LEU:H	1.28	0.96
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.44	0.96
2:B:149:LEU:HG	20:B:513:CLA:HBC1	1.46	0.96
13:O:45:CYS:HB2	13:O:46:PRO:HD2	1.47	0.96
13:O:179:THR:HG22	13:O:181:ASN:H	1.30	0.95
20:C:493:CLA:H191	20:C:493:CLA:HMD2	1.49	0.95
15:U:113:THR:HG22	15:U:114:VAL:N	1.84	0.93
3:C:269:GLU:HG2	3:C:448:ALA:HB2	1.50	0.93
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.49	0.92
8:I:34:ARG:NE	8:I:34:ARG:H	1.67	0.92
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.52	0.92
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.52	0.91
8:I:33:LYS:HA	8:I:34:ARG:HH21	1.34	0.91
10:K:39:TRP:HE1	17:X:31:UNK:HG3	1.33	0.91
20:B:515:CLA:H141	20:B:520:CLA:HMA2	1.54	0.90
24:D:357:BCR:H403	9:J:25:VAL:HG21	1.52	0.89
17:X:86:UNK:O	17:X:87:UNK:HB2	1.73	0.89
4:D:186:GLN:HB2	20:D:354:CLA:HBC1	1.52	0.89
18:Z:36:SER:HA	18:Z:39:LEU:HD12	1.53	0.89
1:A:225:ARG:HH12	2:B:483:ASP:HA	1.35	0.89
8:I:34:ARG:HE	8:I:34:ARG:H	0.92	0.89
15:U:50:ALA:CB	15:U:113:THR:HG21	2.04	0.89
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.54	0.88
17:X:12:UNK:HG3	18:Z:17:PHE:CE1	2.10	0.87
3:C:254:THR:HG22	3:C:255:THR:H	1.40	0.87
3:C:473:ASP:HB3	14:T:26:PRO:CB	2.04	0.87
17:X:6:UNK:NE2	17:X:6:UNK:CG	2.43	0.87
20:B:518:CLA:HAB	4:D:123:ILE:HG23	1.55	0.86
10:K:28:ILE:HA	10:K:31:LEU:HD12	1.57	0.86
2:B:271:THR:H	2:B:274:GLN:HE21	1.17	0.86
28:D:360:MGE:H6D2	11:L:15:THR:HG21	1.57	0.86
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.04	0.86
2:B:327:THR:HG22	20:B:517:CLA:H12	1.58	0.86
13:O:145:LEU:HD23	13:O:175:PRO:HG2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:159:GLY:O	16:V:161:VAL:N	2.08	0.86
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.05	0.86
13:O:145:LEU:CD2	13:O:175:PRO:HG2	2.06	0.86
17:X:26:UNK:NE2	17:X:26:UNK:CG	2.44	0.86
10:K:45:PHE:O	10:K:46:ARG:OXT	1.95	0.85
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.42	0.85
16:V:38:LEU:HD13	16:V:45:ILE:HD11	1.57	0.84
1:A:306:VAL:O	1:A:306:VAL:HG23	1.77	0.84
1:A:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
14:T:29:ILE:HD12	14:T:29:ILE:H	1.43	0.84
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
20:C:493:CLA:HBA1	20:C:493:CLA:HBD	1.59	0.83
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.60	0.83
18:Z:5:PHE:HA	18:Z:57:LEU:HD13	1.59	0.83
1:A:279:PRO:HB2	21:A:561:PHO:HBC1	1.58	0.83
7:H:38:PHE:HB2	24:H:107:BCR:H10C	1.61	0.83
3:C:209:ILE:HG23	24:C:506:BCR:H382	1.61	0.83
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.58	0.83
8:I:34:ARG:HE	8:I:34:ARG:N	1.76	0.83
20:B:518:CLA:H42	4:D:127:LEU:HD11	1.60	0.83
2:B:263:THR:HG22	2:B:448:ARG:HH22	1.44	0.83
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.60	0.82
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.62	0.82
3:C:293:ASN:ND2	3:C:296:VAL:HG22	1.94	0.82
13:O:151:LEU:HD13	13:O:223:ILE:HD11	1.59	0.82
13:O:45:CYS:H	13:O:72:GLN:NE2	1.77	0.82
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.62	0.81
3:C:406:SER:O	3:C:418:ASN:HB2	1.78	0.81
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
4:D:192:THR:HG23	20:D:354:CLA:HBC2	1.60	0.81
5:E:18:ARG:HG2	5:E:22:ILE:HD11	1.62	0.81
24:C:504:BCR:H353	24:X:130:BCR:H321	1.62	0.81
3:C:116:VAL:HG11	24:C:505:BCR:H323	1.62	0.80
6:F:21:VAL:O	6:F:25:THR:HG23	1.80	0.80
3:C:464:GLU:HB2	3:C:467:LEU:HD12	1.61	0.80
4:D:351:ALA:O	4:D:352:LEU:OXT	1.99	0.80
20:C:491:CLA:HMB3	24:C:506:BCR:H403	1.62	0.80
13:O:73:PRO:HG3	13:O:102:THR:HB	1.63	0.80
1:A:201:GLY:HA3	1:A:286:THR:HG23	1.62	0.80
4:D:27:PHE:HD2	4:D:28:VAL:HG23	1.45	0.80
1:A:60:ILE:HG23	1:A:61:ASP:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:49:ALA:O	18:Z:53:VAL:HG23	1.82	0.79
1:A:41:LEU:O	1:A:45:THR:HG22	1.82	0.79
1:A:225:ARG:NH1	2:B:483:ASP:HA	1.96	0.79
4:D:161:PRO:HG2	4:D:170:ALA:HB2	1.63	0.79
3:C:27:ASP:HB2	20:C:501:CLA:HED2	1.64	0.79
13:O:56:TYR:O	13:O:161:SER:HA	1.82	0.79
3:C:365:TRP:HB3	3:C:391:ARG:HD3	1.65	0.78
15:U:58:ASN:ND2	15:U:114:VAL:HG13	1.98	0.78
1:A:190:HIS:HA	1:A:298:ASN:ND2	1.98	0.78
13:O:98:THR:HG22	13:O:99:ARG:N	1.99	0.78
15:U:94:ILE:HB	15:U:97:LEU:HD11	1.66	0.78
3:C:42:LEU:HD21	20:C:501:CLA:H2A	1.66	0.78
3:C:405:ASN:HD22	30:C:509:DGD:HD5	1.48	0.78
3:C:346:THR:O	13:O:40:GLY:HA2	1.84	0.78
14:T:4:ILE:HG13	24:T:5104:BCR:H383	1.65	0.78
4:D:266:TRP:HD1	28:D:360:MGE:H3D	1.48	0.77
8:I:16:VAL:O	8:I:20:VAL:HG23	1.82	0.77
17:X:12:UNK:HG3	18:Z:17:PHE:HE1	1.49	0.77
5:E:18:ARG:O	5:E:22:ILE:HG13	1.85	0.77
3:C:39:ASN:HB2	20:C:498:CLA:HBA1	1.66	0.77
3:C:186:TYR:O	3:C:230:LEU:HD11	1.84	0.77
3:C:282:MET:HA	3:C:285:ILE:HD12	1.67	0.77
2:B:116:VAL:HG21	24:B:529:BCR:H271	1.67	0.77
13:O:155:THR:HG22	13:O:167:ASP:O	1.86	0.77
1:A:142:TRP:HZ2	3:C:447:ARG:HD2	1.50	0.76
15:U:88:VAL:O	15:U:91:VAL:HG23	1.85	0.76
17:X:126:UNK:O	17:X:127:UNK:HB2	1.86	0.76
2:B:68:ARG:NH2	20:B:514:CLA:HED1	2.00	0.76
16:V:64:ALA:O	16:V:68:VAL:HG13	1.86	0.76
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.68	0.76
1:A:257:ARG:HH11	1:A:257:ARG:HG3	1.51	0.76
2:B:263:THR:HG21	2:B:448:ARG:NH1	1.99	0.76
15:U:113:THR:CG2	15:U:114:VAL:H	1.94	0.76
6:F:19:ARG:O	6:F:23:VAL:HG23	1.85	0.76
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.21	0.75
3:C:298:PRO:O	3:C:299:SER:HB3	1.85	0.75
3:C:276:LEU:HD21	20:C:498:CLA:HBB1	1.69	0.75
4:D:266:TRP:CD1	28:D:360:MGE:H3D	2.22	0.75
6:F:34:LEU:HD22	9:J:24:ILE:HD13	1.69	0.75
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.69	0.75
4:D:337:GLU:HG2	4:D:339:PHE:CZ	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:206:PHE:HB2	1.87	0.74
13:O:52:ALA:HB1	13:O:230:VAL:H	1.52	0.74
3:C:103:GLY:HA3	3:C:301:PHE:HE1	1.51	0.74
3:C:419:PHE:HA	30:C:508:DGD:HE5	1.70	0.74
20:A:558:CLA:HBB1	20:D:354:CLA:NB	2.02	0.74
2:B:150:CYS:HB2	20:B:513:CLA:HMC3	1.69	0.74
3:C:204:LEU:O	3:C:205:ASP:HB3	1.85	0.74
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	0.73
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.70	0.73
3:C:449:ARG:HH22	8:I:27:ASP:HB3	1.51	0.73
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.53	0.73
15:U:50:ALA:HB3	15:U:113:THR:HG21	1.70	0.73
1:A:309:ALA:HB3	16:V:28:GLU:HG3	1.68	0.73
2:B:27:THR:O	20:B:515:CLA:HBC1	1.89	0.73
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.19	0.72
13:O:144:LEU:HD23	13:O:144:LEU:H	1.54	0.72
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.71	0.72
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.71	0.72
3:C:204:LEU:CD2	3:C:204:LEU:H	2.02	0.72
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	0.72
21:A:562:PHO:HBC1	4:D:275:PRO:HB2	1.71	0.72
5:E:17:VAL:O	5:E:21:VAL:HG23	1.89	0.72
20:B:518:CLA:HMD1	20:B:520:CLA:HAB	1.70	0.72
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.54	0.72
3:C:337:LEU:HD23	13:O:131:PRO:HG3	1.71	0.72
3:C:464:GLU:CB	3:C:467:LEU:HD12	2.20	0.72
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.20	0.72
24:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	0.72
3:C:29:GLU:HB3	10:K:46:ARG:O	1.89	0.72
3:C:293:ASN:ND2	3:C:296:VAL:H	1.87	0.71
3:C:334:PRO:HA	13:O:179:THR:HB	1.72	0.71
15:U:66:ILE:HG12	15:U:72:TYR:CG	2.25	0.71
2:B:271:THR:HG23	2:B:273:TYR:H	1.56	0.71
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.25	0.71
1:A:224:ILE:HG22	2:B:484:PRO:HG3	1.71	0.71
10:K:17:ILE:HD11	18:Z:6:GLN:HE21	1.56	0.71
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.26	0.71
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.25	0.71
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.55	0.71
4:D:36:LEU:O	4:D:39:PRO:HD2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:THR:CG2	2:B:448:ARG:HH12	2.02	0.70
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.19	0.70
1:A:306:VAL:HG21	1:A:316:THR:HG23	1.74	0.70
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.26	0.70
12:M:25:LEU:O	12:M:28:GLN:HG3	1.92	0.69
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.56	0.69
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.07	0.69
2:B:271:THR:CG2	2:B:273:TYR:H	2.04	0.69
2:B:371:THR:HG22	2:B:377:VAL:HA	1.73	0.69
21:A:562:PHO:H42	4:D:41:ALA:HB1	1.74	0.69
3:C:42:LEU:HD13	20:C:501:CLA:HMA3	1.74	0.69
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.74	0.69
10:K:17:ILE:CD1	18:Z:6:GLN:HE21	2.05	0.69
3:C:241:GLY:C	3:C:243:ILE:H	1.96	0.69
18:Z:21:ILE:O	18:Z:25:VAL:HG23	1.91	0.69
13:O:73:PRO:CG	13:O:102:THR:HB	2.22	0.69
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.75	0.69
20:C:495:CLA:HBD	20:C:495:CLA:HBA1	1.75	0.69
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
3:C:214:LEU:H	3:C:214:LEU:HD23	1.58	0.69
7:H:11:LEU:C	7:H:13:PRO:HD2	2.14	0.69
11:L:14:ARG:HG2	12:M:26:TYR:HE1	1.58	0.69
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.68
18:Z:15:LEU:HD23	18:Z:50:LEU:HD12	1.75	0.68
20:A:559:CLA:HED2	4:D:198:MET:SD	2.33	0.68
2:B:126:PRO:HG3	7:H:12:ARG:NH2	2.09	0.68
3:C:84:GLN:HB2	3:C:86:LEU:HD22	1.75	0.68
1:A:22:THR:HG23	1:A:136:ARG:HH11	1.59	0.68
3:C:363:GLY:O	3:C:367:GLU:HG2	1.93	0.68
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	0.68
2:B:344:ALA:HB2	2:B:401:PHE:CE1	2.29	0.68
4:D:84:SER:HB2	5:E:68:ASP:HA	1.74	0.68
5:E:58:GLN:HE22	16:V:28:GLU:HA	1.58	0.68
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.11	0.68
24:C:505:BCR:H312	18:Z:55:GLY:HA2	1.75	0.68
1:A:270:SER:HA	4:D:232:PHE:CE2	2.29	0.68
13:O:36:ILE:HG23	13:O:41:LEU:HB2	1.76	0.68
1:A:47:CYS:SG	1:A:114:LEU:HD23	2.34	0.67
5:E:4:THR:HG23	17:X:90:UNK:CD2	2.24	0.67
2:B:231:MET:HG3	20:B:520:CLA:HAC2	1.75	0.67
20:B:515:CLA:HMB3	20:B:516:CLA:H11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PRO:HG3	7:H:27:THR:H	1.60	0.67
3:C:124:VAL:HB	24:C:505:BCR:H362	1.77	0.67
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	0.67
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.24	0.67
4:D:261:PHE:O	4:D:262:SER:HB3	1.94	0.67
2:B:191:ASN:HD22	2:B:192:PRO:CD	2.07	0.67
4:D:89:LEU:HG	7:H:50:ASN:OD1	1.95	0.67
13:O:234:THR:OG1	13:O:236:GLU:HG2	1.95	0.67
13:O:163:THR:H	13:O:166:THR:HG23	1.60	0.67
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.75	0.67
3:C:150:ASP:O	3:C:153:ASP:HB3	1.96	0.67
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	0.67
5:E:40:THR:HG21	17:X:102:UNK:CB	2.25	0.67
17:X:54:UNK:HB1	17:X:57:UNK:CG2	2.25	0.67
3:C:153:ASP:O	3:C:155:ASN:N	2.28	0.66
3:C:210:PHE:O	3:C:213:LEU:HB2	1.95	0.66
2:B:353:GLU:HB3	2:B:373:LYS:NZ	2.10	0.66
1:A:60:ILE:HG23	1:A:61:ASP:N	2.09	0.66
10:K:35:LEU:HD22	17:X:17:UNK:CB	2.26	0.66
13:O:32:THR:H	13:O:35:ASP:HB2	1.61	0.66
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.78	0.66
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.78	0.66
3:C:56:HIS:C	3:C:58:GLY:H	1.99	0.66
14:T:4:ILE:HD13	14:T:4:ILE:C	2.16	0.66
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.11	0.66
2:B:297:THR:CB	2:B:300:GLU:HG3	2.26	0.65
2:B:463:PHE:HZ	20:B:518:CLA:HBB1	1.61	0.65
4:D:267:LEU:HD23	4:D:267:LEU:C	2.17	0.65
5:E:10:PHE:O	5:E:13:ILE:HG22	1.95	0.65
13:O:77:LEU:N	13:O:77:LEU:HD12	2.10	0.65
24:X:130:BCR:H331	24:X:130:BCR:HC8	1.78	0.65
10:K:23:ASP:OD2	17:X:6:UNK:NE2	2.34	0.65
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.25	0.65
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.25	0.65
5:E:22:ILE:HG23	17:X:116:UNK:HA	1.78	0.65
1:A:270:SER:HA	4:D:232:PHE:HE2	1.61	0.65
3:C:466:VAL:HA	3:C:469:MET:HE3	1.79	0.65
10:K:28:ILE:O	10:K:31:LEU:HB2	1.97	0.65
1:A:76:ASN:ND2	1:A:79:THR:H	1.95	0.65
2:B:176:GLY:HA3	2:B:266:GLU:OE1	1.96	0.65
17:X:51:UNK:O	17:X:52:UNK:C	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:558:CLA:H143	21:A:561:PHO:H62	1.78	0.65
2:B:392:PHE:O	2:B:393:GLU:HB2	1.96	0.65
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.62	0.65
1:A:94:TYR:OH	1:A:104:GLU:HG2	1.97	0.65
5:E:78:THR:O	5:E:82:GLN:HG2	1.97	0.65
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.80	0.64
20:C:501:CLA:H151	18:Z:20:VAL:HG13	1.78	0.64
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.33	0.64
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.80	0.64
3:C:265:ILE:HD13	20:C:495:CLA:HED1	1.78	0.64
3:C:449:ARG:NH2	8:I:27:ASP:HB3	2.12	0.64
1:A:305:SER:O	1:A:306:VAL:C	2.35	0.64
2:B:223:GLN:HE22	2:B:227:LYS:HD3	1.62	0.64
3:C:279:LEU:HA	3:C:282:MET:HE3	1.80	0.64
4:D:210:LEU:HD21	22:D:356:PQ9:H17	1.80	0.64
6:F:37:ILE:HG22	9:J:28:PHE:CE1	2.33	0.64
20:C:495:CLA:CMD	20:C:497:CLA:HAB	2.27	0.64
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.33	0.64
2:B:223:GLN:HE22	2:B:227:LYS:CD	2.10	0.64
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.80	0.64
1:A:134:SER:HB2	1:A:139:MET:HG3	1.79	0.63
1:A:187:GLN:HG3	1:A:325:ASN:OD1	1.98	0.63
16:V:95:ILE:O	16:V:99:VAL:HG23	1.97	0.63
24:C:504:BCR:H311	24:C:504:BCR:H343	1.81	0.63
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	0.63
7:H:12:ARG:N	7:H:13:PRO:HD2	2.13	0.63
24:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
13:O:184:ASP:HB2	13:O:185:PRO:HD2	1.80	0.63
1:A:243:GLU:HA	4:D:241:GLU:HA	1.80	0.63
20:B:519:CLA:HMC2	24:H:107:BCR:H343	1.81	0.63
2:B:120:LEU:HD13	20:B:526:CLA:HMD2	1.79	0.63
4:D:229:ALA:O	4:D:231:THR:HG23	1.97	0.63
16:V:49:GLU:O	16:V:53:LEU:HG	1.98	0.63
4:D:36:LEU:C	4:D:39:PRO:HD2	2.19	0.63
3:C:248:GLY:O	3:C:252:ILE:HG13	1.97	0.63
3:C:343:ARG:HB2	13:O:101:THR:HG23	1.80	0.63
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	0.63
2:B:208:VAL:HG21	20:B:512:CLA:HMC1	1.81	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	0.63
4:D:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63
7:H:43:LEU:HD23	17:X:60:UNK:CZ	2.29	0.63
16:V:38:LEU:HD13	16:V:45:ILE:CD1	2.29	0.63
1:A:16:ARG:HD3	1:A:17:PHE:N	2.14	0.63
3:C:417:VAL:O	3:C:417:VAL:HG22	1.99	0.63
3:C:52:ALA:HA	20:C:501:CLA:HMB3	1.80	0.63
13:O:45:CYS:HB2	13:O:46:PRO:CD	2.27	0.63
15:U:82:ASN:HB2	15:U:85:TYR:OH	1.99	0.63
3:C:158:THR:HG22	3:C:251:HIS:O	1.99	0.63
7:H:6:TRP:O	7:H:10:ILE:HG13	1.99	0.63
2:B:246:PHE:CD1	2:B:246:PHE:C	2.72	0.62
5:E:23:HIS:C	5:E:25:ILE:H	2.02	0.62
15:U:89:GLU:CD	15:U:89:GLU:H	2.02	0.62
5:E:57:ALA:O	5:E:59:GLU:N	2.32	0.62
16:V:135:GLU:O	16:V:139:VAL:HG23	1.98	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.81	0.62
13:O:110:GLU:O	13:O:110:GLU:HG3	1.99	0.62
1:A:40:THR:HG21	1:A:121:LEU:HB3	1.81	0.62
13:O:45:CYS:H	13:O:72:GLN:HE22	1.48	0.62
20:C:501:CLA:H171	18:Z:20:VAL:HA	1.79	0.62
1:A:72:LEU:HD23	14:T:3:THR:HG21	1.82	0.62
2:B:2:GLY:HA3	11:L:11:GLU:OE1	2.00	0.62
4:D:103:ARG:NH1	5:E:77:GLU:HG3	2.15	0.62
13:O:183:LEU:HD22	13:O:187:GLY:O	1.99	0.62
3:C:55:ALA:HB1	24:C:504:BCR:H373	1.82	0.62
4:D:90:LEU:HD23	4:D:109:GLY:HA2	1.81	0.62
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.30	0.62
13:O:46:PRO:HB2	13:O:266:TYR:CG	2.35	0.62
1:A:253:GLY:O	1:A:257:ARG:HD2	2.00	0.61
2:B:357:ARG:NH2	4:D:337:GLU:HG3	2.14	0.61
17:X:28:UNK:CG2	18:Z:29:SER:HA	2.30	0.61
1:A:49:VAL:O	1:A:53:ILE:HG13	2.00	0.61
6:F:41:GLN:HE21	6:F:41:GLN:HA	1.64	0.61
2:B:329:PRO:CB	20:B:517:CLA:HED1	2.26	0.61
3:C:35:TRP:NE1	3:C:36:TRP:HD1	1.99	0.61
17:X:26:UNK:HG2	17:X:26:UNK:NE2	2.20	0.61
1:A:25:ASP:HB3	4:D:251:ARG:HH22	1.65	0.61
6:F:41:GLN:NE2	6:F:41:GLN:HA	2.15	0.61
3:C:90:PRO:O	3:C:94:THR:HG23	2.01	0.61
6:F:31:ILE:HG13	32:F:51:HEM:HMC2	1.82	0.61
16:V:39:ASN:HD21	16:V:41:GLU:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:O	2:B:251:VAL:HG23	2.00	0.61
3:C:298:PRO:O	3:C:299:SER:CB	2.48	0.61
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
5:E:10:PHE:HA	5:E:13:ILE:HG22	1.83	0.61
7:H:21:VAL:HG22	7:H:22:ALA:O	2.01	0.61
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.01	0.61
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.82	0.61
2:B:31:ALA:HB2	20:B:515:CLA:HBC3	1.83	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	0.61
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
1:A:64:ARG:C	1:A:66:PRO:HD3	2.21	0.61
2:B:185:TRP:HH2	2:B:203:ILE:HG21	1.66	0.61
29:C:474:UNK:C15	22:D:356:PQ9:H293	2.31	0.61
13:O:128:ASP:OD2	13:O:149:LYS:HG2	2.01	0.60
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.31	0.60
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.16	0.60
2:B:271:THR:HG22	2:B:274:GLN:H	1.64	0.60
5:E:56:TYR:HB3	5:E:60:GLN:HG3	1.83	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	0.60
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.83	0.60
15:U:66:ILE:HG22	15:U:66:ILE:O	2.01	0.60
5:E:36:LEU:HA	5:E:39:SER:HB3	1.82	0.60
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.16	0.60
2:B:137:LYS:O	2:B:141:ILE:HG13	2.02	0.60
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.15	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	0.60
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
9:J:8:ILE:H	9:J:8:ILE:HD12	1.66	0.60
14:T:21:ILE:HD12	24:T:5104:BCR:H332	1.83	0.60
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	0.60
7:H:49:TYR:CD2	30:H:208:DGD:HB22	2.37	0.60
1:A:315:ASN:O	4:D:63:LEU:HB3	2.02	0.60
2:B:10:THR:O	2:B:13:ILE:HG13	2.02	0.60
15:U:117:VAL:HG13	15:U:122:VAL:HG21	1.82	0.60
2:B:229:LEU:O	2:B:231:MET:N	2.35	0.60
3:C:230:LEU:O	3:C:234:VAL:HG23	2.01	0.59
4:D:337:GLU:HG2	4:D:339:PHE:CE2	2.36	0.59
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
5:E:60:GLN:O	5:E:60:GLN:HG3	2.01	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:55:ALA:O	13:O:57:PRO:HD3	2.02	0.59
3:C:428:THR:HG22	3:C:429:SER:N	2.17	0.59
3:C:458:GLY:HA2	4:D:222:LEU:O	2.02	0.59
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.32	0.59
13:O:112:LYS:HE2	13:O:114:ASN:HB3	1.84	0.59
13:O:179:THR:CG2	13:O:180:ALA:N	2.65	0.59
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.84	0.59
16:V:147:VAL:O	16:V:150:LYS:HB2	2.02	0.59
4:D:60:THR:HG23	4:D:61:HIS:N	2.18	0.59
18:Z:14:ILE:O	18:Z:18:VAL:HG23	2.02	0.59
1:A:326:LEU:CD2	3:C:412:THR:HB	2.33	0.59
18:Z:16:SER:O	18:Z:20:VAL:HG23	2.03	0.59
7:H:62:TRP:CD1	30:H:208:DGD:HE5	2.37	0.59
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.84	0.59
2:B:384:ARG:NH1	15:U:132:LEU:HD22	2.18	0.59
7:H:29:PRO:O	7:H:33:VAL:HG23	2.02	0.59
13:O:230:VAL:HG12	13:O:231:ASP:N	2.17	0.59
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.38	0.59
1:A:307:ILE:HD11	1:A:311:GLY:O	2.00	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD22	20:D:354:CLA:HBA2	1.85	0.58
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.84	0.58
4:D:39:PRO:O	4:D:43:LEU:HB2	2.03	0.58
13:O:204:LYS:HB3	13:O:206:GLU:HG2	1.85	0.58
3:C:265:ILE:HG22	3:C:270:ALA:CB	2.33	0.58
3:C:315:MET:O	3:C:319:ILE:HG13	2.04	0.58
3:C:465:PRO:C	3:C:469:MET:HE2	2.23	0.58
1:A:131:TRP:CE3	1:A:132:GLU:N	2.72	0.58
3:C:456:GLU:N	3:C:456:GLU:OE1	2.35	0.58
13:O:76:PHE:C	13:O:77:LEU:HD12	2.23	0.58
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.85	0.58
18:Z:5:PHE:CA	18:Z:57:LEU:HD13	2.32	0.58
4:D:102:THR:O	4:D:105:CYS:HB2	2.04	0.58
4:D:120:PHE:HA	4:D:123:ILE:HD12	1.85	0.58
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.39	0.58
17:X:7:UNK:O	17:X:11:UNK:HG2	2.04	0.58
21:A:562:PHO:CMC	4:D:279:LEU:HD11	2.34	0.58
2:B:471:ALA:O	2:B:475:PHE:HB2	2.04	0.58
2:B:24:LEU:HD21	20:B:526:CLA:HAB	1.86	0.58
2:B:149:LEU:HG	20:B:513:CLA:CBC	2.28	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ARG:HD3	4:D:106:GLN:OE1	2.04	0.58
4:D:110:LEU:O	4:D:114:ILE:HG13	2.04	0.58
13:O:152:VAL:HG13	13:O:152:VAL:O	2.04	0.58
13:O:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
1:A:54:ALA:O	1:A:55:ALA:HB2	2.03	0.57
1:A:62:GLY:HA3	3:C:356:MET:SD	2.44	0.57
3:C:452:ALA:C	3:C:454:GLY:N	2.56	0.57
13:O:65:ARG:HA	13:O:111:LEU:H	1.68	0.57
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.69	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	0.57
3:C:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
5:E:60:GLN:C	5:E:62:SER:H	2.07	0.57
1:A:217:SER:HA	4:D:272:LEU:HD12	1.86	0.57
4:D:343:GLU:HG2	16:V:161:VAL:HG11	1.86	0.57
6:F:34:LEU:HD22	9:J:24:ILE:CD1	2.32	0.57
13:O:142:ILE:HD12	13:O:142:ILE:N	2.19	0.57
8:I:27:ASP:N	8:I:28:PRO:CD	2.67	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	1.85	0.57
9:J:14:ALA:HB1	24:X:130:BCR:H393	1.85	0.57
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.57
2:B:150:CYS:HA	20:B:513:CLA:HBC2	1.87	0.57
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.04	0.57
18:Z:39:LEU:O	18:Z:42:LEU:HB3	2.05	0.57
3:C:44:ASN:O	3:C:45:LEU:HG	2.04	0.57
3:C:428:THR:CG2	30:C:508:DGD:HA91	2.35	0.57
4:D:239:GLN:O	4:D:240:ALA:HB3	2.05	0.57
4:D:261:PHE:HB2	22:D:356:PQ9:H92	1.84	0.57
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	0.57
4:D:273:PHE:CZ	28:L:210:MGE:H3B2	2.40	0.57
4:D:239:GLN:O	4:D:240:ALA:CB	2.53	0.57
5:E:15:THR:HG23	9:J:8:ILE:O	2.04	0.57
10:K:18:PHE:O	10:K:19:ASP:C	2.43	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	0.57
13:O:168:PHE:CD1	13:O:168:PHE:N	2.71	0.57
14:T:4:ILE:O	14:T:4:ILE:HD13	2.04	0.57
20:B:518:CLA:HMA1	4:D:130:PHE:CE1	2.40	0.57
4:D:14:TRP:HD1	4:D:15:PHE:N	2.03	0.57
13:O:172:PHE:CE2	13:O:223:ILE:HG12	2.39	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:MET:HA	6:F:43:ILE:HG13	1.84	0.57
9:J:15:THR:HG22	10:K:38:VAL:HG22	1.85	0.57
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.35	0.57
4:D:348:ARG:NH2	4:D:352:LEU:OXT	2.37	0.57
13:O:73:PRO:HG2	13:O:102:THR:OG1	2.05	0.57
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
2:B:138:MET:SD	20:B:525:CLA:HAC1	2.45	0.56
2:B:391:SER:OG	2:B:394:GLN:HB2	2.05	0.56
13:O:145:LEU:O	13:O:147:THR:HG22	2.05	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	0.56
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	0.56
4:D:221:THR:HG22	4:D:245:SER:H	1.69	0.56
13:O:163:THR:H	13:O:166:THR:CG2	2.18	0.56
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.26	0.56
1:A:213:ALA:O	1:A:217:SER:HB2	2.06	0.56
8:I:19:PHE:CE1	8:I:23:PHE:HE2	2.24	0.56
16:V:39:ASN:ND2	16:V:41:GLU:HB2	2.20	0.56
3:C:198:VAL:HG12	3:C:200:THR:HG23	1.87	0.56
3:C:27:ASP:O	10:K:46:ARG:HD3	2.06	0.56
3:C:72:LEU:HD11	3:C:108:THR:OG1	2.05	0.56
3:C:56:HIS:C	3:C:58:GLY:N	2.59	0.56
1:A:29:TYR:HD1	1:A:133:LEU:HB2	1.69	0.56
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.41	0.56
2:B:55:MET:HE3	2:B:80:ILE:HG12	1.87	0.56
3:C:315:MET:CE	3:C:319:ILE:HD11	2.35	0.56
8:I:11:VAL:O	8:I:15:PHE:HD1	1.89	0.56
15:U:77:LYS:O	15:U:81:LYS:HB2	2.06	0.56
16:V:81:ARG:HH11	16:V:81:ARG:HG3	1.71	0.56
2:B:353:GLU:HB3	2:B:373:LYS:HZ3	1.71	0.56
4:D:103:ARG:HH12	5:E:77:GLU:HG3	1.70	0.56
9:J:33:TYR:O	9:J:34:ALA:HB3	2.04	0.56
1:A:13:LEU:N	1:A:13:LEU:HD23	2.21	0.56
3:C:293:ASN:HD21	3:C:296:VAL:H	1.51	0.56
4:D:178:ILE:HG22	4:D:179:PHE:N	2.21	0.56
2:B:63:LEU:N	2:B:64:PRO:HD2	2.21	0.56
2:B:467:ILE:HD13	4:D:126:MET:SD	2.46	0.56
1:A:221:SER:HA	4:D:139:ARG:HB2	1.86	0.56
3:C:194:GLY:O	3:C:195:ASP:HB2	2.06	0.55
3:C:332:GLN:HA	3:C:338:GLY:HA2	1.88	0.55
16:V:107:THR:HG22	16:V:108:TYR:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.41	0.55
3:C:260:ALA:O	3:C:264:PHE:HD2	1.89	0.55
3:C:348:GLU:OE2	13:O:37:VAL:HA	2.06	0.55
3:C:400:PRO:C	3:C:401:LEU:HD23	2.26	0.55
10:K:39:TRP:O	10:K:43:VAL:HG23	2.05	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.89	0.55
16:V:103:LYS:O	16:V:122:ARG:HG3	2.07	0.55
3:C:284:PHE:HB3	30:C:507:DGD:HA51	1.87	0.55
13:O:163:THR:HG23	13:O:165:SER:H	1.71	0.55
16:V:124:ALA:HB1	16:V:131:ARG:HG3	1.87	0.55
1:A:38:ILE:O	1:A:42:LEU:HG	2.07	0.55
2:B:283:GLU:OE1	2:B:286:ARG:HD2	2.07	0.55
4:D:176:ALA:C	4:D:178:ILE:H	2.10	0.55
5:E:13:ILE:HD13	32:F:51:HEM:O1D	2.07	0.55
6:F:18:VAL:HG13	6:F:19:ARG:N	2.22	0.55
15:U:72:TYR:CB	15:U:73:PRO:CD	2.84	0.55
1:A:224:ILE:CG2	2:B:484:PRO:HG3	2.35	0.55
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.34	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
2:B:233:ASN:C	2:B:233:ASN:HD22	2.10	0.55
1:A:264:SER:OG	1:A:265:PHE:N	2.40	0.55
2:B:229:LEU:O	2:B:230:ARG:C	2.44	0.55
3:C:42:LEU:CD1	20:C:501:CLA:HMA3	2.36	0.55
3:C:209:ILE:CG2	24:C:506:BCR:H382	2.35	0.55
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.89	0.55
2:B:18:ARG:HG3	2:B:18:ARG:HH11	1.70	0.55
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.55
20:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
13:O:47:THR:HG22	13:O:48:LEU:N	2.22	0.55
16:V:159:GLY:O	16:V:160:LYS:C	2.45	0.55
10:K:39:TRP:NE1	17:X:31:UNK:HG3	2.12	0.55
18:Z:23:VAL:HB	18:Z:24:PRO:HD3	1.89	0.55
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.70	0.55
3:C:466:VAL:HA	3:C:469:MET:CE	2.36	0.55
3:C:37:ALA:HA	20:C:498:CLA:O1A	2.06	0.55
13:O:145:LEU:HD23	13:O:175:PRO:CG	2.34	0.55
3:C:416:SER:O	3:C:417:VAL:CG1	2.55	0.54
9:J:14:ALA:CB	24:X:130:BCR:H393	2.38	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.71	0.54
2:B:10:THR:C	2:B:12:LEU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:346:LEU:O	4:D:348:ARG:HG3	2.07	0.54
13:O:75:THR:HG22	13:O:77:LEU:HD11	1.88	0.54
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.82	0.54
24:B:527:BCR:H322	28:B:530:MGE:H2G	1.89	0.54
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.37	0.54
3:C:91:HIS:HB3	20:C:493:CLA:HBA2	1.88	0.54
30:C:509:DGD:HD2	9:J:32:ALA:O	2.06	0.54
10:K:43:VAL:HG12	10:K:46:ARG:HG3	1.90	0.54
3:C:405:ASN:HD22	30:C:509:DGD:C5D	2.19	0.54
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.89	0.54
3:C:55:ALA:HB1	24:C:504:BCR:C37	2.37	0.54
4:D:325:ILE:O	4:D:329:MET:HB3	2.08	0.54
5:E:25:ILE:O	5:E:29:ALA:HB2	2.08	0.54
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.35	0.54
2:B:221:PRO:O	7:H:21:VAL:HG23	2.08	0.54
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.43	0.54
3:C:418:ASN:HB3	30:C:509:DGD:HE2	1.89	0.54
3:C:52:ALA:HB1	20:C:499:CLA:HAB	1.89	0.54
3:C:75:PHE:CE2	3:C:77:PRO:HA	2.43	0.54
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	0.54
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	0.54
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.33	0.54
2:B:392:PHE:O	2:B:393:GLU:CB	2.54	0.54
15:U:57:LEU:HD22	15:U:79:ILE:CG2	2.37	0.54
1:A:174:LEU:HD22	21:A:561:PHO:H152	1.89	0.54
5:E:76:VAL:O	5:E:79:PHE:HB2	2.07	0.54
10:K:45:PHE:O	10:K:46:ARG:C	2.46	0.54
3:C:201:ASN:N	3:C:202:PRO:HD3	2.22	0.54
4:D:100:ASP:OD1	4:D:102:THR:HG22	2.07	0.54
3:C:276:LEU:CD2	20:C:498:CLA:HBB1	2.37	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	0.54
4:D:67:TYR:CD2	4:D:76:VAL:HG11	2.43	0.54
12:M:26:TYR:O	12:M:29:THR:HB	2.08	0.54
3:C:99:VAL:HG23	3:C:100:GLY:H	1.72	0.53
4:D:45:LEU:HD13	4:D:49:LEU:HD12	1.90	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.89	0.53
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.89	0.53
1:A:159:LEU:O	1:A:163:ILE:HG13	2.08	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.53
1:A:76:ASN:HD22	1:A:76:ASN:C	2.11	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.44	0.53
17:X:72:UNK:O	17:X:73:UNK:C	2.57	0.53
2:B:124:ARG:O	7:H:12:ARG:NH2	2.42	0.53
3:C:158:THR:O	3:C:251:HIS:HB3	2.07	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.90	0.53
3:C:84:GLN:HB2	3:C:86:LEU:CD2	2.37	0.53
11:L:11:GLU:HG2	11:L:12:LEU:N	2.24	0.53
11:L:14:ARG:HG3	11:L:14:ARG:NH1	2.22	0.53
14:T:29:ILE:CD1	14:T:29:ILE:H	2.18	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.28	0.53
4:D:14:TRP:HD1	4:D:15:PHE:H	1.55	0.53
5:E:51:ARG:O	5:E:53:ASP:N	2.41	0.53
10:K:14:ALA:HB2	18:Z:61:VAL:HG11	1.90	0.53
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.37	0.53
1:A:286:THR:HB	20:A:558:CLA:O1D	2.09	0.53
2:B:12:LEU:HB2	20:B:522:CLA:HMC2	1.90	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CD2	2.44	0.53
3:C:48:LYS:HE2	3:C:133:ALA:HA	1.90	0.53
13:O:162:ILE:HA	13:O:166:THR:HG21	1.90	0.53
17:X:122:UNK:C	17:X:124:UNK:N	2.70	0.53
1:A:314:ILE:CG2	1:A:314:ILE:O	2.55	0.53
1:A:40:THR:HG22	1:A:118:HIS:O	2.09	0.53
3:C:193:GLY:O	3:C:194:GLY:C	2.47	0.53
4:D:172:SER:O	4:D:173:PHE:HB2	2.08	0.53
16:V:74:THR:O	16:V:75:ASN:HB2	2.07	0.53
1:A:124:SER:O	1:A:127:MET:HB3	2.09	0.53
1:A:238:LYS:O	1:A:241:GLN:HB3	2.09	0.53
3:C:29:GLU:HG3	3:C:30:SER:N	2.22	0.53
4:D:221:THR:HG22	4:D:221:THR:O	2.08	0.53
15:U:72:TYR:O	15:U:73:PRO:C	2.46	0.53
1:A:183:MET:HA	20:A:558:CLA:HMD2	1.90	0.53
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.44	0.53
3:C:377:LEU:HB2	13:O:106:GLN:HG2	1.91	0.53
1:A:141:PRO:O	1:A:143:ILE:N	2.38	0.53
1:A:176:ILE:HD13	20:A:559:CLA:HED3	1.91	0.53
21:A:561:PHO:NC	4:D:209:LEU:HD12	2.24	0.53
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.75	0.52
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HA	24:B:528:BCR:C40	2.39	0.52
2:B:476:ARG:HG3	2:B:476:ARG:HH11	1.74	0.52
2:B:152:GLY:C	20:B:516:CLA:HMC3	2.30	0.52
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.71	0.52
20:C:492:CLA:H111	20:C:493:CLA:HMB2	1.90	0.52
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
28:D:360:MGE:H241	14:T:13:ILE:HG21	1.90	0.52
5:E:32:ILE:O	5:E:36:LEU:HG	2.10	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.09	0.52
10:K:31:LEU:HB3	24:X:130:BCR:C15	2.39	0.52
13:O:33:TYR:C	13:O:35:ASP:H	2.12	0.52
3:C:318:LEU:HD23	3:C:318:LEU:O	2.10	0.52
3:C:63:TRP:O	3:C:64:ALA:C	2.47	0.52
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
2:B:263:THR:O	2:B:263:THR:HG22	2.08	0.52
2:B:391:SER:OG	2:B:394:GLN:NE2	2.43	0.52
3:C:103:GLY:HA3	3:C:301:PHE:CE1	2.37	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
1:A:103:ASP:OD1	1:A:103:ASP:N	2.40	0.52
3:C:56:HIS:O	3:C:58:GLY:N	2.42	0.52
4:D:93:TRP:HZ2	20:D:355:CLA:O1A	1.93	0.52
5:E:69:ARG:O	5:E:70:PHE:HB2	2.09	0.52
17:X:12:UNK:CG	18:Z:17:PHE:CE1	2.90	0.52
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.45	0.52
4:D:348:ARG:HH21	4:D:352:LEU:C	2.12	0.52
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.24	0.52
2:B:220:ARG:HD2	7:H:20:LYS:O	2.10	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	0.52
3:C:29:GLU:C	3:C:31:SER:H	2.13	0.52
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.52
13:O:206:GLU:CD	13:O:206:GLU:H	2.13	0.52
14:T:1:MET:C	14:T:4:ILE:HG22	2.30	0.52
2:B:214:LEU:O	2:B:218:LEU:HG	2.09	0.52
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.44	0.52
8:I:13:THR:O	8:I:17:LEU:HG	2.09	0.52
16:V:134:THR:HG23	16:V:137:ASP:OD2	2.10	0.52
1:A:63:ILE:CG2	3:C:335:THR:HG21	2.40	0.52
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.45	0.52
2:B:262:THR:C	2:B:264:PRO:HD3	2.30	0.52
2:B:362:PHE:HE2	4:D:164:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
1:A:27:ARG:NH1	1:A:27:ARG:O	2.43	0.52
1:A:64:ARG:O	1:A:66:PRO:HD3	2.10	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
3:C:116:VAL:HG21	24:C:505:BCR:C32	2.40	0.52
20:C:503:CLA:HMC2	24:C:505:BCR:H372	1.91	0.52
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.91	0.52
2:B:137:LYS:HD2	7:H:14:LEU:O	2.10	0.52
11:L:2:GLU:HB3	11:L:3:PRO:HD2	1.92	0.52
13:O:118:SER:HB3	13:O:157:PRO:HA	1.90	0.52
16:V:33:VAL:HG12	16:V:33:VAL:O	2.10	0.52
1:A:257:ARG:HH12	1:A:261:GLN:CD	2.13	0.51
4:D:14:TRP:CD1	4:D:15:PHE:N	2.78	0.51
9:J:24:ILE:HG23	9:J:25:VAL:N	2.24	0.51
13:O:110:GLU:OE2	13:O:112:LYS:HB2	2.10	0.51
18:Z:57:LEU:O	18:Z:61:VAL:HG23	2.10	0.51
2:B:413:ASP:OD1	2:B:415:PRO:HD2	2.09	0.51
4:D:223:PHE:CZ	4:D:245:SER:HB3	2.44	0.51
13:O:144:LEU:N	13:O:144:LEU:HD23	2.23	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
2:B:463:PHE:CZ	20:B:518:CLA:HBB1	2.43	0.51
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
13:O:172:PHE:HE2	13:O:223:ILE:HG12	1.75	0.51
16:V:59:PHE:HA	16:V:63:CYS:SG	2.50	0.51
1:A:192:ILE:HG23	1:A:193:LEU:N	2.25	0.51
2:B:212:ALA:HB2	20:B:519:CLA:HMC3	1.91	0.51
20:C:493:CLA:HBA1	20:C:493:CLA:CBP	2.37	0.51
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.91	0.51
17:X:76:UNK:O	17:X:77:UNK:C	2.57	0.51
1:A:326:LEU:HD21	3:C:412:THR:HB	1.93	0.51
2:B:229:LEU:HD11	20:B:519:CLA:O1A	2.11	0.51
2:B:380:ASP:OD2	2:B:380:ASP:C	2.47	0.51
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
14:T:4:ILE:HB	27:T:217:LMT:O6'	2.11	0.51
15:U:69:ARG:O	15:U:70:GLY:C	2.47	0.51
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.45	0.51
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ASN:ND2	2:B:235:GLU:H	2.08	0.51
10:K:39:TRP:HE1	17:X:31:UNK:CG	2.14	0.51
14:T:29:ILE:HD12	14:T:29:ILE:N	2.18	0.51
14:T:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
3:C:438:LEU:HD11	20:C:495:CLA:HBB1	1.92	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
20:C:495:CLA:HMD3	20:C:497:CLA:HAB	1.92	0.51
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.93	0.51
2:B:31:ALA:O	2:B:32:GLY:C	2.49	0.51
3:C:226:SER:HA	30:C:507:DGD:HE62	1.93	0.51
3:C:438:LEU:CD2	30:C:507:DGD:HAH2	2.41	0.51
3:C:449:ARG:HG3	3:C:449:ARG:O	2.10	0.51
6:F:11:VAL:HG12	6:F:12:SER:N	2.26	0.51
2:B:175:THR:O	2:B:175:THR:HG22	2.11	0.51
3:C:48:LYS:HE2	3:C:132:HIS:O	2.11	0.51
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.51
8:I:4:LEU:O	8:I:8:VAL:HG23	2.11	0.51
2:B:233:ASN:C	2:B:233:ASN:ND2	2.64	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HH11	1.75	0.50
20:B:517:CLA:H202	11:L:27:LEU:HD11	1.93	0.50
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.09	0.50
17:X:85:UNK:C	17:X:86:UNK:OD1	2.59	0.50
20:B:525:CLA:H112	20:B:525:CLA:H162	1.93	0.50
3:C:140:LEU:HB2	3:C:148:GLY:HA2	1.93	0.50
3:C:146:PHE:HD2	3:C:147:PHE:CE1	2.29	0.50
3:C:372:PRO:O	13:O:36:ILE:HD12	2.11	0.50
4:D:63:LEU:N	4:D:63:LEU:HD12	2.26	0.50
6:F:45:ARG:HG2	6:F:45:ARG:OXT	2.11	0.50
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
3:C:150:ASP:HB3	3:C:153:ASP:CB	2.32	0.50
3:C:241:GLY:C	3:C:243:ILE:N	2.64	0.50
20:A:560:CLA:HAB	20:D:354:CLA:H72	1.93	0.50
15:U:64:ALA:O	15:U:67:GLN:HG2	2.10	0.50
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.32	0.50
29:C:484:UNK:HG1	29:C:485:UNK:C	2.40	0.50
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:145:LEU:CD2	13:O:175:PRO:CG	2.86	0.50
14:T:15:ALA:HB2	24:T:5104:BCR:H14C	1.92	0.50
1:A:22:THR:HG23	1:A:136:ARG:NH1	2.26	0.50
1:A:62:GLY:O	1:A:63:ILE:O	2.29	0.50
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.93	0.50
2:B:368:VAL:HG11	2:B:381:ILE:CD1	2.37	0.50
3:C:245:ILE:O	3:C:249:ILE:HD13	2.12	0.50
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.93	0.50
10:K:19:ASP:N	10:K:20:PRO:HD2	2.26	0.50
10:K:37:PHE:HB3	24:X:130:BCR:C40	2.42	0.50
2:B:231:MET:C	2:B:233:ASN:H	2.15	0.50
10:K:43:VAL:HG21	17:X:31:UNK:HG3	1.93	0.50
12:M:15:VAL:O	12:M:19:SER:HB2	2.12	0.50
18:Z:36:SER:CA	18:Z:39:LEU:HD12	2.35	0.50
1:A:72:LEU:HD22	27:T:217:LMT:O3'	2.12	0.50
2:B:15:ASP:O	2:B:17:GLY:N	2.45	0.50
2:B:341:LYS:O	2:B:406:LEU:HB2	2.11	0.50
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.50
3:C:178:LYS:HD2	3:C:182:PHE:O	2.11	0.50
4:D:60:THR:HG23	4:D:61:HIS:H	1.77	0.50
13:O:147:THR:HG21	13:O:175:PRO:HD2	1.93	0.50
1:A:299:GLY:O	3:C:403:SER:HB2	2.11	0.50
2:B:463:PHE:CZ	2:B:467:ILE:HD12	2.46	0.50
13:O:216:PHE:C	13:O:216:PHE:CD2	2.85	0.50
16:V:128:PRO:O	16:V:130:MET:N	2.45	0.50
2:B:31:ALA:HB2	20:B:515:CLA:CBC	2.42	0.49
4:D:176:ALA:C	4:D:178:ILE:N	2.66	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.11	0.49
4:D:35:ILE:O	4:D:35:ILE:HG22	2.12	0.49
7:H:59:ASN:OD1	7:H:59:ASN:O	2.29	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
2:B:246:PHE:HD1	2:B:246:PHE:C	2.15	0.49
2:B:286:ARG:HD3	2:B:286:ARG:C	2.33	0.49
3:C:416:SER:O	3:C:417:VAL:HG12	2.11	0.49
13:O:73:PRO:CG	13:O:102:THR:CB	2.90	0.49
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.46	0.49
16:V:144:HIS:CE1	16:V:148:GLU:OE2	2.65	0.49
2:B:474:LEU:HD11	20:B:518:CLA:HAA1	1.94	0.49
3:C:46:SER:HA	3:C:49:LEU:HB3	1.93	0.49
3:C:67:MET:HE1	20:C:494:CLA:NC	2.26	0.49
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:VAL:HG12	4:D:56:THR:N	2.26	0.49
5:E:47:PHE:O	5:E:49:THR:N	2.45	0.49
9:J:12:ILE:O	9:J:16:VAL:HG23	2.12	0.49
16:V:104:ASN:HD21	16:V:113:GLU:CD	2.14	0.49
3:C:188:THR:HG23	3:C:300:GLU:OE2	2.13	0.49
3:C:277:GLY:C	20:C:495:CLA:HBC2	2.33	0.49
4:D:102:THR:CG2	4:D:103:ARG:N	2.74	0.49
13:O:216:PHE:C	13:O:216:PHE:HD2	2.15	0.49
13:O:51:THR:O	13:O:52:ALA:O	2.30	0.49
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.28	0.49
2:B:124:ARG:HD3	2:B:131:PRO:N	2.28	0.49
2:B:13:ILE:HG22	2:B:13:ILE:O	2.11	0.49
2:B:145:LEU:CD1	20:B:525:CLA:HMB2	2.43	0.49
2:B:165:GLY:HA3	2:B:179:GLN:O	2.11	0.49
2:B:222:PRO:HG3	7:H:27:THR:N	2.26	0.49
3:C:199:ILE:N	3:C:199:ILE:HD12	2.27	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.92	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	0.49
13:O:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
1:A:78:ILE:O	1:A:177:SER:HB2	2.12	0.49
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.95	0.49
2:B:271:THR:HB	2:B:274:GLN:HG3	1.95	0.49
3:C:78:GLU:OE2	3:C:78:GLU:HA	2.12	0.49
13:O:65:ARG:HG2	13:O:66:ILE:N	2.27	0.49
1:A:232:SER:OG	1:A:235:TYR:CD1	2.65	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
3:C:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
10:K:43:VAL:O	10:K:43:VAL:HG12	2.13	0.49
13:O:101:THR:O	13:O:101:THR:HG22	2.13	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.32	0.49
3:C:250:TRP:HE1	20:C:496:CLA:HED1	1.78	0.49
3:C:281:MET:HG3	28:I:201:MGE:H231	1.94	0.49
8:I:24:LEU:C	8:I:26:GLY:H	2.16	0.49
18:Z:28:ALA:O	18:Z:30:PRO:HD3	2.12	0.49
6:F:40:MET:O	6:F:42:PHE:N	2.46	0.49
24:T:5104:BCR:H403	24:T:5104:BCR:H23C	1.95	0.49
15:U:73:PRO:HD2	16:V:109:ASP:HB3	1.94	0.49
1:A:58:VAL:O	1:A:60:ILE:N	2.46	0.49
2:B:28:ALA:O	2:B:104:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:PHE:N	20:B:516:CLA:HMC3	2.27	0.49
3:C:162:GLY:O	3:C:166:ILE:HG13	2.12	0.49
3:C:269:GLU:CG	3:C:448:ALA:HB2	2.34	0.49
16:V:128:PRO:O	16:V:129:LYS:C	2.51	0.49
1:A:153:SER:CB	20:A:558:CLA:H43	2.43	0.48
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.48
3:C:342:MET:HE3	3:C:353:GLY:H	1.78	0.48
3:C:369:LEU:HD21	3:C:384:ILE:HG12	1.95	0.48
4:D:57:SER:O	4:D:63:LEU:O	2.31	0.48
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.30	0.48
13:O:154:SER:O	13:O:168:PHE:HA	2.13	0.48
13:O:259:VAL:HG12	13:O:260:LYS:N	2.28	0.48
13:O:33:TYR:O	13:O:37:VAL:HG23	2.13	0.48
13:O:75:THR:HG22	13:O:77:LEU:CD1	2.43	0.48
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	0.48
1:A:140:ARG:NH2	25:A:567:LHG:O5	2.46	0.48
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.94	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
12:M:33:GLN:C	12:M:35:SER:H	2.16	0.48
15:U:72:TYR:CG	15:U:73:PRO:N	2.79	0.48
11:L:14:ARG:HG2	12:M:26:TYR:CE1	2.44	0.48
1:A:228:THR:OG1	1:A:231:GLU:HG2	2.13	0.48
2:B:18:ARG:NH1	2:B:18:ARG:HG3	2.28	0.48
20:B:520:CLA:OBD	20:B:520:CLA:H151	2.13	0.48
10:K:15:TYR:C	10:K:17:ILE:H	2.17	0.48
13:O:264:VAL:HG12	13:O:265:PHE:N	2.29	0.48
13:O:83:LYS:O	13:O:84:ASN:CB	2.60	0.48
20:B:513:CLA:H2	20:B:515:CLA:H91	1.95	0.48
3:C:48:LYS:HB3	20:C:501:CLA:HMA2	1.95	0.48
4:D:312:GLU:HB2	13:O:185:PRO:HB3	1.96	0.48
16:V:39:ASN:OD1	16:V:43:LYS:N	2.46	0.48
18:Z:15:LEU:O	18:Z:19:MET:HG2	2.13	0.48
2:B:124:ARG:HD3	2:B:130:GLU:C	2.33	0.48
4:D:180:ARG:HD3	4:D:180:ARG:C	2.33	0.48
4:D:246:MET:HE3	4:D:263:ASN:H	1.78	0.48
28:L:210:MGE:H5A2	12:M:22:LEU:HD21	1.94	0.48
2:B:353:GLU:HB3	2:B:373:LYS:HZ1	1.78	0.48
2:B:86:ILE:C	2:B:86:ILE:HD12	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:TYR:CE2	4:D:76:VAL:HG11	2.48	0.48
10:K:17:ILE:HG22	10:K:17:ILE:O	2.14	0.48
3:C:116:VAL:HG13	3:C:117:VAL:N	2.29	0.48
4:D:126:MET:HE1	4:D:147:SER:HA	1.95	0.48
28:D:358:MGE:O3D	9:J:37:GLY:HA3	2.14	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.49	0.48
16:V:160:LYS:O	16:V:161:VAL:C	2.52	0.48
17:X:86:UNK:N	17:X:86:UNK:OD1	2.45	0.48
1:A:153:SER:HB3	20:A:558:CLA:H43	1.96	0.48
3:C:229:ASN:HD22	3:C:231:GLU:HG2	1.79	0.48
3:C:254:THR:HG22	3:C:255:THR:N	2.19	0.48
3:C:435:PHE:O	3:C:438:LEU:N	2.47	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.13	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	0.48
13:O:33:TYR:C	13:O:35:ASP:N	2.66	0.48
1:A:191:ASN:ND2	1:A:194:MET:HB2	2.28	0.48
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
2:B:61:PHE:CZ	20:B:517:CLA:HBB1	2.49	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48
7:H:45:ILE:O	7:H:46:LEU:C	2.51	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
1:A:77:ILE:HD13	11:L:29:LEU:HG	1.96	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.14	0.48
15:U:73:PRO:HG2	16:V:109:ASP:N	2.29	0.48
18:Z:20:VAL:O	18:Z:24:PRO:HG2	2.14	0.48
18:Z:5:PHE:HE1	18:Z:54:VAL:HG13	1.79	0.48
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
4:D:272:LEU:HD23	4:D:272:LEU:C	2.35	0.47
13:O:67:ALA:HB3	13:O:268:SER:OG	2.14	0.47
17:X:3:UNK:C	17:X:5:UNK:N	2.76	0.47
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.48	0.47
3:C:59:LEU:HD13	20:C:500:CLA:HMD2	1.96	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.47	0.47
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	0.47
9:J:18:GLY:O	9:J:22:ILE:HG12	2.14	0.47
11:L:14:ARG:HG3	11:L:14:ARG:HH11	1.78	0.47
13:O:73:PRO:HG2	13:O:102:THR:CB	2.45	0.47
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HD13	11:L:33:SER:HB2	1.96	0.47
2:B:12:LEU:HD12	20:B:522:CLA:HBB1	1.96	0.47
1:A:303:ASN:O	3:C:415:ASN:OD1	2.32	0.47
25:A:567:LHG:HC61	3:C:443:TRP:HH2	1.77	0.47
2:B:191:ASN:HD22	2:B:192:PRO:N	2.12	0.47
2:B:262:THR:O	2:B:262:THR:CG2	2.61	0.47
3:C:152:LYS:O	3:C:154:LYS:N	2.47	0.47
3:C:293:ASN:HD21	3:C:295:THR:HB	1.79	0.47
3:C:459:ILE:HD12	4:D:245:SER:OG	2.13	0.47
3:C:449:ARG:HD3	20:C:495:CLA:HED1	1.95	0.47
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.36	0.47
4:D:213:ILE:HG23	4:D:214:HIS:N	2.28	0.47
6:F:11:VAL:HG12	6:F:12:SER:H	1.79	0.47
3:C:62:PHE:CE2	10:K:28:ILE:HB	2.50	0.47
11:L:12:LEU:HD12	12:M:25:LEU:HD12	1.95	0.47
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.28	0.47
1:A:213:ALA:O	1:A:217:SER:CB	2.63	0.47
1:A:314:ILE:HG22	1:A:314:ILE:O	2.14	0.47
2:B:228:ALA:O	2:B:230:ARG:NH1	2.47	0.47
4:D:49:LEU:HD13	24:D:357:BCR:C15	2.45	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
7:H:12:ARG:HG3	7:H:12:ARG:NH1	2.30	0.47
11:L:14:ARG:HD3	12:M:26:TYR:OH	2.15	0.47
13:O:147:THR:OG1	13:O:148:VAL:N	2.47	0.47
13:O:169:LYS:HG2	13:O:224:SER:HB2	1.96	0.47
14:T:4:ILE:HB	27:T:217:LMT:C6'	2.44	0.47
15:U:105:LEU:O	15:U:109:LEU:HG	2.15	0.47
16:V:134:THR:N	16:V:137:ASP:OD2	2.45	0.47
16:V:144:HIS:HE1	16:V:148:GLU:OE2	1.97	0.47
1:A:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
2:B:179:GLN:HE21	2:B:179:GLN:HA	1.78	0.47
20:B:518:CLA:HMB1	4:D:126:MET:HB3	1.97	0.47
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.95	0.47
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.47
1:A:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:7:ARG:NH2	28:D:359:MGE:O3D	2.47	0.47
20:A:558:CLA:H201	28:D:360:MGE:H232	1.96	0.47
7:H:12:ARG:HH11	7:H:12:ARG:HG3	1.80	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:111:UNK:C	17:X:113:UNK:N	2.76	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HE3	1.96	0.47
4:D:251:ARG:HE	4:D:255:GLN:NE2	2.12	0.47
9:J:33:TYR:CD2	9:J:33:TYR:N	2.83	0.47
20:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47
13:O:79:LYS:HA	13:O:90:GLU:O	2.15	0.47
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.91	0.47
17:X:75:UNK:O	17:X:79:UNK:HG2	2.15	0.47
1:A:29:TYR:CD1	1:A:133:LEU:HB2	2.49	0.47
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.15	0.47
2:B:145:LEU:HD11	20:B:525:CLA:HMB2	1.96	0.47
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.30	0.47
4:D:102:THR:HG23	4:D:103:ARG:N	2.29	0.47
6:F:41:GLN:HE21	6:F:41:GLN:CA	2.26	0.47
16:V:162:TYR:O	16:V:163:TYR:OXT	2.33	0.47
1:A:140:ARG:HH22	25:A:567:LHG:P	2.38	0.47
1:A:306:VAL:O	1:A:306:VAL:CG2	2.49	0.47
2:B:29:LEU:HD12	20:B:524:CLA:HBB2	1.95	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	0.47
3:C:55:ALA:C	24:C:504:BCR:H373	2.35	0.47
4:D:40:CYS:O	4:D:41:ALA:C	2.53	0.47
4:D:68:LEU:HD21	5:E:44:TYR:CD1	2.50	0.47
3:C:201:ASN:OD1	3:C:201:ASN:O	2.33	0.47
1:A:296:ASN:HB2	3:C:400:PRO:O	2.15	0.47
4:D:214:HIS:HA	22:D:356:PQ9:O4	2.15	0.47
14:T:1:MET:O	14:T:1:MET:HG2	2.14	0.47
15:U:73:PRO:HG2	16:V:109:ASP:H	1.80	0.47
16:V:133:LEU:H	16:V:133:LEU:HD23	1.80	0.47
17:X:114:UNK:O	17:X:117:UNK:HB1	2.15	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
2:B:169:SER:HA	2:B:176:GLY:HA2	1.97	0.46
3:C:255:THR:HG23	3:C:256:PRO:CD	2.41	0.46
8:I:6:ILE:O	8:I:10:ILE:HG12	2.15	0.46
13:O:225:LEU:HD12	13:O:225:LEU:N	2.29	0.46
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.46
2:B:390:TYR:CD1	2:B:390:TYR:N	2.83	0.46
20:B:513:CLA:H162	7:H:38:PHE:HE2	1.80	0.46
3:C:180:MET:CE	3:C:202:PRO:HG2	2.45	0.46
3:C:415:ASN:O	3:C:416:SER:CB	2.64	0.46
3:C:453:ALA:CB	8:I:31:ASN:ND2	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:460:ASP:O	3:C:461:ARG:C	2.52	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
13:O:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
3:C:290:VAL:HG23	3:C:297:TYR:CE1	2.50	0.46
3:C:89:ILE:N	3:C:90:PRO:CD	2.79	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.50	0.46
4:D:222:LEU:HA	4:D:244:TYR:HA	1.97	0.46
8:I:32:PRO:O	8:I:33:LYS:HG3	2.14	0.46
9:J:21:VAL:HA	9:J:24:ILE:HG22	1.97	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	1.97	0.46
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	0.46
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.46
1:A:60:ILE:CG2	1:A:61:ASP:H	2.23	0.46
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.51	0.46
6:F:25:THR:O	6:F:29:PRO:HG2	2.15	0.46
13:O:47:THR:HG22	13:O:48:LEU:H	1.80	0.46
13:O:80:GLU:O	13:O:81:GLU:C	2.53	0.46
15:U:98:THR:C	15:U:100:ARG:H	2.16	0.46
17:X:126:UNK:N	17:X:126:UNK:CD	2.77	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
1:A:183:MET:HB3	20:A:558:CLA:HBC2	1.98	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
15:U:113:THR:O	15:U:114:VAL:HG23	2.16	0.46
18:Z:5:PHE:HA	18:Z:57:LEU:CD1	2.40	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
2:B:263:THR:CG2	2:B:448:ARG:NH1	2.70	0.46
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.46
3:C:39:ASN:OD1	20:C:499:CLA:HBB2	2.16	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
6:F:45:ARG:CG	6:F:45:ARG:OXT	2.64	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
12:M:9:ILE:N	12:M:9:ILE:HD12	2.30	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
14:T:11:ALA:HB3	24:T:5104:BCR:H363	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:497:CLA:H142	24:C:506:BCR:H362	1.96	0.46
4:D:106:GLN:NE2	5:E:48:GLY:HA3	2.31	0.46
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.46
5:E:23:HIS:C	5:E:25:ILE:N	2.69	0.46
5:E:59:GLU:O	5:E:60:GLN:C	2.53	0.46
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
15:U:59:ASN:O	15:U:60:THR:C	2.54	0.46
17:X:112:UNK:C	17:X:114:UNK:N	2.79	0.46
1:A:210:LEU:O	1:A:210:LEU:HD12	2.16	0.46
1:A:57:PRO:HA	1:A:68:SER:HA	1.97	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
2:B:10:THR:O	2:B:12:LEU:N	2.49	0.46
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.46	0.46
2:B:462:PHE:CE1	20:B:523:CLA:HMB3	2.50	0.46
1:A:63:ILE:HG21	3:C:335:THR:HG21	1.97	0.46
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
17:X:117:UNK:NZ	17:X:117:UNK:HB1	2.31	0.46
2:B:249:ALA:O	2:B:252:VAL:HG22	2.16	0.46
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.46
2:B:149:LEU:HB2	20:B:514:CLA:H203	1.97	0.46
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.97	0.46
1:A:26:ASN:O	1:A:27:ARG:C	2.54	0.46
1:A:60:ILE:CG2	1:A:61:ASP:N	2.79	0.46
20:B:518:CLA:H51	20:B:519:CLA:H101	1.97	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.46
4:D:229:ALA:O	4:D:231:THR:N	2.49	0.46
13:O:116:ASP:O	13:O:158:ASN:N	2.35	0.46
1:A:126:TYR:O	1:A:130:GLN:HG3	2.16	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
2:B:356:VAL:HA	2:B:370:LEU:HD23	1.96	0.45
3:C:400:PRO:O	3:C:401:LEU:HD23	2.15	0.45
3:C:410:VAL:HG12	3:C:412:THR:H	1.80	0.45
1:A:163:ILE:HD13	30:C:507:DGD:HB22	1.97	0.45
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.45
20:D:355:CLA:H3A	20:D:355:CLA:HBA2	1.53	0.45
7:H:44:ILE:O	7:H:48:ILE:HG13	2.16	0.45
13:O:114:ASN:O	13:O:115:SER:O	2.33	0.45
13:O:151:LEU:HD12	13:O:171:GLU:O	2.17	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:PRO:HD3	20:B:517:CLA:HED2	1.98	0.45
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.97	0.45
6:F:30:THR:HG22	6:F:34:LEU:HD12	1.98	0.45
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
13:O:70:CYS:SG	13:O:71:LEU:N	2.89	0.45
13:O:98:THR:CG2	13:O:99:ARG:H	2.04	0.45
1:A:306:VAL:HG21	1:A:316:THR:CG2	2.42	0.45
22:A:564:PQ9:H91	22:A:564:PQ9:H61	1.69	0.45
2:B:215:PHE:C	2:B:215:PHE:CD2	2.89	0.45
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.45
2:B:156:PHE:HB2	20:B:516:CLA:HAC1	1.99	0.45
3:C:331:ALA:O	3:C:338:GLY:HA2	2.17	0.45
3:C:453:ALA:HB1	8:I:31:ASN:HD22	1.81	0.45
20:B:511:CLA:CAA	24:H:107:BCR:H19C	2.47	0.45
11:L:14:ARG:CG	11:L:14:ARG:HH11	2.29	0.45
15:U:115:THR:HG22	15:U:116:GLU:N	2.32	0.45
1:A:22:THR:HG22	1:A:22:THR:O	2.16	0.45
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.52	0.45
2:B:235:GLU:O	2:B:235:GLU:HG2	2.16	0.45
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.45
3:C:334:PRO:HG2	4:D:350:ASN:ND2	2.32	0.45
13:O:265:PHE:C	13:O:265:PHE:CD1	2.90	0.45
1:A:131:TRP:CZ2	20:C:495:CLA:HAA1	2.51	0.45
2:B:193:TYR:CE1	2:B:260:SER:N	2.84	0.45
3:C:139:THR:O	3:C:139:THR:HG23	2.16	0.45
3:C:299:SER:OG	3:C:304:PRO:HA	2.17	0.45
4:D:213:ILE:CG2	4:D:214:HIS:N	2.79	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	0.45
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.45
9:J:8:ILE:N	9:J:8:ILE:HD12	2.30	0.45
1:A:210:LEU:HD13	21:A:562:PHO:ND	2.31	0.45
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.97	0.45
3:C:250:TRP:HE1	20:C:496:CLA:CED	2.30	0.45
4:D:179:PHE:O	4:D:183:LEU:HG	2.17	0.45
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	0.45
13:O:70:CYS:O	13:O:265:PHE:HB2	2.16	0.45
2:B:271:THR:HG22	2:B:274:GLN:N	2.31	0.45
4:D:96:GLU:H	4:D:96:GLU:CD	2.20	0.45
10:K:46:ARG:HH22	17:X:31:UNK:CG2	2.30	0.45
15:U:50:ALA:O	15:U:53:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:92:LEU:HD11	15:U:109:LEU:HD11	1.98	0.45
18:Z:2:THR:O	18:Z:3:ILE:C	2.55	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.78	0.45
2:B:124:ARG:NH1	2:B:124:ARG:CG	2.77	0.45
2:B:124:ARG:HE	2:B:131:PRO:HG3	1.82	0.45
2:B:98:LEU:O	2:B:99:ALA:C	2.55	0.45
3:C:264:PHE:CD2	3:C:264:PHE:N	2.85	0.45
7:H:55:LEU:HB2	7:H:58:VAL:HG21	1.98	0.45
3:C:349:ILE:HD13	13:O:127:ILE:CD1	2.47	0.45
13:O:139:GLY:O	13:O:140:GLU:O	2.34	0.45
13:O:160:THR:O	13:O:161:SER:O	2.34	0.45
13:O:166:THR:O	13:O:167:ASP:HB3	2.16	0.45
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	0.45
1:A:40:THR:CG2	1:A:118:HIS:O	2.65	0.45
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.99	0.45
20:A:559:CLA:H61	21:A:561:PHO:HMB3	1.99	0.45
20:B:514:CLA:O1A	20:B:515:CLA:HBA1	2.16	0.45
3:C:305:THR:CG2	3:C:307:PRO:HD2	2.31	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	0.45
4:D:68:LEU:HB2	6:F:40:MET:HE1	1.99	0.45
13:O:59:ASP:C	13:O:61:SER:H	2.21	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.82	0.45
2:B:10:THR:HG23	2:B:13:ILE:HD11	1.99	0.45
2:B:171:PRO:HD3	7:H:65:LEU:C	2.37	0.45
2:B:297:THR:H	2:B:300:GLU:CD	2.20	0.45
20:B:519:CLA:HBA2	7:H:31:MET:SD	2.57	0.45
2:B:7:ARG:O	2:B:8:VAL:C	2.55	0.45
4:D:130:PHE:HE2	4:D:140:PRO:HB2	1.81	0.45
4:D:244:TYR:OH	4:D:264:LYS:HD3	2.17	0.45
6:F:18:VAL:CG1	6:F:19:ARG:N	2.80	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.52	0.44
20:B:517:CLA:HBA2	20:B:517:CLA:H3A	1.71	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
32:F:51:HEM:HAD2	32:F:51:HEM:HHA	1.67	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
4:D:100:ASP:C	4:D:100:ASP:OD1	2.55	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
8:I:17:LEU:O	8:I:18:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:31:SER:C	12:M:33:GLN:H	2.21	0.44
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.44
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.51	0.44
4:D:302:GLU:OE1	13:O:186:LYS:CE	2.65	0.44
12:M:33:GLN:O	12:M:35:SER:N	2.50	0.44
1:A:323:ARG:HD2	1:A:323:ARG:HA	1.64	0.44
1:A:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
2:B:124:ARG:HA	2:B:131:PRO:HA	1.99	0.44
3:C:265:ILE:HB	20:C:495:CLA:HED3	1.98	0.44
24:C:504:BCR:H11C	24:X:130:BCR:H322	1.99	0.44
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.52	0.44
5:E:60:GLN:C	5:E:62:SER:N	2.71	0.44
13:O:81:GLU:O	13:O:82:PRO:C	2.56	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	0.44
15:U:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.19	0.44
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.00	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.44
3:C:116:VAL:O	3:C:117:VAL:C	2.56	0.44
3:C:257:PHE:CD1	3:C:257:PHE:N	2.85	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
4:D:85:MET:HE3	4:D:107:LEU:HB3	1.99	0.44
5:E:28:PRO:O	5:E:32:ILE:HG13	2.18	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.82	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
16:V:63:CYS:SG	32:V:552:HEM:HAB	2.57	0.44
16:V:64:ALA:O	16:V:66:CYS:N	2.51	0.44
17:X:126:UNK:HB2	17:X:127:UNK:H	1.41	0.44
20:A:558:CLA:HBD	20:A:559:CLA:HAC2	1.99	0.44
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.00	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	0.44
3:C:42:LEU:HD11	20:C:501:CLA:C1A	2.48	0.44
3:C:292:PHE:HB3	30:C:507:DGD:HD62	1.99	0.44
4:D:60:THR:CG2	4:D:61:HIS:H	2.31	0.44
10:K:17:ILE:CD1	18:Z:6:GLN:NE2	2.78	0.44
17:X:128:UNK:O	17:X:129:UNK:C	2.66	0.44
10:K:21:LEU:HD11	24:X:130:BCR:HC42	1.99	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
21:A:561:PHO:HED2	4:D:257:PHE:CE2	2.52	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:ALA:C	3:C:454:GLY:H	2.21	0.44
5:E:26:THR:O	5:E:29:ALA:HB3	2.18	0.44
5:E:17:VAL:HA	9:J:8:ILE:HD11	2.00	0.44
10:K:13:GLU:O	10:K:16:ALA:HB3	2.18	0.44
13:O:241:PHE:CD1	13:O:241:PHE:C	2.90	0.44
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.44
2:B:450:TRP:O	2:B:451:PHE:C	2.55	0.44
2:B:476:ARG:HG3	2:B:476:ARG:NH1	2.33	0.44
3:C:135:ARG:O	3:C:136:GLY:O	2.35	0.44
5:E:51:ARG:O	5:E:54:SER:N	2.48	0.44
15:U:98:THR:C	15:U:100:ARG:N	2.71	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.44	0.44
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.99	0.44
3:C:405:ASN:HB2	30:C:509:DGD:HG32	2.00	0.44
20:C:501:CLA:HMD2	10:K:40:GLN:CD	2.37	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.48	0.44
13:O:52:ALA:HA	13:O:230:VAL:O	2.18	0.44
2:B:341:LYS:HB3	2:B:406:LEU:HD12	2.00	0.43
2:B:450:TRP:O	2:B:453:PHE:N	2.51	0.43
3:C:225:VAL:O	3:C:225:VAL:HG12	2.18	0.43
4:D:21:TRP:CE2	4:D:26:ARG:NH2	2.78	0.43
10:K:15:TYR:OH	18:Z:58:ASN:HB2	2.17	0.43
11:L:7:ARG:HA	11:L:7:ARG:HD2	1.69	0.43
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	0.43
3:C:321:ASP:OD2	15:U:129:ASN:HB2	2.18	0.43
1:A:48:PHE:HA	1:A:115:ILE:CD1	2.48	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.91	0.43
2:B:193:TYR:HE1	2:B:260:SER:N	2.17	0.43
2:B:217:ILE:HG22	2:B:218:LEU:HD23	1.99	0.43
2:B:36:SER:OG	24:B:528:BCR:H362	2.18	0.43
3:C:134:ILE:HD11	20:C:501:CLA:H92	2.00	0.43
20:C:498:CLA:H122	20:C:500:CLA:HED1	2.00	0.43
4:D:256:ILE:HG12	4:D:256:ILE:O	2.19	0.43
4:D:263:ASN:HB3	28:D:360:MGE:O3D	2.19	0.43
4:D:93:TRP:CZ2	20:D:355:CLA:O1A	2.71	0.43
7:H:19:GLY:O	7:H:21:VAL:HG12	2.17	0.43
16:V:117:VAL:O	16:V:117:VAL:HG12	2.17	0.43
2:B:31:ALA:N	20:B:515:CLA:HBC3	2.33	0.43
20:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:HB	3:C:308:GLU:HB2	1.99	0.43
24:D:357:BCR:H383	28:D:358:MGE:H6B1	2.00	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.54	0.43
13:O:231:ASP:O	13:O:232:GLY:C	2.56	0.43
15:U:78:LEU:HD13	15:U:97:LEU:HD21	2.01	0.43
18:Z:12:LEU:HA	18:Z:50:LEU:HD13	1.99	0.43
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.43
1:A:76:ASN:HD21	1:A:79:THR:H	1.66	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
2:B:318:ASN:ND2	2:B:361:ALA:HB2	2.34	0.43
2:B:332:LYS:HG3	2:B:444:ARG:HH21	1.84	0.43
20:B:520:CLA:H122	20:B:522:CLA:H43	2.00	0.43
20:C:491:CLA:H42	20:C:492:CLA:HMD1	2.00	0.43
4:D:120:PHE:CD1	4:D:123:ILE:HD12	2.53	0.43
4:D:157:PHE:CE2	4:D:171:PRO:HB2	2.53	0.43
22:D:356:PQ9:H61	22:D:356:PQ9:H91	1.75	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
3:C:33:PHE:HE1	4:D:229:ALA:HB2	1.82	0.43
5:E:6:GLY:O	5:E:7:GLU:HG2	2.18	0.43
1:A:32:TRP:CE2	8:I:22:GLY:HA3	2.53	0.43
13:O:153:ALA:HB1	13:O:168:PHE:HB3	2.00	0.43
17:X:102:UNK:O	17:X:103:UNK:C	2.66	0.43
24:X:130:BCR:HC31	18:Z:13:VAL:HG13	2.00	0.43
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.54	0.43
1:A:225:ARG:NH1	2:B:484:PRO:HD3	2.34	0.43
1:A:284:TRP:O	1:A:287:ALA:HB3	2.18	0.43
2:B:188:ASP:C	2:B:190:PHE:H	2.22	0.43
2:B:191:ASN:HD22	2:B:191:ASN:C	2.20	0.43
2:B:271:THR:HG22	2:B:273:TYR:N	2.34	0.43
20:C:498:CLA:H191	30:C:509:DGD:HA91	2.00	0.43
4:D:148:ALA:CB	4:D:149:PRO:HD3	2.35	0.43
1:A:25:ASP:HA	4:D:251:ARG:NH2	2.32	0.43
4:D:246:MET:HE3	4:D:263:ASN:N	2.34	0.43
6:F:22:ALA:O	6:F:24:HIS:N	2.52	0.43
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
1:A:35:VAL:HG22	24:A:566:BCR:HC42	2.00	0.43
2:B:208:VAL:HG21	20:B:512:CLA:CMC	2.48	0.43
2:B:403:GLY:O	2:B:407:ASN:HB2	2.18	0.43
3:C:206:PRO:O	3:C:207:ARG:C	2.57	0.43
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.43
4:D:53:THR:HG22	4:D:67:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:127:UNK:CG	17:X:128:UNK:N	2.81	0.43
2:B:360:PRO:O	2:B:362:PHE:N	2.51	0.43
2:B:368:VAL:O	2:B:368:VAL:HG13	2.19	0.43
3:C:205:ASP:OD2	3:C:205:ASP:C	2.57	0.43
3:C:214:LEU:HD23	3:C:214:LEU:N	2.31	0.43
20:C:491:CLA:CAD	20:C:493:CLA:H12	2.49	0.43
4:D:178:ILE:CG2	4:D:179:PHE:N	2.81	0.43
13:O:231:ASP:OD1	13:O:231:ASP:O	2.37	0.43
14:T:4:ILE:CD1	14:T:4:ILE:C	2.85	0.43
3:C:168:LEU:HD13	20:C:497:CLA:H2	2.01	0.43
3:C:180:MET:SD	3:C:202:PRO:HG2	2.57	0.43
3:C:385:GLN:HB2	3:C:387:TRP:CD1	2.54	0.43
4:D:134:ARG:HA	4:D:134:ARG:NE	2.34	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	0.43
24:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
2:B:221:PRO:O	2:B:222:PRO:C	2.56	0.43
2:B:464:PHE:HD2	20:B:521:CLA:HAC2	1.83	0.43
20:B:515:CLA:CHA	20:B:515:CLA:HBA1	2.48	0.43
3:C:323:LYS:O	3:C:324:LEU:HB2	2.19	0.43
3:C:394:GLU:O	3:C:398:HIS:HD2	2.02	0.43
3:C:404:LEU:C	3:C:406:SER:H	2.23	0.43
4:D:35:ILE:O	4:D:39:PRO:HG2	2.18	0.43
13:O:32:THR:H	13:O:35:ASP:CB	2.28	0.43
14:T:22:PHE:O	14:T:23:PHE:CD2	2.71	0.43
15:U:66:ILE:HD11	15:U:72:TYR:CZ	2.54	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.00	0.42
3:C:201:ASN:O	3:C:202:PRO:C	2.58	0.42
3:C:417:VAL:O	3:C:417:VAL:HG13	2.18	0.42
3:C:87:ILE:C	3:C:90:PRO:HD2	2.39	0.42
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.79	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.54	0.42
1:A:206:PHE:CD1	21:A:562:PHO:HBB2	2.54	0.42
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.01	0.42
2:B:271:THR:CG2	2:B:273:TYR:N	2.79	0.42
2:B:271:THR:HG22	2:B:273:TYR:H	1.82	0.42
2:B:31:ALA:CA	20:B:515:CLA:HBC3	2.49	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
3:C:104:GLU:O	3:C:105:VAL:C	2.57	0.42
3:C:29:GLU:O	3:C:31:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:ALA:O	3:C:454:GLY:N	2.52	0.42
4:D:313:THR:C	4:D:315:TYR:N	2.72	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.42
13:O:120:THR:OG1	13:O:154:SER:HB3	2.19	0.42
17:X:118:UNK:C	17:X:120:UNK:N	2.80	0.42
2:B:314:TYR:CZ	2:B:316:GLY:HA3	2.55	0.42
20:B:518:CLA:HBD	20:B:518:CLA:HBA1	2.00	0.42
2:B:90:PHE:CZ	2:B:98:LEU:HD23	2.55	0.42
3:C:201:ASN:N	3:C:202:PRO:CD	2.82	0.42
4:D:246:MET:CE	4:D:264:LYS:HG3	2.49	0.42
4:D:40:CYS:O	4:D:43:LEU:N	2.52	0.42
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.85	0.42
11:L:12:LEU:CD1	12:M:25:LEU:HD12	2.49	0.42
13:O:30:THR:HG22	13:O:31:LEU:N	2.33	0.42
1:A:225:ARG:HH12	2:B:483:ASP:CA	2.19	0.42
1:A:261:GLN:O	1:A:264:SER:HB3	2.19	0.42
1:A:69:GLY:O	1:A:80:GLY:HA2	2.19	0.42
20:B:524:CLA:H102	24:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:N	3:C:147:PHE:CD1	2.85	0.42
4:D:103:ARG:HA	4:D:103:ARG:HD3	1.81	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
2:B:125:ASP:O	2:B:128:THR:O	2.38	0.42
2:B:214:LEU:O	2:B:217:ILE:HB	2.18	0.42
2:B:271:THR:HG22	2:B:274:GLN:HG3	2.02	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	0.42
4:D:47:GLY:HA2	24:D:357:BCR:H332	2.01	0.42
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.42
20:B:516:CLA:H72	24:B:529:BCR:H311	2.02	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.25	0.42
3:C:113:VAL:O	3:C:117:VAL:HG23	2.20	0.42
3:C:171:GLY:HA3	20:C:502:CLA:H41	2.01	0.42
3:C:472:LEU:H	3:C:472:LEU:HD12	1.84	0.42
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.79	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	0.42
16:V:64:ALA:O	16:V:65:SER:C	2.57	0.42
17:X:23:UNK:CG2	18:Z:25:VAL:HG11	2.50	0.42
17:X:54:UNK:O	17:X:55:UNK:C	2.66	0.42
1:A:33:PHE:CE1	1:A:128:GLY:HA3	2.55	0.42
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.42
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	0.42
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.49	0.42
1:A:184:ILE:HA	20:A:558:CLA:HBC1	2.02	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:103:LEU:HD21	20:B:515:CLA:HMC3	2.01	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
3:C:168:LEU:CD1	20:C:497:CLA:H2	2.49	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42
7:H:54:ILE:O	7:H:55:LEU:HD23	2.20	0.42
12:M:15:VAL:O	12:M:19:SER:CB	2.68	0.42
14:T:2:GLU:O	14:T:3:THR:C	2.57	0.42
32:V:552:HEM:HAD2	32:V:552:HEM:HHA	1.56	0.42
1:A:257:ARG:HH12	1:A:261:GLN:NE2	2.18	0.42
2:B:30:VAL:O	2:B:30:VAL:HG12	2.19	0.42
20:B:515:CLA:H152	20:B:520:CLA:HED1	2.02	0.42
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.82	0.42
7:H:12:ARG:N	7:H:13:PRO:CD	2.82	0.42
11:L:12:LEU:HD13	12:M:25:LEU:HB2	2.02	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.83	0.42
16:V:29:LEU:O	16:V:29:LEU:HG	2.18	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
3:C:138:GLU:O	3:C:139:THR:HB	2.20	0.42
3:C:405:ASN:ND2	30:C:509:DGD:HD5	2.26	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.20	0.42
4:D:274:VAL:HG13	22:D:356:PQ9:H251	2.02	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	0.42
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
5:E:37:PHE:CD1	5:E:42:LEU:HD23	2.55	0.42
13:O:44:LYS:HA	13:O:72:GLN:CD	2.40	0.42
13:O:98:THR:CG2	13:O:99:ARG:N	2.70	0.42
1:A:314:ILE:O	1:A:315:ASN:O	2.38	0.41
2:B:462:PHE:CZ	20:B:523:CLA:HMB3	2.55	0.41
20:C:493:CLA:H171	20:C:500:CLA:HBB2	2.01	0.41
20:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:PHE:HZ	22:D:356:PQ9:H243	1.85	0.41
13:O:266:TYR:CG	13:O:267:ALA:N	2.88	0.41
13:O:45:CYS:CB	13:O:46:PRO:HD2	2.31	0.41
25:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.41
3:C:322:GLN:O	3:C:324:LEU:N	2.49	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
3:C:61:VAL:O	3:C:62:PHE:C	2.57	0.41
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
4:D:267:LEU:CD2	4:D:267:LEU:C	2.88	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
2:B:10:THR:C	2:B:12:LEU:N	2.73	0.41
3:C:120:ILE:C	3:C:122:SER:H	2.23	0.41
3:C:120:ILE:C	3:C:122:SER:N	2.73	0.41
6:F:40:MET:C	6:F:42:PHE:N	2.74	0.41
8:I:33:LYS:HA	8:I:34:ARG:NH2	2.16	0.41
13:O:106:GLN:HE21	13:O:106:GLN:N	2.18	0.41
15:U:69:ARG:HG3	15:U:70:GLY:N	2.33	0.41
16:V:75:ASN:N	16:V:76:PRO:HD3	2.35	0.41
1:A:76:ASN:ND2	1:A:76:ASN:C	2.73	0.41
3:C:334:PRO:O	13:O:182:PHE:HB2	2.19	0.41
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.55	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.52	0.41
17:X:52:UNK:O	17:X:54:UNK:N	2.54	0.41
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.41
1:A:292:THR:C	1:A:294:ALA:H	2.23	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.20	0.41
2:B:208:VAL:HG12	2:B:208:VAL:O	2.20	0.41
20:B:513:CLA:H3A	20:B:513:CLA:CGA	2.50	0.41
3:C:166:ILE:HG23	3:C:245:ILE:CG2	2.42	0.41
3:C:190:ALA:HB3	3:C:193:GLY:C	2.41	0.41
3:C:419:PHE:CD1	3:C:419:PHE:C	2.93	0.41
4:D:178:ILE:O	4:D:181:PHE:N	2.54	0.41
4:D:259:ILE:HG22	4:D:260:ALA:N	2.34	0.41
8:I:27:ASP:O	8:I:28:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:UNK:C	17:X:122:UNK:N	2.82	0.41
1:A:54:ALA:O	1:A:55:ALA:CB	2.69	0.41
2:B:359:MET:HB2	2:B:425:ILE:HG23	2.02	0.41
20:B:521:CLA:C4	20:B:524:CLA:HBC3	2.50	0.41
3:C:75:PHE:CE2	3:C:105:VAL:HG11	2.56	0.41
3:C:95:LEU:O	3:C:185:LEU:HD23	2.21	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
24:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
13:O:77:LEU:N	13:O:77:LEU:CD1	2.81	0.41
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.01	0.41
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.41
7:H:46:LEU:HD11	30:H:208:DGD:HA22	2.02	0.41
16:V:59:PHE:CD1	16:V:63:CYS:HB2	2.56	0.41
16:V:64:ALA:HB1	16:V:68:VAL:HG12	2.03	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.21	0.41
2:B:61:PHE:HZ	20:B:517:CLA:HBB1	1.85	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	0.41
3:C:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
3:C:418:ASN:HB3	30:C:509:DGD:C2E	2.51	0.41
4:D:159:ILE:O	4:D:160:TYR:C	2.58	0.41
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.20	0.41
17:X:4:UNK:O	17:X:5:UNK:C	2.69	0.41
3:C:229:ASN:HD22	3:C:231:GLU:CG	2.34	0.41
3:C:416:SER:C	3:C:417:VAL:HG12	2.41	0.41
3:C:56:HIS:O	3:C:59:LEU:N	2.53	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	0.41
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
1:A:321:ILE:HG22	1:A:322:ASN:N	2.35	0.41
2:B:272:ARG:HH12	4:D:164:GLN:HG3	1.86	0.41
3:C:42:LEU:HG	20:C:501:CLA:O1D	2.20	0.41
20:C:502:CLA:HBA2	20:C:502:CLA:O2D	2.20	0.41
10:K:17:ILE:HD11	18:Z:6:GLN:NE2	2.31	0.41
10:K:43:VAL:HG21	17:X:31:UNK:CG	2.51	0.41
1:A:13:LEU:CD2	1:A:13:LEU:H	2.33	0.41
1:A:78:ILE:HD12	1:A:78:ILE:N	2.36	0.41
2:B:410:THR:HG22	2:B:411:PHE:N	2.36	0.41
3:C:109:PHE:O	3:C:110:PRO:C	2.59	0.41
3:C:146:PHE:CD2	3:C:147:PHE:CE1	3.09	0.41
3:C:438:LEU:HD21	30:C:507:DGD:HAH2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:SER:OG	5:E:19:TYR:HB2	2.21	0.41
10:K:18:PHE:CD1	10:K:18:PHE:N	2.89	0.41
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.28	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.40
1:A:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	0.40
20:B:518:CLA:CHA	20:B:518:CLA:HBA1	2.51	0.40
2:B:68:ARG:HH12	20:B:514:CLA:CED	2.33	0.40
2:B:87:ASP:O	2:B:88:PRO:C	2.58	0.40
3:C:173:LEU:HD23	3:C:173:LEU:HA	1.86	0.40
20:C:494:CLA:CHA	20:C:494:CLA:HBA1	2.52	0.40
4:D:38:PHE:HZ	4:D:128:ARG:NH2	2.18	0.40
12:M:17:VAL:HG12	12:M:18:PRO:N	2.35	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
21:A:561:PHO:HND	4:D:209:LEU:HD12	1.87	0.40
2:B:12:LEU:CD1	20:B:522:CLA:HBB1	2.51	0.40
2:B:74:SER:C	2:B:76:SER:N	2.74	0.40
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.89	0.40
8:I:31:ASN:HB2	8:I:32:PRO:HD2	2.03	0.40
10:K:45:PHE:C	10:K:46:ARG:OXT	2.58	0.40
13:O:142:ILE:CD1	13:O:142:ILE:N	2.84	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.40
8:I:30:ARG:HG2	8:I:30:ARG:H	1.60	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
15:U:69:ARG:HB2	15:U:69:ARG:HE	1.69	0.40
1:A:206:PHE:HD2	1:A:206:PHE:HA	1.75	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.40
2:B:230:ARG:NH1	2:B:474:LEU:HD22	2.36	0.40
2:B:450:TRP:HB3	20:B:517:CLA:HMB2	2.04	0.40
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.79	0.40
2:B:164:PRO:HD3	20:B:516:CLA:O1D	2.22	0.40
20:C:491:CLA:HMA1	24:C:506:BCR:H401	2.02	0.40
4:D:103:ARG:O	4:D:106:GLN:N	2.55	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
28:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:22:PHE:O	14:T:23:PHE:CG	2.75	0.40
17:X:62:UNK:O	17:X:66:UNK:N	2.55	0.40
17:X:85:UNK:N	17:X:85:UNK:OD1	2.54	0.40
1:A:131:TRP:CD2	1:A:132:GLU:N	2.89	0.40
1:A:255:PHE:CE2	22:A:564:PQ9:H151	2.57	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
3:C:252:ILE:HG22	3:C:252:ILE:O	2.21	0.40
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.40
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
4:D:34:GLY:C	4:D:36:LEU:H	2.25	0.40
8:I:24:LEU:O	8:I:26:GLY:N	2.48	0.40
15:U:54:LYS:HB3	15:U:111:HIS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	2	14
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	12
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	3	17
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	3	20
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	10
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	1	10
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	2	14
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	16
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	5
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	0	2
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	0	2
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	0	3
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	0	3
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	10
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	10
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	9
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	1	9
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	5
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	5
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	1	5
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1	5
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	12
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	12
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	6
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	6
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	2	11

All (269) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN

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Mol	Chain	Res	Type
2	B	230	ARG
2	B	260	SER
2	B	362	PHE
2	B	488	PRO
3	C	154	LYS
3	C	324	LEU
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	257	PHE
4	D	262	SER
5	E	7	GLU
5	E	58	GLN
5	E	60	GLN
7	H	18	TYR
7	H	64	ALA
13	O	46	PRO
13	O	52	ALA
13	O	86	ARG
13	O	115	SER
13	O	140	GLU
13	O	175	PRO
15	U	72	TYR
15	U	73	PRO
15	U	83	ALA
16	V	133	LEU
16	V	160	LYS
1	a	5011	ALA
1	a	5012	ASN
1	a	5063	ILE
1	a	5141	PRO
1	a	5142	TRP
1	a	5315	ASN
2	b	5230	ARG
2	b	5260	SER
2	b	5362	PHE
2	b	5488	PRO
3	c	5154	LYS
3	c	5226	SER
3	c	5324	LEU
3	c	5416	SER
4	d	5239	GLN

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Mol	Chain	Res	Type
4	d	5240	ALA
4	d	5262	SER
5	e	5007	GLU
5	e	5058	GLN
5	e	5060	GLN
7	h	5018	TYR
7	h	5064	ALA
13	o	5046	PRO
13	o	5052	ALA
13	o	5086	ARG
13	o	5115	SER
13	o	5140	GLU
13	o	5175	PRO
15	u	5072	TYR
15	u	5073	PRO
15	u	5083	ALA
16	v	5133	LEU
16	v	5160	LYS
1	A	12	ASN
1	A	130	GLN
1	A	261	GLN
1	A	266	ASN
2	B	11	VAL
2	B	85	GLY
2	B	176	GLY
2	B	231	MET
3	C	57	ALA
3	C	136	GLY
3	C	139	THR
3	C	141	GLU
3	C	144	SER
3	C	207	ARG
3	C	209	ILE
3	C	226	SER
3	C	242	LEU
4	D	92	LEU
4	D	263	ASN
5	E	48	GLY
7	H	26	GLY
8	I	25	SER
9	J	35	GLY
10	K	13	GLU

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Mol	Chain	Res	Type
10	K	16	ALA
12	M	34	LYS
13	O	50	ASP
13	O	84	ASN
13	O	88	GLU
13	O	138	GLY
13	O	161	SER
15	U	70	GLY
18	Z	31	GLN
18	Z	32	ASP
1	a	5055	ALA
1	a	5130	GLN
1	a	5242	GLU
1	a	5266	ASN
2	b	5011	VAL
2	b	5085	GLY
3	c	5136	GLY
3	c	5141	GLU
3	c	5144	SER
3	c	5207	ARG
3	c	5209	ILE
4	d	5092	LEU
4	d	5192	THR
4	d	5252	PHE
4	d	5257	PHE
4	d	5263	ASN
5	e	5048	GLY
6	f	5041	GLN
7	h	5026	GLY
8	i	5025	SER
9	j	5035	GLY
10	k	5013	GLU
10	k	5016	ALA
12	m	5034	LYS
13	o	5050	ASP
13	o	5084	ASN
13	o	5088	GLU
13	o	5138	GLY
13	o	5161	SER
13	o	5233	ARG
15	u	5070	GLY
18	z	5031	GLN

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Mol	Chain	Res	Type
18	z	5032	ASP
1	A	55	ALA
1	A	59	ASP
1	A	242	GLU
1	A	306	VAL
2	B	228	ALA
3	C	39	ASN
3	C	194	GLY
3	C	221	GLU
4	D	25	ASP
4	D	192	THR
4	D	252	PHE
4	D	351	ALA
5	E	52	PRO
6	F	41	GLN
7	H	3	ARG
7	H	59	ASN
9	J	14	ALA
11	L	5	PRO
11	L	7	ARG
13	O	233	ARG
15	U	88	VAL
16	V	75	ASN
1	a	5059	ASP
1	a	5261	GLN
1	a	5306	VAL
2	b	5176	GLY
2	b	5228	ALA
3	c	5039	ASN
3	c	5057	ALA
3	c	5139	THR
3	c	5221	GLU
3	c	5242	LEU
4	d	5025	ASP
4	d	5041	ALA
4	d	5351	ALA
5	e	5052	PRO
7	h	5059	ASN
9	j	5011	TRP
11	l	5005	PRO
11	l	5007	ARG
13	o	5167	ASP

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Mol	Chain	Res	Type
13	o	5232	GLY
15	u	5088	VAL
16	v	5064	ALA
1	A	232	SER
1	A	260	PHE
2	B	91	TRP
2	B	485	GLU
3	C	30	SER
3	C	38	GLY
3	C	77	PRO
3	C	205	ASP
3	C	298	PRO
4	D	41	ALA
4	D	177	ALA
4	D	261	PHE
9	J	11	TRP
13	O	167	ASP
13	O	232	GLY
15	U	60	THR
16	V	65	SER
1	a	5260	PHE
2	b	5231	MET
2	b	5485	GLU
3	c	5194	GLY
3	c	5205	ASP
4	d	5062	GLY
7	h	5003	ARG
9	j	5014	ALA
16	v	5129	LYS
2	B	16	PRO
2	B	89	GLY
2	B	386	ALA
3	C	227	VAL
3	C	382	ASN
4	D	29	PHE
4	D	62	GLY
12	M	17	VAL
13	O	139	GLY
16	V	129	LYS
1	a	5172	MET
1	a	5217	SER
2	b	5089	GLY

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Mol	Chain	Res	Type
2	b	5122	LEU
2	b	5361	ALA
3	c	5030	SER
3	c	5077	PRO
3	c	5153	ASP
3	c	5227	VAL
3	c	5298	PRO
3	c	5382	ASN
4	d	5177	ALA
16	v	5075	ASN
2	B	361	ALA
3	C	243	ILE
13	O	185	PRO
3	c	5038	GLY
3	c	5134	ILE
4	d	5264	LYS
12	m	5017	VAL
13	o	5139	GLY
16	v	5065	SER
2	B	8	VAL
6	F	23	VAL
18	Z	24	PRO
2	b	5016	PRO
3	c	5243	ILE
13	o	5185	PRO
15	u	5066	ILE
2	B	414	PRO
3	C	105	VAL
3	C	134	ILE
13	O	117	GLY
2	b	5008	VAL
2	b	5414	PRO
18	z	5003	ILE
4	D	80	THR
18	Z	3	ILE
1	a	5060	ILE
3	c	5105	VAL
6	f	5023	VAL
7	h	5058	VAL
18	z	5024	PRO
2	B	86	ILE
2	B	232	GLY

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Mol	Chain	Res	Type
7	H	58	VAL
15	U	66	ILE
16	V	71	ILE
16	V	161	VAL
2	b	5086	ILE
10	k	5012	PRO
13	o	5117	GLY
5	E	25	ILE
5	e	5025	ILE
11	l	5003	PRO
15	u	5062	ILE
16	v	5071	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	251 (93%)	18 (7%)	16	49
1	a	269/280 (96%)	252 (94%)	17 (6%)	18	51
2	B	378/407 (93%)	361 (96%)	17 (4%)	27	64
2	b	378/407 (93%)	360 (95%)	18 (5%)	25	62
3	C	341/374 (91%)	320 (94%)	21 (6%)	18	52
3	c	341/374 (91%)	320 (94%)	21 (6%)	18	52
4	D	273/283 (96%)	259 (95%)	14 (5%)	24	60
4	d	273/283 (96%)	258 (94%)	15 (6%)	21	57
5	E	68/73 (93%)	65 (96%)	3 (4%)	28	65
5	e	68/73 (93%)	66 (97%)	2 (3%)	42	76
6	F	27/39 (69%)	26 (96%)	1 (4%)	34	70
6	f	27/39 (69%)	26 (96%)	1 (4%)	34	70
7	H	50/55 (91%)	42 (84%)	8 (16%)	2	12
7	h	50/55 (91%)	43 (86%)	7 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	27 (84%)	5 (16%)	2	13
8	i	32/35 (91%)	27 (84%)	5 (16%)	2	13
9	J	22/28 (79%)	21 (96%)	1 (4%)	27	64
9	j	22/28 (79%)	21 (96%)	1 (4%)	27	64
10	K	29/30 (97%)	28 (97%)	1 (3%)	37	72
10	k	29/30 (97%)	28 (97%)	1 (3%)	37	72
11	L	34/35 (97%)	31 (91%)	3 (9%)	10	36
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	36
12	M	32/33 (97%)	32 (100%)	0	100	100
12	m	32/33 (97%)	32 (100%)	0	100	100
13	O	181/208 (87%)	171 (94%)	10 (6%)	21	57
13	o	181/208 (87%)	172 (95%)	9 (5%)	24	60
14	T	26/29 (90%)	25 (96%)	1 (4%)	33	69
14	t	26/29 (90%)	25 (96%)	1 (4%)	33	69
15	U	83/89 (93%)	80 (96%)	3 (4%)	35	70
15	u	83/89 (93%)	80 (96%)	3 (4%)	35	70
16	V	117/117 (100%)	113 (97%)	4 (3%)	37	72
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	60
18	Z	43/52 (83%)	42 (98%)	1 (2%)	50	80
18	z	43/52 (83%)	42 (98%)	1 (2%)	50	80
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	21	57

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	16	ARG
1	A	24	THR
1	A	25	ASP
1	A	30	VAL
1	A	76	ASN
1	A	103	ASP
1	A	131	TRP
1	A	155	PHE

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Mol	Chain	Res	Type
1	A	177	SER
1	A	206	PHE
1	A	232	SER
1	A	241	GLN
1	A	286	THR
1	A	292	THR
1	A	297	LEU
1	A	308	ASP
2	B	36	SER
2	B	124	ARG
2	B	137	LYS
2	B	179	GLN
2	B	191	ASN
2	B	222	PRO
2	B	231	MET
2	B	233	ASN
2	B	246	PHE
2	B	262	THR
2	B	271	THR
2	B	309	LEU
2	B	350	GLU
2	B	354	LEU
2	B	362	PHE
2	B	414	PRO
2	B	478	VAL
3	C	27	ASP
3	C	29	GLU
3	C	67	MET
3	C	86	LEU
3	C	97	TRP
3	C	155	ASN
3	C	165	LEU
3	C	191	PRO
3	C	214	LEU
3	C	244	CYS
3	C	254	THR
3	C	262	ARG
3	C	289	PHE
3	C	298	PRO
3	C	355	THR
3	C	377	LEU
3	C	383	ASP

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Mol	Chain	Res	Type
3	C	419	PHE
3	C	428	THR
3	C	472	LEU
3	C	473	ASP
4	D	14	TRP
4	D	63	LEU
4	D	130	PHE
4	D	164	GLN
4	D	178	ILE
4	D	180	ARG
4	D	191	TRP
4	D	241	GLU
4	D	246	MET
4	D	250	ASN
4	D	294	ARG
4	D	304	ARG
4	D	323	GLU
4	D	346	LEU
5	E	4	THR
5	E	17	VAL
5	E	52	PRO
6	F	17	THR
7	H	12	ARG
7	H	21	VAL
7	H	27	THR
7	H	41	PHE
7	H	49	TYR
7	H	50	ASN
7	H	53	LEU
7	H	59	ASN
8	I	2	GLU
8	I	27	ASP
8	I	30	ARG
8	I	32	PRO
8	I	34	ARG
9	J	29	PHE
10	K	11	LEU
11	L	3	PRO
11	L	14	ARG
11	L	16	SER
13	O	46	PRO
13	O	50	ASP

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Mol	Chain	Res	Type
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	120	THR
13	O	168	PHE
13	O	206	GLU
13	O	216	PHE
13	O	223	ILE
14	T	4	ILE
15	U	46	LYS
15	U	61	ASN
15	U	90	ASP
16	V	81	ARG
16	V	111	GLU
16	V	122	ARG
16	V	128	PRO
18	Z	58	ASN
1	a	5012	ASN
1	a	5013	LEU
1	a	5016	ARG
1	a	5025	ASP
1	a	5030	VAL
1	a	5076	ASN
1	a	5103	ASP
1	a	5131	TRP
1	a	5155	PHE
1	a	5177	SER
1	a	5206	PHE
1	a	5232	SER
1	a	5241	GLN
1	a	5286	THR
1	a	5292	THR
1	a	5297	LEU
1	a	5308	ASP
2	b	5016	PRO
2	b	5036	SER
2	b	5124	ARG
2	b	5137	LYS
2	b	5179	GLN
2	b	5191	ASN
2	b	5222	PRO
2	b	5231	MET

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Mol	Chain	Res	Type
2	b	5233	ASN
2	b	5245	VAL
2	b	5246	PHE
2	b	5262	THR
2	b	5271	THR
2	b	5309	LEU
2	b	5350	GLU
2	b	5362	PHE
2	b	5467	ILE
2	b	5478	VAL
3	c	5027	ASP
3	c	5029	GLU
3	c	5067	MET
3	c	5086	LEU
3	c	5097	TRP
3	c	5155	ASN
3	c	5165	LEU
3	c	5191	PRO
3	c	5214	LEU
3	c	5244	CYS
3	c	5254	THR
3	c	5262	ARG
3	c	5289	PHE
3	c	5298	PRO
3	c	5355	THR
3	c	5377	LEU
3	c	5383	ASP
3	c	5419	PHE
3	c	5428	THR
3	c	5472	LEU
3	c	5473	ASP
4	d	5014	TRP
4	d	5063	LEU
4	d	5090	LEU
4	d	5130	PHE
4	d	5164	GLN
4	d	5178	ILE
4	d	5180	ARG
4	d	5191	TRP
4	d	5241	GLU
4	d	5246	MET
4	d	5250	ASN

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Mol	Chain	Res	Type
4	d	5294	ARG
4	d	5304	ARG
4	d	5323	GLU
4	d	5346	LEU
5	e	5017	VAL
5	e	5052	PRO
6	f	5017	THR
7	h	5012	ARG
7	h	5021	VAL
7	h	5027	THR
7	h	5041	PHE
7	h	5049	TYR
7	h	5050	ASN
7	h	5059	ASN
8	i	5002	GLU
8	i	5027	ASP
8	i	5030	ARG
8	i	5032	PRO
8	i	5034	ARG
9	j	5029	PHE
10	k	5011	LEU
11	l	5010	VAL
11	l	5014	ARG
11	l	5016	SER
13	o	5046	PRO
13	o	5050	ASP
13	o	5097	VAL
13	o	5106	GLN
13	o	5114	ASN
13	o	5120	THR
13	o	5168	PHE
13	o	5216	PHE
13	o	5223	ILE
14	t	5004	ILE
15	u	5046	LYS
15	u	5061	ASN
15	u	5090	ASP
16	v	5035	THR
16	v	5037	PRO
16	v	5081	ARG
16	v	5111	GLU
16	v	5122	ARG

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Mol	Chain	Res	Type
16	v	5128	PRO
18	z	5058	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	75	ASN
1	A	76	ASN
1	A	118	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	234	ASN
1	A	241	GLN
1	A	272	HIS
1	A	296	ASN
1	A	298	ASN
1	A	304	HIS
1	A	322	ASN
2	B	157	HIS
2	B	179	GLN
2	B	191	ASN
2	B	223	GLN
2	B	233	ASN
2	B	274	GLN
2	B	394	GLN
2	B	438	ASN
3	C	155	ASN
3	C	201	ASN
3	C	229	ASN
3	C	293	ASN
3	C	322	GLN
3	C	332	GLN
3	C	398	HIS
3	C	415	ASN
4	D	61	HIS
4	D	98	GLN
4	D	224	GLN
4	D	250	ASN
4	D	255	GLN

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Mol	Chain	Res	Type
5	E	58	GLN
6	F	41	GLN
7	H	15	ASN
12	M	5	GLN
13	O	72	GLN
13	O	106	GLN
13	O	114	ASN
13	O	130	GLN
13	O	262	GLN
15	U	108	ASN
16	V	104	ASN
16	V	144	HIS
18	Z	6	GLN
1	a	5012	ASN
1	a	5019	ASN
1	a	5075	ASN
1	a	5076	ASN
1	a	5118	HIS
1	a	5165	GLN
1	a	5241	GLN
1	a	5272	HIS
1	a	5296	ASN
1	a	5298	ASN
1	a	5304	HIS
1	a	5322	ASN
2	b	5157	HIS
2	b	5179	GLN
2	b	5191	ASN
2	b	5223	GLN
2	b	5233	ASN
2	b	5274	GLN
2	b	5289	GLN
2	b	5394	GLN
2	b	5438	ASN
3	c	5155	ASN
3	c	5201	ASN
3	c	5229	ASN
3	c	5293	ASN
3	c	5332	GLN
3	c	5398	HIS
3	c	5415	ASN
4	d	5061	HIS

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Mol	Chain	Res	Type
4	d	5098	GLN
4	d	5164	GLN
4	d	5224	GLN
4	d	5250	ASN
4	d	5255	GLN
5	e	5058	GLN
6	f	5041	GLN
7	h	5015	ASN
7	h	5059	ASN
12	m	5005	GLN
13	o	5072	GLN
13	o	5106	GLN
13	o	5114	ASN
13	o	5130	GLN
13	o	5262	GLN
15	u	5108	ASN
16	v	5104	ASN
16	v	5144	HIS
18	z	5006	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 34 are unknown and 4 are monoatomic - leaving 142 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$
20	CLA	B	522	-	59,73,73	1.33	6 (10%)	67,113,113	1.91	10 (14%)
20	CLA	C	503	3	44,58,73	1.89	8 (18%)	49,95,113	2.31	12 (24%)
20	CLA	b	5517	-	59,73,73	1.56	7 (11%)	67,113,113	2.03	12 (17%)
20	CLA	B	512	2	59,73,73	1.30	5 (8%)	67,113,113	1.88	14 (20%)
20	CLA	c	5495	-	59,73,73	1.72	9 (15%)	67,113,113	2.12	16 (23%)
20	CLA	b	5526	-	59,73,73	1.57	11 (18%)	67,113,113	2.03	14 (20%)
27	LMT	T	217	-	36,36,36	1.40	6 (16%)	47,47,47	1.02	4 (8%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.97	3 (5%)
20	CLA	b	5522	-	59,73,73	1.37	6 (10%)	67,113,113	1.93	9 (13%)
20	CLA	C	495	-	59,73,73	1.56	8 (13%)	67,113,113	2.07	15 (22%)
20	CLA	d	5354	4	59,73,73	1.26	8 (13%)	67,113,113	1.88	13 (19%)
20	CLA	c	5492	3	54,68,73	1.37	9 (16%)	61,107,113	2.10	12 (19%)
20	CLA	B	518	2	59,73,73	1.47	7 (11%)	67,113,113	2.07	11 (16%)
21	PHO	A	562	-	67,69,69	1.05	6 (8%)	85,99,99	1.49	14 (16%)
27	LMT	A	569	-	36,36,36	1.53	6 (16%)	47,47,47	1.07	1 (2%)
20	CLA	c	5497	-	59,73,73	1.36	8 (13%)	67,113,113	1.99	14 (20%)
27	LMT	M	5216	-	36,36,36	1.46	8 (22%)	47,47,47	0.91	2 (4%)
24	BCR	d	5357	-	41,41,41	1.97	8 (19%)	56,56,56	2.28	21 (37%)
20	CLA	a	5559	-	59,73,73	1.17	5 (8%)	67,113,113	1.86	10 (14%)
24	BCR	B	529	-	41,41,41	1.81	8 (19%)	56,56,56	2.17	20 (35%)
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.53	8 (11%)
21	PHO	A	561	-	67,69,69	1.03	4 (5%)	85,99,99	1.44	14 (16%)
20	CLA	c	5503	3	44,58,73	1.93	9 (20%)	49,95,113	2.31	10 (20%)
20	CLA	c	5494	-	40,54,73	1.48	6 (15%)	44,90,113	2.29	11 (25%)
28	MGE	L	210	-	48,48,48	0.98	3 (6%)	56,56,56	1.17	4 (7%)
31	BCT	d	5353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	C	496	3	59,73,73	1.52	10 (16%)	67,113,113	2.01	14 (20%)
20	CLA	B	520	-	59,73,73	1.32	9 (15%)	67,113,113	1.91	14 (20%)
22	PQ9	A	564	-	30,30,45	0.87	1 (3%)	38,39,57	1.50	8 (21%)
20	CLA	C	494	-	40,54,73	1.58	6 (15%)	44,90,113	2.46	11 (25%)
22	PQ9	D	356	-	30,30,45	0.89	1 (3%)	38,39,57	1.67	9 (23%)
28	MGE	d	5360	-	41,41,48	1.20	6 (14%)	49,49,56	1.05	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	5527	-	41,41,41	1.54	8 (19%)	56,56,56	1.95	14 (25%)
20	CLA	C	491	3	59,73,73	1.31	7 (11%)	67,113,113	1.83	9 (13%)
30	DGD	C	508	-	48,48,67	1.44	9 (18%)	62,62,81	1.70	11 (17%)
20	CLA	b	5520	-	59,73,73	1.40	9 (15%)	67,113,113	1.90	13 (19%)
20	CLA	C	500	-	59,73,73	1.37	8 (13%)	67,113,113	1.91	12 (17%)
20	CLA	C	493	3	59,73,73	1.33	7 (11%)	67,113,113	2.03	14 (20%)
20	CLA	b	5514	2	59,73,73	1.47	6 (10%)	67,113,113	2.09	13 (19%)
32	HEM	V	552	16	27,50,50	1.99	9 (33%)	17,82,82	2.28	5 (29%)
24	BCR	T	5104	-	41,41,41	1.53	8 (19%)	56,56,56	2.26	22 (39%)
20	CLA	B	519	-	59,73,73	1.64	7 (11%)	67,113,113	1.95	13 (19%)
20	CLA	D	354	4	59,73,73	1.23	7 (11%)	67,113,113	1.83	12 (17%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.12	5 (8%)
26	SQD	A	5212	-	25,26,54	2.80	12 (48%)	34,37,65	2.72	11 (32%)
20	CLA	B	516	-	59,73,73	1.53	7 (11%)	67,113,113	2.05	12 (17%)
24	BCR	B	527	-	41,41,41	1.71	8 (19%)	56,56,56	2.03	16 (28%)
20	CLA	b	5512	2	59,73,73	1.26	7 (11%)	67,113,113	1.85	13 (19%)
20	CLA	B	513	2	59,73,73	1.37	8 (13%)	67,113,113	1.93	14 (20%)
24	BCR	c	5505	-	41,41,41	1.95	8 (19%)	56,56,56	2.09	18 (32%)
20	CLA	c	5499	-	41,55,73	1.65	10 (24%)	45,91,113	2.28	12 (26%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.55	9 (13%)
20	CLA	A	560	-	59,73,73	1.34	6 (10%)	67,113,113	1.97	14 (20%)
20	CLA	d	5355	-	44,58,73	1.76	8 (18%)	49,95,113	2.27	11 (22%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.47	6 (8%)
21	PHO	a	5561	-	67,69,69	1.04	5 (7%)	85,99,99	1.38	11 (12%)
27	LMT	m	216	-	36,36,36	1.46	7 (19%)	47,47,47	0.98	3 (6%)
20	CLA	B	525	-	59,73,73	1.34	7 (11%)	67,113,113	1.99	11 (16%)
20	CLA	c	5500	-	59,73,73	1.32	7 (11%)	67,113,113	1.92	14 (20%)
20	CLA	b	5518	2	59,73,73	1.50	6 (10%)	67,113,113	2.06	17 (25%)
22	PQ9	d	5356	-	30,30,45	0.81	0	38,39,57	1.66	6 (15%)
24	BCR	A	566	-	41,41,41	1.58	8 (19%)	56,56,56	2.09	21 (37%)
24	BCR	x	5130	-	41,41,41	1.95	10 (24%)	56,56,56	2.47	23 (41%)
26	SQD	L	5213	-	46,47,54	2.70	24 (52%)	55,58,65	2.44	13 (23%)
26	SQD	d	5358	-	53,54,54	2.44	27 (50%)	62,65,65	2.57	19 (30%)
20	CLA	B	524	2	50,64,73	1.57	5 (10%)	56,102,113	2.23	11 (19%)
20	CLA	B	515	-	59,73,73	1.31	9 (15%)	67,113,113	1.98	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	HEM	f	5051	5,6	27,50,50	1.99	8 (29%)	17,82,82	2.64	8 (47%)
20	CLA	b	5525	-	59,73,73	1.28	6 (10%)	67,113,113	2.02	11 (16%)
24	BCR	b	5528	-	41,41,41	1.70	6 (14%)	56,56,56	2.00	17 (30%)
20	CLA	C	502	-	45,59,73	1.93	11 (24%)	50,96,113	2.33	12 (24%)
24	BCR	C	505	-	41,41,41	1.92	9 (21%)	56,56,56	2.08	16 (28%)
20	CLA	a	5558	1	59,73,73	1.32	9 (15%)	67,113,113	1.78	12 (17%)
20	CLA	B	511	-	35,49,73	2.21	12 (34%)	38,84,113	2.34	10 (26%)
20	CLA	B	526	-	59,73,73	1.53	12 (20%)	67,113,113	2.01	13 (19%)
28	MGE	D	360	-	48,48,48	0.92	4 (8%)	56,56,56	1.11	4 (7%)
24	BCR	c	5504	-	41,41,41	2.12	6 (14%)	56,56,56	2.13	22 (39%)
20	CLA	b	5519	-	59,73,73	1.48	9 (15%)	67,113,113	1.96	13 (19%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.17	6 (10%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.08	4 (7%)
20	CLA	b	5516	-	59,73,73	1.59	7 (11%)	67,113,113	2.09	12 (17%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	0.99	3 (6%)
24	BCR	a	5566	-	41,41,41	1.65	8 (19%)	56,56,56	2.09	22 (39%)
20	CLA	b	5513	2	59,73,73	1.31	8 (13%)	67,113,113	1.89	14 (20%)
30	DGD	C	507	-	54,54,67	1.36	8 (14%)	68,68,81	1.48	6 (8%)
20	CLA	c	5502	-	45,59,73	1.95	8 (17%)	50,96,113	2.33	12 (24%)
22	PQ9	a	5564	-	30,30,45	0.91	1 (3%)	38,39,57	1.46	8 (21%)
20	CLA	b	5523	-	59,73,73	1.23	7 (11%)	67,113,113	2.06	13 (19%)
20	CLA	a	5563	-	49,63,73	1.63	9 (18%)	55,101,113	1.97	11 (20%)
25	LHG	A	567	-	38,38,48	1.94	5 (13%)	41,44,54	1.50	4 (9%)
30	DGD	c	5509	-	58,58,67	1.35	9 (15%)	72,72,81	1.39	5 (6%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	3 (6%)
28	MGE	l	5210	-	48,48,48	0.89	3 (6%)	56,56,56	1.14	4 (7%)
26	SQD	a	212	-	25,26,54	3.06	14 (56%)	34,37,65	2.83	13 (38%)
30	DGD	c	5508	-	48,48,67	1.48	9 (18%)	62,62,81	1.74	11 (17%)
24	BCR	C	504	-	41,41,41	1.84	7 (17%)	56,56,56	2.16	22 (39%)
32	HEM	v	5552	16	27,50,50	2.17	8 (29%)	17,82,82	2.36	6 (35%)
20	CLA	b	5515	-	59,73,73	1.30	10 (16%)	67,113,113	1.95	15 (22%)
31	BCT	D	353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	c	5493	3	59,73,73	1.48	7 (11%)	67,113,113	2.01	15 (22%)
24	BCR	h	5107	-	41,41,41	1.99	8 (19%)	56,56,56	2.24	25 (44%)
26	SQD	A	568	-	53,54,54	2.46	28 (52%)	62,65,65	2.61	19 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	5529	-	41,41,41	1.69	8 (19%)	56,56,56	2.09	18 (32%)
20	CLA	B	523	-	59,73,73	1.29	6 (10%)	67,113,113	2.01	12 (17%)
20	CLA	c	5496	-	59,73,73	1.50	10 (16%)	67,113,113	1.96	13 (19%)
20	CLA	b	5511	-	35,49,73	2.19	10 (28%)	38,84,113	2.42	10 (26%)
20	CLA	C	498	3	59,73,73	1.40	6 (10%)	67,113,113	1.97	11 (16%)
30	DGD	C	509	-	58,58,67	1.12	6 (10%)	72,72,81	1.40	6 (8%)
20	CLA	A	563	-	49,63,73	1.47	8 (16%)	55,101,113	2.08	15 (27%)
20	CLA	b	5521	2	59,73,73	1.27	6 (10%)	67,113,113	1.99	14 (20%)
24	BCR	B	528	-	41,41,41	1.88	6 (14%)	56,56,56	1.96	14 (25%)
24	BCR	H	107	-	41,41,41	2.09	7 (17%)	56,56,56	2.23	24 (42%)
20	CLA	A	559	-	59,73,73	1.17	6 (10%)	67,113,113	1.84	9 (13%)
20	CLA	A	558	1	59,73,73	1.29	6 (10%)	67,113,113	1.86	14 (20%)
32	HEM	F	51	5,6	27,50,50	2.00	8 (29%)	17,82,82	2.65	6 (35%)
20	CLA	B	517	-	59,73,73	1.56	6 (10%)	67,113,113	2.13	14 (20%)
26	SQD	t	213	-	46,47,54	2.70	23 (50%)	55,58,65	2.54	15 (27%)
20	CLA	a	5560	-	59,73,73	1.45	8 (13%)	67,113,113	1.97	12 (17%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.05	2 (3%)
20	CLA	C	501	3	59,73,73	1.64	8 (13%)	67,113,113	2.06	11 (16%)
24	BCR	C	506	-	41,41,41	1.73	9 (21%)	56,56,56	2.18	21 (37%)
24	BCR	c	5506	-	41,41,41	1.93	9 (21%)	56,56,56	2.10	20 (35%)
27	LMT	a	5568	-	36,36,36	1.45	6 (16%)	47,47,47	1.09	1 (2%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
25	LHG	a	5567	-	38,38,48	1.98	5 (13%)	41,44,54	1.45	4 (9%)
20	CLA	D	355	-	44,58,73	1.77	8 (18%)	49,95,113	2.29	11 (22%)
24	BCR	D	357	-	41,41,41	1.92	9 (21%)	56,56,56	2.22	20 (35%)
20	CLA	C	499	-	41,55,73	1.66	9 (21%)	45,91,113	2.33	13 (28%)
23	OEC	A	565	1,3	0,0,13	0.00	-	-	-	-
20	CLA	b	5524	2	50,64,73	1.46	6 (12%)	56,102,113	2.10	10 (17%)
24	BCR	X	130	-	41,41,41	1.91	10 (24%)	56,56,56	2.49	23 (41%)
20	CLA	c	5498	3	59,73,73	1.65	8 (13%)	67,113,113	2.01	10 (14%)
20	CLA	c	5491	3	59,73,73	1.51	8 (13%)	67,113,113	2.04	10 (14%)
23	OEC	a	5565	1,3	0,0,13	0.00	-	-	-	-
20	CLA	B	521	2	59,73,73	1.34	9 (15%)	67,113,113	2.07	13 (19%)
20	CLA	C	492	3	54,68,73	1.42	10 (18%)	61,107,113	2.09	14 (22%)
20	CLA	c	5501	3	59,73,73	1.61	8 (13%)	67,113,113	2.05	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	C	497	-	59,73,73	1.36	7 (11%)	67,113,113	2.12	12 (17%)
24	BCR	t	104	-	41,41,41	1.65	10 (24%)	56,56,56	2.22	22 (39%)
21	PHO	a	5562	-	67,69,69	1.06	6 (8%)	85,99,99	1.49	14 (16%)
28	MGE	i	5201	-	48,48,48	1.25	8 (16%)	56,56,56	1.09	4 (7%)
20	CLA	B	514	2	59,73,73	1.47	7 (11%)	67,113,113	2.05	12 (17%)

