



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:27 AM EDT

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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

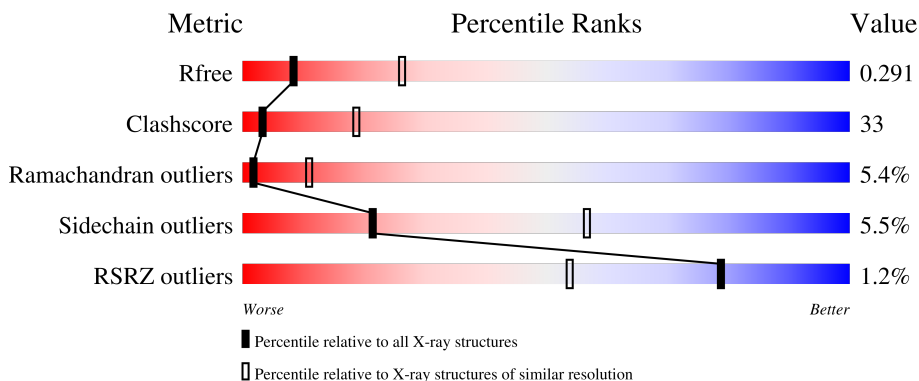
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



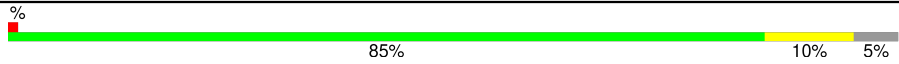
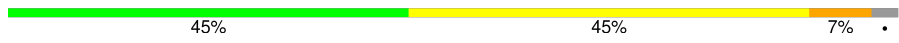

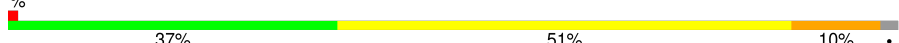
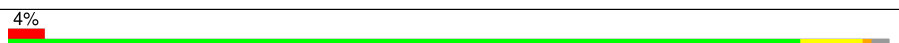
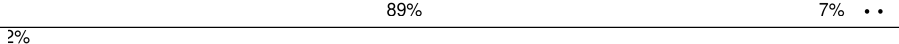
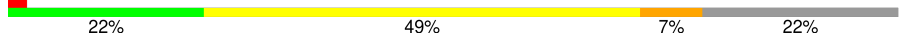




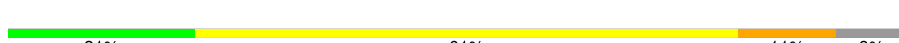
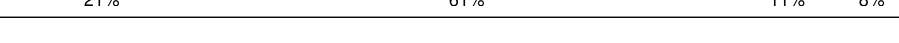

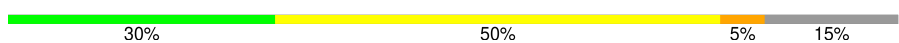
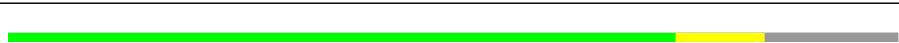
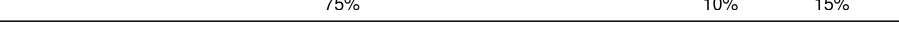
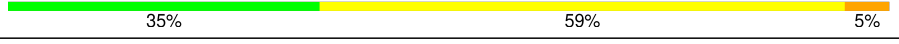


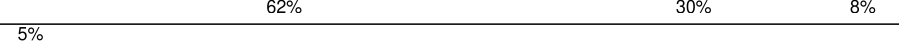



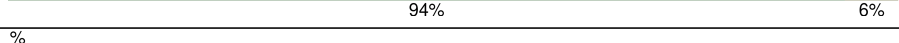
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	473	

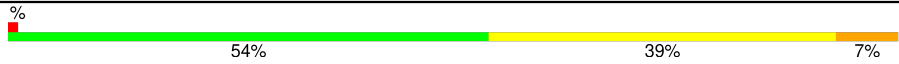
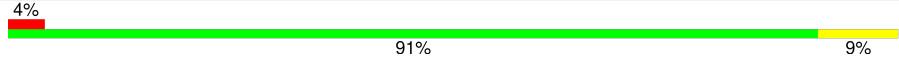


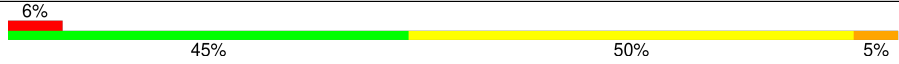
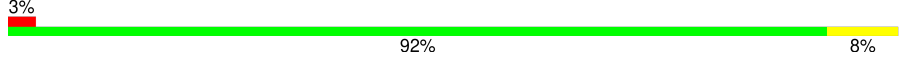
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	473	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	498	X	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	X	-	-	-
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	2623	1718	432	458	15	0	0	0
1	a	335	2623	1718	432	458	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	3800	2498	632	657	13	0	0	0
2	b	488	3800	2498	632	657	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	3421	2244	571	593	13	0	0	0
3	c	447	3421	2244	571	593	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	2696	1789	436	459	12	0	0	0
4	d	340	2696	1789	436	459	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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Unassigned subunits.

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

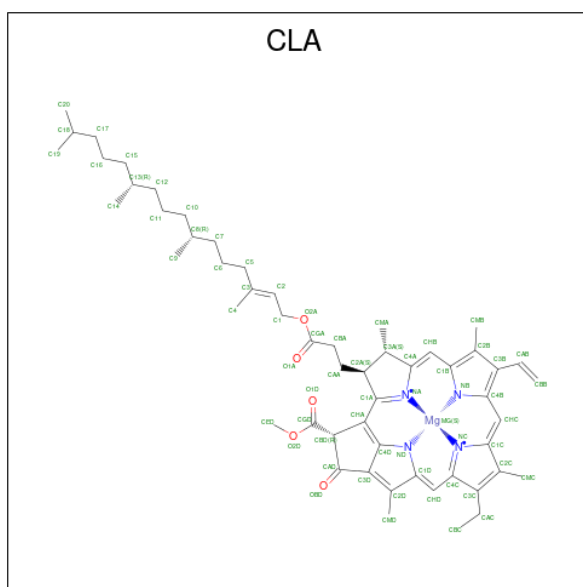
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

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

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

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

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



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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
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	56	46	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	C	1	65	55	1	4	5	0	0
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

Continued on next page...

Continued from previous page...

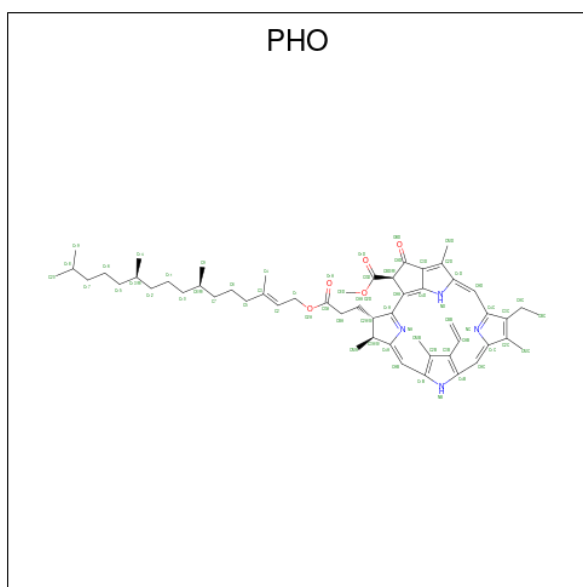
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

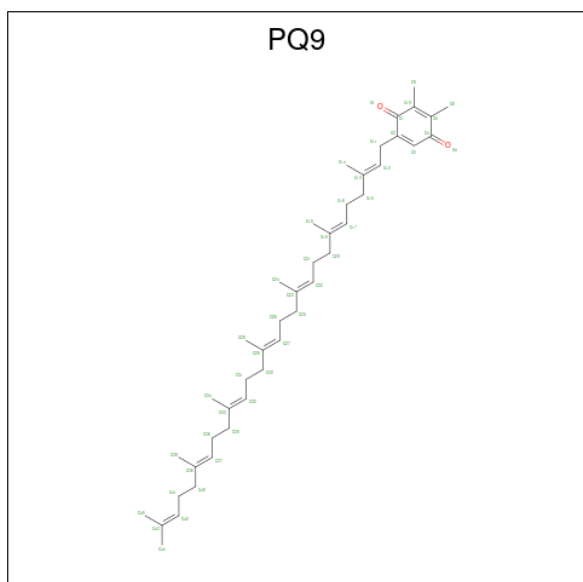
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			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		

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



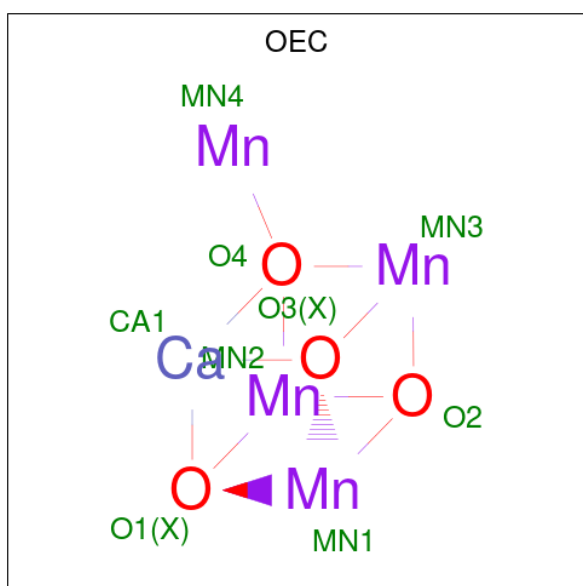
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- 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).



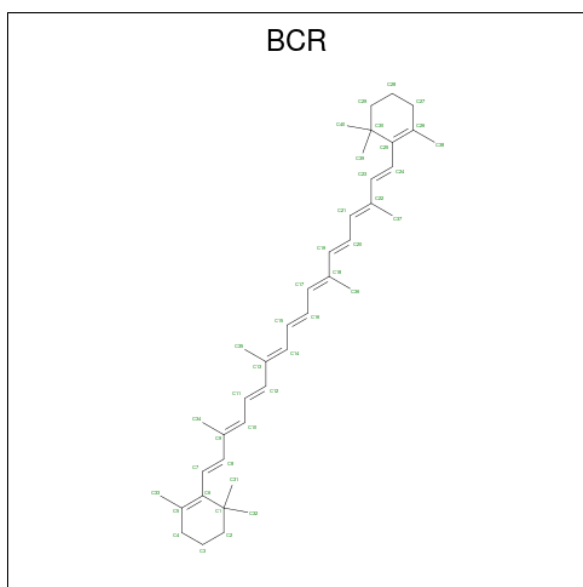
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- 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: $\text{C}_{40}\text{H}_{56}$).



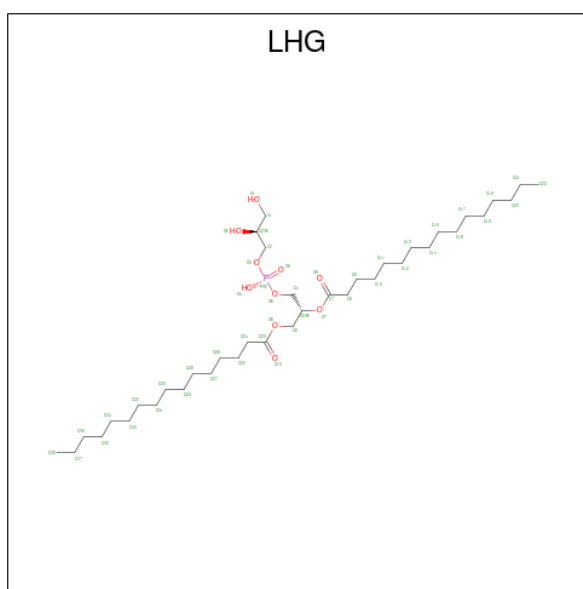
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total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

Continued on next page...

Continued from previous page...

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

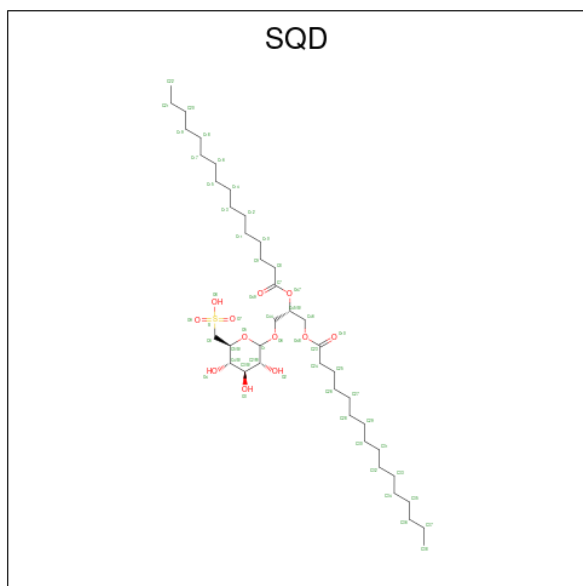
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

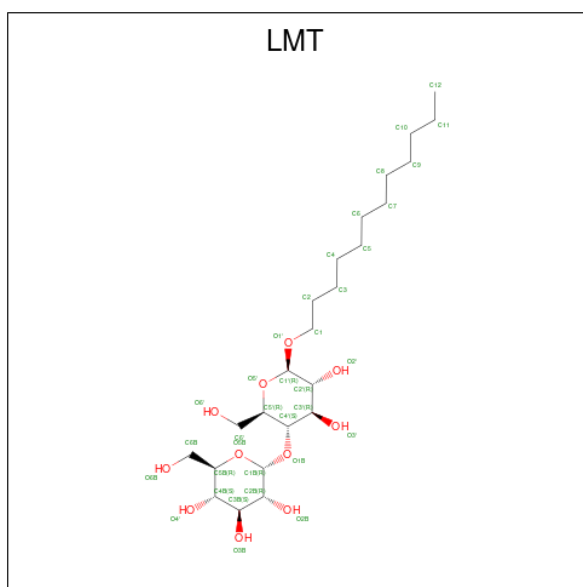
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



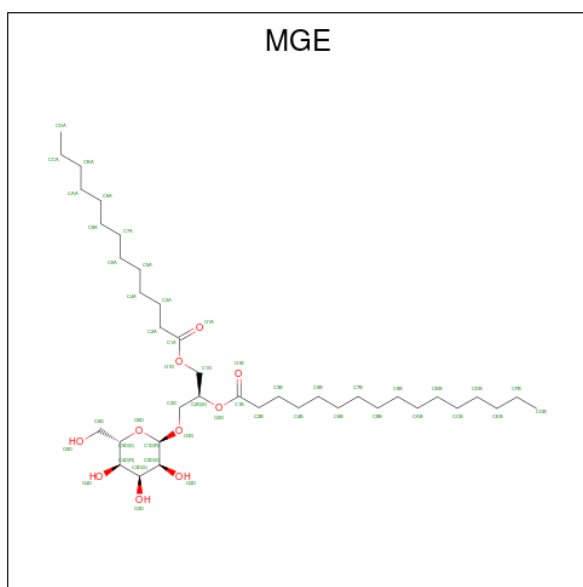
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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).

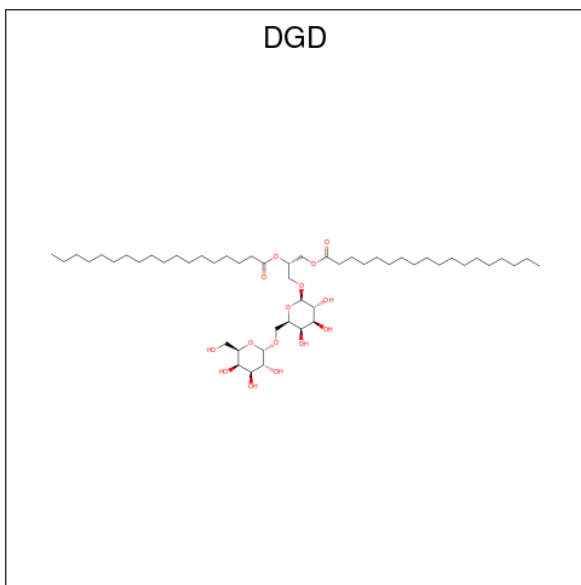


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total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

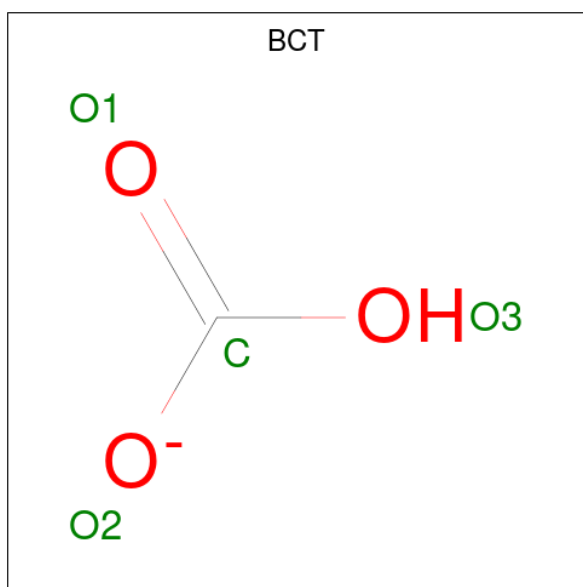
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

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



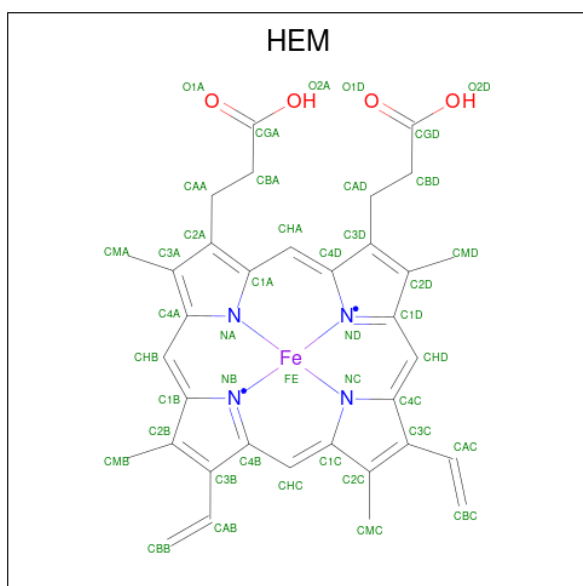
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total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

- 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		

Continued on next page...

Continued from previous page...

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		

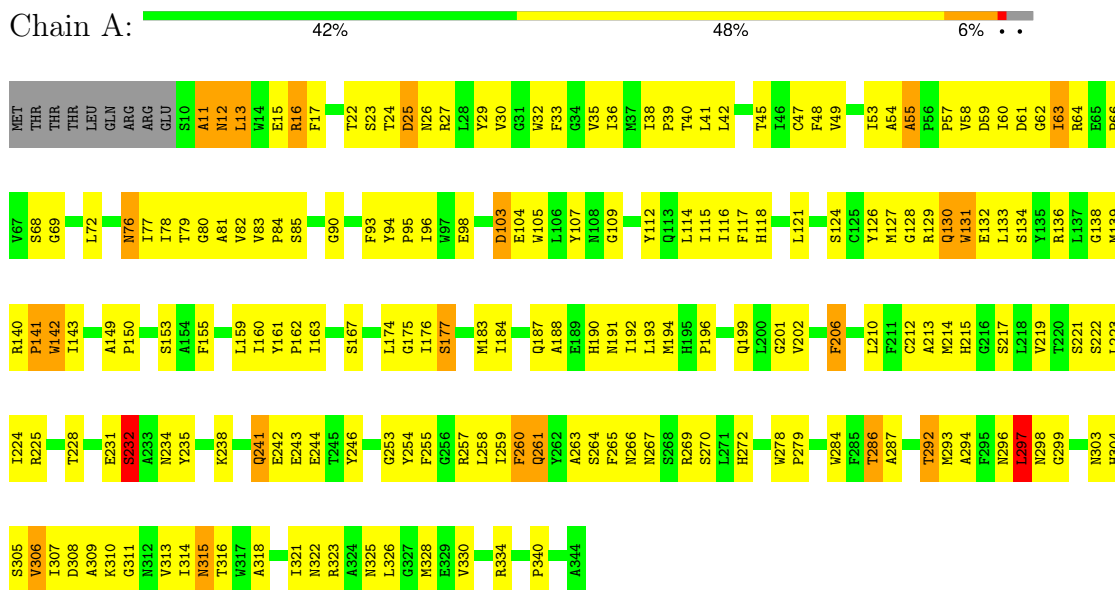
- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

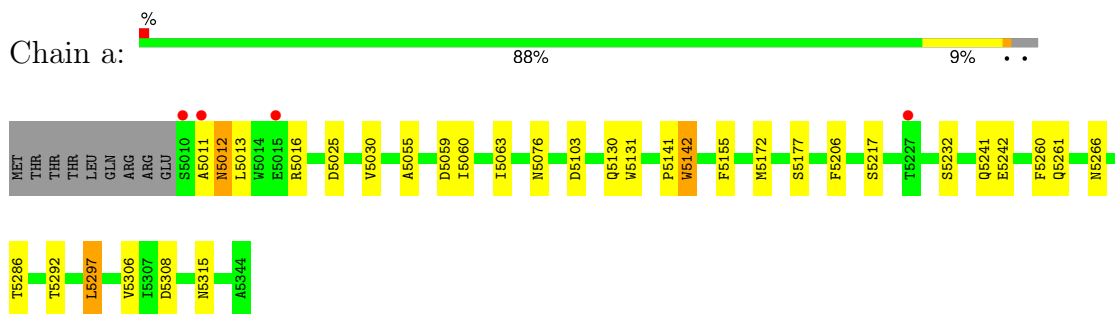
3 Residue-property plots

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

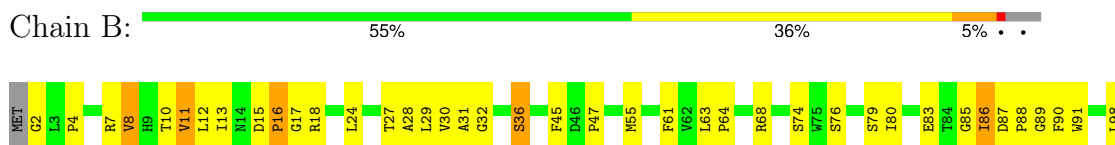
- Molecule 1: Photosystem Q(B) protein

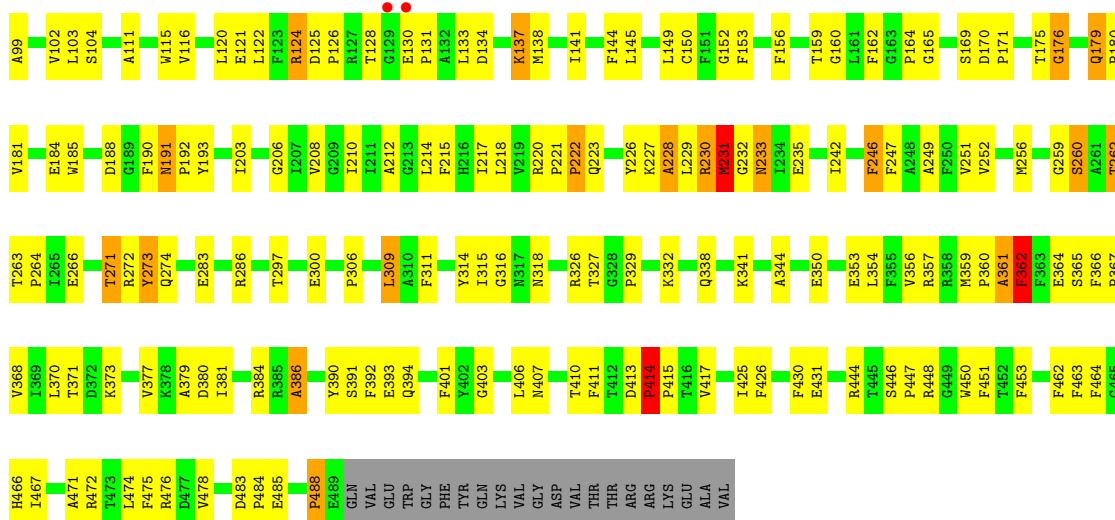


- Molecule 1: Photosystem Q(B) protein

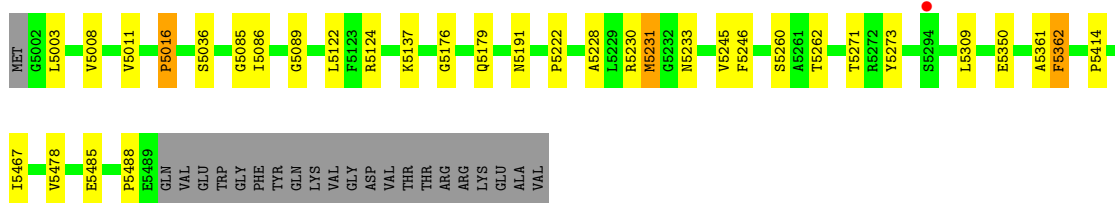
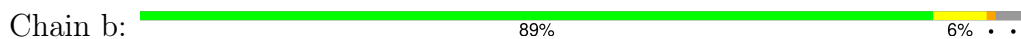


- Molecule 2: CP47 protein

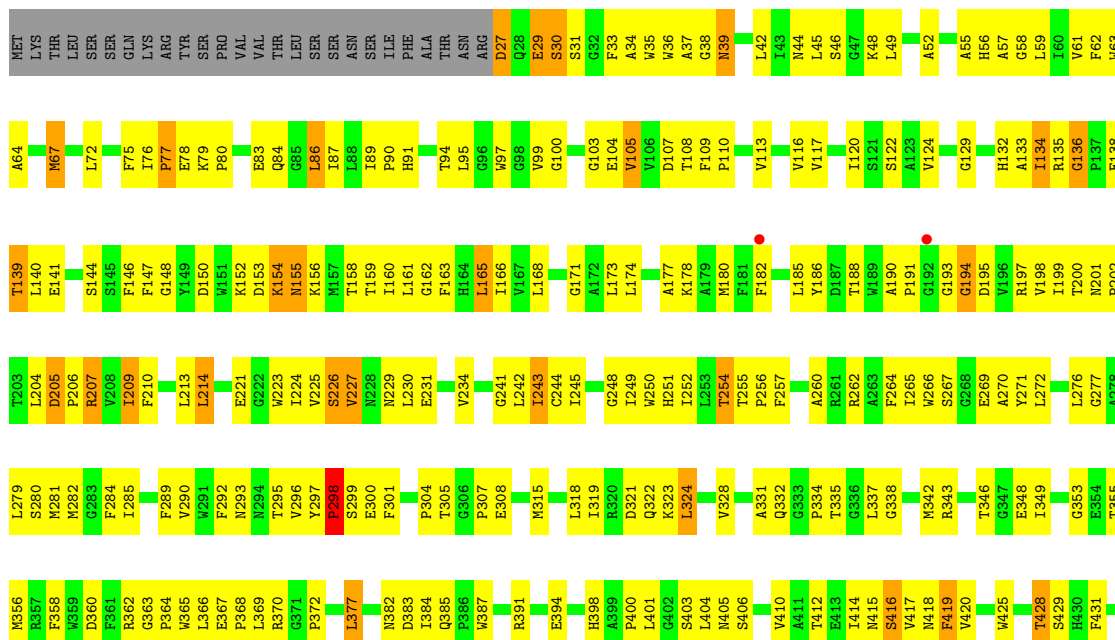


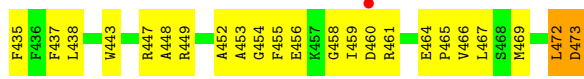


• Molecule 2: CP47 protein

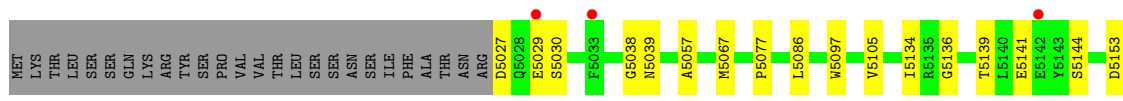
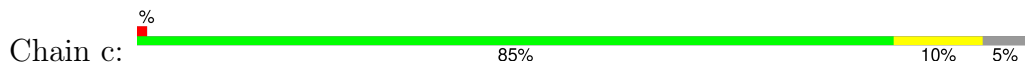


• Molecule 3: photosystem II CP43 protein

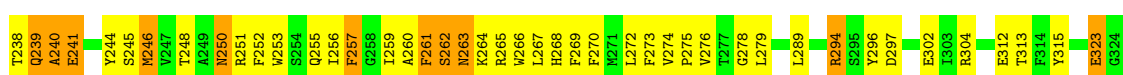
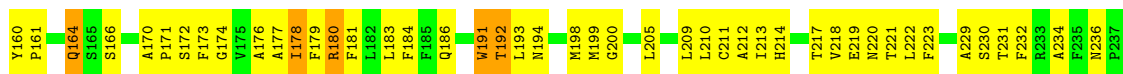
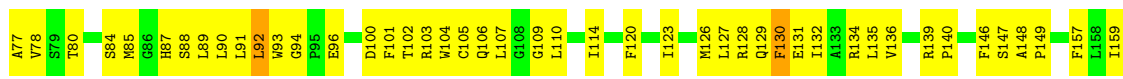
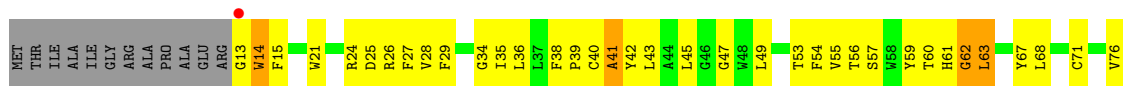




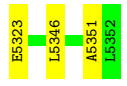
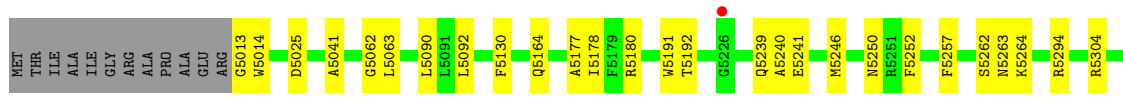
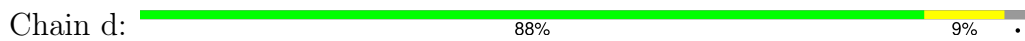
• Molecule 3: photosystem II CP43 protein



• Molecule 4: photosystem II reaction center D2 protein

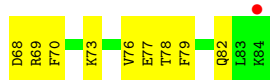
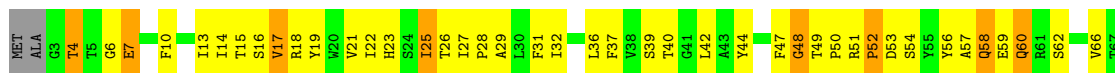


• Molecule 4: photosystem II reaction center D2 protein

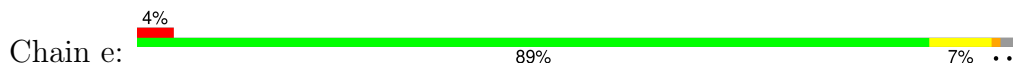


• Molecule 5: Cytochrome b559 alpha subunit





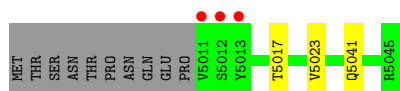
• Molecule 5: Cytochrome b559 alpha subunit



• Molecule 6: Cytochrome b559 beta subunit



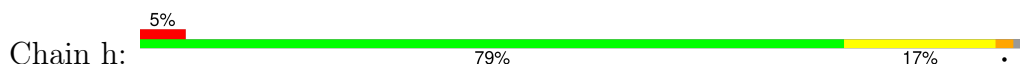
• Molecule 6: Cytochrome b559 beta subunit



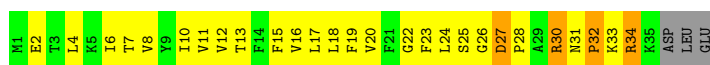
• Molecule 7: Photosystem II reaction center H protein



• Molecule 7: Photosystem II reaction center H protein

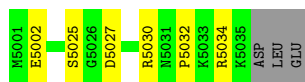


• Molecule 8: Photosystem II reaction center I protein



- 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%

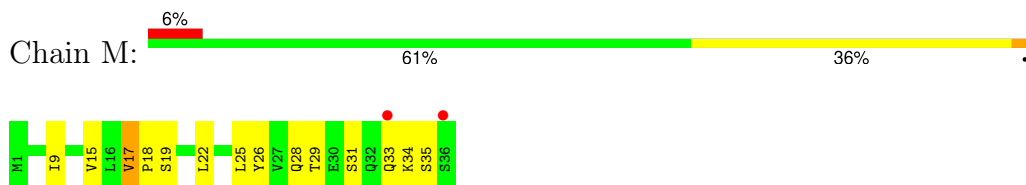


- Molecule 11: Photosystem II reaction center L protein

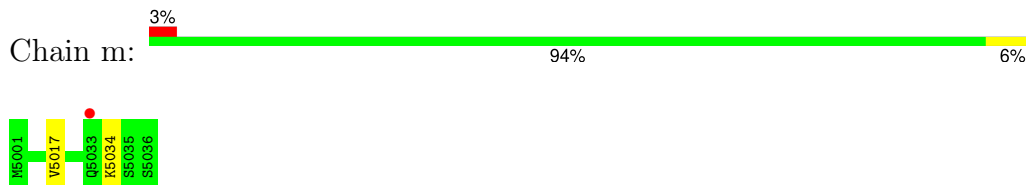
Chain l:  5% 84% 16%



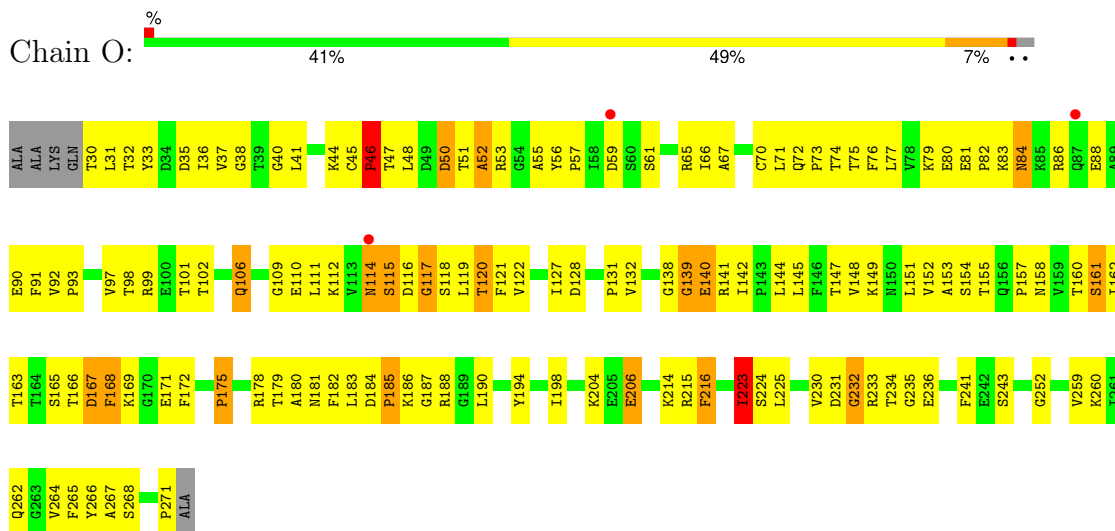
- Molecule 12: Photosystem II reaction center M protein



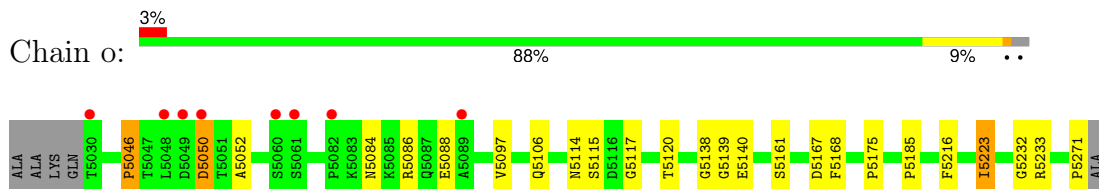
- Molecule 12: Photosystem II reaction center M protein



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



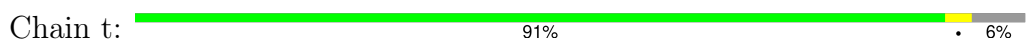
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

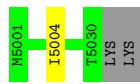


- Molecule 14: Photosystem II reaction center T protein

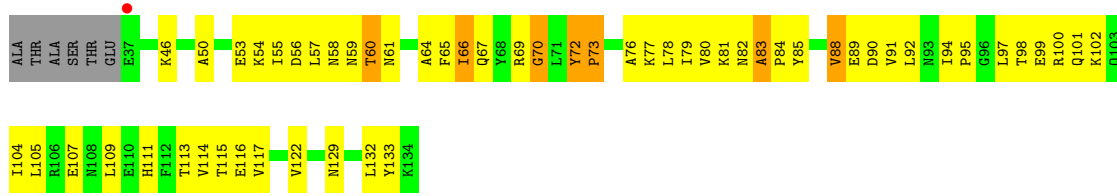


- Molecule 14: Photosystem II reaction center T protein

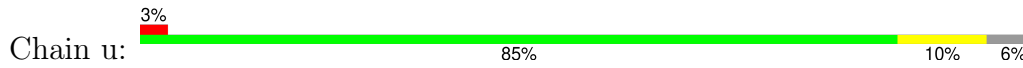




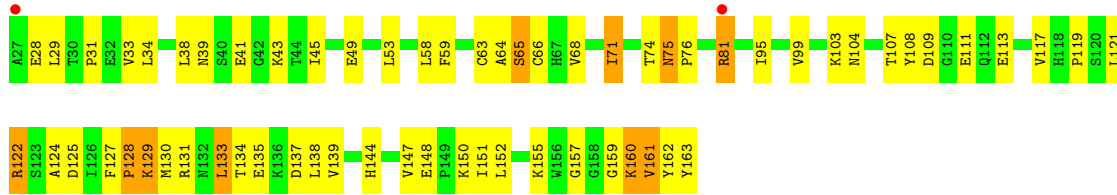
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



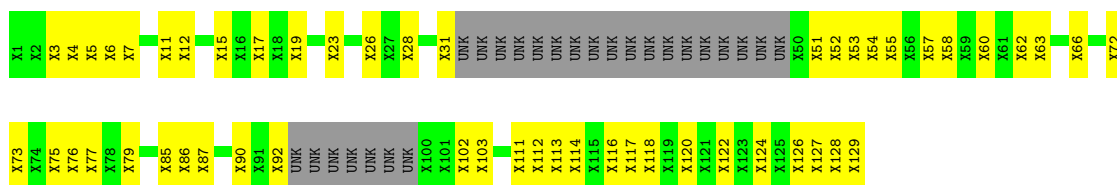
- Molecule 16: Cytochrome c-550



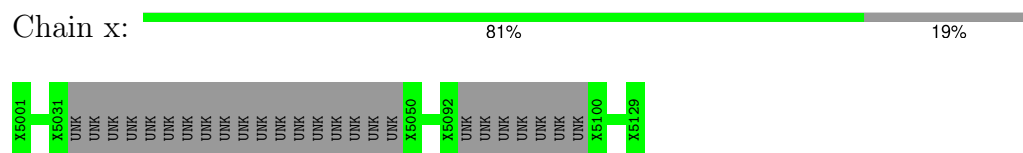
- Molecule 16: Cytochrome c-550



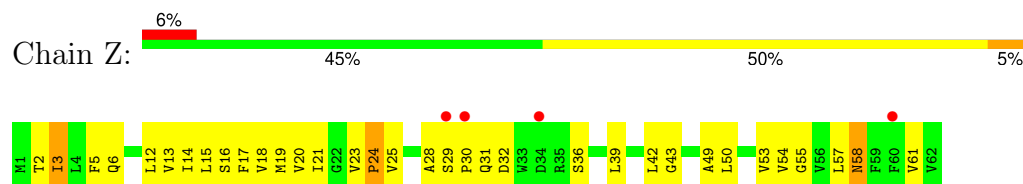
- Molecule 17: Unassigned subunits



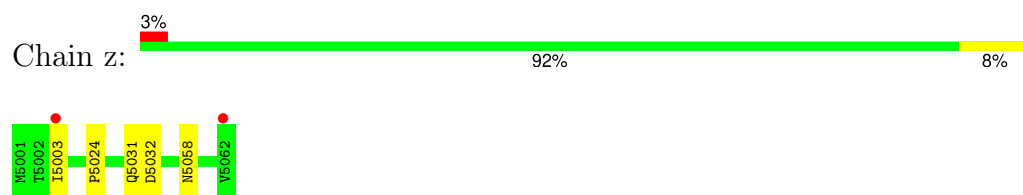
- Molecule 17: Unassigned subunits



- 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 , 0.291	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

5.1 Standard geometry

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:NE2	17:X:26:UNK:CD	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

Continued on next page...

Continued from previous page...

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:HMD2	20:C:493:CLA:H191	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:H	8:I:34:ARG:NE	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:H	8:I:34:ARG:HE	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

Continued on next page...

Continued from previous page...

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:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
1:A:306:VAL:HG23	1:A:306:VAL:O	1.77	0.84
14:T:29:ILE:H	14:T:29:ILE:HD12	1.43	0.84
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
20:C:493:CLA:HBD	20:C:493:CLA:HBA1	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:45:CYS:H	13:O:72:GLN:NE2	1.77	0.82
13:O:151:LEU:HD13	13:O:223:ILE:HD11	1.59	0.82
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
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
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

Continued on next page...

Continued from previous page...

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:HG3	1:A:257:ARG:HH11	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

Continued on next page...

Continued from previous page...

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
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	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:H	13:O:144:LEU:HD23	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
21:A:562:PHO:HBC1	4:D:275:PRO:HB2	1.71	0.72
3:C:204:LEU:H	3:C:204:LEU:CD2	2.02	0.72
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	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
3:C:29:GLU:HB3	10:K:46:ARG:O	1.89	0.72
24:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	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

Continued on next page...

Continued from previous page...

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:HH11	13:O:178:ARG:HG3	1.56	0.69
2:B:124:ARG:HG3	2:B:124:ARG:NH1	2.07	0.69
21:A:562:PHO:H42	4:D:41:ALA:HB1	1.74	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
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
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
20:C:495:CLA:HBD	20:C:495:CLA:HBA1	1.75	0.69
3:C:214:LEU:HD23	3:C:214:LEU:H	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
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	0.68
3:C:363:GLY:O	3:C:367:GLU:HG2	1.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	0.67
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
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
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	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
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:C	14:T:4:ILE:HD13	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:HD12	13:O:77:LEU:N	2.10	0.65
24:X:130:BCR:HC8	24:X:130:BCR:H331	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

Continued on next page...

Continued from previous page...

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:133:LEU:HA	7:H:15:ASN:HD21	1.62	0.65
2:B:392:PHE:O	2:B:393:GLU:HB2	1.96	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
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	0.63
24:C:504:BCR:H343	24:C:504:BCR:H311	1.81	0.63
24:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
7:H:12:ARG:N	7:H:13:PRO:HD2	2.13	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
2:B:120:LEU:HD13	20:B:526:CLA:HMD2	1.79	0.63
20:B:519:CLA:HMC2	24:H:107:BCR:H343	1.81	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
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	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
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:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	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:52:ALA:HA	20:C:501:CLA:HMB3	1.80	0.63
3:C:417:VAL:HG22	3:C:417:VAL:O	1.99	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:HG3	13:O:110:GLU:O	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:NE2	17:X:26:UNK:HG2	2.20	0.61
1:A:25:ASP:HB3	4:D:251:ARG:HH22	1.65	0.61
6:F:41:GLN:HA	6:F:41:GLN:NE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
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
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
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	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:HG3	1:A:257:ARG:NH1	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
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	0.60
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.83	0.60
15:U:66:ILE:O	15:U:66:ILE:HG22	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
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	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:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
4:D:337:GLU:HG2	4:D:339:PHE:CE2	2.36	0.59
5:E:60:GLN:HG3	5:E:60:GLN:O	2.01	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59

Continued on next page...

Continued from previous page...

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:24:LEU:HD21	20:B:526:CLA:HAB	1.86	0.58
2:B:471:ALA:O	2:B:475:PHE:HB2	2.04	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58
2:B:149:LEU:HG	20:B:513:CLA:CBC	2.28	0.58

Continued on next page...

Continued from previous page...

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:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
13:O:152:VAL:O	13:O:152:VAL:HG13	2.04	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:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	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
9:J:14:ALA:HB1	24:X:130:BCR:H393	1.85	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	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
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	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
4:D:273:PHE:CZ	28:L:210:MGE:H3B2	2.40	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	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
13:O:168:PHE:N	13:O:168:PHE:CD1	2.71	0.57
14:T:4:ILE:HD13	14:T:4:ILE:O	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:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57

Continued on next page...

Continued from previous page...

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
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
13:O:73:PRO:HG2	13:O:102:THR:OG1	2.05	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
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
4:D:221:THR:HG22	4:D:245:SER:H	1.69	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	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: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:198:VAL:HG12	3:C:200:THR:HG23	1.87	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:55:MET:HE3	2:B:80:ILE:HG12	1.87	0.56
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.41	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:HG3	16:V:81:ARG:HH11	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
1:A:221:SER:HA	4:D:139:ARG:HB2	1.86	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
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

Continued on next page...

Continued from previous page...

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:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
2:B:233:ASN:HD22	2:B:233:ASN:C	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:HH11	2:B:18:ARG:HG3	1.70	0.55
20:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.55
10:K:39:TRP:NE1	17:X:31:UNK:HG3	2.12	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
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:37:ALA:HA	20:C:498:CLA:O1A	2.06	0.55
3:C:466:VAL:HA	3:C:469:MET:CE	2.36	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

Continued on next page...

Continued from previous page...

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
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.37	0.54
24:B:527:BCR:H322	28:B:530:MGE:H2G	1.89	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
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.89	0.54
3:C:405:ASN:HD22	30:C:509:DGD:C5D	2.19	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
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	0.54
2:B:221:PRO:O	7:H:21:VAL:HG23	2.08	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
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
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	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:67:TYR:CD2	4:D:76:VAL:HG11	2.43	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	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:68:LEU:HD13	6:F:40:MET:HE2	1.89	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	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
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	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:84:GLN:HB2	3:C:86:LEU:CD2	2.37	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
11:L:11:GLU:HG2	11:L:12:LEU:N	2.24	0.53
11:L:14:ARG:NH1	11:L:14:ARG:HG3	2.22	0.53
14:T:29:ILE:H	14:T:29:ILE:CD1	2.18	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
3:C:318:LEU:HD23	3:C:318:LEU:C	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:40:THR:HG22	1:A:118:HIS:O	2.09	0.53
1:A:314:ILE:O	1:A:314:ILE:CG2	2.55	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
2:B:102:VAL:HA	24:B:528:BCR:C40	2.39	0.52
2:B:152:GLY:C	20:B:516:CLA:HMC3	2.30	0.52
2:B:476:ARG:HH11	2:B:476:ARG:HG3	1.74	0.52
3:C:362:ARG:HH11	3:C:362:ARG:HG3	1.71	0.52
20:C:492:CLA:H111	20:C:493:CLA:HMB2	1.90	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:63:TRP:O	3:C:64:ALA:C	2.47	0.52
3:C:318:LEU:HD23	3:C:318:LEU:O	2.10	0.52
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
2:B:263:THR:HG22	2:B:263:THR:O	2.08	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	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
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:29:GLU:C	3:C:31:SER:H	2.13	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	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
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
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
3:C:116:VAL:HG21	24:C:505:BCR:C32	2.40	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
20:C:503:CLA:HMC2	24:C:505:BCR:H372	1.91	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:O	16:V:33:VAL:HG12	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:HD23	13:O:144:LEU:N	2.23	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
2:B:463:PHE:CZ	20:B:518:CLA:HBB1	2.43	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
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
20:C:493:CLA:HBA1	20:C:493:CLA:CBF	2.37	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:C	2:B:380:ASP:OD2	2.47	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	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

Continued on next page...

Continued from previous page...

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:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
14:T:29:ILE:HD12	14:T:29:ILE:N	2.18	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
3:C:438:LEU:HD11	20:C:495:CLA:HBB1	1.92	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
20:C:495:CLA:HMD3	20:C:497:CLA:HAB	1.92	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
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.51
2:B:175:THR:HG22	2:B:175:THR:O	2.11	0.51
3:C:48:LYS:HE2	3:C:132:HIS:O	2.11	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:HD12	4:D:63:LEU:N	2.26	0.50
6:F:45:ARG:OXT	6:F:45:ARG:HG2	2.11	0.50
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
20:A:560:CLA:HAB	20:D:354:CLA:H72	1.93	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
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

Continued on next page...

Continued from previous page...

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:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.50
2:B:341:LYS:O	2:B:406:LEU:HB2	2.11	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:35:ILE:HG22	4:D:35:ILE:O	2.12	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
7:H:59:ASN:O	7:H:59:ASN:OD1	2.29	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
2:B:246:PHE:C	2:B:246:PHE:HD1	2.15	0.49
2:B:286:ARG:C	2:B:286:ARG:HD3	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:55:VAL:HG12	4:D:56:THR:N	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	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:51:THR:O	13:O:52:ALA:O	2.30	0.49
13:O:216:PHE:C	13:O:216:PHE:HD2	2.15	0.49
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.28	0.49
2:B:13:ILE:O	2:B:13:ILE:HG22	2.11	0.49
2:B:124:ARG:HD3	2:B:131:PRO:N	2.28	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:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	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:HA	3:C:78:GLU:OE2	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:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
10:K:43:VAL:HG12	10:K:43:VAL:O	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:H23C	24:T:5104:BCR:H403	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

Continued on next page...

Continued from previous page...

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
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	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: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
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
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
1:A:140:ARG:NH2	25:A:567:LHG:O5	2.46	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.94	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:HG3	2:B:18:ARG:NH1	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:83:LYS:O	13:O:84:ASN:CB	2.60	0.48
13:O:264:VAL:HG12	13:O:265:PHE:N	2.29	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:C	4:D:180:ARG:HD3	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:86:ILE:C	2:B:86:ILE:HD12	2.33	0.48
2:B:353:GLU:HB3	2:B:373:LYS:HZ1	1.78	0.48

Continued on next page...

Continued from previous page...

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:O	10:K:17:ILE:HG22	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:OD1	17:X:86:UNK:N	2.45	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	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:O	4:D:193:LEU:HG	2.13	0.48
13:O:33:TYR:C	13:O:35:ASP:N	2.66	0.48
1:A:77:ILE:HD13	11:L:29:LEU:HG	1.96	0.48
1:A:191:ASN:ND2	1:A:194:MET:HB2	2.28	0.48
2:B:61:PHE:CZ	20:B:517:CLA:HBB1	2.49	0.48
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
7:H:45:ILE:O	7:H:46:LEU:C	2.51	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:5:PHE:HE1	18:Z:54:VAL:HG13	1.79	0.48
18:Z:20:VAL:O	18:Z:24:PRO:HG2	2.14	0.48
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	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
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	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
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:78:ILE:HD13	11:L:33:SER:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:HB3	1:A:162:PRO:HD3	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:12:LEU:HD12	20:B:522:CLA:HBB1	1.96	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:62:PHE:CE2	10:K:28:ILE:HB	2.50	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:449:ARG:HD3	20:C:495:CLA:HED1	1.95	0.47
3:C:459:ILE:HD12	4:D:245:SER:OG	2.13	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
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:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
1:A:314:ILE:O	1:A:314:ILE:HG22	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 ⁷	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
2:B:179:GLN:HA	2:B:179:GLN:HE21	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:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47
20:A:558:CLA:H201	28:D:360:MGE:H232	1.96	0.47
2:B:7:ARG:NH2	28:D:359:MGE:O3D	2.47	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	0.47
20:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:H:12:ARG:HG3	7:H:12:ARG:HH11	1.80	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47
9:J:33:TYR:CD2	9:J:33:TYR:N	2.83	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
17:X:111:UNK:C	17:X:113:UNK:N	2.76	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:55:ALA:C	24:C:504:BCR:H373	2.35	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	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
1:A:296:ASN:HB2	3:C:400:PRO:O	2.15	0.47
3:C:201:ASN:OD1	3:C:201:ASN:O	2.33	0.47
4:D:214:HIS:HA	22:D:356:PQ9:O4	2.15	0.47
14:T:1:MET:HG2	14:T:1:MET:O	2.14	0.47
15:U:73:PRO:HG2	16:V:109:ASP:H	1.80	0.47
16:V:133:LEU:HD23	16:V:133:LEU:H	1.80	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
17:X:114:UNK:O	17:X:117:UNK:HB1	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:N	13:O:225:LEU:HD12	2.29	0.46
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.46
2:B:390:TYR:N	2:B:390:TYR:CD1	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

Continued on next page...

Continued from previous page...

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:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	1.97	0.46
3:C:89:ILE:N	3:C:90:PRO:CD	2.79	0.46
3:C:290:VAL:HG23	3:C:297:TYR:CE1	2.50	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
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
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	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:CD	17:X:126:UNK:N	2.77	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
1:A:183:MET:HB3	20:A:558:CLA:HBC2	1.98	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	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:39:ASN:OD1	20:C:499:CLA:HBB2	2.16	0.46
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
6:F:45:ARG:OXT	6:F:45:ARG:CG	2.64	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
12:M:9:ILE:HD12	12:M:9:ILE:N	2.30	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
14:T:11:ALA:HB3	24:T:5104:BCR:H363	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
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
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	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
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:57:PRO:HA	1:A:68:SER:HA	1.97	0.46
1:A:63:ILE:HG21	3:C:335:THR:HG21	1.97	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
1:A:210:LEU:HD12	1:A:210:LEU:O	2.16	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
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
17:X:117:UNK:HB1	17:X:117:UNK:NZ	2.31	0.46
2:B:149:LEU:HB2	20:B:514:CLA:H203	1.97	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
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
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.46
20:B:518:CLA:H51	20:B:519:CLA:H101	1.97	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:163:ILE:HD13	30:C:507:DGD:HB22	1.97	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	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
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
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

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
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
6:F:30:THR:HG22	6:F:34:LEU:HD12	1.98	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:H61	22:A:564:PQ9:H91	1.69	0.45
2:B:156:PHE:HB2	20:B:516:CLA:HAC1	1.99	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
20:B:511:CLA:CAA	24:H:107:BCR:H19C	2.47	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
11:L:14:ARG:HH11	11:L:14:ARG:CG	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:HG2	2:B:235:GLU:O	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:CD1	13:O:265:PHE:C	2.90	0.45
1:A:131:TRP:CZ2	20:C:495:CLA:HAA1	2.51	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	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
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.45
9:J:8:ILE:HD12	9:J:8:ILE:N	2.30	0.45
1:A:210:LEU:HD13	21:A:562:PHO:ND	2.31	0.45
3:C:250:TRP:HE1	20:C:496:CLA:CED	2.30	0.45
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.97	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	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
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:CD	4:D:96:GLU:H	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

Continued on next page...

Continued from previous page...

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:27:ARG:HA	1:A:27:ARG:HD2	1.78	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
2:B:98:LEU:O	2:B:99:ALA:C	2.55	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
3:C:264:PHE:CD2	3:C:264:PHE:N	2.85	0.45
3:C:349:ILE:HD13	13:O:127:ILE:CD1	2.47	0.45
7:H:55:LEU:HB2	7:H:58:VAL:HG21	1.98	0.45
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	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
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:68:LEU:HB2	6:F:40:MET:HE1	1.99	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	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:7:ARG:O	2:B:8:VAL:C	2.55	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
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:H3A	20:B:517:CLA:HBA2	1.71	0.44
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
32:F:51:HEM:HHA	32:F:51:HEM:HAD2	1.67	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
4:D:100:ASP:OD1	4:D:100:ASP:C	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

Continued on next page...

Continued from previous page...

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:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.64	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:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	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:N	3:C:257:PHE:CD1	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:42:LEU:HD11	20:C:501:CLA:C1A	2.48	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	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
10:K:21:LEU:HD11	24:X:130:BCR:HC42	1.99	0.44
17:X:128:UNK:O	17:X:129:UNK:C	2.66	0.44
1:A:13:LEU:HD23	1:A:13:LEU:H	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

Continued on next page...

Continued from previous page...

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:17:VAL:HA	9:J:8:ILE:HD11	2.00	0.44
5:E:26:THR:O	5:E:29:ALA:HB3	2.18	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
3:C:321:ASP:OD2	15:U:129:ASN:HB2	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:HD2	11:L:7:ARG:HA	1.69	0.43
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	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:36:SER:OG	24:B:528:BCR:H362	2.18	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
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:93:TRP:CZ2	20:D:355:CLA:O1A	2.71	0.43
4:D:256:ILE:O	4:D:256:ILE:HG12	2.19	0.43
4:D:263:ASN:HB3	28:D:360:MGE:O3D	2.19	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
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43
20:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43

Continued on next page...

Continued from previous page...

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: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
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	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:H91	22:D:356:PQ9:H61	1.75	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
1:A:32:TRP:CE2	8:I:22:GLY:HA3	2.53	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
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:25:ASP:HA	4:D:251:ARG:NH2	2.32	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
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

Continued on next page...

Continued from previous page...

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:O	13:O:231:ASP:OD1	2.37	0.43
14:T:4:ILE:C	14:T:4:ILE:CD1	2.85	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	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
24:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
4:D:134:ARG:NE	4:D:134:ARG:HA	2.34	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	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:HBA1	20:B:515:CLA:CHA	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:87:ILE:C	3:C:90:PRO:HD2	2.39	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
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.79	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:31:ALA:CA	20:B:515:CLA:HBC3	2.49	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:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
3:C:29:GLU:O	3:C:31:SER:N	2.52	0.42
3:C:104:GLU:O	3:C:105:VAL:C	2.57	0.42

Continued on next page...

Continued from previous page...

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:90:PHE:CZ	2:B:98:LEU:HD23	2.55	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
3:C:201:ASN:N	3:C:202:PRO:CD	2.82	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
4:D:246:MET:CE	4:D:264:LYS:HG3	2.49	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:69:GLY:O	1:A:80:GLY:HA2	2.19	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
20:B:524:CLA:H102	24:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:CD1	3:C:147:PHE:N	2.85	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
4:D:103:ARG:HD3	4:D:103:ARG:HA	1.81	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	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
4:D:47:GLY:HA2	24:D:357:BCR:H332	2.01	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.25	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
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:64:ALA:O	16:V:65:SER:C	2.57	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	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
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.42
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	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:103:LEU:HD21	20:B:515:CLA:HMC3	2.01	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
3:C:168:LEU:CD1	20:C:497:CLA:H2	2.49	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	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:HHA	32:V:552:HEM:HAD2	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:HG	16:V:29:LEU:O	2.18	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	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:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	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
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
20:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	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

Continued on next page...

Continued from previous page...

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:45:CYS:CB	13:O:46:PRO:HD2	2.31	0.41
13:O:266:TYR:CG	13:O:267:ALA:N	2.88	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
25:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.41
3:C:61:VAL:O	3:C:62:PHE:C	2.57	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
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
4:D:267:LEU:C	4:D:267:LEU:CD2	2.88	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	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:O	2:B:208:VAL:HG12	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

Continued on next page...

Continued from previous page...

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
24:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	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:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	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
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	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
3:C:56:HIS:O	3:C:59:LEU:N	2.53	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
20:C:502:CLA:HBA2	20:C:502:CLA:O2D	2.20	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	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
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
1:A:13:LEU:H	1:A:13:LEU:CD2	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

Continued on next page...

Continued from previous page...

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:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	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
20:B:518:CLA:HBA1	20:B:518:CLA:CHA	2.51	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:N	13:O:142:ILE:CD1	2.84	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.40
8:I:30:ARG:H	8:I:30:ARG:HG2	1.60	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
15:U:69:ARG:HE	15:U:69:ARG:HB2	1.69	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
1:A:206:PHE:HD2	1:A:206:PHE:HA	1.75	0.40
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.40
2:B:164:PRO:HD3	20:B:516:CLA:O1D	2.22	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
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
28:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40

Continued on next page...

Continued from previous page...

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:OD1	17:X:85:UNK:N	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
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.40
3:C:252:ILE:O	3:C:252:ILE:HG22	2.21	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 4 are monoatomic and 34 are unknown - 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
24	BCR	h	5107	-	41,41,41	2.04	7 (17%)	56,56,56	2.30	25 (44%)
31	BCT	d	5353	19	3,3,3	2.70	1 (33%)	2,3,3	0.35	0
24	BCR	B	527	-	41,41,41	1.74	8 (19%)	56,56,56	2.08	16 (28%)
20	CLA	B	512	2	63,73,73	1.67	7 (11%)	74,113,113	1.73	12 (16%)
20	CLA	b	5526	-	63,73,73	2.01	11 (17%)	74,113,113	1.86	11 (14%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	1.00	3 (6%)
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.55	8 (11%)
22	PQ9	d	5356	-	30,30,45	0.82	0	38,39,57	1.66	6 (15%)
24	BCR	t	104	-	41,41,41	1.67	10 (24%)	56,56,56	2.28	23 (41%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.46	6 (8%)
21	PHO	A	561	-	50,69,69	1.12	3 (6%)	48,99,99	1.69	12 (25%)
28	MGE	L	210	-	48,48,48	0.99	3 (6%)	56,56,56	1.15	5 (8%)
20	CLA	b	5514	2	63,73,73	1.99	9 (14%)	74,113,113	1.92	10 (13%)
32	HEM	V	552	16	42,50,50	2.00	14 (33%)	46,82,82	2.34	13 (28%)
20	CLA	A	560	-	63,73,73	1.74	9 (14%)	74,113,113	1.82	12 (16%)
24	BCR	C	504	-	41,41,41	1.87	6 (14%)	56,56,56	2.21	22 (39%)
24	BCR	d	5357	-	41,41,41	2.02	8 (19%)	56,56,56	2.33	21 (37%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.07	4 (7%)
20	CLA	B	526	-	63,73,73	1.94	14 (22%)	74,113,113	1.84	10 (13%)
20	CLA	c	5495	-	63,73,73	2.06	9 (14%)	74,113,113	1.95	13 (17%)
26	SQD	a	212	-	24,26,54	3.09	13 (54%)	34,37,65	2.73	13 (38%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.12	4 (7%)
24	BCR	D	357	-	41,41,41	1.96	8 (19%)	56,56,56	2.27	20 (35%)
24	BCR	c	5505	-	41,41,41	2.01	8 (19%)	56,56,56	2.14	19 (33%)
28	MGE	i	5201	-	48,48,48	1.24	7 (14%)	56,56,56	1.08	4 (7%)
24	BCR	a	5566	-	41,41,41	1.68	7 (17%)	56,56,56	2.14	23 (41%)
24	BCR	H	107	-	41,41,41	2.11	6 (14%)	56,56,56	2.29	24 (42%)
32	HEM	f	5051	5,6	42,50,50	2.08	14 (33%)	46,82,82	2.49	14 (30%)
20	CLA	B	524	2	54,64,73	2.01	6 (11%)	63,102,113	2.04	9 (14%)
24	BCR	C	505	-	41,41,41	1.98	9 (21%)	56,56,56	2.13	18 (32%)
24	BCR	b	5528	-	41,41,41	1.74	6 (14%)	56,56,56	2.06	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMT	M	5216	-	36,36,36	1.45	8 (22%)	47,47,47	0.92	2 (4%)
20	CLA	C	498	3	63,73,73	1.69	6 (9%)	74,113,113	1.84	10 (13%)
24	BCR	c	5504	-	41,41,41	2.18	5 (12%)	56,56,56	2.18	23 (41%)
20	CLA	B	525	-	63,73,73	1.82	7 (11%)	74,113,113	1.84	9 (12%)
20	CLA	c	5494	-	44,54,73	2.00	6 (13%)	51,90,113	2.05	9 (17%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.67	11 (17%)
24	BCR	B	529	-	41,41,41	1.79	6 (14%)	56,56,56	2.22	21 (37%)
20	CLA	c	5503	3	48,58,73	2.38	9 (18%)	56,95,113	2.08	6 (10%)
20	CLA	C	501	3	63,73,73	2.06	9 (14%)	74,113,113	1.94	11 (14%)
28	MGE	d	5360	-	41,41,48	1.19	6 (14%)	49,49,56	1.05	4 (8%)
20	CLA	a	5560	-	63,73,73	1.78	9 (14%)	74,113,113	1.84	11 (14%)
24	BCR	x	5130	-	41,41,41	1.95	9 (21%)	56,56,56	2.52	24 (42%)
20	CLA	b	5513	2	63,73,73	1.70	9 (14%)	74,113,113	1.73	14 (18%)
20	CLA	A	563	-	53,63,73	1.82	10 (18%)	62,101,113	1.86	11 (17%)
20	CLA	b	5519	-	63,73,73	1.92	8 (12%)	74,113,113	1.81	12 (16%)
27	LMT	a	5568	-	36,36,36	1.46	6 (16%)	47,47,47	1.09	1 (2%)
20	CLA	C	494	-	44,54,73	1.97	7 (15%)	51,90,113	2.23	9 (17%)
20	CLA	c	5493	3	63,73,73	1.81	7 (11%)	74,113,113	1.90	13 (17%)
24	BCR	b	5529	-	41,41,41	1.66	6 (14%)	56,56,56	2.15	21 (37%)
25	LHG	a	5567	-	38,38,48	2.02	5 (13%)	41,44,54	1.46	4 (9%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.56	9 (13%)
20	CLA	B	519	-	63,73,73	2.00	8 (12%)	74,113,113	1.82	11 (14%)
20	CLA	b	5512	2	63,73,73	1.67	7 (11%)	74,113,113	1.69	10 (13%)
24	BCR	b	5527	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
21	PHO	a	5561	-	50,69,69	1.13	5 (10%)	48,99,99	1.57	11 (22%)
20	CLA	c	5500	-	63,73,73	1.76	8 (12%)	74,113,113	1.79	12 (16%)
27	LMT	A	569	-	36,36,36	1.54	6 (16%)	47,47,47	1.07	1 (2%)
20	CLA	b	5520	-	63,73,73	1.81	11 (17%)	74,113,113	1.75	11 (14%)
22	PQ9	D	356	-	30,30,45	0.91	1 (3%)	38,39,57	1.68	9 (23%)
20	CLA	d	5354	4	63,73,73	1.64	10 (15%)	74,113,113	1.75	11 (14%)
20	CLA	C	496	3	63,73,73	1.89	11 (17%)	74,113,113	1.87	13 (17%)
20	CLA	b	5516	-	63,73,73	1.94	7 (11%)	74,113,113	1.94	8 (10%)
20	CLA	c	5501	3	63,73,73	1.89	7 (11%)	74,113,113	1.91	8 (10%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.47	7 (10%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.06	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	c	5498	3	63,73,73	1.86	8 (12%)	74,113,113	1.88	12 (16%)
20	CLA	C	500	-	63,73,73	1.66	10 (15%)	74,113,113	1.78	12 (16%)
30	DGD	c	5508	-	48,48,67	1.48	8 (16%)	62,62,81	1.71	10 (16%)
20	CLA	C	495	-	63,73,73	2.08	11 (17%)	74,113,113	1.92	12 (16%)
24	BCR	A	566	-	41,41,41	1.63	8 (19%)	56,56,56	2.14	22 (39%)
20	CLA	a	5558	1	63,73,73	1.67	11 (17%)	74,113,113	1.66	12 (16%)
20	CLA	C	491	3	63,73,73	1.76	7 (11%)	74,113,113	1.70	8 (10%)
20	CLA	d	5355	-	48,58,73	2.30	9 (18%)	56,95,113	2.05	9 (16%)
32	HEM	F	51	5,6	42,50,50	2.06	15 (35%)	46,82,82	2.41	15 (32%)
20	CLA	b	5515	-	63,73,73	1.71	11 (17%)	74,113,113	1.83	15 (20%)
24	BCR	T	5104	-	41,41,41	1.55	9 (21%)	56,56,56	2.31	25 (44%)
20	CLA	c	5496	-	63,73,73	1.78	9 (14%)	74,113,113	1.81	11 (14%)
20	CLA	b	5518	2	63,73,73	1.91	6 (9%)	74,113,113	1.89	11 (14%)
20	CLA	c	5499	-	45,55,73	2.04	8 (17%)	52,91,113	2.04	8 (15%)
20	CLA	B	523	-	63,73,73	1.98	8 (12%)	74,113,113	1.86	11 (14%)
20	CLA	a	5563	-	53,63,73	1.84	9 (16%)	62,101,113	1.80	11 (17%)
24	BCR	C	506	-	41,41,41	1.74	8 (19%)	56,56,56	2.23	21 (37%)
20	CLA	C	493	3	63,73,73	1.81	8 (12%)	74,113,113	1.91	13 (17%)
20	CLA	A	559	-	63,73,73	1.73	7 (11%)	74,113,113	1.72	8 (10%)
20	CLA	b	5524	2	54,64,73	1.91	6 (11%)	63,102,113	1.93	8 (12%)
25	LHG	A	567	-	38,38,48	1.98	5 (13%)	41,44,54	1.51	4 (9%)
27	LMT	m	216	-	36,36,36	1.45	7 (19%)	47,47,47	0.98	3 (6%)
20	CLA	B	521	2	63,73,73	1.85	9 (14%)	74,113,113	1.90	11 (14%)
20	CLA	C	502	-	49,59,73	2.16	10 (20%)	56,96,113	2.13	11 (19%)
26	SQD	t	213	-	45,47,54	2.81	23 (51%)	55,58,65	2.49	14 (25%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.11	6 (10%)
32	HEM	v	5552	16	42,50,50	2.11	15 (35%)	46,82,82	2.34	15 (32%)
20	CLA	B	511	-	39,49,73	2.25	11 (28%)	46,84,113	2.11	9 (19%)
31	BCT	D	353	19	3,3,3	2.28	1 (33%)	2,3,3	0.32	0
30	DGD	c	5509	-	58,58,67	1.35	7 (12%)	72,72,81	1.39	6 (8%)
26	SQD	A	5212	-	24,26,54	2.85	13 (54%)	34,37,65	2.65	11 (32%)
20	CLA	D	354	4	63,73,73	1.70	8 (12%)	74,113,113	1.68	10 (13%)
20	CLA	D	355	-	48,58,73	2.30	11 (22%)	56,95,113	2.07	11 (19%)
20	CLA	b	5511	-	39,49,73	2.46	10 (25%)	46,84,113	2.18	9 (19%)
27	LMT	T	217	-	36,36,36	1.40	5 (13%)	47,47,47	1.03	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	514	2	63,73,73	1.98	9 (14%)	74,113,113	1.89	10 (13%)
20	CLA	C	499	-	45,55,73	2.28	9 (20%)	52,91,113	2.09	10 (19%)
20	CLA	B	513	2	63,73,73	1.87	11 (17%)	74,113,113	1.76	11 (14%)
20	CLA	b	5523	-	63,73,73	1.87	10 (15%)	74,113,113	1.89	11 (14%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	4 (8%)
20	CLA	b	5521	2	63,73,73	1.56	6 (9%)	74,113,113	1.84	12 (16%)
26	SQD	A	568	-	52,54,54	2.59	31 (59%)	62,65,65	2.55	18 (29%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.96	3 (5%)
22	PQ9	A	564	-	30,30,45	0.85	0	38,39,57	1.50	8 (21%)
20	CLA	B	516	-	63,73,73	1.82	6 (9%)	74,113,113	1.90	8 (10%)
20	CLA	B	515	-	63,73,73	1.78	10 (15%)	74,113,113	1.86	14 (18%)
26	SQD	d	5358	-	52,54,54	2.58	29 (55%)	62,65,65	2.53	18 (29%)
20	CLA	a	5559	-	63,73,73	1.61	6 (9%)	74,113,113	1.75	10 (13%)
20	CLA	B	518	2	63,73,73	1.91	6 (9%)	74,113,113	1.91	9 (12%)
20	CLA	B	517	-	63,73,73	2.03	7 (11%)	74,113,113	1.96	12 (16%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.16	6 (10%)
21	PHO	A	562	-	50,69,69	1.12	3 (6%)	48,99,99	1.66	10 (20%)
20	CLA	c	5491	3	63,73,73	1.90	7 (11%)	74,113,113	1.91	10 (13%)
24	BCR	c	5506	-	41,41,41	1.95	7 (17%)	56,56,56	2.16	20 (35%)
20	CLA	c	5492	3	58,68,73	1.76	9 (15%)	68,107,113	1.93	9 (13%)
30	DGD	C	509	-	58,58,67	1.12	7 (12%)	72,72,81	1.40	5 (6%)
20	CLA	C	497	-	63,73,73	1.78	9 (14%)	74,113,113	1.95	11 (14%)
20	CLA	B	520	-	63,73,73	1.71	10 (15%)	74,113,113	1.76	12 (16%)
20	CLA	b	5522	-	63,73,73	1.87	8 (12%)	74,113,113	1.76	7 (9%)
21	PHO	a	5562	-	50,69,69	1.09	3 (6%)	48,99,99	1.64	11 (22%)
20	CLA	C	503	3	48,58,73	2.28	8 (16%)	56,95,113	2.08	10 (17%)
22	PQ9	a	5564	-	30,30,45	0.86	1 (3%)	38,39,57	1.46	6 (15%)
20	CLA	B	522	-	63,73,73	1.83	7 (11%)	74,113,113	1.75	9 (12%)
24	BCR	B	528	-	41,41,41	1.93	6 (14%)	56,56,56	2.02	17 (30%)
28	MGE	l	5210	-	48,48,48	0.90	4 (8%)	56,56,56	1.12	5 (8%)
24	BCR	X	130	-	41,41,41	1.93	8 (19%)	56,56,56	2.54	23 (41%)
20	CLA	c	5502	-	49,59,73	2.29	10 (20%)	56,96,113	2.17	11 (19%)
20	CLA	c	5497	-	63,73,73	1.81	10 (15%)	74,113,113	1.85	11 (14%)
20	CLA	b	5525	-	63,73,73	1.85	6 (9%)	74,113,113	1.87	9 (12%)
26	SQD	L	5213	-	45,47,54	2.81	24 (53%)	55,58,65	2.42	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	C	492	3	58,68,73	1.75	9 (15%)	68,107,113	1.91	11 (16%)
20	CLA	A	558	1	63,73,73	1.70	8 (12%)	74,113,113	1.71	10 (13%)
20	CLA	b	5517	-	63,73,73	1.82	8 (12%)	74,113,113	1.86	9 (12%)

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
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	B	512	2	1/1/15/20	10/37/115/115	-
20	CLA	b	5526	-	1/1/15/20	10/37/115/115	-
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	A	561	-	-	12/37/103/103	0/5/6/6
28	MGE	L	210	-	-	23/43/63/63	0/1/1/1
20	CLA	b	5514	2	1/1/15/20	12/37/115/115	-
32	HEM	V	552	16	-	4/12/54/54	-
20	CLA	A	560	-	1/1/15/20	7/37/115/115	-
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
28	MGE	d	5359	-	-	13/42/62/63	0/1/1/1
28	MGE	I	201	-	-	24/43/63/63	0/1/1/1
20	CLA	B	526	-	1/1/15/20	10/37/115/115	-
20	CLA	c	5495	-	1/1/15/20	16/37/115/115	-
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
32	HEM	f	5051	5,6	-	2/12/54/54	-
20	CLA	B	524	2	1/1/13/20	7/27/105/115	-
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
20	CLA	C	498	3	1/1/15/20	16/37/115/115	-
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
20	CLA	B	525	-	1/1/15/20	12/37/115/115	-
20	CLA	c	5494	-	1/1/11/20	7/15/93/115	-
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
24	BCR	B	529	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5503	3	1/1/12/20	5/19/97/115	-
20	CLA	C	501	3	1/1/15/20	13/37/115/115	-
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
20	CLA	a	5560	-	1/1/15/20	7/37/115/115	-
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5513	2	1/1/15/20	10/37/115/115	-
20	CLA	A	563	-	1/1/13/20	5/25/103/115	-
20	CLA	b	5519	-	1/1/15/20	11/37/115/115	-
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
20	CLA	C	494	-	1/1/11/20	7/15/93/115	-
20	CLA	c	5493	3	1/1/15/20	10/37/115/115	-
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
25	LHG	a	5567	-	-	14/43/43/53	-
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	B	519	-	1/1/15/20	11/37/115/115	-
20	CLA	b	5512	2	1/1/15/20	10/37/115/115	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
21	PHO	a	5561	-	-	12/37/103/103	0/5/6/6
20	CLA	c	5500	-	1/1/15/20	11/37/115/115	-
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
20	CLA	b	5520	-	1/1/15/20	11/37/115/115	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
20	CLA	d	5354	4	1/1/15/20	8/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	C	496	3	1/1/15/20	11/37/115/115	-
20	CLA	b	5516	-	1/1/15/20	13/37/115/115	-
20	CLA	c	5501	3	1/1/15/20	11/37/115/115	-
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	c	5498	3	1/1/15/20	16/37/115/115	-
20	CLA	C	500	-	1/1/15/20	11/37/115/115	-
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
20	CLA	C	495	-	1/1/15/20	16/37/115/115	-
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
20	CLA	a	5558	1	1/1/15/20	9/37/115/115	-
20	CLA	C	491	3	1/1/15/20	7/37/115/115	-
20	CLA	d	5355	-	1/1/12/20	9/19/97/115	-
32	HEM	F	51	5,6	-	2/12/54/54	-
20	CLA	b	5515	-	1/1/15/20	17/37/115/115	-
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5496	-	1/1/15/20	11/37/115/115	-
20	CLA	b	5518	2	1/1/15/20	14/37/115/115	-
20	CLA	c	5499	-	1/1/11/20	6/16/94/115	-
20	CLA	B	523	-	1/1/15/20	13/37/115/115	-
20	CLA	a	5563	-	1/1/13/20	5/25/103/115	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
20	CLA	C	493	3	1/1/15/20	10/37/115/115	-
20	CLA	A	559	-	1/1/15/20	12/37/115/115	-
20	CLA	b	5524	2	1/1/13/20	7/27/105/115	-
25	LHG	A	567	-	-	16/43/43/53	-
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	B	521	2	1/1/15/20	7/37/115/115	-
20	CLA	C	502	-	1/1/12/20	7/21/99/115	-
26	SQD	t	213	-	-	20/42/62/69	0/1/1/1
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
32	HEM	v	5552	16	-	4/12/54/54	-
20	CLA	B	511	-	1/1/10/20	2/8/86/115	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	5212	-	-	5/19/39/69	0/1/1/1
20	CLA	D	354	4	1/1/15/20	10/37/115/115	-
20	CLA	D	355	-	1/1/12/20	9/19/97/115	-
20	CLA	b	5511	-	1/1/10/20	2/8/86/115	-
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
20	CLA	B	514	2	1/1/15/20	11/37/115/115	-
20	CLA	C	499	-	1/1/11/20	6/16/94/115	-
20	CLA	B	513	2	1/1/15/20	12/37/115/115	-
20	CLA	b	5523	-	1/1/15/20	13/37/115/115	-
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
20	CLA	b	5521	2	1/1/15/20	7/37/115/115	-
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	516	-	1/1/15/20	13/37/115/115	-
20	CLA	B	515	-	1/1/15/20	17/37/115/115	-
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
20	CLA	a	5559	-	1/1/15/20	12/37/115/115	-
20	CLA	B	518	2	1/1/15/20	14/37/115/115	-
20	CLA	B	517	-	1/1/15/20	12/37/115/115	-
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
21	PHO	A	562	-	-	9/37/103/103	0/5/6/6
20	CLA	c	5491	3	1/1/15/20	9/37/115/115	-
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5492	3	1/1/14/20	9/31/109/115	-
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
20	CLA	C	497	-	1/1/15/20	7/37/115/115	-
20	CLA	B	520	-	1/1/15/20	13/37/115/115	-
20	CLA	b	5522	-	1/1/15/20	12/37/115/115	-
21	PHO	a	5562	-	-	9/37/103/103	0/5/6/6
20	CLA	C	503	3	1/1/12/20	5/19/97/115	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	522	-	1/1/15/20	12/37/115/115	-
24	BCR	B	528	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	MGE	l	5210	-	-	23/43/63/63	0/1/1/1
24	BCR	X	130	-	-	5/29/63/63	0/2/2/2
20	CLA	c	5502	-	1/1/12/20	6/21/99/115	-
20	CLA	c	5497	-	1/1/15/20	8/37/115/115	-
20	CLA	b	5525	-	1/1/15/20	12/37/115/115	-
26	SQD	L	5213	-	-	21/42/62/69	0/1/1/1
20	CLA	C	492	3	1/1/14/20	9/31/109/115	-
20	CLA	A	558	1	1/1/15/20	8/37/115/115	-
20	CLA	b	5517	-	1/1/15/20	12/37/115/115	-