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
20	CLA	b	5526	-	3/3/20/25	11/37/135/135	-
20	CLA	C	503	3	3/3/17/25	5/19/117/135	-
20	CLA	b	5517	-	3/3/20/25	14/37/135/135	-
20	CLA	B	512	2	3/3/20/25	14/37/135/135	-
20	CLA	c	5495	-	3/3/20/25	16/37/135/135	-
20	CLA	B	522	-	3/3/20/25	13/37/135/135	-
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
20	CLA	b	5522	-	3/3/20/25	12/37/135/135	-
20	CLA	C	495	-	3/3/20/25	16/37/135/135	-
20	CLA	d	5354	4	3/3/20/25	10/37/135/135	-
20	CLA	c	5492	3	3/3/19/25	10/31/129/135	-
20	CLA	B	518	2	3/3/20/25	15/37/135/135	-
21	PHO	A	562	-	-	10/53/103/103	0/5/6/6
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
20	CLA	c	5497	-	3/3/20/25	7/37/135/135	-
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
20	CLA	a	5559	-	3/3/20/25	17/37/135/135	-
24	BCR	B	529	-	-	4/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	c	5503	3	3/3/17/25	5/19/117/135	-
28	MGE	L	210	-	-	24/43/63/63	0/1/1/1
20	CLA	C	496	3	3/3/20/25	14/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5524	2	3/3/18/25	9/27/125/135	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
20	CLA	C	494	-	3/3/16/25	7/15/113/135	-
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
20	CLA	C	491	3	3/3/20/25	8/37/135/135	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
20	CLA	B	524	2	3/3/18/25	10/27/125/135	-
20	CLA	C	500	-	3/3/20/25	12/37/135/135	-
20	CLA	C	493	3	3/3/20/25	12/37/135/135	-
20	CLA	b	5514	2	3/3/20/25	12/37/135/135	-
32	HEM	V	552	16	-	0/6/54/54	-
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
20	CLA	B	519	-	3/3/20/25	13/37/135/135	-
20	CLA	D	354	4	3/3/20/25	11/37/135/135	-
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
26	SQD	A	5212	-	-	6/19/39/69	0/1/1/1
20	CLA	B	516	-	3/3/20/25	13/37/135/135	-
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	b	5512	2	3/3/20/25	13/37/135/135	-
20	CLA	B	513	2	3/3/20/25	11/37/135/135	-
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5499	-	3/3/16/25	7/16/114/135	-
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	A	560	-	3/3/20/25	10/37/135/135	-
20	CLA	d	5355	-	3/3/17/25	9/19/117/135	-
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	a	5561	-	-	16/53/103/103	0/5/6/6
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	b	5521	2	3/3/20/25	8/37/135/135	-
20	CLA	c	5500	-	3/3/20/25	12/37/135/135	-
20	CLA	b	5518	2	3/3/20/25	14/37/135/135	-
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
26	SQD	L	5213	-	-	20/42/62/69	0/1/1/1
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
20	CLA	b	5520	-	3/3/20/25	15/37/135/135	-
20	CLA	B	515	-	3/3/20/25	18/37/135/135	-
32	HEM	f	5051	5,6	-	0/6/54/54	-
20	CLA	B	521	2	3/3/20/25	7/37/135/135	-
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
20	CLA	C	502	-	3/3/17/25	9/21/119/135	-
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
20	CLA	a	5558	1	3/3/20/25	10/37/135/135	-
20	CLA	B	511	-	3/3/15/25	2/8/106/135	-
20	CLA	B	526	-	3/3/20/25	12/37/135/135	-
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
20	CLA	b	5519	-	3/3/20/25	12/37/135/135	-
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
28	MGE	I	201	-	-	23/43/63/63	0/1/1/1
20	CLA	b	5516	-	3/3/20/25	14/37/135/135	-
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5513	2	3/3/20/25	10/37/135/135	-
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5502	-	3/3/17/25	9/21/119/135	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
20	CLA	b	5523	-	3/3/20/25	15/37/135/135	-
20	CLA	a	5563	-	3/3/18/25	5/25/123/135	-
25	LHG	A	567	-	-	17/43/43/53	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
28	MGE	l	5210	-	-	24/43/63/63	0/1/1/1
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
32	HEM	v	5552	16	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5515	-	3/3/20/25	18/37/135/135	-
20	CLA	c	5494	-	3/3/16/25	7/15/113/135	-
20	CLA	c	5493	3	3/3/20/25	12/37/135/135	-
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
20	CLA	B	523	-	3/3/20/25	16/37/135/135	-
20	CLA	c	5496	-	3/3/20/25	14/37/135/135	-
20	CLA	b	5511	-	3/3/15/25	2/8/106/135	-
20	CLA	C	498	3	3/3/20/25	20/37/135/135	-
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
20	CLA	A	563	-	3/3/18/25	5/25/123/135	-
20	CLA	B	525	-	3/3/20/25	13/37/135/135	-
24	BCR	B	528	-	-	2/29/63/63	0/2/2/2
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
20	CLA	A	559	-	3/3/20/25	17/37/135/135	-
20	CLA	A	558	1	3/3/20/25	8/37/135/135	-
32	HEM	F	51	5,6	-	0/6/54/54	-
20	CLA	B	517	-	3/3/20/25	14/37/135/135	-
26	SQD	t	213	-	-	19/42/62/69	0/1/1/1
20	CLA	a	5560	-	3/3/20/25	10/37/135/135	-
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	C	501	3	3/3/20/25	14/37/135/135	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
28	MGE	d	5359	-	-	14/42/62/63	0/1/1/1
25	LHG	a	5567	-	-	16/43/43/53	-
20	CLA	D	355	-	3/3/17/25	9/19/117/135	-
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
20	CLA	C	499	-	3/3/16/25	7/16/114/135	-
21	PHO	A	561	-	-	16/53/103/103	0/5/6/6
20	CLA	B	520	-	3/3/20/25	18/37/135/135	-
24	BCR	X	130	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	5498	3	3/3/20/25	19/37/135/135	-
20	CLA	c	5491	3	3/3/20/25	7/37/135/135	-
23	OEC	a	5565	1,3	-	-	0/1/0/5
20	CLA	b	5525	-	3/3/20/25	14/37/135/135	-
20	CLA	C	492	3	3/3/19/25	10/31/129/135	-
20	CLA	c	5501	3	3/3/20/25	13/37/135/135	-
20	CLA	C	497	-	3/3/20/25	7/37/135/135	-
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	a	5562	-	-	10/53/103/103	0/5/6/6
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
20	CLA	B	514	2	3/3/20/25	12/37/135/135	-

All (1085) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5495	CLA	MG-NA	8.38	2.26	2.06
26	A	568	SQD	C4-C3	8.18	1.73	1.52
26	t	213	SQD	C4-C3	8.14	1.73	1.52
20	B	517	CLA	MG-NA	8.14	2.25	2.06
26	a	212	SQD	C4-C3	8.11	1.73	1.52
25	A	567	LHG	P-O5	8.02	1.79	1.50
25	a	5567	LHG	P-O5	7.93	1.79	1.50
20	c	5503	CLA	MG-NA	7.88	2.25	2.06
20	C	503	CLA	MG-NA	7.88	2.25	2.06
26	d	5358	SQD	C4-C3	7.84	1.72	1.52
26	L	5213	SQD	C4-C3	7.78	1.72	1.52
24	c	5504	BCR	C1-C6	7.65	1.64	1.53
20	B	511	CLA	C4B-NB	7.61	1.42	1.35
20	b	5516	CLA	MG-NA	7.52	2.24	2.06
20	C	495	CLA	MG-NA	7.46	2.24	2.06
20	C	501	CLA	MG-NA	7.40	2.23	2.06
20	c	5498	CLA	MG-NA	7.30	2.23	2.06
26	A	5212	SQD	C4-C3	7.25	1.70	1.52
20	D	355	CLA	MG-NA	7.17	2.23	2.06
20	B	516	CLA	MG-NA	7.16	2.23	2.06
20	c	5491	CLA	MG-NA	7.12	2.23	2.06
20	B	524	CLA	MG-NA	7.02	2.23	2.06
20	b	5514	CLA	MG-NA	6.92	2.22	2.06
20	b	5518	CLA	MG-NA	6.73	2.22	2.06
24	c	5504	BCR	C30-C25	6.69	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	5107	BCR	C30-C25	6.67	1.62	1.53
20	c	5501	CLA	MG-NA	6.65	2.22	2.06
20	B	519	CLA	MG-NA	6.65	2.22	2.06
20	B	518	CLA	MG-NA	6.64	2.22	2.06
24	H	107	BCR	C30-C25	6.61	1.62	1.53
20	c	5502	CLA	MG-NA	6.54	2.21	2.06
20	B	514	CLA	MG-NA	6.50	2.21	2.06
20	C	499	CLA	MG-NA	6.47	2.21	2.06
20	b	5517	CLA	MG-NA	6.44	2.21	2.06
20	b	5511	CLA	C4B-NB	6.38	1.40	1.35
20	d	5355	CLA	MG-NA	6.29	2.21	2.06
24	B	528	BCR	C30-C25	6.27	1.62	1.53
26	L	5213	SQD	O7-S	6.20	1.63	1.45
24	d	5357	BCR	C1-C6	6.17	1.62	1.53
20	C	502	CLA	MG-NA	6.14	2.20	2.06
20	C	502	CLA	C4B-NB	6.08	1.40	1.35
24	C	505	BCR	C30-C25	6.01	1.62	1.53
24	c	5505	BCR	C30-C25	5.95	1.61	1.53
24	C	504	BCR	C1-C6	5.88	1.61	1.53
26	t	213	SQD	O7-S	5.87	1.62	1.45
20	C	496	CLA	MG-NA	5.79	2.20	2.06
26	d	5358	SQD	O7-S	5.79	1.62	1.45
20	c	5502	CLA	C4B-NB	5.76	1.40	1.35
24	b	5528	BCR	C30-C25	5.67	1.61	1.53
30	H	208	DGD	O3G-C1D	5.62	1.49	1.40
24	B	528	BCR	C1-C6	5.60	1.61	1.53
26	a	212	SQD	O47-C7	5.60	1.47	1.35
20	C	498	CLA	MG-NA	5.59	2.19	2.06
24	A	566	BCR	C1-C6	5.56	1.61	1.53
20	b	5519	CLA	MG-NA	5.54	2.19	2.06
20	b	5522	CLA	MG-NA	5.44	2.19	2.06
20	b	5524	CLA	MG-NA	5.43	2.19	2.06
24	H	107	BCR	C1-C6	5.42	1.61	1.53
20	b	5511	CLA	MG-NA	5.41	2.19	2.06
20	a	5560	CLA	MG-NA	5.36	2.19	2.06
24	B	527	BCR	C30-C25	5.33	1.61	1.53
26	A	5212	SQD	O7-S	5.29	1.60	1.45
20	c	5499	CLA	MG-NA	5.26	2.18	2.06
24	D	357	BCR	C30-C25	5.20	1.60	1.53
24	h	5107	BCR	C1-C6	5.16	1.60	1.53
20	B	526	CLA	MG-NA	5.15	2.18	2.06
20	C	493	CLA	MG-NA	5.15	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5493	CLA	C4B-NB	5.12	1.39	1.35
24	H	107	BCR	C29-C30	5.04	1.65	1.54
26	t	213	SQD	C1-C2	5.04	1.67	1.52
24	c	5506	BCR	C30-C25	5.01	1.60	1.53
24	a	5566	BCR	C1-C6	5.01	1.60	1.53
24	C	504	BCR	C30-C25	4.98	1.60	1.53
30	h	5208	DGD	O3G-C1D	4.96	1.48	1.40
20	B	523	CLA	MG-NA	4.94	2.18	2.06
20	c	5493	CLA	MG-NA	4.94	2.18	2.06
24	B	529	BCR	C30-C25	4.93	1.60	1.53
24	x	5130	BCR	C1-C6	4.90	1.60	1.53
24	x	5130	BCR	C30-C25	4.90	1.60	1.53
24	X	130	BCR	C1-C6	4.89	1.60	1.53
26	a	212	SQD	O7-S	4.88	1.59	1.45
24	X	130	BCR	C5-C6	4.83	1.42	1.34
24	b	5527	BCR	C30-C25	4.81	1.60	1.53
20	B	519	CLA	C4B-NB	4.79	1.39	1.35
20	a	5563	CLA	MG-NA	4.77	2.17	2.06
24	c	5505	BCR	C1-C6	4.77	1.60	1.53
24	X	130	BCR	C30-C25	4.77	1.60	1.53
24	b	5529	BCR	C30-C25	4.76	1.60	1.53
26	A	5212	SQD	O47-C7	4.71	1.45	1.35
24	x	5130	BCR	C5-C6	4.70	1.42	1.34
20	c	5492	CLA	MG-NA	4.68	2.17	2.06
20	B	525	CLA	C4B-NB	4.68	1.39	1.35
25	a	5567	LHG	P-O3	4.66	1.78	1.59
26	A	568	SQD	O7-S	4.61	1.58	1.45
27	A	569	LMT	O1'-C1'	4.60	1.48	1.40
24	c	5506	BCR	C1-C6	4.60	1.60	1.53
20	C	492	CLA	MG-NA	4.59	2.17	2.06
24	D	357	BCR	C26-C25	4.58	1.42	1.34
20	A	560	CLA	MG-NA	4.57	2.17	2.06
20	c	5498	CLA	C4B-NB	4.56	1.39	1.35
24	B	527	BCR	C26-C25	4.51	1.42	1.34
26	L	5213	SQD	O48-C23	4.51	1.46	1.33
26	t	213	SQD	O5-C5	4.50	1.55	1.44
20	B	522	CLA	C4B-NB	4.50	1.39	1.35
32	f	5051	HEM	CAA-C2A	4.48	1.58	1.52
20	c	5501	CLA	C1B-NB	4.44	1.39	1.35
20	c	5497	CLA	MG-NC	4.43	2.16	2.06
24	c	5505	BCR	C26-C25	4.40	1.42	1.34
20	C	497	CLA	MG-NA	4.40	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	51	HEM	CAA-C2A	4.39	1.58	1.52
24	C	505	BCR	C26-C25	4.36	1.42	1.34
24	a	5566	BCR	C30-C25	4.34	1.59	1.53
20	B	515	CLA	MG-NA	4.33	2.16	2.06
24	B	529	BCR	C26-C25	4.33	1.41	1.34
26	a	212	SQD	C1-C2	4.32	1.64	1.52
30	c	5509	DGD	O3G-C1D	4.30	1.47	1.40
20	C	501	CLA	C4B-NB	4.30	1.39	1.35
24	d	5357	BCR	C5-C6	4.30	1.41	1.34
20	B	513	CLA	MG-NA	4.29	2.16	2.06
32	v	5552	HEM	CAD-C3D	-4.28	1.44	1.52
20	b	5511	CLA	C1B-NB	4.26	1.39	1.35
20	b	5517	CLA	C4B-NB	4.26	1.39	1.35
24	C	506	BCR	C30-C25	4.26	1.59	1.53
20	b	5521	CLA	C4B-NB	4.25	1.39	1.35
30	c	5508	DGD	O6D-C1D	4.25	1.52	1.41
20	b	5526	CLA	MG-NA	4.24	2.16	2.06
24	H	107	BCR	C26-C25	4.24	1.41	1.34
24	h	5107	BCR	C26-C25	4.24	1.41	1.34
32	v	5552	HEM	CAA-C2A	4.21	1.58	1.52
24	B	529	BCR	C1-C6	4.20	1.59	1.53
24	C	506	BCR	C2-C1	4.20	1.63	1.54
20	B	521	CLA	MG-NA	4.20	2.16	2.06
20	A	563	CLA	MG-NA	4.20	2.16	2.06
20	c	5496	CLA	C4B-NB	4.19	1.39	1.35
24	c	5506	BCR	C5-C6	4.19	1.41	1.34
20	a	5563	CLA	C4B-NB	4.17	1.38	1.35
20	B	522	CLA	MG-NA	4.17	2.16	2.06
20	a	5560	CLA	C4B-NB	4.16	1.38	1.35
28	B	530	MGE	O3G-C1D	4.16	1.47	1.40
20	c	5495	CLA	C4B-NB	4.15	1.38	1.35
24	D	357	BCR	C5-C6	4.14	1.41	1.34
27	a	5568	LMT	O1'-C1'	4.14	1.47	1.40
20	A	558	CLA	MG-NA	4.13	2.16	2.06
27	M	5216	LMT	O1'-C1'	4.13	1.47	1.40
24	d	5357	BCR	C26-C25	4.12	1.41	1.34
20	B	525	CLA	MG-NA	4.11	2.16	2.06
20	C	500	CLA	MG-NA	4.11	2.16	2.06
24	c	5506	BCR	C26-C25	4.10	1.41	1.34
24	b	5528	BCR	C1-C6	4.09	1.59	1.53
24	c	5504	BCR	C29-C30	4.09	1.63	1.54
26	d	5358	SQD	C1-C2	4.08	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	511	CLA	MG-NA	4.07	2.15	2.06
26	L	5213	SQD	O5-C5	4.06	1.54	1.44
24	h	5107	BCR	C29-C30	4.03	1.63	1.54
24	C	505	BCR	C1-C6	4.03	1.59	1.53
24	x	5130	BCR	C29-C30	4.02	1.63	1.54
26	A	568	SQD	C1-C2	4.02	1.64	1.52
20	A	560	CLA	CAA-C2A	4.01	1.61	1.54
26	d	5358	SQD	O47-C7	4.00	1.45	1.34
26	A	568	SQD	O48-C23	4.00	1.45	1.33
26	d	5358	SQD	O48-C23	4.00	1.45	1.33
30	c	5507	DGD	O5D-C1E	4.00	1.47	1.40
24	t	104	BCR	C30-C25	4.00	1.59	1.53
20	B	511	CLA	MG-NC	3.99	2.15	2.06
24	h	5107	BCR	C2-C1	3.99	1.63	1.54
26	L	5213	SQD	C1-C2	3.99	1.64	1.52
20	C	496	CLA	C4B-NB	3.98	1.38	1.35
24	c	5506	BCR	C2-C1	3.97	1.63	1.54
20	b	5513	CLA	MG-NA	3.97	2.15	2.06
24	C	505	BCR	C2-C1	3.97	1.63	1.54
32	v	5552	HEM	C1A-NA	3.96	1.44	1.36
32	v	5552	HEM	CBC-CAC	3.96	1.55	1.29
20	C	500	CLA	C4B-NB	3.96	1.38	1.35
30	c	5507	DGD	C4D-C3D	3.96	1.62	1.52
28	D	359	MGE	O3G-C1D	3.94	1.46	1.40
20	c	5494	CLA	CAA-C2A	3.93	1.61	1.54
24	D	357	BCR	C29-C30	3.92	1.63	1.54
26	t	213	SQD	O48-C23	3.91	1.44	1.33
20	C	497	CLA	MG-NC	3.91	2.15	2.06
20	B	511	CLA	C1B-NB	3.91	1.38	1.35
26	A	568	SQD	O47-C7	3.90	1.45	1.34
24	T	5104	BCR	C2-C1	3.89	1.63	1.54
20	B	512	CLA	MG-NA	3.88	2.15	2.06
20	C	499	CLA	C4B-NB	3.88	1.38	1.35
32	V	552	HEM	CBC-CAC	3.87	1.55	1.29
32	f	5051	HEM	C1A-NA	3.87	1.44	1.36
30	c	5508	DGD	O3G-C1D	3.86	1.46	1.40
20	C	494	CLA	MG-NA	3.85	2.15	2.06
32	f	5051	HEM	CBC-CAC	3.82	1.54	1.29
20	C	491	CLA	MG-NA	3.82	2.15	2.06
20	C	494	CLA	C4B-NB	3.82	1.38	1.35
20	b	5519	CLA	C4B-NB	3.82	1.38	1.35
20	D	355	CLA	CAA-C2A	3.82	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5500	CLA	C4B-NB	3.81	1.38	1.35
25	A	567	LHG	P-O3	3.80	1.74	1.59
20	b	5520	CLA	C4B-NB	3.80	1.38	1.35
26	a	212	SQD	O5-C5	3.79	1.53	1.44
27	T	217	LMT	O1'-C1'	3.79	1.46	1.40
32	F	51	HEM	CBC-CAC	3.78	1.54	1.29
20	c	5496	CLA	MG-NA	3.77	2.15	2.06
24	d	5357	BCR	C29-C30	3.77	1.62	1.54
20	C	494	CLA	CAA-C2A	3.77	1.61	1.54
24	X	130	BCR	C29-C30	3.76	1.62	1.54
24	T	5104	BCR	C5-C6	3.76	1.40	1.34
25	A	567	LHG	O8-C23	3.75	1.44	1.33
24	t	104	BCR	C1-C6	3.73	1.58	1.53
24	B	528	BCR	C29-C30	3.73	1.62	1.54
30	C	507	DGD	C4D-C3D	3.73	1.61	1.52
32	V	552	HEM	CAD-C3D	-3.72	1.45	1.52
24	H	107	BCR	C2-C1	3.71	1.62	1.54
20	B	519	CLA	CAA-C2A	3.71	1.61	1.54
20	b	5522	CLA	C4B-NB	3.71	1.38	1.35
20	c	5498	CLA	C1B-NB	3.70	1.38	1.35
24	d	5357	BCR	C30-C25	3.70	1.58	1.53
24	c	5504	BCR	C2-C1	3.70	1.62	1.54
20	c	5501	CLA	CAA-C2A	3.70	1.61	1.54
28	d	5361	MGE	O6D-C1D	3.70	1.51	1.41
28	L	210	MGE	O6D-C1D	3.69	1.51	1.41
24	C	504	BCR	C29-C30	3.68	1.62	1.54
26	A	568	SQD	O3-C3	3.68	1.51	1.43
20	b	5518	CLA	C4B-NB	3.68	1.38	1.35
25	a	5567	LHG	P-O6	3.68	1.74	1.59
20	c	5499	CLA	C4B-NB	3.67	1.38	1.35
32	V	552	HEM	C1A-NA	3.67	1.43	1.36
20	a	5558	CLA	CHC-C1C	3.65	1.44	1.35
20	C	503	CLA	CAA-C2A	3.62	1.60	1.54
20	b	5512	CLA	MG-NA	3.61	2.14	2.06
30	C	507	DGD	O5D-C1E	3.61	1.46	1.40
26	t	213	SQD	O8-S	3.61	1.60	1.47
26	L	5213	SQD	O8-S	3.60	1.60	1.47
26	t	213	SQD	O47-C7	3.60	1.44	1.34
20	A	563	CLA	C1B-CHB	-3.60	1.31	1.41
26	a	212	SQD	O8-S	3.60	1.60	1.47
24	D	357	BCR	C1-C6	3.60	1.58	1.53
20	B	522	CLA	CHC-C1C	3.60	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	5509	DGD	O6D-C1D	3.60	1.51	1.41
20	c	5500	CLA	MG-NA	3.59	2.14	2.06
32	V	552	HEM	CAA-C2A	3.58	1.57	1.52
20	b	5525	CLA	MG-NA	3.58	2.14	2.06
20	B	516	CLA	CAA-C2A	3.58	1.60	1.54
24	C	506	BCR	C5-C6	3.57	1.40	1.34
30	C	509	DGD	O3G-C1D	3.57	1.46	1.40
25	a	5567	LHG	O8-C23	3.57	1.43	1.33
24	D	357	BCR	C2-C1	3.57	1.62	1.54
20	D	354	CLA	C1B-CHB	-3.57	1.31	1.41
20	b	5520	CLA	MG-NC	3.56	2.14	2.06
25	A	567	LHG	P-O6	3.56	1.73	1.59
28	D	358	MGE	O6D-C1D	3.55	1.50	1.41
28	D	358	MGE	O3G-C1D	3.55	1.46	1.40
24	A	566	BCR	C5-C6	3.55	1.40	1.34
28	L	210	MGE	O3G-C1D	3.55	1.46	1.40
20	B	513	CLA	CAA-C2A	3.54	1.60	1.54
32	v	5552	HEM	C1C-C2C	3.54	1.50	1.42
20	C	497	CLA	C4B-NB	3.53	1.38	1.35
24	C	504	BCR	C26-C25	3.53	1.40	1.34
26	A	5212	SQD	O5-C5	3.53	1.52	1.44
26	d	5358	SQD	O5-C5	3.53	1.52	1.44
24	b	5529	BCR	C29-C30	3.52	1.62	1.54
24	b	5528	BCR	C29-C30	3.52	1.62	1.54
20	B	518	CLA	CAA-C2A	3.52	1.60	1.54
26	A	5212	SQD	O8-S	3.52	1.60	1.47
20	c	5503	CLA	CAA-C2A	3.52	1.60	1.54
20	b	5519	CLA	MG-NC	3.52	2.14	2.06
24	x	5130	BCR	C2-C1	3.52	1.62	1.54
24	C	505	BCR	C29-C30	3.52	1.62	1.54
24	C	506	BCR	C1-C6	3.51	1.58	1.53
20	c	5501	CLA	C4B-NB	3.51	1.38	1.35
20	C	492	CLA	C4B-NB	3.51	1.38	1.35
30	H	208	DGD	C4E-C5E	3.50	1.60	1.53
20	c	5493	CLA	MG-NC	3.49	2.14	2.06
24	t	104	BCR	C5-C6	3.49	1.40	1.34
20	b	5526	CLA	CAA-C2A	3.46	1.60	1.54
20	a	5563	CLA	C1B-NB	3.46	1.38	1.35
20	B	522	CLA	CAA-C2A	3.46	1.60	1.54
25	A	567	LHG	O7-C7	3.46	1.44	1.34
20	c	5497	CLA	C4B-NB	3.45	1.38	1.35
20	c	5503	CLA	C1B-NB	3.45	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	566	BCR	C2-C1	3.45	1.62	1.54
24	C	506	BCR	C26-C25	3.45	1.40	1.34
25	a	5567	LHG	O7-C7	3.45	1.44	1.34
32	f	5051	HEM	CAD-C3D	-3.44	1.46	1.52
32	F	51	HEM	CAD-C3D	-3.44	1.46	1.52
20	c	5494	CLA	C4B-NB	3.44	1.38	1.35
24	c	5505	BCR	C2-C1	3.44	1.62	1.54
20	C	503	CLA	C4B-NB	3.44	1.38	1.35
24	B	527	BCR	C29-C30	3.44	1.62	1.54
26	A	5212	SQD	O3-C3	3.44	1.51	1.43
26	A	5212	SQD	C1-C2	3.43	1.62	1.52
30	c	5509	DGD	O5D-C1E	3.43	1.46	1.40
24	B	528	BCR	C26-C25	3.43	1.40	1.34
20	b	5522	CLA	CAA-C2A	3.42	1.60	1.54
24	b	5529	BCR	C2-C1	3.42	1.62	1.54
28	b	5530	MGE	O6D-C1D	3.42	1.50	1.41
20	C	498	CLA	CHC-C1C	3.42	1.43	1.35
20	b	5525	CLA	C4B-NB	3.42	1.38	1.35
26	L	5213	SQD	O3-C3	3.42	1.51	1.43
20	b	5526	CLA	C4-C3	3.42	1.59	1.50
24	b	5527	BCR	C29-C30	3.42	1.62	1.54
24	T	5104	BCR	C1-C6	3.41	1.58	1.53
20	c	5502	CLA	C1B-NB	3.40	1.38	1.35
20	b	5515	CLA	C4B-NB	3.39	1.38	1.35
20	c	5496	CLA	CAA-C2A	3.39	1.60	1.54
20	a	5563	CLA	C1B-CHB	-3.39	1.31	1.41
20	c	5498	CLA	CHC-C1C	3.39	1.43	1.35
20	c	5499	CLA	CAA-C2A	3.39	1.60	1.54
24	B	529	BCR	C2-C1	3.39	1.61	1.54
20	B	520	CLA	C4B-NB	3.38	1.38	1.35
27	t	5217	LMT	O1'-C1'	3.38	1.46	1.40
20	b	5526	CLA	C5-C3	3.38	1.58	1.51
20	b	5518	CLA	C1B-NB	3.38	1.38	1.35
26	a	212	SQD	O3-C3	3.38	1.50	1.43
20	a	5559	CLA	MG-NA	3.38	2.14	2.06
28	B	530	MGE	O6D-C1D	3.37	1.50	1.41
24	d	5357	BCR	C2-C1	3.37	1.61	1.54
20	c	5491	CLA	C4B-NB	3.37	1.38	1.35
20	b	5520	CLA	MG-NA	3.36	2.14	2.06
24	c	5505	BCR	C5-C6	3.36	1.40	1.34
20	d	5354	CLA	C1B-CHB	-3.36	1.31	1.41
26	t	213	SQD	O3-C3	3.35	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5517	CLA	CAA-C2A	3.35	1.60	1.54
20	C	501	CLA	C1B-NB	3.35	1.38	1.35
24	c	5505	BCR	C29-C30	3.32	1.61	1.54
20	b	5514	CLA	CHC-C1C	3.32	1.43	1.35
24	b	5529	BCR	C1-C6	3.31	1.58	1.53
20	b	5522	CLA	CHC-C1C	3.31	1.43	1.35
20	c	5502	CLA	CHC-C1C	3.31	1.43	1.35
20	a	5558	CLA	MG-NA	3.31	2.14	2.06
20	C	493	CLA	C4B-NB	3.30	1.38	1.35
24	B	527	BCR	C5-C6	3.30	1.40	1.34
26	L	5213	SQD	O47-C7	3.29	1.43	1.34
32	F	51	HEM	CMA-C3A	3.29	1.58	1.51
20	d	5355	CLA	CHC-C1C	3.28	1.43	1.35
28	i	5201	MGE	O6D-C5D	3.28	1.52	1.44
20	A	559	CLA	C4B-NB	3.27	1.38	1.35
20	c	5502	CLA	MG-NC	3.27	2.14	2.06
20	B	526	CLA	C5-C3	3.27	1.58	1.51
20	B	512	CLA	C1B-CHB	-3.27	1.31	1.41
20	B	519	CLA	MG-NC	3.26	2.14	2.06
20	b	5515	CLA	MG-NA	3.26	2.14	2.06
20	C	491	CLA	C4B-NB	3.26	1.38	1.35
20	C	495	CLA	CHC-C1C	3.25	1.43	1.35
20	A	558	CLA	CHC-C1C	3.25	1.43	1.35
26	a	212	SQD	O6-C1	3.25	1.45	1.40
20	a	5558	CLA	C1B-CHB	-3.25	1.32	1.41
30	c	5507	DGD	O6D-C1D	3.25	1.50	1.41
20	D	354	CLA	CHC-C1C	3.24	1.43	1.35
20	D	355	CLA	C4B-NB	3.24	1.38	1.35
20	b	5518	CLA	CHC-C1C	3.24	1.43	1.35
30	C	508	DGD	O6D-C1D	3.24	1.50	1.41
20	C	502	CLA	CHC-C1C	3.23	1.43	1.35
20	C	491	CLA	CAA-C2A	3.23	1.60	1.54
24	X	130	BCR	C2-C1	3.22	1.61	1.54
20	B	516	CLA	C4B-NB	3.22	1.38	1.35
24	c	5506	BCR	C29-C30	3.22	1.61	1.54
24	t	104	BCR	C2-C1	3.22	1.61	1.54
30	C	508	DGD	O5D-C1E	3.22	1.45	1.40
28	D	360	MGE	O3G-C1D	3.21	1.45	1.40
20	b	5523	CLA	MG-NA	3.21	2.13	2.06
20	c	5495	CLA	CHC-C1C	3.20	1.43	1.35
20	b	5512	CLA	MG-NC	3.20	2.13	2.06
20	c	5495	CLA	CAA-C2A	3.20	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	520	CLA	MG-NA	3.20	2.13	2.06
20	c	5494	CLA	CHC-C1C	3.20	1.43	1.35
20	B	512	CLA	MG-NC	3.20	2.13	2.06
20	A	563	CLA	CHC-C1C	3.19	1.43	1.35
28	b	5530	MGE	O3G-C1D	3.19	1.45	1.40
20	b	5525	CLA	CHC-C1C	3.18	1.43	1.35
20	b	5516	CLA	CAA-C2A	3.18	1.60	1.54
20	c	5501	CLA	CHC-C1C	3.18	1.43	1.35
20	A	560	CLA	C1B-CHB	-3.18	1.32	1.41
20	B	518	CLA	CHC-C1C	3.18	1.43	1.35
28	d	5359	MGE	O3G-C1D	3.18	1.45	1.40
20	c	5493	CLA	CHC-C1C	3.17	1.43	1.35
20	b	5511	CLA	MG-NC	3.17	2.13	2.06
20	B	515	CLA	C4B-NB	3.17	1.38	1.35
20	b	5517	CLA	CHC-C1C	3.17	1.43	1.35
20	B	519	CLA	C1B-NB	3.17	1.38	1.35
20	a	5558	CLA	C4B-NB	3.16	1.38	1.35
28	D	359	MGE	O6D-C1D	3.16	1.49	1.41
20	b	5515	CLA	CAA-C2A	3.16	1.60	1.54
20	c	5501	CLA	MG-NC	3.15	2.13	2.06
26	A	568	SQD	O6-C44	-3.15	1.38	1.43
20	b	5514	CLA	CAA-C2A	3.15	1.60	1.54
20	c	5494	CLA	MG-NC	3.15	2.13	2.06
21	A	562	PHO	CHB-C1B	-3.15	1.32	1.38
26	A	568	SQD	O5-C5	3.14	1.52	1.44
28	d	5361	MGE	O3G-C1D	3.14	1.45	1.40
27	m	216	LMT	C3B-C2B	3.14	1.60	1.52
24	B	528	BCR	C2-C1	3.13	1.61	1.54
24	B	529	BCR	C29-C30	3.13	1.61	1.54
20	B	521	CLA	CHC-C1C	3.13	1.43	1.35
20	C	498	CLA	C1B-CHB	-3.13	1.32	1.41
20	C	501	CLA	CHC-C1C	3.12	1.43	1.35
24	H	107	BCR	C14-C13	3.12	1.39	1.35
20	A	558	CLA	C1B-CHB	-3.12	1.32	1.41
20	b	5521	CLA	C1B-CHB	-3.12	1.32	1.41
28	l	5210	MGE	O6D-C1D	3.12	1.49	1.41
24	d	5357	BCR	C38-C26	3.12	1.56	1.50
20	b	5524	CLA	CHC-C1C	3.11	1.42	1.35
20	C	500	CLA	CAA-C2A	3.11	1.59	1.54
26	t	213	SQD	C20-C19	-3.11	1.34	1.51
24	a	5566	BCR	C5-C6	3.11	1.39	1.34
32	F	51	HEM	C1A-NA	3.11	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	524	CLA	CHC-C1C	3.10	1.42	1.35
20	C	502	CLA	MG-NC	3.10	2.13	2.06
20	b	5516	CLA	C4B-NB	3.10	1.38	1.35
26	d	5358	SQD	O3-C3	3.10	1.50	1.43
20	a	5563	CLA	CAA-C2A	3.09	1.59	1.54
20	B	513	CLA	C1B-CHB	-3.08	1.32	1.41
20	b	5520	CLA	C1B-NB	3.08	1.38	1.35
24	c	5505	BCR	C38-C26	3.08	1.56	1.50
24	a	5566	BCR	C2-C1	3.07	1.61	1.54
20	D	355	CLA	CHC-C1C	3.07	1.42	1.35
20	B	517	CLA	CAA-C2A	3.06	1.59	1.54
20	b	5515	CLA	C1B-CHB	-3.06	1.32	1.41
30	C	507	DGD	O6D-C1D	3.06	1.49	1.41
24	C	504	BCR	C2-C1	3.06	1.61	1.54
20	b	5512	CLA	C1B-CHB	-3.05	1.32	1.41
24	b	5527	BCR	C2-C1	3.05	1.61	1.54
28	d	5359	MGE	O6D-C1D	3.05	1.49	1.41
20	c	5496	CLA	MG-NC	3.05	2.13	2.06
20	B	520	CLA	CAA-C2A	3.05	1.59	1.54
20	b	5525	CLA	MG-NC	3.05	2.13	2.06
24	A	566	BCR	C30-C25	3.04	1.57	1.53
20	b	5513	CLA	CAA-C2A	3.04	1.59	1.54
24	c	5504	BCR	C26-C25	3.04	1.39	1.34
26	L	5213	SQD	C12-C11	-3.04	1.34	1.51
20	C	498	CLA	C4B-NB	3.03	1.37	1.35
20	B	520	CLA	C1B-CHB	-3.03	1.32	1.41
20	d	5354	CLA	CAA-CBA	-3.03	1.43	1.52
20	d	5354	CLA	CHC-C1C	3.03	1.42	1.35
32	f	5051	HEM	C3C-CAC	3.02	1.54	1.47
20	C	502	CLA	C1B-NB	3.02	1.37	1.35
20	B	517	CLA	CHC-C1C	3.02	1.42	1.35
20	C	497	CLA	CHC-C1C	3.02	1.42	1.35
20	a	5560	CLA	CAA-C2A	3.02	1.59	1.54
26	L	5213	SQD	C6-S	3.02	1.88	1.77
20	b	5519	CLA	CAA-C2A	3.02	1.59	1.54
26	L	5213	SQD	O5-C1	3.01	1.49	1.41
20	D	354	CLA	CAA-CBA	-3.01	1.43	1.52
26	L	5213	SQD	C17-C16	-3.01	1.34	1.51
26	L	5213	SQD	C11-C10	-3.01	1.34	1.51
20	B	526	CLA	CAA-C2A	3.01	1.59	1.54
20	C	502	CLA	CAA-C2A	3.01	1.59	1.54
21	a	5562	PHO	CHB-C1B	-3.00	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	51	HEM	C1C-C2C	3.00	1.49	1.42
20	B	524	CLA	C4B-NB	3.00	1.37	1.35
30	C	508	DGD	O1G-C1A	3.00	1.42	1.33
20	b	5511	CLA	C4C-C3C	3.00	1.50	1.45
20	B	521	CLA	CAA-C2A	2.99	1.59	1.54
20	B	526	CLA	C1B-CHB	-2.99	1.32	1.41
20	c	5497	CLA	CHC-C1C	2.99	1.42	1.35
20	a	5558	CLA	MG-NC	2.99	2.13	2.06
20	c	5503	CLA	C4B-NB	2.99	1.37	1.35
20	b	5511	CLA	C1C-C2C	2.98	1.50	1.44
20	c	5496	CLA	C1B-CHB	-2.98	1.32	1.41
24	b	5528	BCR	C2-C1	2.98	1.61	1.54
21	a	5561	PHO	C4-C3	2.98	1.58	1.50
26	L	5213	SQD	C20-C19	-2.98	1.34	1.51
20	b	5523	CLA	CAA-C2A	2.98	1.59	1.54
20	B	525	CLA	CHC-C1C	2.98	1.42	1.35
20	B	515	CLA	C1B-CHB	-2.97	1.32	1.41
27	a	5568	LMT	O5'-C1'	2.97	1.49	1.41
20	c	5500	CLA	MG-NC	2.97	2.13	2.06
20	C	503	CLA	CHC-C1C	2.97	1.42	1.35
20	C	495	CLA	C1C-C2C	2.96	1.50	1.44
24	X	130	BCR	C26-C25	2.96	1.39	1.34
24	C	505	BCR	C5-C6	2.95	1.39	1.34
24	t	104	BCR	C29-C30	2.95	1.60	1.54
28	D	358	MGE	C4D-C3D	2.94	1.59	1.52
32	V	552	HEM	C1C-C2C	2.94	1.49	1.42
24	C	506	BCR	C29-C30	2.94	1.60	1.54
28	d	5360	MGE	O6D-C1D	2.94	1.49	1.41
20	c	5496	CLA	C4C-C3C	2.94	1.50	1.45
20	B	526	CLA	C4-C3	2.94	1.58	1.50
28	d	5360	MGE	C4D-C3D	2.94	1.59	1.52
20	C	503	CLA	C1B-NB	2.93	1.37	1.35
26	t	213	SQD	C19-C18	-2.93	1.35	1.51
20	c	5494	CLA	C1B-CHB	-2.93	1.32	1.41
26	A	5212	SQD	O6-C1	2.92	1.45	1.40
28	D	358	MGE	O6D-C5D	2.92	1.51	1.44
20	C	494	CLA	C1B-CHB	-2.92	1.32	1.41
20	c	5491	CLA	CAA-C2A	2.92	1.59	1.54
27	A	569	LMT	C1'-C2'	2.92	1.60	1.52
27	A	569	LMT	O5'-C1'	2.92	1.49	1.41
20	C	503	CLA	MG-NC	2.91	2.13	2.06
20	D	354	CLA	MG-NC	2.91	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	5355	CLA	C4B-NB	2.91	1.37	1.35
20	c	5500	CLA	CAA-C2A	2.91	1.59	1.54
20	C	494	CLA	CHC-C1C	2.91	1.42	1.35
26	L	5213	SQD	O6-C1	2.91	1.45	1.40
28	i	5201	MGE	C4D-C5D	2.91	1.59	1.53
26	t	213	SQD	C14-C13	-2.90	1.35	1.51
20	B	516	CLA	CHC-C1C	2.90	1.42	1.35
20	C	500	CLA	C1B-CHB	-2.90	1.32	1.41
20	c	5493	CLA	CAA-C2A	2.90	1.59	1.54
20	a	5559	CLA	C1B-CHB	-2.89	1.32	1.41
20	C	493	CLA	CHC-C1C	2.89	1.42	1.35
20	a	5560	CLA	C1B-CHB	-2.89	1.33	1.41
20	B	525	CLA	C1B-CHB	-2.89	1.33	1.41
26	L	5213	SQD	C19-C18	-2.89	1.35	1.51
24	B	529	BCR	C14-C13	2.89	1.39	1.35
30	c	5507	DGD	C3E-C2E	2.89	1.59	1.52
26	d	5358	SQD	O6-C44	-2.89	1.38	1.43
20	b	5521	CLA	CAA-C2A	2.88	1.59	1.54
20	b	5526	CLA	C4B-NB	2.88	1.37	1.35
20	a	5563	CLA	CHC-C1C	2.88	1.42	1.35
20	b	5518	CLA	CAA-C2A	2.88	1.59	1.54
30	H	208	DGD	O5D-C1E	2.87	1.45	1.40
30	C	508	DGD	C4E-C3E	2.87	1.59	1.52
20	a	5560	CLA	MG-NC	2.87	2.13	2.06
20	C	496	CLA	CHC-C1C	2.87	1.42	1.35
24	x	5130	BCR	C26-C25	2.87	1.39	1.34
20	b	5524	CLA	MG-NC	2.87	2.13	2.06
30	c	5508	DGD	C4D-C3D	2.86	1.59	1.52
20	B	519	CLA	CHC-C1C	2.86	1.42	1.35
20	B	512	CLA	C4B-NB	2.86	1.37	1.35
20	c	5497	CLA	C1B-CHB	-2.86	1.33	1.41
30	C	508	DGD	O3G-C1D	2.86	1.45	1.40
22	a	5564	PQ9	C11-C2	2.86	1.54	1.51
20	b	5526	CLA	CHC-C1C	2.86	1.42	1.35
20	b	5514	CLA	C4B-NB	2.86	1.37	1.35
20	b	5521	CLA	MG-NC	2.85	2.13	2.06
21	a	5562	PHO	C3B-C4B	2.85	1.49	1.43
20	B	517	CLA	C1B-CHB	-2.84	1.33	1.41
20	b	5526	CLA	C1-C2	2.84	1.57	1.49
20	b	5519	CLA	CHC-C1C	2.84	1.42	1.35
30	h	5208	DGD	O6D-C5D	2.84	1.51	1.44
24	b	5529	BCR	C14-C13	2.84	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	568	SQD	C17-C16	-2.84	1.35	1.51
20	b	5516	CLA	C1B-CHB	-2.84	1.33	1.41
27	t	5217	LMT	O1B-C1B	2.84	1.49	1.41
26	t	213	SQD	C15-C14	-2.83	1.35	1.51
26	L	5213	SQD	C18-C17	-2.83	1.35	1.51
20	b	5521	CLA	MG-NA	2.83	2.13	2.06
24	t	104	BCR	C26-C25	2.83	1.39	1.34
20	c	5496	CLA	CHC-C1C	2.83	1.42	1.35
20	c	5500	CLA	CHC-C1C	2.83	1.42	1.35
20	C	500	CLA	CHC-C1C	2.83	1.42	1.35
24	D	357	BCR	C19-C18	-2.82	1.39	1.45
20	b	5522	CLA	C1B-CHB	-2.82	1.33	1.41
24	b	5527	BCR	C5-C6	2.82	1.39	1.34
20	b	5526	CLA	C1B-CHB	-2.82	1.33	1.41
20	d	5355	CLA	CAA-C2A	2.82	1.59	1.54
20	B	514	CLA	CHC-C1C	2.81	1.42	1.35
30	C	509	DGD	O6D-C1D	2.81	1.49	1.41
26	L	5213	SQD	C13-C12	-2.81	1.35	1.51
24	H	107	BCR	C5-C6	2.81	1.39	1.34
20	C	492	CLA	C1B-NB	2.81	1.37	1.35
28	b	5530	MGE	O6D-C5D	2.81	1.51	1.44
21	A	561	PHO	CAA-CBA	-2.81	1.44	1.52
20	B	521	CLA	C1B-CHB	-2.80	1.33	1.41
20	B	518	CLA	C4B-NB	2.80	1.37	1.35
30	c	5507	DGD	O3G-C1D	2.80	1.45	1.40
28	i	5201	MGE	O2G-C1B	2.80	1.42	1.34
20	B	518	CLA	C1B-NB	2.79	1.37	1.35
21	A	562	PHO	C3B-C4B	2.79	1.49	1.43
20	b	5526	CLA	C1B-NB	2.79	1.37	1.35
20	b	5516	CLA	CHC-C1C	2.79	1.42	1.35
30	C	507	DGD	O3G-C1D	2.78	1.44	1.40
28	d	5359	MGE	C4D-C3D	2.78	1.59	1.52
20	A	563	CLA	MG-NC	2.78	2.12	2.06
20	c	5497	CLA	CAA-C2A	2.78	1.59	1.54
26	t	213	SQD	C12-C11	-2.78	1.36	1.51
26	t	213	SQD	C11-C10	-2.78	1.36	1.51
20	c	5493	CLA	C1B-CHB	-2.77	1.33	1.41
20	B	515	CLA	CHC-C1C	2.77	1.42	1.35
20	C	492	CLA	C1B-CHB	-2.77	1.33	1.41
20	B	523	CLA	CHC-C1C	2.77	1.42	1.35
20	A	560	CLA	MG-NC	2.77	2.12	2.06
20	b	5523	CLA	CHC-C1C	2.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	5208	DGD	O6E-C1E	2.77	1.48	1.41
20	A	559	CLA	MG-NA	2.77	2.12	2.06
20	A	558	CLA	MG-NC	2.77	2.12	2.06
20	B	521	CLA	C4B-NB	2.77	1.37	1.35
20	B	517	CLA	C4B-NB	2.76	1.37	1.35
20	b	5520	CLA	CHC-C1C	2.76	1.42	1.35
20	c	5503	CLA	C1C-C2C	2.76	1.49	1.44
24	B	527	BCR	C2-C1	2.76	1.60	1.54
28	d	5360	MGE	O1G-C1A	2.76	1.41	1.33
26	A	568	SQD	C12-C11	-2.75	1.36	1.51
20	b	5517	CLA	C1B-CHB	-2.75	1.33	1.41
26	t	213	SQD	C17-C16	-2.75	1.36	1.51
20	B	513	CLA	C5-C3	2.75	1.57	1.51
20	B	512	CLA	CHC-C1C	2.75	1.42	1.35
24	b	5527	BCR	C26-C25	2.75	1.39	1.34
26	A	568	SQD	O8-S	2.75	1.57	1.47
20	B	514	CLA	C4B-NB	2.75	1.37	1.35
20	C	496	CLA	MG-NC	2.75	2.12	2.06
20	B	514	CLA	CAA-C2A	2.75	1.59	1.54
20	b	5515	CLA	CHC-C1C	2.75	1.42	1.35
20	B	521	CLA	MG-NC	2.74	2.12	2.06
20	B	525	CLA	MG-NC	2.74	2.12	2.06
30	C	508	DGD	C1E-C2E	2.74	1.60	1.52
20	B	522	CLA	MG-NC	2.74	2.12	2.06
20	b	5525	CLA	CAA-C2A	2.74	1.59	1.54
20	C	501	CLA	C1C-C2C	2.74	1.49	1.44
20	b	5525	CLA	C1B-CHB	-2.74	1.33	1.41
20	d	5355	CLA	MG-NC	2.73	2.12	2.06
20	C	495	CLA	CAA-C2A	2.73	1.59	1.54
20	B	511	CLA	C4C-C3C	2.73	1.49	1.45
27	t	5217	LMT	O5B-C1B	2.73	1.48	1.41
20	B	513	CLA	MG-NC	2.73	2.12	2.06
20	A	560	CLA	CHC-C1C	2.73	1.42	1.35
20	d	5355	CLA	C1B-CHB	-2.72	1.33	1.41
21	A	562	PHO	CHC-C1C	2.72	1.44	1.38
20	D	354	CLA	C4B-NB	2.72	1.37	1.35
20	b	5513	CLA	C1B-CHB	-2.72	1.33	1.41
24	A	566	BCR	C29-C30	2.72	1.60	1.54
26	d	5358	SQD	O8-S	2.71	1.57	1.47
30	c	5508	DGD	O1G-C1A	2.71	1.41	1.33
24	t	104	BCR	C23-C22	-2.71	1.40	1.45
26	L	5213	SQD	C15-C14	-2.71	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	m	216	LMT	O1'-C1'	2.71	1.44	1.40
24	b	5529	BCR	C26-C25	2.70	1.39	1.34
20	b	5524	CLA	C1B-CHB	-2.70	1.33	1.41
20	C	493	CLA	CAA-C2A	2.70	1.59	1.54
20	c	5499	CLA	CHC-C1C	2.70	1.41	1.35
30	C	507	DGD	C3E-C2E	2.70	1.59	1.52
20	C	491	CLA	C1B-CHB	-2.70	1.33	1.41
20	C	496	CLA	C4C-C3C	2.70	1.49	1.45
30	H	208	DGD	O6D-C1D	2.70	1.48	1.41
28	I	201	MGE	O2G-C1B	2.70	1.41	1.34
20	C	491	CLA	CHC-C1C	2.69	1.41	1.35
20	b	5511	CLA	CHC-C1C	2.69	1.41	1.35
30	C	508	DGD	C3D-C2D	2.69	1.59	1.52
26	t	213	SQD	C13-C12	-2.69	1.36	1.51
24	b	5528	BCR	C5-C6	2.69	1.39	1.34
24	C	504	BCR	C5-C6	2.69	1.39	1.34
24	C	505	BCR	C38-C26	2.69	1.55	1.50
20	d	5354	CLA	MG-NA	2.68	2.12	2.06
26	L	5213	SQD	C16-C15	-2.68	1.36	1.51
20	c	5491	CLA	C1B-NB	2.68	1.37	1.35
26	A	568	SQD	C16-C15	-2.68	1.36	1.51
20	c	5502	CLA	CAA-C2A	2.68	1.59	1.54
28	d	5360	MGE	O6D-C5D	2.68	1.50	1.44
28	D	359	MGE	C4D-C3D	2.68	1.59	1.52
20	C	500	CLA	MG-NC	2.67	2.12	2.06
20	c	5491	CLA	CHC-C1C	2.67	1.41	1.35
26	A	5212	SQD	O5-C1	2.67	1.48	1.41
20	B	524	CLA	C1B-CHB	-2.67	1.33	1.41
24	b	5529	BCR	C5-C6	2.67	1.39	1.34
32	F	51	HEM	C3C-CAC	2.67	1.53	1.47
20	A	558	CLA	CAA-CBA	-2.66	1.44	1.52
26	d	5358	SQD	C17-C16	-2.66	1.36	1.51
30	h	5208	DGD	O5D-C1E	2.66	1.44	1.40
24	x	5130	BCR	C14-C13	2.66	1.39	1.35
26	L	5213	SQD	C14-C13	-2.66	1.36	1.51
20	a	5558	CLA	CAA-C2A	2.66	1.59	1.54
20	C	501	CLA	MG-NC	2.66	2.12	2.06
20	c	5495	CLA	C1B-NB	2.66	1.37	1.35
20	C	496	CLA	CAA-C2A	2.66	1.59	1.54
26	A	568	SQD	C15-C14	-2.66	1.36	1.51
20	A	559	CLA	C1B-CHB	-2.65	1.33	1.41
30	H	208	DGD	C1E-C2E	2.65	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	509	DGD	O6D-C5D	2.65	1.50	1.44
30	C	508	DGD	C4D-C3D	2.65	1.59	1.52
30	H	208	DGD	O6D-C5D	2.65	1.50	1.44
30	c	5507	DGD	C1E-C2E	2.65	1.60	1.52
20	c	5496	CLA	C1C-C2C	2.63	1.49	1.44
26	A	568	SQD	C11-C10	-2.63	1.36	1.51
30	c	5509	DGD	O6D-C5D	2.63	1.50	1.44
26	a	212	SQD	O5-C1	2.63	1.48	1.41
20	C	501	CLA	CAA-C2A	2.63	1.59	1.54
20	b	5517	CLA	MG-NC	2.63	2.12	2.06
20	a	5563	CLA	C5-C3	2.63	1.56	1.51
24	B	529	BCR	C5-C6	2.63	1.39	1.34
20	c	5492	CLA	C4-C3	2.63	1.57	1.50
27	T	217	LMT	O5B-C1B	2.63	1.48	1.41
28	I	201	MGE	O6D-C5D	2.63	1.50	1.44
20	B	511	CLA	CHC-C1C	2.63	1.41	1.35
20	b	5512	CLA	CHC-C1C	2.63	1.41	1.35
20	a	5559	CLA	C4B-NB	2.62	1.37	1.35
20	B	514	CLA	MG-NC	2.62	2.12	2.06
24	B	529	BCR	C10-C9	2.62	1.39	1.35
20	a	5558	CLA	CAA-CBA	-2.62	1.44	1.52
24	T	5104	BCR	C29-C30	2.62	1.60	1.54
26	t	213	SQD	C16-C15	-2.62	1.36	1.51
20	b	5520	CLA	C1B-CHB	-2.62	1.33	1.41
20	c	5492	CLA	C1B-NB	2.62	1.37	1.35
20	c	5503	CLA	CHC-C1C	2.61	1.41	1.35
20	B	525	CLA	CAA-C2A	2.61	1.58	1.54
28	i	5201	MGE	O6D-C1D	2.61	1.48	1.41
20	c	5494	CLA	MG-NA	2.61	2.12	2.06
20	c	5492	CLA	C1B-CHB	-2.61	1.33	1.41
26	t	213	SQD	O5-C1	2.60	1.48	1.41
20	B	520	CLA	C4C-C3C	2.60	1.49	1.45
30	c	5508	DGD	C1E-C2E	2.60	1.60	1.52
20	c	5498	CLA	C1B-CHB	-2.60	1.33	1.41
28	d	5359	MGE	O6D-C5D	2.60	1.50	1.44
26	t	213	SQD	C18-C17	-2.60	1.37	1.51
27	A	569	LMT	O5B-C5B	2.60	1.50	1.44
20	B	516	CLA	C1B-CHB	-2.59	1.33	1.41
20	B	516	CLA	MG-NC	2.59	2.12	2.06
24	b	5529	BCR	C10-C9	2.59	1.39	1.35
20	B	523	CLA	C1B-CHB	-2.58	1.33	1.41
20	A	559	CLA	CAA-C2A	2.58	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	562	PHO	C4-C3	2.58	1.57	1.50
20	b	5516	CLA	OBD-CAD	2.58	1.25	1.22
20	C	493	CLA	C1B-CHB	-2.58	1.33	1.41
30	C	507	DGD	O6D-C5D	2.57	1.50	1.44
26	a	212	SQD	C8-C7	2.57	1.58	1.49
28	B	530	MGE	O2G-C1B	2.56	1.41	1.34
20	b	5512	CLA	C4B-NB	2.56	1.37	1.35
20	a	5560	CLA	CHC-C1C	2.56	1.41	1.35
28	B	530	MGE	C1D-C2D	2.56	1.59	1.52
26	d	5358	SQD	O5-C1	2.56	1.48	1.41
24	c	5506	BCR	C19-C18	-2.55	1.40	1.45
32	f	5051	HEM	CMA-C3A	2.55	1.56	1.51
24	b	5527	BCR	C19-C18	-2.55	1.40	1.45
20	b	5520	CLA	CAA-C2A	2.54	1.58	1.54
20	c	5498	CLA	CAA-C2A	2.54	1.58	1.54
20	B	526	CLA	C1B-NB	2.53	1.37	1.35
28	D	360	MGE	O6D-C1D	2.53	1.48	1.41
28	B	530	MGE	O6D-C5D	2.53	1.50	1.44
20	B	511	CLA	C1C-C2C	2.52	1.49	1.44
27	T	217	LMT	O1B-C1B	2.52	1.48	1.41
30	H	208	DGD	O6E-C1E	2.52	1.48	1.41
24	T	5104	BCR	C29-C28	-2.52	1.46	1.52
21	A	561	PHO	CHD-C1D	2.52	1.43	1.38
20	c	5500	CLA	C4-C3	2.52	1.57	1.50
20	C	492	CLA	CHC-C1C	2.52	1.41	1.35
20	B	520	CLA	CHC-C1C	2.52	1.41	1.35
20	b	5524	CLA	C4B-NB	2.52	1.37	1.35
20	c	5501	CLA	C1C-C2C	2.52	1.49	1.44
20	B	526	CLA	MG-NC	2.52	2.12	2.06
26	d	5358	SQD	C32-C31	-2.51	1.37	1.51
27	t	5217	LMT	C1B-C2B	2.51	1.59	1.52
20	c	5500	CLA	C1B-CHB	-2.51	1.34	1.41
20	C	498	CLA	C1B-NB	2.51	1.37	1.35
26	A	568	SQD	C13-C12	-2.50	1.37	1.51
20	d	5354	CLA	MG-NC	2.50	2.12	2.06
20	b	5513	CLA	MG-NC	2.50	2.12	2.06
20	B	522	CLA	C1B-CHB	-2.50	1.34	1.41
20	b	5521	CLA	CHC-C1C	2.50	1.41	1.35
27	A	569	LMT	C1B-C2B	2.50	1.59	1.52
20	A	563	CLA	C4B-NB	2.49	1.37	1.35
26	d	5358	SQD	C20-C19	-2.49	1.37	1.51
27	A	569	LMT	O5B-C1B	2.49	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	568	SQD	C14-C13	-2.49	1.37	1.51
21	a	5562	PHO	CHC-C1C	2.49	1.43	1.38
27	a	5568	LMT	C1'-C2'	2.49	1.59	1.52
24	a	5566	BCR	C29-C30	2.48	1.59	1.54
20	C	499	CLA	OBD-CAD	2.48	1.25	1.22
24	t	104	BCR	C29-C28	-2.48	1.46	1.52
20	c	5492	CLA	CHC-C1C	2.48	1.41	1.35
24	T	5104	BCR	C23-C22	-2.48	1.40	1.45
20	B	511	CLA	C3C-C2C	2.47	1.42	1.36
20	b	5526	CLA	MG-NC	2.47	2.12	2.06
24	A	566	BCR	C26-C25	2.47	1.38	1.34
20	b	5523	CLA	MG-NC	2.47	2.12	2.06
20	C	502	CLA	C1B-CHB	-2.47	1.34	1.41
20	B	513	CLA	CHC-C1C	2.47	1.41	1.35
20	b	5519	CLA	C1B-NB	2.47	1.37	1.35
21	a	5561	PHO	CAA-CBA	-2.46	1.45	1.52
20	c	5499	CLA	C1B-CHB	-2.46	1.34	1.41
20	b	5513	CLA	C4-C3	2.46	1.57	1.50
20	b	5511	CLA	C3C-C2C	2.46	1.41	1.36
20	C	491	CLA	MG-NC	2.46	2.12	2.06
26	L	5213	SQD	O6-C44	-2.45	1.39	1.43
20	A	563	CLA	C5-C3	2.45	1.56	1.51
20	B	514	CLA	C1B-CHB	-2.45	1.34	1.41
20	c	5496	CLA	C1B-NB	2.45	1.37	1.35
20	C	494	CLA	MG-NC	2.45	2.12	2.06
28	I	201	MGE	O6D-C1D	2.44	1.48	1.41
20	b	5515	CLA	MG-NC	2.44	2.12	2.06
26	d	5358	SQD	C11-C10	-2.44	1.37	1.51
20	C	500	CLA	C4C-C3C	2.44	1.49	1.45
20	c	5502	CLA	C1B-CHB	-2.44	1.34	1.41
27	t	5217	LMT	O1B-C4'	2.43	1.50	1.43
20	c	5495	CLA	C1C-C2C	2.43	1.49	1.44
26	A	568	SQD	O5-C1	2.43	1.48	1.41
26	d	5358	SQD	C12-C11	-2.43	1.38	1.51
26	d	5358	SQD	C33-C32	-2.42	1.38	1.51
28	I	201	MGE	O3G-C1D	2.42	1.44	1.40
20	A	559	CLA	CHC-C1C	2.42	1.41	1.35
24	X	130	BCR	C33-C5	2.42	1.54	1.50
27	M	5216	LMT	O5'-C1'	2.42	1.48	1.41
20	B	523	CLA	C4B-NB	2.42	1.37	1.35
20	B	511	CLA	C3B-C2B	2.41	1.43	1.40
26	d	5358	SQD	C15-C14	-2.41	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	5507	DGD	O6D-C5D	2.41	1.50	1.44
27	T	217	LMT	O1B-C4'	2.41	1.50	1.43
20	A	563	CLA	C4-C3	2.40	1.56	1.50
30	c	5508	DGD	O5D-C1E	2.40	1.44	1.40
20	b	5523	CLA	C1B-CHB	-2.40	1.34	1.41
20	a	5560	CLA	C1B-NB	2.40	1.37	1.35
20	B	520	CLA	C4-C3	2.40	1.56	1.50
20	B	526	CLA	C4B-NB	2.40	1.37	1.35
27	m	216	LMT	O5'-C1'	2.40	1.48	1.41
26	d	5358	SQD	C19-C18	-2.40	1.38	1.51
20	c	5495	CLA	MG-NC	2.40	2.12	2.06
28	I	201	MGE	C4D-C3D	2.39	1.58	1.52
20	C	497	CLA	C4-C3	2.39	1.56	1.50
26	d	5358	SQD	C8-C7	2.39	1.57	1.50
24	b	5527	BCR	C1-C6	2.39	1.57	1.53
20	b	5515	CLA	C4-C3	2.38	1.56	1.50
26	A	568	SQD	C33-C32	-2.38	1.38	1.51
24	h	5107	BCR	C14-C13	2.38	1.38	1.35
26	d	5358	SQD	C16-C15	-2.38	1.38	1.51
26	a	212	SQD	O6-C44	-2.38	1.39	1.43
20	C	497	CLA	C1B-CHB	-2.37	1.34	1.41
30	c	5509	DGD	C4E-C5E	2.37	1.58	1.53
28	d	5361	MGE	O6D-C5D	2.37	1.50	1.44
26	t	213	SQD	C21-C20	-2.37	1.34	1.51
20	c	5491	CLA	C1B-CHB	-2.37	1.34	1.41
27	m	216	LMT	O5B-C1B	2.37	1.47	1.41
32	V	552	HEM	C3C-CAC	2.37	1.52	1.47
30	C	507	DGD	C4D-C5D	2.37	1.58	1.53
32	v	5552	HEM	C1B-C2B	2.37	1.47	1.42
20	b	5514	CLA	C1B-CHB	-2.37	1.34	1.41
20	C	492	CLA	C4-C3	2.37	1.56	1.50
20	b	5519	CLA	C1B-CHB	-2.36	1.34	1.41
20	c	5492	CLA	C3D-C2D	2.36	1.43	1.39
20	c	5502	CLA	C4-C3	2.35	1.56	1.50
20	C	491	CLA	C4-C3	2.35	1.56	1.50
20	B	513	CLA	C4-C3	2.35	1.56	1.50
24	c	5504	BCR	C10-C9	2.35	1.38	1.35
32	f	5051	HEM	C1C-C2C	2.35	1.47	1.42
20	B	514	CLA	C4-C3	2.34	1.56	1.50
28	b	5530	MGE	C4D-C5D	2.34	1.58	1.53
20	C	499	CLA	CHC-C1C	2.34	1.41	1.35
24	B	528	BCR	C5-C6	2.34	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	568	SQD	C32-C31	-2.34	1.38	1.51
20	C	492	CLA	CAA-C2A	2.34	1.58	1.54
20	b	5519	CLA	C1C-C2C	2.34	1.49	1.44
30	C	509	DGD	O1G-C1A	2.33	1.40	1.33
20	D	355	CLA	MG-NC	2.33	2.11	2.06
30	c	5508	DGD	C4E-C3E	2.33	1.58	1.52
20	c	5496	CLA	C4-C3	2.33	1.56	1.50
20	b	5513	CLA	CHC-C1C	2.33	1.40	1.35
20	b	5513	CLA	C5-C3	2.33	1.56	1.51
20	c	5499	CLA	MG-NC	2.33	2.11	2.06
24	c	5506	BCR	C10-C9	2.33	1.38	1.35
20	c	5499	CLA	C4C-C3C	2.32	1.49	1.45
28	i	5201	MGE	C2A-C1A	2.32	1.57	1.50
30	c	5507	DGD	O6E-C5E	2.32	1.50	1.44
20	c	5503	CLA	C4-C3	2.32	1.56	1.50
24	T	5104	BCR	C30-C25	2.32	1.56	1.53
20	b	5520	CLA	C4C-C3C	2.31	1.49	1.45
26	A	5212	SQD	O6-C44	-2.31	1.39	1.43
26	A	568	SQD	C8-C7	2.31	1.57	1.50
24	B	527	BCR	C1-C6	2.31	1.56	1.53
32	v	5552	HEM	C2A-C3A	2.31	1.44	1.37
32	V	552	HEM	CMA-C3A	2.31	1.56	1.51
28	D	360	MGE	O6D-C5D	2.31	1.50	1.44
20	a	5559	CLA	CHC-C1C	2.31	1.40	1.35
20	c	5492	CLA	C1C-NC	-2.31	1.34	1.37
26	a	212	SQD	O48-C23	2.31	1.44	1.33
20	d	5355	CLA	C1C-C2C	2.30	1.49	1.44
20	b	5518	CLA	C1B-CHB	-2.30	1.34	1.41
20	b	5512	CLA	CAA-CBA	-2.30	1.45	1.52
20	B	526	CLA	CHC-C1C	2.30	1.40	1.35
20	B	525	CLA	C1B-NB	2.30	1.37	1.35
26	d	5358	SQD	C14-C13	-2.30	1.38	1.51
26	d	5358	SQD	C24-C23	2.30	1.57	1.50
32	V	552	HEM	C3B-CAB	2.29	1.52	1.47
26	A	568	SQD	C19-C18	-2.29	1.38	1.51
20	B	515	CLA	CAA-C2A	2.29	1.58	1.54
26	d	5358	SQD	C36-C35	-2.29	1.38	1.51
28	l	5210	MGE	C4D-C3D	2.29	1.58	1.52
20	B	523	CLA	CAA-C2A	2.29	1.58	1.54
30	h	5208	DGD	C1D-C2D	2.29	1.59	1.52
21	a	5561	PHO	CHD-C1D	2.28	1.43	1.38
20	c	5503	CLA	C1-C2	2.28	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	5561	PHO	CHB-C1B	-2.28	1.34	1.38
27	M	5216	LMT	C1B-C2B	2.27	1.59	1.52
20	c	5497	CLA	MG-NA	2.27	2.11	2.06
26	A	568	SQD	C18-C17	-2.27	1.38	1.51
20	b	5523	CLA	C5-C3	2.27	1.56	1.51
21	a	5562	PHO	C4-C3	2.27	1.56	1.50
28	b	5530	MGE	C4D-C3D	2.27	1.58	1.52
24	B	527	BCR	C19-C18	-2.27	1.41	1.45
28	d	5360	MGE	O3G-C1D	2.27	1.44	1.40
30	C	507	DGD	O6E-C5E	2.27	1.49	1.44
30	h	5208	DGD	C3E-C2E	2.26	1.58	1.52
28	b	5530	MGE	O2G-C1B	2.26	1.40	1.34
27	M	5216	LMT	C3B-C2B	2.26	1.58	1.52
28	i	5201	MGE	O3G-C1D	2.26	1.44	1.40
20	c	5497	CLA	C4-C3	2.26	1.56	1.50
20	c	5492	CLA	CAA-C2A	2.26	1.58	1.54
27	a	5568	LMT	O5B-C1B	2.26	1.47	1.41
26	A	568	SQD	C35-C34	-2.26	1.38	1.51
24	a	5566	BCR	C14-C13	2.25	1.38	1.35
20	B	520	CLA	MG-NC	2.25	2.11	2.06
26	L	5213	SQD	C21-C20	-2.25	1.35	1.51
20	C	499	CLA	C1B-CHB	-2.25	1.34	1.41
20	C	492	CLA	C5-C3	2.25	1.56	1.51
24	h	5107	BCR	C5-C6	2.25	1.38	1.34
21	A	561	PHO	C4-C3	2.24	1.56	1.50
27	M	5216	LMT	C1'-C2'	2.24	1.59	1.52
20	B	524	CLA	CAA-C2A	2.24	1.58	1.54
28	L	210	MGE	C4D-C3D	2.24	1.58	1.52
26	A	568	SQD	C34-C33	-2.24	1.39	1.51
24	B	527	BCR	C38-C26	2.24	1.54	1.50
20	C	493	CLA	C3D-CAD	-2.24	1.40	1.46
20	c	5498	CLA	C1C-C2C	2.24	1.48	1.44
20	c	5491	CLA	C4-C3	2.24	1.56	1.50
20	d	5354	CLA	C1B-NB	2.24	1.37	1.35
20	C	493	CLA	MG-NC	2.24	2.11	2.06
20	D	355	CLA	C1C-C2C	2.24	1.48	1.44
20	A	563	CLA	CAA-C2A	2.24	1.58	1.54
28	B	530	MGE	C4D-C5D	2.23	1.57	1.53
22	A	564	PQ9	C11-C2	2.23	1.53	1.51
30	h	5208	DGD	O6D-C1D	2.23	1.47	1.41
26	d	5358	SQD	C13-C12	-2.23	1.39	1.51
30	C	509	DGD	O2G-C1B	2.23	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	526	CLA	C1-C2	2.23	1.55	1.49
32	v	5552	HEM	CMA-C3A	2.22	1.56	1.51
26	t	213	SQD	O6-C1	2.22	1.44	1.40
20	C	496	CLA	C1C-C2C	2.22	1.48	1.44
20	c	5503	CLA	MG-NC	2.22	2.11	2.06
28	b	5530	MGE	C1D-C2D	2.22	1.58	1.52
24	a	5566	BCR	C26-C25	2.22	1.38	1.34
20	c	5495	CLA	C1B-CHB	-2.22	1.34	1.41
20	B	515	CLA	MG-NC	2.22	2.11	2.06
20	c	5498	CLA	C4-C3	2.22	1.56	1.50
28	b	5530	MGE	O1G-C1G	-2.22	1.40	1.45
26	A	568	SQD	C20-C19	-2.22	1.39	1.51
20	b	5511	CLA	OBD-CAD	2.21	1.25	1.22
20	C	496	CLA	C1B-CHB	-2.21	1.34	1.41
20	b	5513	CLA	C4B-NB	2.21	1.37	1.35
26	d	5358	SQD	C35-C34	-2.21	1.39	1.51
27	a	5568	LMT	C1B-C2B	2.21	1.58	1.52
24	C	506	BCR	C35-C13	2.21	1.55	1.50
20	b	5520	CLA	C1C-C2C	2.21	1.48	1.44
20	C	495	CLA	C4C-C3C	2.20	1.48	1.45
24	t	104	BCR	C35-C13	2.20	1.55	1.50
24	C	504	BCR	C14-C13	2.20	1.38	1.35
24	D	357	BCR	C38-C26	2.20	1.54	1.50
20	d	5354	CLA	C3A-C4A	-2.20	1.44	1.51
20	D	355	CLA	C1B-CHB	-2.20	1.34	1.41
30	c	5508	DGD	O6D-C5D	2.20	1.49	1.44
28	D	359	MGE	O1G-C1A	2.20	1.39	1.33
20	B	511	CLA	CMD-C2D	2.20	1.56	1.51
30	h	5208	DGD	C4E-C3E	2.19	1.57	1.52
26	A	568	SQD	O6-C1	2.19	1.43	1.40
30	c	5507	DGD	C4D-C5D	2.19	1.57	1.53
20	C	499	CLA	MG-NC	2.19	2.11	2.06
20	c	5499	CLA	C1C-C2C	2.19	1.48	1.44
30	H	208	DGD	C1D-C2D	2.19	1.58	1.52
26	A	568	SQD	C36-C35	-2.19	1.39	1.51
20	B	511	CLA	C1B-CHB	-2.19	1.34	1.41
24	C	506	BCR	C14-C13	2.18	1.38	1.35
28	d	5361	MGE	O2G-C1B	2.18	1.40	1.34
20	B	526	CLA	C2-C3	2.18	1.38	1.33
27	m	216	LMT	O5'-C5'	2.18	1.49	1.44
20	b	5514	CLA	MG-NC	2.18	2.11	2.06
22	D	356	PQ9	C3-C4	2.18	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	496	CLA	OBD-CAD	2.18	1.25	1.22
26	d	5358	SQD	C34-C33	-2.17	1.39	1.51
24	X	130	BCR	C14-C13	2.17	1.38	1.35
20	C	503	CLA	C4-C3	2.17	1.56	1.50
28	d	5359	MGE	C4D-C5D	2.17	1.57	1.53
20	b	5515	CLA	C3A-C2A	-2.17	1.48	1.54
27	m	216	LMT	C4B-C3B	2.17	1.57	1.52
28	D	359	MGE	O6D-C5D	2.17	1.49	1.44
20	D	354	CLA	C1C-C2C	2.17	1.48	1.44
20	B	511	CLA	CMC-C2C	2.16	1.55	1.50
20	A	558	CLA	CAA-C2A	2.16	1.58	1.54
26	a	212	SQD	C6-S	2.16	1.85	1.77
20	D	355	CLA	C4-C3	2.16	1.56	1.50
24	c	5505	BCR	C19-C18	-2.16	1.41	1.45
20	B	513	CLA	C4B-NB	2.16	1.37	1.35
20	c	5495	CLA	C4-C3	2.16	1.56	1.50
27	a	5568	LMT	O5B-C5B	2.16	1.49	1.44
20	c	5492	CLA	MG-NC	2.16	2.11	2.06
20	b	5526	CLA	CAA-CBA	-2.16	1.46	1.52
20	c	5491	CLA	MG-NC	2.15	2.11	2.06
28	D	358	MGE	O2G-C1B	2.15	1.40	1.34
20	a	5558	CLA	CBA-CGA	-2.15	1.44	1.50
20	C	492	CLA	OBD-CAD	2.15	1.25	1.22
20	a	5559	CLA	CAA-C2A	2.15	1.58	1.54
20	b	5517	CLA	C1-C2	2.15	1.55	1.49
26	d	5358	SQD	C18-C17	-2.14	1.39	1.51
20	c	5493	CLA	CMB-C2B	2.14	1.56	1.51
20	C	499	CLA	CAA-C2A	2.14	1.58	1.54
20	C	497	CLA	CAA-C2A	2.14	1.58	1.54
20	a	5560	CLA	C4-C3	2.14	1.56	1.50
21	A	561	PHO	CHB-C1B	-2.13	1.34	1.38
20	C	502	CLA	C4-C3	2.13	1.56	1.50
30	C	509	DGD	C3D-C2D	2.13	1.57	1.52
20	B	519	CLA	C1B-CHB	-2.13	1.35	1.41
20	B	521	CLA	CBA-CGA	-2.13	1.44	1.50
20	C	503	CLA	C1B-CHB	-2.13	1.35	1.41
20	A	559	CLA	MG-NC	2.12	2.11	2.06
27	M	5216	LMT	C4B-C5B	2.12	1.57	1.53
27	M	5216	LMT	O5B-C1B	2.12	1.47	1.41
20	b	5515	CLA	CAA-CBA	-2.12	1.46	1.52
26	L	5213	SQD	C8-C7	2.12	1.56	1.50
28	i	5201	MGE	C3D-C2D	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	208	DGD	C4E-C3E	2.12	1.57	1.52
20	B	518	CLA	C4-C3	2.12	1.56	1.50
30	H	208	DGD	O6E-C5E	2.12	1.49	1.44
24	D	357	BCR	C14-C13	2.11	1.38	1.35
24	A	566	BCR	C19-C18	-2.11	1.41	1.45
24	T	5104	BCR	C37-C22	2.11	1.55	1.50
26	A	5212	SQD	C44-C45	2.11	1.57	1.50
20	C	495	CLA	MG-NC	2.11	2.11	2.06
26	a	212	SQD	C44-C45	2.11	1.57	1.50
20	C	498	CLA	CAA-C2A	2.11	1.58	1.54
20	B	518	CLA	OBD-CAD	2.10	1.25	1.22
30	C	508	DGD	O6D-C5D	2.10	1.49	1.44
24	d	5357	BCR	C19-C18	-2.10	1.41	1.45
28	D	360	MGE	O2G-C1B	2.10	1.40	1.34
27	m	216	LMT	C1'-C2'	2.10	1.58	1.52
20	C	499	CLA	C1B-NB	2.10	1.37	1.35
20	B	515	CLA	C4-C3	2.10	1.56	1.50
28	l	5210	MGE	O6D-C5D	2.10	1.49	1.44
28	d	5360	MGE	O2G-C1B	2.10	1.40	1.34
20	B	526	CLA	CAA-CBA	-2.10	1.46	1.52
24	C	505	BCR	C19-C18	-2.10	1.41	1.45
20	b	5511	CLA	CMD-C2D	2.10	1.56	1.51
21	a	5561	PHO	CBA-CGA	-2.09	1.44	1.50
20	B	521	CLA	C1C-C2C	2.09	1.48	1.44
24	C	506	BCR	C19-C18	-2.09	1.41	1.45
21	A	562	PHO	C1D-C2D	-2.09	1.41	1.45
21	A	562	PHO	CHD-C1D	2.09	1.42	1.38
24	b	5527	BCR	C23-C22	-2.09	1.41	1.45
20	C	502	CLA	CMB-C2B	2.09	1.56	1.51
20	d	5354	CLA	CBA-CGA	-2.09	1.44	1.50
26	A	5212	SQD	C8-C7	2.09	1.56	1.49
20	B	516	CLA	C3D-C2D	2.09	1.43	1.39
20	b	5512	CLA	C4C-C3C	2.08	1.48	1.45
24	b	5528	BCR	C26-C25	2.08	1.38	1.34
20	a	5558	CLA	C1C-C2C	2.08	1.48	1.44
20	C	502	CLA	C4C-C3C	2.08	1.48	1.45
20	C	502	CLA	C1C-C2C	2.08	1.48	1.44
20	c	5501	CLA	C1B-CHB	-2.08	1.35	1.41
21	a	5562	PHO	C1D-C2D	-2.08	1.41	1.45
20	B	521	CLA	C4-C3	2.08	1.56	1.50
21	a	5562	PHO	CMD-C2D	2.07	1.55	1.50
30	h	5208	DGD	C4E-C5E	2.07	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	495	CLA	C4B-NB	2.07	1.37	1.35
20	A	560	CLA	C4C-C3C	2.07	1.48	1.45
20	C	501	CLA	C1B-CHB	-2.06	1.35	1.41
24	X	130	BCR	C24-C23	2.06	1.39	1.33
27	M	5216	LMT	O5B-C5B	2.06	1.49	1.44
24	x	5130	BCR	C24-C23	2.06	1.39	1.33
20	B	515	CLA	C3A-C2A	-2.06	1.48	1.54
24	x	5130	BCR	C35-C13	2.06	1.55	1.50
20	b	5516	CLA	C1B-NB	2.06	1.37	1.35
24	X	130	BCR	C10-C9	2.06	1.38	1.35
20	b	5522	CLA	C4-C3	2.05	1.56	1.50
30	c	5509	DGD	O1G-C1A	2.05	1.39	1.33
20	C	496	CLA	C1B-NB	2.05	1.37	1.35
20	B	520	CLA	C3D-CAD	-2.05	1.40	1.46
24	A	566	BCR	C29-C28	-2.05	1.47	1.52
27	T	217	LMT	C1B-C2B	2.05	1.58	1.52
20	b	5524	CLA	C1B-NB	2.05	1.37	1.35
20	B	515	CLA	C1B-NB	2.05	1.37	1.35
20	a	5563	CLA	C4-C3	2.05	1.55	1.50
20	C	499	CLA	C4C-C3C	2.04	1.48	1.45
26	t	213	SQD	C6-S	2.04	1.84	1.77
26	A	568	SQD	C24-C23	2.04	1.56	1.50
20	b	5519	CLA	C5-C3	2.04	1.55	1.51
20	C	500	CLA	C3D-CAD	-2.04	1.40	1.46
24	x	5130	BCR	C33-C5	2.03	1.54	1.50
24	c	5506	BCR	C14-C13	2.03	1.38	1.35
24	h	5107	BCR	C38-C26	2.03	1.54	1.50
32	V	552	HEM	C2A-C3A	2.03	1.43	1.37
30	c	5509	DGD	O6E-C5E	2.03	1.49	1.44
26	t	213	SQD	O6-C44	-2.03	1.40	1.43
24	a	5566	BCR	C29-C28	-2.03	1.47	1.52
27	T	217	LMT	C3B-C2B	2.02	1.57	1.52
20	c	5499	CLA	C1B-NB	2.02	1.37	1.35
24	t	104	BCR	C19-C18	-2.02	1.41	1.45
20	C	495	CLA	C4-C3	2.02	1.55	1.50
20	C	492	CLA	MG-NC	2.02	2.11	2.06
20	D	354	CLA	C3B-C2B	-2.02	1.37	1.40
32	f	5051	HEM	C2A-C3A	2.02	1.43	1.37
20	d	5355	CLA	C1-C2	2.02	1.55	1.49
20	b	5523	CLA	CAA-CBA	-2.02	1.46	1.52
20	a	5563	CLA	MG-NC	2.02	2.11	2.06
30	c	5508	DGD	C3D-C2D	2.01	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	5509	DGD	C3D-C2D	2.01	1.57	1.52
20	b	5515	CLA	C5-C3	2.01	1.55	1.51
30	c	5509	DGD	C4E-C3E	2.01	1.57	1.52
20	c	5497	CLA	C4C-C3C	2.01	1.48	1.45
20	B	523	CLA	C5-C3	2.01	1.55	1.51
20	c	5499	CLA	C3D-C2D	2.01	1.43	1.39
28	i	5201	MGE	C4D-C3D	2.00	1.57	1.52
24	C	505	BCR	C23-C22	-2.00	1.41	1.45
32	F	51	HEM	C2A-C3A	2.00	1.43	1.37
20	B	517	CLA	CMB-C2B	2.00	1.55	1.51