All (1145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	523	CLA	CHB-C4A	11.56	1.43	1.33
20	C	501	CLA	CHB-C4A	11.29	1.43	1.33
20	b	5525	CLA	CHB-C4A	11.17	1.43	1.33
20	C	495	CLA	CHB-C4A	11.16	1.43	1.33
20	b	5511	CLA	CHB-C4A	10.99	1.43	1.33
20	C	499	CLA	CHB-C4A	10.93	1.43	1.33
20	c	5503	CLA	CHB-C4A	10.89	1.43	1.33
20	d	5355	CLA	CHB-C4A	10.88	1.43	1.33
20	B	525	CLA	CHB-C4A	10.84	1.43	1.33
20	c	5502	CLA	CHB-C4A	10.82	1.43	1.33
20	B	519	CLA	CHB-C4A	10.72	1.43	1.33
20	D	355	CLA	CHB-C4A	10.72	1.43	1.33
20	b	5523	CLA	CHB-C4A	10.69	1.43	1.33
20	B	514	CLA	CHB-C4A	10.66	1.43	1.33
20	b	5526	CLA	CHB-C4A	10.49	1.42	1.33
20	b	5519	CLA	CHB-C4A	10.49	1.42	1.33
20	B	522	CLA	CHB-C4A	10.39	1.42	1.33
20	b	5514	CLA	CHB-C4A	10.38	1.42	1.33
20	B	517	CLA	CHB-C4A	10.35	1.42	1.33
20	B	521	CLA	CHB-C4A	10.29	1.42	1.33
20	A	559	CLA	CHB-C4A	10.28	1.42	1.33
20	b	5520	CLA	CHB-C4A	10.13	1.42	1.33
20	b	5522	CLA	CHB-C4A	10.00	1.42	1.33
20	C	496	CLA	CHB-C4A	9.99	1.42	1.33
20	b	5518	CLA	CHB-C4A	9.98	1.42	1.33
20	c	5495	CLA	CHB-C4A	9.97	1.42	1.33
20	C	493	CLA	CHB-C4A	9.97	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	518	CLA	CHB-C4A	9.94	1.42	1.33
20	C	503	CLA	CHB-C4A	9.86	1.42	1.33
20	B	515	CLA	CHB-C4A	9.79	1.42	1.33
20	c	5491	CLA	CHB-C4A	9.77	1.42	1.33
20	C	491	CLA	CHB-C4A	9.75	1.42	1.33
20	c	5497	CLA	CHB-C4A	9.74	1.42	1.33
20	C	502	CLA	CHB-C4A	9.74	1.42	1.33
20	c	5500	CLA	CHB-C4A	9.67	1.42	1.33
20	B	511	CLA	CHB-C4A	9.65	1.42	1.33
20	B	526	CLA	CHB-C4A	9.61	1.42	1.33
20	c	5501	CLA	CHB-C4A	9.61	1.42	1.33
20	B	524	CLA	CHB-C4A	9.60	1.42	1.33
20	c	5493	CLA	CHB-C4A	9.57	1.42	1.33
20	c	5494	CLA	CHB-C4A	9.49	1.41	1.33
20	C	497	CLA	CHB-C4A	9.42	1.41	1.33
20	b	5516	CLA	CHB-C4A	9.33	1.41	1.33
20	B	513	CLA	CHB-C4A	9.31	1.41	1.33
20	c	5499	CLA	CHB-C4A	9.28	1.41	1.33
20	b	5524	CLA	CHB-C4A	9.26	1.41	1.33
20	D	354	CLA	CHB-C4A	9.23	1.41	1.33
20	a	5559	CLA	CHB-C4A	9.03	1.41	1.33
20	c	5496	CLA	CHB-C4A	8.97	1.41	1.33
20	b	5515	CLA	CHB-C4A	8.96	1.41	1.33
20	B	520	CLA	CHB-C4A	8.95	1.41	1.33
20	c	5498	CLA	CHB-C4A	8.94	1.41	1.33
20	b	5512	CLA	CHB-C4A	8.88	1.41	1.33
20	c	5492	CLA	CHB-C4A	8.85	1.41	1.33
20	C	494	CLA	CHB-C4A	8.83	1.41	1.33
20	C	492	CLA	CHB-C4A	8.82	1.41	1.33
20	a	5560	CLA	CHB-C4A	8.78	1.41	1.33
20	B	516	CLA	CHB-C4A	8.73	1.41	1.33
20	A	560	CLA	CHB-C4A	8.58	1.41	1.33
20	A	558	CLA	CHB-C4A	8.53	1.41	1.33
20	b	5513	CLA	CHB-C4A	8.40	1.40	1.33
20	c	5495	CLA	MG-NA	8.38	2.26	2.06
20	b	5517	CLA	CHB-C4A	8.38	1.40	1.33
20	B	512	CLA	CHB-C4A	8.35	1.40	1.33
20	d	5354	CLA	CHB-C4A	8.28	1.40	1.33
20	C	498	CLA	CHB-C4A	8.24	1.40	1.33
25	A	567	LHG	P-O5	8.23	1.79	1.50
24	c	5504	BCR	C1-C6	8.20	1.64	1.53
20	B	517	CLA	MG-NA	8.14	2.25	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	5567	LHG	P-O5	8.13	1.79	1.50
20	b	5521	CLA	CHB-C4A	8.13	1.40	1.33
20	a	5558	CLA	CHB-C4A	8.04	1.40	1.33
26	A	568	SQD	C4-C3	8.02	1.73	1.52
26	t	213	SQD	C4-C3	7.98	1.73	1.52
26	a	212	SQD	C4-C3	7.96	1.73	1.52
20	c	5503	CLA	MG-NA	7.88	2.25	2.06
20	C	503	CLA	MG-NA	7.88	2.25	2.06
20	C	500	CLA	CHB-C4A	7.79	1.40	1.33
20	a	5563	CLA	CHB-C4A	7.77	1.40	1.33
26	d	5358	SQD	C4-C3	7.69	1.72	1.52
26	L	5213	SQD	C4-C3	7.63	1.72	1.52
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	A	563	CLA	CHB-C4A	7.46	1.40	1.33
20	C	501	CLA	MG-NA	7.40	2.23	2.06
20	c	5498	CLA	MG-NA	7.30	2.23	2.06
20	D	355	CLA	MG-NA	7.17	2.23	2.06
20	B	516	CLA	MG-NA	7.16	2.23	2.06
24	c	5504	BCR	C30-C25	7.16	1.62	1.53
24	h	5107	BCR	C30-C25	7.14	1.62	1.53
20	c	5491	CLA	MG-NA	7.12	2.23	2.06
26	A	5212	SQD	C4-C3	7.11	1.70	1.52
24	H	107	BCR	C30-C25	7.07	1.62	1.53
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	B	528	BCR	C30-C25	6.71	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	d	5357	BCR	C1-C6	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
26	L	5213	SQD	O7-S	6.45	1.63	1.45
20	b	5517	CLA	MG-NA	6.44	2.21	2.06
24	C	505	BCR	C30-C25	6.43	1.62	1.53
24	c	5505	BCR	C30-C25	6.37	1.61	1.53
24	C	504	BCR	C1-C6	6.29	1.61	1.53
20	d	5355	CLA	MG-NA	6.29	2.21	2.06
32	F	51	HEM	C3C-C4C	6.19	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	502	CLA	MG-NA	6.14	2.20	2.06
26	t	213	SQD	O7-S	6.11	1.62	1.45
24	b	5528	BCR	C30-C25	6.06	1.61	1.53
26	d	5358	SQD	O7-S	6.03	1.62	1.45
24	B	528	BCR	C1-C6	5.99	1.61	1.53
24	A	566	BCR	C1-C6	5.94	1.61	1.53
24	H	107	BCR	C1-C6	5.80	1.61	1.53
20	C	496	CLA	MG-NA	5.79	2.20	2.06
30	H	208	DGD	O3G-C1D	5.76	1.49	1.40
26	a	212	SQD	O47-C7	5.72	1.47	1.35
24	B	527	BCR	C30-C25	5.70	1.61	1.53
20	C	498	CLA	MG-NA	5.59	2.19	2.06
24	D	357	BCR	C30-C25	5.57	1.60	1.53
20	b	5519	CLA	MG-NA	5.54	2.19	2.06
24	h	5107	BCR	C1-C6	5.52	1.60	1.53
26	A	5212	SQD	O7-S	5.51	1.60	1.45
20	b	5522	CLA	MG-NA	5.44	2.19	2.06
20	b	5524	CLA	MG-NA	5.43	2.19	2.06
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	c	5506	BCR	C30-C25	5.36	1.60	1.53
24	a	5566	BCR	C1-C6	5.36	1.60	1.53
24	C	504	BCR	C30-C25	5.33	1.60	1.53
32	v	5552	HEM	C3C-C4C	5.29	1.49	1.41
24	B	529	BCR	C30-C25	5.28	1.60	1.53
20	c	5499	CLA	MG-NA	5.26	2.18	2.06
24	x	5130	BCR	C1-C6	5.24	1.60	1.53
24	x	5130	BCR	C30-C25	5.24	1.60	1.53
24	X	130	BCR	C1-C6	5.23	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
24	b	5527	BCR	C30-C25	5.15	1.60	1.53
32	V	552	HEM	C3C-C4C	5.14	1.49	1.41
24	c	5505	BCR	C1-C6	5.10	1.60	1.53
24	X	130	BCR	C30-C25	5.10	1.60	1.53
24	H	107	BCR	C29-C30	5.09	1.65	1.54
24	b	5529	BCR	C30-C25	5.09	1.60	1.53
32	f	5051	HEM	C3C-C4C	5.08	1.48	1.41
30	h	5208	DGD	O3G-C1D	5.08	1.48	1.40
26	a	212	SQD	O7-S	5.07	1.59	1.45
20	B	523	CLA	MG-NA	4.94	2.18	2.06
26	t	213	SQD	C1-C2	4.94	1.67	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5493	CLA	MG-NA	4.94	2.18	2.06
24	X	130	BCR	C5-C6	4.94	1.42	1.34
24	c	5506	BCR	C1-C6	4.92	1.60	1.53
26	A	5212	SQD	O47-C7	4.82	1.45	1.35
24	x	5130	BCR	C5-C6	4.80	1.42	1.34
26	A	568	SQD	O7-S	4.79	1.58	1.45
25	a	5567	LHG	P-O3	4.79	1.78	1.59
20	a	5563	CLA	MG-NA	4.77	2.17	2.06
27	A	569	LMT	O1'-C1'	4.71	1.48	1.40
20	c	5492	CLA	MG-NA	4.68	2.17	2.06
24	D	357	BCR	C26-C25	4.68	1.42	1.34
31	d	5353	BCT	O1-C	4.65	1.41	1.25
24	a	5566	BCR	C30-C25	4.64	1.59	1.53
24	B	527	BCR	C26-C25	4.61	1.42	1.34
20	C	492	CLA	MG-NA	4.59	2.17	2.06
20	A	560	CLA	MG-NA	4.57	2.17	2.06
24	C	506	BCR	C30-C25	4.55	1.59	1.53
26	L	5213	SQD	O48-C23	4.52	1.46	1.33
24	c	5505	BCR	C26-C25	4.50	1.42	1.34
24	B	529	BCR	C1-C6	4.49	1.59	1.53
24	C	505	BCR	C26-C25	4.46	1.42	1.34
26	t	213	SQD	O5-C5	4.45	1.55	1.44
20	c	5497	CLA	MG-NC	4.43	2.16	2.06
24	B	529	BCR	C26-C25	4.42	1.41	1.34
30	c	5509	DGD	O3G-C1D	4.41	1.47	1.40
20	C	497	CLA	MG-NA	4.40	2.16	2.06
24	d	5357	BCR	C5-C6	4.39	1.41	1.34
24	b	5528	BCR	C1-C6	4.38	1.59	1.53
20	B	515	CLA	MG-NA	4.33	2.16	2.06
24	H	107	BCR	C26-C25	4.33	1.41	1.34
24	h	5107	BCR	C26-C25	4.32	1.41	1.34
32	f	5051	HEM	C4D-ND	-4.31	1.32	1.40
24	C	505	BCR	C1-C6	4.30	1.59	1.53
20	B	513	CLA	MG-NA	4.29	2.16	2.06
24	c	5506	BCR	C5-C6	4.28	1.41	1.34
24	t	104	BCR	C30-C25	4.27	1.59	1.53
28	B	530	MGE	O3G-C1D	4.26	1.47	1.40
21	a	5562	PHO	C3A-C2A	-4.25	1.51	1.54
24	C	506	BCR	C2-C1	4.25	1.63	1.54
20	b	5526	CLA	MG-NA	4.24	2.16	2.06
27	a	5568	LMT	O1'-C1'	4.24	1.47	1.40
26	a	212	SQD	C1-C2	4.24	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	562	PHO	C3A-C2A	-4.23	1.51	1.54
27	M	5216	LMT	O1'-C1'	4.23	1.47	1.40
24	D	357	BCR	C5-C6	4.23	1.41	1.34
30	c	5508	DGD	O6D-C1D	4.21	1.52	1.41
24	d	5357	BCR	C26-C25	4.20	1.41	1.34
20	B	521	CLA	MG-NA	4.20	2.16	2.06
20	A	563	CLA	MG-NA	4.20	2.16	2.06
32	v	5552	HEM	CBC-CAC	4.19	1.55	1.29
24	c	5506	BCR	C26-C25	4.19	1.41	1.34
20	B	522	CLA	MG-NA	4.17	2.16	2.06
20	A	558	CLA	MG-NA	4.13	2.16	2.06
24	c	5504	BCR	C29-C30	4.13	1.63	1.54
20	B	525	CLA	MG-NA	4.11	2.16	2.06
20	C	500	CLA	MG-NA	4.11	2.16	2.06
32	V	552	HEM	CBC-CAC	4.10	1.55	1.29
20	A	560	CLA	CAA-C2A	4.10	1.61	1.54
30	c	5507	DGD	O5D-C1E	4.09	1.47	1.40
24	h	5107	BCR	C29-C30	4.07	1.63	1.54
20	B	511	CLA	MG-NA	4.07	2.15	2.06
24	x	5130	BCR	C29-C30	4.06	1.63	1.54
32	f	5051	HEM	CBC-CAC	4.05	1.54	1.29
24	h	5107	BCR	C2-C1	4.04	1.63	1.54
28	D	359	MGE	O3G-C1D	4.03	1.46	1.40
20	c	5494	CLA	CAA-C2A	4.02	1.61	1.54
24	c	5506	BCR	C2-C1	4.02	1.63	1.54
26	L	5213	SQD	O5-C5	4.02	1.54	1.44
24	C	505	BCR	C2-C1	4.01	1.63	1.54
26	A	568	SQD	O48-C23	4.01	1.45	1.33
26	d	5358	SQD	O47-C7	4.01	1.45	1.34
26	d	5358	SQD	O48-C23	4.00	1.45	1.33
26	d	5358	SQD	C1-C2	4.00	1.64	1.52
32	F	51	HEM	CBC-CAC	4.00	1.54	1.29
20	B	511	CLA	MG-NC	3.99	2.15	2.06
24	t	104	BCR	C1-C6	3.99	1.58	1.53
20	a	5558	CLA	CHC-C1C	3.97	1.44	1.34
20	b	5513	CLA	MG-NA	3.97	2.15	2.06
24	D	357	BCR	C29-C30	3.96	1.63	1.54
24	d	5357	BCR	C30-C25	3.96	1.58	1.53
21	A	561	PHO	C3A-C2A	-3.96	1.51	1.54
30	c	5508	DGD	O3G-C1D	3.95	1.46	1.40
26	A	568	SQD	C1-C2	3.94	1.64	1.52
24	T	5104	BCR	C2-C1	3.94	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	353	BCT	O1-C	3.93	1.39	1.25
26	t	213	SQD	O48-C23	3.92	1.44	1.33
32	v	5552	HEM	C1A-NA	3.92	1.44	1.36
26	L	5213	SQD	C1-C2	3.91	1.64	1.52
20	C	497	CLA	MG-NC	3.91	2.15	2.06
20	B	522	CLA	CHC-C1C	3.91	1.44	1.34
25	A	567	LHG	P-O3	3.91	1.74	1.59
26	A	568	SQD	O47-C7	3.91	1.45	1.34
20	D	355	CLA	CAA-C2A	3.90	1.61	1.54
20	B	512	CLA	MG-NA	3.88	2.15	2.06
27	T	217	LMT	O1'-C1'	3.88	1.46	1.40
30	c	5507	DGD	C4D-C3D	3.88	1.62	1.52
20	C	494	CLA	MG-NA	3.85	2.15	2.06
20	C	494	CLA	CAA-C2A	3.85	1.61	1.54
21	a	5561	PHO	C3A-C2A	-3.84	1.51	1.54
24	D	357	BCR	C1-C6	3.84	1.58	1.53
24	T	5104	BCR	C5-C6	3.83	1.40	1.34
32	f	5051	HEM	C1A-NA	3.83	1.44	1.36
20	C	491	CLA	MG-NA	3.82	2.15	2.06
24	d	5357	BCR	C29-C30	3.81	1.62	1.54
24	X	130	BCR	C29-C30	3.81	1.62	1.54
20	B	519	CLA	CAA-C2A	3.79	1.61	1.54
20	c	5501	CLA	CAA-C2A	3.78	1.61	1.54
24	B	528	BCR	C29-C30	3.78	1.62	1.54
25	a	5567	LHG	P-O6	3.78	1.74	1.59
20	c	5496	CLA	MG-NA	3.77	2.15	2.06
26	a	212	SQD	O5-C5	3.75	1.53	1.44
24	C	506	BCR	C1-C6	3.75	1.58	1.53
24	H	107	BCR	C2-C1	3.75	1.62	1.54
25	A	567	LHG	O8-C23	3.75	1.44	1.33
24	c	5504	BCR	C2-C1	3.75	1.62	1.54
20	C	498	CLA	CHC-C1C	3.73	1.43	1.34
24	C	504	BCR	C29-C30	3.72	1.62	1.54
32	f	5051	HEM	CBD-CAD	3.71	1.64	1.51
20	C	503	CLA	CAA-C2A	3.70	1.60	1.54
20	c	5498	CLA	CHC-C1C	3.69	1.43	1.34
30	C	507	DGD	O5D-C1E	3.69	1.46	1.40
32	V	552	HEM	CHA-C4D	3.68	1.43	1.34
28	d	5361	MGE	O6D-C1D	3.66	1.51	1.41
32	F	51	HEM	C4D-ND	-3.66	1.33	1.40
20	B	516	CLA	CAA-C2A	3.66	1.60	1.54
25	A	567	LHG	P-O6	3.66	1.73	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	507	DGD	C4D-C3D	3.65	1.61	1.52
30	C	509	DGD	O3G-C1D	3.65	1.46	1.40
28	L	210	MGE	O6D-C1D	3.65	1.51	1.41
24	T	5104	BCR	C1-C6	3.64	1.58	1.53
24	C	506	BCR	C5-C6	3.64	1.40	1.34
28	D	358	MGE	O3G-C1D	3.63	1.46	1.40
28	L	210	MGE	O3G-C1D	3.63	1.46	1.40
32	V	552	HEM	C1A-NA	3.62	1.43	1.36
20	B	513	CLA	CAA-C2A	3.62	1.60	1.54
20	b	5514	CLA	CHC-C1C	3.62	1.43	1.34
20	b	5522	CLA	CHC-C1C	3.62	1.43	1.34
20	b	5512	CLA	MG-NA	3.61	2.14	2.06
20	c	5502	CLA	CHC-C1C	3.61	1.43	1.34
24	A	566	BCR	C5-C6	3.61	1.40	1.34
20	b	5518	CLA	C1D-ND	-3.61	1.33	1.37
24	D	357	BCR	C2-C1	3.61	1.62	1.54
32	v	5552	HEM	C2C-C1C	3.61	1.50	1.42
26	t	213	SQD	O47-C7	3.61	1.44	1.34
20	B	518	CLA	CAA-C2A	3.60	1.60	1.54
20	c	5503	CLA	CAA-C2A	3.60	1.60	1.54
20	A	563	CLA	C1B-CHB	-3.60	1.31	1.41
24	C	504	BCR	C26-C25	3.59	1.40	1.34
20	c	5500	CLA	MG-NA	3.59	2.14	2.06
20	b	5526	CLA	C4-C3	3.58	1.59	1.50
20	d	5355	CLA	CHC-C1C	3.58	1.43	1.34
20	b	5525	CLA	MG-NA	3.58	2.14	2.06
20	B	523	CLA	C1D-ND	-3.57	1.33	1.37
25	a	5567	LHG	O8-C23	3.57	1.43	1.33
24	b	5529	BCR	C29-C30	3.57	1.62	1.54
24	b	5528	BCR	C29-C30	3.57	1.62	1.54
20	D	354	CLA	C1B-CHB	-3.57	1.31	1.41
30	c	5509	DGD	O6D-C1D	3.56	1.51	1.41
20	b	5520	CLA	MG-NC	3.56	2.14	2.06
24	C	505	BCR	C29-C30	3.56	1.62	1.54
24	x	5130	BCR	C2-C1	3.56	1.62	1.54
20	C	495	CLA	CHC-C1C	3.55	1.43	1.34
24	t	104	BCR	C5-C6	3.55	1.40	1.34
20	A	558	CLA	CHC-C1C	3.55	1.43	1.34
26	t	213	SQD	C20-C19	-3.55	1.34	1.51
20	D	354	CLA	CHC-C1C	3.54	1.43	1.34
20	b	5526	CLA	CAA-C2A	3.54	1.60	1.54
24	b	5529	BCR	C1-C6	3.54	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	522	CLA	CAA-C2A	3.53	1.60	1.54
20	b	5518	CLA	CHC-C1C	3.53	1.43	1.34
32	v	5552	HEM	C4D-ND	-3.53	1.34	1.40
20	C	502	CLA	CHC-C1C	3.53	1.43	1.34
32	v	5552	HEM	CHA-C4D	3.53	1.43	1.34
28	D	358	MGE	O6D-C1D	3.52	1.50	1.41
20	b	5519	CLA	MG-NC	3.52	2.14	2.06
24	C	506	BCR	C26-C25	3.51	1.40	1.34
30	c	5509	DGD	O5D-C1E	3.51	1.46	1.40
26	t	213	SQD	O8-S	3.51	1.60	1.47
26	A	568	SQD	O3-C3	3.51	1.51	1.43
26	L	5213	SQD	O8-S	3.50	1.60	1.47
20	c	5495	CLA	CHC-C1C	3.50	1.43	1.34
20	b	5522	CLA	CAA-C2A	3.50	1.60	1.54
26	a	212	SQD	O8-S	3.50	1.60	1.47
24	A	566	BCR	C2-C1	3.50	1.62	1.54
20	c	5493	CLA	MG-NC	3.49	2.14	2.06
20	c	5494	CLA	CHC-C1C	3.49	1.43	1.34
26	A	5212	SQD	O5-C5	3.49	1.52	1.44
20	A	563	CLA	CHC-C1C	3.49	1.43	1.34
26	d	5358	SQD	O5-C5	3.49	1.52	1.44
24	B	528	BCR	C26-C25	3.49	1.40	1.34
24	c	5505	BCR	C2-C1	3.49	1.62	1.54
24	B	527	BCR	C29-C30	3.48	1.62	1.54
20	b	5525	CLA	CHC-C1C	3.48	1.43	1.34
20	c	5501	CLA	CHC-C1C	3.48	1.43	1.34
20	B	518	CLA	CHC-C1C	3.48	1.43	1.34
20	c	5493	CLA	CHC-C1C	3.47	1.43	1.34
26	L	5213	SQD	C12-C11	-3.47	1.34	1.51
20	c	5496	CLA	CAA-C2A	3.47	1.60	1.54
20	b	5517	CLA	CHC-C1C	3.47	1.43	1.34
24	b	5529	BCR	C2-C1	3.46	1.62	1.54
20	c	5499	CLA	CAA-C2A	3.46	1.60	1.54
27	t	5217	LMT	O1'-C1'	3.46	1.46	1.40
25	A	567	LHG	O7-C7	3.46	1.44	1.34
24	b	5527	BCR	C29-C30	3.46	1.62	1.54
30	H	208	DGD	C4E-C5E	3.46	1.60	1.53
25	a	5567	LHG	O7-C7	3.46	1.44	1.34
32	F	51	HEM	CMA-C3A	3.44	1.58	1.51
26	L	5213	SQD	C17-C16	-3.44	1.34	1.51
26	L	5213	SQD	C11-C10	-3.44	1.34	1.51
20	b	5517	CLA	CAA-C2A	3.43	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	529	BCR	C2-C1	3.43	1.61	1.54
26	A	5212	SQD	O8-S	3.43	1.60	1.47
20	B	521	CLA	CHC-C1C	3.42	1.43	1.34
24	c	5505	BCR	C5-C6	3.42	1.40	1.34
20	C	501	CLA	CHC-C1C	3.42	1.43	1.34
24	d	5357	BCR	C2-C1	3.41	1.61	1.54
20	b	5526	CLA	C5-C3	3.41	1.58	1.51
20	b	5524	CLA	CHC-C1C	3.41	1.42	1.34
26	L	5213	SQD	C20-C19	-3.40	1.34	1.51
20	B	524	CLA	CHC-C1C	3.40	1.42	1.34
20	B	513	CLA	C1D-ND	-3.40	1.33	1.37
20	a	5563	CLA	C1B-CHB	-3.39	1.31	1.41
28	b	5530	MGE	O6D-C1D	3.39	1.50	1.41
20	a	5559	CLA	MG-NA	3.38	2.14	2.06
26	A	5212	SQD	C1-C2	3.37	1.62	1.52
24	c	5505	BCR	C29-C30	3.37	1.61	1.54
20	b	5520	CLA	MG-NA	3.36	2.14	2.06
20	D	355	CLA	CHC-C1C	3.36	1.42	1.34
24	B	527	BCR	C5-C6	3.36	1.40	1.34
20	d	5354	CLA	C1B-CHB	-3.36	1.31	1.41
20	b	5523	CLA	C1D-ND	-3.35	1.33	1.37
26	t	213	SQD	C19-C18	-3.35	1.35	1.51
28	B	530	MGE	O6D-C1D	3.34	1.50	1.41
26	a	212	SQD	O6-C1	3.32	1.45	1.40
26	A	568	SQD	O6-C44	-3.32	1.38	1.43
20	d	5354	CLA	CHC-C1C	3.32	1.42	1.34
26	t	213	SQD	C14-C13	-3.31	1.35	1.51
20	B	517	CLA	CHC-C1C	3.31	1.42	1.34
20	a	5558	CLA	MG-NA	3.31	2.14	2.06
20	C	497	CLA	CHC-C1C	3.31	1.42	1.34
20	C	491	CLA	CAA-C2A	3.30	1.60	1.54
26	L	5213	SQD	C19-C18	-3.30	1.35	1.51
26	L	5213	SQD	O47-C7	3.30	1.43	1.34
30	C	508	DGD	O5D-C1E	3.29	1.45	1.40
20	B	526	CLA	C5-C3	3.29	1.58	1.51
28	D	360	MGE	O3G-C1D	3.29	1.45	1.40
26	A	5212	SQD	O3-C3	3.28	1.51	1.43
20	c	5495	CLA	CAA-C2A	3.28	1.60	1.54
20	c	5497	CLA	CHC-C1C	3.28	1.42	1.34
20	c	5502	CLA	MG-NC	3.27	2.14	2.06
20	B	512	CLA	C1B-CHB	-3.27	1.31	1.41
24	X	130	BCR	C2-C1	3.26	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	525	CLA	CHC-C1C	3.26	1.42	1.34
28	b	5530	MGE	O3G-C1D	3.26	1.45	1.40
24	c	5506	BCR	C29-C30	3.26	1.61	1.54
24	t	104	BCR	C2-C1	3.26	1.61	1.54
20	B	519	CLA	MG-NC	3.26	2.14	2.06
26	L	5213	SQD	O3-C3	3.26	1.51	1.43
20	b	5515	CLA	MG-NA	3.26	2.14	2.06
20	C	503	CLA	CHC-C1C	3.25	1.42	1.34
20	b	5516	CLA	CAA-C2A	3.25	1.60	1.54
28	d	5359	MGE	O3G-C1D	3.25	1.45	1.40
24	A	566	BCR	C30-C25	3.25	1.57	1.53
20	a	5558	CLA	C1B-CHB	-3.25	1.32	1.41
28	i	5201	MGE	O6D-C5D	3.25	1.52	1.44
26	A	568	SQD	C17-C16	-3.24	1.35	1.51
26	t	213	SQD	C15-C14	-3.24	1.35	1.51
26	L	5213	SQD	C18-C17	-3.24	1.35	1.51
20	b	5515	CLA	CAA-C2A	3.23	1.60	1.54
20	b	5514	CLA	CAA-C2A	3.22	1.60	1.54
26	a	212	SQD	O3-C3	3.22	1.50	1.43
30	c	5507	DGD	O6D-C1D	3.21	1.50	1.41
24	d	5357	BCR	C38-C26	3.21	1.56	1.50
28	d	5361	MGE	O3G-C1D	3.21	1.45	1.40
26	L	5213	SQD	C13-C12	-3.21	1.35	1.51
20	b	5523	CLA	MG-NA	3.21	2.13	2.06
30	C	508	DGD	O6D-C1D	3.20	1.50	1.41
20	b	5512	CLA	MG-NC	3.20	2.13	2.06
20	B	520	CLA	MG-NA	3.20	2.13	2.06
26	t	213	SQD	O3-C3	3.20	1.50	1.43
20	B	512	CLA	MG-NC	3.20	2.13	2.06
20	C	494	CLA	CHC-C1C	3.19	1.42	1.34
20	b	5522	CLA	C1D-ND	-3.19	1.33	1.37
20	B	516	CLA	CHC-C1C	3.19	1.42	1.34
20	d	5354	CLA	CAA-CBA	-3.19	1.43	1.52
20	C	500	CLA	CAA-C2A	3.18	1.59	1.54
20	A	560	CLA	C1B-CHB	-3.18	1.32	1.41
20	C	493	CLA	CHC-C1C	3.18	1.42	1.34
26	t	213	SQD	C12-C11	-3.17	1.36	1.51
26	t	213	SQD	C11-C10	-3.17	1.36	1.51
24	B	528	BCR	C2-C1	3.17	1.61	1.54
20	b	5511	CLA	MG-NC	3.17	2.13	2.06
24	c	5505	BCR	C38-C26	3.17	1.56	1.50
24	B	529	BCR	C29-C30	3.17	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	354	CLA	CAA-CBA	-3.17	1.43	1.52
20	a	5563	CLA	CHC-C1C	3.16	1.42	1.34
20	a	5563	CLA	CAA-C2A	3.16	1.59	1.54
24	a	5566	BCR	C5-C6	3.16	1.39	1.34
20	C	496	CLA	CHC-C1C	3.16	1.42	1.34
20	c	5501	CLA	MG-NC	3.15	2.13	2.06
20	c	5494	CLA	MG-NC	3.15	2.13	2.06
20	B	519	CLA	CHC-C1C	3.15	1.42	1.34
26	A	568	SQD	C12-C11	-3.15	1.36	1.51
26	t	213	SQD	C17-C16	-3.14	1.36	1.51
20	b	5526	CLA	CHC-C1C	3.14	1.42	1.34
32	f	5051	HEM	CHA-C4D	3.14	1.42	1.34
20	B	517	CLA	CAA-C2A	3.13	1.59	1.54
28	D	359	MGE	O6D-C1D	3.13	1.49	1.41
20	C	498	CLA	C1B-CHB	-3.13	1.32	1.41
21	a	5561	PHO	C4-C3	3.13	1.58	1.50
20	b	5519	CLA	CHC-C1C	3.12	1.42	1.34
20	A	558	CLA	C1B-CHB	-3.12	1.32	1.41
20	b	5521	CLA	C1B-CHB	-3.12	1.32	1.41
20	B	520	CLA	CAA-C2A	3.12	1.59	1.54
24	a	5566	BCR	C2-C1	3.11	1.61	1.54
20	c	5496	CLA	CHC-C1C	3.11	1.42	1.34
20	b	5513	CLA	CAA-C2A	3.11	1.59	1.54
20	c	5500	CLA	CHC-C1C	3.11	1.42	1.34
20	C	500	CLA	CHC-C1C	3.11	1.42	1.34
26	A	568	SQD	O5-C5	3.10	1.52	1.44
20	C	502	CLA	MG-NC	3.10	2.13	2.06
24	C	504	BCR	C2-C1	3.10	1.61	1.54
26	L	5213	SQD	C15-C14	-3.10	1.36	1.51
20	B	514	CLA	CHC-C1C	3.09	1.42	1.34
24	b	5527	BCR	C2-C1	3.09	1.61	1.54
28	l	5210	MGE	O6D-C1D	3.09	1.49	1.41
24	c	5504	BCR	C26-C25	3.09	1.39	1.34
20	a	5560	CLA	CAA-C2A	3.08	1.59	1.54
20	b	5519	CLA	CAA-C2A	3.08	1.59	1.54
20	B	513	CLA	C1B-CHB	-3.08	1.32	1.41
20	C	499	CLA	C1D-ND	-3.08	1.33	1.37
20	B	513	CLA	C1D-C2D	-3.08	1.39	1.45
20	B	526	CLA	C4-C3	3.08	1.58	1.50
20	B	526	CLA	CAA-C2A	3.08	1.59	1.54
26	t	213	SQD	C13-C12	-3.08	1.36	1.51
20	C	502	CLA	CAA-C2A	3.07	1.59	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	m	216	LMT	C3B-C2B	3.07	1.60	1.52
20	b	5516	CLA	CHC-C1C	3.07	1.42	1.34
26	L	5213	SQD	C16-C15	-3.07	1.36	1.51
26	A	568	SQD	C16-C15	-3.07	1.36	1.51
20	B	521	CLA	CAA-C2A	3.06	1.59	1.54
20	b	5515	CLA	C1B-CHB	-3.06	1.32	1.41
32	F	51	HEM	C2C-C1C	3.06	1.49	1.42
20	b	5512	CLA	C1B-CHB	-3.05	1.32	1.41
20	B	515	CLA	CHC-C1C	3.05	1.42	1.34
20	B	523	CLA	CHC-C1C	3.05	1.42	1.34
20	c	5496	CLA	MG-NC	3.05	2.13	2.06
20	b	5523	CLA	CHC-C1C	3.05	1.42	1.34
32	F	51	HEM	C1A-NA	3.05	1.42	1.36
20	b	5523	CLA	CAA-C2A	3.05	1.59	1.54
26	d	5358	SQD	C17-C16	-3.05	1.36	1.51
20	b	5525	CLA	MG-NC	3.05	2.13	2.06
26	d	5358	SQD	O6-C44	-3.04	1.38	1.43
26	L	5213	SQD	C14-C13	-3.04	1.36	1.51
20	b	5514	CLA	C1D-C2D	-3.04	1.39	1.45
20	b	5511	CLA	C4C-C3C	3.04	1.50	1.45
20	b	5520	CLA	CHC-C1C	3.04	1.42	1.34
26	A	568	SQD	C15-C14	-3.04	1.36	1.51
20	B	520	CLA	C1B-CHB	-3.03	1.32	1.41
30	C	507	DGD	O6D-C1D	3.03	1.49	1.41
20	B	512	CLA	CHC-C1C	3.03	1.42	1.34
28	d	5359	MGE	O6D-C1D	3.02	1.49	1.41
20	b	5515	CLA	CHC-C1C	3.02	1.42	1.34
24	b	5528	BCR	C2-C1	3.02	1.61	1.54
26	A	568	SQD	C11-C10	-3.01	1.36	1.51
32	V	552	HEM	C2C-C1C	3.00	1.49	1.42
20	A	560	CLA	CHC-C1C	3.00	1.42	1.34
20	a	5559	CLA	C1D-ND	-3.00	1.33	1.37
24	X	130	BCR	C26-C25	3.00	1.39	1.34
30	C	508	DGD	O1G-C1A	3.00	1.42	1.33
26	t	213	SQD	C16-C15	-2.99	1.36	1.51
24	C	505	BCR	C5-C6	2.99	1.39	1.34
20	B	526	CLA	C1B-CHB	-2.99	1.32	1.41
26	A	5212	SQD	O6-C1	2.99	1.45	1.40
20	c	5491	CLA	CAA-C2A	2.99	1.59	1.54
24	t	104	BCR	C29-C30	2.99	1.60	1.54
26	L	5213	SQD	O5-C1	2.99	1.49	1.41
20	a	5558	CLA	MG-NC	2.99	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5496	CLA	C4C-C3C	2.98	1.50	1.45
20	c	5496	CLA	C1B-CHB	-2.98	1.32	1.41
20	c	5499	CLA	CHC-C1C	2.98	1.41	1.34
24	C	506	BCR	C29-C30	2.98	1.60	1.54
20	c	5500	CLA	CAA-C2A	2.98	1.59	1.54
26	L	5213	SQD	O6-C1	2.97	1.45	1.40
20	C	491	CLA	CHC-C1C	2.97	1.41	1.34
26	t	213	SQD	C18-C17	-2.97	1.37	1.51
20	B	515	CLA	C1B-CHB	-2.97	1.32	1.41
20	b	5511	CLA	CHC-C1C	2.97	1.41	1.34
20	c	5500	CLA	MG-NC	2.97	2.13	2.06
20	b	5526	CLA	C1-C2	2.96	1.57	1.49
20	c	5493	CLA	CAA-C2A	2.96	1.59	1.54
26	d	5358	SQD	O3-C3	2.95	1.50	1.43
21	A	561	PHO	CAA-CBA	-2.95	1.44	1.52
20	b	5521	CLA	CAA-C2A	2.95	1.59	1.54
20	c	5491	CLA	CHC-C1C	2.95	1.41	1.34
27	a	5568	LMT	O5'-C1'	2.94	1.49	1.41
20	b	5518	CLA	CAA-C2A	2.94	1.59	1.54
20	B	511	CLA	CMD-C2D	2.94	1.56	1.50
30	H	208	DGD	O5D-C1E	2.94	1.45	1.40
20	B	518	CLA	C1D-ND	-2.94	1.34	1.37
20	c	5494	CLA	C1B-CHB	-2.93	1.32	1.41
30	C	508	DGD	O3G-C1D	2.93	1.45	1.40
20	C	494	CLA	C1B-CHB	-2.92	1.32	1.41
32	V	552	HEM	C4D-ND	-2.91	1.35	1.40
20	C	503	CLA	MG-NC	2.91	2.13	2.06
20	D	354	CLA	MG-NC	2.91	2.13	2.06
28	d	5360	MGE	O6D-C1D	2.91	1.49	1.41
24	x	5130	BCR	C26-C25	2.91	1.39	1.34
20	B	511	CLA	CHC-C1C	2.90	1.41	1.34
20	b	5512	CLA	CHC-C1C	2.90	1.41	1.34
20	C	500	CLA	C1B-CHB	-2.90	1.32	1.41
20	a	5559	CLA	C1B-CHB	-2.89	1.32	1.41
20	a	5560	CLA	C1B-CHB	-2.89	1.33	1.41
20	B	525	CLA	C1B-CHB	-2.89	1.33	1.41
28	D	358	MGE	O6D-C5D	2.89	1.51	1.44
27	A	569	LMT	O5'-C1'	2.89	1.49	1.41
28	D	358	MGE	C4D-C3D	2.88	1.59	1.52
20	c	5503	CLA	CHC-C1C	2.88	1.41	1.34
20	d	5355	CLA	CAA-C2A	2.88	1.59	1.54
28	d	5360	MGE	C4D-C3D	2.88	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	i	5201	MGE	C4D-C5D	2.87	1.59	1.53
26	d	5358	SQD	C32-C31	-2.87	1.37	1.51
20	a	5560	CLA	MG-NC	2.87	2.13	2.06
24	t	104	BCR	C26-C25	2.87	1.39	1.34
20	b	5524	CLA	MG-NC	2.87	2.13	2.06
20	b	5511	CLA	C1C-C2C	2.87	1.50	1.44
26	A	568	SQD	C13-C12	-2.86	1.37	1.51
20	c	5497	CLA	C1B-CHB	-2.86	1.33	1.41
24	b	5527	BCR	C5-C6	2.86	1.39	1.34
30	c	5507	DGD	O3G-C1D	2.86	1.45	1.40
27	A	569	LMT	C1'-C2'	2.86	1.60	1.52
20	b	5521	CLA	MG-NC	2.85	2.13	2.06
26	d	5358	SQD	C20-C19	-2.85	1.37	1.51
26	A	568	SQD	C14-C13	-2.85	1.37	1.51
24	H	107	BCR	C5-C6	2.85	1.39	1.34
20	C	495	CLA	C1C-C2C	2.85	1.50	1.44
30	C	507	DGD	O3G-C1D	2.85	1.44	1.40
20	B	517	CLA	C1B-CHB	-2.84	1.33	1.41
20	c	5497	CLA	CAA-C2A	2.84	1.59	1.54
24	D	357	BCR	C19-C18	-2.84	1.39	1.46
32	f	5051	HEM	C3C-CAC	2.84	1.54	1.47
20	b	5516	CLA	C1B-CHB	-2.84	1.33	1.41
20	a	5560	CLA	CHC-C1C	2.83	1.41	1.34
30	c	5507	DGD	C3E-C2E	2.83	1.59	1.52
20	b	5521	CLA	MG-NA	2.83	2.13	2.06
27	t	5217	LMT	O1B-C1B	2.83	1.49	1.41
20	b	5522	CLA	C1B-CHB	-2.82	1.33	1.41
20	b	5511	CLA	CMD-C2D	2.82	1.56	1.50
20	b	5526	CLA	C1B-CHB	-2.82	1.33	1.41
30	C	508	DGD	C4E-C3E	2.82	1.59	1.52
30	h	5208	DGD	O6D-C5D	2.81	1.51	1.44
20	B	514	CLA	CAA-C2A	2.81	1.59	1.54
30	c	5508	DGD	C4D-C3D	2.81	1.59	1.52
20	A	558	CLA	CAA-CBA	-2.80	1.44	1.52
28	i	5201	MGE	O2G-C1B	2.80	1.42	1.34
20	B	521	CLA	C1B-CHB	-2.80	1.33	1.41
20	b	5525	CLA	CAA-C2A	2.80	1.59	1.54
24	B	527	BCR	C2-C1	2.80	1.60	1.54
20	C	495	CLA	CAA-C2A	2.79	1.59	1.54
26	d	5358	SQD	C11-C10	-2.79	1.37	1.51
20	C	492	CLA	CHC-C1C	2.79	1.41	1.34
20	B	520	CLA	CHC-C1C	2.79	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	5527	BCR	C26-C25	2.79	1.39	1.34
30	C	509	DGD	O6D-C1D	2.78	1.49	1.41
20	A	563	CLA	MG-NC	2.78	2.12	2.06
26	d	5358	SQD	C12-C11	-2.78	1.38	1.51
26	d	5358	SQD	C33-C32	-2.78	1.38	1.51
28	b	5530	MGE	O6D-C5D	2.77	1.51	1.44
20	c	5493	CLA	C1B-CHB	-2.77	1.33	1.41
20	C	492	CLA	C1B-CHB	-2.77	1.33	1.41
20	A	560	CLA	MG-NC	2.77	2.12	2.06
20	B	513	CLA	C5-C3	2.77	1.57	1.51
20	B	511	CLA	C4C-C3C	2.77	1.49	1.45
20	b	5514	CLA	C1D-ND	-2.77	1.34	1.37
24	C	505	BCR	C38-C26	2.77	1.55	1.50
20	A	559	CLA	MG-NA	2.77	2.12	2.06
20	C	493	CLA	CAA-C2A	2.77	1.59	1.54
27	m	216	LMT	O1'-C1'	2.77	1.44	1.40
20	A	558	CLA	MG-NC	2.77	2.12	2.06
20	b	5521	CLA	CHC-C1C	2.76	1.41	1.34
26	d	5358	SQD	C15-C14	-2.76	1.38	1.51
28	d	5360	MGE	O1G-C1A	2.76	1.41	1.33
20	a	5558	CLA	CAA-CBA	-2.76	1.44	1.52
20	c	5492	CLA	C4-C3	2.76	1.57	1.50
24	A	566	BCR	C29-C30	2.75	1.60	1.54
20	b	5517	CLA	C1B-CHB	-2.75	1.33	1.41
20	c	5492	CLA	CHC-C1C	2.75	1.41	1.34
20	C	496	CLA	MG-NC	2.75	2.12	2.06
26	d	5358	SQD	C19-C18	-2.74	1.38	1.51
20	B	521	CLA	MG-NC	2.74	2.12	2.06
30	h	5208	DGD	O6E-C1E	2.74	1.48	1.41
20	B	525	CLA	MG-NC	2.74	2.12	2.06
24	b	5529	BCR	C26-C25	2.74	1.39	1.34
20	c	5502	CLA	CAA-C2A	2.74	1.59	1.54
20	C	496	CLA	C4C-C3C	2.74	1.49	1.45
20	B	522	CLA	MG-NC	2.74	2.12	2.06
20	B	513	CLA	CHC-C1C	2.74	1.41	1.34
20	b	5525	CLA	C1B-CHB	-2.74	1.33	1.41
20	d	5355	CLA	MG-NC	2.73	2.12	2.06
26	A	568	SQD	C33-C32	-2.73	1.38	1.51
20	B	513	CLA	MG-NC	2.73	2.12	2.06
26	t	213	SQD	C21-C20	-2.73	1.34	1.51
24	C	504	BCR	C5-C6	2.72	1.39	1.34
24	b	5528	BCR	C5-C6	2.72	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	5359	MGE	C4D-C3D	2.72	1.59	1.52
30	h	5208	DGD	O5D-C1E	2.72	1.44	1.40
20	d	5355	CLA	C1B-CHB	-2.72	1.33	1.41
24	t	104	BCR	C23-C22	-2.72	1.40	1.46
26	d	5358	SQD	C16-C15	-2.72	1.38	1.51
20	a	5558	CLA	CAA-C2A	2.72	1.59	1.54
20	C	496	CLA	CAA-C2A	2.72	1.59	1.54
20	b	5513	CLA	C1B-CHB	-2.72	1.33	1.41
30	c	5508	DGD	O1G-C1A	2.71	1.41	1.33
20	a	5560	CLA	CHD-C1D	2.71	1.43	1.38
26	A	568	SQD	O8-S	2.71	1.57	1.47
20	b	5524	CLA	C1B-CHB	-2.70	1.33	1.41
28	I	201	MGE	O2G-C1B	2.70	1.41	1.34
24	b	5529	BCR	C5-C6	2.70	1.39	1.34
27	t	5217	LMT	O5B-C1B	2.70	1.48	1.41
21	A	562	PHO	C4-C3	2.70	1.57	1.50
20	C	491	CLA	C1B-CHB	-2.70	1.33	1.41
20	C	501	CLA	CAA-C2A	2.69	1.59	1.54
32	f	5051	HEM	CAA-C2A	2.69	1.58	1.52
20	A	559	CLA	CHC-C1C	2.69	1.41	1.34
20	d	5354	CLA	MG-NA	2.68	2.12	2.06
30	C	508	DGD	C1E-C2E	2.68	1.60	1.52
26	A	568	SQD	C32-C31	-2.68	1.38	1.51
26	d	5358	SQD	O8-S	2.68	1.57	1.47
30	H	208	DGD	O6D-C1D	2.67	1.48	1.41
20	C	500	CLA	MG-NC	2.67	2.12	2.06
32	f	5051	HEM	CMA-C3A	2.67	1.56	1.51
20	B	524	CLA	C1B-CHB	-2.67	1.33	1.41
32	F	51	HEM	CHA-C4D	2.67	1.41	1.34
20	B	525	CLA	CAA-C2A	2.67	1.58	1.54
24	B	529	BCR	C5-C6	2.66	1.39	1.34
26	a	212	SQD	C8-C7	2.66	1.58	1.49
20	C	501	CLA	MG-NC	2.66	2.12	2.06
20	c	5502	CLA	CMD-C2D	2.66	1.56	1.50
24	T	5104	BCR	C29-C30	2.66	1.60	1.54
20	A	559	CLA	C1B-CHB	-2.65	1.33	1.41
20	B	519	CLA	CMD-C2D	2.65	1.56	1.50
20	c	5503	CLA	C1C-C2C	2.65	1.49	1.44
20	a	5563	CLA	C5-C3	2.65	1.56	1.51
30	C	507	DGD	C3E-C2E	2.65	1.59	1.52
26	A	5212	SQD	O5-C1	2.65	1.48	1.41
28	d	5360	MGE	O6D-C5D	2.65	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5500	CLA	C4-C3	2.64	1.57	1.50
20	B	520	CLA	C4C-C3C	2.64	1.49	1.45
24	T	5104	BCR	C29-C28	-2.64	1.46	1.52
20	A	559	CLA	CAA-C2A	2.64	1.58	1.54
20	B	522	CLA	C1D-ND	-2.64	1.34	1.37
30	C	508	DGD	C3D-C2D	2.64	1.59	1.52
26	d	5358	SQD	C14-C13	-2.64	1.38	1.51
20	b	5517	CLA	MG-NC	2.63	2.12	2.06
32	F	51	HEM	CBD-CAD	2.63	1.61	1.51
20	C	501	CLA	C1C-C2C	2.63	1.49	1.44
32	F	51	HEM	CAA-C2A	2.63	1.58	1.52
21	A	562	PHO	C4A-C3A	-2.63	1.46	1.51
26	A	568	SQD	C19-C18	-2.62	1.38	1.51
26	d	5358	SQD	C36-C35	-2.62	1.38	1.51
20	B	514	CLA	MG-NC	2.62	2.12	2.06
30	C	509	DGD	O6D-C5D	2.62	1.50	1.44
28	D	359	MGE	C4D-C3D	2.62	1.59	1.52
20	b	5520	CLA	C1B-CHB	-2.62	1.33	1.41
30	H	208	DGD	O6D-C5D	2.62	1.50	1.44
26	a	212	SQD	O5-C1	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
27	T	217	LMT	O5B-C1B	2.60	1.48	1.41
26	A	568	SQD	C18-C17	-2.60	1.38	1.51
20	C	499	CLA	CHC-C1C	2.60	1.41	1.34
30	c	5509	DGD	O6D-C5D	2.60	1.50	1.44
20	B	517	CLA	C1D-ND	-2.60	1.34	1.37
20	b	5520	CLA	CAA-C2A	2.60	1.58	1.54
20	c	5498	CLA	CAA-C2A	2.60	1.58	1.54
24	t	104	BCR	C29-C28	-2.60	1.46	1.52
20	c	5498	CLA	C1B-CHB	-2.60	1.33	1.41
30	H	208	DGD	C1E-C2E	2.60	1.60	1.52
28	I	201	MGE	O6D-C5D	2.60	1.50	1.44
20	B	516	CLA	C1B-CHB	-2.59	1.33	1.41
21	a	5561	PHO	CAA-CBA	-2.59	1.45	1.52
30	C	508	DGD	C4D-C3D	2.59	1.59	1.52
20	b	5513	CLA	CHC-C1C	2.59	1.40	1.34
30	c	5507	DGD	C1E-C2E	2.59	1.60	1.52
20	B	516	CLA	MG-NC	2.59	2.12	2.06
26	L	5213	SQD	O6-C44	-2.59	1.39	1.43
26	L	5213	SQD	C21-C20	-2.59	1.35	1.51
26	A	568	SQD	C35-C34	-2.58	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	i	5201	MGE	O6D-C1D	2.58	1.48	1.41
20	B	523	CLA	C1B-CHB	-2.58	1.33	1.41
26	t	213	SQD	O5-C1	2.58	1.48	1.41
20	b	5513	CLA	C4-C3	2.58	1.57	1.50
20	C	493	CLA	C1B-CHB	-2.58	1.33	1.41
28	B	530	MGE	O2G-C1B	2.57	1.41	1.34
20	C	500	CLA	CMD-C2D	2.57	1.56	1.50
26	A	568	SQD	C34-C33	-2.57	1.39	1.51
32	v	5552	HEM	CAD-C3D	-2.57	1.44	1.51
20	a	5559	CLA	CHC-C1C	2.57	1.40	1.34
24	c	5506	BCR	C19-C18	-2.57	1.40	1.46
28	d	5359	MGE	O6D-C5D	2.57	1.50	1.44
27	A	569	LMT	O5B-C5B	2.57	1.50	1.44
24	b	5527	BCR	C19-C18	-2.56	1.40	1.46
20	B	526	CLA	CHC-C1C	2.56	1.40	1.34
26	d	5358	SQD	C13-C12	-2.56	1.39	1.51
20	B	523	CLA	C1D-C2D	-2.56	1.40	1.45
30	c	5508	DGD	C1E-C2E	2.55	1.60	1.52
24	b	5527	BCR	C1-C6	2.55	1.57	1.53
30	C	507	DGD	O6D-C5D	2.54	1.50	1.44
26	A	568	SQD	C20-C19	-2.54	1.39	1.51
26	d	5358	SQD	O5-C1	2.54	1.48	1.41
20	c	5496	CLA	C1C-C2C	2.53	1.49	1.44
26	d	5358	SQD	C35-C34	-2.53	1.39	1.51
20	D	354	CLA	C1D-C2D	-2.52	1.40	1.45
32	v	5552	HEM	CAA-C2A	2.52	1.58	1.52
32	F	51	HEM	C3C-CAC	2.52	1.53	1.47
24	a	5566	BCR	C29-C30	2.52	1.59	1.54
20	A	563	CLA	C4-C3	2.52	1.56	1.50
27	T	217	LMT	O1B-C1B	2.52	1.48	1.41
20	B	526	CLA	MG-NC	2.52	2.12	2.06
20	B	520	CLA	C4-C3	2.51	1.56	1.50
32	v	5552	HEM	CBA-CGA	-2.51	1.44	1.50
28	D	360	MGE	O6D-C1D	2.51	1.48	1.41
20	C	493	CLA	C1D-ND	-2.51	1.34	1.37
28	B	530	MGE	C1D-C2D	2.51	1.59	1.52
26	A	568	SQD	C36-C35	-2.51	1.39	1.51
20	B	514	CLA	C1D-C2D	-2.51	1.40	1.45
20	C	497	CLA	C4-C3	2.51	1.56	1.50
26	a	212	SQD	O6-C44	-2.51	1.39	1.43
20	c	5500	CLA	C1B-CHB	-2.51	1.34	1.41
20	C	495	CLA	C1D-C2D	-2.50	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	530	MGE	O6D-C5D	2.50	1.50	1.44
20	b	5513	CLA	MG-NC	2.50	2.12	2.06
20	d	5354	CLA	MG-NC	2.50	2.12	2.06
30	H	208	DGD	O6E-C1E	2.50	1.48	1.41
24	A	566	BCR	C26-C25	2.50	1.38	1.34
20	b	5515	CLA	C4-C3	2.50	1.56	1.50
20	B	522	CLA	C1B-CHB	-2.50	1.34	1.41
26	d	5358	SQD	C34-C33	-2.49	1.39	1.51
24	T	5104	BCR	C23-C22	-2.49	1.40	1.46
24	X	130	BCR	C33-C5	2.49	1.54	1.50
27	t	5217	LMT	O1B-C4'	2.49	1.50	1.43
20	A	563	CLA	C1D-ND	-2.49	1.34	1.37
20	d	5355	CLA	CMD-C2D	2.49	1.55	1.50
20	C	492	CLA	C4-C3	2.48	1.56	1.50
28	I	201	MGE	O3G-C1D	2.48	1.44	1.40
20	C	500	CLA	C4C-C3C	2.48	1.49	1.45
20	c	5500	CLA	CMD-C2D	2.48	1.55	1.50
32	v	5552	HEM	CBD-CAD	2.47	1.60	1.51
20	b	5526	CLA	MG-NC	2.47	2.12	2.06
20	B	511	CLA	C3B-C2B	2.47	1.43	1.40
20	A	563	CLA	C5-C3	2.47	1.56	1.51
20	b	5523	CLA	MG-NC	2.47	2.12	2.06
20	C	502	CLA	C1B-CHB	-2.47	1.34	1.41
24	T	5104	BCR	C30-C25	2.47	1.56	1.53
27	A	569	LMT	O5B-C1B	2.47	1.48	1.41
24	B	527	BCR	C1-C6	2.47	1.56	1.53
20	c	5502	CLA	C4-C3	2.46	1.56	1.50
20	c	5499	CLA	C1B-CHB	-2.46	1.34	1.41
26	d	5358	SQD	C18-C17	-2.46	1.39	1.51
20	C	491	CLA	C4-C3	2.46	1.56	1.50
20	B	513	CLA	C4-C3	2.46	1.56	1.50
27	T	217	LMT	O1B-C4'	2.46	1.50	1.43
20	B	514	CLA	C4-C3	2.46	1.56	1.50
20	C	491	CLA	MG-NC	2.46	2.12	2.06
30	c	5508	DGD	O5D-C1E	2.45	1.44	1.40
27	t	5217	LMT	C1B-C2B	2.45	1.59	1.52
20	B	514	CLA	C1B-CHB	-2.45	1.34	1.41
20	C	494	CLA	MG-NC	2.45	2.12	2.06
20	c	5496	CLA	C4-C3	2.44	1.56	1.50
27	A	569	LMT	C1B-C2B	2.44	1.59	1.52
20	b	5515	CLA	MG-NC	2.44	2.12	2.06
26	A	5212	SQD	O6-C44	-2.44	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5502	CLA	C1B-CHB	-2.44	1.34	1.41
27	a	5568	LMT	C1'-C2'	2.43	1.59	1.52
32	v	5552	HEM	C3B-C2B	2.43	1.42	1.37
20	B	511	CLA	C1C-C2C	2.43	1.49	1.44
20	b	5512	CLA	CAA-CBA	-2.43	1.45	1.52
28	I	201	MGE	O6D-C1D	2.42	1.48	1.41
20	A	559	CLA	C1D-ND	-2.42	1.34	1.37
20	c	5501	CLA	C1C-C2C	2.42	1.49	1.44
32	V	552	HEM	CMA-C3A	2.42	1.56	1.51
26	d	5358	SQD	C8-C7	2.41	1.57	1.50
20	d	5354	CLA	C1D-C2D	-2.41	1.40	1.45
20	B	511	CLA	C3C-C2C	2.41	1.42	1.36
26	A	568	SQD	O5-C1	2.41	1.48	1.41
20	b	5523	CLA	C1B-CHB	-2.40	1.34	1.41
32	f	5051	HEM	C2C-C1C	2.40	1.47	1.42
27	M	5216	LMT	O5'-C1'	2.40	1.48	1.41
20	c	5495	CLA	MG-NC	2.40	2.12	2.06
20	b	5511	CLA	C3C-C2C	2.39	1.41	1.36
20	C	492	CLA	CAA-C2A	2.39	1.58	1.54
21	a	5562	PHO	C4A-C3A	-2.39	1.47	1.51
30	c	5507	DGD	O6D-C5D	2.38	1.50	1.44
21	a	5562	PHO	C4-C3	2.38	1.56	1.50
27	m	216	LMT	O5'-C1'	2.38	1.48	1.41
20	B	512	CLA	CHD-C1D	2.38	1.43	1.38
20	C	497	CLA	C1B-CHB	-2.37	1.34	1.41
20	c	5491	CLA	C1B-CHB	-2.37	1.34	1.41
20	c	5503	CLA	C1-C2	2.37	1.55	1.49
32	F	51	HEM	O2A-CGA	2.37	1.38	1.30
26	a	212	SQD	O48-C23	2.37	1.44	1.33
20	b	5514	CLA	C1B-CHB	-2.37	1.34	1.41
20	c	5497	CLA	C4-C3	2.36	1.56	1.50
24	B	528	BCR	C5-C6	2.36	1.38	1.34
20	b	5519	CLA	C1B-CHB	-2.36	1.34	1.41
20	c	5499	CLA	C4C-C3C	2.36	1.49	1.45
27	m	216	LMT	O5B-C1B	2.35	1.47	1.41
21	A	561	PHO	C4-C3	2.35	1.56	1.50
20	c	5503	CLA	CMD-C2D	2.35	1.55	1.50
30	c	5509	DGD	C4E-C5E	2.35	1.58	1.53
20	b	5520	CLA	C4C-C3C	2.35	1.49	1.45
20	b	5513	CLA	C5-C3	2.35	1.56	1.51
28	d	5361	MGE	O6D-C5D	2.35	1.50	1.44
20	c	5491	CLA	C4-C3	2.34	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	507	DGD	C4D-C5D	2.34	1.58	1.53
20	B	515	CLA	CAA-C2A	2.34	1.58	1.54
28	I	201	MGE	C4D-C3D	2.34	1.58	1.52
20	B	523	CLA	CAA-C2A	2.34	1.58	1.54
20	c	5495	CLA	C1C-C2C	2.34	1.49	1.44
28	i	5201	MGE	C2A-C1A	2.34	1.57	1.50
20	D	355	CLA	MG-NC	2.33	2.11	2.06
30	C	509	DGD	O1G-C1A	2.33	1.40	1.33
26	A	568	SQD	C8-C7	2.33	1.57	1.50
32	v	5552	HEM	CMA-C3A	2.33	1.56	1.51
20	D	355	CLA	CHD-C1D	2.33	1.42	1.38
20	c	5499	CLA	MG-NC	2.33	2.11	2.06
20	A	558	CLA	C1D-C2D	-2.33	1.40	1.45
20	c	5498	CLA	C4-C3	2.32	1.56	1.50
28	b	5530	MGE	C4D-C5D	2.32	1.58	1.53
20	c	5503	CLA	C4-C3	2.32	1.56	1.50
26	d	5358	SQD	C24-C23	2.32	1.57	1.50
28	d	5360	MGE	O3G-C1D	2.32	1.44	1.40
20	B	526	CLA	C1-C2	2.31	1.55	1.49
32	V	552	HEM	CBD-CAD	2.31	1.60	1.51
32	v	5552	HEM	C2A-C3A	2.31	1.44	1.37
20	c	5492	CLA	CAA-C2A	2.31	1.58	1.54
24	B	527	BCR	C38-C26	2.31	1.54	1.50
28	i	5201	MGE	O3G-C1D	2.31	1.44	1.40
20	b	5518	CLA	C1B-CHB	-2.30	1.34	1.41
20	B	514	CLA	C1D-ND	-2.30	1.34	1.37
20	C	500	CLA	C1D-ND	-2.30	1.34	1.37
20	B	524	CLA	CAA-C2A	2.30	1.58	1.54
20	b	5523	CLA	C1D-C2D	-2.29	1.40	1.45
20	c	5497	CLA	C1D-C2D	-2.29	1.40	1.45
20	b	5515	CLA	C1D-ND	-2.29	1.34	1.37
30	c	5507	DGD	O6E-C5E	2.29	1.50	1.44
20	A	563	CLA	CAA-C2A	2.29	1.58	1.54
20	b	5523	CLA	C5-C3	2.29	1.56	1.51
30	c	5508	DGD	C4E-C3E	2.28	1.58	1.52
20	b	5524	CLA	C1D-ND	-2.28	1.34	1.37
28	D	360	MGE	O6D-C5D	2.28	1.50	1.44
24	B	527	BCR	C19-C18	-2.28	1.41	1.46
24	C	506	BCR	C35-C13	2.27	1.55	1.50
20	b	5526	CLA	CAA-CBA	-2.27	1.46	1.52
20	c	5497	CLA	MG-NA	2.27	2.11	2.06
28	b	5530	MGE	O2G-C1B	2.27	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	213	SQD	O6-C1	2.27	1.44	1.40
24	t	104	BCR	C35-C13	2.27	1.55	1.50
24	D	357	BCR	C38-C26	2.27	1.54	1.50
28	b	5530	MGE	O1G-C1G	-2.27	1.40	1.45
24	h	5107	BCR	C5-C6	2.26	1.38	1.34
20	C	492	CLA	C5-C3	2.26	1.56	1.51
20	c	5495	CLA	C4-C3	2.26	1.56	1.50
32	V	552	HEM	C3C-CAC	2.26	1.52	1.47
26	A	568	SQD	C37-C36	-2.26	1.37	1.51
20	B	520	CLA	MG-NC	2.25	2.11	2.06
20	d	5354	CLA	C1D-ND	-2.25	1.34	1.37
20	b	5519	CLA	C1C-C2C	2.25	1.49	1.44
20	c	5492	CLA	C1C-NC	-2.25	1.34	1.37
20	C	499	CLA	C1B-CHB	-2.25	1.34	1.41
20	B	511	CLA	CMC-C2C	2.25	1.55	1.50
20	b	5515	CLA	C3A-C2A	-2.25	1.48	1.54
20	c	5493	CLA	CMB-C2B	2.24	1.56	1.51
28	l	5210	MGE	C4D-C3D	2.24	1.58	1.52
32	f	5051	HEM	CBD-CGD	2.24	1.55	1.50
20	b	5515	CLA	CAA-CBA	-2.24	1.46	1.52
26	A	568	SQD	O6-C1	2.24	1.43	1.40
22	a	5564	PQ9	C11-C2	2.24	1.54	1.51
30	C	507	DGD	O6E-C5E	2.24	1.49	1.44
30	h	5208	DGD	C1D-C2D	2.24	1.59	1.52
20	a	5560	CLA	C4-C3	2.24	1.56	1.50
20	B	526	CLA	C2-C3	2.24	1.38	1.33
20	C	493	CLA	MG-NC	2.24	2.11	2.06
20	C	495	CLA	C4C-C3C	2.24	1.48	1.45
27	a	5568	LMT	O5B-C1B	2.24	1.47	1.41
30	C	509	DGD	O2G-C1B	2.24	1.40	1.34
24	a	5566	BCR	C26-C25	2.23	1.38	1.34
20	C	502	CLA	C4-C3	2.23	1.56	1.50
20	b	5517	CLA	C1-C2	2.23	1.55	1.49
27	M	5216	LMT	C1B-C2B	2.23	1.59	1.52
22	D	356	PQ9	C3-C4	2.22	1.50	1.44
20	b	5520	CLA	C1D-C2D	-2.22	1.40	1.45
28	b	5530	MGE	C4D-C3D	2.22	1.58	1.52
20	d	5355	CLA	C1C-C2C	2.22	1.49	1.44
20	c	5503	CLA	MG-NC	2.22	2.11	2.06
20	B	518	CLA	C4-C3	2.22	1.56	1.50
20	c	5495	CLA	C1D-C2D	-2.22	1.40	1.45
20	C	499	CLA	C1D-C2D	-2.22	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	5208	DGD	C3E-C2E	2.22	1.58	1.52
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	A	558	CLA	CAA-C2A	2.21	1.58	1.54
20	C	496	CLA	C1B-CHB	-2.21	1.34	1.41
20	B	526	CLA	CHD-C1D	2.21	1.42	1.38
27	M	5216	LMT	C3B-C2B	2.21	1.58	1.52
28	B	530	MGE	C4D-C5D	2.21	1.57	1.53
30	h	5208	DGD	O6D-C1D	2.21	1.47	1.41
20	B	526	CLA	CAA-CBA	-2.21	1.46	1.52
20	B	515	CLA	C1D-ND	-2.21	1.35	1.37
20	b	5513	CLA	C1D-ND	-2.21	1.35	1.37
20	d	5354	CLA	C3A-C4A	-2.20	1.44	1.51
32	F	51	HEM	FE-NB	2.20	2.10	1.98
20	D	355	CLA	C1B-CHB	-2.20	1.34	1.41
20	a	5559	CLA	CAA-C2A	2.20	1.58	1.54
20	B	515	CLA	C4-C3	2.20	1.56	1.50
28	D	359	MGE	O1G-C1A	2.20	1.39	1.33
27	M	5216	LMT	C1'-C2'	2.20	1.59	1.52
28	L	210	MGE	C4D-C3D	2.20	1.58	1.52
28	d	5361	MGE	O2G-C1B	2.19	1.40	1.34
20	C	502	CLA	CMB-C2B	2.19	1.56	1.51
20	C	492	CLA	C1D-C2D	-2.19	1.41	1.45
20	C	499	CLA	MG-NC	2.19	2.11	2.06
32	V	552	HEM	CAD-C3D	-2.19	1.45	1.51
20	C	497	CLA	CAA-C2A	2.19	1.58	1.54
20	C	499	CLA	CAA-C2A	2.19	1.58	1.54
32	F	51	HEM	CMD-C2D	2.19	1.55	1.50
20	B	511	CLA	C1B-CHB	-2.19	1.34	1.41
20	b	5517	CLA	C1D-ND	-2.19	1.35	1.37
20	B	513	CLA	C3D-C4D	-2.18	1.39	1.44
20	b	5514	CLA	MG-NC	2.18	2.11	2.06
24	T	5104	BCR	C37-C22	2.17	1.55	1.50
20	B	521	CLA	C4-C3	2.17	1.56	1.50
20	B	520	CLA	C1D-ND	-2.17	1.35	1.37
20	C	503	CLA	C4-C3	2.17	1.56	1.50
24	c	5505	BCR	C19-C18	-2.17	1.41	1.46
30	c	5508	DGD	O6D-C5D	2.17	1.49	1.44
26	t	213	SQD	C22-C21	-2.17	1.34	1.50
28	b	5530	MGE	C1D-C2D	2.17	1.58	1.52
30	c	5507	DGD	C4D-C5D	2.17	1.57	1.53
20	a	5558	CLA	CBA-CGA	-2.17	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	5212	SQD	C8-C7	2.16	1.56	1.49
28	D	358	MGE	O2G-C1B	2.16	1.40	1.34
27	a	5568	LMT	C1B-C2B	2.16	1.58	1.52
32	v	5552	HEM	CMB-C2B	2.16	1.55	1.50
20	D	355	CLA	C4-C3	2.16	1.56	1.50
20	c	5492	CLA	MG-NC	2.16	2.11	2.06
20	c	5498	CLA	C1C-C2C	2.16	1.48	1.44
20	C	498	CLA	CAA-C2A	2.16	1.58	1.54
20	c	5491	CLA	MG-NC	2.15	2.11	2.06
20	c	5492	CLA	C1D-C2D	-2.15	1.41	1.45
20	D	355	CLA	C1C-C2C	2.15	1.48	1.44
27	m	216	LMT	O5'-C5'	2.15	1.49	1.44
28	d	5359	MGE	C4D-C5D	2.15	1.57	1.53
32	V	552	HEM	CAA-C2A	2.15	1.57	1.52
20	b	5522	CLA	C4-C3	2.15	1.56	1.50
24	A	566	BCR	C29-C28	-2.15	1.47	1.52
30	h	5208	DGD	C4E-C3E	2.15	1.57	1.52
20	C	494	CLA	CMD-C2D	2.15	1.55	1.50
20	B	521	CLA	CBA-CGA	-2.15	1.44	1.50
20	a	5560	CLA	C1D-ND	-2.15	1.35	1.37
30	H	208	DGD	C1D-C2D	2.14	1.58	1.52
26	t	213	SQD	O6-C44	-2.14	1.40	1.43
20	a	5563	CLA	C4-C3	2.14	1.55	1.50
32	f	5051	HEM	FE-NB	2.14	2.10	1.98
28	D	359	MGE	O6D-C5D	2.14	1.49	1.44
20	C	496	CLA	C1C-C2C	2.14	1.48	1.44
26	L	5213	SQD	C8-C7	2.14	1.56	1.50
20	B	520	CLA	C1D-C2D	-2.14	1.41	1.45
20	C	503	CLA	CHD-C1D	2.14	1.42	1.38
20	B	515	CLA	C3A-C2A	-2.13	1.48	1.54
20	b	5523	CLA	CAA-CBA	-2.13	1.46	1.52
20	B	519	CLA	C1B-CHB	-2.13	1.35	1.41
27	a	5568	LMT	O5B-C5B	2.13	1.49	1.44
20	C	503	CLA	C1B-CHB	-2.13	1.35	1.41
20	b	5520	CLA	C1C-C2C	2.13	1.48	1.44
20	A	559	CLA	MG-NC	2.12	2.11	2.06
24	a	5566	BCR	C29-C28	-2.12	1.47	1.52
24	A	566	BCR	C19-C18	-2.12	1.41	1.46
27	m	216	LMT	C4B-C3B	2.12	1.57	1.52
24	x	5130	BCR	C35-C13	2.12	1.55	1.50
20	C	495	CLA	C4-C3	2.12	1.55	1.50
20	b	5512	CLA	C4C-C3C	2.12	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	5357	BCR	C19-C18	-2.12	1.41	1.46
20	C	502	CLA	C4C-C3C	2.11	1.48	1.45
32	V	552	HEM	C1D-C2D	-2.11	1.40	1.44
28	D	360	MGE	O2G-C1B	2.11	1.40	1.34
20	A	563	CLA	CHD-C1D	2.11	1.42	1.38
20	C	501	CLA	CMD-C2D	2.11	1.55	1.50
20	c	5499	CLA	C1C-C2C	2.11	1.48	1.44
21	a	5561	PHO	CBA-CGA	-2.11	1.44	1.50
24	C	505	BCR	C19-C18	-2.11	1.41	1.46
20	C	497	CLA	C1D-C2D	-2.11	1.41	1.45
28	d	5360	MGE	O2G-C1B	2.11	1.40	1.34
27	M	5216	LMT	O5B-C1B	2.11	1.47	1.41
20	C	495	CLA	MG-NC	2.11	2.11	2.06
24	C	506	BCR	C19-C18	-2.11	1.41	1.46
20	d	5354	CLA	CBA-CGA	-2.10	1.44	1.50
27	M	5216	LMT	C4B-C5B	2.10	1.57	1.53
26	d	5358	SQD	C37-C36	-2.10	1.38	1.51
24	b	5527	BCR	C23-C22	-2.10	1.41	1.46
20	D	355	CLA	CMD-C2D	2.10	1.55	1.50
20	A	560	CLA	C4C-C3C	2.10	1.48	1.45
20	B	517	CLA	CMB-C2B	2.10	1.55	1.51
20	d	5355	CLA	C1-C2	2.10	1.55	1.49
24	b	5528	BCR	C26-C25	2.10	1.38	1.34
32	V	552	HEM	C3D-C2D	2.10	1.41	1.36
26	A	568	SQD	C21-C20	-2.09	1.38	1.51
20	C	500	CLA	C4-C3	2.09	1.55	1.50
24	x	5130	BCR	C33-C5	2.09	1.54	1.50
24	h	5107	BCR	C38-C26	2.09	1.54	1.50
30	H	208	DGD	O6E-C5E	2.09	1.49	1.44
20	c	5502	CLA	CMB-C2B	2.09	1.55	1.51
20	C	496	CLA	CHD-C1D	2.09	1.42	1.38
20	D	354	CLA	C1C-C2C	2.09	1.48	1.44
30	C	509	DGD	C3D-C2D	2.09	1.57	1.52
20	c	5502	CLA	CHD-C1D	2.09	1.42	1.38
20	a	5563	CLA	C1D-ND	-2.09	1.35	1.37
24	X	130	BCR	C24-C23	2.08	1.39	1.33
24	x	5130	BCR	C24-C23	2.08	1.39	1.33
28	i	5201	MGE	C3D-C2D	2.08	1.57	1.52
20	c	5501	CLA	C1B-CHB	-2.08	1.35	1.41
20	C	499	CLA	C4C-C3C	2.08	1.48	1.45
30	C	508	DGD	O6D-C5D	2.08	1.49	1.44
30	H	208	DGD	C4E-C3E	2.08	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	354	CLA	C3B-C2B	-2.07	1.37	1.40
20	b	5511	CLA	C3A-C2A	-2.07	1.52	1.54
20	A	560	CLA	C4-C3	2.07	1.55	1.50
28	l	5210	MGE	O6D-C5D	2.07	1.49	1.44
20	C	498	CLA	C4-C3	2.07	1.55	1.50
20	B	512	CLA	CAA-CBA	-2.07	1.46	1.52
20	b	5520	CLA	C4-C3	2.07	1.55	1.50
20	B	519	CLA	C4-C3	2.07	1.55	1.50
20	C	501	CLA	C1B-CHB	-2.06	1.35	1.41
32	v	5552	HEM	C1D-C2D	-2.06	1.40	1.44
20	b	5516	CLA	C1D-ND	-2.06	1.35	1.37
26	A	568	SQD	C24-C23	2.06	1.56	1.50
20	b	5519	CLA	C5-C3	2.06	1.55	1.51
27	m	216	LMT	C1'-C2'	2.06	1.58	1.52
20	C	496	CLA	C1-C2	2.05	1.55	1.49
30	h	5208	DGD	C4E-C5E	2.05	1.57	1.53
30	c	5509	DGD	O1G-C1A	2.05	1.39	1.33
20	C	496	CLA	C2-C3	2.04	1.37	1.33
20	a	5558	CLA	C1D-ND	-2.04	1.35	1.37
20	B	526	CLA	CMD-C2D	2.04	1.55	1.50
20	c	5497	CLA	C4C-C3C	2.04	1.48	1.45
20	b	5520	CLA	CMD-C2D	2.04	1.55	1.50
20	c	5497	CLA	C1-C2	2.04	1.55	1.49
21	a	5561	PHO	C1-C2	2.04	1.55	1.49
20	b	5514	CLA	C4-C3	2.04	1.55	1.50
27	M	5216	LMT	O5B-C5B	2.04	1.49	1.44
26	d	5358	SQD	C21-C20	-2.04	1.39	1.51
24	t	104	BCR	C19-C18	-2.04	1.41	1.46
20	C	497	CLA	CHD-C1D	2.03	1.42	1.38
26	A	568	SQD	C22-C21	-2.03	1.35	1.50
28	l	5210	MGE	O3G-C1D	2.03	1.43	1.40
20	b	5511	CLA	CMC-C2C	2.03	1.54	1.50
26	A	5212	SQD	C44-C45	2.03	1.57	1.50
26	a	212	SQD	C44-C45	2.03	1.57	1.50
26	A	5212	SQD	C24-C23	2.03	1.56	1.49
32	V	552	HEM	C2A-C3A	2.03	1.43	1.37
20	C	495	CLA	C1D-ND	-2.03	1.35	1.37
20	B	525	CLA	CMD-C2D	2.03	1.54	1.50
20	B	524	CLA	C1D-ND	-2.03	1.35	1.37
20	b	5515	CLA	C5-C3	2.03	1.55	1.51
20	C	493	CLA	C4-C3	2.02	1.55	1.50
20	b	5526	CLA	C2-C3	2.02	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	492	CLA	MG-NC	2.02	2.11	2.06
20	B	523	CLA	C5-C3	2.02	1.55	1.51
32	f	5051	HEM	C2A-C3A	2.02	1.43	1.37
26	L	5213	SQD	C22-C21	-2.02	1.35	1.50
20	b	5522	CLA	CMD-C2D	2.02	1.54	1.50
20	B	521	CLA	C1C-C2C	2.02	1.48	1.44
20	B	526	CLA	CMB-C2B	2.02	1.55	1.51
20	c	5498	CLA	C1D-ND	-2.02	1.35	1.37
20	a	5563	CLA	MG-NC	2.02	2.11	2.06
20	C	495	CLA	C5-C3	2.01	1.55	1.51
20	D	355	CLA	C1-C2	2.01	1.54	1.49
24	C	505	BCR	C23-C22	-2.01	1.41	1.46
30	C	509	DGD	O5D-C1E	2.01	1.43	1.40
20	B	515	CLA	CAA-CBA	-2.01	1.46	1.52
20	b	5516	CLA	C1D-C2D	-2.01	1.41	1.45
20	a	5558	CLA	C1C-C2C	2.01	1.48	1.44
24	T	5104	BCR	C26-C25	2.01	1.37	1.34
20	C	502	CLA	C1C-C2C	2.01	1.48	1.44
20	A	560	CLA	CHD-C1D	2.01	1.42	1.38
27	T	217	LMT	C1B-C2B	2.01	1.58	1.52
20	a	5558	CLA	C1D-C2D	-2.00	1.41	1.45
32	f	5051	HEM	CAD-C3D	-2.00	1.46	1.51
30	c	5509	DGD	O6E-C5E	2.00	1.49	1.44
32	F	51	HEM	CAD-C3D	-2.00	1.46	1.51
20	C	501	CLA	C4-C3	2.00	1.55	1.50
32	F	51	HEM	C2A-C3A	2.00	1.43	1.37