All (1635) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5501	CLA	C4A-NA-C1A	13.09	112.59	106.71
20	b	5514	CLA	C4A-NA-C1A	13.03	112.56	106.71
20	C	501	CLA	C4A-NA-C1A	12.97	112.54	106.71
20	B	514	CLA	C4A-NA-C1A	12.87	112.49	106.71
20	B	524	CLA	C4A-NA-C1A	12.65	112.39	106.71
20	c	5491	CLA	C4A-NA-C1A	12.55	112.35	106.71
20	c	5503	CLA	C4A-NA-C1A	12.46	112.31	106.71
20	b	5516	CLA	C4A-NA-C1A	12.33	112.25	106.71
20	C	497	CLA	C4A-NA-C1A	12.33	112.25	106.71
20	C	503	CLA	C4A-NA-C1A	12.28	112.23	106.71
20	B	518	CLA	C4A-NA-C1A	12.26	112.22	106.71
20	B	521	CLA	C4A-NA-C1A	12.25	112.21	106.71
20	b	5525	CLA	C4A-NA-C1A	12.22	112.20	106.71
20	c	5502	CLA	C4A-NA-C1A	12.21	112.20	106.71
20	B	517	CLA	C4A-NA-C1A	12.20	112.19	106.71
20	c	5492	CLA	C4A-NA-C1A	12.20	112.19	106.71
20	B	523	CLA	C4A-NA-C1A	12.15	112.17	106.71
20	c	5498	CLA	C4A-NA-C1A	12.12	112.15	106.71
20	b	5523	CLA	C4A-NA-C1A	12.10	112.15	106.71
20	c	5495	CLA	C4A-NA-C1A	12.08	112.14	106.71
20	B	516	CLA	C4A-NA-C1A	12.07	112.13	106.71
20	C	494	CLA	C4A-NA-C1A	12.02	112.11	106.71
20	d	5355	CLA	C4A-NA-C1A	11.99	112.10	106.71
20	b	5518	CLA	C4A-NA-C1A	11.92	112.07	106.71
20	D	355	CLA	C4A-NA-C1A	11.83	112.03	106.71
20	C	502	CLA	C4A-NA-C1A	11.82	112.02	106.71
20	C	493	CLA	C4A-NA-C1A	11.76	112.00	106.71
20	b	5511	CLA	C4A-NA-C1A	11.71	111.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	492	CLA	C4A-NA-C1A	11.69	111.96	106.71
20	C	498	CLA	C4A-NA-C1A	11.67	111.95	106.71
20	C	496	CLA	C4A-NA-C1A	11.65	111.94	106.71
20	b	5524	CLA	C4A-NA-C1A	11.64	111.94	106.71
20	B	525	CLA	C4A-NA-C1A	11.64	111.94	106.71
20	C	499	CLA	C4A-NA-C1A	11.60	111.92	106.71
20	b	5521	CLA	C4A-NA-C1A	11.54	111.89	106.71
20	b	5517	CLA	C4A-NA-C1A	11.52	111.89	106.71
20	c	5493	CLA	C4A-NA-C1A	11.48	111.87	106.71
20	C	495	CLA	C4A-NA-C1A	11.48	111.87	106.71
20	B	526	CLA	C4A-NA-C1A	11.38	111.82	106.71
20	c	5499	CLA	C4A-NA-C1A	11.31	111.79	106.71
20	c	5496	CLA	C4A-NA-C1A	11.27	111.77	106.71
20	B	519	CLA	C4A-NA-C1A	11.23	111.75	106.71
20	b	5522	CLA	C4A-NA-C1A	11.21	111.75	106.71
20	b	5519	CLA	C4A-NA-C1A	11.16	111.72	106.71
20	a	5560	CLA	C4A-NA-C1A	11.13	111.71	106.71
20	c	5497	CLA	C4A-NA-C1A	11.07	111.68	106.71
20	B	511	CLA	C4A-NA-C1A	11.02	111.66	106.71
20	C	500	CLA	C4A-NA-C1A	10.98	111.64	106.71
20	b	5526	CLA	C4A-NA-C1A	10.97	111.64	106.71
20	c	5500	CLA	C4A-NA-C1A	10.91	111.61	106.71
20	B	522	CLA	C4A-NA-C1A	10.83	111.57	106.71
20	A	560	CLA	C4A-NA-C1A	10.71	111.52	106.71
20	c	5494	CLA	C4A-NA-C1A	10.70	111.52	106.71
20	B	520	CLA	C4A-NA-C1A	10.67	111.50	106.71
20	a	5559	CLA	C4A-NA-C1A	10.56	111.45	106.71
20	C	491	CLA	C4A-NA-C1A	10.50	111.43	106.71
20	b	5520	CLA	C4A-NA-C1A	10.45	111.41	106.71
20	A	559	CLA	C4A-NA-C1A	10.44	111.40	106.71
20	A	563	CLA	C4A-NA-C1A	10.35	111.36	106.71
20	B	513	CLA	C4A-NA-C1A	10.30	111.34	106.71
20	B	515	CLA	C4A-NA-C1A	10.25	111.31	106.71
20	d	5354	CLA	C4A-NA-C1A	10.22	111.30	106.71
20	B	512	CLA	C4A-NA-C1A	10.00	111.20	106.71
20	b	5515	CLA	C4A-NA-C1A	9.85	111.13	106.71
20	a	5563	CLA	C4A-NA-C1A	9.76	111.09	106.71
20	b	5513	CLA	C4A-NA-C1A	9.69	111.06	106.71
20	A	558	CLA	C4A-NA-C1A	9.62	111.03	106.71
20	b	5512	CLA	C4A-NA-C1A	9.50	110.98	106.71
20	D	354	CLA	C4A-NA-C1A	9.28	110.88	106.71
20	a	5558	CLA	C4A-NA-C1A	9.14	110.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	5212	SQD	O5-C1-O6	8.78	130.76	109.97
26	a	212	SQD	O5-C1-O6	8.40	129.88	109.97
26	A	568	SQD	O5-C1-O6	8.38	129.81	109.97
26	d	5358	SQD	O5-C1-O6	8.10	129.16	109.97
26	L	5213	SQD	O5-C1-O6	8.07	129.09	109.97
26	t	213	SQD	O5-C1-O6	7.73	128.28	109.97
30	c	5507	DGD	O6E-C5E-C4E	7.66	123.60	109.69
26	t	213	SQD	O6-C1-C2	7.64	120.22	108.30
30	H	208	DGD	O6E-C5E-C4E	7.49	123.29	109.69
30	c	5508	DGD	O6E-C5E-C4E	7.42	123.17	109.69
26	L	5213	SQD	O6-C1-C2	7.27	119.65	108.30
30	C	507	DGD	O6E-C5E-C4E	7.26	122.88	109.69
30	C	508	DGD	O6E-C5E-C4E	7.26	122.87	109.69
26	d	5358	SQD	O6-C1-C2	7.19	119.53	108.30
30	C	509	DGD	O6E-C5E-C4E	7.16	122.70	109.69
30	c	5509	DGD	O6E-C5E-C4E	7.14	122.66	109.69
30	h	5208	DGD	O6E-C5E-C4E	7.13	122.65	109.69
26	A	568	SQD	O6-C1-C2	7.03	119.27	108.30
26	a	212	SQD	O6-C1-C2	6.66	118.71	108.30
24	D	357	BCR	C38-C26-C25	6.48	131.80	124.53
24	X	130	BCR	C33-C5-C6	6.47	131.79	124.53
24	T	5104	BCR	C38-C26-C25	6.45	131.77	124.53
26	A	5212	SQD	O6-C1-C2	6.44	118.36	108.30
24	d	5357	BCR	C33-C5-C6	6.28	131.58	124.53
24	c	5505	BCR	C38-C26-C25	6.26	131.55	124.53
24	d	5357	BCR	C38-C26-C25	6.24	131.54	124.53
24	B	529	BCR	C38-C26-C25	6.22	131.51	124.53
32	F	51	HEM	CBD-CAD-C3D	-6.20	101.06	112.48
24	x	5130	BCR	C33-C5-C6	6.19	131.48	124.53
25	A	567	LHG	C25-C24-C23	6.18	136.10	113.62
26	d	5358	SQD	C25-C24-C23	6.18	136.09	113.62
26	A	568	SQD	C10-C9-C8	6.14	135.25	113.19
24	t	104	BCR	C38-C26-C25	6.11	131.39	124.53
26	t	213	SQD	C10-C9-C8	6.09	135.07	113.19
25	a	5567	LHG	C25-C24-C23	6.08	135.74	113.62
26	d	5358	SQD	C10-C9-C8	6.07	135.02	113.19
26	L	5213	SQD	C10-C9-C8	6.06	134.96	113.19
26	A	568	SQD	O7-S-C6	5.97	114.04	106.94
24	D	357	BCR	C33-C5-C6	5.96	131.22	124.53
32	f	5051	HEM	CBD-CAD-C3D	-5.90	101.61	112.48
26	t	213	SQD	C25-C24-C23	5.90	135.06	113.62
24	B	527	BCR	C38-C26-C25	5.85	131.09	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	5213	SQD	C25-C24-C23	5.81	134.76	113.62
26	A	568	SQD	C25-C24-C23	5.81	134.74	113.62
24	B	528	BCR	C38-C26-C25	5.76	131.00	124.53
24	C	505	BCR	C38-C26-C25	5.76	131.00	124.53
24	C	506	BCR	C38-C26-C25	5.68	130.90	124.53
26	a	212	SQD	O7-S-C6	5.66	113.66	106.94
24	h	5107	BCR	C38-C26-C25	5.65	130.87	124.53
32	v	5552	HEM	CBD-CAD-C3D	-5.63	102.11	112.48
24	c	5506	BCR	C38-C26-C25	5.56	130.77	124.53
24	B	527	BCR	C33-C5-C6	5.56	130.77	124.53
24	X	130	BCR	C7-C8-C9	5.56	134.63	126.23
24	A	566	BCR	C33-C5-C6	5.53	130.73	124.53
24	C	504	BCR	C38-C26-C25	5.52	130.73	124.53
24	b	5527	BCR	C33-C5-C6	5.50	130.71	124.53
24	b	5528	BCR	C38-C26-C25	5.49	130.70	124.53
24	t	104	BCR	C33-C5-C6	5.49	130.70	124.53
24	T	5104	BCR	C33-C5-C6	5.49	130.69	124.53
22	d	5356	PQ9	C11-C2-C1	5.47	121.32	116.88
24	a	5566	BCR	C38-C26-C25	5.44	130.63	124.53
24	b	5529	BCR	C38-C26-C25	5.43	130.63	124.53
24	A	566	BCR	C38-C26-C25	5.43	130.62	124.53
24	x	5130	BCR	C7-C8-C9	5.41	134.40	126.23
24	B	529	BCR	C33-C5-C6	5.40	130.59	124.53
24	a	5566	BCR	C33-C5-C6	5.38	130.57	124.53
24	H	107	BCR	C38-C26-C25	5.37	130.56	124.53
32	f	5051	HEM	CAD-C3D-C2D	5.37	142.66	127.25
24	c	5504	BCR	C38-C26-C25	5.32	130.51	124.53
24	b	5527	BCR	C38-C26-C25	5.30	130.49	124.53
24	C	506	BCR	C33-C5-C6	5.30	130.48	124.53
24	X	130	BCR	C11-C10-C9	5.28	134.85	127.31
24	C	505	BCR	C33-C5-C6	5.24	130.41	124.53
32	F	51	HEM	CAD-C3D-C2D	5.22	142.26	127.25
24	x	5130	BCR	C38-C26-C25	5.20	130.36	124.53
32	V	552	HEM	CBD-CAD-C3D	-5.19	102.91	112.48
20	B	515	CLA	CAA-C2A-C3A	-5.19	98.56	112.78
24	c	5506	BCR	C33-C5-C6	5.18	130.35	124.53
26	A	568	SQD	O8-S-C6	-5.18	97.49	105.74
32	V	552	HEM	CAD-C3D-C2D	5.18	142.12	127.25
24	X	130	BCR	C38-C26-C25	5.13	130.29	124.53
32	v	5552	HEM	CAD-C3D-C2D	5.09	141.87	127.25
22	D	356	PQ9	C11-C2-C1	5.05	120.98	116.88
24	H	107	BCR	C33-C5-C6	4.99	130.13	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5505	BCR	C33-C5-C6	4.92	130.06	124.53
26	t	213	SQD	O7-S-C6	4.91	112.78	106.94
24	b	5529	BCR	C33-C5-C6	4.90	130.03	124.53
26	a	212	SQD	O8-S-C6	-4.87	97.98	105.74
24	h	5107	BCR	C33-C5-C6	4.86	129.99	124.53
20	b	5515	CLA	CAA-C2A-C3A	-4.86	99.47	112.78
24	x	5130	BCR	C11-C10-C9	4.82	134.19	127.31
26	d	5358	SQD	O8-S-C6	-4.82	98.07	105.74
26	d	5358	SQD	O7-S-C6	4.81	112.66	106.94
26	A	5212	SQD	O7-S-C6	4.81	112.66	106.94
24	C	504	BCR	C33-C5-C6	4.80	129.92	124.53
26	a	212	SQD	C44-O6-C1	4.78	123.07	113.74
24	b	5528	BCR	C33-C5-C6	4.77	129.88	124.53
30	c	5508	DGD	C3G-O3G-C1D	-4.71	104.53	113.74
20	C	494	CLA	CED-O2D-CGD	4.56	126.25	115.94
24	c	5504	BCR	C33-C5-C6	4.55	129.64	124.53
24	B	528	BCR	C33-C5-C6	4.52	129.60	124.53
21	A	561	PHO	C4A-NA-C1A	4.49	111.77	108.14
24	T	5104	BCR	C29-C30-C25	4.49	117.39	110.48
20	b	5523	CLA	C1D-CHD-C4C	4.47	128.46	122.56
21	a	5561	PHO	C4A-NA-C1A	4.44	111.73	108.14
21	A	562	PHO	C4A-NA-C1A	4.40	111.69	108.14
24	X	130	BCR	C8-C9-C10	-4.38	112.22	118.94
28	L	210	MGE	C3G-O3G-C1D	-4.38	105.18	113.74
21	a	5562	PHO	C4A-NA-C1A	4.38	111.68	108.14
28	l	5210	MGE	C3G-O3G-C1D	-4.37	105.20	113.74
26	t	213	SQD	O8-S-C6	-4.34	98.83	105.74
24	x	5130	BCR	C8-C9-C10	-4.32	112.31	118.94
26	A	5212	SQD	C44-O6-C1	4.32	122.17	113.74
28	D	360	MGE	O6D-C5D-C6D	4.28	117.08	106.44
21	A	562	PHO	CBD-CHA-C4D	-4.27	103.73	108.54
30	C	508	DGD	C3G-O3G-C1D	-4.26	105.42	113.74
21	A	561	PHO	C1-C2-C3	4.23	133.36	126.04
24	T	5104	BCR	C33-C5-C4	-4.22	105.51	113.62
24	T	5104	BCR	C38-C26-C27	-4.21	105.53	113.62
24	b	5529	BCR	C29-C30-C25	4.19	116.94	110.48
24	x	5130	BCR	C33-C5-C4	-4.18	105.58	113.62
24	B	529	BCR	C38-C26-C27	-4.18	105.58	113.62
24	c	5505	BCR	C23-C24-C25	4.17	138.93	127.20
24	D	357	BCR	C38-C26-C27	-4.16	105.62	113.62
24	d	5357	BCR	C38-C26-C27	-4.16	105.63	113.62
20	c	5494	CLA	CED-O2D-CGD	4.15	125.33	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	5562	PHO	CBD-CHA-C4D	-4.12	103.90	108.54
20	b	5526	CLA	CED-O2D-CGD	4.12	125.26	115.94
24	D	357	BCR	C33-C5-C4	-4.11	105.72	113.62
24	X	130	BCR	C33-C5-C4	-4.10	105.73	113.62
24	C	505	BCR	C23-C24-C25	4.10	138.71	127.20
24	t	104	BCR	C29-C30-C25	4.10	116.79	110.48
26	A	5212	SQD	O8-S-C6	-4.09	99.22	105.74
24	t	104	BCR	C33-C5-C4	-4.06	105.81	113.62
24	C	506	BCR	C8-C7-C6	4.06	138.60	127.20
20	A	563	CLA	OBD-CAD-CBD	-4.06	120.10	125.89
30	C	509	DGD	O6D-C5D-C6D	4.05	114.84	106.67
24	d	5357	BCR	C33-C5-C4	-4.04	105.85	113.62
20	B	517	CLA	OBD-CAD-CBD	-4.04	120.12	125.89
28	D	360	MGE	O2G-C1B-C2B	4.02	120.16	111.50
24	C	504	BCR	C38-C26-C27	-4.01	105.91	113.62
20	C	497	CLA	C7-C6-C5	-4.01	102.48	113.36
27	a	5568	LMT	C1-O1'-C1'	-4.00	107.21	113.84
24	C	505	BCR	C33-C5-C4	-3.99	105.95	113.62
30	h	5208	DGD	O3G-C1D-C2D	3.99	114.53	108.30
24	C	506	BCR	C38-C26-C27	-3.97	105.99	113.62
32	F	51	HEM	CAA-CBA-CGA	3.97	119.33	112.67
27	A	569	LMT	C1-O1'-C1'	-3.96	107.27	113.84
20	B	523	CLA	C1D-CHD-C4C	3.95	127.77	122.56
20	c	5502	CLA	CAA-C2A-C3A	-3.95	101.96	112.78
24	H	107	BCR	C38-C26-C27	-3.95	106.03	113.62
24	d	5357	BCR	C29-C30-C25	3.95	116.56	110.48
30	c	5509	DGD	O6D-C5D-C6D	3.94	114.62	106.67
20	C	495	CLA	CAA-C2A-C3A	-3.92	102.03	112.78
24	B	528	BCR	C38-C26-C27	-3.92	106.08	113.62
24	x	5130	BCR	C29-C30-C25	3.91	116.50	110.48
20	c	5495	CLA	CAA-C2A-C3A	-3.90	102.09	112.78
20	B	511	CLA	CAA-C2A-C3A	-3.90	107.00	116.10
26	d	5358	SQD	C31-C30-C29	3.90	134.21	114.42
28	d	5361	MGE	O2G-C1B-C2B	3.90	119.90	111.50
20	b	5511	CLA	CAA-C2A-C3A	-3.89	107.01	116.10
28	d	5361	MGE	O6D-C5D-C6D	3.89	116.12	106.44
24	x	5130	BCR	C23-C24-C25	3.89	138.13	127.20
24	C	504	BCR	C33-C5-C4	-3.88	106.16	113.62
24	X	130	BCR	C23-C24-C25	3.88	138.10	127.20
20	B	517	CLA	C1D-CHD-C4C	3.87	127.67	122.56
32	f	5051	HEM	CAA-CBA-CGA	3.87	119.16	112.67
20	b	5517	CLA	OBD-CAD-CBD	-3.87	120.37	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	BCR	C24-C23-C22	3.86	132.07	126.23
21	a	5561	PHO	CBD-CHA-C4D	-3.86	104.19	108.54
20	C	494	CLA	CAA-C2A-C3A	-3.86	102.21	112.78
24	h	5107	BCR	C29-C30-C25	3.85	116.41	110.48
20	D	354	CLA	C1-C2-C3	3.85	132.70	126.04
24	X	130	BCR	C2-C1-C6	3.84	116.40	110.48
20	b	5519	CLA	CED-O2D-CGD	3.84	124.63	115.94
26	L	5213	SQD	O48-C23-C24	3.83	123.94	111.91
24	C	506	BCR	C33-C5-C4	-3.83	106.25	113.62
24	c	5506	BCR	C8-C7-C6	3.83	137.95	127.20
24	c	5506	BCR	C38-C26-C27	-3.82	106.27	113.62
24	B	528	BCR	C30-C25-C26	-3.82	117.23	122.61
22	A	564	PQ9	C11-C12-C13	-3.82	120.43	126.79
20	c	5493	CLA	CAA-C2A-C3A	-3.82	102.32	112.78
20	c	5494	CLA	CAA-C2A-C3A	-3.81	102.33	112.78
21	A	561	PHO	CBD-CHA-C4D	-3.81	104.25	108.54
26	A	568	SQD	C31-C30-C29	3.81	133.77	114.42
24	c	5504	BCR	C38-C26-C27	-3.81	106.30	113.62
20	C	493	CLA	CAA-C2A-C3A	-3.80	102.37	112.78
24	t	104	BCR	C8-C7-C6	3.79	137.84	127.20
20	c	5500	CLA	C1D-CHD-C4C	3.79	127.56	122.56
20	c	5491	CLA	CED-O2D-CGD	3.79	124.50	115.94
24	A	566	BCR	C38-C26-C27	-3.79	106.34	113.62
26	t	213	SQD	O48-C23-C24	3.78	123.78	111.91
24	b	5527	BCR	C38-C26-C27	-3.78	106.35	113.62
30	H	208	DGD	O3G-C1D-C2D	3.78	114.21	108.30
20	c	5497	CLA	C7-C6-C5	-3.78	103.09	113.36
24	A	566	BCR	C33-C5-C4	-3.77	106.37	113.62
24	a	5566	BCR	C38-C26-C27	-3.77	106.37	113.62
24	h	5107	BCR	C38-C26-C27	-3.77	106.37	113.62
20	C	502	CLA	CAA-C2A-C3A	-3.76	102.47	112.78
24	c	5505	BCR	C38-C26-C27	-3.76	106.39	113.62
24	c	5506	BCR	C33-C5-C4	-3.76	106.39	113.62
24	X	130	BCR	C29-C30-C25	3.76	116.27	110.48
24	C	505	BCR	C2-C1-C6	3.76	116.26	110.48
20	C	496	CLA	CED-O2D-CGD	3.75	124.42	115.94
24	C	505	BCR	C29-C30-C25	3.75	116.25	110.48
24	c	5505	BCR	C29-C30-C25	3.74	116.25	110.48
24	b	5528	BCR	C29-C30-C25	3.74	116.24	110.48
26	A	568	SQD	C11-C10-C9	3.73	133.38	114.42
20	c	5492	CLA	CED-O2D-CGD	3.73	124.37	115.94
24	a	5566	BCR	C29-C30-C25	3.73	116.22	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5520	CLA	C7-C6-C5	-3.72	103.25	113.36
24	x	5130	BCR	C2-C1-C6	3.72	116.21	110.48
20	B	513	CLA	C1D-CHD-C4C	3.72	127.47	122.56
24	T	5104	BCR	C24-C23-C22	3.72	131.85	126.23
20	B	522	CLA	C1D-CHD-C4C	3.72	127.46	122.56
20	c	5503	CLA	CED-O2D-CGD	3.72	124.34	115.94
24	c	5505	BCR	C33-C5-C4	-3.71	106.48	113.62
24	B	527	BCR	C38-C26-C27	-3.71	106.49	113.62
24	X	130	BCR	C38-C26-C27	-3.71	106.49	113.62
24	c	5504	BCR	C24-C23-C22	3.70	131.83	126.23
24	b	5529	BCR	C38-C26-C27	-3.70	106.51	113.62
24	b	5529	BCR	C2-C1-C6	3.70	116.17	110.48
24	b	5527	BCR	C33-C5-C4	-3.70	106.52	113.62
28	B	530	MGE	C3G-O3G-C1D	-3.69	106.53	113.74
24	H	107	BCR	C33-C5-C4	-3.69	106.53	113.62
24	t	104	BCR	C38-C26-C27	-3.68	106.54	113.62
24	d	5357	BCR	C30-C25-C26	-3.68	117.42	122.61
24	T	5104	BCR	C30-C25-C26	-3.68	117.43	122.61
21	a	5562	PHO	C7-C6-C5	-3.68	103.37	113.36
24	B	527	BCR	C33-C5-C4	-3.68	106.55	113.62
20	b	5526	CLA	OBD-CAD-CBD	-3.67	120.65	125.89
24	b	5528	BCR	C2-C1-C6	3.66	116.12	110.48
24	d	5357	BCR	C1-C6-C5	-3.66	117.46	122.61
24	x	5130	BCR	C38-C26-C27	-3.66	106.58	113.62
26	t	213	SQD	C11-C10-C9	3.66	133.00	114.42
22	d	5356	PQ9	C24-C23-C25	3.66	121.42	115.27
26	d	5358	SQD	C11-C10-C9	3.65	132.98	114.42
24	A	566	BCR	C29-C30-C25	3.65	116.10	110.48
26	L	5213	SQD	O8-S-C6	-3.65	99.93	105.74
24	h	5107	BCR	C11-C10-C9	3.64	132.51	127.31
25	A	567	LHG	O8-C23-C24	3.64	123.35	111.91
20	C	501	CLA	C1D-CHD-C4C	3.64	127.36	122.56
24	T	5104	BCR	C8-C7-C6	3.64	137.42	127.20
24	H	107	BCR	C11-C10-C9	3.64	132.50	127.31
24	b	5529	BCR	C33-C5-C4	-3.64	106.63	113.62
20	C	502	CLA	C1D-CHD-C4C	3.63	127.36	122.56
30	h	5208	DGD	C1E-O6E-C5E	3.63	120.81	113.69
20	C	500	CLA	C1D-CHD-C4C	3.62	127.34	122.56
28	d	5360	MGE	O6D-C5D-C6D	3.61	115.42	106.44
24	D	357	BCR	C2-C1-C6	3.61	116.04	110.48
24	B	529	BCR	C33-C5-C4	-3.61	106.69	113.62
24	H	107	BCR	C29-C30-C25	3.61	116.03	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	518	CLA	O2A-CGA-CBA	3.60	123.22	111.91
30	C	508	DGD	O5D-C1E-C2E	3.60	113.92	108.30
20	D	355	CLA	C1D-CHD-C4C	3.60	127.31	122.56
20	C	492	CLA	CED-O2D-CGD	3.59	124.07	115.94
24	c	5504	BCR	C1-C6-C5	-3.59	117.55	122.61
24	a	5566	BCR	C33-C5-C4	-3.59	106.72	113.62
24	D	357	BCR	C1-C6-C5	-3.59	117.56	122.61
20	b	5514	CLA	OBD-CAD-CBD	-3.59	120.77	125.89
24	B	529	BCR	C29-C30-C25	3.59	116.00	110.48
30	c	5508	DGD	O5D-C6D-C5D	3.59	115.68	109.05
20	b	5518	CLA	O2A-CGA-CBA	3.58	123.15	111.91
20	b	5522	CLA	C1D-CHD-C4C	3.58	127.28	122.56
26	d	5358	SQD	O48-C23-C24	3.57	123.12	111.91
24	B	529	BCR	C2-C1-C6	3.57	115.98	110.48
24	H	107	BCR	C30-C25-C26	-3.57	117.58	122.61
24	c	5504	BCR	C33-C5-C4	-3.57	106.76	113.62
24	C	504	BCR	C1-C6-C5	-3.57	117.59	122.61
24	c	5506	BCR	C29-C30-C25	3.57	115.97	110.48
28	d	5359	MGE	O2G-C1B-C2B	3.57	119.19	111.50
26	L	5213	SQD	O7-S-C6	3.56	111.17	106.94
22	D	356	PQ9	C24-C23-C25	3.56	121.26	115.27
20	c	5495	CLA	C1D-CHD-C4C	3.56	127.26	122.56
20	B	525	CLA	C1D-CHD-C4C	3.56	127.26	122.56
20	b	5521	CLA	C7-C6-C5	-3.56	103.69	113.36
24	D	357	BCR	C30-C25-C26	-3.56	117.60	122.61
30	C	507	DGD	C1E-O6E-C5E	3.55	120.66	113.69
20	B	513	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
20	C	496	CLA	C1D-CHD-C4C	3.55	127.24	122.56
20	B	513	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
20	b	5516	CLA	O2A-CGA-CBA	3.55	123.03	111.91
26	A	5212	SQD	C45-O47-C7	3.54	124.50	117.90
20	C	497	CLA	C1-C2-C3	3.54	132.17	126.04
24	b	5528	BCR	C30-C25-C26	-3.54	117.63	122.61
24	x	5130	BCR	C16-C17-C18	3.54	132.36	127.31
20	B	517	CLA	C1-C2-C3	3.54	132.16	126.04
20	A	563	CLA	C1D-CHD-C4C	3.53	127.22	122.56
32	f	5051	HEM	CAD-CBD-CGD	3.53	118.60	112.67
20	A	560	CLA	C1D-CHD-C4C	3.53	127.22	122.56
30	c	5508	DGD	O2G-C1B-C2B	3.53	119.11	111.50
20	C	495	CLA	C1D-CHD-C4C	3.53	127.21	122.56
20	B	521	CLA	C7-C6-C5	-3.53	103.78	113.36
20	D	354	CLA	OBD-CAD-CBD	-3.52	120.86	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	522	CLA	OBD-CAD-CBD	-3.52	120.87	125.89
24	h	5107	BCR	C33-C5-C4	-3.52	106.86	113.62
20	C	503	CLA	OBD-CAD-CBD	-3.52	120.87	125.89
20	b	5517	CLA	C1D-CHD-C4C	3.52	127.20	122.56
20	b	5513	CLA	C1D-CHD-C4C	3.52	127.20	122.56
20	B	520	CLA	C7-C6-C5	-3.51	103.82	113.36
24	c	5506	BCR	C30-C25-C26	-3.51	117.67	122.61
20	B	526	CLA	OBD-CAD-CBD	-3.51	120.88	125.89
20	c	5496	CLA	CED-O2D-CGD	3.51	123.87	115.94
20	B	518	CLA	C1D-CHD-C4C	3.51	127.19	122.56
20	a	5560	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
20	c	5493	CLA	CED-O2D-CGD	3.50	123.85	115.94
26	L	5213	SQD	C11-C10-C9	3.50	132.18	114.42
24	b	5528	BCR	C38-C26-C27	-3.50	106.90	113.62
24	C	505	BCR	C38-C26-C27	-3.49	106.90	113.62
20	b	5521	CLA	C1D-CHD-C4C	3.49	127.17	122.56
24	b	5528	BCR	C33-C5-C4	-3.49	106.91	113.62
20	B	521	CLA	C1D-CHD-C4C	3.49	127.17	122.56
24	C	506	BCR	C2-C1-C6	3.49	115.86	110.48
20	c	5500	CLA	C7-C6-C5	-3.49	103.88	113.36
24	d	5357	BCR	C2-C1-C6	3.49	115.85	110.48
20	c	5491	CLA	C1D-CHD-C4C	3.48	127.16	122.56
24	C	506	BCR	C23-C24-C25	3.48	136.99	127.20
21	a	5561	PHO	C1-C2-C3	3.48	132.06	126.04
20	c	5501	CLA	C7-C6-C5	-3.48	103.91	113.36
24	t	104	BCR	C30-C25-C26	-3.48	117.71	122.61
20	c	5501	CLA	C1D-CHD-C4C	3.48	127.15	122.56
24	X	130	BCR	C30-C25-C26	-3.48	117.71	122.61
20	A	560	CLA	CAA-C2A-C3A	-3.48	103.26	112.78
24	x	5130	BCR	C30-C25-C26	-3.47	117.72	122.61
20	B	517	CLA	O2A-CGA-CBA	3.47	122.80	111.91
20	C	499	CLA	C1D-CHD-C4C	3.47	127.14	122.56
20	B	514	CLA	C1D-CHD-C4C	3.47	127.13	122.56
20	C	503	CLA	CED-O2D-CGD	3.47	123.78	115.94
20	B	519	CLA	CED-O2D-CGD	3.46	123.77	115.94
20	b	5518	CLA	C1D-CHD-C4C	3.46	127.13	122.56
20	c	5503	CLA	C1D-CHD-C4C	3.46	127.12	122.56
30	C	508	DGD	O5D-C6D-C5D	3.46	115.45	109.05
20	B	526	CLA	CED-O2D-CGD	3.46	123.76	115.94
24	c	5505	BCR	C2-C1-C6	3.45	115.80	110.48
20	b	5516	CLA	CED-O2D-CGD	3.45	123.75	115.94
20	a	5558	CLA	CED-O2D-CGD	3.45	123.74	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	516	CLA	C1-C2-C3	3.44	131.99	126.04
20	d	5355	CLA	C1-C2-C3	3.44	132.32	126.75
21	a	5562	PHO	CAB-C3B-C2B	-3.44	117.27	128.60
24	C	506	BCR	C29-C30-C25	3.44	115.77	110.48
30	c	5509	DGD	C1E-O6E-C5E	3.43	120.42	113.69
24	a	5566	BCR	C30-C25-C26	-3.43	117.78	122.61
20	b	5522	CLA	OBD-CAD-CBD	-3.43	121.00	125.89
20	A	558	CLA	C1-C2-C3	3.43	131.97	126.04
24	b	5527	BCR	C2-C1-C6	3.43	115.76	110.48
20	b	5519	CLA	C1D-CHD-C4C	3.43	127.08	122.56
24	h	5107	BCR	C23-C24-C25	3.43	136.82	127.20
20	B	521	CLA	OBD-CAD-CBD	-3.42	121.00	125.89
20	c	5502	CLA	C1D-CHD-C4C	3.42	127.07	122.56
20	b	5524	CLA	C1D-CHD-C4C	3.42	127.07	122.56
20	b	5514	CLA	C1D-CHD-C4C	3.41	127.06	122.56
24	h	5107	BCR	C30-C25-C26	-3.41	117.81	122.61
25	a	5567	LHG	O8-C23-C24	3.41	122.60	111.91
20	C	503	CLA	C1D-CHD-C4C	3.41	127.05	122.56
26	a	212	SQD	C45-O47-C7	3.41	124.24	117.90
20	a	5559	CLA	C1D-CHD-C4C	3.40	127.05	122.56
26	A	568	SQD	O48-C23-C24	3.40	122.58	111.91
20	a	5563	CLA	OBD-CAD-CBD	-3.40	121.04	125.89
28	b	5530	MGE	C3G-O3G-C1D	-3.40	107.10	113.74
20	B	524	CLA	C1D-CHD-C4C	3.39	127.03	122.56
30	C	507	DGD	O6D-C5D-C6D	3.39	113.50	106.67
30	C	508	DGD	O2G-C1B-C2B	3.38	118.80	111.50
20	a	5559	CLA	CED-O2D-CGD	3.38	123.59	115.94
30	c	5507	DGD	O6D-C5D-C6D	3.38	113.49	106.67
20	d	5355	CLA	C1D-CHD-C4C	3.37	127.01	122.56
20	c	5498	CLA	C1D-CHD-C4C	3.37	127.01	122.56
20	C	491	CLA	C1D-CHD-C4C	3.37	127.01	122.56
20	c	5495	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
20	b	5512	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
24	A	566	BCR	C30-C25-C26	-3.36	117.88	122.61
20	B	516	CLA	O2A-CGA-CBA	3.36	122.46	111.91
20	b	5513	CLA	CAA-C2A-C3A	-3.36	103.57	112.78
21	A	562	PHO	CAB-C3B-C2B	-3.36	117.53	128.60
24	c	5504	BCR	C2-C1-C6	3.36	115.65	110.48
20	c	5503	CLA	OBD-CAD-CBD	-3.35	121.10	125.89
30	C	509	DGD	C1E-O6E-C5E	3.35	120.27	113.69
24	D	357	BCR	C29-C30-C25	3.35	115.64	110.48
30	c	5508	DGD	O5D-C1E-C2E	3.35	113.53	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	561	PHO	CED-O2D-CGD	3.35	123.51	115.94
20	C	497	CLA	C1D-CHD-C4C	3.35	126.97	122.56
24	x	5130	BCR	C12-C13-C14	-3.35	113.81	118.94
30	H	208	DGD	O2G-C1B-C2B	3.34	118.71	111.50
28	i	5201	MGE	O2G-C1B-C2B	3.34	118.70	111.50
28	I	201	MGE	O2G-C1B-C2B	3.34	118.70	111.50
21	A	562	PHO	C7-C6-C5	-3.34	104.28	113.36
20	b	5512	CLA	CAA-C2A-C3A	-3.33	103.65	112.78
20	b	5526	CLA	C1D-CHD-C4C	3.33	126.95	122.56
24	b	5529	BCR	C30-C25-C26	-3.33	117.93	122.61
20	b	5511	CLA	CMA-C3A-C2A	-3.33	108.33	116.10
20	b	5525	CLA	C1D-CHD-C4C	3.32	126.94	122.56
20	c	5496	CLA	C1D-CHD-C4C	3.32	126.94	122.56
20	D	354	CLA	C1D-CHD-C4C	3.32	126.94	122.56
26	t	213	SQD	C44-O6-C1	3.32	120.23	113.74
24	B	529	BCR	C30-C25-C26	-3.32	117.94	122.61
20	b	5517	CLA	O2A-CGA-CBA	3.32	122.33	111.91
24	B	528	BCR	C2-C1-C6	3.32	115.59	110.48
24	H	107	BCR	C23-C24-C25	3.32	136.52	127.20
24	D	357	BCR	C23-C24-C25	3.31	136.51	127.20
20	b	5512	CLA	CED-O2D-CGD	3.31	123.43	115.94
22	a	5564	PQ9	C11-C12-C13	-3.31	121.28	126.79
20	B	520	CLA	C1D-CHD-C4C	3.31	126.93	122.56
20	b	5526	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
24	a	5566	BCR	C24-C23-C22	3.30	131.22	126.23
30	h	5208	DGD	O6D-C5D-C6D	3.30	113.33	106.67
20	C	492	CLA	OBD-CAD-CBD	-3.30	121.18	125.89
24	b	5527	BCR	C23-C24-C25	3.30	136.46	127.20
20	c	5494	CLA	C1D-CHD-C4C	3.30	126.91	122.56
20	C	502	CLA	O2A-CGA-CBA	3.29	122.24	111.91
20	B	512	CLA	OBD-CAD-CBD	-3.29	121.19	125.89
28	B	530	MGE	O2G-C1B-C2B	3.29	118.60	111.50
30	C	508	DGD	C3G-C2G-C1G	-3.29	104.00	111.79
24	B	528	BCR	C29-C30-C25	3.29	115.55	110.48
28	D	359	MGE	O6D-C5D-C6D	3.29	114.62	106.44
20	b	5522	CLA	C7-C6-C5	-3.29	104.42	113.36
22	d	5356	PQ9	C11-C2-C3	-3.29	118.97	123.30
28	D	359	MGE	O2G-C1B-C2B	3.29	118.59	111.50
20	c	5493	CLA	C1D-CHD-C4C	3.29	126.90	122.56
20	d	5354	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
28	D	358	MGE	O2G-C1B-C2B	3.28	118.58	111.50
20	B	522	CLA	O2A-CGA-CBA	3.28	122.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	498	CLA	C1D-CHD-C4C	3.27	126.87	122.56
20	d	5354	CLA	C1-C2-C3	3.27	131.69	126.04
20	c	5494	CLA	OBD-CAD-CBD	-3.27	121.23	125.89
24	h	5107	BCR	C8-C7-C6	3.27	136.37	127.20
24	C	504	BCR	C2-C1-C6	3.27	115.51	110.48
20	C	492	CLA	C1D-CHD-C4C	3.27	126.87	122.56
32	F	51	HEM	CAD-CBD-CGD	3.26	118.15	112.67
20	C	493	CLA	C1D-CHD-C4C	3.26	126.86	122.56
24	d	5357	BCR	C24-C23-C22	3.26	131.16	126.23
20	A	559	CLA	C1D-CHD-C4C	3.26	126.86	122.56
20	B	524	CLA	OBD-CAD-CBD	-3.26	121.24	125.89
20	B	513	CLA	O2A-CGA-CBA	3.26	122.13	111.91
20	C	494	CLA	C1D-CHD-C4C	3.26	126.86	122.56
24	t	104	BCR	C24-C23-C22	3.26	131.16	126.23
20	A	560	CLA	OBD-CAD-CBD	-3.26	121.24	125.89
20	B	512	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
20	B	526	CLA	C1D-CHD-C4C	3.25	126.85	122.56
20	b	5517	CLA	C1-C2-C3	3.25	131.67	126.04
20	b	5518	CLA	OBD-CAD-CBD	-3.25	121.25	125.89
28	l	5210	MGE	O6D-C5D-C6D	3.25	114.52	106.44
20	c	5496	CLA	OBD-CAD-CBD	-3.25	121.25	125.89
24	H	107	BCR	C2-C1-C6	3.25	115.48	110.48
24	C	504	BCR	C30-C25-C26	-3.25	118.04	122.61
20	B	511	CLA	CMA-C3A-C2A	-3.24	108.53	116.10
28	b	5530	MGE	O2G-C1B-C2B	3.24	118.48	111.50
20	C	501	CLA	C7-C6-C5	-3.24	104.56	113.36
30	C	507	DGD	O2G-C1B-C2B	3.24	118.48	111.50
20	c	5502	CLA	O2A-CGA-CBA	3.24	122.07	111.91
20	B	519	CLA	C1D-CHD-C4C	3.24	126.83	122.56
20	b	5520	CLA	C1D-CHD-C4C	3.24	126.83	122.56
24	b	5528	BCR	C23-C24-C25	3.24	136.29	127.20
20	c	5493	CLA	O2A-CGA-CBA	3.23	122.06	111.91
20	C	493	CLA	O2A-CGA-CBA	3.23	122.06	111.91
30	c	5508	DGD	C3G-C2G-C1G	-3.23	104.14	111.79
30	C	507	DGD	O5D-C6D-C5D	3.23	115.02	109.05
20	d	5355	CLA	OBD-CAD-CBD	-3.23	121.28	125.89
24	B	528	BCR	C23-C24-C25	3.23	136.26	127.20
20	a	5560	CLA	C1D-CHD-C4C	3.23	126.81	122.56
20	c	5502	CLA	CED-O2D-CGD	3.22	123.22	115.94
20	b	5513	CLA	O2A-CGA-CBA	3.22	122.01	111.91
24	A	566	BCR	C24-C23-C22	3.22	131.10	126.23
20	c	5497	CLA	O2A-CGA-CBA	3.22	122.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	BCR	C30-C25-C26	-3.22	118.08	122.61
24	B	529	BCR	C23-C24-C25	3.22	136.24	127.20
20	B	524	CLA	CED-O2D-CGD	3.21	123.20	115.94
20	b	5512	CLA	C1D-CHD-C4C	3.21	126.79	122.56
21	a	5562	PHO	O2A-CGA-CBA	3.21	121.98	111.91
24	c	5506	BCR	C23-C24-C25	3.21	136.21	127.20
20	b	5515	CLA	CED-O2D-CGD	3.20	123.18	115.94
24	c	5506	BCR	C2-C1-C6	3.20	115.41	110.48
24	H	107	BCR	C1-C6-C5	-3.20	118.11	122.61
20	D	355	CLA	C1-C2-C3	3.20	131.93	126.75
20	B	511	CLA	C1D-CHD-C4C	3.19	126.77	122.56
20	A	559	CLA	CAA-C2A-C3A	-3.19	104.04	112.78
20	A	563	CLA	C1-C2-C3	3.18	131.55	126.04
20	C	491	CLA	CED-O2D-CGD	3.18	123.13	115.94
24	b	5528	BCR	C1-C6-C5	-3.18	118.13	122.61
21	A	562	PHO	O2A-CGA-CBA	3.18	121.89	111.91
30	c	5507	DGD	O2G-C1B-C2B	3.18	118.35	111.50
24	h	5107	BCR	C1-C6-C5	-3.18	118.14	122.61
20	c	5492	CLA	C1D-CHD-C4C	3.18	126.75	122.56
22	D	356	PQ9	C11-C2-C3	-3.18	119.12	123.30
20	D	354	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
20	b	5513	CLA	OBD-CAD-CBD	-3.18	121.36	125.89
30	h	5208	DGD	O2G-C1B-C2B	3.18	118.34	111.50
24	B	528	BCR	C33-C5-C4	-3.17	107.52	113.62
20	d	5354	CLA	C1D-CHD-C4C	3.17	126.75	122.56
20	C	496	CLA	C1-C2-C3	3.17	131.52	126.04
20	b	5521	CLA	OBD-CAD-CBD	-3.16	121.38	125.89
20	a	5559	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
30	c	5508	DGD	C1E-O6E-C5E	3.16	119.90	113.69
26	d	5358	SQD	C45-O47-C7	3.16	125.58	117.79
20	a	5560	CLA	OBD-CAD-CBD	-3.16	121.38	125.89
24	b	5529	BCR	C23-C24-C25	3.16	136.07	127.20
24	C	504	BCR	C29-C30-C25	3.16	115.34	110.48
24	h	5107	BCR	C2-C1-C6	3.16	115.34	110.48
20	b	5515	CLA	O2A-CGA-CBA	3.16	121.81	111.91
20	B	518	CLA	CED-O2D-CGD	3.15	123.07	115.94
20	c	5497	CLA	C1-C2-C3	3.15	131.49	126.04
30	c	5507	DGD	C1E-O6E-C5E	3.15	119.87	113.69
24	H	107	BCR	C15-C14-C13	3.15	131.80	127.31
20	b	5522	CLA	O2A-CGA-CBA	3.14	121.77	111.91
20	b	5516	CLA	C1-C2-C3	3.14	131.48	126.04
30	c	5507	DGD	O5D-C6D-C5D	3.14	114.86	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	495	CLA	C7-C6-C5	-3.14	104.83	113.36
24	B	527	BCR	C30-C25-C26	-3.14	118.19	122.61
20	a	5558	CLA	C1D-CHD-C4C	3.14	126.70	122.56
20	B	514	CLA	OBD-CAD-CBD	-3.13	121.42	125.89
24	C	505	BCR	C16-C17-C18	3.13	131.78	127.31
20	c	5497	CLA	C1D-CHD-C4C	3.13	126.69	122.56
24	b	5529	BCR	C1-C6-C5	-3.13	118.21	122.61
20	a	5558	CLA	C7-C6-C5	-3.13	104.87	113.36
24	B	527	BCR	C2-C1-C6	3.12	115.29	110.48
20	B	525	CLA	C7-C6-C5	-3.12	104.87	113.36
20	B	512	CLA	C1D-CHD-C4C	3.12	126.68	122.56
20	B	522	CLA	CED-O2D-CGD	3.12	123.00	115.94
20	D	355	CLA	OBD-CAD-CBD	-3.12	121.44	125.89
28	I	201	MGE	O6D-C5D-C6D	3.12	114.19	106.44
20	b	5522	CLA	CED-O2D-CGD	3.12	123.00	115.94
20	B	520	CLA	OBD-CAD-CBD	-3.12	121.44	125.89
21	a	5561	PHO	C7-C6-C5	-3.12	104.89	113.36
20	B	516	CLA	CED-O2D-CGD	3.12	122.99	115.94
28	L	210	MGE	O6D-C5D-C6D	3.12	114.19	106.44
20	B	522	CLA	C7-C6-C5	-3.11	104.90	113.36
24	C	506	BCR	C35-C13-C12	3.11	122.98	118.08
24	H	107	BCR	C12-C13-C14	-3.11	114.17	118.94
24	x	5130	BCR	C1-C6-C5	-3.11	118.23	122.61
20	B	512	CLA	CED-O2D-CGD	3.11	122.97	115.94
24	H	107	BCR	C24-C23-C22	3.11	130.93	126.23
21	A	561	PHO	CAB-C3B-C2B	-3.11	118.36	128.60
24	D	357	BCR	C8-C7-C6	3.11	135.93	127.20
20	B	526	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
20	A	558	CLA	C1D-CHD-C4C	3.10	126.65	122.56
26	L	5213	SQD	C44-O6-C1	3.10	119.80	113.74
20	B	520	CLA	CED-O2D-CGD	3.10	122.95	115.94
30	c	5509	DGD	O2G-C1B-C2B	3.10	118.18	111.50
24	c	5505	BCR	C35-C13-C12	3.10	122.96	118.08
20	c	5495	CLA	CBA-CAA-C2A	3.09	123.00	113.86
20	C	493	CLA	CED-O2D-CGD	3.09	122.94	115.94
20	B	521	CLA	CED-O2D-CGD	3.09	122.93	115.94
20	b	5523	CLA	OBD-CAD-CBD	-3.09	121.48	125.89
28	d	5360	MGE	O2G-C1B-C2B	3.09	118.16	111.50
20	b	5511	CLA	C1D-CHD-C4C	3.09	126.64	122.56
24	X	130	BCR	C1-C6-C5	-3.09	118.27	122.61
20	c	5493	CLA	C7-C6-C5	-3.08	104.99	113.36
20	b	5516	CLA	OBD-CAD-CBD	-3.08	121.49	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	558	CLA	C7-C6-C5	-3.08	104.99	113.36
24	C	506	BCR	C16-C17-C18	3.08	131.71	127.31
20	b	5524	CLA	CED-O2D-CGD	3.08	122.90	115.94
24	b	5527	BCR	C1-C6-C5	-3.07	118.28	122.61
24	d	5357	BCR	C23-C24-C25	3.07	135.83	127.20
20	C	495	CLA	CBA-CAA-C2A	3.07	122.93	113.86
20	a	5563	CLA	C1D-CHD-C4C	3.07	126.61	122.56
24	x	5130	BCR	C34-C9-C8	3.07	122.91	118.08
20	C	497	CLA	O2A-CGA-CBA	3.07	121.53	111.91
20	C	502	CLA	OBD-CAD-CBD	-3.07	121.51	125.89
21	a	5562	PHO	C2A-C1A-NA	-3.06	108.34	111.86
21	a	5561	PHO	CED-O2D-CGD	3.06	122.86	115.94
30	C	509	DGD	O2G-C1B-C2B	3.06	118.10	111.50
26	A	568	SQD	C32-C31-C30	3.06	129.96	114.42
21	a	5562	PHO	CED-O2D-CGD	3.06	122.85	115.94
20	C	502	CLA	CED-O2D-CGD	3.06	122.85	115.94
24	b	5527	BCR	C29-C30-C25	3.05	115.18	110.48
24	B	529	BCR	C24-C23-C22	3.05	130.85	126.23
20	a	5563	CLA	C1-C2-C3	3.05	131.32	126.04
26	A	5212	SQD	C3-C4-C5	-3.05	104.79	110.24
30	C	508	DGD	C1E-O6E-C5E	3.05	119.68	113.69
20	B	515	CLA	C1D-CHD-C4C	3.05	126.58	122.56
24	c	5504	BCR	C32-C1-C6	3.05	115.25	110.30
20	d	5355	CLA	CED-O2D-CGD	3.05	122.83	115.94
24	H	107	BCR	C8-C7-C6	3.05	135.76	127.20
20	B	516	CLA	OBD-CAD-CBD	-3.05	121.54	125.89
30	H	208	DGD	O6D-C5D-C6D	3.05	112.81	106.67
20	B	511	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
20	C	497	CLA	OBD-CAD-CBD	-3.04	121.55	125.89
24	B	527	BCR	C23-C24-C25	3.04	135.75	127.20
20	c	5495	CLA	C7-C6-C5	-3.04	105.10	113.36
20	C	495	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
20	b	5520	CLA	O2A-CGA-CBA	3.04	121.45	111.91
20	d	5354	CLA	O2A-CGA-CBA	3.04	121.45	111.91
20	B	525	CLA	OBD-CAD-CBD	-3.04	121.56	125.89
20	b	5515	CLA	C1D-CHD-C4C	3.03	126.56	122.56
24	B	529	BCR	C1-C6-C5	-3.03	118.34	122.61
20	b	5514	CLA	O2A-CGA-CBA	3.03	121.42	111.91
20	a	5563	CLA	CED-O2D-CGD	3.03	122.79	115.94
20	c	5491	CLA	O2A-CGA-CBA	3.03	121.41	111.91
25	A	567	LHG	O7-C7-C8	3.03	118.02	111.50
26	a	212	SQD	C3-C4-C5	-3.02	104.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	5354	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
24	B	527	BCR	C29-C30-C25	3.02	115.13	110.48
24	h	5107	BCR	C32-C1-C6	3.02	115.20	110.30
20	c	5499	CLA	C1D-CHD-C4C	3.02	126.54	122.56
30	H	208	DGD	C1E-O6E-C5E	3.01	119.60	113.69
24	h	5107	BCR	C24-C23-C22	3.01	130.79	126.23
24	b	5529	BCR	C8-C7-C6	3.01	135.65	127.20
21	a	5561	PHO	CAB-C3B-C2B	-3.01	118.69	128.60
24	A	566	BCR	C23-C24-C25	3.01	135.65	127.20
20	C	500	CLA	C7-C6-C5	-3.01	105.19	113.36
20	C	499	CLA	OBD-CAD-CBD	-3.01	121.60	125.89
20	C	493	CLA	C7-C6-C5	-3.01	105.20	113.36
24	X	130	BCR	C34-C9-C8	3.00	122.81	118.08
30	C	507	DGD	O5D-C1E-C2E	3.00	112.99	108.30
20	A	558	CLA	OBD-CAD-CBD	-3.00	121.61	125.89
20	c	5493	CLA	C1-C2-C3	3.00	131.23	126.04
24	t	104	BCR	C11-C10-C9	3.00	131.59	127.31
20	c	5500	CLA	C1-C2-C3	3.00	131.23	126.04
24	B	527	BCR	C35-C13-C12	3.00	122.80	118.08
20	c	5499	CLA	OBD-CAD-CBD	-3.00	121.61	125.89
20	b	5519	CLA	OBD-CAD-CBD	-3.00	121.61	125.89
24	d	5357	BCR	C8-C7-C6	2.99	135.60	127.20
24	c	5504	BCR	C30-C25-C26	-2.99	118.40	122.61
20	c	5498	CLA	CED-O2D-CGD	2.98	122.68	115.94
24	c	5505	BCR	C1-C6-C5	-2.98	118.41	122.61
24	t	104	BCR	C35-C13-C12	2.98	122.77	118.08
20	c	5496	CLA	C1-C2-C3	2.97	131.19	126.04
20	c	5499	CLA	CED-O2D-CGD	2.97	122.66	115.94
20	C	495	CLA	O2A-CGA-CBA	2.97	121.23	111.91
20	B	524	CLA	C7-C6-C5	-2.97	105.30	113.36
20	C	494	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
24	t	104	BCR	C2-C1-C6	2.96	115.04	110.48
20	B	518	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
20	B	515	CLA	C7-C6-C5	-2.96	105.32	113.36
28	i	5201	MGE	O6D-C5D-C6D	2.96	113.80	106.44
24	a	5566	BCR	C23-C24-C25	2.96	135.51	127.20
20	b	5516	CLA	C1D-CHD-C4C	2.95	126.46	122.56
20	c	5491	CLA	C7-C6-C5	-2.95	105.36	113.36
20	b	5518	CLA	CED-O2D-CGD	2.94	122.59	115.94
20	b	5512	CLA	O2A-CGA-CBA	2.94	121.13	111.91
24	c	5504	BCR	C23-C24-C25	2.93	135.44	127.20
20	b	5517	CLA	C7-C6-C5	-2.93	105.39	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	495	CLA	OBD-CAD-CBD	-2.93	121.71	125.89
20	C	495	CLA	C1-C2-C3	2.93	131.11	126.04
30	c	5507	DGD	O5D-C1E-C2E	2.93	112.88	108.30
24	C	506	BCR	C1-C6-C5	-2.93	118.49	122.61
27	m	216	LMT	C1-O1'-C1'	-2.93	108.99	113.84
20	D	355	CLA	CED-O2D-CGD	2.93	122.55	115.94
24	B	528	BCR	C8-C7-C6	2.92	135.42	127.20
20	C	498	CLA	O2D-CGD-CBD	2.92	116.47	111.27
20	C	501	CLA	C1-C2-C3	2.92	131.10	126.04
20	C	496	CLA	OBD-CAD-CBD	-2.92	121.72	125.89
24	C	504	BCR	C23-C24-C25	2.92	135.40	127.20
24	h	5107	BCR	C12-C13-C14	-2.92	114.46	118.94
20	b	5524	CLA	C7-C6-C5	-2.92	105.43	113.36
24	B	528	BCR	C24-C23-C22	2.92	130.64	126.23
25	a	5567	LHG	O7-C7-C8	2.92	117.79	111.50
20	c	5495	CLA	C1-C2-C3	2.91	131.08	126.04
20	c	5498	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
20	D	354	CLA	O2A-CGA-CBA	2.91	121.05	111.91
20	b	5525	CLA	O2A-CGA-CBA	2.91	121.04	111.91
20	b	5525	CLA	CED-O2D-CGD	2.91	122.52	115.94
24	c	5504	BCR	C29-C30-C25	2.91	114.96	110.48
20	B	525	CLA	CED-O2D-CGD	2.91	122.51	115.94
20	C	496	CLA	O2A-CGA-CBA	2.91	121.03	111.91
20	c	5496	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
24	B	528	BCR	C1-C6-C5	-2.90	118.53	122.61
20	c	5498	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
24	X	130	BCR	C12-C13-C14	-2.90	114.50	118.94
20	b	5518	CLA	CAA-C2A-C3A	-2.90	104.85	112.78
24	D	357	BCR	C12-C13-C14	-2.89	114.50	118.94
20	A	558	CLA	CED-O2D-CGD	2.89	122.48	115.94
20	B	520	CLA	O2A-CGA-CBA	2.89	120.98	111.91
20	a	5558	CLA	C1-C2-C3	2.89	131.04	126.04
20	C	496	CLA	C7-C6-C5	-2.89	105.51	113.36
20	c	5494	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
24	b	5527	BCR	C30-C25-C26	-2.89	118.55	122.61
20	C	499	CLA	O2A-CGA-CBA	2.89	120.97	111.91
20	c	5499	CLA	O2A-CGA-CBA	2.89	120.97	111.91
20	b	5525	CLA	C7-C6-C5	-2.88	105.53	113.36
20	b	5513	CLA	CED-O2D-CGD	2.88	122.45	115.94
20	b	5523	CLA	C1-C2-C3	2.88	131.02	126.04
24	T	5104	BCR	C35-C13-C12	2.88	122.61	118.08
20	b	5520	CLA	OBD-CAD-CBD	-2.88	121.78	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	492	CLA	O2A-CGA-CBA	2.88	120.93	111.91
20	C	497	CLA	CED-O2D-CGD	2.88	122.44	115.94
20	A	559	CLA	CED-O2D-CGD	2.87	122.44	115.94
20	B	515	CLA	O2A-CGA-CBA	2.87	120.92	111.91
26	d	5358	SQD	C32-C31-C30	2.87	129.01	114.42
20	A	563	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
22	a	5564	PQ9	C19-C18-C20	2.87	120.10	115.27
22	a	5564	PQ9	C24-C23-C25	2.87	120.10	115.27
20	c	5495	CLA	O2A-CGA-CBA	2.87	120.91	111.91
24	B	529	BCR	C7-C8-C9	2.87	130.57	126.23
20	c	5497	CLA	CED-O2D-CGD	2.87	122.42	115.94
26	A	5212	SQD	O47-C7-C8	2.86	116.36	111.09
24	c	5504	BCR	C40-C30-C25	2.86	114.94	110.30
20	c	5501	CLA	CED-O2D-CGD	2.86	122.41	115.94
24	C	504	BCR	C35-C13-C12	2.86	122.58	118.08
24	c	5504	BCR	C1-C6-C7	2.86	123.86	115.78
20	a	5560	CLA	CAA-CBA-CGA	2.86	121.60	113.25
24	b	5528	BCR	C8-C7-C6	2.86	135.22	127.20
20	a	5560	CLA	C7-C6-C5	-2.86	105.60	113.36
20	B	514	CLA	O2A-CGA-CBA	2.86	120.87	111.91
20	C	493	CLA	C1-C2-C3	2.85	130.98	126.04
20	B	516	CLA	C1D-CHD-C4C	2.85	126.32	122.56
26	A	568	SQD	C45-O47-C7	2.85	124.81	117.79
20	b	5526	CLA	C1-O2A-CGA	2.85	123.92	116.44
20	B	512	CLA	C7-C6-C5	-2.85	105.62	113.36
20	b	5525	CLA	OBD-CAD-CBD	-2.85	121.83	125.89
20	C	491	CLA	OBD-CAD-CBD	-2.85	121.83	125.89
20	B	513	CLA	CED-O2D-CGD	2.84	122.37	115.94
24	b	5529	BCR	C24-C23-C22	2.84	130.53	126.23
28	D	358	MGE	O6D-C5D-C6D	2.84	113.49	106.44
20	A	560	CLA	CED-O2D-CGD	2.84	122.36	115.94
20	b	5520	CLA	CED-O2D-CGD	2.84	122.35	115.94
20	C	500	CLA	C1-C2-C3	2.83	130.95	126.04
26	a	212	SQD	O47-C7-C8	2.83	116.30	111.09
20	C	497	CLA	O2D-CGD-CBD	2.83	116.30	111.27
24	d	5357	BCR	C37-C22-C23	2.83	122.54	118.08
20	c	5496	CLA	C7-C6-C5	-2.83	105.67	113.36
20	B	518	CLA	C7-C6-C5	-2.83	105.68	113.36
22	A	564	PQ9	C16-C17-C18	-2.83	120.86	127.66
20	B	512	CLA	O2A-CGA-CBA	2.82	120.77	111.91
20	B	516	CLA	C7-C6-C5	-2.82	105.70	113.36
20	c	5495	CLA	CMB-C2B-C1B	-2.82	124.13	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5519	CLA	C7-C6-C5	-2.82	105.71	113.36
21	A	562	PHO	C2A-C1A-NA	-2.82	108.63	111.86
20	a	5563	CLA	O2A-CGA-CBA	2.82	120.75	111.91
20	a	5559	CLA	O2A-CGA-CBA	2.81	120.74	111.91
20	c	5499	CLA	O2D-CGD-CBD	2.81	116.27	111.27
20	C	503	CLA	O2A-CGA-CBA	2.81	120.74	111.91
20	B	515	CLA	OBD-CAD-CBD	-2.81	121.88	125.89
24	H	107	BCR	C32-C1-C6	2.81	114.86	110.30
20	B	525	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	c	5505	BCR	C30-C25-C26	-2.81	118.66	122.61
24	B	529	BCR	C8-C7-C6	2.81	135.09	127.20
20	B	519	CLA	OBD-CAD-CBD	-2.81	121.89	125.89
22	D	356	PQ9	C19-C18-C20	2.80	119.99	115.27
20	b	5523	CLA	O2A-CGA-CBA	2.80	120.71	111.91
20	A	563	CLA	O2A-CGA-CBA	2.80	120.71	111.91
20	b	5524	CLA	OBD-CAD-CBD	-2.80	121.89	125.89
27	T	217	LMT	C1-O1'-C1'	-2.80	109.19	113.84
22	A	564	PQ9	C19-C18-C20	2.80	119.98	115.27
20	B	526	CLA	O2A-CGA-CBA	2.80	120.70	111.91
22	A	564	PQ9	C24-C23-C25	2.80	119.98	115.27
24	T	5104	BCR	C23-C22-C21	-2.80	114.65	118.94
20	B	515	CLA	C2A-C3A-C4A	2.80	106.39	101.87
28	L	210	MGE	O2G-C1B-C2B	2.80	117.53	111.50
24	C	504	BCR	C32-C1-C6	2.80	114.83	110.30
20	C	501	CLA	CED-O2D-CGD	2.79	122.26	115.94
20	B	515	CLA	CED-O2D-CGD	2.79	122.25	115.94
20	a	5560	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
21	A	562	PHO	CED-O2D-CGD	2.79	122.25	115.94
24	T	5104	BCR	C2-C1-C6	2.79	114.78	110.48
22	a	5564	PQ9	C16-C17-C18	-2.79	120.94	127.66
20	B	514	CLA	C7-C6-C5	-2.79	105.79	113.36
26	d	5358	SQD	C36-C35-C34	2.79	128.58	114.42
20	B	519	CLA	C7-C6-C5	-2.79	105.79	113.36
24	C	505	BCR	C1-C6-C5	-2.78	118.69	122.61
20	C	498	CLA	C7-C6-C5	-2.78	105.80	113.36
20	b	5514	CLA	C1-C2-C3	2.78	130.86	126.04
27	t	5217	LMT	C1-O1'-C1'	-2.78	109.23	113.84
20	B	517	CLA	C7-C6-C5	-2.78	105.81	113.36
24	c	5505	BCR	C16-C17-C18	2.78	131.27	127.31
20	C	499	CLA	O2D-CGD-CBD	2.78	116.20	111.27
24	t	104	BCR	C1-C6-C5	-2.78	118.70	122.61
20	b	5526	CLA	C1-C2-C3	2.78	130.84	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	5562	PHO	CBD-CHA-C1A	2.77	132.83	126.40
20	b	5511	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
20	A	558	CLA	O2A-CGA-CBA	2.77	120.61	111.91
20	C	499	CLA	C2A-C1A-CHA	2.77	128.70	123.86
21	A	562	PHO	CBD-CHA-C1A	2.77	132.82	126.40
26	A	568	SQD	C36-C35-C34	2.77	128.47	114.42
20	C	498	CLA	CED-O2D-CGD	2.76	122.19	115.94
24	B	527	BCR	C1-C6-C5	-2.76	118.72	122.61
20	B	516	CLA	CBA-CAA-C2A	2.76	122.02	113.86
24	C	505	BCR	C35-C13-C12	2.76	122.43	118.08
24	T	5104	BCR	C1-C6-C5	-2.76	118.73	122.61
20	A	560	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
24	b	5527	BCR	C16-C17-C18	2.76	131.24	127.31
20	b	5512	CLA	C7-C6-C5	-2.75	105.89	113.36
20	D	355	CLA	O2A-CGA-CBA	2.75	120.54	111.91
21	A	562	PHO	CAA-C2A-C3A	-2.75	105.25	112.78
21	A	561	PHO	C7-C6-C5	-2.75	105.89	113.36
24	d	5357	BCR	C36-C18-C19	2.75	122.41	118.08
24	h	5107	BCR	C15-C14-C13	2.75	131.23	127.31
28	l	5210	MGE	O2G-C1B-C2B	2.75	117.42	111.50
24	T	5104	BCR	C11-C10-C9	2.74	131.22	127.31
20	C	499	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
20	A	560	CLA	CAA-CBA-CGA	2.74	121.26	113.25
20	C	494	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
20	b	5523	CLA	C2A-C3A-C4A	2.74	106.29	101.87
20	a	5558	CLA	O2A-CGA-CBA	2.73	120.49	111.91
20	b	5517	CLA	OBD-CAD-C3D	2.73	132.52	127.98
21	a	5562	PHO	CAA-C2A-C3A	-2.73	105.30	112.78
20	a	5563	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
20	B	526	CLA	C1-C2-C3	2.73	130.76	126.04
30	h	5208	DGD	O6D-C5D-C4D	2.73	114.64	109.69
20	d	5354	CLA	O2D-CGD-CBD	2.73	116.11	111.27
24	c	5506	BCR	C35-C13-C12	2.72	122.36	118.08
30	H	208	DGD	O6D-C5D-C4D	2.72	114.63	109.69
24	C	505	BCR	C19-C18-C17	-2.72	114.77	118.94
20	C	493	CLA	OBD-CAD-CBD	-2.72	122.01	125.89
20	C	491	CLA	O2A-CGA-CBA	2.72	120.44	111.91
20	b	5513	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
20	b	5518	CLA	C7-C6-C5	-2.72	105.98	113.36
24	D	357	BCR	C24-C23-C22	2.71	130.34	126.23
20	c	5502	CLA	C1-C2-C3	2.71	130.74	126.04
24	B	527	BCR	C24-C23-C22	2.71	130.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	5566	BCR	C8-C7-C6	2.71	134.81	127.20
20	b	5516	CLA	CBA-CAA-C2A	2.71	121.86	113.86
20	b	5526	CLA	C7-C6-C5	-2.71	106.01	113.36
20	C	498	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
20	C	502	CLA	C2A-C3A-C4A	2.70	106.24	101.87
20	b	5515	CLA	C7-C6-C5	-2.70	106.03	113.36
24	X	130	BCR	C16-C17-C18	2.70	131.16	127.31
20	b	5515	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
20	C	496	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
24	b	5529	BCR	C35-C13-C12	2.69	122.32	118.08
20	C	498	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
20	b	5516	CLA	C7-C6-C5	-2.69	106.06	113.36
26	A	568	SQD	O8-S-O7	2.68	117.83	111.27
24	d	5357	BCR	C12-C13-C14	-2.68	114.82	118.94
24	B	527	BCR	C8-C7-C6	2.68	134.74	127.20
20	b	5526	CLA	O2A-CGA-CBA	2.68	120.31	111.91
24	b	5528	BCR	C24-C23-C22	2.68	130.28	126.23
20	b	5521	CLA	CED-O2D-CGD	2.68	121.99	115.94
20	C	500	CLA	C2A-C3A-C4A	2.67	106.19	101.87
20	B	519	CLA	C1-C2-C3	2.67	130.67	126.04
28	d	5360	MGE	C3G-O3G-C1D	-2.67	108.52	113.74
24	C	506	BCR	C19-C18-C17	-2.67	114.85	118.94
24	D	357	BCR	C35-C13-C12	2.67	122.28	118.08
20	B	512	CLA	C1-C2-C3	2.67	130.66	126.04
20	C	499	CLA	CED-O2D-CGD	2.67	121.97	115.94
20	a	5559	CLA	OBD-CAD-CBD	-2.67	122.09	125.89
20	B	519	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
30	c	5509	DGD	C3G-C2G-C1G	-2.66	105.49	111.79
20	c	5499	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	b	5521	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	A	560	CLA	C7-C6-C5	-2.66	106.13	113.36
26	A	5212	SQD	O48-C23-C24	2.66	123.98	112.38
20	b	5523	CLA	C7-C6-C5	-2.66	106.14	113.36
24	t	104	BCR	C23-C22-C21	-2.66	114.86	118.94
24	C	506	BCR	C12-C13-C14	-2.66	114.86	118.94
20	A	558	CLA	CAA-C2A-C3A	-2.66	105.51	112.78
28	b	5530	MGE	O6D-C5D-C6D	2.65	113.03	106.44
24	x	5130	BCR	C35-C13-C12	2.65	122.26	118.08
20	c	5497	CLA	O2D-CGD-CBD	2.65	115.98	111.27
20	b	5514	CLA	C2A-C3A-C4A	2.65	106.15	101.87
20	a	5563	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
24	C	505	BCR	C30-C25-C26	-2.65	118.88	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	562	PHO	CAB-C3B-C4B	2.65	136.00	126.21
24	C	504	BCR	C23-C22-C21	-2.65	114.88	118.94
20	B	517	CLA	OBD-CAD-C3D	2.65	132.38	127.98
24	C	504	BCR	C1-C6-C7	2.65	123.26	115.78
26	t	213	SQD	C31-C30-C29	2.65	133.50	113.42
30	c	5508	DGD	O6D-C5D-C6D	2.64	112.00	106.67
20	A	560	CLA	C2A-C3A-C4A	2.64	106.14	101.87
28	B	530	MGE	O3G-C1D-C2D	2.64	112.43	108.30
20	B	517	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
20	B	524	CLA	O2A-CGA-CBA	2.64	120.20	111.91
21	a	5562	PHO	CAB-C3B-C4B	2.64	135.97	126.21
20	a	5558	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
20	B	520	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
24	A	566	BCR	C36-C18-C19	2.63	122.23	118.08
24	t	104	BCR	C7-C8-C9	2.63	130.21	126.23
20	B	523	CLA	C1-C2-C3	2.63	130.59	126.04
24	c	5506	BCR	C37-C22-C23	2.63	122.22	118.08
25	A	567	LHG	P-O6-C4	-2.63	106.26	121.68
20	b	5518	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
21	a	5561	PHO	CBD-CHA-C1A	2.63	132.50	126.40
20	B	523	CLA	O2A-CGA-CBA	2.63	120.15	111.91
26	d	5358	SQD	O9-S-C6	-2.63	103.82	106.94
20	b	5523	CLA	CMB-C2B-C1B	-2.63	124.43	128.46
24	A	566	BCR	C35-C13-C12	2.63	122.21	118.08
20	C	491	CLA	C7-C6-C5	-2.62	106.23	113.36
20	a	5560	CLA	CED-O2D-CGD	2.62	121.87	115.94
24	c	5504	BCR	C35-C13-C12	2.62	122.21	118.08
24	h	5107	BCR	C35-C13-C12	2.62	122.21	118.08
24	A	566	BCR	C16-C17-C18	2.62	131.05	127.31
26	A	568	SQD	C44-O6-C1	2.62	118.86	113.74
32	F	51	HEM	C4C-C3C-C2C	-2.62	105.07	106.90
20	C	500	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
20	c	5493	CLA	OBD-CAD-CBD	-2.62	122.16	125.89
20	c	5502	CLA	C2A-C3A-C4A	2.61	106.09	101.87
24	c	5506	BCR	C30-C25-C24	2.61	123.17	115.78
26	d	5358	SQD	C15-C14-C13	2.61	127.69	114.42
24	c	5506	BCR	C40-C30-C29	-2.61	98.46	108.91
20	A	559	CLA	O2A-CGA-CBA	2.61	120.11	111.91
20	c	5492	CLA	OBD-CAD-CBD	-2.61	122.16	125.89
24	a	5566	BCR	C37-C22-C23	2.61	122.19	118.08
20	B	525	CLA	O2D-CGD-CBD	2.61	115.91	111.27
26	a	212	SQD	O48-C23-C24	2.61	123.76	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5526	CLA	OBD-CAD-C3D	2.61	132.31	127.98
20	B	523	CLA	C7-C6-C5	-2.61	106.28	113.36
24	B	527	BCR	C16-C17-C18	2.60	131.03	127.31
20	b	5519	CLA	C1-C2-C3	2.60	130.54	126.04
24	d	5357	BCR	C7-C8-C9	2.60	130.16	126.23
24	B	529	BCR	C35-C13-C12	2.59	122.17	118.08
26	A	568	SQD	O9-S-C6	-2.59	103.86	106.94
24	A	566	BCR	C1-C6-C5	-2.59	118.96	122.61
24	c	5506	BCR	C16-C17-C18	2.59	131.01	127.31
20	B	513	CLA	C1-C2-C3	2.59	130.53	126.04
26	L	5213	SQD	C3-C4-C5	-2.59	105.62	110.24
24	c	5506	BCR	C24-C23-C22	2.59	130.14	126.23
20	B	519	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
20	c	5498	CLA	O2D-CGD-CBD	2.58	115.86	111.27
20	C	500	CLA	O2A-CGA-CBA	2.58	120.01	111.91
24	c	5506	BCR	C1-C6-C5	-2.58	118.98	122.61
20	b	5520	CLA	C1-C2-C3	2.58	130.51	126.04
24	C	504	BCR	C37-C22-C23	2.58	122.14	118.08
20	B	523	CLA	OBD-CAD-CBD	-2.58	122.21	125.89
20	A	563	CLA	CED-O2D-CGD	2.58	121.77	115.94
20	B	520	CLA	C1-C2-C3	2.58	130.50	126.04
20	C	494	CLA	CBA-CAA-C2A	2.58	121.47	113.86
21	A	561	PHO	O2D-CGD-CBD	2.58	115.84	111.27
20	d	5354	CLA	CED-O2D-CGD	2.57	121.76	115.94
22	D	356	PQ9	C16-C17-C18	-2.57	121.46	127.66
20	C	501	CLA	O2A-CGA-CBA	2.57	119.98	111.91
20	b	5513	CLA	O2D-CGD-CBD	2.57	115.84	111.27
24	c	5505	BCR	C8-C7-C6	2.57	134.42	127.20
28	d	5359	MGE	O6D-C5D-C6D	2.57	112.83	106.44
20	A	563	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
22	d	5356	PQ9	C14-C13-C15	2.57	119.59	115.27
20	c	5498	CLA	C7-C6-C5	-2.57	106.39	113.36
24	X	130	BCR	C24-C23-C22	2.57	130.11	126.23
20	C	499	CLA	C2A-C3A-C4A	2.57	106.01	101.87
30	C	509	DGD	C3G-C2G-C1G	-2.57	105.72	111.79
20	c	5496	CLA	O2A-CGA-CBA	2.56	119.96	111.91
21	A	561	PHO	CBD-CHA-C1A	2.56	132.34	126.40
24	c	5504	BCR	C37-C22-C23	2.56	122.11	118.08
20	b	5520	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
21	A	561	PHO	CAB-C3B-C4B	2.56	135.67	126.21
20	b	5513	CLA	C1-C2-C3	2.56	130.47	126.04
20	b	5517	CLA	CMB-C2B-C1B	-2.56	124.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	BCR	C40-C30-C29	-2.56	98.68	108.91
20	b	5521	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
24	b	5527	BCR	C8-C7-C6	2.56	134.38	127.20
20	C	503	CLA	CMB-C2B-C1B	-2.56	124.54	128.46
20	D	355	CLA	O2D-CGD-CBD	2.55	115.81	111.27
20	c	5498	CLA	O2A-CGA-CBA	2.55	119.92	111.91
20	b	5517	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
20	b	5521	CLA	C6-C5-C3	2.55	120.15	113.45
20	b	5519	CLA	C1-O2A-CGA	2.55	123.13	116.44
20	d	5355	CLA	O2A-CGA-CBA	2.54	119.89	111.91
30	H	208	DGD	O5D-C1E-C2E	2.54	112.27	108.30
24	a	5566	BCR	C1-C6-C5	-2.54	119.03	122.61
24	A	566	BCR	C7-C8-C9	2.54	130.08	126.23
26	d	5358	SQD	C44-O6-C1	2.54	118.70	113.74
24	a	5566	BCR	C36-C18-C19	2.53	122.07	118.08
20	a	5558	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
20	C	494	CLA	C2A-C3A-C4A	2.53	105.95	101.87
24	H	107	BCR	C16-C17-C18	2.53	130.92	127.31
20	c	5497	CLA	OBD-CAD-CBD	-2.53	122.28	125.89
26	L	5213	SQD	C31-C30-C29	2.52	132.59	113.42
20	B	512	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
20	A	558	CLA	C2A-C3A-C4A	2.52	105.94	101.87
20	B	518	CLA	OBD-CAD-CBD	-2.52	122.29	125.89
20	C	495	CLA	CED-O2D-CGD	2.52	121.63	115.94
32	v	5552	HEM	CMB-C2B-C3B	2.51	129.38	124.68
20	B	526	CLA	C7-C6-C5	-2.51	106.53	113.36
20	C	492	CLA	C6-C5-C3	2.51	120.04	113.45
20	C	495	CLA	C6-C5-C3	2.51	120.04	113.45
24	C	505	BCR	C12-C13-C14	-2.51	115.10	118.94
24	D	357	BCR	C37-C22-C23	2.50	122.02	118.08
20	A	560	CLA	C1-C2-C3	2.50	130.37	126.04
20	b	5519	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
24	b	5529	BCR	C7-C8-C9	2.50	130.01	126.23
20	d	5354	CLA	C7-C6-C5	-2.50	106.57	113.36
20	c	5498	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
20	B	517	CLA	C2A-C1A-CHA	2.50	128.23	123.86
24	b	5529	BCR	C32-C1-C6	2.50	114.35	110.30
24	b	5527	BCR	C35-C13-C12	2.50	122.01	118.08
20	c	5502	CLA	OBD-CAD-CBD	-2.50	122.33	125.89
20	c	5491	CLA	OBD-CAD-CBD	-2.50	122.33	125.89
20	B	514	CLA	C2A-C3A-C4A	2.50	105.90	101.87
20	C	492	CLA	C4D-C3D-CAD	-2.49	107.08	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	558	CLA	CBA-CAA-C2A	2.49	121.22	113.86
24	c	5506	BCR	C19-C18-C17	-2.49	115.12	118.94
24	t	104	BCR	C12-C13-C14	-2.49	115.12	118.94
20	B	521	CLA	C2A-C3A-C4A	2.49	105.89	101.87
20	b	5512	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
24	T	5104	BCR	C40-C30-C29	-2.49	98.95	108.91
20	a	5558	CLA	OBD-CAD-CBD	-2.49	122.34	125.89
20	b	5512	CLA	C1-C2-C3	2.49	130.34	126.04
20	B	523	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
20	B	513	CLA	C7-C6-C5	-2.48	106.62	113.36
20	A	559	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
25	a	5567	LHG	P-O6-C4	-2.48	107.14	121.68
28	i	5201	MGE	C3G-O3G-C1D	-2.48	108.90	113.74
20	c	5495	CLA	C2A-C1A-CHA	2.48	128.19	123.86
30	C	508	DGD	O6D-C5D-C6D	2.48	111.66	106.67
20	B	524	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
24	a	5566	BCR	C2-C1-C6	2.47	114.29	110.48
24	B	527	BCR	C36-C18-C19	2.47	121.97	118.08
20	A	560	CLA	CMB-C2B-C3B	2.47	129.30	124.68
20	A	559	CLA	OBD-CAD-CBD	-2.47	122.36	125.89
20	b	5525	CLA	O2D-CGD-CBD	2.47	115.66	111.27
24	h	5107	BCR	C1-C6-C7	2.47	122.77	115.78
20	b	5524	CLA	O2A-CGA-CBA	2.47	119.66	111.91
20	D	354	CLA	C2A-C3A-C4A	2.47	105.86	101.87
22	a	5564	PQ9	C14-C13-C15	2.47	119.42	115.27
20	b	5524	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
22	A	564	PQ9	C14-C13-C15	2.47	119.42	115.27
20	C	498	CLA	O2A-CGA-CBA	2.47	119.65	111.91
20	C	495	CLA	CMB-C2B-C3B	2.47	129.29	124.68
24	h	5107	BCR	C16-C17-C18	2.46	130.83	127.31
20	B	521	CLA	O2D-CGD-CBD	2.46	115.64	111.27
20	b	5519	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
20	c	5500	CLA	O2A-CGA-CBA	2.46	119.63	111.91
20	b	5525	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
20	A	563	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
20	A	559	CLA	C2A-C3A-C4A	2.46	105.83	101.87
24	X	130	BCR	C35-C13-C12	2.45	121.94	118.08
24	a	5566	BCR	C16-C17-C18	2.45	130.81	127.31
20	c	5494	CLA	CBA-CAA-C2A	2.45	121.10	113.86
21	a	5561	PHO	CAB-C3B-C4B	2.45	135.26	126.21
20	a	5558	CLA	C2A-C3A-C4A	2.45	105.83	101.87
24	C	504	BCR	C7-C8-C9	2.45	129.94	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	5104	BCR	C7-C8-C9	2.45	129.93	126.23
26	d	5358	SQD	O8-S-O7	2.45	117.25	111.27
20	C	502	CLA	C1-C2-C3	2.44	130.27	126.04
20	C	494	CLA	C2A-C1A-CHA	2.44	128.13	123.86
24	t	104	BCR	C8-C9-C10	-2.44	115.19	118.94
32	V	552	HEM	C4A-C3A-C2A	2.44	108.69	107.00
24	d	5357	BCR	C16-C17-C18	2.44	130.79	127.31
28	I	201	MGE	O1G-C1G-C2G	-2.44	101.33	108.43
20	C	502	CLA	C2A-C1A-CHA	2.44	128.13	123.86
28	i	5201	MGE	O1G-C1G-C2G	-2.44	101.33	108.43
24	X	130	BCR	C37-C22-C23	2.44	121.92	118.08
20	c	5493	CLA	C2A-C3A-C4A	2.44	105.81	101.87
24	D	357	BCR	C16-C17-C18	2.44	130.79	127.31
27	t	5217	LMT	C3'-C4'-C5'	-2.44	105.33	110.93
24	A	566	BCR	C37-C22-C23	2.44	121.92	118.08
20	b	5523	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	a	5558	CLA	CBA-CAA-C2A	2.44	121.06	113.86
20	B	523	CLA	C6-C5-C3	2.44	119.85	113.45
20	b	5513	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	D	355	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
21	A	562	PHO	O2D-CGD-CBD	2.44	115.60	111.27
26	A	568	SQD	C3-C4-C5	-2.44	105.89	110.24
20	C	498	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
20	B	523	CLA	C2A-C3A-C4A	2.43	105.80	101.87
24	C	505	BCR	C36-C18-C19	2.43	121.91	118.08
24	A	566	BCR	C2-C1-C6	2.43	114.22	110.48
26	A	568	SQD	C15-C14-C13	2.43	126.76	114.42
20	D	354	CLA	C7-C6-C5	-2.43	106.76	113.36
20	c	5502	CLA	C2A-C1A-CHA	2.43	128.11	123.86
20	b	5515	CLA	C12-C11-C10	-2.43	102.08	113.24
24	B	528	BCR	C32-C1-C6	2.43	114.24	110.30
20	c	5493	CLA	C12-C11-C10	-2.43	102.09	113.24
24	T	5104	BCR	C37-C22-C23	2.43	121.90	118.08
20	D	354	CLA	CED-O2D-CGD	2.42	121.42	115.94
20	c	5492	CLA	C7-C6-C5	-2.42	106.78	113.36
24	C	506	BCR	C36-C18-C19	2.42	121.89	118.08
24	C	505	BCR	C8-C7-C6	2.42	134.00	127.20
20	B	518	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
20	c	5492	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
20	a	5560	CLA	C2A-C3A-C4A	2.42	105.77	101.87
26	t	213	SQD	C3-C4-C5	-2.42	105.93	110.24
20	C	494	CLA	CMB-C2B-C3B	2.42	129.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	566	BCR	C8-C7-C6	2.42	133.99	127.20
26	d	5358	SQD	C3-C4-C5	-2.42	105.93	110.24
20	b	5514	CLA	C7-C6-C5	-2.41	106.80	113.36
24	X	130	BCR	C30-C25-C24	2.41	122.61	115.78
20	c	5492	CLA	O2A-CGA-CBA	2.41	119.48	111.91
20	B	521	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
20	C	503	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
20	B	526	CLA	C1-O2A-CGA	2.41	122.76	116.44
20	b	5516	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
24	c	5504	BCR	C23-C22-C21	-2.41	115.25	118.94
20	b	5522	CLA	C2A-C3A-C4A	2.41	105.76	101.87
24	c	5505	BCR	C12-C13-C14	-2.41	115.25	118.94
20	B	511	CLA	CMB-C2B-C3B	2.41	129.18	124.68
20	a	5559	CLA	C2A-C3A-C4A	2.40	105.75	101.87
24	C	506	BCR	C30-C25-C24	2.40	122.57	115.78
24	B	527	BCR	C12-C13-C14	-2.40	115.26	118.94
24	c	5504	BCR	C12-C13-C14	-2.40	115.26	118.94
28	B	530	MGE	O6D-C5D-C6D	2.40	112.39	106.44
20	B	526	CLA	OBD-CAD-C3D	2.40	131.96	127.98
24	C	506	BCR	C37-C22-C23	2.39	121.85	118.08
24	C	504	BCR	C32-C1-C2	-2.39	99.33	108.91
20	B	520	CLA	CMB-C2B-C3B	2.39	129.15	124.68
20	c	5500	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
20	c	5494	CLA	O2A-CGA-CBA	2.39	121.67	112.23
20	A	558	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
24	d	5357	BCR	C35-C13-C12	2.39	121.83	118.08
20	b	5515	CLA	C6-C5-C3	2.38	119.71	113.45
20	c	5495	CLA	CED-O2D-CGD	2.38	121.32	115.94
28	B	530	MGE	O1G-C1G-C2G	-2.38	101.51	108.43
20	c	5501	CLA	O2A-CGA-CBA	2.38	119.38	111.91
20	b	5515	CLA	C2A-C3A-C4A	2.38	105.71	101.87
22	d	5356	PQ9	C16-C17-C18	-2.37	121.94	127.66
20	C	494	CLA	O2A-CGA-CBA	2.37	121.61	112.23
20	B	524	CLA	C1-C2-C3	2.37	130.15	126.04
20	B	524	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
20	B	526	CLA	C2A-C3A-C4A	2.37	105.70	101.87
20	c	5499	CLA	C2A-C1A-CHA	2.37	128.01	123.86
20	c	5495	CLA	CMB-C2B-C3B	2.37	129.12	124.68
20	c	5494	CLA	CMB-C2B-C3B	2.37	129.12	124.68
22	D	356	PQ9	C11-C12-C13	-2.37	122.85	126.79
20	b	5516	CLA	OBD-CAD-C3D	2.37	131.91	127.98
24	c	5506	BCR	C12-C13-C14	-2.37	115.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	130	BCR	C32-C1-C2	-2.37	99.44	108.91
20	c	5496	CLA	C2A-C3A-C4A	2.37	105.69	101.87
21	A	562	PHO	C3D-C4D-CHA	2.37	115.87	109.49
24	b	5529	BCR	C12-C13-C14	-2.37	115.31	118.94
20	c	5500	CLA	CED-O2D-CGD	2.36	121.29	115.94
28	d	5359	MGE	C3G-C2G-C1G	-2.36	106.20	111.79
20	B	514	CLA	CED-O2D-CGD	2.36	121.28	115.94
20	C	493	CLA	C2A-C3A-C4A	2.36	105.68	101.87
24	B	529	BCR	C12-C13-C14	-2.36	115.32	118.94
21	A	561	PHO	O2A-CGA-CBA	2.36	119.31	111.91
24	H	107	BCR	C35-C13-C12	2.36	121.79	118.08
20	C	492	CLA	C1-C2-C3	2.36	130.12	126.04
20	A	563	CLA	OBD-CAD-C3D	2.36	131.90	127.98
24	B	528	BCR	C1-C6-C7	2.36	122.45	115.78
22	d	5356	PQ9	C19-C18-C20	2.36	119.23	115.27
20	b	5518	CLA	OBD-CAD-C3D	2.35	131.89	127.98
20	C	492	CLA	OBD-CAD-C3D	2.35	131.89	127.98
20	c	5502	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
24	c	5504	BCR	C30-C25-C24	2.35	122.44	115.78
24	T	5104	BCR	C12-C13-C14	-2.35	115.33	118.94
20	b	5514	CLA	CED-O2D-CGD	2.35	121.25	115.94
28	B	530	MGE	C3G-C2G-C1G	-2.35	106.24	111.79
20	B	515	CLA	C12-C11-C10	-2.35	102.46	113.24
20	D	354	CLA	O2D-CGD-CBD	2.34	115.44	111.27
24	C	504	BCR	C40-C30-C25	2.34	114.10	110.30
24	t	104	BCR	C36-C18-C19	2.34	121.77	118.08
20	C	491	CLA	O2D-CGD-CBD	2.34	115.43	111.27
20	B	519	CLA	C2A-C3A-C4A	2.34	105.66	101.87
20	B	523	CLA	CED-O2D-CGD	2.34	121.24	115.94
20	B	513	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
24	t	104	BCR	C37-C22-C23	2.34	121.77	118.08
22	D	356	PQ9	C21-C22-C23	-2.34	122.03	127.66
20	B	521	CLA	C6-C5-C3	2.34	119.58	113.45
24	B	529	BCR	C40-C30-C25	2.34	114.09	110.30
20	c	5500	CLA	C2A-C3A-C4A	2.34	105.64	101.87
20	C	492	CLA	C2A-C3A-C4A	2.33	105.64	101.87
24	b	5528	BCR	C1-C6-C7	2.33	122.38	115.78
24	h	5107	BCR	C37-C22-C23	2.33	121.75	118.08
24	a	5566	BCR	C32-C1-C6	2.33	114.08	110.30
20	C	493	CLA	O2D-CGD-CBD	2.33	115.41	111.27
20	c	5491	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
20	b	5520	CLA	CMB-C2B-C3B	2.33	129.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	522	CLA	C2A-C3A-C4A	2.33	105.63	101.87
24	A	566	BCR	C19-C18-C17	-2.33	115.37	118.94
21	a	5561	PHO	O2D-CGD-CBD	2.33	115.40	111.27
26	A	5212	SQD	O8-S-O7	2.32	116.95	111.27
20	c	5501	CLA	OBD-CAD-CBD	-2.32	122.58	125.89
20	c	5495	CLA	OBD-CAD-C3D	2.32	131.84	127.98
24	c	5506	BCR	C36-C18-C19	2.32	121.74	118.08
20	c	5499	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
20	b	5519	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	T	5104	BCR	C36-C18-C19	2.32	121.73	118.08
20	d	5354	CLA	C2A-C3A-C4A	2.32	105.61	101.87
20	b	5518	CLA	O2D-CGD-CBD	2.32	115.39	111.27
20	c	5503	CLA	O2A-CGA-CBA	2.32	119.18	111.91
24	B	529	BCR	C32-C1-C6	2.32	114.05	110.30
24	b	5528	BCR	C32-C1-C6	2.31	114.05	110.30
24	T	5104	BCR	C23-C24-C25	2.31	133.69	127.20
20	c	5492	CLA	C6-C5-C3	2.31	119.52	113.45
20	b	5512	CLA	CMB-C2B-C3B	2.31	129.00	124.68
20	c	5493	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
20	B	511	CLA	CED-O2D-CGD	2.31	121.16	115.94
24	H	107	BCR	C1-C6-C7	2.31	122.31	115.78
20	a	5559	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
24	x	5130	BCR	C30-C25-C24	2.31	122.30	115.78
21	a	5561	PHO	C3D-C4D-CHA	2.30	115.71	109.49
24	t	104	BCR	C23-C24-C25	2.30	133.67	127.20
20	B	525	CLA	C2A-C3A-C4A	2.30	105.59	101.87
30	h	5208	DGD	O5D-C1E-C2E	2.30	111.90	108.30
24	a	5566	BCR	C30-C25-C24	2.30	122.29	115.78
24	c	5505	BCR	C36-C18-C19	2.30	121.70	118.08
20	c	5497	CLA	C2A-C3A-C4A	2.30	105.59	101.87
28	I	201	MGE	C3G-O3G-C1D	-2.30	109.25	113.74
24	c	5506	BCR	C23-C22-C21	-2.30	115.41	118.94
20	a	5560	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	H	107	BCR	C36-C18-C19	2.30	121.70	118.08
20	B	517	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
24	a	5566	BCR	C35-C13-C12	2.30	121.69	118.08
20	C	495	CLA	C2A-C3A-C4A	2.30	105.58	101.87
24	t	104	BCR	C40-C30-C29	-2.30	99.73	108.91
20	A	563	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	c	5491	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	c	5497	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
20	C	492	CLA	CAA-C2A-C3A	-2.29	106.50	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5521	CLA	OBD-CAD-C3D	2.29	131.79	127.98
20	b	5526	CLA	O2D-CGD-CBD	2.29	115.34	111.27
20	c	5495	CLA	C6-C5-C3	2.29	119.46	113.45
21	A	562	PHO	C2A-C3A-C4A	2.29	105.87	101.34
21	A	561	PHO	C2A-C3A-C4A	2.29	105.87	101.34
20	C	500	CLA	CED-O2D-CGD	2.29	121.12	115.94
26	L	5213	SQD	C15-C14-C13	2.29	126.05	114.42
20	C	501	CLA	C2A-C1A-CHA	2.29	127.86	123.86
20	B	523	CLA	CMB-C2B-C3B	2.29	128.96	124.68
20	a	5563	CLA	C2A-C3A-C4A	2.29	105.56	101.87
20	c	5503	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
20	C	499	CLA	OBD-CAD-C3D	2.29	131.78	127.98
20	B	516	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
20	a	5563	CLA	O2D-CGD-CBD	2.29	115.33	111.27
20	B	519	CLA	C2A-C1A-CHA	2.29	127.86	123.86
20	c	5501	CLA	C12-C11-C10	-2.28	102.75	113.24
20	B	512	CLA	C2A-C3A-C4A	2.28	105.55	101.87
20	b	5511	CLA	CED-O2D-CGD	2.28	121.09	115.94
20	B	513	CLA	O2D-CGD-CBD	2.28	115.32	111.27
32	V	552	HEM	CMB-C2B-C3B	2.28	128.94	124.68
24	D	357	BCR	C23-C22-C21	-2.28	115.44	118.94
20	c	5500	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
30	C	508	DGD	C6E-C5E-C4E	-2.28	107.67	113.00
20	C	492	CLA	O2D-CGD-CBD	2.28	115.31	111.27
20	C	493	CLA	C2A-C1A-CHA	2.27	127.84	123.86
24	t	104	BCR	C34-C9-C8	2.27	121.66	118.08
20	c	5501	CLA	C1-C2-C3	2.27	129.97	126.04
24	B	529	BCR	C15-C14-C13	2.27	130.55	127.31
20	c	5494	CLA	C2A-C3A-C4A	2.27	105.54	101.87
20	C	499	CLA	C1-O2A-CGA	2.27	123.32	116.73
20	a	5560	CLA	C3C-C4C-NC	-2.27	108.03	110.57
20	C	501	CLA	C1-O2A-CGA	2.27	122.39	116.44
20	b	5515	CLA	C1-C2-C3	2.27	129.96	126.04
20	C	495	CLA	C2A-C1A-CHA	2.27	127.82	123.86
24	C	504	BCR	C11-C10-C9	2.26	130.54	127.31
20	C	501	CLA	OBD-CAD-CBD	-2.26	122.66	125.89
20	B	515	CLA	C6-C5-C3	2.26	119.39	113.45
28	D	359	MGE	C3G-O3G-C1D	-2.26	109.32	113.74
24	h	5107	BCR	C34-C9-C8	2.26	121.64	118.08
24	X	130	BCR	C19-C18-C17	-2.26	115.48	118.94
20	B	515	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
20	c	5499	CLA	C4D-C3D-CAD	-2.26	107.21	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	502	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
24	C	506	BCR	C23-C22-C21	-2.25	115.48	118.94
21	a	5562	PHO	C3D-C4D-CHA	2.25	115.57	109.49
20	b	5521	CLA	O2D-CGD-CBD	2.25	115.27	111.27
20	C	503	CLA	C1-C2-C3	2.25	130.40	126.75
20	D	355	CLA	C1-O2A-CGA	2.25	122.35	116.44
24	a	5566	BCR	C12-C13-C14	-2.25	115.49	118.94
26	d	5358	SQD	C34-C33-C32	2.25	125.85	114.42
20	B	521	CLA	O2A-CGA-CBA	2.25	118.96	111.91
20	C	501	CLA	C12-C11-C10	-2.25	102.92	113.24
20	b	5524	CLA	O2D-CGD-CBD	2.24	115.26	111.27
21	A	561	PHO	C3D-C4D-CHA	2.24	115.54	109.49
20	C	493	CLA	C12-C11-C10	-2.24	102.94	113.24
20	b	5511	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	C	504	BCR	C12-C13-C14	-2.24	115.50	118.94
24	X	130	BCR	C36-C18-C19	2.24	121.61	118.08
20	B	512	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	A	566	BCR	C12-C13-C14	-2.24	115.50	118.94
20	b	5523	CLA	C6-C5-C3	2.24	119.33	113.45
20	B	522	CLA	OBD-CAD-C3D	2.24	131.70	127.98
24	C	506	BCR	C24-C23-C22	2.24	129.62	126.23
27	T	217	LMT	C3'-C4'-C5'	-2.24	105.80	110.93
24	c	5504	BCR	C32-C1-C2	-2.24	99.96	108.91
28	b	5530	MGE	O1G-C1G-C2G	-2.24	101.92	108.43
20	b	5521	CLA	C1-C2-C3	2.24	129.91	126.04
20	d	5355	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
20	B	521	CLA	C1-C2-C3	2.23	129.91	126.04
22	A	564	PQ9	C21-C22-C23	-2.23	122.28	127.66
20	B	519	CLA	C1-O2A-CGA	2.23	122.30	116.44
20	B	516	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
24	D	357	BCR	C40-C30-C25	2.23	113.92	110.30
26	a	212	SQD	O8-S-O7	2.23	116.73	111.27
21	a	5562	PHO	C2A-C3A-C4A	2.23	105.75	101.34
20	b	5514	CLA	OBD-CAD-C3D	2.23	131.69	127.98
26	d	5358	SQD	C17-C16-C15	2.23	125.75	114.42
20	a	5563	CLA	CMB-C2B-C3B	2.23	128.85	124.68
28	l	5210	MGE	O1G-C1G-C2G	-2.23	101.94	108.43
24	x	5130	BCR	C37-C22-C23	2.23	121.59	118.08
26	t	213	SQD	C15-C14-C13	2.23	125.74	114.42
20	b	5513	CLA	C7-C6-C5	-2.22	107.32	113.36
24	x	5130	BCR	C36-C18-C19	2.22	121.58	118.08
20	A	559	CLA	CAA-CBA-CGA	2.22	119.75	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5521	CLA	O2A-CGA-CBA	2.22	118.88	111.91
24	d	5357	BCR	C19-C18-C17	-2.22	115.53	118.94
20	b	5526	CLA	C2A-C3A-C4A	2.22	105.45	101.87
24	H	107	BCR	C7-C8-C9	2.22	129.58	126.23
20	b	5514	CLA	C2A-C1A-CHA	2.21	127.73	123.86
20	b	5517	CLA	C2A-C1A-CHA	2.21	127.73	123.86
32	v	5552	HEM	CBA-CAA-C2A	2.21	116.57	112.49
24	c	5504	BCR	C11-C10-C9	2.21	130.47	127.31
20	B	512	CLA	O2D-CGD-CBD	2.21	115.20	111.27
27	M	5216	LMT	C1-O1'-C1'	-2.21	110.17	113.84
20	B	518	CLA	C6-C7-C8	2.21	123.07	115.92
20	C	500	CLA	O2D-CGD-CBD	2.21	115.19	111.27
20	B	514	CLA	C2A-C1A-CHA	2.21	127.72	123.86
20	B	519	CLA	O2A-CGA-CBA	2.21	118.84	111.91
20	c	5498	CLA	C2A-C3A-C4A	2.21	105.43	101.87
20	a	5560	CLA	O2A-CGA-CBA	2.21	118.83	111.91
22	D	356	PQ9	C14-C13-C15	2.20	118.98	115.27
20	a	5558	CLA	CMB-C2B-C3B	2.20	128.80	124.68
20	b	5512	CLA	O2D-CGD-CBD	2.20	115.18	111.27
20	b	5524	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
20	b	5525	CLA	C2A-C3A-C4A	2.20	105.42	101.87
24	D	357	BCR	C7-C8-C9	2.20	129.56	126.23
20	d	5355	CLA	O2D-CGD-CBD	2.20	115.18	111.27
26	A	568	SQD	C34-C33-C32	2.20	125.59	114.42
20	c	5503	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
24	H	107	BCR	C28-C27-C26	2.20	118.00	114.08
20	C	503	CLA	CMB-C2B-C3B	2.20	128.79	124.68
24	a	5566	BCR	C34-C9-C8	2.20	121.54	118.08
20	C	497	CLA	C12-C11-C10	-2.20	103.15	113.24
20	B	515	CLA	O2D-CGD-CBD	2.20	115.17	111.27
22	A	564	PQ9	C11-C2-C1	2.20	118.66	116.88
20	B	525	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
27	t	5217	LMT	O1B-C1B-C2B	2.20	113.79	108.10
24	x	5130	BCR	C32-C1-C2	-2.20	100.12	108.91
24	c	5505	BCR	C7-C8-C9	2.20	129.55	126.23
26	t	213	SQD	O9-S-C6	-2.19	104.33	106.94
20	C	500	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
20	b	5521	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
20	b	5512	CLA	C2A-C3A-C4A	2.19	105.41	101.87
20	c	5496	CLA	CBA-CAA-C2A	2.19	120.33	113.86
24	b	5527	BCR	C12-C13-C14	-2.19	115.58	118.94
20	c	5493	CLA	C2A-C1A-CHA	2.19	127.69	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5519	CLA	C2A-C1A-CHA	2.19	127.69	123.86
24	c	5504	BCR	C7-C8-C9	2.19	129.54	126.23
20	b	5518	CLA	CBA-CAA-C2A	2.19	120.32	113.86
28	L	210	MGE	O1G-C1G-C2G	-2.19	102.07	108.43
20	b	5511	CLA	C2A-C3A-C4A	2.19	104.57	101.78
20	B	513	CLA	C2A-C3A-C4A	2.19	105.40	101.87
20	b	5520	CLA	O2D-CGD-CBD	2.19	115.15	111.27
20	c	5500	CLA	CBA-CAA-C2A	2.18	120.31	113.86
20	C	496	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
20	C	502	CLA	O2D-CGD-CBD	2.18	115.14	111.27
24	H	107	BCR	C37-C22-C23	2.18	121.51	118.08
20	b	5520	CLA	C2A-C3A-C4A	2.18	105.39	101.87
20	c	5502	CLA	CBA-CAA-C2A	2.18	120.30	113.86
20	B	521	CLA	C12-C11-C10	-2.18	103.22	113.24
21	a	5562	PHO	C1-C2-C3	2.18	129.81	126.04
24	B	527	BCR	C19-C18-C17	-2.18	115.60	118.94
24	a	5566	BCR	C8-C9-C10	-2.18	115.60	118.94
20	b	5522	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
20	c	5503	CLA	OBD-CAD-C3D	2.18	131.59	127.98
21	a	5561	PHO	O2A-CGA-CBA	2.18	118.73	111.91
20	b	5520	CLA	C12-C11-C10	-2.17	103.25	113.24
22	A	564	PQ9	C6-C5-C4	2.17	119.44	114.99
20	D	354	CLA	OBD-CAD-C3D	2.17	131.59	127.98
20	c	5497	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
20	b	5514	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
20	C	492	CLA	C7-C6-C5	-2.17	107.46	113.36
24	d	5357	BCR	C23-C22-C21	-2.17	115.61	118.94
20	B	516	CLA	C2A-C3A-C4A	2.17	105.38	101.87
20	C	498	CLA	C2A-C3A-C4A	2.17	105.37	101.87
20	c	5492	CLA	O2D-CGD-CBD	2.17	115.12	111.27
20	b	5523	CLA	O2D-CGD-CBD	2.17	115.12	111.27
30	H	208	DGD	C3G-C2G-C1G	-2.17	106.66	111.79
20	C	499	CLA	CMB-C2B-C3B	2.17	128.73	124.68
20	c	5497	CLA	C12-C11-C10	-2.17	103.28	113.24
20	B	526	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
20	B	514	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
20	C	497	CLA	CMB-C2B-C1B	-2.17	125.14	128.46
20	b	5515	CLA	CBA-CAA-C2A	2.17	120.25	113.86
20	A	563	CLA	O2D-CGD-CBD	2.16	115.11	111.27
20	B	515	CLA	C2A-C1A-CHA	2.16	127.64	123.86
26	A	5212	SQD	O47-C45-C44	2.16	116.23	108.40
22	a	5564	PQ9	C21-C22-C23	-2.16	122.45	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	562	PHO	CMD-C2D-C1D	2.16	128.39	125.06
20	B	517	CLA	CBA-CAA-C2A	2.16	120.24	113.86
20	b	5511	CLA	OBD-CAD-CBD	-2.16	122.81	125.89
20	B	518	CLA	CBA-CAA-C2A	2.16	120.24	113.86
20	d	5355	CLA	C2A-C3A-C4A	2.16	105.36	101.87
24	b	5528	BCR	C7-C8-C9	2.16	129.50	126.23
20	B	525	CLA	C2A-C1A-CHA	2.16	127.63	123.86
20	C	498	CLA	C12-C11-C10	-2.16	103.33	113.24
20	c	5496	CLA	OBD-CAD-C3D	2.16	131.56	127.98
20	c	5493	CLA	O2D-CGD-CBD	2.16	115.10	111.27
20	c	5491	CLA	O2D-CGD-CBD	2.16	115.10	111.27
20	C	501	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
24	T	5104	BCR	C34-C9-C8	2.15	121.47	118.08
27	T	217	LMT	O1B-C1B-C2B	2.15	113.68	108.10
26	a	212	SQD	O10-C23-C24	-2.15	116.98	124.81
30	C	508	DGD	O3G-C3G-C2G	2.15	116.08	110.90
20	B	511	CLA	C2A-C1A-CHA	2.15	127.60	123.85
27	T	217	LMT	C1B-O1B-C4'	-2.15	112.65	117.96
20	b	5521	CLA	C12-C11-C10	-2.15	103.38	113.24
20	C	496	CLA	OBD-CAD-C3D	2.15	131.54	127.98
20	b	5518	CLA	C6-C7-C8	2.14	122.85	115.92
20	c	5492	CLA	C1-C2-C3	2.14	129.75	126.04
20	b	5514	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
24	c	5505	BCR	C34-C9-C8	2.14	121.45	118.08
24	h	5107	BCR	C36-C18-C19	2.14	121.45	118.08
24	h	5107	BCR	C28-C27-C26	2.14	117.89	114.08
20	c	5497	CLA	C6-C5-C3	2.14	119.06	113.45
20	B	520	CLA	C2A-C3A-C4A	2.14	105.32	101.87
20	c	5500	CLA	CMB-C2B-C3B	2.14	128.67	124.68
32	v	5552	HEM	C1D-C2D-C3D	-2.13	105.51	107.00
24	X	130	BCR	C8-C7-C6	2.13	133.19	127.20
24	b	5528	BCR	C35-C13-C12	2.13	121.44	118.08
24	C	504	BCR	C30-C25-C24	2.13	121.81	115.78
26	t	213	SQD	O8-S-O7	2.13	116.48	111.27
20	c	5494	CLA	C2A-C1A-CHA	2.13	127.58	123.86
24	C	504	BCR	C16-C17-C18	2.13	130.35	127.31
20	b	5518	CLA	O2A-C1-C2	2.13	114.23	108.64
24	b	5528	BCR	C32-C1-C2	-2.13	100.39	108.91
24	a	5566	BCR	C7-C8-C9	2.13	129.45	126.23
32	f	5051	HEM	CBA-CAA-C2A	-2.13	108.56	112.49
20	B	513	CLA	OBD-CAD-C3D	2.13	131.51	127.98
20	b	5512	CLA	OBD-CAD-C3D	2.13	131.51	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5517	CLA	CMB-C2B-C3B	2.13	128.66	124.68
20	b	5517	CLA	C2A-C3A-C4A	2.13	105.31	101.87
20	B	513	CLA	C6-C5-C3	2.13	119.03	113.45
32	f	5051	HEM	C4C-C3C-C2C	-2.13	105.41	106.90
20	A	563	CLA	CMA-C3A-C2A	-2.13	105.25	113.83
24	B	529	BCR	C36-C18-C19	2.13	121.43	118.08
20	b	5511	CLA	C2A-C1A-CHA	2.13	127.56	123.85
32	v	5552	HEM	C4A-C3A-C2A	2.12	108.47	107.00
24	C	505	BCR	C7-C8-C9	2.12	129.44	126.23
20	B	520	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
20	B	519	CLA	CMB-C2B-C3B	2.12	128.65	124.68
20	b	5516	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	C	506	BCR	C32-C1-C6	2.12	113.74	110.30
24	t	104	BCR	C16-C17-C18	2.12	130.34	127.31
20	B	514	CLA	C1-C2-C3	2.12	129.71	126.04
24	d	5357	BCR	C34-C9-C8	2.12	121.41	118.08
20	A	560	CLA	O2A-CGA-CBA	2.12	118.55	111.91
24	b	5529	BCR	C1-C6-C7	2.12	121.77	115.78
24	T	5104	BCR	C8-C9-C10	-2.12	115.69	118.94
20	a	5559	CLA	C1-C2-C3	2.12	129.70	126.04
20	C	493	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
24	B	528	BCR	C40-C30-C25	2.11	113.73	110.30
20	b	5518	CLA	CMB-C2B-C3B	2.11	128.63	124.68
20	c	5493	CLA	CBA-CAA-C2A	2.11	120.10	113.86
20	C	497	CLA	C6-C5-C3	2.11	119.00	113.45
30	C	509	DGD	C3G-O3G-C1D	-2.11	109.61	113.74
20	b	5526	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
20	c	5495	CLA	C2A-C3A-C4A	2.11	105.28	101.87
20	A	558	CLA	OBD-CAD-C3D	2.11	131.49	127.98
21	A	561	PHO	C1-O2A-CGA	2.11	121.98	116.44
20	b	5523	CLA	OBD-CAD-C3D	2.11	131.49	127.98
20	C	502	CLA	CBA-CAA-C2A	2.11	120.09	113.86
32	f	5051	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
20	b	5525	CLA	CMB-C2B-C3B	2.11	128.62	124.68
20	a	5559	CLA	CAA-CBA-CGA	2.11	119.41	113.25
26	A	568	SQD	C17-C16-C15	2.11	125.13	114.42
20	c	5497	CLA	CMB-C2B-C3B	2.11	128.62	124.68
20	b	5520	CLA	C4D-C3D-CAD	-2.11	107.30	108.47
22	D	356	PQ9	C30-C28-C29	2.11	119.26	114.60
24	x	5130	BCR	C8-C7-C6	2.11	133.12	127.20
20	B	514	CLA	CMB-C2B-C1B	-2.11	125.23	128.46
24	b	5529	BCR	C15-C14-C13	2.10	130.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5522	CLA	OBD-CAD-C3D	2.10	131.47	127.98
20	D	355	CLA	CBA-CAA-C2A	2.10	120.07	113.86
20	B	511	CLA	C2A-C3A-C4A	2.10	104.47	101.78
20	A	563	CLA	C7-C6-C5	-2.10	107.65	113.36
28	D	360	MGE	O1G-C1A-C2A	2.10	118.50	111.91
20	B	514	CLA	C1-O2A-CGA	2.10	121.96	116.44
20	b	5518	CLA	C2A-C3A-C4A	2.10	105.26	101.87
20	b	5525	CLA	C2A-C1A-CHA	2.10	127.53	123.86
20	A	558	CLA	CMA-C3A-C2A	-2.10	105.36	113.83
20	b	5515	CLA	CMA-C3A-C2A	-2.10	105.36	113.83
20	c	5491	CLA	C2A-C1A-CHA	2.10	127.53	123.86
24	c	5504	BCR	C34-C9-C8	2.10	121.38	118.08
20	C	496	CLA	C2A-C3A-C4A	2.10	105.26	101.87
21	a	5562	PHO	O2D-CGD-CBD	2.10	114.99	111.27
26	a	212	SQD	O47-C45-C44	2.10	115.99	108.40
24	h	5107	BCR	C30-C25-C24	2.10	121.71	115.78
20	C	499	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
20	B	518	CLA	C2A-C3A-C4A	2.09	105.25	101.87
20	c	5500	CLA	OBD-CAD-CBD	-2.09	122.91	125.89
24	d	5357	BCR	C32-C1-C6	2.09	113.69	110.30
20	B	524	CLA	C2A-C3A-C4A	2.09	105.24	101.87
30	h	5208	DGD	C3G-C2G-C1G	-2.09	106.85	111.79
20	A	558	CLA	CMB-C2B-C3B	2.09	128.58	124.68
20	C	491	CLA	CBA-CAA-C2A	2.09	120.03	113.86
24	B	529	BCR	C11-C10-C9	2.09	130.29	127.31
20	b	5515	CLA	O2D-CGD-CBD	2.09	114.98	111.27
20	B	517	CLA	O2D-CGD-CBD	2.09	114.98	111.27
22	a	5564	PQ9	C6-C5-C4	2.09	119.26	114.99
24	c	5505	BCR	C19-C18-C17	-2.08	115.74	118.94
20	c	5499	CLA	CMB-C2B-C3B	2.08	128.58	124.68
20	c	5501	CLA	C2A-C1A-CHA	2.08	127.50	123.86
24	D	357	BCR	C34-C9-C8	2.08	121.36	118.08
20	C	500	CLA	CMB-C2B-C3B	2.08	128.58	124.68
24	b	5528	BCR	C30-C25-C24	2.08	121.67	115.78
20	C	491	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
28	D	358	MGE	C3G-C2G-C1G	-2.08	106.87	111.79
24	H	107	BCR	C30-C25-C24	2.08	121.66	115.78
20	B	520	CLA	C2A-C1A-CHA	2.08	127.50	123.86
20	B	511	CLA	OBD-CAD-CBD	-2.08	122.93	125.89
24	D	357	BCR	C36-C18-C19	2.08	121.35	118.08
20	B	515	CLA	CBA-CAA-C2A	2.08	119.99	113.86
24	H	107	BCR	C34-C9-C8	2.08	121.35	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	355	CLA	C2A-C3A-C4A	2.08	105.22	101.87
20	C	493	CLA	CBA-CAA-C2A	2.08	119.99	113.86
20	C	496	CLA	C1-O2A-CGA	2.08	121.89	116.44
20	C	496	CLA	C2A-C1A-CHA	2.07	127.48	123.86
20	A	560	CLA	O2D-CGD-CBD	2.07	114.95	111.27
32	V	552	HEM	CBA-CAA-C2A	2.07	116.31	112.49
20	B	524	CLA	OBD-CAD-C3D	2.07	131.42	127.98
20	B	521	CLA	OBD-CAD-C3D	2.07	131.42	127.98
24	A	566	BCR	C34-C9-C8	2.07	121.34	118.08
24	T	5104	BCR	C19-C18-C17	-2.07	115.77	118.94
20	b	5513	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	C	497	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	c	5499	CLA	C1-O2A-CGA	2.06	122.73	116.73
20	b	5526	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	A	566	BCR	C1-C6-C7	2.06	121.61	115.78
28	d	5360	MGE	O1G-C1A-C2A	2.06	118.37	111.91
21	A	561	PHO	CMD-C2D-C1D	2.06	128.23	125.06
20	c	5503	CLA	C1-O2A-CGA	2.06	121.84	116.44
20	b	5513	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
20	B	526	CLA	CMB-C2B-C3B	2.05	128.52	124.68
30	c	5508	DGD	C6E-C5E-C4E	-2.05	108.19	113.00
20	D	354	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
20	c	5500	CLA	O2D-CGD-CBD	2.05	114.92	111.27
24	b	5527	BCR	C19-C18-C17	-2.05	115.79	118.94
24	a	5566	BCR	C19-C18-C17	-2.05	115.80	118.94
20	d	5355	CLA	C1-O2A-CGA	2.05	121.82	116.44
28	D	360	MGE	O1G-C1G-C2G	-2.05	102.47	108.43
20	B	525	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	x	5130	BCR	C24-C23-C22	2.05	129.33	126.23
27	M	5216	LMT	C6B-C5B-C4B	-2.05	108.20	113.00
20	A	560	CLA	OBD-CAD-C3D	2.05	131.38	127.98
20	c	5492	CLA	CMD-C2D-C3D	2.05	128.51	124.68
30	c	5508	DGD	O1G-C1A-C2A	2.05	118.33	111.91
20	d	5354	CLA	C2A-C1A-CHA	2.05	127.44	123.86
20	c	5495	CLA	C1-O2A-CGA	2.04	121.81	116.44
24	c	5505	BCR	C40-C30-C25	2.04	113.61	110.30
20	c	5502	CLA	CMB-C2B-C3B	2.04	128.50	124.68
20	B	517	CLA	CMB-C2B-C3B	2.04	128.50	124.68
26	L	5213	SQD	O8-S-O7	2.04	116.26	111.27
24	h	5107	BCR	C11-C12-C13	2.04	132.15	126.42
20	C	503	CLA	O2D-CGD-CBD	2.04	114.89	111.27
20	b	5514	CLA	C1-O2A-CGA	2.04	121.79	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	566	BCR	C30-C25-C24	2.03	121.53	115.78
30	c	5508	DGD	O3G-C3G-C2G	2.03	115.80	110.90
20	B	520	CLA	C12-C11-C10	-2.03	103.90	113.24
24	h	5107	BCR	C8-C9-C10	-2.03	115.82	118.94
20	b	5519	CLA	CMB-C2B-C3B	2.03	128.48	124.68
20	B	520	CLA	O2D-CGD-CBD	2.03	114.88	111.27
20	b	5523	CLA	CBA-CAA-C2A	2.03	119.85	113.86
20	d	5354	CLA	OBD-CAD-C3D	2.03	131.35	127.98
22	a	5564	PQ9	C11-C2-C1	2.03	118.52	116.88
20	B	517	CLA	C2A-C3A-C4A	2.03	105.14	101.87
20	d	5355	CLA	OBD-CAD-C3D	2.03	131.35	127.98
20	c	5496	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
20	d	5354	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
26	a	212	SQD	O5-C5-C4	2.02	113.37	109.69
20	c	5496	CLA	O2D-CGD-CBD	2.02	114.86	111.27
20	B	523	CLA	CBA-CAA-C2A	2.02	119.83	113.86
20	B	512	CLA	OBD-CAD-C3D	2.02	131.34	127.98
28	b	5530	MGE	C3G-C2G-C1G	-2.02	107.01	111.79
20	c	5501	CLA	C2A-C3A-C4A	2.02	105.13	101.87
20	B	522	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
26	t	213	SQD	O48-C23-O10	-2.02	118.49	123.59
20	b	5518	CLA	C16-C15-C13	2.02	122.45	115.92
27	m	216	LMT	C4B-C3B-C2B	-2.02	107.30	110.82
27	m	216	LMT	C1B-O1B-C4'	-2.02	112.97	117.96
32	f	5051	HEM	C4A-C3A-C2A	2.02	108.40	107.00
20	C	496	CLA	CBA-CAA-C2A	2.02	119.81	113.86
20	B	516	CLA	OBD-CAD-C3D	2.02	131.33	127.98
24	x	5130	BCR	C19-C18-C17	-2.01	115.85	118.94
20	C	500	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
20	C	495	CLA	OBD-CAD-C3D	2.01	131.32	127.98
20	b	5518	CLA	C6-C5-C3	2.01	118.73	113.45
30	C	508	DGD	O1G-C1A-C2A	2.01	118.22	111.91
20	c	5500	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
20	c	5492	CLA	C2A-C1A-CHA	2.01	127.38	123.86
20	B	512	CLA	C2A-C1A-CHA	2.01	127.38	123.86
24	b	5529	BCR	C36-C18-C19	2.01	121.25	118.08
20	B	515	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
20	b	5513	CLA	C6-C5-C3	2.01	118.73	113.45
20	c	5503	CLA	CMB-C2B-C3B	2.01	128.44	124.68
24	B	529	BCR	C1-C6-C7	2.01	121.46	115.78
20	b	5516	CLA	CMB-C2B-C3B	2.01	128.44	124.68
20	C	503	CLA	OBD-CAD-C3D	2.01	131.32	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5493	CLA	CMB-C2B-C3B	2.01	128.44	124.68
20	b	5519	CLA	C2A-C3A-C4A	2.01	105.11	101.87
20	C	492	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
30	h	5208	DGD	O3G-C3G-C2G	2.01	115.74	110.90
20	b	5515	CLA	C2A-C1A-CHA	2.00	127.36	123.86
32	F	51	HEM	C1D-C2D-C3D	-2.00	105.60	107.00
20	C	503	CLA	C2A-C3A-C4A	2.00	105.11	101.87
20	b	5524	CLA	CMB-C2B-C3B	2.00	128.43	124.68
20	A	563	CLA	CMB-C2B-C3B	2.00	128.42	124.68
20	B	513	CLA	CMA-C3A-C2A	-2.00	105.75	113.83
20	B	522	CLA	CBA-CAA-C2A	2.00	119.77	113.86

All (234) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	b	5526	CLA	NC
20	b	5526	CLA	ND
20	b	5526	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	ND
20	C	503	CLA	NA
20	b	5517	CLA	NC
20	b	5517	CLA	ND
20	b	5517	CLA	NA
20	B	512	CLA	NC
20	B	512	CLA	ND
20	B	512	CLA	NA
20	c	5495	CLA	NC
20	c	5495	CLA	ND
20	c	5495	CLA	NA
20	B	526	CLA	NC
20	B	526	CLA	ND
20	B	526	CLA	NA
20	C	495	CLA	NC
20	C	495	CLA	ND
20	C	495	CLA	NA
20	d	5354	CLA	NC
20	d	5354	CLA	ND
20	d	5354	CLA	NA
20	c	5492	CLA	NC
20	c	5492	CLA	ND
20	c	5492	CLA	NA

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Mol	Chain	Res	Type	Atom
20	B	518	CLA	NC
20	B	518	CLA	ND
20	B	518	CLA	NA
20	c	5497	CLA	NC
20	c	5497	CLA	ND
20	c	5497	CLA	NA
20	c	5496	CLA	NC
20	c	5496	CLA	ND
20	c	5496	CLA	NA
20	a	5559	CLA	NC
20	a	5559	CLA	ND
20	a	5559	CLA	NA
20	c	5503	CLA	NC
20	c	5503	CLA	ND
20	c	5503	CLA	NA
20	C	496	CLA	NC
20	C	496	CLA	ND
20	C	496	CLA	NA
20	B	520	CLA	NC
20	B	520	CLA	ND
20	B	520	CLA	NA
20	C	494	CLA	NC
20	C	494	CLA	ND
20	C	494	CLA	NA
20	C	491	CLA	NC
20	C	491	CLA	ND
20	C	491	CLA	NA
20	b	5520	CLA	NC
20	b	5520	CLA	ND
20	b	5520	CLA	NA
20	C	500	CLA	NC
20	C	500	CLA	ND
20	C	500	CLA	NA
20	C	493	CLA	NC
20	C	493	CLA	ND
20	C	493	CLA	NA
20	b	5514	CLA	NC
20	b	5514	CLA	ND
20	b	5514	CLA	NA
20	B	519	CLA	NC
20	B	519	CLA	ND
20	B	519	CLA	NA

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Mol	Chain	Res	Type	Atom
20	D	354	CLA	NC
20	D	354	CLA	ND
20	D	354	CLA	NA
20	B	516	CLA	NC
20	B	516	CLA	ND
20	B	516	CLA	NA
20	b	5512	CLA	NC
20	b	5512	CLA	ND
20	b	5512	CLA	NA
20	B	513	CLA	NC
20	B	513	CLA	ND
20	B	513	CLA	NA
20	c	5499	CLA	NC
20	c	5499	CLA	ND
20	c	5499	CLA	NA
30	h	5208	DGD	C2D
30	h	5208	DGD	C5D
30	h	5208	DGD	C5E
20	A	560	CLA	NC
20	A	560	CLA	ND
20	A	560	CLA	NA
20	d	5355	CLA	NC
20	d	5355	CLA	ND
20	d	5355	CLA	NA
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D
30	c	5507	DGD	C5E
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
20	B	525	CLA	NC
20	B	525	CLA	ND
20	B	525	CLA	NA
20	c	5500	CLA	NC
20	c	5500	CLA	ND
20	c	5500	CLA	NA
20	b	5518	CLA	NC
20	b	5518	CLA	ND
20	b	5518	CLA	NA
20	B	524	CLA	NC
20	B	524	CLA	ND
20	B	524	CLA	NA

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Mol	Chain	Res	Type	Atom
20	B	515	CLA	NC
20	B	515	CLA	ND
20	B	515	CLA	NA
20	b	5525	CLA	NC
20	b	5525	CLA	ND
20	b	5525	CLA	NA
30	C	508	DGD	C2D
30	C	508	DGD	C5D
30	C	508	DGD	C5E
20	C	502	CLA	NC
20	C	502	CLA	ND
20	C	502	CLA	NA
20	a	5558	CLA	NC
20	a	5558	CLA	ND
20	a	5558	CLA	NA
20	B	511	CLA	NC
20	B	511	CLA	ND
20	B	511	CLA	NA
20	b	5522	CLA	NC
20	b	5522	CLA	ND
20	b	5522	CLA	NA
20	b	5519	CLA	NC
20	b	5519	CLA	ND
20	b	5519	CLA	NA
20	B	522	CLA	NC
20	B	522	CLA	ND
20	B	522	CLA	NA
20	b	5516	CLA	NC
20	b	5516	CLA	ND
20	b	5516	CLA	NA
20	b	5513	CLA	NC
20	b	5513	CLA	ND
20	b	5513	CLA	NA
30	C	507	DGD	C2D
30	C	507	DGD	C5D
30	C	507	DGD	C5E
20	c	5502	CLA	NC
20	c	5502	CLA	ND
20	c	5502	CLA	NA
20	b	5523	CLA	NC
20	b	5523	CLA	ND
20	b	5523	CLA	NA

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Mol	Chain	Res	Type	Atom
20	a	5563	CLA	NC
20	a	5563	CLA	ND
20	a	5563	CLA	NA
30	c	5509	DGD	C2D
30	c	5509	DGD	C5D
30	c	5509	DGD	C5E
30	c	5508	DGD	C2D
30	c	5508	DGD	C5D
30	c	5508	DGD	C5E
20	b	5515	CLA	NC
20	b	5515	CLA	ND
20	b	5515	CLA	NA
20	c	5494	CLA	NC
20	c	5494	CLA	ND
20	c	5494	CLA	NA
20	c	5493	CLA	NC
20	c	5493	CLA	ND
20	c	5493	CLA	NA
20	B	523	CLA	NC
20	B	523	CLA	ND
20	B	523	CLA	NA
20	b	5511	CLA	NC
20	b	5511	CLA	ND
20	b	5511	CLA	NA
20	C	498	CLA	NC
20	C	498	CLA	ND
20	C	498	CLA	NA
30	C	509	DGD	C2D
30	C	509	DGD	C5D
30	C	509	DGD	C5E
20	A	563	CLA	NC
20	A	563	CLA	ND
20	A	563	CLA	NA
20	b	5521	CLA	NC
20	b	5521	CLA	ND
20	b	5521	CLA	NA
20	A	559	CLA	NC
20	A	559	CLA	ND
20	A	559	CLA	NA
20	A	558	CLA	NC
20	A	558	CLA	ND
20	A	558	CLA	NA

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Mol	Chain	Res	Type	Atom
20	B	517	CLA	NC
20	B	517	CLA	ND
20	B	517	CLA	NA
20	a	5560	CLA	NC
20	a	5560	CLA	ND
20	a	5560	CLA	NA
20	C	501	CLA	NC
20	C	501	CLA	ND
20	C	501	CLA	NA
20	D	355	CLA	NC
20	D	355	CLA	ND
20	D	355	CLA	NA
20	C	499	CLA	NC
20	C	499	CLA	ND
20	C	499	CLA	NA
20	b	5524	CLA	NC
20	b	5524	CLA	ND
20	b	5524	CLA	NA
20	c	5498	CLA	NC
20	c	5498	CLA	ND
20	c	5498	CLA	NA
20	c	5491	CLA	NC
20	c	5491	CLA	ND
20	c	5491	CLA	NA
20	B	521	CLA	NC
20	B	521	CLA	ND
20	B	521	CLA	NA
20	C	492	CLA	NC
20	C	492	CLA	ND
20	C	492	CLA	NA
20	c	5501	CLA	NC
20	c	5501	CLA	ND
20	c	5501	CLA	NA
20	C	497	CLA	NC
20	C	497	CLA	ND
20	C	497	CLA	NA
20	B	514	CLA	NC
20	B	514	CLA	ND
20	B	514	CLA	NA