All (1544) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5501	CLA	C4A-NA-C1A	12.96	112.59	106.68
20	b	5514	CLA	C4A-NA-C1A	12.90	112.56	106.68
20	C	501	CLA	C4A-NA-C1A	12.84	112.54	106.68
20	B	514	CLA	C4A-NA-C1A	12.74	112.49	106.68
20	B	524	CLA	C4A-NA-C1A	12.52	112.39	106.68
20	c	5491	CLA	C4A-NA-C1A	12.43	112.35	106.68
20	c	5503	CLA	C4A-NA-C1A	12.34	112.31	106.68
20	C	497	CLA	C4A-NA-C1A	12.21	112.25	106.68
20	b	5516	CLA	C4A-NA-C1A	12.21	112.25	106.68
20	C	503	CLA	C4A-NA-C1A	12.17	112.23	106.68
20	B	518	CLA	C4A-NA-C1A	12.15	112.22	106.68
20	B	521	CLA	C4A-NA-C1A	12.13	112.21	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5525	CLA	C4A-NA-C1A	12.10	112.20	106.68
20	c	5502	CLA	C4A-NA-C1A	12.09	112.20	106.68
20	B	517	CLA	C4A-NA-C1A	12.08	112.19	106.68
20	c	5492	CLA	C4A-NA-C1A	12.08	112.19	106.68
20	B	523	CLA	C4A-NA-C1A	12.04	112.17	106.68
20	c	5498	CLA	C4A-NA-C1A	12.00	112.15	106.68
20	b	5523	CLA	C4A-NA-C1A	11.99	112.15	106.68
20	c	5495	CLA	C4A-NA-C1A	11.97	112.14	106.68
20	B	516	CLA	C4A-NA-C1A	11.95	112.13	106.68
20	C	494	CLA	C4A-NA-C1A	11.90	112.11	106.68
20	d	5355	CLA	C4A-NA-C1A	11.88	112.10	106.68
20	b	5518	CLA	C4A-NA-C1A	11.81	112.07	106.68
20	D	355	CLA	C4A-NA-C1A	11.72	112.03	106.68
20	C	502	CLA	C4A-NA-C1A	11.70	112.02	106.68
20	C	493	CLA	C4A-NA-C1A	11.65	112.00	106.68
20	b	5511	CLA	C4A-NA-C1A	11.60	111.97	106.68
20	C	492	CLA	C4A-NA-C1A	11.58	111.96	106.68
20	C	498	CLA	C4A-NA-C1A	11.56	111.95	106.68
20	C	496	CLA	C4A-NA-C1A	11.54	111.94	106.68
20	b	5524	CLA	C4A-NA-C1A	11.53	111.94	106.68
20	B	525	CLA	C4A-NA-C1A	11.53	111.94	106.68
20	C	499	CLA	C4A-NA-C1A	11.49	111.92	106.68
20	b	5521	CLA	C4A-NA-C1A	11.43	111.89	106.68
20	b	5517	CLA	C4A-NA-C1A	11.41	111.89	106.68
20	c	5493	CLA	C4A-NA-C1A	11.38	111.87	106.68
20	C	495	CLA	C4A-NA-C1A	11.37	111.87	106.68
20	B	526	CLA	C4A-NA-C1A	11.27	111.82	106.68
20	c	5499	CLA	C4A-NA-C1A	11.20	111.79	106.68
20	c	5496	CLA	C4A-NA-C1A	11.16	111.77	106.68
20	B	519	CLA	C4A-NA-C1A	11.12	111.75	106.68
20	b	5522	CLA	C4A-NA-C1A	11.11	111.75	106.68
20	b	5519	CLA	C4A-NA-C1A	11.05	111.72	106.68
20	a	5560	CLA	C4A-NA-C1A	11.03	111.71	106.68
20	c	5497	CLA	C4A-NA-C1A	10.97	111.68	106.68
20	B	511	CLA	C4A-NA-C1A	10.92	111.66	106.68
20	C	500	CLA	C4A-NA-C1A	10.88	111.64	106.68
20	b	5526	CLA	C4A-NA-C1A	10.87	111.64	106.68
20	c	5500	CLA	C4A-NA-C1A	10.81	111.61	106.68
20	B	522	CLA	C4A-NA-C1A	10.73	111.57	106.68
20	A	560	CLA	C4A-NA-C1A	10.61	111.52	106.68
20	c	5494	CLA	C4A-NA-C1A	10.60	111.52	106.68
20	B	520	CLA	C4A-NA-C1A	10.57	111.50	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	5559	CLA	C4A-NA-C1A	10.46	111.45	106.68
20	C	491	CLA	C4A-NA-C1A	10.41	111.43	106.68
20	b	5520	CLA	C4A-NA-C1A	10.36	111.41	106.68
20	A	559	CLA	C4A-NA-C1A	10.35	111.40	106.68
20	A	563	CLA	C4A-NA-C1A	10.26	111.36	106.68
20	B	513	CLA	C4A-NA-C1A	10.21	111.34	106.68
20	B	515	CLA	C4A-NA-C1A	10.16	111.31	106.68
20	d	5354	CLA	C4A-NA-C1A	10.13	111.30	106.68
20	B	512	CLA	C4A-NA-C1A	9.91	111.20	106.68
20	b	5515	CLA	C4A-NA-C1A	9.76	111.13	106.68
20	a	5563	CLA	C4A-NA-C1A	9.68	111.09	106.68
20	b	5513	CLA	C4A-NA-C1A	9.60	111.06	106.68
20	A	558	CLA	C4A-NA-C1A	9.53	111.03	106.68
20	b	5512	CLA	C4A-NA-C1A	9.42	110.98	106.68
20	D	354	CLA	C4A-NA-C1A	9.20	110.88	106.68
20	a	5558	CLA	C4A-NA-C1A	9.07	110.82	106.68
26	A	5212	SQD	O5-C1-O6	8.77	130.76	110.04
26	a	212	SQD	O5-C1-O6	8.39	129.88	110.04
26	A	568	SQD	O5-C1-O6	8.36	129.81	110.04
26	d	5358	SQD	O5-C1-O6	8.09	129.16	110.04
26	L	5213	SQD	O5-C1-O6	8.06	129.09	110.04
32	f	5051	HEM	CAD-C3D-C2D	7.90	142.66	127.87
26	t	213	SQD	O6-C1-C2	7.87	120.22	108.27
26	t	213	SQD	O5-C1-O6	7.72	128.28	110.04
30	c	5507	DGD	O6E-C5E-C4E	7.71	123.60	109.70
32	F	51	HEM	CAD-C3D-C2D	7.68	142.26	127.87
32	V	552	HEM	CAD-C3D-C2D	7.61	142.12	127.87
30	H	208	DGD	O6E-C5E-C4E	7.54	123.29	109.70
26	L	5213	SQD	O6-C1-C2	7.49	119.65	108.27
32	v	5552	HEM	CAD-C3D-C2D	7.48	141.87	127.87
30	c	5508	DGD	O6E-C5E-C4E	7.47	123.17	109.70
26	d	5358	SQD	O6-C1-C2	7.41	119.53	108.27
32	f	5051	HEM	CAD-C3D-C4D	-7.40	111.81	124.70
30	C	507	DGD	O6E-C5E-C4E	7.31	122.88	109.70
30	C	508	DGD	O6E-C5E-C4E	7.31	122.87	109.70
26	A	568	SQD	O6-C1-C2	7.24	119.27	108.27
30	C	509	DGD	O6E-C5E-C4E	7.22	122.70	109.70
30	c	5509	DGD	O6E-C5E-C4E	7.19	122.66	109.70
30	h	5208	DGD	O6E-C5E-C4E	7.19	122.65	109.70
32	F	51	HEM	CAD-C3D-C4D	-7.11	112.31	124.70
32	V	552	HEM	CAD-C3D-C4D	-7.09	112.35	124.70
32	v	5552	HEM	CAD-C3D-C4D	-7.02	112.46	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	212	SQD	O6-C1-C2	6.87	118.71	108.27
24	D	357	BCR	C38-C26-C25	6.71	131.80	124.48
24	X	130	BCR	C33-C5-C6	6.70	131.79	124.48
24	T	5104	BCR	C38-C26-C25	6.67	131.77	124.48
26	A	5212	SQD	O6-C1-C2	6.64	118.36	108.27
24	d	5357	BCR	C33-C5-C6	6.51	131.58	124.48
24	c	5505	BCR	C38-C26-C25	6.48	131.55	124.48
24	d	5357	BCR	C38-C26-C25	6.46	131.54	124.48
24	B	529	BCR	C38-C26-C25	6.44	131.51	124.48
24	x	5130	BCR	C33-C5-C6	6.41	131.48	124.48
24	t	104	BCR	C38-C26-C25	6.33	131.39	124.48
24	D	357	BCR	C33-C5-C6	6.17	131.22	124.48
25	A	567	LHG	C25-C24-C23	6.12	136.10	113.69
26	d	5358	SQD	C25-C24-C23	6.11	136.09	113.69
24	B	527	BCR	C38-C26-C25	6.06	131.09	124.48
26	A	568	SQD	C10-C9-C8	6.02	135.25	113.13
25	a	5567	LHG	C25-C24-C23	6.02	135.74	113.69
24	B	528	BCR	C38-C26-C25	5.97	131.00	124.48
26	t	213	SQD	C10-C9-C8	5.97	135.07	113.13
24	C	505	BCR	C38-C26-C25	5.97	131.00	124.48
26	d	5358	SQD	C10-C9-C8	5.96	135.02	113.13
26	L	5213	SQD	C10-C9-C8	5.94	134.96	113.13
24	C	506	BCR	C38-C26-C25	5.88	130.90	124.48
24	h	5107	BCR	C38-C26-C25	5.85	130.87	124.48
26	t	213	SQD	C25-C24-C23	5.83	135.06	113.69
24	c	5506	BCR	C38-C26-C25	5.76	130.77	124.48
24	B	527	BCR	C33-C5-C6	5.76	130.77	124.48
26	L	5213	SQD	C25-C24-C23	5.75	134.76	113.69
26	A	568	SQD	C25-C24-C23	5.74	134.74	113.69
24	A	566	BCR	C33-C5-C6	5.73	130.73	124.48
24	C	504	BCR	C38-C26-C25	5.72	130.73	124.48
24	b	5527	BCR	C33-C5-C6	5.70	130.71	124.48
24	b	5528	BCR	C38-C26-C25	5.69	130.70	124.48
24	t	104	BCR	C33-C5-C6	5.69	130.70	124.48
24	T	5104	BCR	C33-C5-C6	5.69	130.69	124.48
24	X	130	BCR	C7-C8-C9	5.67	134.63	126.23
24	a	5566	BCR	C38-C26-C25	5.64	130.63	124.48
24	b	5529	BCR	C38-C26-C25	5.63	130.63	124.48
24	A	566	BCR	C38-C26-C25	5.63	130.62	124.48
24	B	529	BCR	C33-C5-C6	5.60	130.59	124.48
24	a	5566	BCR	C33-C5-C6	5.58	130.57	124.48
24	H	107	BCR	C38-C26-C25	5.57	130.56	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	5130	BCR	C7-C8-C9	5.52	134.40	126.23
24	c	5504	BCR	C38-C26-C25	5.52	130.51	124.48
24	b	5527	BCR	C38-C26-C25	5.50	130.49	124.48
24	C	506	BCR	C33-C5-C6	5.50	130.48	124.48
24	C	505	BCR	C33-C5-C6	5.43	130.41	124.48
24	X	130	BCR	C11-C10-C9	5.40	134.85	127.28
24	x	5130	BCR	C38-C26-C25	5.39	130.36	124.48
24	c	5506	BCR	C33-C5-C6	5.38	130.35	124.48
22	d	5356	PQ9	C11-C2-C1	5.35	121.32	116.91
20	B	515	CLA	CAA-C2A-C3A	-5.34	98.56	113.00
24	X	130	BCR	C38-C26-C25	5.32	130.29	124.48
32	f	5051	HEM	CHA-C4D-ND	5.29	130.92	124.37
24	H	107	BCR	C33-C5-C6	5.17	130.13	124.48
24	c	5505	BCR	C33-C5-C6	5.11	130.06	124.48
24	b	5529	BCR	C33-C5-C6	5.08	130.03	124.48
32	F	51	HEM	C4C-CHD-C1D	5.05	129.23	122.56
24	h	5107	BCR	C33-C5-C6	5.04	129.99	124.48
20	b	5515	CLA	CAA-C2A-C3A	-5.01	99.47	113.00
24	C	504	BCR	C33-C5-C6	4.98	129.92	124.48
32	V	552	HEM	CHA-C4D-ND	4.97	130.53	124.37
22	D	356	PQ9	C11-C2-C1	4.95	120.98	116.91
24	b	5528	BCR	C33-C5-C6	4.94	129.88	124.48
24	x	5130	BCR	C11-C10-C9	4.93	134.19	127.28
32	f	5051	HEM	C4C-CHD-C1D	4.88	129.00	122.56
26	A	568	SQD	O7-S-C6	4.88	114.04	106.76
24	T	5104	BCR	C29-C30-C25	4.79	117.39	110.44
32	v	5552	HEM	CHA-C4D-ND	4.72	130.23	124.37
24	c	5504	BCR	C33-C5-C6	4.72	129.64	124.48
24	B	528	BCR	C33-C5-C6	4.69	129.60	124.48
26	a	212	SQD	O7-S-C6	4.63	113.66	106.76
20	C	494	CLA	CED-O2D-CGD	4.56	126.25	115.92
24	b	5529	BCR	C29-C30-C25	4.47	116.94	110.44
24	c	5505	BCR	C23-C24-C25	4.47	138.93	127.00
21	A	561	PHO	O2D-CGD-CBD	4.46	115.84	110.95
26	A	568	SQD	O8-S-C6	-4.40	97.49	105.97
24	C	505	BCR	C23-C24-C25	4.39	138.71	127.00
21	A	561	PHO	C1-C2-C3	4.37	133.36	126.20
24	t	104	BCR	C29-C30-C25	4.37	116.79	110.44
24	C	506	BCR	C8-C7-C6	4.34	138.60	127.00
26	a	212	SQD	C44-O6-C1	4.33	123.07	113.80
30	c	5508	DGD	C3G-O3G-C1D	-4.32	104.53	113.80
24	X	130	BCR	C8-C9-C10	-4.32	112.22	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	360	MGE	O6D-C5D-C6D	4.29	117.08	106.44
32	v	5552	HEM	C4C-CHD-C1D	4.29	128.22	122.56
24	x	5130	BCR	C8-C9-C10	-4.26	112.31	119.01
21	A	562	PHO	O2D-CGD-CBD	4.23	115.60	110.95
24	d	5357	BCR	C29-C30-C25	4.21	116.56	110.44
24	x	5130	BCR	C29-C30-C25	4.18	116.50	110.44
24	x	5130	BCR	C23-C24-C25	4.17	138.13	127.00
24	X	130	BCR	C23-C24-C25	4.16	138.10	127.00
32	F	51	HEM	CHA-C4D-ND	4.16	129.52	124.37
20	c	5494	CLA	CED-O2D-CGD	4.15	125.33	115.92
32	F	51	HEM	CBD-CAD-C3D	-4.15	101.06	112.53
26	a	212	SQD	O8-S-C6	-4.14	97.98	105.97
20	b	5526	CLA	CED-O2D-CGD	4.12	125.26	115.92
30	h	5208	DGD	O3G-C1D-C2D	4.12	114.53	108.27
24	h	5107	BCR	C29-C30-C25	4.11	116.41	110.44
30	C	509	DGD	O6D-C5D-C6D	4.11	114.84	106.69
24	X	130	BCR	C2-C1-C6	4.10	116.40	110.44
24	c	5506	BCR	C8-C7-C6	4.10	137.95	127.00
26	d	5358	SQD	O8-S-C6	-4.09	98.07	105.97
20	c	5502	CLA	CAA-C2A-C3A	-4.09	101.96	113.00
24	t	104	BCR	C8-C7-C6	4.06	137.84	127.00
20	C	495	CLA	CAA-C2A-C3A	-4.06	102.03	113.00
21	a	5561	PHO	O2D-CGD-CBD	4.05	115.40	110.95
20	C	497	CLA	C7-C6-C5	-4.05	102.48	113.26
20	c	5495	CLA	CAA-C2A-C3A	-4.04	102.09	113.00
26	t	213	SQD	O7-S-C6	4.03	112.78	106.76
20	B	511	CLA	CAA-C2A-C3A	-4.03	107.00	116.23
20	b	5511	CLA	CAA-C2A-C3A	-4.02	107.01	116.23
28	L	210	MGE	C3G-O3G-C1D	-4.02	105.18	113.80
24	X	130	BCR	C29-C30-C25	4.01	116.27	110.44
28	D	360	MGE	O2G-C1B-C2B	4.01	120.16	111.48
28	l	5210	MGE	C3G-O3G-C1D	-4.01	105.20	113.80
24	C	505	BCR	C2-C1-C6	4.01	116.26	110.44
24	C	505	BCR	C29-C30-C25	4.00	116.25	110.44
30	c	5509	DGD	O6D-C5D-C6D	4.00	114.62	106.69
24	c	5505	BCR	C29-C30-C25	4.00	116.25	110.44
24	b	5528	BCR	C29-C30-C25	4.00	116.24	110.44
20	C	494	CLA	CAA-C2A-C3A	-3.99	102.21	113.00
24	a	5566	BCR	C29-C30-C25	3.98	116.22	110.44
24	x	5130	BCR	C2-C1-C6	3.97	116.21	110.44
20	D	354	CLA	C1-C2-C3	3.97	132.70	126.20
26	L	5213	SQD	O48-C23-C24	3.97	123.94	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	528	BCR	C30-C25-C26	-3.96	117.23	122.64
32	f	5051	HEM	CBD-CAD-C3D	-3.95	101.61	112.53
26	d	5358	SQD	O7-S-C6	3.95	112.66	106.76
26	A	5212	SQD	O7-S-C6	3.95	112.66	106.76
20	c	5493	CLA	CAA-C2A-C3A	-3.95	102.32	113.00
24	b	5529	BCR	C2-C1-C6	3.95	116.17	110.44
20	c	5494	CLA	CAA-C2A-C3A	-3.95	102.33	113.00
24	C	504	BCR	C24-C23-C22	3.95	132.07	126.23
20	C	493	CLA	CAA-C2A-C3A	-3.93	102.37	113.00
26	d	5358	SQD	C31-C30-C29	3.93	134.21	114.37
26	t	213	SQD	O48-C23-C24	3.92	123.78	111.83
24	b	5528	BCR	C2-C1-C6	3.91	116.12	110.44
30	H	208	DGD	O3G-C1D-C2D	3.91	114.21	108.27
26	A	5212	SQD	C44-O6-C1	3.91	122.17	113.80
30	C	508	DGD	C3G-O3G-C1D	-3.91	105.42	113.80
28	d	5361	MGE	O6D-C5D-C6D	3.90	116.12	106.44
24	T	5104	BCR	C8-C7-C6	3.90	137.42	127.00
24	A	566	BCR	C29-C30-C25	3.90	116.10	110.44
20	C	502	CLA	CAA-C2A-C3A	-3.90	102.47	113.00
28	d	5361	MGE	O2G-C1B-C2B	3.89	119.90	111.48
24	D	357	BCR	C2-C1-C6	3.85	116.04	110.44
24	H	107	BCR	C29-C30-C25	3.85	116.03	110.44
20	b	5519	CLA	CED-O2D-CGD	3.84	124.63	115.92
26	A	568	SQD	C31-C30-C29	3.84	133.77	114.37
32	v	5552	HEM	C4B-CHC-C1C	3.84	127.62	122.56
32	V	552	HEM	C4C-CHD-C1D	3.83	127.62	122.56
24	B	529	BCR	C29-C30-C25	3.83	116.00	110.44
20	c	5497	CLA	C7-C6-C5	-3.82	103.09	113.26
24	B	529	BCR	C2-C1-C6	3.81	115.98	110.44
24	d	5357	BCR	C30-C25-C26	-3.81	117.42	122.64
24	T	5104	BCR	C30-C25-C26	-3.81	117.43	122.64
24	c	5506	BCR	C29-C30-C25	3.81	115.97	110.44
32	f	5051	HEM	C4B-CHC-C1C	3.80	127.57	122.56
24	T	5104	BCR	C24-C23-C22	3.80	131.85	126.23
24	T	5104	BCR	C33-C5-C4	-3.79	105.51	113.60
32	V	552	HEM	C4B-CHC-C1C	3.79	127.56	122.56
24	d	5357	BCR	C1-C6-C5	-3.79	117.46	122.64
27	a	5568	LMT	C1-O1'-C1'	-3.79	107.21	113.68
20	c	5491	CLA	CED-O2D-CGD	3.79	124.50	115.92
24	T	5104	BCR	C38-C26-C27	-3.78	105.53	113.60
24	c	5504	BCR	C24-C23-C22	3.78	131.83	126.23
25	A	567	LHG	O8-C23-C24	3.78	123.35	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	v	5552	HEM	CBD-CAD-C3D	-3.77	102.11	112.53
26	A	5212	SQD	C45-O47-C7	3.77	124.50	117.85
26	A	568	SQD	C11-C10-C9	3.76	133.38	114.37
24	x	5130	BCR	C33-C5-C4	-3.76	105.58	113.60
24	B	529	BCR	C38-C26-C27	-3.76	105.58	113.60
20	b	5520	CLA	C7-C6-C5	-3.76	103.25	113.26
27	A	569	LMT	C1-O1'-C1'	-3.75	107.27	113.68
20	C	496	CLA	CED-O2D-CGD	3.75	124.42	115.92
22	d	5356	PQ9	C11-C2-C3	-3.75	118.97	123.39
24	D	357	BCR	C38-C26-C27	-3.74	105.62	113.60
24	C	506	BCR	C23-C24-C25	3.74	136.99	127.00
24	d	5357	BCR	C38-C26-C27	-3.74	105.63	113.60
20	B	518	CLA	O2A-CGA-CBA	3.73	123.22	111.83
24	h	5107	BCR	C11-C10-C9	3.73	132.51	127.28
24	C	506	BCR	C2-C1-C6	3.73	115.86	110.44
20	c	5492	CLA	CED-O2D-CGD	3.73	124.37	115.92
24	d	5357	BCR	C2-C1-C6	3.73	115.85	110.44
24	H	107	BCR	C11-C10-C9	3.72	132.50	127.28
24	c	5504	BCR	C1-C6-C5	-3.72	117.55	122.64
30	C	508	DGD	O5D-C1E-C2E	3.72	113.92	108.27
24	D	357	BCR	C1-C6-C5	-3.72	117.56	122.64
20	c	5503	CLA	CED-O2D-CGD	3.71	124.34	115.92
22	A	564	PQ9	C11-C12-C13	-3.71	120.43	126.83
20	b	5518	CLA	O2A-CGA-CBA	3.71	123.15	111.83
21	a	5562	PHO	C7-C6-C5	-3.71	103.37	113.26
26	d	5358	SQD	O48-C23-C24	3.70	123.12	111.83
26	t	213	SQD	O8-S-C6	-3.70	98.83	105.97
24	H	107	BCR	C30-C25-C26	-3.70	117.58	122.64
32	F	51	HEM	C4B-CHC-C1C	3.70	127.44	122.56
24	C	504	BCR	C1-C6-C5	-3.70	117.59	122.64
24	D	357	BCR	C33-C5-C4	-3.69	105.72	113.60
24	c	5505	BCR	C2-C1-C6	3.69	115.80	110.44
24	X	130	BCR	C33-C5-C4	-3.69	105.73	113.60
26	t	213	SQD	C11-C10-C9	3.69	133.00	114.37
24	D	357	BCR	C30-C25-C26	-3.68	117.60	122.64
21	a	5562	PHO	O2D-CGD-CBD	3.68	114.99	110.95
26	d	5358	SQD	C11-C10-C9	3.68	132.98	114.37
24	h	5107	BCR	C23-C24-C25	3.68	136.82	127.00
20	B	513	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
20	b	5516	CLA	O2A-CGA-CBA	3.67	123.03	111.83
24	C	506	BCR	C29-C30-C25	3.67	115.77	110.44
24	b	5528	BCR	C30-C25-C26	-3.67	117.63	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5527	BCR	C2-C1-C6	3.66	115.76	110.44
24	t	104	BCR	C33-C5-C4	-3.65	105.81	113.60
20	C	497	CLA	C1-C2-C3	3.65	132.17	126.20
20	B	517	CLA	C1-C2-C3	3.64	132.16	126.20
24	c	5506	BCR	C30-C25-C26	-3.64	117.67	122.64
24	d	5357	BCR	C33-C5-C4	-3.63	105.85	113.60
30	h	5208	DGD	C1E-O6E-C5E	3.63	120.81	113.72
20	a	5560	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
24	x	5130	BCR	C16-C17-C18	3.63	132.36	127.28
28	d	5360	MGE	O6D-C5D-C6D	3.63	115.42	106.44
26	a	212	SQD	C45-O47-C7	3.62	124.24	117.85
22	D	356	PQ9	C11-C2-C3	-3.62	119.12	123.39
24	C	504	BCR	C38-C26-C27	-3.60	105.91	113.60
20	A	560	CLA	CAA-C2A-C3A	-3.60	103.26	113.00
24	t	104	BCR	C30-C25-C26	-3.60	117.71	122.64
24	X	130	BCR	C30-C25-C26	-3.60	117.71	122.64
24	x	5130	BCR	C30-C25-C26	-3.60	117.72	122.64
20	B	517	CLA	O2A-CGA-CBA	3.60	122.80	111.83
20	C	492	CLA	CED-O2D-CGD	3.59	124.07	115.92
20	b	5521	CLA	C7-C6-C5	-3.59	103.69	113.26
24	c	5504	BCR	C2-C1-C6	3.59	115.65	110.44
24	C	505	BCR	C33-C5-C4	-3.59	105.95	113.60
24	D	357	BCR	C29-C30-C25	3.58	115.64	110.44
21	a	5561	PHO	C1-C2-C3	3.58	132.06	126.20
22	d	5356	PQ9	C24-C23-C25	3.57	121.42	115.23
24	C	506	BCR	C38-C26-C27	-3.57	105.99	113.60
24	H	107	BCR	C23-C24-C25	3.56	136.52	127.00
28	d	5359	MGE	O2G-C1B-C2B	3.56	119.19	111.48
24	D	357	BCR	C23-C24-C25	3.56	136.51	127.00
20	B	521	CLA	C7-C6-C5	-3.56	103.78	113.26
30	C	507	DGD	C1E-O6E-C5E	3.56	120.66	113.72
24	a	5566	BCR	C30-C25-C26	-3.55	117.78	122.64
24	H	107	BCR	C38-C26-C27	-3.55	106.03	113.60
24	B	528	BCR	C2-C1-C6	3.54	115.59	110.44
20	B	520	CLA	C7-C6-C5	-3.54	103.82	113.26
24	b	5527	BCR	C23-C24-C25	3.54	136.46	127.00
20	B	516	CLA	C1-C2-C3	3.54	131.99	126.20
24	h	5107	BCR	C30-C25-C26	-3.53	117.81	122.64
25	a	5567	LHG	O8-C23-C24	3.53	122.60	111.83
30	c	5508	DGD	O2G-C1B-C2B	3.53	119.11	111.48
20	A	558	CLA	C1-C2-C3	3.53	131.97	126.20
26	A	568	SQD	O48-C23-C24	3.52	122.58	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	528	BCR	C38-C26-C27	-3.52	106.08	113.60
26	L	5213	SQD	C11-C10-C9	3.52	132.18	114.37
20	c	5500	CLA	C7-C6-C5	-3.52	103.88	113.26
24	B	528	BCR	C29-C30-C25	3.52	115.55	110.44
24	h	5107	BCR	C8-C7-C6	3.51	136.37	127.00
20	c	5501	CLA	C7-C6-C5	-3.51	103.91	113.26
20	c	5496	CLA	CED-O2D-CGD	3.51	123.87	115.92
20	c	5493	CLA	CED-O2D-CGD	3.50	123.85	115.92
26	A	5212	SQD	O8-S-C6	-3.50	99.22	105.97
24	C	504	BCR	C2-C1-C6	3.49	115.51	110.44
20	b	5513	CLA	CAA-C2A-C3A	-3.49	103.57	113.00
24	C	504	BCR	C33-C5-C4	-3.49	106.16	113.60
20	B	516	CLA	O2A-CGA-CBA	3.48	122.46	111.83
24	A	566	BCR	C30-C25-C26	-3.48	117.88	122.64
32	V	552	HEM	CBD-CAD-C3D	-3.48	102.91	112.53
24	b	5528	BCR	C23-C24-C25	3.48	136.29	127.00
22	D	356	PQ9	C24-C23-C25	3.48	121.26	115.23
24	H	107	BCR	C2-C1-C6	3.47	115.48	110.44
24	B	528	BCR	C23-C24-C25	3.47	136.26	127.00
20	C	503	CLA	CED-O2D-CGD	3.46	123.78	115.92
30	c	5508	DGD	O5D-C1E-C2E	3.46	113.53	108.27
20	B	519	CLA	CED-O2D-CGD	3.46	123.77	115.92
24	B	529	BCR	C23-C24-C25	3.46	136.24	127.00
20	b	5512	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
20	B	526	CLA	CED-O2D-CGD	3.46	123.76	115.92
20	b	5516	CLA	CED-O2D-CGD	3.45	123.75	115.92
20	a	5558	CLA	CED-O2D-CGD	3.45	123.74	115.92
24	b	5529	BCR	C30-C25-C26	-3.45	117.93	122.64
24	c	5506	BCR	C23-C24-C25	3.45	136.21	127.00
24	C	506	BCR	C33-C5-C4	-3.44	106.25	113.60
20	b	5511	CLA	CMA-C3A-C2A	-3.44	108.33	116.23
20	b	5517	CLA	O2A-CGA-CBA	3.44	122.33	111.83
24	B	529	BCR	C30-C25-C26	-3.44	117.94	122.64
24	c	5506	BCR	C38-C26-C27	-3.44	106.27	113.60
20	b	5526	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
30	c	5509	DGD	C1E-O6E-C5E	3.43	120.42	113.72
20	d	5355	CLA	C1-C2-C3	3.43	132.32	126.76
30	C	507	DGD	O6D-C5D-C6D	3.43	113.50	106.69
30	c	5507	DGD	O6D-C5D-C6D	3.43	113.49	106.69
24	c	5504	BCR	C38-C26-C27	-3.42	106.30	113.60
24	c	5506	BCR	C2-C1-C6	3.42	115.41	110.44
20	C	502	CLA	O2A-CGA-CBA	3.41	122.24	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	5354	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
24	A	566	BCR	C38-C26-C27	-3.40	106.34	113.60
24	b	5527	BCR	C38-C26-C27	-3.40	106.35	113.60
20	B	522	CLA	O2A-CGA-CBA	3.40	122.19	111.83
24	b	5529	BCR	C23-C24-C25	3.40	136.07	127.00
24	A	566	BCR	C33-C5-C4	-3.39	106.37	113.60
24	a	5566	BCR	C38-C26-C27	-3.39	106.37	113.60
24	h	5107	BCR	C38-C26-C27	-3.39	106.37	113.60
28	B	530	MGE	C3G-O3G-C1D	-3.39	106.53	113.80
20	a	5559	CLA	CED-O2D-CGD	3.38	123.59	115.92
30	C	508	DGD	O2G-C1B-C2B	3.38	118.80	111.48
20	B	512	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
24	c	5505	BCR	C38-C26-C27	-3.38	106.39	113.60
24	c	5506	BCR	C33-C5-C4	-3.38	106.39	113.60
20	B	513	CLA	O2A-CGA-CBA	3.38	122.13	111.83
24	C	504	BCR	C29-C30-C25	3.37	115.34	110.44
24	h	5107	BCR	C2-C1-C6	3.37	115.34	110.44
24	a	5566	BCR	C24-C23-C22	3.37	131.22	126.23
21	A	562	PHO	C7-C6-C5	-3.37	104.28	113.26
24	C	504	BCR	C30-C25-C26	-3.36	118.04	122.64
20	B	511	CLA	CMA-C3A-C2A	-3.36	108.53	116.23
20	c	5502	CLA	O2A-CGA-CBA	3.36	122.07	111.83
20	d	5354	CLA	C1-C2-C3	3.35	131.69	126.20
30	C	509	DGD	C1E-O6E-C5E	3.35	120.27	113.72
20	c	5493	CLA	O2A-CGA-CBA	3.35	122.06	111.83
20	C	493	CLA	O2A-CGA-CBA	3.35	122.06	111.83
21	A	561	PHO	CED-O2D-CGD	3.35	123.51	115.92
30	h	5208	DGD	O6D-C5D-C6D	3.35	113.33	106.69
24	D	357	BCR	C8-C7-C6	3.34	135.93	127.00
20	b	5517	CLA	C1-C2-C3	3.34	131.67	126.20
30	H	208	DGD	O2G-C1B-C2B	3.34	118.71	111.48
24	B	527	BCR	C2-C1-C6	3.34	115.29	110.44
28	i	5201	MGE	O2G-C1B-C2B	3.34	118.70	111.48
28	I	201	MGE	O2G-C1B-C2B	3.34	118.70	111.48
20	b	5513	CLA	O2A-CGA-CBA	3.34	122.01	111.83
30	C	508	DGD	C3G-C2G-C1G	-3.34	104.00	111.78
24	c	5505	BCR	C33-C5-C4	-3.34	106.48	113.60
20	c	5497	CLA	O2A-CGA-CBA	3.34	122.00	111.83
24	B	527	BCR	C38-C26-C27	-3.33	106.49	113.60
24	C	506	BCR	C30-C25-C26	-3.33	118.08	122.64
24	d	5357	BCR	C24-C23-C22	3.33	131.16	126.23
24	X	130	BCR	C38-C26-C27	-3.33	106.49	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	104	BCR	C24-C23-C22	3.33	131.16	126.23
21	a	5562	PHO	O2A-CGA-CBA	3.33	121.98	111.83
24	b	5529	BCR	C38-C26-C27	-3.32	106.51	113.60
24	b	5527	BCR	C33-C5-C4	-3.32	106.52	113.60
20	A	559	CLA	CAA-C2A-C3A	-3.32	104.04	113.00
20	b	5522	CLA	C7-C6-C5	-3.32	104.42	113.26
24	H	107	BCR	C1-C6-C5	-3.31	118.11	122.64
20	b	5512	CLA	CED-O2D-CGD	3.31	123.43	115.92
24	H	107	BCR	C33-C5-C4	-3.31	106.53	113.60
24	t	104	BCR	C38-C26-C27	-3.31	106.54	113.60
24	x	5130	BCR	C12-C13-C14	-3.31	113.81	119.01
24	d	5357	BCR	C23-C24-C25	3.31	135.83	127.00
24	B	527	BCR	C33-C5-C4	-3.30	106.55	113.60
20	D	354	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
28	D	359	MGE	O6D-C5D-C6D	3.30	114.62	106.44
21	A	562	PHO	O2A-CGA-CBA	3.30	121.89	111.83
24	b	5528	BCR	C1-C6-C5	-3.30	118.13	122.64
24	h	5107	BCR	C1-C6-C5	-3.29	118.14	122.64
28	B	530	MGE	O2G-C1B-C2B	3.29	118.60	111.48
24	x	5130	BCR	C38-C26-C27	-3.29	106.58	113.60
20	a	5559	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
24	A	566	BCR	C24-C23-C22	3.29	131.10	126.23
28	D	359	MGE	O2G-C1B-C2B	3.29	118.59	111.48
24	H	107	BCR	C8-C7-C6	3.28	135.76	127.00
28	D	358	MGE	O2G-C1B-C2B	3.28	118.58	111.48
30	c	5508	DGD	C3G-C2G-C1G	-3.28	104.14	111.78
24	B	527	BCR	C23-C24-C25	3.28	135.75	127.00
20	b	5515	CLA	O2A-CGA-CBA	3.27	121.81	111.83
20	A	563	CLA	C1-C2-C3	3.27	131.55	126.20
24	b	5529	BCR	C33-C5-C4	-3.27	106.63	113.60
24	b	5527	BCR	C29-C30-C25	3.27	115.18	110.44
20	C	501	CLA	C7-C6-C5	-3.26	104.56	113.26
28	l	5210	MGE	O6D-C5D-C6D	3.26	114.52	106.44
20	b	5522	CLA	O2A-CGA-CBA	3.26	121.77	111.83
24	B	527	BCR	C30-C25-C26	-3.25	118.19	122.64
26	d	5358	SQD	C45-O47-C7	3.25	125.58	117.80
20	C	496	CLA	C1-C2-C3	3.25	131.52	126.20
24	B	529	BCR	C33-C5-C4	-3.24	106.69	113.60
24	b	5529	BCR	C1-C6-C5	-3.24	118.21	122.64
24	b	5529	BCR	C8-C7-C6	3.24	135.65	127.00
24	A	566	BCR	C23-C24-C25	3.24	135.65	127.00
28	b	5530	MGE	O2G-C1B-C2B	3.24	118.48	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	507	DGD	O2G-C1B-C2B	3.24	118.48	111.48
20	c	5497	CLA	C1-C2-C3	3.23	131.49	126.20
20	B	526	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
24	B	527	BCR	C29-C30-C25	3.23	115.13	110.44
24	a	5566	BCR	C33-C5-C4	-3.23	106.72	113.60
22	a	5564	PQ9	C11-C12-C13	-3.22	121.28	126.83
20	b	5516	CLA	C1-C2-C3	3.22	131.48	126.20
24	H	107	BCR	C15-C14-C13	3.22	131.80	127.28
24	x	5130	BCR	C1-C6-C5	-3.22	118.23	122.64
24	d	5357	BCR	C8-C7-C6	3.22	135.60	127.00
20	c	5502	CLA	CED-O2D-CGD	3.22	123.22	115.92
32	f	5051	HEM	CHA-C4D-C3D	-3.22	119.29	125.23
20	B	524	CLA	CED-O2D-CGD	3.21	123.20	115.92
24	C	505	BCR	C16-C17-C18	3.21	131.78	127.28
24	c	5504	BCR	C33-C5-C4	-3.21	106.76	113.60
20	b	5515	CLA	CED-O2D-CGD	3.20	123.18	115.92
24	C	506	BCR	C35-C13-C12	3.20	122.98	118.09
24	X	130	BCR	C1-C6-C5	-3.20	118.27	122.64
24	c	5504	BCR	C32-C1-C6	3.19	115.25	110.24
20	D	355	CLA	C1-C2-C3	3.19	131.93	126.76
20	B	511	CLA	CMB-C2B-C1B	-3.19	123.78	128.46
24	c	5505	BCR	C35-C13-C12	3.19	122.96	118.09
24	a	5566	BCR	C23-C24-C25	3.19	135.51	127.00
20	C	495	CLA	CMB-C2B-C1B	-3.18	123.79	128.46
24	b	5527	BCR	C1-C6-C5	-3.18	118.28	122.64
20	C	491	CLA	CED-O2D-CGD	3.18	123.13	115.92
20	C	497	CLA	O2A-CGA-CBA	3.18	121.53	111.83
21	A	561	PHO	C4A-C3A-C2A	3.18	105.87	102.84
21	A	562	PHO	C4A-C3A-C2A	3.18	105.87	102.84
30	c	5507	DGD	O2G-C1B-C2B	3.18	118.35	111.48
24	H	107	BCR	C24-C23-C22	3.17	130.93	126.23
30	h	5208	DGD	O2G-C1B-C2B	3.17	118.34	111.48
24	t	104	BCR	C2-C1-C6	3.17	115.04	110.44
20	C	495	CLA	C7-C6-C5	-3.17	104.83	113.26
30	c	5508	DGD	C1E-O6E-C5E	3.16	119.90	113.72
24	h	5107	BCR	C33-C5-C4	-3.16	106.86	113.60
24	c	5504	BCR	C23-C24-C25	3.16	135.44	127.00
24	h	5107	BCR	C32-C1-C6	3.16	115.20	110.24
24	C	506	BCR	C16-C17-C18	3.16	131.71	127.28
24	x	5130	BCR	C34-C9-C8	3.16	122.91	118.09
20	B	518	CLA	CED-O2D-CGD	3.15	123.07	115.92
20	b	5520	CLA	O2A-CGA-CBA	3.15	121.45	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	5354	CLA	O2A-CGA-CBA	3.15	121.45	111.83
24	B	528	BCR	C8-C7-C6	3.15	135.42	127.00
20	a	5558	CLA	C7-C6-C5	-3.15	104.87	113.26
20	B	525	CLA	C7-C6-C5	-3.15	104.87	113.26
30	c	5507	DGD	C1E-O6E-C5E	3.15	119.87	113.72
24	C	504	BCR	C23-C24-C25	3.15	135.40	127.00
20	b	5514	CLA	O2A-CGA-CBA	3.14	121.42	111.83
24	b	5528	BCR	C38-C26-C27	-3.14	106.90	113.60
21	a	5561	PHO	C7-C6-C5	-3.14	104.89	113.26
24	B	529	BCR	C1-C6-C5	-3.14	118.34	122.64
20	c	5491	CLA	O2A-CGA-CBA	3.14	121.41	111.83
24	C	505	BCR	C38-C26-C27	-3.14	106.90	113.60
20	B	522	CLA	C7-C6-C5	-3.14	104.90	113.26
24	b	5528	BCR	C33-C5-C4	-3.14	106.91	113.60
26	L	5213	SQD	O8-S-C6	-3.13	99.93	105.97
28	I	201	MGE	O6D-C5D-C6D	3.13	114.19	106.44
20	a	5563	CLA	C1-C2-C3	3.13	131.32	126.20
28	L	210	MGE	O6D-C5D-C6D	3.13	114.19	106.44
20	B	522	CLA	CED-O2D-CGD	3.12	123.00	115.92
28	b	5530	MGE	C3G-O3G-C1D	-3.12	107.10	113.80
20	b	5522	CLA	CED-O2D-CGD	3.12	123.00	115.92
24	B	529	BCR	C24-C23-C22	3.12	130.85	126.23
20	B	516	CLA	CED-O2D-CGD	3.12	122.99	115.92
24	c	5504	BCR	C29-C30-C25	3.11	114.96	110.44
20	B	512	CLA	CED-O2D-CGD	3.11	122.97	115.92
30	C	507	DGD	O5D-C1E-C2E	3.11	112.99	108.27
20	C	494	CLA	CMB-C2B-C1B	-3.10	123.91	128.46
20	c	5493	CLA	C7-C6-C5	-3.10	104.99	113.26
20	A	558	CLA	C7-C6-C5	-3.10	104.99	113.26
20	B	520	CLA	CED-O2D-CGD	3.10	122.95	115.92
24	c	5504	BCR	C30-C25-C26	-3.10	118.40	122.64
32	F	51	HEM	CAB-C3B-C2B	-3.10	118.36	128.43
30	c	5509	DGD	O2G-C1B-C2B	3.09	118.18	111.48
20	C	493	CLA	CED-O2D-CGD	3.09	122.94	115.92
20	c	5495	CLA	CBA-CAA-C2A	3.09	123.00	113.79
20	B	521	CLA	CED-O2D-CGD	3.09	122.93	115.92
24	X	130	BCR	C34-C9-C8	3.09	122.81	118.09
24	c	5505	BCR	C1-C6-C5	-3.09	118.41	122.64
28	d	5360	MGE	O2G-C1B-C2B	3.09	118.16	111.48
30	H	208	DGD	O6D-C5D-C6D	3.09	112.81	106.69
24	B	527	BCR	C35-C13-C12	3.09	122.80	118.09
26	A	568	SQD	C32-C31-C30	3.08	129.96	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	495	CLA	O2A-CGA-CBA	3.08	121.23	111.83
20	B	518	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
24	b	5528	BCR	C8-C7-C6	3.08	135.22	127.00
24	h	5107	BCR	C24-C23-C22	3.08	130.79	126.23
24	H	107	BCR	C12-C13-C14	-3.08	114.17	119.01
20	b	5524	CLA	CED-O2D-CGD	3.08	122.90	115.92
24	t	104	BCR	C11-C10-C9	3.08	131.59	127.28
20	c	5493	CLA	C1-C2-C3	3.07	131.23	126.20
20	c	5500	CLA	C1-C2-C3	3.07	131.23	126.20
32	f	5051	HEM	CAB-C3B-C2B	-3.07	118.45	128.43
20	C	495	CLA	CBA-CAA-C2A	3.07	122.93	113.79
21	a	5561	PHO	CED-O2D-CGD	3.06	122.86	115.92
24	t	104	BCR	C35-C13-C12	3.06	122.77	118.09
20	c	5495	CLA	C7-C6-C5	-3.06	105.10	113.26
30	C	509	DGD	O2G-C1B-C2B	3.06	118.10	111.48
21	a	5562	PHO	C4A-C3A-C2A	3.06	105.75	102.84
21	a	5562	PHO	CED-O2D-CGD	3.06	122.85	115.92
20	C	502	CLA	CED-O2D-CGD	3.06	122.85	115.92
30	C	508	DGD	C1E-O6E-C5E	3.05	119.68	113.72
20	d	5355	CLA	CED-O2D-CGD	3.05	122.83	115.92
20	b	5512	CLA	O2A-CGA-CBA	3.05	121.13	111.83
20	c	5496	CLA	C1-C2-C3	3.05	131.19	126.20
24	C	506	BCR	C1-C6-C5	-3.03	118.49	122.64
20	c	5498	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
30	c	5507	DGD	O5D-C1E-C2E	3.03	112.88	108.27
20	a	5563	CLA	CED-O2D-CGD	3.03	122.79	115.92
24	B	529	BCR	C8-C7-C6	3.03	135.09	127.00
20	C	500	CLA	C7-C6-C5	-3.03	105.19	113.26
24	c	5504	BCR	C1-C6-C7	3.03	123.86	115.65
20	c	5494	CLA	CMB-C2B-C1B	-3.03	124.02	128.46
20	C	493	CLA	C7-C6-C5	-3.03	105.20	113.26
25	A	567	LHG	O7-C7-C8	3.02	118.02	111.48
20	c	5496	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
20	D	354	CLA	O2A-CGA-CBA	3.02	121.05	111.83
20	b	5525	CLA	O2A-CGA-CBA	3.02	121.04	111.83
20	b	5518	CLA	CAA-C2A-C3A	-3.02	104.85	113.00
20	C	496	CLA	O2A-CGA-CBA	3.01	121.03	111.83
30	H	208	DGD	C1E-O6E-C5E	3.01	119.60	113.72
24	B	528	BCR	C1-C6-C5	-3.00	118.53	122.64
20	b	5526	CLA	C1-O2A-CGA	3.00	123.92	116.65
20	B	520	CLA	O2A-CGA-CBA	3.00	120.98	111.83
20	C	495	CLA	C1-C2-C3	3.00	131.11	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	213	SQD	C44-O6-C1	3.00	120.23	113.80
26	A	5212	SQD	C3-C4-C5	-3.00	104.79	110.23
24	c	5504	BCR	C40-C30-C25	3.00	114.94	110.24
20	C	499	CLA	O2A-CGA-CBA	3.00	120.97	111.83
20	c	5499	CLA	O2A-CGA-CBA	2.99	120.97	111.83
20	C	498	CLA	O2D-CGD-CBD	2.99	116.47	111.23
24	b	5527	BCR	C30-C25-C26	-2.99	118.55	122.64
20	C	501	CLA	C1-C2-C3	2.99	131.10	126.20
20	A	563	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
20	B	524	CLA	C7-C6-C5	-2.99	105.30	113.26
24	T	5104	BCR	C2-C1-C6	2.99	114.78	110.44
20	C	492	CLA	O2A-CGA-CBA	2.98	120.93	111.83
26	t	213	SQD	C31-C30-C29	2.98	133.50	113.36
20	c	5495	CLA	C1-C2-C3	2.98	131.08	126.20
20	c	5498	CLA	CED-O2D-CGD	2.98	122.68	115.92
20	B	515	CLA	O2A-CGA-CBA	2.98	120.92	111.83
20	B	515	CLA	C7-C6-C5	-2.98	105.32	113.26
24	B	528	BCR	C24-C23-C22	2.98	130.64	126.23
20	c	5495	CLA	O2A-CGA-CBA	2.98	120.91	111.83
20	c	5499	CLA	CED-O2D-CGD	2.97	122.66	115.92
26	a	212	SQD	C3-C4-C5	-2.97	104.84	110.23
32	F	51	HEM	O2A-CGA-CBA	2.97	123.38	114.00
28	i	5201	MGE	O6D-C5D-C6D	2.97	113.80	106.44
20	c	5491	CLA	C7-C6-C5	-2.97	105.36	113.26
20	B	514	CLA	O2A-CGA-CBA	2.96	120.87	111.83
24	T	5104	BCR	C35-C13-C12	2.96	122.61	118.09
26	L	5213	SQD	O7-S-C6	2.96	111.17	106.76
20	a	5558	CLA	C1-C2-C3	2.96	131.04	126.20
20	a	5560	CLA	CAA-CBA-CGA	2.96	121.60	113.21
22	A	564	PQ9	C16-C17-C18	-2.96	120.86	127.62
26	A	5212	SQD	O47-C7-C8	2.96	116.36	111.09
20	b	5517	CLA	C7-C6-C5	-2.95	105.39	113.26
20	c	5495	CLA	CMB-C2B-C1B	-2.95	124.13	128.46
20	b	5523	CLA	C1-C2-C3	2.95	131.02	126.20
24	H	107	BCR	C32-C1-C6	2.94	114.86	110.24
24	C	504	BCR	C35-C13-C12	2.94	122.58	118.09
20	b	5518	CLA	CED-O2D-CGD	2.94	122.59	115.92
20	b	5524	CLA	C7-C6-C5	-2.94	105.43	113.26
20	B	512	CLA	O2A-CGA-CBA	2.93	120.77	111.83
24	B	529	BCR	C7-C8-C9	2.93	130.57	126.23
26	A	568	SQD	C45-O47-C7	2.93	124.81	117.80
24	C	504	BCR	C32-C1-C6	2.93	114.83	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	355	CLA	CED-O2D-CGD	2.93	122.55	115.92
21	A	561	PHO	OBD-CAD-CBD	-2.93	121.53	125.82
26	a	212	SQD	O47-C7-C8	2.92	116.30	111.09
24	a	5566	BCR	C8-C7-C6	2.92	134.81	127.00
20	a	5560	CLA	CMB-C2B-C1B	-2.92	124.17	128.46
20	a	5563	CLA	O2A-CGA-CBA	2.92	120.75	111.83
20	a	5559	CLA	O2A-CGA-CBA	2.92	120.74	111.83
22	a	5564	PQ9	C16-C17-C18	-2.92	120.94	127.62
20	C	503	CLA	O2A-CGA-CBA	2.92	120.74	111.83
20	C	493	CLA	C1-C2-C3	2.92	130.98	126.20
20	B	525	CLA	O2A-CGA-CBA	2.92	120.73	111.83
25	a	5567	LHG	O7-C7-C8	2.92	117.79	111.48
24	d	5357	BCR	C37-C22-C23	2.91	122.54	118.09
24	c	5505	BCR	C30-C25-C26	-2.91	118.66	122.64
20	b	5525	CLA	CED-O2D-CGD	2.91	122.52	115.92
20	b	5523	CLA	O2A-CGA-CBA	2.91	120.71	111.83
20	A	563	CLA	O2A-CGA-CBA	2.91	120.71	111.83
20	C	496	CLA	C7-C6-C5	-2.91	105.51	113.26
20	B	525	CLA	CED-O2D-CGD	2.91	122.51	115.92
20	B	526	CLA	O2A-CGA-CBA	2.91	120.70	111.83
20	b	5511	CLA	CMB-C2B-C1B	-2.90	124.20	128.46
24	b	5529	BCR	C24-C23-C22	2.90	130.53	126.23
20	C	497	CLA	O2D-CGD-CBD	2.90	116.30	111.23
20	b	5525	CLA	C7-C6-C5	-2.90	105.53	113.26
20	C	500	CLA	C1-C2-C3	2.90	130.95	126.20
24	B	527	BCR	C8-C7-C6	2.90	134.74	127.00
26	d	5358	SQD	C32-C31-C30	2.90	129.01	114.37
20	A	558	CLA	CED-O2D-CGD	2.89	122.48	115.92
24	h	5107	BCR	C12-C13-C14	-2.89	114.46	119.01
20	A	560	CLA	CMB-C2B-C1B	-2.89	124.23	128.46
24	C	505	BCR	C1-C6-C5	-2.89	118.69	122.64
20	c	5499	CLA	O2D-CGD-CBD	2.88	116.27	111.23
20	b	5513	CLA	CED-O2D-CGD	2.88	122.45	115.92
24	t	104	BCR	C1-C6-C5	-2.88	118.70	122.64
20	C	497	CLA	CED-O2D-CGD	2.88	122.44	115.92
20	A	558	CLA	O2A-CGA-CBA	2.88	120.61	111.83
20	A	559	CLA	CED-O2D-CGD	2.87	122.44	115.92
20	a	5560	CLA	C7-C6-C5	-2.87	105.60	113.26
20	C	499	CLA	CMB-C2B-C1B	-2.87	124.25	128.46
21	A	562	PHO	CAA-C2A-C3A	-2.87	105.25	113.00
24	X	130	BCR	C12-C13-C14	-2.87	114.50	119.01
20	c	5497	CLA	CED-O2D-CGD	2.87	122.42	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	512	CLA	C7-C6-C5	-2.87	105.62	113.26
24	D	357	BCR	C12-C13-C14	-2.87	114.50	119.01
24	B	527	BCR	C1-C6-C5	-2.86	118.72	122.64
20	c	5501	CLA	CED-O2D-CGD	2.86	122.41	115.92
24	T	5104	BCR	C1-C6-C5	-2.86	118.73	122.64
20	D	355	CLA	O2A-CGA-CBA	2.86	120.54	111.83
21	A	562	PHO	OBD-CAD-CBD	-2.85	121.64	125.82
21	a	5562	PHO	CAA-C2A-C3A	-2.85	105.30	113.00
20	a	5563	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
24	B	528	BCR	C33-C5-C4	-2.85	107.52	113.60
20	c	5496	CLA	C7-C6-C5	-2.85	105.67	113.26
24	c	5505	BCR	C16-C17-C18	2.85	131.27	127.28
26	L	5213	SQD	C31-C30-C29	2.85	132.59	113.36
28	D	358	MGE	O6D-C5D-C6D	2.85	113.49	106.44
20	B	518	CLA	C7-C6-C5	-2.85	105.68	113.26
20	B	513	CLA	CED-O2D-CGD	2.85	122.37	115.92
20	b	5513	CLA	CMB-C2B-C1B	-2.84	124.29	128.46
20	b	5514	CLA	C1-C2-C3	2.84	130.86	126.20
20	C	499	CLA	O2D-CGD-CBD	2.84	116.20	111.23
24	C	505	BCR	C35-C13-C12	2.84	122.43	118.09
20	A	560	CLA	CED-O2D-CGD	2.84	122.36	115.92
20	b	5520	CLA	CED-O2D-CGD	2.84	122.35	115.92
20	B	516	CLA	C7-C6-C5	-2.84	105.70	113.26
20	a	5558	CLA	O2A-CGA-CBA	2.84	120.49	111.83
32	F	51	HEM	CHA-C4D-C3D	-2.84	120.00	125.23
20	b	5526	CLA	C1-C2-C3	2.84	130.84	126.20
20	b	5519	CLA	C7-C6-C5	-2.83	105.71	113.26
20	A	560	CLA	CAA-CBA-CGA	2.83	121.26	113.21
24	b	5527	BCR	C16-C17-C18	2.83	131.24	127.28
24	d	5357	BCR	C36-C18-C19	2.83	122.41	118.09
21	a	5561	PHO	OBD-CAD-CBD	-2.83	121.68	125.82
20	C	498	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
20	C	491	CLA	O2A-CGA-CBA	2.82	120.44	111.83
24	h	5107	BCR	C15-C14-C13	2.82	131.23	127.28
20	C	498	CLA	CMB-C2B-C1B	-2.82	124.33	128.46
24	T	5104	BCR	C11-C10-C9	2.81	131.22	127.28
20	C	496	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
26	d	5358	SQD	C36-C35-C34	2.81	128.58	114.37
24	C	504	BCR	C1-C6-C7	2.81	123.26	115.65
22	a	5564	PQ9	C19-C18-C20	2.81	120.10	115.23
22	a	5564	PQ9	C24-C23-C25	2.81	120.10	115.23
20	B	514	CLA	C7-C6-C5	-2.81	105.79	113.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	519	CLA	C7-C6-C5	-2.80	105.79	113.26
24	c	5506	BCR	C35-C13-C12	2.80	122.36	118.09
20	C	498	CLA	C7-C6-C5	-2.80	105.80	113.26
26	L	5213	SQD	C44-O6-C1	2.80	119.80	113.80
20	B	517	CLA	C7-C6-C5	-2.80	105.81	113.26
20	B	515	CLA	C2A-C3A-C4A	2.80	106.39	101.87
20	C	501	CLA	CED-O2D-CGD	2.80	122.26	115.92
28	L	210	MGE	O2G-C1B-C2B	2.79	117.53	111.48
20	B	515	CLA	CED-O2D-CGD	2.79	122.25	115.92
32	V	552	HEM	CHA-C4D-C3D	-2.79	120.08	125.23
20	d	5354	CLA	O2D-CGD-CBD	2.79	116.11	111.23
21	A	562	PHO	CED-O2D-CGD	2.79	122.25	115.92
26	A	568	SQD	C36-C35-C34	2.79	128.47	114.37
20	B	519	CLA	CMB-C2B-C1B	-2.79	124.37	128.46
20	B	526	CLA	C1-C2-C3	2.78	130.76	126.20
20	C	499	CLA	C2A-C1A-CHA	2.78	128.70	123.87
20	b	5526	CLA	O2A-CGA-CBA	2.78	120.31	111.83
24	c	5505	BCR	C8-C7-C6	2.78	134.42	127.00
30	c	5508	DGD	O5D-C6D-C5D	2.78	115.68	109.42
20	a	5563	CLA	CMB-C2B-C1B	-2.77	124.39	128.46
20	A	558	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
24	c	5506	BCR	C30-C25-C24	2.77	123.17	115.65
24	D	357	BCR	C24-C23-C22	2.77	130.34	126.23
24	T	5104	BCR	C23-C22-C21	-2.77	114.65	119.01
20	c	5502	CLA	C1-C2-C3	2.77	130.74	126.20
24	b	5529	BCR	C35-C13-C12	2.77	122.32	118.09
24	B	527	BCR	C24-C23-C22	2.77	130.33	126.23
20	b	5512	CLA	C7-C6-C5	-2.77	105.89	113.26
24	X	130	BCR	C16-C17-C18	2.77	131.16	127.28
21	A	561	PHO	C7-C6-C5	-2.77	105.89	113.26
20	C	498	CLA	CED-O2D-CGD	2.76	122.19	115.92
20	B	516	CLA	CBA-CAA-C2A	2.76	122.02	113.79
24	b	5527	BCR	C8-C7-C6	2.76	134.38	127.00
20	B	520	CLA	CMB-C2B-C1B	-2.76	124.41	128.46
20	B	517	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
20	a	5558	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
20	b	5518	CLA	CMB-C2B-C1B	-2.75	124.42	128.46
20	b	5523	CLA	CMB-C2B-C1B	-2.75	124.43	128.46
24	C	505	BCR	C30-C25-C26	-2.75	118.88	122.64
27	m	216	LMT	C1-O1'-C1'	-2.75	108.99	113.68
24	D	357	BCR	C35-C13-C12	2.74	122.28	118.09
30	h	5208	DGD	O6D-C5D-C4D	2.74	114.64	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	5210	MGE	O2G-C1B-C2B	2.74	117.42	111.48
20	B	524	CLA	O2A-CGA-CBA	2.74	120.20	111.83
20	b	5521	CLA	C6-C5-C3	2.74	120.15	113.47
22	D	356	PQ9	C19-C18-C20	2.74	119.99	115.23
22	A	564	PQ9	C19-C18-C20	2.74	119.98	115.23
20	C	500	CLA	CMB-C2B-C1B	-2.74	124.44	128.46
22	A	564	PQ9	C24-C23-C25	2.74	119.98	115.23
30	H	208	DGD	O6D-C5D-C4D	2.74	114.63	109.70
28	B	530	MGE	O3G-C1D-C2D	2.74	112.43	108.27
20	b	5523	CLA	C2A-C3A-C4A	2.74	106.29	101.87
32	v	5552	HEM	CHA-C4D-C3D	-2.74	120.18	125.23
24	b	5528	BCR	C24-C23-C22	2.73	130.28	126.23
24	c	5506	BCR	C40-C30-C29	-2.73	98.46	108.95
26	A	5212	SQD	O48-C23-C24	2.73	123.98	112.38
20	b	5518	CLA	C7-C6-C5	-2.73	105.98	113.26
24	x	5130	BCR	C35-C13-C12	2.73	122.26	118.09
20	B	523	CLA	O2A-CGA-CBA	2.73	120.15	111.83
20	B	519	CLA	C1-C2-C3	2.73	130.67	126.20
32	V	552	HEM	O2A-CGA-CBA	2.72	122.61	114.00
20	b	5526	CLA	C7-C6-C5	-2.72	106.01	113.26
20	B	512	CLA	C1-C2-C3	2.72	130.66	126.20
20	c	5497	CLA	O2D-CGD-CBD	2.72	115.98	111.23
20	b	5515	CLA	C7-C6-C5	-2.71	106.03	113.26
20	A	559	CLA	O2A-CGA-CBA	2.71	120.11	111.83
20	b	5516	CLA	CBA-CAA-C2A	2.71	121.86	113.79
24	A	566	BCR	C36-C18-C19	2.71	122.23	118.09
24	c	5506	BCR	C37-C22-C23	2.71	122.22	118.09
20	C	502	CLA	C2A-C3A-C4A	2.70	106.24	101.87
20	b	5516	CLA	C7-C6-C5	-2.70	106.06	113.26
20	B	519	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
24	A	566	BCR	C35-C13-C12	2.70	122.21	118.09
20	C	492	CLA	C6-C5-C3	2.70	120.04	113.47
30	c	5509	DGD	C3G-C2G-C1G	-2.70	105.49	111.78
24	c	5504	BCR	C35-C13-C12	2.70	122.21	118.09
24	C	505	BCR	C19-C18-C17	-2.70	114.77	119.01
20	C	495	CLA	C6-C5-C3	2.70	120.04	113.47
24	h	5107	BCR	C35-C13-C12	2.70	122.21	118.09
22	D	356	PQ9	C16-C17-C18	-2.69	121.46	127.62
24	A	566	BCR	C1-C6-C5	-2.69	118.96	122.64
24	A	566	BCR	C16-C17-C18	2.69	131.05	127.28
24	t	104	BCR	C7-C8-C9	2.69	130.21	126.23
24	a	5566	BCR	C37-C22-C23	2.69	122.19	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	523	CLA	C1-C2-C3	2.68	130.59	126.20
26	a	212	SQD	O48-C23-C24	2.68	123.76	112.38
20	C	500	CLA	O2A-CGA-CBA	2.68	120.01	111.83
20	b	5520	CLA	CMB-C2B-C1B	-2.68	124.53	128.46
20	b	5517	CLA	CMB-C2B-C1B	-2.68	124.53	128.46
21	a	5562	PHO	OBD-CAD-CBD	-2.68	121.89	125.82
24	c	5506	BCR	C1-C6-C5	-2.68	118.98	122.64
30	c	5508	DGD	O6D-C5D-C6D	2.68	112.00	106.69
20	b	5519	CLA	C1-O2A-CGA	2.68	123.13	116.65
20	b	5521	CLA	CED-O2D-CGD	2.68	121.99	115.92
20	B	525	CLA	O2D-CGD-CBD	2.68	115.91	111.23
20	C	503	CLA	CMB-C2B-C1B	-2.68	124.54	128.46
20	A	560	CLA	C7-C6-C5	-2.68	106.13	113.26
24	C	506	BCR	C40-C30-C29	-2.67	98.68	108.95
30	C	508	DGD	O5D-C6D-C5D	2.67	115.45	109.42
20	C	500	CLA	C2A-C3A-C4A	2.67	106.19	101.87
20	b	5523	CLA	C7-C6-C5	-2.67	106.14	113.26
24	B	527	BCR	C16-C17-C18	2.67	131.03	127.28
20	C	501	CLA	O2A-CGA-CBA	2.67	119.98	111.83
20	b	5521	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
24	B	529	BCR	C35-C13-C12	2.67	122.17	118.09
20	b	5517	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
20	C	499	CLA	CED-O2D-CGD	2.67	121.97	115.92
20	c	5496	CLA	O2A-CGA-CBA	2.66	119.96	111.83
20	b	5521	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	c	5499	CLA	C2A-C3A-C4A	2.66	106.17	101.87
24	d	5357	BCR	C12-C13-C14	-2.66	114.82	119.01
24	c	5506	BCR	C16-C17-C18	2.66	131.01	127.28
28	b	5530	MGE	O6D-C5D-C6D	2.66	113.03	106.44
20	c	5493	CLA	CMD-C2D-C1D	2.66	129.41	124.73
20	a	5558	CLA	CMB-C2B-C1B	-2.65	124.57	128.46
24	C	504	BCR	C37-C22-C23	2.65	122.14	118.09
20	b	5519	CLA	C1-C2-C3	2.65	130.54	126.20
24	d	5357	BCR	C7-C8-C9	2.65	130.16	126.23
20	c	5498	CLA	O2A-CGA-CBA	2.65	119.92	111.83
20	b	5514	CLA	C2A-C3A-C4A	2.65	106.15	101.87
24	a	5566	BCR	C2-C1-C6	2.65	114.29	110.44
20	c	5498	CLA	O2D-CGD-CBD	2.65	115.86	111.23
24	C	506	BCR	C19-C18-C17	-2.65	114.85	119.01
21	A	561	PHO	O1D-CGD-CBD	-2.64	120.71	124.72
20	A	560	CLA	C2A-C3A-C4A	2.64	106.14	101.87
20	d	5355	CLA	O2A-CGA-CBA	2.64	119.89	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5506	BCR	C24-C23-C22	2.64	130.14	126.23
20	B	513	CLA	C1-C2-C3	2.64	130.53	126.20
20	B	512	CLA	CMB-C2B-C1B	-2.64	124.59	128.46
20	C	491	CLA	C7-C6-C5	-2.64	106.23	113.26
24	a	5566	BCR	C1-C6-C5	-2.64	119.03	122.64
20	b	5513	CLA	O2D-CGD-CBD	2.64	115.84	111.23
24	t	104	BCR	C23-C22-C21	-2.64	114.86	119.01
26	d	5358	SQD	C15-C14-C13	2.64	127.69	114.37
24	c	5504	BCR	C37-C22-C23	2.63	122.11	118.09
30	H	208	DGD	O5D-C1E-C2E	2.63	112.27	108.27
24	C	506	BCR	C12-C13-C14	-2.63	114.86	119.01
25	A	567	LHG	P-O6-C4	-2.63	106.26	121.35
20	b	5520	CLA	C1-C2-C3	2.63	130.51	126.20
20	a	5559	CLA	CMD-C2D-C1D	2.63	129.36	124.73
32	v	5552	HEM	O2A-CGA-CBA	2.63	122.30	114.00
27	T	217	LMT	C1-O1'-C1'	-2.63	109.19	113.68
24	C	504	BCR	C23-C22-C21	-2.63	114.88	119.01
20	a	5560	CLA	CED-O2D-CGD	2.63	121.87	115.92
20	B	520	CLA	C1-C2-C3	2.63	130.50	126.20
24	h	5107	BCR	C1-C6-C7	2.62	122.77	115.65
24	C	505	BCR	C8-C7-C6	2.62	134.00	127.00
24	X	130	BCR	C24-C23-C22	2.62	130.11	126.23
24	b	5529	BCR	C32-C1-C6	2.62	114.35	110.24
20	B	523	CLA	C7-C6-C5	-2.62	106.28	113.26
20	b	5519	CLA	CMB-C2B-C1B	-2.62	124.62	128.46
20	B	523	CLA	C6-C5-C3	2.62	119.85	113.47
20	D	355	CLA	O2D-CGD-CBD	2.62	115.81	111.23
20	c	5498	CLA	CMB-C2B-C1B	-2.62	124.62	128.46
32	F	51	HEM	C2C-C3C-C4C	-2.62	105.07	106.90
24	A	566	BCR	C8-C7-C6	2.62	133.99	127.00
20	c	5502	CLA	C2A-C3A-C4A	2.61	106.09	101.87
20	b	5513	CLA	C1-C2-C3	2.61	130.47	126.20
27	t	5217	LMT	C1-O1'-C1'	-2.61	109.23	113.68
24	a	5566	BCR	C36-C18-C19	2.61	122.07	118.09
20	b	5512	CLA	CMB-C2B-C1B	-2.61	124.64	128.46
24	A	566	BCR	C2-C1-C6	2.60	114.22	110.44
24	T	5104	BCR	C40-C30-C29	-2.60	98.95	108.95
30	C	509	DGD	C3G-C2G-C1G	-2.60	105.72	111.78
20	B	523	CLA	CMB-C2B-C1B	-2.60	124.65	128.46
24	A	566	BCR	C7-C8-C9	2.60	130.08	126.23
24	H	107	BCR	C16-C17-C18	2.60	130.92	127.28
20	A	559	CLA	CMB-C2B-C1B	-2.60	124.65	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	524	CLA	CMB-C2B-C1B	-2.59	124.66	128.46
20	b	5515	CLA	CMD-C2D-C1D	2.59	129.28	124.73
20	b	5524	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
20	c	5498	CLA	C7-C6-C5	-2.58	106.39	113.26
20	A	563	CLA	CED-O2D-CGD	2.58	121.77	115.92
20	C	494	CLA	CBA-CAA-C2A	2.58	121.47	113.79
20	d	5354	CLA	CED-O2D-CGD	2.58	121.76	115.92
28	d	5359	MGE	O6D-C5D-C6D	2.58	112.83	106.44
20	b	5519	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
24	D	357	BCR	C37-C22-C23	2.57	122.02	118.09
20	b	5525	CLA	CMB-C2B-C1B	-2.57	124.69	128.46
20	C	493	CLA	CMD-C2D-C1D	2.57	129.26	124.73
26	A	568	SQD	O8-S-O7	2.57	117.83	111.40
32	f	5051	HEM	O2A-CGA-CBA	2.57	122.12	114.00
20	A	563	CLA	CMB-C2B-C1B	-2.57	124.69	128.46
24	b	5527	BCR	C35-C13-C12	2.57	122.01	118.09
20	C	499	CLA	C2A-C3A-C4A	2.57	106.01	101.87
20	b	5524	CLA	O2A-CGA-CBA	2.57	119.66	111.83
24	X	130	BCR	C30-C25-C24	2.57	122.61	115.65
20	C	498	CLA	O2A-CGA-CBA	2.56	119.65	111.83
20	b	5515	CLA	C6-C5-C3	2.56	119.71	113.47
20	c	5500	CLA	O2A-CGA-CBA	2.56	119.63	111.83
24	b	5529	BCR	C7-C8-C9	2.56	130.01	126.23
21	a	5561	PHO	O1D-CGD-CBD	-2.55	120.85	124.72
20	D	355	CLA	CMB-C2B-C1B	-2.55	124.72	128.46
24	C	506	BCR	C30-C25-C24	2.55	122.57	115.65
20	A	560	CLA	C1-C2-C3	2.55	130.37	126.20
24	B	528	BCR	C32-C1-C6	2.55	114.24	110.24
26	L	5213	SQD	C3-C4-C5	-2.55	105.62	110.23
20	b	5511	CLA	C2A-C3A-C4A	2.54	104.57	101.59
24	B	527	BCR	C36-C18-C19	2.54	121.97	118.09
20	c	5492	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
20	B	518	CLA	CMB-C2B-C1B	-2.53	124.74	128.46
20	b	5525	CLA	O2D-CGD-CBD	2.53	115.66	111.23
24	h	5107	BCR	C16-C17-C18	2.53	130.83	127.28
20	b	5512	CLA	C1-C2-C3	2.53	130.34	126.20
20	C	494	CLA	C2A-C3A-C4A	2.53	105.95	101.87
20	B	521	CLA	O2D-CGD-CBD	2.53	115.64	111.23
20	B	521	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
20	B	526	CLA	C1-O2A-CGA	2.53	122.76	116.65
20	B	526	CLA	C7-C6-C5	-2.52	106.53	113.26
24	X	130	BCR	C35-C13-C12	2.52	121.94	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	t	5217	LMT	C3'-C4'-C5'	-2.52	105.33	110.93
20	c	5494	CLA	O2A-CGA-CBA	2.52	121.67	112.14
20	C	503	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
20	A	558	CLA	C2A-C3A-C4A	2.52	105.94	101.87
20	b	5516	CLA	CMB-C2B-C1B	-2.52	124.76	128.46
20	C	495	CLA	CED-O2D-CGD	2.52	121.63	115.92
20	a	5560	CLA	CMD-C2D-C1D	2.52	129.16	124.73
24	a	5566	BCR	C16-C17-C18	2.52	130.81	127.28
20	B	517	CLA	C2A-C1A-CHA	2.51	128.23	123.87
22	d	5356	PQ9	C14-C13-C15	2.51	119.59	115.23
20	d	5354	CLA	C7-C6-C5	-2.51	106.57	113.26
20	B	521	CLA	C6-C5-C3	2.51	119.58	113.47
32	f	5051	HEM	CMD-C2D-C1D	2.51	128.96	125.03
24	X	130	BCR	C37-C22-C23	2.51	121.92	118.09
24	A	566	BCR	C37-C22-C23	2.51	121.92	118.09
24	d	5357	BCR	C16-C17-C18	2.51	130.79	127.28
20	c	5492	CLA	O2A-CGA-CBA	2.51	119.48	111.83
24	T	5104	BCR	C23-C24-C25	2.51	133.69	127.00
20	C	494	CLA	O2A-CGA-CBA	2.51	121.61	112.14
24	B	528	BCR	C1-C6-C7	2.51	122.45	115.65
24	D	357	BCR	C16-C17-C18	2.51	130.79	127.28
30	C	508	DGD	O6D-C5D-C6D	2.51	111.66	106.69
24	C	504	BCR	C32-C1-C2	-2.50	99.33	108.95
20	c	5500	CLA	CMB-C2B-C1B	-2.50	124.79	128.46
24	c	5504	BCR	C30-C25-C24	2.50	122.44	115.65
24	C	505	BCR	C36-C18-C19	2.50	121.91	118.09
24	C	504	BCR	C7-C8-C9	2.50	129.94	126.23
24	T	5104	BCR	C7-C8-C9	2.50	129.93	126.23
24	t	104	BCR	C23-C24-C25	2.50	133.67	127.00
20	A	558	CLA	CMB-C2B-C1B	-2.50	124.80	128.46
20	b	5515	CLA	C12-C11-C10	-2.50	102.08	113.28
20	A	558	CLA	CBA-CAA-C2A	2.50	121.22	113.79
20	c	5493	CLA	C12-C11-C10	-2.50	102.09	113.28
20	B	514	CLA	C2A-C3A-C4A	2.50	105.90	101.87
24	T	5104	BCR	C37-C22-C23	2.49	121.90	118.09
20	B	513	CLA	C7-C6-C5	-2.49	106.62	113.26
24	C	506	BCR	C36-C18-C19	2.49	121.89	118.09
20	c	5495	CLA	C2A-C1A-CHA	2.49	128.19	123.87
20	B	521	CLA	C2A-C3A-C4A	2.49	105.89	101.87
24	C	505	BCR	C12-C13-C14	-2.49	115.10	119.01
20	B	524	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
20	C	502	CLA	C1-C2-C3	2.49	130.27	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	507	DGD	O5D-C6D-C5D	2.48	115.02	109.42
20	c	5492	CLA	C6-C5-C3	2.48	119.52	113.47
22	d	5356	PQ9	C16-C17-C18	-2.48	121.94	127.62
24	b	5528	BCR	C1-C6-C7	2.48	122.38	115.65
25	a	5567	LHG	P-O6-C4	-2.48	107.14	121.35
24	X	130	BCR	C32-C1-C2	-2.48	99.44	108.95
20	c	5501	CLA	O2A-CGA-CBA	2.47	119.38	111.83
24	c	5506	BCR	C19-C18-C17	-2.47	115.12	119.01
24	t	104	BCR	C12-C13-C14	-2.47	115.12	119.01
20	D	354	CLA	C2A-C3A-C4A	2.47	105.86	101.87
20	c	5502	CLA	CMB-C2B-C1B	-2.46	124.85	128.46
24	C	506	BCR	C37-C22-C23	2.46	121.85	118.09
24	C	504	BCR	C40-C30-C25	2.46	114.10	110.24
20	c	5495	CLA	C6-C5-C3	2.46	119.46	113.47
28	d	5360	MGE	C3G-O3G-C1D	-2.46	108.52	113.80
20	C	494	CLA	C2A-C1A-CHA	2.46	128.13	123.87
20	C	502	CLA	C2A-C1A-CHA	2.46	128.13	123.87
20	A	559	CLA	C2A-C3A-C4A	2.46	105.83	101.87
20	c	5494	CLA	CBA-CAA-C2A	2.45	121.10	113.79
24	H	107	BCR	C1-C6-C7	2.45	122.31	115.65
24	x	5130	BCR	C30-C25-C24	2.45	122.30	115.65
24	d	5357	BCR	C35-C13-C12	2.45	121.83	118.09
20	B	511	CLA	C2A-C3A-C4A	2.45	104.47	101.59
28	I	201	MGE	O1G-C1G-C2G	-2.45	101.33	108.40
24	B	529	BCR	C40-C30-C25	2.45	114.09	110.24
26	A	568	SQD	C15-C14-C13	2.45	126.76	114.37
28	i	5201	MGE	O1G-C1G-C2G	-2.45	101.33	108.40
21	A	561	PHO	O2A-CGA-CBA	2.45	119.31	111.83
20	B	513	CLA	CMB-C2B-C1B	-2.45	124.87	128.46
20	a	5558	CLA	C2A-C3A-C4A	2.45	105.83	101.87
24	a	5566	BCR	C32-C1-C6	2.45	114.08	110.24
24	a	5566	BCR	C30-C25-C24	2.45	122.29	115.65
22	D	356	PQ9	C21-C22-C23	-2.45	122.03	127.62
20	c	5502	CLA	C2A-C1A-CHA	2.44	128.11	123.87
32	V	552	HEM	C4A-C3A-C2A	2.44	108.69	107.00
20	a	5558	CLA	CBA-CAA-C2A	2.44	121.06	113.79
20	c	5491	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
20	D	354	CLA	C7-C6-C5	-2.44	106.76	113.26
20	c	5493	CLA	C2A-C3A-C4A	2.44	105.81	101.87
20	C	491	CLA	CMD-C2D-C1D	2.44	129.02	124.73
20	B	523	CLA	C2A-C3A-C4A	2.43	105.80	101.87
20	c	5499	CLA	CMB-C2B-C1B	-2.43	124.89	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5492	CLA	C7-C6-C5	-2.43	106.78	113.26
20	B	515	CLA	C6-C5-C3	2.43	119.39	113.47
24	B	529	BCR	C32-C1-C6	2.43	114.05	110.24
24	b	5528	BCR	C32-C1-C6	2.43	114.05	110.24
24	t	104	BCR	C8-C9-C10	-2.43	115.19	119.01
20	D	354	CLA	CED-O2D-CGD	2.43	121.42	115.92
24	H	107	BCR	C35-C13-C12	2.43	121.79	118.09
20	b	5514	CLA	C7-C6-C5	-2.42	106.80	113.26
20	c	5493	CLA	CMB-C2B-C1B	-2.42	124.92	128.46
20	a	5560	CLA	C2A-C3A-C4A	2.42	105.77	101.87
22	a	5564	PQ9	C14-C13-C15	2.42	119.42	115.23
22	A	564	PQ9	C14-C13-C15	2.42	119.42	115.23
20	a	5559	CLA	CMB-C2B-C1B	-2.41	124.92	128.46
20	B	515	CLA	C12-C11-C10	-2.41	102.46	113.28
30	c	5507	DGD	O5D-C6D-C5D	2.41	114.86	109.42
20	b	5519	CLA	O2A-CGA-CBA	2.41	119.19	111.83
20	B	524	CLA	C1-C2-C3	2.41	130.15	126.20
24	t	104	BCR	C36-C18-C19	2.41	121.77	118.09
20	c	5503	CLA	O2A-CGA-CBA	2.41	119.18	111.83
24	t	104	BCR	C37-C22-C23	2.41	121.77	118.09
20	b	5522	CLA	C2A-C3A-C4A	2.41	105.76	101.87
20	C	492	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
20	b	5523	CLA	C6-C5-C3	2.41	119.33	113.47
20	D	354	CLA	O2D-CGD-CBD	2.41	115.44	111.23
20	C	491	CLA	O2D-CGD-CBD	2.40	115.43	111.23
20	B	517	CLA	CMB-C2B-C1B	-2.40	124.93	128.46
20	a	5559	CLA	C2A-C3A-C4A	2.40	105.75	101.87
24	t	104	BCR	C40-C30-C29	-2.40	99.73	108.95
20	c	5497	CLA	CMB-C2B-C1B	-2.40	124.94	128.46
28	B	530	MGE	O6D-C5D-C6D	2.40	112.39	106.44
20	c	5503	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
24	h	5107	BCR	C37-C22-C23	2.40	121.75	118.09
32	v	5552	HEM	CBA-CAA-C2A	2.40	116.57	112.54
28	d	5359	MGE	C3G-C2G-C1G	-2.40	106.20	111.78
20	C	492	CLA	C1-C2-C3	2.40	130.12	126.20
26	A	568	SQD	C3-C4-C5	-2.39	105.89	110.23
24	c	5504	BCR	C23-C22-C21	-2.39	115.25	119.01
20	C	493	CLA	O2D-CGD-CBD	2.39	115.41	111.23
20	c	5500	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
28	B	530	MGE	O1G-C1G-C2G	-2.39	101.51	108.40
24	c	5505	BCR	C12-C13-C14	-2.39	115.25	119.01
24	c	5506	BCR	C36-C18-C19	2.39	121.74	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	5208	DGD	O5D-C1E-C2E	2.39	111.90	108.27
24	T	5104	BCR	C36-C18-C19	2.39	121.73	118.09
20	c	5499	CLA	C2A-C1A-CHA	2.39	128.01	123.87
20	c	5495	CLA	CED-O2D-CGD	2.38	121.32	115.92
24	B	527	BCR	C12-C13-C14	-2.38	115.26	119.01
24	c	5504	BCR	C12-C13-C14	-2.38	115.26	119.01
21	A	561	PHO	CMA-C3A-C4A	-2.38	109.48	114.61
28	B	530	MGE	C3G-C2G-C1G	-2.38	106.24	111.78
20	b	5518	CLA	O2D-CGD-CBD	2.38	115.39	111.23
20	b	5515	CLA	C2A-C3A-C4A	2.38	105.71	101.87
26	t	213	SQD	C3-C4-C5	-2.37	105.93	110.23
26	d	5358	SQD	C3-C4-C5	-2.37	105.93	110.23
20	B	526	CLA	C2A-C3A-C4A	2.37	105.70	101.87
20	C	501	CLA	C1-O2A-CGA	2.37	122.39	116.65
20	c	5500	CLA	CED-O2D-CGD	2.37	121.29	115.92
20	c	5496	CLA	C2A-C3A-C4A	2.37	105.69	101.87
24	c	5505	BCR	C36-C18-C19	2.37	121.70	118.09
32	f	5051	HEM	CBA-CAA-C2A	-2.37	108.56	112.54
32	F	51	HEM	CAB-C3B-C4B	2.37	134.84	124.39
20	B	514	CLA	CED-O2D-CGD	2.36	121.28	115.92
24	H	107	BCR	C36-C18-C19	2.36	121.70	118.09
20	B	515	CLA	CMB-C2B-C1B	-2.36	125.00	128.46
24	a	5566	BCR	C35-C13-C12	2.36	121.69	118.09
20	C	502	CLA	CMB-C2B-C1B	-2.36	125.00	128.46
26	A	568	SQD	C44-O6-C1	2.36	118.86	113.80
20	C	493	CLA	C2A-C3A-C4A	2.36	105.68	101.87
20	D	355	CLA	C1-O2A-CGA	2.36	122.35	116.65
24	c	5506	BCR	C12-C13-C14	-2.35	115.31	119.01
20	b	5514	CLA	CED-O2D-CGD	2.35	121.25	115.92
20	b	5526	CLA	O2D-CGD-CBD	2.35	115.34	111.23
24	b	5529	BCR	C12-C13-C14	-2.35	115.31	119.01
20	c	5501	CLA	C12-C11-C10	-2.35	102.75	113.28
32	f	5051	HEM	CAB-C3B-C4B	2.35	134.76	124.39
20	B	523	CLA	CED-O2D-CGD	2.35	121.24	115.92
20	a	5563	CLA	O2D-CGD-CBD	2.34	115.33	111.23
24	B	529	BCR	C12-C13-C14	-2.34	115.32	119.01
24	D	357	BCR	C40-C30-C25	2.34	113.92	110.24
20	B	519	CLA	C2A-C3A-C4A	2.34	105.66	101.87
21	a	5561	PHO	C4A-C3A-C2A	2.34	105.07	102.84
21	A	562	PHO	CHA-C4D-C3D	2.34	115.87	111.19
20	C	499	CLA	C1-O2A-CGA	2.34	123.32	116.67
24	c	5504	BCR	C32-C1-C2	-2.34	99.96	108.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	559	CLA	CMD-C2D-C1D	2.34	128.85	124.73
20	B	513	CLA	O2D-CGD-CBD	2.34	115.32	111.23
20	d	5355	CLA	CMB-C2B-C1B	-2.34	125.03	128.46
24	t	104	BCR	C34-C9-C8	2.34	121.66	118.09
26	d	5358	SQD	O8-S-O7	2.34	117.25	111.40
20	B	516	CLA	CMB-C2B-C1B	-2.34	125.03	128.46
20	B	521	CLA	O2A-CGA-CBA	2.34	118.96	111.83
20	c	5500	CLA	C2A-C3A-C4A	2.34	105.64	101.87
24	T	5104	BCR	C12-C13-C14	-2.34	115.33	119.01
20	B	519	CLA	C1-O2A-CGA	2.34	122.30	116.65
20	C	492	CLA	O2D-CGD-CBD	2.33	115.31	111.23
22	A	564	PQ9	C21-C22-C23	-2.33	122.28	127.62
20	C	492	CLA	C2A-C3A-C4A	2.33	105.64	101.87
24	B	529	BCR	C15-C14-C13	2.33	130.55	127.28
20	B	522	CLA	C2A-C3A-C4A	2.33	105.63	101.87
20	C	500	CLA	CMA-C3A-C2A	-2.33	104.98	113.98
24	C	504	BCR	C11-C10-C9	2.33	130.54	127.28
24	h	5107	BCR	C34-C9-C8	2.33	121.64	118.09
24	X	130	BCR	C8-C7-C6	2.32	133.19	127.00
20	d	5354	CLA	C2A-C3A-C4A	2.32	105.61	101.87
27	t	5217	LMT	O1B-C1B-C2B	2.32	113.79	108.09
27	T	217	LMT	C3'-C4'-C5'	-2.32	105.80	110.93
20	b	5521	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	A	566	BCR	C19-C18-C17	-2.31	115.37	119.01
22	D	356	PQ9	C11-C12-C13	-2.31	122.85	126.83
20	A	560	CLA	CMB-C2B-C3B	2.31	129.30	124.68
20	B	511	CLA	CED-O2D-CGD	2.31	121.16	115.92
26	L	5213	SQD	C15-C14-C13	2.31	126.05	114.37
20	C	501	CLA	C12-C11-C10	-2.31	102.92	113.28
20	b	5521	CLA	O2A-CGA-CBA	2.31	118.88	111.83
22	d	5356	PQ9	C19-C18-C20	2.31	119.23	115.23
20	C	493	CLA	C12-C11-C10	-2.31	102.94	113.28
20	c	5501	CLA	C1-C2-C3	2.31	129.97	126.20
20	C	495	CLA	CMB-C2B-C3B	2.31	129.29	124.68
20	b	5524	CLA	CMB-C2B-C1B	-2.30	125.08	128.46
24	X	130	BCR	C36-C18-C19	2.30	121.61	118.09
20	B	525	CLA	C2A-C3A-C4A	2.30	105.59	101.87
20	b	5524	CLA	O2D-CGD-CBD	2.30	115.26	111.23
20	A	559	CLA	CAA-CBA-CGA	2.30	119.75	113.21
20	c	5503	CLA	CMB-C2B-C1B	-2.30	125.08	128.46
20	C	501	CLA	C2A-C1A-CHA	2.30	127.86	123.87
20	c	5497	CLA	C2A-C3A-C4A	2.30	105.59	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	5130	BCR	C32-C1-C2	-2.30	100.12	108.95
20	B	525	CLA	CMB-C2B-C1B	-2.30	125.09	128.46
20	A	560	CLA	CMD-C2D-C1D	2.30	128.78	124.73
20	B	519	CLA	C2A-C1A-CHA	2.30	127.86	123.87
20	b	5515	CLA	C1-C2-C3	2.30	129.96	126.20
21	A	562	PHO	CMA-C3A-C4A	-2.30	109.66	114.61
20	B	519	CLA	O2A-CGA-CBA	2.30	118.84	111.83
20	C	495	CLA	C2A-C3A-C4A	2.30	105.58	101.87
20	b	5521	CLA	CMB-C2B-C1B	-2.30	125.09	128.46
20	B	511	CLA	CMD-C2D-C1D	2.30	128.77	124.73
20	c	5497	CLA	C6-C5-C3	2.30	119.06	113.47
20	a	5560	CLA	O2A-CGA-CBA	2.30	118.83	111.83
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	500	CLA	CED-O2D-CGD	2.29	121.12	115.92
24	x	5130	BCR	C37-C22-C23	2.29	121.59	118.09
24	x	5130	BCR	C8-C7-C6	2.29	133.12	127.00
26	d	5358	SQD	C44-O6-C1	2.29	118.70	113.80
20	C	493	CLA	C2A-C1A-CHA	2.29	127.84	123.87
20	a	5563	CLA	C2A-C3A-C4A	2.29	105.56	101.87
24	c	5506	BCR	C23-C22-C21	-2.29	115.41	119.01
24	x	5130	BCR	C36-C18-C19	2.29	121.58	118.09
20	c	5497	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
24	C	506	BCR	C24-C23-C22	2.28	129.62	126.23
20	C	496	CLA	CMB-C2B-C1B	-2.28	125.11	128.46
20	B	513	CLA	C6-C5-C3	2.28	119.03	113.47
28	i	5201	MGE	C3G-O3G-C1D	-2.28	108.90	113.80
20	b	5511	CLA	CED-O2D-CGD	2.28	121.09	115.92
20	B	512	CLA	C2A-C3A-C4A	2.28	105.55	101.87
20	b	5523	CLA	CMB-C2B-C3B	2.28	129.24	124.68
20	b	5513	CLA	CMB-C2B-C3B	2.28	129.24	124.68
20	b	5522	CLA	CMB-C2B-C1B	-2.28	125.12	128.46
20	C	495	CLA	C2A-C1A-CHA	2.28	127.82	123.87
20	B	514	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
20	B	522	CLA	CMD-C2D-C1D	2.27	128.73	124.73
24	c	5504	BCR	C11-C10-C9	2.27	130.47	127.28
20	b	5514	CLA	CMB-C2B-C1B	-2.27	125.13	128.46
20	B	515	CLA	CMD-C2D-C1D	2.27	128.73	124.73
20	b	5511	CLA	CMD-C2D-C1D	2.27	128.73	124.73
24	C	504	BCR	C30-C25-C24	2.27	121.81	115.65
27	T	217	LMT	O1B-C1B-C2B	2.27	113.68	108.09
26	d	5358	SQD	C34-C33-C32	2.27	125.85	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	512	CLA	O2D-CGD-CBD	2.27	115.20	111.23
20	c	5494	CLA	C2A-C3A-C4A	2.27	105.54	101.87
20	C	497	CLA	C6-C5-C3	2.27	119.00	113.47
20	B	526	CLA	CMB-C2B-C1B	-2.27	125.13	128.46
24	D	357	BCR	C23-C22-C21	-2.27	115.44	119.01
20	C	500	CLA	O2D-CGD-CBD	2.27	115.19	111.23
20	C	497	CLA	CMB-C2B-C1B	-2.27	125.14	128.46
20	a	5558	CLA	CMD-C2D-C1D	2.27	128.72	124.73
20	b	5521	CLA	C1-C2-C3	2.27	129.91	126.20
20	B	521	CLA	C1-C2-C3	2.27	129.91	126.20
21	a	5561	PHO	O2A-CGA-CBA	2.26	118.73	111.83
24	H	107	BCR	C7-C8-C9	2.26	129.58	126.23
21	a	5561	PHO	CMA-C3A-C4A	-2.26	109.74	114.61
20	C	497	CLA	C12-C11-C10	-2.26	103.15	113.28
20	b	5512	CLA	O2D-CGD-CBD	2.26	115.18	111.23
20	C	494	CLA	CMB-C2B-C3B	2.26	129.20	124.68
22	a	5564	PQ9	C21-C22-C23	-2.26	122.45	127.62
24	a	5566	BCR	C34-C9-C8	2.26	121.54	118.09
21	a	5561	PHO	CHA-C4D-C3D	2.26	115.71	111.19
20	A	563	CLA	CMA-C3A-C2A	-2.26	105.25	113.98
20	c	5491	CLA	CMD-C2D-C1D	2.26	128.70	124.73
20	d	5355	CLA	O2D-CGD-CBD	2.26	115.18	111.23
20	C	501	CLA	CMB-C2B-C1B	-2.26	125.15	128.46
24	b	5529	BCR	C1-C6-C7	2.25	121.77	115.65
20	B	515	CLA	O2D-CGD-CBD	2.25	115.17	111.23
20	d	5354	CLA	CMD-C2D-C1D	2.25	128.69	124.73
20	b	5514	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
26	d	5358	SQD	C17-C16-C15	2.25	125.75	114.37
20	B	511	CLA	CMB-C2B-C3B	2.25	129.18	124.68
26	t	213	SQD	C15-C14-C13	2.25	125.74	114.37
27	T	217	LMT	C1B-O1B-C4'	-2.25	112.65	117.98
24	D	357	BCR	C7-C8-C9	2.25	129.56	126.23
20	C	503	CLA	C1-C2-C3	2.25	130.40	126.76
24	X	130	BCR	C19-C18-C17	-2.25	115.48	119.01
28	b	5530	MGE	O1G-C1G-C2G	-2.25	101.92	108.40
20	b	5520	CLA	O2D-CGD-CBD	2.24	115.15	111.23
20	B	521	CLA	C12-C11-C10	-2.24	103.22	113.28
24	C	506	BCR	C23-C22-C21	-2.24	115.48	119.01
32	V	552	HEM	CBA-CAA-C2A	2.24	116.31	112.54
24	c	5505	BCR	C7-C8-C9	2.24	129.55	126.23
24	H	107	BCR	C37-C22-C23	2.24	121.51	118.09
20	C	502	CLA	O2D-CGD-CBD	2.24	115.14	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5520	CLA	C12-C11-C10	-2.24	103.25	113.28
28	l	5210	MGE	O1G-C1G-C2G	-2.24	101.94	108.40
24	a	5566	BCR	C12-C13-C14	-2.24	115.49	119.01
20	c	5498	CLA	C4D-CHA-C1A	2.24	123.91	121.24
20	B	520	CLA	CMB-C2B-C3B	2.24	129.15	124.68
24	c	5504	BCR	C7-C8-C9	2.24	129.54	126.23
20	B	520	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
24	h	5107	BCR	C30-C25-C24	2.23	121.71	115.65
20	c	5497	CLA	C12-C11-C10	-2.23	103.28	113.28
20	b	5513	CLA	C7-C6-C5	-2.23	107.32	113.26
24	b	5528	BCR	C32-C1-C2	-2.23	100.39	108.95
20	A	558	CLA	CMA-C3A-C2A	-2.23	105.36	113.98
20	b	5515	CLA	CMA-C3A-C2A	-2.23	105.36	113.98
24	C	504	BCR	C12-C13-C14	-2.23	115.50	119.01
24	A	566	BCR	C12-C13-C14	-2.23	115.50	119.01
24	C	506	BCR	C32-C1-C6	2.23	113.74	110.24
32	V	552	HEM	CAB-C3B-C2B	-2.23	121.19	128.43
20	b	5514	CLA	C2A-C1A-CHA	2.23	127.73	123.87
20	b	5523	CLA	O2D-CGD-CBD	2.23	115.12	111.23
20	c	5492	CLA	O2D-CGD-CBD	2.23	115.12	111.23
20	b	5517	CLA	C2A-C1A-CHA	2.23	127.73	123.87
32	F	51	HEM	CBA-CAA-C2A	-2.22	108.80	112.54
20	A	563	CLA	O2D-CGD-CBD	2.22	115.11	111.23
24	B	528	BCR	C40-C30-C25	2.22	113.73	110.24
20	C	498	CLA	C12-C11-C10	-2.22	103.33	113.28
26	A	568	SQD	C34-C33-C32	2.22	125.59	114.37
20	B	514	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	A	5212	SQD	O8-S-O7	2.22	116.95	111.40
24	b	5528	BCR	C30-C25-C24	2.22	121.67	115.65
20	c	5494	CLA	CMB-C2B-C3B	2.22	129.12	124.68
20	c	5495	CLA	CMB-C2B-C3B	2.22	129.12	124.68
20	b	5526	CLA	C2A-C3A-C4A	2.22	105.45	101.87
24	H	107	BCR	C30-C25-C24	2.22	121.66	115.65
24	H	107	BCR	C28-C27-C26	2.21	118.00	114.06
24	T	5104	BCR	C34-C9-C8	2.21	121.47	118.09
20	c	5493	CLA	O2D-CGD-CBD	2.21	115.10	111.23
20	C	493	CLA	CMB-C2B-C1B	-2.21	125.21	128.46
20	c	5491	CLA	O2D-CGD-CBD	2.21	115.10	111.23
32	F	51	HEM	O1A-CGA-CBA	-2.21	116.08	123.09
20	b	5521	CLA	C12-C11-C10	-2.21	103.38	113.28
24	d	5357	BCR	C19-C18-C17	-2.21	115.53	119.01
20	A	563	CLA	CMD-C2D-C1D	2.21	128.62	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5498	CLA	C2A-C3A-C4A	2.21	105.43	101.87
21	a	5562	PHO	C1-C2-C3	2.21	129.81	126.20
20	C	499	CLA	CAA-C2A-C3A	-2.20	107.04	113.00
24	b	5528	BCR	C7-C8-C9	2.20	129.50	126.23
20	B	514	CLA	CMB-C2B-C1B	-2.20	125.23	128.46
21	A	561	PHO	C1-O2A-CGA	2.20	121.98	116.65
20	A	560	CLA	O2A-CGA-CBA	2.20	118.55	111.83
20	c	5493	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	c	5505	BCR	C34-C9-C8	2.20	121.45	118.09
26	a	212	SQD	O10-C23-C24	-2.20	116.98	124.77
20	b	5525	CLA	C2A-C3A-C4A	2.20	105.42	101.87
24	h	5107	BCR	C36-C18-C19	2.20	121.45	118.09
20	b	5519	CLA	C2A-C1A-CHA	2.20	127.69	123.87
26	A	5212	SQD	O47-C45-C44	2.20	116.23	108.34
24	d	5357	BCR	C32-C1-C6	2.20	113.69	110.24
30	H	208	DGD	C3G-C2G-C1G	-2.20	106.66	111.78
32	v	5552	HEM	CAB-C3B-C2B	-2.20	121.29	128.43
20	c	5496	CLA	CBA-CAA-C2A	2.20	120.33	113.79
24	A	566	BCR	C1-C6-C7	2.20	121.61	115.65
28	L	210	MGE	O1G-C1G-C2G	-2.20	102.07	108.40
20	b	5518	CLA	CBA-CAA-C2A	2.19	120.32	113.79
21	A	562	PHO	O1D-CGD-CBD	-2.19	121.40	124.72
24	b	5528	BCR	C35-C13-C12	2.19	121.44	118.09
20	B	514	CLA	C1-O2A-CGA	2.19	121.96	116.65
20	b	5512	CLA	C2A-C3A-C4A	2.19	105.41	101.87
21	a	5562	PHO	CHA-C4D-C3D	2.19	115.57	111.19
24	C	504	BCR	C16-C17-C18	2.19	130.35	127.28
20	C	491	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
20	c	5500	CLA	CBA-CAA-C2A	2.19	120.31	113.79
28	D	360	MGE	O1G-C1A-C2A	2.19	118.50	111.83
20	b	5524	CLA	CMD-C2D-C1D	2.19	128.58	124.73
20	B	513	CLA	C2A-C3A-C4A	2.19	105.40	101.87
20	a	5559	CLA	CAA-CBA-CGA	2.19	119.41	113.21
20	c	5502	CLA	CBA-CAA-C2A	2.19	120.30	113.79
20	b	5513	CLA	CMA-C3A-C2A	-2.19	105.53	113.98
24	B	529	BCR	C36-C18-C19	2.19	121.43	118.09
24	b	5527	BCR	C12-C13-C14	-2.18	115.58	119.01
20	b	5520	CLA	C2A-C3A-C4A	2.18	105.39	101.87
24	t	104	BCR	C16-C17-C18	2.18	130.34	127.28
30	C	508	DGD	C6E-C5E-C4E	-2.18	107.67	113.02
20	b	5520	CLA	CMB-C2B-C3B	2.18	129.03	124.68
20	b	5516	CLA	O2D-CGD-CBD	2.18	115.04	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	5357	BCR	C34-C9-C8	2.18	121.41	118.09
20	C	492	CLA	C7-C6-C5	-2.18	107.46	113.26
21	A	561	PHO	CHA-C4D-C3D	2.18	115.54	111.19
20	B	515	CLA	C2A-C1A-CHA	2.18	127.64	123.87
24	a	5566	BCR	C7-C8-C9	2.17	129.45	126.23
20	b	5515	CLA	CBA-CAA-C2A	2.17	120.25	113.79
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
24	C	505	BCR	C7-C8-C9	2.17	129.44	126.23
20	B	525	CLA	C2A-C1A-CHA	2.17	127.63	123.87
20	c	5492	CLA	C1-C2-C3	2.17	129.75	126.20
24	B	527	BCR	C19-C18-C17	-2.17	115.60	119.01
24	a	5566	BCR	C8-C9-C10	-2.17	115.60	119.01
24	A	566	BCR	C30-C25-C24	2.17	121.53	115.65
20	B	517	CLA	CBA-CAA-C2A	2.17	120.24	113.79
20	B	518	CLA	CBA-CAA-C2A	2.17	120.24	113.79
30	C	508	DGD	O3G-C3G-C2G	2.17	116.08	110.82
24	b	5529	BCR	C15-C14-C13	2.16	130.31	127.28
20	C	496	CLA	C1-O2A-CGA	2.16	121.89	116.65
20	B	517	CLA	CMD-C2D-C1D	2.16	128.53	124.73
22	D	356	PQ9	C14-C13-C15	2.16	118.98	115.23
24	d	5357	BCR	C23-C22-C21	-2.16	115.61	119.01
20	b	5518	CLA	C6-C5-C3	2.16	118.73	113.47
20	b	5512	CLA	CMB-C2B-C3B	2.16	129.00	124.68
20	B	511	CLA	C2A-C1A-CHA	2.16	127.60	123.86
20	b	5513	CLA	C6-C5-C3	2.16	118.73	113.47
20	d	5355	CLA	C2A-C3A-C4A	2.16	105.36	101.87
24	c	5504	BCR	C34-C9-C8	2.16	121.38	118.09
20	b	5526	CLA	CMB-C2B-C1B	-2.16	125.30	128.46
24	h	5107	BCR	C28-C27-C26	2.15	117.89	114.06
20	D	354	CLA	CMD-C2D-C1D	2.15	128.52	124.73
24	c	5505	BCR	C40-C30-C25	2.15	113.61	110.24
20	a	5560	CLA	CMB-C2B-C3B	2.15	128.98	124.68
20	D	354	CLA	CMB-C2B-C1B	-2.15	125.31	128.46
24	B	529	BCR	C11-C10-C9	2.15	130.29	127.28
20	c	5503	CLA	C1-O2A-CGA	2.14	121.84	116.65
20	b	5515	CLA	O2D-CGD-CBD	2.14	114.98	111.23
28	d	5360	MGE	O1G-C1A-C2A	2.14	118.37	111.83
20	B	517	CLA	O2D-CGD-CBD	2.14	114.98	111.23
24	B	529	BCR	C1-C6-C7	2.14	121.46	115.65
24	D	357	BCR	C34-C9-C8	2.14	121.36	118.09
20	c	5494	CLA	C2A-C1A-CHA	2.14	127.58	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	514	CLA	C1-C2-C3	2.14	129.71	126.20
20	B	523	CLA	CMB-C2B-C3B	2.14	128.96	124.68
20	c	5500	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
20	a	5559	CLA	C1-C2-C3	2.14	129.70	126.20
20	B	515	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
20	B	520	CLA	C2A-C3A-C4A	2.14	105.32	101.87
20	b	5511	CLA	C2A-C1A-CHA	2.14	127.56	123.86
20	B	518	CLA	C6-C7-C8	2.14	123.07	115.97
20	d	5355	CLA	C1-O2A-CGA	2.14	121.82	116.65
24	D	357	BCR	C36-C18-C19	2.14	121.35	118.09
20	B	517	CLA	C2D-C1D-ND	2.13	112.24	110.13
24	H	107	BCR	C34-C9-C8	2.13	121.35	118.09
20	c	5496	CLA	CMD-C2D-C1D	2.13	128.49	124.73
20	c	5499	CLA	C1-O2A-CGA	2.13	122.73	116.67
20	c	5495	CLA	C1-O2A-CGA	2.13	121.81	116.65
26	a	212	SQD	O47-C45-C44	2.13	115.99	108.34
26	a	212	SQD	O8-S-O7	2.13	116.73	111.40
30	c	5508	DGD	O1G-C1A-C2A	2.13	118.33	111.83
20	B	513	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
20	A	560	CLA	O2D-CGD-CBD	2.13	114.95	111.23
26	A	568	SQD	C17-C16-C15	2.13	125.13	114.37
20	b	5517	CLA	C2A-C3A-C4A	2.13	105.31	101.87
20	B	526	CLA	C6-C5-C3	2.13	118.65	113.47
32	f	5051	HEM	C2C-C3C-C4C	-2.13	105.41	106.90
24	A	566	BCR	C34-C9-C8	2.13	121.34	118.09
22	A	564	PQ9	C11-C2-C1	2.13	118.66	116.91
24	b	5529	BCR	C30-C25-C24	2.12	121.41	115.65
32	v	5552	HEM	C4A-C3A-C2A	2.12	108.47	107.00
20	C	500	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
28	I	201	MGE	C3G-O3G-C1D	-2.12	109.25	113.80
20	b	5517	CLA	CMD-C2D-C1D	2.12	128.47	124.73
20	b	5514	CLA	C1-O2A-CGA	2.12	121.79	116.65
20	c	5493	CLA	CBA-CAA-C2A	2.12	120.10	113.79
20	c	5496	CLA	CMB-C2B-C1B	-2.12	125.35	128.46
20	d	5354	CLA	CMB-C2B-C1B	-2.12	125.35	128.46
20	b	5526	CLA	C6-C5-C3	2.12	118.63	113.47
20	c	5498	CLA	CMD-C2D-C1D	2.12	128.46	124.73
20	C	502	CLA	CBA-CAA-C2A	2.12	120.09	113.79
30	h	5208	DGD	C3G-C2G-C1G	-2.12	106.85	111.78
21	a	5562	PHO	CMA-C3A-C4A	-2.12	110.05	114.61
20	B	522	CLA	CMB-C2B-C1B	-2.11	125.36	128.46
20	c	5495	CLA	C2A-C3A-C4A	2.11	105.28	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	528	BCR	C30-C25-C24	2.11	121.38	115.65
27	m	216	LMT	C1B-O1B-C4'	-2.11	112.97	117.98
20	b	5525	CLA	C2A-C1A-CHA	2.11	127.53	123.87
20	D	355	CLA	CBA-CAA-C2A	2.11	120.07	113.79
24	h	5107	BCR	C11-C12-C13	2.11	132.15	126.36
20	c	5500	CLA	O2D-CGD-CBD	2.11	114.92	111.23
20	c	5491	CLA	C2A-C1A-CHA	2.11	127.53	123.87
28	D	358	MGE	C3G-C2G-C1G	-2.11	106.87	111.78
24	T	5104	BCR	C8-C9-C10	-2.11	115.69	119.01
20	A	563	CLA	C7-C6-C5	-2.11	107.65	113.26
20	b	5518	CLA	C2A-C3A-C4A	2.10	105.26	101.87
20	C	492	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
32	V	552	HEM	C4B-C3B-C2B	-2.10	105.35	107.28
20	C	496	CLA	C2A-C3A-C4A	2.10	105.26	101.87
24	A	566	BCR	C32-C1-C6	2.10	113.53	110.24
20	a	5558	CLA	CMA-C3A-C2A	-2.10	105.88	113.98
30	C	508	DGD	O1G-C1A-C2A	2.10	118.22	111.83
20	b	5511	CLA	CMB-C2B-C3B	2.10	128.87	124.68
20	c	5501	CLA	C2A-C1A-CHA	2.10	127.50	123.87
20	B	512	CLA	CMB-C2B-C3B	2.09	128.87	124.68
20	C	491	CLA	CBA-CAA-C2A	2.09	120.03	113.79
20	B	518	CLA	C2A-C3A-C4A	2.09	105.25	101.87
24	x	5130	BCR	C24-C23-C22	2.09	129.33	126.23
32	F	51	HEM	CMD-C2D-C1D	2.09	128.30	125.03
20	C	503	CLA	O2D-CGD-CBD	2.09	114.89	111.23
20	B	520	CLA	C12-C11-C10	-2.09	103.90	113.28
20	C	496	CLA	CMD-C2D-C1D	2.09	128.41	124.73
20	B	520	CLA	C2A-C1A-CHA	2.09	127.50	123.87
20	B	524	CLA	CMD-C2D-C1D	2.09	128.41	124.73
20	C	492	CLA	CMB-C2B-C1B	-2.09	125.39	128.46
20	B	524	CLA	C2A-C3A-C4A	2.09	105.24	101.87
28	D	359	MGE	C3G-O3G-C1D	-2.09	109.32	113.80
20	B	523	CLA	CMA-C3A-C2A	-2.09	105.91	113.98
20	a	5563	CLA	CMB-C2B-C3B	2.09	128.85	124.68
20	B	520	CLA	O2D-CGD-CBD	2.09	114.88	111.23
20	C	496	CLA	C2A-C1A-CHA	2.08	127.48	123.87
20	a	5563	CLA	CMD-C2D-C1D	2.08	128.40	124.73
20	B	515	CLA	CBA-CAA-C2A	2.08	119.99	113.79
20	B	522	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
20	C	493	CLA	CBA-CAA-C2A	2.08	119.99	113.79
20	b	5525	CLA	CMD-C2D-C1D	2.08	128.39	124.73
20	d	5355	CLA	CMD-C2D-C1D	2.08	128.39	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5496	CLA	O2D-CGD-CBD	2.08	114.86	111.23
24	c	5505	BCR	C19-C18-C17	-2.08	115.74	119.01
20	D	355	CLA	C2A-C3A-C4A	2.08	105.22	101.87
20	b	5523	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
24	T	5104	BCR	C30-C25-C24	2.07	121.28	115.65
20	c	5502	CLA	CMD-C2D-C1D	2.07	128.38	124.73
20	b	5518	CLA	C6-C7-C8	2.07	122.85	115.97
32	v	5552	HEM	C4B-C3B-C2B	-2.07	105.38	107.28
21	a	5561	PHO	CMA-C3A-C2A	-2.07	106.14	114.13
24	b	5529	BCR	C36-C18-C19	2.07	121.25	118.09
20	C	497	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	b	5513	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	B	525	CLA	CMD-C2D-C1D	2.06	128.36	124.73
20	b	5521	CLA	CMD-C2D-C1D	2.06	128.36	124.73
24	t	104	BCR	C30-C25-C24	2.06	121.24	115.65
24	B	528	BCR	C32-C1-C2	-2.06	101.03	108.95
20	a	5558	CLA	CMB-C2B-C3B	2.06	128.80	124.68
24	C	505	BCR	C1-C6-C7	2.06	121.24	115.65
24	T	5104	BCR	C19-C18-C17	-2.06	115.77	119.01
28	D	360	MGE	O1G-C1G-C2G	-2.06	102.47	108.40
20	d	5354	CLA	C2A-C1A-CHA	2.06	127.44	123.87
20	C	503	CLA	CMB-C2B-C3B	2.06	128.79	124.68
20	D	355	CLA	CMD-C2D-C1D	2.06	128.35	124.73
20	a	5563	CLA	CMA-C3A-C2A	-2.05	106.04	113.98
32	v	5552	HEM	CMA-C3A-C4A	-2.05	125.45	128.46
27	M	5216	LMT	C1-O1'-C1'	-2.05	110.17	113.68
20	C	501	CLA	O2D-CGD-CBD	2.05	114.82	111.23
20	c	5498	CLA	C12-C11-C10	-2.05	104.08	113.28
26	t	213	SQD	O48-C23-O10	-2.05	118.49	123.63
20	c	5500	CLA	C12-C11-C10	-2.05	104.08	113.28
24	c	5505	BCR	C1-C6-C7	2.05	121.22	115.65
32	V	552	HEM	CAB-C3B-C4B	2.05	133.46	124.39
20	C	501	CLA	C2D-C1D-ND	2.05	112.16	110.13
28	b	5530	MGE	C3G-C2G-C1G	-2.05	107.01	111.78
20	b	5522	CLA	CMD-C2D-C1D	2.05	128.34	124.73
30	c	5508	DGD	O3G-C3G-C2G	2.05	115.80	110.82
28	L	210	MGE	O1G-C1A-C2A	2.05	118.08	111.83
24	b	5527	BCR	C19-C18-C17	-2.05	115.79	119.01
21	a	5562	PHO	CMA-C3A-C2A	-2.04	106.23	114.13
28	b	5530	MGE	O1G-C1A-C2A	2.04	118.06	111.83
24	a	5566	BCR	C19-C18-C17	-2.04	115.80	119.01
24	c	5504	BCR	C8-C7-C6	2.04	132.45	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	5216	LMT	C1B-O1B-C4'	-2.04	113.14	117.98
32	F	51	HEM	CAA-CBA-CGA	2.04	119.33	113.83
20	c	5502	CLA	CMA-C3A-C2A	-2.04	106.10	113.98
24	T	5104	BCR	C16-C17-C18	2.04	130.13	127.28
20	b	5523	CLA	CBA-CAA-C2A	2.04	119.85	113.79
24	x	5130	BCR	C40-C30-C29	-2.04	101.13	108.95
20	C	496	CLA	O2D-CGD-CBD	2.04	114.79	111.23
20	B	512	CLA	C1-O2A-CGA	2.04	121.58	116.65
26	a	212	SQD	O5-C5-C4	2.04	113.37	109.70
32	v	5552	HEM	C1B-NB-C4B	2.03	107.62	105.21
20	B	521	CLA	CMB-C2B-C1B	-2.03	125.48	128.46
26	t	213	SQD	O8-S-O7	2.03	116.48	111.40
20	b	5519	CLA	C6-C5-C3	2.03	118.42	113.47
20	b	5515	CLA	CMB-C2B-C1B	-2.03	125.48	128.46
20	B	523	CLA	CBA-CAA-C2A	2.03	119.83	113.79
20	a	5560	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	A	564	PQ9	C6-C5-C4	2.03	119.44	115.28
20	c	5498	CLA	C2D-C1D-ND	2.03	112.13	110.13
20	b	5520	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
20	b	5513	CLA	CMD-C2D-C1D	2.03	128.30	124.73
22	D	356	PQ9	C30-C28-C29	2.03	119.26	114.59
24	a	5566	BCR	C1-C6-C7	2.03	121.15	115.65
24	b	5529	BCR	C37-C22-C23	2.03	121.19	118.09
20	C	499	CLA	CMB-C2B-C3B	2.03	128.73	124.68
20	B	517	CLA	C2A-C3A-C4A	2.03	105.14	101.87
20	c	5491	CLA	CMA-C3A-C2A	-2.03	106.15	113.98
24	b	5527	BCR	C37-C22-C23	2.03	121.18	118.09
24	h	5107	BCR	C8-C9-C10	-2.02	115.82	119.01
20	C	498	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
32	v	5552	HEM	CAB-C3B-C4B	2.02	133.33	124.39
20	c	5492	CLA	C2A-C1A-CHA	2.02	127.38	123.87
20	C	496	CLA	CBA-CAA-C2A	2.02	119.81	113.79
20	B	512	CLA	C2A-C1A-CHA	2.02	127.38	123.87
30	h	5208	DGD	O3G-C3G-C2G	2.02	115.74	110.82
20	c	5501	CLA	C2A-C3A-C4A	2.02	105.13	101.87
28	l	5210	MGE	O1G-C1A-C2A	2.02	117.99	111.83
20	C	503	CLA	CMD-C2D-C1D	2.02	128.28	124.73
30	c	5509	DGD	O1G-C1A-C2A	2.02	117.99	111.83
20	C	502	CLA	CMD-C2D-C1D	2.02	128.28	124.73
32	f	5051	HEM	C4A-C3A-C2A	2.02	108.40	107.00
20	D	355	CLA	CMA-C3A-C2A	-2.02	106.19	113.98
20	b	5515	CLA	C2A-C1A-CHA	2.01	127.36	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	528	BCR	C7-C8-C9	2.01	129.21	126.23
20	b	5519	CLA	O2D-CGD-CBD	2.01	114.75	111.23
24	C	505	BCR	C37-C22-C23	2.01	121.16	118.09
27	m	216	LMT	C4B-C3B-C2B	-2.01	107.30	110.83
21	A	561	PHO	CMA-C3A-C2A	-2.01	106.36	114.13
20	C	500	CLA	C1-O2A-CGA	2.01	121.52	116.65
24	b	5529	BCR	C11-C10-C9	2.01	130.10	127.28
20	B	519	CLA	O2D-CGD-CBD	2.01	114.74	111.23
24	x	5130	BCR	C19-C18-C17	-2.01	115.85	119.01
20	C	500	CLA	C12-C11-C10	-2.01	104.28	113.28
20	C	497	CLA	C2A-C1A-CHA	2.01	127.35	123.87
24	B	529	BCR	C16-C17-C18	2.01	130.09	127.28
20	B	522	CLA	CBA-CAA-C2A	2.01	119.77	113.79
20	b	5519	CLA	C2A-C3A-C4A	2.01	105.11	101.87
28	D	359	MGE	O1G-C1A-C2A	2.01	117.95	111.83
20	a	5559	CLA	CHD-C1D-ND	-2.01	121.98	124.80
20	C	503	CLA	C2A-C3A-C4A	2.00	105.11	101.87
24	T	5104	BCR	C32-C1-C6	2.00	113.38	110.24
30	C	507	DGD	O6D-C1D-C2D	2.00	114.48	110.37
20	b	5513	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (94) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	558	CLA	ND
20	A	559	CLA	ND
20	A	560	CLA	ND
20	A	563	CLA	ND
20	B	511	CLA	ND
20	B	512	CLA	ND
20	B	513	CLA	ND
20	B	514	CLA	ND
20	B	515	CLA	ND
20	B	516	CLA	ND
20	B	517	CLA	ND
20	B	518	CLA	ND
20	B	519	CLA	ND
20	B	520	CLA	ND
20	B	521	CLA	ND
20	B	522	CLA	ND
20	B	523	CLA	ND
20	B	524	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	B	525	CLA	ND
20	B	526	CLA	ND
20	C	491	CLA	ND
20	C	492	CLA	ND
20	C	493	CLA	ND
20	C	494	CLA	ND
20	C	495	CLA	ND
20	C	496	CLA	ND
20	C	497	CLA	ND
20	C	498	CLA	ND
20	C	499	CLA	ND
20	C	500	CLA	ND
20	C	501	CLA	ND
20	C	502	CLA	ND
20	C	503	CLA	ND
20	D	354	CLA	ND
20	D	355	CLA	ND
20	a	5558	CLA	ND
20	a	5559	CLA	ND
20	a	5560	CLA	ND
20	a	5563	CLA	ND
20	b	5511	CLA	ND
20	b	5512	CLA	ND
20	b	5513	CLA	ND
20	b	5514	CLA	ND
20	b	5515	CLA	ND
20	b	5516	CLA	ND
20	b	5517	CLA	ND
20	b	5518	CLA	ND
20	b	5519	CLA	ND
20	b	5520	CLA	ND
20	b	5521	CLA	ND
20	b	5522	CLA	ND
20	b	5523	CLA	ND
20	b	5524	CLA	ND
20	b	5525	CLA	ND
20	b	5526	CLA	ND
20	c	5491	CLA	ND
20	c	5492	CLA	ND
20	c	5493	CLA	ND
20	c	5494	CLA	ND
20	c	5495	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	c	5496	CLA	ND
20	c	5497	CLA	ND
20	c	5498	CLA	ND
20	c	5499	CLA	ND
20	c	5500	CLA	ND
20	c	5501	CLA	ND
20	c	5502	CLA	ND
20	c	5503	CLA	ND
20	d	5354	CLA	ND
20	d	5355	CLA	ND
30	C	507	DGD	C5E
30	C	507	DGD	C2D
30	C	507	DGD	C5D
30	C	508	DGD	C5E
30	C	508	DGD	C2D
30	C	508	DGD	C5D
30	C	509	DGD	C5E
30	C	509	DGD	C2D
30	C	509	DGD	C5D
30	H	208	DGD	C5E
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	c	5507	DGD	C5E
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D
30	c	5508	DGD	C5E
30	c	5508	DGD	C2D
30	c	5508	DGD	C5D
30	c	5509	DGD	C5E
30	c	5509	DGD	C2D
30	c	5509	DGD	C5D
30	h	5208	DGD	C5E
30	h	5208	DGD	C2D
30	h	5208	DGD	C5D

All (1400) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	511	CLA	CBD-CGD-O2D-CED
20	B	515	CLA	C2-C3-C5-C6
20	B	515	CLA	C4-C3-C5-C6
20	B	516	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	516	CLA	C3A-C2A-CAA-CBA
20	B	516	CLA	C1-C2-C3-C4
20	B	516	CLA	C1-C2-C3-C5
20	B	517	CLA	C1A-C2A-CAA-CBA
20	B	517	CLA	C3A-C2A-CAA-CBA
20	B	518	CLA	C1A-C2A-CAA-CBA
20	B	518	CLA	C3A-C2A-CAA-CBA
20	B	518	CLA	C1-C2-C3-C5
20	B	518	CLA	C6-C7-C8-C9
20	B	525	CLA	C1-C2-C3-C5
20	B	526	CLA	C1A-C2A-CAA-CBA
20	C	492	CLA	C1-C2-C3-C5
20	C	494	CLA	C1A-C2A-CAA-CBA
20	C	495	CLA	C1A-C2A-CAA-CBA
20	C	495	CLA	CBD-CGD-O2D-CED
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	C	496	CLA	C1A-C2A-CAA-CBA
20	C	496	CLA	CBD-CGD-O2D-CED
20	C	500	CLA	C1-C2-C3-C5
20	C	501	CLA	C1-C2-C3-C5
20	C	502	CLA	C1A-C2A-CAA-CBA
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	D	354	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C5
20	D	355	CLA	C1A-C2A-CAA-CBA
20	D	355	CLA	C3A-C2A-CAA-CBA
20	D	355	CLA	C1-C2-C3-C4
20	D	355	CLA	C1-C2-C3-C5
20	a	5558	CLA	CBD-CGD-O2D-CED
20	b	5511	CLA	CBD-CGD-O2D-CED
20	b	5515	CLA	C2-C3-C5-C6
20	b	5515	CLA	C4-C3-C5-C6
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
20	b	5517	CLA	C1A-C2A-CAA-CBA
20	b	5517	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	b	5518	CLA	C1A-C2A-CAA-CBA
20	b	5518	CLA	C3A-C2A-CAA-CBA
20	b	5518	CLA	C1-C2-C3-C5
20	b	5518	CLA	C6-C7-C8-C9
20	b	5520	CLA	C1-C2-C3-C4
20	b	5525	CLA	C1-C2-C3-C5
20	b	5526	CLA	C1A-C2A-CAA-CBA
20	c	5491	CLA	C1A-C2A-CAA-CBA
20	c	5492	CLA	C1-C2-C3-C5
20	c	5494	CLA	C1A-C2A-CAA-CBA
20	c	5495	CLA	C1A-C2A-CAA-CBA
20	c	5495	CLA	CBD-CGD-O2D-CED
20	c	5495	CLA	C1-C2-C3-C5
20	c	5495	CLA	C2-C3-C5-C6
20	c	5495	CLA	C4-C3-C5-C6
20	c	5496	CLA	C1A-C2A-CAA-CBA
20	c	5496	CLA	CBD-CGD-O2D-CED
20	c	5500	CLA	CBD-CGD-O2D-CED
20	c	5500	CLA	C1-C2-C3-C5
20	c	5501	CLA	C1-C2-C3-C5
20	c	5502	CLA	C1A-C2A-CAA-CBA
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	d	5354	CLA	C1-C2-C3-C4
20	d	5354	CLA	C1-C2-C3-C5
20	d	5355	CLA	C1A-C2A-CAA-CBA
20	d	5355	CLA	C3A-C2A-CAA-CBA
20	d	5355	CLA	C1-C2-C3-C4
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	D	356	PQ9	C16-C17-C18-C19
22	D	356	PQ9	C16-C17-C18-C20
22	D	356	PQ9	C21-C22-C23-C25
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
22	d	5356	PQ9	C16-C17-C18-C19
22	d	5356	PQ9	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	d	5356	PQ9	C21-C22-C23-C25
24	A	566	BCR	C5-C6-C7-C8
24	B	527	BCR	C6-C7-C8-C9
24	B	528	BCR	C6-C7-C8-C9
24	B	529	BCR	C6-C7-C8-C9
24	B	529	BCR	C23-C24-C25-C26
24	C	504	BCR	C1-C6-C7-C8
24	C	504	BCR	C5-C6-C7-C8
24	C	504	BCR	C6-C7-C8-C9
24	C	505	BCR	C6-C7-C8-C9
24	C	506	BCR	C22-C23-C24-C25
24	C	506	BCR	C23-C24-C25-C26
24	D	357	BCR	C6-C7-C8-C9
24	T	5104	BCR	C6-C7-C8-C9
24	b	5527	BCR	C6-C7-C8-C9
24	b	5528	BCR	C6-C7-C8-C9
24	b	5529	BCR	C6-C7-C8-C9
24	b	5529	BCR	C23-C24-C25-C26
24	c	5504	BCR	C1-C6-C7-C8
24	c	5504	BCR	C5-C6-C7-C8
24	c	5504	BCR	C6-C7-C8-C9
24	c	5505	BCR	C6-C7-C8-C9
24	c	5506	BCR	C22-C23-C24-C25
24	c	5506	BCR	C23-C24-C25-C26
24	d	5357	BCR	C6-C7-C8-C9
24	t	104	BCR	C6-C7-C8-C9
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
26	A	5212	SQD	O5-C1-O6-C44
26	A	5212	SQD	O6-C44-C45-O47
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	a	212	SQD	O5-C1-O6-C44
26	a	212	SQD	O6-C44-C45-O47
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
26	t	213	SQD	O5-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	t	213	SQD	O5-C5-C6-S
28	B	530	MGE	C2B-C1B-O2G-C2G
28	B	530	MGE	C2D-C1D-O3G-C3G
28	B	530	MGE	O6D-C1D-O3G-C3G
28	D	358	MGE	C2B-C1B-O2G-C2G
28	D	359	MGE	C2B-C1B-O2G-C2G
28	D	360	MGE	C2B-C1B-O2G-C2G
28	I	201	MGE	O1A-C1A-O1G-C1G
28	I	201	MGE	C2B-C1B-O2G-C2G
28	b	5530	MGE	C2B-C1B-O2G-C2G
28	b	5530	MGE	C2D-C1D-O3G-C3G
28	b	5530	MGE	O6D-C1D-O3G-C3G
28	d	5359	MGE	C2B-C1B-O2G-C2G
28	d	5360	MGE	C2B-C1B-O2G-C2G
28	d	5361	MGE	C2B-C1B-O2G-C2G
28	i	5201	MGE	C2B-C1B-O2G-C2G
30	C	507	DGD	C2D-C1D-O3G-C3G
30	C	507	DGD	C2E-C1E-O5D-C6D
30	C	508	DGD	C2B-C1B-O2G-C2G
30	C	508	DGD	O6E-C1E-O5D-C6D
30	H	208	DGD	O6D-C1D-O3G-C3G
30	H	208	DGD	C2E-C1E-O5D-C6D
30	c	5507	DGD	C2E-C1E-O5D-C6D
30	c	5508	DGD	C2B-C1B-O2G-C2G
30	c	5508	DGD	O1B-C1B-O2G-C2G
30	c	5508	DGD	O6E-C1E-O5D-C6D
30	h	5208	DGD	O6D-C1D-O3G-C3G
30	h	5208	DGD	C2E-C1E-O5D-C6D
32	F	51	HEM	C2B-C3B-CAB-CBB
32	F	51	HEM	C4B-C3B-CAB-CBB
32	V	552	HEM	C2B-C3B-CAB-CBB
32	f	5051	HEM	C2B-C3B-CAB-CBB
32	f	5051	HEM	C4B-C3B-CAB-CBB
32	v	5552	HEM	C2B-C3B-CAB-CBB
20	A	558	CLA	O1D-CGD-O2D-CED
20	a	5558	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	A	558	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	CBD-CGD-O2D-CED
20	B	514	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	517	CLA	CBD-CGD-O2D-CED
20	B	526	CLA	CBD-CGD-O2D-CED
20	C	493	CLA	CBD-CGD-O2D-CED
20	C	494	CLA	CBD-CGD-O2D-CED
20	C	499	CLA	CBD-CGD-O2D-CED
20	C	500	CLA	CBD-CGD-O2D-CED
20	C	502	CLA	CBD-CGD-O2D-CED
20	D	355	CLA	CBD-CGD-O2D-CED
20	b	5513	CLA	CBD-CGD-O2D-CED
20	b	5514	CLA	CBD-CGD-O2D-CED
20	b	5517	CLA	CBD-CGD-O2D-CED
20	b	5524	CLA	CBD-CGD-O2D-CED
20	b	5526	CLA	CBD-CGD-O2D-CED
20	c	5493	CLA	CBD-CGD-O2D-CED
20	c	5494	CLA	CBD-CGD-O2D-CED
20	c	5499	CLA	CBD-CGD-O2D-CED
20	d	5355	CLA	CBD-CGD-O2D-CED
21	A	562	PHO	CBD-CGD-O2D-CED
21	a	5562	PHO	CBD-CGD-O2D-CED
28	D	360	MGE	O1A-C1A-O1G-C1G
28	i	5201	MGE	O1A-C1A-O1G-C1G
20	C	495	CLA	O1D-CGD-O2D-CED
20	c	5494	CLA	O1D-CGD-O2D-CED
20	c	5495	CLA	O1D-CGD-O2D-CED
22	A	564	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C30
20	B	526	CLA	O1D-CGD-O2D-CED
20	b	5526	CLA	O1D-CGD-O2D-CED
20	c	5499	CLA	O1D-CGD-O2D-CED
26	L	5213	SQD	C24-C23-O48-C46
26	t	213	SQD	C24-C23-O48-C46
28	I	201	MGE	C2A-C1A-O1G-C1G
20	B	515	CLA	CBD-CGD-O2D-CED
20	b	5515	CLA	CBD-CGD-O2D-CED
26	t	213	SQD	O10-C23-O48-C46
28	D	359	MGE	O1A-C1A-O1G-C1G
28	L	210	MGE	O1A-C1A-O1G-C1G
28	d	5360	MGE	O1A-C1A-O1G-C1G
28	d	5361	MGE	O1A-C1A-O1G-C1G
28	l	5210	MGE	O1A-C1A-O1G-C1G
20	B	511	CLA	O1D-CGD-O2D-CED
20	C	493	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	499	CLA	O1D-CGD-O2D-CED
20	C	500	CLA	O1D-CGD-O2D-CED
20	c	5493	CLA	O1D-CGD-O2D-CED
20	c	5496	CLA	O1D-CGD-O2D-CED
20	c	5500	CLA	O1D-CGD-O2D-CED
20	C	496	CLA	O1D-CGD-O2D-CED
26	A	5212	SQD	O10-C23-O48-C46
20	B	524	CLA	CBD-CGD-O2D-CED
20	c	5502	CLA	CBD-CGD-O2D-CED
28	B	530	MGE	O1B-C1B-O2G-C2G
28	D	358	MGE	O1B-C1B-O2G-C2G
28	D	359	MGE	O1B-C1B-O2G-C2G
28	I	201	MGE	O1B-C1B-O2G-C2G
28	b	5530	MGE	O1B-C1B-O2G-C2G
28	d	5359	MGE	O1B-C1B-O2G-C2G
28	d	5360	MGE	O1B-C1B-O2G-C2G
28	i	5201	MGE	O1B-C1B-O2G-C2G
30	C	508	DGD	O1B-C1B-O2G-C2G
22	D	356	PQ9	C26-C27-C28-C29
22	a	5564	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C29
20	B	512	CLA	C3-C5-C6-C7
20	B	523	CLA	C3-C5-C6-C7
20	b	5512	CLA	C3-C5-C6-C7
20	b	5523	CLA	C3-C5-C6-C7
21	A	562	PHO	C3-C5-C6-C7
21	a	5562	PHO	C3-C5-C6-C7
21	A	562	PHO	O1D-CGD-O2D-CED
28	D	359	MGE	C2A-C1A-O1G-C1G
28	D	360	MGE	C2A-C1A-O1G-C1G
28	L	210	MGE	C2A-C1A-O1G-C1G
28	d	5360	MGE	C2A-C1A-O1G-C1G
28	i	5201	MGE	C2A-C1A-O1G-C1G
28	l	5210	MGE	C2A-C1A-O1G-C1G
20	A	563	CLA	CBD-CGD-O2D-CED
20	B	519	CLA	CBD-CGD-O2D-CED
20	B	525	CLA	CBD-CGD-O2D-CED
20	C	498	CLA	CBD-CGD-O2D-CED
20	b	5519	CLA	CBD-CGD-O2D-CED
20	b	5523	CLA	CBD-CGD-O2D-CED
20	b	5525	CLA	CBD-CGD-O2D-CED
20	c	5498	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	513	CLA	O1D-CGD-O2D-CED
20	b	5511	CLA	O1D-CGD-O2D-CED
21	a	5562	PHO	O1D-CGD-O2D-CED
26	a	212	SQD	O10-C23-O48-C46
20	d	5355	CLA	C2A-CAA-CBA-CGA
22	A	564	PQ9	C26-C27-C28-C30
22	D	356	PQ9	C26-C27-C28-C30
22	a	5564	PQ9	C26-C27-C28-C30
20	B	518	CLA	C3-C5-C6-C7
20	b	5518	CLA	C3-C5-C6-C7
28	d	5361	MGE	C2A-C1A-O1G-C1G
22	D	356	PQ9	C21-C22-C23-C24
22	d	5356	PQ9	C21-C22-C23-C24
30	c	5508	DGD	C4D-C5D-C6D-O5D
28	D	360	MGE	O1B-C1B-O2G-C2G
28	d	5361	MGE	O1B-C1B-O2G-C2G
20	b	5513	CLA	O1D-CGD-O2D-CED
20	B	523	CLA	CBD-CGD-O2D-CED
20	a	5563	CLA	CBD-CGD-O2D-CED
20	B	517	CLA	O1D-CGD-O2D-CED
20	d	5355	CLA	O1D-CGD-O2D-CED
28	D	360	MGE	O6D-C5D-C6D-O5D
30	C	508	DGD	C4D-C5D-C6D-O5D
30	C	507	DGD	C4E-C5E-C6E-O5E
30	c	5507	DGD	C4E-C5E-C6E-O5E
20	D	355	CLA	O1D-CGD-O2D-CED
20	b	5517	CLA	O1D-CGD-O2D-CED
30	C	508	DGD	O6D-C5D-C6D-O5D
30	c	5508	DGD	O6D-C5D-C6D-O5D
20	B	515	CLA	C3-C5-C6-C7
28	b	5530	MGE	C2A-C1A-O1G-C1G
28	d	5361	MGE	O6D-C5D-C6D-O5D
20	C	502	CLA	O1D-CGD-O2D-CED
28	I	201	MGE	O6D-C5D-C6D-O5D
20	C	498	CLA	C2A-CAA-CBA-CGA
20	D	355	CLA	C2A-CAA-CBA-CGA
20	b	5520	CLA	C2A-CAA-CBA-CGA
20	c	5498	CLA	C2A-CAA-CBA-CGA
20	c	5501	CLA	C2A-CAA-CBA-CGA
20	B	514	CLA	O1D-CGD-O2D-CED
20	b	5524	CLA	O1D-CGD-O2D-CED
28	I	201	MGE	O6D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	i	5201	MGE	O6D-C1D-O3G-C3G
30	C	507	DGD	O6D-C1D-O3G-C3G
30	C	507	DGD	O6E-C1E-O5D-C6D
30	H	208	DGD	O6E-C1E-O5D-C6D
30	c	5507	DGD	O6D-C1D-O3G-C3G
30	h	5208	DGD	O6E-C1E-O5D-C6D
28	B	530	MGE	C2A-C1A-O1G-C1G
20	B	522	CLA	CBD-CGD-O2D-CED
20	b	5522	CLA	CBD-CGD-O2D-CED
28	b	5530	MGE	O1A-C1A-O1G-C1G
30	C	507	DGD	C4D-C5D-C6D-O5D
28	D	359	MGE	O6D-C5D-C6D-O5D
28	d	5360	MGE	O6D-C5D-C6D-O5D
20	b	5514	CLA	O1D-CGD-O2D-CED
28	D	359	MGE	C4D-C5D-C6D-O5D
20	C	491	CLA	CBD-CGD-O2D-CED
20	c	5491	CLA	CBD-CGD-O2D-CED
28	B	530	MGE	O1A-C1A-O1G-C1G
20	c	5502	CLA	O1D-CGD-O2D-CED
25	a	5567	LHG	C24-C23-O8-C6
26	A	568	SQD	C24-C23-O48-C46
26	d	5358	SQD	C24-C23-O48-C46
28	i	5201	MGE	O6D-C5D-C6D-O5D
20	C	501	CLA	CBD-CGD-O2D-CED
20	b	5518	CLA	CBD-CGD-O2D-CED
30	C	507	DGD	O6D-C5D-C6D-O5D
30	c	5507	DGD	O6D-C5D-C6D-O5D
30	c	5507	DGD	C4D-C5D-C6D-O5D
20	B	515	CLA	O1D-CGD-O2D-CED
20	B	524	CLA	O1D-CGD-O2D-CED
20	b	5515	CLA	O1D-CGD-O2D-CED
28	d	5360	MGE	C4D-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
20	A	558	CLA	C14-C13-C15-C16
20	B	514	CLA	C6-C7-C8-C9
20	B	518	CLA	C14-C13-C15-C16
20	B	522	CLA	C6-C7-C8-C9
20	C	501	CLA	C6-C7-C8-C9
20	a	5558	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	b	5514	CLA	C6-C7-C8-C9
20	b	5518	CLA	C14-C13-C15-C16
20	b	5522	CLA	C6-C7-C8-C9
20	c	5501	CLA	C6-C7-C8-C9
28	I	201	MGE	C2D-C1D-O3G-C3G
28	i	5201	MGE	C2D-C1D-O3G-C3G
30	H	208	DGD	C2D-C1D-O3G-C3G
30	c	5507	DGD	C2D-C1D-O3G-C3G
30	h	5208	DGD	C2D-C1D-O3G-C3G
30	h	5208	DGD	O6D-C5D-C6D-O5D
25	A	567	LHG	C24-C23-O8-C6
26	d	5358	SQD	O10-C23-O48-C46
20	b	5525	CLA	O1D-CGD-O2D-CED
20	B	520	CLA	C2A-CAA-CBA-CGA
20	C	501	CLA	C2A-CAA-CBA-CGA
30	H	208	DGD	O6D-C5D-C6D-O5D
20	b	5523	CLA	O1D-CGD-O2D-CED
20	B	525	CLA	O1D-CGD-O2D-CED
20	c	5498	CLA	O1D-CGD-O2D-CED
22	A	564	PQ9	C21-C22-C23-C24
20	C	491	CLA	C15-C16-C17-C18
20	C	498	CLA	O1D-CGD-O2D-CED
28	B	530	MGE	C1B-C2B-C3B-C4B
20	C	493	CLA	C13-C15-C16-C17
20	B	520	CLA	C6-C7-C8-C10
20	b	5520	CLA	C6-C7-C8-C10
20	b	5519	CLA	O1D-CGD-O2D-CED
22	D	356	PQ9	C18-C20-C21-C22
22	d	5356	PQ9	C18-C20-C21-C22
20	b	5515	CLA	C3-C5-C6-C7
20	b	5517	CLA	C10-C11-C12-C13
20	c	5491	CLA	C15-C16-C17-C18
20	c	5493	CLA	C13-C15-C16-C17
28	D	358	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	C1B-C2B-C3B-C4B
30	c	5507	DGD	C1A-C2A-C3A-C4A
25	A	567	LHG	O10-C23-O8-C6
25	a	5567	LHG	O10-C23-O8-C6
26	A	568	SQD	O10-C23-O48-C46
20	A	558	CLA	C10-C11-C12-C13
20	B	517	CLA	C10-C11-C12-C13
20	b	5513	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	c	5497	CLA	C15-C16-C17-C18
21	A	562	PHO	C10-C11-C12-C13
21	A	562	PHO	C13-C15-C16-C17
21	a	5562	PHO	C13-C15-C16-C17
28	d	5361	MGE	C4D-C5D-C6D-O5D
20	C	494	CLA	C2A-CAA-CBA-CGA
20	C	496	CLA	C2A-CAA-CBA-CGA
20	c	5494	CLA	C2A-CAA-CBA-CGA
20	c	5502	CLA	C2A-CAA-CBA-CGA
20	A	563	CLA	C5-C6-C7-C8
20	C	500	CLA	C5-C6-C7-C8
20	c	5493	CLA	C10-C11-C12-C13
21	a	5562	PHO	C10-C11-C12-C13
30	c	5508	DGD	C4E-C5E-C6E-O5E
28	b	5530	MGE	C1B-C2B-C3B-C4B
30	C	507	DGD	C1A-C2A-C3A-C4A
30	c	5507	DGD	O6E-C1E-O5D-C6D
30	C	508	DGD	C4E-C5E-C6E-O5E
20	A	559	CLA	C15-C16-C17-C18
20	B	513	CLA	C5-C6-C7-C8
20	B	519	CLA	C15-C16-C17-C18
20	B	523	CLA	C10-C11-C12-C13
20	C	497	CLA	C15-C16-C17-C18
20	a	5558	CLA	C10-C11-C12-C13
20	a	5563	CLA	C5-C6-C7-C8
20	b	5519	CLA	C15-C16-C17-C18
20	b	5522	CLA	C10-C11-C12-C13
30	C	509	DGD	C2A-C1A-O1G-C1G
20	b	5516	CLA	CBD-CGD-O2D-CED
28	D	360	MGE	C4D-C5D-C6D-O5D
28	d	5360	MGE	C1B-C2B-C3B-C4B
20	b	5516	CLA	C13-C15-C16-C17
20	c	5500	CLA	C5-C6-C7-C8
22	a	5564	PQ9	C21-C22-C23-C24
20	A	563	CLA	O1D-CGD-O2D-CED
20	B	522	CLA	C10-C11-C12-C13
20	a	5559	CLA	C15-C16-C17-C18
20	b	5523	CLA	C10-C11-C12-C13
30	c	5507	DGD	O6E-C5E-C6E-O5E
28	D	358	MGE	C1A-C2A-C3A-C4A
28	D	359	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	C1A-C2A-C3A-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	519	CLA	O1D-CGD-O2D-CED
20	B	523	CLA	O1D-CGD-O2D-CED
20	B	519	CLA	C10-C11-C12-C13
20	B	516	CLA	CBD-CGD-O2D-CED
20	B	520	CLA	CBD-CGD-O2D-CED
28	L	210	MGE	C2B-C1B-O2G-C2G
20	B	516	CLA	C13-C15-C16-C17
20	c	5493	CLA	C5-C6-C7-C8
20	B	526	CLA	C13-C15-C16-C17
20	C	493	CLA	C10-C11-C12-C13
20	b	5516	CLA	C10-C11-C12-C13
20	b	5517	CLA	C5-C6-C7-C8
30	C	507	DGD	O6E-C5E-C6E-O5E
30	c	5507	DGD	O1B-C1B-O2G-C2G
20	C	502	CLA	C2A-CAA-CBA-CGA
20	c	5496	CLA	C2A-CAA-CBA-CGA
30	c	5509	DGD	C2A-C1A-O1G-C1G
20	C	493	CLA	C5-C6-C7-C8
20	b	5512	CLA	C15-C16-C17-C18
20	b	5515	CLA	C13-C15-C16-C17
20	b	5526	CLA	C13-C15-C16-C17
20	c	5500	CLA	C15-C16-C17-C18
20	a	5563	CLA	O1D-CGD-O2D-CED
20	B	512	CLA	C15-C16-C17-C18
20	B	522	CLA	C13-C15-C16-C17
20	b	5522	CLA	C13-C15-C16-C17
20	c	5495	CLA	C15-C16-C17-C18
20	B	515	CLA	C13-C15-C16-C17
20	B	516	CLA	C10-C11-C12-C13
20	B	517	CLA	C5-C6-C7-C8
20	B	523	CLA	C5-C6-C7-C8
20	C	495	CLA	C10-C11-C12-C13
20	C	495	CLA	C15-C16-C17-C18
20	a	5560	CLA	C10-C11-C12-C13
20	b	5519	CLA	C10-C11-C12-C13
20	b	5523	CLA	C5-C6-C7-C8
20	c	5498	CLA	C13-C15-C16-C17
20	A	560	CLA	C10-C11-C12-C13
20	B	517	CLA	C8-C10-C11-C12
20	c	5495	CLA	C10-C11-C12-C13
20	d	5355	CLA	C1-C2-C3-C5
20	c	5501	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	l	5210	MGE	C2B-C1B-O2G-C2G
30	c	5507	DGD	C2B-C1B-O2G-C2G
28	L	210	MGE	O1B-C1B-O2G-C2G
28	l	5210	MGE	O1B-C1B-O2G-C2G
30	C	507	DGD	O1B-C1B-O2G-C2G
30	c	5509	DGD	O1B-C1B-O2G-C2G
28	L	210	MGE	C2D-C1D-O3G-C3G
28	l	5210	MGE	C2D-C1D-O3G-C3G
30	C	508	DGD	C2E-C1E-O5D-C6D
30	c	5508	DGD	C2E-C1E-O5D-C6D
20	C	498	CLA	C13-C15-C16-C17
20	b	5517	CLA	C8-C10-C11-C12
30	C	509	DGD	O1A-C1A-O1G-C1G
20	B	517	CLA	C2A-CAA-CBA-CGA
20	b	5517	CLA	C2A-CAA-CBA-CGA
20	A	559	CLA	C5-C6-C7-C8
20	C	500	CLA	C15-C16-C17-C18
20	a	5559	CLA	C5-C6-C7-C8
25	A	567	LHG	O1-C1-C2-C3
30	c	5509	DGD	O1A-C1A-O1G-C1G
28	L	210	MGE	O6D-C1D-O3G-C3G
28	l	5210	MGE	O6D-C1D-O3G-C3G
30	C	507	DGD	C2B-C1B-O2G-C2G
30	c	5509	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C4D-C5D-C6D-O5D
20	b	5520	CLA	C5-C6-C7-C8
20	c	5492	CLA	C11-C12-C13-C14
20	B	520	CLA	C5-C6-C7-C8
30	h	5208	DGD	C4D-C5D-C6D-O5D
26	L	5213	SQD	C11-C12-C13-C14
28	B	530	MGE	C9A-CAA-CBA-CCA
28	D	359	MGE	C3B-C4B-C5B-C6B
28	L	210	MGE	CCB-CDB-CEB-CFB
28	i	5201	MGE	C9A-CAA-CBA-CCA
30	H	208	DGD	C5B-C6B-C7B-C8B
25	a	5567	LHG	C30-C31-C32-C33
26	t	213	SQD	C9-C10-C11-C12
28	b	5530	MGE	C9A-CAA-CBA-CCA
26	t	213	SQD	C11-C12-C13-C14
28	l	5210	MGE	C5B-C6B-C7B-C8B
30	h	5208	DGD	C5B-C6B-C7B-C8B
30	h	5208	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	5360	MGE	C3B-C4B-C5B-C6B
28	l	5210	MGE	CCB-CDB-CEB-CFB
30	H	208	DGD	C5A-C6A-C7A-C8A
30	h	5208	DGD	C5A-C6A-C7A-C8A
25	A	567	LHG	C30-C31-C32-C33
28	D	359	MGE	C8B-C9B-CAB-CBB
28	L	210	MGE	C3B-C4B-C5B-C6B
28	L	210	MGE	C5B-C6B-C7B-C8B
28	d	5360	MGE	C8B-C9B-CAB-CBB
28	l	5210	MGE	C3B-C4B-C5B-C6B
30	C	507	DGD	C9A-CAA-CBA-CCA
20	C	492	CLA	C11-C12-C13-C14
20	C	492	CLA	C11-C12-C13-C15
20	c	5492	CLA	C11-C12-C13-C15
30	C	509	DGD	C8B-C9B-CAB-CBB
26	A	568	SQD	C8-C7-O47-C45
26	d	5358	SQD	C8-C7-O47-C45
20	A	560	CLA	C11-C12-C13-C15
20	a	5560	CLA	C11-C12-C13-C15
26	d	5358	SQD	C32-C33-C34-C35
28	I	201	MGE	C9A-CAA-CBA-CCA
20	C	495	CLA	C5-C6-C7-C8
28	B	530	MGE	C3B-C4B-C5B-C6B
30	C	509	DGD	C7A-C8A-C9A-CAA
30	C	509	DGD	C9B-CAB-CBB-CCB
30	c	5507	DGD	C9A-CAA-CBA-CCA
30	c	5509	DGD	C8B-C9B-CAB-CBB
30	c	5509	DGD	C9B-CAB-CBB-CCB
20	B	512	CLA	C3A-C2A-CAA-CBA
20	B	515	CLA	C3A-C2A-CAA-CBA
20	C	494	CLA	C3A-C2A-CAA-CBA
20	C	495	CLA	C3A-C2A-CAA-CBA
20	C	496	CLA	C3A-C2A-CAA-CBA
20	D	354	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	C3A-C2A-CAA-CBA
20	c	5496	CLA	C3A-C2A-CAA-CBA
20	d	5354	CLA	C3A-C2A-CAA-CBA
20	B	522	CLA	O1D-CGD-O2D-CED
26	A	568	SQD	C32-C33-C34-C35
26	L	5213	SQD	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	L	210	MGE	C4B-C5B-C6B-C7B
30	c	5509	DGD	C7A-C8A-C9A-CAA
20	c	5495	CLA	C5-C6-C7-C8
20	b	5522	CLA	O1D-CGD-O2D-CED
28	L	210	MGE	CAB-CBB-CCB-CDB
28	b	5530	MGE	C4A-C5A-C6A-C7A
28	b	5530	MGE	C3B-C4B-C5B-C6B
28	B	530	MGE	C4A-C5A-C6A-C7A
28	D	358	MGE	C7A-C8A-C9A-CAA
28	d	5359	MGE	C7A-C8A-C9A-CAA
28	d	5361	MGE	C4B-C5B-C6B-C7B
28	D	358	MGE	C7B-C8B-C9B-CAB
28	D	360	MGE	C6B-C7B-C8B-C9B
28	l	5210	MGE	C4B-C5B-C6B-C7B
28	l	5210	MGE	C9B-CAB-CBB-CCB
20	A	560	CLA	C13-C15-C16-C17
28	D	360	MGE	C4B-C5B-C6B-C7B
28	L	210	MGE	C9B-CAB-CBB-CCB
28	d	5359	MGE	C7B-C8B-C9B-CAB
28	d	5361	MGE	C6B-C7B-C8B-C9B
30	H	208	DGD	C3B-C4B-C5B-C6B
26	L	5213	SQD	C12-C13-C14-C15
28	d	5359	MGE	C4B-C5B-C6B-C7B
28	l	5210	MGE	CAB-CBB-CCB-CDB
30	C	507	DGD	C3B-C4B-C5B-C6B
30	h	5208	DGD	C3B-C4B-C5B-C6B
20	c	5491	CLA	O1D-CGD-O2D-CED
26	t	213	SQD	C12-C13-C14-C15
28	D	358	MGE	C4B-C5B-C6B-C7B
20	C	491	CLA	O1D-CGD-O2D-CED
30	h	5208	DGD	O1A-C1A-O1G-C1G
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	B	529	BCR	C23-C24-C25-C30
24	C	506	BCR	C23-C24-C25-C30
24	D	357	BCR	C5-C6-C7-C8
24	T	5104	BCR	C23-C24-C25-C26
24	T	5104	BCR	C23-C24-C25-C30
24	X	130	BCR	C23-C24-C25-C26
24	X	130	BCR	C23-C24-C25-C30
24	a	5566	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	5566	BCR	C5-C6-C7-C8
24	a	5566	BCR	C23-C24-C25-C26
24	a	5566	BCR	C23-C24-C25-C30
24	b	5529	BCR	C23-C24-C25-C30
24	c	5504	BCR	C23-C24-C25-C30
24	c	5506	BCR	C23-C24-C25-C30
24	d	5357	BCR	C5-C6-C7-C8
24	h	5107	BCR	C1-C6-C7-C8
24	t	104	BCR	C23-C24-C25-C26
24	t	104	BCR	C23-C24-C25-C30
24	x	5130	BCR	C23-C24-C25-C26
24	x	5130	BCR	C23-C24-C25-C30
28	I	201	MGE	C9B-CAB-CBB-CCB
30	C	509	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C2A-C1A-O1G-C1G
20	B	514	CLA	C3-C5-C6-C7
20	C	498	CLA	C3-C5-C6-C7
28	D	358	MGE	C4A-C5A-C6A-C7A
28	D	358	MGE	C8B-C9B-CAB-CBB
28	d	5359	MGE	C8B-C9B-CAB-CBB
28	i	5201	MGE	C9B-CAB-CBB-CCB
26	A	568	SQD	C12-C13-C14-C15
28	B	530	MGE	CBB-CCB-CDB-CEB
30	c	5507	DGD	C4A-C5A-C6A-C7A
30	c	5507	DGD	C3B-C4B-C5B-C6B
28	b	5530	MGE	CBB-CCB-CDB-CEB
28	d	5359	MGE	C4A-C5A-C6A-C7A
30	H	208	DGD	C4B-C5B-C6B-C7B
30	h	5208	DGD	C4B-C5B-C6B-C7B
28	b	5530	MGE	C7B-C8B-C9B-CAB
28	i	5201	MGE	C3B-C4B-C5B-C6B
26	A	568	SQD	O49-C7-O47-C45
26	d	5358	SQD	O49-C7-O47-C45
30	C	509	DGD	O1B-C1B-O2G-C2G
20	B	523	CLA	C4-C3-C5-C6
28	B	530	MGE	C7B-C8B-C9B-CAB
30	H	208	DGD	CBA-CCA-CDA-CEA
28	I	201	MGE	C3B-C4B-C5B-C6B
28	d	5359	MGE	C5A-C6A-C7A-C8A
30	C	507	DGD	C4A-C5A-C6A-C7A
20	A	559	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	a	5559	CLA	C6-C7-C8-C9
21	a	5561	PHO	C11-C10-C8-C9
26	d	5358	SQD	C12-C13-C14-C15
30	h	5208	DGD	CBA-CCA-CDA-CEA
20	D	354	CLA	C13-C15-C16-C17
28	D	358	MGE	C5A-C6A-C7A-C8A
28	i	5201	MGE	C7A-C8A-C9A-CAA
28	I	201	MGE	C2A-C3A-C4A-C5A
30	C	509	DGD	CBB-CCB-CDB-CEB
28	l	5210	MGE	C6B-C7B-C8B-C9B
30	c	5509	DGD	CBB-CCB-CDB-CEB
20	b	5514	CLA	C3-C5-C6-C7
20	c	5498	CLA	C3-C5-C6-C7
25	A	567	LHG	C8-C7-O7-C5
25	a	5567	LHG	C8-C7-O7-C5
26	L	5213	SQD	C8-C7-O47-C45
26	t	213	SQD	C8-C7-O47-C45
30	h	5208	DGD	C2B-C1B-O2G-C2G
20	a	5560	CLA	C13-C15-C16-C17
20	b	5516	CLA	C5-C6-C7-C8
21	A	561	PHO	C8-C10-C11-C12
25	A	567	LHG	O9-C7-O7-C5
28	I	201	MGE	C3A-C4A-C5A-C6A
28	l	5210	MGE	C7A-C8A-C9A-CAA
20	b	5520	CLA	CBD-CGD-O2D-CED
20	B	516	CLA	C5-C6-C7-C8
20	b	5526	CLA	C15-C16-C17-C18
28	L	210	MGE	C7A-C8A-C9A-CAA
30	C	508	DGD	C5D-C6D-O5D-C1E
30	c	5508	DGD	C5D-C6D-O5D-C1E
28	i	5201	MGE	C2A-C3A-C4A-C5A
21	A	561	PHO	C16-C17-C18-C20
21	a	5561	PHO	C16-C17-C18-C20
20	B	518	CLA	CBD-CGD-O2D-CED
28	I	201	MGE	C7A-C8A-C9A-CAA
28	L	210	MGE	C6B-C7B-C8B-C9B
20	b	5523	CLA	C4-C3-C5-C6
20	B	526	CLA	C15-C16-C17-C18
20	C	497	CLA	C5-C6-C7-C8
20	c	5495	CLA	C13-C15-C16-C17
20	d	5354	CLA	C13-C15-C16-C17
21	a	5561	PHO	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	i	5201	MGE	C3A-C4A-C5A-C6A
28	d	5361	MGE	C1B-C2B-C3B-C4B
30	h	5208	DGD	C1B-C2B-C3B-C4B
30	C	509	DGD	C2A-C3A-C4A-C5A
30	c	5509	DGD	CCB-CDB-CEB-CFB
20	C	495	CLA	C13-C15-C16-C17
32	V	552	HEM	C4B-C3B-CAB-CBB
32	v	5552	HEM	C4B-C3B-CAB-CBB
30	H	208	DGD	O1A-C1A-O1G-C1G
20	C	501	CLA	O1D-CGD-O2D-CED
30	H	208	DGD	C1B-C2B-C3B-C4B
28	D	360	MGE	O2G-C2G-C3G-O3G
28	d	5361	MGE	O2G-C2G-C3G-O3G
28	D	360	MGE	C7A-C8A-C9A-CAA
30	C	509	DGD	CCB-CDB-CEB-CFB
26	d	5358	SQD	C25-C26-C27-C28
28	D	360	MGE	C5B-C6B-C7B-C8B
28	d	5361	MGE	C8B-C9B-CAB-CBB
30	c	5509	DGD	C2A-C3A-C4A-C5A
28	D	359	MGE	CAB-CBB-CCB-CDB
28	B	530	MGE	C8B-C9B-CAB-CBB
28	d	5361	MGE	C5B-C6B-C7B-C8B
30	C	508	DGD	C5A-C6A-C7A-C8A
26	A	568	SQD	C25-C26-C27-C28
28	d	5360	MGE	CBB-CCB-CDB-CEB
28	d	5361	MGE	C7A-C8A-C9A-CAA
30	H	208	DGD	O1B-C1B-O2G-C2G
30	h	5208	DGD	O1B-C1B-O2G-C2G
20	C	503	CLA	C2A-CAA-CBA-CGA
25	A	567	LHG	C28-C29-C30-C31
28	D	359	MGE	CBB-CCB-CDB-CEB
28	D	360	MGE	C7B-C8B-C9B-CAB
21	a	5561	PHO	C16-C17-C18-C19
28	D	360	MGE	C8B-C9B-CAB-CBB
20	B	515	CLA	C1A-C2A-CAA-CBA
20	C	491	CLA	C1A-C2A-CAA-CBA
20	D	354	CLA	C1A-C2A-CAA-CBA
20	b	5515	CLA	C1A-C2A-CAA-CBA
20	d	5354	CLA	C1A-C2A-CAA-CBA
20	c	5497	CLA	C5-C6-C7-C8
28	d	5360	MGE	CAB-CBB-CCB-CDB
20	d	5355	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	568	SQD	C17-C18-C19-C20
28	d	5361	MGE	C7B-C8B-C9B-CAB
30	c	5508	DGD	C5A-C6A-C7A-C8A
21	a	5561	PHO	C5-C6-C7-C8
25	a	5567	LHG	O9-C7-O7-C5
26	L	5213	SQD	O49-C7-O47-C45
20	A	558	CLA	C11-C10-C8-C7
20	A	558	CLA	C12-C13-C15-C16
20	A	559	CLA	C12-C13-C15-C16
20	B	514	CLA	C11-C10-C8-C7
20	B	522	CLA	C11-C10-C8-C7
20	B	525	CLA	C11-C10-C8-C7
20	C	493	CLA	C11-C12-C13-C15
20	C	495	CLA	C11-C10-C8-C7
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	a	5558	CLA	C11-C10-C8-C7
20	a	5558	CLA	C12-C13-C15-C16
20	a	5559	CLA	C12-C13-C15-C16
20	b	5514	CLA	C11-C10-C8-C7
20	b	5522	CLA	C11-C10-C8-C7
20	b	5525	CLA	C11-C10-C8-C7
20	c	5493	CLA	C11-C12-C13-C15
20	c	5495	CLA	C11-C10-C8-C7
20	c	5496	CLA	C11-C10-C8-C7
20	c	5496	CLA	C12-C13-C15-C16
20	c	5500	CLA	C11-C10-C8-C7
20	c	5501	CLA	C11-C10-C8-C7
21	A	562	PHO	C11-C10-C8-C7
21	A	561	PHO	C16-C17-C18-C19
20	b	5515	CLA	C15-C16-C17-C18
21	A	562	PHO	C15-C16-C17-C18
25	a	5567	LHG	C28-C29-C30-C31
20	A	558	CLA	C2A-CAA-CBA-CGA
20	a	5558	CLA	C2A-CAA-CBA-CGA
20	B	513	CLA	C14-C13-C15-C16
20	B	514	CLA	C11-C10-C8-C9
20	B	525	CLA	C6-C7-C8-C9
20	B	525	CLA	C11-C10-C8-C9
20	C	493	CLA	C6-C7-C8-C9
20	C	493	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	500	CLA	C11-C10-C8-C9
20	C	501	CLA	C11-C10-C8-C9
20	a	5559	CLA	C14-C13-C15-C16
20	b	5513	CLA	C14-C13-C15-C16
20	b	5514	CLA	C11-C10-C8-C9
20	b	5519	CLA	C14-C13-C15-C16
20	b	5520	CLA	C6-C7-C8-C9
20	b	5525	CLA	C6-C7-C8-C9
20	b	5525	CLA	C11-C10-C8-C9
20	c	5493	CLA	C11-C12-C13-C14
20	c	5500	CLA	C11-C10-C8-C9
21	A	562	PHO	C11-C10-C8-C9
21	a	5562	PHO	C11-C10-C8-C9
28	D	359	MGE	C9B-CAB-CBB-CCB
28	i	5201	MGE	C4A-C5A-C6A-C7A
21	A	561	PHO	C5-C6-C7-C8
20	b	5521	CLA	C15-C16-C17-C18
20	b	5518	CLA	O1D-CGD-O2D-CED
28	D	359	MGE	C1G-C2G-C3G-O3G
28	d	5360	MGE	C1G-C2G-C3G-O3G
26	L	5213	SQD	C25-C26-C27-C28
20	B	515	CLA	C15-C16-C17-C18
20	C	491	CLA	C13-C15-C16-C17
28	b	5530	MGE	C8B-C9B-CAB-CBB
30	C	509	DGD	C7B-C8B-C9B-CAB
30	h	5208	DGD	C7A-C8A-C9A-CAA
26	d	5358	SQD	C17-C18-C19-C20
20	D	355	CLA	C2C-C3C-CAC-CBC
27	A	569	LMT	C3-C4-C5-C6
30	H	208	DGD	CAA-CBA-CCA-CDA
30	c	5509	DGD	C7B-C8B-C9B-CAB
28	I	201	MGE	C4A-C5A-C6A-C7A
30	H	208	DGD	C7A-C8A-C9A-CAA
28	D	358	MGE	O6D-C5D-C6D-O5D
30	c	5508	DGD	C4A-C5A-C6A-C7A
28	d	5359	MGE	O6D-C5D-C6D-O5D
26	t	213	SQD	C25-C26-C27-C28
26	L	5213	SQD	C17-C18-C19-C20
30	C	508	DGD	C4A-C5A-C6A-C7A
25	A	567	LHG	C26-C27-C28-C29
28	B	530	MGE	C5A-C6A-C7A-C8A
28	i	5201	MGE	C6A-C7A-C8A-C9A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	5360	MGE	C9B-CAB-CBB-CCB
30	h	5208	DGD	CAA-CBA-CCA-CDA
30	C	507	DGD	CBA-CCA-CDA-CEA
28	l	5210	MGE	CDB-CEB-CFB-CGB
28	b	5530	MGE	C5A-C6A-C7A-C8A
28	L	210	MGE	CDB-CEB-CFB-CGB
27	a	5568	LMT	C3-C4-C5-C6
28	d	5361	MGE	C2A-C3A-C4A-C5A
25	a	5567	LHG	C35-C36-C37-C38
28	I	201	MGE	C6A-C7A-C8A-C9A
28	l	5210	MGE	CBB-CCB-CDB-CEB
25	A	567	LHG	C35-C36-C37-C38
30	c	5507	DGD	CBA-CCA-CDA-CEA
26	t	213	SQD	O49-C7-O47-C45
25	a	5567	LHG	C26-C27-C28-C29
30	c	5509	DGD	CDB-CEB-CFB-CGB
25	a	5567	LHG	C27-C28-C29-C30
26	t	213	SQD	C17-C18-C19-C20
28	d	5361	MGE	C5A-C6A-C7A-C8A
26	A	568	SQD	C27-C28-C29-C30
28	D	360	MGE	C5A-C6A-C7A-C8A
20	B	521	CLA	C15-C16-C17-C18
20	b	5522	CLA	C5-C6-C7-C8
20	c	5491	CLA	C13-C15-C16-C17
20	B	520	CLA	O1D-CGD-O2D-CED
20	A	563	CLA	C4-C3-C5-C6
20	b	5513	CLA	C4-C3-C5-C6
30	C	509	DGD	CDB-CEB-CFB-CGB
28	D	360	MGE	C1B-C2B-C3B-C4B
26	d	5358	SQD	C28-C29-C30-C31
26	d	5358	SQD	C27-C28-C29-C30
20	A	558	CLA	C11-C10-C8-C9
20	A	559	CLA	C14-C13-C15-C16
20	B	512	CLA	C11-C10-C8-C9
20	B	515	CLA	C14-C13-C15-C16
20	B	519	CLA	C14-C13-C15-C16
20	B	520	CLA	C6-C7-C8-C9
20	B	522	CLA	C11-C10-C8-C9
20	C	495	CLA	C11-C10-C8-C9
20	C	496	CLA	C11-C10-C8-C9
20	C	496	CLA	C14-C13-C15-C16
20	D	354	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	a	5558	CLA	C11-C10-C8-C9
20	b	5512	CLA	C11-C10-C8-C9
20	b	5515	CLA	C14-C13-C15-C16
20	b	5522	CLA	C11-C10-C8-C9
20	b	5524	CLA	C6-C7-C8-C9
20	c	5493	CLA	C6-C7-C8-C9
20	c	5495	CLA	C11-C10-C8-C9
20	c	5496	CLA	C11-C10-C8-C9
20	c	5496	CLA	C14-C13-C15-C16
20	c	5501	CLA	C11-C10-C8-C9
20	d	5354	CLA	C14-C13-C15-C16
21	A	561	PHO	C6-C7-C8-C9
21	A	561	PHO	C11-C10-C8-C9
21	a	5561	PHO	C6-C7-C8-C9
20	c	5501	CLA	O1D-CGD-O2D-CED
20	B	525	CLA	C5-C6-C7-C8
21	a	5562	PHO	C15-C16-C17-C18
20	b	5516	CLA	C2A-CAA-CBA-CGA
20	A	560	CLA	C11-C10-C8-C7
20	B	512	CLA	C11-C10-C8-C7
20	B	513	CLA	C11-C10-C8-C7
20	B	513	CLA	C12-C13-C15-C16
20	B	518	CLA	C6-C7-C8-C10
20	B	519	CLA	C12-C13-C15-C16
20	B	524	CLA	C6-C7-C8-C10
20	B	525	CLA	C6-C7-C8-C10
20	C	493	CLA	C6-C7-C8-C10
20	C	501	CLA	C11-C10-C8-C7
20	D	354	CLA	C12-C13-C15-C16
20	a	5559	CLA	C11-C10-C8-C7
20	a	5560	CLA	C11-C10-C8-C7
20	b	5512	CLA	C11-C10-C8-C7
20	b	5513	CLA	C12-C13-C15-C16
20	b	5518	CLA	C6-C7-C8-C10
20	b	5524	CLA	C6-C7-C8-C10
20	b	5525	CLA	C6-C7-C8-C10
20	c	5493	CLA	C6-C7-C8-C10
20	c	5501	CLA	C6-C7-C8-C10
20	d	5354	CLA	C12-C13-C15-C16
21	A	561	PHO	C6-C7-C8-C10
21	a	5561	PHO	C6-C7-C8-C10
21	a	5562	PHO	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	522	CLA	C8-C10-C11-C12
20	b	5518	CLA	C5-C6-C7-C8
20	b	5521	CLA	C8-C10-C11-C12
20	c	5501	CLA	C10-C11-C12-C13
30	H	208	DGD	CCA-CDA-CEA-CFA
30	c	5509	DGD	C4A-C5A-C6A-C7A
20	B	519	CLA	C4-C3-C5-C6
20	B	526	CLA	C3A-C2A-CAA-CBA
20	a	5563	CLA	C4-C3-C5-C6
20	b	5512	CLA	C3A-C2A-CAA-CBA
20	b	5519	CLA	C4-C3-C5-C6
20	b	5526	CLA	C3A-C2A-CAA-CBA
20	B	522	CLA	C5-C6-C7-C8
20	b	5525	CLA	C5-C6-C7-C8
30	C	509	DGD	C4A-C5A-C6A-C7A
30	h	5208	DGD	CCA-CDA-CEA-CFA
20	C	501	CLA	C5-C6-C7-C8
28	L	210	MGE	CBB-CCB-CDB-CEB
26	A	568	SQD	O6-C44-C45-C46
26	A	5212	SQD	O6-C44-C45-C46
26	L	5213	SQD	C44-C45-C46-O48
26	a	212	SQD	O6-C44-C45-C46
26	d	5358	SQD	O6-C44-C45-C46
26	t	213	SQD	C44-C45-C46-O48
28	D	360	MGE	C1G-C2G-C3G-O3G
28	d	5361	MGE	C1G-C2G-C3G-O3G
28	d	5360	MGE	C6B-C7B-C8B-C9B
20	b	5522	CLA	C8-C10-C11-C12
20	B	515	CLA	C1-C2-C3-C4
20	B	518	CLA	C1-C2-C3-C4
20	B	522	CLA	C1-C2-C3-C4
20	B	525	CLA	C1-C2-C3-C4
20	B	526	CLA	C1-C2-C3-C4
20	C	492	CLA	C1-C2-C3-C4
20	C	495	CLA	C1-C2-C3-C4
20	C	500	CLA	C1-C2-C3-C4
20	C	501	CLA	C1-C2-C3-C4
20	b	5515	CLA	C1-C2-C3-C4
20	b	5517	CLA	C1-C2-C3-C4
20	b	5518	CLA	C1-C2-C3-C4
20	b	5522	CLA	C1-C2-C3-C4
20	b	5523	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	b	5525	CLA	C1-C2-C3-C4
20	b	5526	CLA	C1-C2-C3-C4
20	c	5492	CLA	C1-C2-C3-C4
20	c	5495	CLA	C1-C2-C3-C4
20	c	5500	CLA	C1-C2-C3-C4
20	c	5501	CLA	C1-C2-C3-C4
20	B	513	CLA	C4-C3-C5-C6
26	A	568	SQD	C10-C11-C12-C13
20	a	5563	CLA	C2-C3-C5-C6
20	b	5519	CLA	C2-C3-C5-C6
20	B	518	CLA	C5-C6-C7-C8
21	A	561	PHO	C15-C16-C17-C18
25	A	567	LHG	C27-C28-C29-C30
30	c	5509	DGD	C4E-C5E-C6E-O5E
24	C	504	BCR	C23-C24-C25-C30
24	C	505	BCR	C1-C6-C7-C8
24	H	107	BCR	C1-C6-C7-C8
24	H	107	BCR	C23-C24-C25-C30
24	X	130	BCR	C5-C6-C7-C8
24	c	5505	BCR	C1-C6-C7-C8
24	d	5357	BCR	C1-C6-C7-C8
24	h	5107	BCR	C23-C24-C25-C30
24	x	5130	BCR	C5-C6-C7-C8
20	c	5501	CLA	C5-C6-C7-C8
20	b	5524	CLA	C11-C10-C8-C9
26	d	5358	SQD	C10-C11-C12-C13
20	b	5515	CLA	C2A-CAA-CBA-CGA
20	b	5514	CLA	C13-C15-C16-C17
26	A	568	SQD	O6-C44-C45-O47
26	d	5358	SQD	O6-C44-C45-O47
28	D	359	MGE	O2G-C2G-C3G-O3G
28	d	5360	MGE	O2G-C2G-C3G-O3G
28	d	5359	MGE	C2A-C3A-C4A-C5A
28	d	5361	MGE	C4A-C5A-C6A-C7A
20	b	5516	CLA	O1D-CGD-O2D-CED
28	i	5201	MGE	C6B-C7B-C8B-C9B
20	B	514	CLA	C13-C15-C16-C17
21	a	5561	PHO	C15-C16-C17-C18
20	A	563	CLA	C2-C3-C5-C6
20	B	519	CLA	C2-C3-C5-C6
30	C	508	DGD	C7A-C8A-C9A-CAA
20	A	559	CLA	C1-C2-C3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	515	CLA	C1-C2-C3-C5
20	B	517	CLA	C1-C2-C3-C5
20	B	519	CLA	C1-C2-C3-C5
20	B	520	CLA	C1-C2-C3-C5
20	B	523	CLA	C1-C2-C3-C5
20	B	526	CLA	C1-C2-C3-C5
20	C	498	CLA	C1-C2-C3-C5
20	a	5559	CLA	C1-C2-C3-C5
20	b	5515	CLA	C1-C2-C3-C5
20	b	5517	CLA	C1-C2-C3-C5
20	b	5519	CLA	C1-C2-C3-C5
20	b	5520	CLA	C1-C2-C3-C5
20	b	5523	CLA	C1-C2-C3-C5
20	b	5526	CLA	C1-C2-C3-C5
20	c	5497	CLA	C1-C2-C3-C5
20	c	5498	CLA	C1-C2-C3-C5
21	A	561	PHO	C1-C2-C3-C5
21	a	5561	PHO	C1-C2-C3-C5
20	A	560	CLA	C11-C10-C8-C9
20	B	516	CLA	C11-C12-C13-C14
20	a	5560	CLA	C11-C10-C8-C9
20	b	5516	CLA	C11-C12-C13-C14
30	H	208	DGD	C2A-C3A-C4A-C5A
28	B	530	MGE	C2A-C3A-C4A-C5A
30	h	5208	DGD	C2A-C3A-C4A-C5A
28	I	201	MGE	C6B-C7B-C8B-C9B
28	D	360	MGE	C9A-CAA-CBA-CCA
20	B	516	CLA	O1D-CGD-O2D-CED
20	C	492	CLA	CBD-CGD-O2D-CED
20	B	521	CLA	C8-C10-C11-C12
28	l	5210	MGE	C2A-C3A-C4A-C5A
20	C	496	CLA	C5-C6-C7-C8
28	D	358	MGE	C2A-C3A-C4A-C5A
20	b	5520	CLA	O1D-CGD-O2D-CED
30	c	5507	DGD	C5A-C6A-C7A-C8A
30	c	5508	DGD	C8A-C9A-CAA-CBA
20	B	516	CLA	C11-C12-C13-C15
20	C	498	CLA	C11-C10-C8-C7
20	C	501	CLA	C6-C7-C8-C10
20	b	5513	CLA	C11-C10-C8-C7
20	b	5516	CLA	C11-C12-C13-C15
20	b	5519	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	514	CLA	C15-C16-C17-C18
20	b	5514	CLA	C15-C16-C17-C18
20	c	5496	CLA	C5-C6-C7-C8
30	C	507	DGD	C5A-C6A-C7A-C8A
30	c	5508	DGD	C7A-C8A-C9A-CAA
28	D	359	MGE	CDB-CEB-CFB-CGB
26	L	5213	SQD	C5-C6-S-O8
26	t	213	SQD	C5-C6-S-O8
30	C	507	DGD	C5D-C6D-O5D-C1E
30	c	5507	DGD	C5D-C6D-O5D-C1E
28	D	360	MGE	C2A-C3A-C4A-C5A
20	c	5503	CLA	C2A-CAA-CBA-CGA
20	B	524	CLA	C11-C10-C8-C9
28	L	210	MGE	C2A-C3A-C4A-C5A
28	L	210	MGE	C4A-C5A-C6A-C7A
20	B	521	CLA	C4-C3-C5-C6
28	i	5201	MGE	CDB-CEB-CFB-CGB
20	B	521	CLA	CBD-CGD-O2D-CED
28	d	5360	MGE	CDB-CEB-CFB-CGB
20	c	5492	CLA	CBD-CGD-O2D-CED
28	d	5361	MGE	C9A-CAA-CBA-CCA
25	a	5567	LHG	C9-C10-C11-C12
28	D	359	MGE	C6B-C7B-C8B-C9B
30	C	509	DGD	C4E-C5E-C6E-O5E
28	i	5201	MGE	C5A-C6A-C7A-C8A
28	l	5210	MGE	C4A-C5A-C6A-C7A
26	d	5358	SQD	C9-C10-C11-C12
20	b	5521	CLA	C4-C3-C5-C6
20	c	5491	CLA	C2A-CAA-CBA-CGA
20	B	523	CLA	C2-C3-C5-C6
20	B	514	CLA	C5-C6-C7-C8
20	b	5525	CLA	C10-C11-C12-C13
28	d	5360	MGE	C7B-C8B-C9B-CAB
26	L	5213	SQD	O47-C45-C46-O48
26	t	213	SQD	O47-C45-C46-O48
28	i	5201	MGE	O1G-C1G-C2G-O2G
20	B	512	CLA	C10-C11-C12-C13
20	B	524	CLA	C6-C7-C8-C9
26	A	568	SQD	C9-C10-C11-C12
30	c	5507	DGD	C5B-C6B-C7B-C8B
30	c	5509	DGD	C6B-C7B-C8B-C9B
20	B	517	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	509	DGD	C6B-C7B-C8B-C9B
26	d	5358	SQD	C24-C25-C26-C27
20	d	5355	CLA	C4C-C3C-CAC-CBC
28	D	359	MGE	C7B-C8B-C9B-CAB
30	C	508	DGD	C8A-C9A-CAA-CBA
25	A	567	LHG	C9-C10-C11-C12
20	C	501	CLA	C10-C11-C12-C13
28	b	5530	MGE	C5B-C6B-C7B-C8B
25	a	5567	LHG	C23-C24-C25-C26
20	b	5514	CLA	C5-C6-C7-C8
20	D	355	CLA	C4C-C3C-CAC-CBC
26	A	568	SQD	C24-C25-C26-C27
20	a	5559	CLA	C1A-C2A-CAA-CBA
30	c	5509	DGD	C4B-C5B-C6B-C7B
28	I	201	MGE	CDB-CEB-CFB-CGB
24	C	506	BCR	C6-C7-C8-C9
30	C	507	DGD	C5B-C6B-C7B-C8B
20	A	559	CLA	C11-C10-C8-C7
20	B	518	CLA	C11-C10-C8-C7
20	B	520	CLA	C11-C10-C8-C7
20	B	526	CLA	C11-C12-C13-C15
20	C	492	CLA	C11-C10-C8-C7
20	b	5518	CLA	C11-C10-C8-C7
20	b	5526	CLA	C11-C12-C13-C15
20	c	5498	CLA	C11-C10-C8-C7
28	D	360	MGE	C4A-C5A-C6A-C7A
28	I	201	MGE	C5A-C6A-C7A-C8A
28	b	5530	MGE	C2A-C3A-C4A-C5A
25	A	567	LHG	C23-C24-C25-C26
28	B	530	MGE	C9B-CAB-CBB-CCB
28	I	201	MGE	O1G-C1G-C2G-O2G
30	c	5508	DGD	C9A-CAA-CBA-CCA
20	b	5512	CLA	C10-C11-C12-C13
20	C	496	CLA	C13-C15-C16-C17
20	B	521	CLA	C2-C3-C5-C6
30	C	508	DGD	C9A-CAA-CBA-CCA
26	L	5213	SQD	C19-C20-C21-C22
20	C	499	CLA	CAD-CBD-CGD-O2D
20	C	500	CLA	CAD-CBD-CGD-O2D
20	c	5499	CLA	CAD-CBD-CGD-O2D
20	c	5500	CLA	CAD-CBD-CGD-O2D
20	C	492	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	516	CLA	C2A-CAA-CBA-CGA
26	t	213	SQD	C19-C20-C21-C22
20	B	525	CLA	C10-C11-C12-C13
30	c	5509	DGD	CAB-CBB-CCB-CDB
20	C	499	CLA	CAD-CBD-CGD-O1D
20	C	500	CLA	CAD-CBD-CGD-O1D
20	c	5499	CLA	CAD-CBD-CGD-O1D
20	c	5500	CLA	CAD-CBD-CGD-O1D
20	a	5559	CLA	C3-C5-C6-C7
24	D	357	BCR	C1-C6-C7-C8
28	B	530	MGE	C5B-C6B-C7B-C8B
30	C	509	DGD	CAB-CBB-CCB-CDB
26	A	568	SQD	C28-C29-C30-C31
30	C	509	DGD	C4B-C5B-C6B-C7B
28	B	530	MGE	C6B-C7B-C8B-C9B
20	A	559	CLA	C3-C5-C6-C7
22	A	564	PQ9	C12-C11-C2-C1
22	a	5564	PQ9	C12-C11-C2-C1
20	c	5496	CLA	C13-C15-C16-C17
25	A	567	LHG	C25-C26-C27-C28
25	A	567	LHG	C6-C5-O7-C7
25	a	5567	LHG	C6-C5-O7-C7
20	B	513	CLA	C2-C3-C5-C6
20	b	5521	CLA	C2-C3-C5-C6
28	L	210	MGE	C3A-C4A-C5A-C6A
28	b	5530	MGE	C9B-CAB-CBB-CCB
28	d	5359	MGE	CAB-CBB-CCB-CDB
20	B	518	CLA	O1D-CGD-O2D-CED
20	b	5515	CLA	C11-C10-C8-C9
20	B	521	CLA	O1D-CGD-O2D-CED
20	B	514	CLA	C6-C7-C8-C10
20	b	5520	CLA	C11-C10-C8-C7
20	b	5523	CLA	C12-C13-C15-C16
20	b	5513	CLA	C2-C3-C5-C6
27	m	216	LMT	C1-C2-C3-C4
30	h	5208	DGD	O2G-C2G-C3G-O3G
28	L	210	MGE	C9A-CAA-CBA-CCA
20	B	515	CLA	C2A-CAA-CBA-CGA
28	B	530	MGE	CAB-CBB-CCB-CDB
25	a	5567	LHG	C25-C26-C27-C28
28	i	5201	MGE	C2G-C3G-O3G-C1D
20	B	519	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	491	CLA	C2A-CAA-CBA-CGA
21	a	5561	PHO	C2A-CAA-CBA-CGA
28	l	5210	MGE	C9A-CAA-CBA-CCA
26	d	5358	SQD	C19-C20-C21-C22
20	B	513	CLA	C11-C10-C8-C9
20	B	515	CLA	C11-C10-C8-C9
20	B	526	CLA	C11-C12-C13-C14
20	a	5559	CLA	C11-C10-C8-C9
20	b	5513	CLA	C11-C10-C8-C9
28	i	5201	MGE	CBB-CCB-CDB-CEB
30	C	509	DGD	C1B-C2B-C3B-C4B
28	B	530	MGE	CAA-CBA-CCA-CDA
28	D	360	MGE	CDB-CEB-CFB-CGB
20	B	515	CLA	C11-C10-C8-C7
20	b	5518	CLA	C12-C13-C15-C16
20	b	5522	CLA	C6-C7-C8-C10
26	L	5213	SQD	C27-C28-C29-C30
20	b	5517	CLA	C13-C15-C16-C17
20	C	502	CLA	C3A-C2A-CAA-CBA
20	C	503	CLA	C3A-C2A-CAA-CBA
27	M	5216	LMT	C1-C2-C3-C4
20	B	514	CLA	C10-C11-C12-C13
20	b	5525	CLA	C13-C15-C16-C17
20	c	5492	CLA	O1D-CGD-O2D-CED
20	B	516	CLA	C15-C16-C17-C18
20	a	5559	CLA	C2-C1-O2A-CGA
20	b	5514	CLA	C10-C11-C12-C13
28	b	5530	MGE	CAB-CBB-CCB-CDB
26	t	213	SQD	C24-C25-C26-C27
22	d	5356	PQ9	C19-C18-C20-C21
26	L	5213	SQD	C24-C25-C26-C27
20	b	5521	CLA	CBD-CGD-O2D-CED
20	b	5526	CLA	C11-C12-C13-C14
28	b	5530	MGE	C6B-C7B-C8B-C9B
20	B	525	CLA	C13-C15-C16-C17
25	A	567	LHG	C4-C5-O7-C7
25	a	5567	LHG	C4-C5-O7-C7
20	A	559	CLA	C1-C2-C3-C4
20	B	517	CLA	C1-C2-C3-C4
20	B	519	CLA	C1-C2-C3-C4
20	B	520	CLA	C1-C2-C3-C4
20	B	523	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	498	CLA	C1-C2-C3-C4
20	a	5559	CLA	C1-C2-C3-C4
20	b	5519	CLA	C1-C2-C3-C4
20	c	5498	CLA	C1-C2-C3-C4
21	A	561	PHO	C1-C2-C3-C4
21	a	5561	PHO	C1-C2-C3-C4
20	b	5523	CLA	C2-C3-C5-C6
20	C	498	CLA	C15-C16-C17-C18
20	c	5498	CLA	C15-C16-C17-C18
26	A	568	SQD	C19-C20-C21-C22
20	b	5512	CLA	C2A-CAA-CBA-CGA
20	A	559	CLA	C1A-C2A-CAA-CBA
20	A	560	CLA	C1A-C2A-CAA-CBA
20	B	512	CLA	C1A-C2A-CAA-CBA
20	b	5512	CLA	C1A-C2A-CAA-CBA
24	C	504	BCR	C23-C24-C25-C26
24	H	107	BCR	C5-C6-C7-C8
24	H	107	BCR	C23-C24-C25-C26
24	c	5504	BCR	C23-C24-C25-C26
24	h	5107	BCR	C5-C6-C7-C8
24	h	5107	BCR	C23-C24-C25-C26
30	c	5509	DGD	C1B-C2B-C3B-C4B
20	c	5500	CLA	C4-C3-C5-C6
22	D	356	PQ9	C19-C18-C20-C21
22	d	5356	PQ9	C17-C18-C20-C21
20	B	522	CLA	C6-C7-C8-C10
20	B	523	CLA	C12-C13-C15-C16
20	b	5514	CLA	C6-C7-C8-C10
20	b	5515	CLA	C11-C10-C8-C7
20	c	5492	CLA	C11-C10-C8-C7
20	B	512	CLA	C2A-CAA-CBA-CGA
27	M	5216	LMT	O1'-C1-C2-C3
30	H	208	DGD	O2G-C2G-C3G-O3G
27	T	217	LMT	C4-C5-C6-C7
30	h	5208	DGD	C6B-C7B-C8B-C9B
28	l	5210	MGE	C3A-C4A-C5A-C6A
26	t	213	SQD	C27-C28-C29-C30
20	B	524	CLA	C11-C10-C8-C7
20	C	498	CLA	C4-C3-C5-C6
20	c	5498	CLA	C2-C3-C5-C6
22	D	356	PQ9	C17-C18-C20-C21
30	C	508	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	522	CLA	C1-C2-C3-C5
20	b	5522	CLA	C1-C2-C3-C5
28	I	201	MGE	CBB-CCB-CDB-CEB
30	c	5509	DGD	C3A-C4A-C5A-C6A
20	C	498	CLA	C8-C10-C11-C12
28	D	358	MGE	CAB-CBB-CCB-CDB
20	c	5498	CLA	C10-C11-C12-C13
24	T	5104	BCR	C22-C23-C24-C25
24	c	5506	BCR	C6-C7-C8-C9
20	c	5498	CLA	C4-C3-C5-C6
20	C	492	CLA	C10-C11-C12-C13
20	b	5519	CLA	C5-C6-C7-C8
28	D	360	MGE	O1G-C1G-C2G-C3G
28	d	5361	MGE	O1G-C1G-C2G-C3G
20	c	5498	CLA	C8-C10-C11-C12
32	V	552	HEM	CAD-CBD-CGD-O2D
25	A	567	LHG	O1-C1-C2-O2
20	C	500	CLA	C4-C3-C5-C6
32	v	5552	HEM	CAD-CBD-CGD-O2D
28	d	5361	MGE	CDB-CEB-CFB-CGB
30	C	509	DGD	C3A-C4A-C5A-C6A
28	B	530	MGE	C1A-C2A-C3A-C4A
20	b	5520	CLA	C13-C15-C16-C17
20	C	498	CLA	C2-C3-C5-C6
20	B	520	CLA	C13-C15-C16-C17
20	C	498	CLA	C10-C11-C12-C13
20	A	559	CLA	C11-C10-C8-C9
20	a	5560	CLA	C11-C12-C13-C14
26	a	212	SQD	C5-C6-S-O8
28	D	359	MGE	C2G-C3G-O3G-C1D
28	I	201	MGE	C2G-C3G-O3G-C1D
28	d	5360	MGE	C2G-C3G-O3G-C1D
20	A	559	CLA	C2-C1-O2A-CGA
20	B	517	CLA	C2-C1-O2A-CGA
20	b	5517	CLA	C2-C1-O2A-CGA
30	H	208	DGD	C6B-C7B-C8B-C9B
20	c	5502	CLA	C3A-C2A-CAA-CBA
20	c	5503	CLA	C3A-C2A-CAA-CBA
20	C	497	CLA	O2A-C1-C2-C3
20	c	5497	CLA	O2A-C1-C2-C3
32	v	5552	HEM	CAD-CBD-CGD-O1D
21	A	561	PHO	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	V	552	HEM	CAD-CBD-CGD-O1D
20	b	5521	CLA	O1D-CGD-O2D-CED
27	m	216	LMT	O1'-C1-C2-C3
24	t	104	BCR	C22-C23-C24-C25
30	c	5508	DGD	C2A-C1A-O1G-C1G
26	t	213	SQD	O6-C44-C45-C46
28	b	5530	MGE	CAA-CBA-CCA-CDA
20	a	5560	CLA	CBD-CGD-O2D-CED
30	c	5508	DGD	O1A-C1A-O1G-C1G
20	c	5497	CLA	CAA-CBA-CGA-O2A
28	L	210	MGE	O2G-C1B-C2B-C3B
28	d	5361	MGE	O2G-C1B-C2B-C3B
20	A	560	CLA	C11-C12-C13-C14
20	B	520	CLA	C11-C10-C8-C9
20	C	498	CLA	C11-C10-C8-C9
20	b	5520	CLA	C11-C10-C8-C9
20	b	5523	CLA	C14-C13-C15-C16
20	c	5498	CLA	C11-C10-C8-C9
28	l	5210	MGE	O2G-C1B-C2B-C3B
27	a	5568	LMT	C1-C2-C3-C4
30	H	208	DGD	C9A-CAA-CBA-CCA
21	A	561	PHO	C2C-C3C-CAC-CBC
21	a	5561	PHO	C2C-C3C-CAC-CBC
26	A	568	SQD	O47-C7-C8-C9
26	d	5358	SQD	O47-C7-C8-C9
28	D	360	MGE	O2G-C1B-C2B-C3B
20	B	518	CLA	C12-C13-C15-C16
20	C	501	CLA	C12-C13-C15-C16
20	b	5523	CLA	C11-C12-C13-C15
20	B	512	CLA	C5-C6-C7-C8
24	C	505	BCR	C5-C6-C7-C8
24	X	130	BCR	C1-C6-C7-C8
24	c	5505	BCR	C5-C6-C7-C8
30	h	5208	DGD	C9A-CAA-CBA-CCA
20	c	5498	CLA	C2-C1-O2A-CGA
20	C	494	CLA	CAA-CBA-CGA-O2A
20	c	5494	CLA	CAA-CBA-CGA-O2A
26	A	568	SQD	C13-C14-C15-C16
26	L	5213	SQD	C45-C46-O48-C23
20	b	5516	CLA	C15-C16-C17-C18
20	B	515	CLA	CAA-CBA-CGA-O2A
20	C	497	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	b	5515	CLA	CAA-CBA-CGA-O2A
20	b	5524	CLA	C11-C10-C8-C7
30	C	507	DGD	O2G-C1B-C2B-C3B
20	C	495	CLA	CAA-CBA-CGA-O2A
20	c	5495	CLA	CAA-CBA-CGA-O2A
20	B	523	CLA	C14-C13-C15-C16
20	c	5492	CLA	C11-C10-C8-C9
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	5492	CLA	C1A-C2A-CAA-CBA
20	b	5525	CLA	C4-C3-C5-C6
24	X	130	BCR	C6-C7-C8-C9
24	x	5130	BCR	C6-C7-C8-C9
20	C	499	CLA	CAA-CBA-CGA-O2A
20	c	5499	CLA	CAA-CBA-CGA-O2A
30	c	5507	DGD	O2G-C1B-C2B-C3B
28	D	358	MGE	C3B-C4B-C5B-C6B
20	B	520	CLA	C15-C16-C17-C18
28	I	201	MGE	C4B-C5B-C6B-C7B
26	L	5213	SQD	C5-C6-S-O7
26	L	5213	SQD	C5-C6-S-O9
26	t	213	SQD	C5-C6-S-O7
26	t	213	SQD	C5-C6-S-O9
20	B	525	CLA	C4-C3-C5-C6
20	B	521	CLA	C2-C1-O2A-CGA
20	C	498	CLA	C2-C1-O2A-CGA
20	C	502	CLA	C2-C1-O2A-CGA
20	D	354	CLA	C2-C1-O2A-CGA
20	b	5521	CLA	C2-C1-O2A-CGA
20	d	5354	CLA	C2-C1-O2A-CGA
20	B	520	CLA	C12-C13-C15-C16
20	B	523	CLA	C11-C12-C13-C15
20	D	354	CLA	C11-C12-C13-C15
20	a	5558	CLA	C11-C12-C13-C15
27	a	5568	LMT	C7-C8-C9-C10
21	A	562	PHO	O2A-C1-C2-C3
30	c	5508	DGD	O6E-C5E-C6E-O5E
28	L	210	MGE	O1B-C1B-C2B-C3B
20	C	493	CLA	C3A-C2A-CAA-CBA
20	c	5491	CLA	C3A-C2A-CAA-CBA
20	c	5493	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	5562	PHO	C4-C3-C5-C6
20	B	515	CLA	CAA-CBA-CGA-O1A
28	d	5361	MGE	O1B-C1B-C2B-C3B
28	l	5210	MGE	O1B-C1B-C2B-C3B
26	d	5358	SQD	C13-C14-C15-C16
28	D	360	MGE	O1B-C1B-C2B-C3B
20	c	5494	CLA	CAA-CBA-CGA-O1A
20	B	518	CLA	C11-C10-C8-C9
20	C	492	CLA	C11-C10-C8-C9
20	C	498	CLA	C6-C7-C8-C9
20	C	501	CLA	C14-C13-C15-C16
20	D	354	CLA	C11-C12-C13-C14
20	b	5518	CLA	C11-C10-C8-C9
20	b	5523	CLA	C11-C12-C13-C14
28	I	201	MGE	C4D-C5D-C6D-O5D
20	c	5495	CLA	CAA-CBA-CGA-O1A
20	b	5512	CLA	C13-C15-C16-C17
30	c	5507	DGD	O1B-C1B-C2B-C3B
20	c	5491	CLA	CAA-CBA-CGA-O2A
20	B	512	CLA	C13-C15-C16-C17
20	C	494	CLA	CAA-CBA-CGA-O1A
20	C	495	CLA	CAA-CBA-CGA-O1A
20	C	497	CLA	CAA-CBA-CGA-O1A
20	C	499	CLA	CAA-CBA-CGA-O1A
20	c	5497	CLA	CAA-CBA-CGA-O1A
26	A	568	SQD	O49-C7-C8-C9
26	d	5358	SQD	O49-C7-C8-C9
20	b	5512	CLA	C5-C6-C7-C8
20	b	5515	CLA	CAA-CBA-CGA-O1A
30	C	507	DGD	O1B-C1B-C2B-C3B
20	B	513	CLA	C2A-CAA-CBA-CGA
20	B	513	CLA	CAD-CBD-CGD-O2D
20	B	523	CLA	CAD-CBD-CGD-O2D
20	C	497	CLA	CAD-CBD-CGD-O2D
20	b	5513	CLA	CAD-CBD-CGD-O2D
20	c	5497	CLA	CAD-CBD-CGD-O2D
20	c	5498	CLA	CAD-CBD-CGD-O2D
28	l	5210	MGE	O1G-C1A-C2A-C3A
28	b	5530	MGE	C1A-C2A-C3A-C4A
20	b	5524	CLA	CAA-CBA-CGA-O2A
20	C	491	CLA	C1-C2-C3-C4
20	C	497	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	502	CLA	C1-C2-C3-C4
20	b	5514	CLA	C1-C2-C3-C4
20	c	5497	CLA	C1-C2-C3-C4
20	c	5502	CLA	C1-C2-C3-C4
20	B	513	CLA	C13-C15-C16-C17
28	L	210	MGE	O1G-C1A-C2A-C3A
20	B	524	CLA	CAA-CBA-CGA-O2A
30	C	509	DGD	O1G-C1A-C2A-C3A
20	c	5491	CLA	CAA-CBA-CGA-O1A
20	c	5499	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	527	BCR	2	0
20	B	512	CLA	2	0
30	H	208	DGD	3	0
21	A	561	PHO	7	0
28	L	210	MGE	2	0
32	V	552	HEM	2	0
20	A	560	CLA	1	0
24	C	504	BCR	7	0
28	I	201	MGE	1	0
20	B	526	CLA	2	0
28	D	360	MGE	7	0
24	D	357	BCR	4	0
24	H	107	BCR	3	0
20	B	524	CLA	4	0
24	C	505	BCR	6	0
20	C	498	CLA	6	0
20	B	525	CLA	4	0
30	C	508	DGD	2	0
24	B	529	BCR	2	0
20	C	501	CLA	13	0
20	C	494	CLA	2	0
20	B	519	CLA	5	0
22	D	356	PQ9	7	0
20	C	496	CLA	2	0
30	C	507	DGD	6	0
20	C	500	CLA	3	0
20	C	495	CLA	9	0