All (1497) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	b	5526	CLA	C1A-C2A-CAA-CBA
20	b	5526	CLA	C1-C2-C3-C4
20	b	5526	CLA	C1-C2-C3-C5
20	C	503	CLA	C1A-C2A-CAA-CBA
20	C	503	CLA	C1-C2-C3-C4
20	C	503	CLA	C1-C2-C3-C5
20	b	5517	CLA	C1A-C2A-CAA-CBA
20	b	5517	CLA	C3A-C2A-CAA-CBA
20	b	5517	CLA	CHA-CBD-CGD-O1D
20	b	5517	CLA	CHA-CBD-CGD-O2D
20	b	5517	CLA	C1-C2-C3-C4
20	b	5517	CLA	C1-C2-C3-C5
20	c	5495	CLA	C1A-C2A-CAA-CBA
20	c	5495	CLA	CBD-CGD-O2D-CED
20	c	5495	CLA	C1-C2-C3-C4
20	c	5495	CLA	C1-C2-C3-C5
20	c	5495	CLA	C2-C3-C5-C6
20	c	5495	CLA	C4-C3-C5-C6
28	D	358	MGE	C2B-C1B-O2G-C2G
20	B	526	CLA	C1A-C2A-CAA-CBA
20	B	526	CLA	C1-C2-C3-C4
20	B	526	CLA	C1-C2-C3-C5
20	C	495	CLA	C1A-C2A-CAA-CBA
20	C	495	CLA	CBD-CGD-O2D-CED
20	C	495	CLA	C1-C2-C3-C4
20	C	495	CLA	C1-C2-C3-C5
20	C	495	CLA	C2-C3-C5-C6
20	C	495	CLA	C4-C3-C5-C6
20	d	5354	CLA	C1-C2-C3-C4
20	d	5354	CLA	C1-C2-C3-C5
20	c	5492	CLA	C1-C2-C3-C4
20	c	5492	CLA	C1-C2-C3-C5
20	B	518	CLA	C1A-C2A-CAA-CBA
20	B	518	CLA	C3A-C2A-CAA-CBA
20	B	518	CLA	C1-C2-C3-C4
20	B	518	CLA	C1-C2-C3-C5
20	B	518	CLA	C6-C7-C8-C9
20	c	5496	CLA	C1A-C2A-CAA-CBA
20	c	5496	CLA	CBD-CGD-O2D-CED
24	d	5357	BCR	C6-C7-C8-C9
20	a	5559	CLA	CHA-CBD-CGD-O1D
20	a	5559	CLA	CHA-CBD-CGD-O2D
20	a	5559	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
24	B	529	BCR	C6-C7-C8-C9
24	B	529	BCR	C23-C24-C25-C26
21	A	561	PHO	C1-C2-C3-C4
20	c	5503	CLA	C1A-C2A-CAA-CBA
20	c	5503	CLA	C1-C2-C3-C4
20	c	5503	CLA	C1-C2-C3-C5
20	C	496	CLA	C1A-C2A-CAA-CBA
20	C	496	CLA	CBD-CGD-O2D-CED
20	B	520	CLA	C2A-CAA-CBA-CGA
22	A	564	PQ9	C11-C12-C13-C14
22	A	564	PQ9	C11-C12-C13-C15
22	A	564	PQ9	C16-C17-C18-C19
22	A	564	PQ9	C16-C17-C18-C20
22	A	564	PQ9	C26-C27-C28-C29
20	C	494	CLA	C1A-C2A-CAA-CBA
22	D	356	PQ9	C16-C17-C18-C19
22	D	356	PQ9	C16-C17-C18-C20
22	D	356	PQ9	C21-C22-C23-C25
28	d	5360	MGE	C2B-C1B-O2G-C2G
24	b	5527	BCR	C6-C7-C8-C9
20	b	5520	CLA	C2A-CAA-CBA-CGA
20	b	5520	CLA	C1-C2-C3-C4
20	C	500	CLA	C1-C2-C3-C4
20	C	500	CLA	C1-C2-C3-C5
24	T	5104	BCR	C6-C7-C8-C9
20	B	519	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C5
28	b	5530	MGE	C2B-C1B-O2G-C2G
28	b	5530	MGE	C2D-C1D-O3G-C3G
28	b	5530	MGE	O6D-C1D-O3G-C3G
26	A	5212	SQD	O5-C1-O6-C44
26	A	5212	SQD	O6-C44-C45-O47
20	B	516	CLA	C1A-C2A-CAA-CBA
20	B	516	CLA	C3A-C2A-CAA-CBA
20	B	516	CLA	C1-C2-C3-C4
20	B	516	CLA	C1-C2-C3-C5
24	B	527	BCR	C6-C7-C8-C9
24	c	5505	BCR	C1-C6-C7-C8
24	c	5505	BCR	C6-C7-C8-C9
30	h	5208	DGD	O6D-C1D-O3G-C3G
30	h	5208	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
30	h	5208	DGD	O6E-C1E-O5D-C6D
20	A	560	CLA	CHA-CBD-CGD-O1D
20	A	560	CLA	CHA-CBD-CGD-O2D
20	d	5355	CLA	C1A-C2A-CAA-CBA
20	d	5355	CLA	C3A-C2A-CAA-CBA
20	d	5355	CLA	C2A-CAA-CBA-CGA
20	d	5355	CLA	C1-C2-C3-C4
30	c	5507	DGD	C2D-C1D-O3G-C3G
30	c	5507	DGD	O6D-C1D-O3G-C3G
30	c	5507	DGD	C2E-C1E-O5D-C6D
30	H	208	DGD	O6D-C1D-O3G-C3G
30	H	208	DGD	C2E-C1E-O5D-C6D
30	H	208	DGD	O6E-C1E-O5D-C6D
21	a	5561	PHO	C1-C2-C3-C4
20	B	525	CLA	C1-C2-C3-C4
20	B	525	CLA	C1-C2-C3-C5
20	c	5500	CLA	CBD-CGD-O2D-CED
20	c	5500	CLA	C1-C2-C3-C4
20	c	5500	CLA	C1-C2-C3-C5
20	b	5518	CLA	C1A-C2A-CAA-CBA
20	b	5518	CLA	C3A-C2A-CAA-CBA
20	b	5518	CLA	C1-C2-C3-C4
20	b	5518	CLA	C6-C7-C8-C9
22	d	5356	PQ9	C16-C17-C18-C19
22	d	5356	PQ9	C16-C17-C18-C20
22	d	5356	PQ9	C21-C22-C23-C25
24	A	566	BCR	C5-C6-C7-C8
26	L	5213	SQD	O5-C1-O6-C44
26	L	5213	SQD	O10-C23-O48-C46
26	L	5213	SQD	O5-C5-C6-S
26	d	5358	SQD	O5-C1-O6-C44
26	d	5358	SQD	C5-C6-S-O7
26	d	5358	SQD	C5-C6-S-O8
26	d	5358	SQD	C5-C6-S-O9
20	B	524	CLA	CHA-CBD-CGD-O1D
20	B	524	CLA	CHA-CBD-CGD-O2D
20	B	515	CLA	C1-C2-C3-C4
20	B	515	CLA	C1-C2-C3-C5
20	B	515	CLA	C2-C3-C5-C6
20	B	515	CLA	C4-C3-C5-C6
20	b	5525	CLA	C1-C2-C3-C4
20	b	5525	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
30	C	508	DGD	C2B-C1B-O2G-C2G
30	C	508	DGD	O6E-C1E-O5D-C6D
24	b	5528	BCR	C6-C7-C8-C9
20	C	502	CLA	C1A-C2A-CAA-CBA
20	C	502	CLA	CHA-CBD-CGD-O1D
20	C	502	CLA	CHA-CBD-CGD-O2D
24	C	505	BCR	C1-C6-C7-C8
24	C	505	BCR	C6-C7-C8-C9
20	a	5558	CLA	CBD-CGD-O2D-CED
20	B	511	CLA	CBD-CGD-O2D-CED
20	b	5522	CLA	C1-C2-C3-C4
28	D	360	MGE	C2B-C1B-O2G-C2G
24	c	5504	BCR	C1-C6-C7-C8
24	c	5504	BCR	C5-C6-C7-C8
24	c	5504	BCR	C6-C7-C8-C9
20	b	5519	CLA	C1-C2-C3-C4
28	B	530	MGE	C2B-C1B-O2G-C2G
28	B	530	MGE	C2D-C1D-O3G-C3G
28	B	530	MGE	O6D-C1D-O3G-C3G
20	B	522	CLA	C1-C2-C3-C4
28	I	201	MGE	O1A-C1A-O1G-C1G
28	I	201	MGE	C2B-C1B-O2G-C2G
28	I	201	MGE	C2D-C1D-O3G-C3G
28	I	201	MGE	O6D-C1D-O3G-C3G
20	b	5516	CLA	C1A-C2A-CAA-CBA
20	b	5516	CLA	C3A-C2A-CAA-CBA
20	b	5516	CLA	C1-C2-C3-C4
20	b	5516	CLA	C1-C2-C3-C5
30	C	507	DGD	C2D-C1D-O3G-C3G
30	C	507	DGD	O6D-C1D-O3G-C3G
30	C	507	DGD	C2E-C1E-O5D-C6D
20	c	5502	CLA	C1A-C2A-CAA-CBA
20	c	5502	CLA	CHA-CBD-CGD-O1D
20	c	5502	CLA	CHA-CBD-CGD-O2D
22	a	5564	PQ9	C11-C12-C13-C14
22	a	5564	PQ9	C11-C12-C13-C15
22	a	5564	PQ9	C16-C17-C18-C19
22	a	5564	PQ9	C16-C17-C18-C20
20	b	5523	CLA	C1-C2-C3-C4
20	b	5523	CLA	C1-C2-C3-C5
28	D	359	MGE	C2B-C1B-O2G-C2G
26	a	212	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
26	a	212	SQD	O6-C44-C45-O47
30	c	5508	DGD	C2B-C1B-O2G-C2G
30	c	5508	DGD	O1B-C1B-O2G-C2G
30	c	5508	DGD	O6E-C1E-O5D-C6D
24	C	504	BCR	C1-C6-C7-C8
24	C	504	BCR	C5-C6-C7-C8
24	C	504	BCR	C6-C7-C8-C9
20	b	5515	CLA	C1-C2-C3-C4
20	b	5515	CLA	C1-C2-C3-C5
20	b	5515	CLA	C2-C3-C5-C6
20	b	5515	CLA	C4-C3-C5-C6
20	c	5494	CLA	C1A-C2A-CAA-CBA
26	A	568	SQD	O5-C1-O6-C44
26	A	568	SQD	C5-C6-S-O7
26	A	568	SQD	C5-C6-S-O8
26	A	568	SQD	C5-C6-S-O9
24	b	5529	BCR	C6-C7-C8-C9
24	b	5529	BCR	C23-C24-C25-C26
20	B	523	CLA	C1-C2-C3-C4
20	b	5511	CLA	CBD-CGD-O2D-CED
20	C	498	CLA	C1-C2-C3-C4
24	B	528	BCR	C6-C7-C8-C9
20	A	559	CLA	CHA-CBD-CGD-O1D
20	A	559	CLA	CHA-CBD-CGD-O2D
20	A	559	CLA	C1-C2-C3-C4
20	B	517	CLA	C1A-C2A-CAA-CBA
20	B	517	CLA	C3A-C2A-CAA-CBA
20	B	517	CLA	CHA-CBD-CGD-O1D
20	B	517	CLA	CHA-CBD-CGD-O2D
20	B	517	CLA	C1-C2-C3-C4
20	B	517	CLA	C1-C2-C3-C5
26	t	213	SQD	O5-C1-O6-C44
26	t	213	SQD	O5-C5-C6-S
20	a	5560	CLA	CHA-CBD-CGD-O1D
20	a	5560	CLA	CHA-CBD-CGD-O2D
28	d	5361	MGE	C2B-C1B-O2G-C2G
20	C	501	CLA	C1-C2-C3-C4
20	C	501	CLA	C1-C2-C3-C5
24	C	506	BCR	C22-C23-C24-C25
24	C	506	BCR	C23-C24-C25-C26
24	c	5506	BCR	C22-C23-C24-C25
24	c	5506	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
28	d	5359	MGE	C2B-C1B-O2G-C2G
20	D	355	CLA	C1A-C2A-CAA-CBA
20	D	355	CLA	C3A-C2A-CAA-CBA
20	D	355	CLA	C2A-CAA-CBA-CGA
20	D	355	CLA	C1-C2-C3-C4
20	D	355	CLA	C1-C2-C3-C5
24	D	357	BCR	C6-C7-C8-C9
20	b	5524	CLA	CHA-CBD-CGD-O1D
20	b	5524	CLA	CHA-CBD-CGD-O2D
20	c	5498	CLA	C1-C2-C3-C4
20	c	5491	CLA	C1A-C2A-CAA-CBA
20	C	492	CLA	C1-C2-C3-C4
20	C	492	CLA	C1-C2-C3-C5
20	c	5501	CLA	C1-C2-C3-C4
20	c	5501	CLA	C1-C2-C3-C5
24	t	104	BCR	C6-C7-C8-C9
28	i	5201	MGE	C2B-C1B-O2G-C2G
28	i	5201	MGE	C2D-C1D-O3G-C3G
28	i	5201	MGE	O6D-C1D-O3G-C3G
20	a	5558	CLA	O1D-CGD-O2D-CED
20	A	558	CLA	O1D-CGD-O2D-CED
20	C	494	CLA	O1D-CGD-O2D-CED
26	A	5212	SQD	C24-C23-O48-C46
26	a	212	SQD	C24-C23-O48-C46
20	b	5526	CLA	CBD-CGD-O2D-CED
20	b	5517	CLA	CBD-CGD-O2D-CED
20	B	526	CLA	CBD-CGD-O2D-CED
21	A	562	PHO	CBD-CGD-O2D-CED
20	C	494	CLA	CBD-CGD-O2D-CED
20	C	500	CLA	CBD-CGD-O2D-CED
20	C	493	CLA	CBD-CGD-O2D-CED
20	b	5514	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	CBD-CGD-O2D-CED
20	c	5499	CLA	CBD-CGD-O2D-CED
20	d	5355	CLA	CBD-CGD-O2D-CED
20	B	524	CLA	CBD-CGD-O2D-CED
20	B	515	CLA	CBD-CGD-O2D-CED
20	C	502	CLA	CBD-CGD-O2D-CED
20	b	5513	CLA	CBD-CGD-O2D-CED
20	c	5502	CLA	CBD-CGD-O2D-CED
20	b	5515	CLA	CBD-CGD-O2D-CED
20	c	5494	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	c	5493	CLA	CBD-CGD-O2D-CED
20	A	558	CLA	CBD-CGD-O2D-CED
20	B	517	CLA	CBD-CGD-O2D-CED
20	D	355	CLA	CBD-CGD-O2D-CED
20	C	499	CLA	CBD-CGD-O2D-CED
20	b	5524	CLA	CBD-CGD-O2D-CED
21	a	5562	PHO	CBD-CGD-O2D-CED
20	B	514	CLA	CBD-CGD-O2D-CED
28	D	360	MGE	O1A-C1A-O1G-C1G
28	i	5201	MGE	O1A-C1A-O1G-C1G
20	b	5526	CLA	O1D-CGD-O2D-CED
20	c	5495	CLA	O1D-CGD-O2D-CED
20	B	526	CLA	O1D-CGD-O2D-CED
20	C	495	CLA	O1D-CGD-O2D-CED
20	c	5499	CLA	O1D-CGD-O2D-CED
20	B	511	CLA	O1D-CGD-O2D-CED
20	c	5494	CLA	O1D-CGD-O2D-CED
20	c	5496	CLA	O1D-CGD-O2D-CED
20	C	500	CLA	O1D-CGD-O2D-CED
20	C	493	CLA	O1D-CGD-O2D-CED
20	c	5500	CLA	O1D-CGD-O2D-CED
20	c	5493	CLA	O1D-CGD-O2D-CED
20	C	499	CLA	O1D-CGD-O2D-CED
26	L	5213	SQD	C24-C23-O48-C46
28	I	201	MGE	C2A-C1A-O1G-C1G
26	t	213	SQD	C24-C23-O48-C46
22	D	356	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C30
22	a	5564	PQ9	C26-C27-C28-C29
20	B	519	CLA	CBD-CGD-O2D-CED
20	B	525	CLA	CBD-CGD-O2D-CED
20	b	5525	CLA	CBD-CGD-O2D-CED
20	b	5519	CLA	CBD-CGD-O2D-CED
20	b	5523	CLA	CBD-CGD-O2D-CED
20	C	498	CLA	CBD-CGD-O2D-CED
20	A	563	CLA	CBD-CGD-O2D-CED
20	c	5498	CLA	CBD-CGD-O2D-CED
28	L	210	MGE	O1A-C1A-O1G-C1G
28	d	5360	MGE	O1A-C1A-O1G-C1G
28	D	359	MGE	O1A-C1A-O1G-C1G
28	l	5210	MGE	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
26	t	213	SQD	O10-C23-O48-C46
28	d	5361	MGE	O1A-C1A-O1G-C1G
20	C	496	CLA	O1D-CGD-O2D-CED
21	A	562	PHO	O1D-CGD-O2D-CED
26	A	5212	SQD	O10-C23-O48-C46
20	a	5563	CLA	CBD-CGD-O2D-CED
20	B	523	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	O1D-CGD-O2D-CED
20	b	5511	CLA	O1D-CGD-O2D-CED
21	a	5562	PHO	O1D-CGD-O2D-CED
28	D	358	MGE	O1B-C1B-O2G-C2G
28	d	5360	MGE	O1B-C1B-O2G-C2G
28	b	5530	MGE	O1B-C1B-O2G-C2G
30	C	508	DGD	O1B-C1B-O2G-C2G
28	B	530	MGE	O1B-C1B-O2G-C2G
28	I	201	MGE	O1B-C1B-O2G-C2G
28	D	359	MGE	O1B-C1B-O2G-C2G
28	d	5359	MGE	O1B-C1B-O2G-C2G
28	i	5201	MGE	O1B-C1B-O2G-C2G
20	B	512	CLA	C3-C5-C6-C7
21	A	562	PHO	C3-C5-C6-C7
20	b	5512	CLA	C3-C5-C6-C7
20	b	5523	CLA	C3-C5-C6-C7
20	B	523	CLA	C3-C5-C6-C7
21	a	5562	PHO	C3-C5-C6-C7
28	L	210	MGE	C2A-C1A-O1G-C1G
28	d	5360	MGE	C2A-C1A-O1G-C1G
28	D	360	MGE	C2A-C1A-O1G-C1G
28	D	359	MGE	C2A-C1A-O1G-C1G
28	l	5210	MGE	C2A-C1A-O1G-C1G
28	i	5201	MGE	C2A-C1A-O1G-C1G
22	A	564	PQ9	C26-C27-C28-C30
22	D	356	PQ9	C26-C27-C28-C30
22	a	5564	PQ9	C26-C27-C28-C30
30	C	508	DGD	O6D-C5D-C6D-O5D
30	c	5508	DGD	O6D-C5D-C6D-O5D
30	C	508	DGD	C4D-C5D-C6D-O5D
30	c	5508	DGD	C4D-C5D-C6D-O5D
26	a	212	SQD	O10-C23-O48-C46
20	C	496	CLA	C2A-CAA-CBA-CGA
20	C	494	CLA	C2A-CAA-CBA-CGA
20	c	5502	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	c	5494	CLA	C2A-CAA-CBA-CGA
20	C	498	CLA	C2A-CAA-CBA-CGA
20	c	5498	CLA	C2A-CAA-CBA-CGA
20	c	5501	CLA	C2A-CAA-CBA-CGA
20	B	518	CLA	C3-C5-C6-C7
20	b	5518	CLA	C3-C5-C6-C7
28	d	5361	MGE	C2A-C1A-O1G-C1G
20	b	5513	CLA	O1D-CGD-O2D-CED
20	b	5518	CLA	C1-C2-C3-C5
20	b	5522	CLA	C1-C2-C3-C5
20	B	522	CLA	C1-C2-C3-C5
20	B	523	CLA	C1-C2-C3-C5
22	D	356	PQ9	C21-C22-C23-C24
22	d	5356	PQ9	C21-C22-C23-C24
20	d	5355	CLA	O1D-CGD-O2D-CED
20	B	517	CLA	O1D-CGD-O2D-CED
28	D	360	MGE	O1B-C1B-O2G-C2G
28	d	5361	MGE	O1B-C1B-O2G-C2G
28	D	360	MGE	O6D-C5D-C6D-O5D
20	b	5522	CLA	CBD-CGD-O2D-CED
20	B	522	CLA	CBD-CGD-O2D-CED
20	b	5517	CLA	O1D-CGD-O2D-CED
20	D	355	CLA	O1D-CGD-O2D-CED
30	C	507	DGD	C4E-C5E-C6E-O5E
20	C	491	CLA	CBD-CGD-O2D-CED
20	b	5518	CLA	CBD-CGD-O2D-CED
20	C	501	CLA	CBD-CGD-O2D-CED
20	c	5491	CLA	CBD-CGD-O2D-CED
30	c	5507	DGD	C4E-C5E-C6E-O5E
20	C	502	CLA	O1D-CGD-O2D-CED
28	I	201	MGE	O6D-C5D-C6D-O5D
30	C	507	DGD	C4D-C5D-C6D-O5D
20	b	5524	CLA	O1D-CGD-O2D-CED
20	B	514	CLA	O1D-CGD-O2D-CED
20	B	515	CLA	C3-C5-C6-C7
28	b	5530	MGE	C2A-C1A-O1G-C1G
28	d	5361	MGE	O6D-C5D-C6D-O5D
22	D	356	PQ9	C24-C23-C25-C26
22	d	5356	PQ9	C24-C23-C25-C26
22	D	356	PQ9	C22-C23-C25-C26
22	d	5356	PQ9	C22-C23-C25-C26
30	h	5208	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
30	c	5507	DGD	O6D-C5D-C6D-O5D
30	C	507	DGD	O6D-C5D-C6D-O5D
20	c	5496	CLA	C2A-CAA-CBA-CGA
20	C	502	CLA	C2A-CAA-CBA-CGA
20	C	501	CLA	C2A-CAA-CBA-CGA
20	b	5514	CLA	O1D-CGD-O2D-CED
30	c	5507	DGD	C4D-C5D-C6D-O5D
28	d	5360	MGE	O6D-C5D-C6D-O5D
28	D	359	MGE	O6D-C5D-C6D-O5D
30	C	507	DGD	O6E-C1E-O5D-C6D
28	B	530	MGE	C2A-C1A-O1G-C1G
20	c	5502	CLA	O1D-CGD-O2D-CED
28	i	5201	MGE	O6D-C5D-C6D-O5D
30	H	208	DGD	O6D-C5D-C6D-O5D
20	B	524	CLA	O1D-CGD-O2D-CED
20	B	515	CLA	O1D-CGD-O2D-CED
20	b	5515	CLA	O1D-CGD-O2D-CED
28	b	5530	MGE	O1A-C1A-O1G-C1G
20	b	5520	CLA	C1-C2-C3-C5
28	D	359	MGE	C4D-C5D-C6D-O5D
28	B	530	MGE	O1A-C1A-O1G-C1G
20	b	5525	CLA	O1D-CGD-O2D-CED
26	d	5358	SQD	C24-C23-O48-C46
26	A	568	SQD	C24-C23-O48-C46
25	a	5567	LHG	C24-C23-O8-C6
28	d	5360	MGE	C4D-C5D-C6D-O5D
20	b	5523	CLA	O1D-CGD-O2D-CED
20	C	491	CLA	C15-C16-C17-C18
30	h	5208	DGD	C2D-C1D-O3G-C3G
30	H	208	DGD	C2D-C1D-O3G-C3G
30	C	508	DGD	C2E-C1E-O5D-C6D
30	c	5508	DGD	C2E-C1E-O5D-C6D
25	A	567	LHG	C24-C23-O8-C6
26	d	5358	SQD	O10-C23-O48-C46
20	B	518	CLA	C14-C13-C15-C16
20	b	5514	CLA	C6-C7-C8-C9
20	b	5518	CLA	C14-C13-C15-C16
20	a	5558	CLA	C14-C13-C15-C16
20	b	5522	CLA	C6-C7-C8-C9
20	B	522	CLA	C6-C7-C8-C9
20	A	558	CLA	C14-C13-C15-C16
20	C	501	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	c	5501	CLA	C6-C7-C8-C9
20	B	514	CLA	C6-C7-C8-C9
20	B	525	CLA	O1D-CGD-O2D-CED
20	c	5498	CLA	O1D-CGD-O2D-CED
20	C	493	CLA	C13-C15-C16-C17
20	C	498	CLA	O1D-CGD-O2D-CED
28	B	530	MGE	C1B-C2B-C3B-C4B
20	b	5517	CLA	C10-C11-C12-C13
21	A	562	PHO	C13-C15-C16-C17
20	A	558	CLA	C10-C11-C12-C13
20	B	517	CLA	C10-C11-C12-C13
21	a	5562	PHO	C13-C15-C16-C17
21	A	562	PHO	C10-C11-C12-C13
20	c	5497	CLA	C15-C16-C17-C18
20	b	5513	CLA	C5-C6-C7-C8
20	c	5493	CLA	C10-C11-C12-C13
20	c	5493	CLA	C13-C15-C16-C17
20	A	563	CLA	C5-C6-C7-C8
20	c	5491	CLA	C15-C16-C17-C18
28	D	358	MGE	C1B-C2B-C3B-C4B
28	d	5360	MGE	C1B-C2B-C3B-C4B
20	b	5519	CLA	O1D-CGD-O2D-CED
20	b	5516	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	C5-C6-C7-C8
20	a	5558	CLA	C10-C11-C12-C13
20	b	5519	CLA	C15-C16-C17-C18
20	a	5563	CLA	C5-C6-C7-C8
20	A	559	CLA	C15-C16-C17-C18
20	B	520	CLA	C1-C2-C3-C5
22	A	564	PQ9	C21-C22-C23-C24
28	D	358	MGE	C1A-C2A-C3A-C4A
28	b	5530	MGE	C1B-C2B-C3B-C4B
30	c	5507	DGD	C1A-C2A-C3A-C4A
28	D	359	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	C1A-C2A-C3A-C4A
28	d	5359	MGE	C1B-C2B-C3B-C4B
20	C	500	CLA	C5-C6-C7-C8
20	B	519	CLA	C15-C16-C17-C18
20	b	5522	CLA	C10-C11-C12-C13
20	B	523	CLA	C10-C11-C12-C13
20	C	497	CLA	C15-C16-C17-C18
21	a	5562	PHO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	a	5559	CLA	C15-C16-C17-C18
20	c	5500	CLA	C5-C6-C7-C8
20	b	5516	CLA	C13-C15-C16-C17
30	C	507	DGD	C1A-C2A-C3A-C4A
20	B	520	CLA	CBD-CGD-O2D-CED
20	B	516	CLA	CBD-CGD-O2D-CED
20	B	522	CLA	C10-C11-C12-C13
20	b	5523	CLA	C10-C11-C12-C13
20	B	520	CLA	C6-C7-C8-C10
20	b	5520	CLA	C6-C7-C8-C10
20	b	5518	CLA	C12-C13-C15-C16
20	B	515	CLA	C11-C10-C8-C7
20	b	5522	CLA	C6-C7-C8-C10
20	B	522	CLA	C6-C7-C8-C10
20	b	5515	CLA	C3-C5-C6-C7
25	A	567	LHG	O10-C23-O8-C6
26	A	568	SQD	O10-C23-O48-C46
25	a	5567	LHG	O10-C23-O8-C6
20	b	5517	CLA	C2A-CAA-CBA-CGA
20	B	517	CLA	C2A-CAA-CBA-CGA
20	B	519	CLA	O1D-CGD-O2D-CED
20	B	523	CLA	O1D-CGD-O2D-CED
20	A	563	CLA	O1D-CGD-O2D-CED
20	c	5493	CLA	C5-C6-C7-C8
28	d	5361	MGE	C4D-C5D-C6D-O5D
30	c	5507	DGD	O6E-C1E-O5D-C6D
20	B	526	CLA	C13-C15-C16-C17
20	C	493	CLA	C10-C11-C12-C13
20	B	519	CLA	C10-C11-C12-C13
20	B	516	CLA	C13-C15-C16-C17
20	b	5516	CLA	C10-C11-C12-C13
22	D	356	PQ9	C18-C20-C21-C22
22	d	5356	PQ9	C18-C20-C21-C22
30	c	5508	DGD	C4E-C5E-C6E-O5E
20	b	5517	CLA	C5-C6-C7-C8
20	b	5512	CLA	C15-C16-C17-C18
20	b	5515	CLA	C13-C15-C16-C17
30	C	509	DGD	C2A-C1A-O1G-C1G
30	C	508	DGD	C4E-C5E-C6E-O5E
28	D	360	MGE	C4D-C5D-C6D-O5D
20	b	5526	CLA	C13-C15-C16-C17
20	B	512	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	c	5495	CLA	C15-C16-C17-C18
20	C	493	CLA	C5-C6-C7-C8
20	c	5500	CLA	C15-C16-C17-C18
20	b	5522	CLA	C13-C15-C16-C17
20	b	5519	CLA	C10-C11-C12-C13
20	B	522	CLA	C13-C15-C16-C17
30	c	5507	DGD	O6E-C5E-C6E-O5E
20	a	5563	CLA	O1D-CGD-O2D-CED
20	c	5501	CLA	CBD-CGD-O2D-CED
28	L	210	MGE	C2B-C1B-O2G-C2G
20	C	495	CLA	C10-C11-C12-C13
20	C	495	CLA	C15-C16-C17-C18
20	B	516	CLA	C10-C11-C12-C13
20	A	560	CLA	C10-C11-C12-C13
20	B	515	CLA	C13-C15-C16-C17
20	b	5523	CLA	C5-C6-C7-C8
20	B	523	CLA	C5-C6-C7-C8
20	C	498	CLA	C13-C15-C16-C17
20	B	517	CLA	C5-C6-C7-C8
20	a	5560	CLA	C10-C11-C12-C13
20	c	5498	CLA	C13-C15-C16-C17
22	a	5564	PQ9	C21-C22-C23-C24
20	c	5495	CLA	C10-C11-C12-C13
20	B	517	CLA	C8-C10-C11-C12
30	c	5507	DGD	O1B-C1B-O2G-C2G
20	b	5517	CLA	C8-C10-C11-C12
30	C	507	DGD	O6E-C5E-C6E-O5E
30	c	5509	DGD	C2A-C1A-O1G-C1G
28	i	5201	MGE	C9A-CAA-CBA-CCA
30	c	5507	DGD	C2B-C1B-O2G-C2G
28	l	5210	MGE	C2B-C1B-O2G-C2G
20	a	5559	CLA	C5-C6-C7-C8
20	C	500	CLA	C15-C16-C17-C18
20	A	559	CLA	C5-C6-C7-C8
28	L	210	MGE	CCB-CDB-CEB-CFB
30	h	5208	DGD	C5B-C6B-C7B-C8B
30	H	208	DGD	C5B-C6B-C7B-C8B
26	L	5213	SQD	C11-C12-C13-C14
28	B	530	MGE	C9A-CAA-CBA-CCA
28	D	359	MGE	C3B-C4B-C5B-C6B
26	t	213	SQD	C9-C10-C11-C12
26	t	213	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	a	5567	LHG	C30-C31-C32-C33
28	L	210	MGE	C5B-C6B-C7B-C8B
28	d	5360	MGE	C3B-C4B-C5B-C6B
28	b	5530	MGE	C9A-CAA-CBA-CCA
30	h	5208	DGD	C5A-C6A-C7A-C8A
30	H	208	DGD	C5A-C6A-C7A-C8A
25	A	567	LHG	C30-C31-C32-C33
28	l	5210	MGE	C3B-C4B-C5B-C6B
30	C	509	DGD	C8B-C9B-CAB-CBB
28	L	210	MGE	O1B-C1B-O2G-C2G
30	C	507	DGD	O1B-C1B-O2G-C2G
30	c	5509	DGD	O1B-C1B-O2G-C2G
28	l	5210	MGE	O1B-C1B-O2G-C2G
20	d	5355	CLA	C1-C2-C3-C5
28	L	210	MGE	C3B-C4B-C5B-C6B
28	I	201	MGE	C9A-CAA-CBA-CCA
28	D	359	MGE	C8B-C9B-CAB-CBB
28	l	5210	MGE	CCB-CDB-CEB-CFB
30	C	509	DGD	O1A-C1A-O1G-C1G
28	d	5360	MGE	C8B-C9B-CAB-CBB
26	L	5213	SQD	C9-C10-C11-C12
30	c	5509	DGD	C8B-C9B-CAB-CBB
28	l	5210	MGE	C5B-C6B-C7B-C8B
30	C	509	DGD	C7A-C8A-C9A-CAA
28	L	210	MGE	CAB-CBB-CCB-CDB
30	C	507	DGD	C9A-CAA-CBA-CCA
30	c	5509	DGD	C7A-C8A-C9A-CAA
28	L	210	MGE	C2D-C1D-O3G-C3G
28	l	5210	MGE	C2D-C1D-O3G-C3G
20	a	5559	CLA	C1-C2-C3-C5
20	A	559	CLA	C1-C2-C3-C5
28	L	210	MGE	C9B-CAB-CBB-CCB
30	c	5507	DGD	C9A-CAA-CBA-CCA
30	H	208	DGD	C3B-C4B-C5B-C6B
28	B	530	MGE	C3B-C4B-C5B-C6B
28	l	5210	MGE	C9B-CAB-CBB-CCB
28	d	5359	MGE	C7B-C8B-C9B-CAB
20	b	5520	CLA	C5-C6-C7-C8
20	c	5492	CLA	C11-C12-C13-C14
28	D	358	MGE	C7B-C8B-C9B-CAB
30	c	5509	DGD	C9B-CAB-CBB-CCB
26	A	568	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	C	509	DGD	C9B-CAB-CBB-CCB
20	a	5559	CLA	C6-C7-C8-C9
21	a	5561	PHO	C11-C10-C8-C9
20	A	559	CLA	C6-C7-C8-C9
28	D	358	MGE	C4A-C5A-C6A-C7A
28	L	210	MGE	C4B-C5B-C6B-C7B
28	b	5530	MGE	C4A-C5A-C6A-C7A
28	b	5530	MGE	C3B-C4B-C5B-C6B
28	b	5530	MGE	C7B-C8B-C9B-CAB
30	h	5208	DGD	C3B-C4B-C5B-C6B
30	c	5507	DGD	C3B-C4B-C5B-C6B
26	d	5358	SQD	C32-C33-C34-C35
28	B	530	MGE	CBB-CCB-CDB-CEB
30	C	507	DGD	C3B-C4B-C5B-C6B
28	l	5210	MGE	CAB-CBB-CCB-CDB
28	d	5359	MGE	C4A-C5A-C6A-C7A
28	d	5359	MGE	C5A-C6A-C7A-C8A
28	d	5359	MGE	C8B-C9B-CAB-CBB
20	B	520	CLA	C5-C6-C7-C8
30	c	5509	DGD	O1A-C1A-O1G-C1G
28	D	358	MGE	C7A-C8A-C9A-CAA
28	D	358	MGE	C8B-C9B-CAB-CBB
28	b	5530	MGE	CBB-CCB-CDB-CEB
28	I	201	MGE	C3B-C4B-C5B-C6B
28	l	5210	MGE	C4B-C5B-C6B-C7B
25	A	567	LHG	O1-C1-C2-C3
30	C	507	DGD	C2B-C1B-O2G-C2G
30	c	5509	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	CBA-CCA-CDA-CEA
28	B	530	MGE	C7B-C8B-C9B-CAB
28	d	5361	MGE	C4B-C5B-C6B-C7B
28	d	5359	MGE	C7A-C8A-C9A-CAA
28	i	5201	MGE	C3B-C4B-C5B-C6B
20	B	522	CLA	O1D-CGD-O2D-CED
28	D	358	MGE	C5A-C6A-C7A-C8A
30	h	5208	DGD	CBA-CCA-CDA-CEA
28	D	360	MGE	C6B-C7B-C8B-C9B
28	B	530	MGE	C4A-C5A-C6A-C7A
28	I	201	MGE	C2A-C3A-C4A-C5A
28	i	5201	MGE	C7A-C8A-C9A-CAA
20	c	5492	CLA	C11-C12-C13-C15
20	C	492	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	C	492	CLA	C11-C12-C13-C15
28	L	210	MGE	O6D-C1D-O3G-C3G
28	l	5210	MGE	O6D-C1D-O3G-C3G
28	D	360	MGE	C4B-C5B-C6B-C7B
30	c	5509	DGD	CBB-CCB-CDB-CEB
28	l	5210	MGE	C6B-C7B-C8B-C9B
30	C	509	DGD	CBB-CCB-CDB-CEB
30	H	208	DGD	C4D-C5D-C6D-O5D
20	b	5522	CLA	O1D-CGD-O2D-CED
28	D	358	MGE	C4B-C5B-C6B-C7B
28	L	210	MGE	C6B-C7B-C8B-C9B
28	I	201	MGE	C7A-C8A-C9A-CAA
20	C	495	CLA	C5-C6-C7-C8
26	L	5213	SQD	C12-C13-C14-C15
30	c	5509	DGD	CCB-CDB-CEB-CFB
28	i	5201	MGE	C2A-C3A-C4A-C5A
26	t	213	SQD	C12-C13-C14-C15
28	d	5361	MGE	C6B-C7B-C8B-C9B
20	C	491	CLA	O1D-CGD-O2D-CED
20	c	5491	CLA	O1D-CGD-O2D-CED
20	B	512	CLA	C3A-C2A-CAA-CBA
20	c	5495	CLA	C3A-C2A-CAA-CBA
20	C	495	CLA	C3A-C2A-CAA-CBA
20	d	5354	CLA	C3A-C2A-CAA-CBA
20	c	5496	CLA	C3A-C2A-CAA-CBA
20	C	496	CLA	C3A-C2A-CAA-CBA
20	C	494	CLA	C3A-C2A-CAA-CBA
20	D	354	CLA	C3A-C2A-CAA-CBA
20	B	515	CLA	C3A-C2A-CAA-CBA
20	b	5515	CLA	C3A-C2A-CAA-CBA
20	c	5494	CLA	C3A-C2A-CAA-CBA
20	c	5495	CLA	C5-C6-C7-C8
30	h	5208	DGD	C4D-C5D-C6D-O5D
28	d	5359	MGE	C4B-C5B-C6B-C7B
30	c	5507	DGD	C4A-C5A-C6A-C7A
30	H	208	DGD	C4B-C5B-C6B-C7B
28	D	360	MGE	C7A-C8A-C9A-CAA
28	I	201	MGE	C9B-CAB-CBB-CCB
26	A	568	SQD	C12-C13-C14-C15
30	h	5208	DGD	C4B-C5B-C6B-C7B
30	C	509	DGD	CCB-CDB-CEB-CFB
28	d	5361	MGE	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	i	5201	MGE	C9B-CAB-CBB-CCB
20	B	514	CLA	C3-C5-C6-C7
26	d	5358	SQD	C12-C13-C14-C15
28	d	5361	MGE	C7A-C8A-C9A-CAA
20	A	560	CLA	C13-C15-C16-C17
30	h	5208	DGD	C2A-C1A-O1G-C1G
26	d	5358	SQD	C8-C7-O47-C45
26	A	568	SQD	C8-C7-O47-C45
28	d	5361	MGE	C5B-C6B-C7B-C8B
21	a	5561	PHO	C1-C2-C3-C5
30	C	508	DGD	C5A-C6A-C7A-C8A
28	D	360	MGE	C5B-C6B-C7B-C8B
28	B	530	MGE	C8B-C9B-CAB-CBB
30	C	507	DGD	C4A-C5A-C6A-C7A
28	D	359	MGE	CAB-CBB-CCB-CDB
28	d	5360	MGE	CBB-CCB-CDB-CEB
26	d	5358	SQD	O49-C7-O47-C45
26	A	568	SQD	O49-C7-O47-C45
30	C	509	DGD	O1B-C1B-O2G-C2G
28	D	360	MGE	C7B-C8B-C9B-CAB
25	A	567	LHG	C28-C29-C30-C31
28	D	359	MGE	CBB-CCB-CDB-CEB
20	D	354	CLA	C13-C15-C16-C17
28	D	360	MGE	C8B-C9B-CAB-CBB
28	I	201	MGE	C3A-C4A-C5A-C6A
28	l	5210	MGE	C7A-C8A-C9A-CAA
24	d	5357	BCR	C5-C6-C7-C8
24	B	529	BCR	C23-C24-C25-C30
20	b	5514	CLA	C3-C5-C6-C7
24	T	5104	BCR	C23-C24-C25-C26
24	T	5104	BCR	C23-C24-C25-C30
24	A	566	BCR	C1-C6-C7-C8
24	A	566	BCR	C23-C24-C25-C26
24	A	566	BCR	C23-C24-C25-C30
24	x	5130	BCR	C5-C6-C7-C8
24	x	5130	BCR	C23-C24-C25-C26
24	x	5130	BCR	C23-C24-C25-C30
24	c	5504	BCR	C23-C24-C25-C26
24	c	5504	BCR	C23-C24-C25-C30
24	a	5566	BCR	C1-C6-C7-C8
24	a	5566	BCR	C5-C6-C7-C8
24	a	5566	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	a	5566	BCR	C23-C24-C25-C30
24	C	504	BCR	C23-C24-C25-C26
24	C	504	BCR	C23-C24-C25-C30
24	h	5107	BCR	C1-C6-C7-C8
24	h	5107	BCR	C5-C6-C7-C8
24	h	5107	BCR	C23-C24-C25-C26
24	h	5107	BCR	C23-C24-C25-C30
24	b	5529	BCR	C23-C24-C25-C30
20	C	498	CLA	C3-C5-C6-C7
24	H	107	BCR	C1-C6-C7-C8
24	H	107	BCR	C5-C6-C7-C8
24	H	107	BCR	C23-C24-C25-C26
24	H	107	BCR	C23-C24-C25-C30
24	C	506	BCR	C23-C24-C25-C30
24	c	5506	BCR	C23-C24-C25-C30
24	D	357	BCR	C5-C6-C7-C8
24	X	130	BCR	C5-C6-C7-C8
24	X	130	BCR	C23-C24-C25-C26
24	X	130	BCR	C23-C24-C25-C30
24	t	104	BCR	C23-C24-C25-C26
24	t	104	BCR	C23-C24-C25-C30
28	L	210	MGE	C7A-C8A-C9A-CAA
30	c	5508	DGD	C5A-C6A-C7A-C8A
26	A	568	SQD	C17-C18-C19-C20
20	b	5526	CLA	C15-C16-C17-C18
21	A	561	PHO	C8-C10-C11-C12
20	B	516	CLA	C5-C6-C7-C8
20	b	5516	CLA	C5-C6-C7-C8
30	H	208	DGD	C2B-C1B-O2G-C2G
30	C	509	DGD	C2B-C1B-O2G-C2G
28	d	5360	MGE	CAB-CBB-CCB-CDB
28	d	5361	MGE	C7B-C8B-C9B-CAB
30	h	5208	DGD	O1A-C1A-O1G-C1G
20	b	5520	CLA	CBD-CGD-O2D-CED
28	i	5201	MGE	C3A-C4A-C5A-C6A
20	c	5495	CLA	C13-C15-C16-C17
20	B	526	CLA	C15-C16-C17-C18
21	a	5561	PHO	C8-C10-C11-C12
20	B	523	CLA	C4-C3-C5-C6
20	B	518	CLA	C12-C13-C15-C16
20	A	560	CLA	C11-C12-C13-C15
20	b	5515	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	a	5560	CLA	C11-C12-C13-C15
20	C	501	CLA	C12-C13-C15-C16
30	C	509	DGD	C2A-C3A-C4A-C5A
20	C	495	CLA	C13-C15-C16-C17
20	d	5354	CLA	C13-C15-C16-C17
20	a	5560	CLA	C13-C15-C16-C17
20	C	497	CLA	C5-C6-C7-C8
20	B	518	CLA	CBD-CGD-O2D-CED
20	C	501	CLA	O1D-CGD-O2D-CED
25	A	567	LHG	O9-C7-O7-C5
30	h	5208	DGD	C1B-C2B-C3B-C4B
28	d	5361	MGE	C1B-C2B-C3B-C4B
30	H	208	DGD	C2A-C1A-O1G-C1G
20	C	503	CLA	C2A-CAA-CBA-CGA
25	a	5567	LHG	C28-C29-C30-C31
28	i	5201	MGE	C4A-C5A-C6A-C7A
30	H	208	DGD	C1B-C2B-C3B-C4B
26	d	5358	SQD	C25-C26-C27-C28
21	A	561	PHO	C2B-C3B-CAB-CBB
21	a	5561	PHO	C2B-C3B-CAB-CBB
20	c	5498	CLA	C3-C5-C6-C7
26	L	5213	SQD	C25-C26-C27-C28
30	c	5509	DGD	C2A-C3A-C4A-C5A
26	A	568	SQD	C25-C26-C27-C28
28	b	5530	MGE	C8B-C9B-CAB-CBB
30	h	5208	DGD	C7A-C8A-C9A-CAA
30	C	509	DGD	C7B-C8B-C9B-CAB
30	h	5208	DGD	C2B-C1B-O2G-C2G
26	L	5213	SQD	C8-C7-O47-C45
25	A	567	LHG	C8-C7-O7-C5
26	t	213	SQD	C8-C7-O47-C45
25	a	5567	LHG	C8-C7-O7-C5
26	d	5358	SQD	C17-C18-C19-C20
21	A	561	PHO	C4B-C3B-CAB-CBB
21	a	5561	PHO	C4B-C3B-CAB-CBB
27	A	569	LMT	C3-C4-C5-C6
30	c	5509	DGD	C7B-C8B-C9B-CAB
30	h	5208	DGD	O1B-C1B-O2G-C2G
30	H	208	DGD	O1B-C1B-O2G-C2G
26	L	5213	SQD	O49-C7-O47-C45
30	H	208	DGD	C7A-C8A-C9A-CAA
28	D	360	MGE	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	d	5361	MGE	O2G-C2G-C3G-O3G
28	I	201	MGE	C4A-C5A-C6A-C7A
30	c	5508	DGD	C4A-C5A-C6A-C7A
20	c	5497	CLA	C5-C6-C7-C8
20	b	5523	CLA	C4-C3-C5-C6
26	L	5213	SQD	C17-C18-C19-C20
30	C	508	DGD	C4A-C5A-C6A-C7A
20	a	5559	CLA	C14-C13-C15-C16
20	C	500	CLA	C11-C10-C8-C9
20	b	5514	CLA	C11-C10-C8-C9
20	B	525	CLA	C11-C10-C8-C9
20	c	5500	CLA	C11-C10-C8-C9
20	B	515	CLA	C11-C10-C8-C9
20	b	5525	CLA	C11-C10-C8-C9
20	b	5515	CLA	C11-C10-C8-C9
20	B	514	CLA	C11-C10-C8-C9
20	a	5558	CLA	C2A-CAA-CBA-CGA
20	A	558	CLA	C2A-CAA-CBA-CGA
26	t	213	SQD	C25-C26-C27-C28
28	B	530	MGE	C5A-C6A-C7A-C8A
28	i	5201	MGE	C6A-C7A-C8A-C9A
30	H	208	DGD	O1A-C1A-O1G-C1G
20	b	5518	CLA	O1D-CGD-O2D-CED
20	d	5354	CLA	C1A-C2A-CAA-CBA
20	C	491	CLA	C1A-C2A-CAA-CBA
20	D	354	CLA	C1A-C2A-CAA-CBA
20	B	515	CLA	C1A-C2A-CAA-CBA
20	b	5515	CLA	C1A-C2A-CAA-CBA
21	A	561	PHO	C16-C17-C18-C20
21	a	5561	PHO	C16-C17-C18-C20
25	a	5567	LHG	O9-C7-O7-C5
25	A	567	LHG	C26-C27-C28-C29
21	A	562	PHO	C15-C16-C17-C18
20	b	5515	CLA	C15-C16-C17-C18
28	D	359	MGE	C9B-CAB-CBB-CCB
21	a	5561	PHO	C5-C6-C7-C8
21	a	5561	PHO	C16-C17-C18-C19
20	d	5355	CLA	C2C-C3C-CAC-CBC
20	b	5521	CLA	C15-C16-C17-C18
20	C	491	CLA	C13-C15-C16-C17
20	B	515	CLA	C15-C16-C17-C18
28	b	5530	MGE	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
21	A	561	PHO	C5-C6-C7-C8
21	A	561	PHO	C16-C17-C18-C19
28	d	5360	MGE	C1G-C2G-C3G-O3G
28	I	201	MGE	C6A-C7A-C8A-C9A
28	D	359	MGE	C1G-C2G-C3G-O3G
30	H	208	DGD	CAA-CBA-CCA-CDA
27	a	5568	LMT	C3-C4-C5-C6
30	c	5507	DGD	C5D-C6D-O5D-C1E
30	C	508	DGD	C5D-C6D-O5D-C1E
30	C	507	DGD	C5D-C6D-O5D-C1E
30	c	5508	DGD	C5D-C6D-O5D-C1E
28	l	5210	MGE	CBB-CCB-CDB-CEB
25	a	5567	LHG	C26-C27-C28-C29
26	t	213	SQD	C17-C18-C19-C20
28	d	5361	MGE	C5A-C6A-C7A-C8A
28	d	5360	MGE	C9B-CAB-CBB-CCB
30	c	5509	DGD	CDB-CEB-CFB-CGB
25	a	5567	LHG	C27-C28-C29-C30
30	h	5208	DGD	CAA-CBA-CCA-CDA
28	D	360	MGE	C5A-C6A-C7A-C8A
30	C	507	DGD	CBA-CCA-CDA-CEA
26	A	568	SQD	C27-C28-C29-C30
20	D	355	CLA	C2C-C3C-CAC-CBC
28	l	5210	MGE	CDB-CEB-CFB-CGB
30	c	5507	DGD	CBA-CCA-CDA-CEA
30	C	509	DGD	CDB-CEB-CFB-CGB
28	L	210	MGE	CDB-CEB-CFB-CGB
25	a	5567	LHG	C35-C36-C37-C38
28	D	358	MGE	O6D-C5D-C6D-O5D
26	t	213	SQD	O49-C7-O47-C45
25	A	567	LHG	C35-C36-C37-C38
28	D	360	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	O6D-C5D-C6D-O5D
26	d	5358	SQD	C27-C28-C29-C30
20	B	520	CLA	O1D-CGD-O2D-CED
20	c	5491	CLA	C13-C15-C16-C17
20	B	521	CLA	C15-C16-C17-C18
28	d	5361	MGE	C2A-C3A-C4A-C5A
20	c	5501	CLA	O1D-CGD-O2D-CED
21	a	5562	PHO	C15-C16-C17-C18
30	c	5509	DGD	C4A-C5A-C6A-C7A
20	c	5495	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	C	495	CLA	C11-C10-C8-C7
21	A	562	PHO	C11-C10-C8-C7
20	c	5496	CLA	C11-C10-C8-C7
20	c	5496	CLA	C12-C13-C15-C16
20	a	5559	CLA	C11-C10-C8-C7
20	a	5559	CLA	C12-C13-C15-C16
20	C	496	CLA	C11-C10-C8-C7
20	C	496	CLA	C12-C13-C15-C16
20	C	500	CLA	C11-C10-C8-C7
20	C	493	CLA	C11-C12-C13-C15
20	b	5514	CLA	C11-C10-C8-C7
20	b	5512	CLA	C11-C12-C13-C15
20	B	513	CLA	C11-C10-C8-C7
20	B	525	CLA	C11-C10-C8-C7
20	c	5500	CLA	C11-C10-C8-C7
20	b	5525	CLA	C11-C10-C8-C7
20	a	5558	CLA	C11-C10-C8-C7
20	a	5558	CLA	C12-C13-C15-C16
20	b	5522	CLA	C11-C10-C8-C7
20	B	522	CLA	C11-C10-C8-C7
20	c	5493	CLA	C11-C12-C13-C15
20	A	559	CLA	C12-C13-C15-C16
20	A	558	CLA	C11-C10-C8-C7
20	A	558	CLA	C12-C13-C15-C16
20	c	5501	CLA	C11-C10-C8-C7
20	B	514	CLA	C11-C10-C8-C7
20	c	5495	CLA	C11-C10-C8-C9
20	C	495	CLA	C11-C10-C8-C9
20	d	5354	CLA	C14-C13-C15-C16
21	A	562	PHO	C11-C10-C8-C9
20	c	5496	CLA	C11-C10-C8-C9
20	c	5496	CLA	C14-C13-C15-C16
21	A	561	PHO	C11-C10-C8-C9
20	C	496	CLA	C11-C10-C8-C9
20	C	496	CLA	C14-C13-C15-C16
20	B	520	CLA	C6-C7-C8-C9
20	b	5520	CLA	C6-C7-C8-C9
20	C	493	CLA	C6-C7-C8-C9
20	C	493	CLA	C11-C12-C13-C14
20	D	354	CLA	C14-C13-C15-C16
20	B	513	CLA	C14-C13-C15-C16
20	B	525	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	515	CLA	C14-C13-C15-C16
20	b	5525	CLA	C6-C7-C8-C9
20	a	5558	CLA	C11-C10-C8-C9
20	b	5522	CLA	C11-C10-C8-C9
20	b	5519	CLA	C14-C13-C15-C16
20	B	522	CLA	C11-C10-C8-C9
20	b	5513	CLA	C14-C13-C15-C16
20	b	5515	CLA	C14-C13-C15-C16
20	c	5493	CLA	C6-C7-C8-C9
20	c	5493	CLA	C11-C12-C13-C14
20	C	498	CLA	C6-C7-C8-C9
20	A	559	CLA	C14-C13-C15-C16
20	A	558	CLA	C11-C10-C8-C9
20	C	501	CLA	C11-C10-C8-C9
20	C	501	CLA	C14-C13-C15-C16
21	a	5562	PHO	C11-C10-C8-C9
26	d	5358	SQD	C28-C29-C30-C31
20	b	5521	CLA	C8-C10-C11-C12
20	c	5501	CLA	C10-C11-C12-C13
20	b	5516	CLA	C2A-CAA-CBA-CGA
30	C	509	DGD	C4A-C5A-C6A-C7A
20	b	5522	CLA	C5-C6-C7-C8
28	L	210	MGE	CBB-CCB-CDB-CEB
30	H	208	DGD	CCA-CDA-CEA-CFA
20	B	525	CLA	C5-C6-C7-C8
20	b	5519	CLA	C4-C3-C5-C6
20	a	5563	CLA	C4-C3-C5-C6
20	A	563	CLA	C4-C3-C5-C6
20	b	5519	CLA	C2-C3-C5-C6
20	b	5524	CLA	C11-C10-C8-C9
26	A	568	SQD	C10-C11-C12-C13
30	h	5208	DGD	CCA-CDA-CEA-CFA
25	A	567	LHG	C27-C28-C29-C30
20	b	5518	CLA	C5-C6-C7-C8
20	B	522	CLA	C8-C10-C11-C12
28	d	5360	MGE	C6B-C7B-C8B-C9B
20	b	5526	CLA	C3A-C2A-CAA-CBA
20	B	526	CLA	C3A-C2A-CAA-CBA
20	b	5512	CLA	C3A-C2A-CAA-CBA
20	b	5525	CLA	C5-C6-C7-C8
20	B	522	CLA	C5-C6-C7-C8
26	d	5358	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	d	5361	MGE	C4A-C5A-C6A-C7A
26	A	5212	SQD	O6-C44-C45-C46
26	L	5213	SQD	C44-C45-C46-O48
26	d	5358	SQD	O6-C44-C45-C46
28	D	360	MGE	C1G-C2G-C3G-O3G
26	a	212	SQD	O6-C44-C45-C46
26	A	568	SQD	O6-C44-C45-C46
26	t	213	SQD	C44-C45-C46-O48
28	d	5361	MGE	C1G-C2G-C3G-O3G
28	d	5359	MGE	C2A-C3A-C4A-C5A
28	i	5201	MGE	C6B-C7B-C8B-C9B
20	b	5516	CLA	O1D-CGD-O2D-CED
20	C	501	CLA	C5-C6-C7-C8
20	B	519	CLA	C4-C3-C5-C6
20	B	513	CLA	C4-C3-C5-C6
20	b	5513	CLA	C4-C3-C5-C6
30	c	5509	DGD	C4E-C5E-C6E-O5E
20	a	5563	CLA	C2-C3-C5-C6
30	C	508	DGD	C7A-C8A-C9A-CAA
20	C	492	CLA	CBD-CGD-O2D-CED
20	b	5522	CLA	C8-C10-C11-C12
30	H	208	DGD	C2A-C3A-C4A-C5A
28	B	530	MGE	C2A-C3A-C4A-C5A
30	h	5208	DGD	C2A-C3A-C4A-C5A
20	B	516	CLA	O1D-CGD-O2D-CED
20	B	518	CLA	C5-C6-C7-C8
21	A	561	PHO	C15-C16-C17-C18
20	c	5501	CLA	C5-C6-C7-C8
28	I	201	MGE	C6B-C7B-C8B-C9B
28	d	5360	MGE	O2G-C2G-C3G-O3G
26	d	5358	SQD	O6-C44-C45-O47
28	D	359	MGE	O2G-C2G-C3G-O3G
26	A	568	SQD	O6-C44-C45-O47
28	D	360	MGE	C9A-CAA-CBA-CCA
28	l	5210	MGE	C2A-C3A-C4A-C5A
20	b	5514	CLA	C13-C15-C16-C17
28	D	359	MGE	CDB-CEB-CFB-CGB
20	b	5520	CLA	O1D-CGD-O2D-CED
20	B	519	CLA	C2-C3-C5-C6
20	A	563	CLA	C2-C3-C5-C6
20	B	521	CLA	C8-C10-C11-C12
20	B	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	561	PHO	C6-C7-C8-C9
20	B	519	CLA	C14-C13-C15-C16
20	b	5512	CLA	C11-C10-C8-C9
21	a	5561	PHO	C6-C7-C8-C9
20	C	498	CLA	C14-C13-C15-C16
20	b	5524	CLA	C6-C7-C8-C9
20	c	5501	CLA	C11-C10-C8-C9
28	D	358	MGE	C2A-C3A-C4A-C5A
20	B	521	CLA	CBD-CGD-O2D-CED
30	c	5507	DGD	C5A-C6A-C7A-C8A
21	a	5561	PHO	C15-C16-C17-C18
20	B	514	CLA	C13-C15-C16-C17
28	d	5360	MGE	CDB-CEB-CFB-CGB
20	c	5503	CLA	C2A-CAA-CBA-CGA
20	b	5515	CLA	C2A-CAA-CBA-CGA
20	c	5492	CLA	CBD-CGD-O2D-CED
24	d	5357	BCR	C1-C6-C7-C8
24	c	5505	BCR	C5-C6-C7-C8
24	C	505	BCR	C5-C6-C7-C8
24	D	357	BCR	C1-C6-C7-C8
30	c	5508	DGD	C8A-C9A-CAA-CBA
25	a	5567	LHG	C9-C10-C11-C12
28	i	5201	MGE	CDB-CEB-CFB-CGB
30	C	507	DGD	C5A-C6A-C7A-C8A
30	c	5508	DGD	C7A-C8A-C9A-CAA
20	b	5514	CLA	C15-C16-C17-C18
20	B	514	CLA	C15-C16-C17-C18
28	L	210	MGE	C2A-C3A-C4A-C5A
28	L	210	MGE	C4A-C5A-C6A-C7A
28	D	360	MGE	C2A-C3A-C4A-C5A
20	B	524	CLA	C11-C10-C8-C9
28	d	5361	MGE	C9A-CAA-CBA-CCA
20	B	512	CLA	C11-C10-C8-C7
20	d	5354	CLA	C12-C13-C15-C16
20	B	518	CLA	C6-C7-C8-C10
20	a	5559	CLA	C6-C7-C8-C10
20	a	5559	CLA	C11-C12-C13-C15
21	A	561	PHO	C6-C7-C8-C10
20	C	493	CLA	C6-C7-C8-C10
20	B	519	CLA	C12-C13-C15-C16
20	D	354	CLA	C12-C13-C15-C16
20	b	5512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	513	CLA	C12-C13-C15-C16
20	A	560	CLA	C11-C10-C8-C7
21	a	5561	PHO	C6-C7-C8-C10
20	B	525	CLA	C6-C7-C8-C10
20	b	5518	CLA	C6-C7-C8-C10
20	B	524	CLA	C6-C7-C8-C10
20	b	5525	CLA	C6-C7-C8-C10
20	b	5513	CLA	C11-C10-C8-C7
20	b	5513	CLA	C12-C13-C15-C16
20	c	5493	CLA	C6-C7-C8-C10
20	C	498	CLA	C6-C7-C8-C10
20	C	498	CLA	C11-C10-C8-C7
20	A	559	CLA	C11-C12-C13-C15
20	a	5560	CLA	C11-C10-C8-C7
20	C	501	CLA	C11-C10-C8-C7
20	b	5524	CLA	C6-C7-C8-C10
20	c	5501	CLA	C6-C7-C8-C10
21	a	5562	PHO	C11-C10-C8-C7
20	c	5497	CLA	C1-C2-C3-C4
20	C	497	CLA	C1-C2-C3-C4
28	D	359	MGE	C6B-C7B-C8B-C9B
28	l	5210	MGE	C4A-C5A-C6A-C7A
26	d	5358	SQD	C9-C10-C11-C12
20	c	5491	CLA	C2A-CAA-CBA-CGA
20	C	496	CLA	C5-C6-C7-C8
28	d	5360	MGE	C7B-C8B-C9B-CAB
20	d	5355	CLA	C4C-C3C-CAC-CBC
28	i	5201	MGE	C5A-C6A-C7A-C8A
20	B	517	CLA	C13-C15-C16-C17
20	c	5497	CLA	CAD-CBD-CGD-O2D
20	b	5523	CLA	CAD-CBD-CGD-O2D
20	B	523	CLA	CAD-CBD-CGD-O2D
20	C	498	CLA	CAD-CBD-CGD-O2D
20	c	5498	CLA	CAD-CBD-CGD-O2D
20	C	497	CLA	CAD-CBD-CGD-O2D
30	c	5507	DGD	C5B-C6B-C7B-C8B
30	c	5509	DGD	C6B-C7B-C8B-C9B
26	A	568	SQD	C9-C10-C11-C12
20	c	5496	CLA	C5-C6-C7-C8
25	a	5567	LHG	C23-C24-C25-C26
20	B	521	CLA	C4-C3-C5-C6
25	A	567	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	C	509	DGD	C4E-C5E-C6E-O5E
30	C	509	DGD	C6B-C7B-C8B-C9B
26	d	5358	SQD	C24-C25-C26-C27
20	C	501	CLA	C10-C11-C12-C13
30	C	508	DGD	C8A-C9A-CAA-CBA
28	D	359	MGE	C7B-C8B-C9B-CAB
20	B	520	CLA	CHA-CBD-CGD-O1D
20	b	5520	CLA	CHA-CBD-CGD-O1D
20	C	500	CLA	CHA-CBD-CGD-O1D
20	C	500	CLA	CHA-CBD-CGD-O2D
20	c	5499	CLA	CHA-CBD-CGD-O1D
20	c	5499	CLA	CHA-CBD-CGD-O2D
20	B	525	CLA	CHA-CBD-CGD-O1D
20	B	525	CLA	CHA-CBD-CGD-O2D
20	c	5500	CLA	CHA-CBD-CGD-O1D
20	c	5500	CLA	CHA-CBD-CGD-O2D
20	b	5525	CLA	CHA-CBD-CGD-O1D
20	b	5525	CLA	CHA-CBD-CGD-O2D
20	C	499	CLA	CHA-CBD-CGD-O1D
20	C	499	CLA	CHA-CBD-CGD-O2D
20	D	355	CLA	C4C-C3C-CAC-CBC
28	I	201	MGE	CDB-CEB-CFB-CGB
26	L	5213	SQD	O47-C45-C46-O48
26	t	213	SQD	O47-C45-C46-O48
28	i	5201	MGE	O1G-C1G-C2G-O2G
21	A	561	PHO	C1-C2-C3-C5
20	b	5521	CLA	C4-C3-C5-C6
28	b	5530	MGE	C5B-C6B-C7B-C8B
20	B	516	CLA	C11-C12-C13-C14
20	A	560	CLA	C11-C10-C8-C9
20	b	5516	CLA	C11-C12-C13-C14
20	a	5560	CLA	C11-C10-C8-C9
30	c	5509	DGD	C4B-C5B-C6B-C7B
30	C	507	DGD	C5B-C6B-C7B-C8B
26	A	568	SQD	C24-C25-C26-C27
20	b	5525	CLA	C10-C11-C12-C13
20	B	514	CLA	C5-C6-C7-C8
26	L	5213	SQD	C5-C6-S-O8
26	t	213	SQD	C5-C6-S-O8
20	B	512	CLA	C10-C11-C12-C13
25	A	567	LHG	C23-C24-C25-C26
20	a	5559	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	a	5559	CLA	C2-C1-O2A-CGA
28	D	360	MGE	C4A-C5A-C6A-C7A
30	c	5508	DGD	C9A-CAA-CBA-CCA
20	B	523	CLA	C2-C3-C5-C6
30	C	508	DGD	C9A-CAA-CBA-CCA
28	I	201	MGE	C5A-C6A-C7A-C8A
20	C	492	CLA	O1D-CGD-O2D-CED
26	L	5213	SQD	C19-C20-C21-C22
28	b	5530	MGE	C2A-C3A-C4A-C5A
26	t	213	SQD	C19-C20-C21-C22
20	C	500	CLA	CAD-CBD-CGD-O1D
20	c	5499	CLA	CAD-CBD-CGD-O1D
20	c	5500	CLA	CAD-CBD-CGD-O1D
26	L	5213	SQD	C5-C6-S-O9
26	t	213	SQD	C5-C6-S-O9
20	C	499	CLA	CAD-CBD-CGD-O1D
20	b	5514	CLA	C5-C6-C7-C8
28	B	530	MGE	C9B-CAB-CBB-CCB
20	b	5526	CLA	C11-C12-C13-C15
20	B	526	CLA	C11-C12-C13-C15
20	B	518	CLA	C11-C10-C8-C7
20	B	520	CLA	C11-C10-C8-C7
20	B	516	CLA	C11-C12-C13-C15
20	b	5518	CLA	C11-C10-C8-C7
20	b	5519	CLA	C12-C13-C15-C16
20	b	5516	CLA	C11-C12-C13-C15
20	A	559	CLA	C11-C10-C8-C7
20	C	501	CLA	C6-C7-C8-C10
20	c	5498	CLA	C11-C10-C8-C7
20	C	492	CLA	C11-C10-C8-C7
30	c	5509	DGD	CAB-CBB-CCB-CDB
20	B	516	CLA	C2A-CAA-CBA-CGA
28	I	201	MGE	O1G-C1G-C2G-O2G
28	B	530	MGE	C5B-C6B-C7B-C8B
30	C	509	DGD	CAB-CBB-CCB-CDB
30	C	509	DGD	C4B-C5B-C6B-C7B
20	B	518	CLA	O1D-CGD-O2D-CED
28	B	530	MGE	C6B-C7B-C8B-C9B
20	B	521	CLA	O1D-CGD-O2D-CED
26	A	568	SQD	C28-C29-C30-C31
20	a	5559	CLA	C11-C12-C13-C14
20	b	5512	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	524	CLA	C6-C7-C8-C9
20	c	5498	CLA	C6-C7-C8-C9
20	c	5498	CLA	C14-C13-C15-C16
20	c	5501	CLA	C14-C13-C15-C16
24	C	506	BCR	C6-C7-C8-C9
28	b	5530	MGE	C9B-CAB-CBB-CCB
28	L	210	MGE	C3A-C4A-C5A-C6A
28	d	5359	MGE	CAB-CBB-CCB-CDB
20	b	5512	CLA	C10-C11-C12-C13
25	A	567	LHG	C25-C26-C27-C28
20	a	5559	CLA	C3-C5-C6-C7
20	C	496	CLA	C13-C15-C16-C17
27	m	216	LMT	C1-C2-C3-C4
20	B	521	CLA	C2-C3-C5-C6
20	B	525	CLA	C10-C11-C12-C13
28	L	210	MGE	C9A-CAA-CBA-CCA
30	C	509	DGD	C1B-C2B-C3B-C4B
20	A	559	CLA	C3-C5-C6-C7
25	A	567	LHG	C6-C5-O7-C7
25	a	5567	LHG	C6-C5-O7-C7
20	C	491	CLA	C2A-CAA-CBA-CGA
20	B	515	CLA	C2A-CAA-CBA-CGA
20	b	5517	CLA	C2-C1-O2A-CGA
20	b	5521	CLA	C2-C1-O2A-CGA
20	A	559	CLA	C2-C1-O2A-CGA
20	B	517	CLA	C2-C1-O2A-CGA
20	c	5498	CLA	C2-C1-O2A-CGA
20	B	521	CLA	C2-C1-O2A-CGA
28	B	530	MGE	CAB-CBB-CCB-CDB
20	c	5496	CLA	C13-C15-C16-C17
20	B	519	CLA	C5-C6-C7-C8
28	l	5210	MGE	C9A-CAA-CBA-CCA
21	a	5561	PHO	C2A-CAA-CBA-CGA
30	h	5208	DGD	O2G-C2G-C3G-O3G
25	A	567	LHG	C3-O3-P-O6
25	a	5567	LHG	C3-O3-P-O6
25	a	5567	LHG	C25-C26-C27-C28
26	d	5358	SQD	C19-C20-C21-C22
28	i	5201	MGE	CBB-CCB-CDB-CEB
20	B	512	CLA	C11-C12-C13-C15
20	b	5520	CLA	C11-C10-C8-C7
20	B	513	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	b	5523	CLA	C12-C13-C15-C16
20	C	498	CLA	C12-C13-C15-C16
20	b	5521	CLA	C2-C3-C5-C6
20	A	559	CLA	C6-C7-C8-C10
20	c	5498	CLA	C6-C7-C8-C10
20	c	5498	CLA	C12-C13-C15-C16
20	c	5501	CLA	C12-C13-C15-C16
20	B	514	CLA	C6-C7-C8-C10
20	B	526	CLA	C11-C12-C13-C14
20	a	5559	CLA	C11-C10-C8-C9
20	B	513	CLA	C11-C10-C8-C9
20	b	5513	CLA	C11-C10-C8-C9
20	A	559	CLA	C11-C12-C13-C14
26	L	5213	SQD	C27-C28-C29-C30
20	c	5492	CLA	O1D-CGD-O2D-CED
28	D	360	MGE	CDB-CEB-CFB-CGB
20	b	5521	CLA	CBD-CGD-O2D-CED
28	B	530	MGE	CAA-CBA-CCA-CDA
20	b	5513	CLA	C2-C3-C5-C6
27	M	5216	LMT	C1-C2-C3-C4
30	c	5509	DGD	C1B-C2B-C3B-C4B
20	b	5517	CLA	C13-C15-C16-C17
28	b	5530	MGE	CAB-CBB-CCB-CDB
26	t	213	SQD	C24-C25-C26-C27
26	L	5213	SQD	C24-C25-C26-C27
28	b	5530	MGE	C6B-C7B-C8B-C9B
20	B	512	CLA	C2A-CAA-CBA-CGA
20	b	5512	CLA	C2A-CAA-CBA-CGA
20	C	503	CLA	C3A-C2A-CAA-CBA
20	C	502	CLA	C3A-C2A-CAA-CBA
26	A	568	SQD	C19-C20-C21-C22
22	A	564	PQ9	C12-C11-C2-C1
22	a	5564	PQ9	C12-C11-C2-C1
20	b	5526	CLA	C11-C12-C13-C14
20	B	512	CLA	C11-C12-C13-C14
28	D	360	MGE	O1G-C1G-C2G-C3G
28	d	5361	MGE	O1G-C1G-C2G-C3G
20	b	5525	CLA	C13-C15-C16-C17
20	B	514	CLA	C10-C11-C12-C13
21	A	562	PHO	O2A-C1-C2-C3
20	c	5497	CLA	O2A-C1-C2-C3
20	C	497	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
20	B	516	CLA	C15-C16-C17-C18
28	l	5210	MGE	C3A-C4A-C5A-C6A
30	h	5208	DGD	C6B-C7B-C8B-C9B
26	t	213	SQD	C27-C28-C29-C30
25	A	567	LHG	C4-C5-O7-C7
25	a	5567	LHG	C4-C5-O7-C7
20	B	512	CLA	C1A-C2A-CAA-CBA
20	b	5512	CLA	C1A-C2A-CAA-CBA
20	A	560	CLA	C1A-C2A-CAA-CBA
20	A	559	CLA	C1A-C2A-CAA-CBA
20	c	5492	CLA	C11-C10-C8-C7
20	b	5514	CLA	C6-C7-C8-C10
20	B	523	CLA	C12-C13-C15-C16
20	b	5514	CLA	C10-C11-C12-C13
28	I	201	MGE	CBB-CCB-CDB-CEB
30	c	5509	DGD	C3A-C4A-C5A-C6A
20	B	525	CLA	C13-C15-C16-C17
27	T	217	LMT	C4-C5-C6-C7
28	D	358	MGE	CAB-CBB-CCB-CDB
20	C	498	CLA	C8-C10-C11-C12
20	c	5498	CLA	C10-C11-C12-C13
28	B	530	MGE	C1A-C2A-C3A-C4A
27	M	5216	LMT	O1'-C1-C2-C3
20	b	5519	CLA	C5-C6-C7-C8
20	C	498	CLA	C15-C16-C17-C18
20	c	5498	CLA	C15-C16-C17-C18
20	C	492	CLA	C10-C11-C12-C13
30	C	508	DGD	O6E-C5E-C6E-O5E
30	H	208	DGD	O2G-C2G-C3G-O3G
20	c	5498	CLA	C8-C10-C11-C12
21	A	561	PHO	C2A-CAA-CBA-CGA
20	d	5354	CLA	C2-C1-O2A-CGA
20	D	354	CLA	C2-C1-O2A-CGA
20	C	502	CLA	C2-C1-O2A-CGA
20	c	5502	CLA	C2-C1-O2A-CGA
20	C	498	CLA	C2-C1-O2A-CGA
21	a	5561	PHO	C2C-C3C-CAC-CBC
20	c	5496	CLA	C6-C7-C8-C9
30	C	509	DGD	C3A-C4A-C5A-C6A
28	d	5361	MGE	CDB-CEB-CFB-CGB
24	B	529	BCR	C1-C6-C7-C8
24	X	130	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	b	5520	CLA	C13-C15-C16-C17
20	c	5500	CLA	C4-C3-C5-C6
22	d	5356	PQ9	C19-C18-C20-C21
20	B	520	CLA	C13-C15-C16-C17
20	C	498	CLA	C10-C11-C12-C13
20	b	5523	CLA	C2-C3-C5-C6
28	i	5201	MGE	C2G-C3G-O3G-C1D
20	b	5521	CLA	O1D-CGD-O2D-CED
30	H	208	DGD	C6B-C7B-C8B-C9B
20	a	5560	CLA	CBD-CGD-O2D-CED
20	b	5519	CLA	C1-C2-C3-C5
20	C	498	CLA	C4-C3-C5-C6
20	B	520	CLA	C1-C2-C3-C4
20	C	491	CLA	C1-C2-C3-C4
20	C	493	CLA	C1-C2-C3-C4
20	b	5514	CLA	C1-C2-C3-C4
20	A	560	CLA	C1-C2-C3-C4
20	C	502	CLA	C1-C2-C3-C4
20	c	5502	CLA	C1-C2-C3-C4
20	c	5493	CLA	C1-C2-C3-C4
20	a	5560	CLA	C1-C2-C3-C4
20	B	514	CLA	C1-C2-C3-C4
20	c	5497	CLA	CAA-CBA-CGA-O2A
28	L	210	MGE	O2G-C1B-C2B-C3B
28	d	5361	MGE	O2G-C1B-C2B-C3B
30	c	5508	DGD	C2A-C1A-O1G-C1G
27	a	5568	LMT	C1-C2-C3-C4
28	l	5210	MGE	O2G-C1B-C2B-C3B
22	D	356	PQ9	C19-C18-C20-C21
20	B	519	CLA	C1-C2-C3-C5
20	C	498	CLA	C1-C2-C3-C5
22	d	5356	PQ9	C17-C18-C20-C21
26	d	5358	SQD	O47-C7-C8-C9
28	D	360	MGE	O2G-C1B-C2B-C3B
26	A	568	SQD	O47-C7-C8-C9
20	B	524	CLA	C11-C10-C8-C7
20	c	5492	CLA	C11-C10-C8-C9
20	C	496	CLA	C6-C7-C8-C9
20	B	520	CLA	C11-C10-C8-C9
20	b	5520	CLA	C11-C10-C8-C9
20	A	560	CLA	C11-C12-C13-C14
20	b	5523	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	523	CLA	C14-C13-C15-C16
20	C	498	CLA	C11-C10-C8-C9
20	A	559	CLA	C11-C10-C8-C9
20	a	5560	CLA	C11-C12-C13-C14
20	c	5498	CLA	C11-C10-C8-C9
28	b	5530	MGE	CAA-CBA-CCA-CDA
20	c	5503	CLA	C3A-C2A-CAA-CBA
20	c	5502	CLA	C3A-C2A-CAA-CBA
30	c	5508	DGD	O1A-C1A-O1G-C1G
20	C	494	CLA	CAA-CBA-CGA-O2A
20	c	5492	CLA	CAD-CBD-CGD-O2D
21	A	562	PHO	CAD-CBD-CGD-O2D
21	A	561	PHO	CAD-CBD-CGD-O2D
20	B	520	CLA	CAD-CBD-CGD-O2D
20	C	491	CLA	CAD-CBD-CGD-O2D
20	b	5520	CLA	CAD-CBD-CGD-O2D
20	C	493	CLA	CAD-CBD-CGD-O2D
21	a	5561	PHO	CAD-CBD-CGD-O2D
20	B	515	CLA	CAD-CBD-CGD-O2D
20	b	5515	CLA	CAD-CBD-CGD-O2D
20	c	5493	CLA	CAD-CBD-CGD-O2D
20	C	492	CLA	CAD-CBD-CGD-O2D
21	a	5562	PHO	CAD-CBD-CGD-O2D
20	B	515	CLA	CAA-CBA-CGA-O2A
20	c	5494	CLA	CAA-CBA-CGA-O2A
20	C	497	CLA	CAA-CBA-CGA-O2A
27	m	216	LMT	O1'-C1-C2-C3
24	T	5104	BCR	C22-C23-C24-C25
24	c	5506	BCR	C6-C7-C8-C9
20	C	500	CLA	C4-C3-C5-C6
20	c	5498	CLA	C4-C3-C5-C6
22	D	356	PQ9	C17-C18-C20-C21
20	c	5498	CLA	C2-C3-C5-C6
30	C	507	DGD	O2G-C1B-C2B-C3B
26	t	213	SQD	O6-C44-C45-C46
20	B	512	CLA	C5-C6-C7-C8
20	b	5515	CLA	CAA-CBA-CGA-O2A
30	H	208	DGD	C9A-CAA-CBA-CCA
20	d	5354	CLA	O2A-C1-C2-C3
20	B	520	CLA	O2A-C1-C2-C3
20	b	5520	CLA	O2A-C1-C2-C3
20	D	354	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
20	b	5523	CLA	O2A-C1-C2-C3
20	B	523	CLA	O2A-C1-C2-C3
21	a	5562	PHO	O2A-C1-C2-C3
30	h	5208	DGD	C9A-CAA-CBA-CCA
21	A	561	PHO	C2C-C3C-CAC-CBC
30	c	5507	DGD	O2G-C1B-C2B-C3B
20	b	5526	CLA	CHA-CBD-CGD-O2D
20	B	512	CLA	CHA-CBD-CGD-O2D
20	B	526	CLA	CHA-CBD-CGD-O1D
20	B	526	CLA	CHA-CBD-CGD-O2D
20	B	520	CLA	CHA-CBD-CGD-O2D
20	b	5520	CLA	CHA-CBD-CGD-O2D
20	B	519	CLA	CHA-CBD-CGD-O1D
20	b	5516	CLA	CHA-CBD-CGD-O2D
20	c	5495	CLA	CAA-CBA-CGA-O2A
20	C	495	CLA	CAA-CBA-CGA-O2A
21	A	561	PHO	C4C-C3C-CAC-CBC
26	A	568	SQD	C13-C14-C15-C16
21	a	5561	PHO	C4C-C3C-CAC-CBC
20	C	499	CLA	CAA-CBA-CGA-O2A
25	A	567	LHG	O1-C1-C2-O2
20	c	5499	CLA	CAA-CBA-CGA-O2A
20	c	5496	CLA	C6-C7-C8-C10
20	b	5523	CLA	C11-C12-C13-C15
20	C	498	CLA	C2-C3-C5-C6
20	B	518	CLA	C11-C10-C8-C9
20	D	354	CLA	C11-C12-C13-C14
20	b	5518	CLA	C11-C10-C8-C9
20	b	5523	CLA	C11-C12-C13-C14
20	C	492	CLA	C11-C10-C8-C9
26	L	5213	SQD	C45-C46-O48-C23
28	L	210	MGE	O1B-C1B-C2B-C3B
28	l	5210	MGE	O1B-C1B-C2B-C3B
26	A	5212	SQD	C5-C6-S-O8
26	a	212	SQD	C5-C6-S-O8
28	d	5361	MGE	O1B-C1B-C2B-C3B
28	D	360	MGE	O1B-C1B-C2B-C3B
20	b	5516	CLA	C15-C16-C17-C18
28	D	358	MGE	C3B-C4B-C5B-C6B
28	I	201	MGE	C4B-C5B-C6B-C7B
20	c	5492	CLA	C1A-C2A-CAA-CBA
20	B	515	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	c	5494	CLA	CAA-CBA-CGA-O1A
20	B	523	CLA	C2-C1-O2A-CGA
20	B	520	CLA	C15-C16-C17-C18
20	C	494	CLA	CAA-CBA-CGA-O1A
26	d	5358	SQD	O49-C7-C8-C9
20	C	497	CLA	CAA-CBA-CGA-O1A
26	L	5213	SQD	O6-C44-C45-C46
28	I	201	MGE	O1G-C1G-C2G-C3G
28	i	5201	MGE	O1G-C1G-C2G-C3G
20	c	5495	CLA	CAA-CBA-CGA-O1A
20	c	5497	CLA	CAA-CBA-CGA-O1A
30	c	5507	DGD	O1B-C1B-C2B-C3B
24	t	104	BCR	C22-C23-C24-C25
28	d	5360	MGE	C2D-C1D-O3G-C3G
28	D	359	MGE	C2D-C1D-O3G-C3G
20	C	495	CLA	CAA-CBA-CGA-O1A
26	A	568	SQD	O49-C7-C8-C9
20	C	499	CLA	CAA-CBA-CGA-O1A
27	a	5568	LMT	C7-C8-C9-C10
24	x	5130	BCR	C1-C6-C7-C8
24	B	528	BCR	C1-C6-C7-C8
28	b	5530	MGE	C1A-C2A-C3A-C4A
30	C	507	DGD	O1B-C1B-C2B-C3B
20	b	5515	CLA	CAA-CBA-CGA-O1A
30	c	5508	DGD	O6E-C5E-C6E-O5E
20	c	5491	CLA	CAA-CBA-CGA-O2A
26	d	5358	SQD	C13-C14-C15-C16
20	c	5496	CLA	CAD-CBD-CGD-O1D
20	C	496	CLA	CAD-CBD-CGD-O1D
20	B	519	CLA	CAD-CBD-CGD-O1D
20	B	513	CLA	CAD-CBD-CGD-O1D
20	b	5519	CLA	CAD-CBD-CGD-O1D
20	b	5513	CLA	CAD-CBD-CGD-O1D
20	C	501	CLA	CAD-CBD-CGD-O1D
20	B	512	CLA	C6-C7-C8-C9
20	d	5354	CLA	C11-C12-C13-C14
20	B	520	CLA	C14-C13-C15-C16
20	b	5512	CLA	C6-C7-C8-C9
20	a	5558	CLA	C11-C12-C13-C14
20	B	522	CLA	C11-C12-C13-C14
20	B	523	CLA	C11-C12-C13-C14
20	b	5521	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	L	210	MGE	O1G-C1A-C2A-C3A
28	l	5210	MGE	O1G-C1A-C2A-C3A
20	b	5524	CLA	CAA-CBA-CGA-O2A
20	B	513	CLA	C2A-CAA-CBA-CGA
20	B	524	CLA	CAA-CBA-CGA-O2A
25	a	5567	LHG	C1-C2-C3-O3
20	b	5525	CLA	C4-C3-C5-C6
20	b	5512	CLA	C5-C6-C7-C8
20	C	496	CLA	C6-C7-C8-C10
20	B	520	CLA	C12-C13-C15-C16
20	C	493	CLA	C3A-C2A-CAA-CBA
20	D	354	CLA	C11-C12-C13-C15
20	a	5558	CLA	C11-C12-C13-C15
20	c	5493	CLA	C3A-C2A-CAA-CBA
20	B	523	CLA	C11-C12-C13-C15
20	c	5499	CLA	CAA-CBA-CGA-O1A
28	l	5210	MGE	O1A-C1A-C2A-C3A
20	b	5524	CLA	CAA-CBA-CGA-O1A
20	B	524	CLA	CAA-CBA-CGA-O1A
28	d	5359	MGE	C3B-C4B-C5B-C6B
28	I	201	MGE	C4D-C5D-C6D-O5D
20	B	512	CLA	C13-C15-C16-C17
20	b	5512	CLA	C13-C15-C16-C17
20	B	518	CLA	CAA-CBA-CGA-O2A
30	C	509	DGD	O1G-C1A-C2A-C3A
28	L	210	MGE	O1A-C1A-C2A-C3A

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	522	CLA	4	0
20	C	503	CLA	1	0
20	B	512	CLA	2	0
27	T	217	LMT	3	0
28	D	358	MGE	2	0
20	C	495	CLA	9	0
20	B	518	CLA	11	0
21	A	562	PHO	5	0
24	B	529	BCR	2	0
30	H	208	DGD	3	0
21	A	561	PHO	7	0

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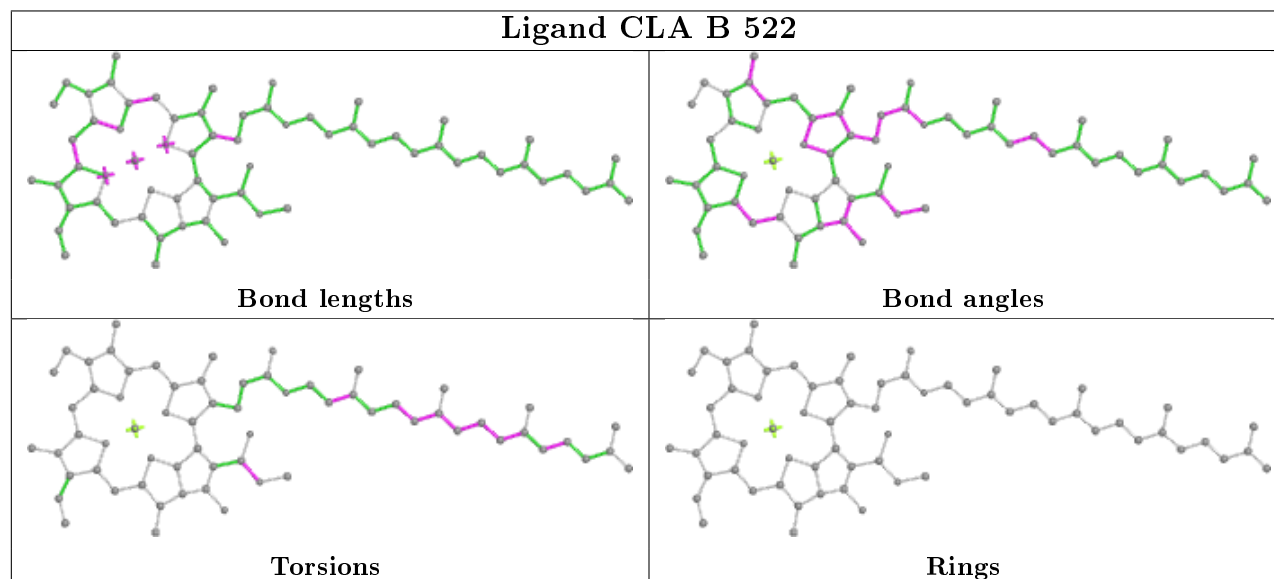
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	L	210	MGE	2	0
20	C	496	CLA	2	0
20	B	520	CLA	6	0
22	A	564	PQ9	2	0
20	C	494	CLA	2	0
22	D	356	PQ9	7	0
20	C	491	CLA	4	0
30	C	508	DGD	2	0
20	C	500	CLA	3	0
20	C	493	CLA	7	0
32	V	552	HEM	2	0
24	T	5104	BCR	5	0
20	B	519	CLA	5	0
20	D	354	CLA	5	0
20	B	516	CLA	6	0
24	B	527	BCR	2	0
20	B	513	CLA	8	0
20	A	560	CLA	1	0
20	B	525	CLA	4	0
24	A	566	BCR	1	0
20	B	524	CLA	4	0
20	B	515	CLA	12	0
20	C	502	CLA	2	0
24	C	505	BCR	6	0
20	B	511	CLA	1	0
20	B	526	CLA	2	0
28	D	360	MGE	7	0
28	B	530	MGE	1	0
28	I	201	MGE	1	0
30	C	507	DGD	6	0
25	A	567	LHG	4	0
28	D	359	MGE	1	0
24	C	504	BCR	7	0
20	B	523	CLA	2	0
20	C	498	CLA	6	0
30	C	509	DGD	10	0
24	B	528	BCR	2	0
24	H	107	BCR	3	0
20	A	559	CLA	5	0
20	A	558	CLA	10	0
32	F	51	HEM	3	0
20	B	517	CLA	9	0

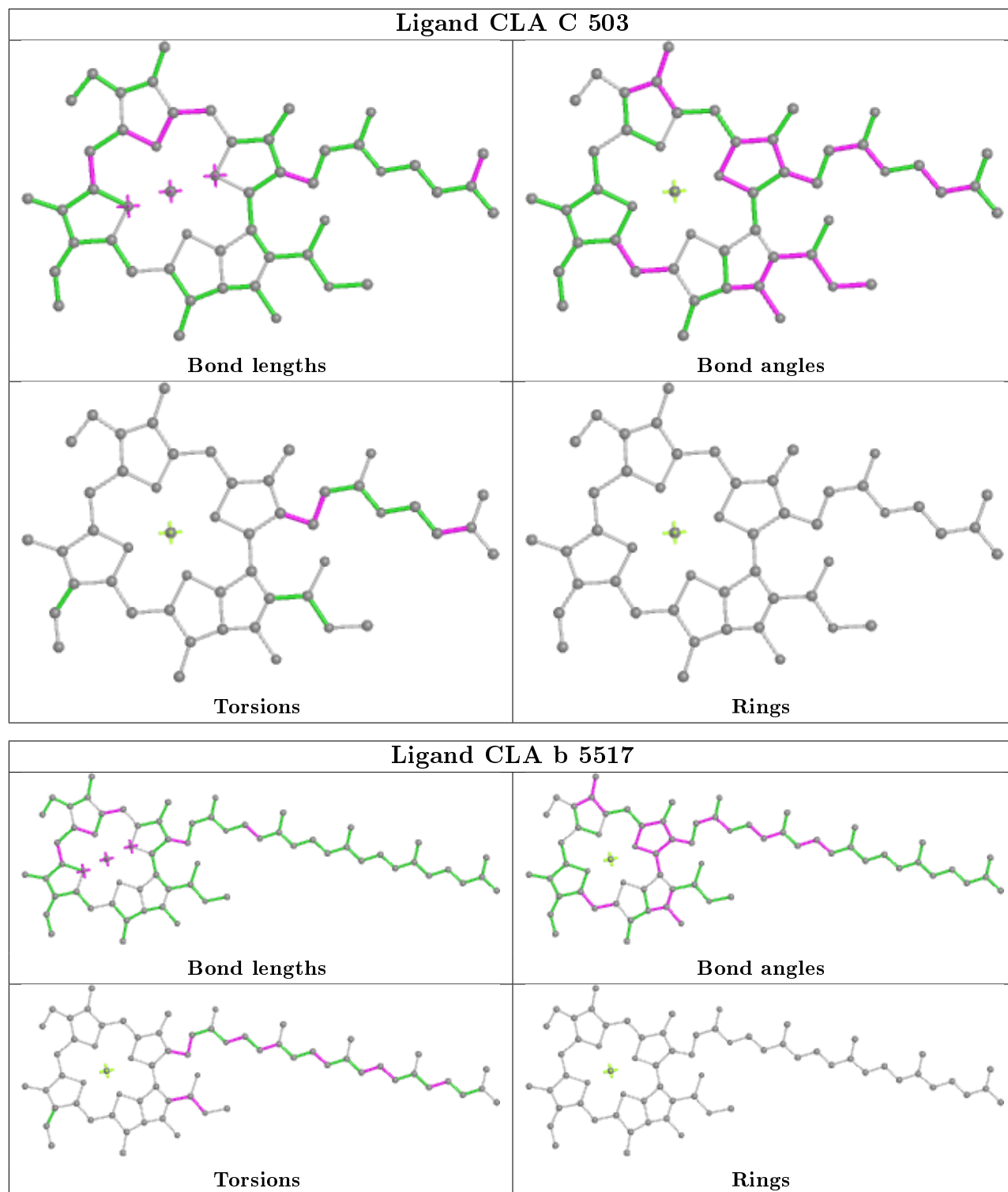
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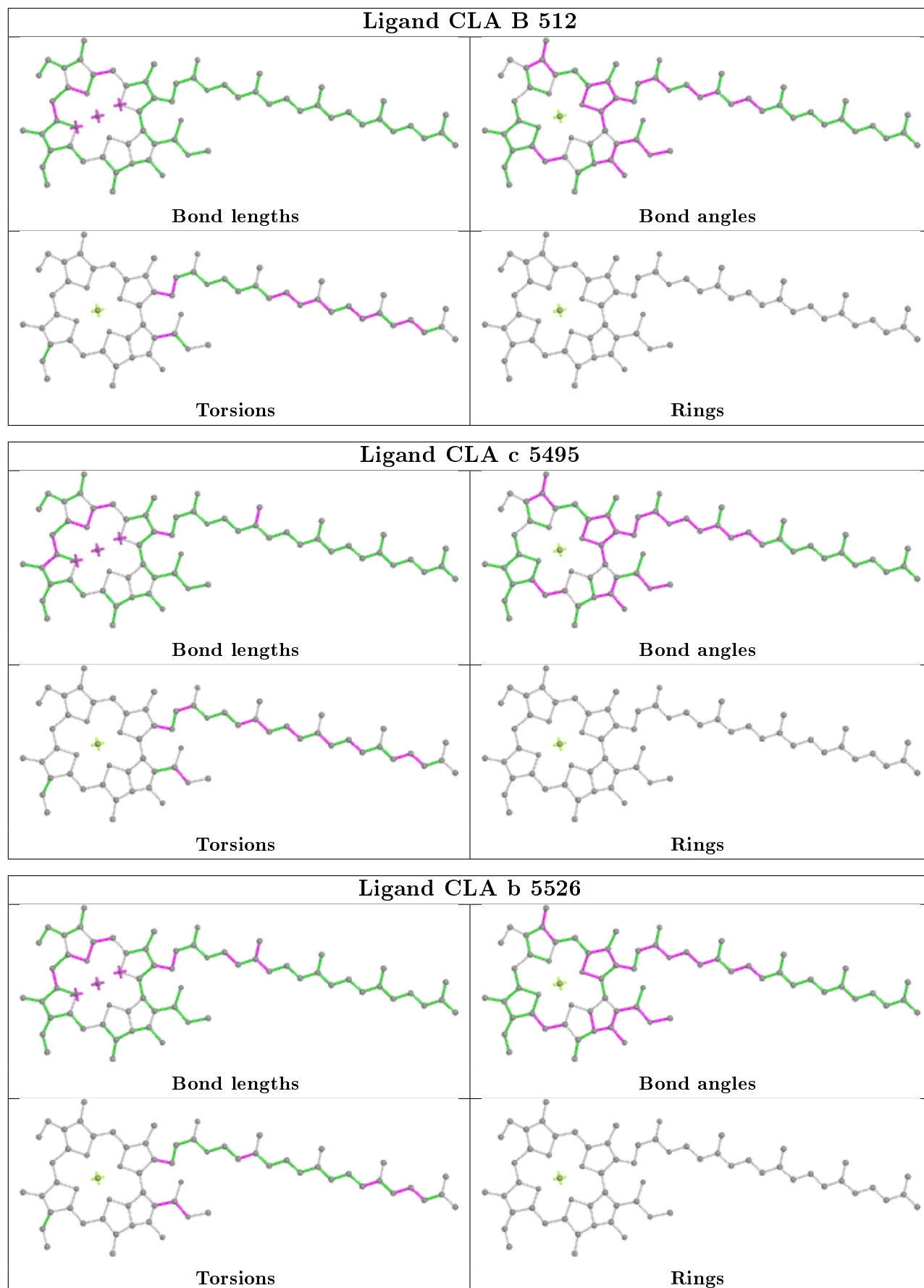
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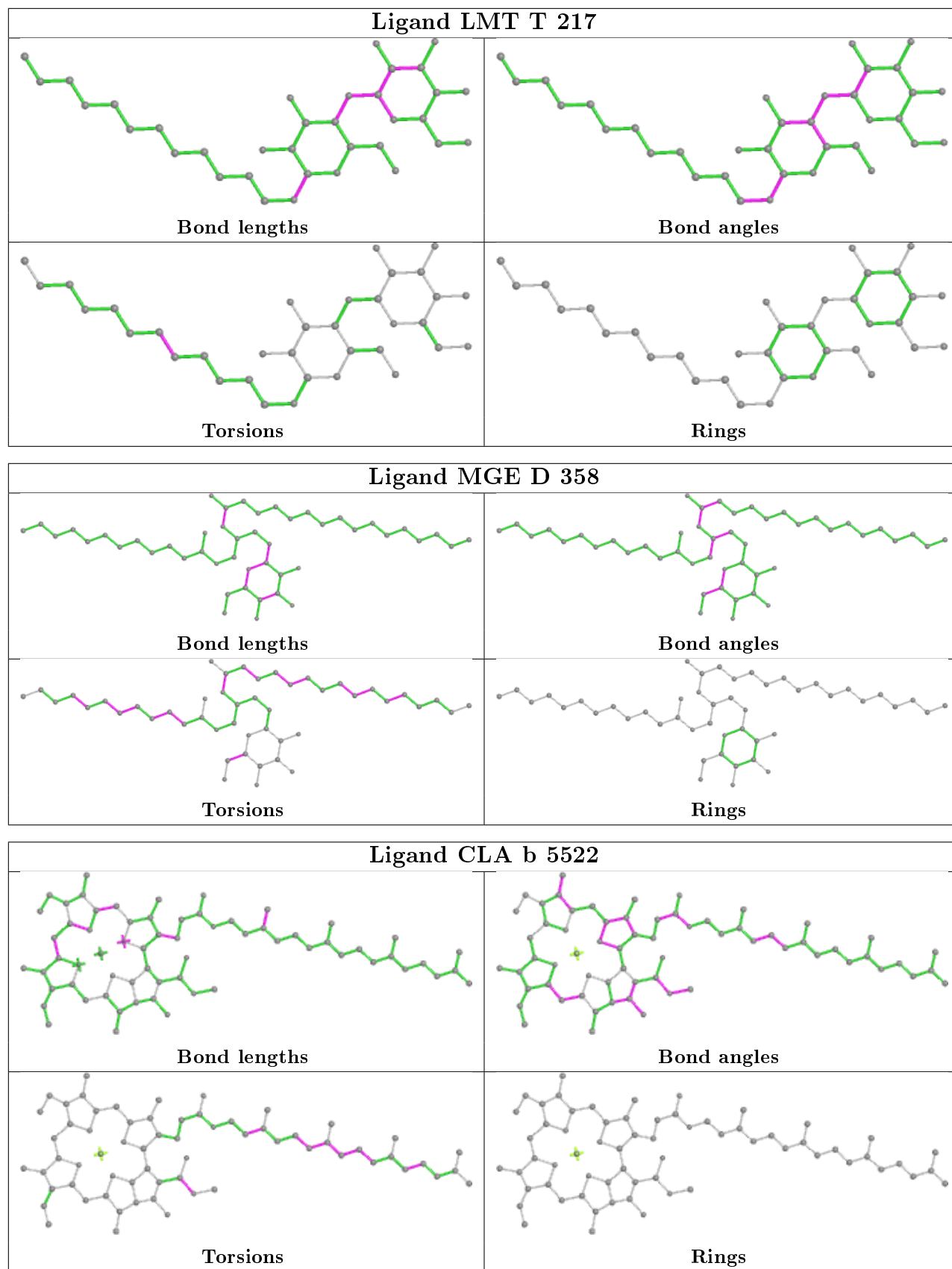
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	501	CLA	13	0
24	C	506	BCR	7	0
20	D	355	CLA	3	0
24	D	357	BCR	4	0
20	C	499	CLA	2	0
24	X	130	BCR	9	0
20	B	521	CLA	2	0
20	C	492	CLA	2	0
20	C	497	CLA	5	0
20	B	514	CLA	5	0

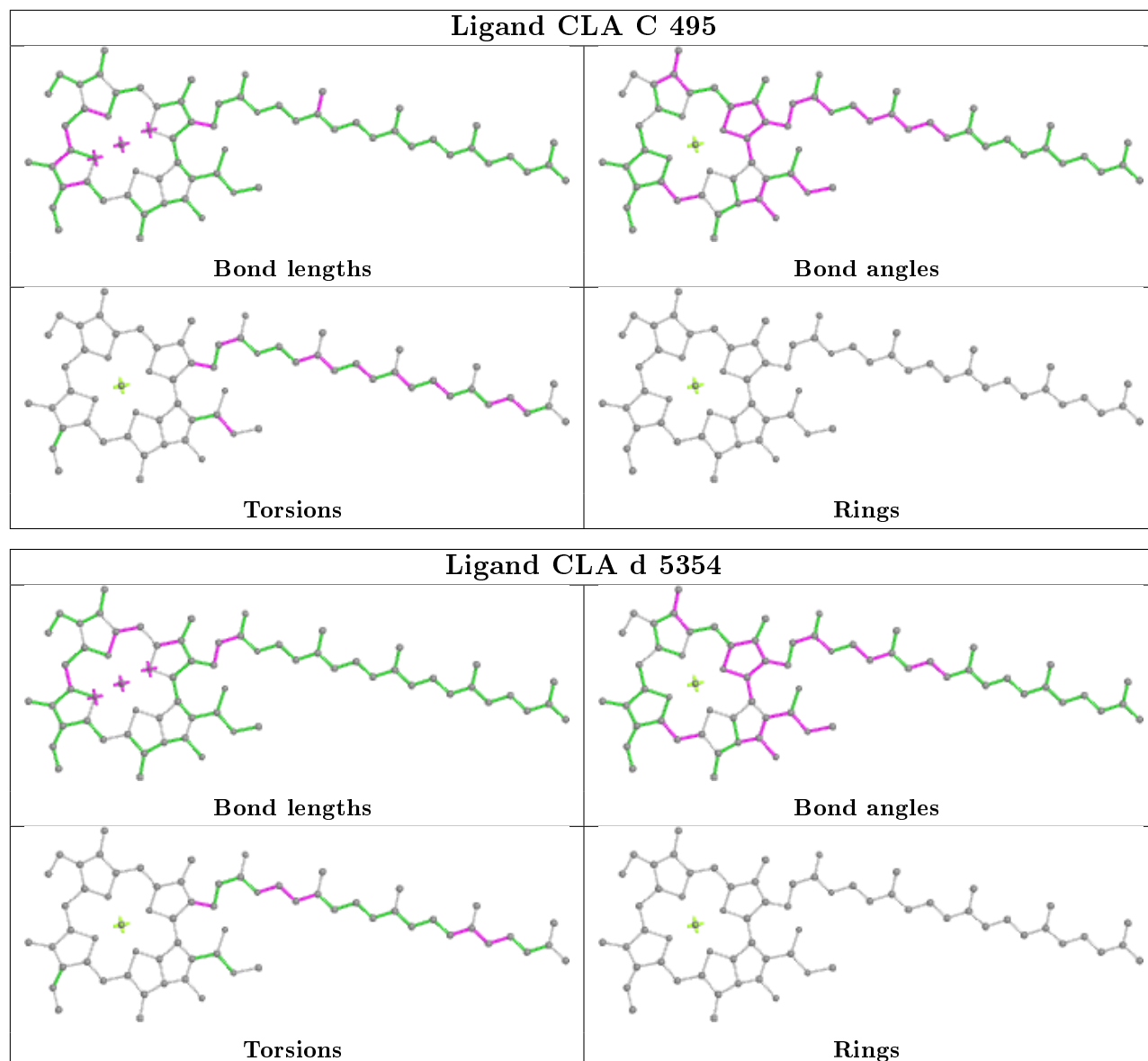
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

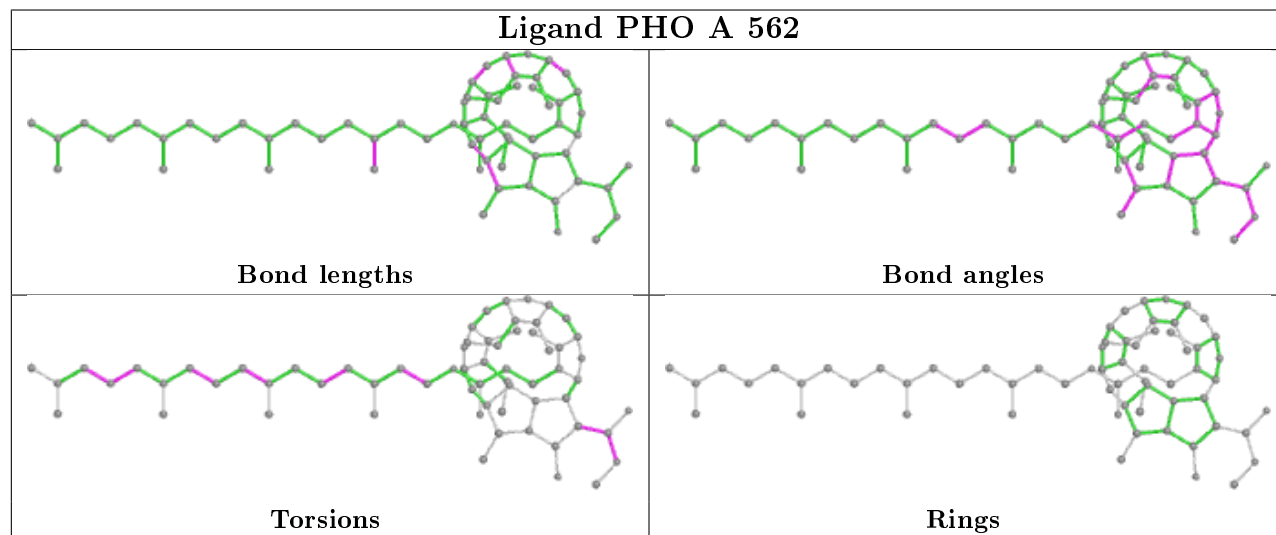
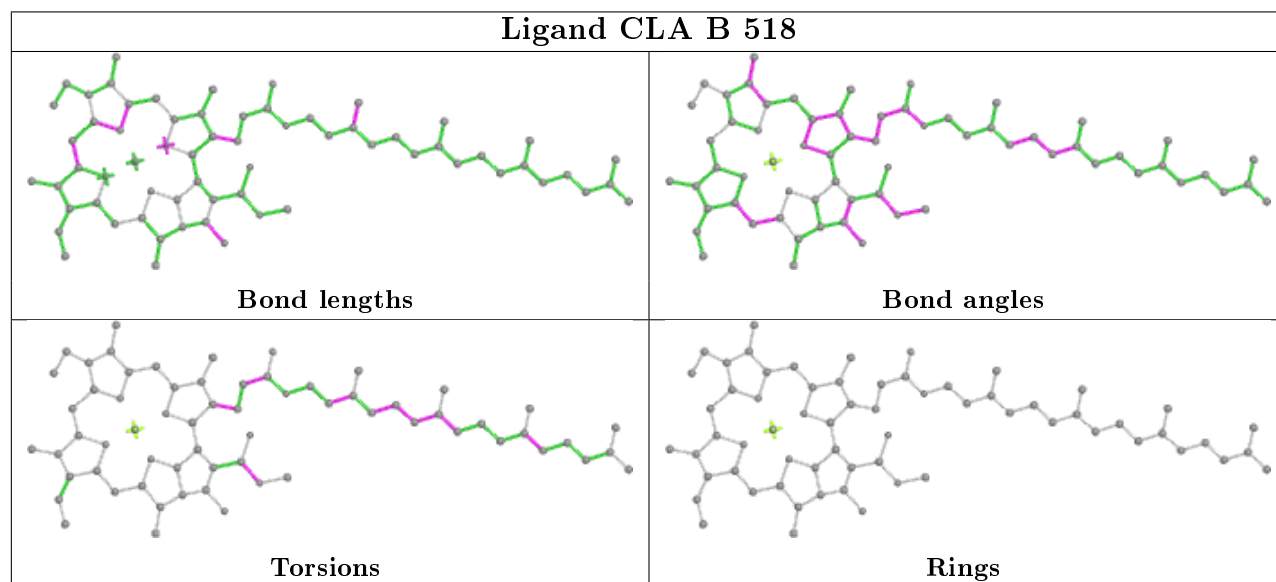
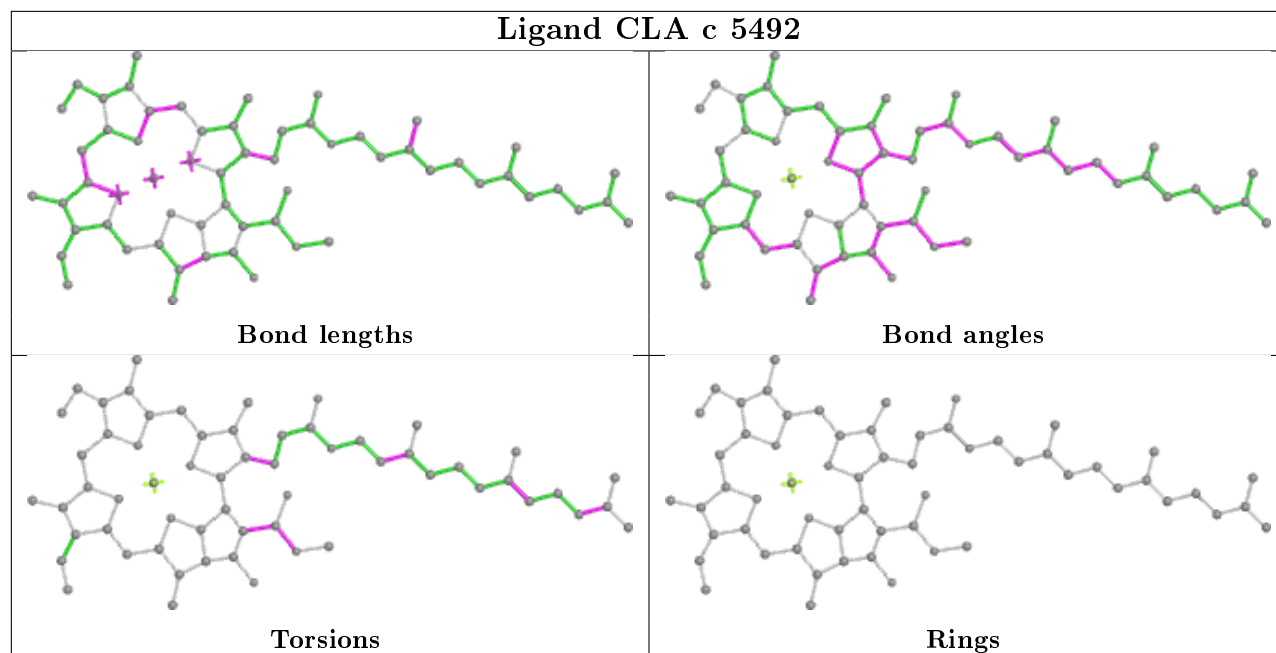


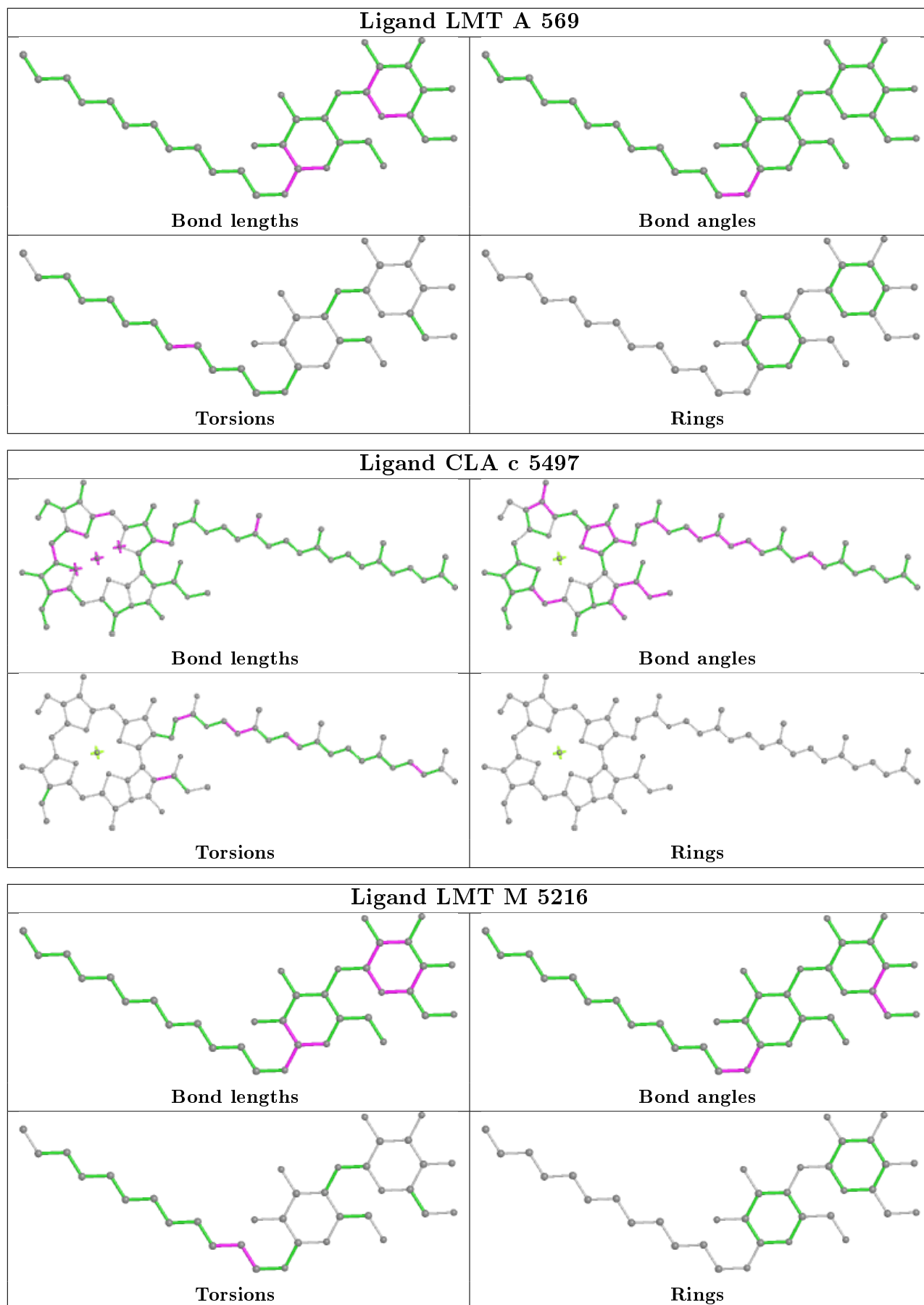


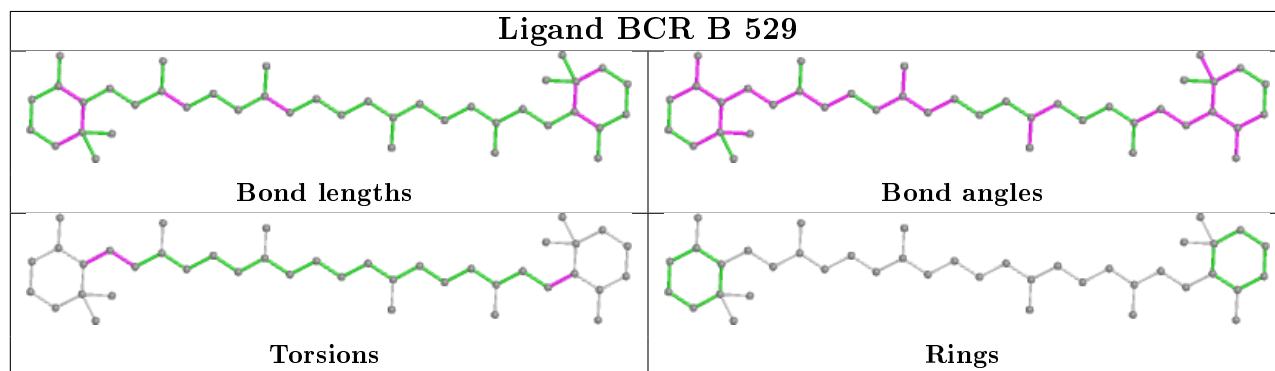
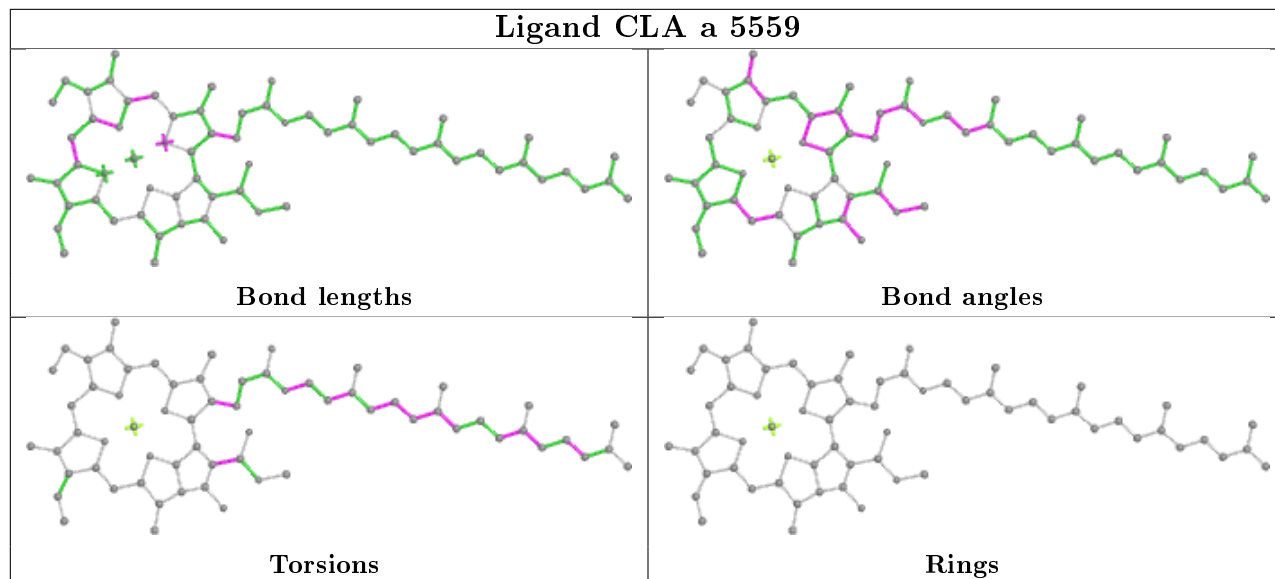
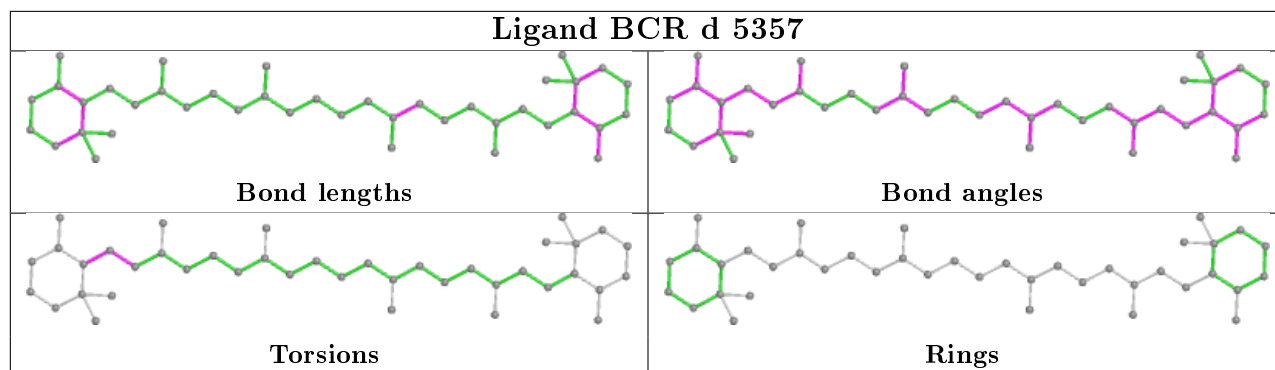


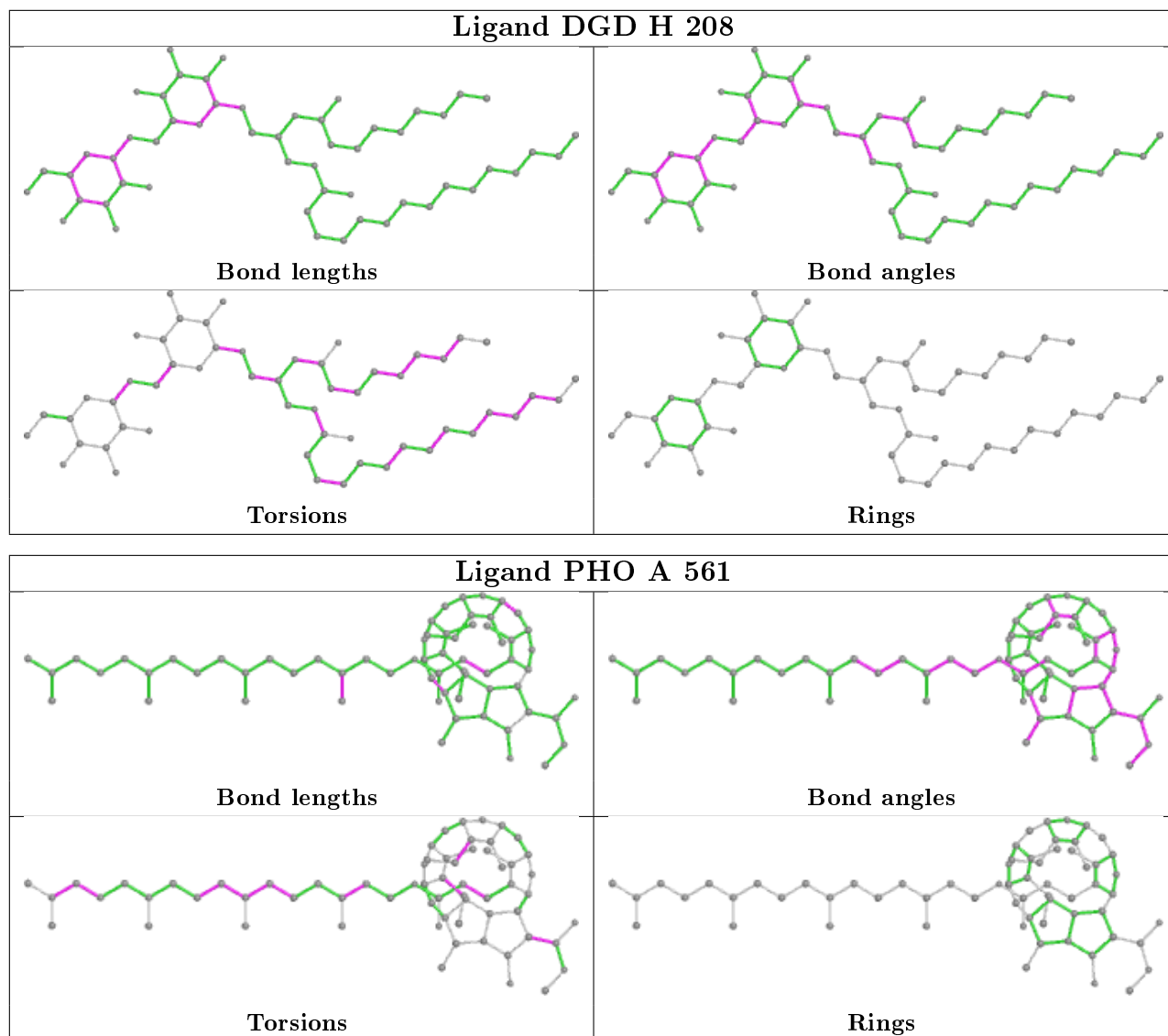


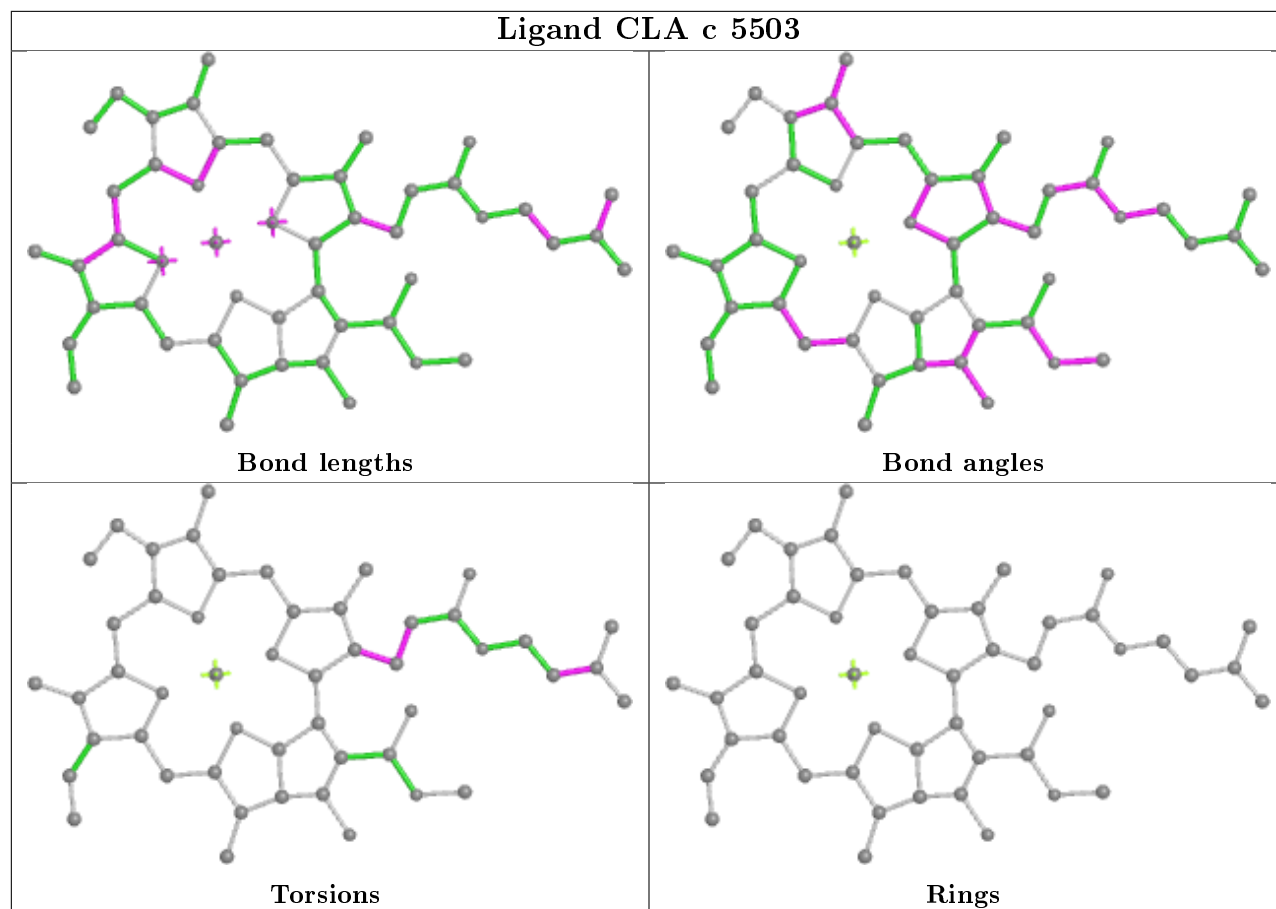


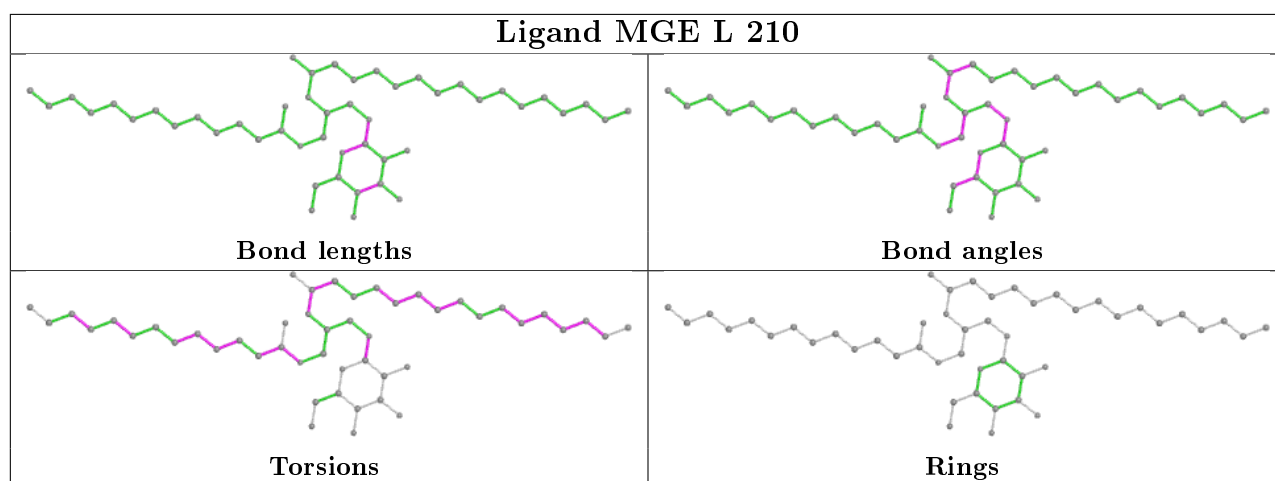
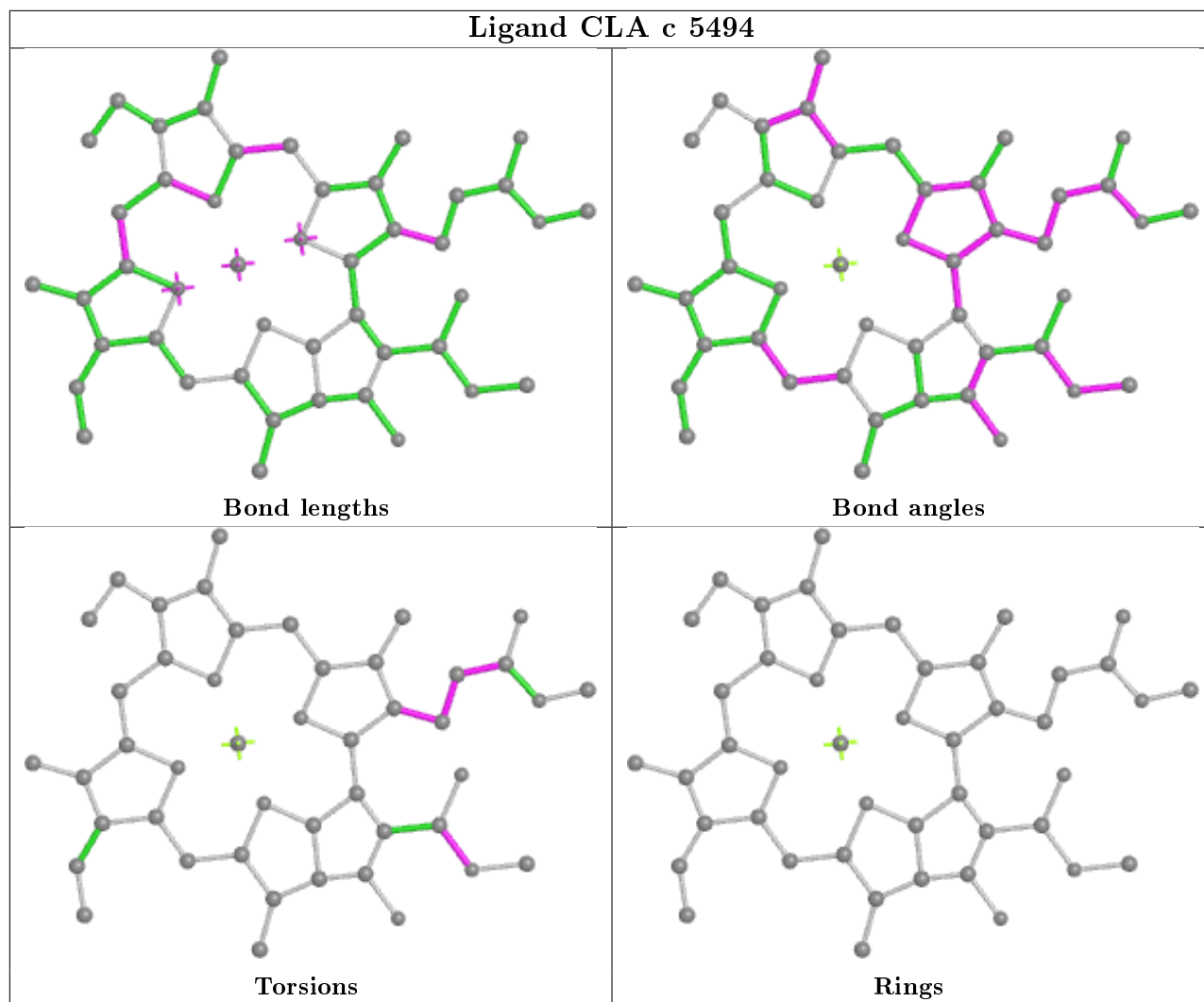