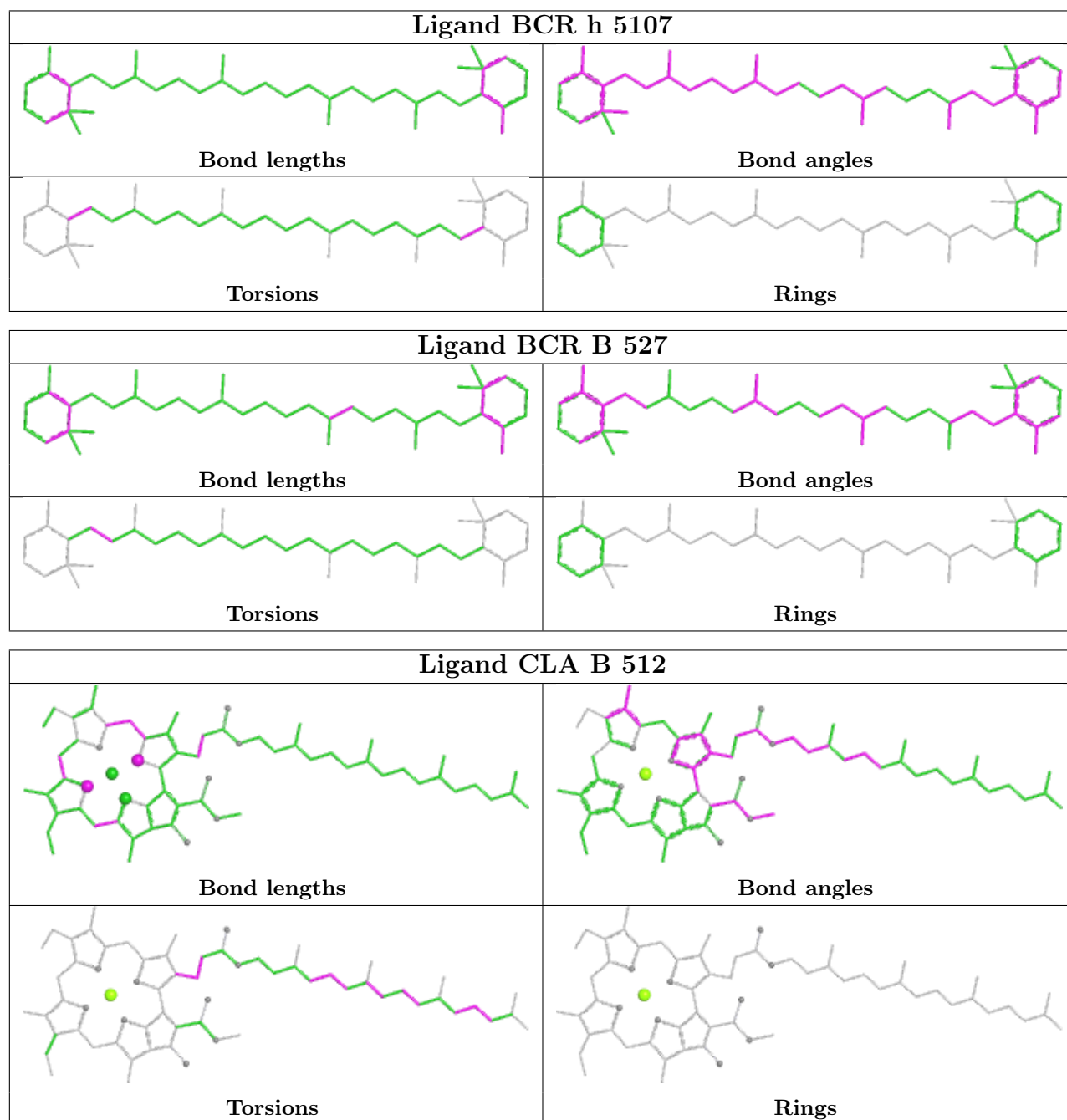
Continued on next page...

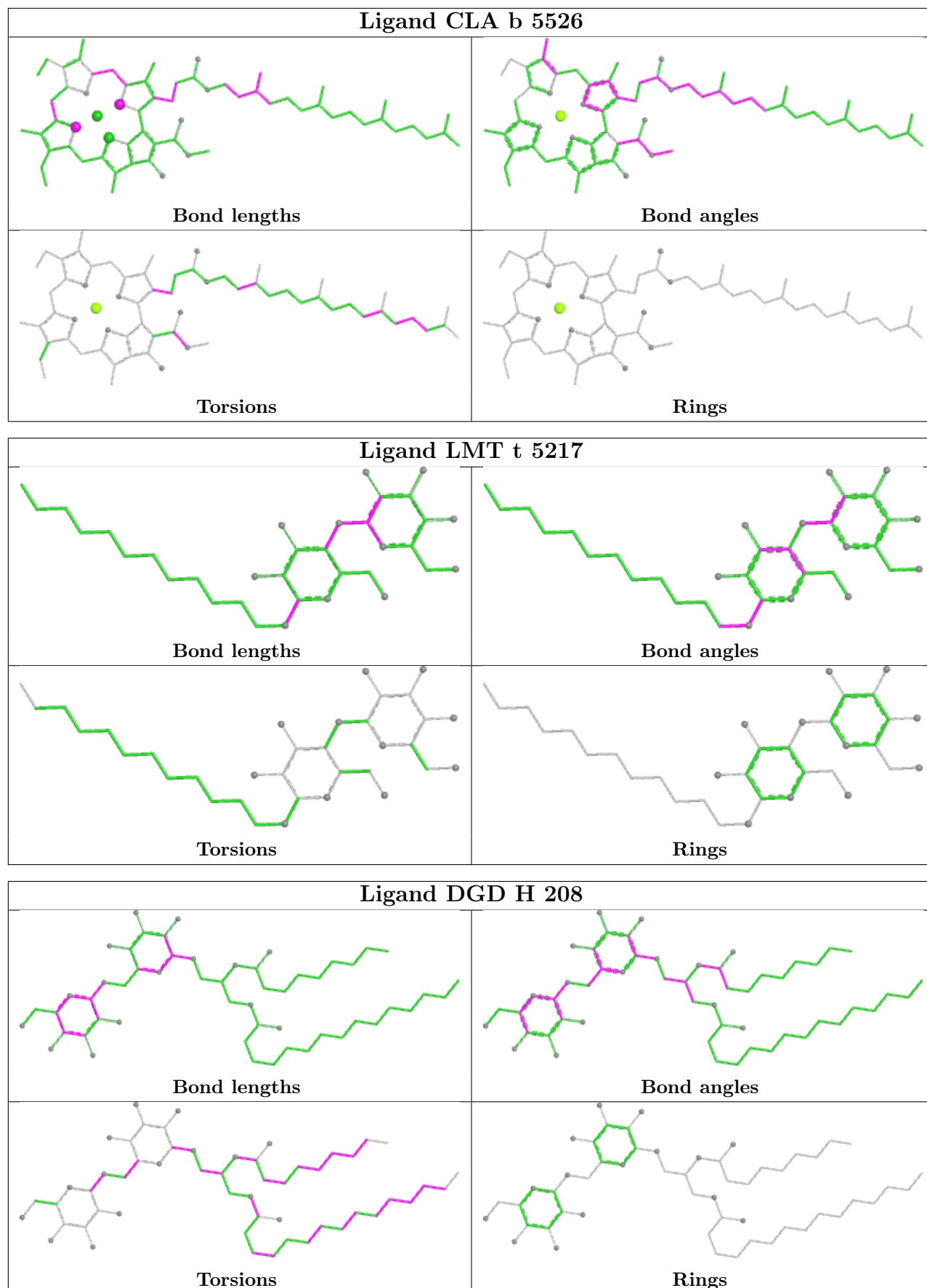
Continued from previous page...

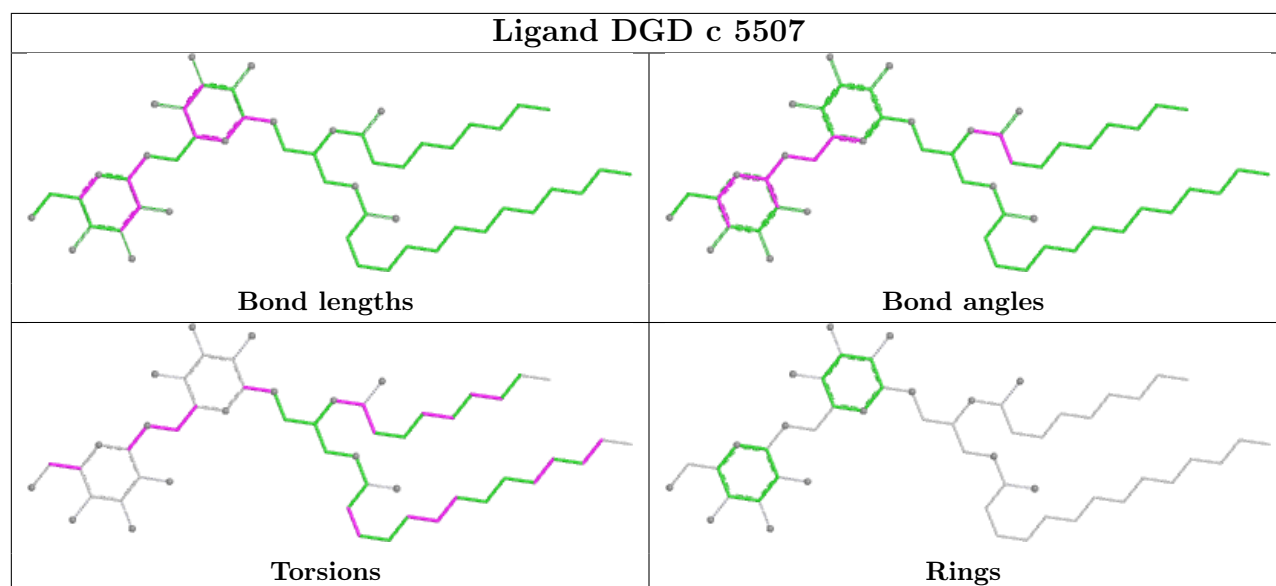
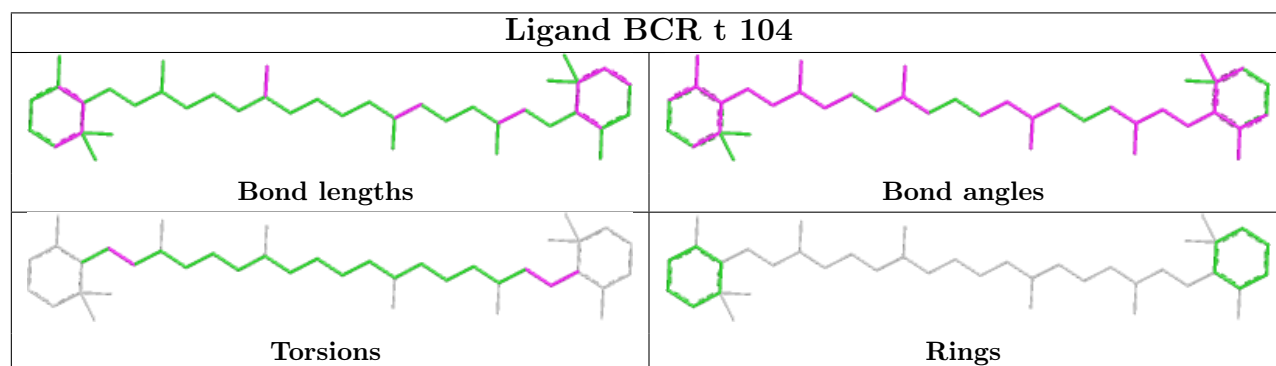
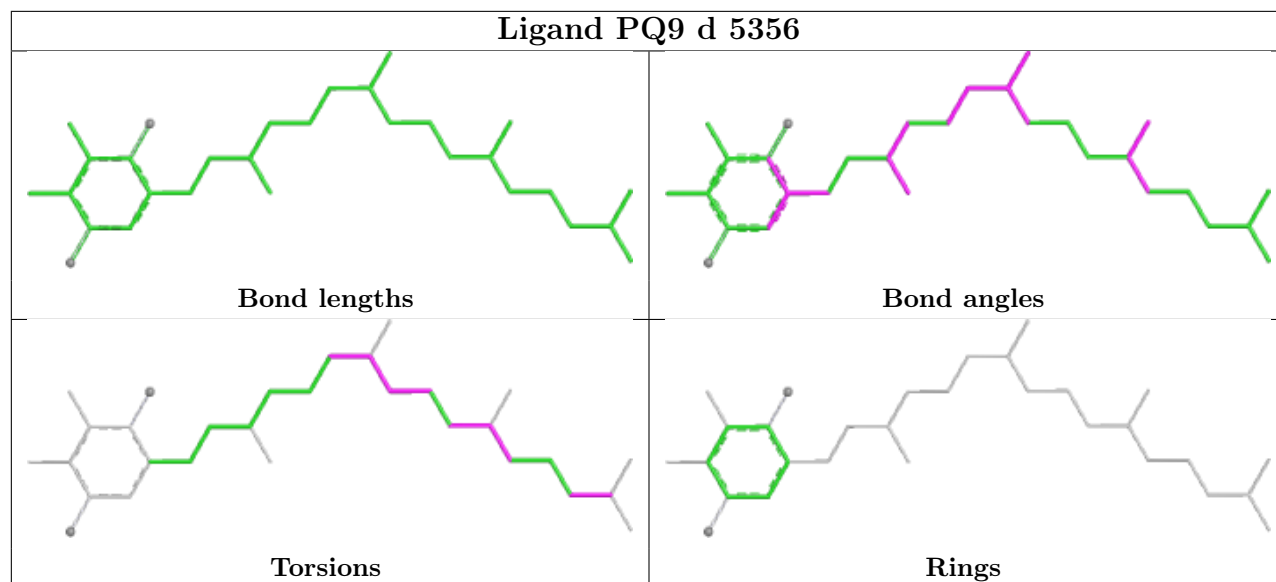
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	566	BCR	1	0
20	C	491	CLA	4	0
32	F	51	HEM	3	0
24	T	5104	BCR	5	0
20	B	523	CLA	2	0
24	C	506	BCR	7	0
20	C	493	CLA	7	0
20	A	559	CLA	5	0
25	A	567	LHG	4	0
20	B	521	CLA	2	0
20	C	502	CLA	2	0
20	B	511	CLA	1	0
20	D	354	CLA	5	0
20	D	355	CLA	3	0
27	T	217	LMT	3	0
20	B	514	CLA	5	0
20	C	499	CLA	2	0
20	B	513	CLA	8	0
28	D	359	MGE	1	0
28	D	358	MGE	2	0
22	A	564	PQ9	2	0
20	B	516	CLA	6	0
20	B	515	CLA	12	0
20	B	518	CLA	11	0
20	B	517	CLA	9	0
28	B	530	MGE	1	0
21	A	562	PHO	5	0
30	C	509	DGD	10	0
20	C	497	CLA	5	0
20	B	520	CLA	6	0
20	C	503	CLA	1	0
20	B	522	CLA	4	0
24	B	528	BCR	2	0
24	X	130	BCR	9	0
20	C	492	CLA	2	0
20	A	558	CLA	10	0

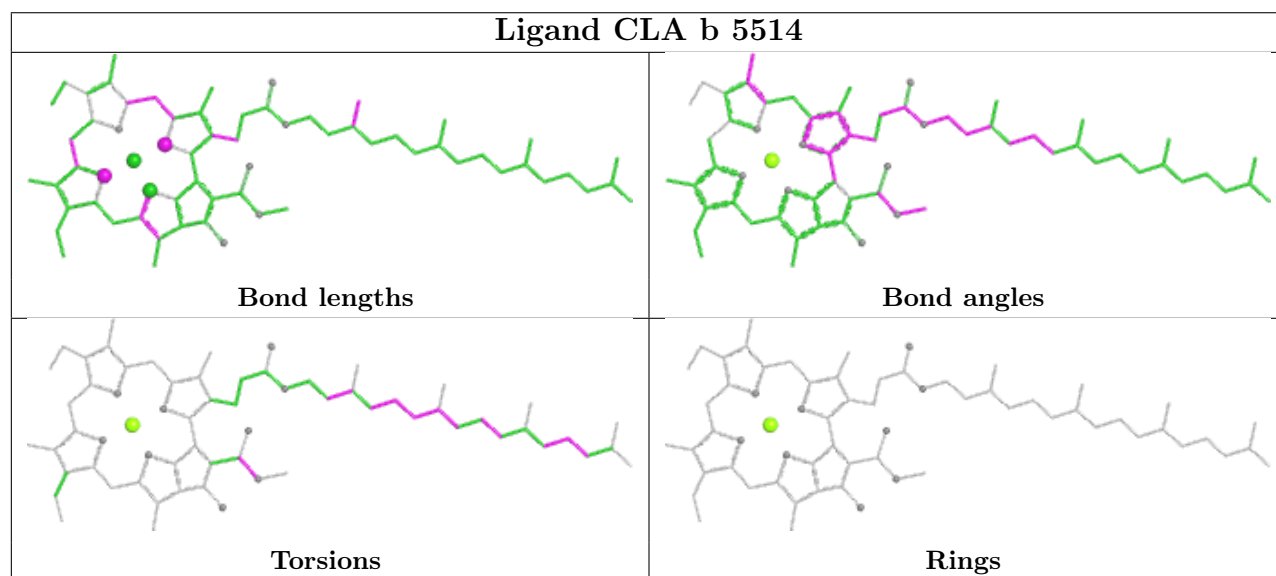
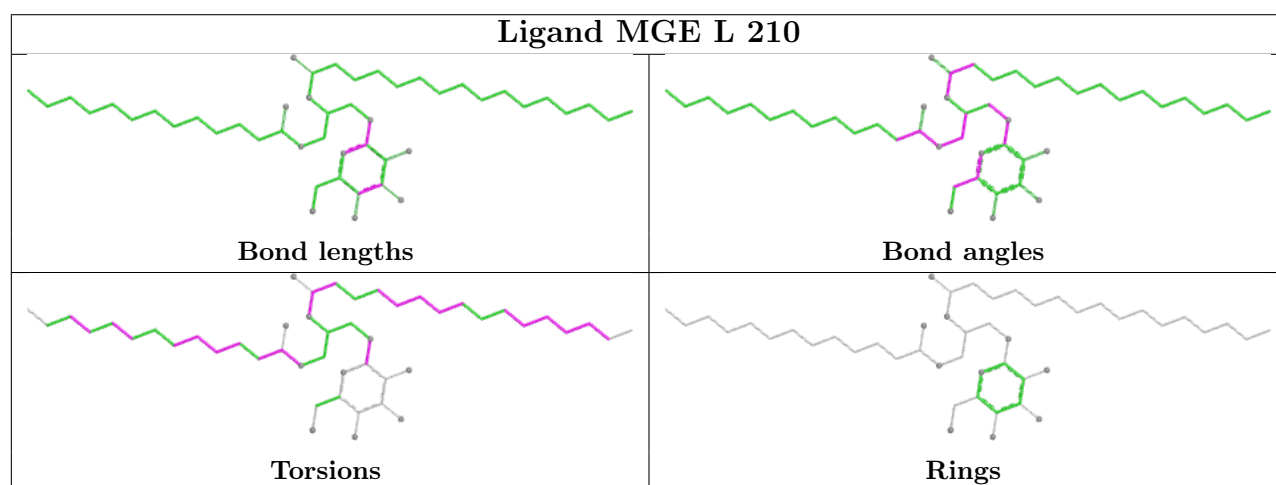
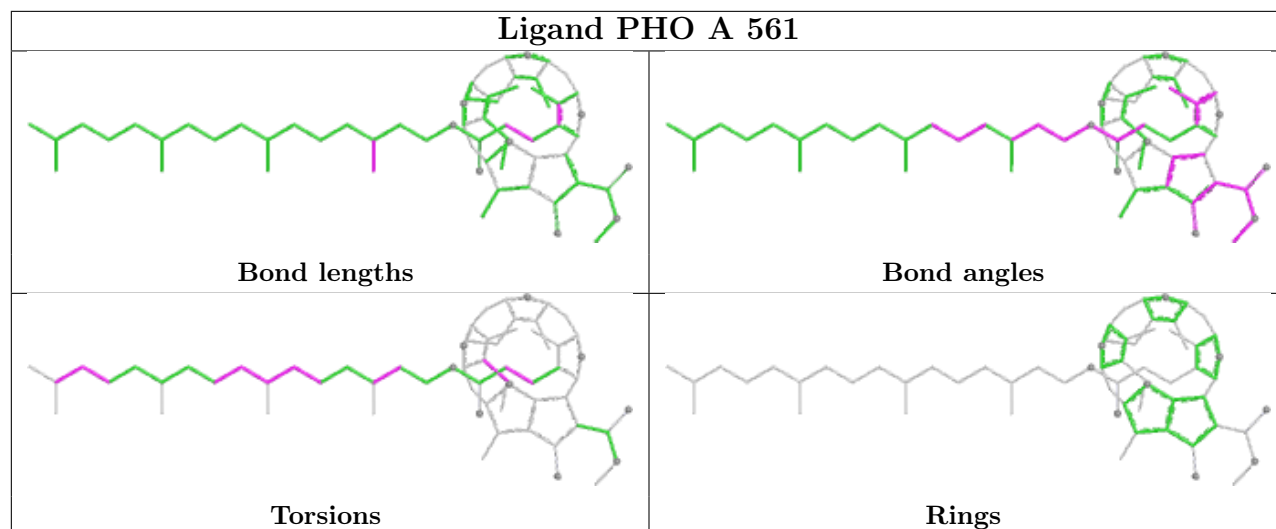
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

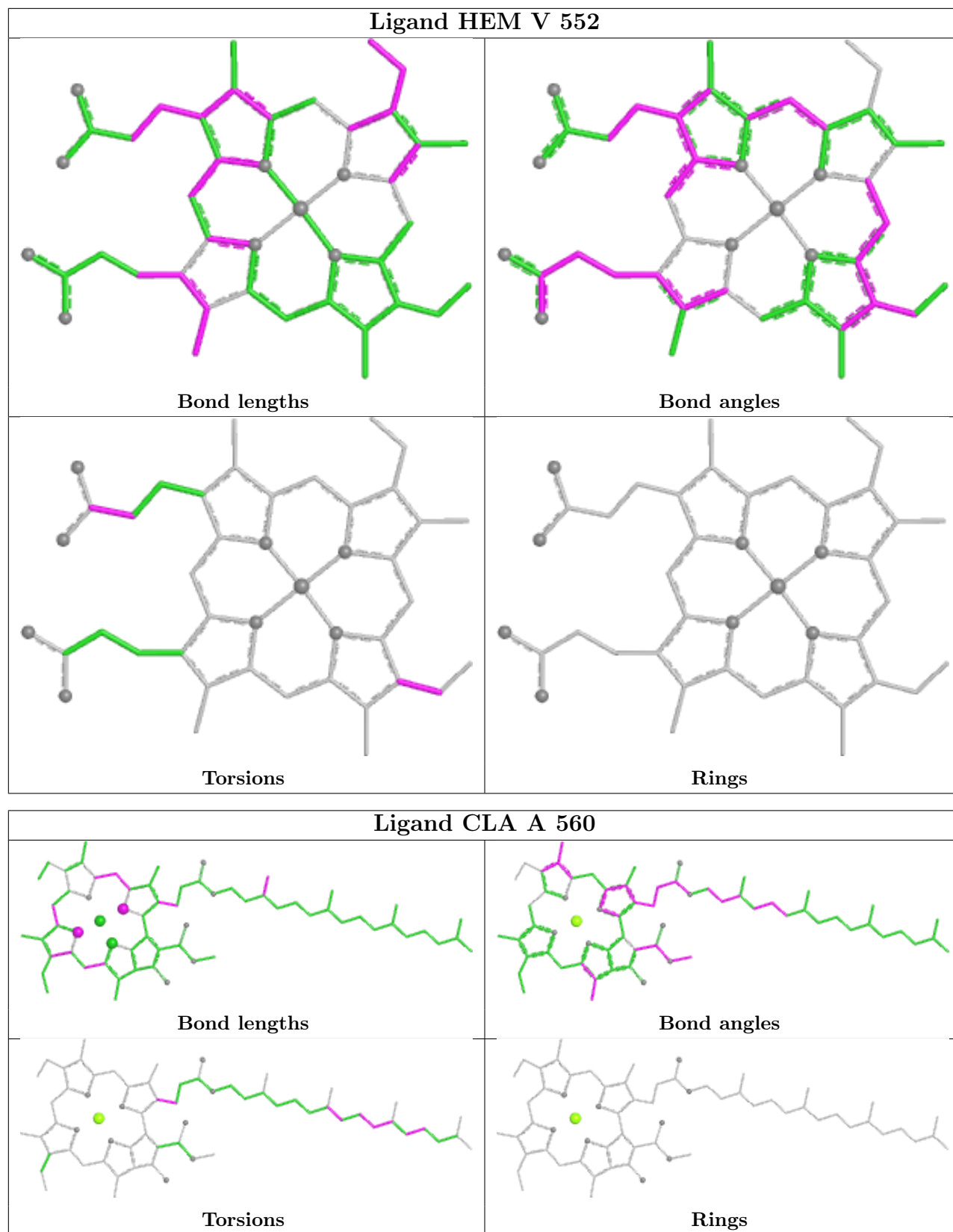
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

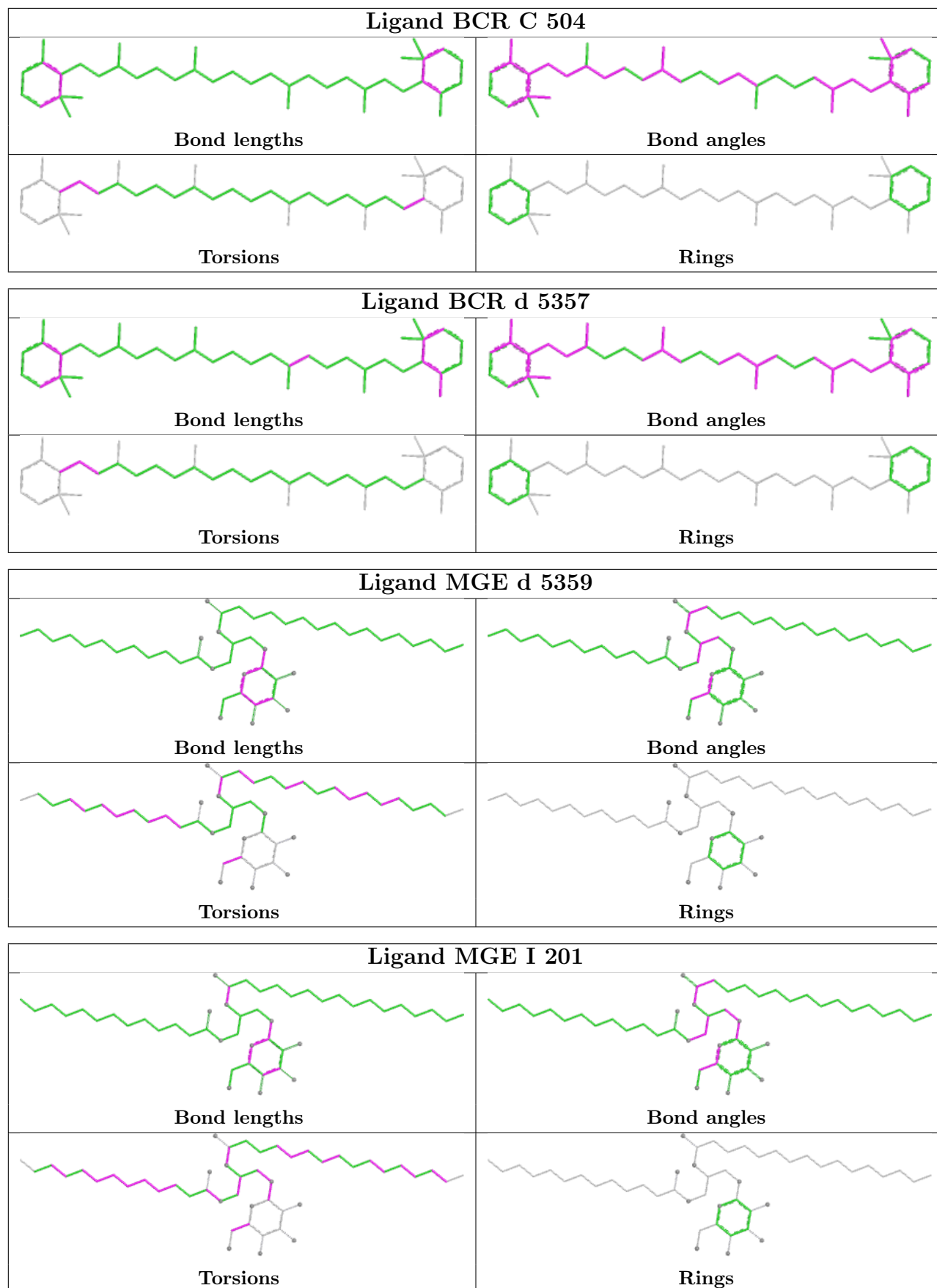


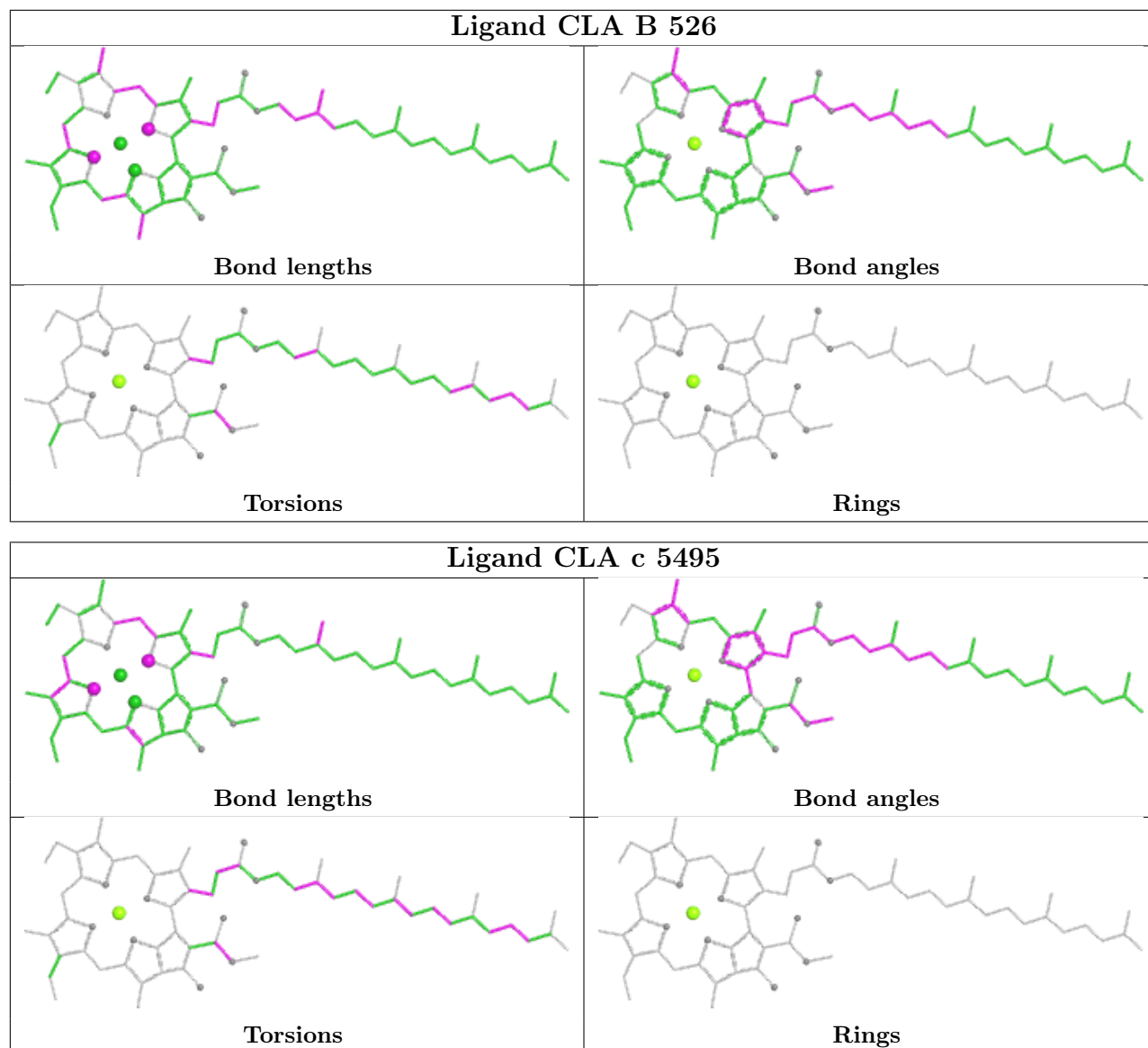


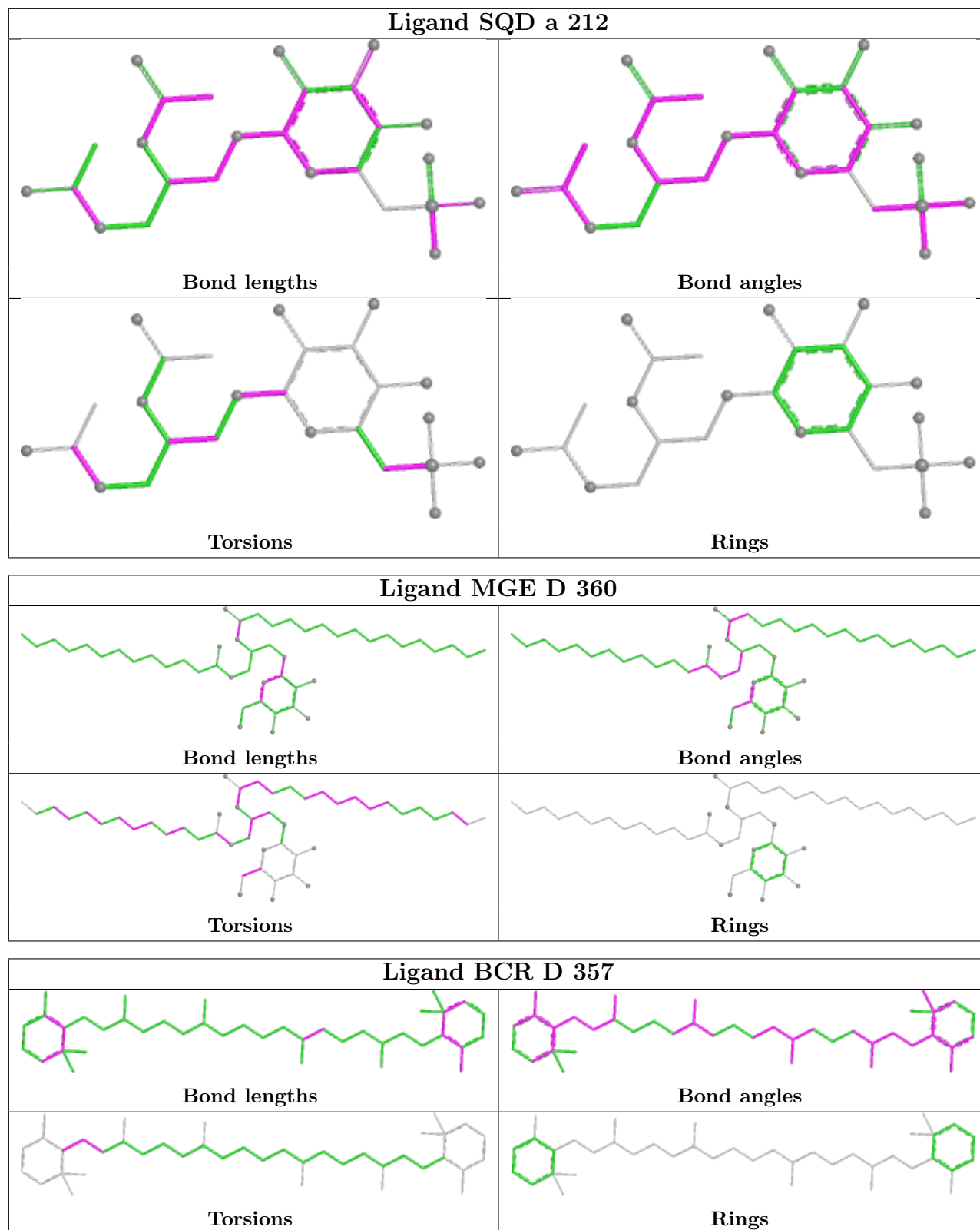


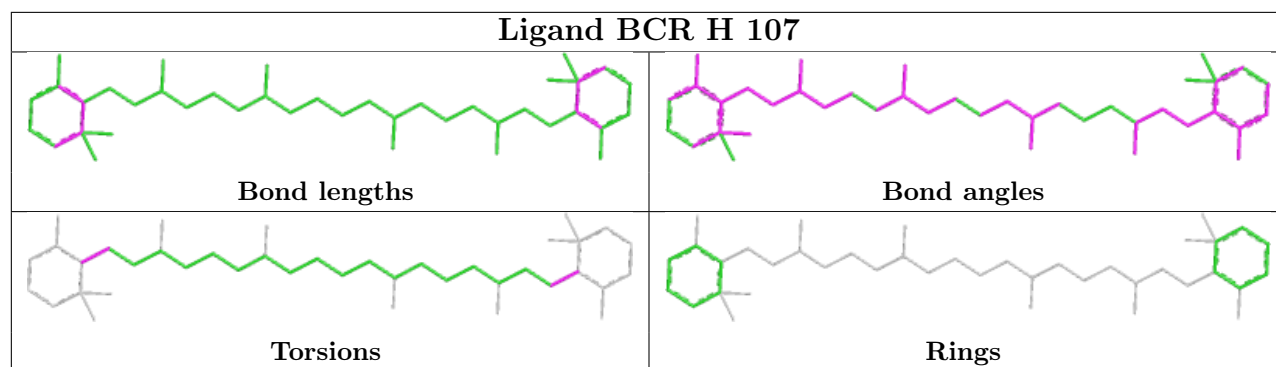
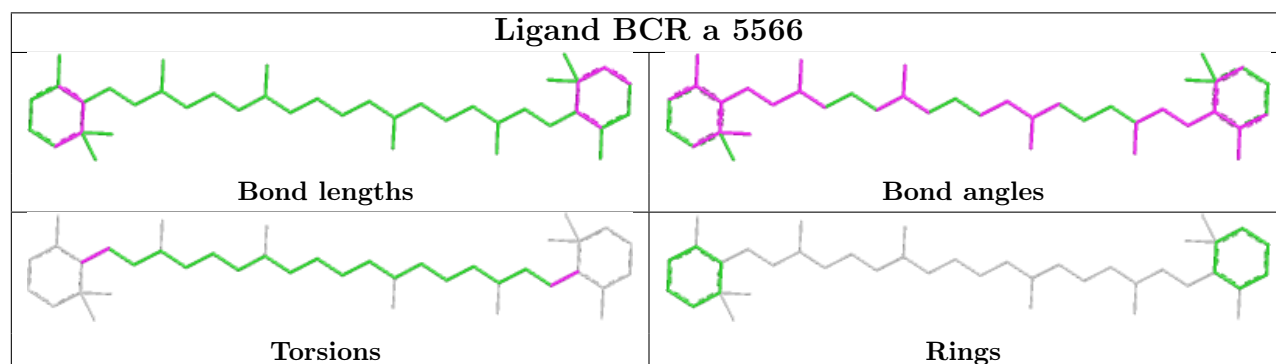
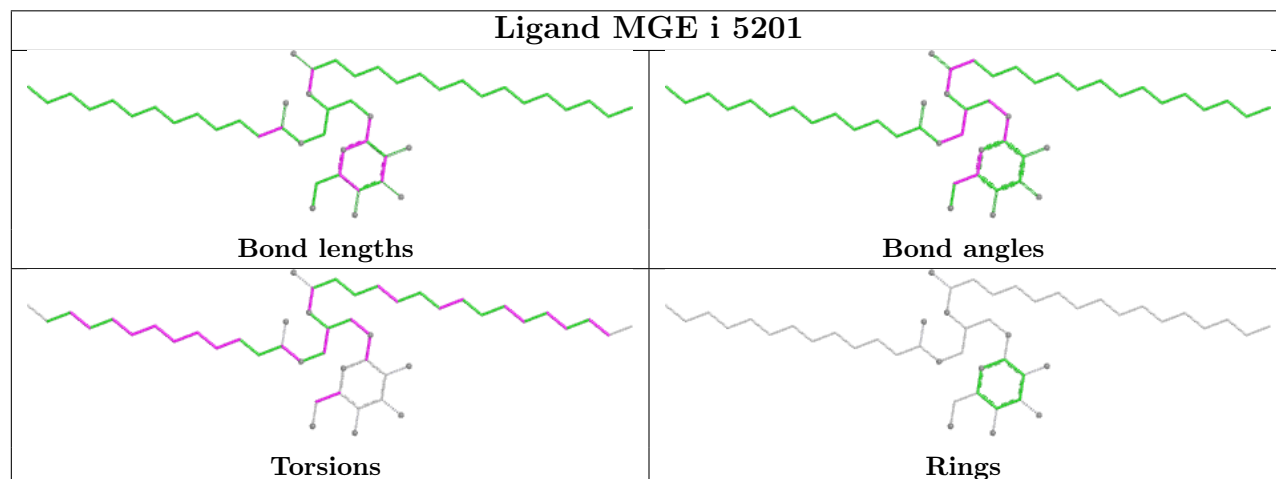
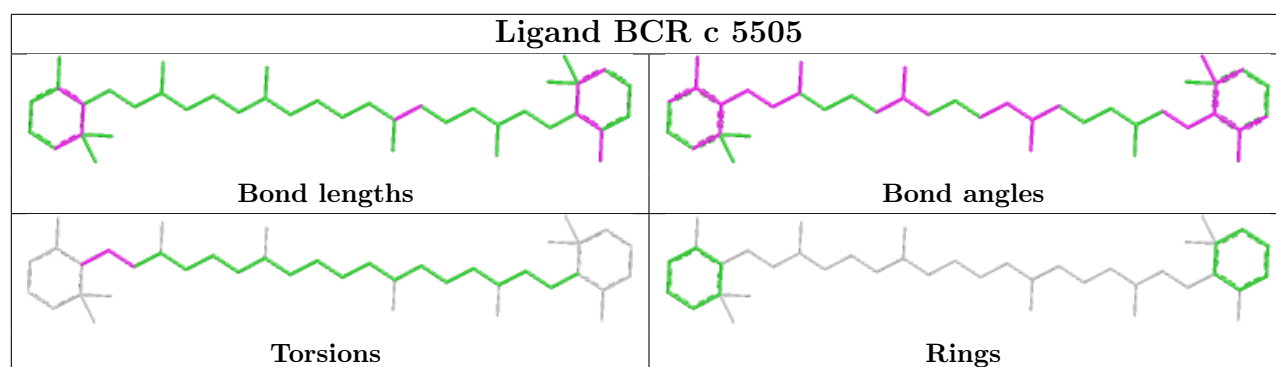


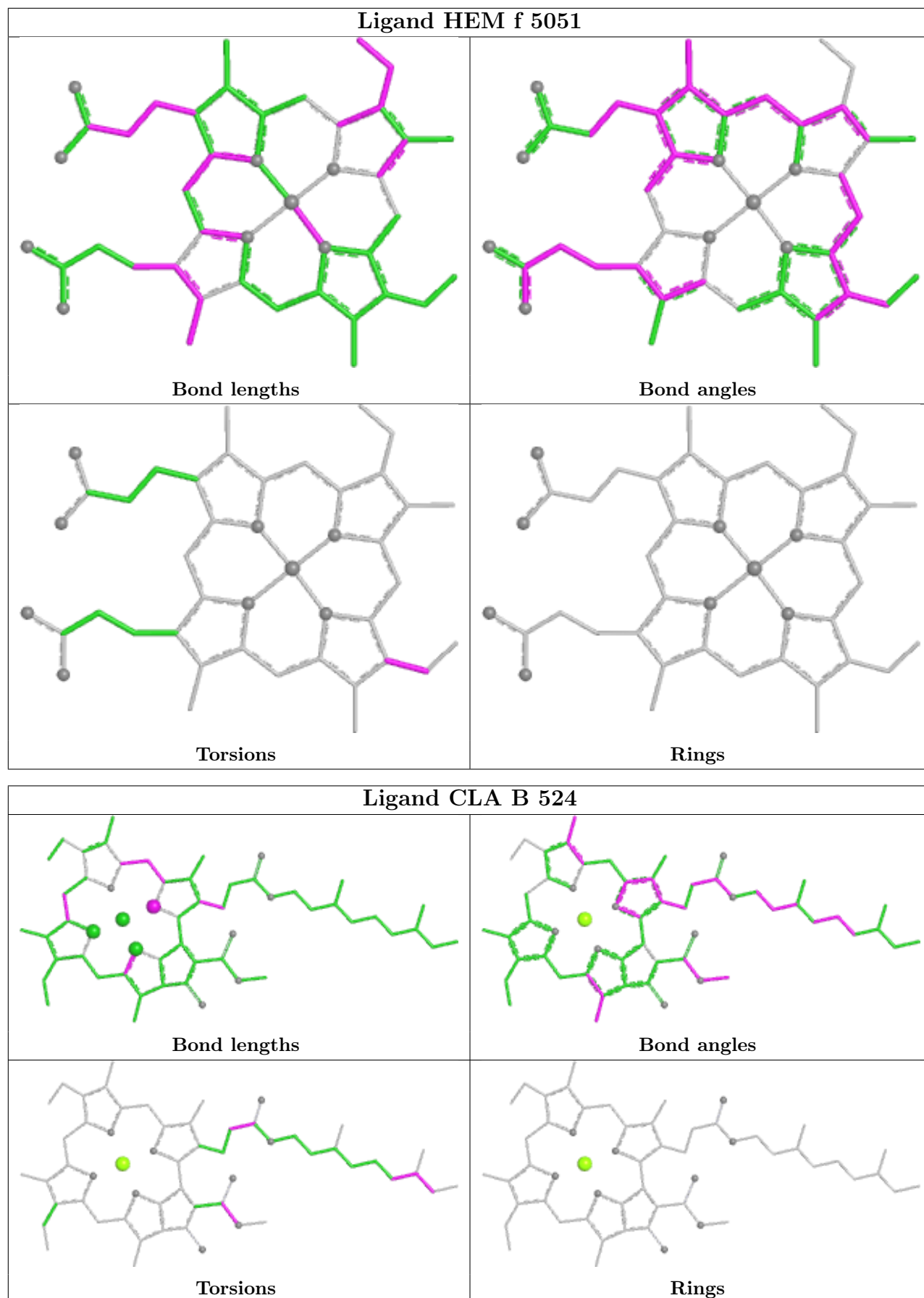


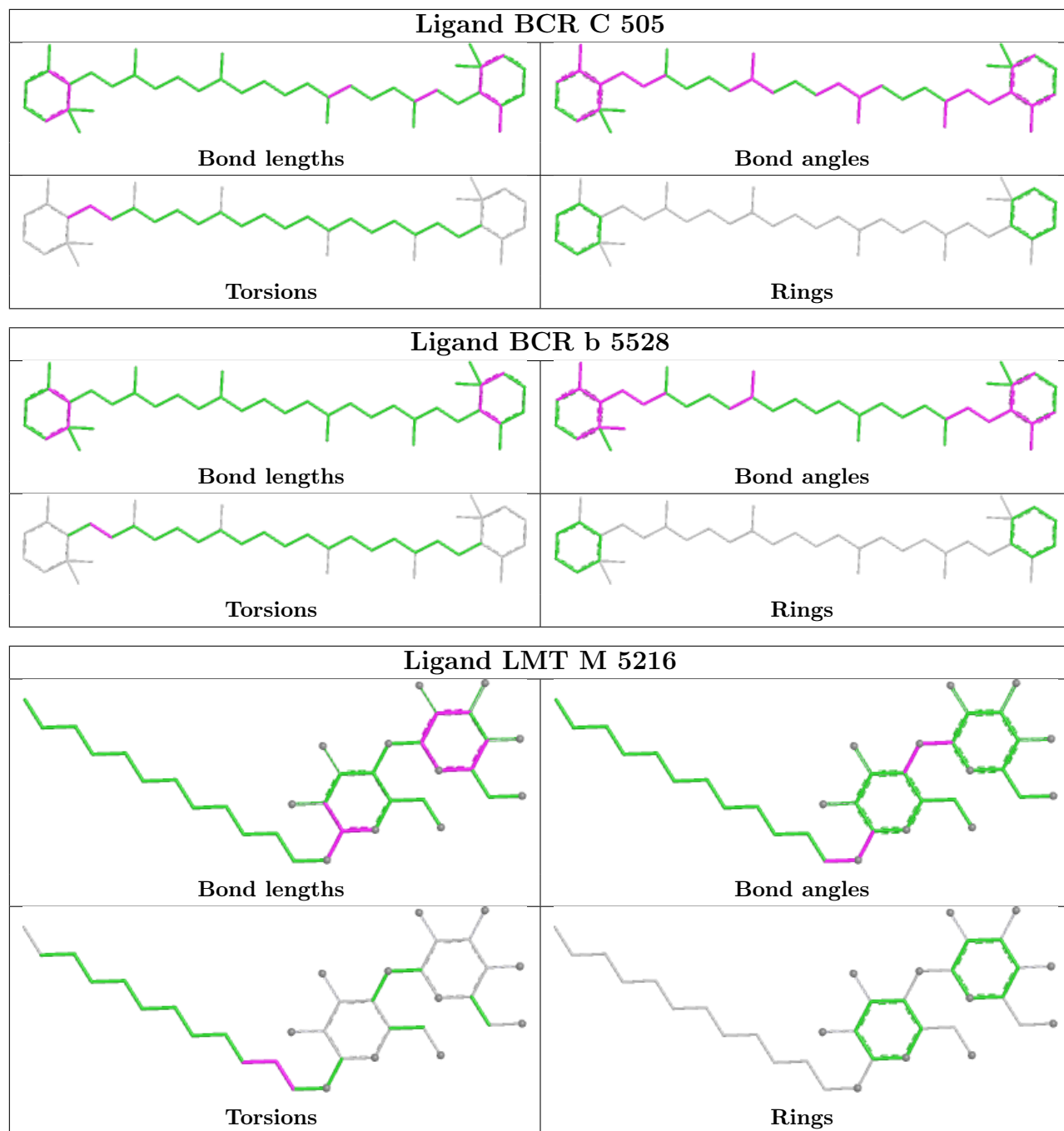


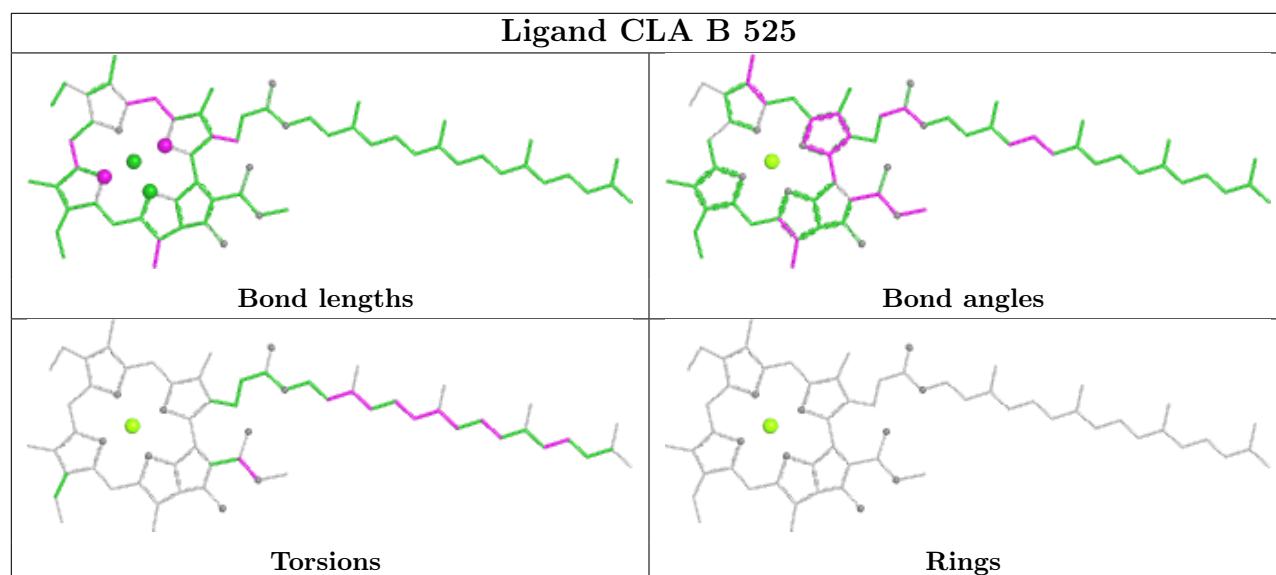
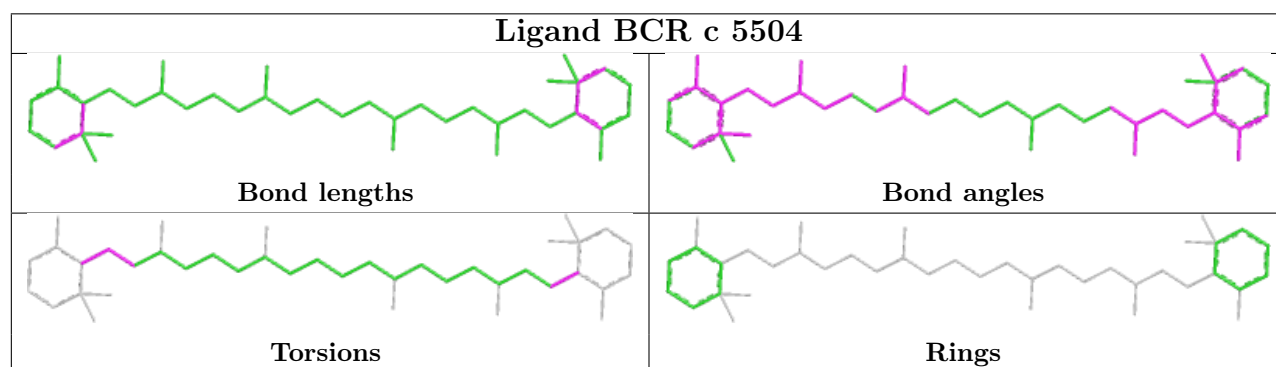
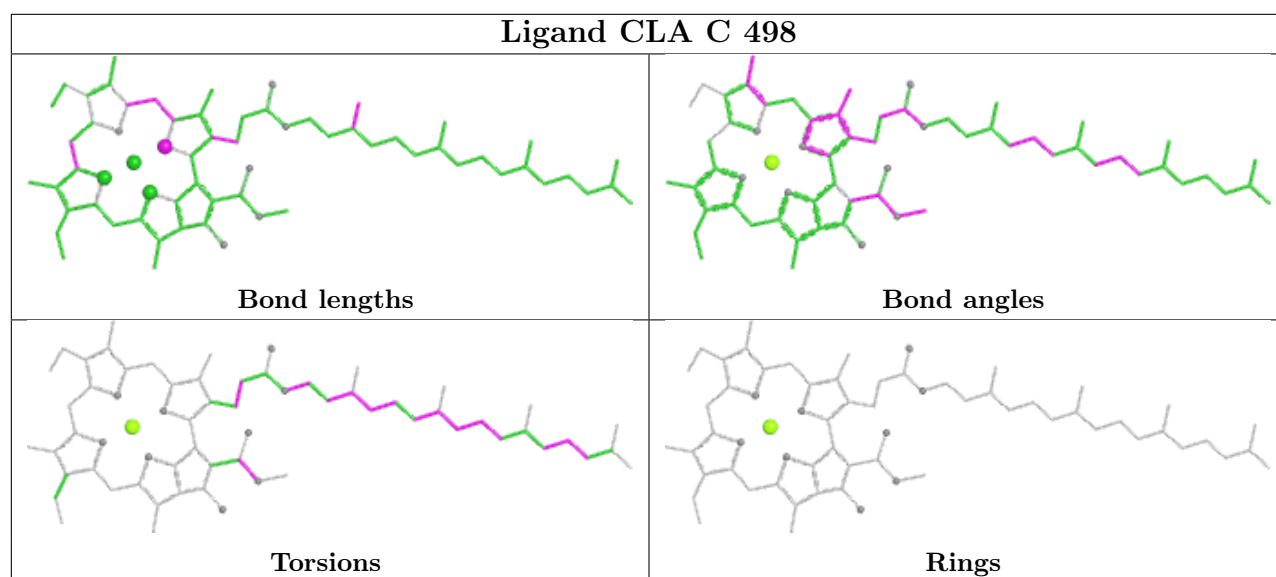


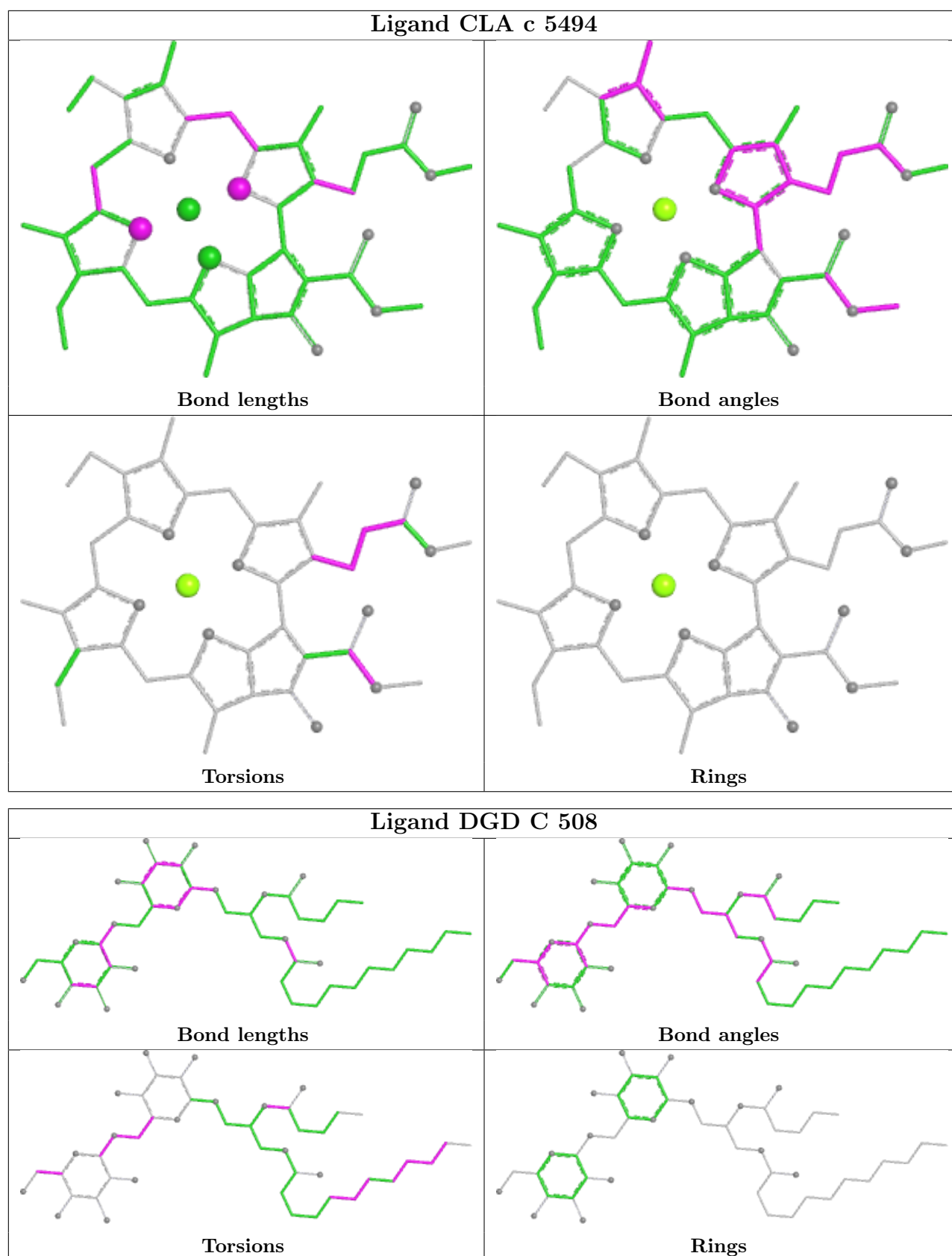


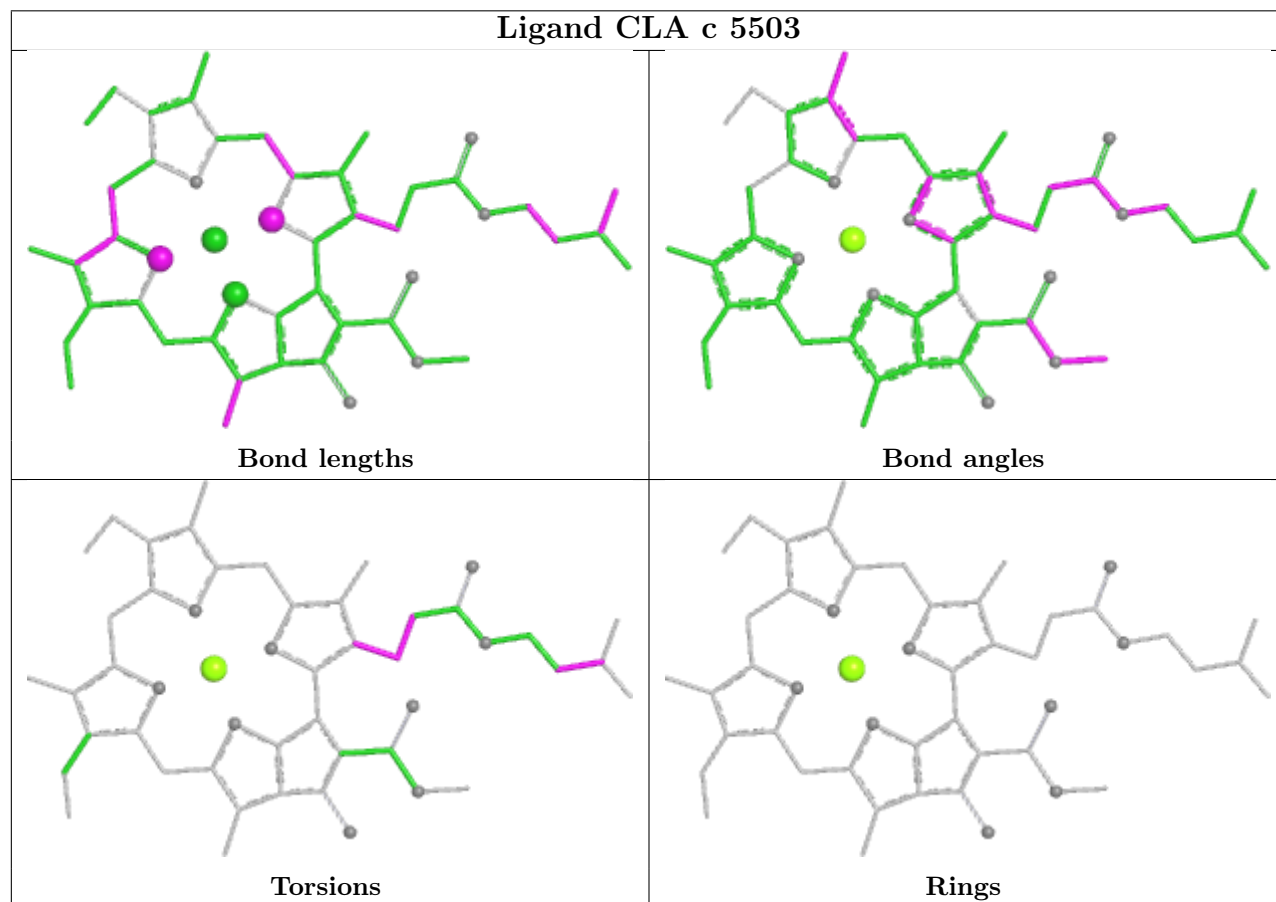
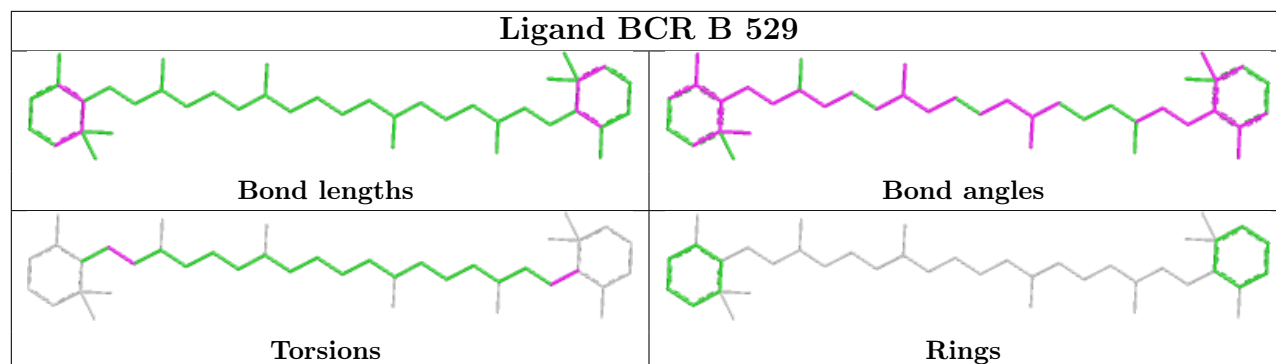


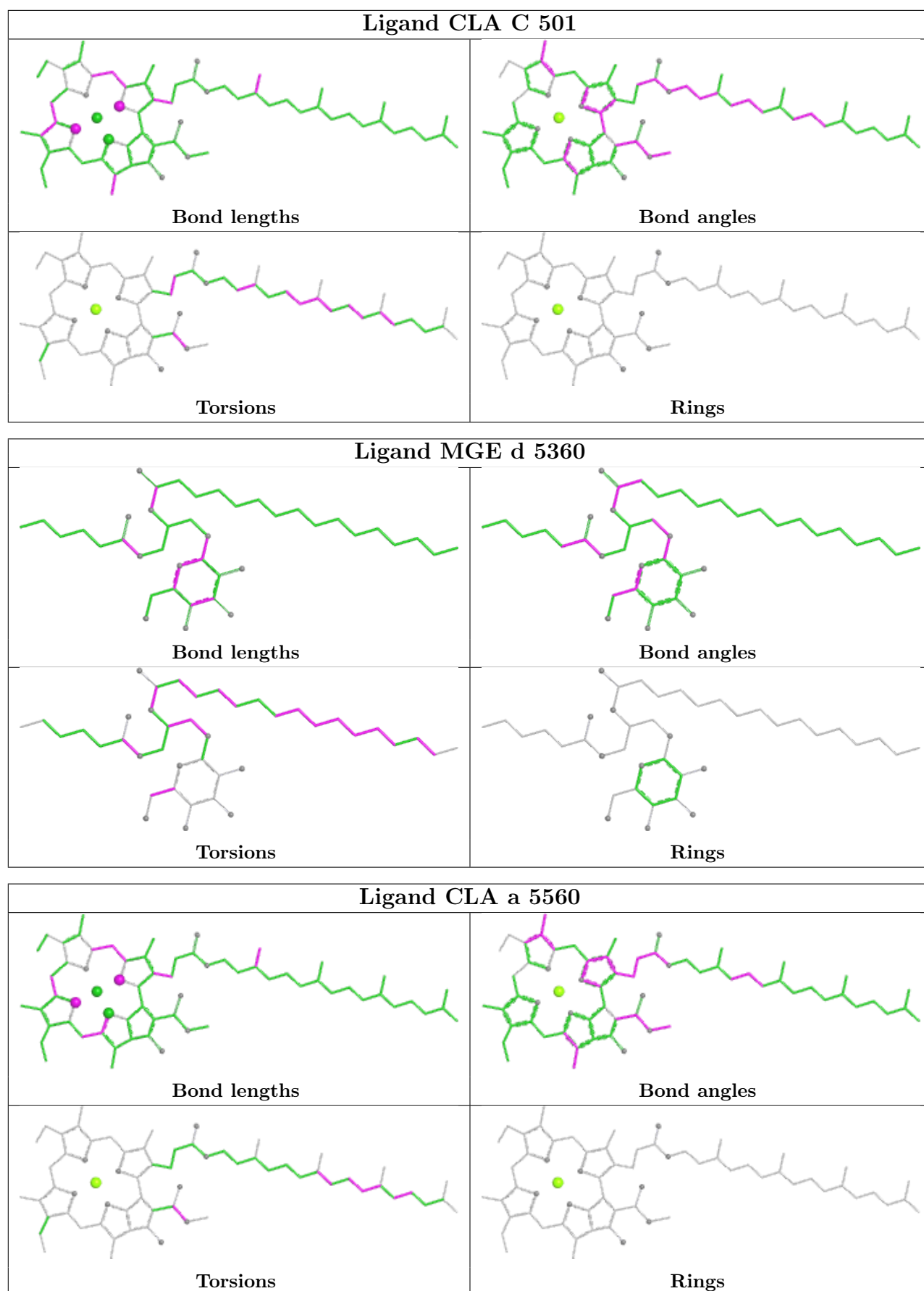


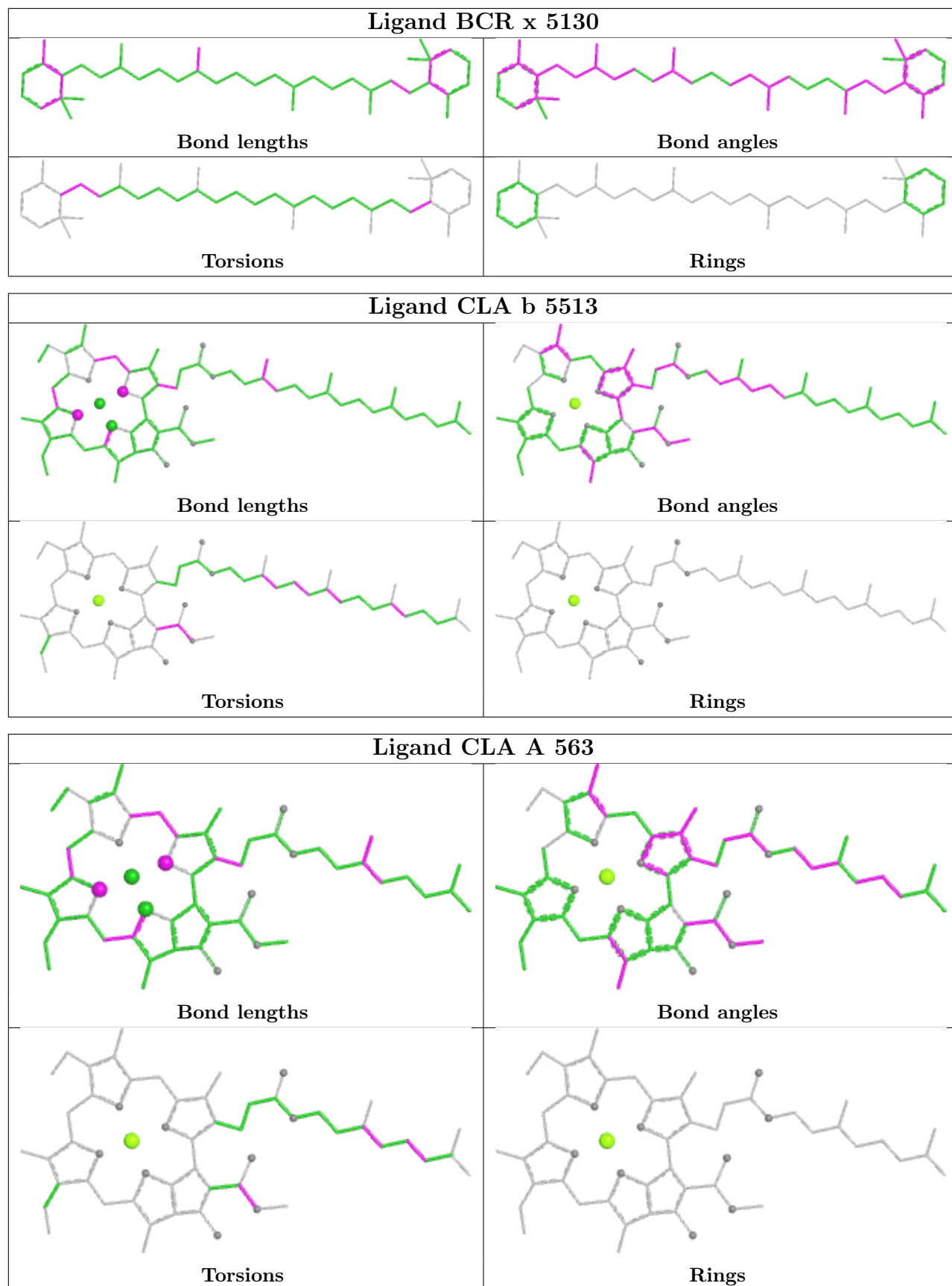


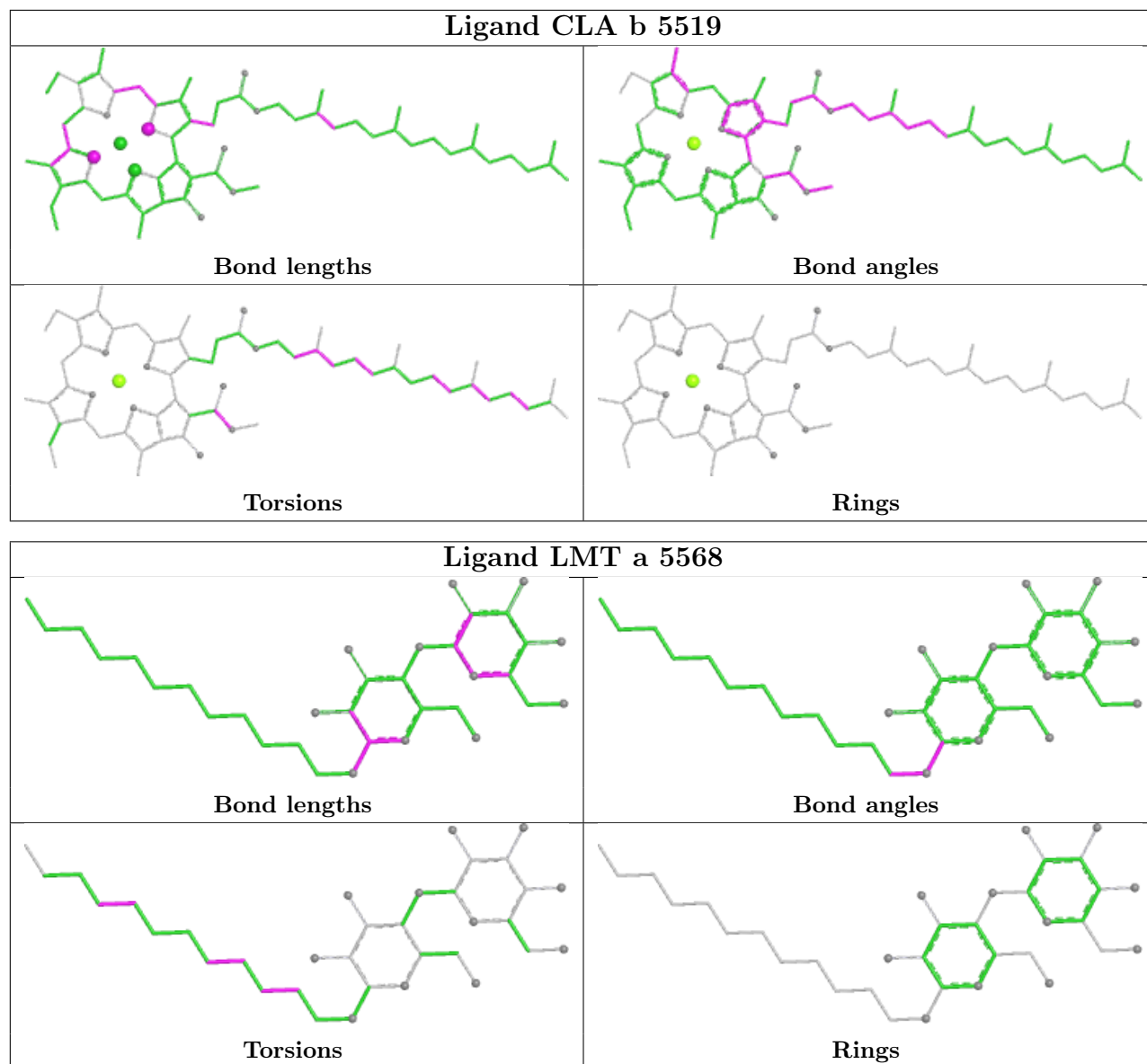


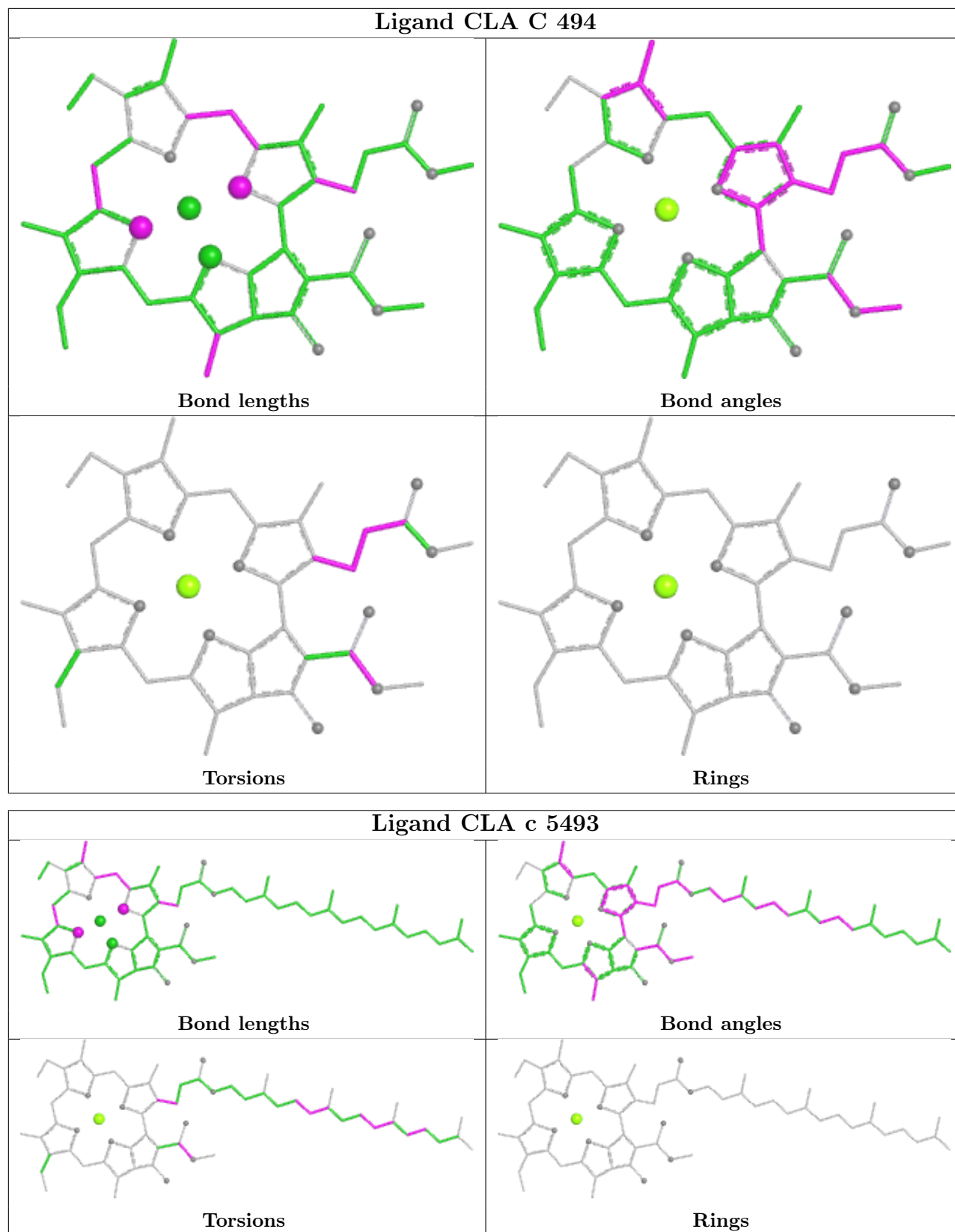


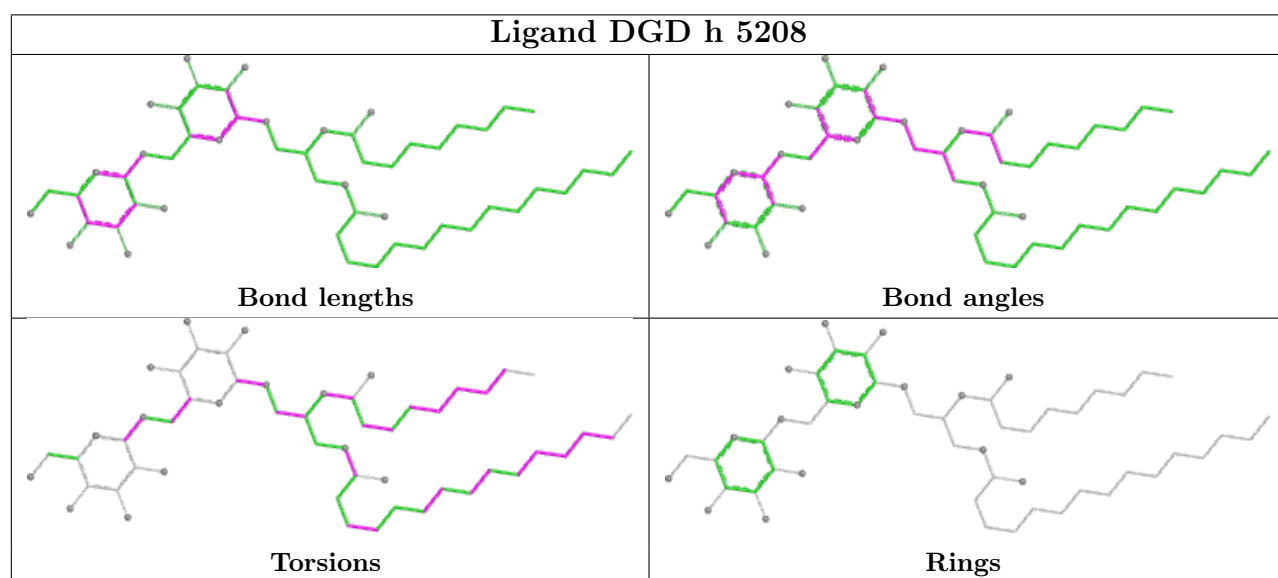
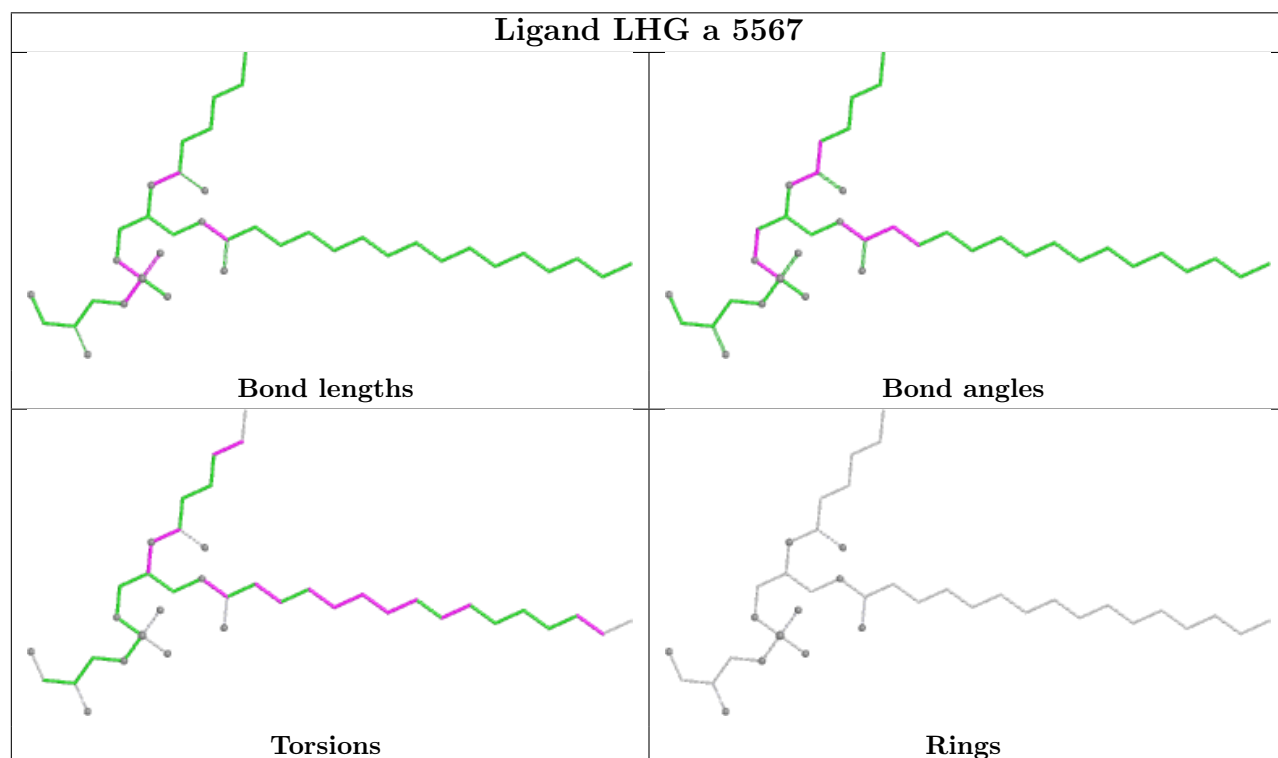
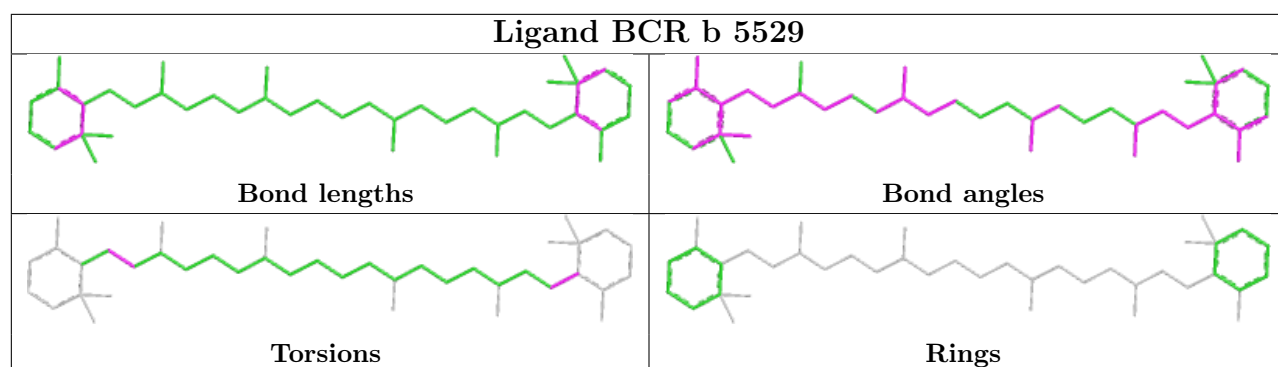


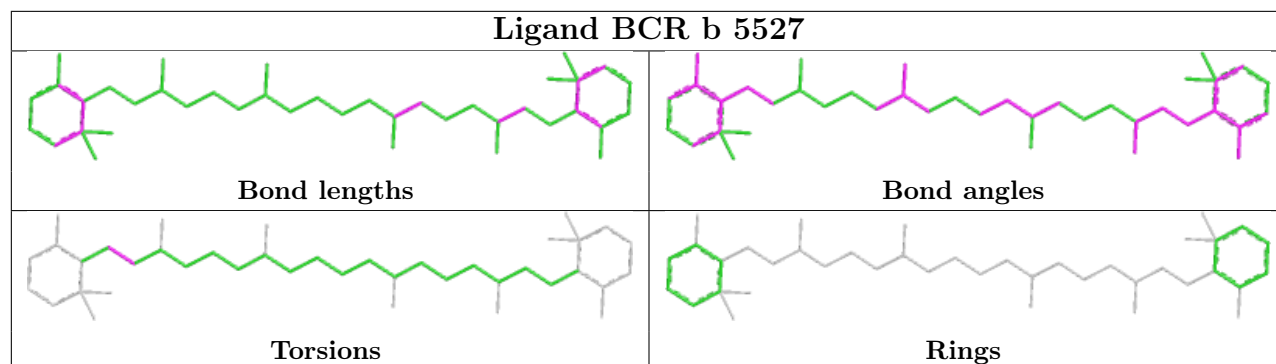
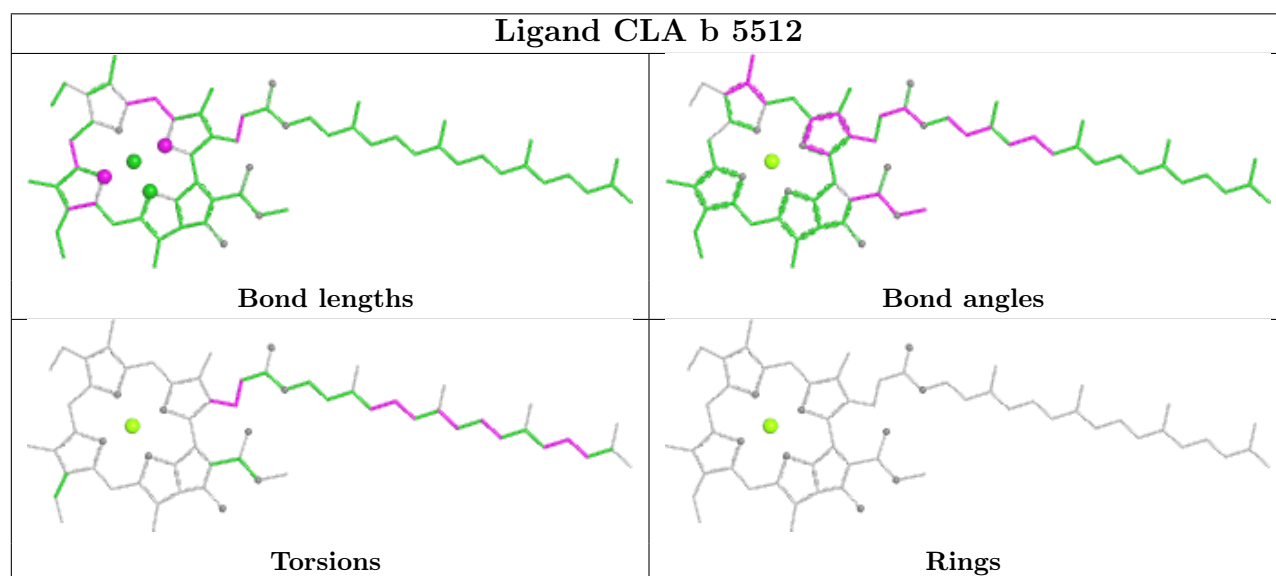
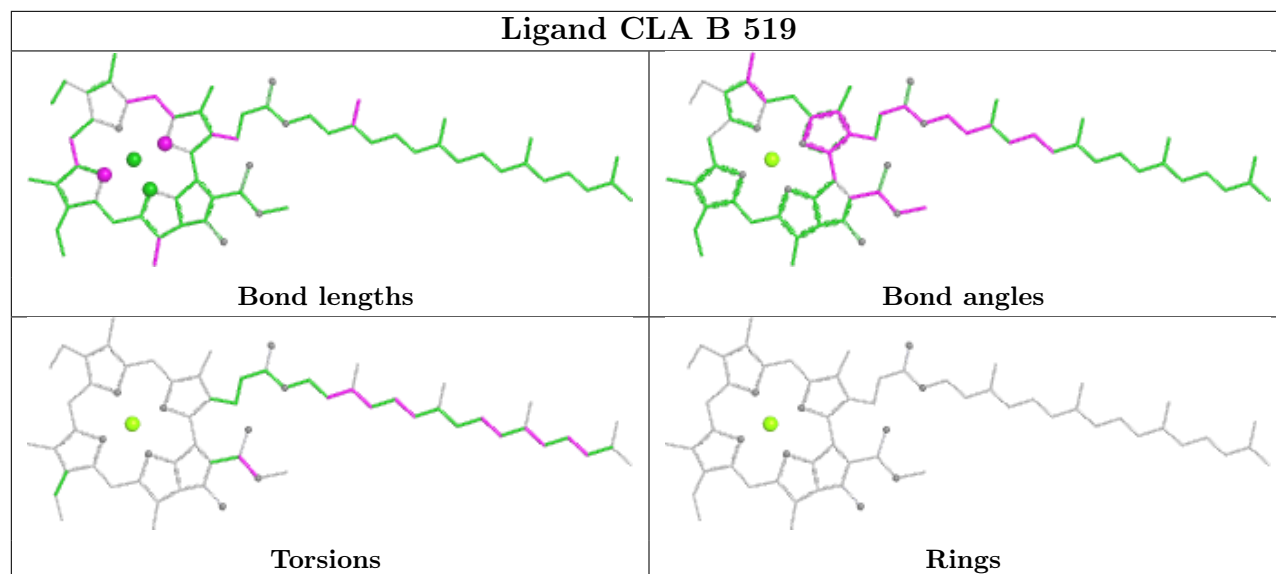


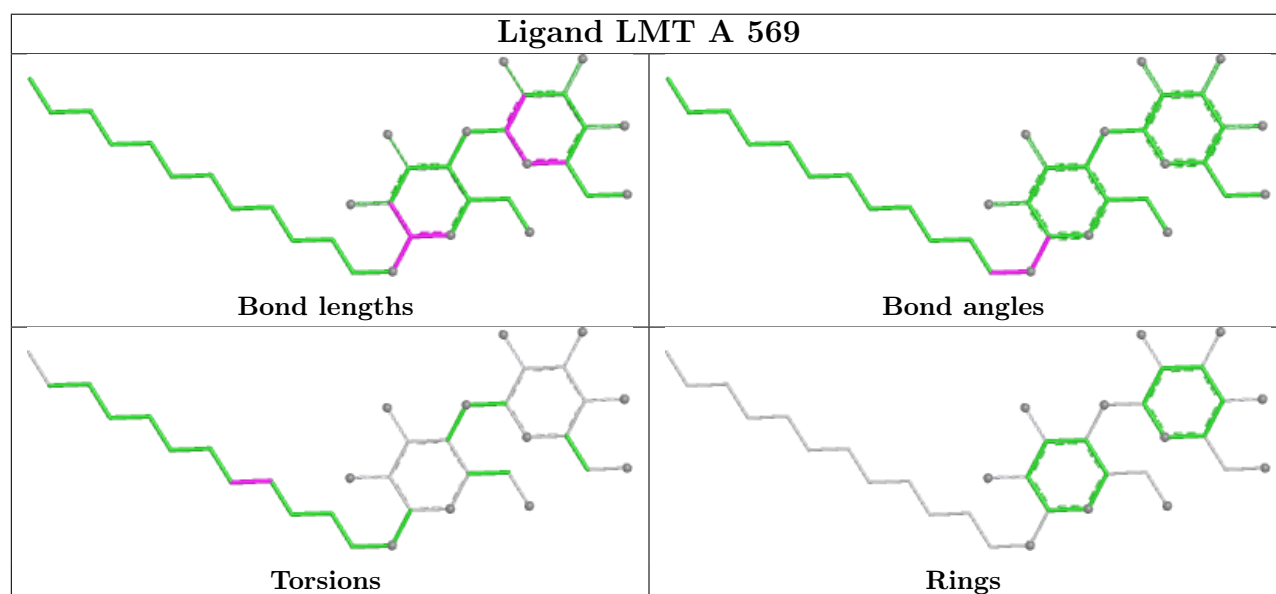
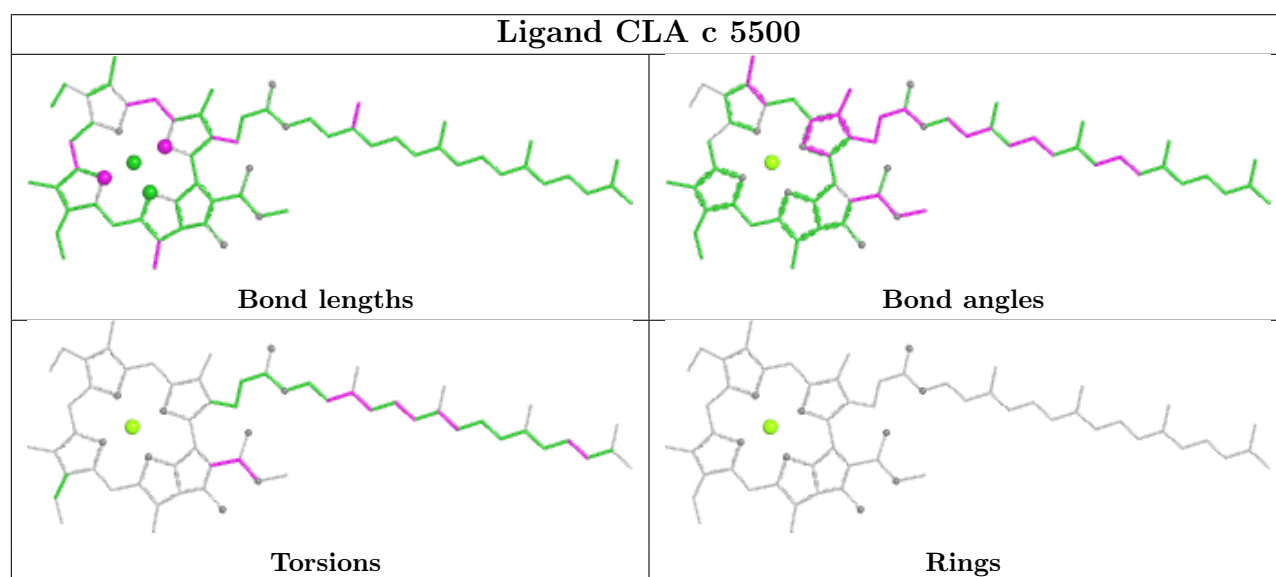
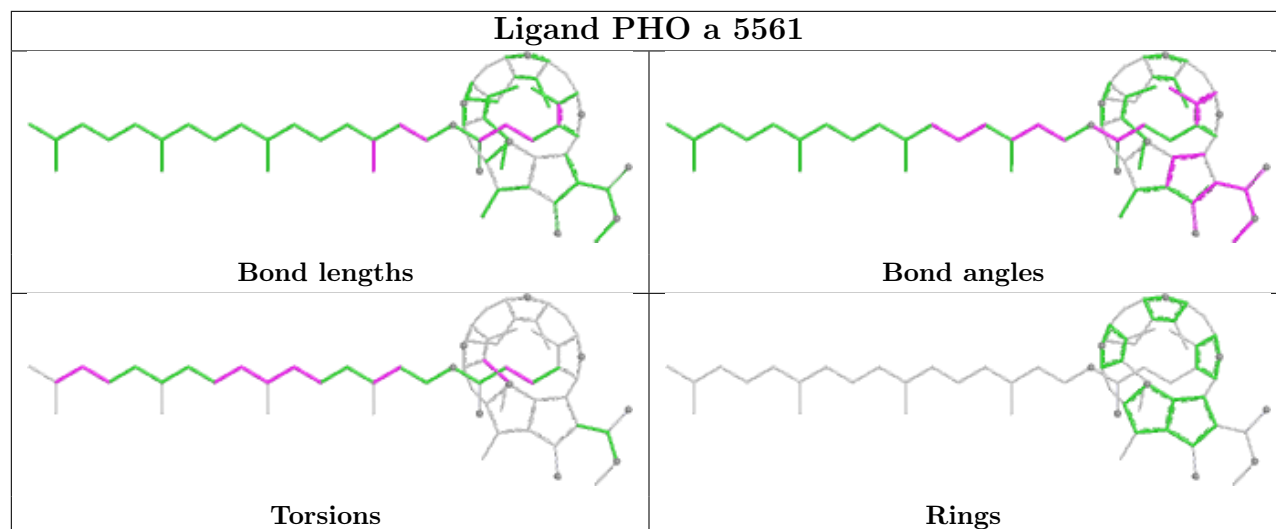


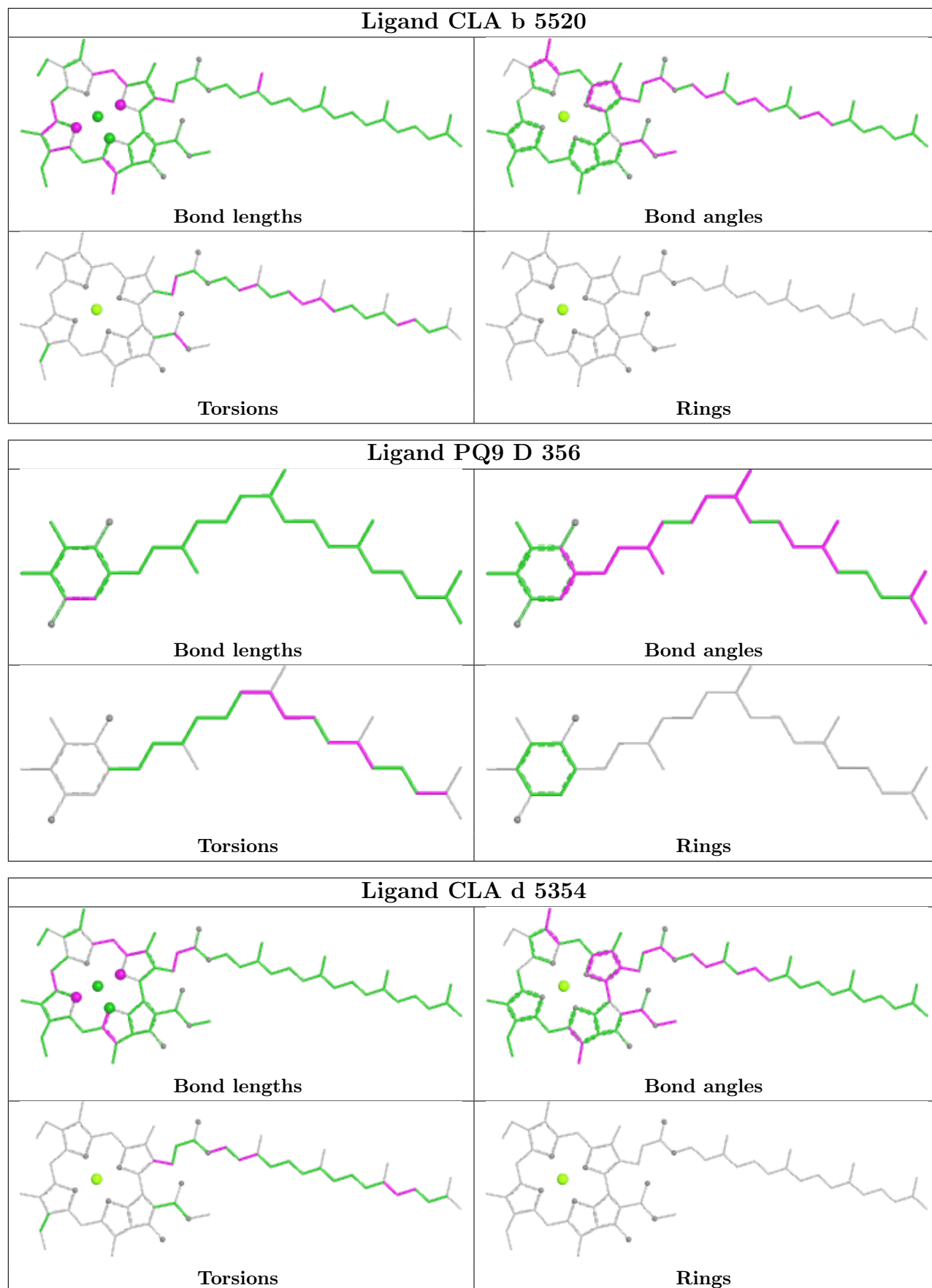


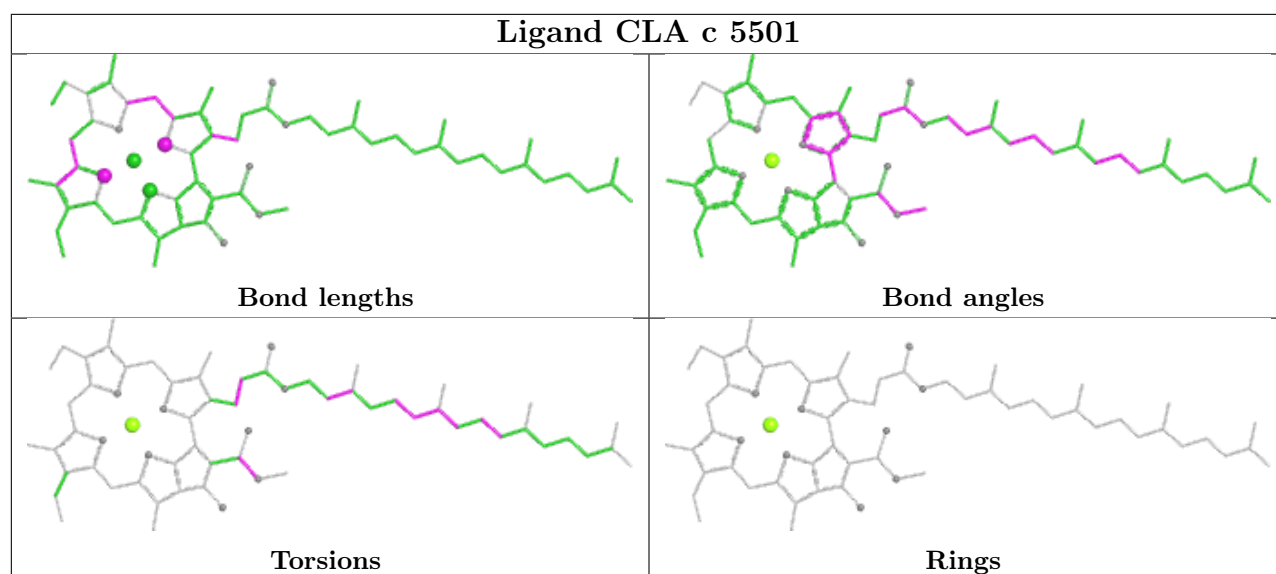
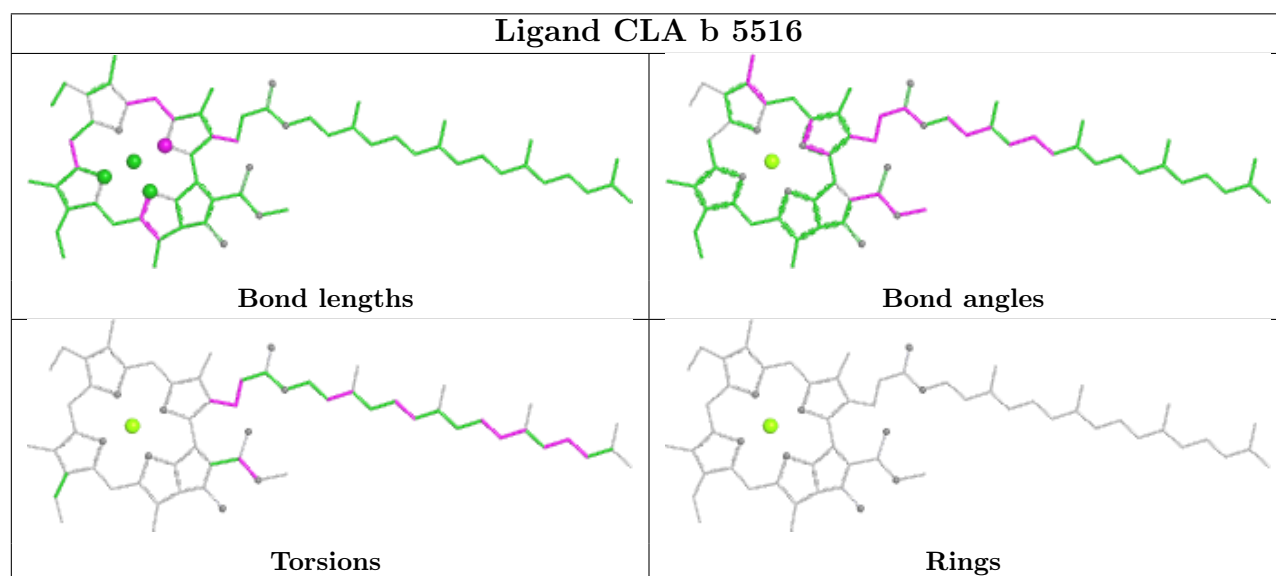
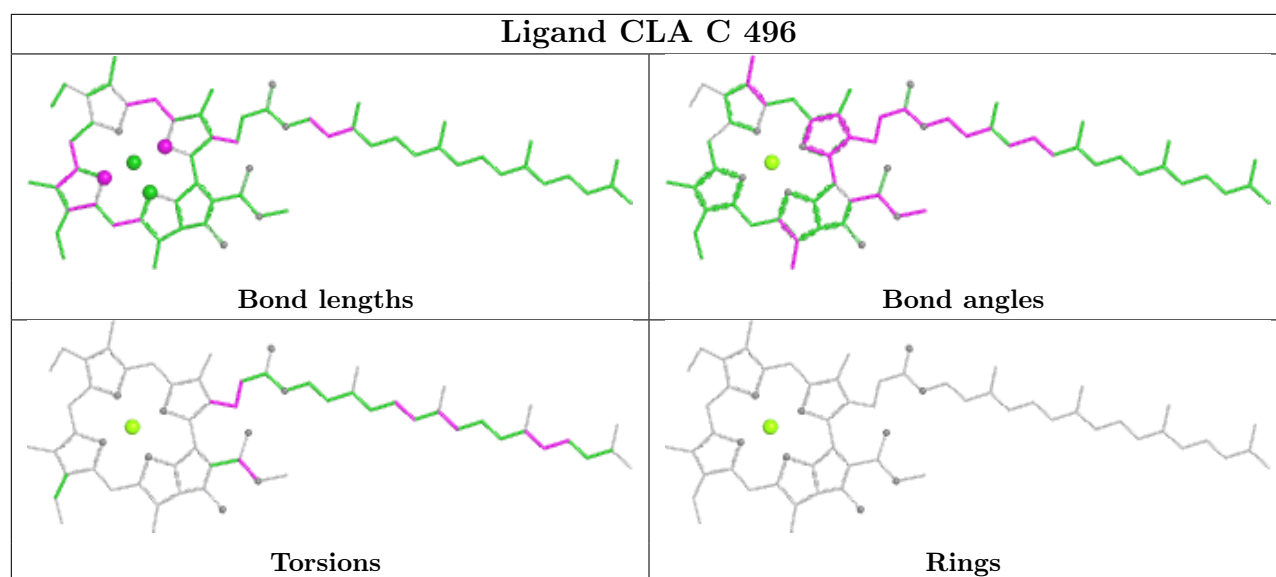


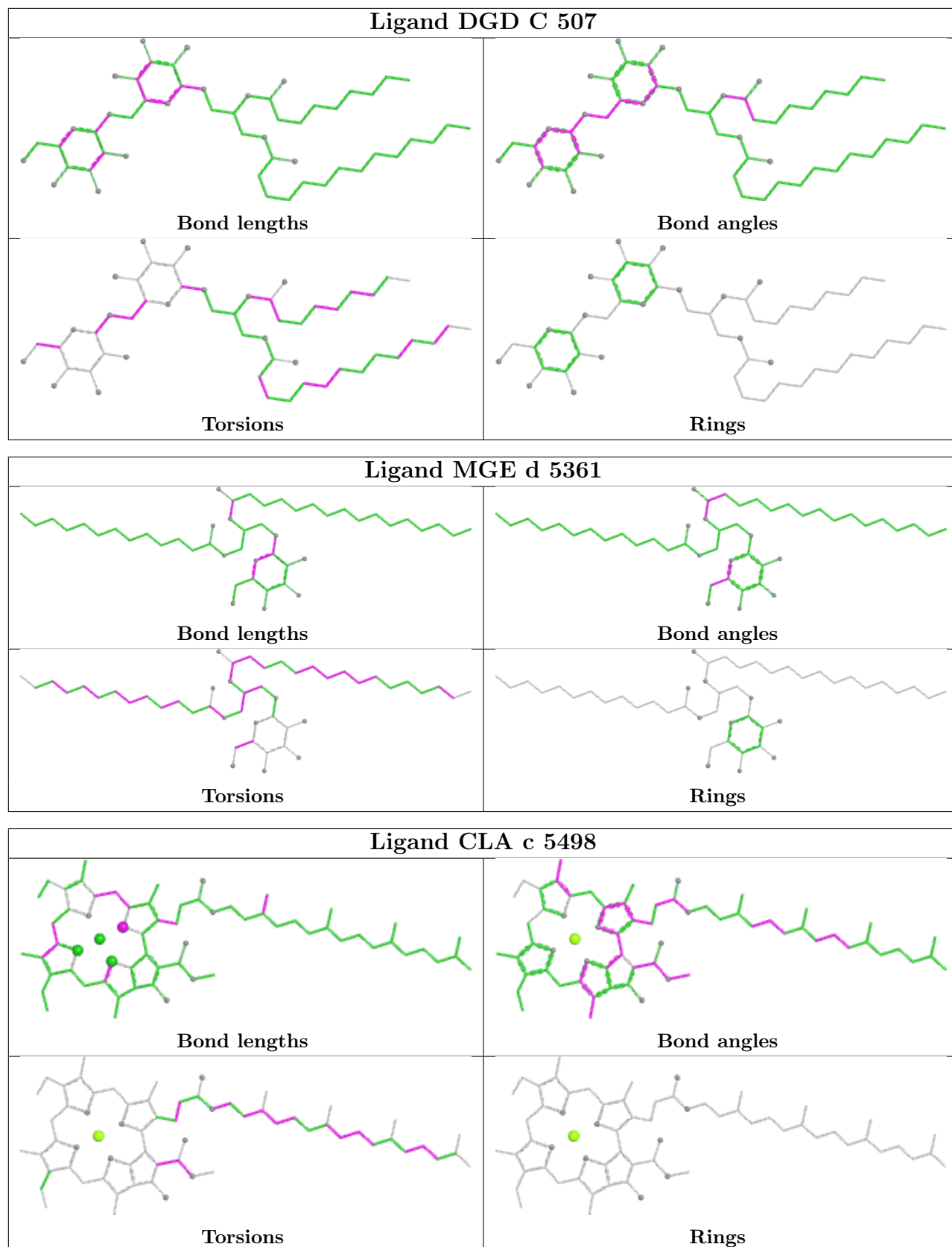


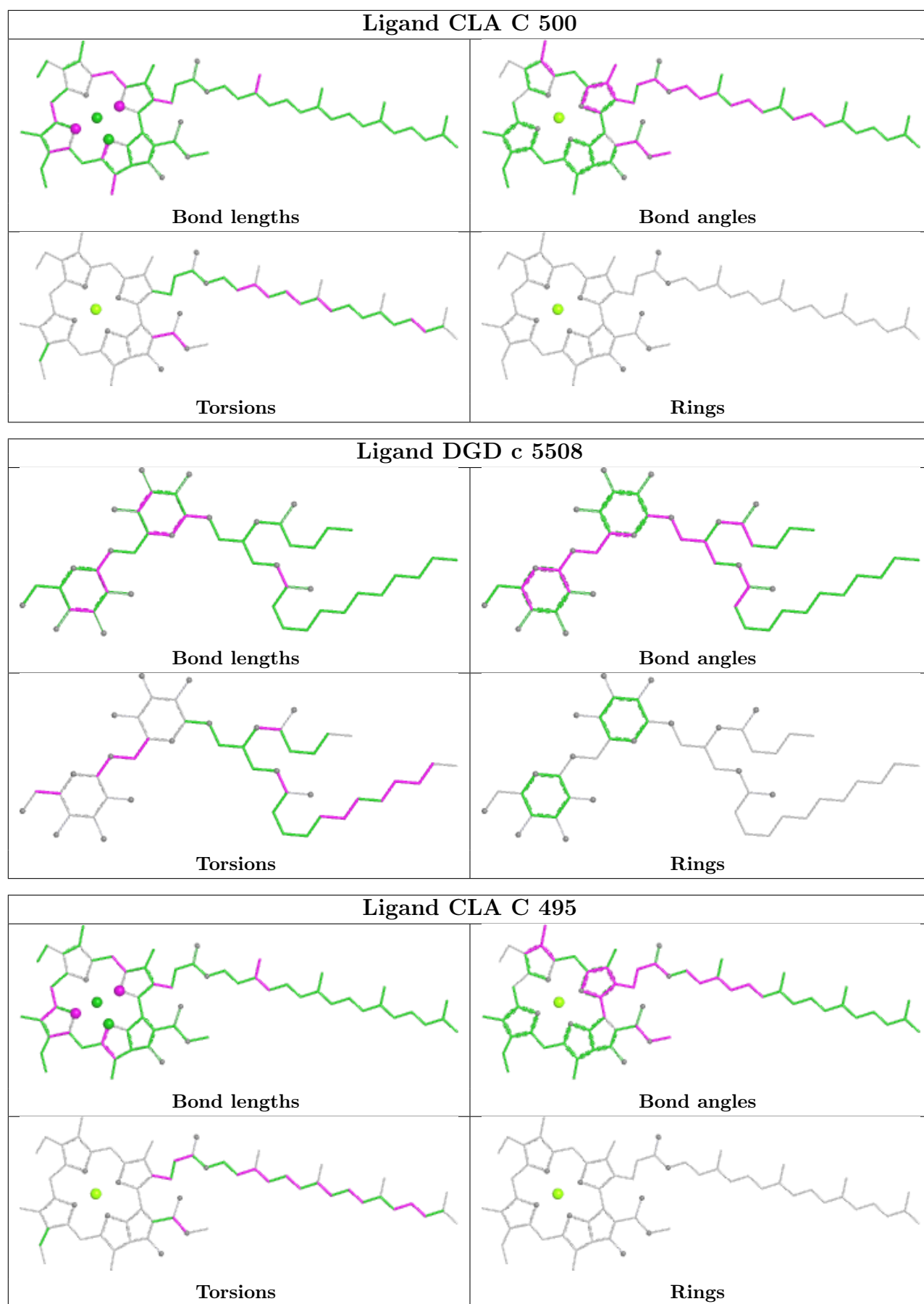


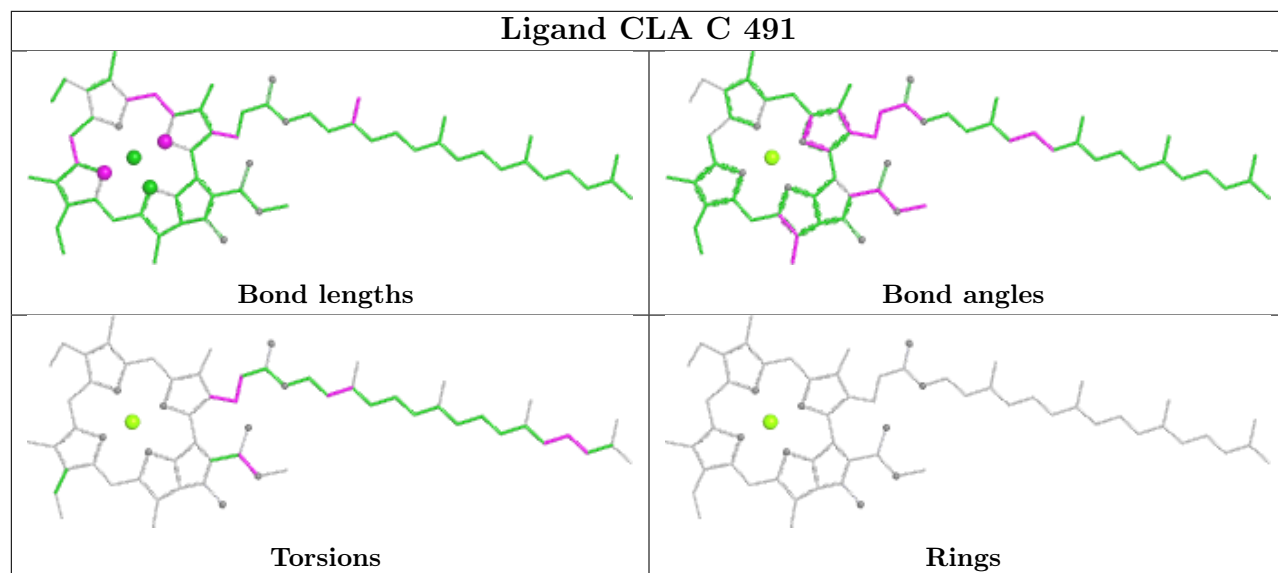
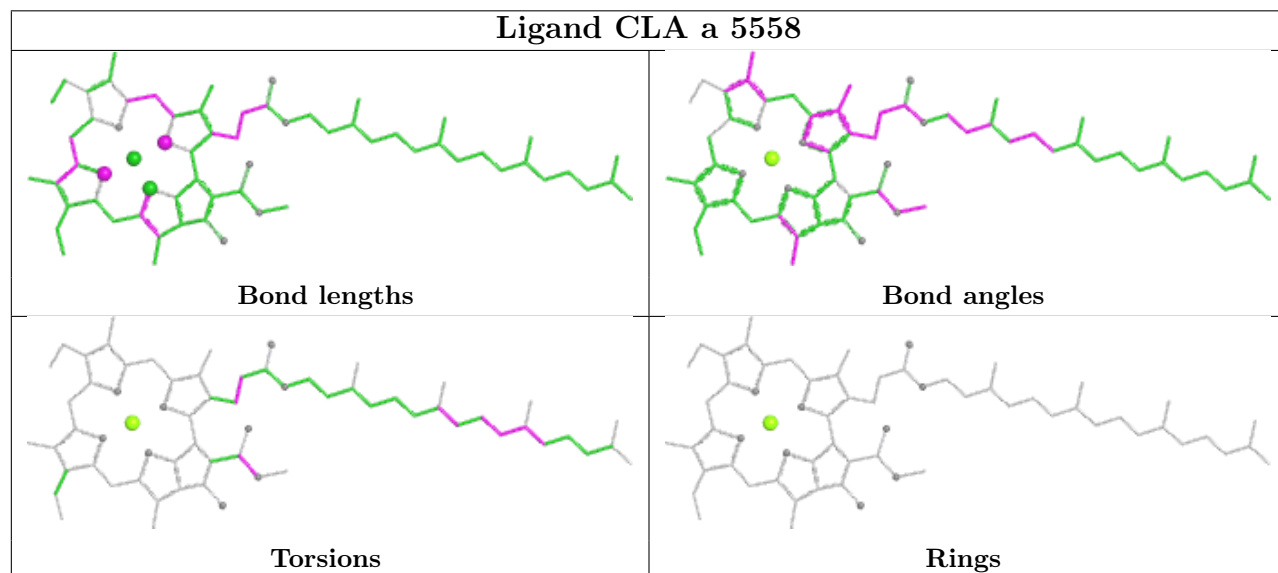
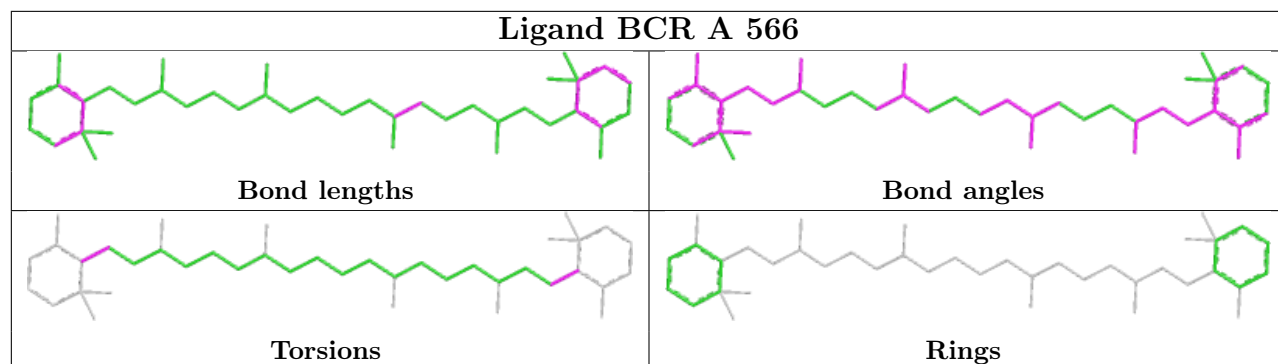