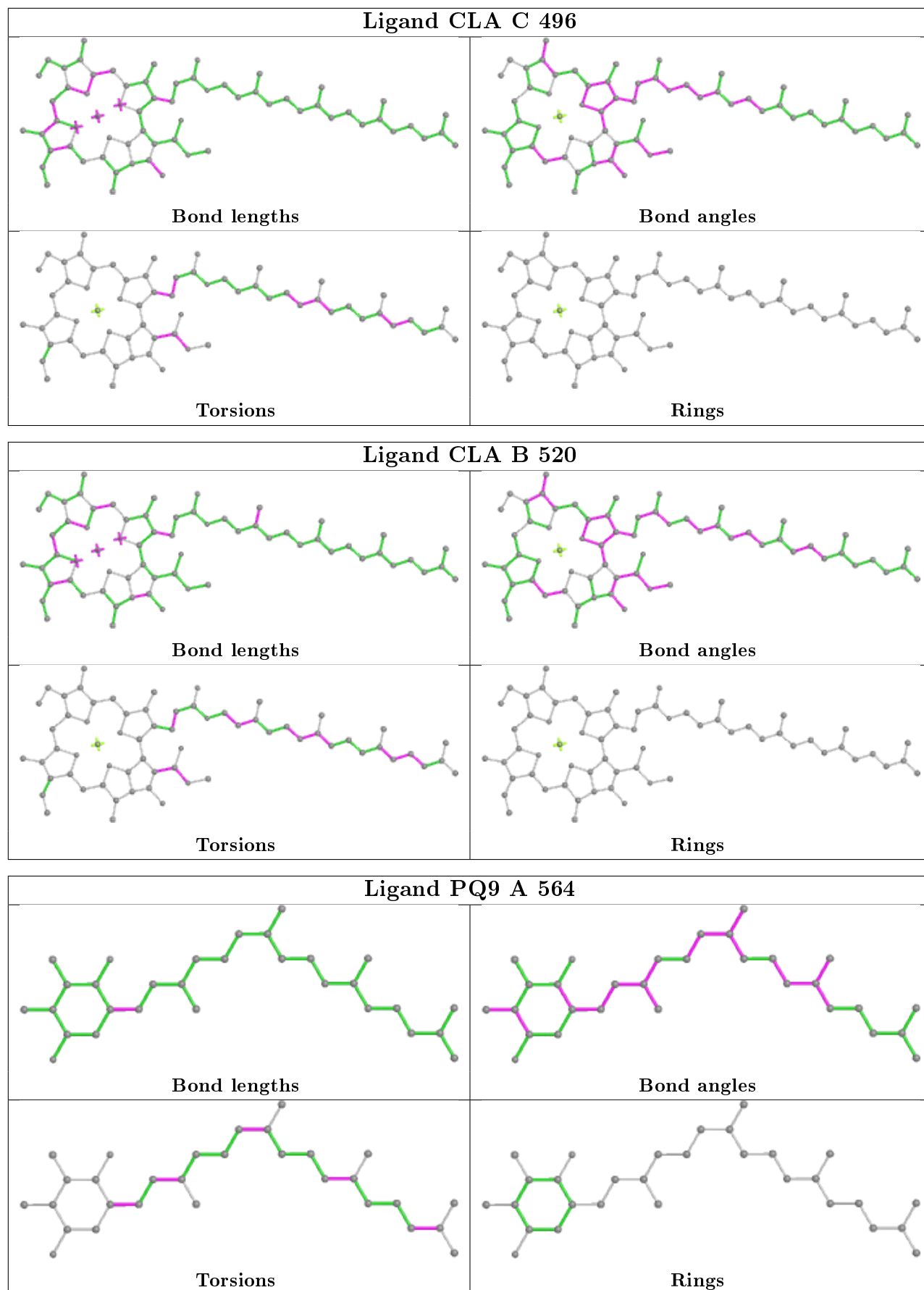


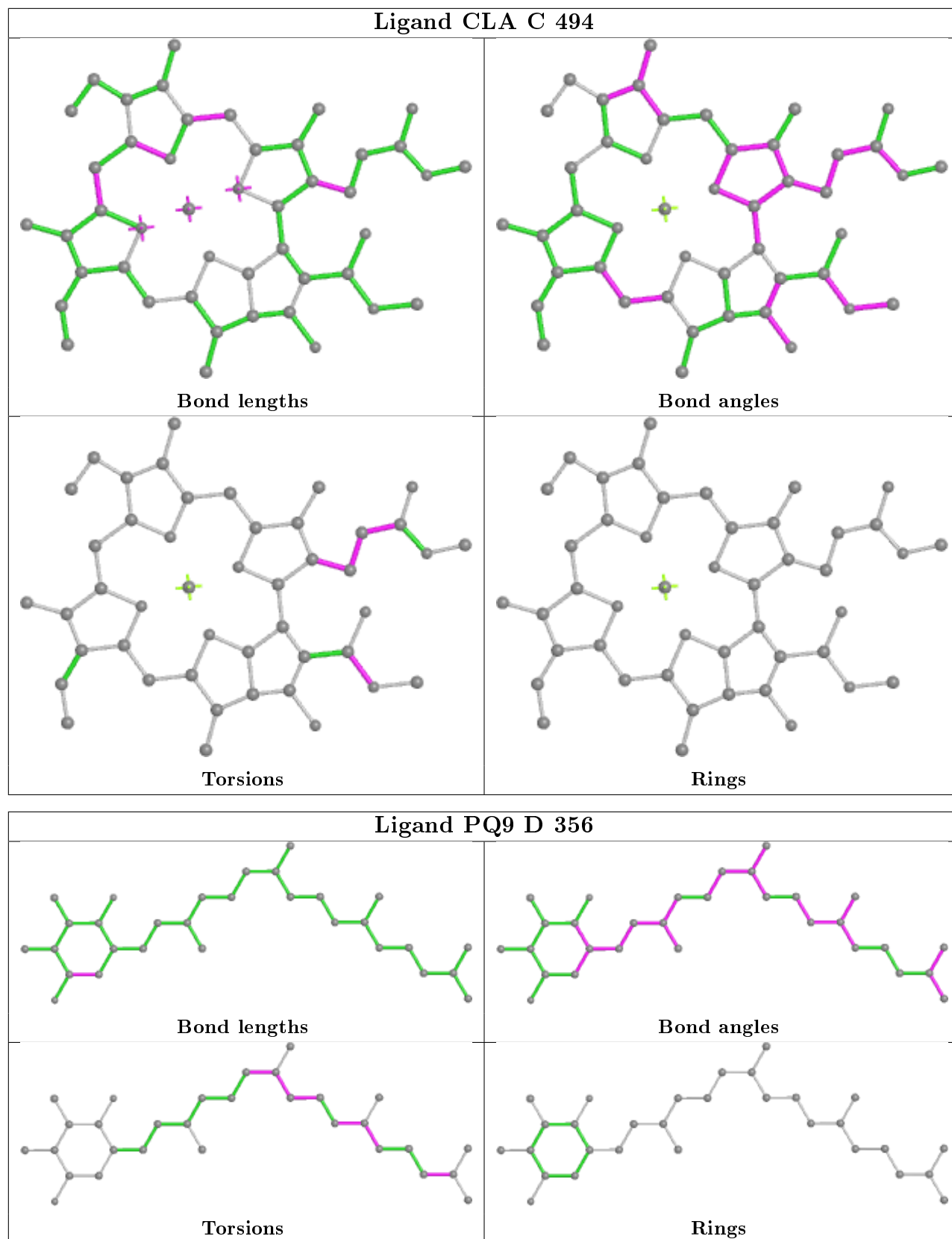


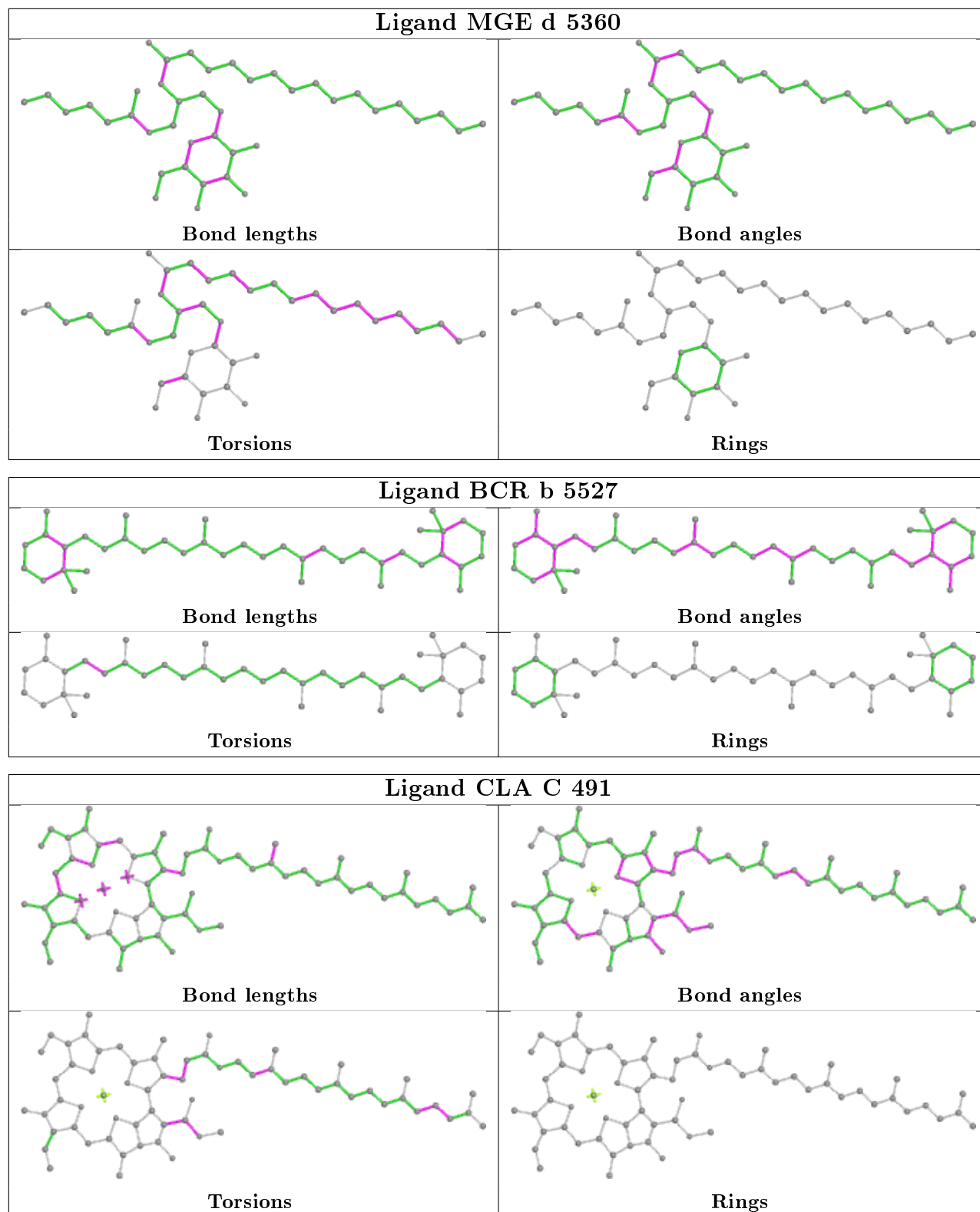


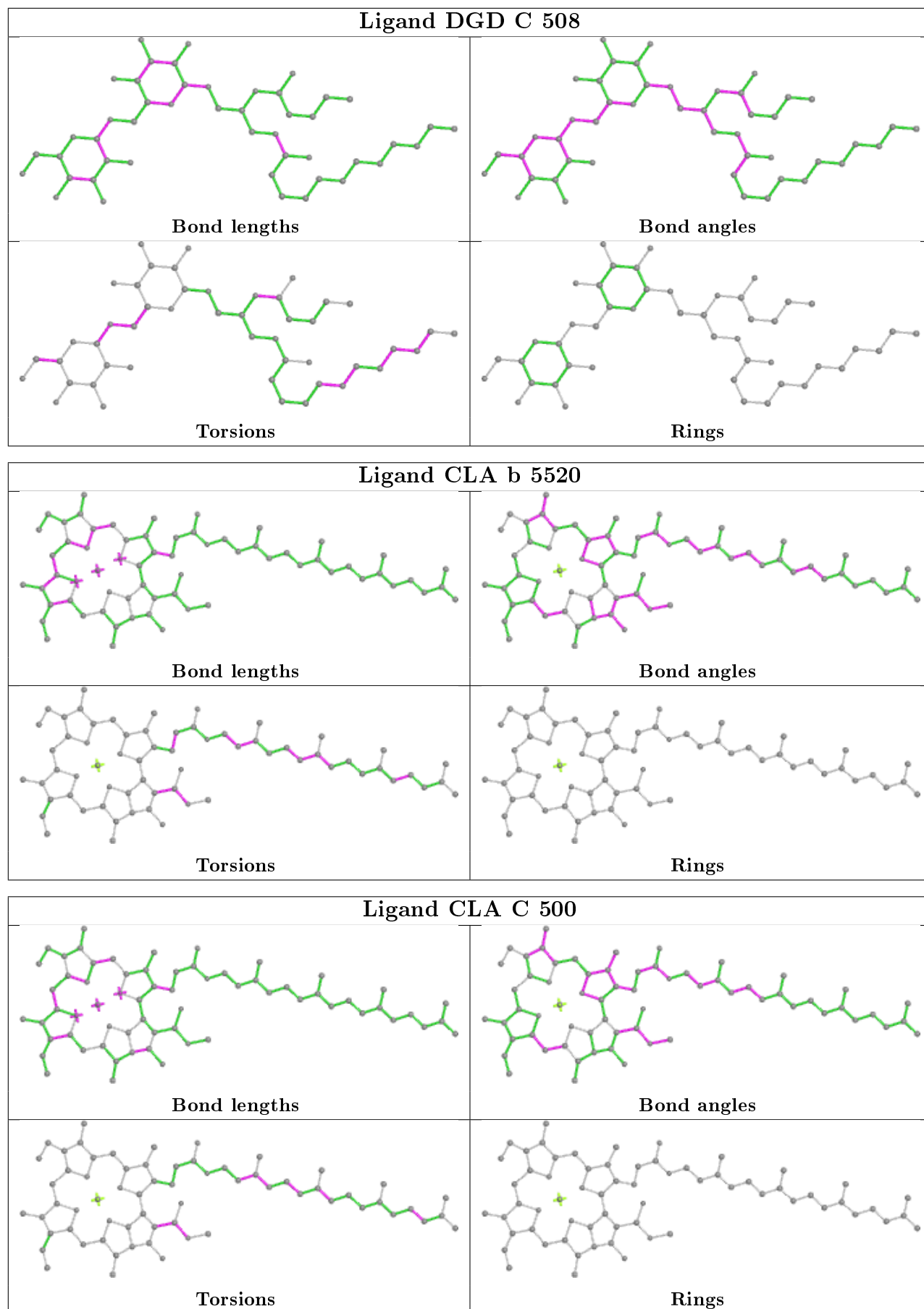


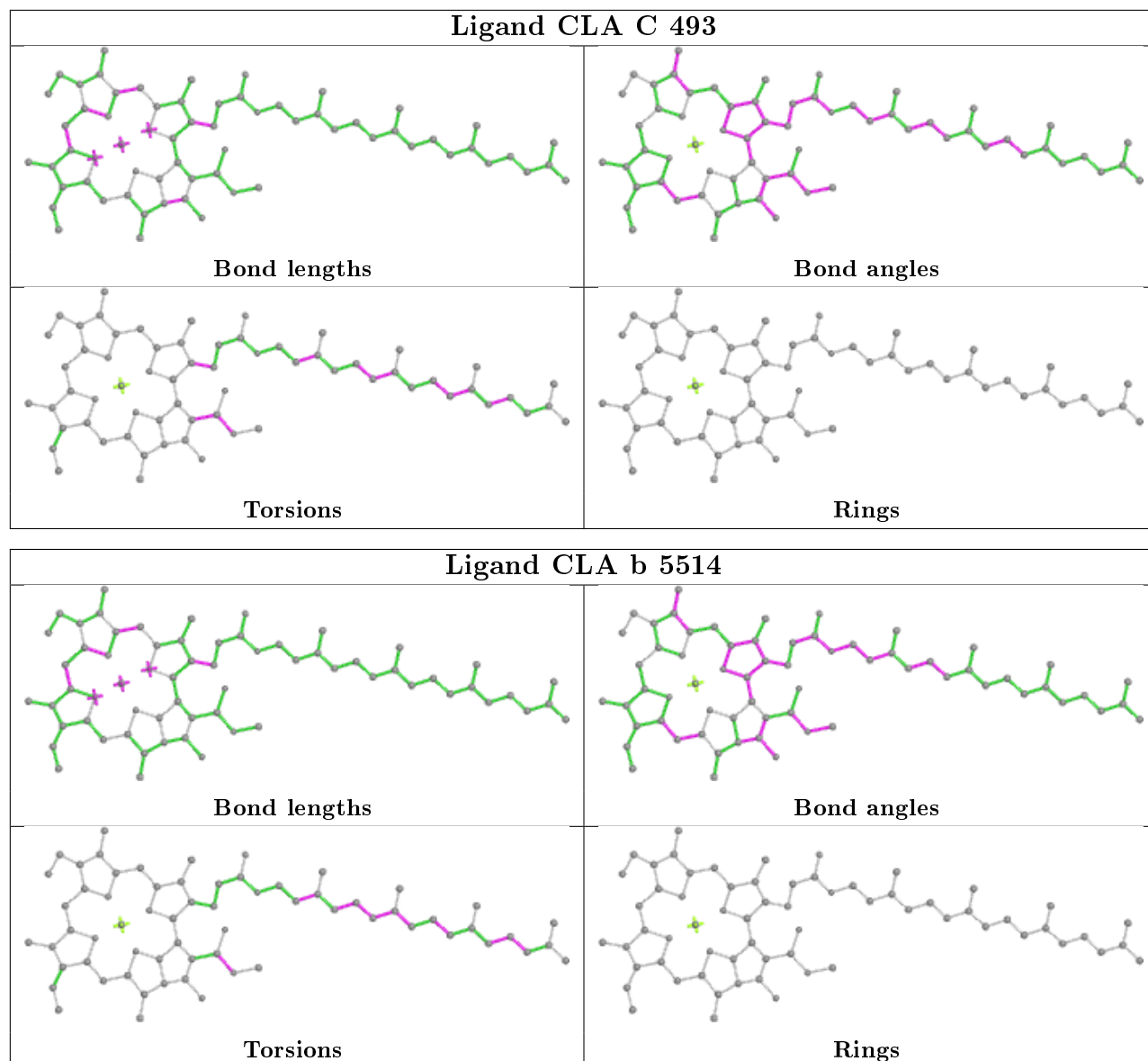


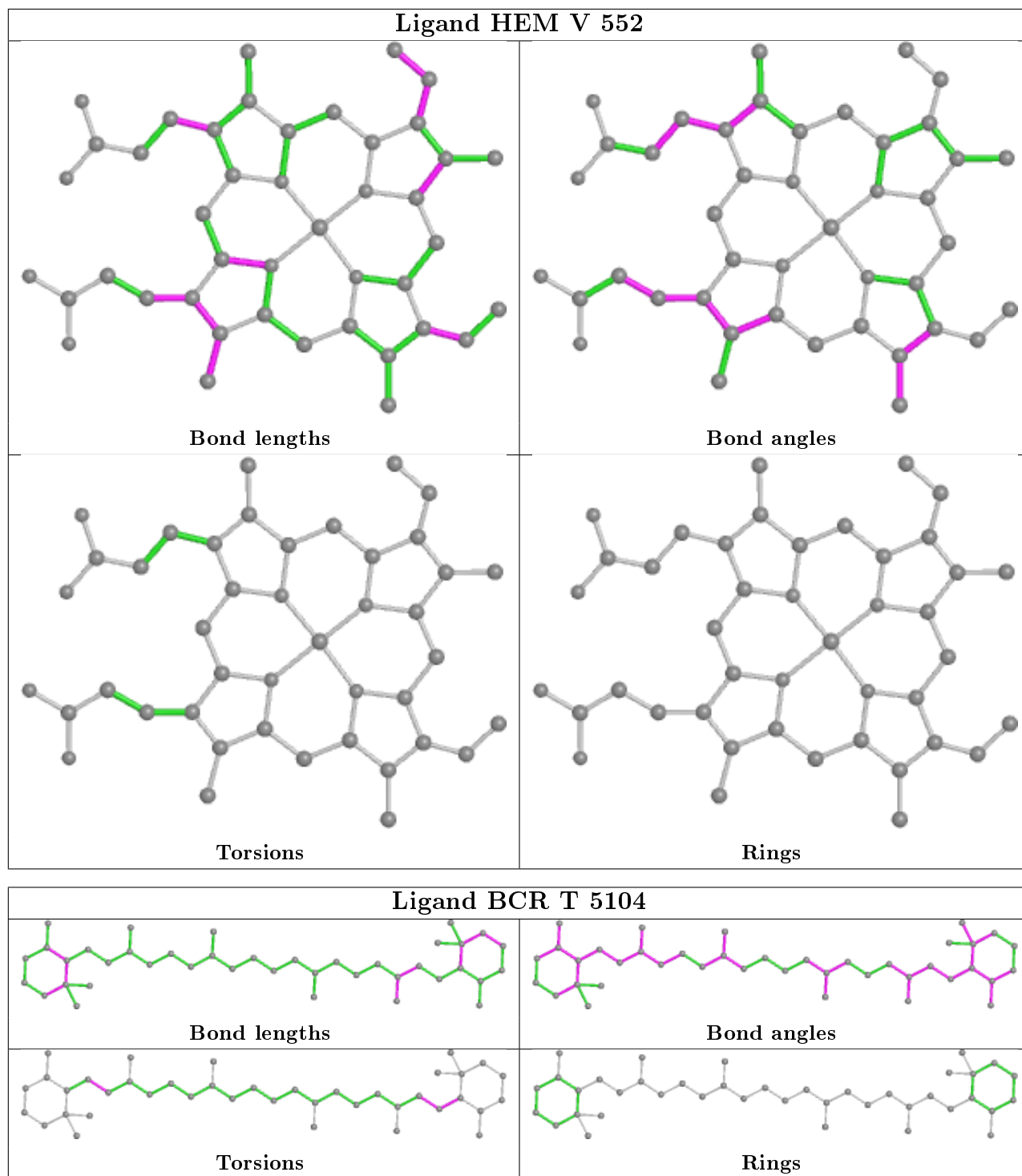


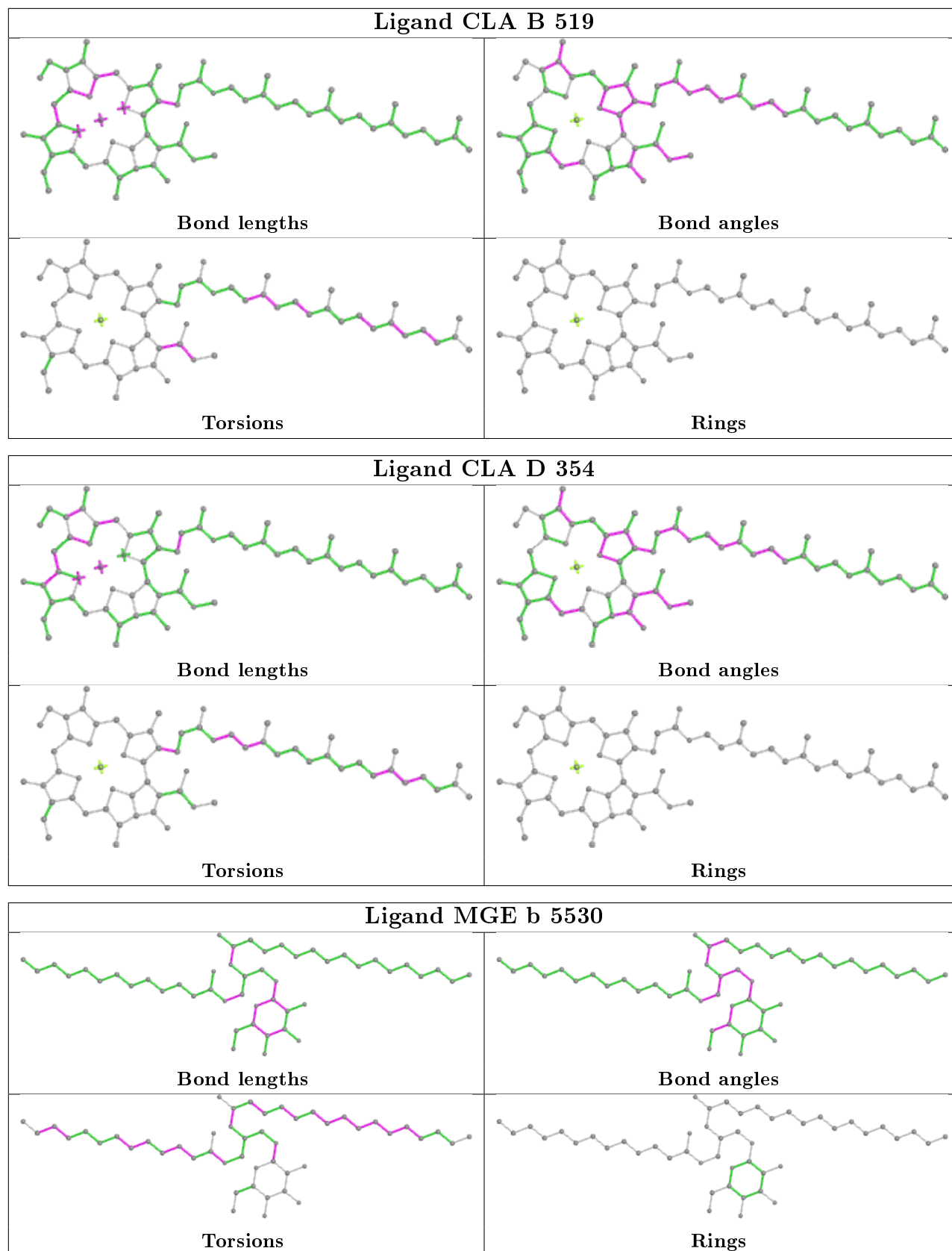


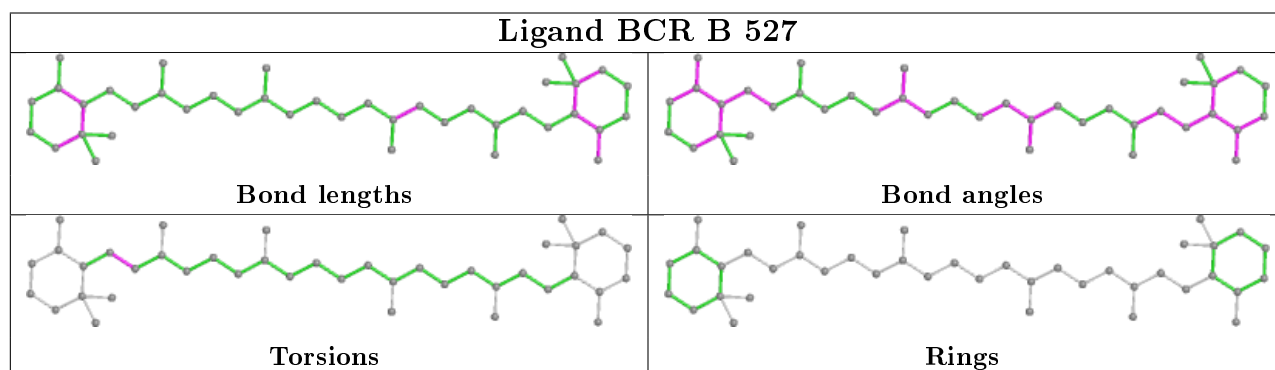
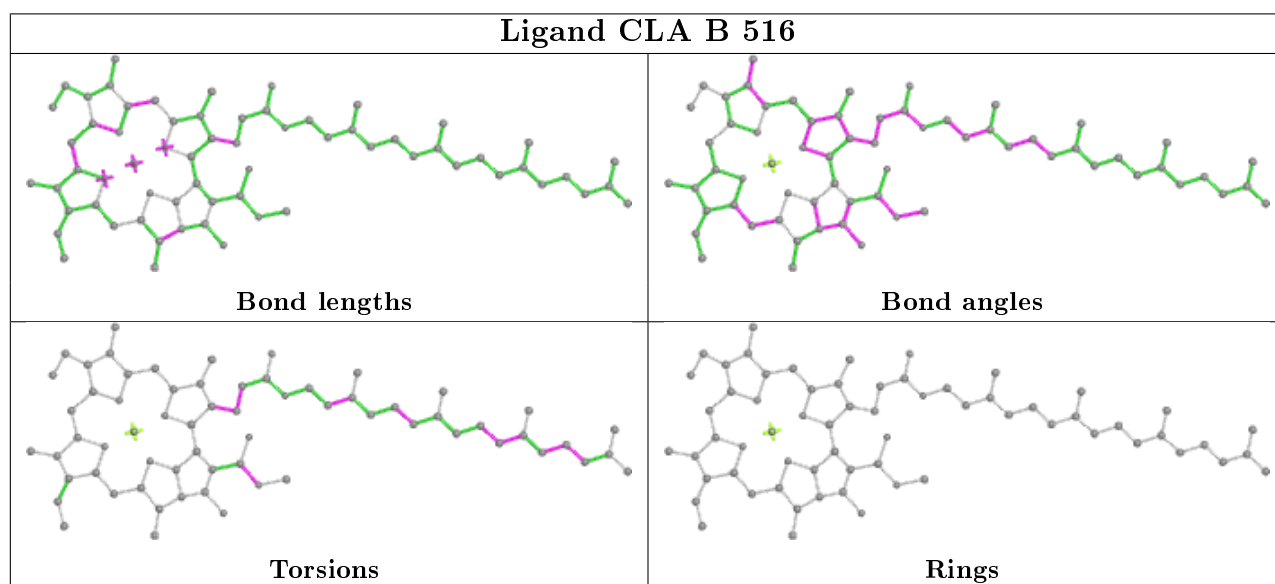
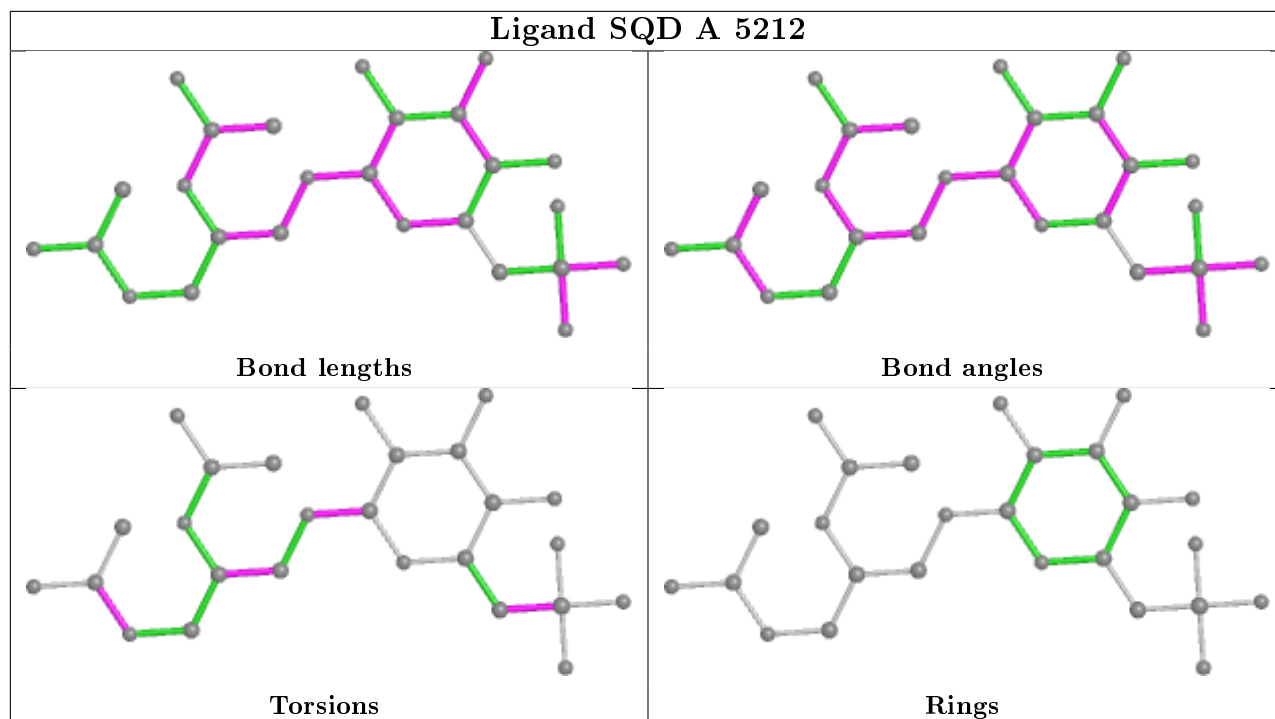


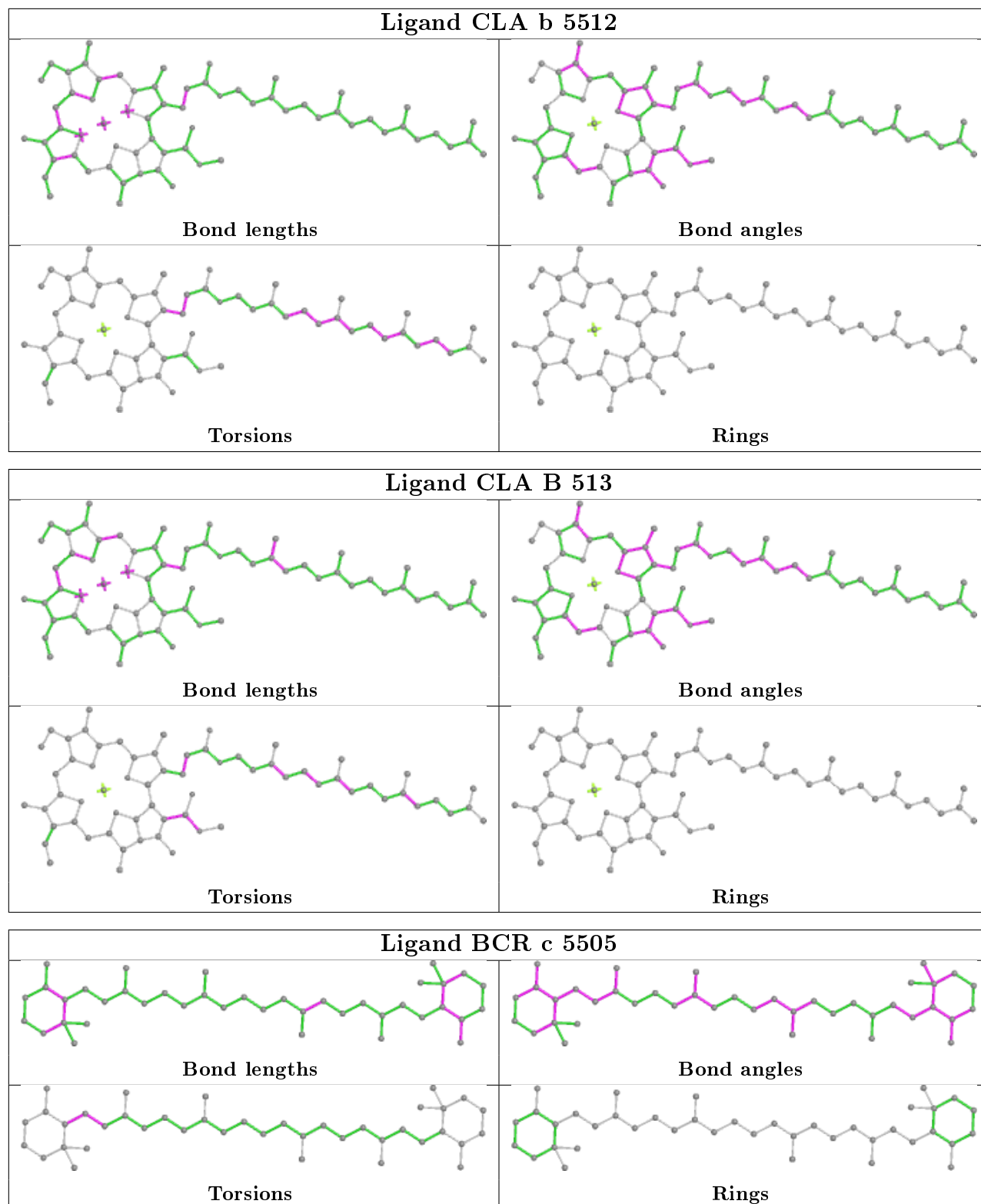


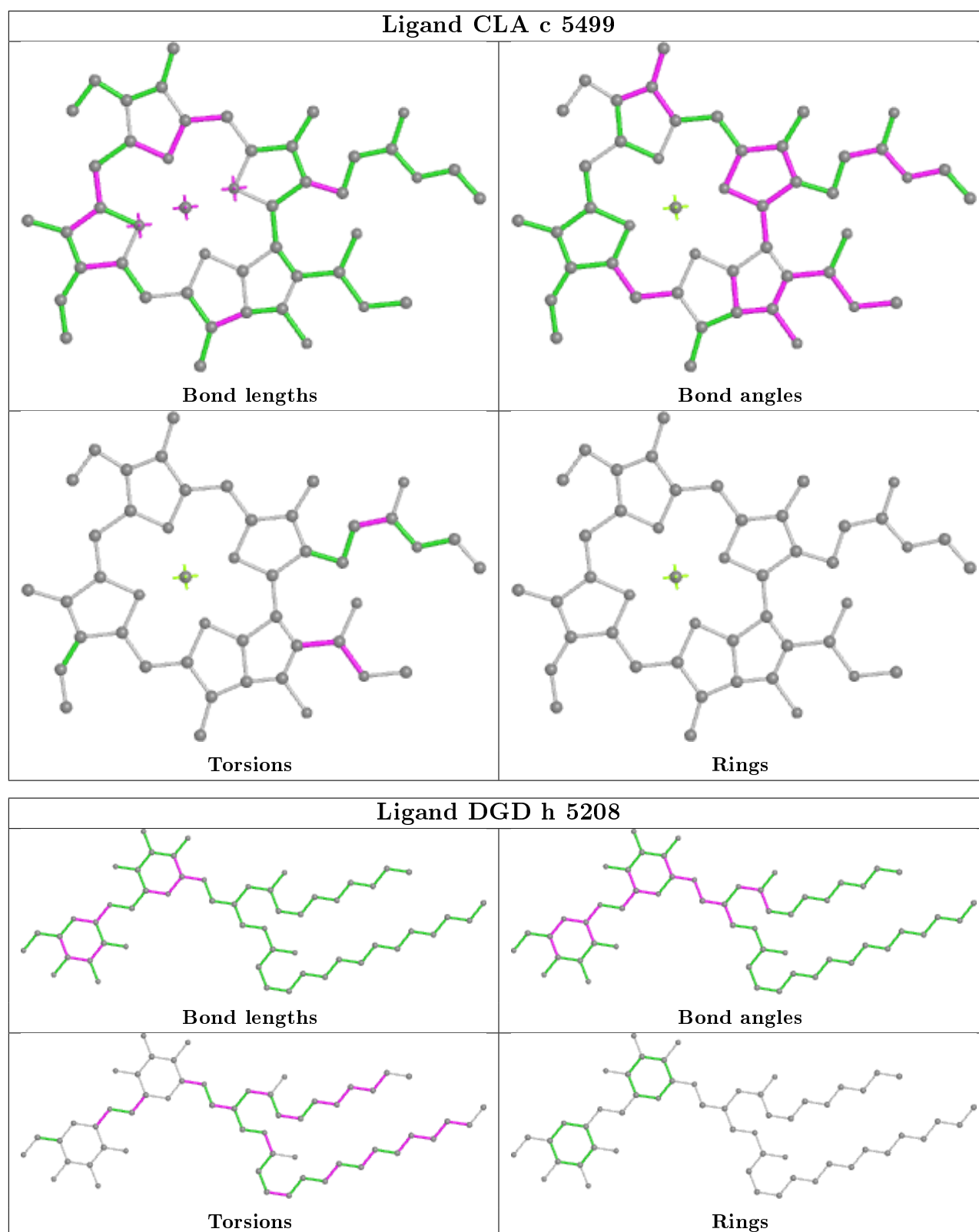


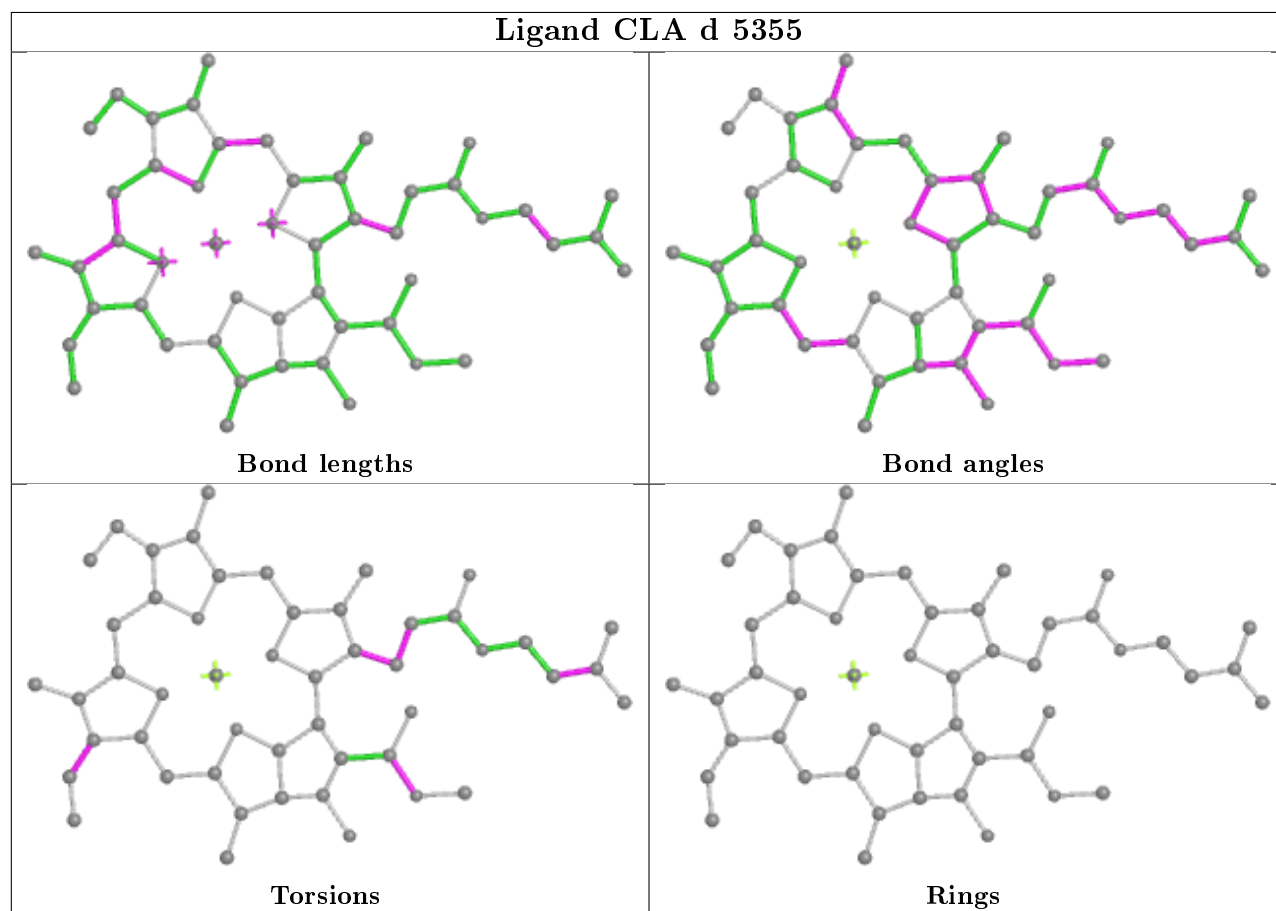
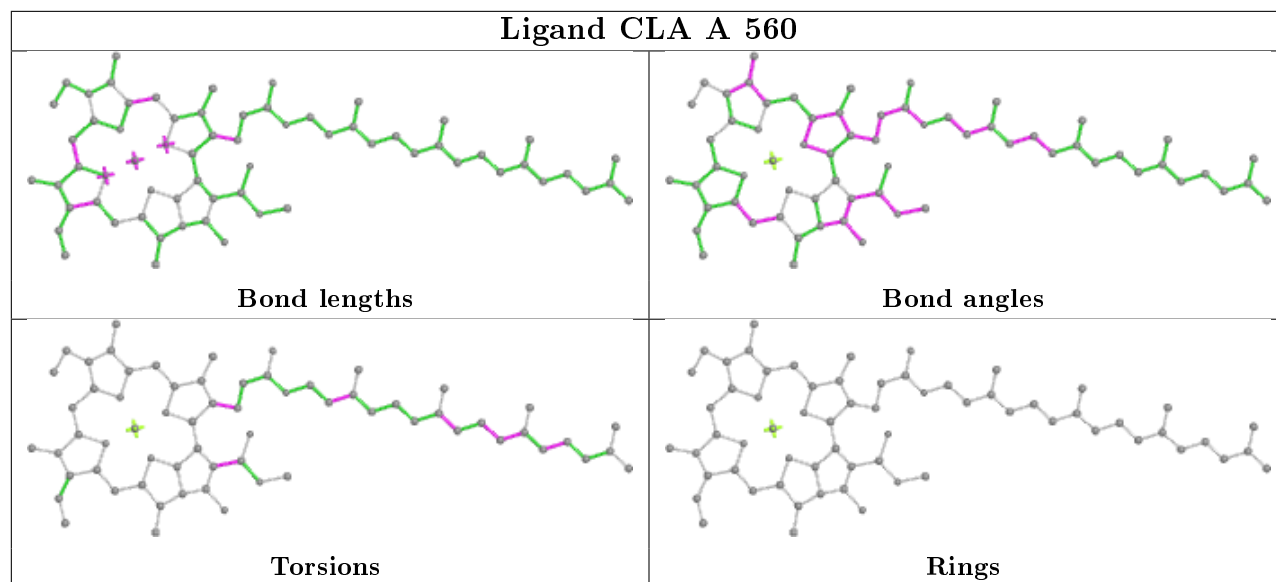


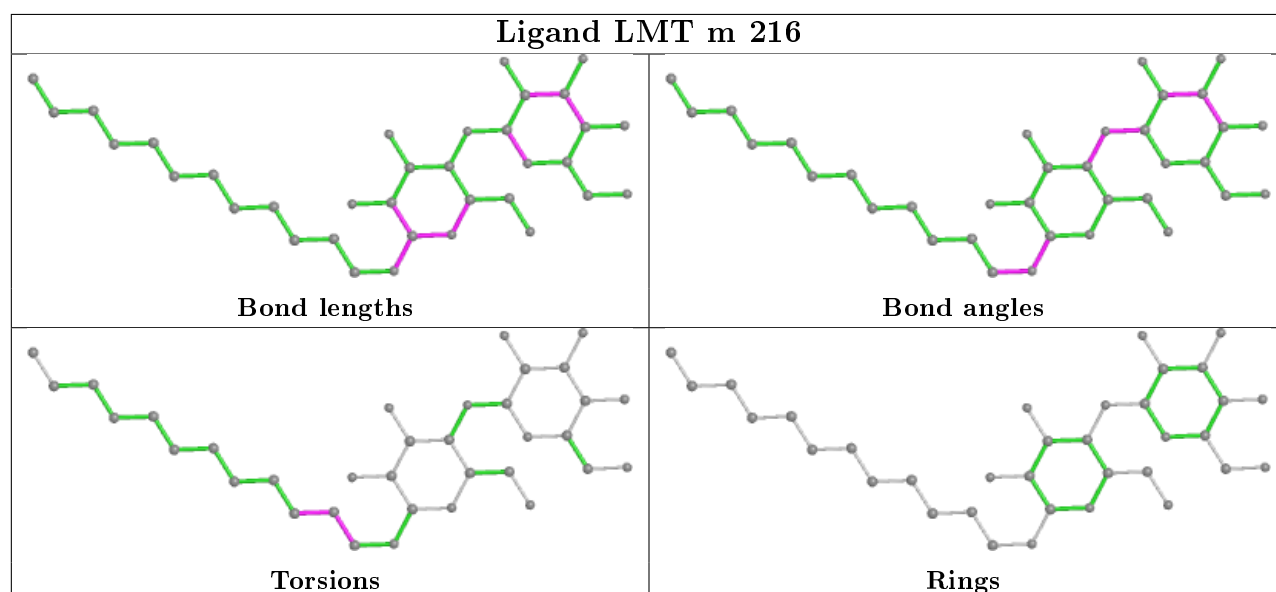
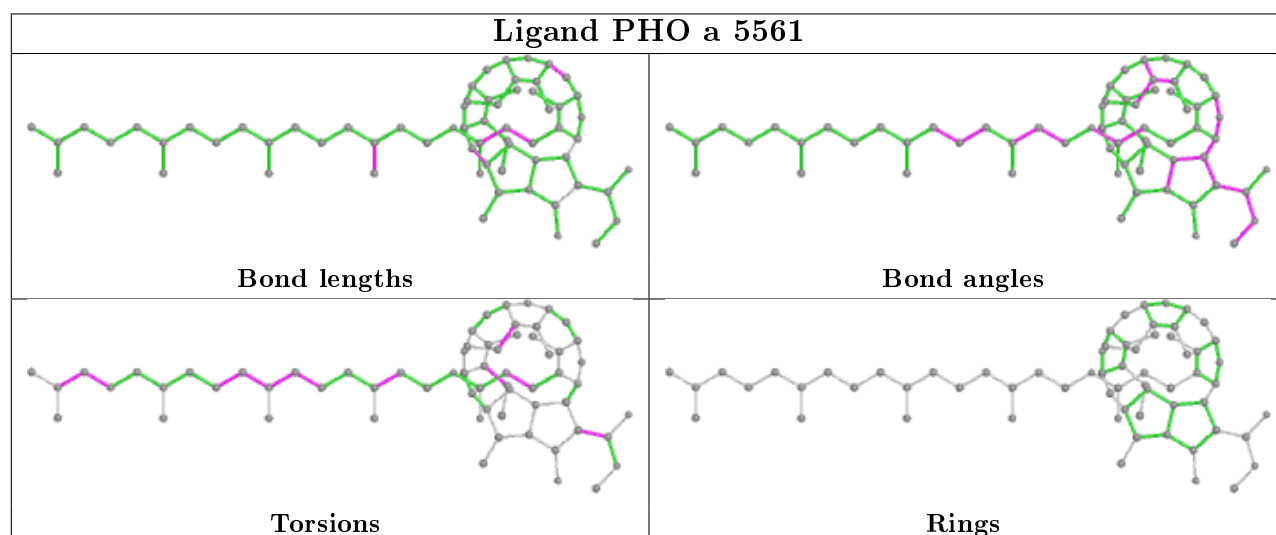
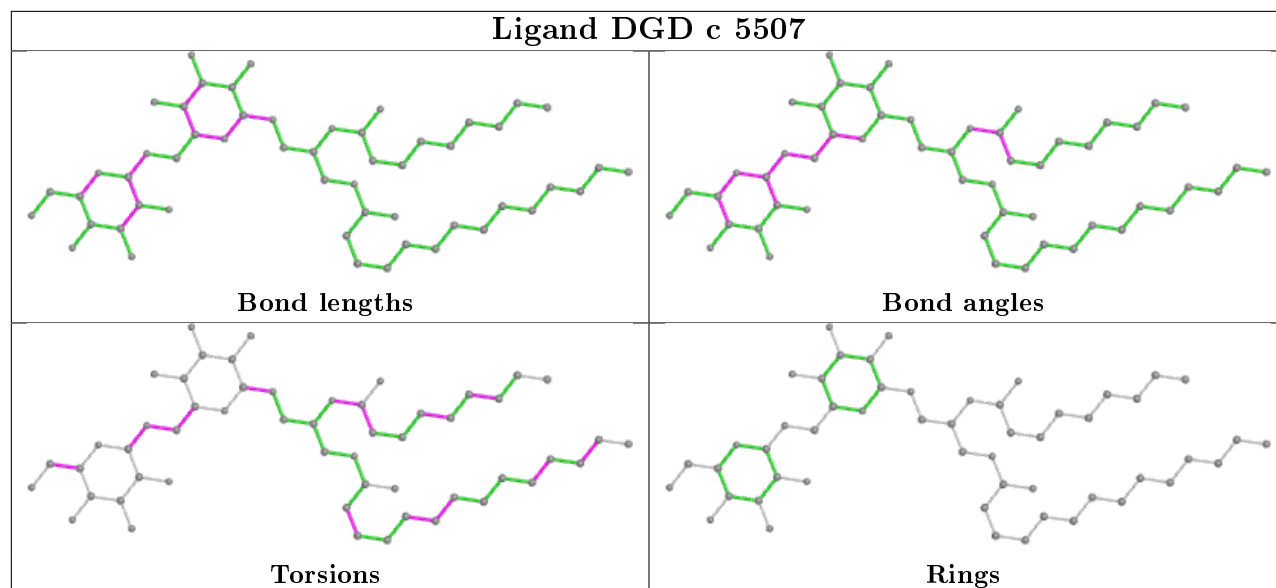


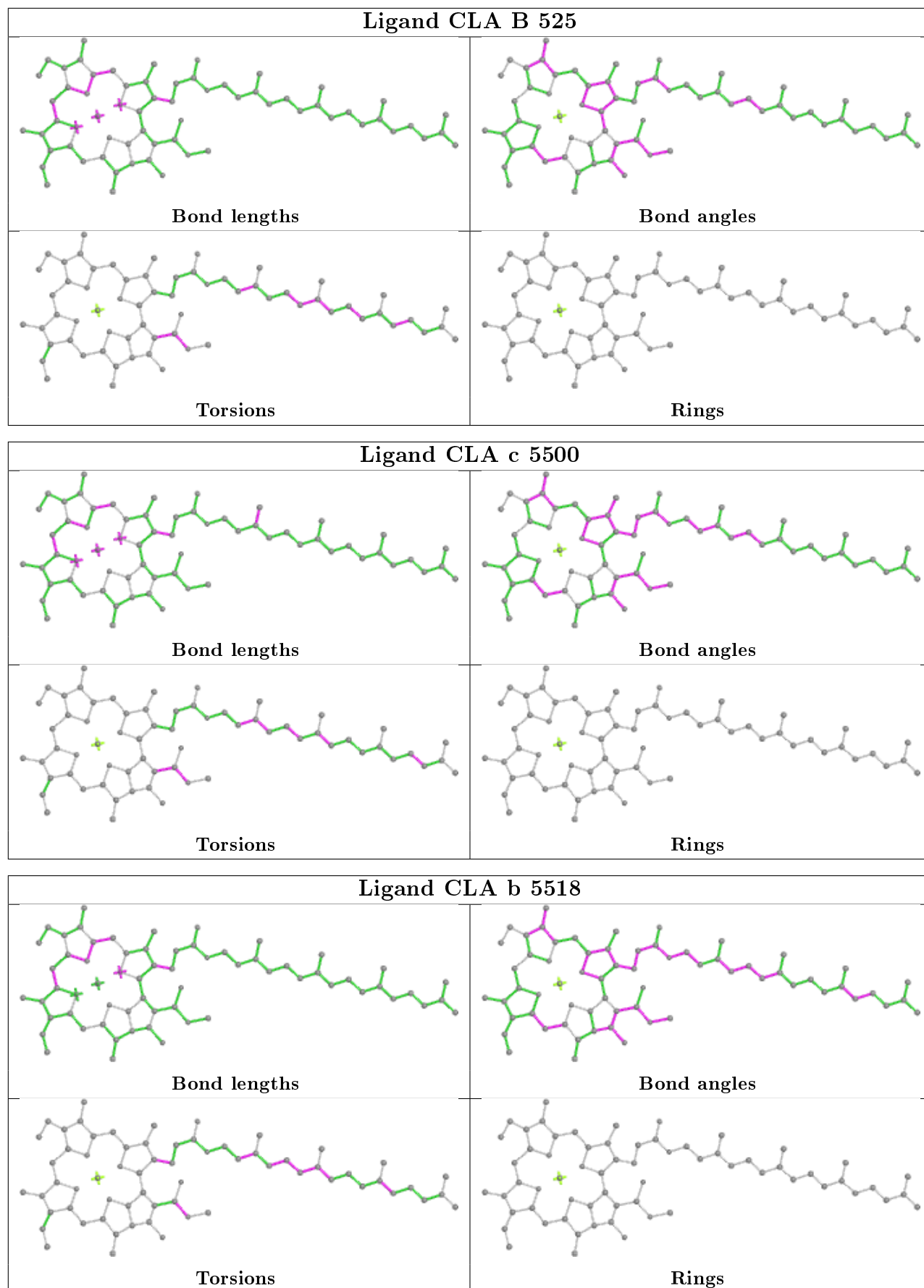


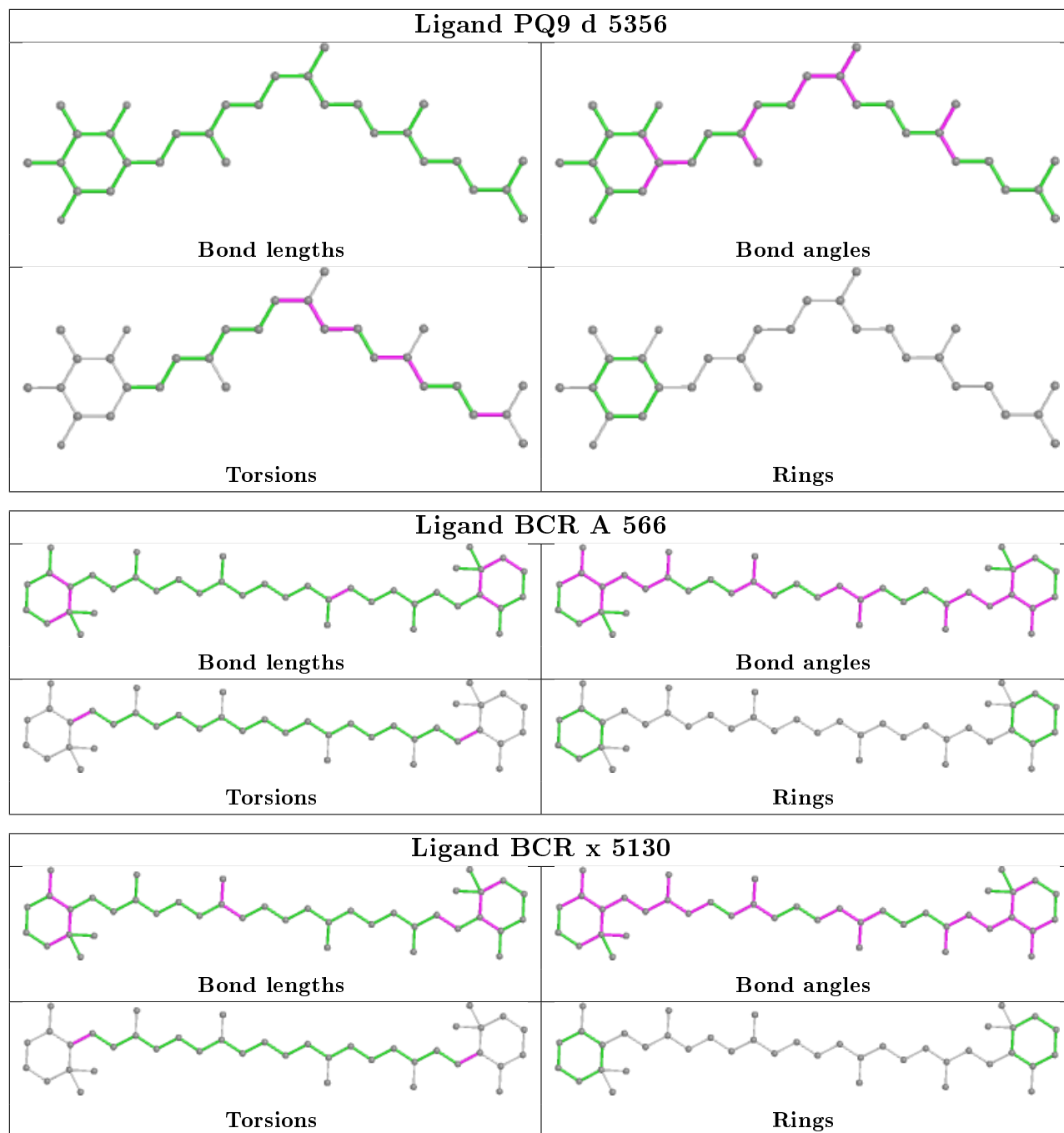


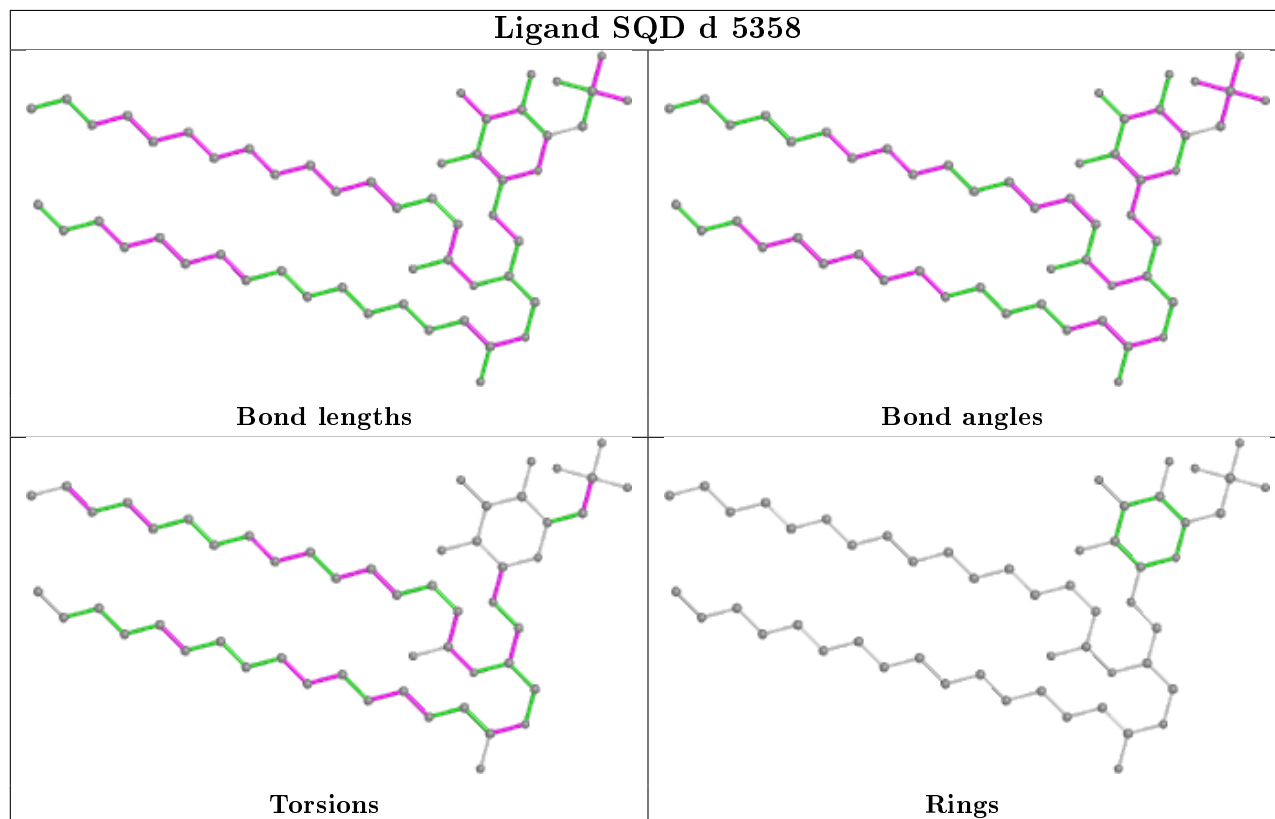
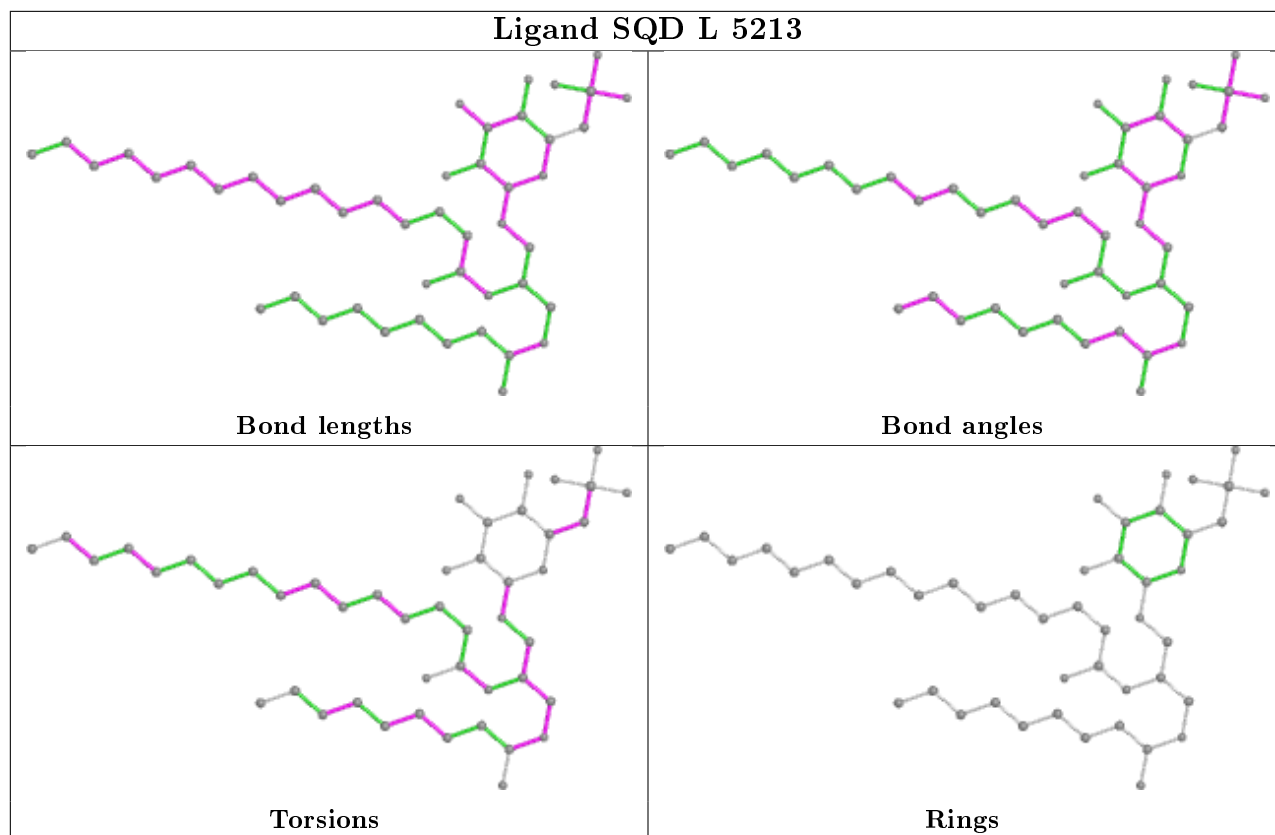


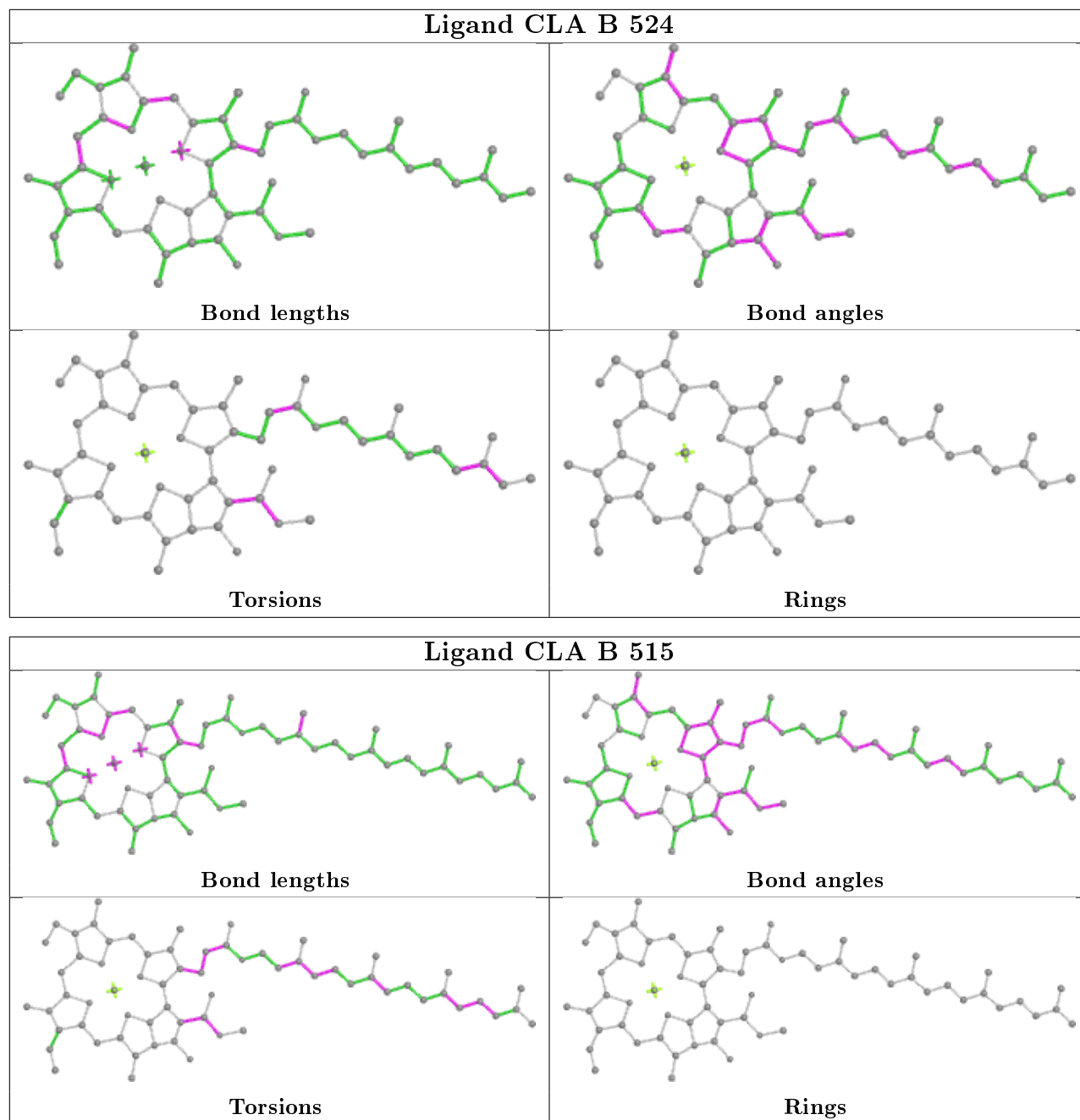


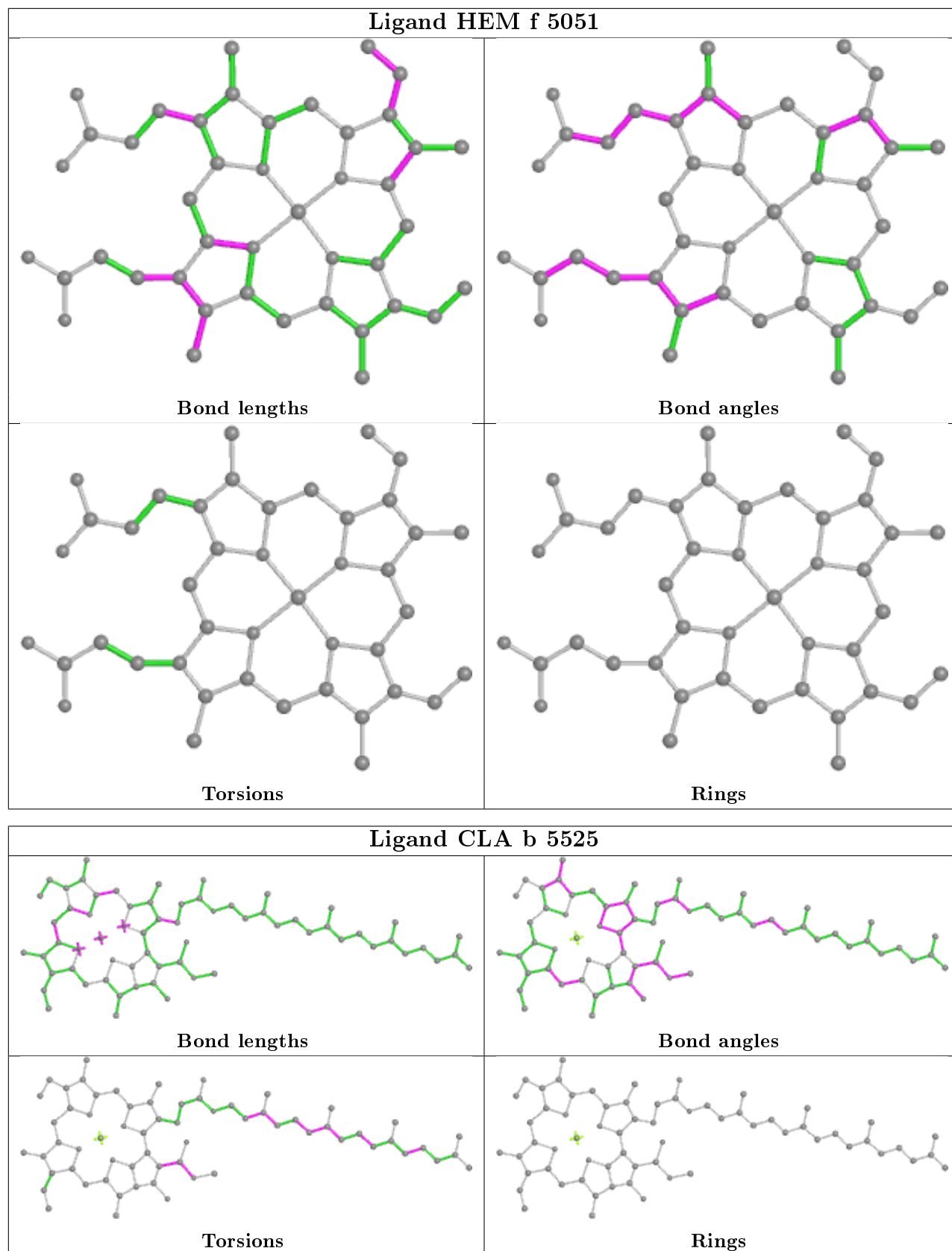


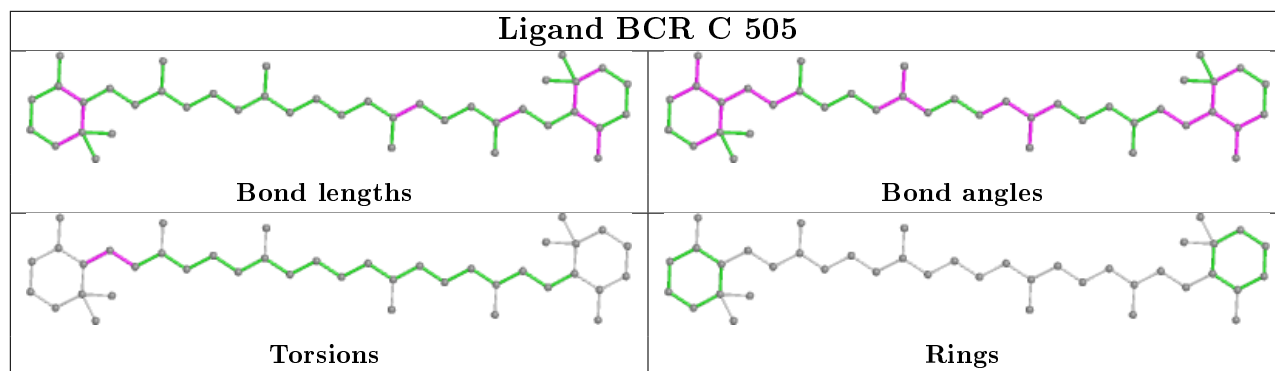
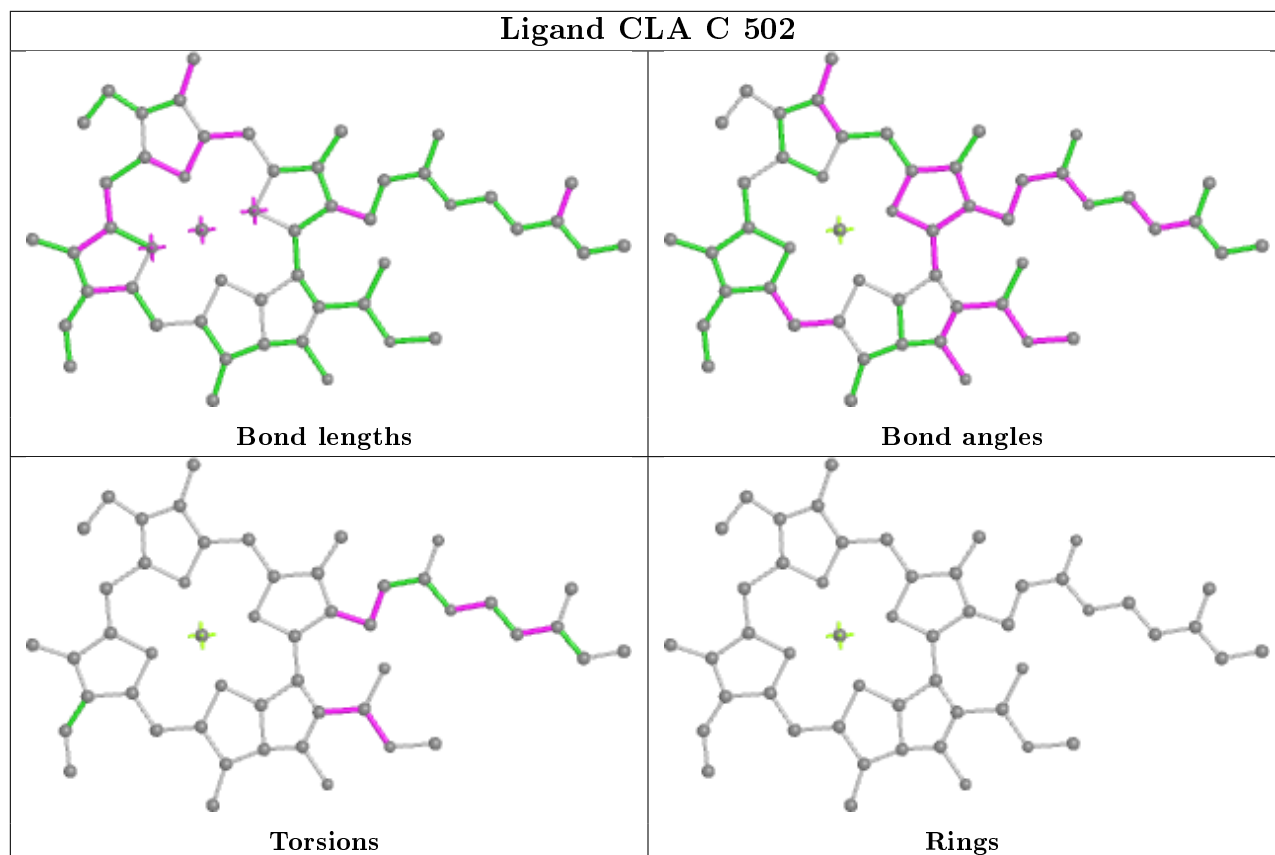
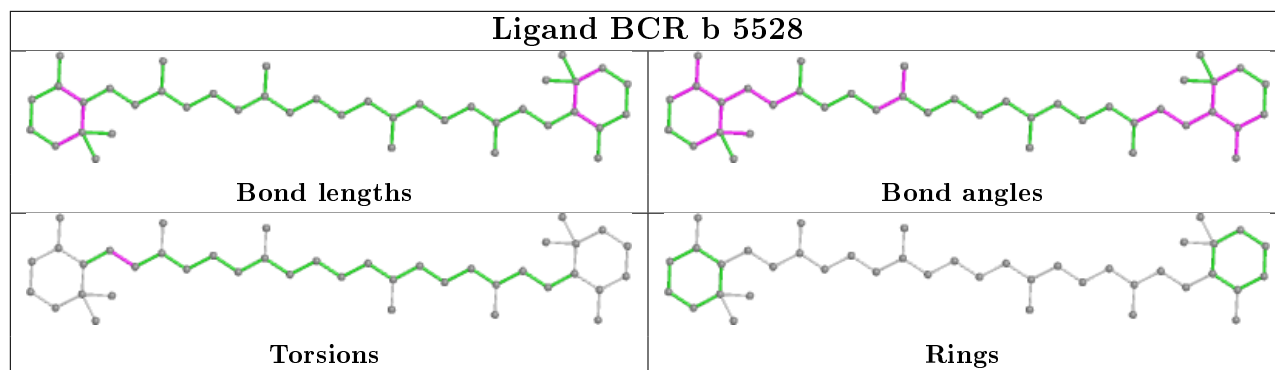


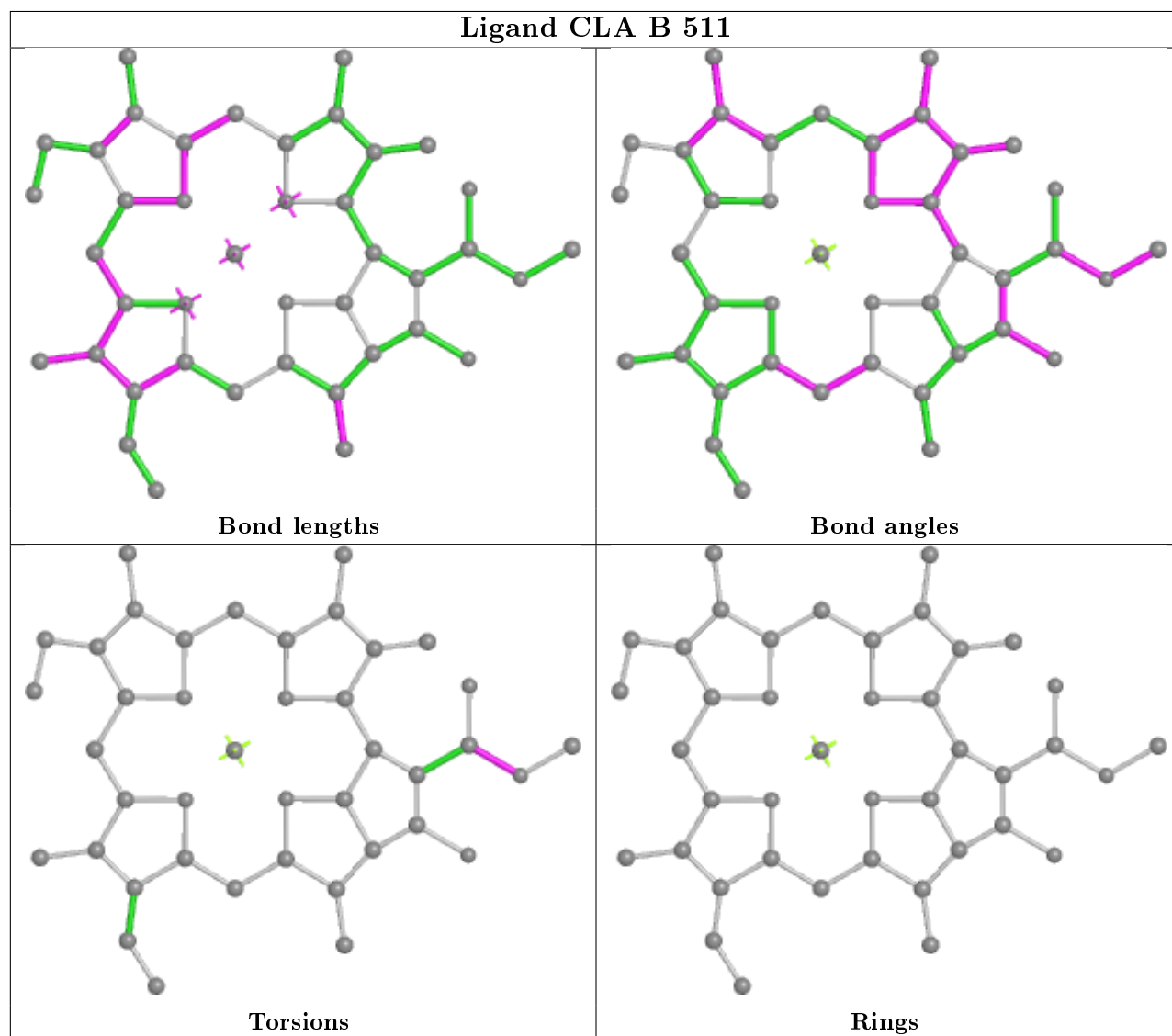
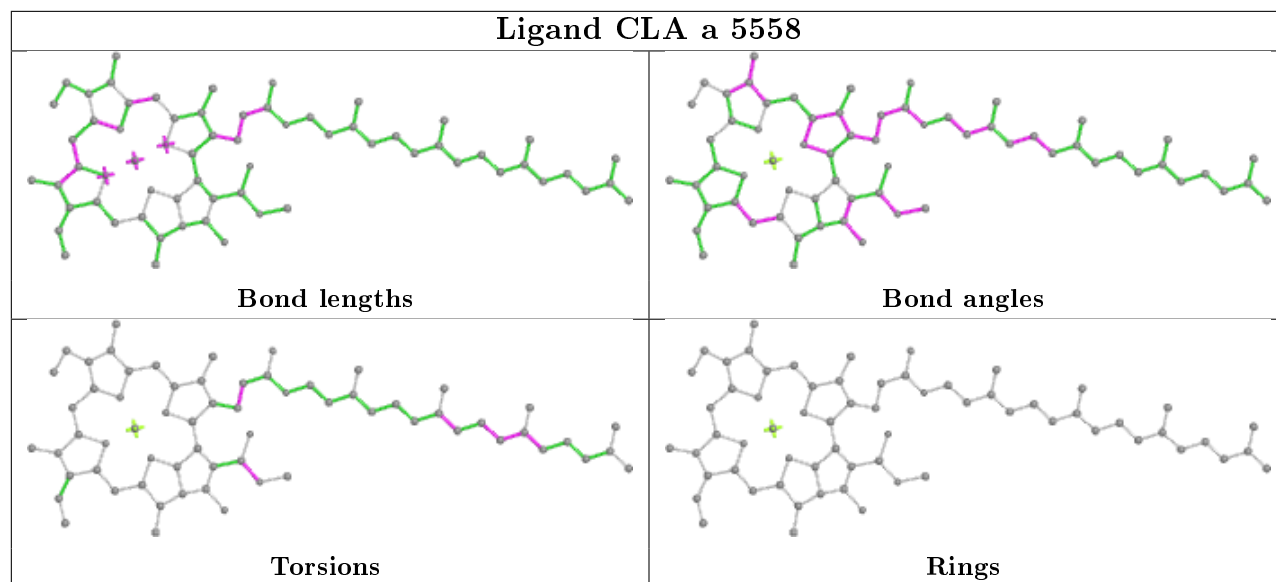


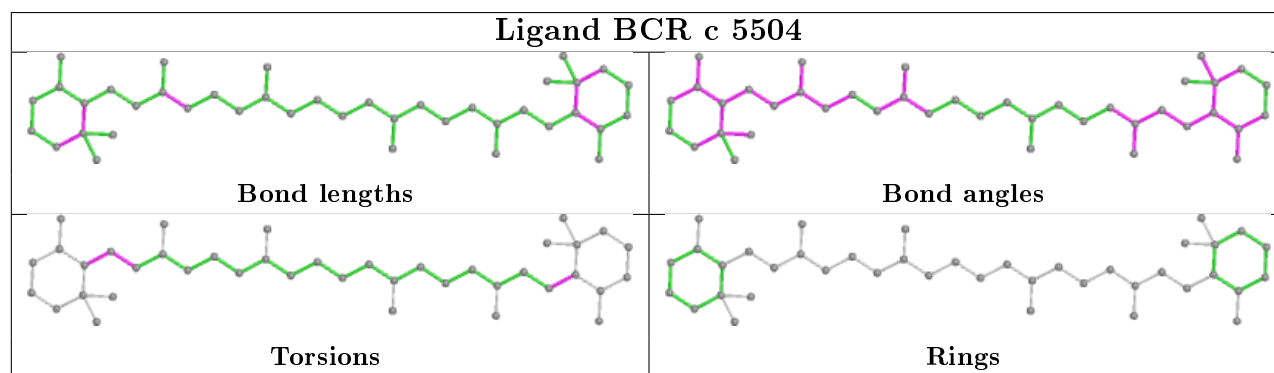
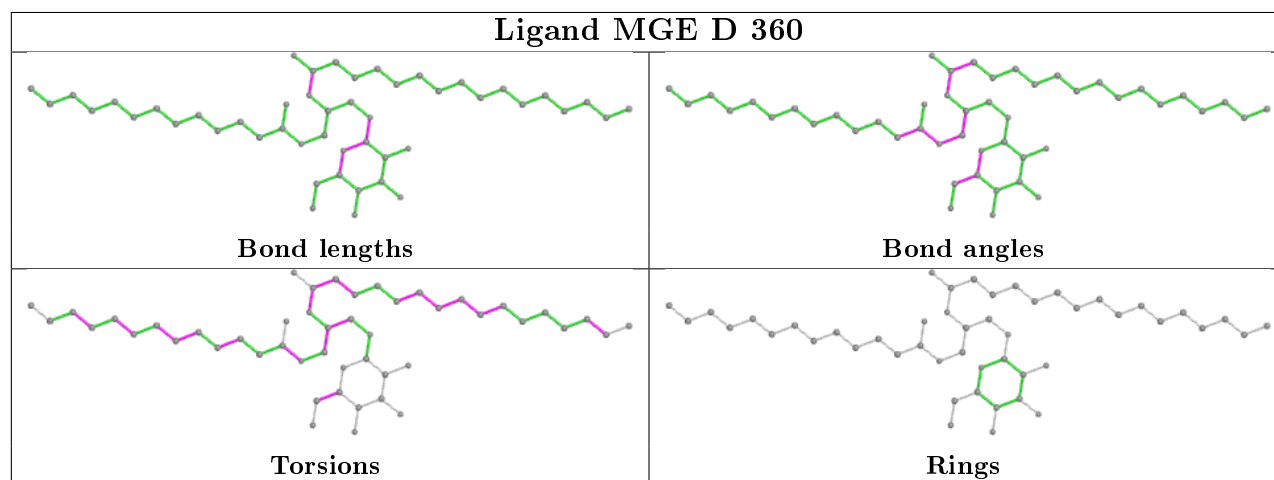
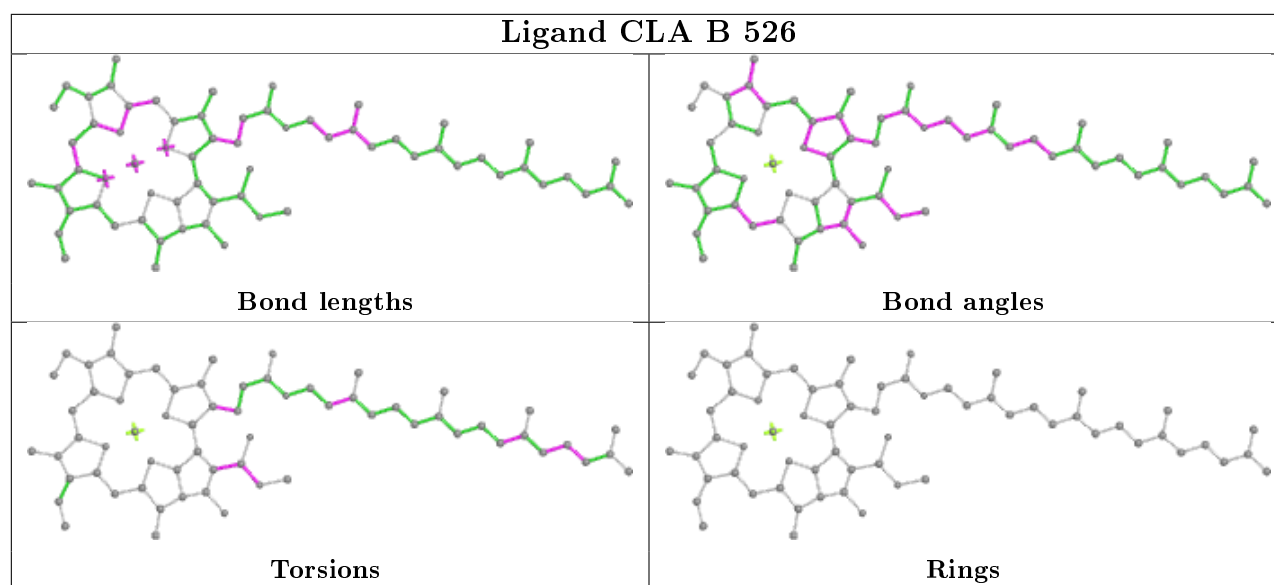


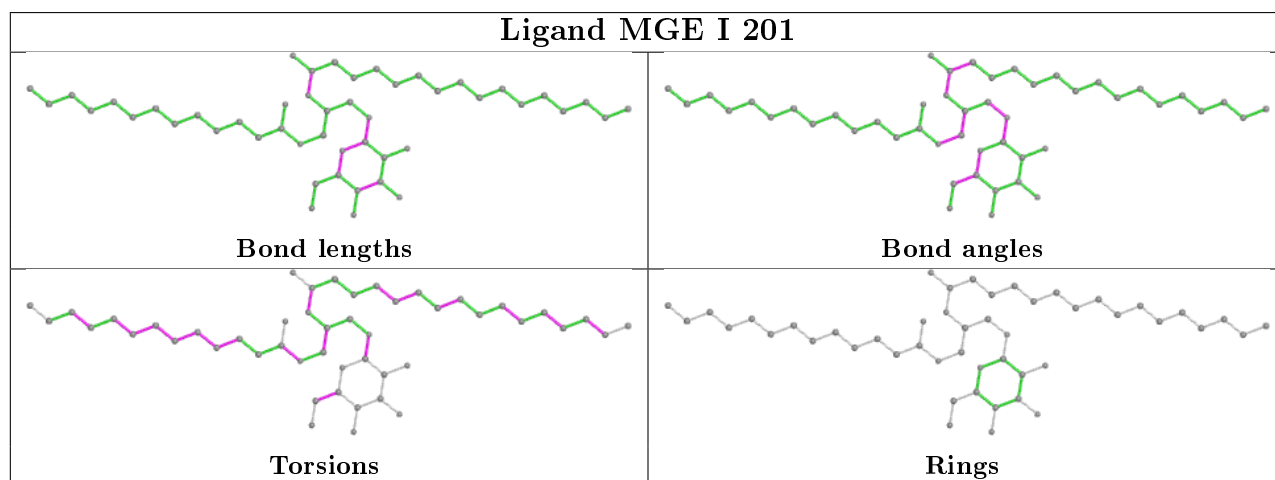
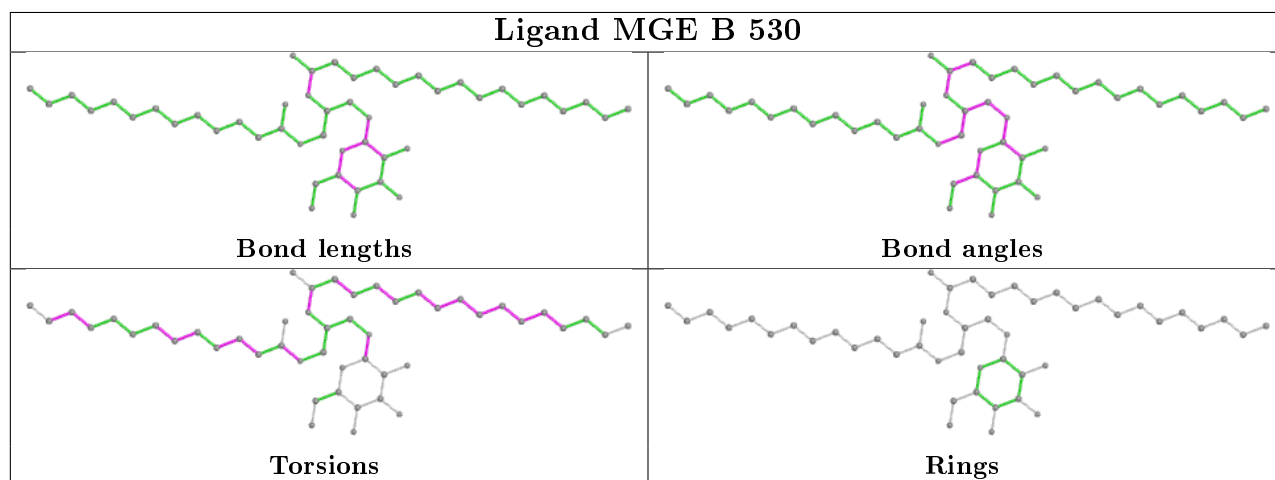
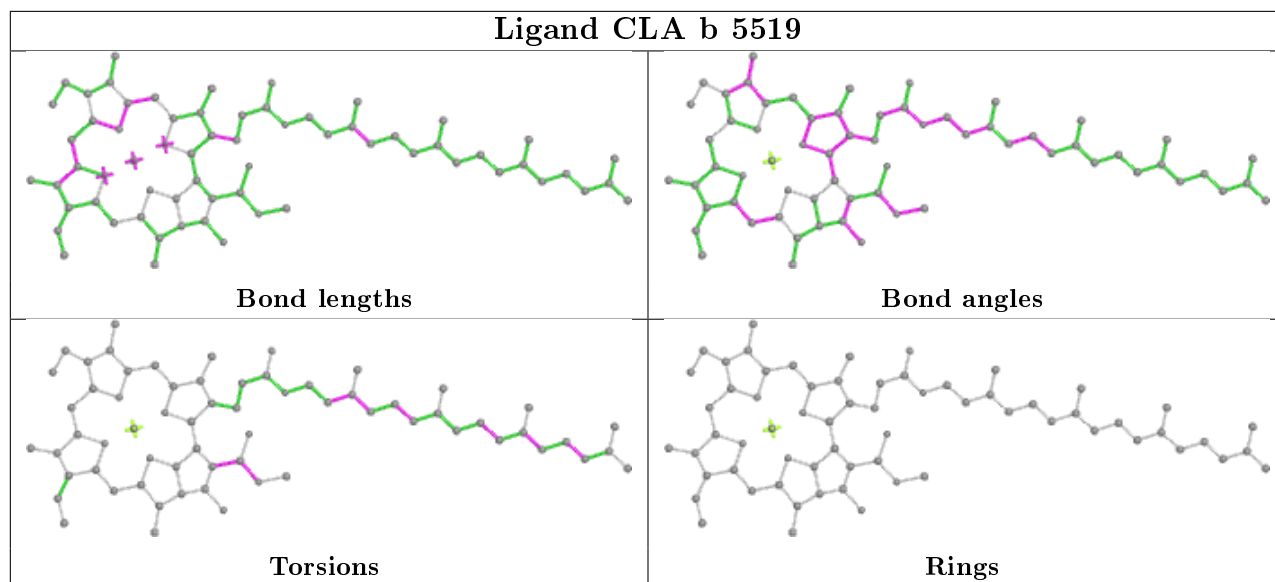


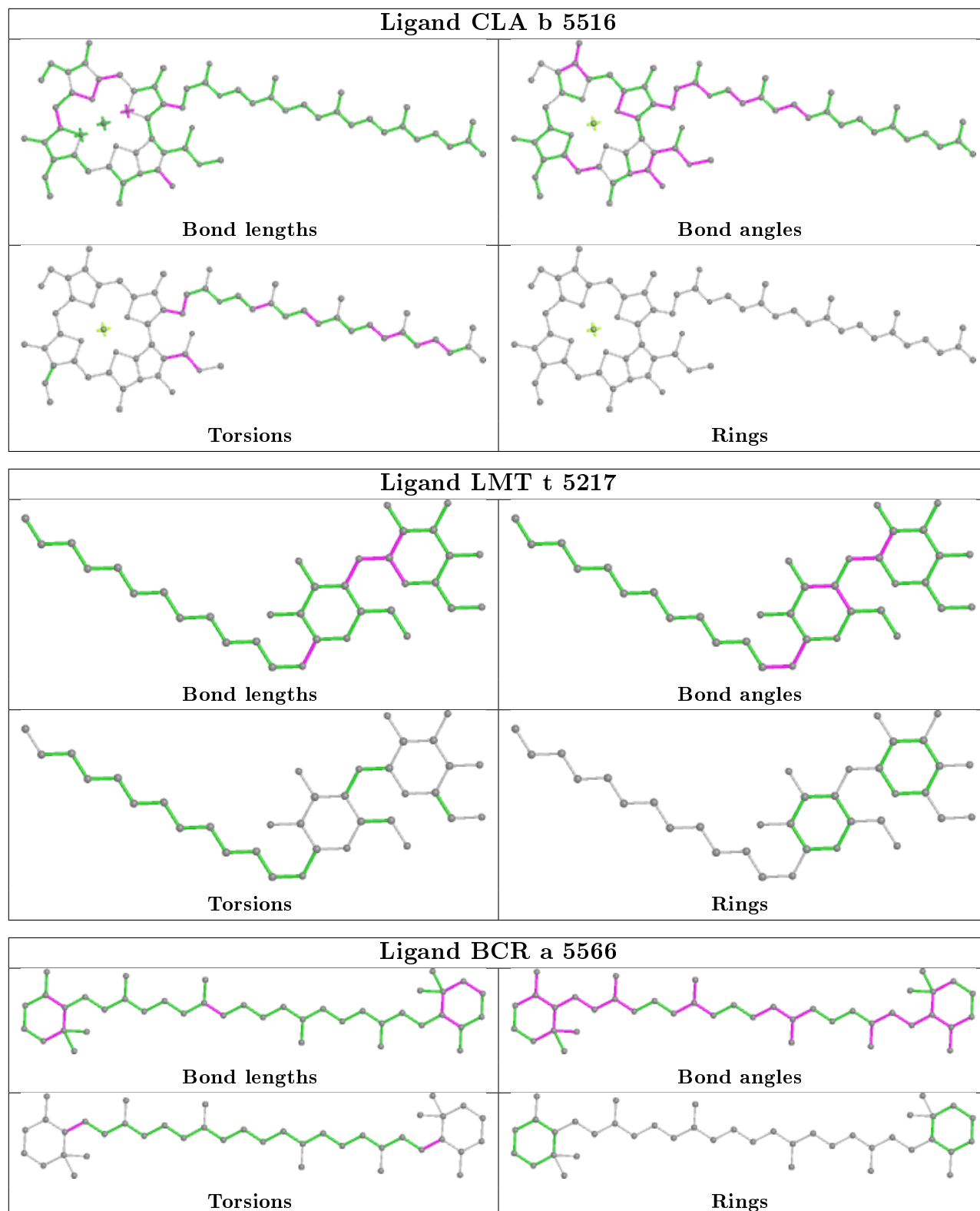


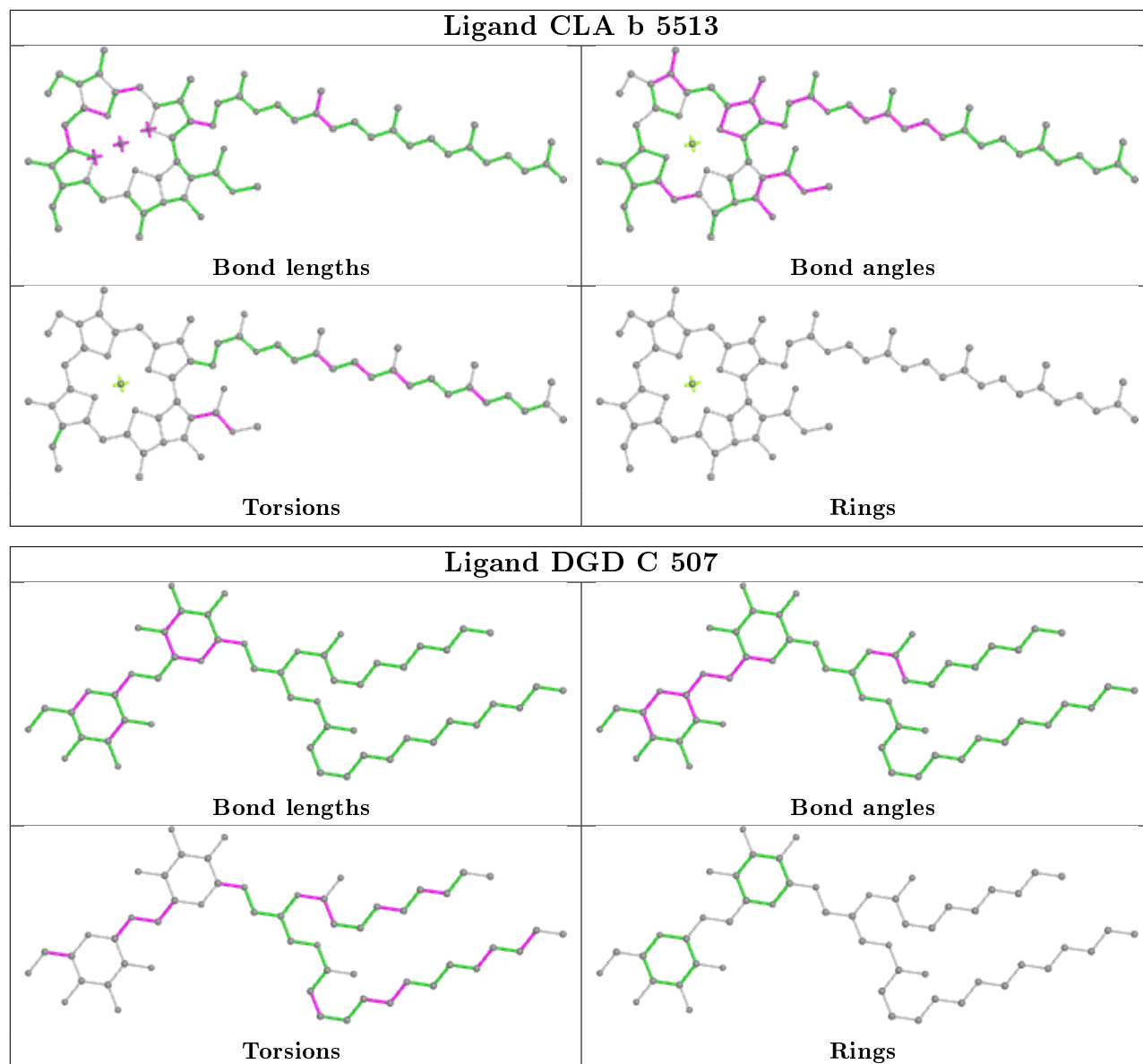


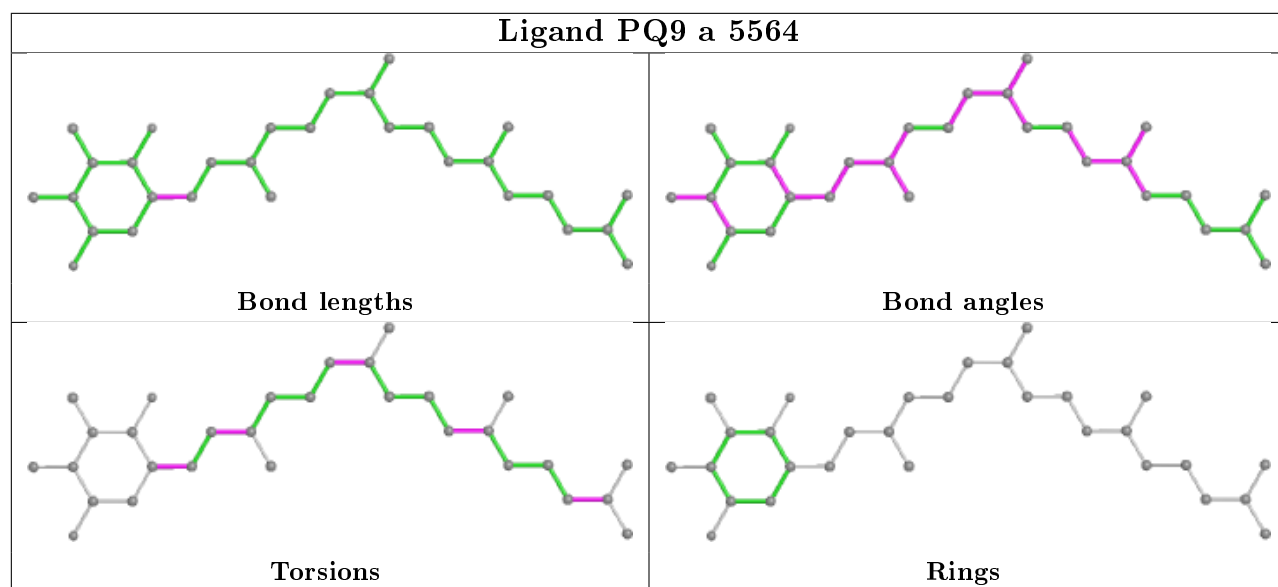
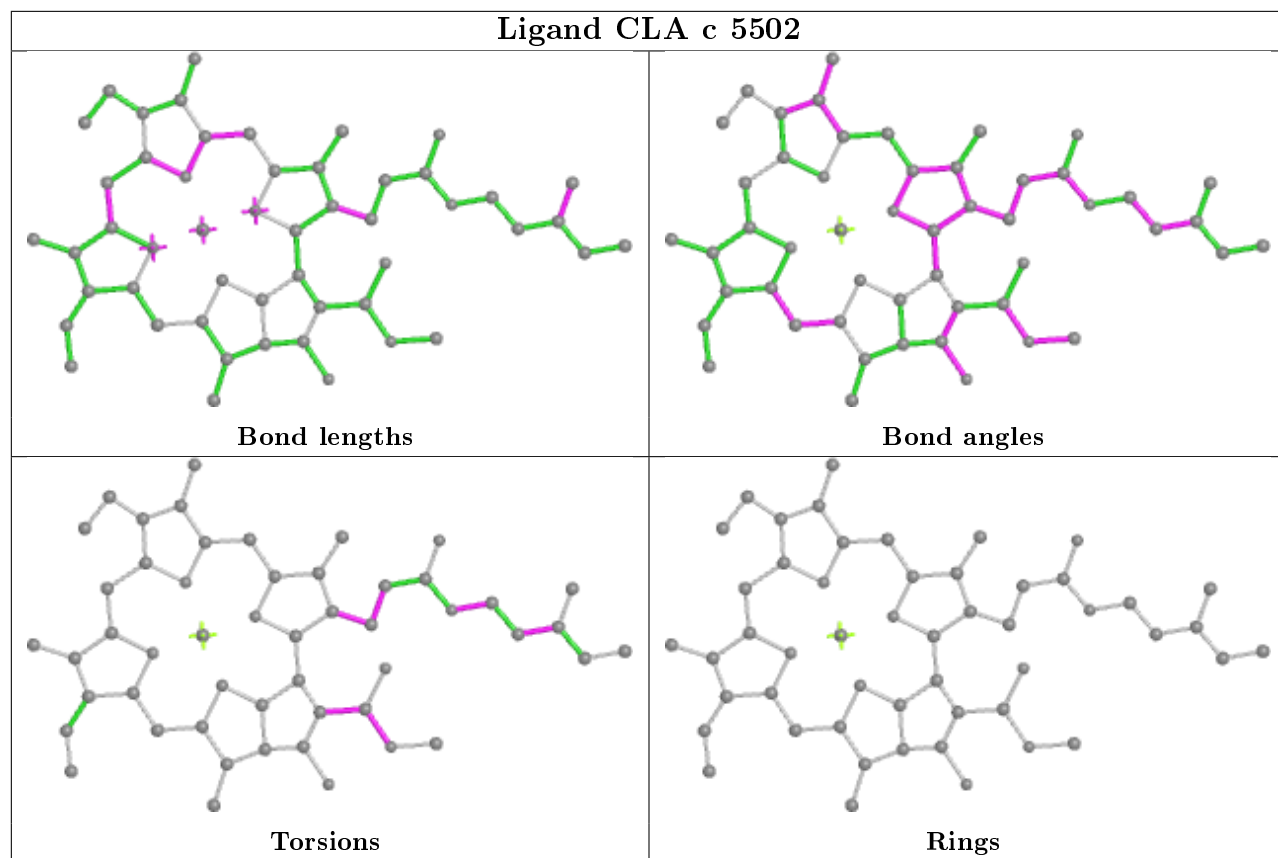


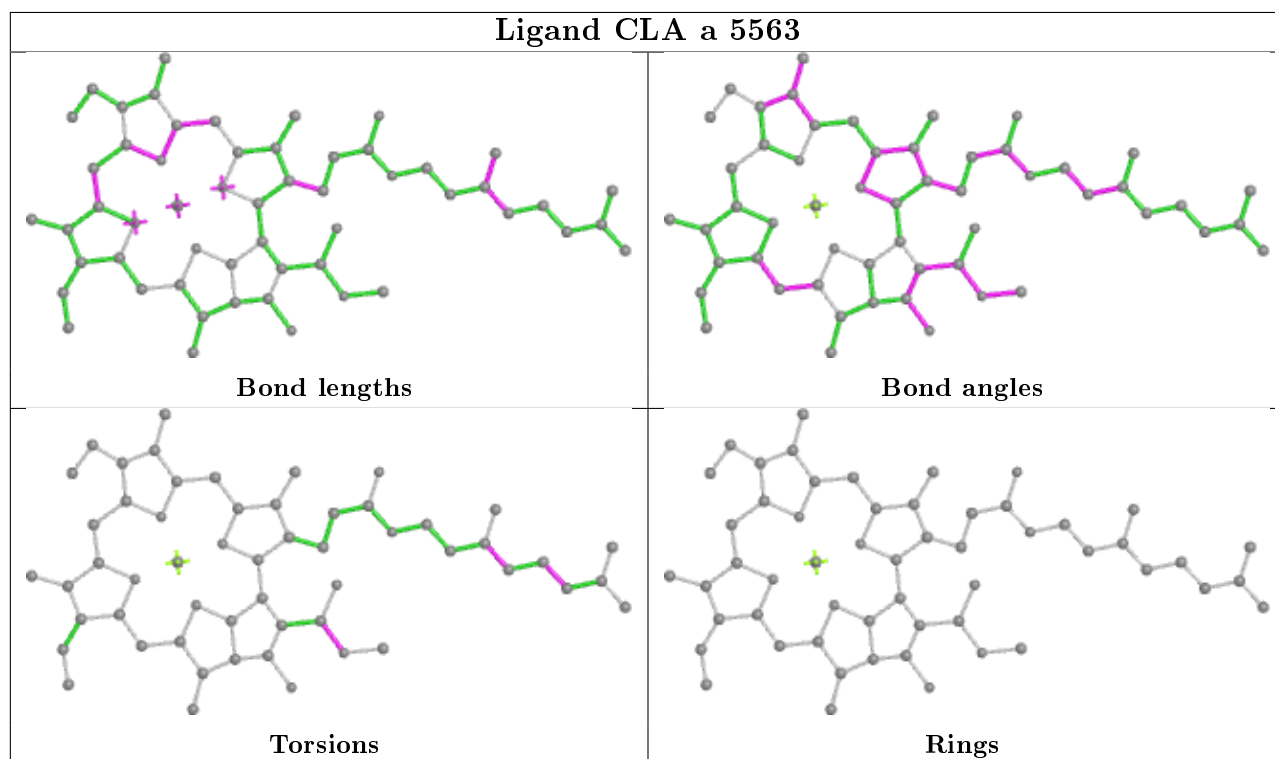
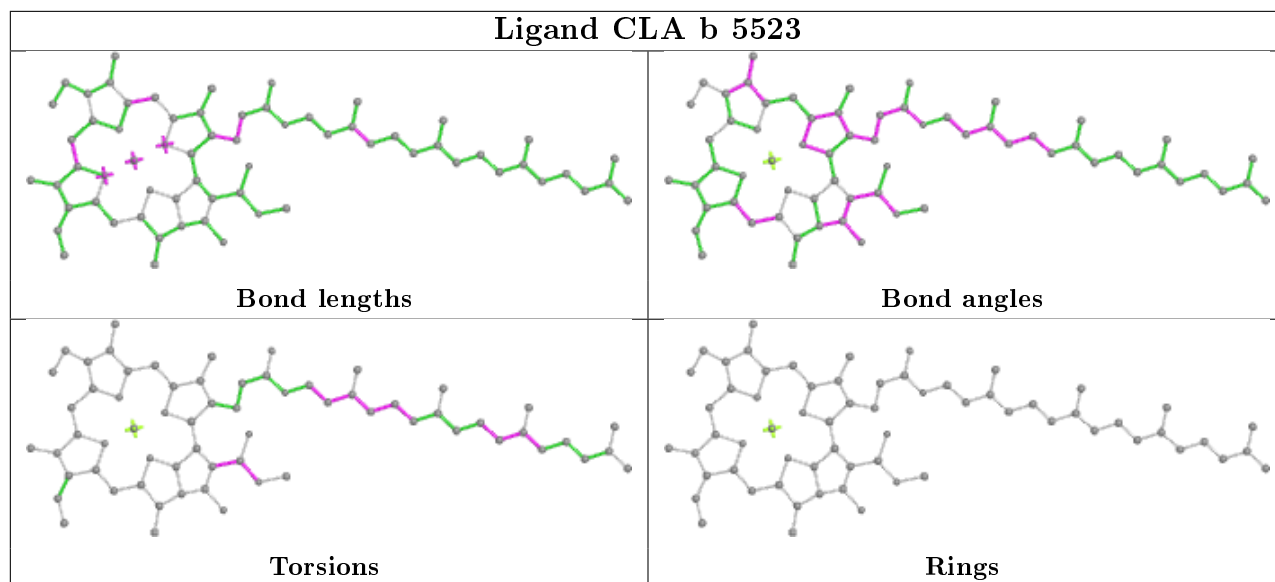


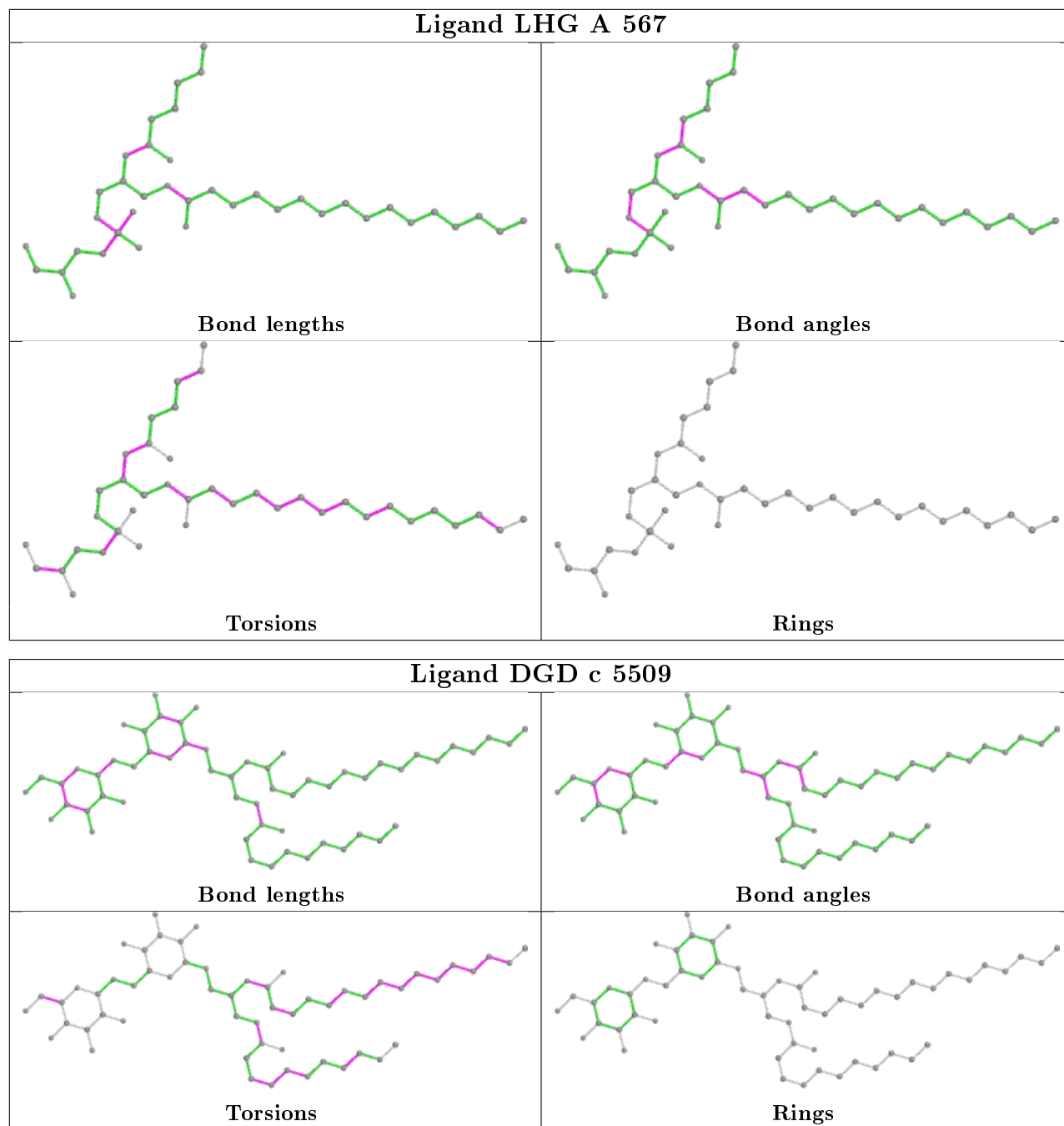


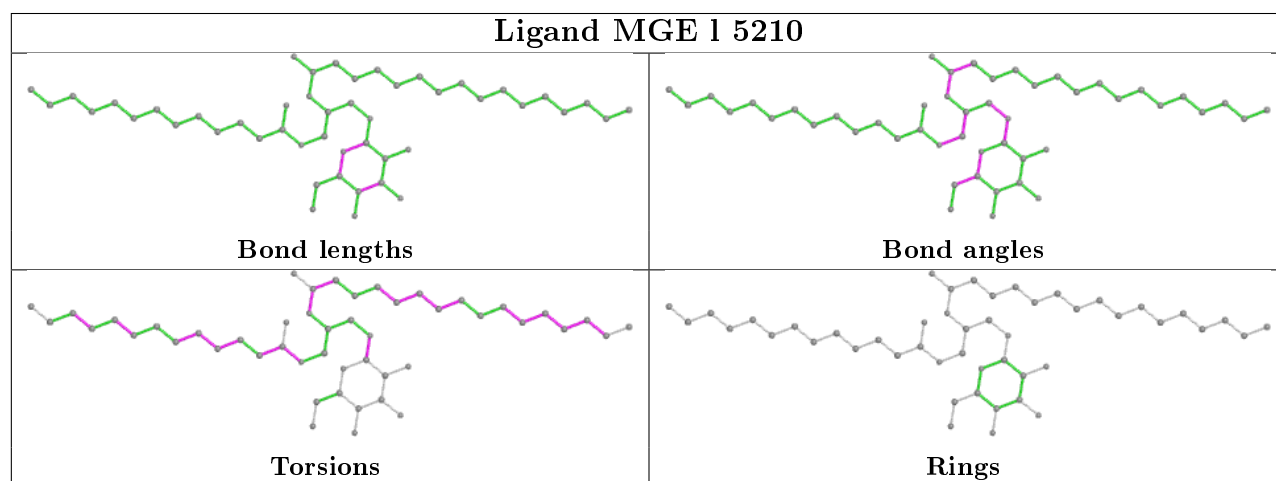
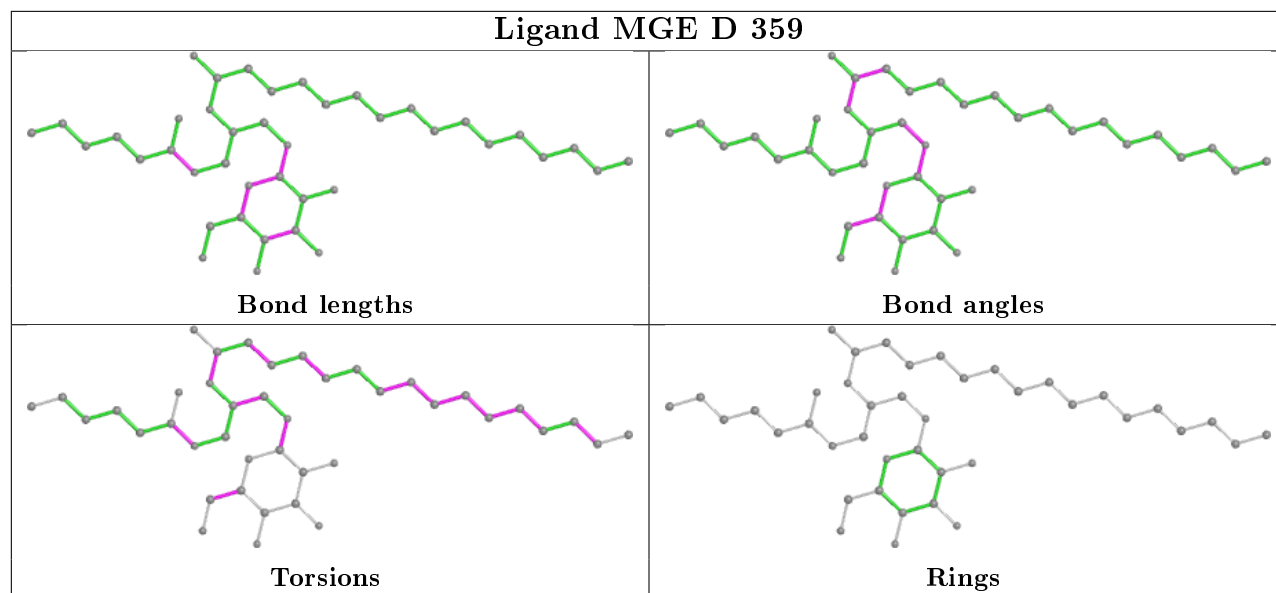


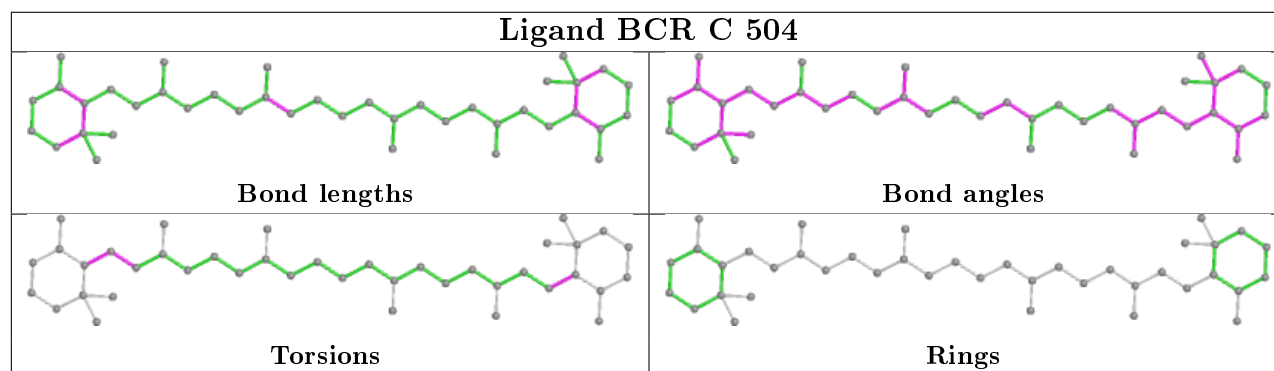
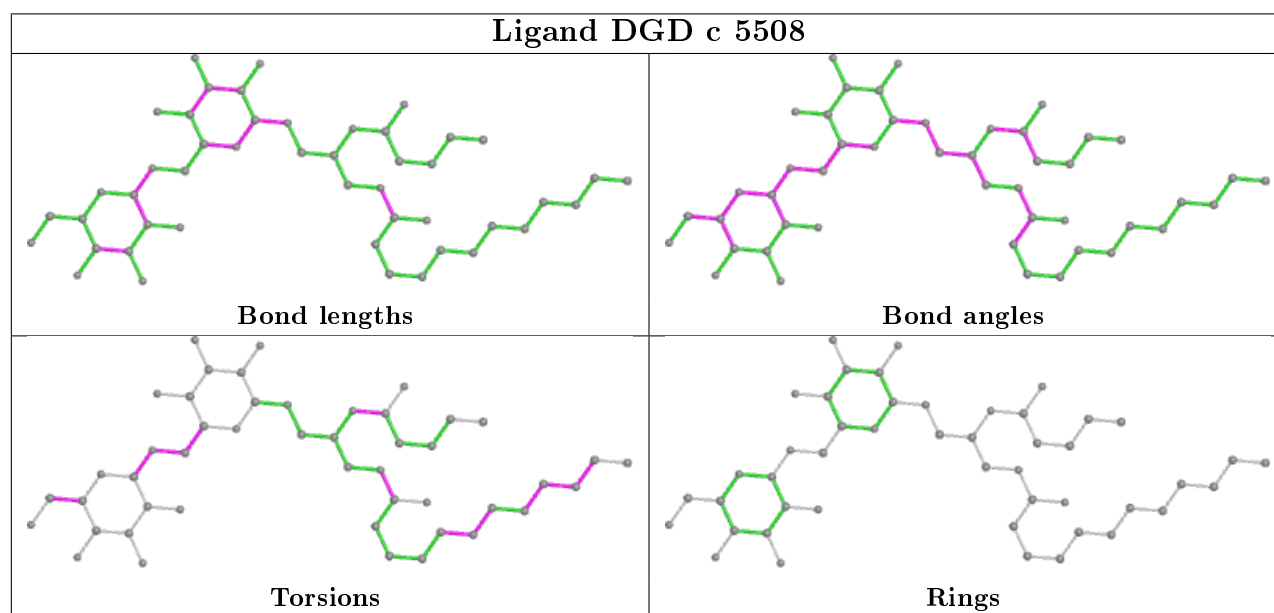
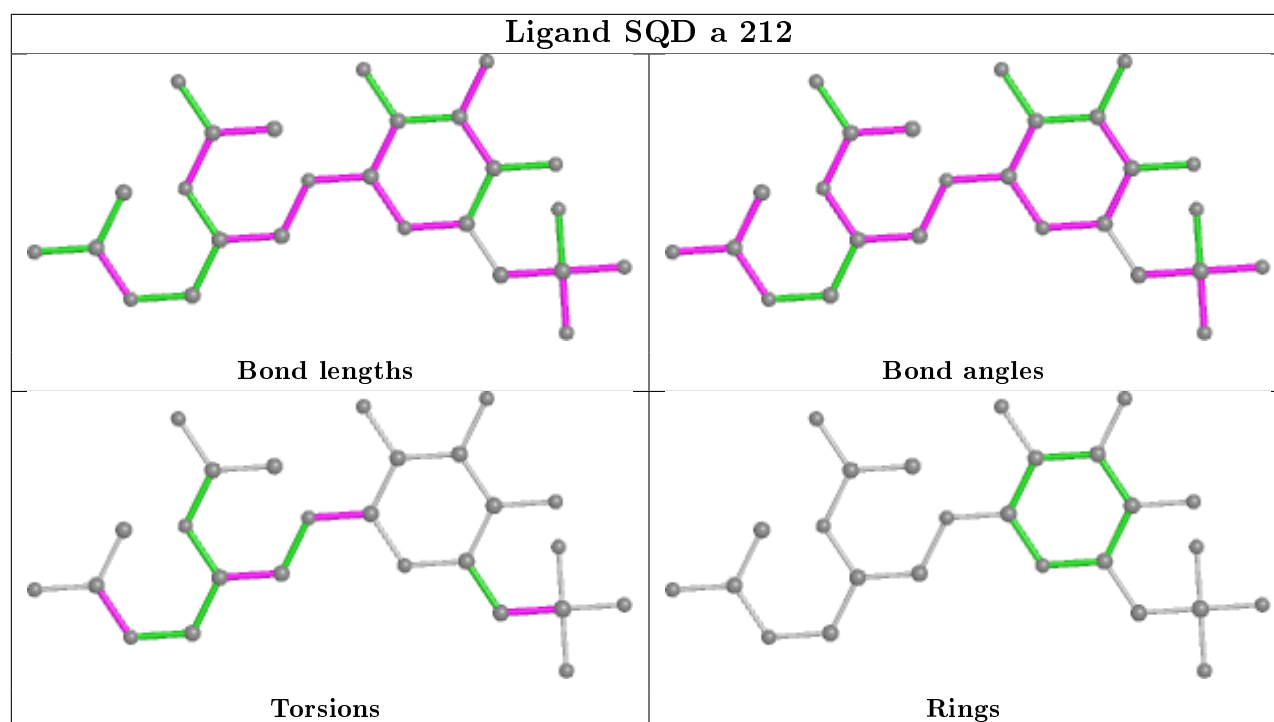


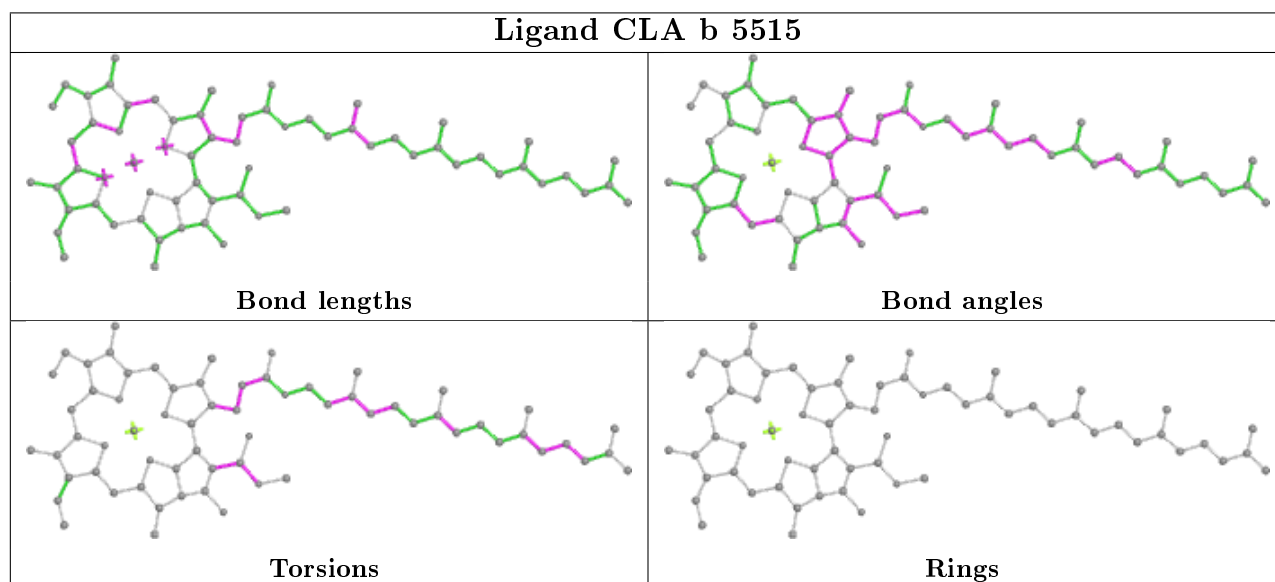
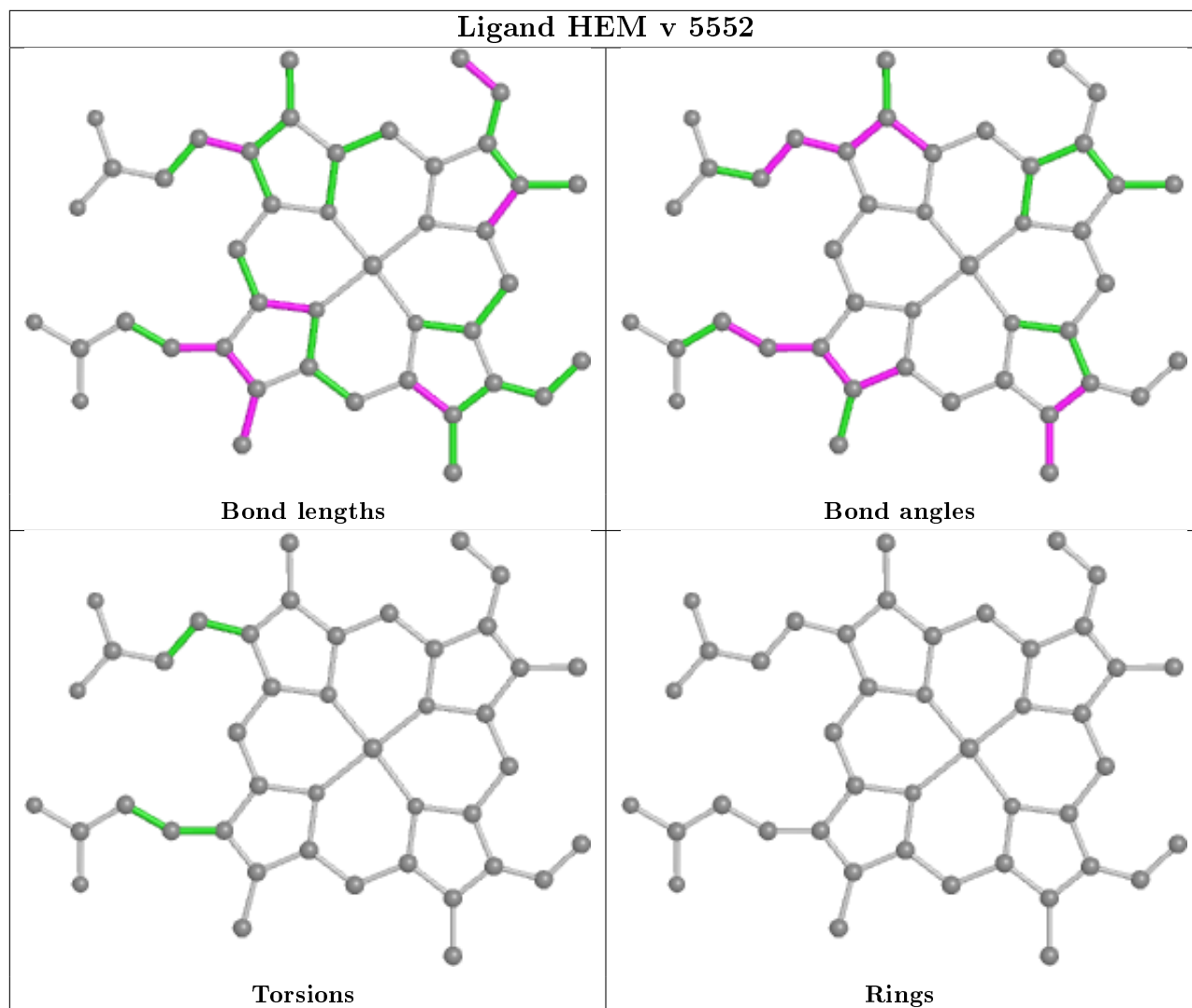