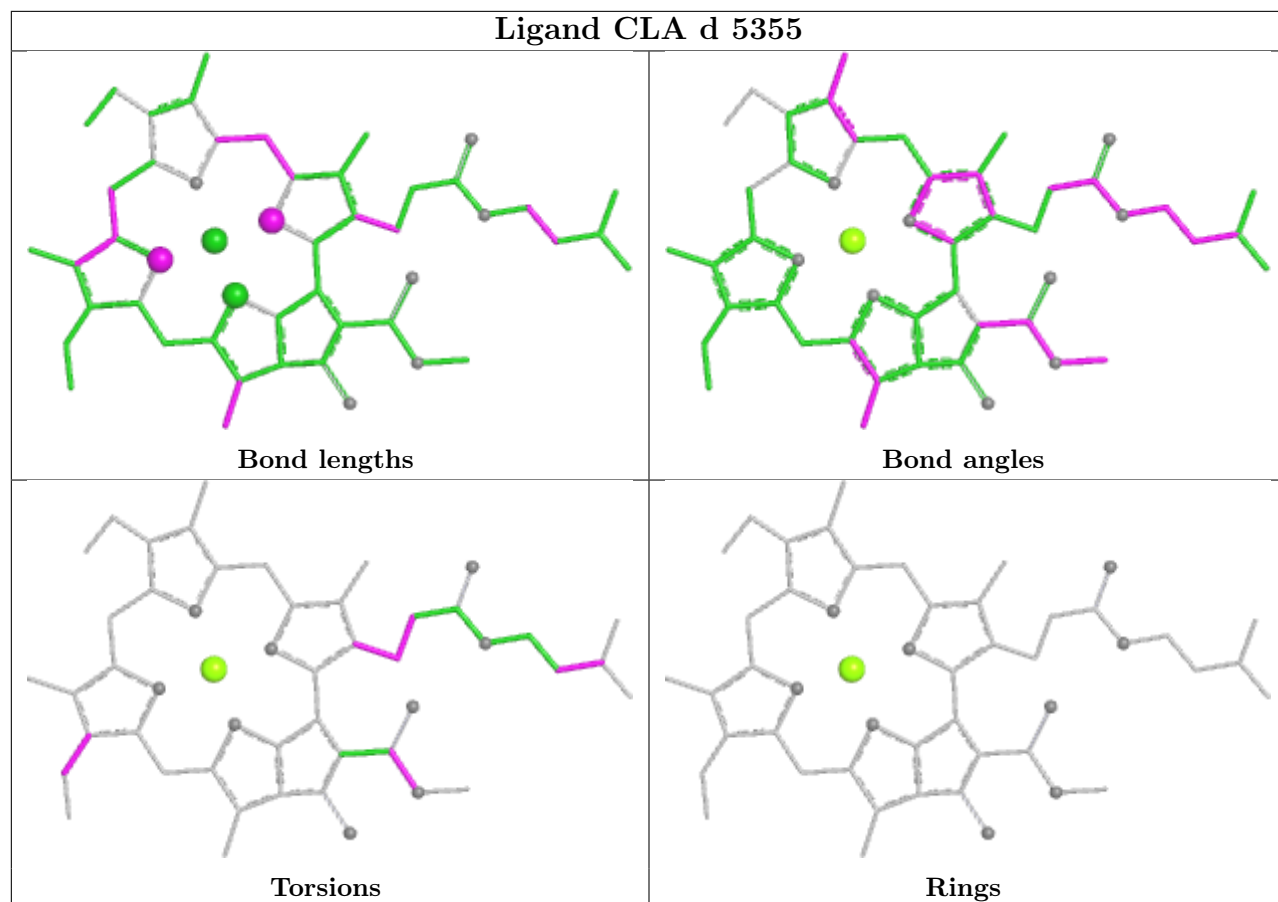


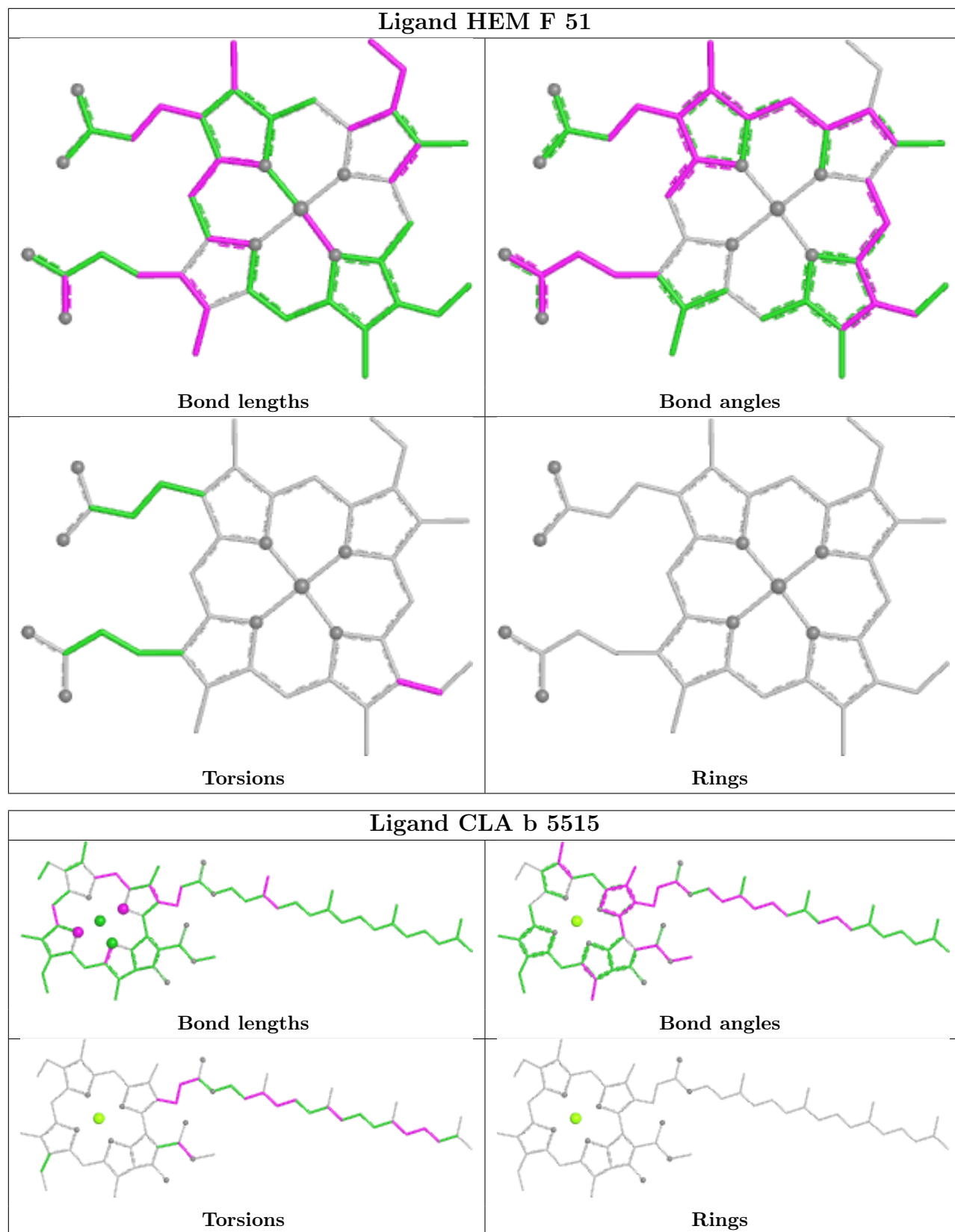


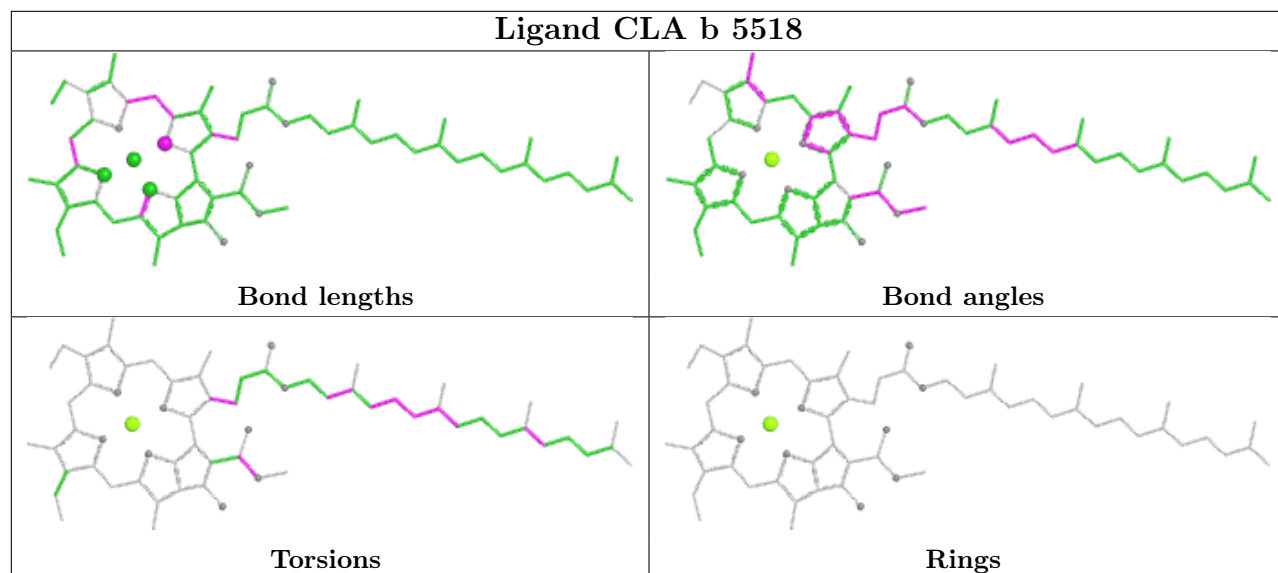
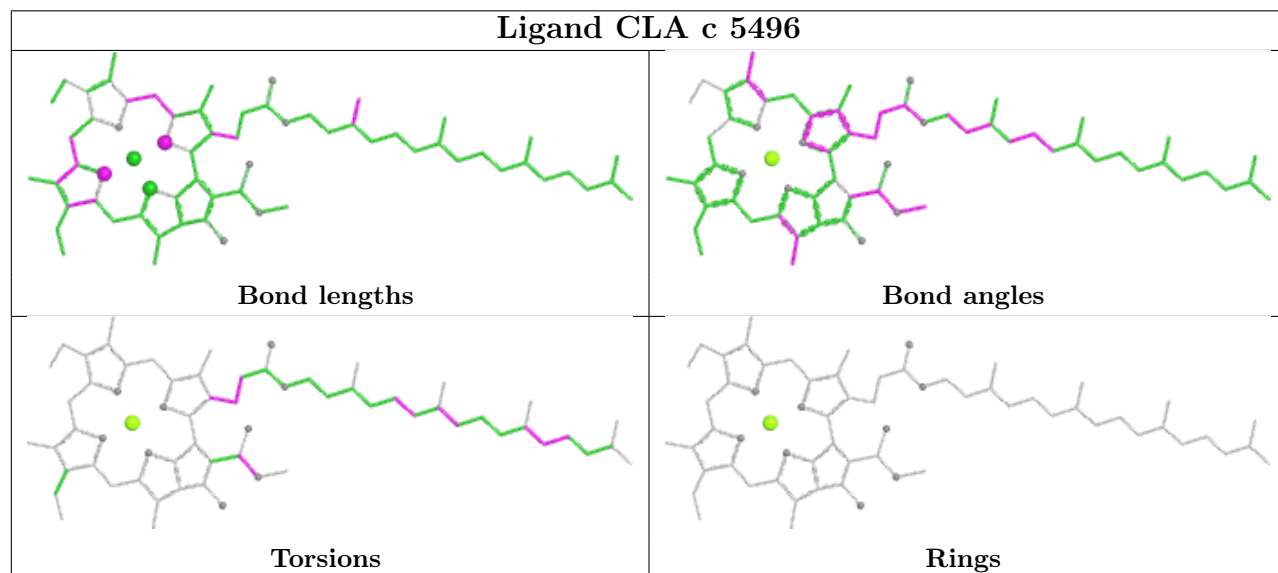
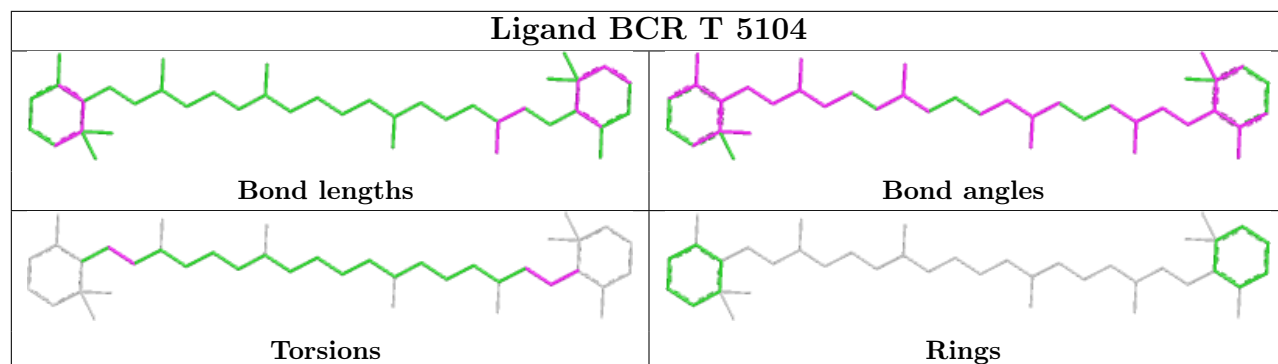


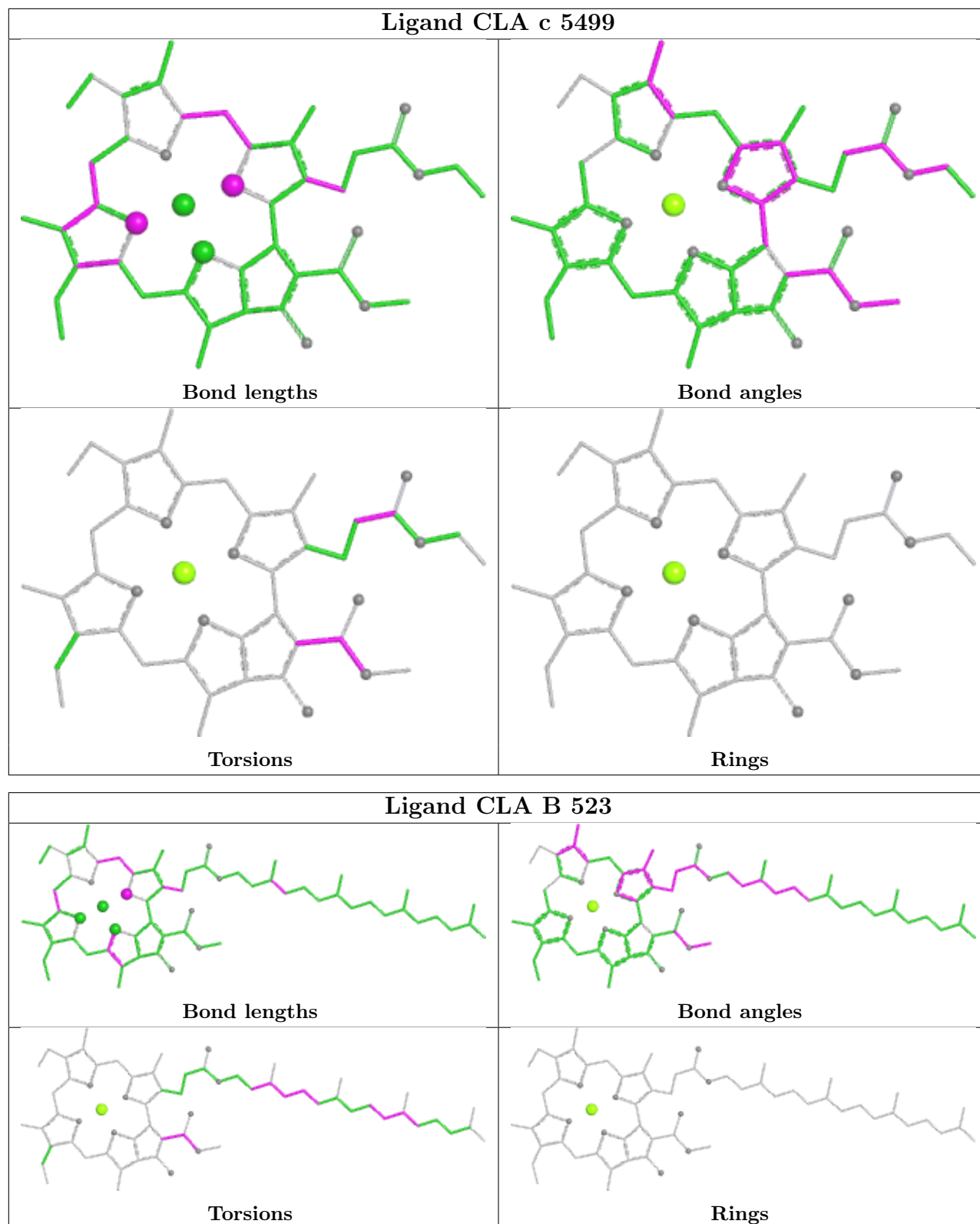


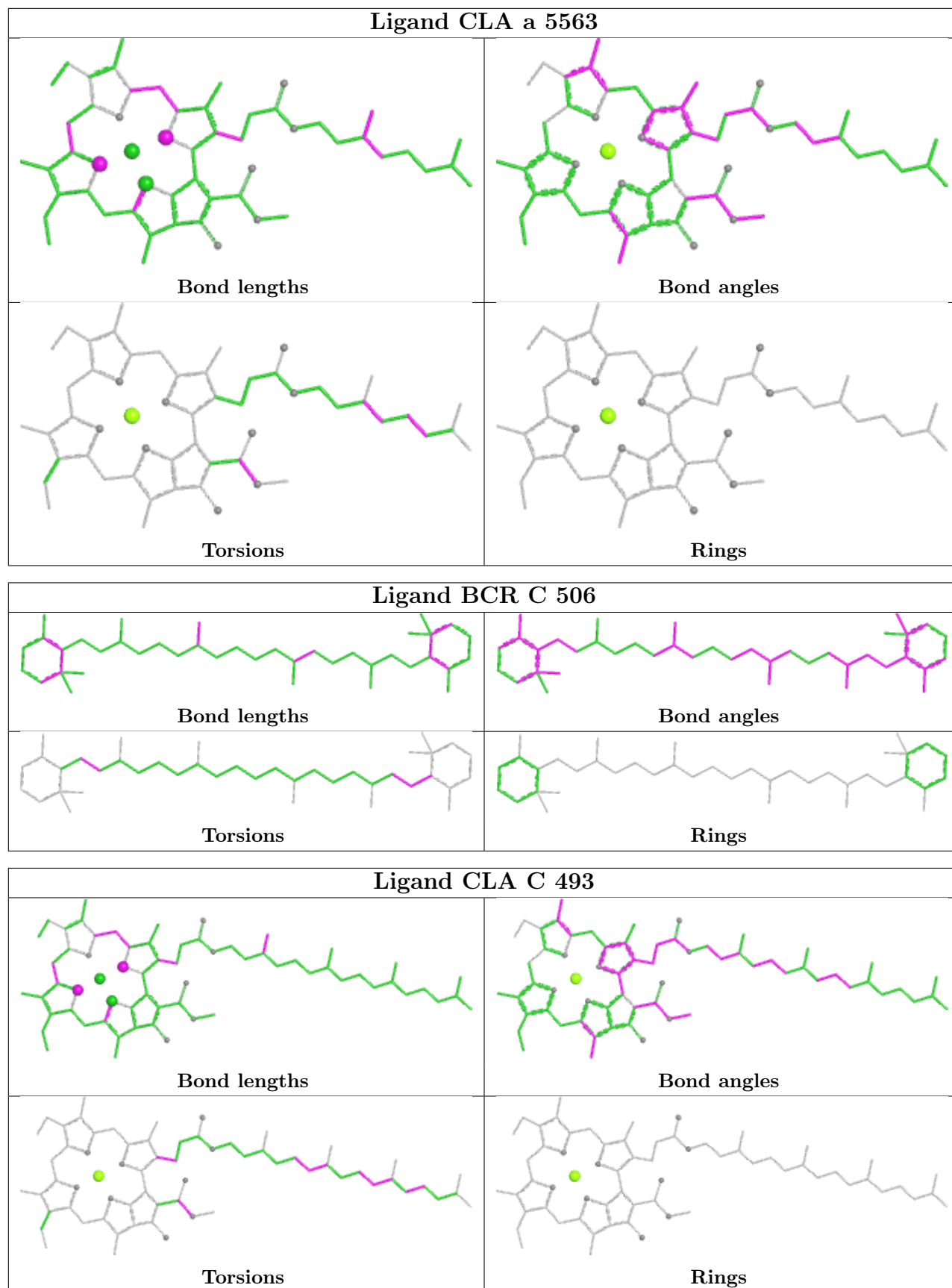


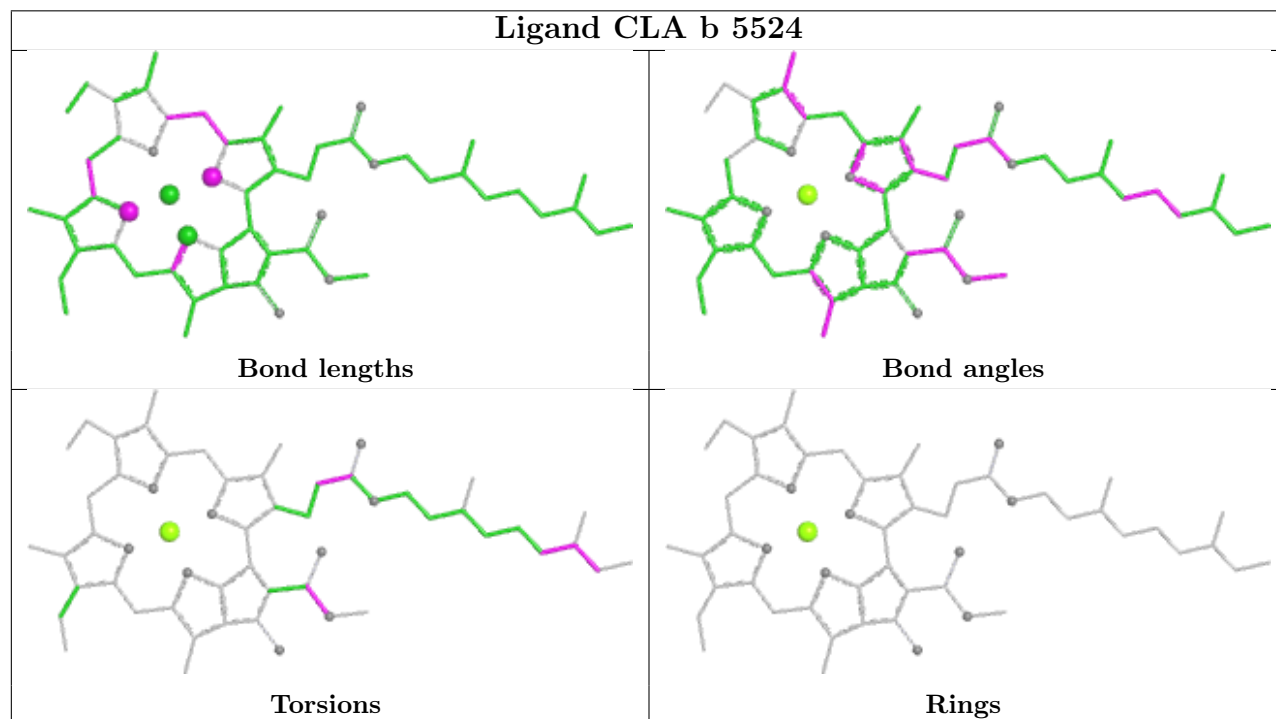
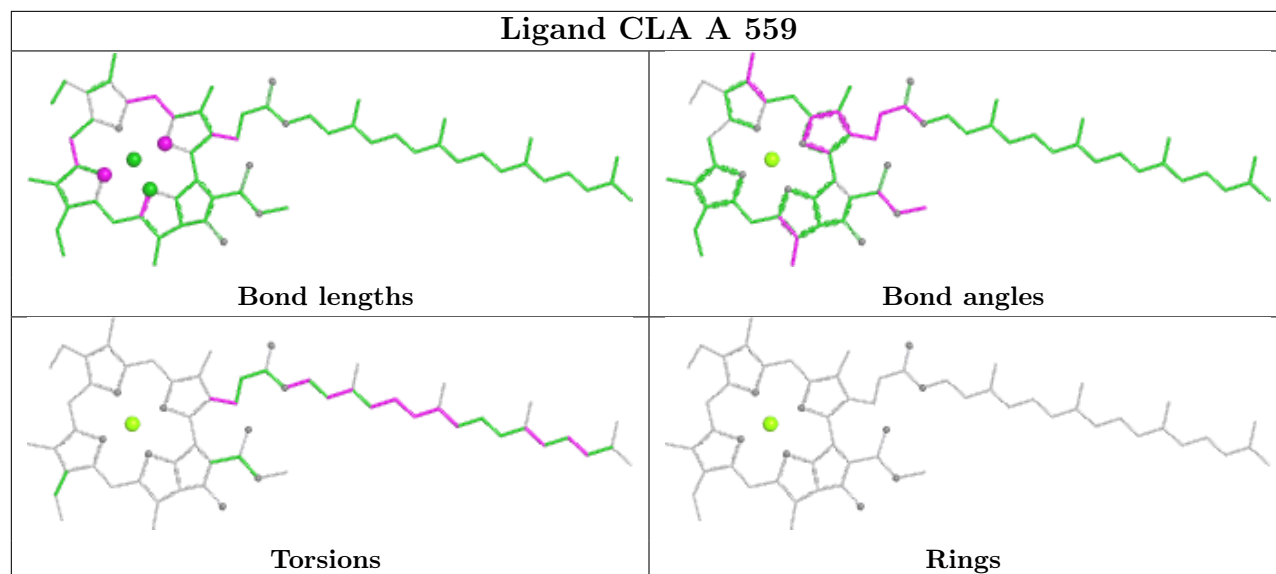


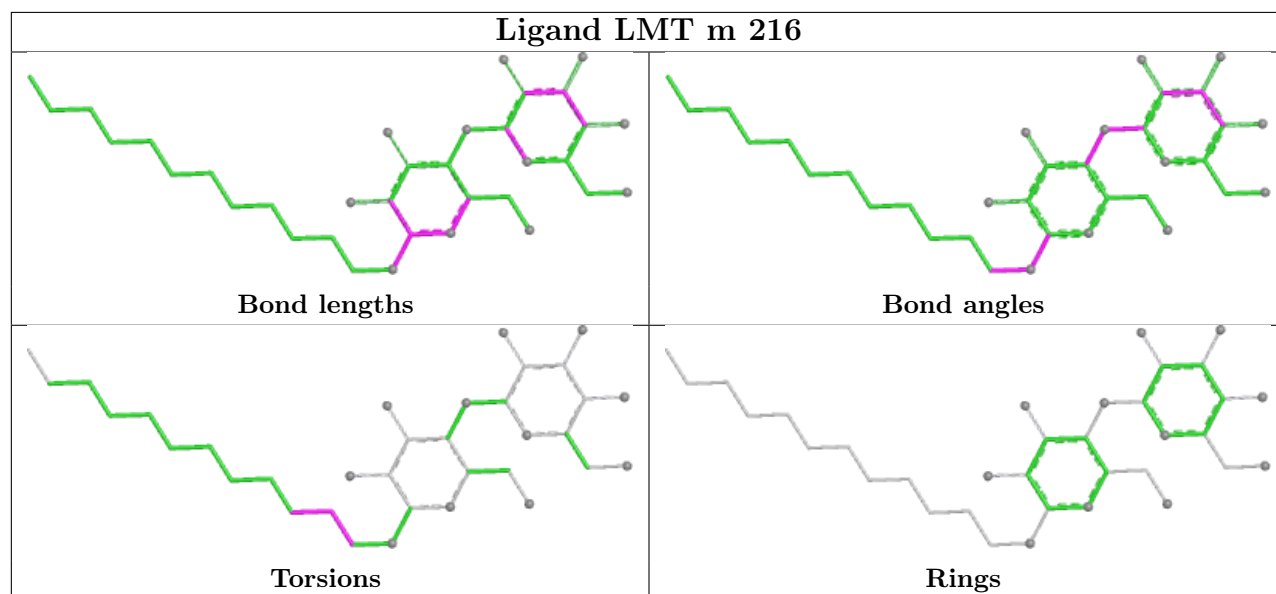
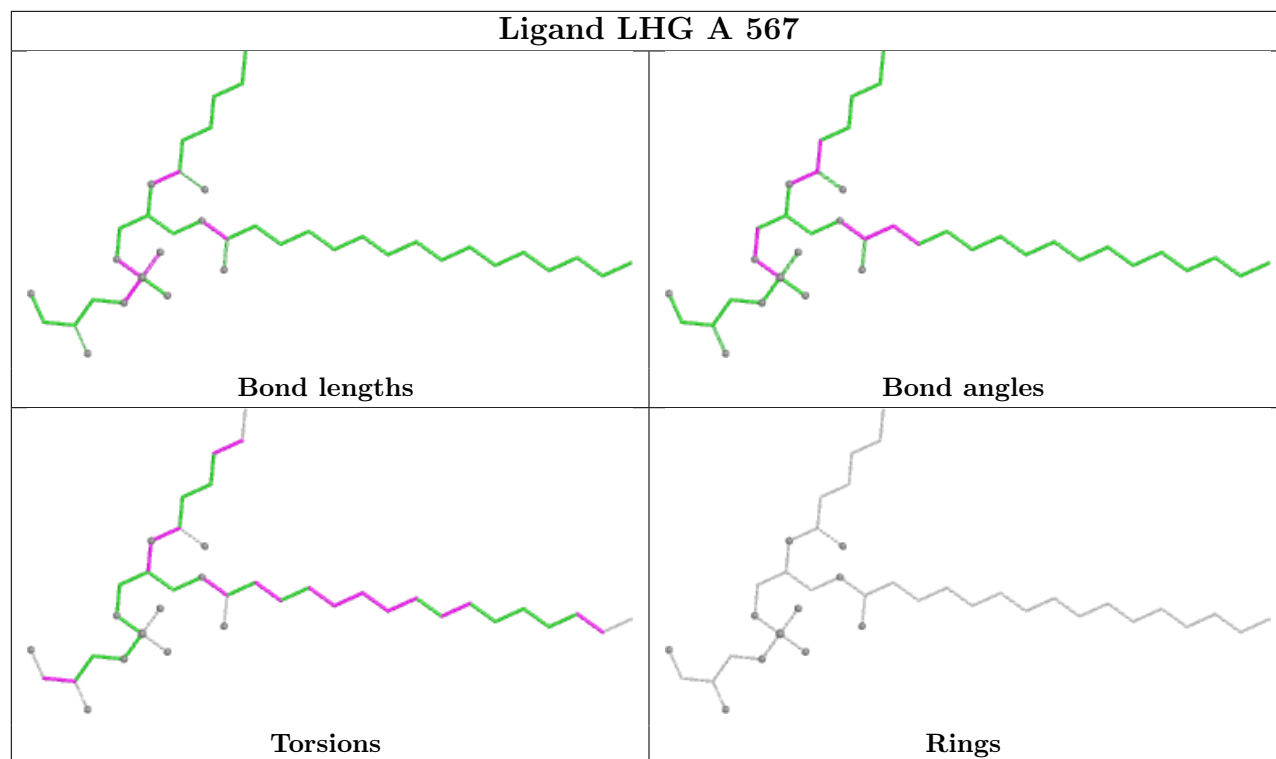


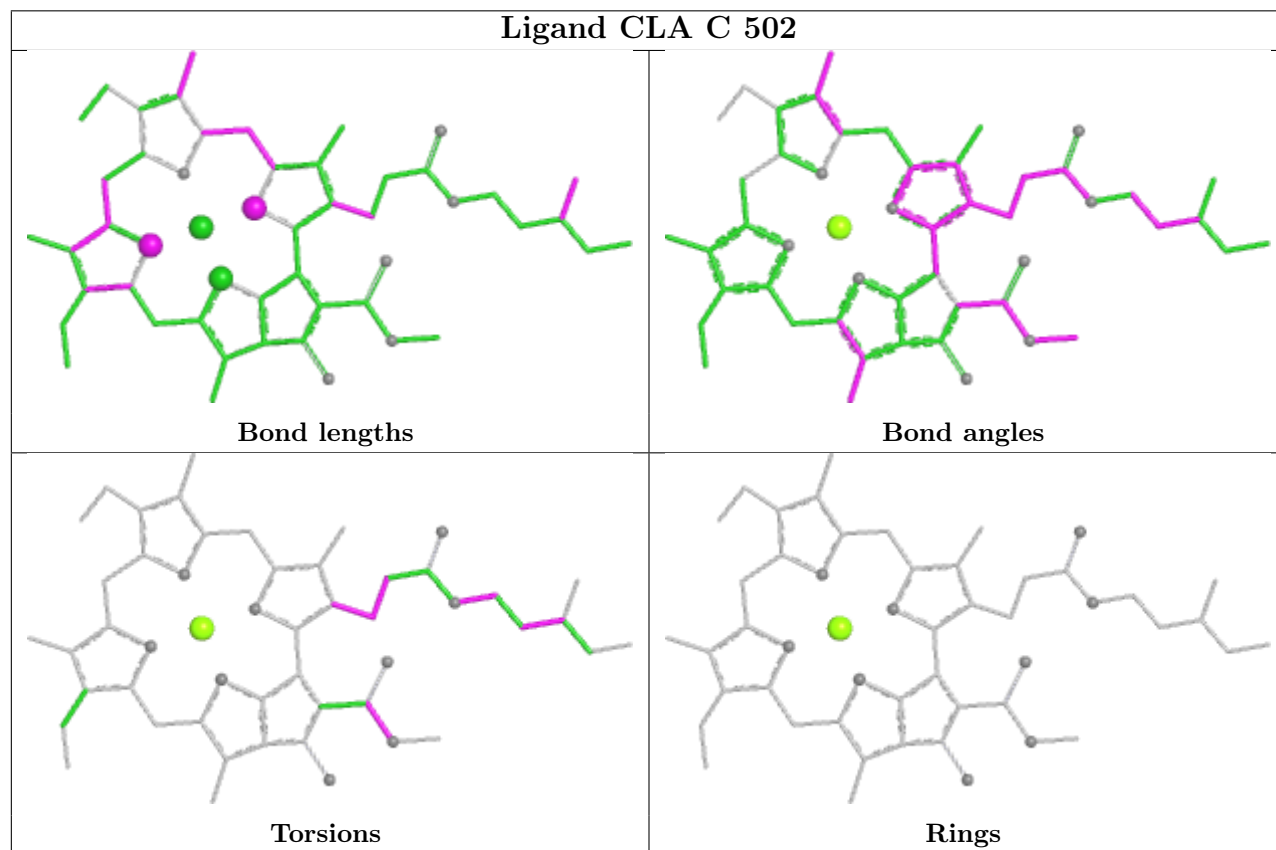
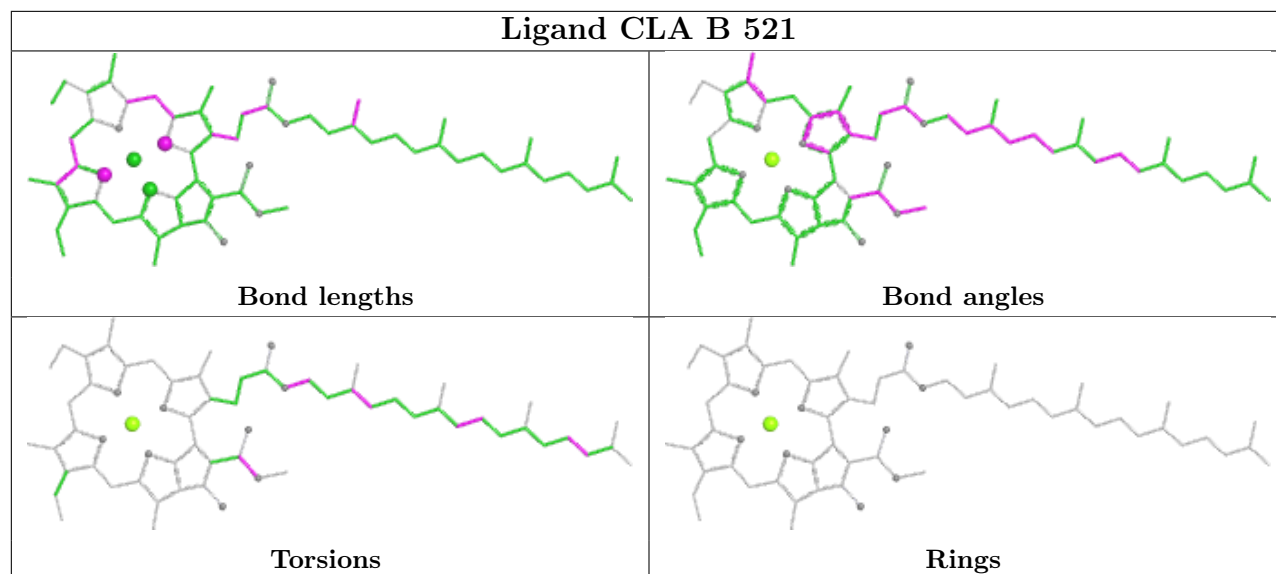


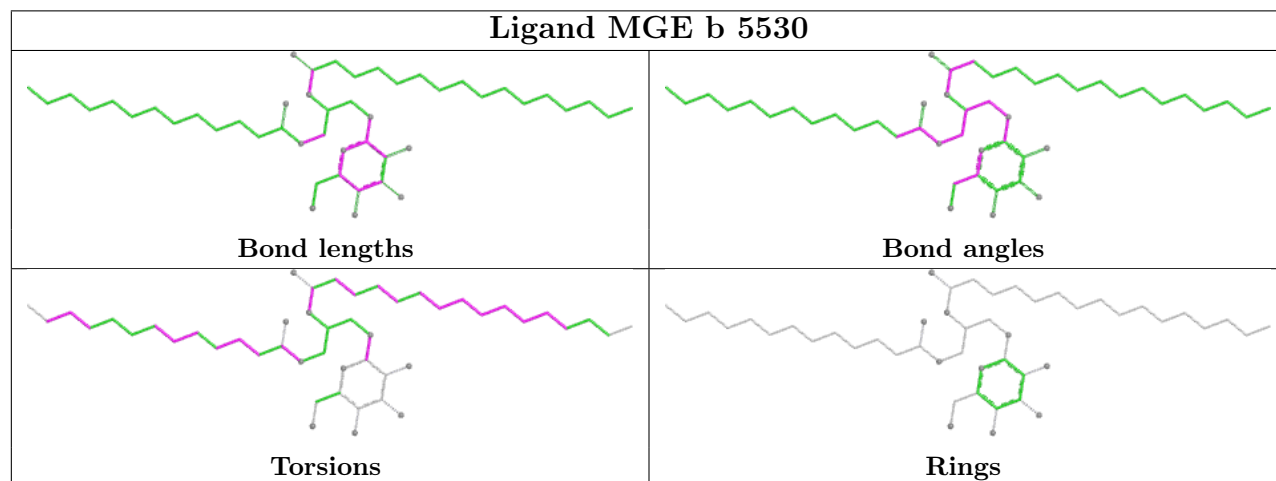
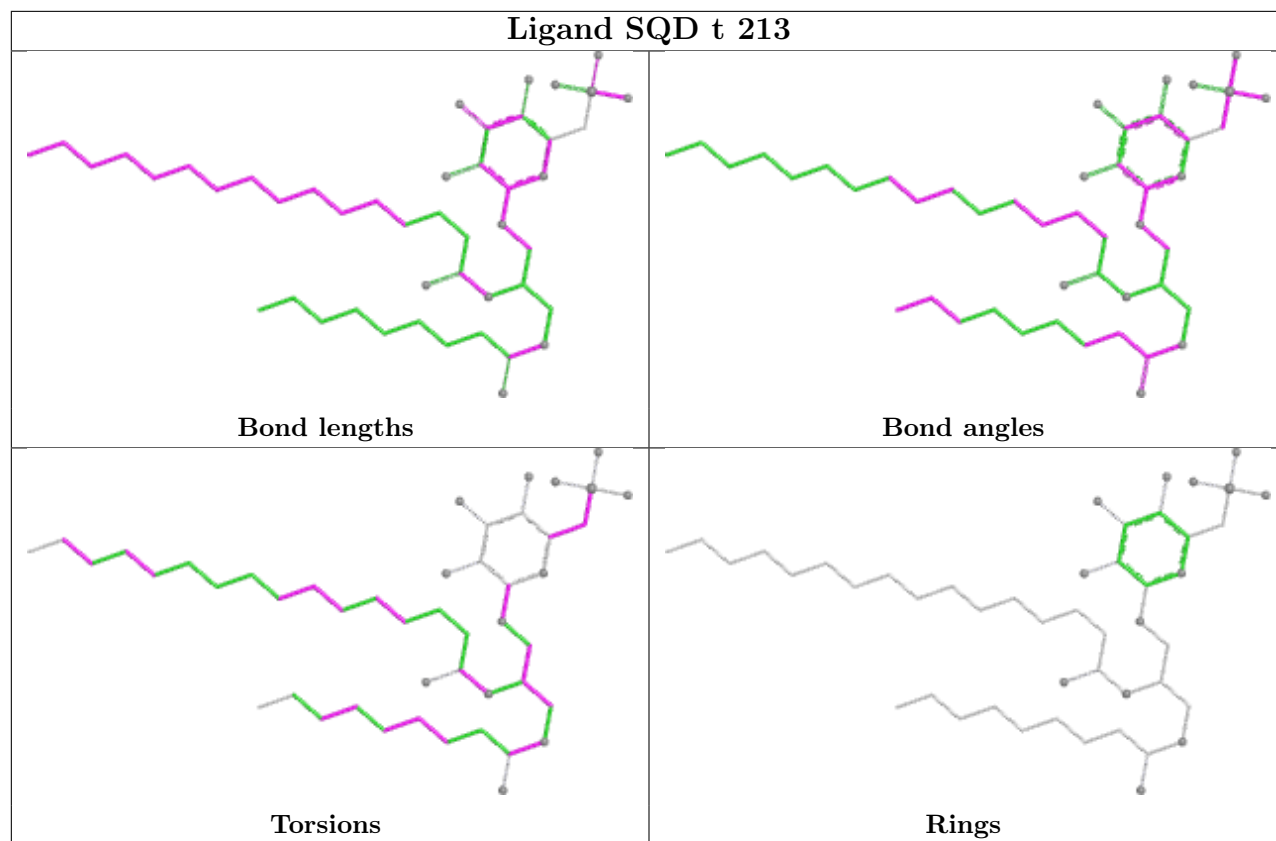


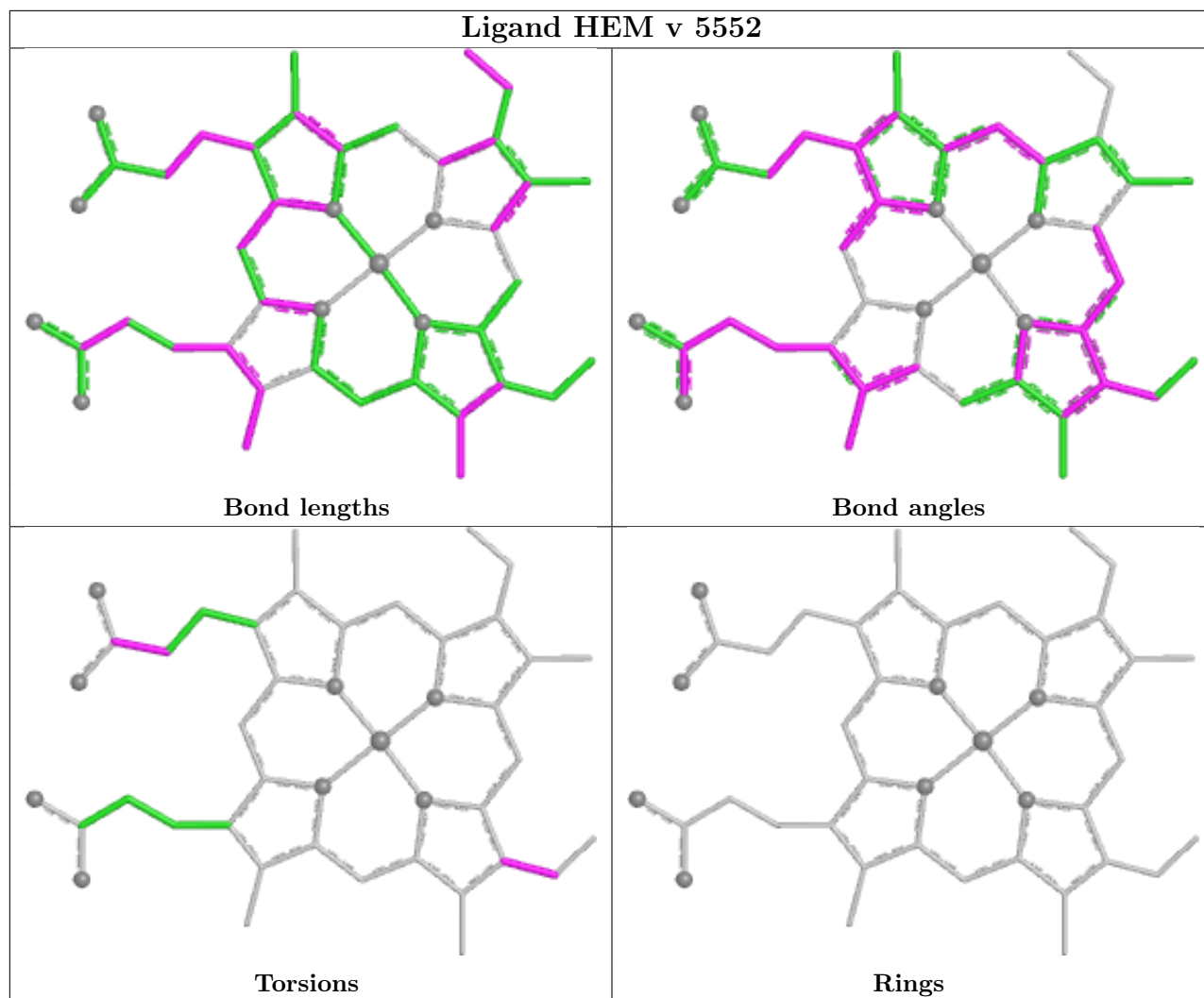


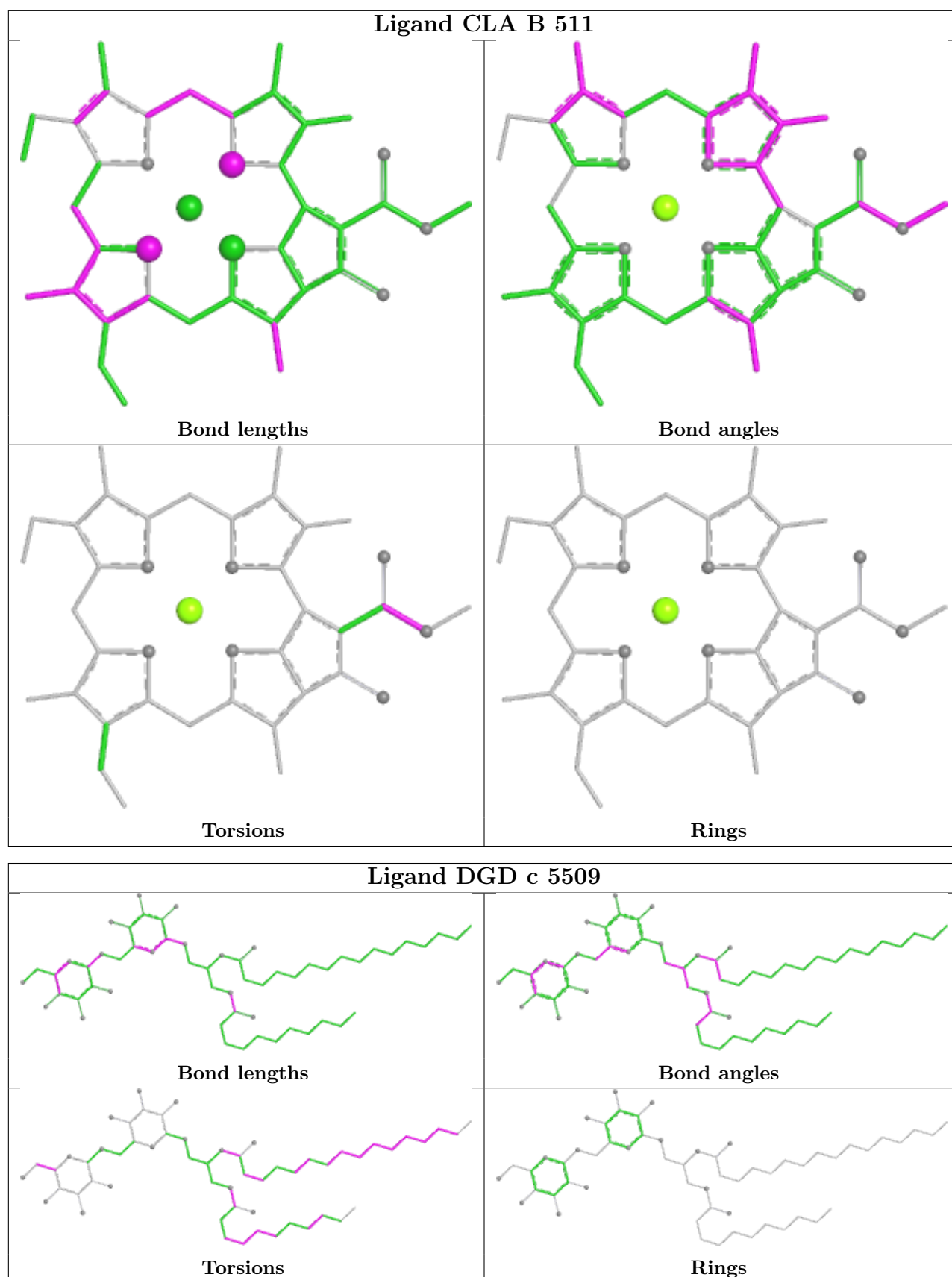


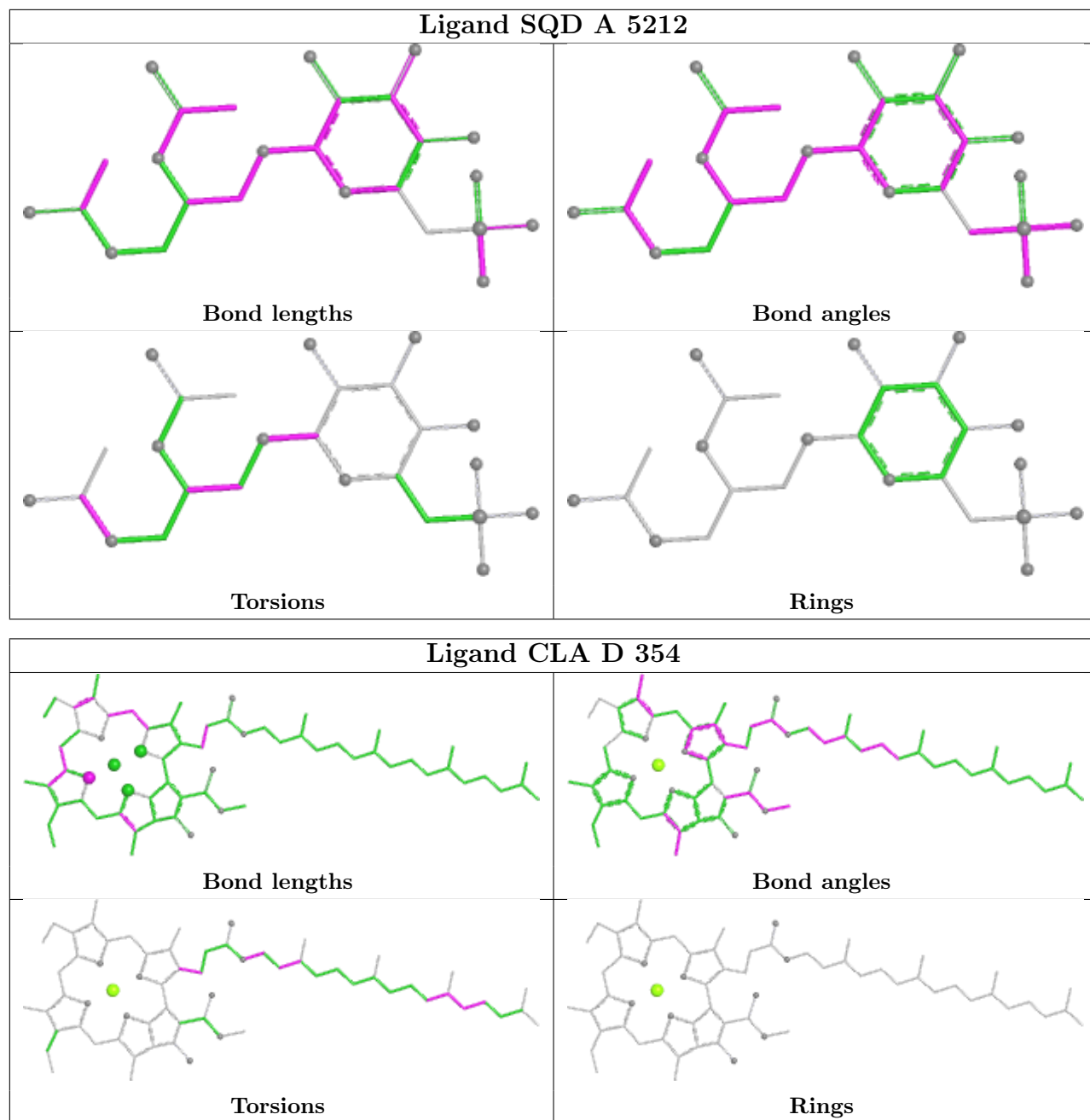


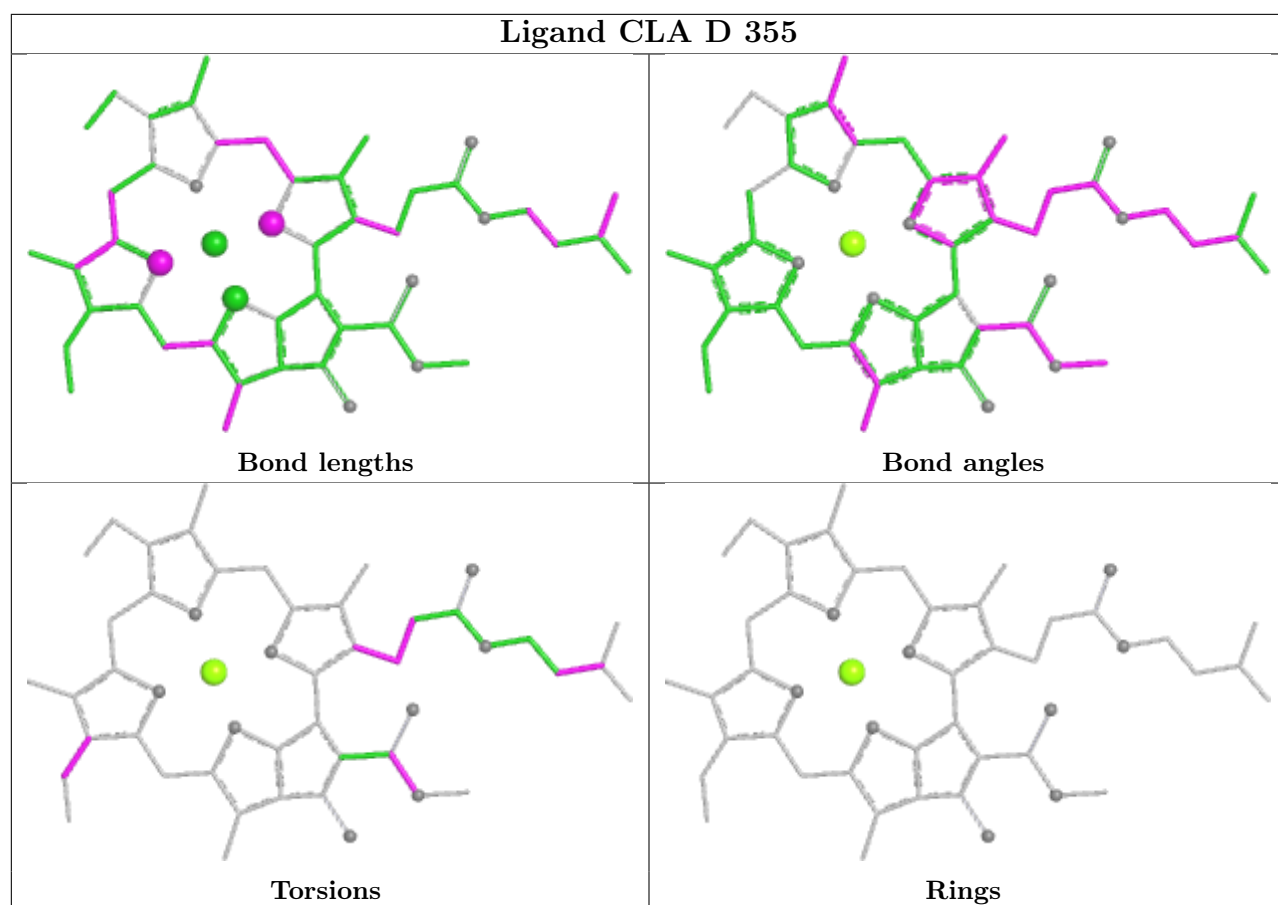


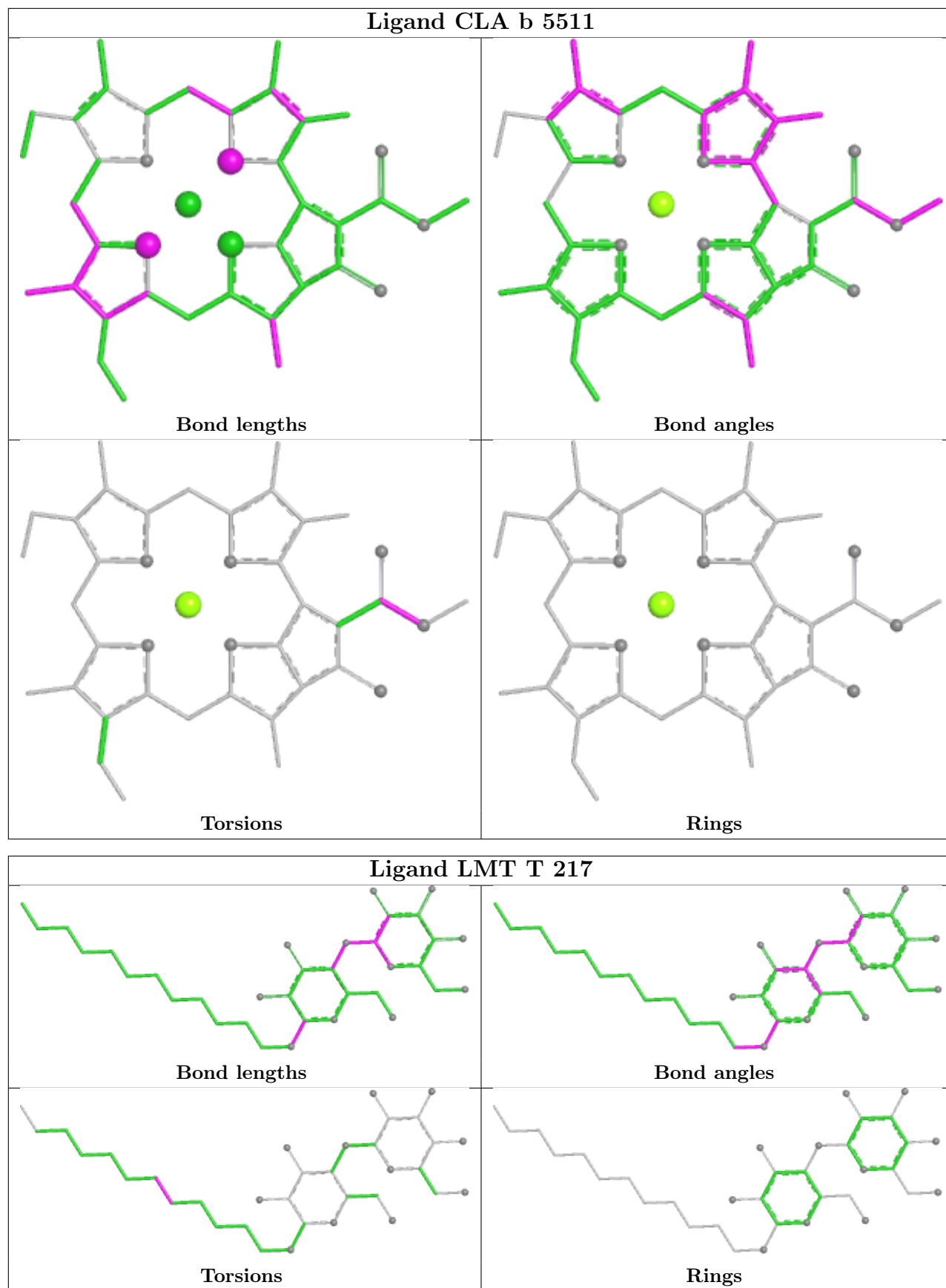


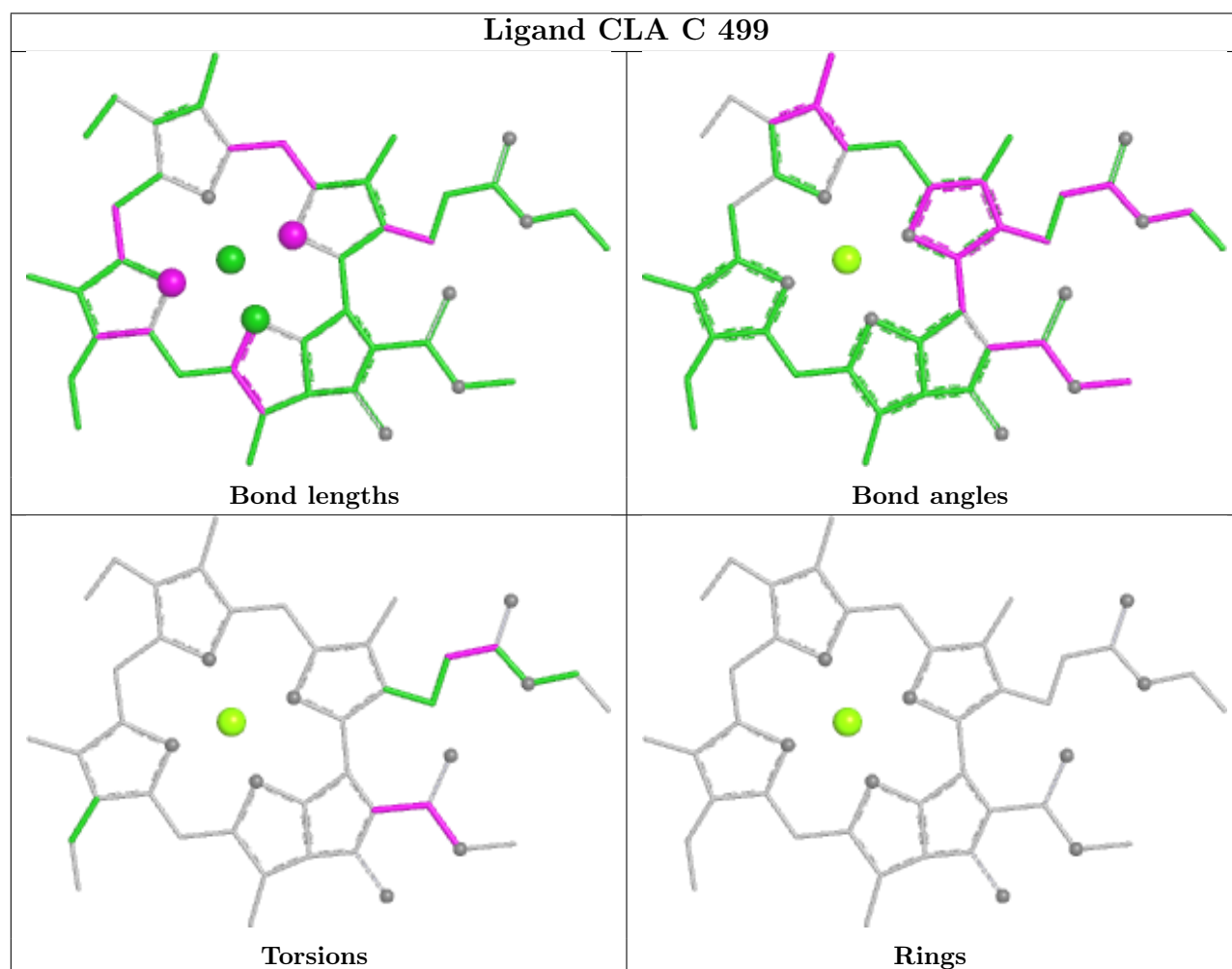
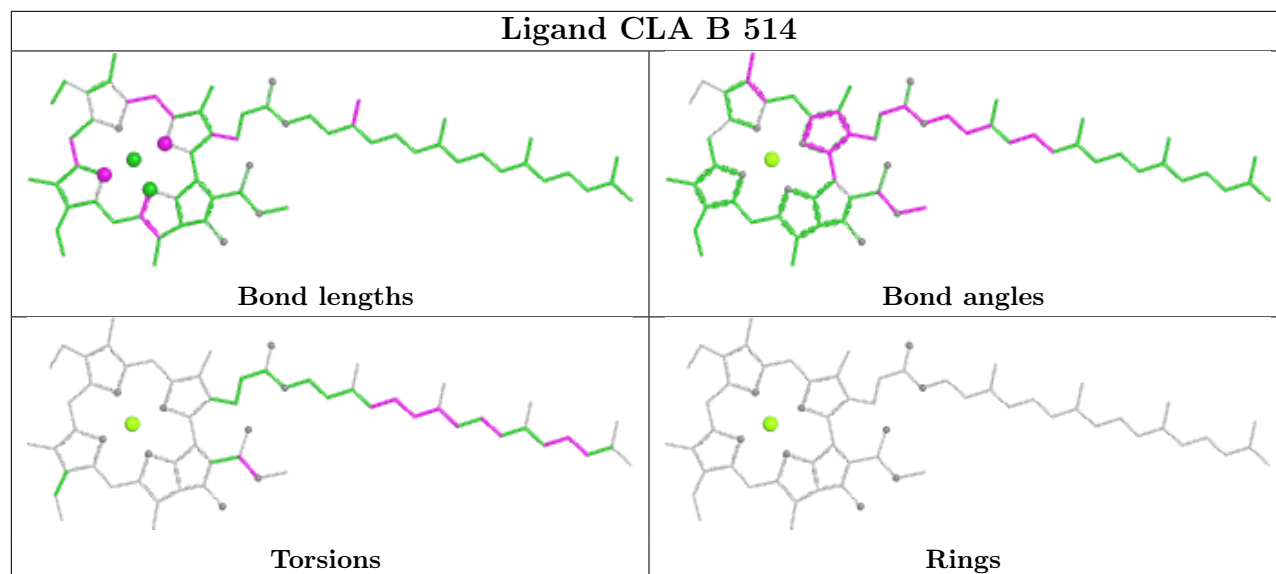


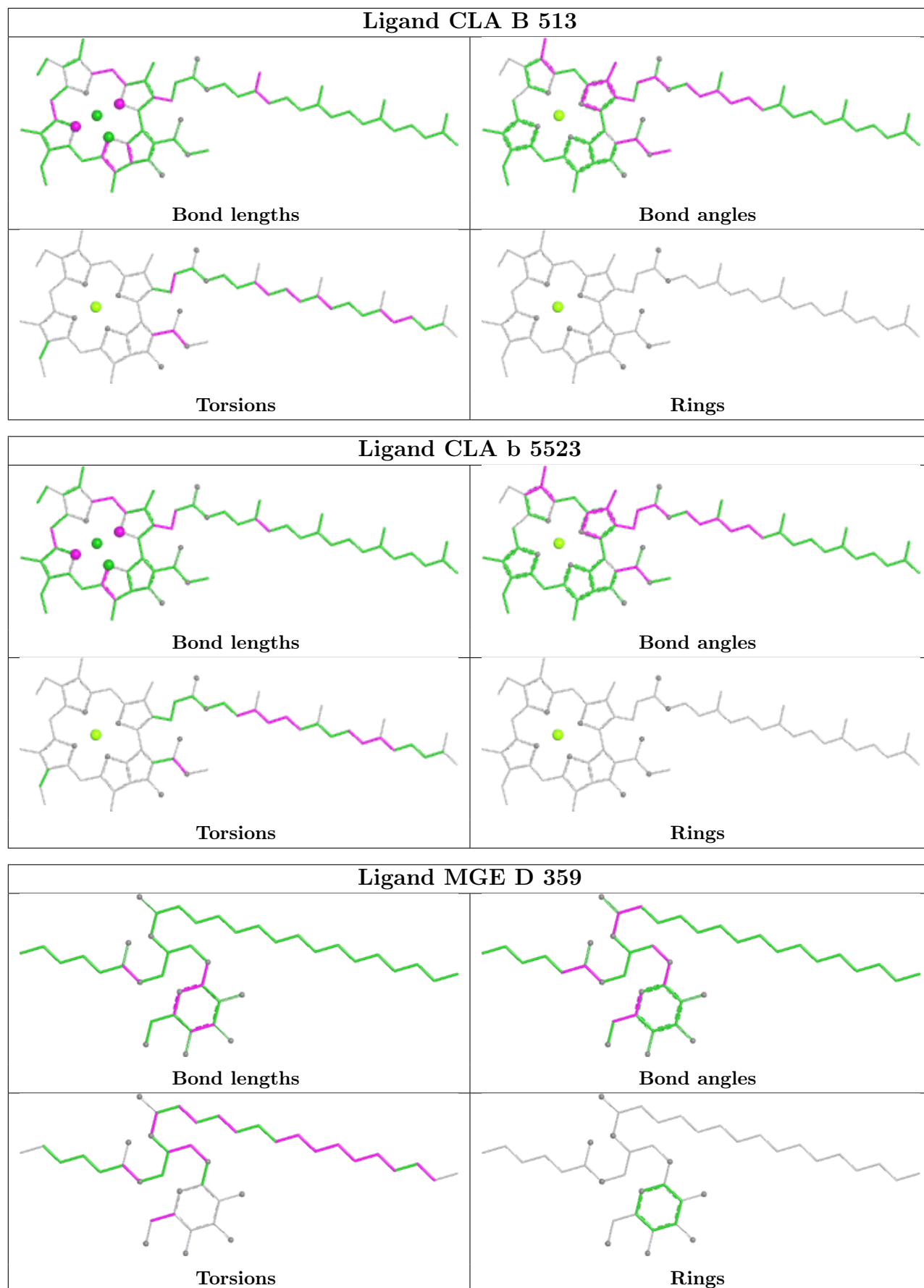


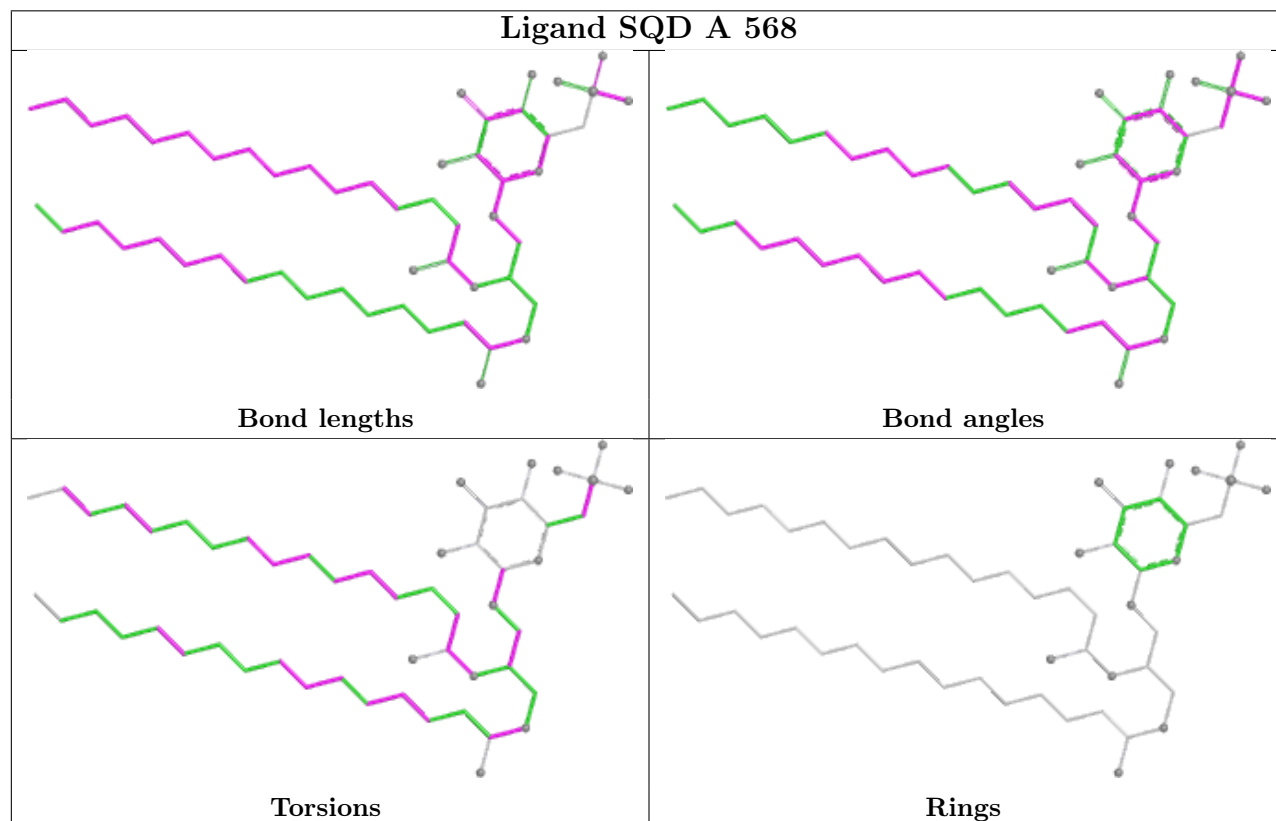
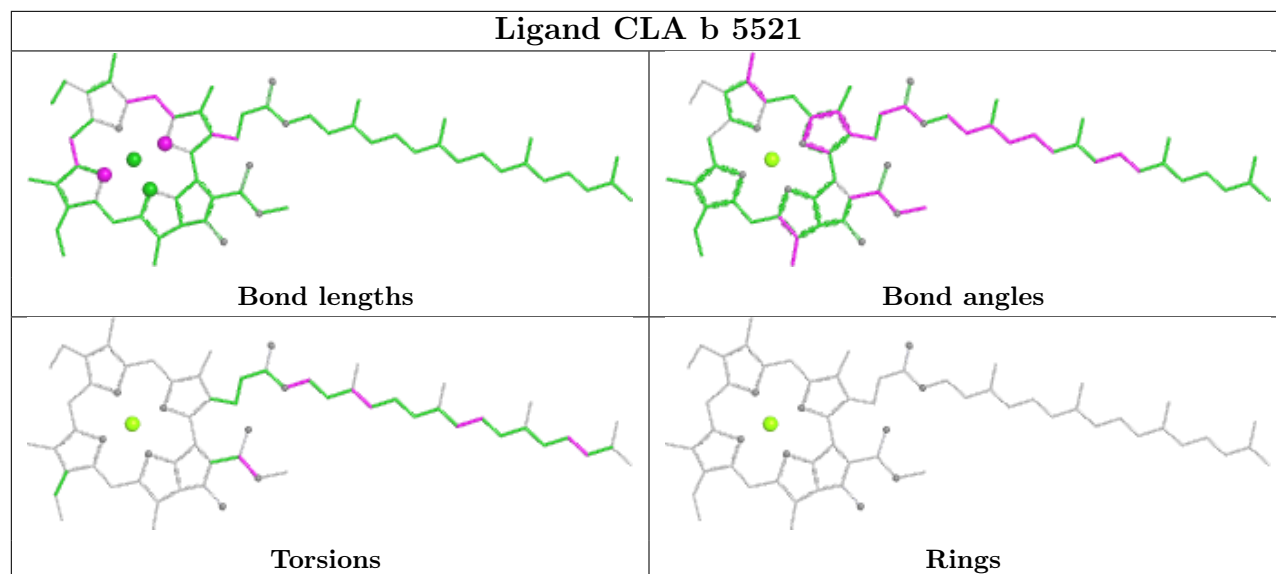