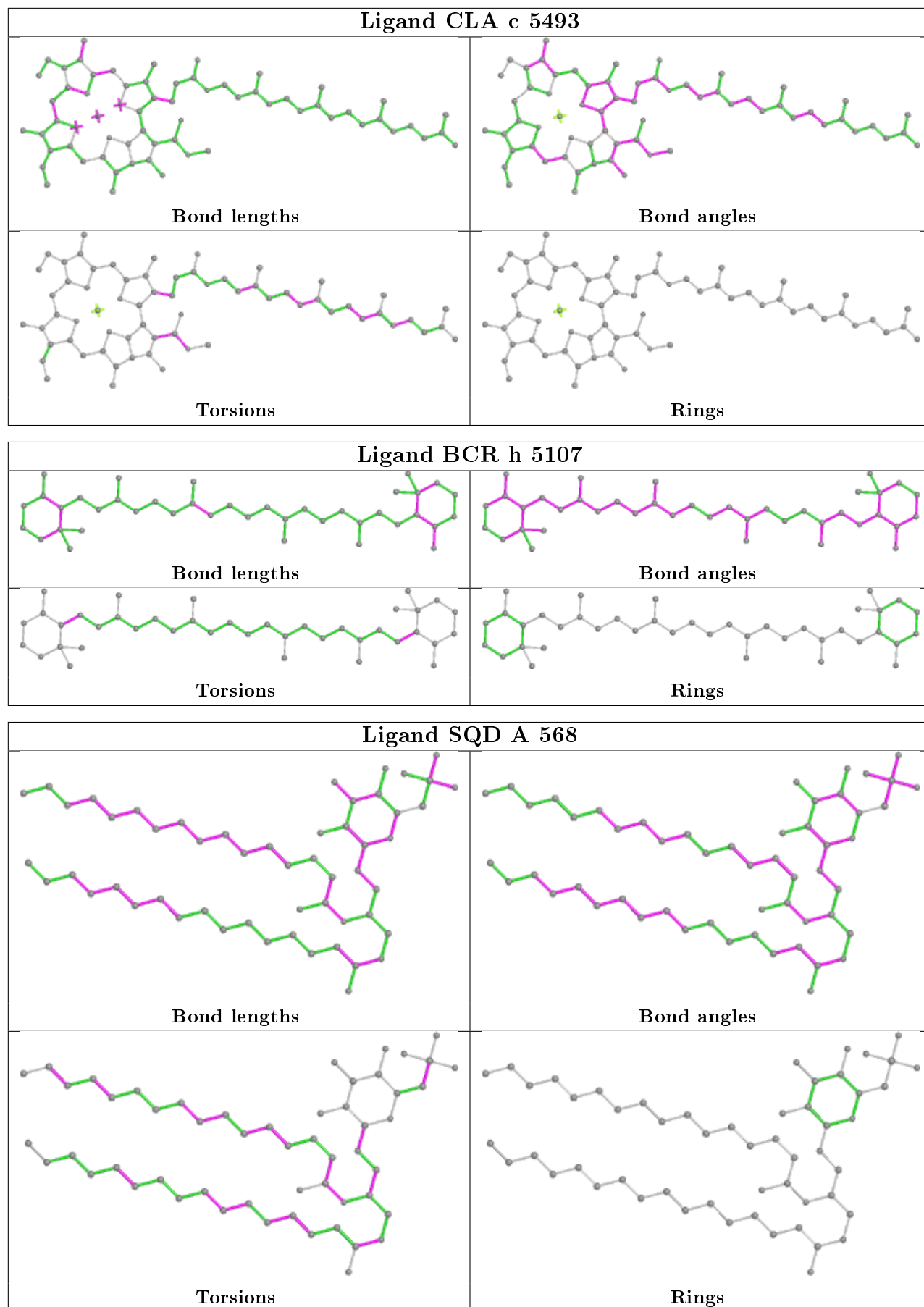


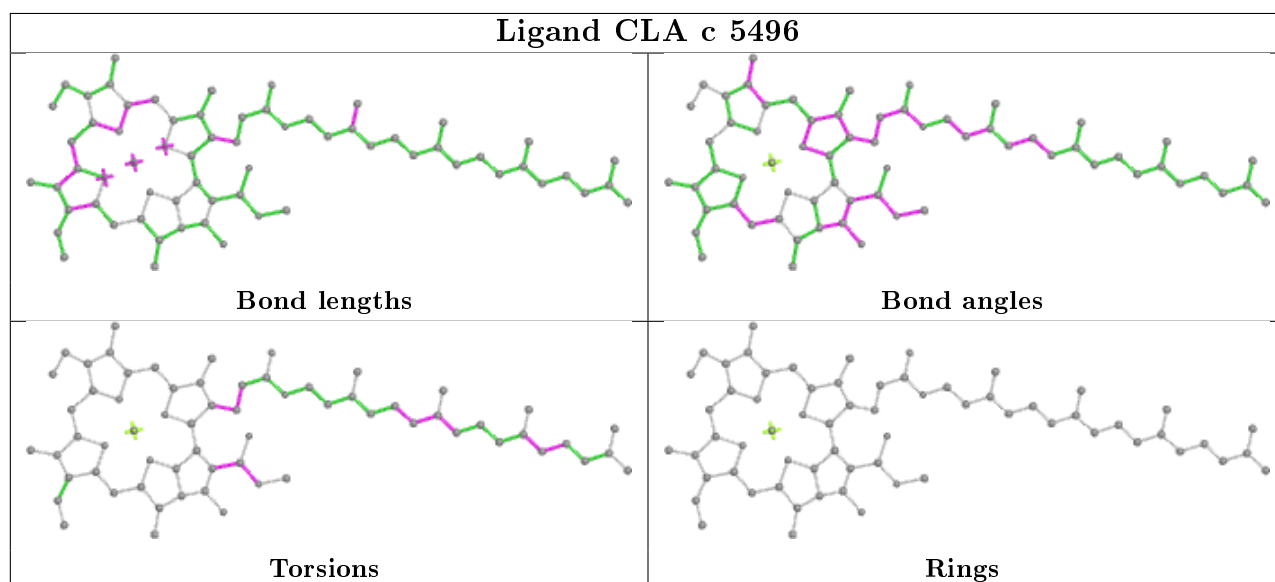
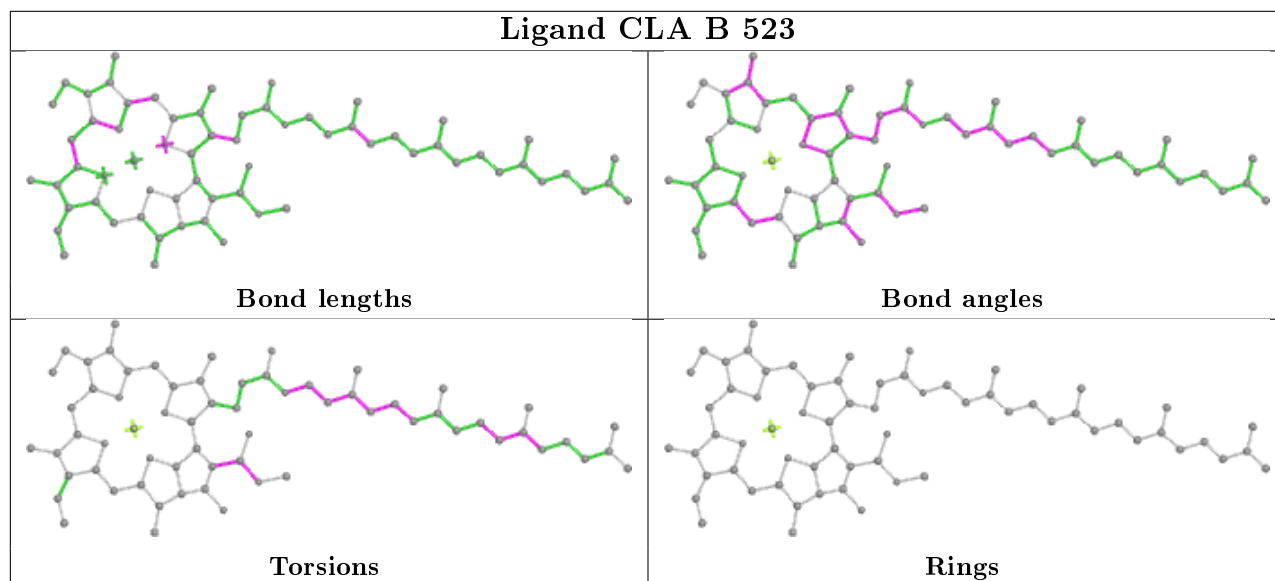
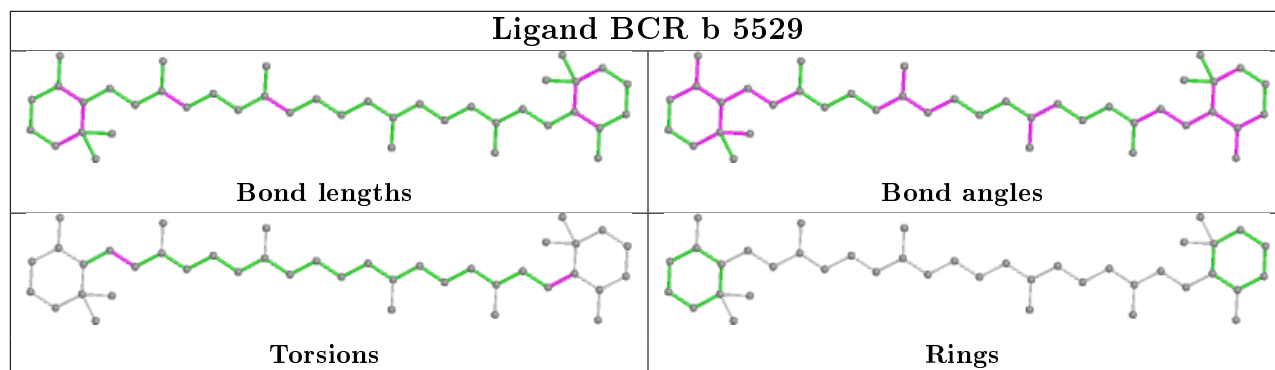


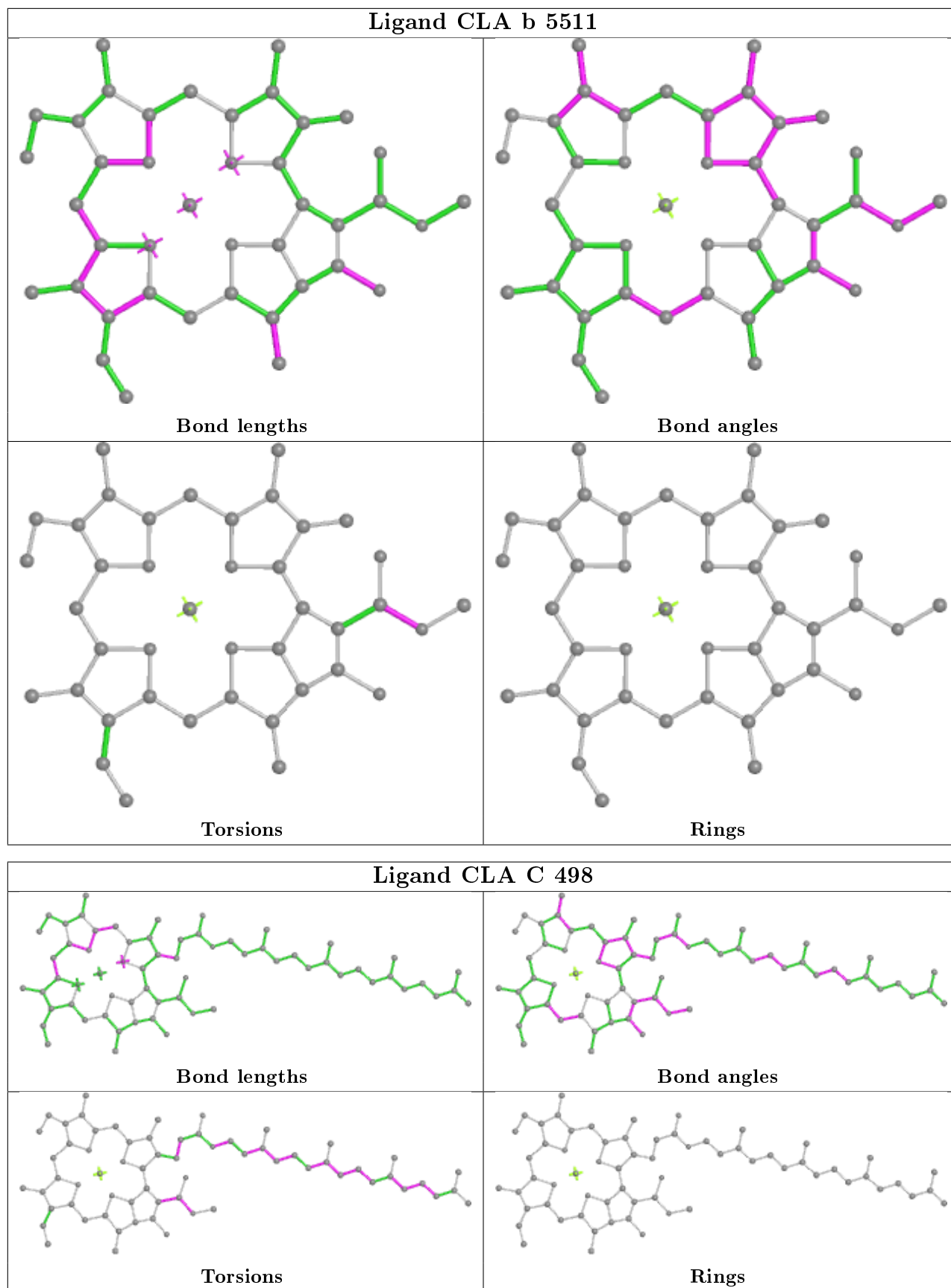


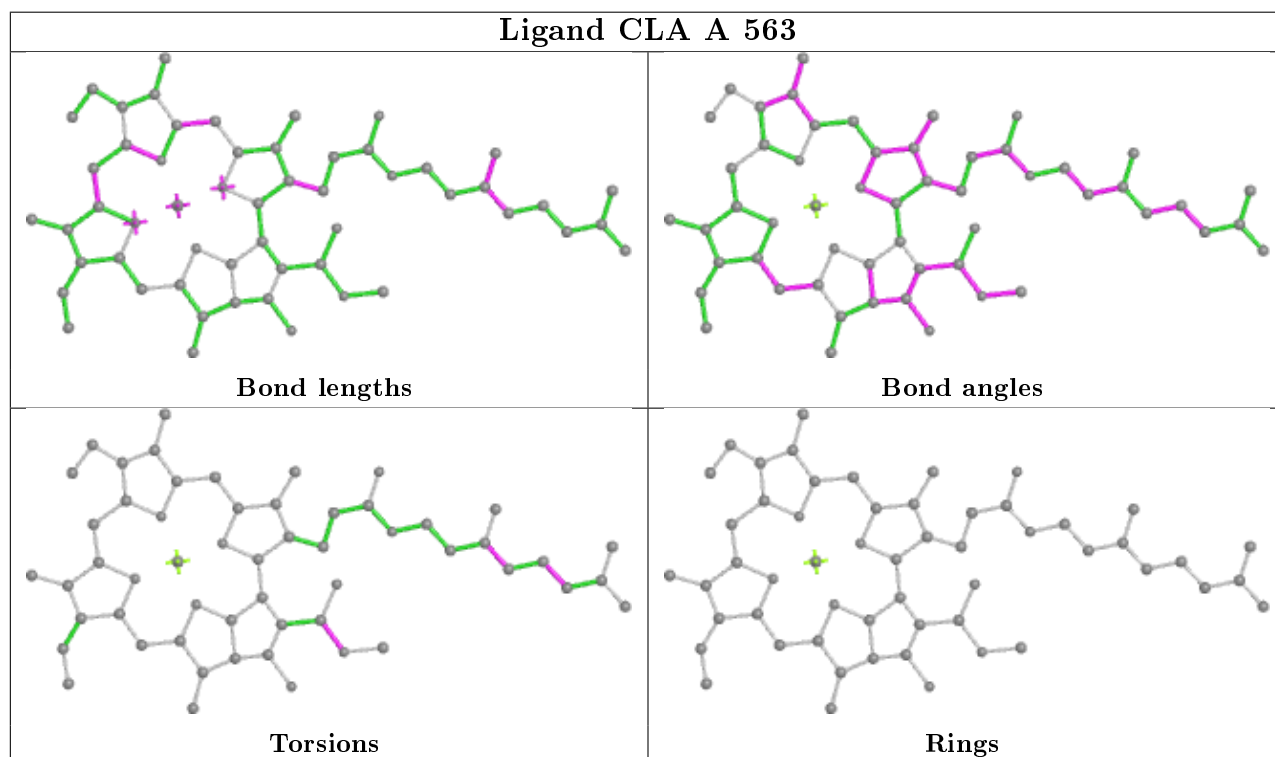
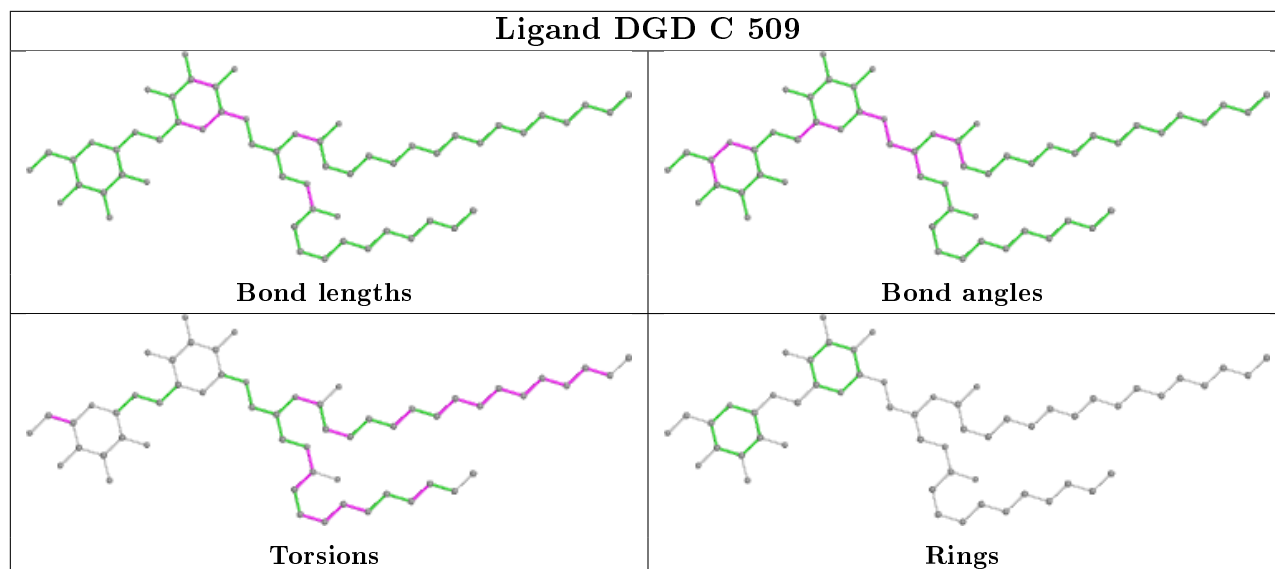


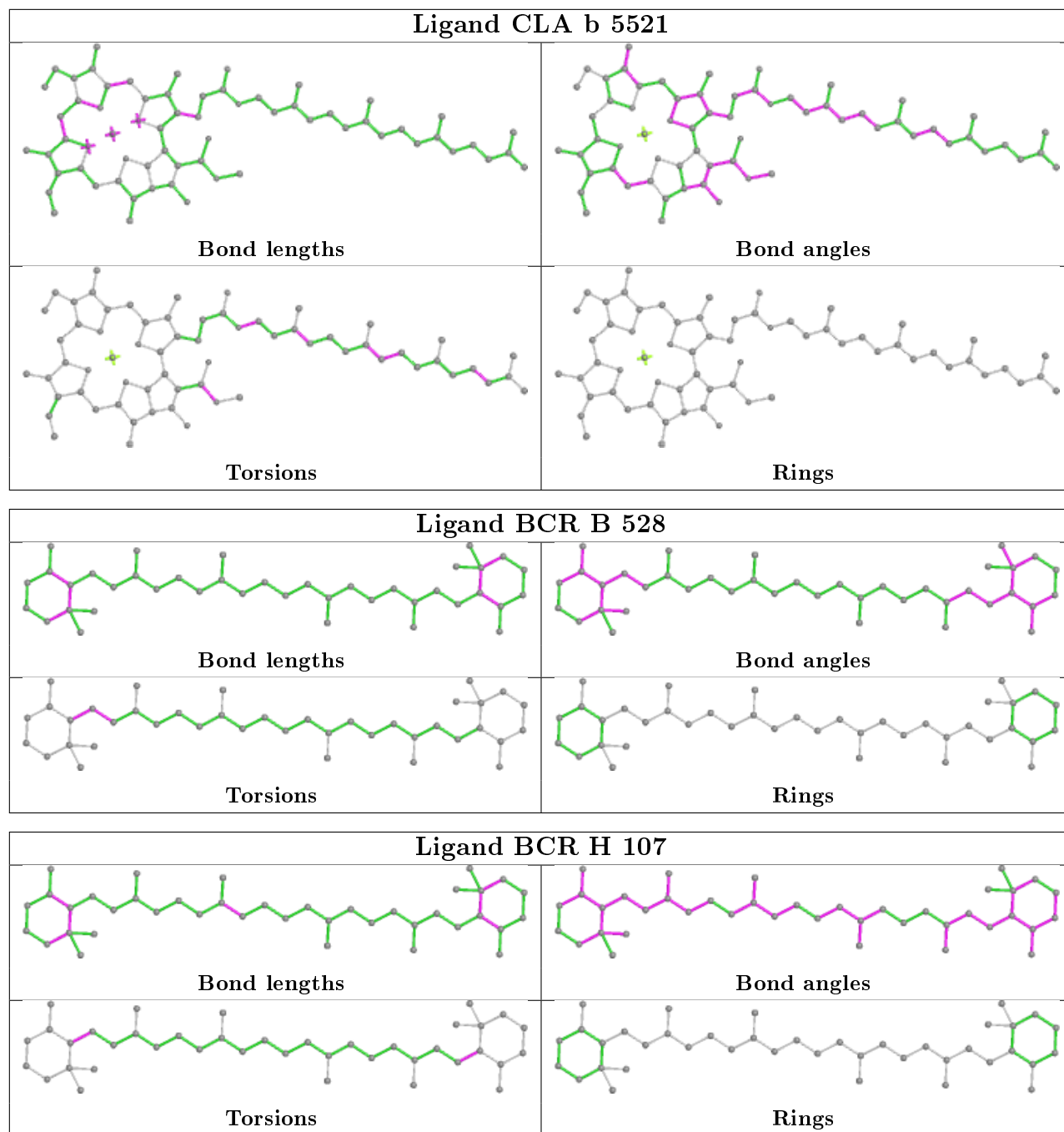


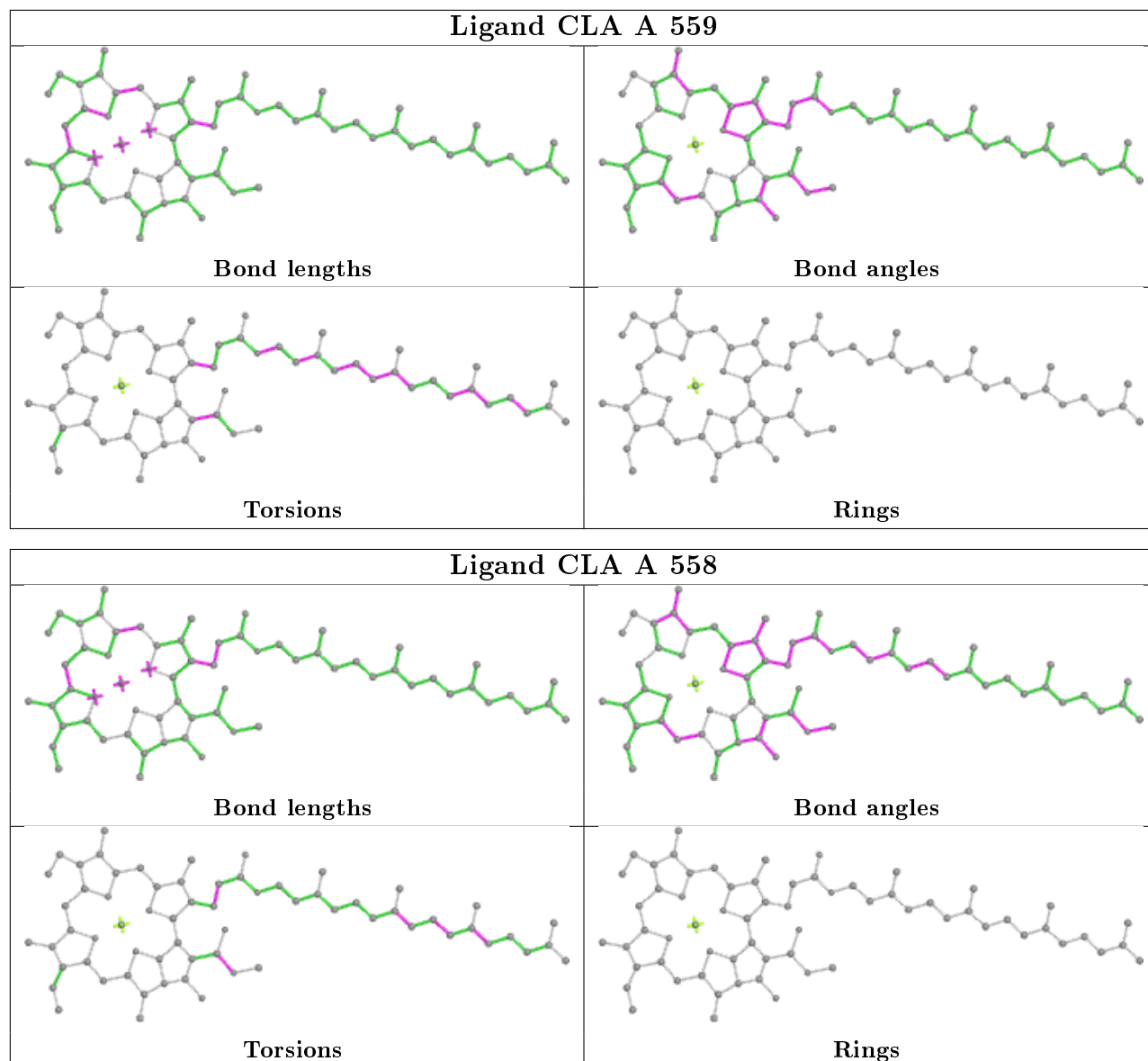


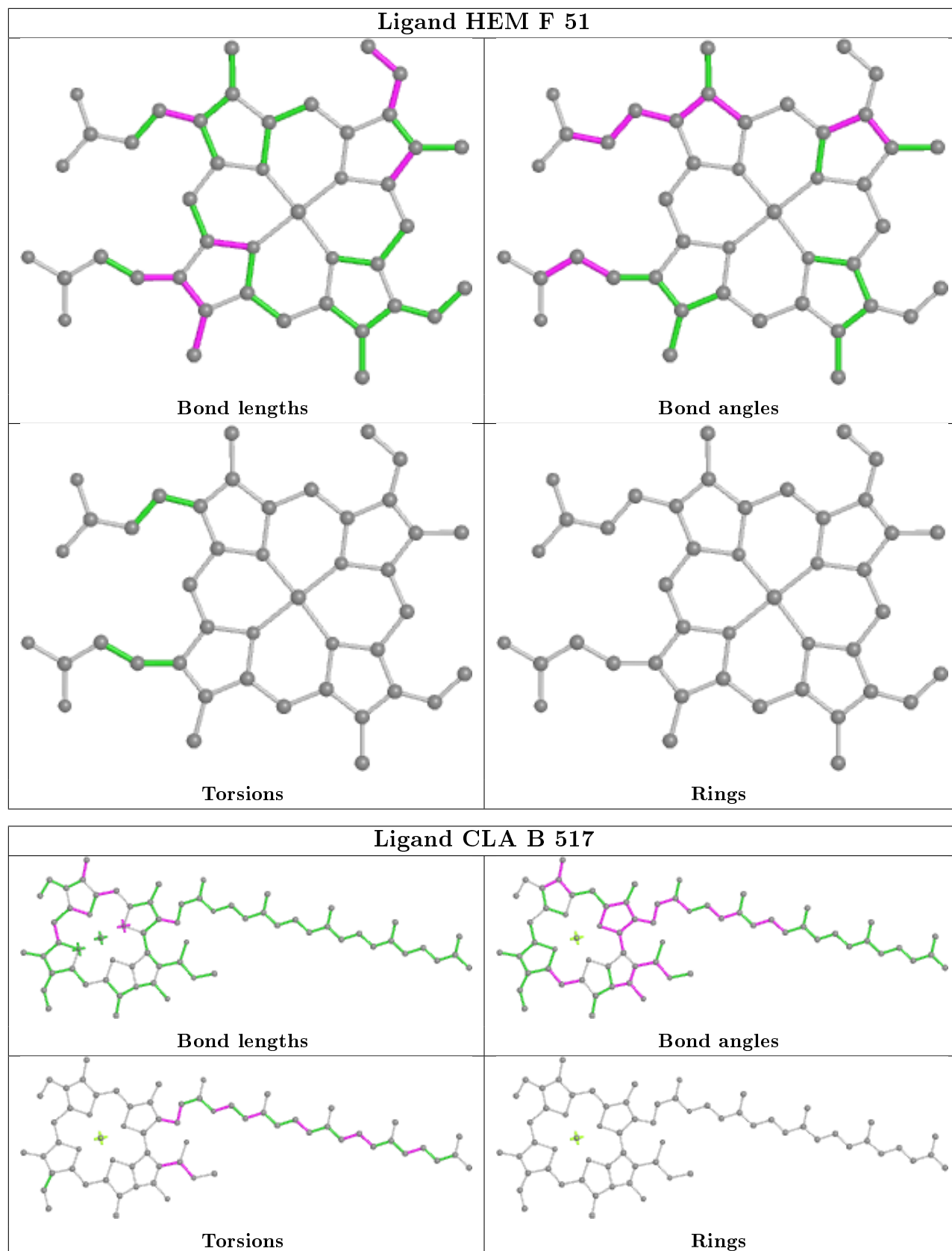


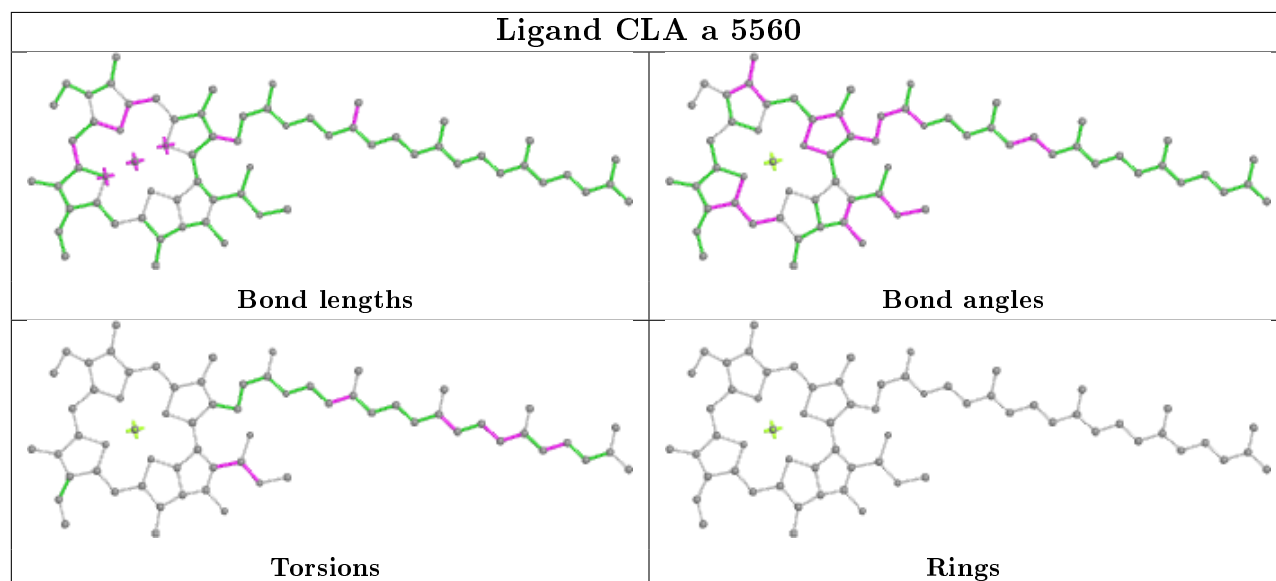
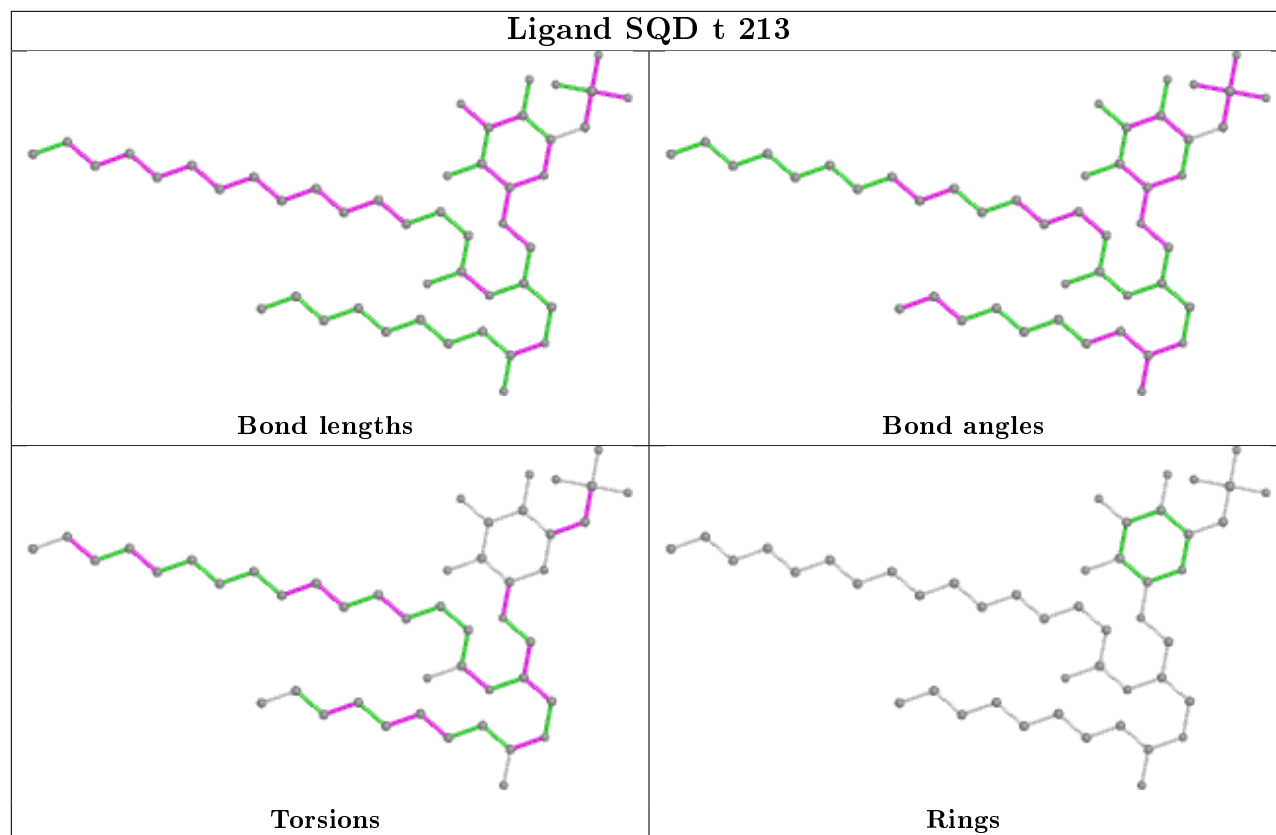


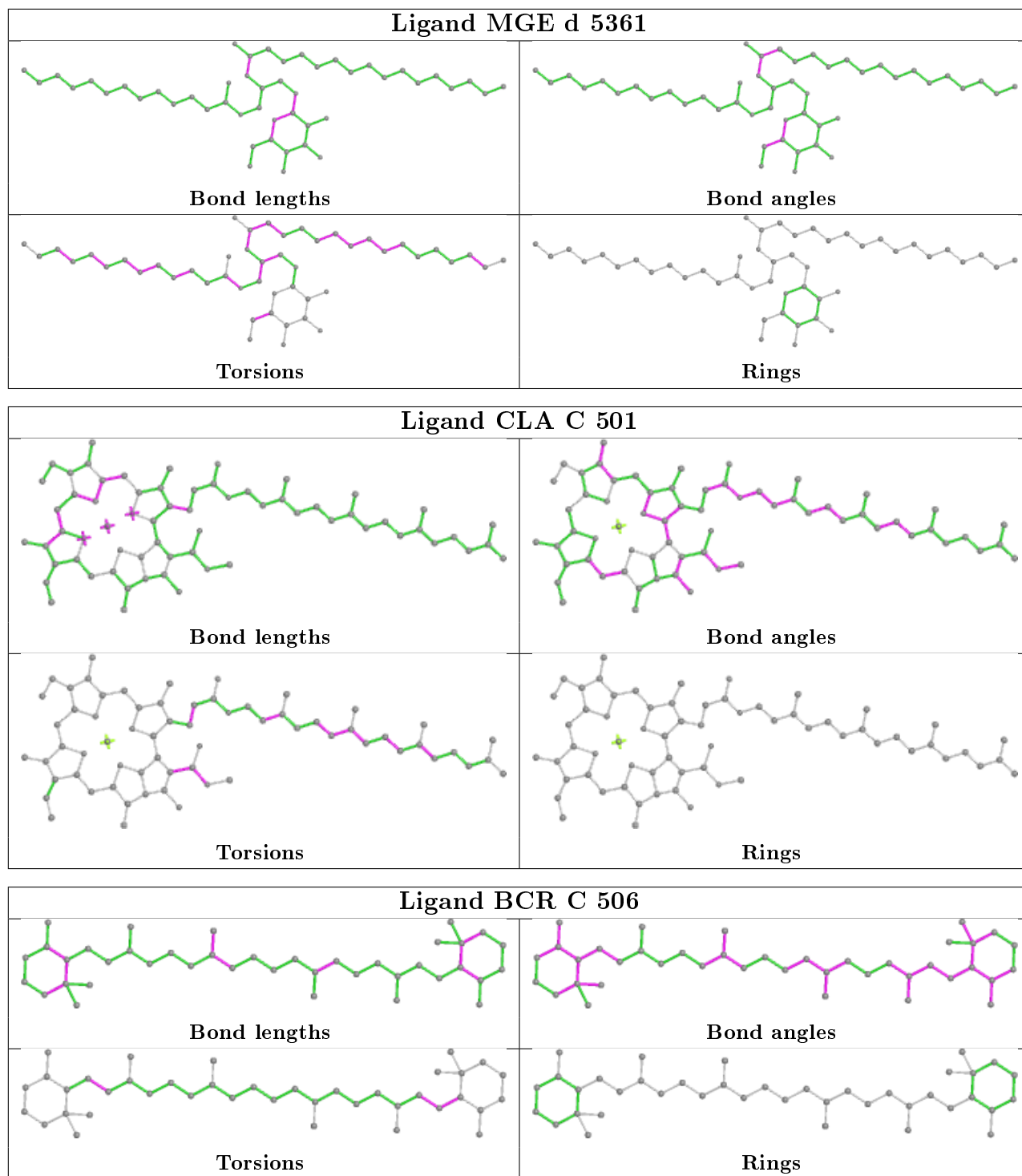


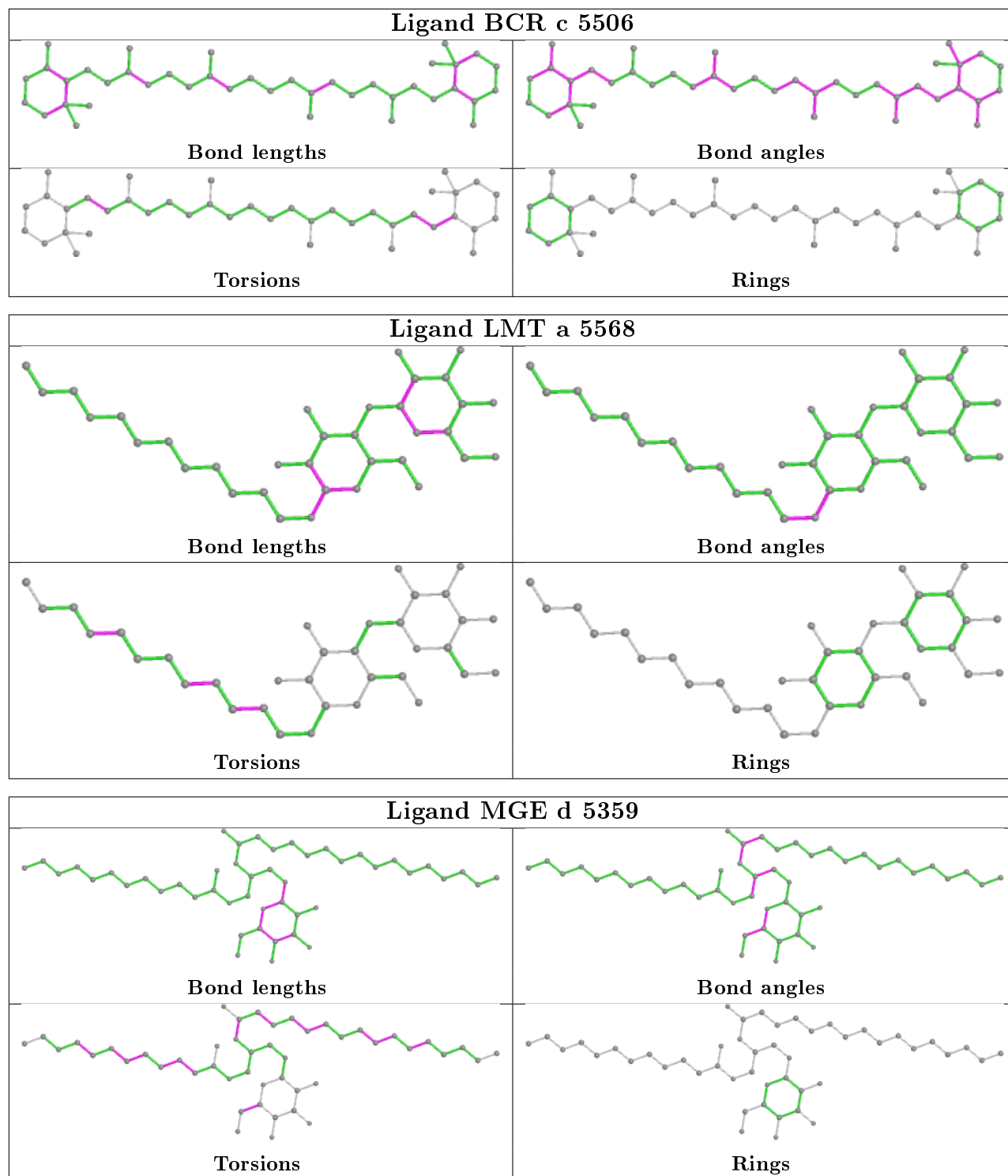


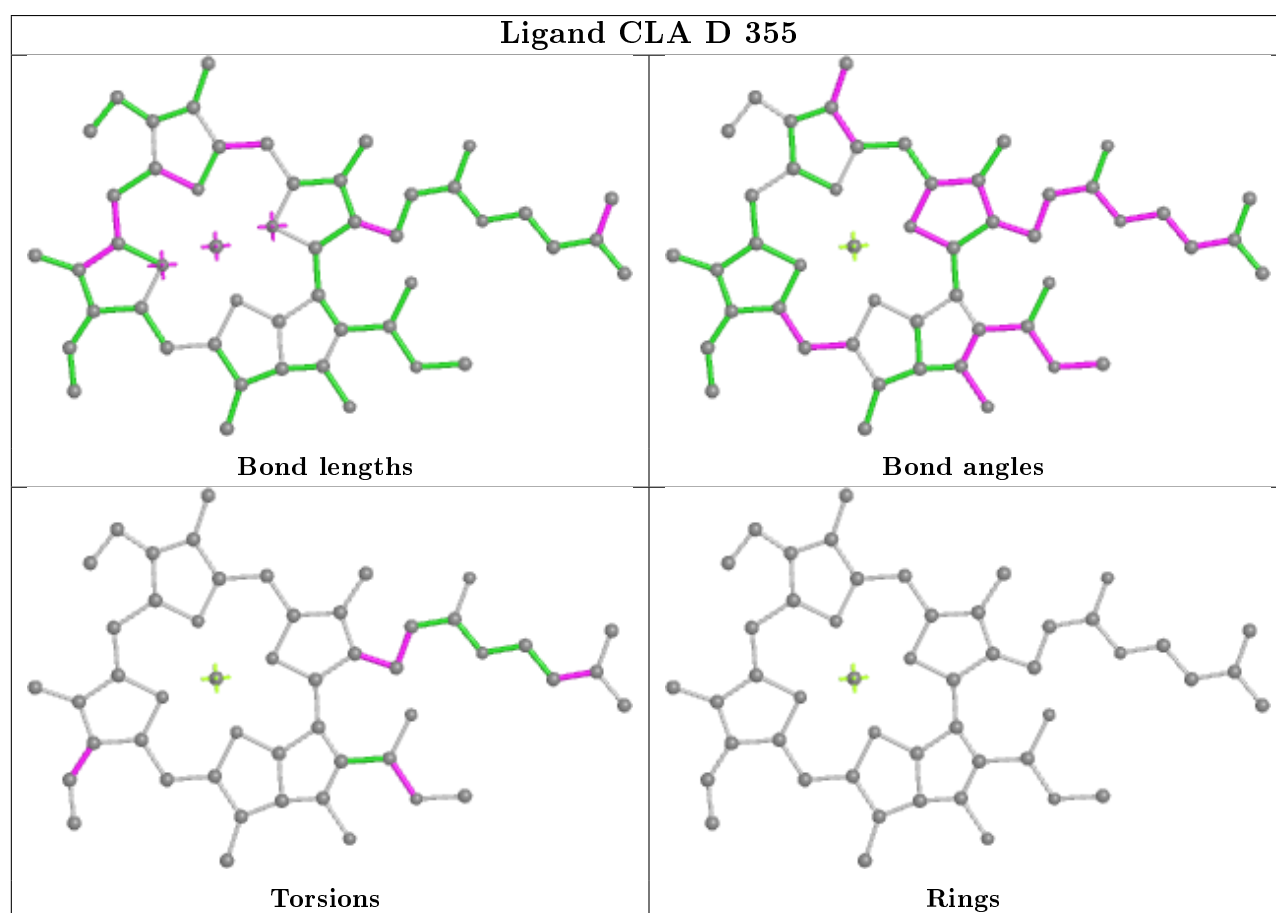
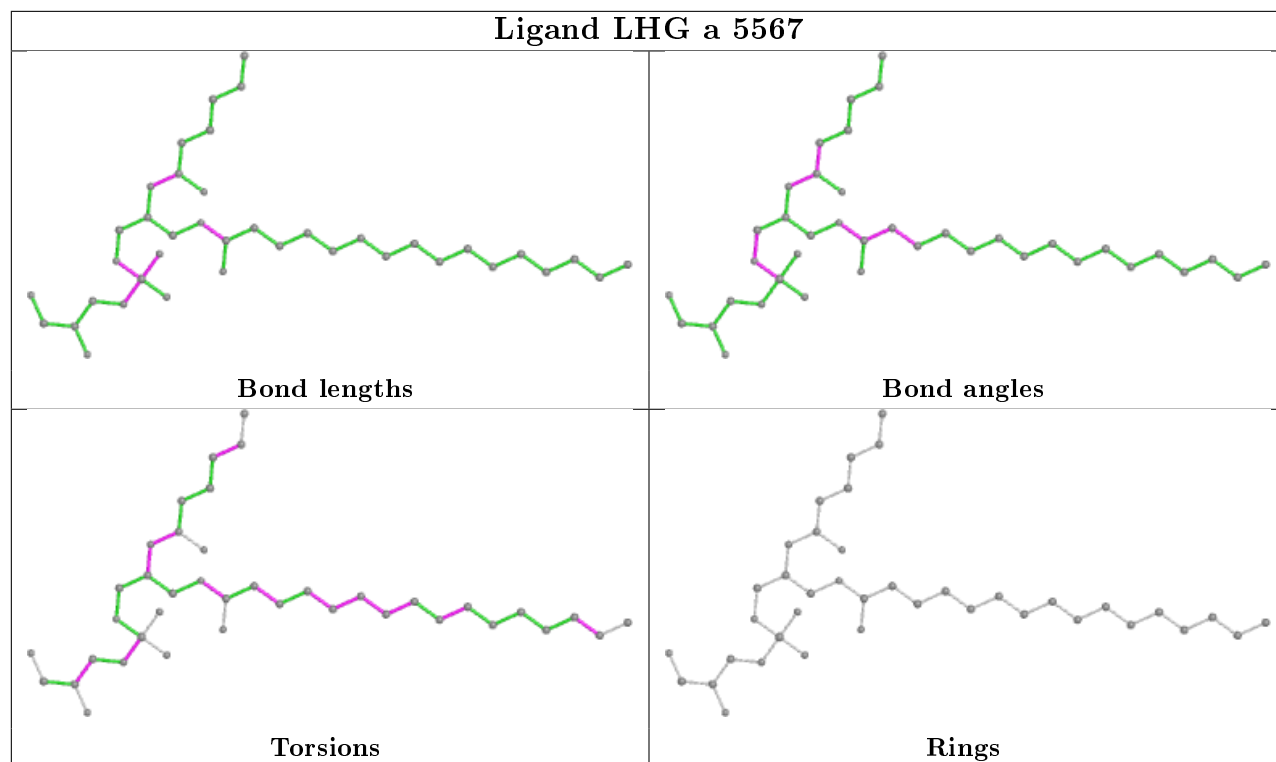


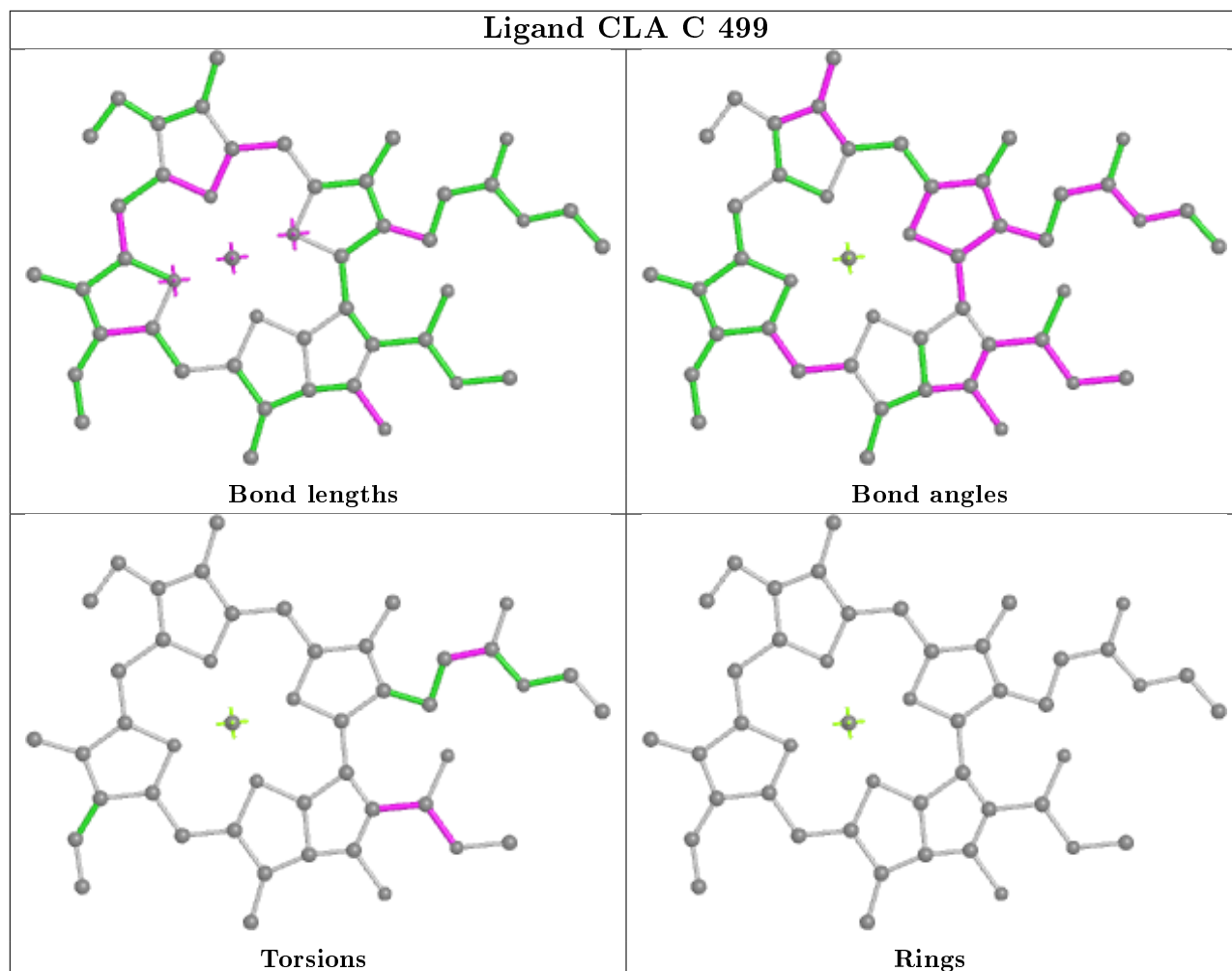
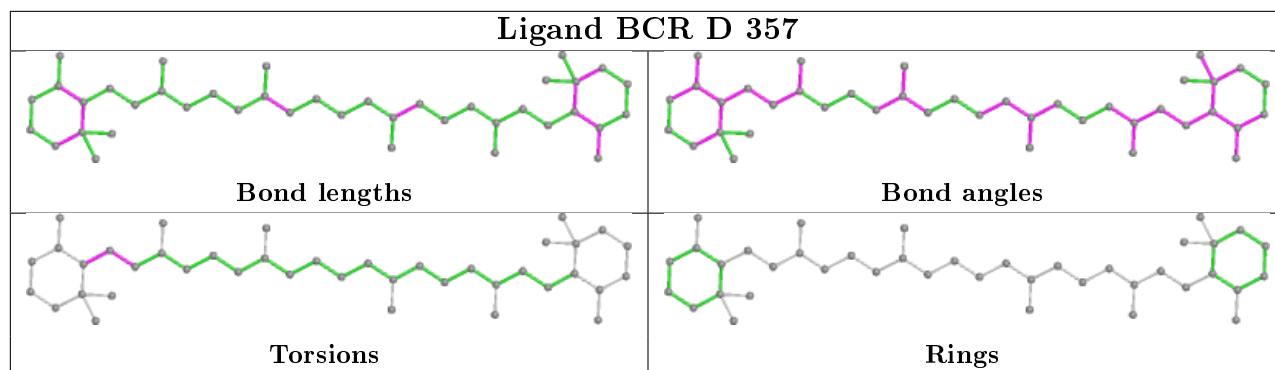


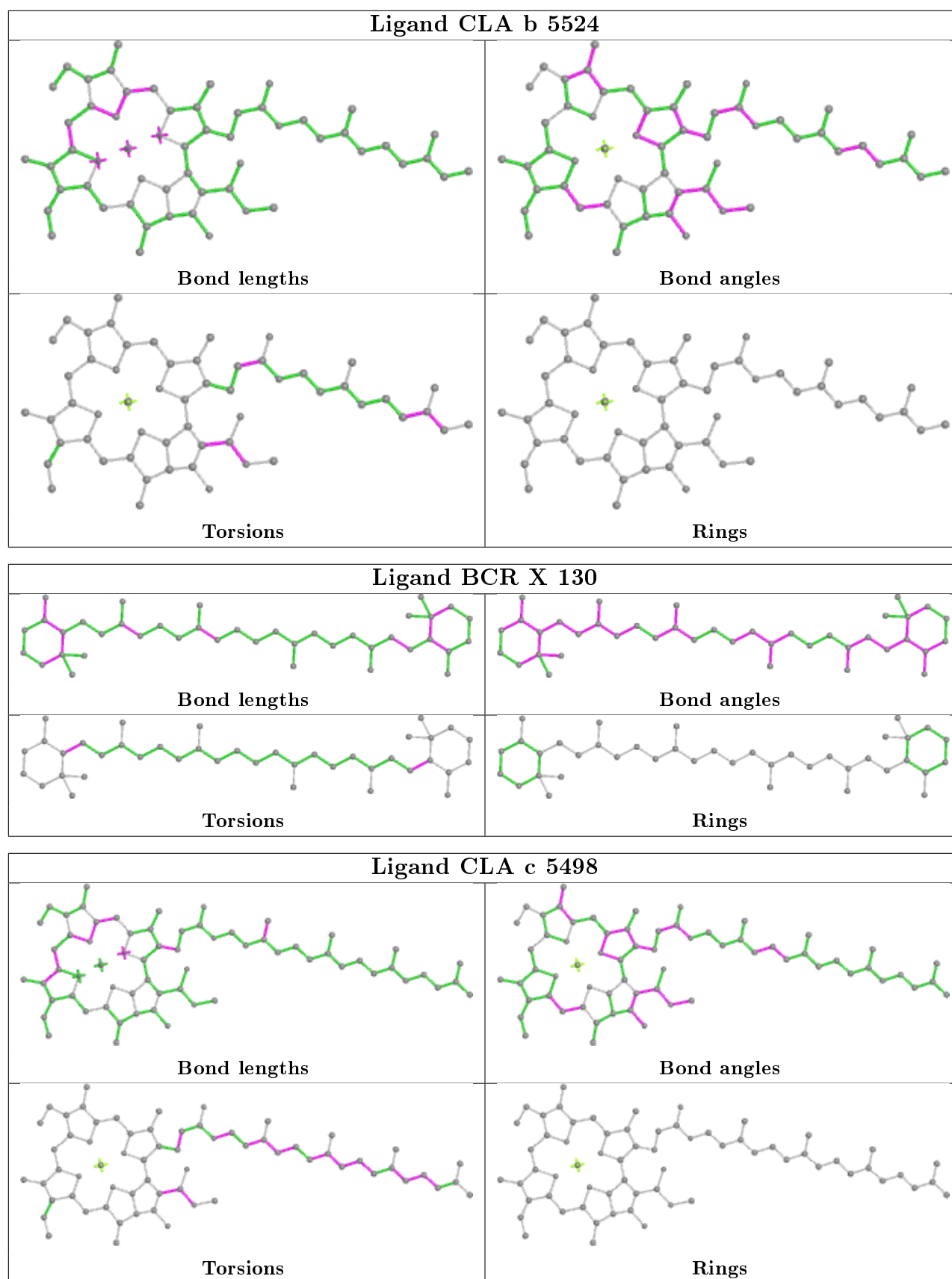


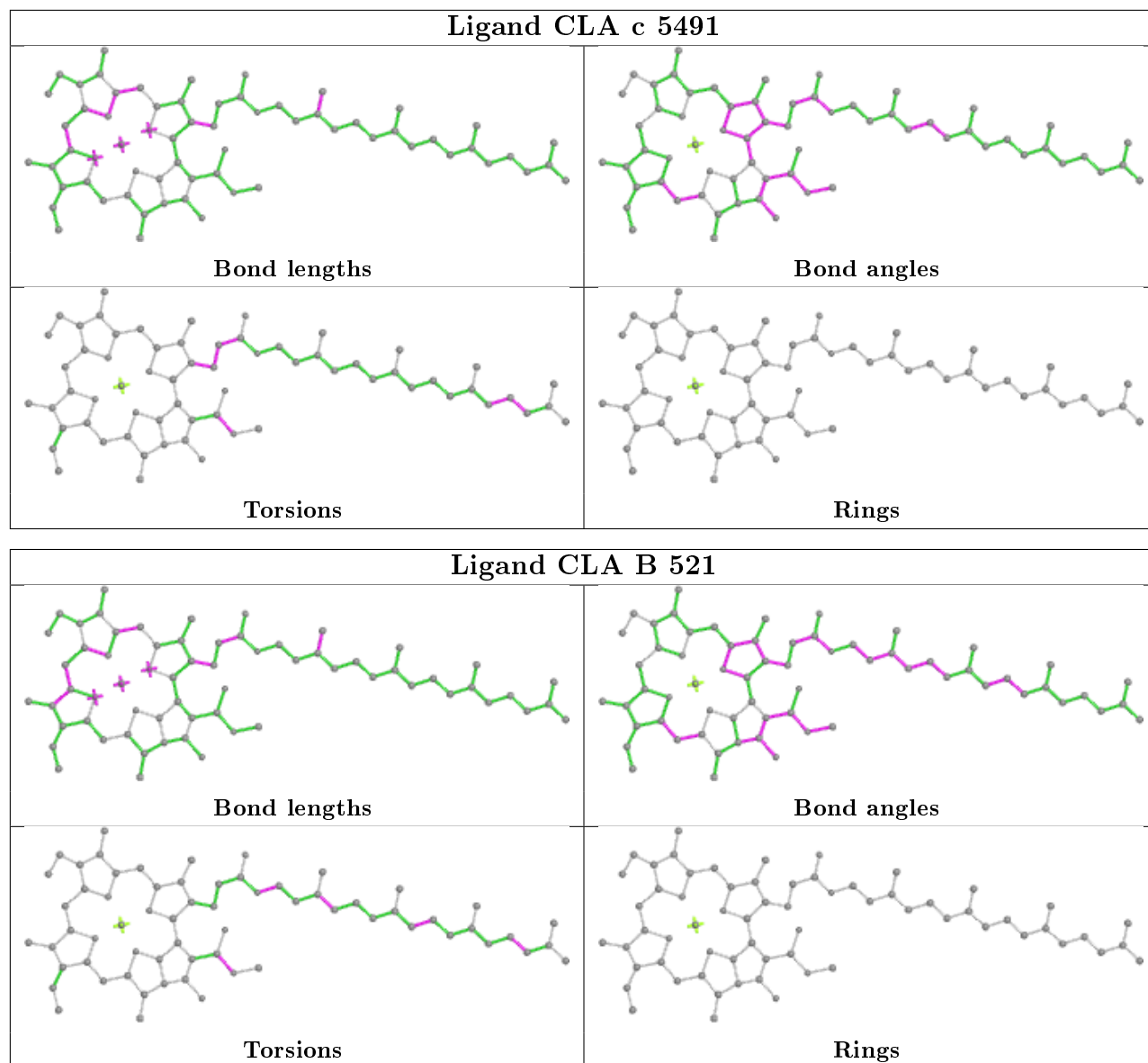


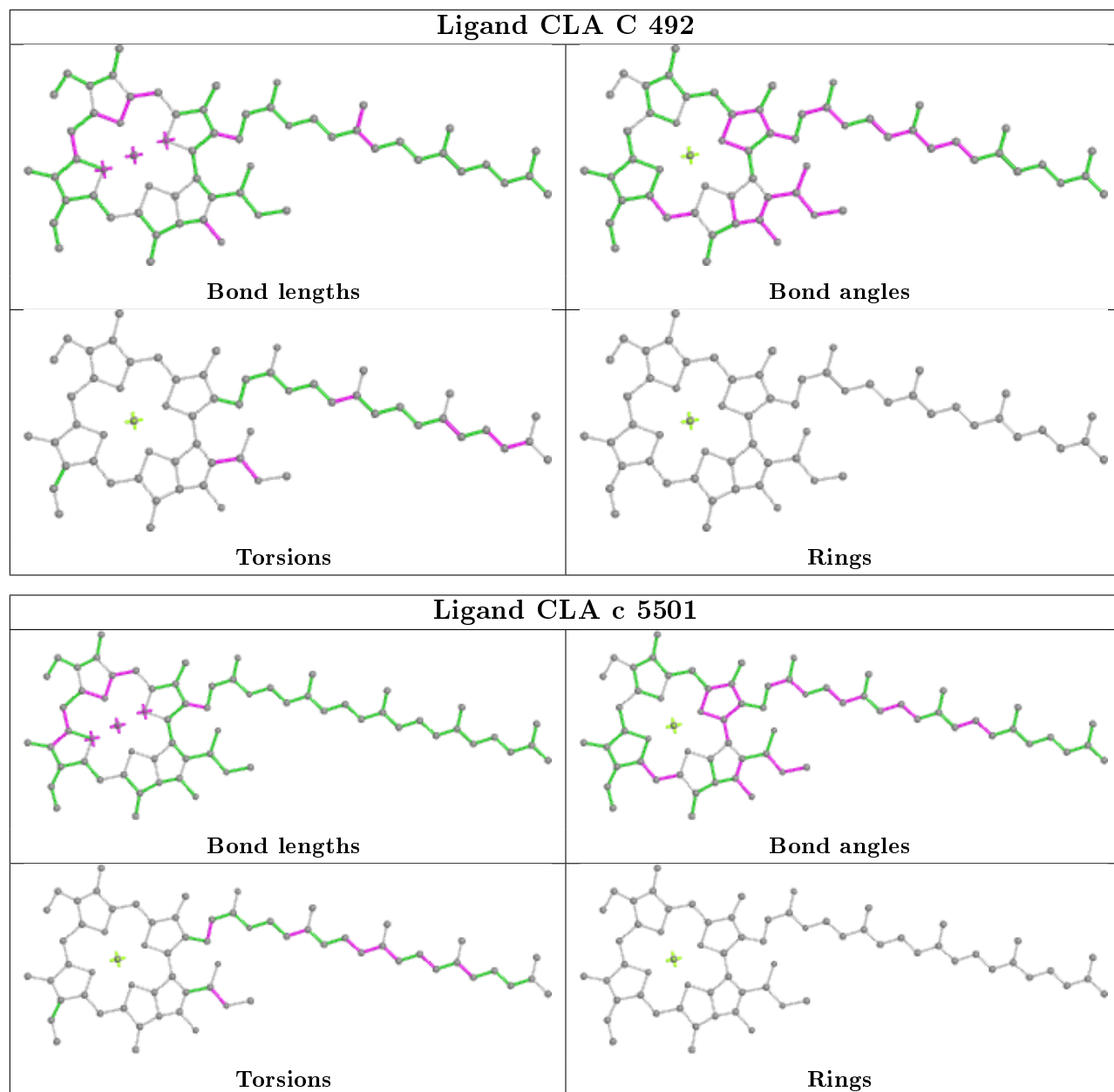


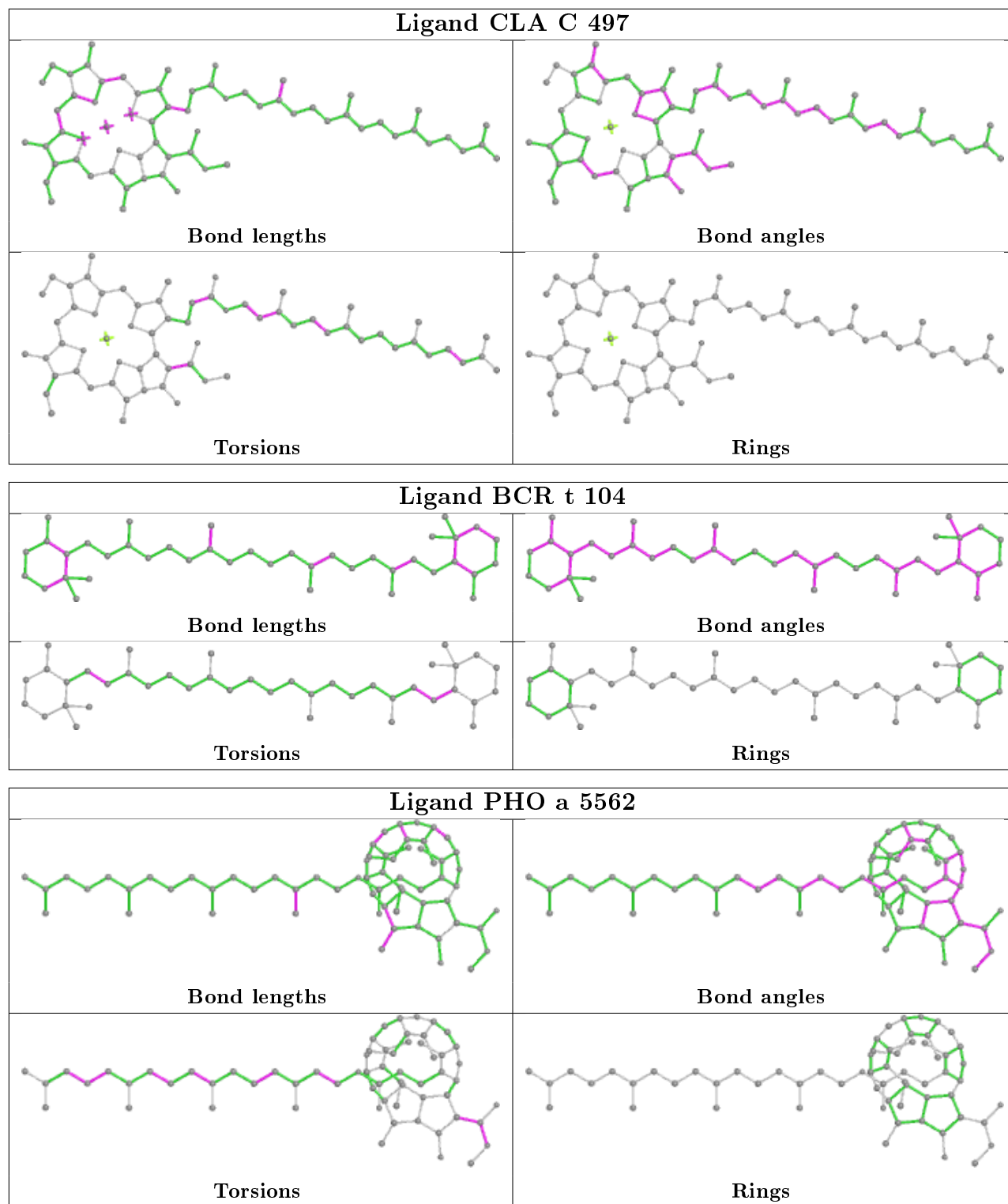


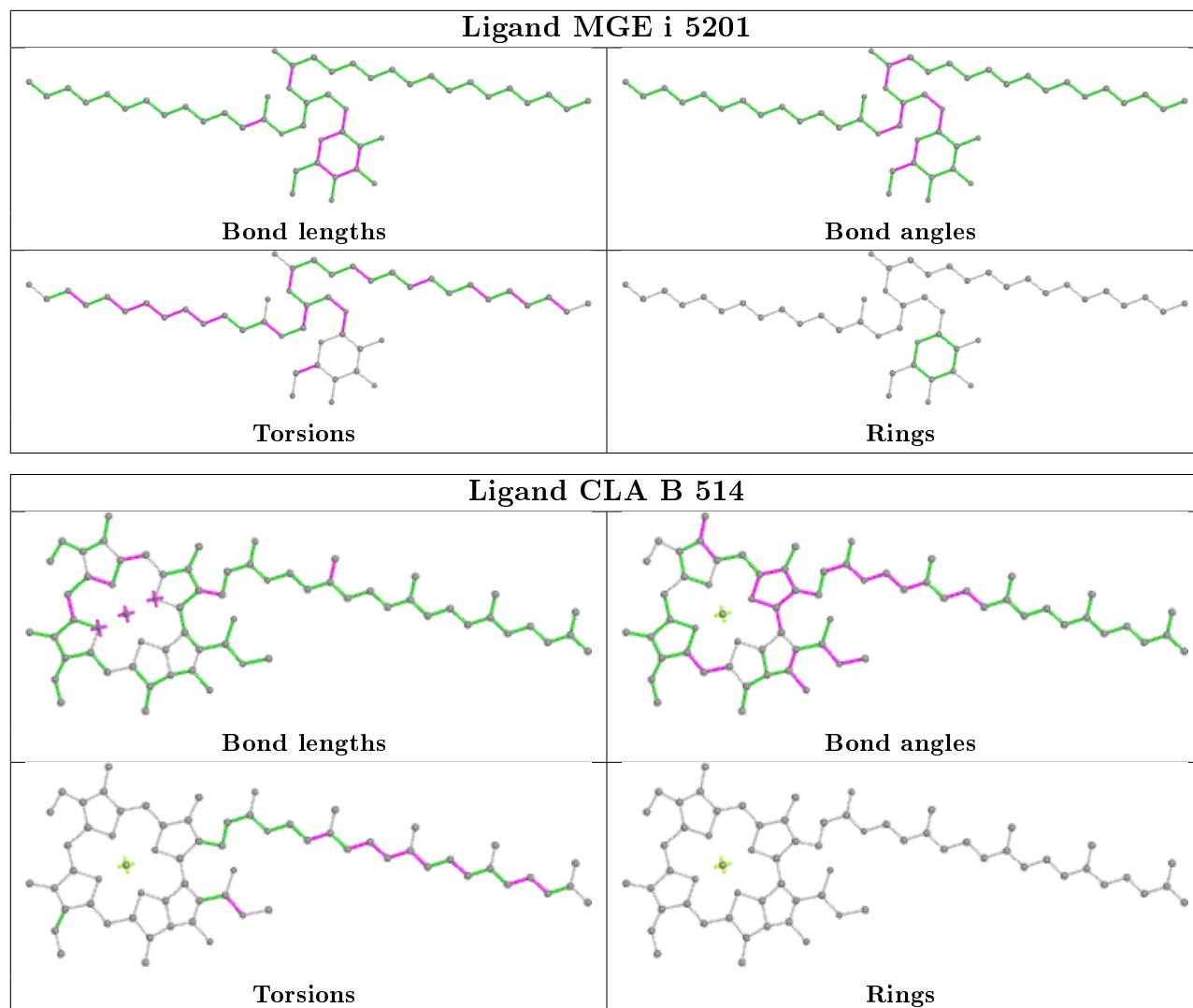












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.59	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.53	4 (1%) 79 54	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.53	2 (0%) 92 79	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.50	1 (0%) 95 87	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.52	3 (0%) 87 69	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.35	5 (1%) 80 56	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 94 84	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.57	1 (0%) 94 84	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.20	1 (1%) 79 54	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.01	3 (3%) 41 17	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.25	1 (2%) 51 23	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	3 (8%) 10 3	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.37	1 (1%) 72 44	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.19	3 (4%) 31 11	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	0 100 100	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.34	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.60	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.52	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.53	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.40	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.15	1 (2%) 54 26	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.36	2 (5%) 25 9	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.42	2 (5%) 24 8	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.34	1 (2%) 53 25	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.39	3 (1%) 79 54	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.30	8 (3%) 46 20	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.48	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.73	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.39	1 (1%) 82 59	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.42	3 (3%) 49 21	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.48	2 (1%) 73 46	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.24	5 (3%) 42 17	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.25	4 (6%) 18 5	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.20	2 (3%) 47 20	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.45	63 (1%) 79 54	35, 66, 85, 101	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5473	ASP	4.5
1	a	5010	SER	4.4
13	o	5049	ASP	4.3
4	D	13	GLY	4.2
11	l	5001	MET	4.0
13	O	114	ASN	3.9
6	f	5013	TYR	3.7
7	h	5065	LEU	3.6
15	U	37	GLU	3.4
11	L	5	PRO	3.3
5	e	5003	GLY	3.3
1	a	5015	GLU	3.3
1	a	5011	ALA	3.3
5	e	5060	GLN	3.2
6	f	5011	VAL	3.2
18	Z	30	PRO	3.2
5	E	84	LYS	3.0
13	o	5050	ASP	3.0
18	z	5062	VAL	2.9
3	c	5029	GLU	2.9
5	e	5017	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
7	h	5064	ALA	2.8
18	Z	60	PHE	2.7
3	C	192	GLY	2.7
13	O	87	GLN	2.6
16	v	5111	GLU	2.6
16	V	27	ALA	2.6
6	f	5012	SER	2.6
16	v	5041	GLU	2.6
13	o	5060	SER	2.6
6	F	12	SER	2.6
12	M	36	SER	2.5
18	z	5003	ILE	2.5
3	C	182	PHE	2.5
13	O	59	ASP	2.5
13	o	5061	SER	2.4
7	h	5006	TRP	2.4
2	B	129	GLY	2.4
13	o	5030	THR	2.4
1	a	5227	THR	2.3
3	C	460	ASP	2.3
3	c	5033	PHE	2.3
15	u	5053	GLU	2.3
3	c	5472	LEU	2.3
16	V	81	ARG	2.3
13	o	5048	LEU	2.2
18	Z	29	SER	2.2
18	Z	34	ASP	2.2
2	b	5294	SER	2.2
11	l	5003	PRO	2.2
4	d	5226	GLY	2.2
15	u	5086	GLU	2.2
15	u	5052	GLY	2.2
2	B	130	GLU	2.1
7	H	26	GLY	2.1
12	m	5033	GLN	2.1
13	o	5082	PRO	2.1
13	o	5089	ALA	2.1
3	c	5142	GLU	2.0
16	v	5027	ALA	2.0
16	v	5039	ASN	2.0
12	M	33	GLN	2.0
16	v	5043	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	b	5511	41/65	0.64	0.39	88,92,95,96	0
27	LMT	t	5217	35/35	0.69	0.45	76,95,104,105	0
29	UNK	c	5478	11/-	0.70	0.40	76,79,81,81	0
29	UNK	c	5490	4/-	0.71	0.33	91,92,92,92	0
29	UNK	C	481	13/-	0.72	0.37	61,64,68,69	0
27	LMT	A	569	35/35	0.73	0.47	80,89,92,93	0
20	CLA	B	511	41/65	0.73	0.41	88,90,92,98	0
29	UNK	C	475	12/-	0.73	0.32	68,69,72,73	0
29	UNK	c	5475	12/-	0.74	0.35	74,78,84,84	0
27	LMT	T	217	35/35	0.75	0.32	83,93,96,97	0
28	MGE	d	5359	47/48	0.76	0.30	72,81,96,98	0
22	PQ9	A	564	30/45	0.77	0.37	54,57,63,64	30
24	BCR	c	5506	40/40	0.77	0.32	75,81,86,86	0
24	BCR	x	5130	40/40	0.78	0.44	77,81,85,86	0
27	LMT	M	5216	35/35	0.78	0.31	58,83,90,90	0
20	CLA	b	5526	65/65	0.79	0.28	66,71,92,95	0
29	UNK	C	489	7/-	0.79	0.42	75,76,77,78	0
29	UNK	c	5489	7/-	0.79	0.39	73,73,74,74	0
26	SQD	d	5358	54/54	0.79	0.29	74,85,106,107	0
26	SQD	a	212	26/54	0.79	0.26	82,94,101,103	0
20	CLA	B	526	65/65	0.80	0.28	71,82,97,98	0
26	SQD	L	5213	47/54	0.80	0.27	52,85,106,108	0
29	UNK	c	5476	9/-	0.80	0.32	58,60,62,62	0
28	MGE	D	358	47/48	0.81	0.24	65,72,79,81	0
27	LMT	m	216	35/35	0.81	0.28	62,87,89,91	0
24	BCR	C	505	40/40	0.81	0.43	75,81,91,92	0
29	UNK	C	486	8/-	0.81	0.36	55,56,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNK	C	476	9/-	0.81	0.29	61,62,63,64	0
27	LMT	a	5568	35/35	0.81	0.43	79,92,94,96	0
20	CLA	b	5516	65/65	0.81	0.28	62,66,84,86	0
26	SQD	A	5212	26/54	0.81	0.23	75,100,107,107	0
24	BCR	d	5357	40/40	0.82	0.37	61,72,86,88	0
20	CLA	B	516	65/65	0.82	0.27	61,76,92,97	0
24	BCR	H	107	40/40	0.82	0.30	77,83,88,89	0
20	CLA	c	5496	65/65	0.82	0.27	79,83,95,97	0
29	UNK	c	5485	5/-	0.83	0.41	68,69,69,70	0
26	SQD	A	568	54/54	0.84	0.32	76,82,90,90	0
20	CLA	C	496	65/65	0.84	0.26	71,78,88,89	0
20	CLA	a	5563	55/65	0.84	0.32	59,65,102,103	0
24	BCR	B	528	40/40	0.84	0.25	54,68,74,75	0
29	UNK	C	478	11/-	0.84	0.24	58,65,66,66	0
29	UNK	c	5484	5/-	0.84	0.52	69,69,70,72	0
24	BCR	h	5107	40/40	0.85	0.28	74,79,82,83	0
26	SQD	t	213	47/54	0.85	0.27	61,95,116,117	0
29	UNK	C	479	11/-	0.85	0.26	58,64,67,67	0
20	CLA	C	503	50/65	0.85	0.27	83,86,88,94	0
20	CLA	c	5503	50/65	0.85	0.28	88,91,92,93	0
29	UNK	C	482	13/-	0.85	0.25	64,66,67,67	0
24	BCR	X	130	40/40	0.85	0.32	68,71,80,81	0
20	CLA	c	5498	65/65	0.85	0.25	81,90,93,93	0
28	MGE	i	5201	48/48	0.85	0.27	67,83,88,90	0
29	UNK	c	5479	11/-	0.85	0.24	76,77,77,77	0
30	DGD	c	5509	57/66	0.86	0.28	67,72,77,78	0
29	UNK	C	487	7/-	0.86	0.24	49,52,52,53	0
29	UNK	C	488	5/-	0.86	0.17	41,45,47,47	0
24	BCR	c	5504	40/40	0.86	0.29	73,80,88,89	0
24	BCR	b	5529	40/40	0.86	0.35	69,72,74,74	0
20	CLA	d	5355	50/65	0.86	0.23	74,77,80,81	0
29	UNK	C	484	5/-	0.86	0.21	47,51,52,53	0
28	MGE	D	359	41/48	0.87	0.23	60,67,76,79	0
20	CLA	B	519	65/65	0.87	0.26	73,82,85,87	0
20	CLA	c	5502	51/65	0.87	0.23	93,96,97,98	0
29	UNK	c	5481	13/-	0.87	0.22	60,62,66,66	0
28	MGE	I	201	48/48	0.87	0.22	73,81,89,90	0
20	CLA	C	498	65/65	0.88	0.22	64,74,98,101	0
20	CLA	A	563	55/65	0.88	0.26	43,49,75,78	0
24	BCR	T	5104	40/40	0.88	0.25	67,71,78,79	0
22	PQ9	a	5564	30/45	0.88	0.32	51,55,62,62	30
24	BCR	c	5505	40/40	0.88	0.31	84,87,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNK	c	5483	13/-	0.88	0.26	71,75,80,82	0
29	UNK	c	5487	7/-	0.88	0.20	57,57,58,58	0
20	CLA	C	502	51/65	0.88	0.21	74,80,83,84	0
24	BCR	C	506	40/40	0.88	0.22	68,72,79,80	0
29	UNK	C	483	13/-	0.89	0.23	61,68,78,78	0
28	MGE	L	210	48/48	0.89	0.24	59,68,73,75	0
30	DGD	c	5507	53/66	0.89	0.23	66,74,90,91	0
20	CLA	b	5519	65/65	0.89	0.24	70,75,80,81	0
20	CLA	C	501	65/65	0.89	0.25	70,78,83,85	0
29	UNK	c	5474	15/-	0.89	0.24	39,50,56,56	0
28	MGE	B	530	48/48	0.89	0.19	55,64,70,72	0
29	UNK	c	5477	7/-	0.89	0.34	67,68,70,70	0
20	CLA	c	5497	65/65	0.89	0.24	66,82,84,87	0
29	UNK	c	5486	8/-	0.89	0.30	63,64,65,66	0
29	UNK	C	474	15/-	0.89	0.18	26,37,40,40	0
24	BCR	D	357	40/40	0.89	0.26	61,66,78,80	0
28	MGE	d	5360	41/48	0.89	0.21	68,72,78,80	0
29	UNK	C	485	5/-	0.89	0.24	57,59,61,61	0
24	BCR	B	529	40/40	0.89	0.25	62,69,80,80	0
20	CLA	c	5501	65/65	0.89	0.26	82,91,94,95	0
20	CLA	C	497	65/65	0.89	0.24	74,78,80,82	0
30	DGD	C	507	53/66	0.89	0.25	55,66,86,88	0
29	UNK	c	5480	7/-	0.89	0.26	65,66,66,67	0
24	BCR	a	5566	40/40	0.90	0.25	59,75,78,79	0
20	CLA	B	520	65/65	0.90	0.23	62,67,76,79	0
25	LHG	a	5567	39/49	0.90	0.26	65,68,74,80	0
29	UNK	c	5482	13/-	0.90	0.19	60,61,71,72	0
20	CLA	a	5560	65/65	0.90	0.22	62,68,100,101	0
28	MGE	d	5361	48/48	0.90	0.21	61,68,78,83	0
28	MGE	l	5210	48/48	0.90	0.21	59,69,78,81	0
30	DGD	H	208	54/66	0.90	0.20	61,69,75,76	0
20	CLA	c	5493	65/65	0.90	0.21	67,81,86,86	0
20	CLA	b	5520	65/65	0.90	0.24	63,72,74,76	0
28	MGE	b	5530	48/48	0.90	0.18	59,64,71,73	0
30	DGD	C	508	47/66	0.91	0.19	61,71,80,83	0
20	CLA	A	560	65/65	0.91	0.21	49,57,86,88	0
20	CLA	B	512	65/65	0.91	0.24	68,75,78,79	0
20	CLA	D	355	50/65	0.91	0.22	63,65,68,70	0
22	PQ9	D	356	30/45	0.91	0.21	49,67,80,83	0
29	UNK	C	480	7/-	0.91	0.22	35,36,38,38	0
28	MGE	D	360	48/48	0.91	0.20	52,60,63,68	0
24	BCR	B	527	40/40	0.91	0.18	58,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	c	5491	65/65	0.91	0.20	70,78,81,86	0
30	DGD	C	509	57/66	0.91	0.20	52,60,69,70	0
20	CLA	c	5495	65/65	0.91	0.21	74,81,86,88	0
24	BCR	t	104	40/40	0.91	0.20	65,72,84,85	0
21	PHO	a	5562	64/64	0.91	0.22	70,75,81,82	0
30	DGD	c	5508	47/66	0.91	0.18	66,76,82,84	0
24	BCR	C	504	40/40	0.91	0.27	57,64,70,70	0
24	BCR	b	5527	40/40	0.92	0.19	58,63,72,72	0
22	PQ9	d	5356	30/45	0.92	0.20	51,57,66,66	0
20	CLA	b	5525	65/65	0.92	0.20	71,77,80,82	0
24	BCR	A	566	40/40	0.92	0.24	50,57,64,66	0
20	CLA	c	5499	47/65	0.92	0.20	60,69,76,78	0
29	UNK	c	5488	5/-	0.92	0.21	59,59,59,60	0
25	LHG	A	567	39/49	0.92	0.23	57,73,79,81	0
20	CLA	C	495	65/65	0.92	0.21	58,68,74,76	0
20	CLA	b	5512	65/65	0.92	0.23	68,72,75,76	0
20	CLA	c	5500	65/65	0.92	0.20	64,69,82,83	0
20	CLA	b	5524	56/65	0.93	0.18	63,68,89,91	0
20	CLA	B	515	65/65	0.93	0.21	55,66,71,72	0
20	CLA	c	5492	60/65	0.93	0.17	57,61,83,84	0
24	BCR	b	5528	40/40	0.93	0.17	61,64,72,73	0
30	DGD	h	5208	54/66	0.93	0.17	57,68,73,75	0
20	CLA	B	522	65/65	0.93	0.21	54,65,75,77	0
20	CLA	B	518	65/65	0.93	0.19	53,64,79,79	0
20	CLA	B	525	65/65	0.93	0.20	67,84,91,92	0
20	CLA	c	5494	46/65	0.93	0.16	72,77,86,88	0
20	CLA	B	514	65/65	0.93	0.21	59,64,82,83	0
20	CLA	B	524	56/65	0.93	0.19	67,72,77,80	0
20	CLA	b	5514	65/65	0.94	0.18	41,51,74,75	0
33	CA	k	5056	1/1	0.94	0.19	119,119,119,119	0
20	CLA	b	5515	65/65	0.94	0.21	46,51,74,76	0
21	PHO	a	5561	64/64	0.94	0.18	51,55,66,68	0
20	CLA	b	5521	65/65	0.94	0.15	48,57,63,64	0
20	CLA	b	5522	65/65	0.94	0.20	60,66,75,76	0
21	PHO	A	562	64/64	0.94	0.17	47,53,63,66	0
20	CLA	B	513	65/65	0.94	0.18	56,61,67,67	0
32	HEM	f	5051	43/43	0.94	0.28	80,84,97,101	0
20	CLA	b	5513	65/65	0.94	0.20	54,61,84,90	0
20	CLA	C	500	65/65	0.94	0.16	59,63,73,74	0
20	CLA	C	493	65/65	0.94	0.18	67,71,77,79	0
20	CLA	C	499	47/65	0.95	0.17	57,60,66,69	0
21	PHO	A	561	64/64	0.95	0.16	32,52,55,59	0

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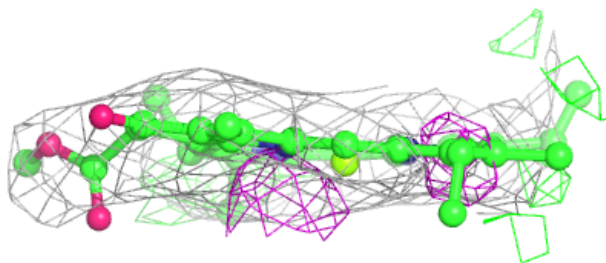
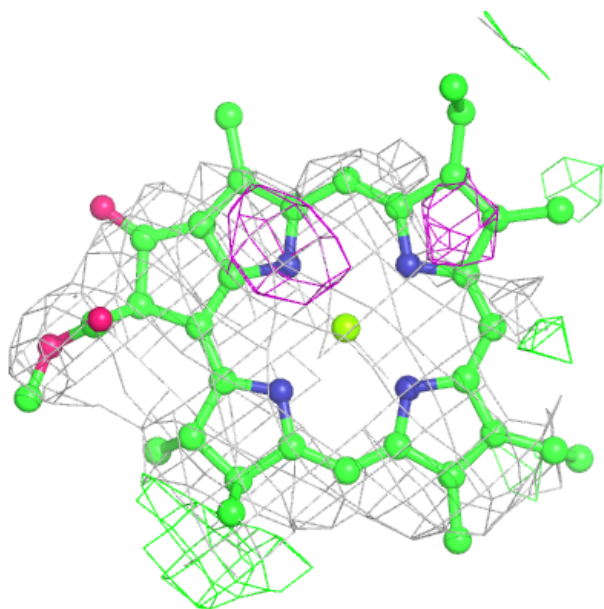
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	B	523	65/65	0.95	0.16	47,56,73,74	0
20	CLA	C	494	46/65	0.95	0.15	59,66,68,72	0
20	CLA	d	5354	65/65	0.95	0.17	39,47,64,65	0
20	CLA	a	5559	65/65	0.95	0.15	42,49,60,60	0
19	FE2	A	557	1/1	0.95	0.05	60,60,60,60	0
20	CLA	B	521	65/65	0.95	0.17	58,63,66,68	0
20	CLA	C	492	60/65	0.95	0.17	53,58,76,77	0
20	CLA	C	491	65/65	0.95	0.18	63,70,77,79	0
20	CLA	b	5518	65/65	0.95	0.17	60,64,69,75	0
20	CLA	b	5523	65/65	0.95	0.15	45,52,74,75	0
20	CLA	a	5558	65/65	0.95	0.16	41,50,55,61	0
20	CLA	b	5517	65/65	0.95	0.15	54,58,66,71	0
20	CLA	D	354	65/65	0.95	0.16	35,43,63,66	0
32	HEM	F	51	43/43	0.95	0.25	78,84,92,95	0
23	OEC	a	5565	5/9	0.96	0.13	63,64,71,87	0
20	CLA	A	558	65/65	0.96	0.14	41,46,50,51	0
29	UNK	C	490	4/-	0.96	0.15	67,67,68,68	0
29	UNK	C	477	7/-	0.96	0.16	47,49,51,51	0
23	OEC	A	565	5/9	0.96	0.13	62,63,65,66	0
20	CLA	B	517	65/65	0.96	0.14	37,44,56,57	0
33	CA	K	56	1/1	0.96	0.09	119,119,119,119	0
32	HEM	v	5552	43/43	0.96	0.21	65,67,70,70	0
20	CLA	A	559	65/65	0.96	0.14	39,43,49,52	0
31	BCT	D	353	4/4	0.96	0.18	72,73,73,74	0
32	HEM	V	552	43/43	0.97	0.18	37,54,58,59	0
31	BCT	d	5353	4/4	0.98	0.15	75,75,76,77	0
19	FE2	a	5557	1/1	1.00	0.11	75,75,75,75	0

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

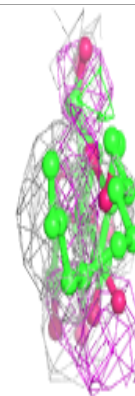
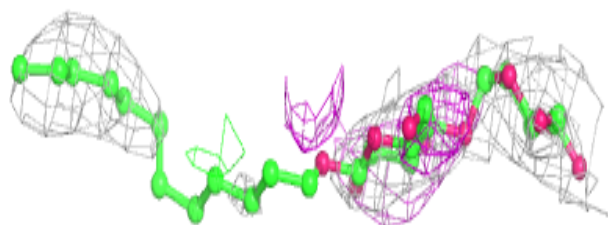
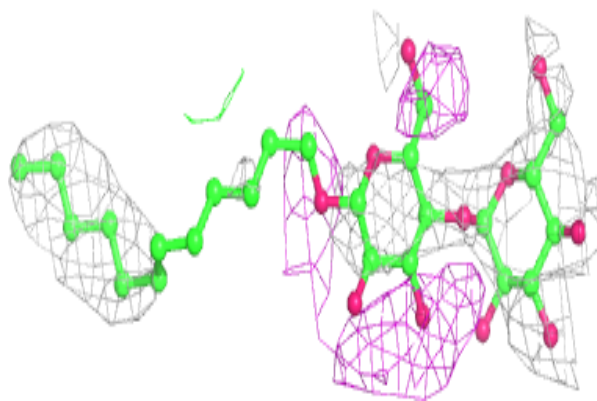
Electron density around CLA b 5511:

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

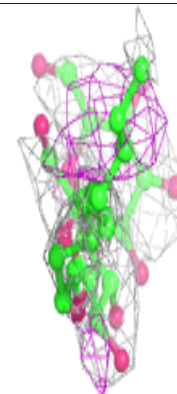
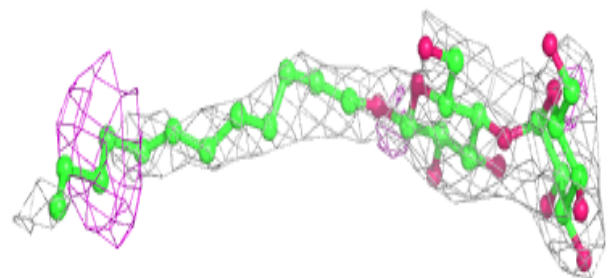
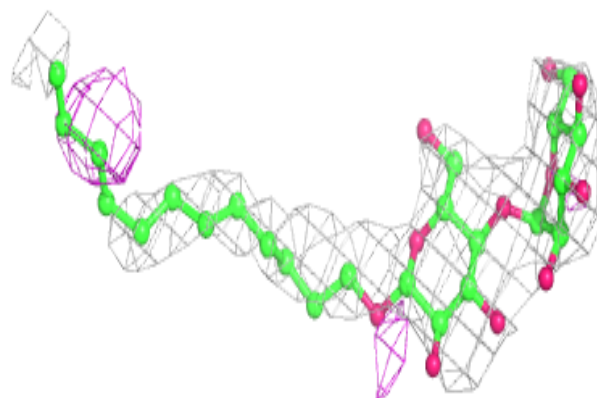


Electron density around LMT t 5217:

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

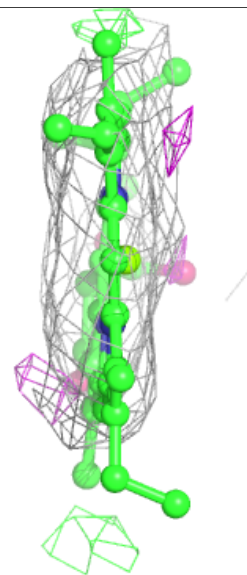
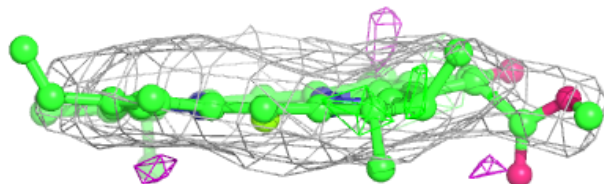
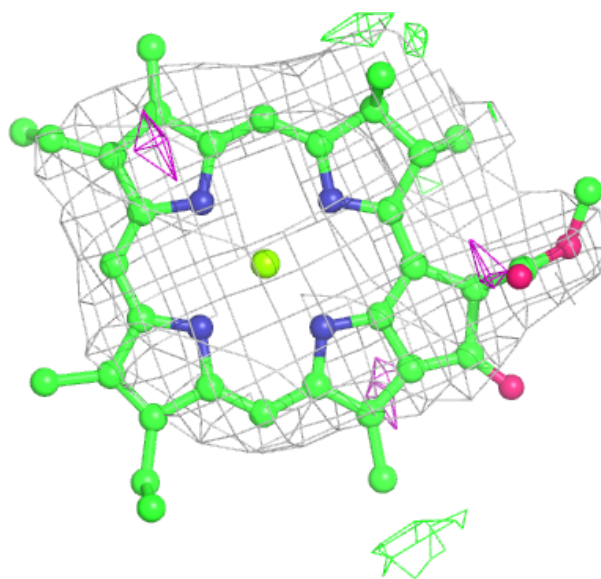
**Electron density around LMT A 569:**

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



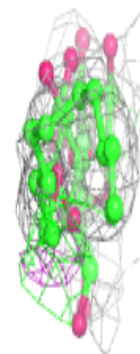
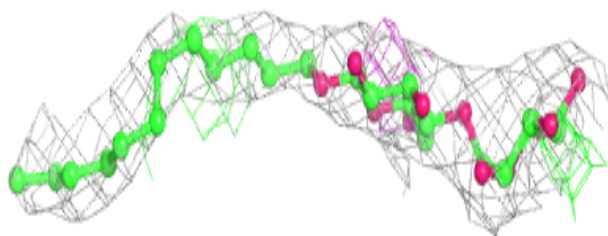
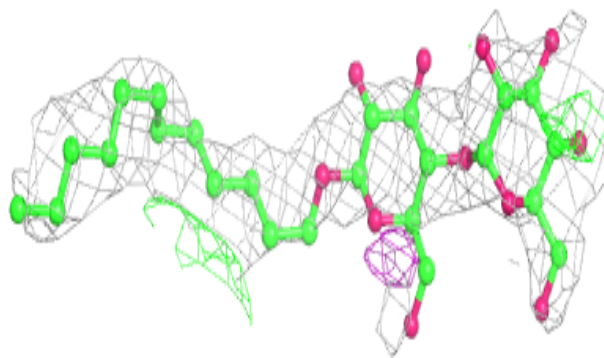
Electron density around CLA B 511:

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

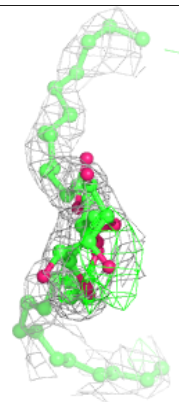
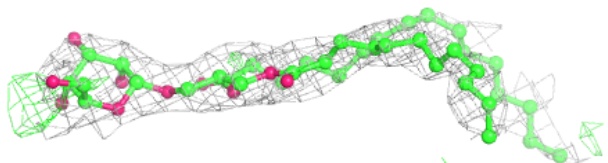
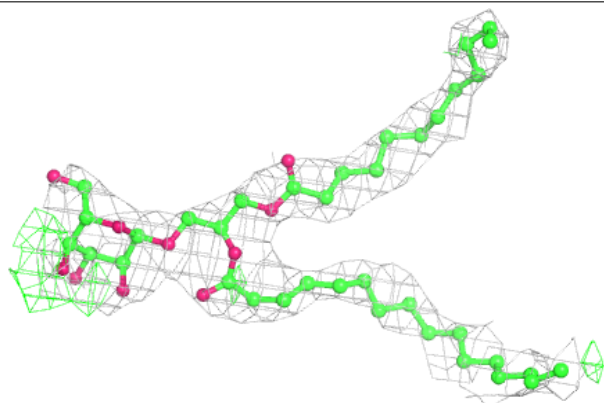


Electron density around LMT T 217:

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

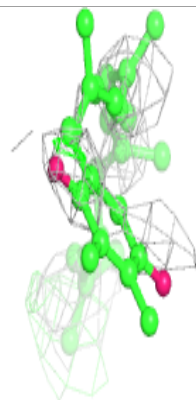
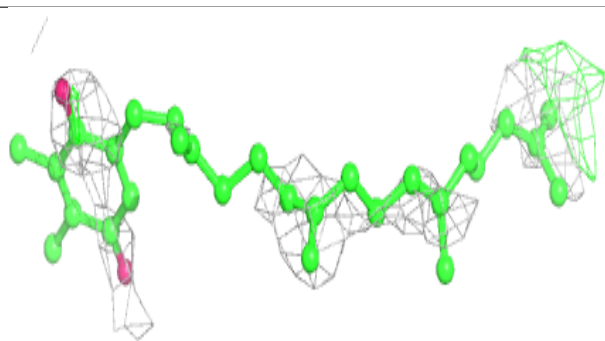
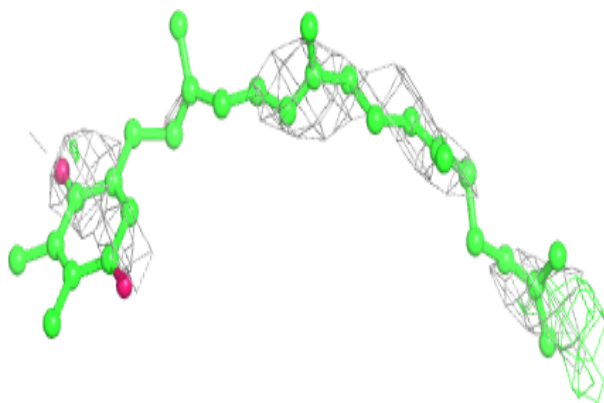
**Electron density around MGE d 5359:**

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

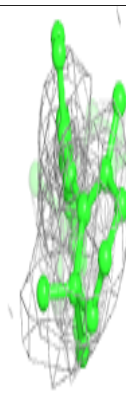
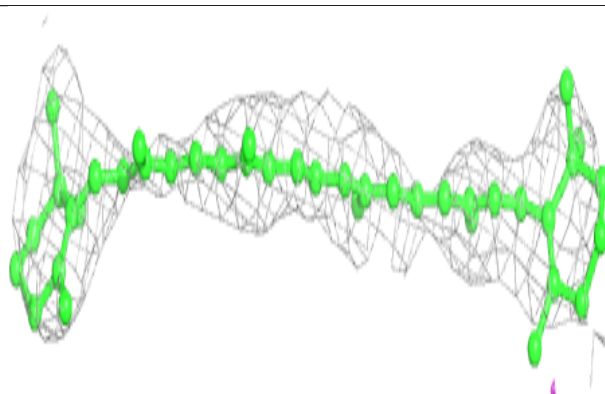
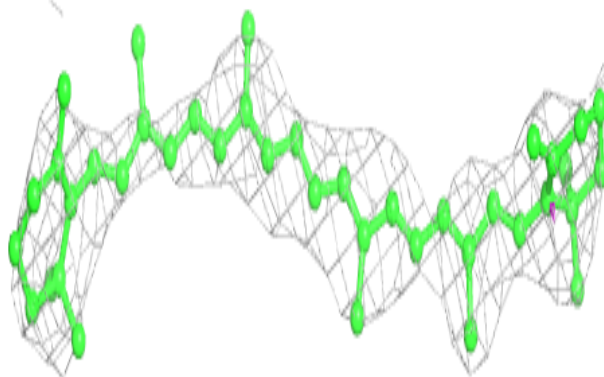


Electron density around PQ9 A 564:

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

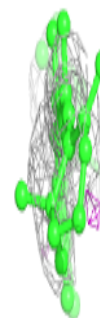
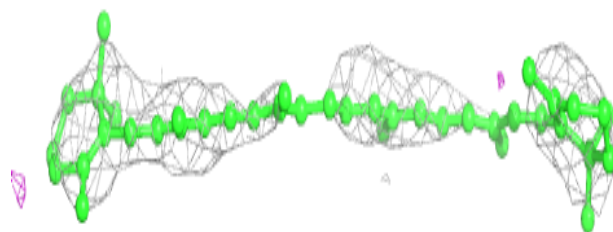
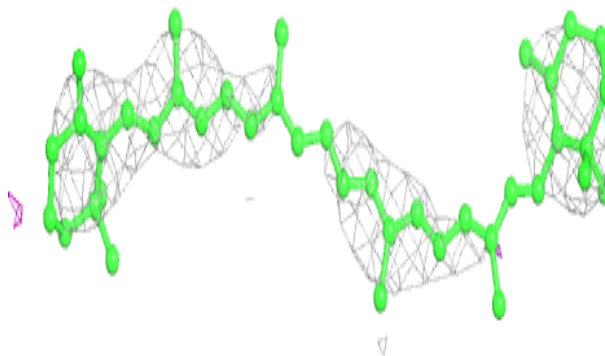
**Electron density around BCR c 5506:**

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

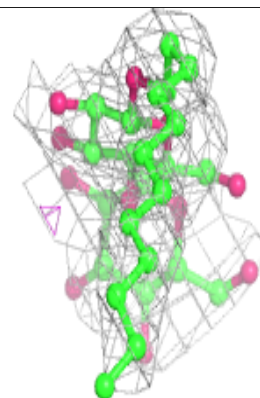
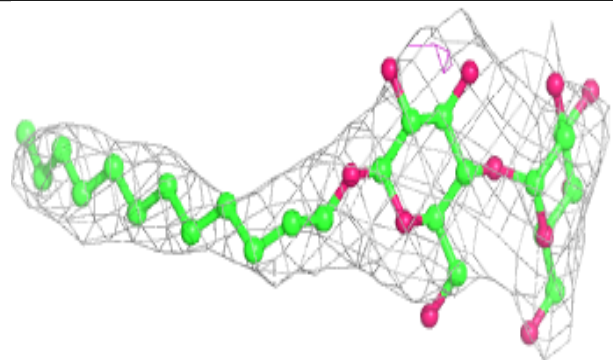
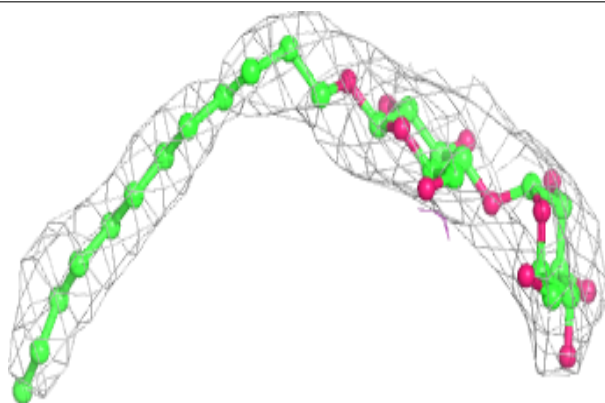


Electron density around BCR x 5130:

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

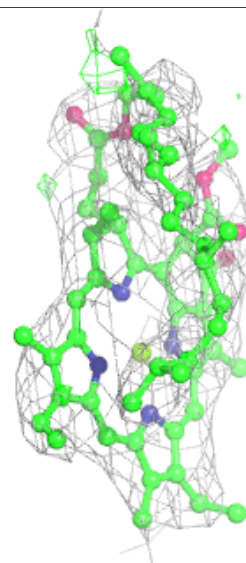
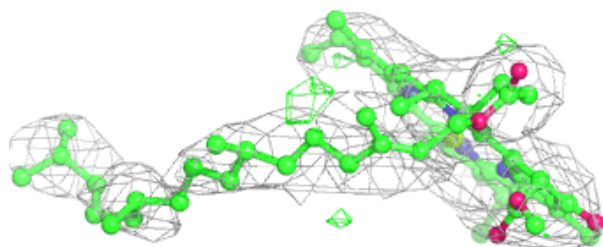
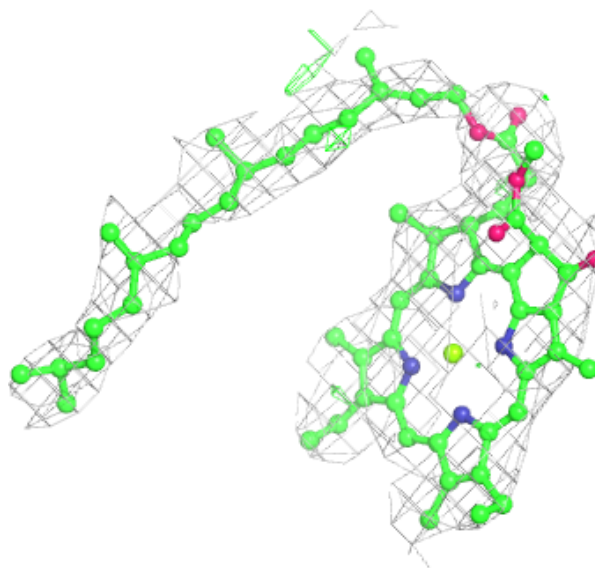
**Electron density around LMT M 5216:**

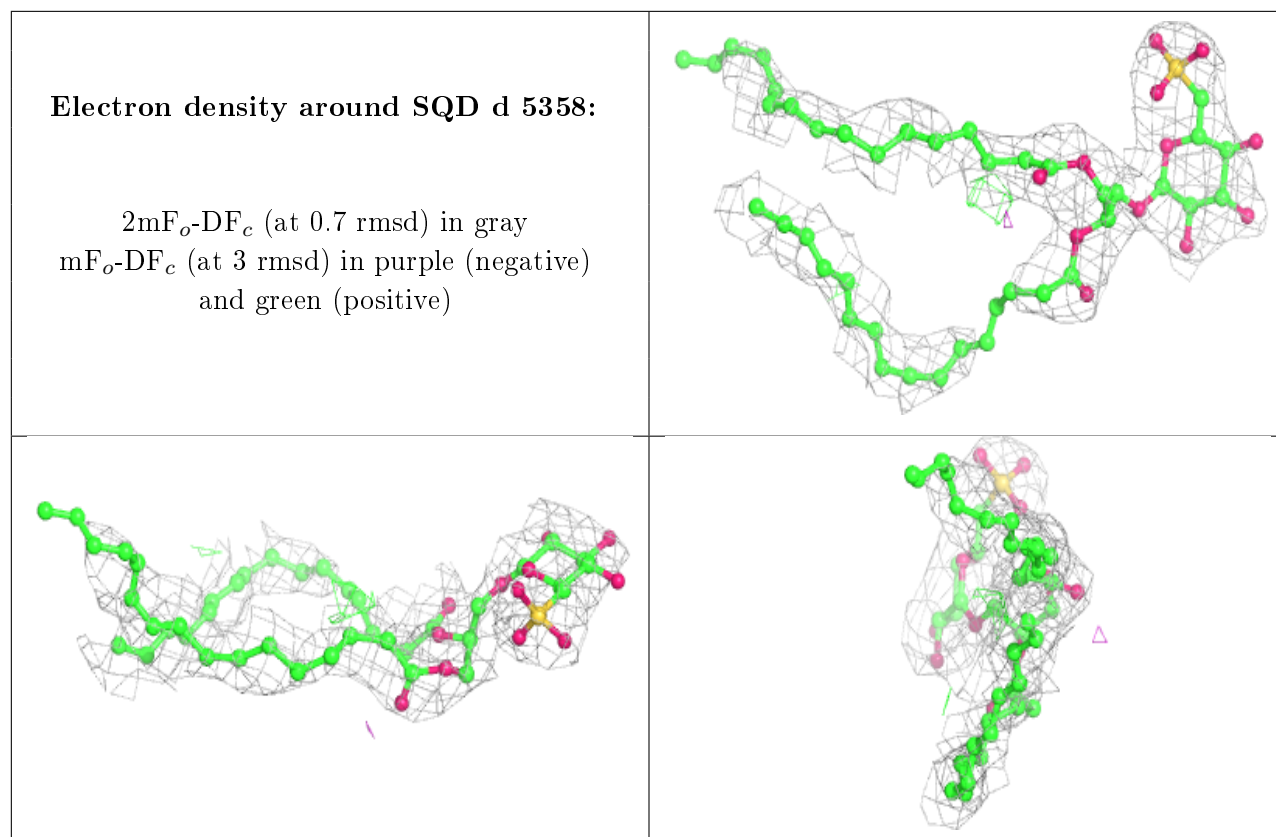
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 5526:

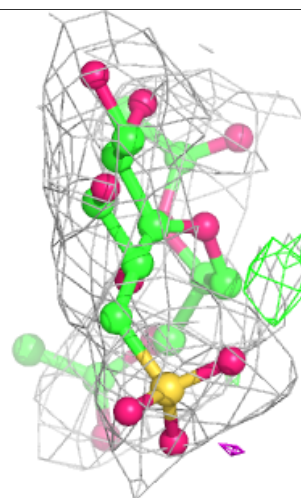
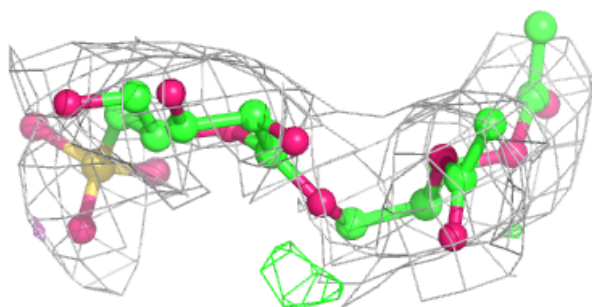
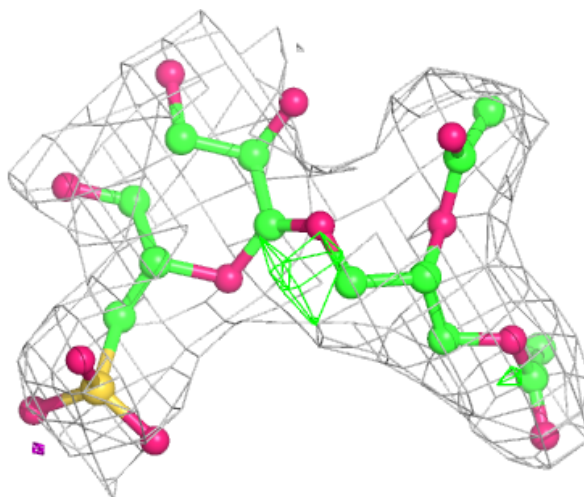
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





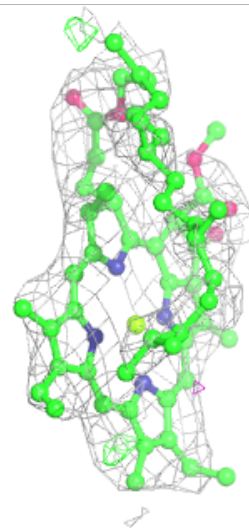
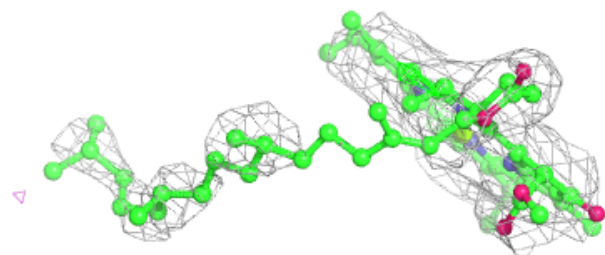
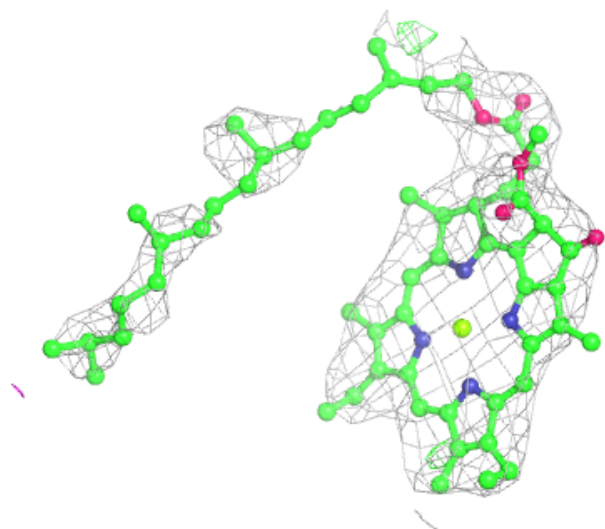
Electron density around SQD a 212:

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



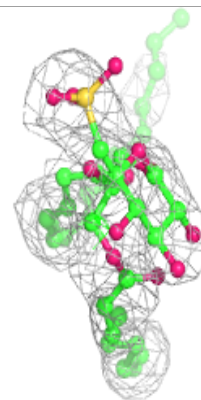
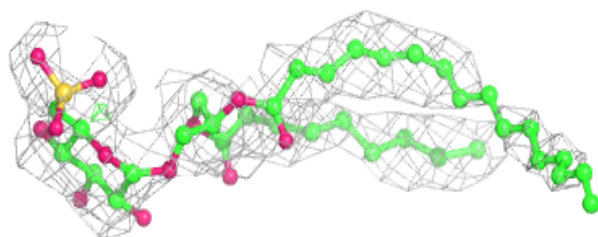
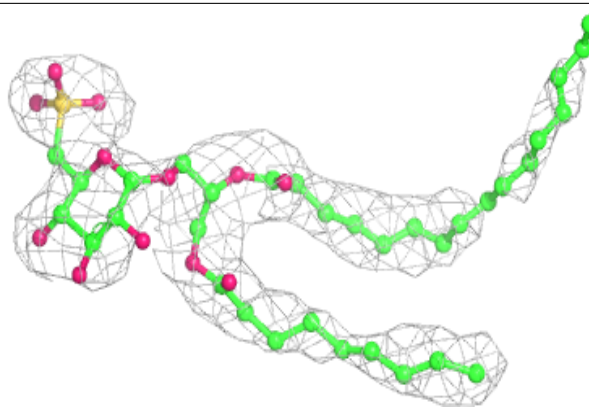
Electron density around CLA B 526:

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

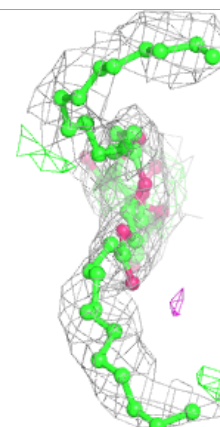
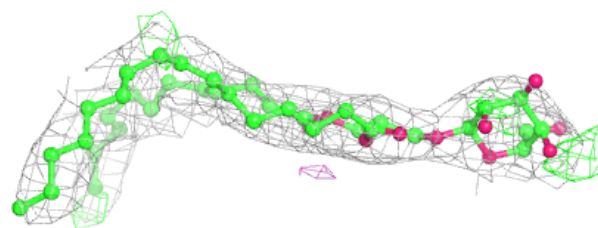
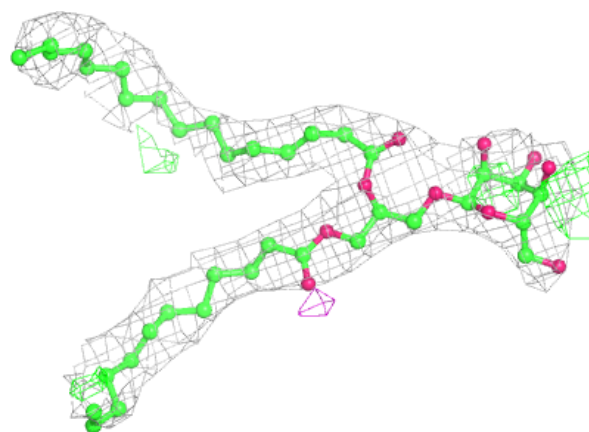


Electron density around SQD L 5213:

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

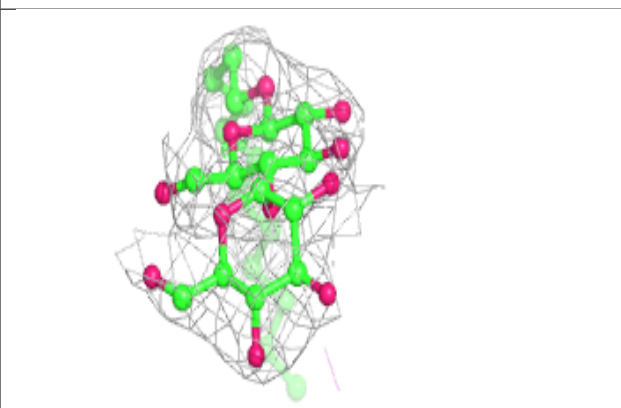
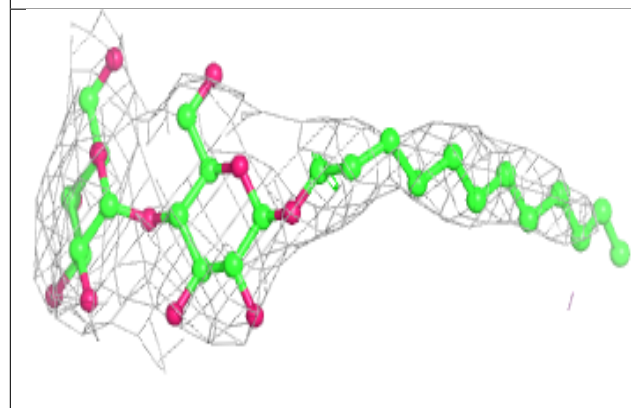
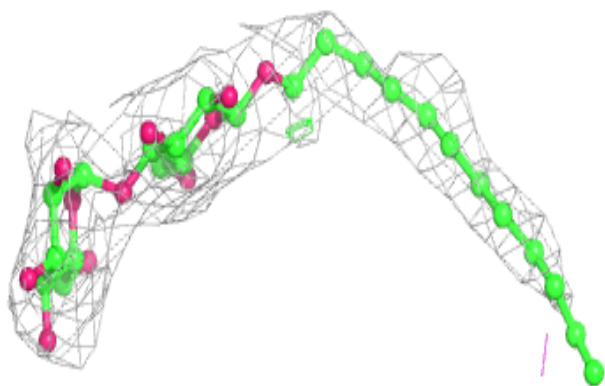
**Electron density around MGE D 358:**

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

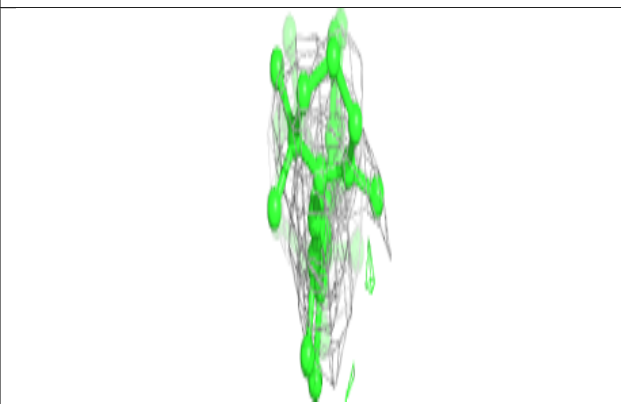
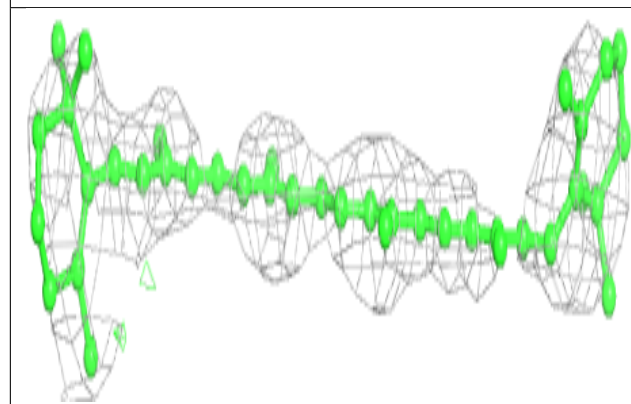
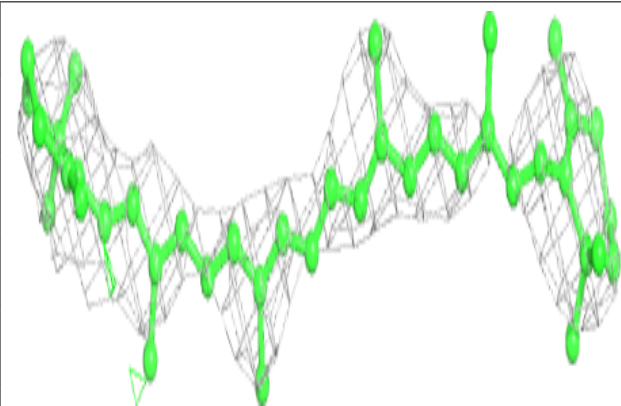


Electron density around LMT m 216:

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

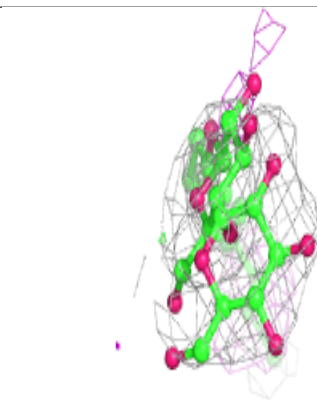
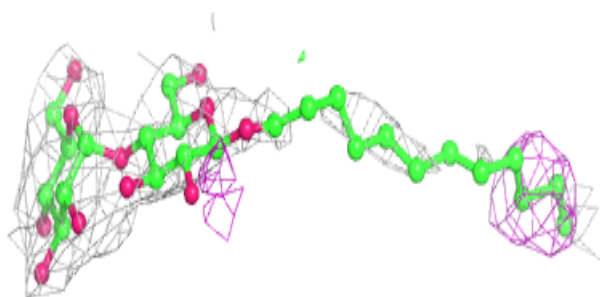
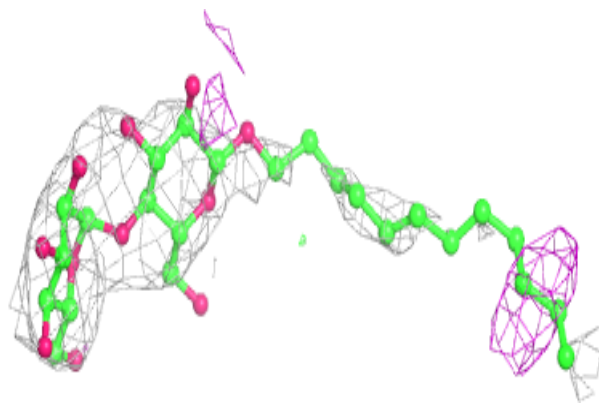
**Electron density around BCR C 505:**

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

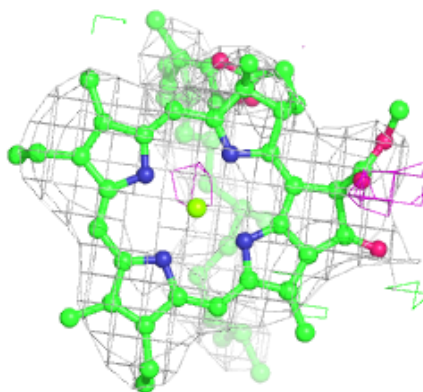
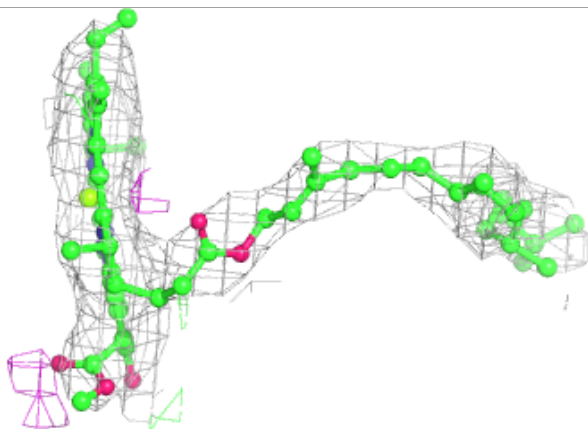
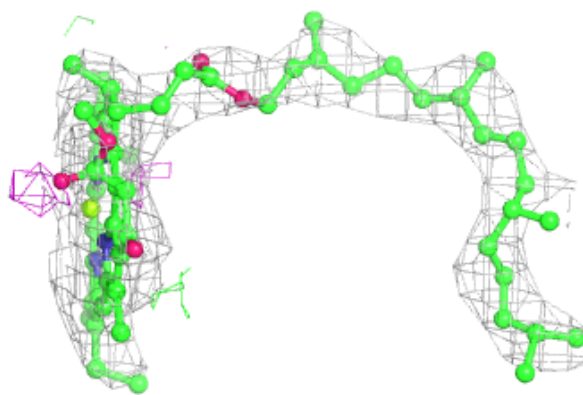


Electron density around LMT a 5568:

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

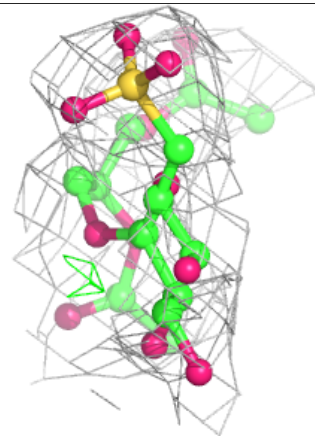
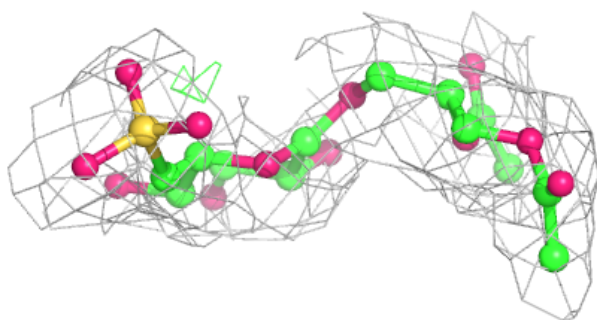
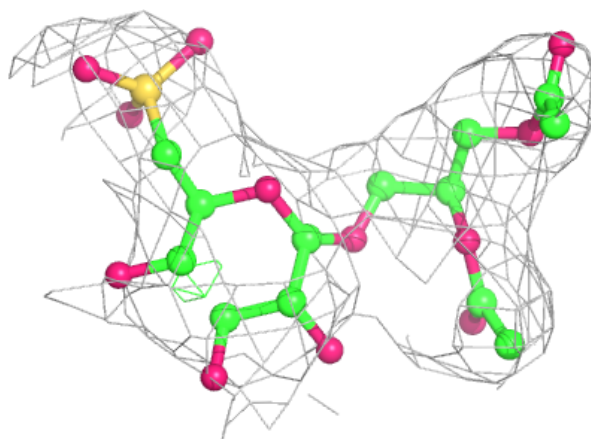
**Electron density around CLA b 5516:**

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

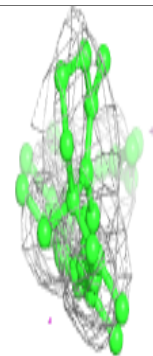
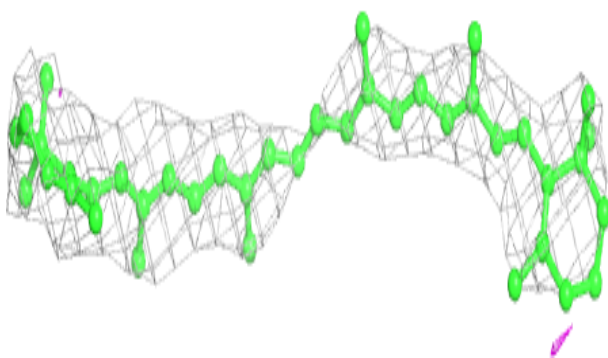
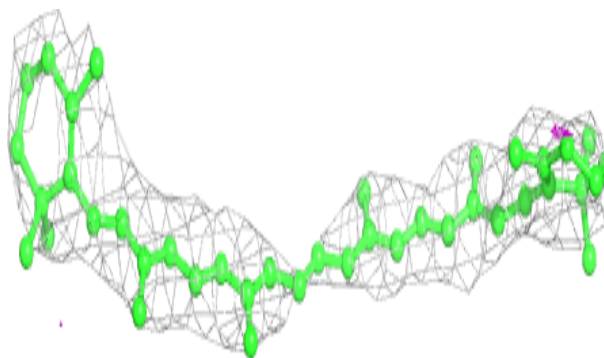


Electron density around SQD A 5212:

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

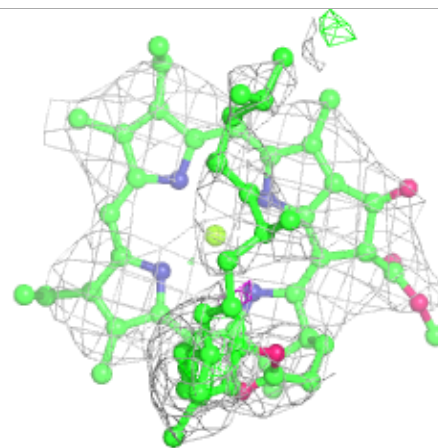
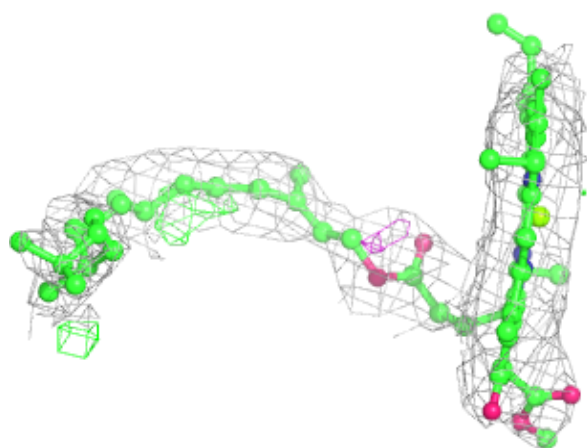
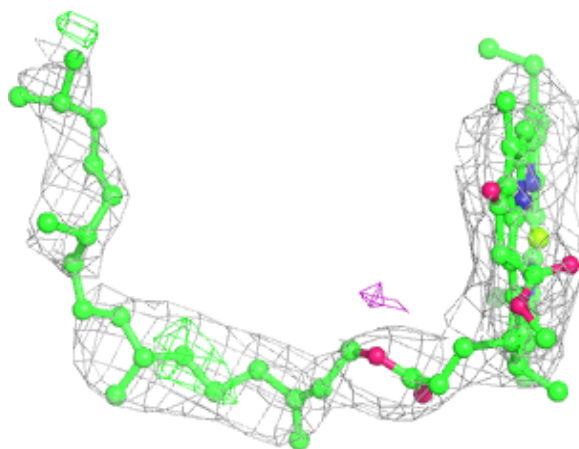
**Electron density around BCR d 5357:**

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



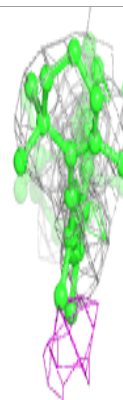
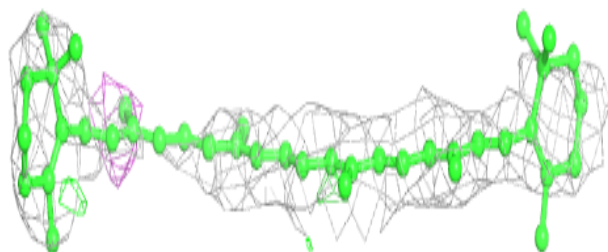
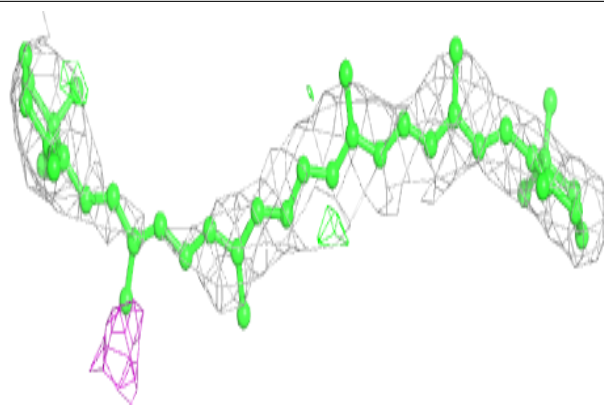
Electron density around CLA B 516:

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

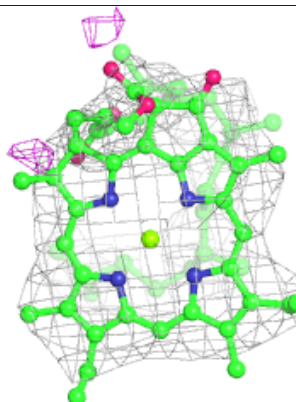
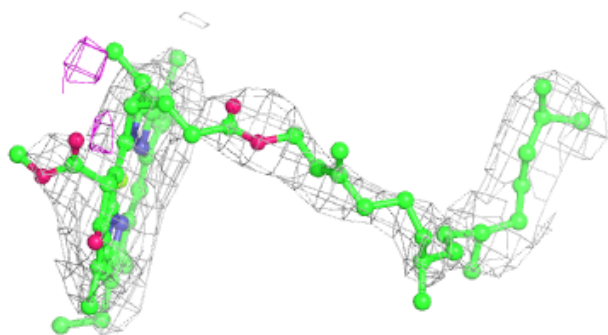
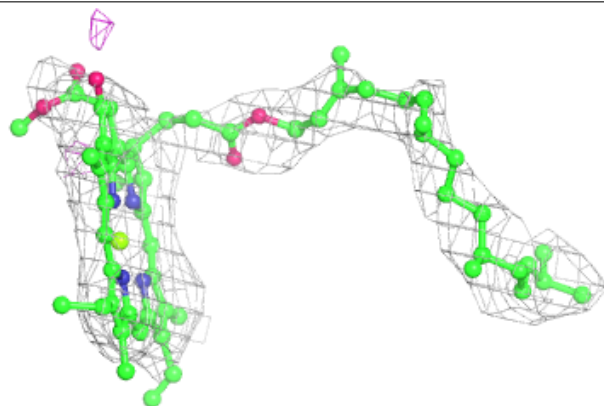


Electron density around BCR H 107:

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

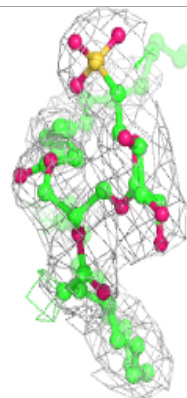
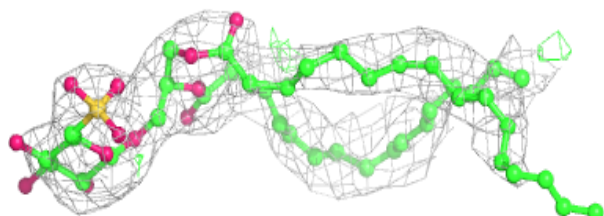
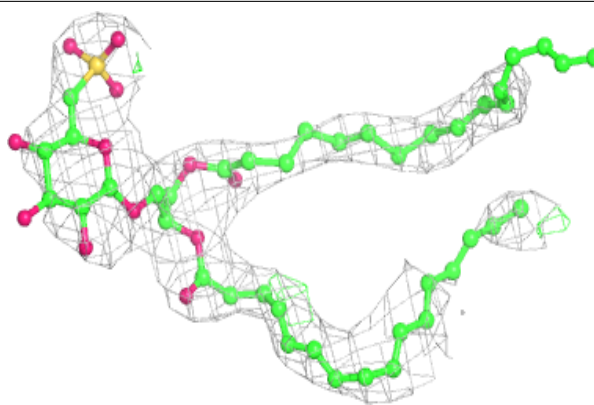
**Electron density around CLA c 5496:**

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

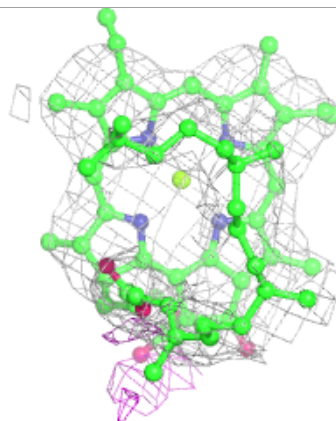
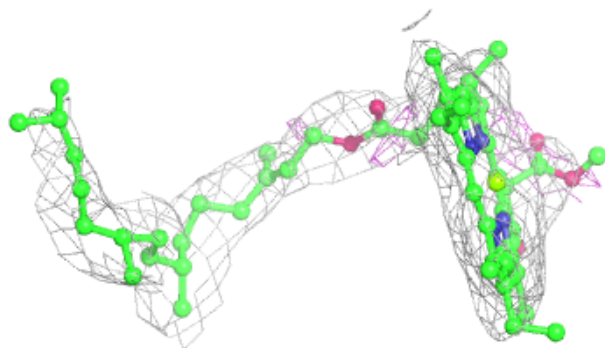
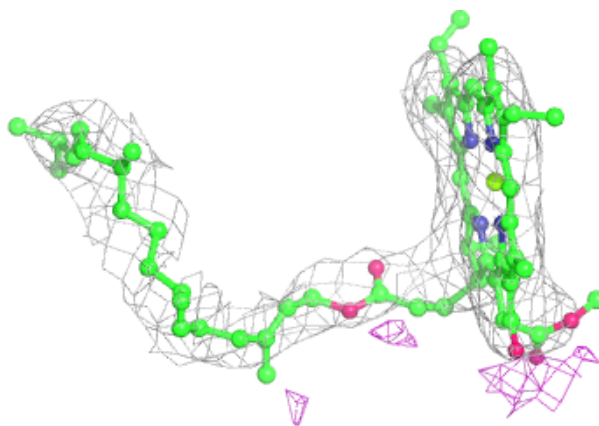


Electron density around SQD A 568:

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

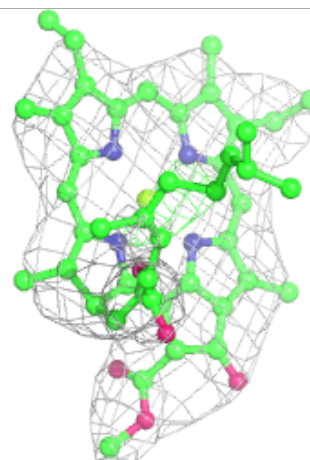
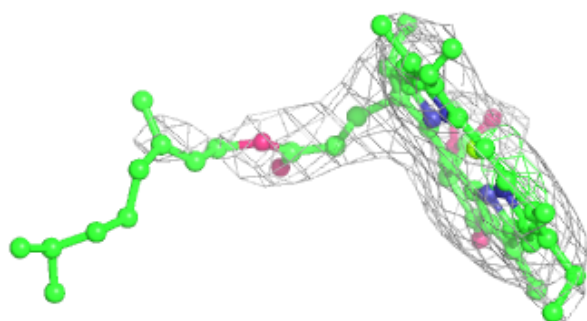
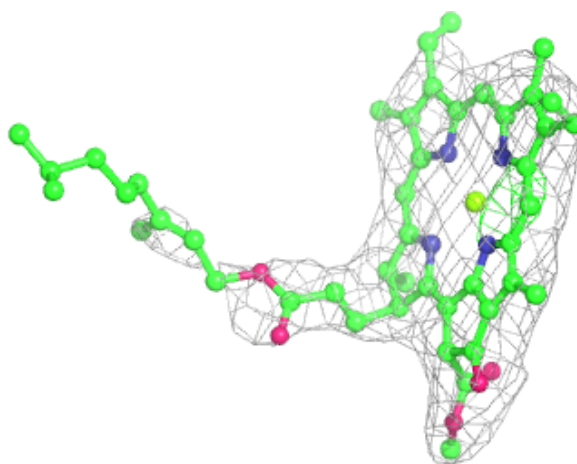
**Electron density around CLA C 496:**

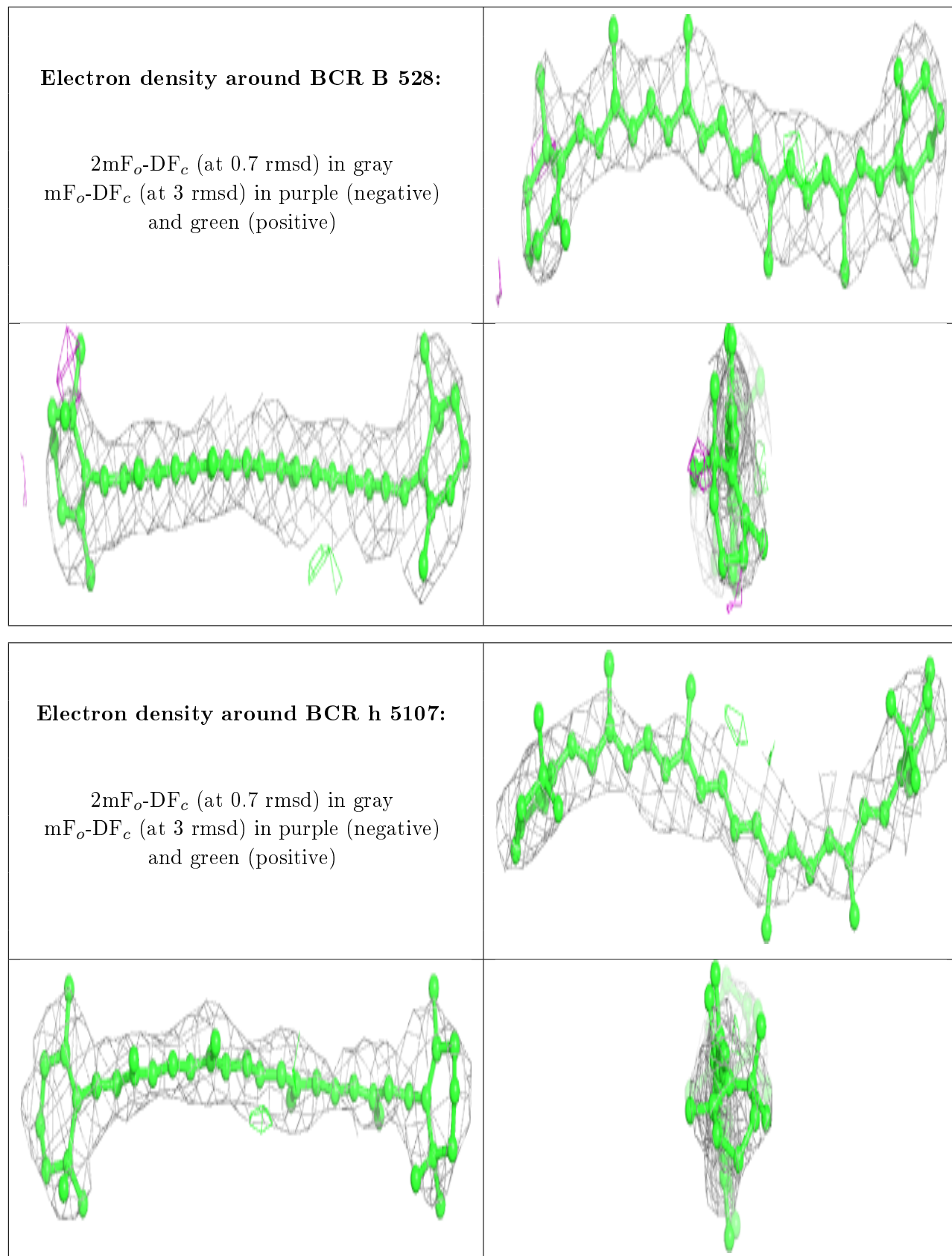
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 5563:

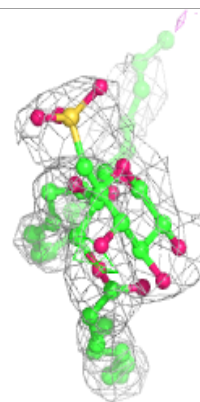
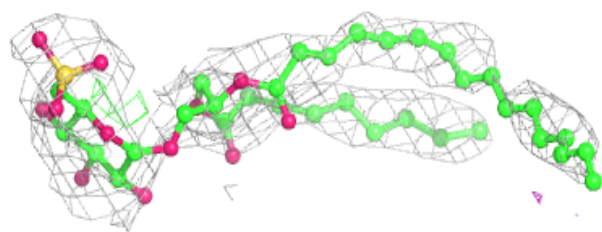
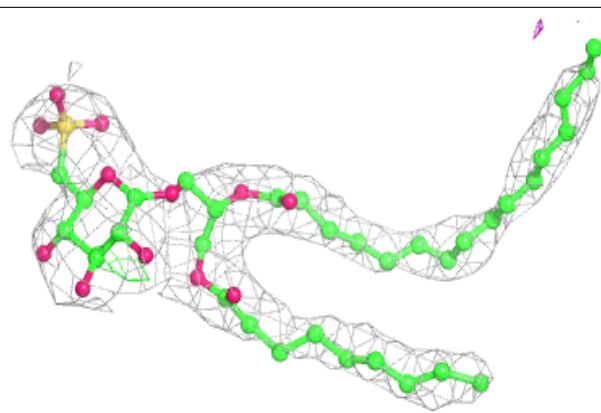
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





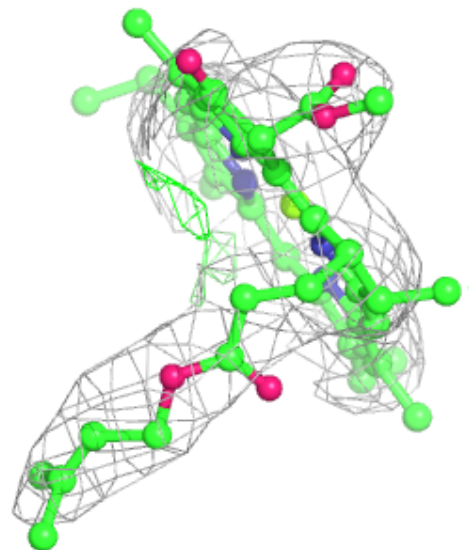
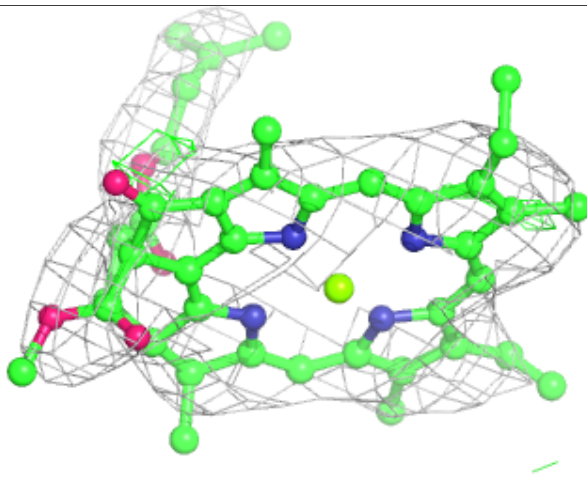
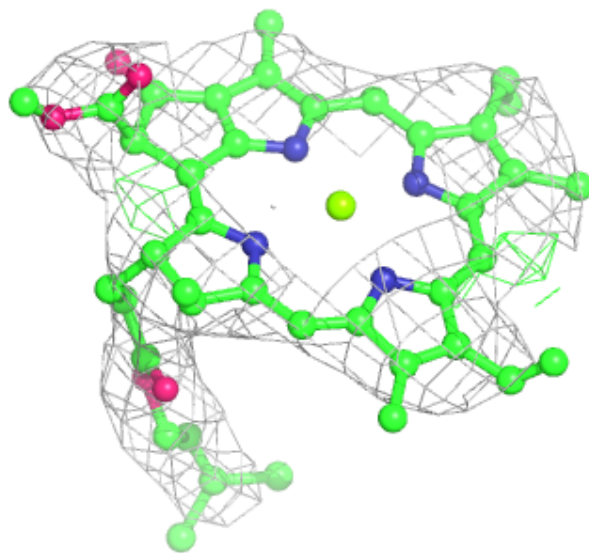
Electron density around SQD t 213:

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



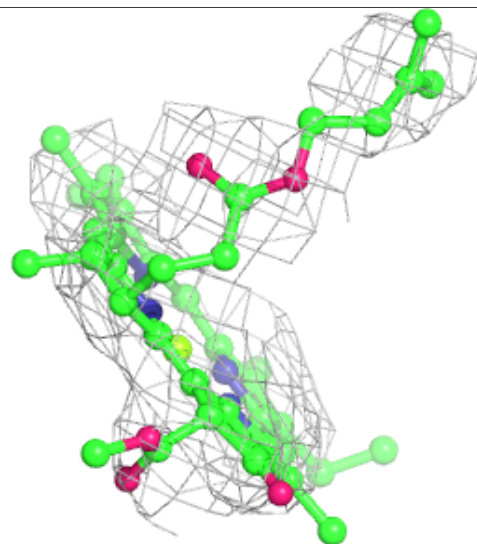
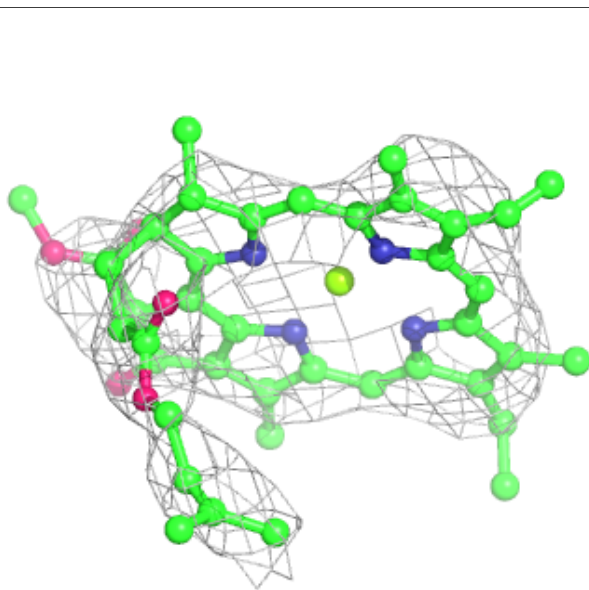
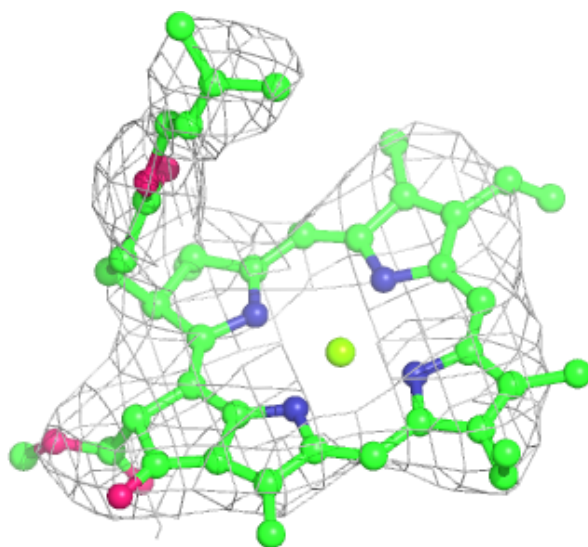
Electron density around CLA C 503:

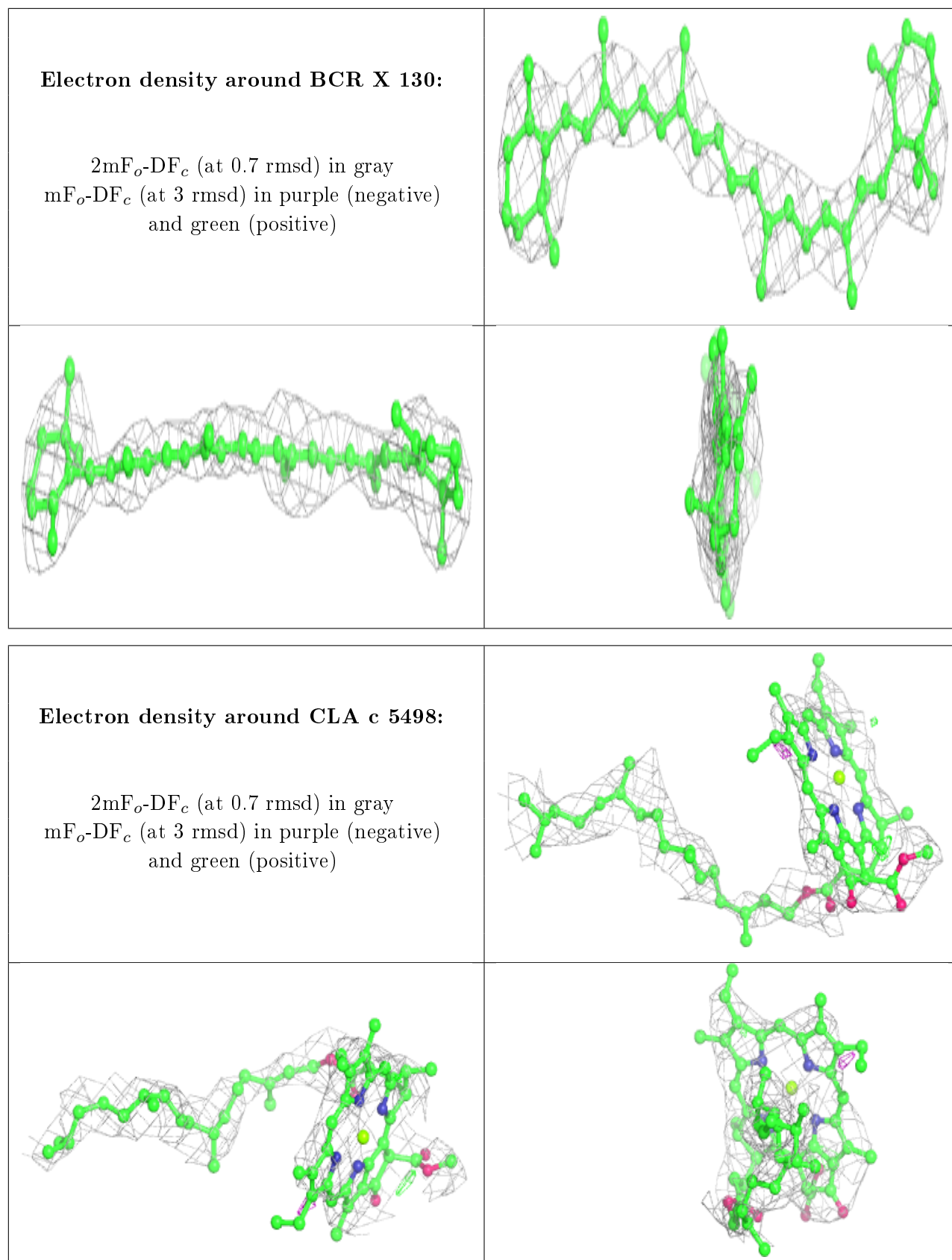
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 5503:

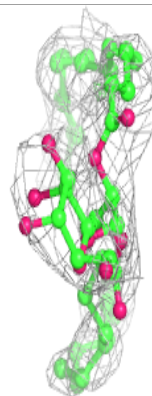
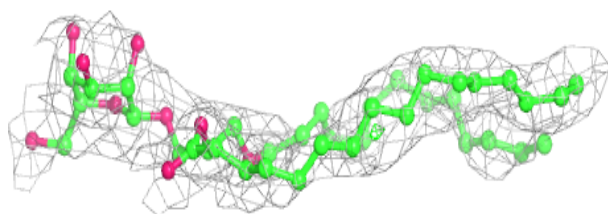
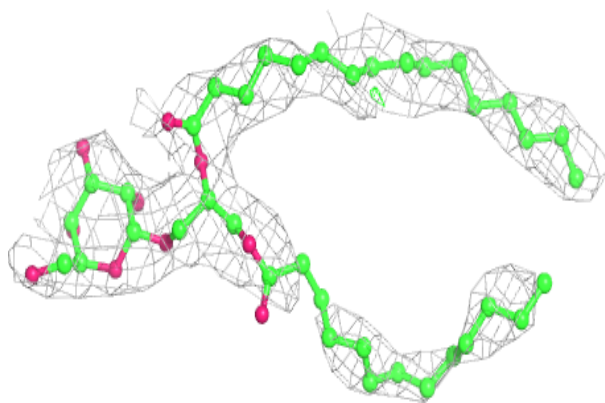
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



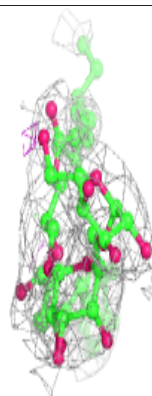
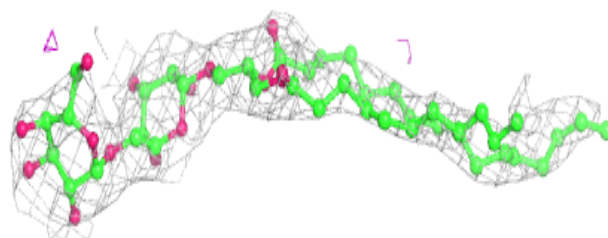
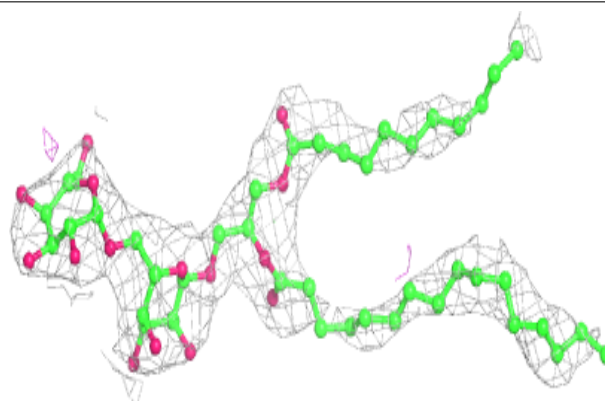


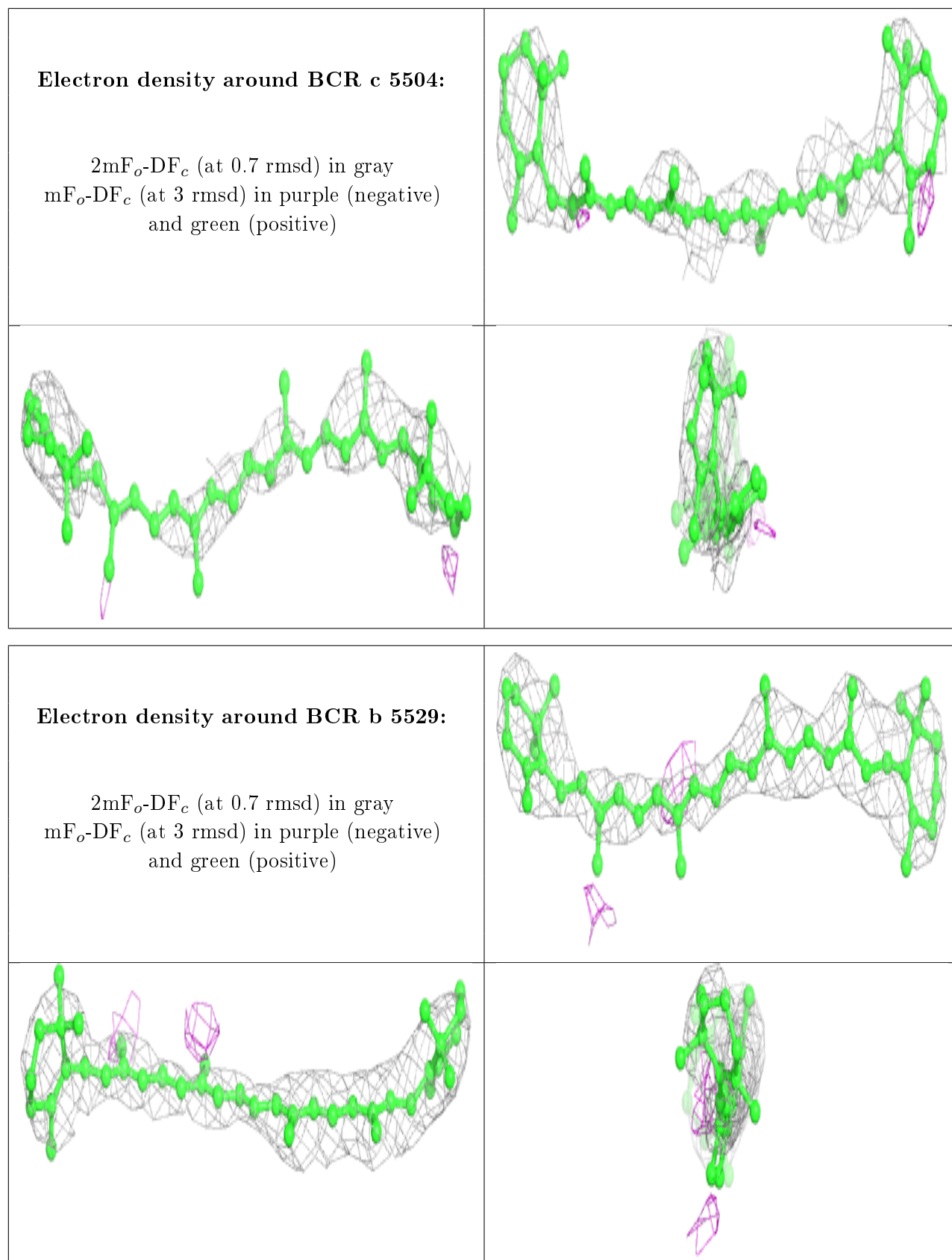
Electron density around MGE i 5201:

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

**Electron density around DGD c 5509:**

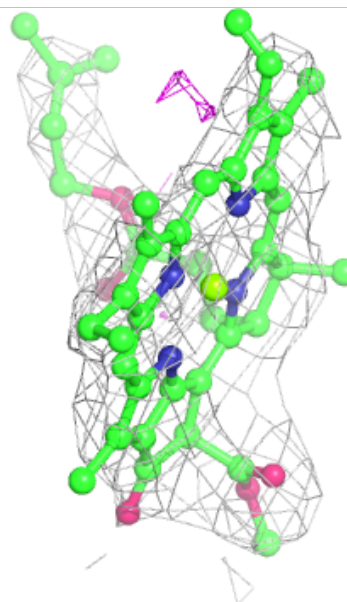
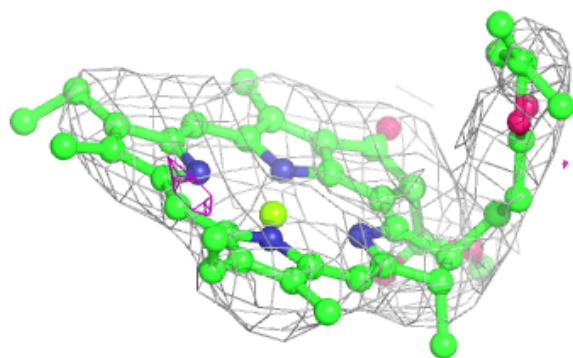
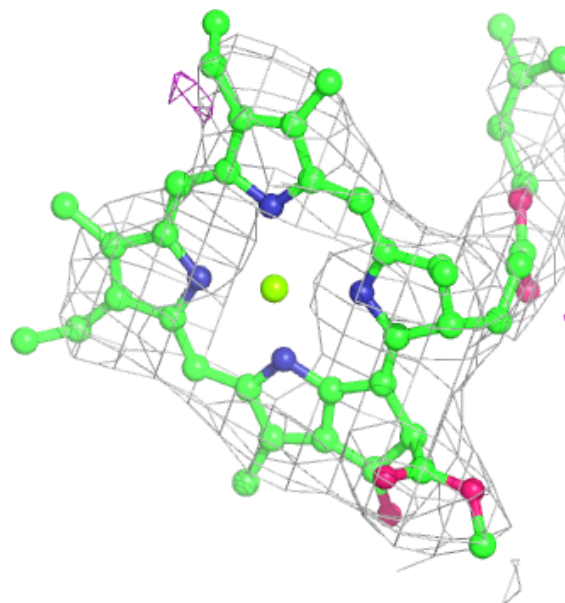
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





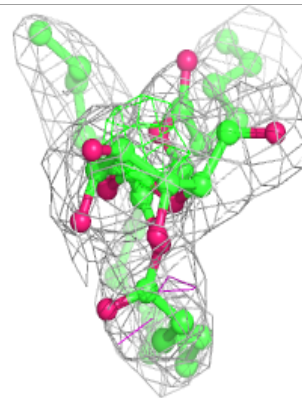
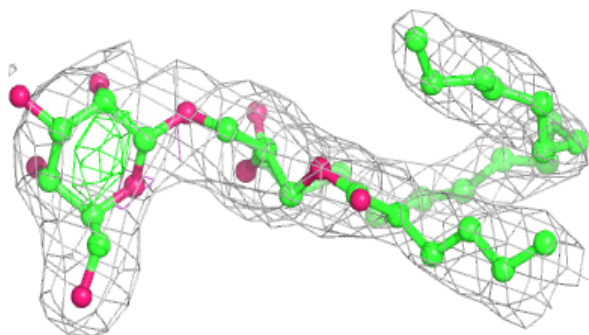
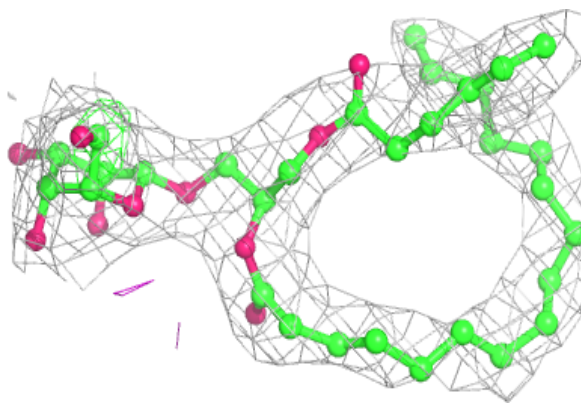
Electron density around CLA d 5355:

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

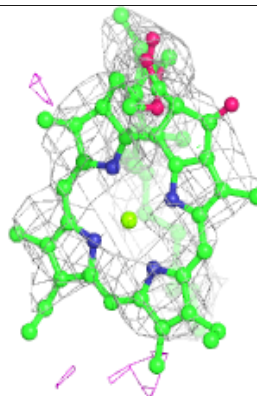
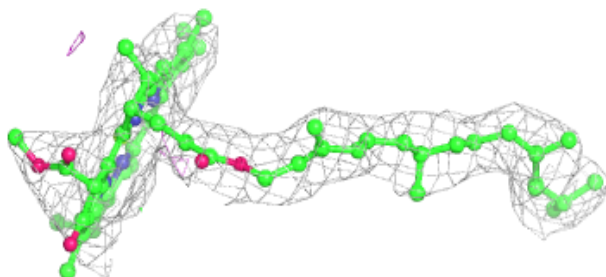
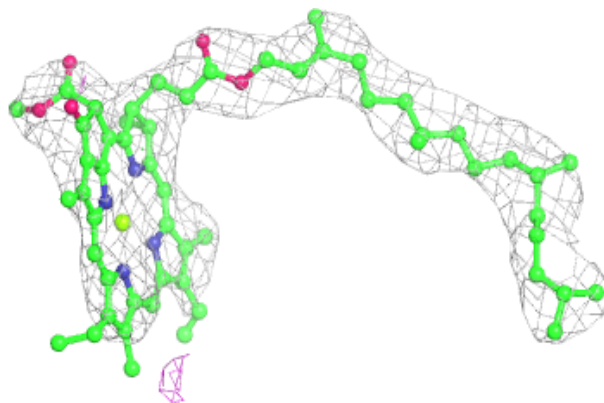


Electron density around MGE D 359:

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

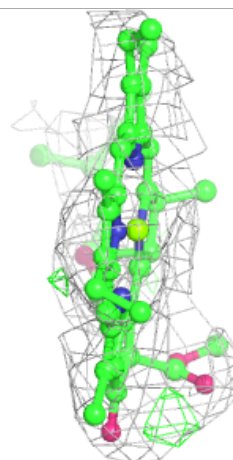
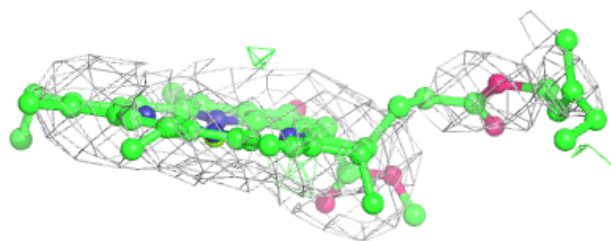
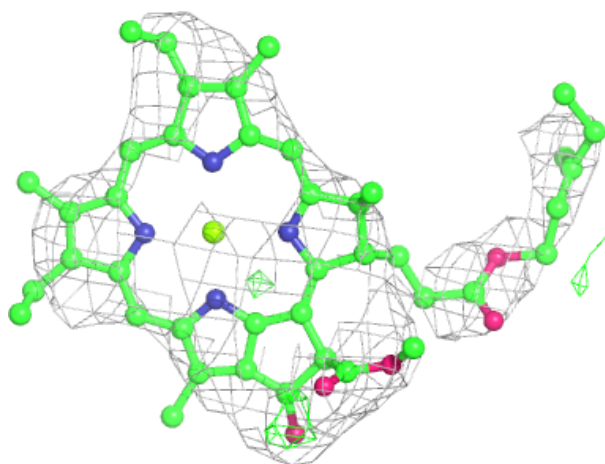
**Electron density around CLA B 519:**

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



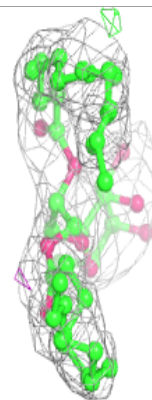
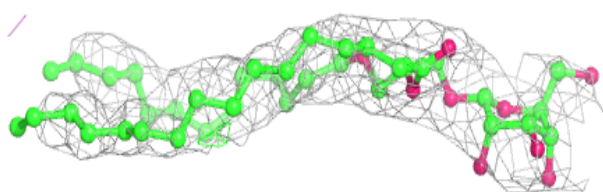
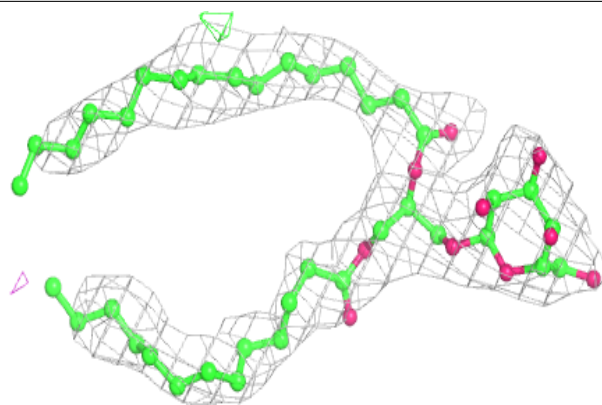
Electron density around CLA c 5502:

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

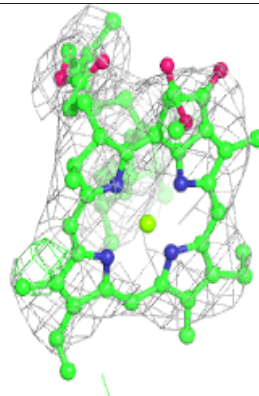
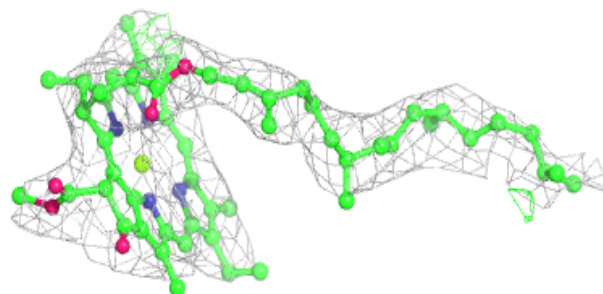
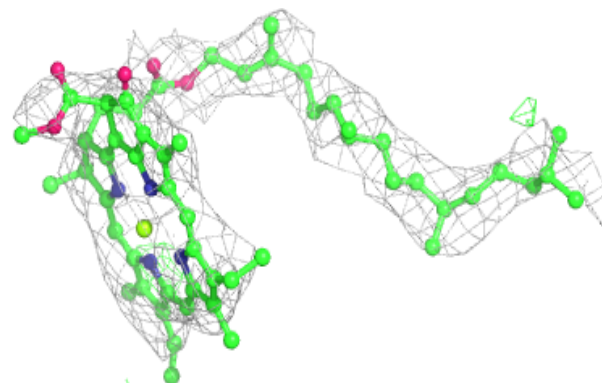


Electron density around MGE I 201:

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

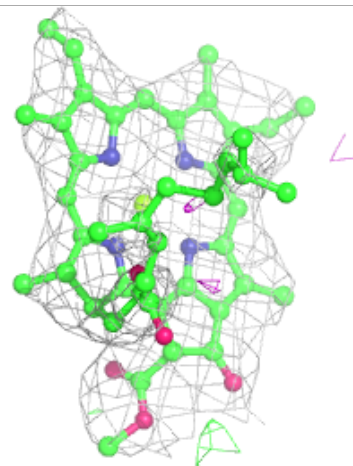
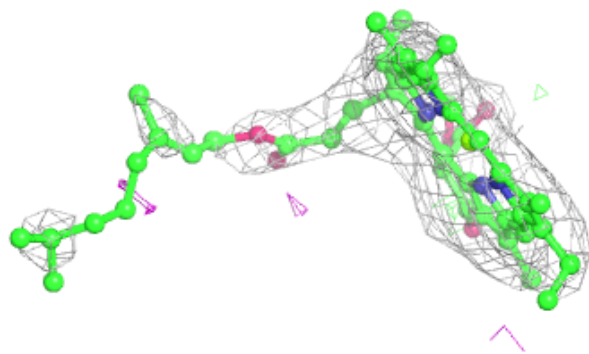
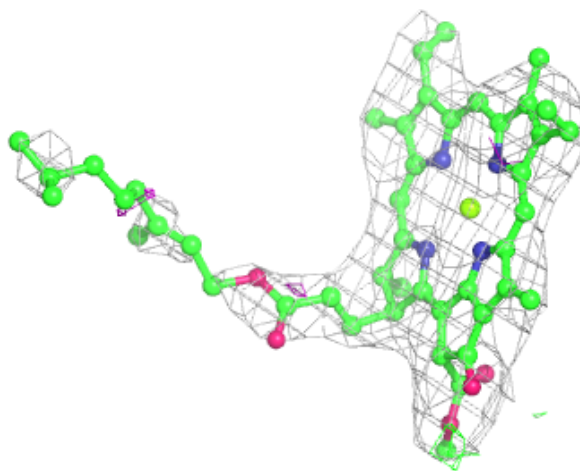
**Electron density around CLA C 498:**

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



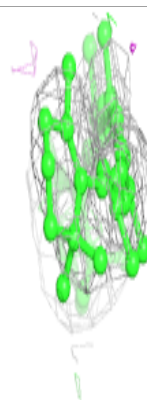
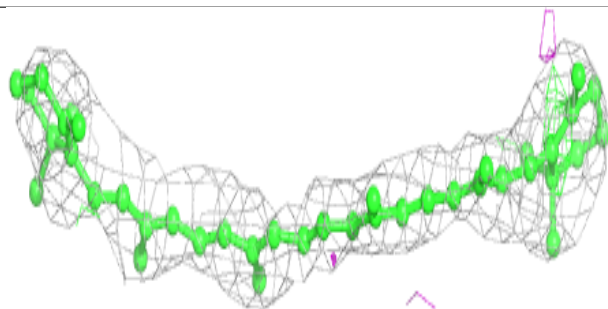
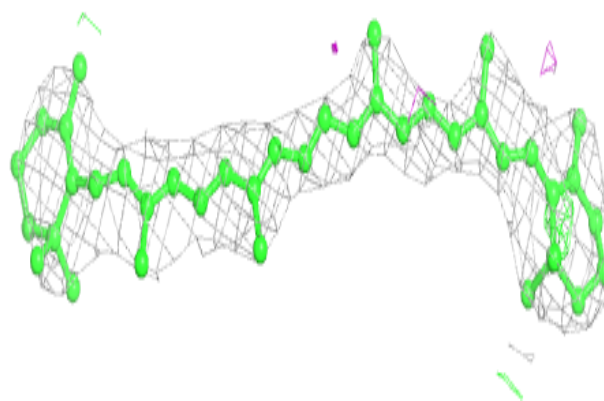
Electron density around CLA A 563:

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

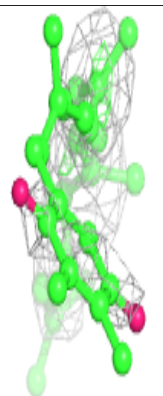
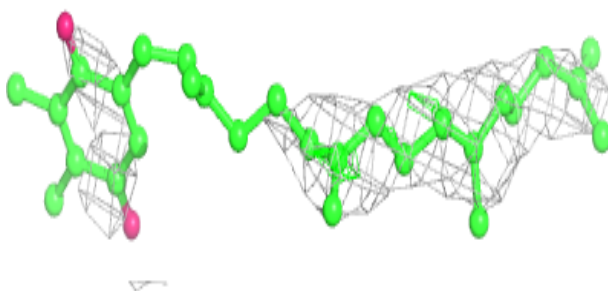
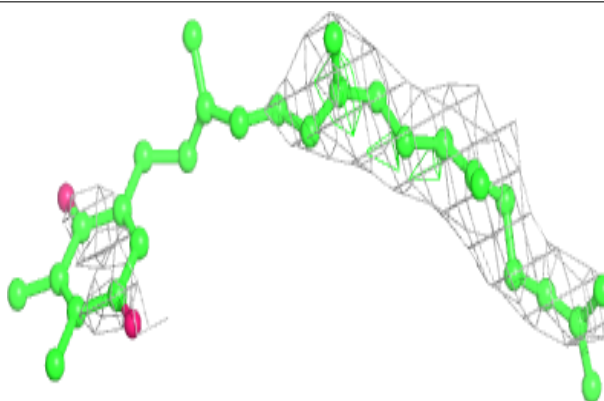


Electron density around BCR T 5104:

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

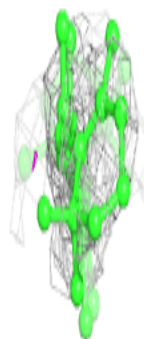
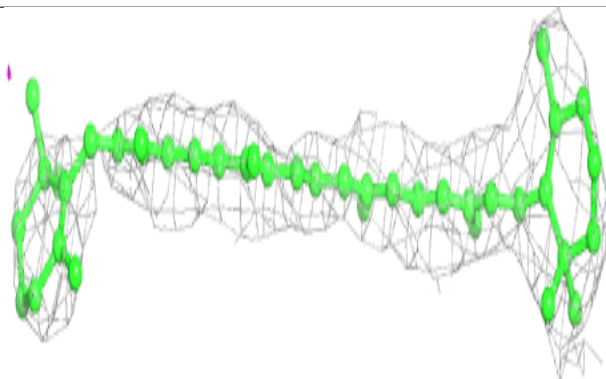
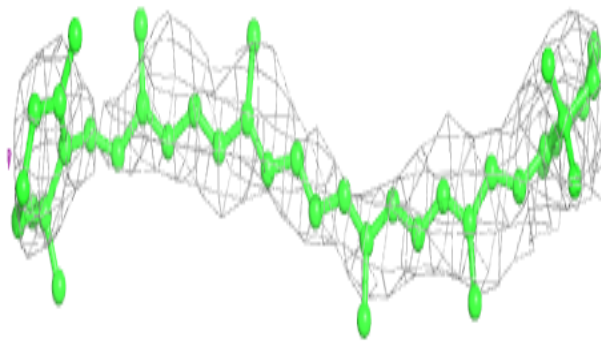
**Electron density around PQ9 a 5564:**

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

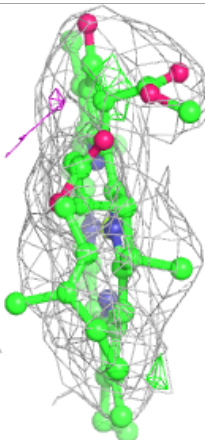
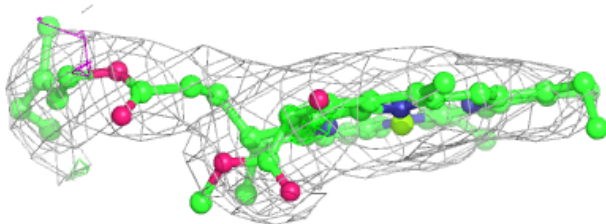
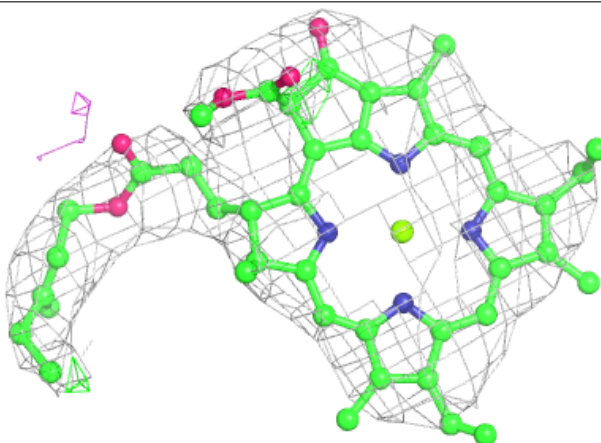


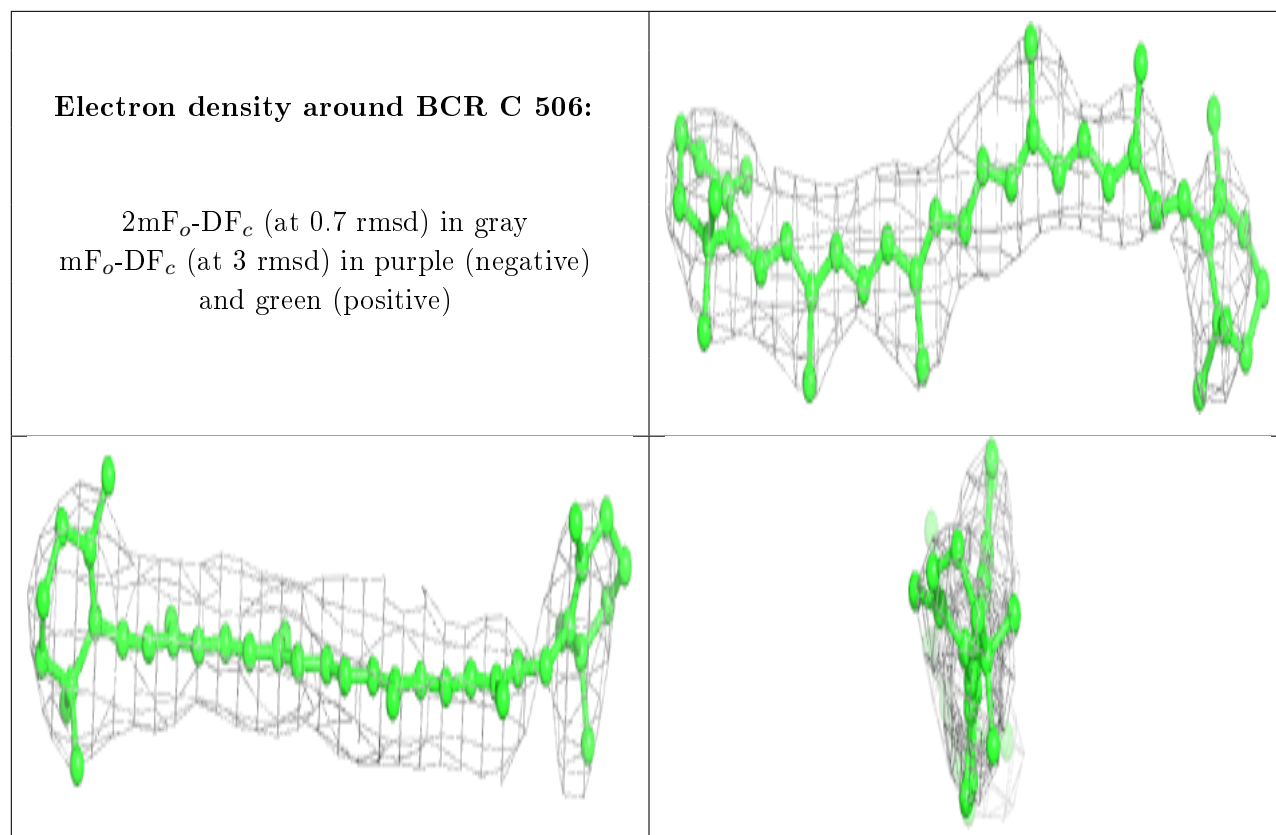
Electron density around BCR c 5505:

$2mF_o-DF_c$ (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:**

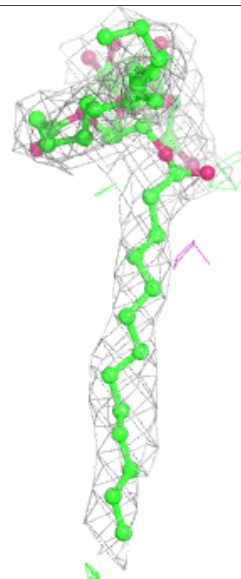
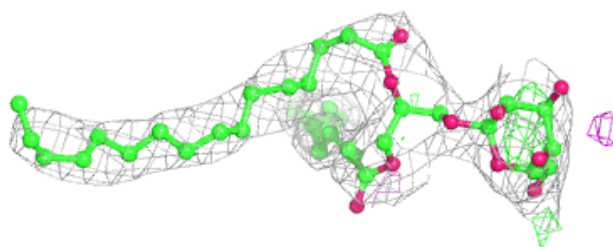
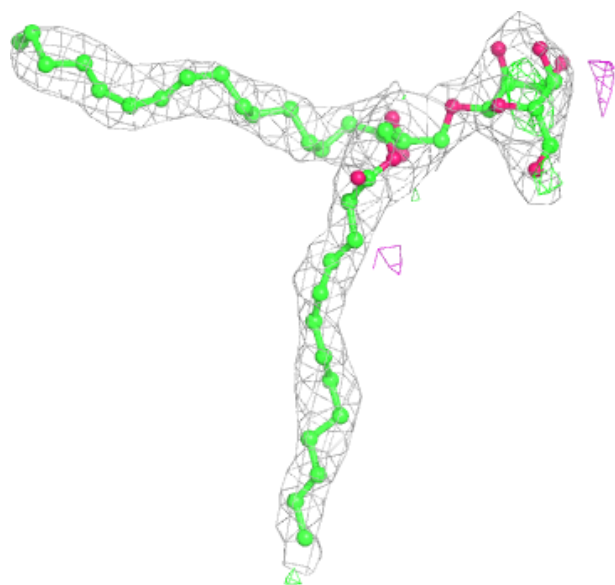
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





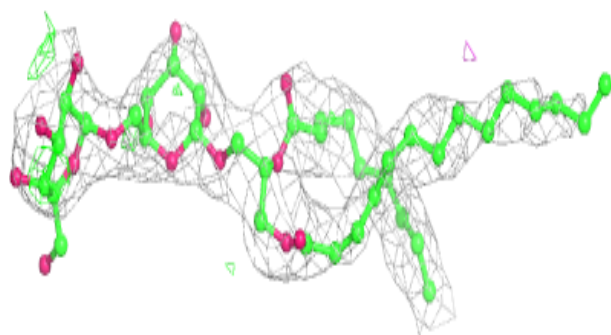
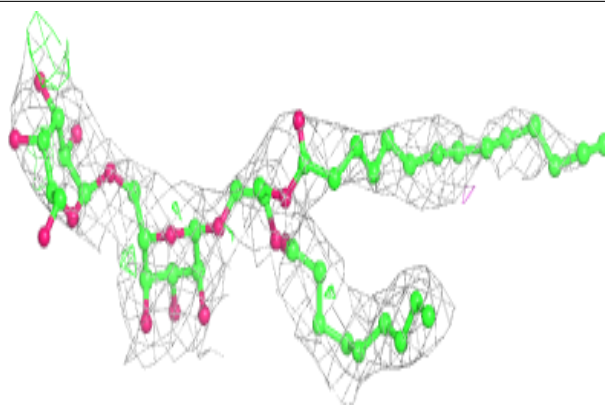
Electron density around MGE L 210:

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

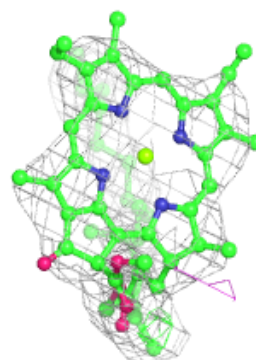
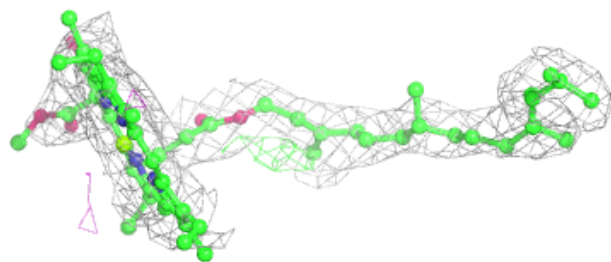
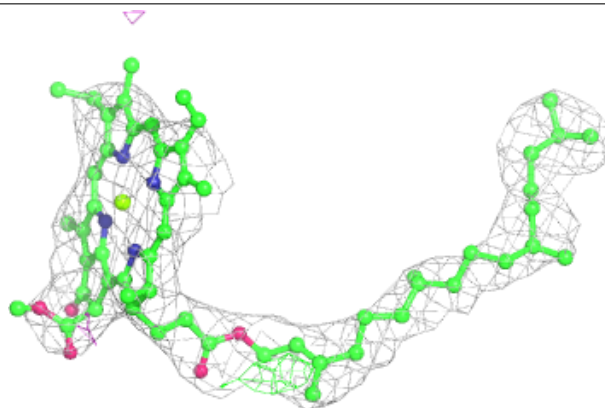


Electron density around DGD c 5507:

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

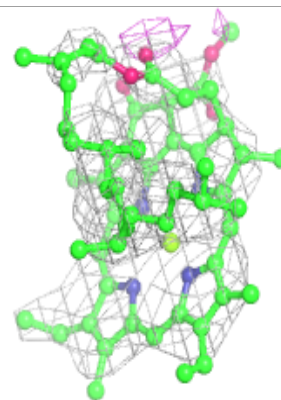
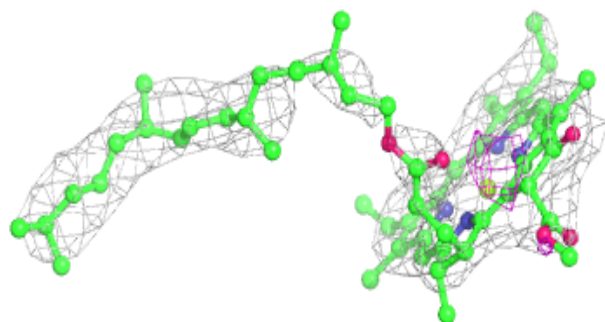
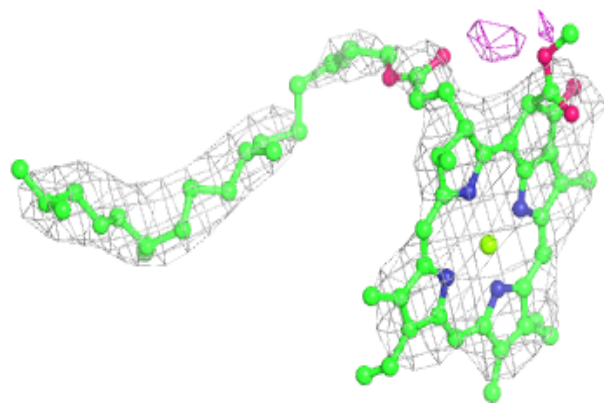
**Electron density around CLA b 5519:**

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



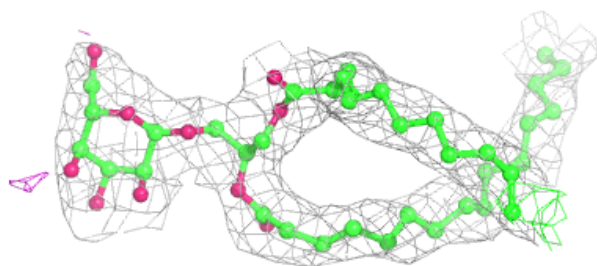
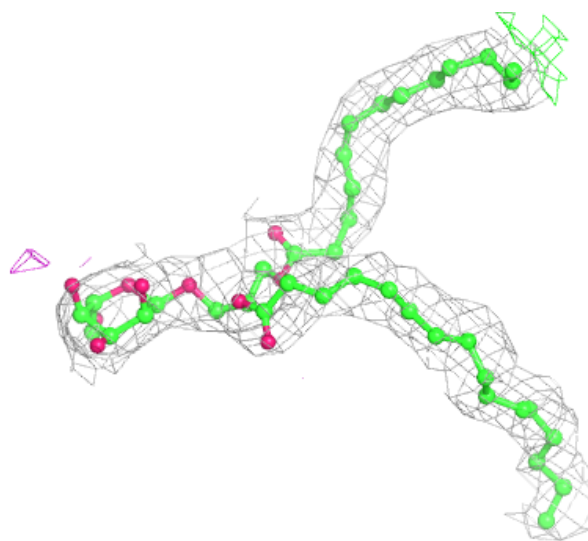
Electron density around CLA C 501:

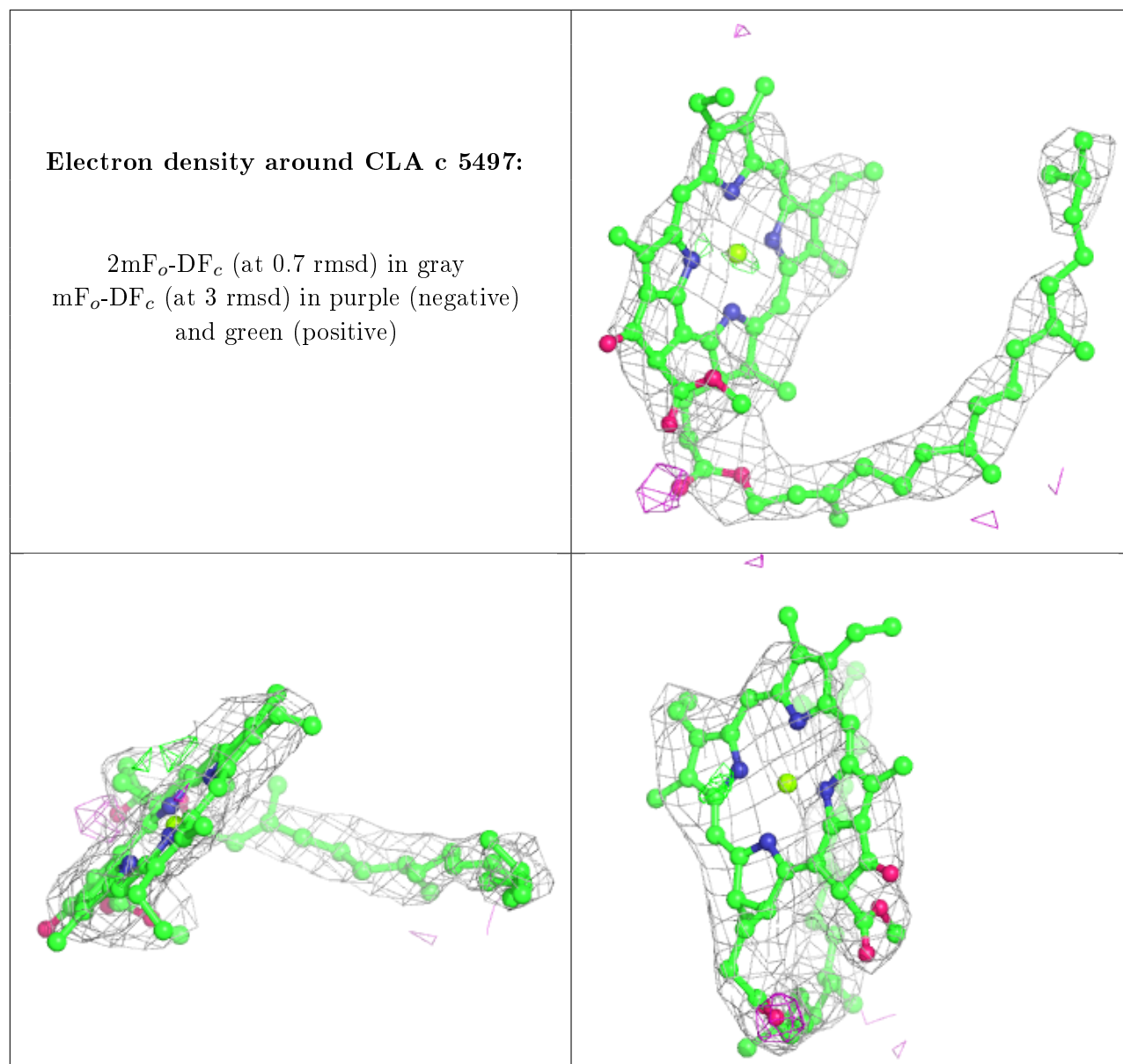
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE B 530:

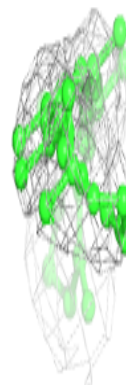
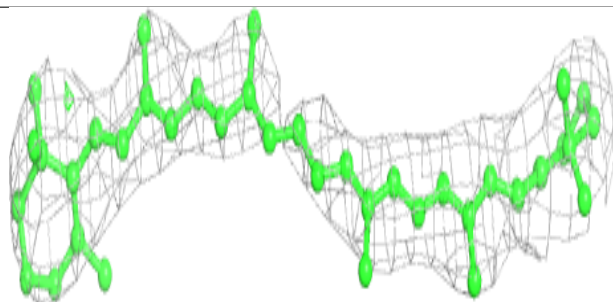
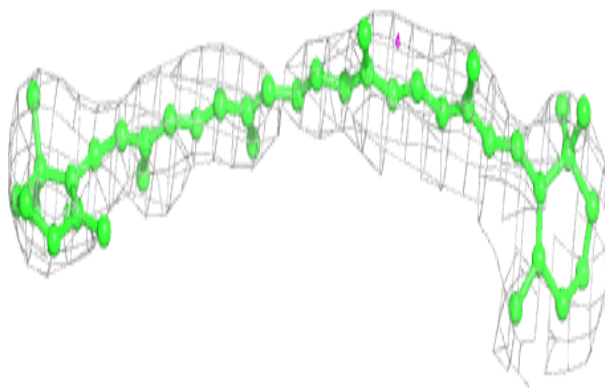
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



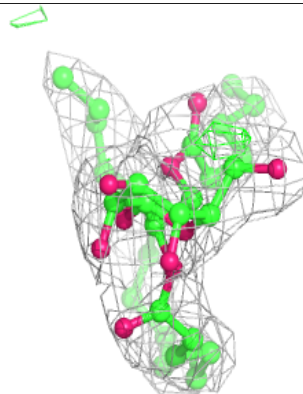
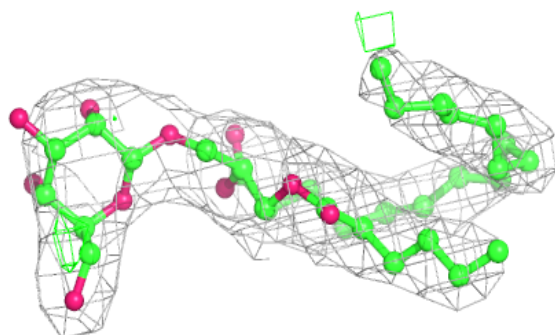
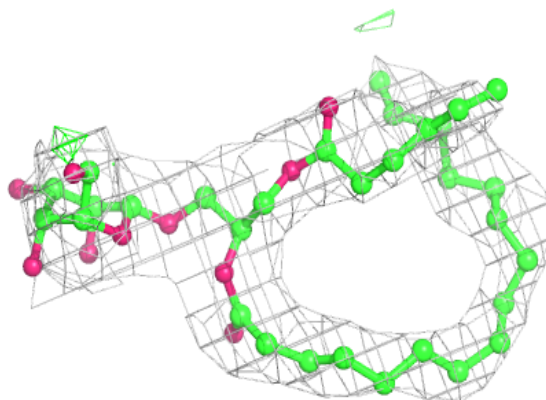


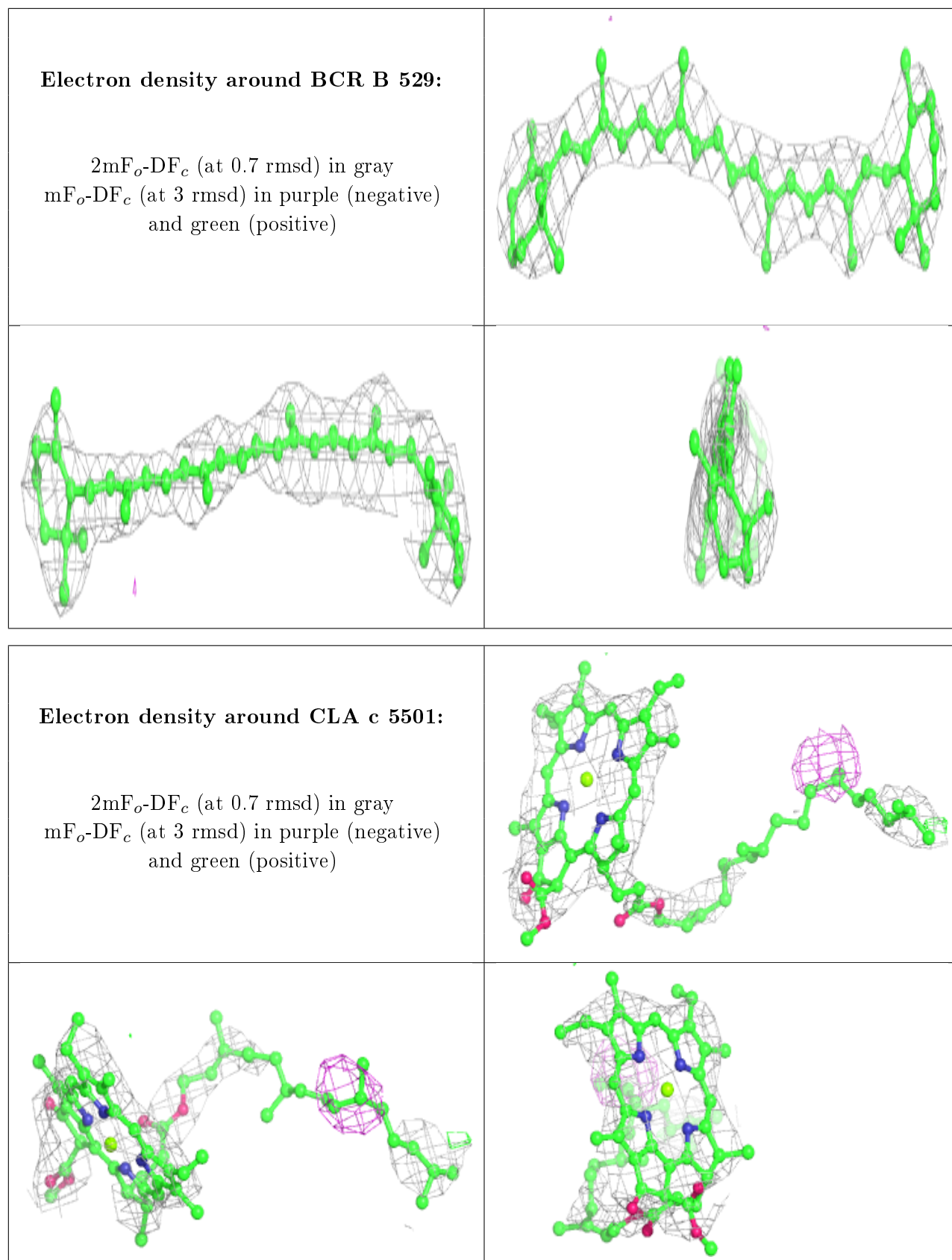
Electron density around BCR D 357:

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

**Electron density around MGE d 5360:**

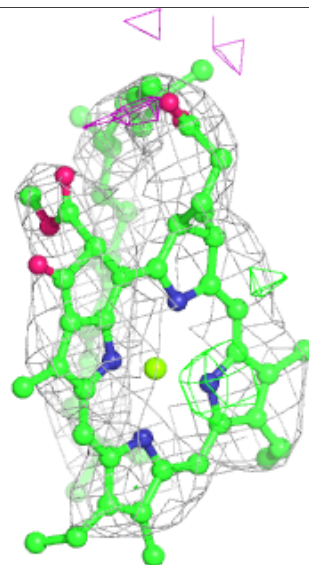
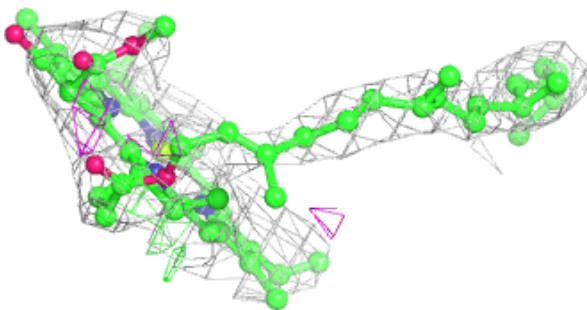
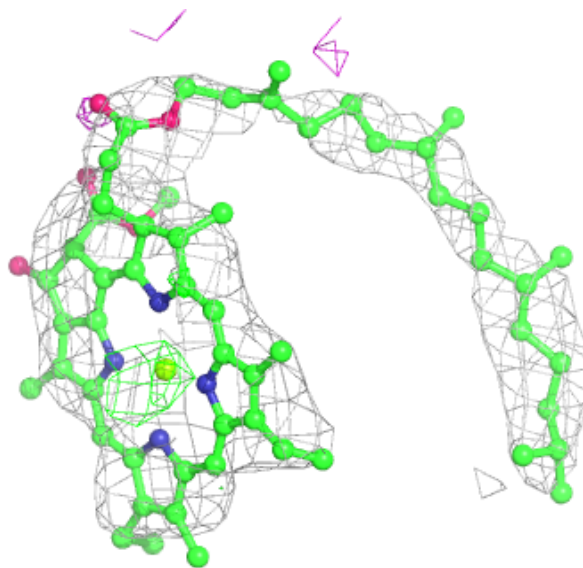
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





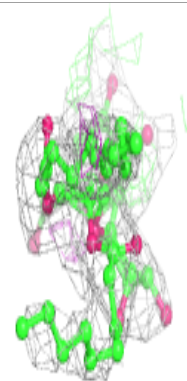
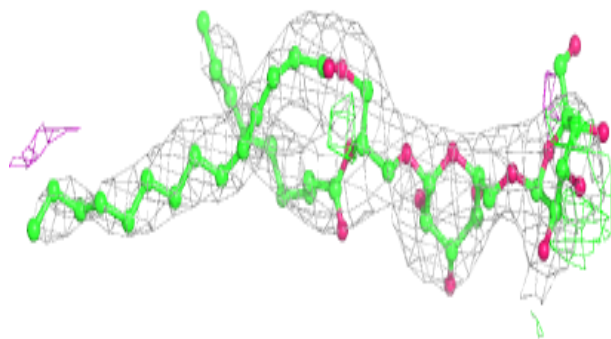
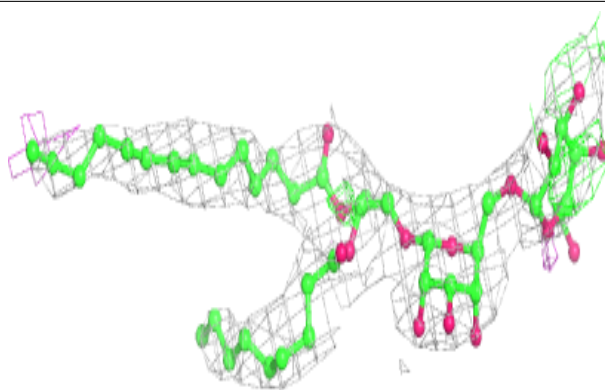
Electron density around CLA C 497:

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

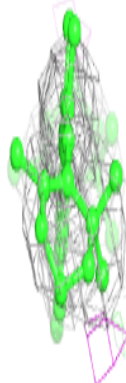
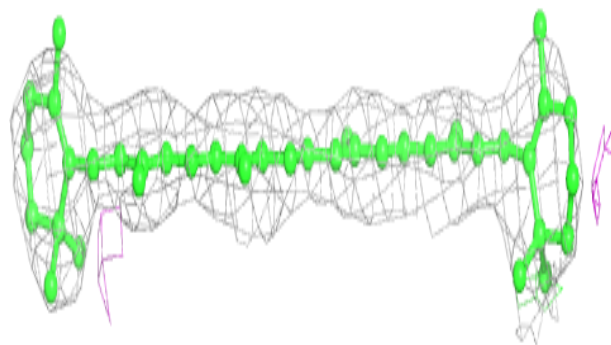
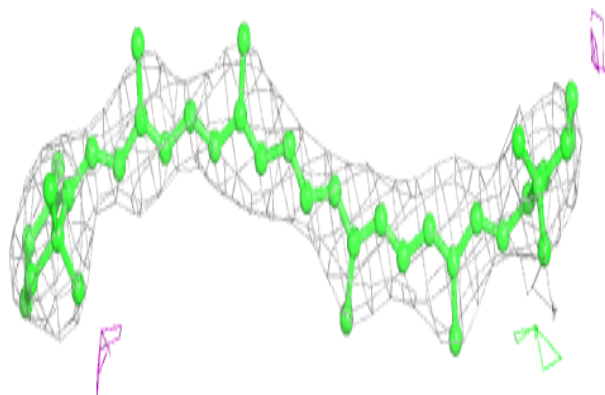


Electron density around DGD C 507:

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

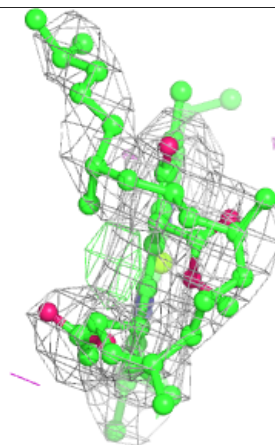
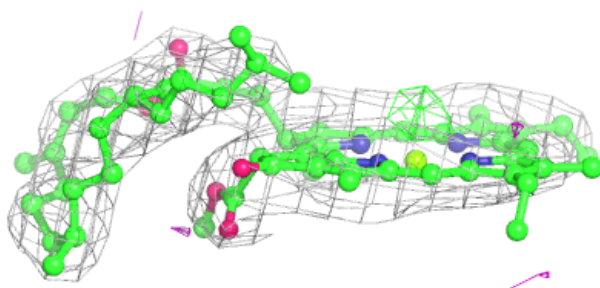
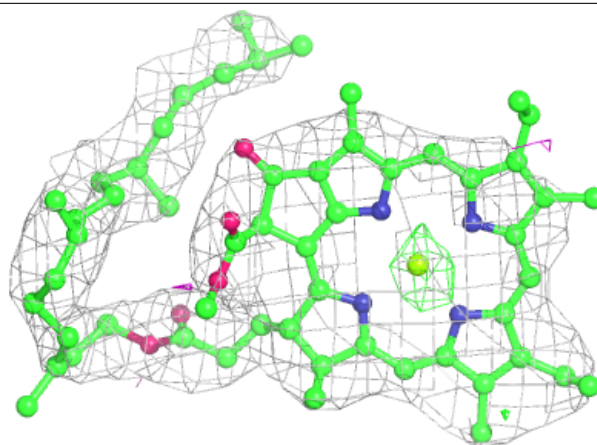
**Electron density around BCR a 5566:**

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

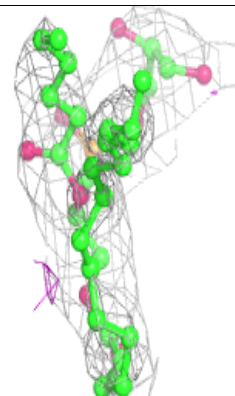
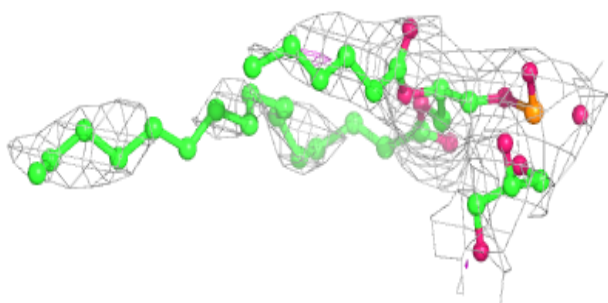
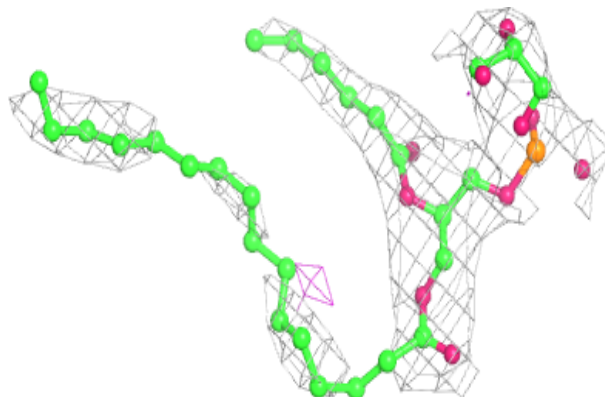


Electron density around CLA B 520:

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

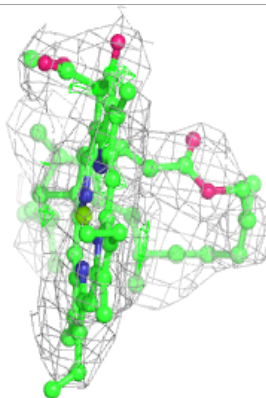
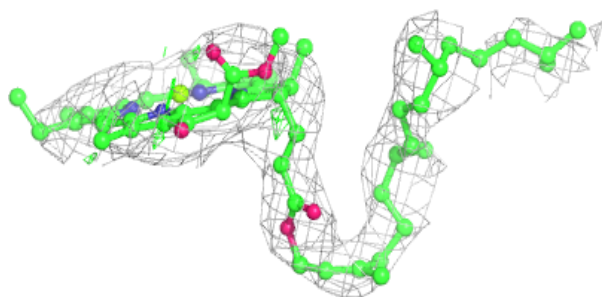
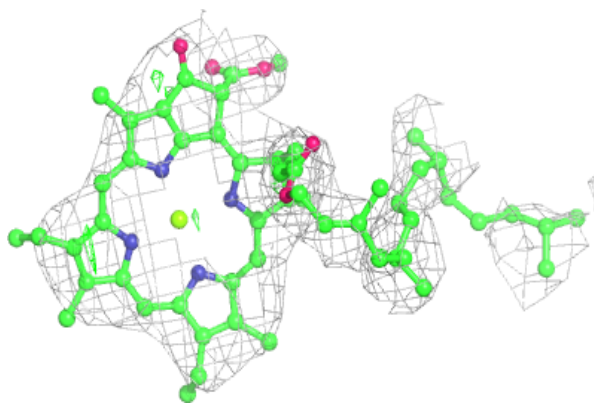
**Electron density around LHG a 5567:**

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

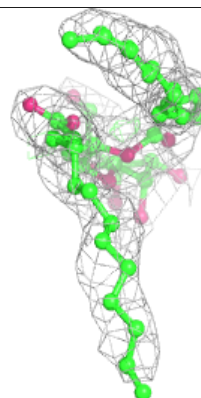
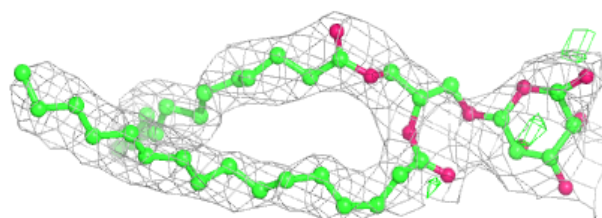
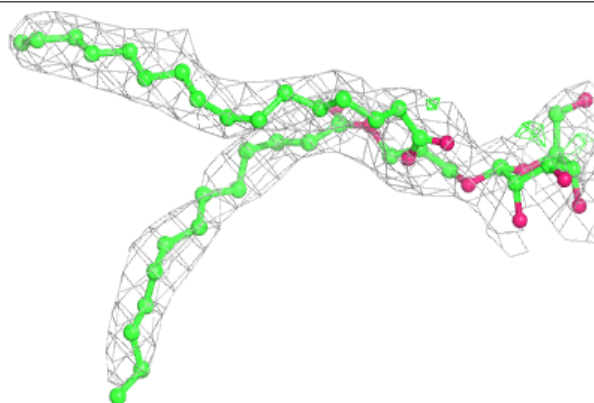


Electron density around CLA a 5560:

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

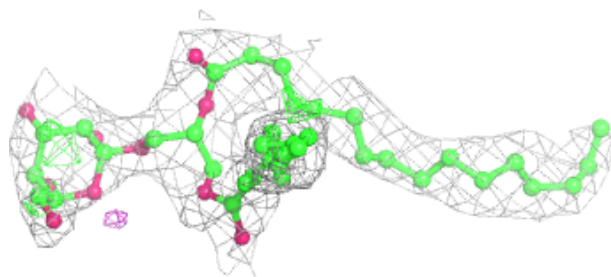
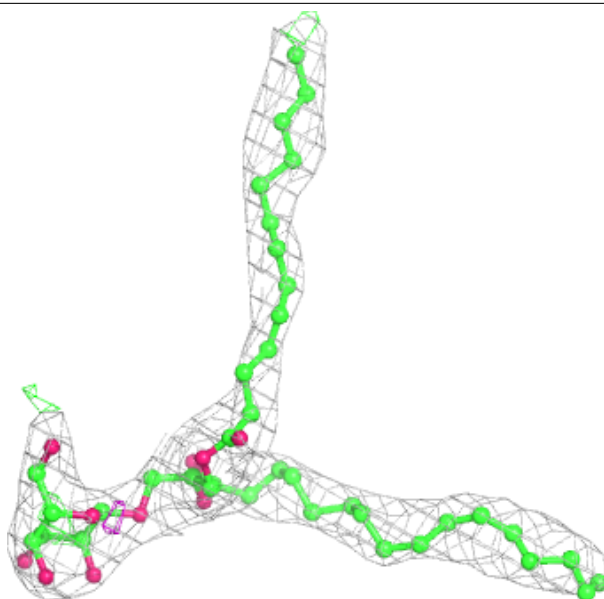
**Electron density around MGE d 5361:**

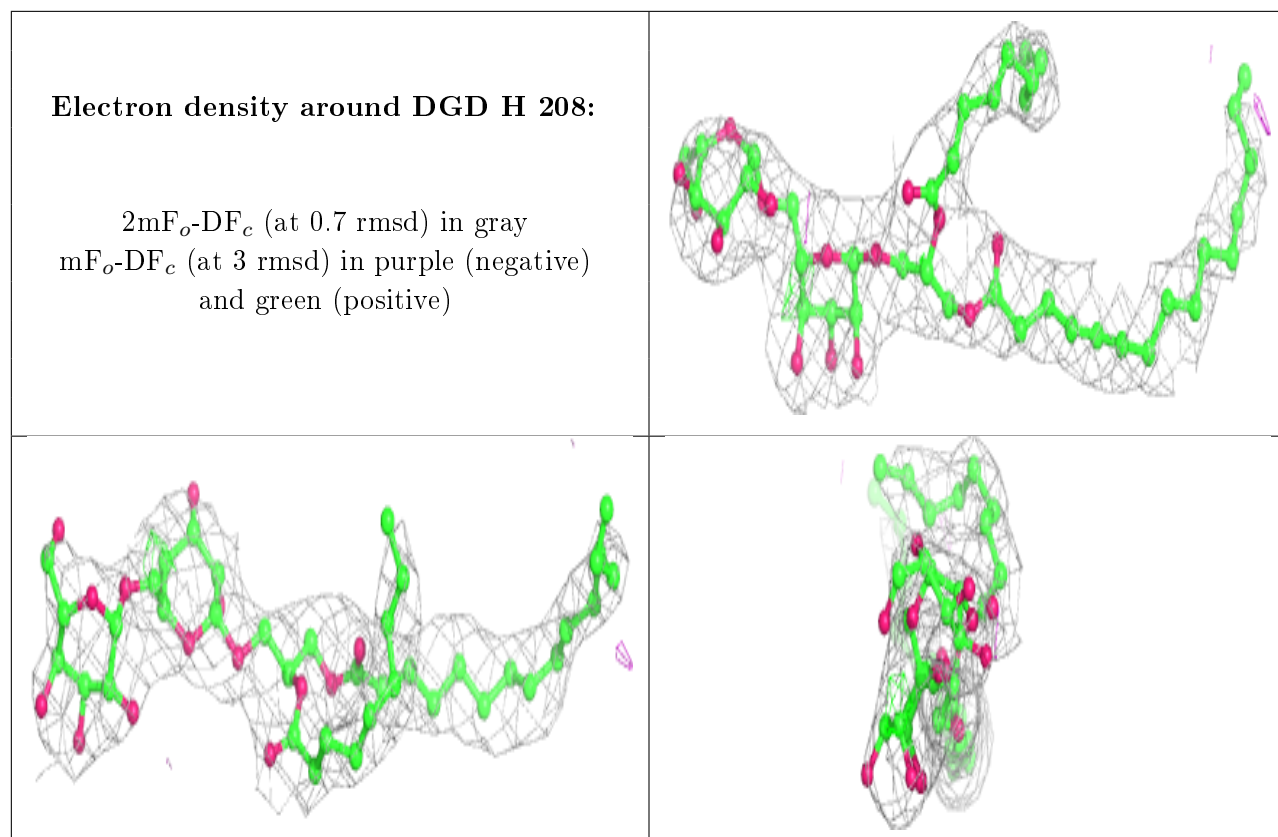
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE 1 5210:

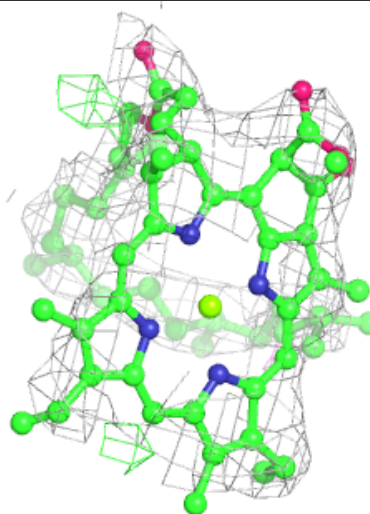
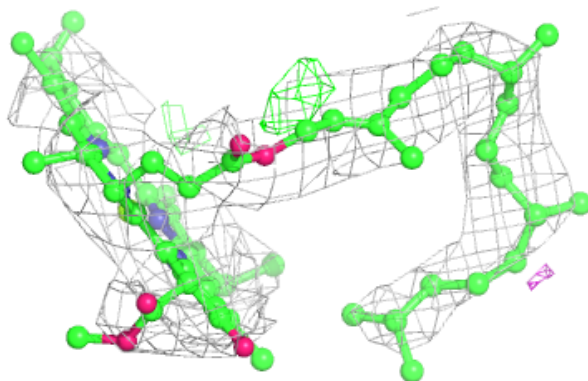
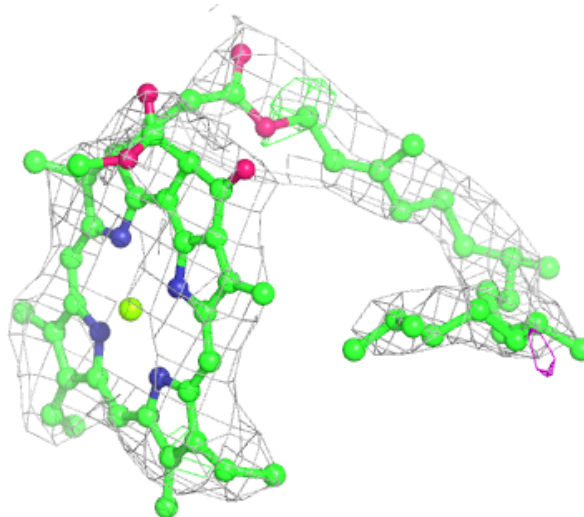
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





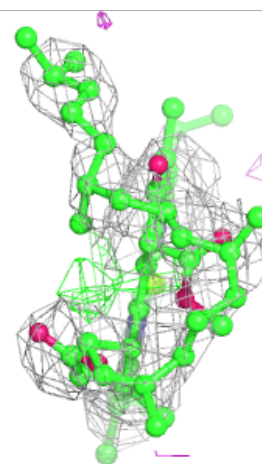
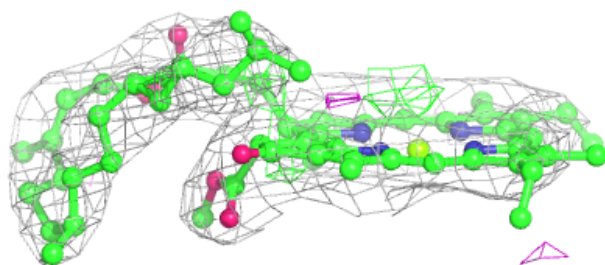
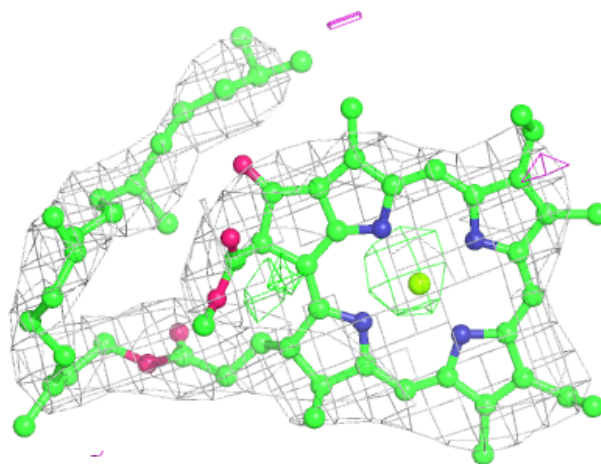
Electron density around CLA c 5493:

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



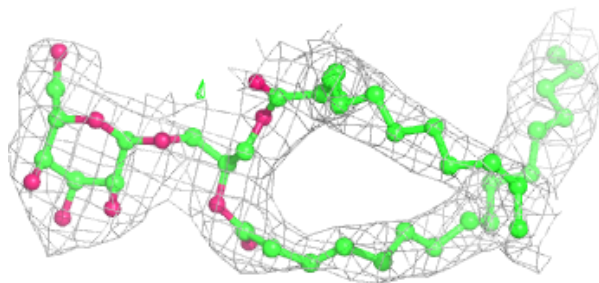
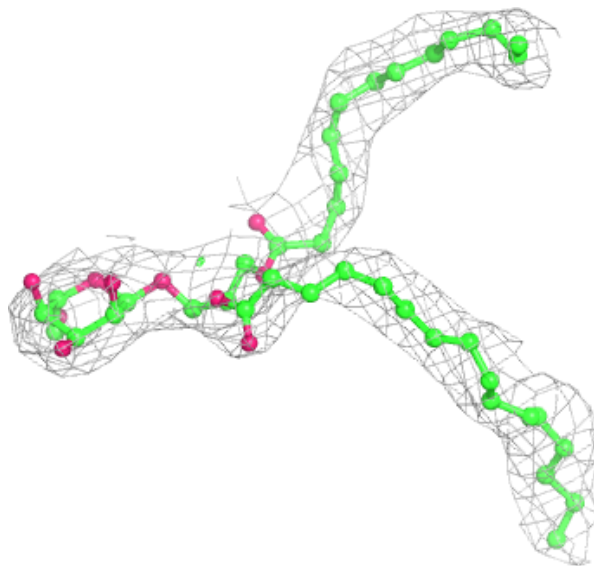
Electron density around CLA b 5520:

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



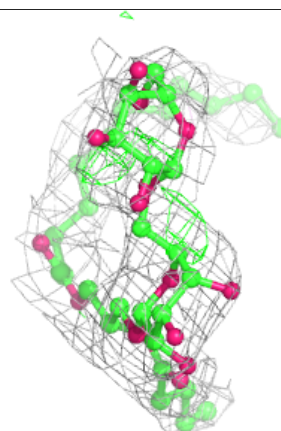
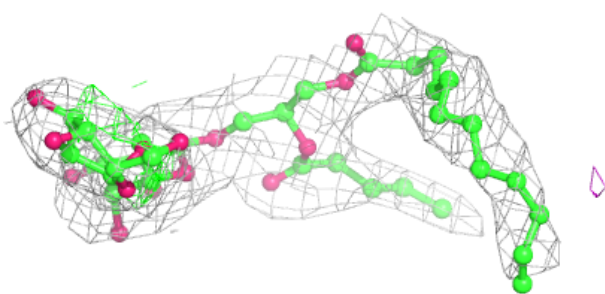
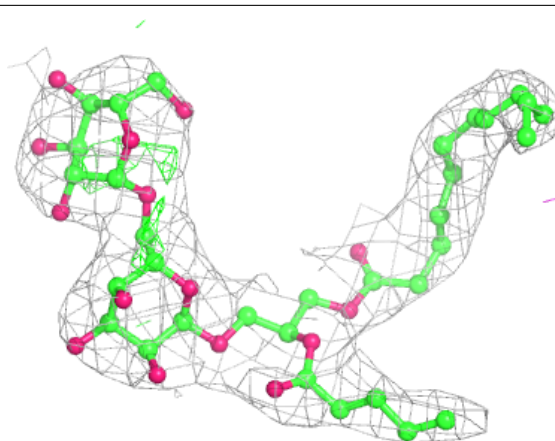
Electron density around MGE b 5530:

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

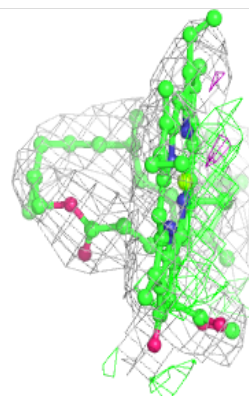
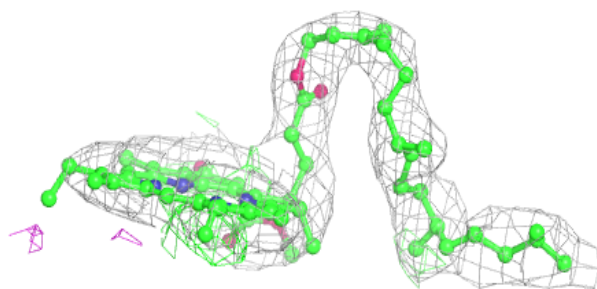
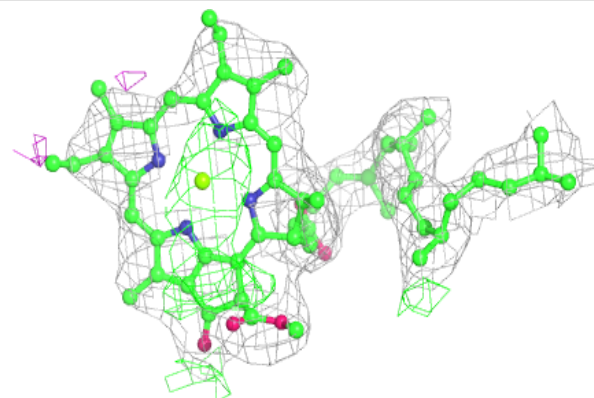


Electron density around DGD C 508:

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

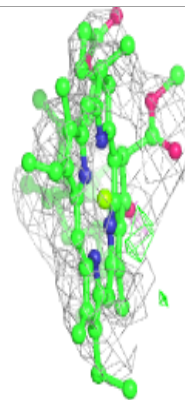
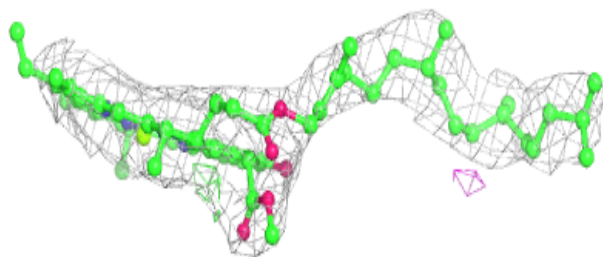
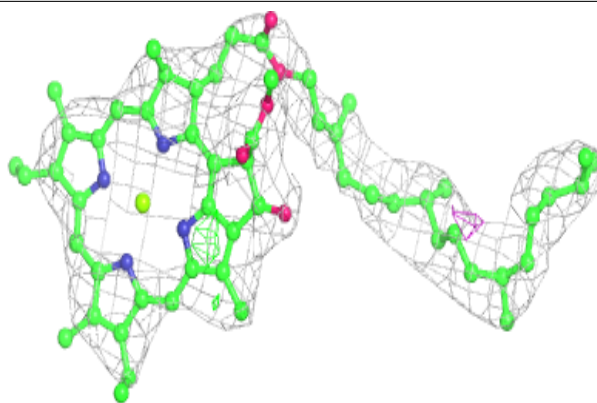
**Electron density around CLA A 560:**

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



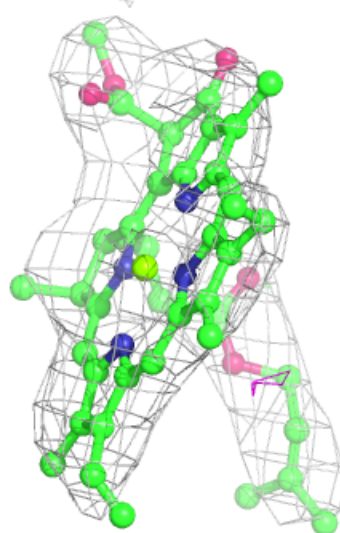
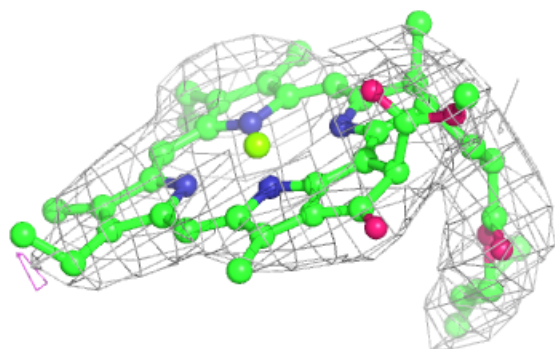
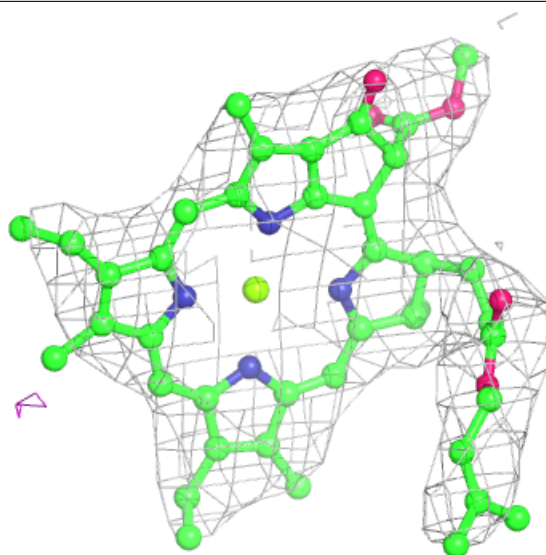
Electron density around CLA B 512:

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



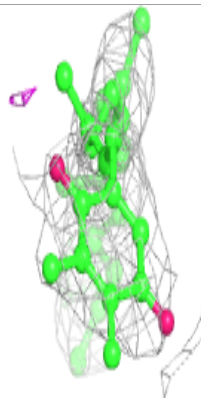
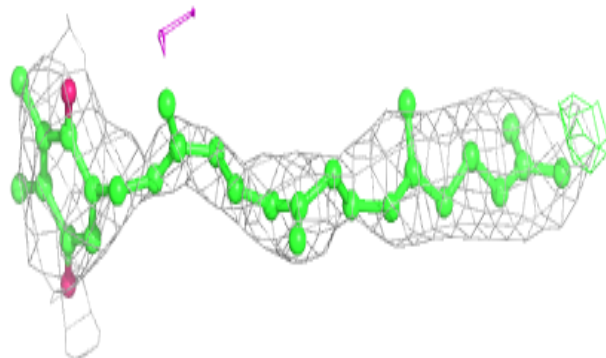
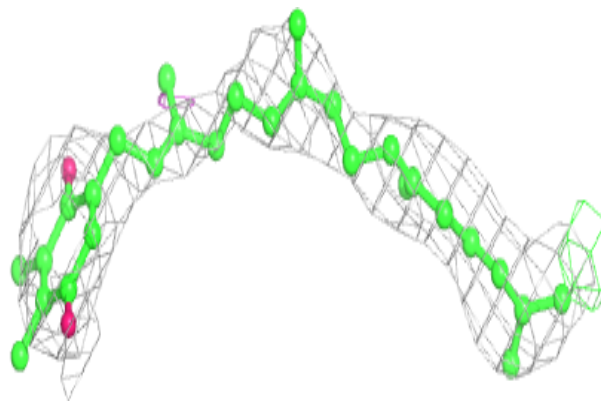
Electron density around CLA D 355:

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

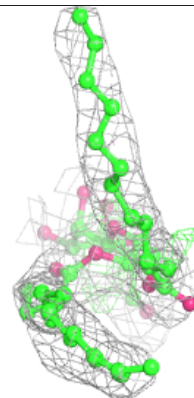
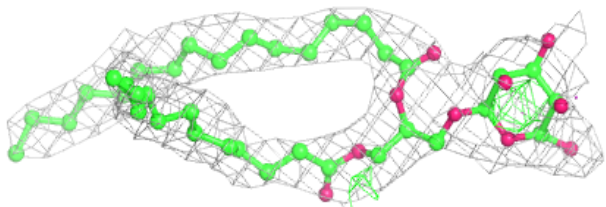
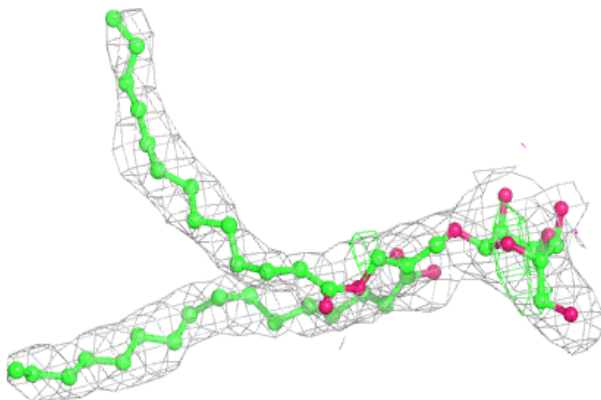


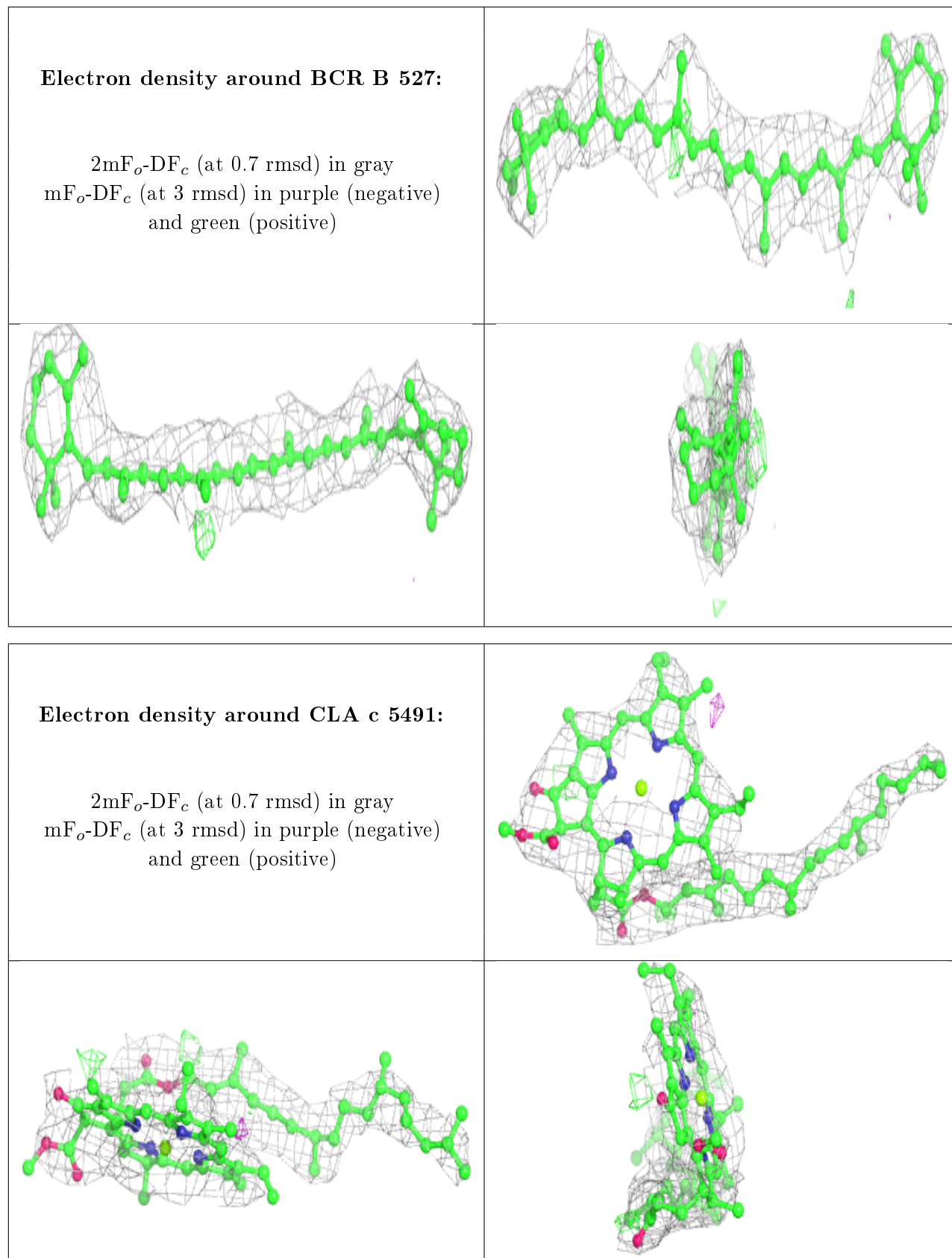
Electron density around PQ9 D 356:

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

**Electron density around MGE D 360:**

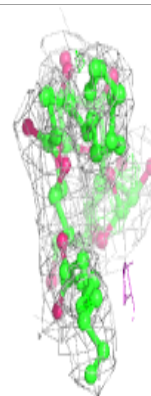
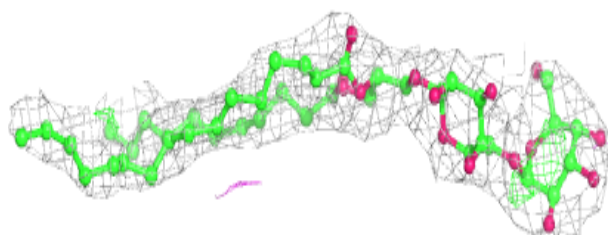
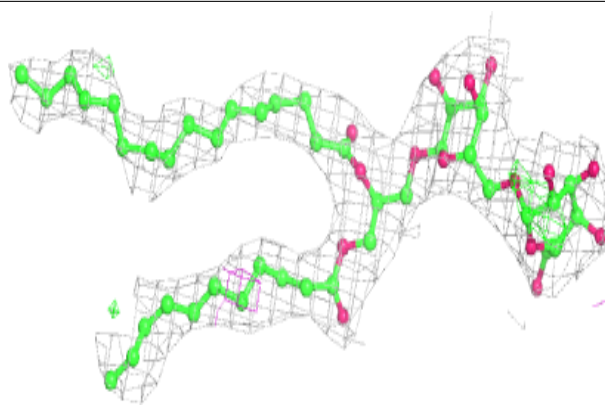
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



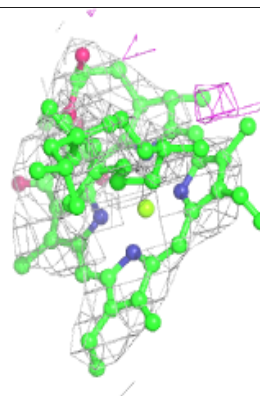
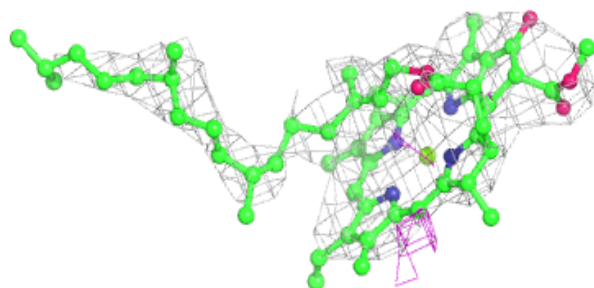
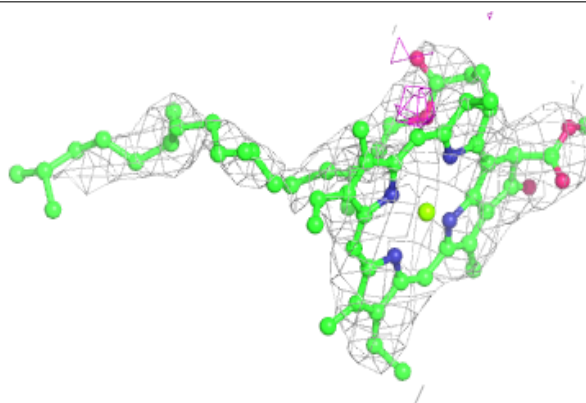


Electron density around DGD C 509:

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

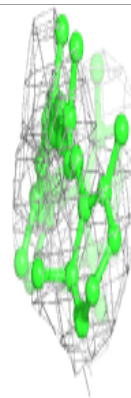
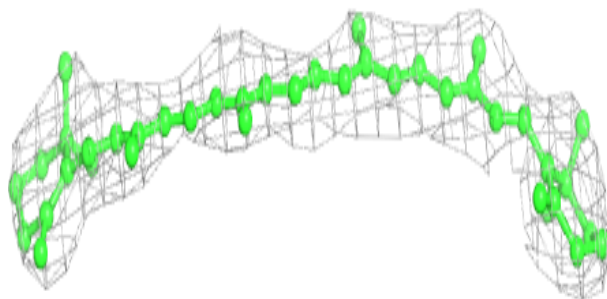
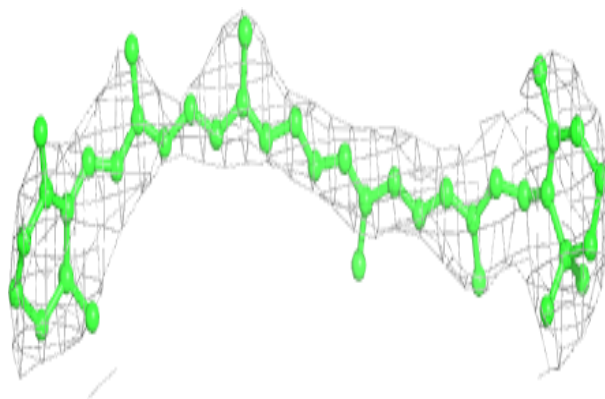
**Electron density around CLA c 5495:**

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



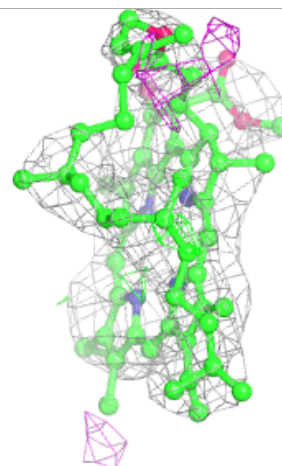
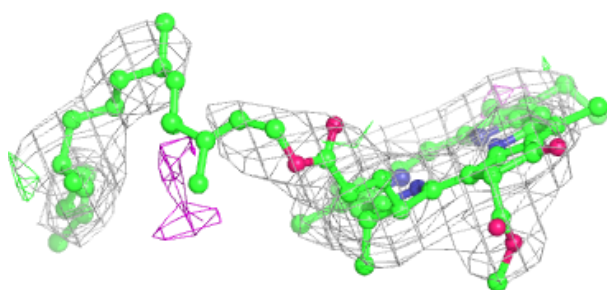
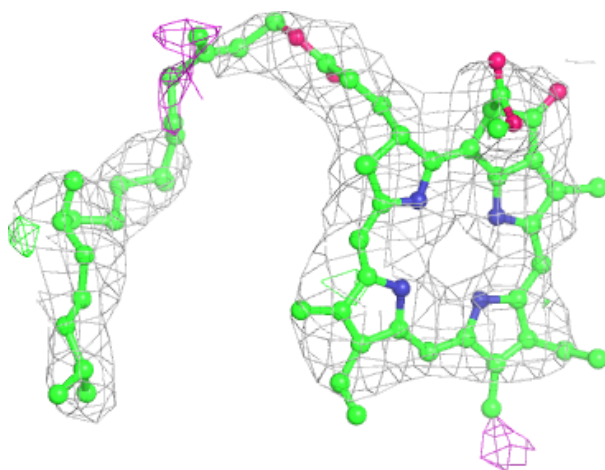
Electron density around BCR t 104:

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



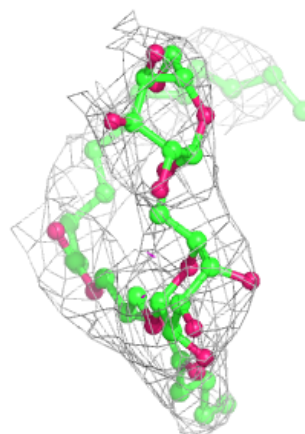
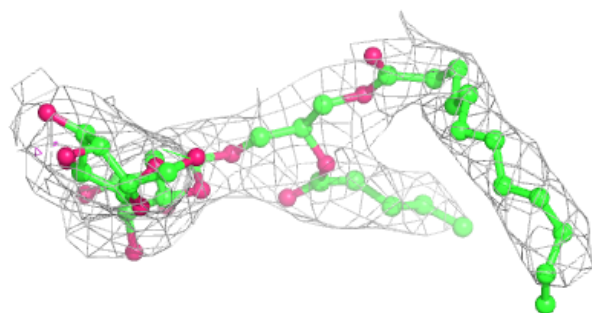
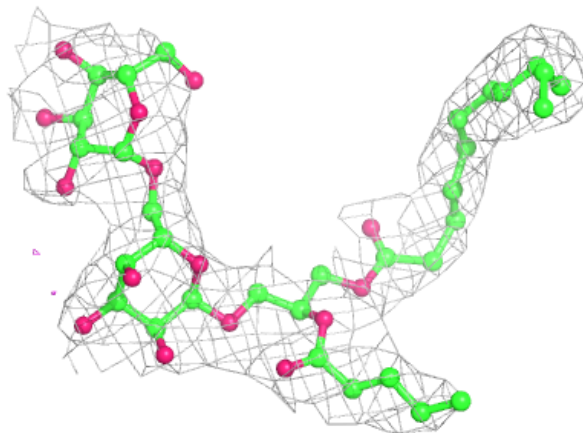
Electron density around PHO a 5562:

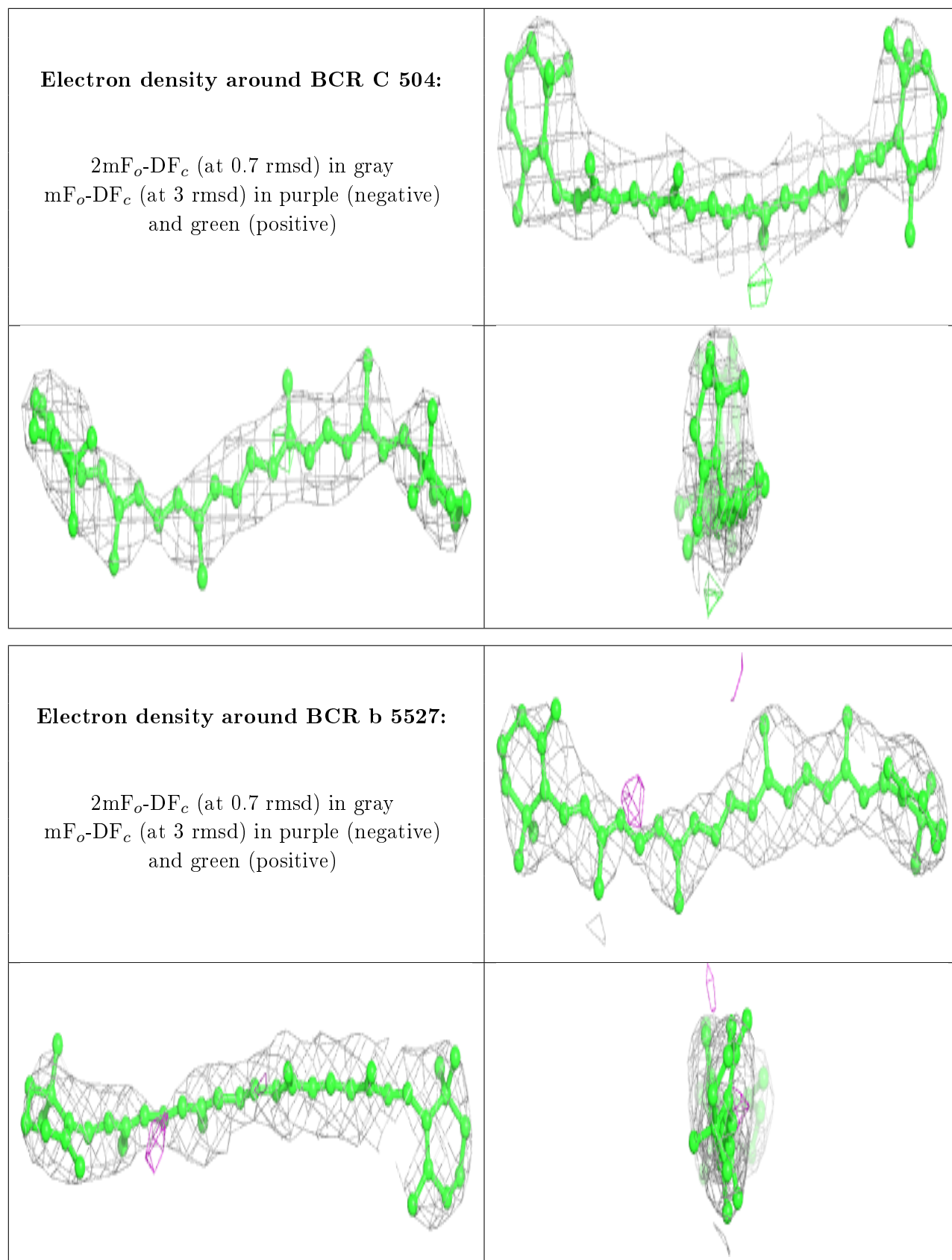
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

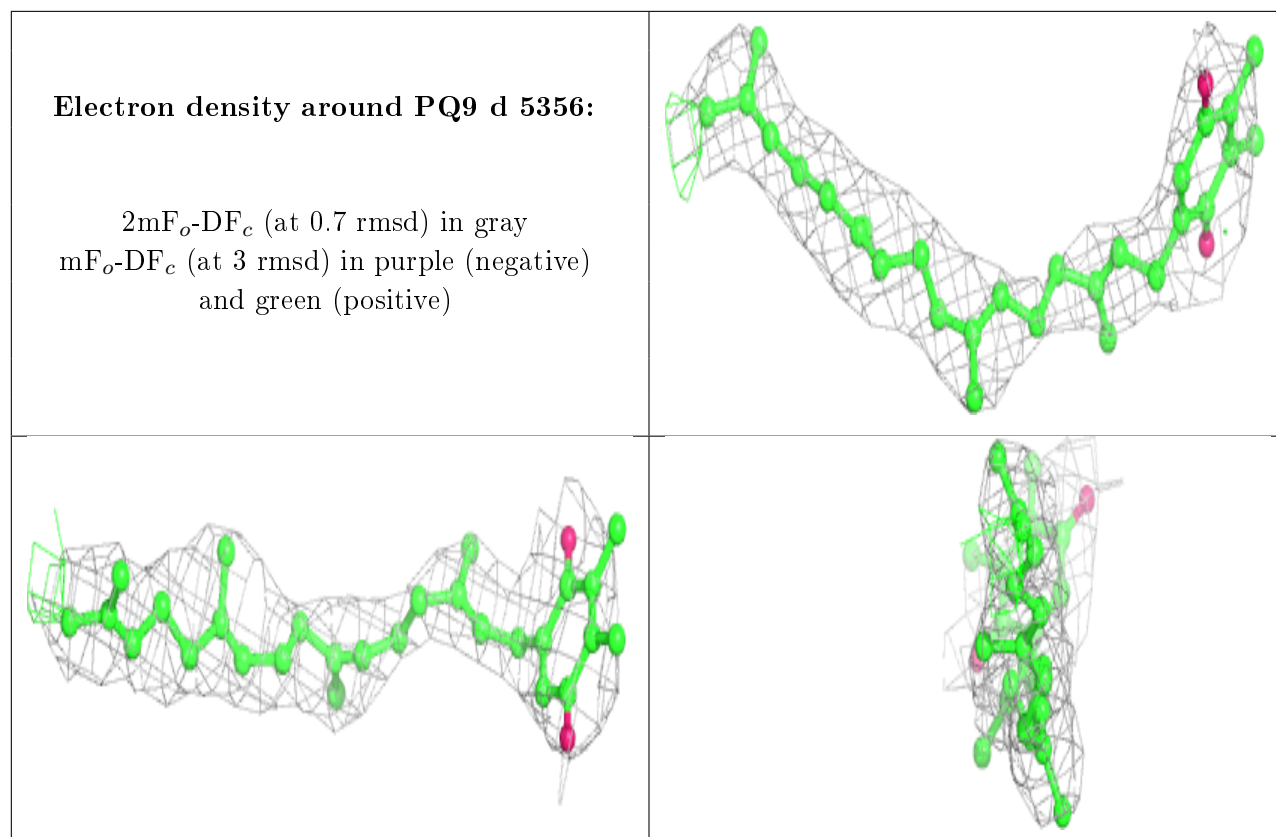


Electron density around DGD c 5508:

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

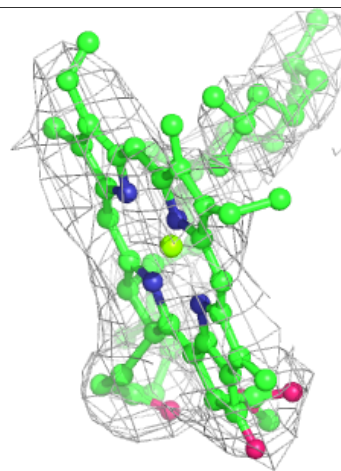
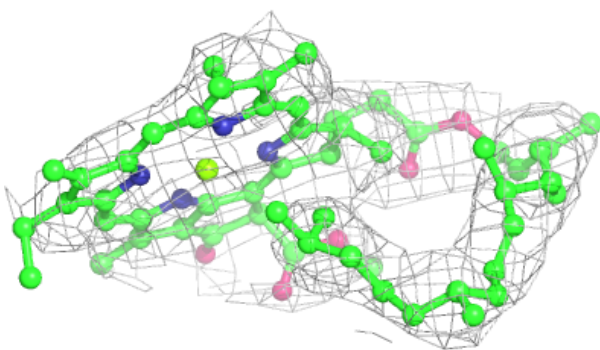
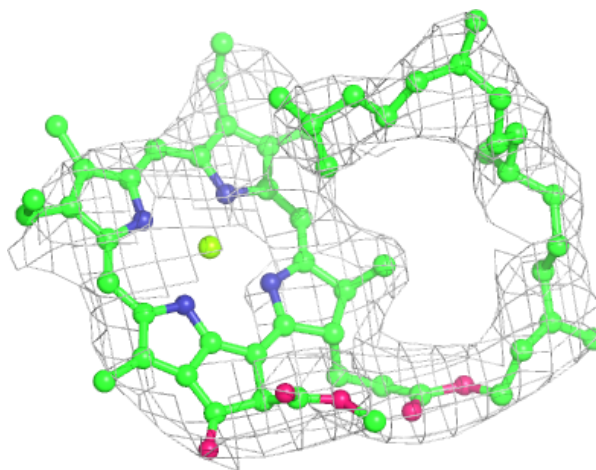


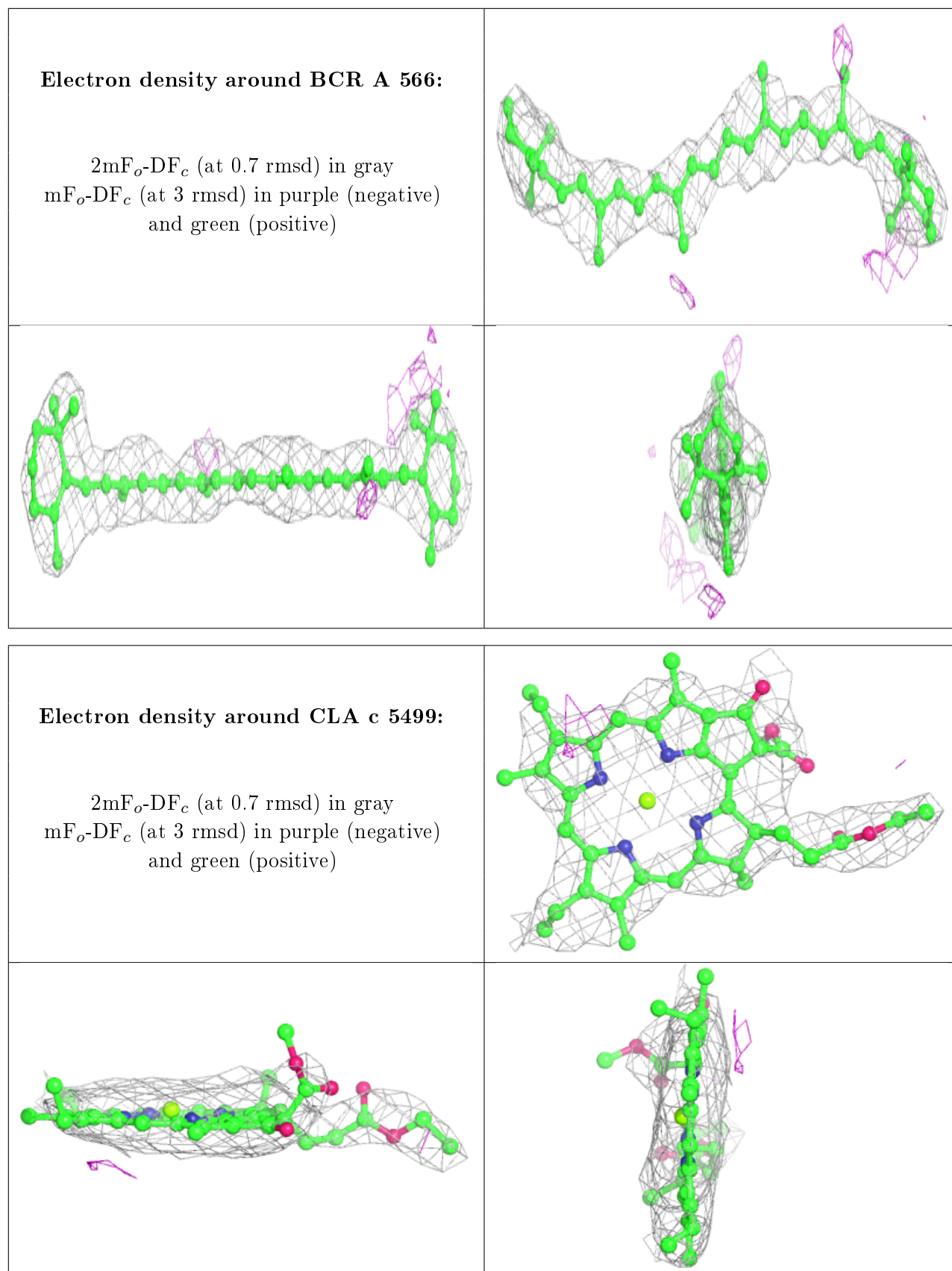


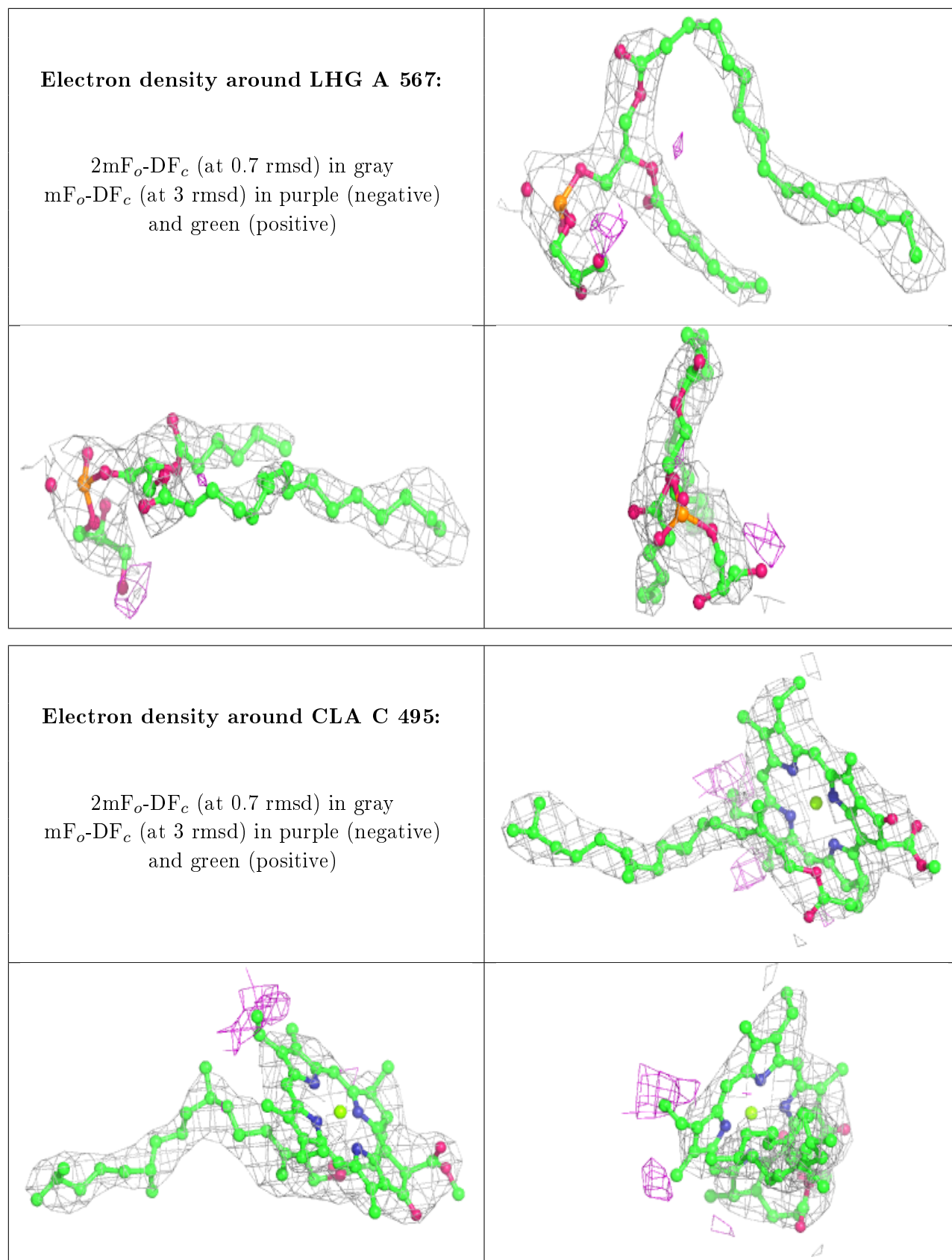


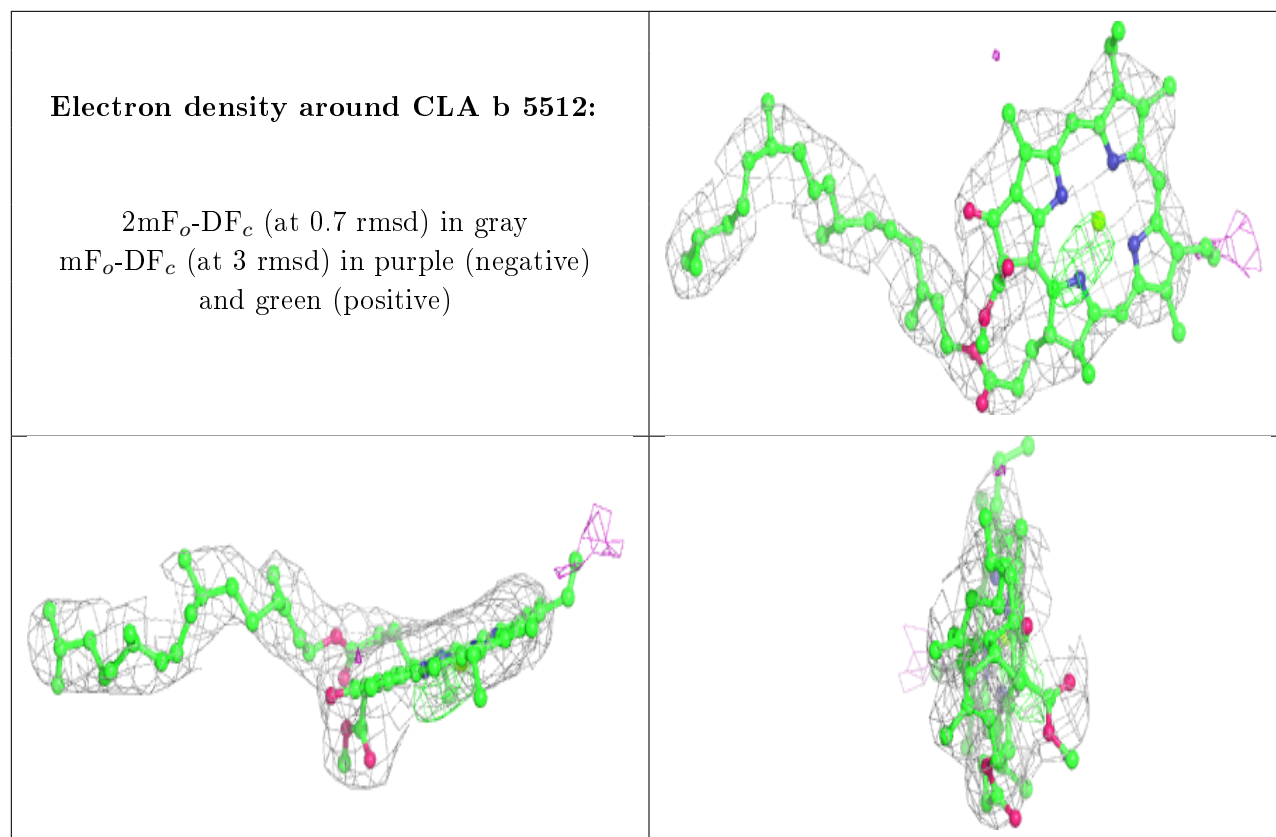
Electron density around CLA b 5525:

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



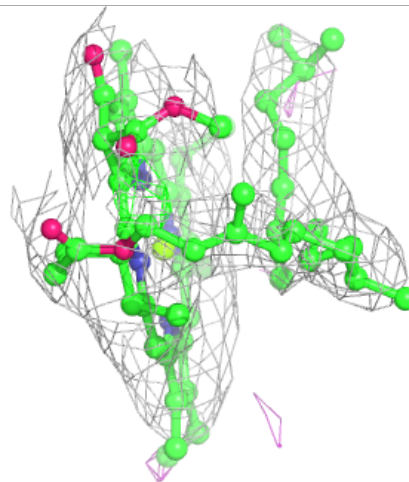
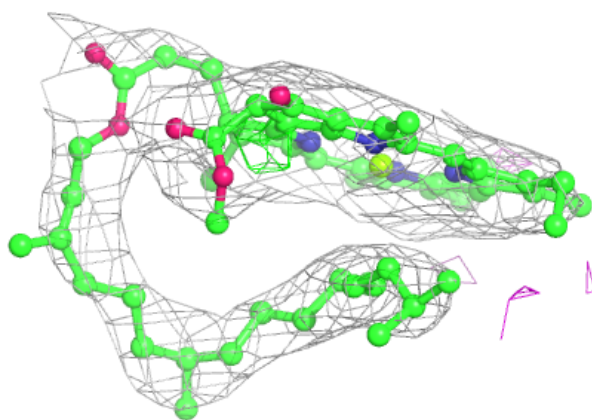
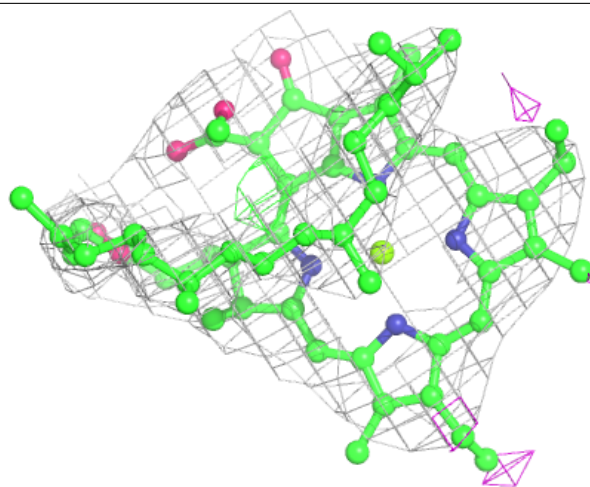






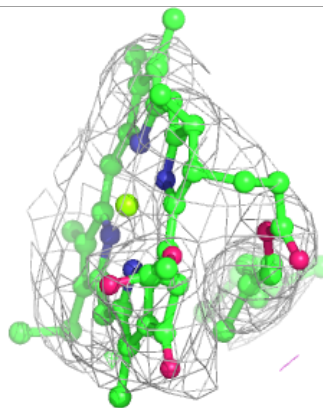
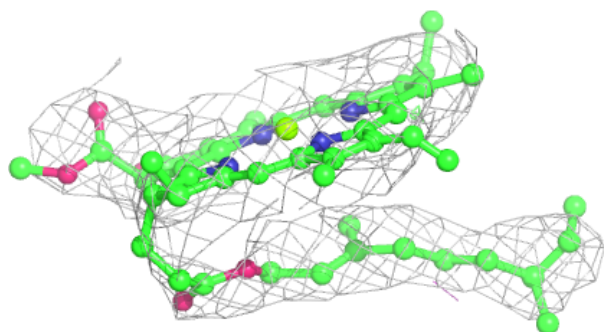
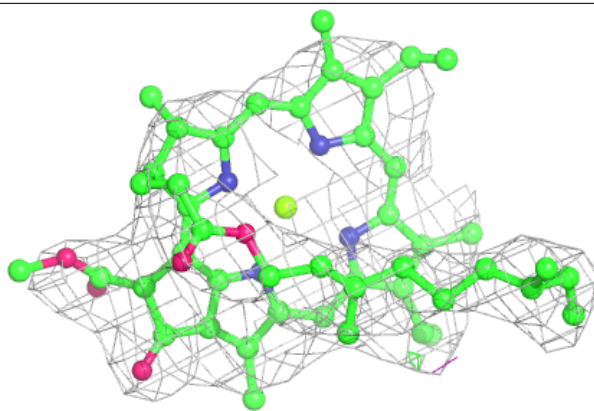
Electron density around CLA c 5500:

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

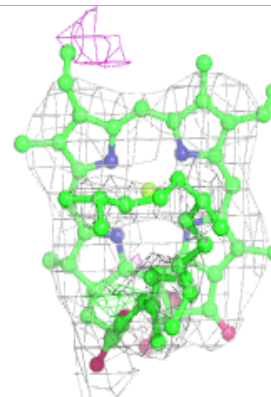
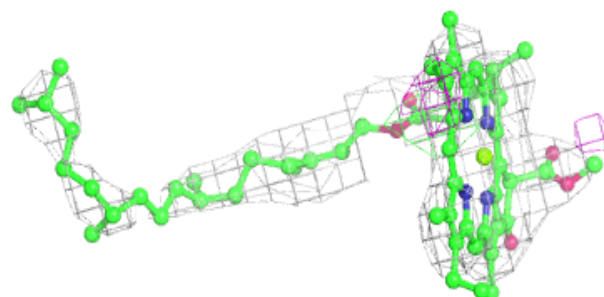
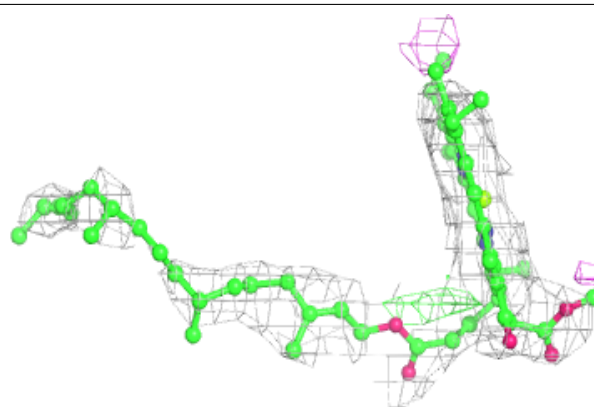


Electron density around CLA b 5524:

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

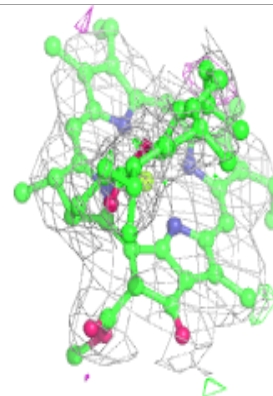
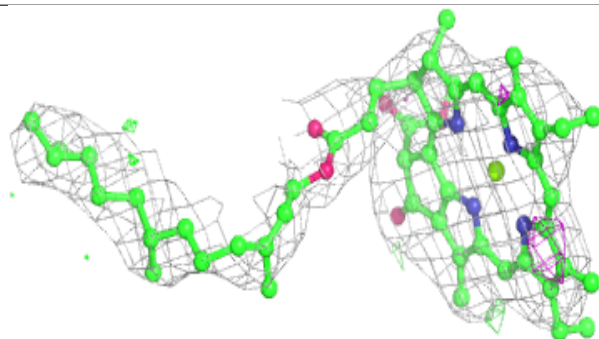
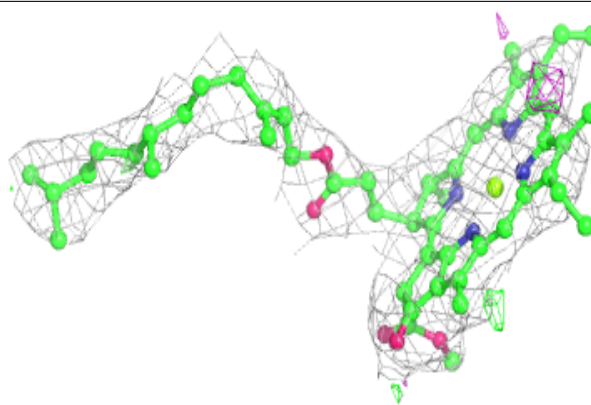
**Electron density around CLA B 515:**

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

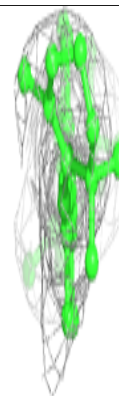
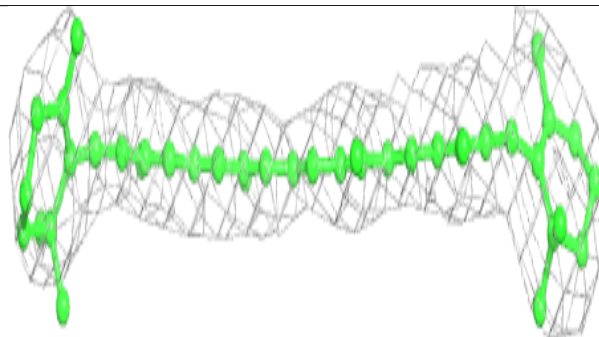
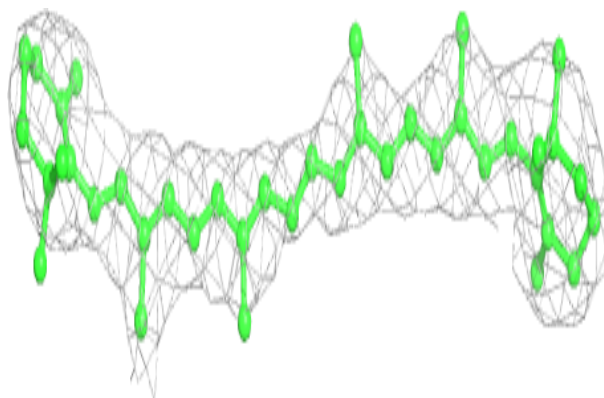


Electron density around CLA c 5492:

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

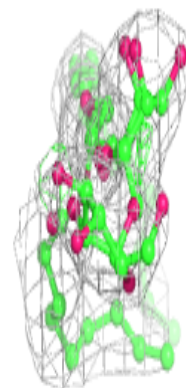
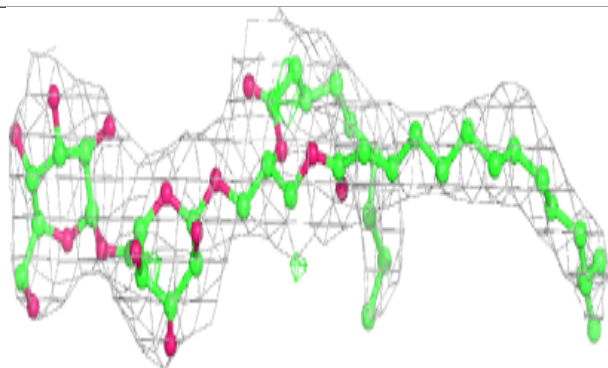
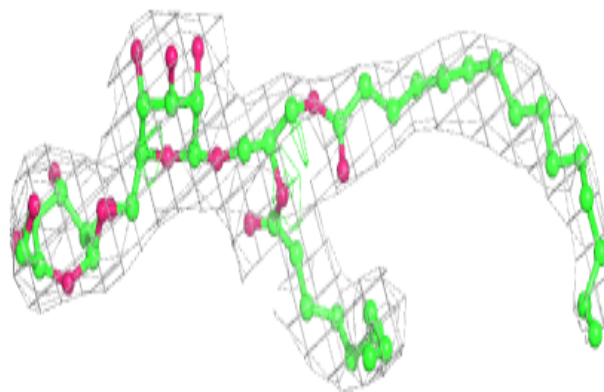
**Electron density around BCR b 5528:**

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

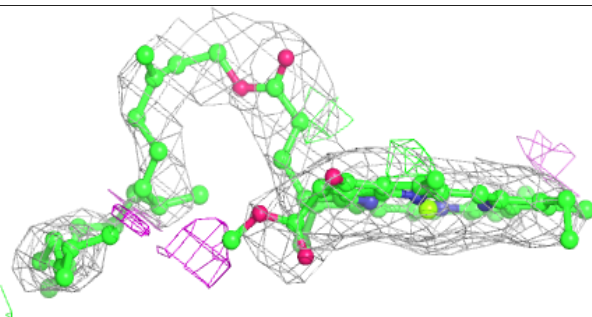
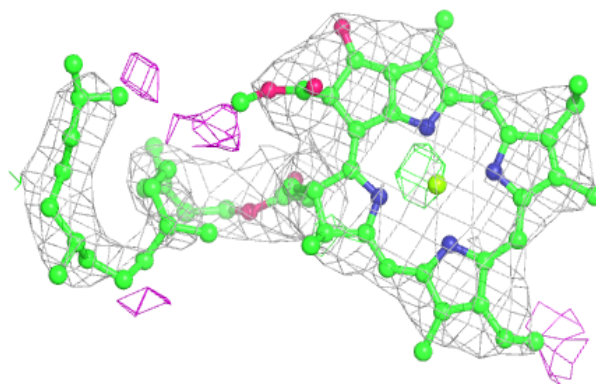


Electron density around DGD h 5208:

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

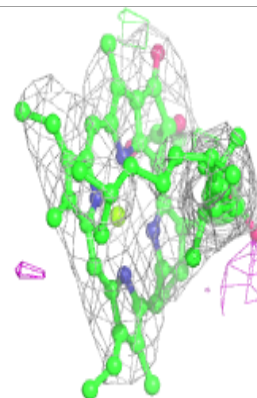
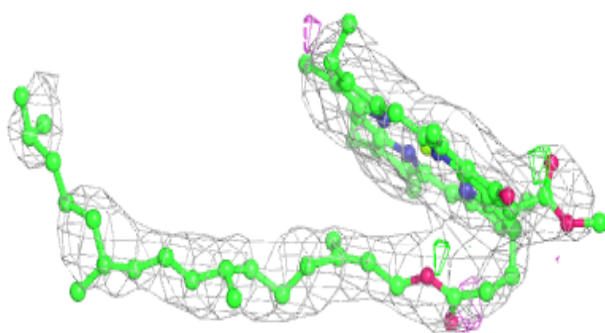
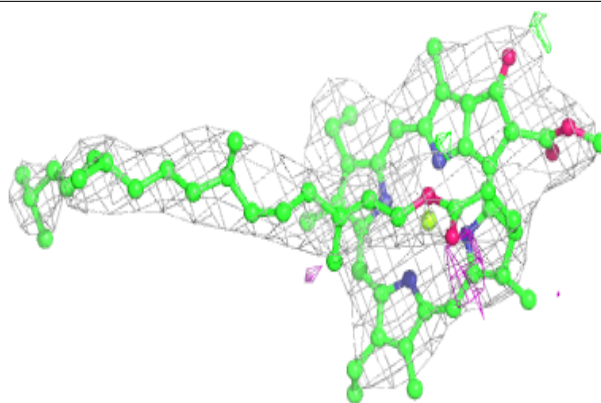
**Electron density around CLA B 522:**

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

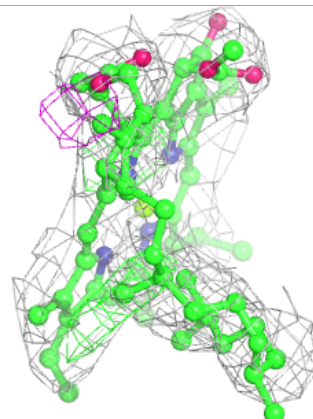
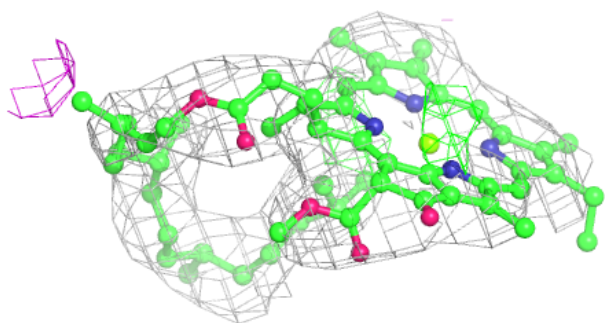
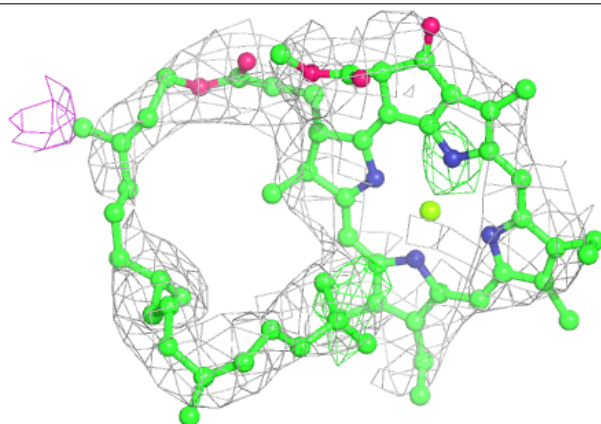


Electron density around CLA B 518:

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

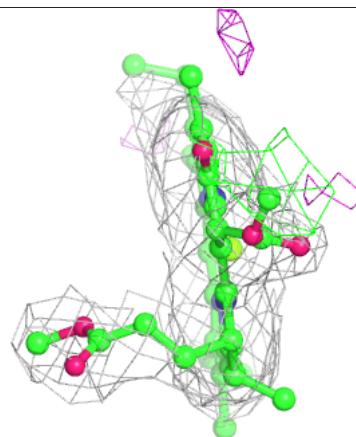
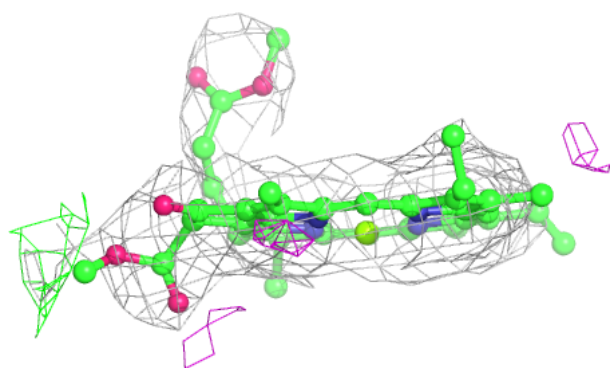
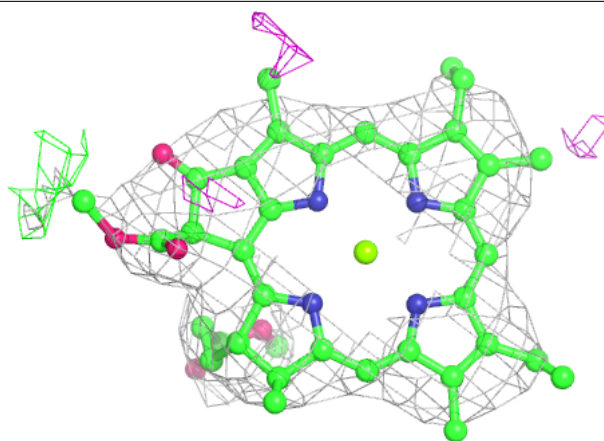
**Electron density around CLA B 525:**

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

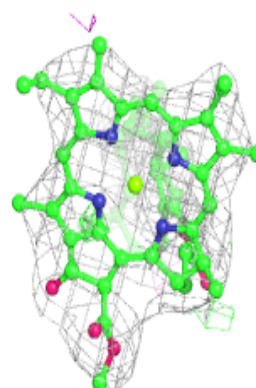
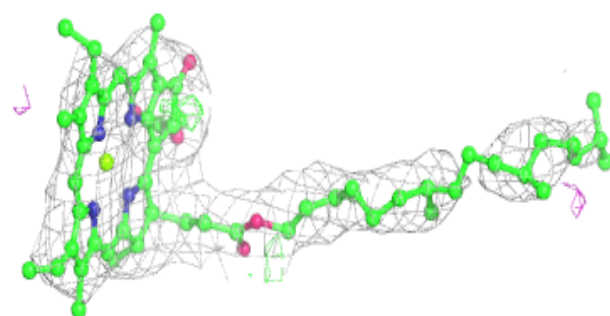
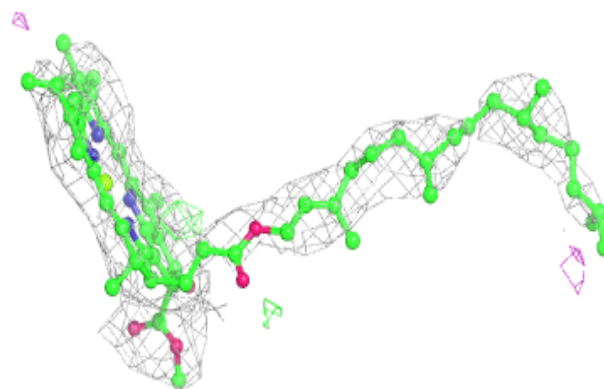


Electron density around CLA c 5494:

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

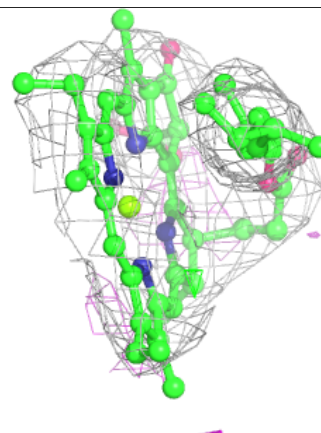
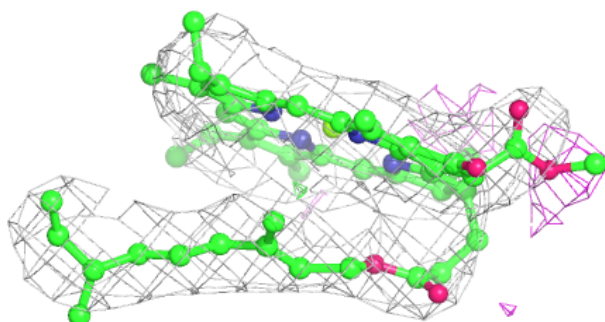
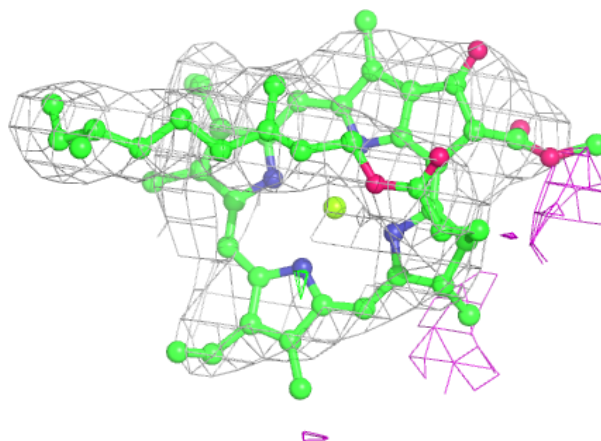
**Electron density around CLA B 514:**

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

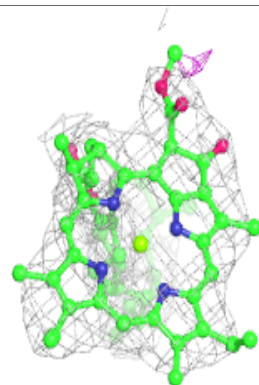
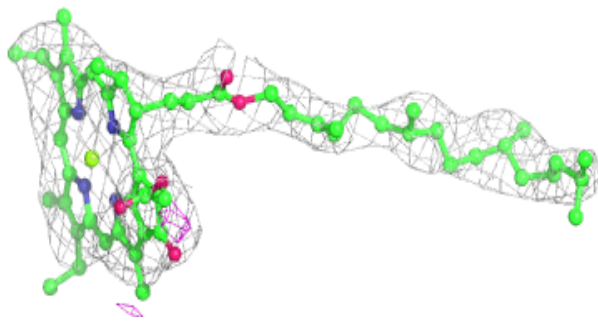
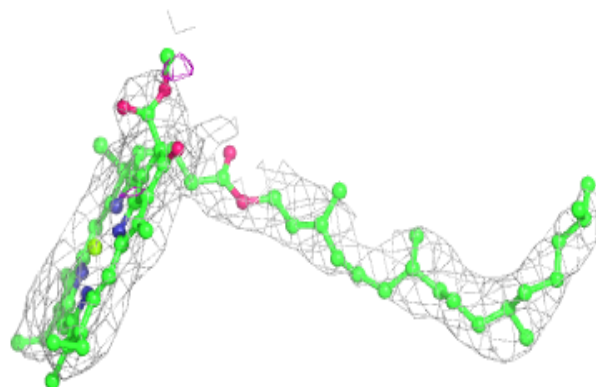


Electron density around CLA B 524:

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

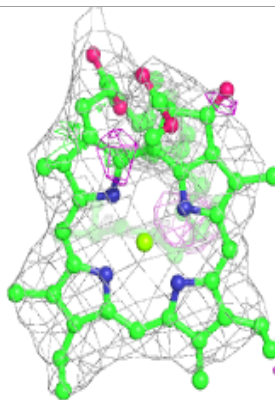
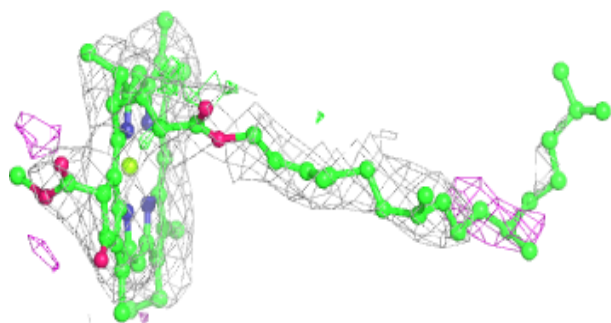
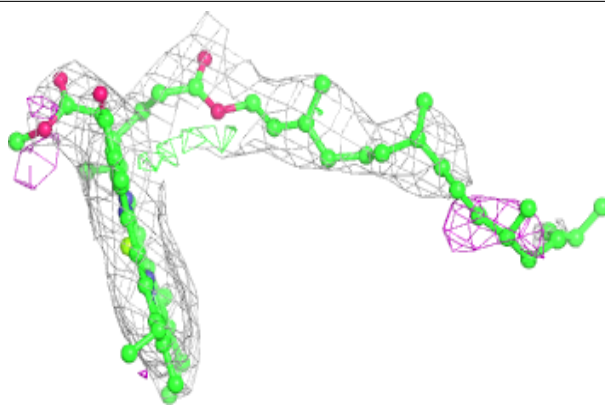
**Electron density around CLA b 5514:**

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

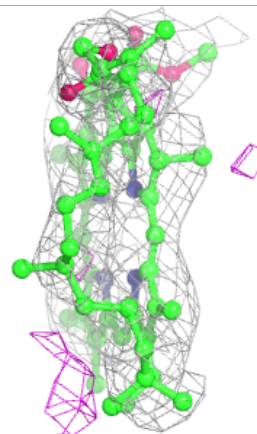
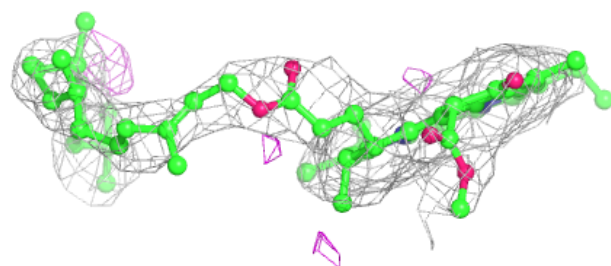
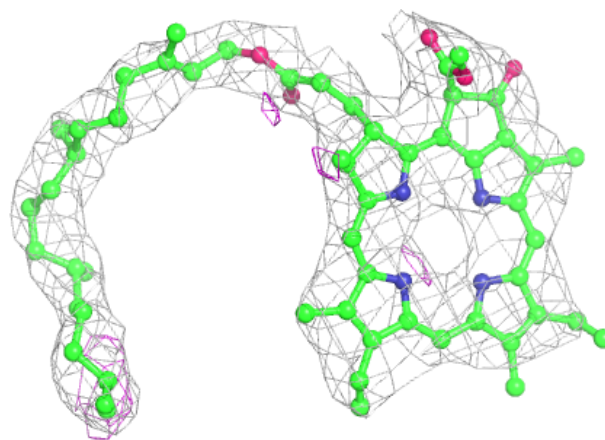


Electron density around CLA b 5515:

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

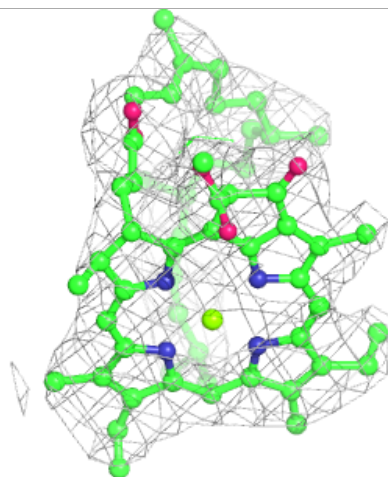
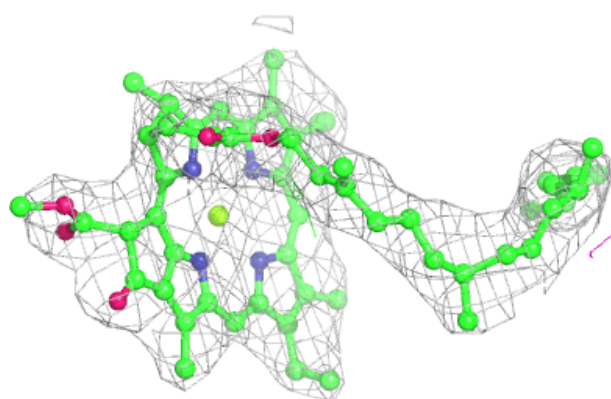
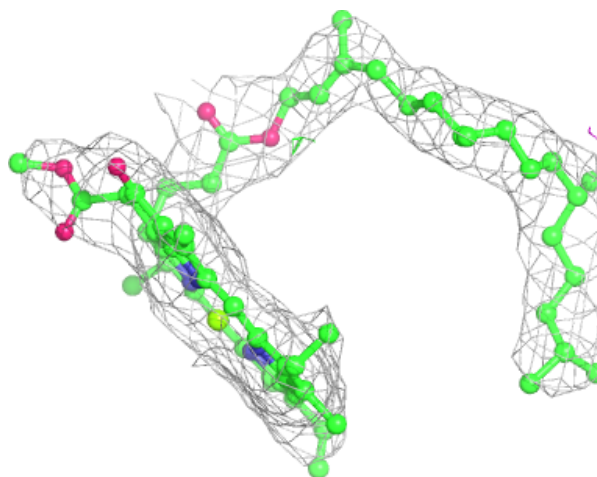
**Electron density around PHO a 5561:**

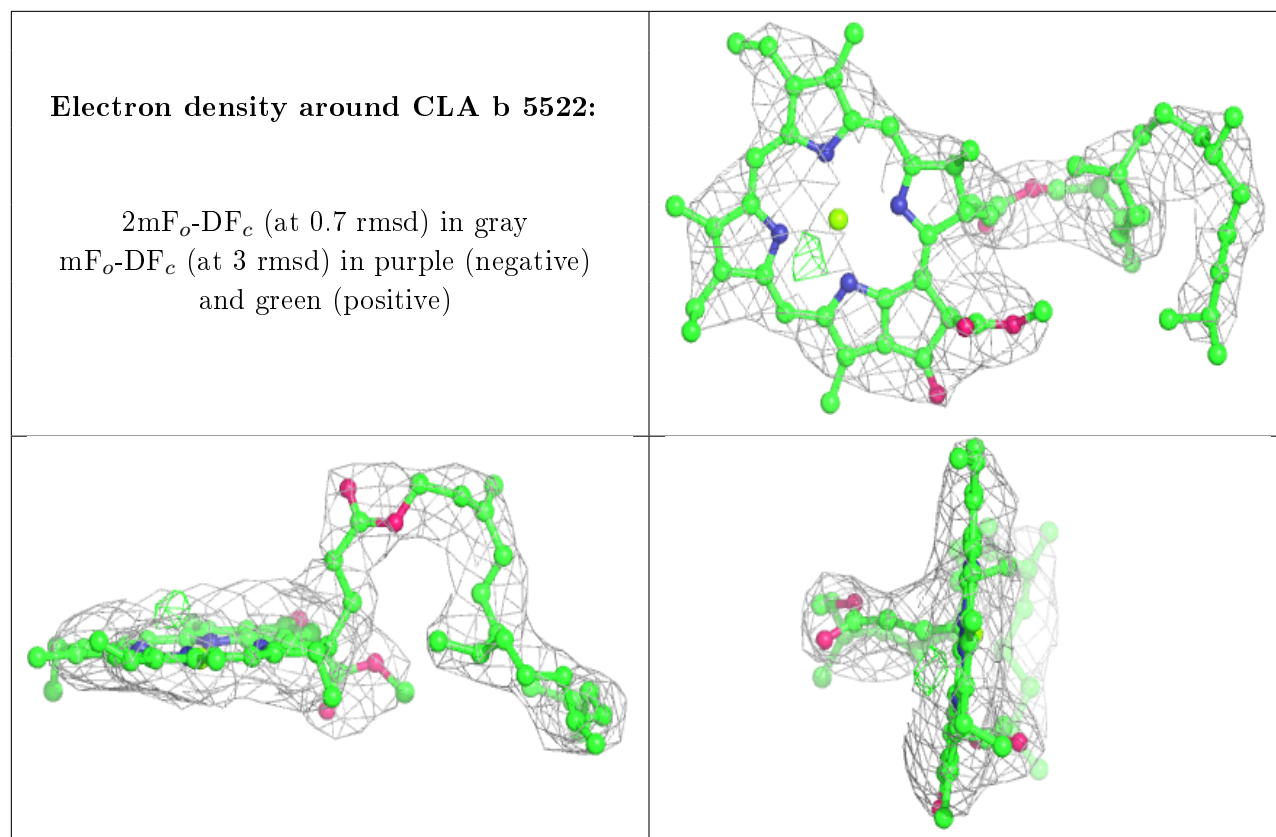
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 5521:

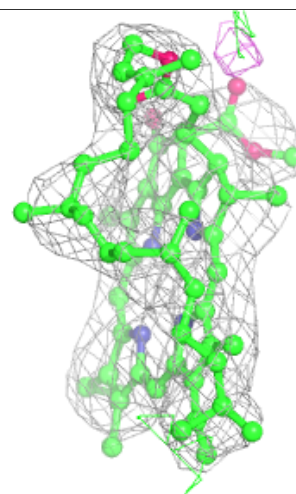
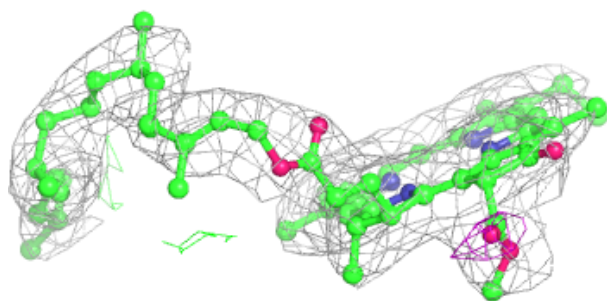
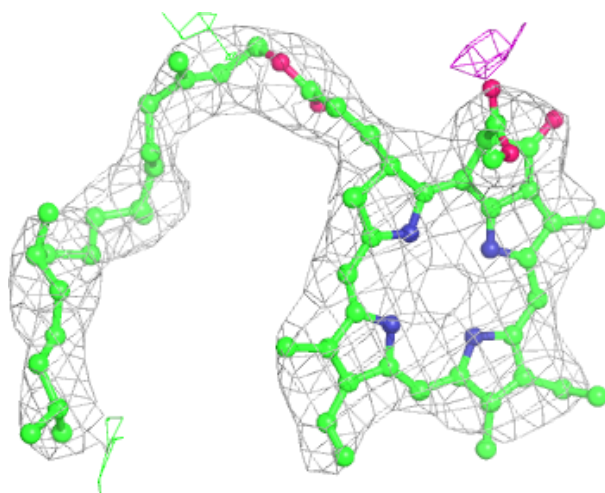
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





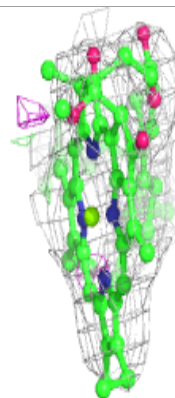
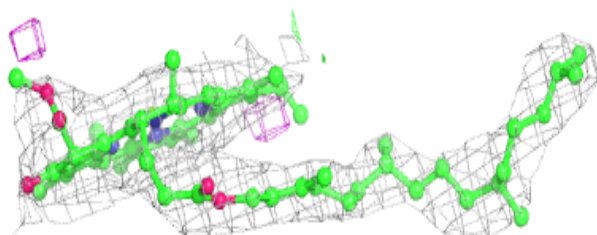
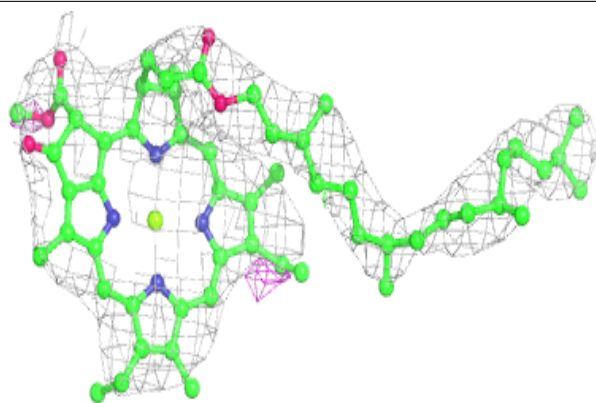
Electron density around PHO A 562:

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

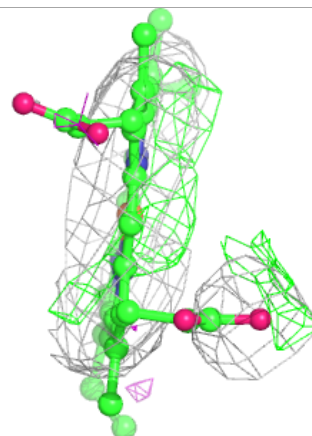
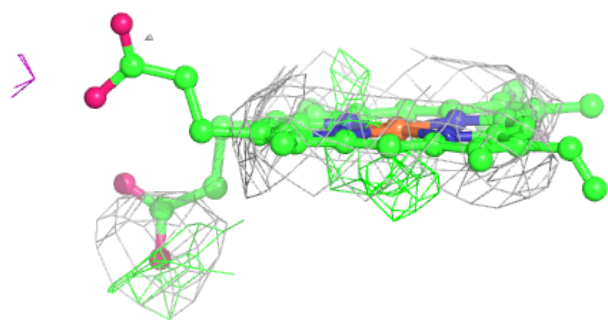
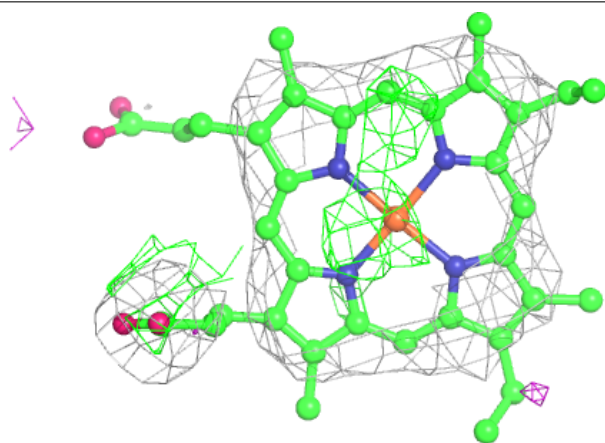


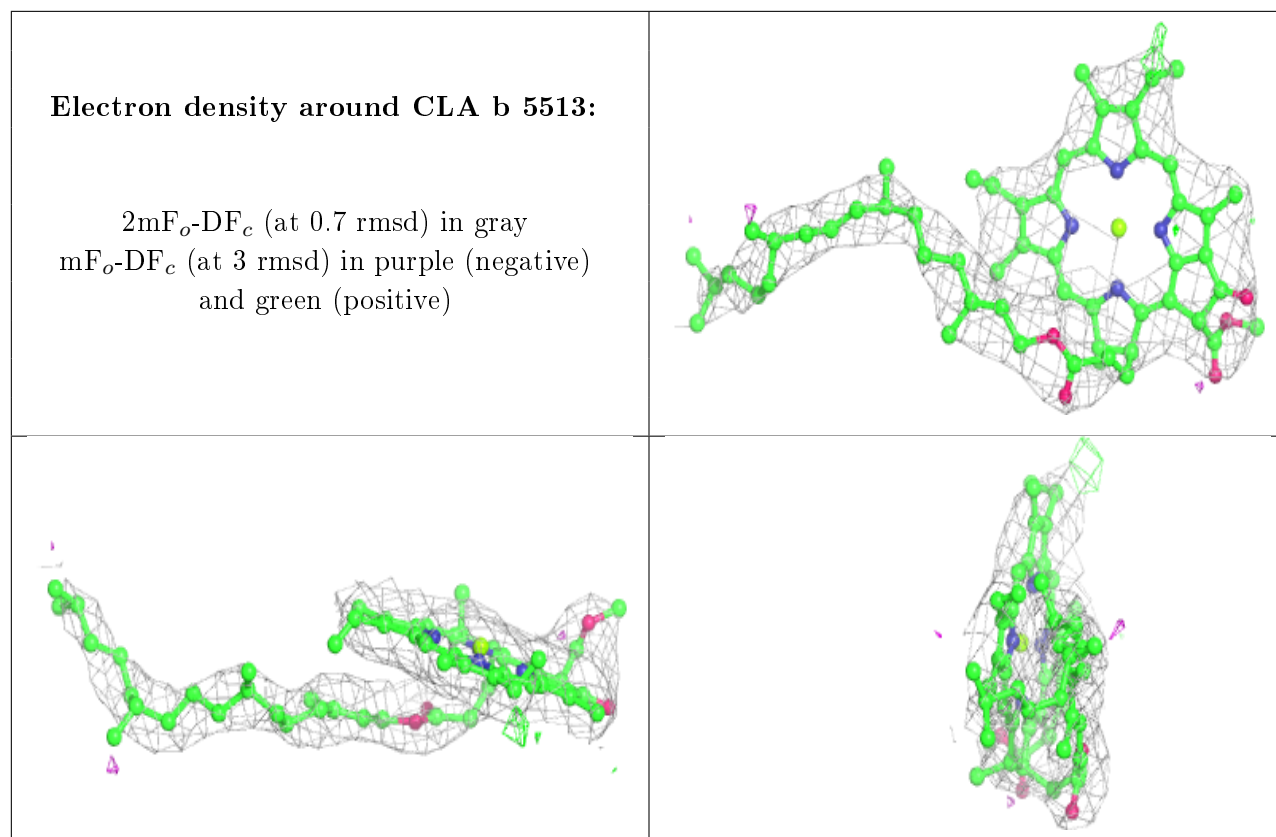
Electron density around CLA B 513:

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

**Electron density around HEM f 5051:**

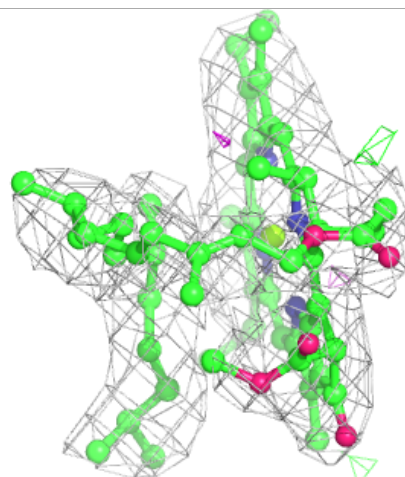
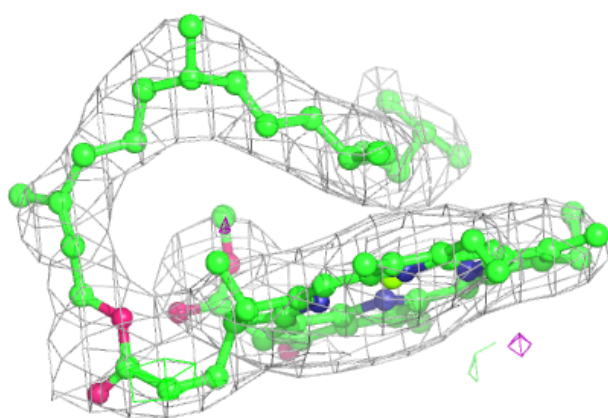
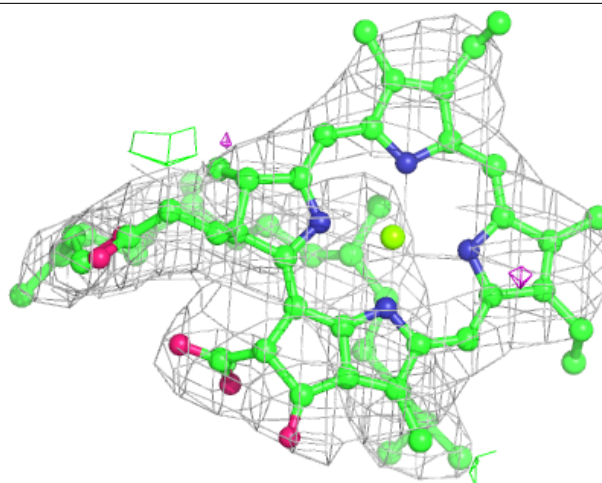
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





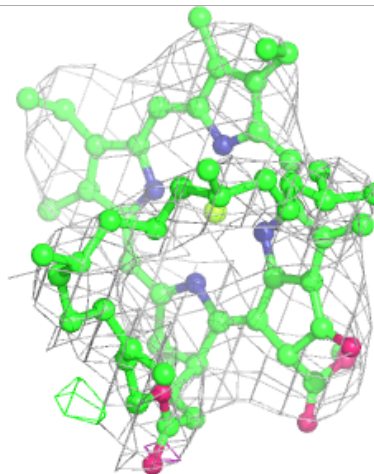
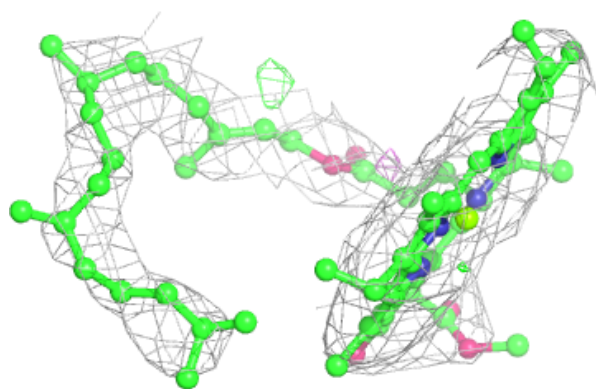
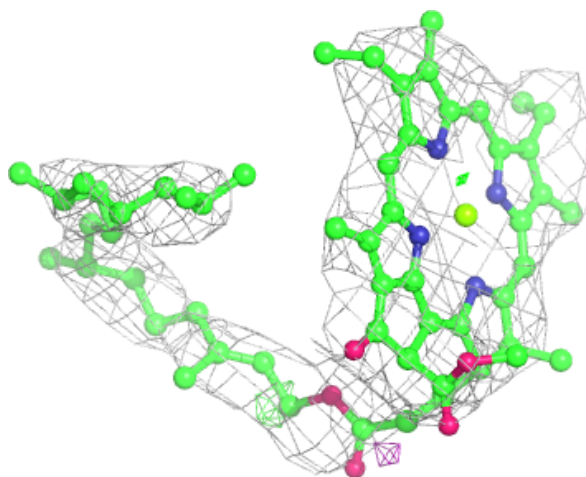
Electron density around CLA C 500:

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



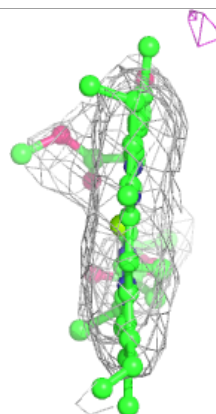
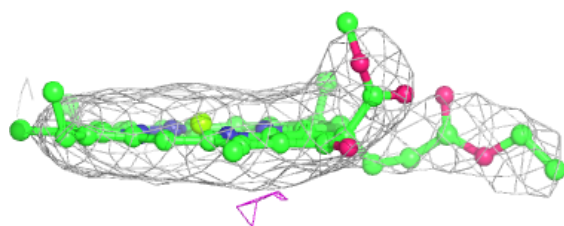
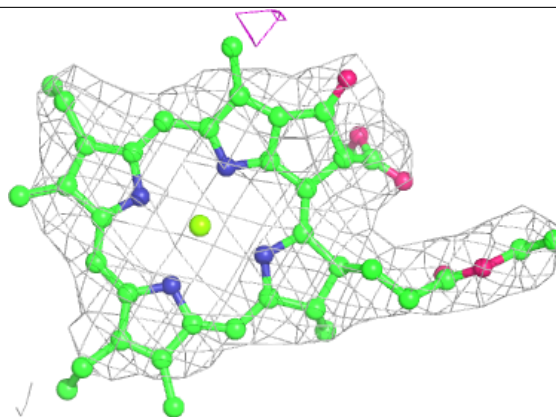
Electron density around CLA C 493:

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

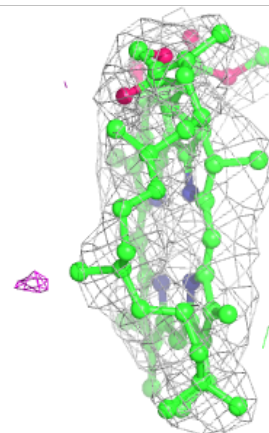
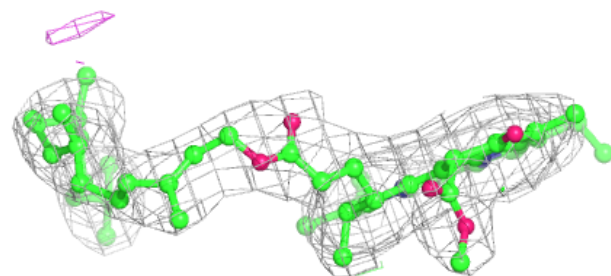
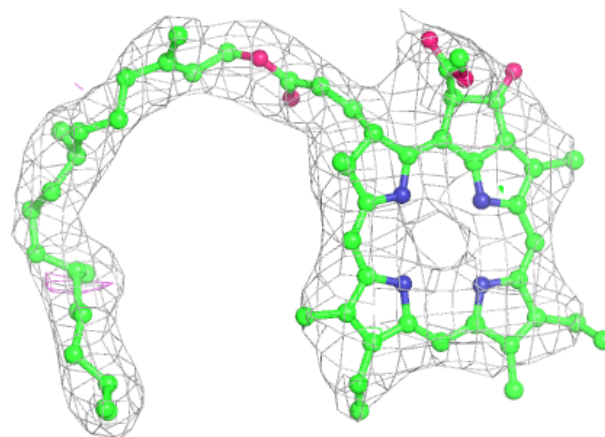


Electron density around CLA C 499:

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

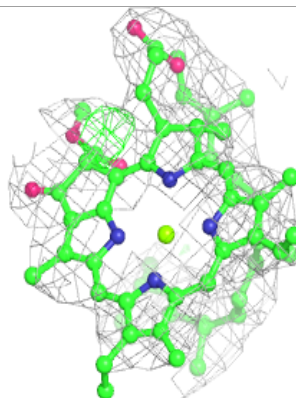
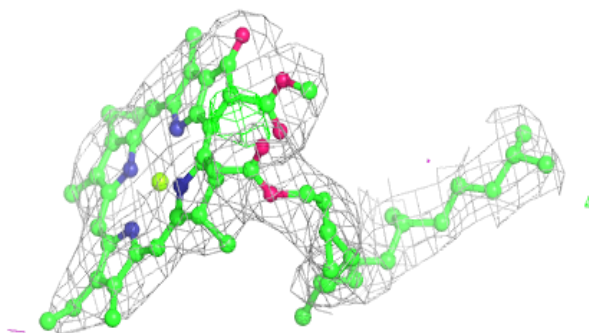
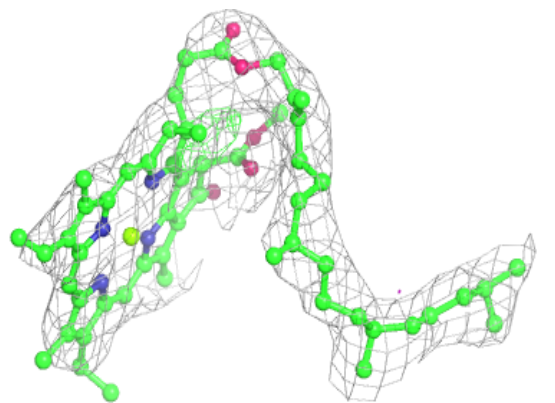
**Electron density around PHO A 561:**

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

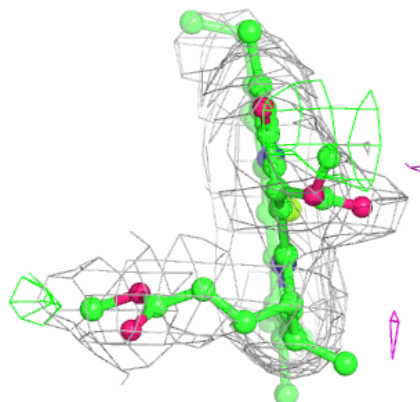
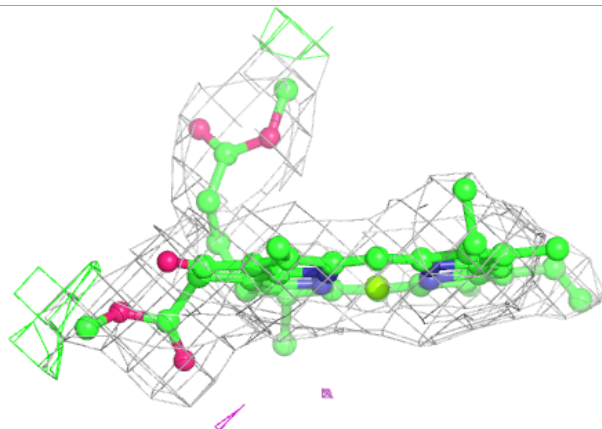
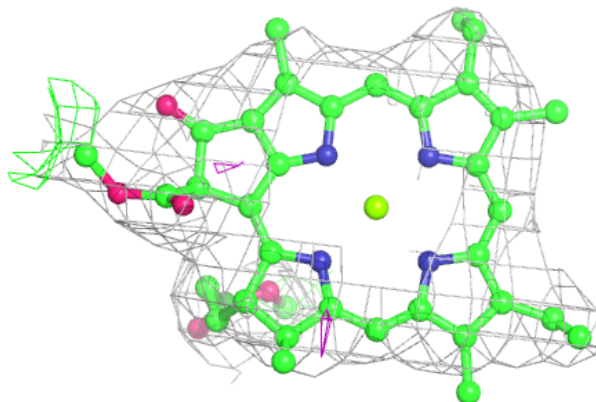


Electron density around CLA B 523:

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

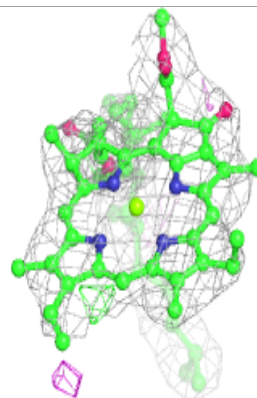
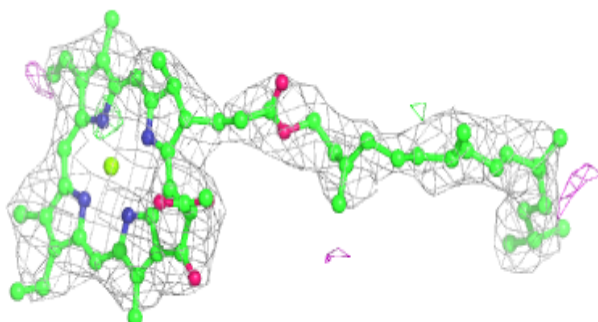
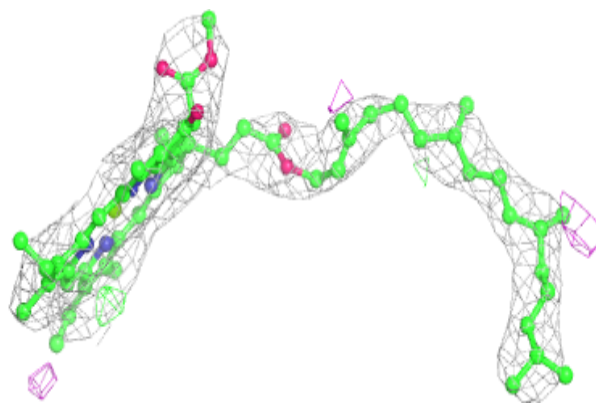
**Electron density around CLA C 494:**

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

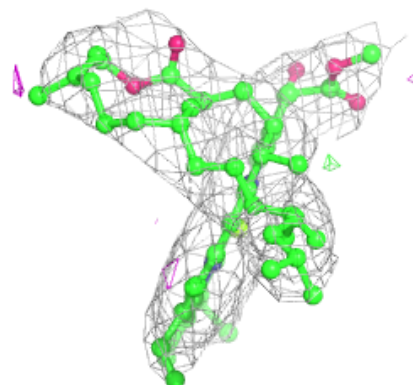
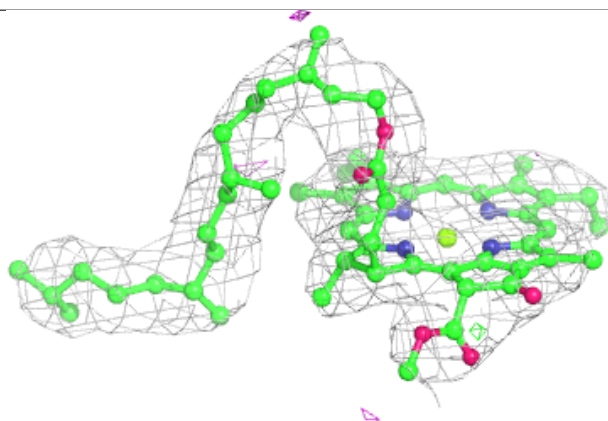
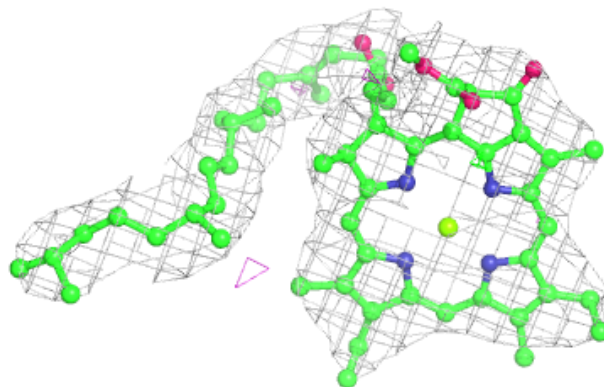


Electron density around CLA d 5354:

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

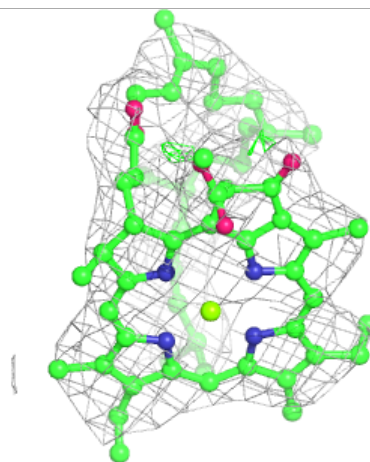
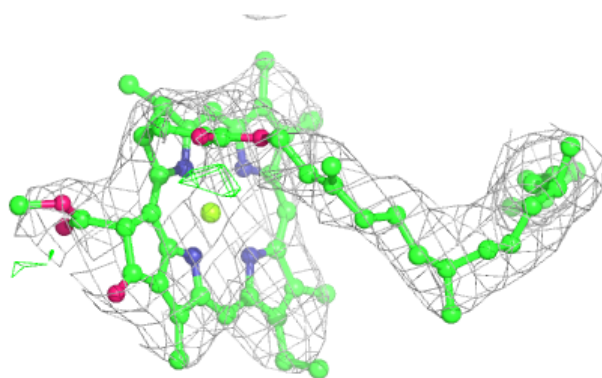
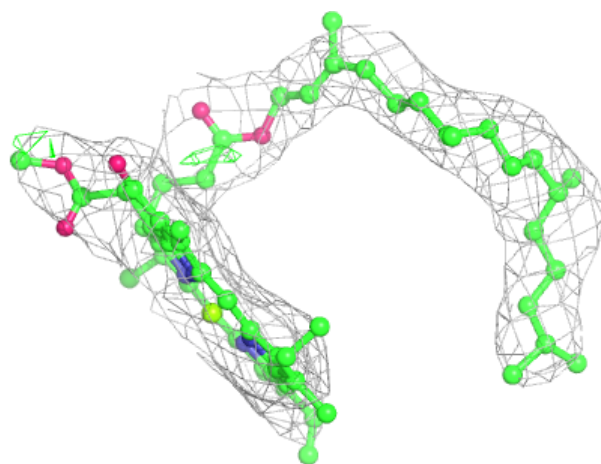
**Electron density around CLA a 5559:**

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



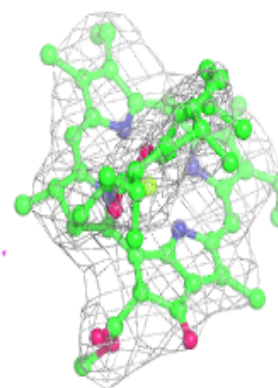
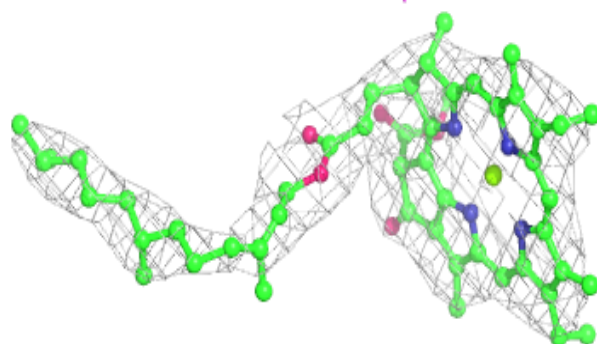
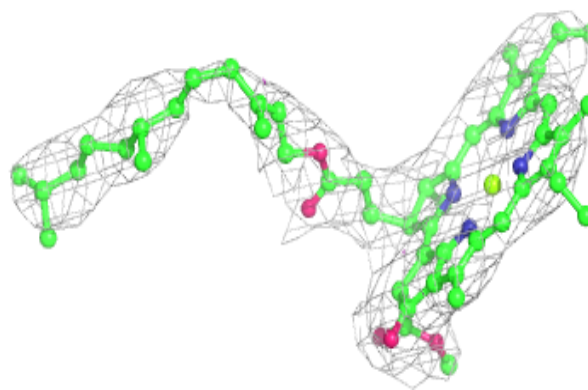
Electron density around CLA B 521:

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

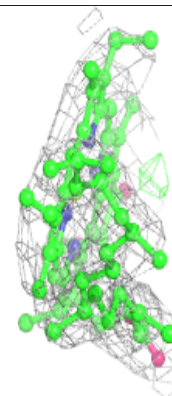
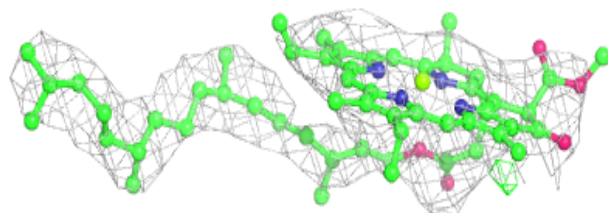
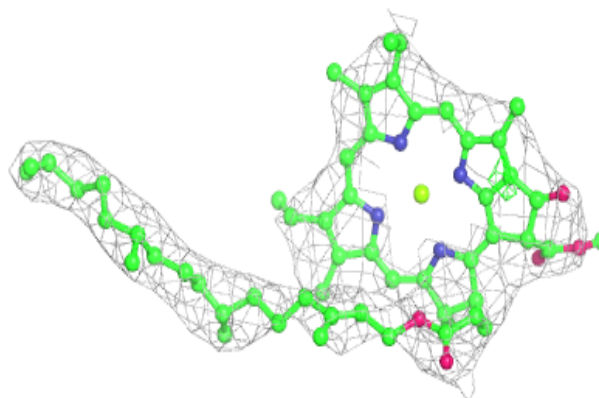


Electron density around CLA C 492:

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

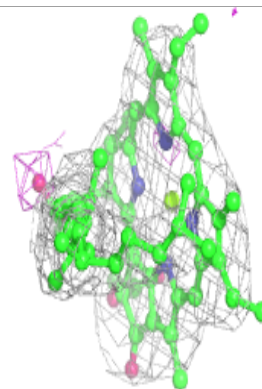
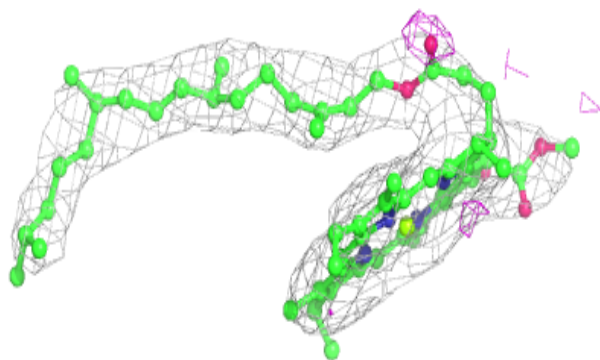
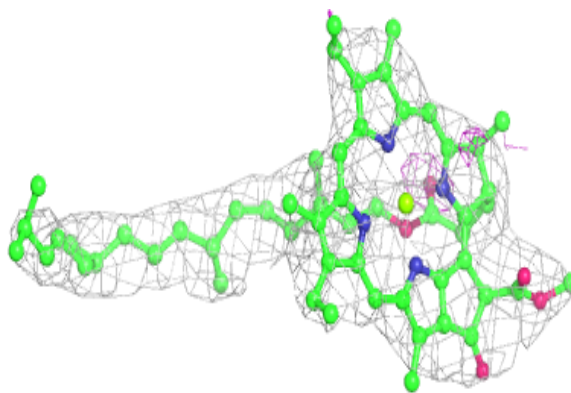
**Electron density around CLA C 491:**

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

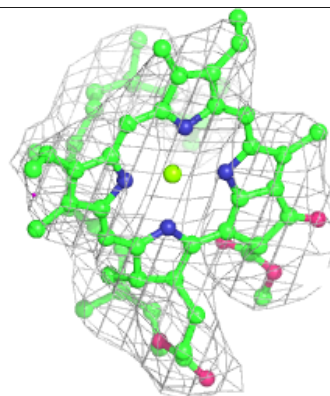
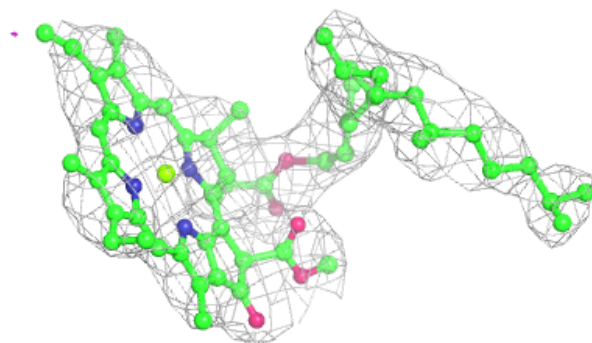
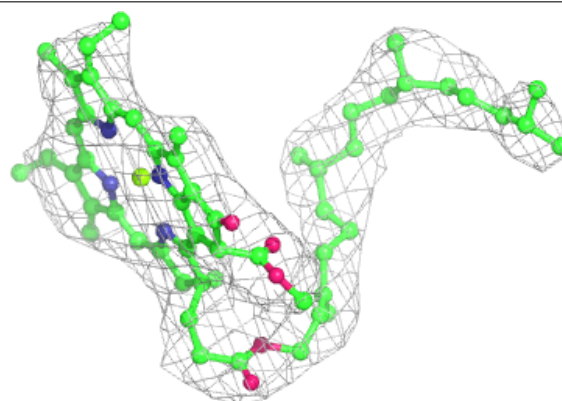


Electron density around CLA b 5518:

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

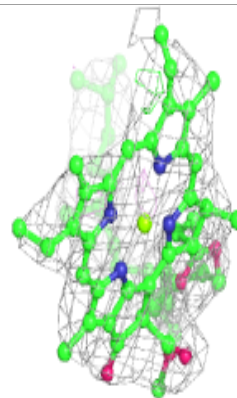
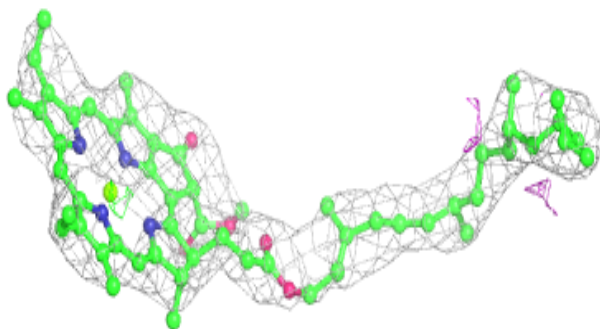
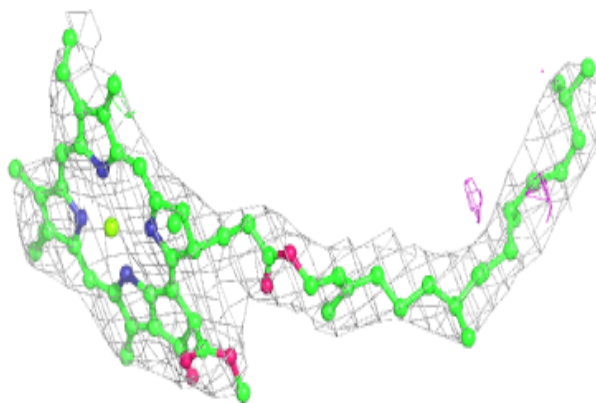
**Electron density around CLA b 5523:**

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

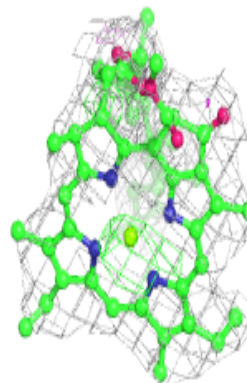
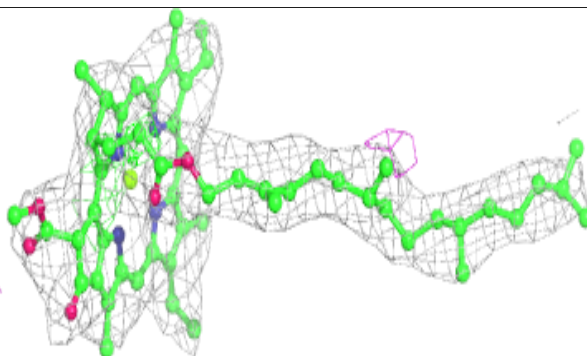
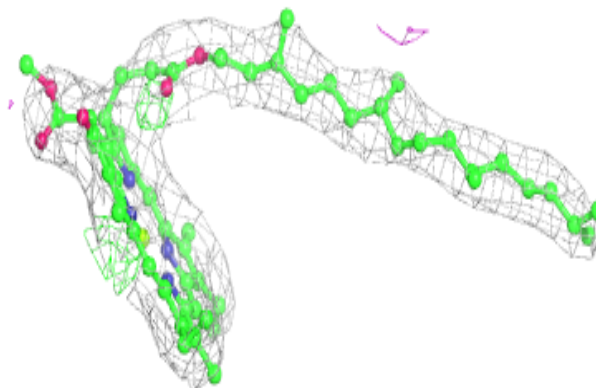


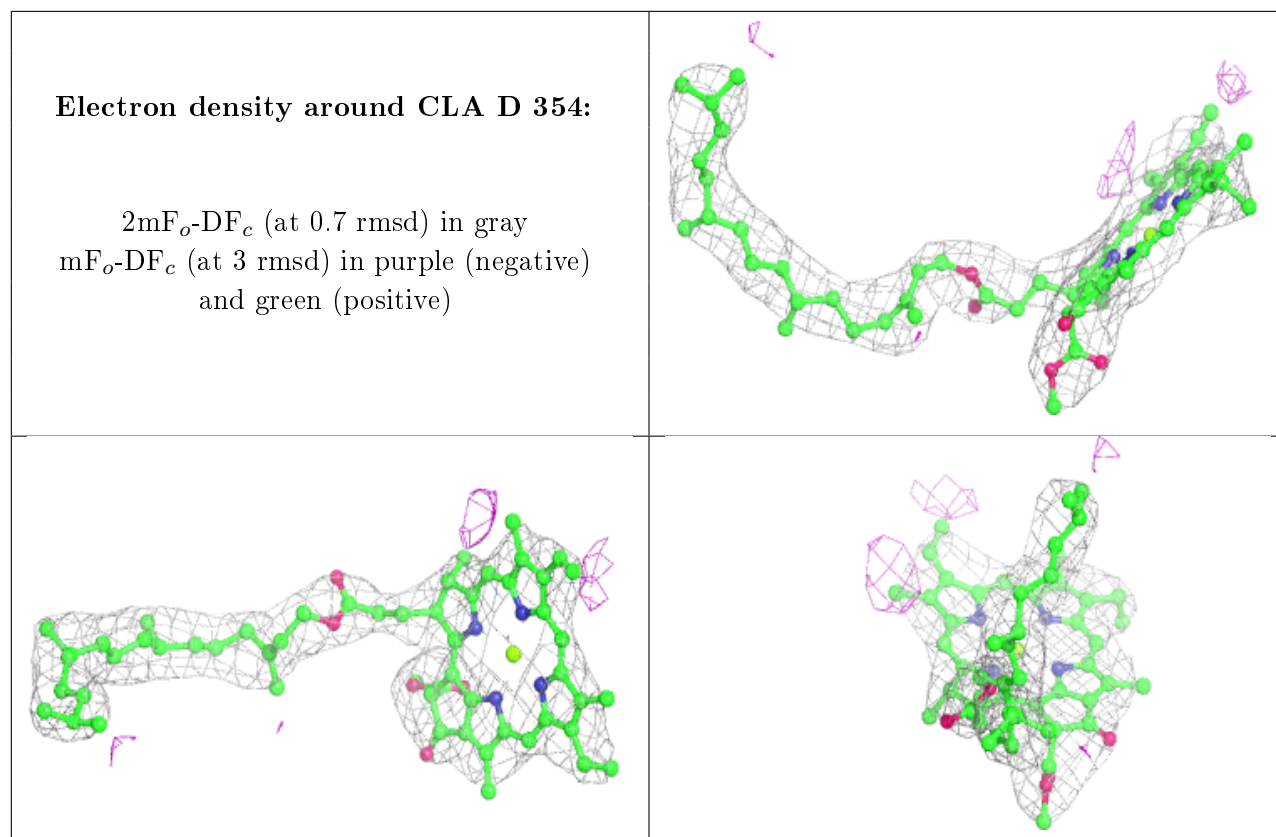
Electron density around CLA a 5558:

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

**Electron density around CLA b 5517:**

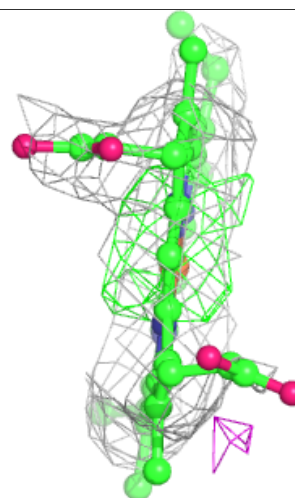
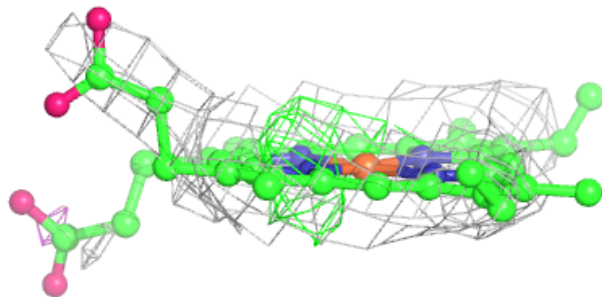
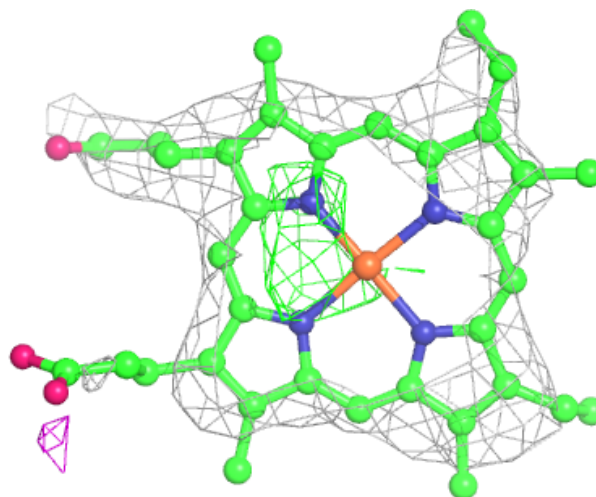
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





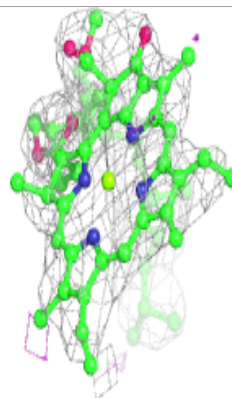
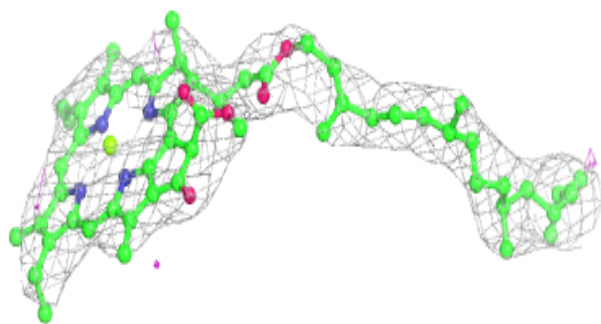
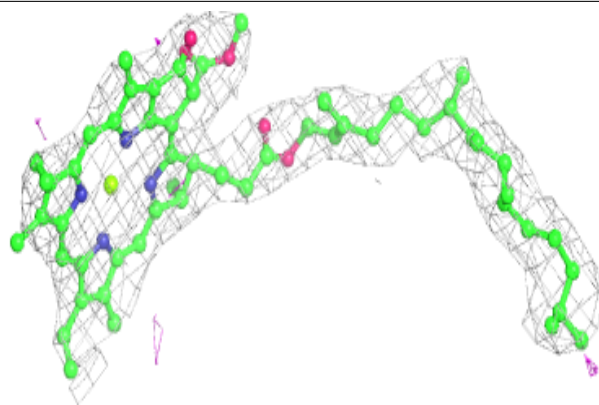
Electron density around HEM F 51:

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

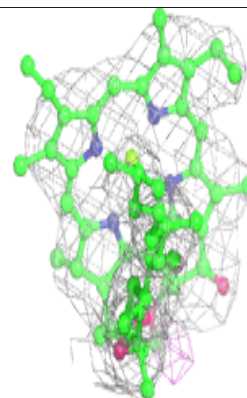
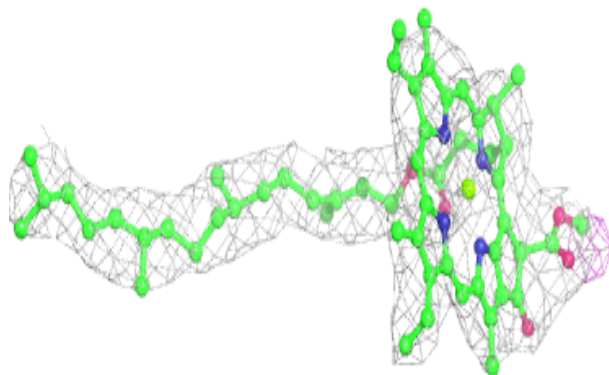
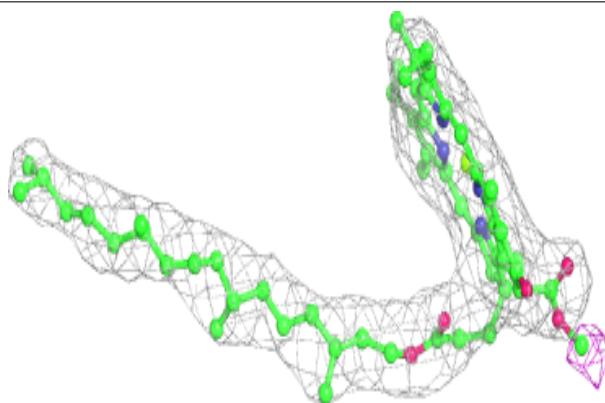


Electron density around CLA A 558:

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

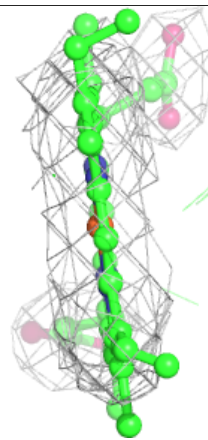
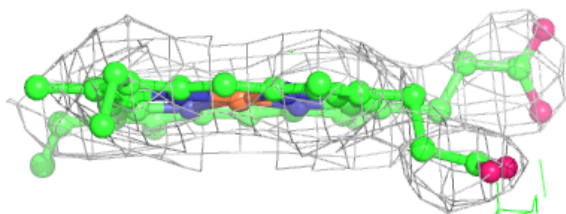
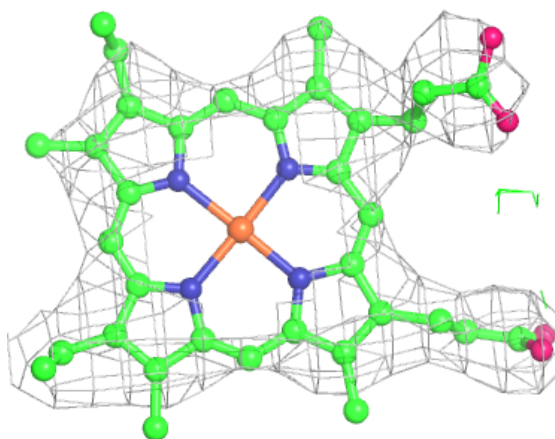
**Electron density around CLA B 517:**

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

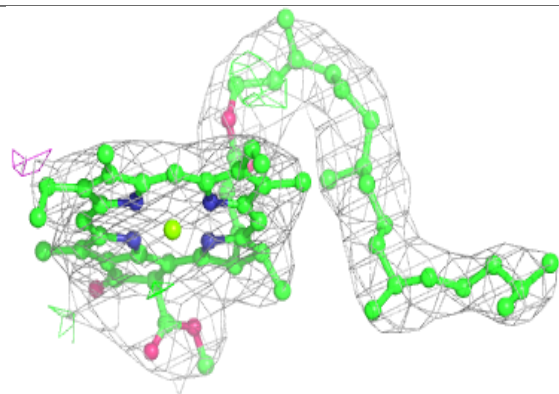
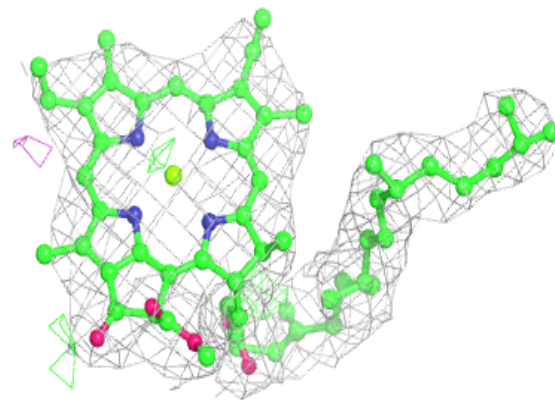


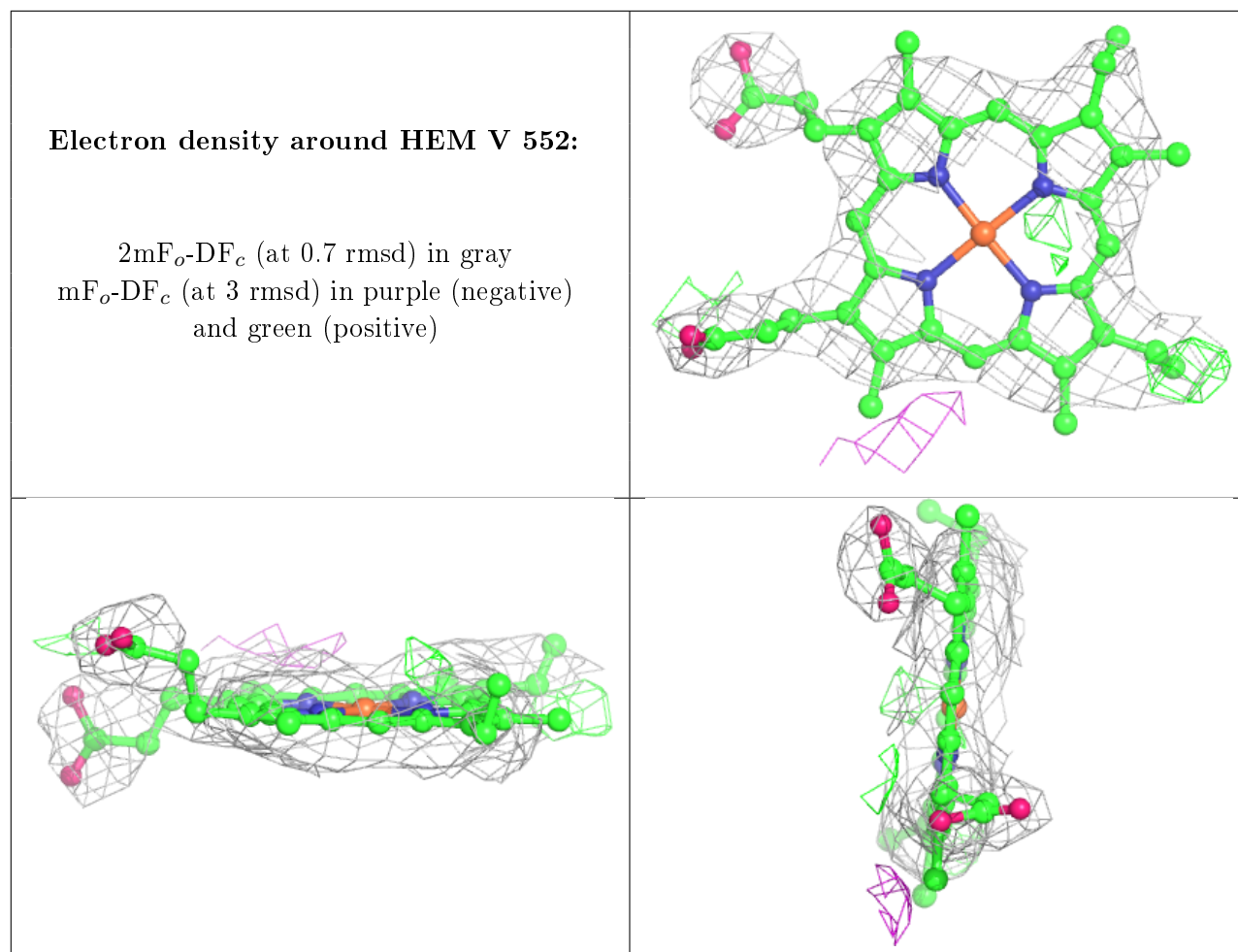
Electron density around HEM v 5552:

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

**Electron density around CLA A 559:**

$2mF_o-DF_c$ (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.