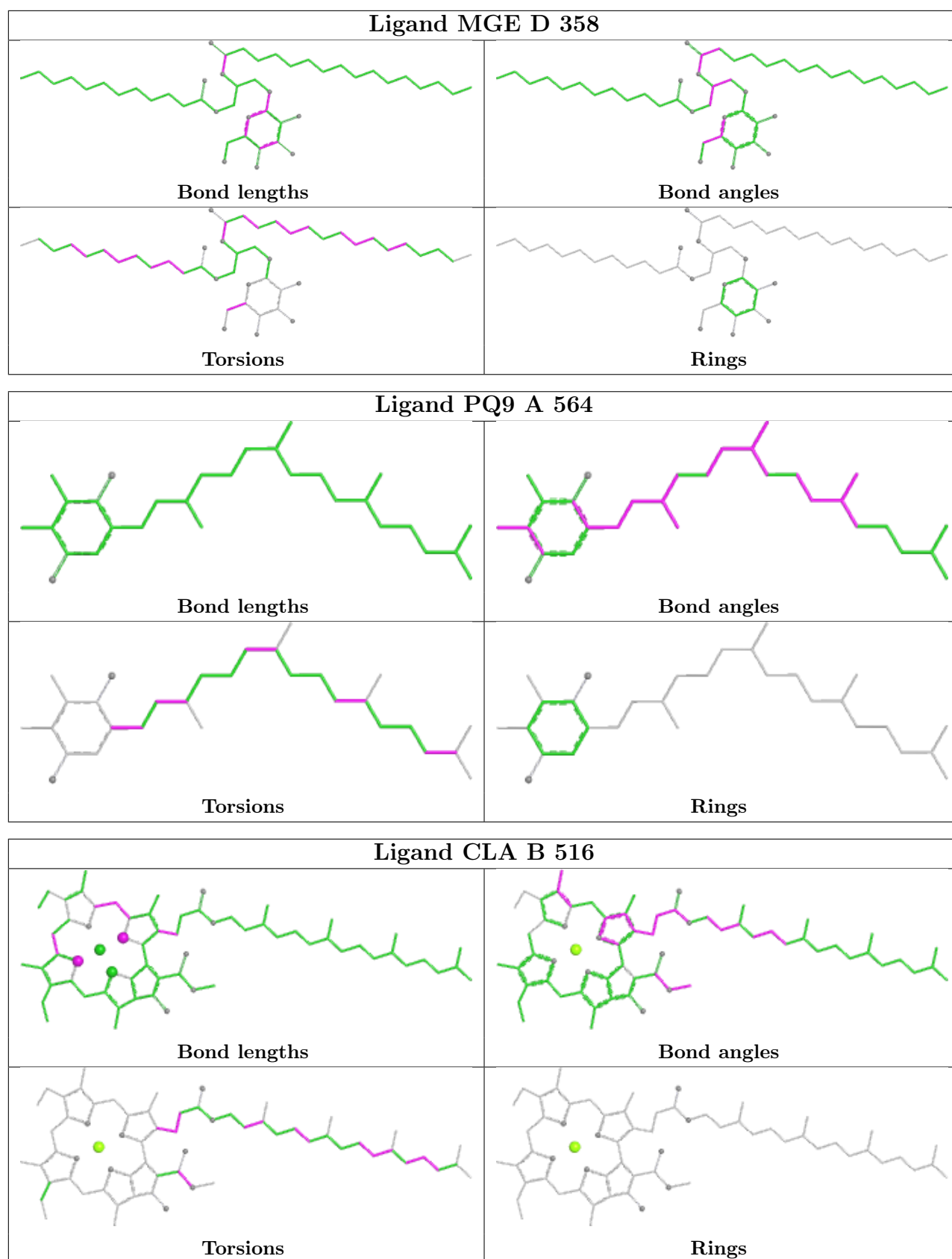


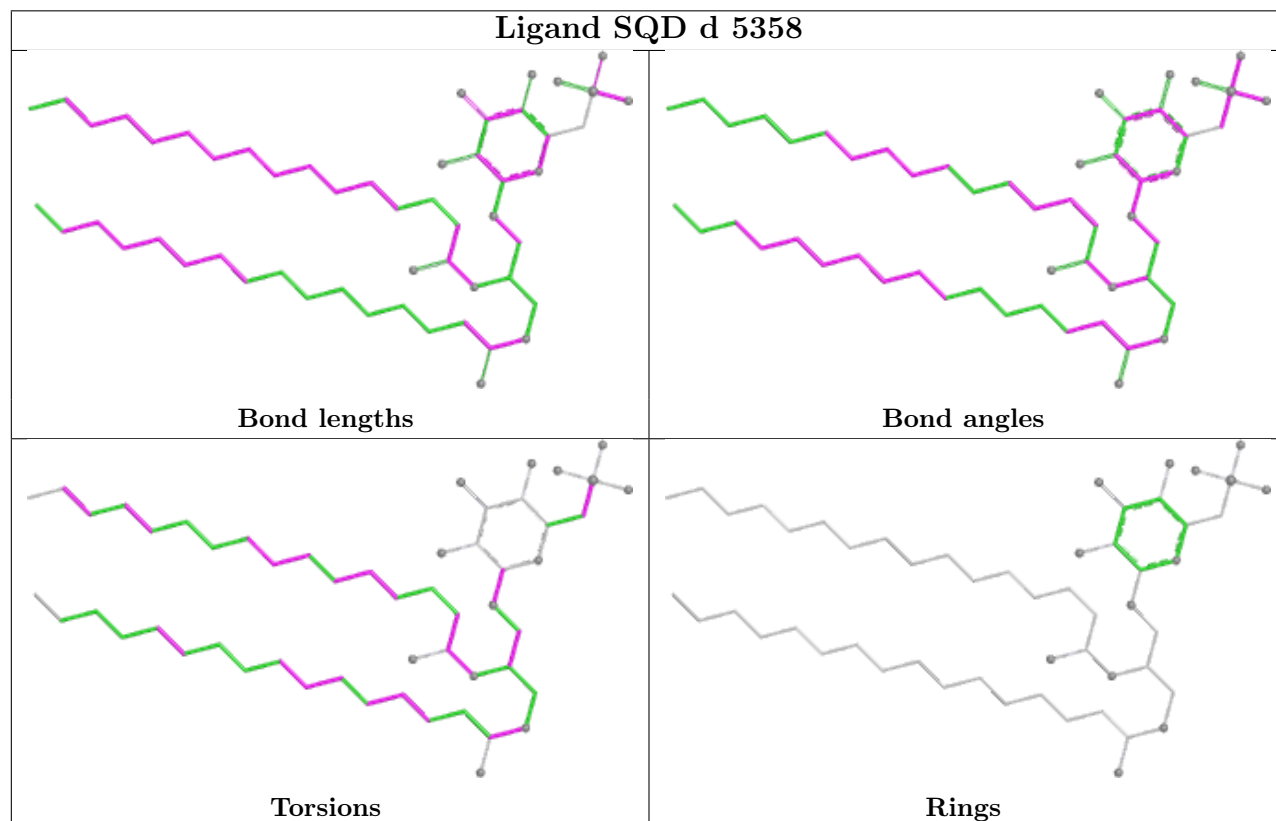
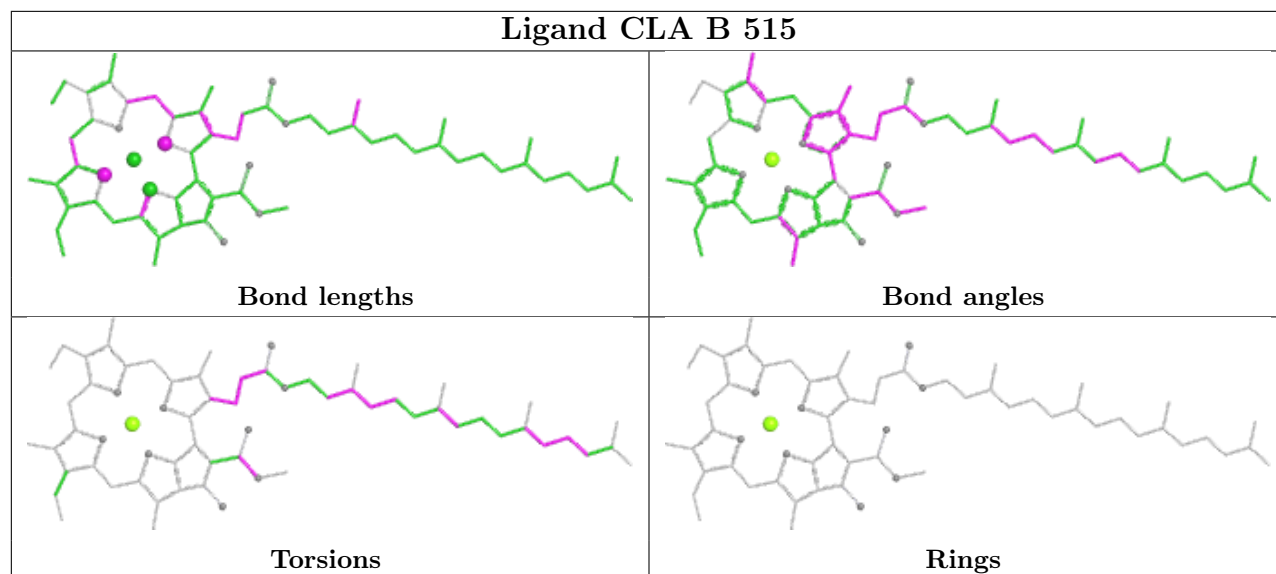


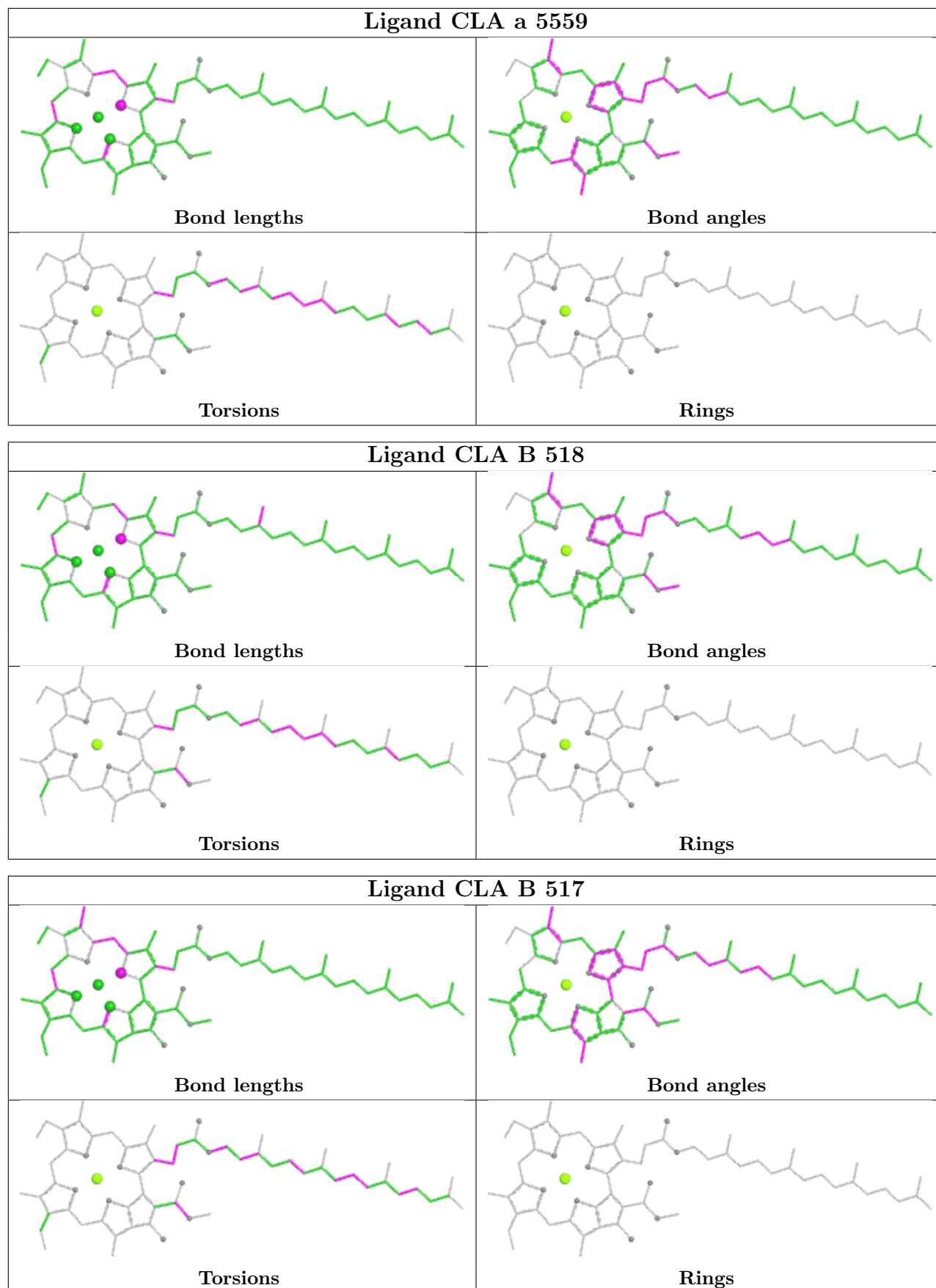


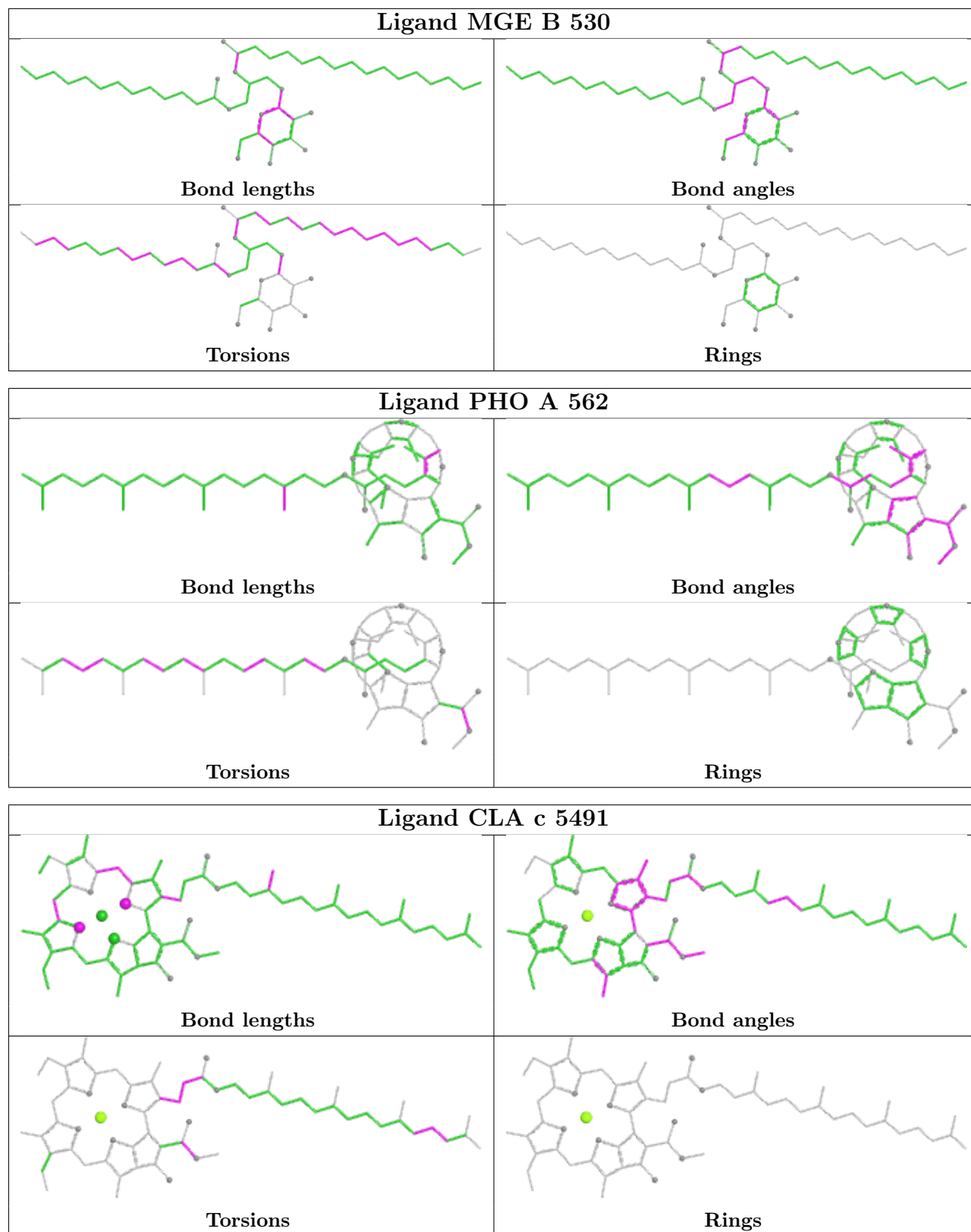


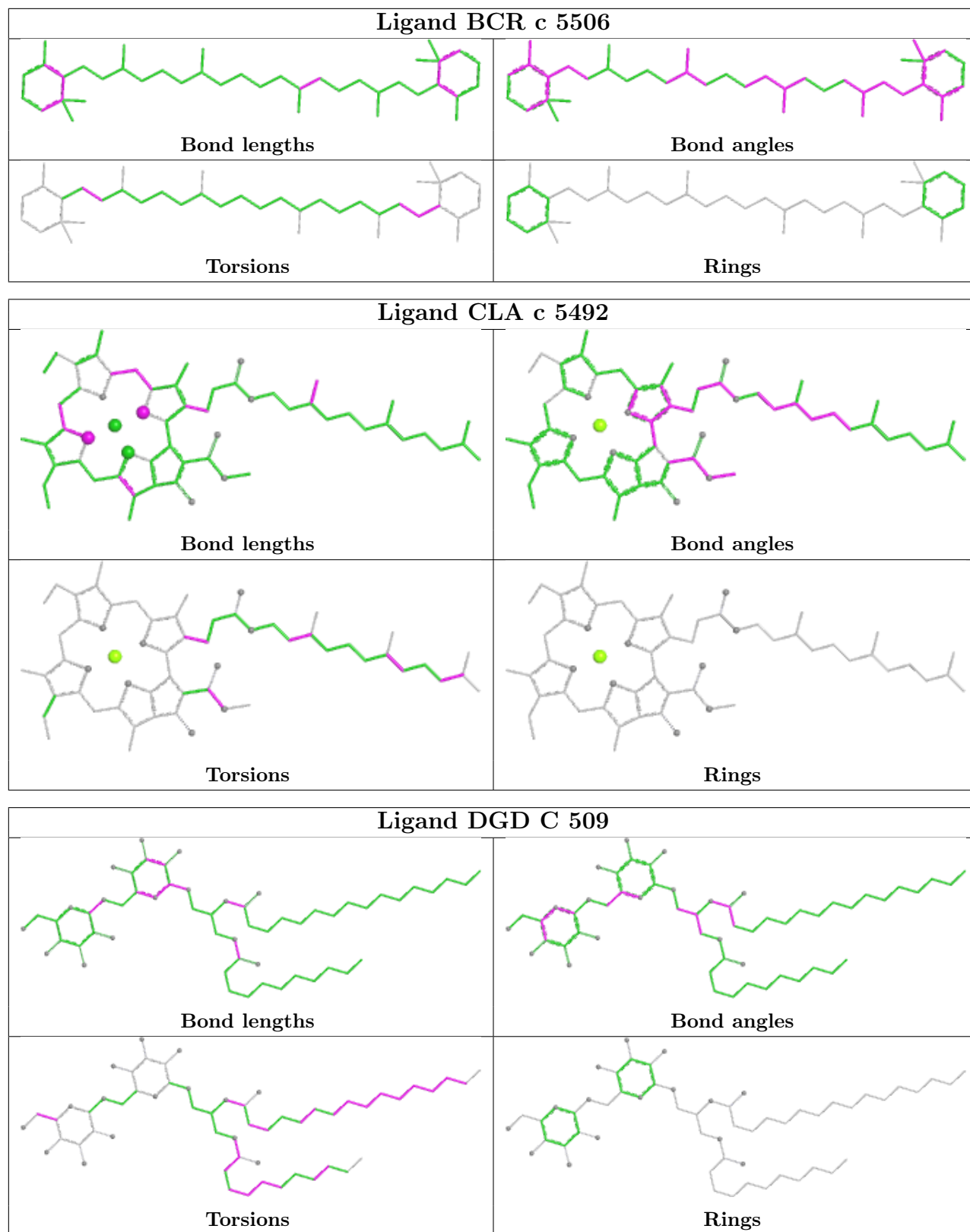


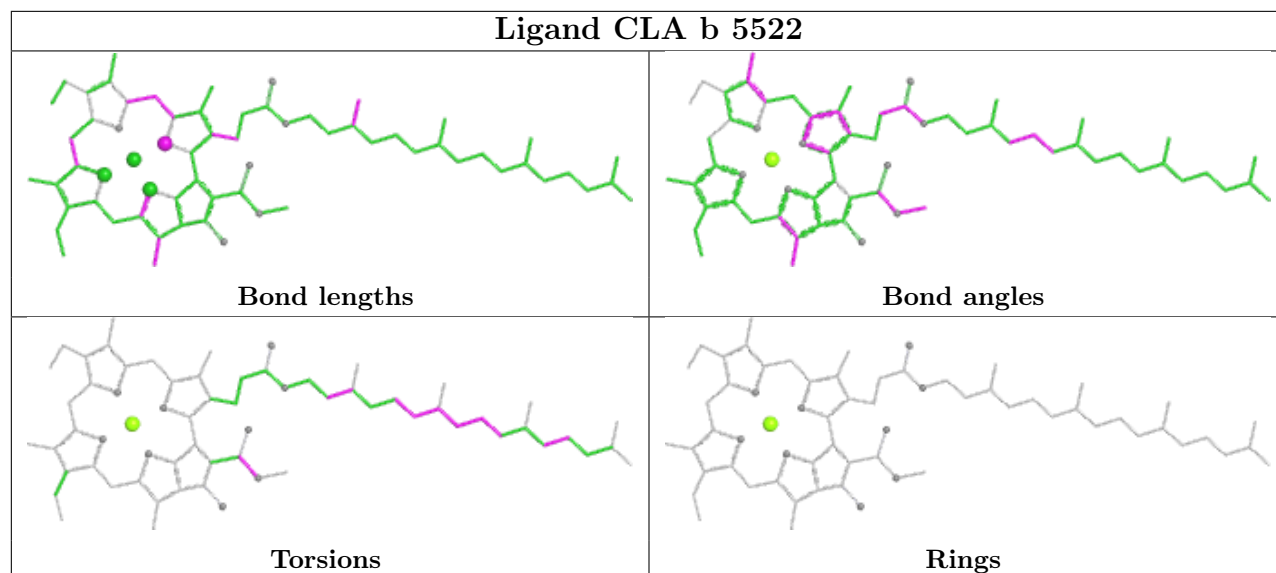
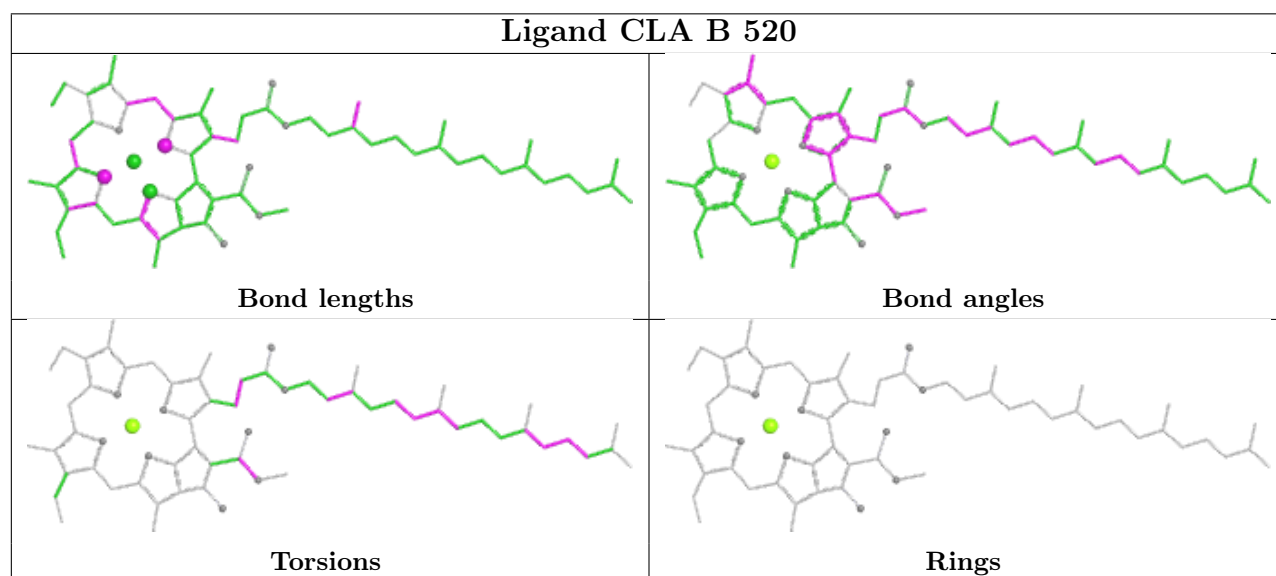
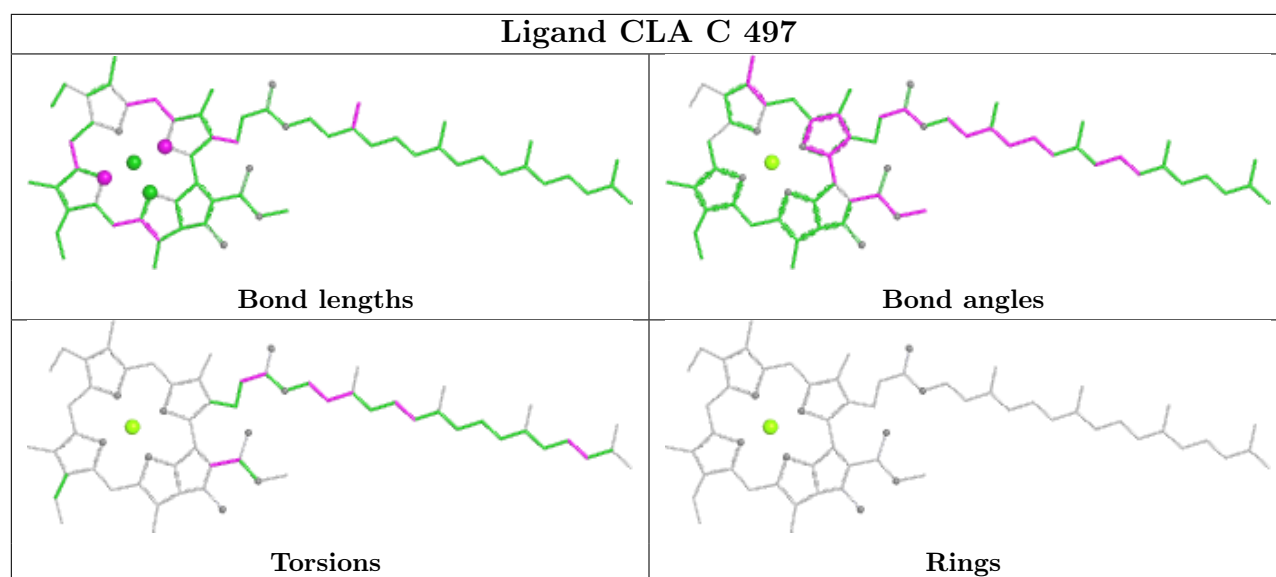


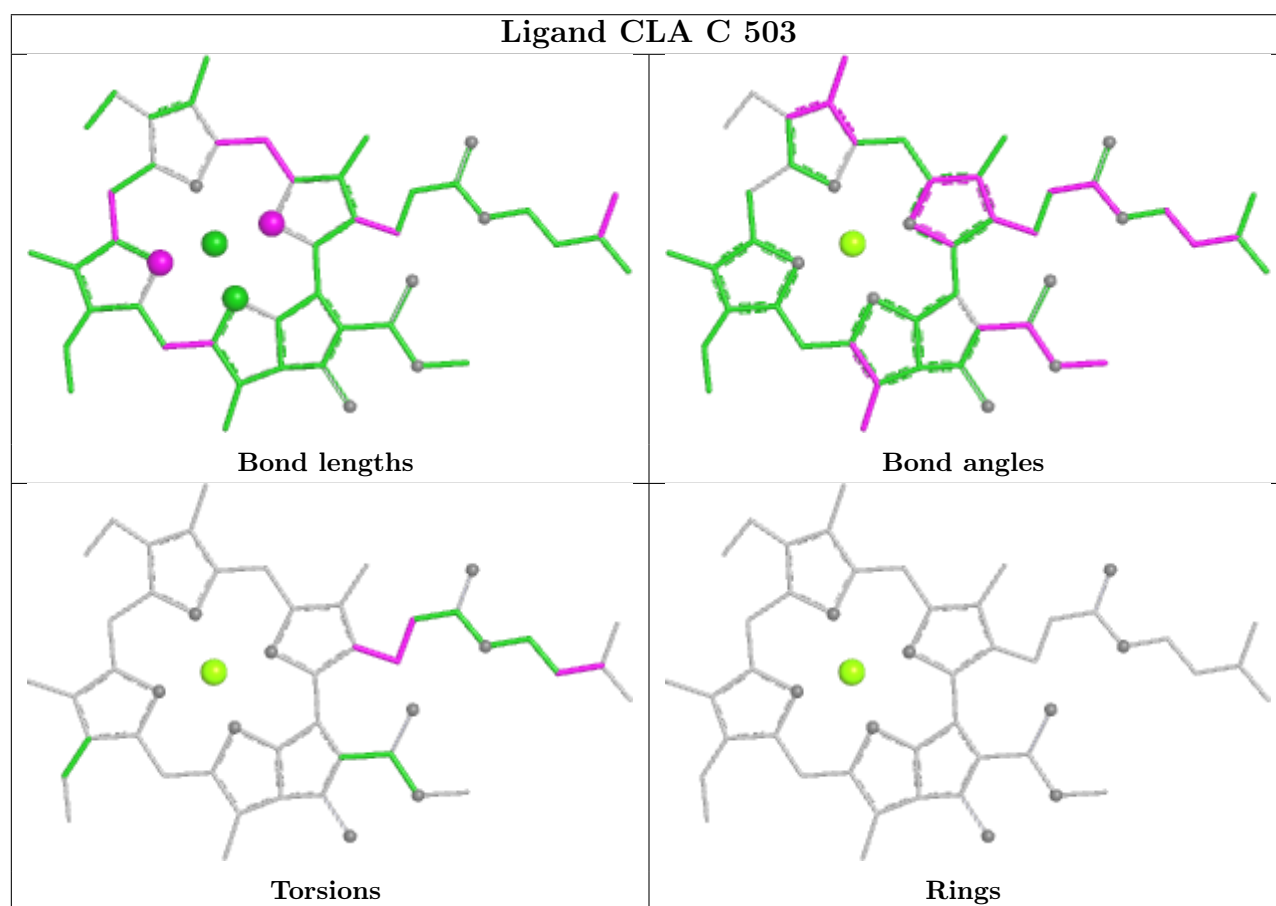
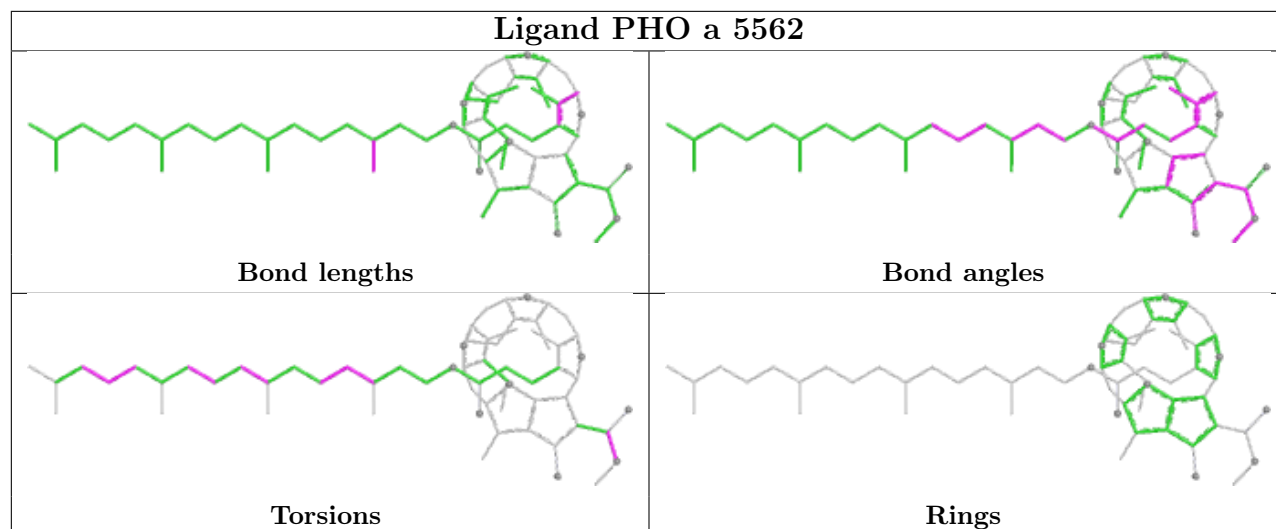


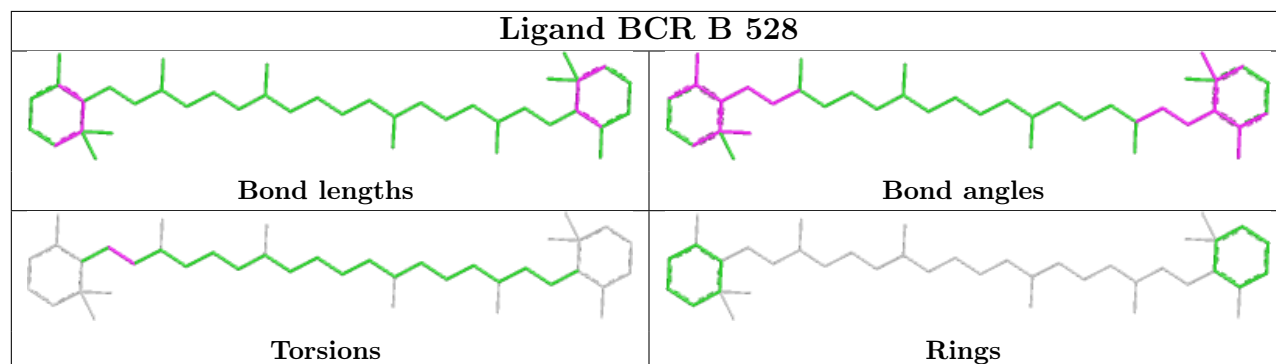
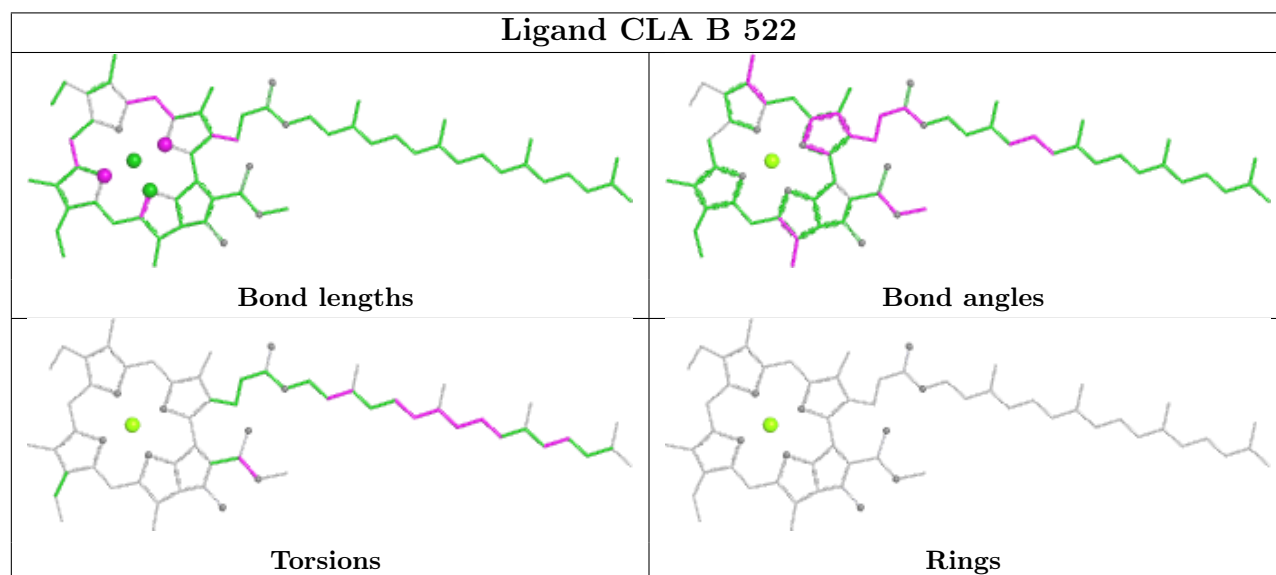
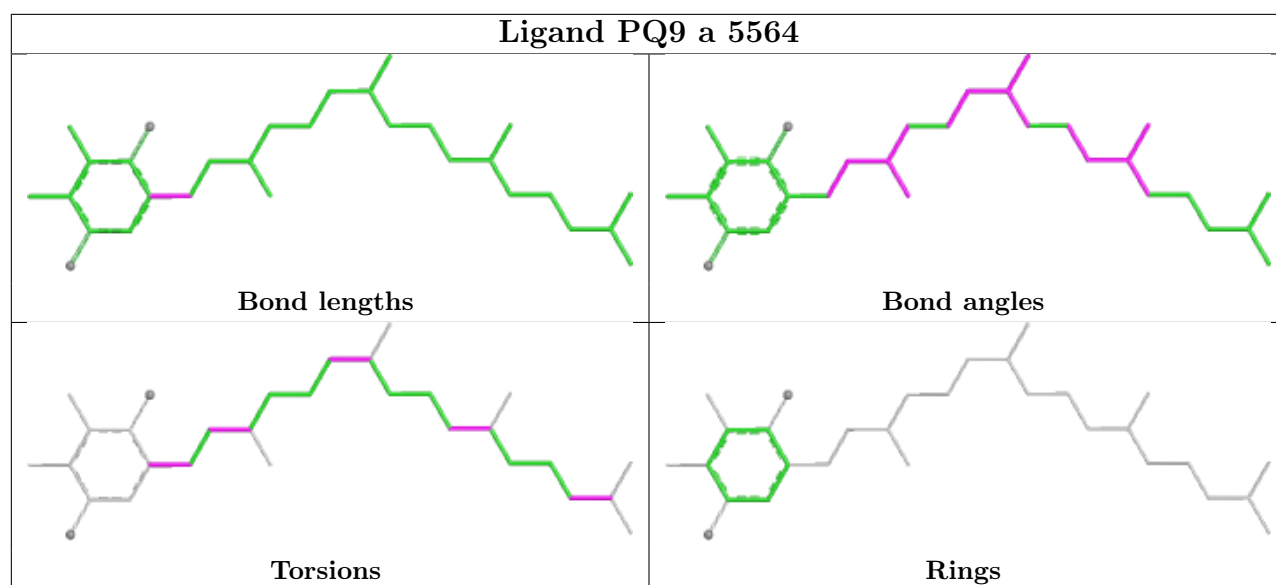


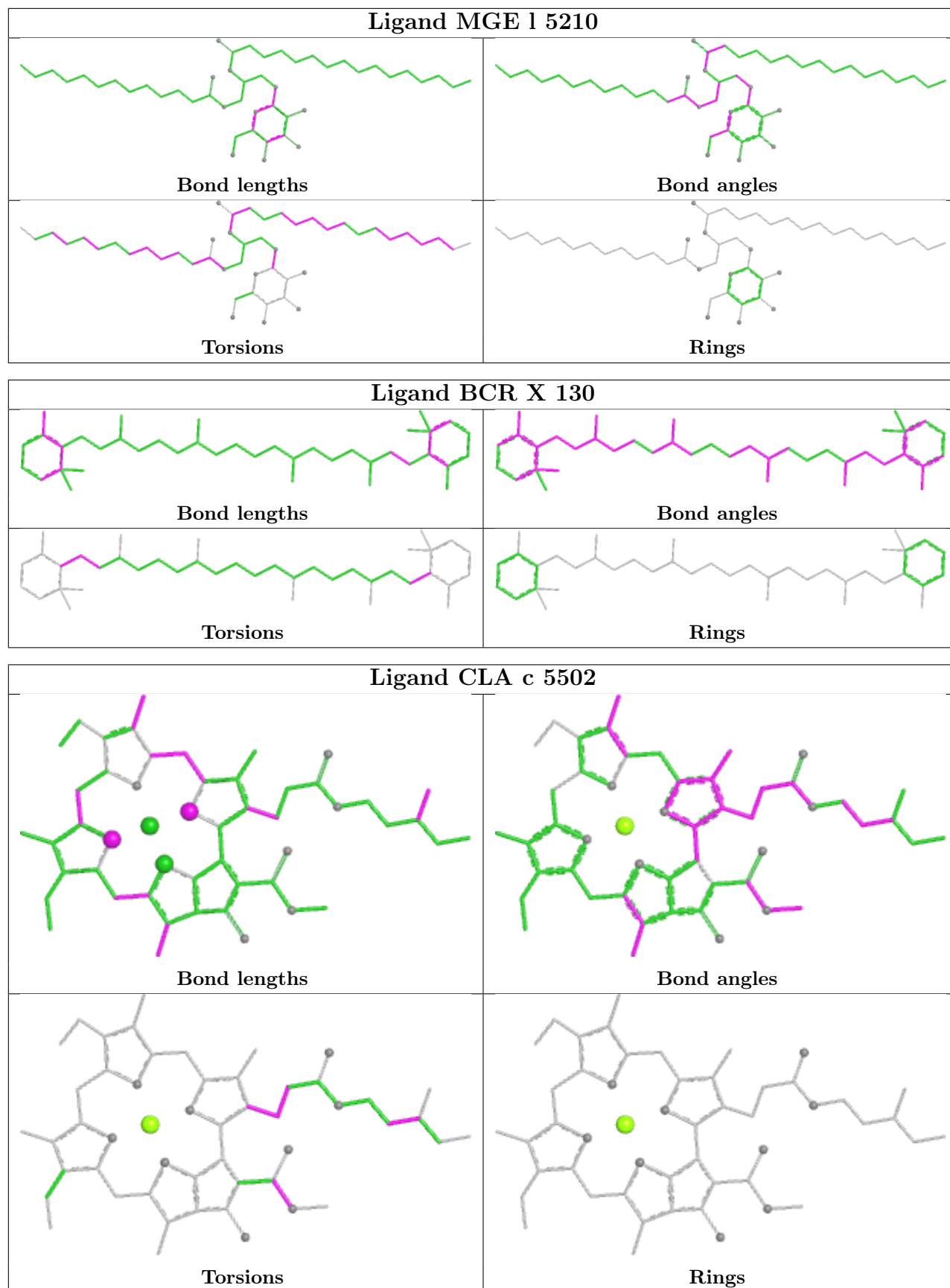


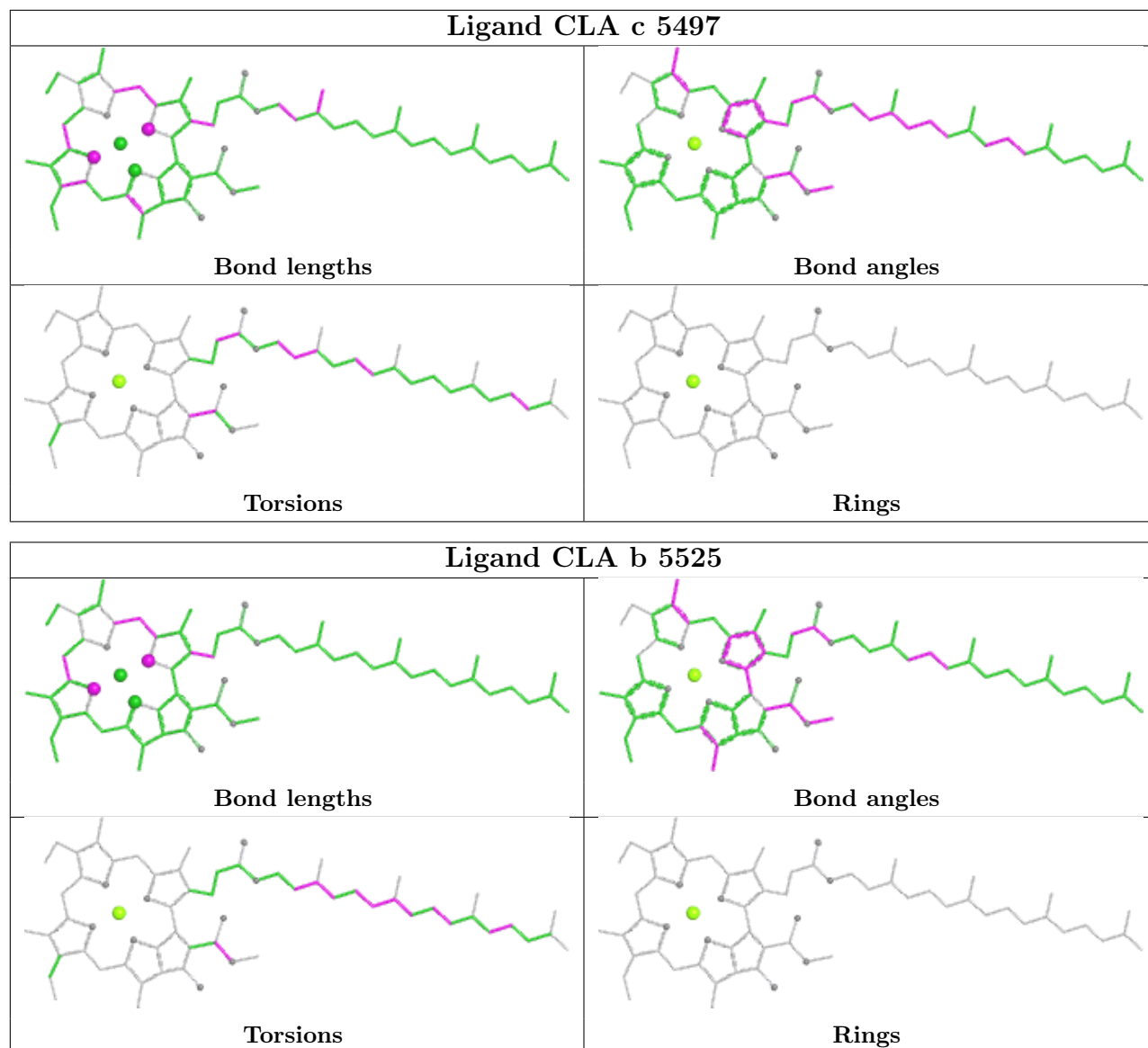


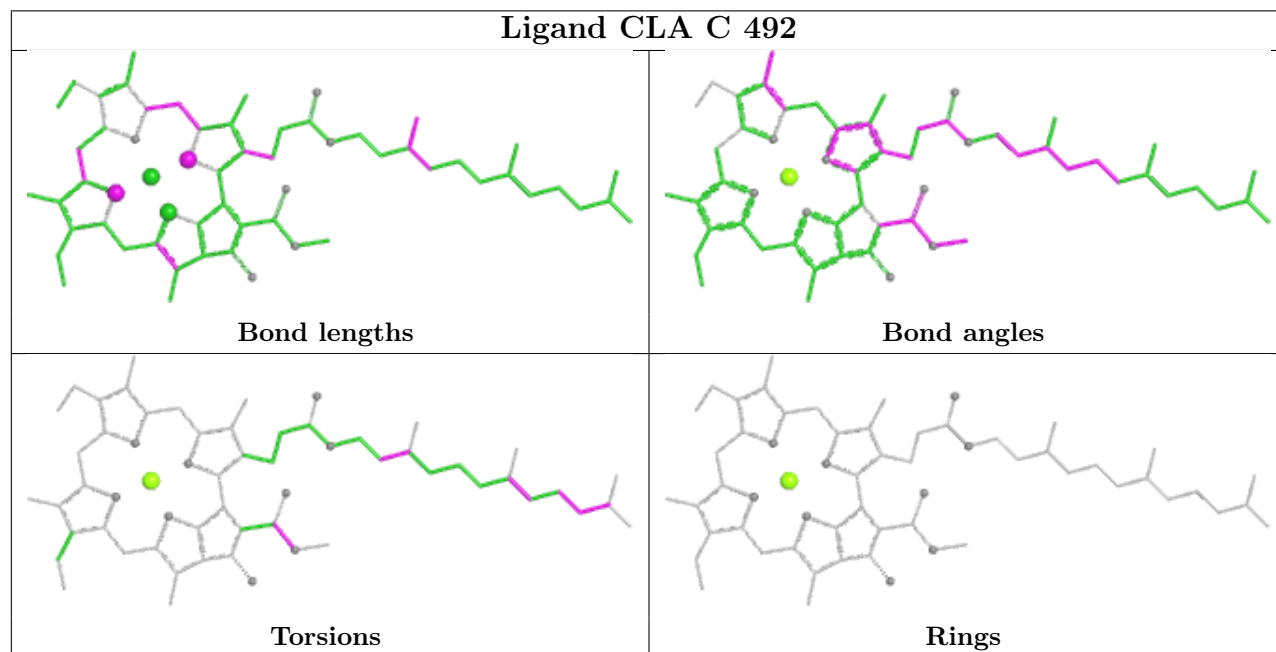
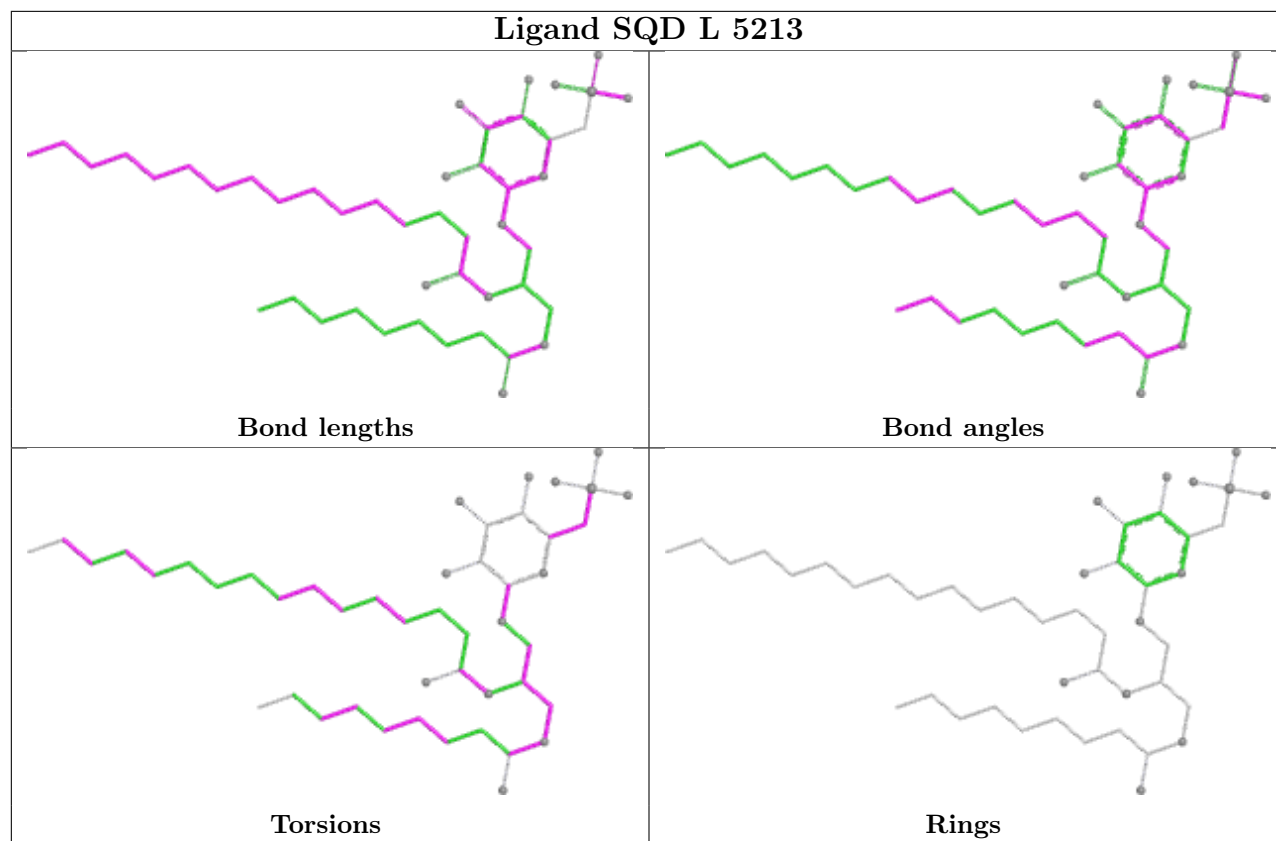


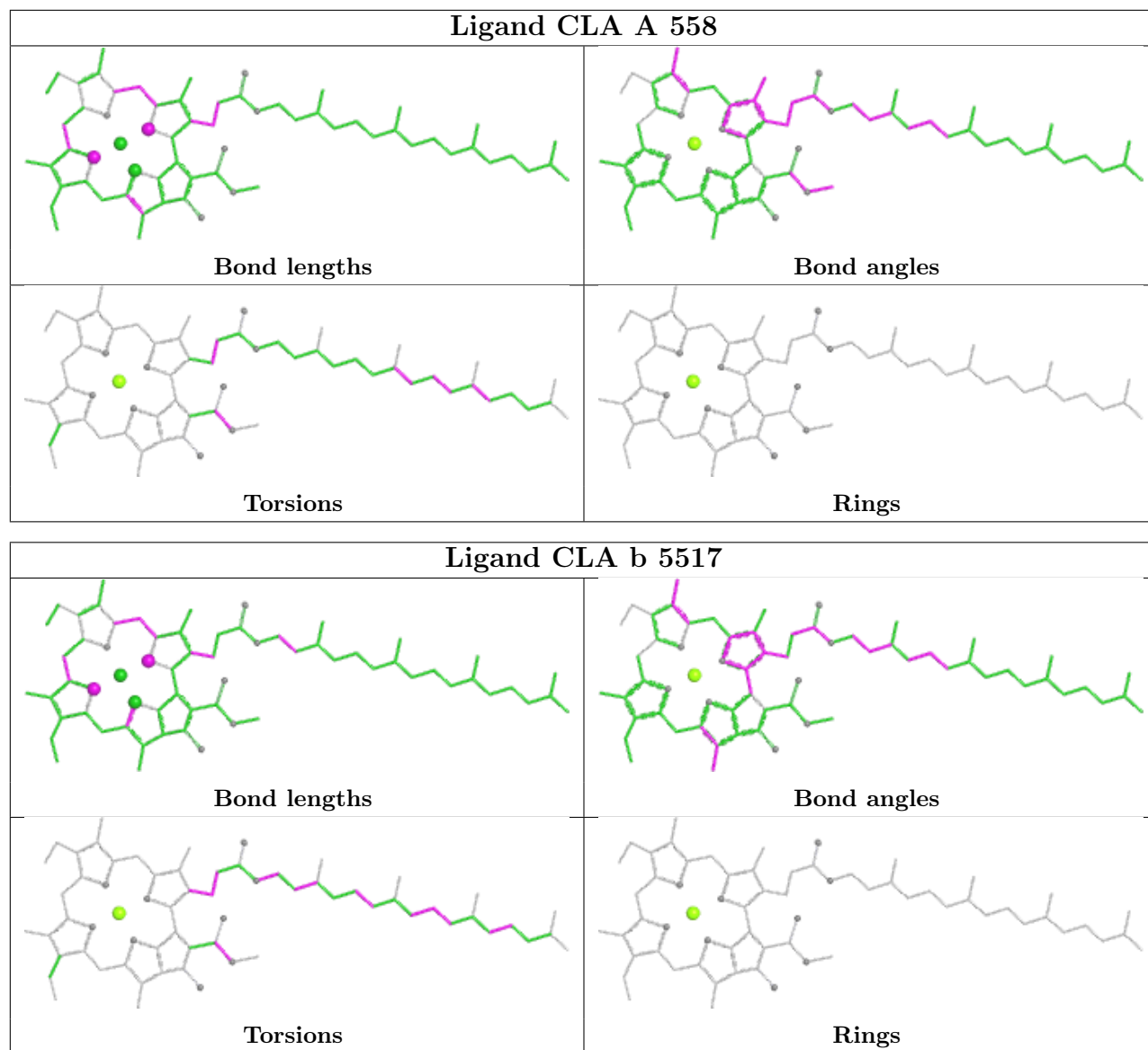












5.7 Other polymers [\(i\)](#)

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, 56, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	5052	GLY	2.2
2	B	130	GLU	2.1
15	u	5086	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
24	BCR	c	5506	40/40	0.77	0.32	75,81,86,86	0
22	PQ9	A	564	30/45	0.77	0.37	54,57,63,64	30
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
29	UNK	C	489	7/-	0.79	0.42	75,76,77,78	0
26	SQD	a	212	26/54	0.79	0.26	82,94,101,103	0
26	SQD	d	5358	54/54	0.79	0.29	74,85,106,107	0
29	UNK	c	5489	7/-	0.79	0.39	73,73,74,74	0
20	CLA	b	5526	65/65	0.79	0.28	66,71,92,95	0
26	SQD	L	5213	47/54	0.80	0.27	52,85,106,108	0
20	CLA	B	526	65/65	0.80	0.28	71,82,97,98	0
29	UNK	c	5476	9/-	0.80	0.32	58,60,62,62	0
27	LMT	a	5568	35/35	0.81	0.43	79,92,94,96	0
29	UNK	C	486	8/-	0.81	0.36	55,56,59,60	0
27	LMT	m	216	35/35	0.81	0.28	62,87,89,91	0
20	CLA	b	5516	65/65	0.81	0.28	62,66,84,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	MGE	D	358	47/48	0.81	0.24	65,72,79,81	0
24	BCR	C	505	40/40	0.81	0.43	75,81,91,92	0
26	SQD	A	5212	26/54	0.81	0.23	75,100,107,107	0
29	UNK	C	476	9/-	0.81	0.29	61,62,63,64	0
24	BCR	d	5357	40/40	0.82	0.37	61,72,86,88	0
20	CLA	c	5496	65/65	0.82	0.27	79,83,95,97	0
24	BCR	H	107	40/40	0.82	0.30	77,83,88,89	0
20	CLA	B	516	65/65	0.82	0.27	61,76,92,97	0
29	UNK	c	5485	5/-	0.83	0.41	68,69,69,70	0
29	UNK	C	478	11/-	0.84	0.24	58,65,66,66	0
20	CLA	C	496	65/65	0.84	0.26	71,78,88,89	0
29	UNK	c	5484	5/-	0.84	0.52	69,69,70,72	0
26	SQD	A	568	54/54	0.84	0.32	76,82,90,90	0
24	BCR	B	528	40/40	0.84	0.25	54,68,74,75	0
20	CLA	a	5563	55/65	0.84	0.32	59,65,102,103	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
20	CLA	c	5503	50/65	0.85	0.28	88,91,92,93	0
24	BCR	h	5107	40/40	0.85	0.28	74,79,82,83	0
29	UNK	c	5479	11/-	0.85	0.24	76,77,77,77	0
20	CLA	C	503	50/65	0.85	0.27	83,86,88,94	0
29	UNK	C	479	11/-	0.85	0.26	58,64,67,67	0
26	SQD	t	213	47/54	0.85	0.27	61,95,116,117	0
29	UNK	C	482	13/-	0.85	0.25	64,66,67,67	0
24	BCR	b	5529	40/40	0.86	0.35	69,72,74,74	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
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
30	DGD	c	5509	57/66	0.86	0.28	67,72,77,78	0
20	CLA	c	5502	51/65	0.87	0.23	93,96,97,98	0
28	MGE	D	359	41/48	0.87	0.23	60,67,76,79	0
28	MGE	I	201	48/48	0.87	0.22	73,81,89,90	0
20	CLA	B	519	65/65	0.87	0.26	73,82,85,87	0
29	UNK	c	5481	13/-	0.87	0.22	60,62,66,66	0
24	BCR	C	506	40/40	0.88	0.22	68,72,79,80	0
20	CLA	C	498	65/65	0.88	0.22	64,74,98,101	0
29	UNK	c	5483	13/-	0.88	0.26	71,75,80,82	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
20	CLA	A	563	55/65	0.88	0.26	43,49,75,78	0
24	BCR	c	5505	40/40	0.88	0.31	84,87,91,92	0
29	UNK	C	474	15/-	0.89	0.18	26,37,40,40	0
29	UNK	c	5474	15/-	0.89	0.24	39,50,56,56	0
24	BCR	D	357	40/40	0.89	0.26	61,66,78,80	0
20	CLA	b	5519	65/65	0.89	0.24	70,75,80,81	0
29	UNK	c	5477	7/-	0.89	0.34	67,68,70,70	0
28	MGE	B	530	48/48	0.89	0.19	55,64,70,72	0
20	CLA	c	5501	65/65	0.89	0.26	82,91,94,95	0
29	UNK	c	5480	7/-	0.89	0.26	65,66,66,67	0
20	CLA	C	501	65/65	0.89	0.25	70,78,83,85	0
24	BCR	B	529	40/40	0.89	0.25	62,69,80,80	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
29	UNK	c	5486	8/-	0.89	0.30	63,64,65,66	0
29	UNK	C	485	5/-	0.89	0.24	57,59,61,61	0
20	CLA	C	497	65/65	0.89	0.24	74,78,80,82	0
28	MGE	d	5360	41/48	0.89	0.21	68,72,78,80	0
30	DGD	C	507	53/66	0.89	0.25	55,66,86,88	0
30	DGD	c	5507	53/66	0.89	0.23	66,74,90,91	0
20	CLA	c	5497	65/65	0.89	0.24	66,82,84,87	0
25	LHG	a	5567	39/49	0.90	0.26	65,68,74,80	0
20	CLA	c	5493	65/65	0.90	0.21	67,81,86,86	0
28	MGE	d	5361	48/48	0.90	0.21	61,68,78,83	0
20	CLA	a	5560	65/65	0.90	0.22	62,68,100,101	0
28	MGE	l	5210	48/48	0.90	0.21	59,69,78,81	0
24	BCR	a	5566	40/40	0.90	0.25	59,75,78,79	0
20	CLA	b	5520	65/65	0.90	0.24	63,72,74,76	0
20	CLA	B	520	65/65	0.90	0.23	62,67,76,79	0
30	DGD	H	208	54/66	0.90	0.20	61,69,75,76	0
28	MGE	b	5530	48/48	0.90	0.18	59,64,71,73	0
29	UNK	c	5482	13/-	0.90	0.19	60,61,71,72	0
24	BCR	C	504	40/40	0.91	0.27	57,64,70,70	0
20	CLA	A	560	65/65	0.91	0.21	49,57,86,88	0
21	PHO	a	5562	64/64	0.91	0.22	70,75,81,82	0
28	MGE	D	360	48/48	0.91	0.20	52,60,63,68	0
20	CLA	c	5491	65/65	0.91	0.20	70,78,81,86	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
24	BCR	t	104	40/40	0.91	0.20	65,72,84,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	CLA	B	512	65/65	0.91	0.24	68,75,78,79	0
30	DGD	C	508	47/66	0.91	0.19	61,71,80,83	0
30	DGD	C	509	57/66	0.91	0.20	52,60,69,70	0
24	BCR	B	527	40/40	0.91	0.18	58,65,68,69	0
20	CLA	c	5495	65/65	0.91	0.21	74,81,86,88	0
30	DGD	c	5508	47/66	0.91	0.18	66,76,82,84	0
20	CLA	D	355	50/65	0.91	0.22	63,65,68,70	0
29	UNK	c	5488	5/-	0.92	0.21	59,59,59,60	0
20	CLA	b	5512	65/65	0.92	0.23	68,72,75,76	0
22	PQ9	d	5356	30/45	0.92	0.20	51,57,66,66	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
20	CLA	c	5500	65/65	0.92	0.20	64,69,82,83	0
20	CLA	C	495	65/65	0.92	0.21	58,68,74,76	0
20	CLA	b	5525	65/65	0.92	0.20	71,77,80,82	0
24	BCR	b	5527	40/40	0.92	0.19	58,63,72,72	0
25	LHG	A	567	39/49	0.92	0.23	57,73,79,81	0
20	CLA	B	525	65/65	0.93	0.20	67,84,91,92	0
20	CLA	B	518	65/65	0.93	0.19	53,64,79,79	0
20	CLA	c	5492	60/65	0.93	0.17	57,61,83,84	0
20	CLA	B	515	65/65	0.93	0.21	55,66,71,72	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
24	BCR	b	5528	40/40	0.93	0.18	61,64,72,73	0
20	CLA	B	522	65/65	0.93	0.21	54,65,75,77	0
20	CLA	b	5524	56/65	0.93	0.18	63,68,89,91	0
20	CLA	B	524	56/65	0.93	0.19	67,72,77,80	0
30	DGD	h	5208	54/66	0.93	0.17	57,68,73,75	0
20	CLA	B	513	65/65	0.94	0.18	56,61,67,67	0
20	CLA	C	493	65/65	0.94	0.18	67,71,77,79	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
20	CLA	b	5513	65/65	0.94	0.20	54,61,84,90	0
21	PHO	A	562	64/64	0.94	0.17	47,53,63,66	0
21	PHO	a	5561	64/64	0.94	0.18	51,55,66,68	0
20	CLA	b	5514	65/65	0.94	0.18	41,51,74,75	0
20	CLA	b	5515	65/65	0.94	0.21	46,51,74,76	0
20	CLA	C	500	65/65	0.94	0.16	59,63,73,74	0
32	HEM	f	5051	43/43	0.94	0.28	80,84,97,101	0
33	CA	k	5056	1/1	0.94	0.19	119,119,119,119	0
20	CLA	C	499	47/65	0.95	0.17	57,60,66,69	0
20	CLA	b	5523	65/65	0.95	0.15	45,52,74,75	0

Continued on next page...

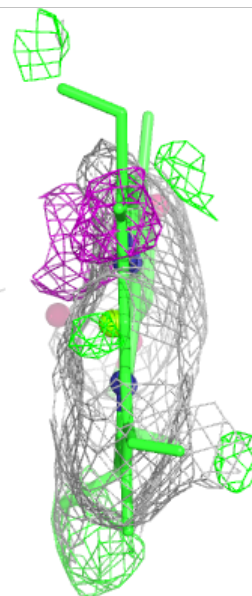
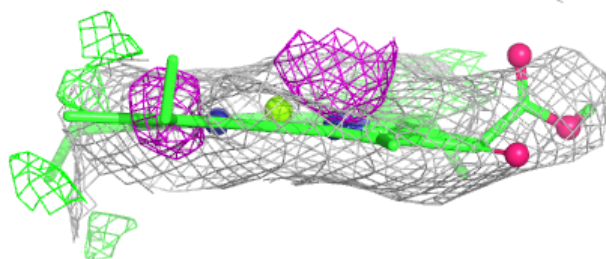
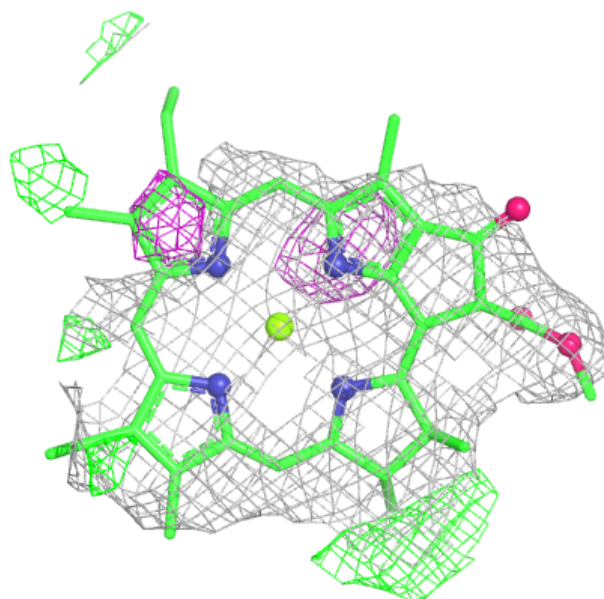
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	B	521	65/65	0.95	0.17	58,63,66,68	0
20	CLA	C	494	46/65	0.95	0.15	59,66,68,72	0
19	FE2	A	557	1/1	0.95	0.05	60,60,60,60	0
20	CLA	d	5354	65/65	0.95	0.17	39,47,64,65	0
20	CLA	B	523	65/65	0.95	0.16	47,56,73,74	0
21	PHO	A	561	64/64	0.95	0.16	32,52,55,59	0
20	CLA	D	354	65/65	0.95	0.16	35,43,63,66	0
20	CLA	C	491	65/65	0.95	0.18	63,70,77,79	0
20	CLA	b	5517	65/65	0.95	0.15	54,58,66,71	0
20	CLA	b	5518	65/65	0.95	0.17	60,64,69,75	0
20	CLA	a	5558	65/65	0.95	0.16	41,50,55,61	0
32	HEM	F	51	43/43	0.95	0.25	78,84,92,95	0
20	CLA	a	5559	65/65	0.95	0.15	42,49,60,60	0
20	CLA	C	492	60/65	0.95	0.17	53,58,76,77	0
20	CLA	B	517	65/65	0.96	0.14	37,44,56,57	0
20	CLA	A	558	65/65	0.96	0.14	41,46,50,51	0
23	OEC	A	565	5/9	0.96	0.13	62,63,65,66	0
23	OEC	a	5565	5/9	0.96	0.13	63,64,71,87	0
31	BCT	D	353	4/4	0.96	0.18	72,73,73,74	0
20	CLA	A	559	65/65	0.96	0.14	39,43,49,52	0
29	UNK	C	477	7/-	0.96	0.16	47,49,51,51	0
32	HEM	v	5552	43/43	0.96	0.21	65,67,70,70	0
33	CA	K	56	1/1	0.96	0.09	119,119,119,119	0
29	UNK	C	490	4/-	0.96	0.15	67,67,68,68	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.

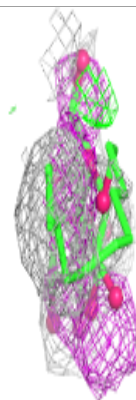
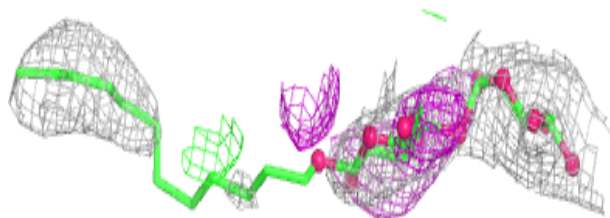
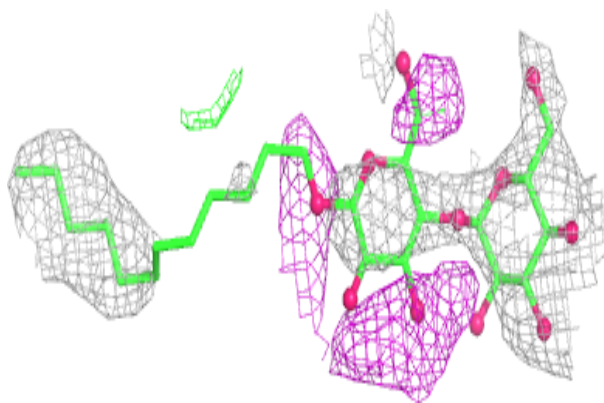
Electron density around CLA b 5511:

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

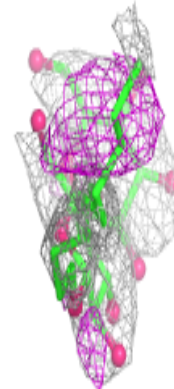
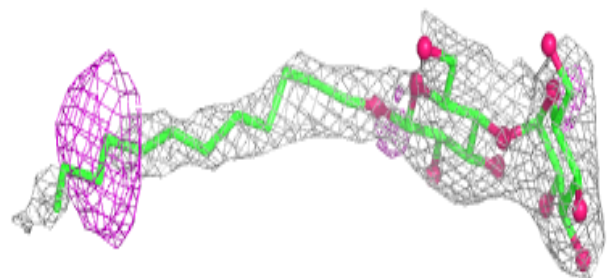
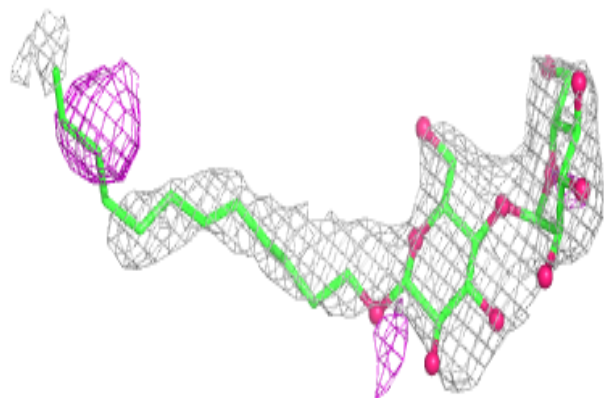


Electron density around LMT t 5217:

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

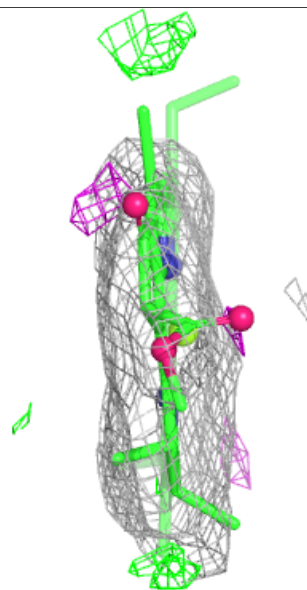
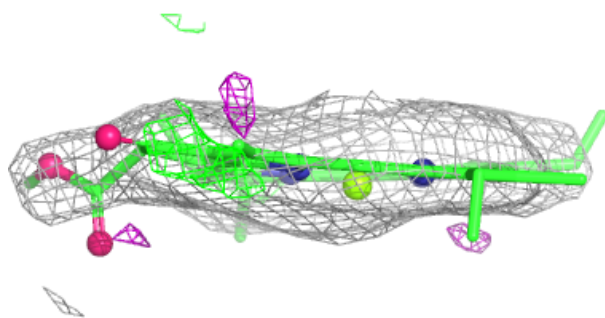
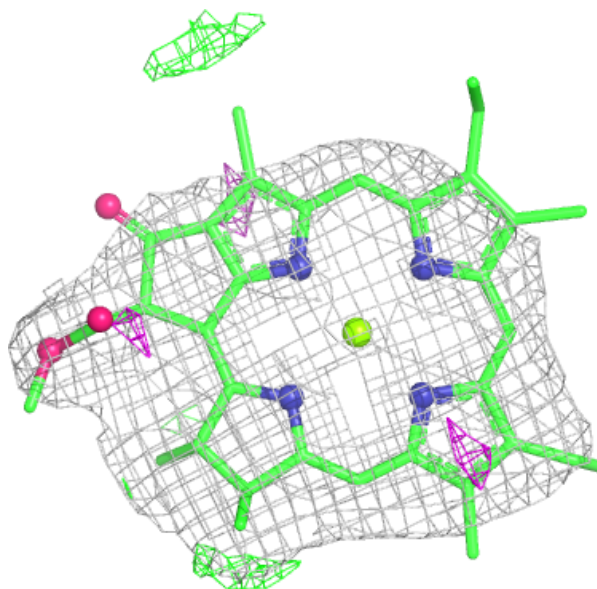
**Electron density around LMT A 569:**

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



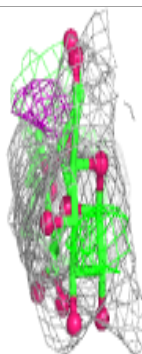
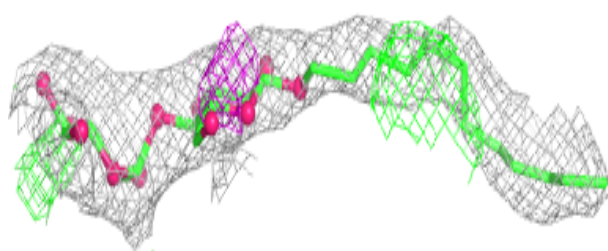
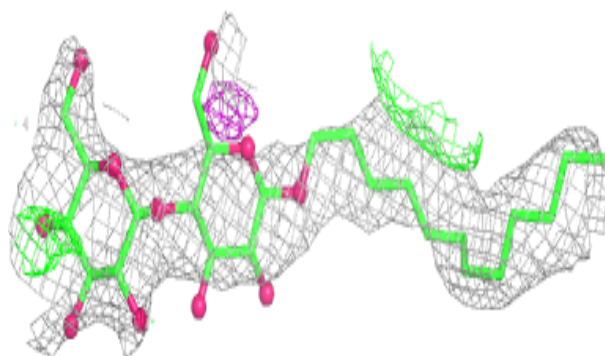
Electron density around CLA B 511:

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

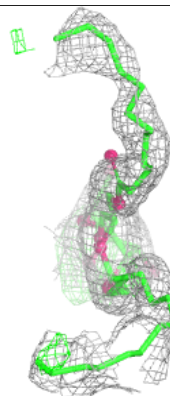
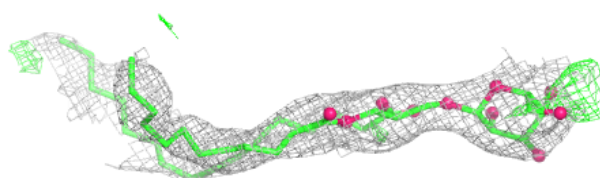
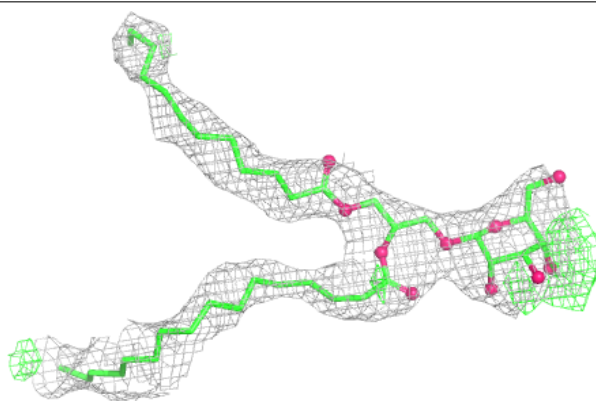


Electron density around LMT T 217:

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

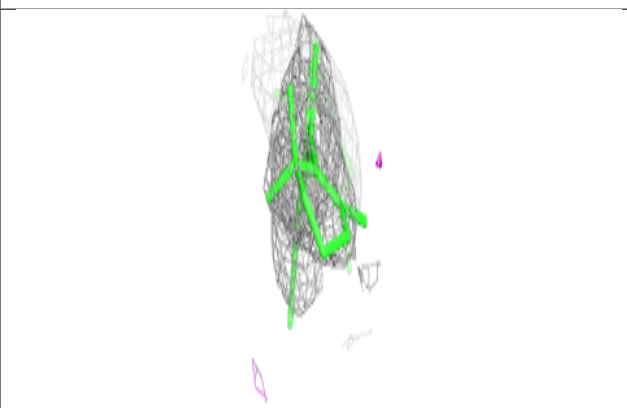
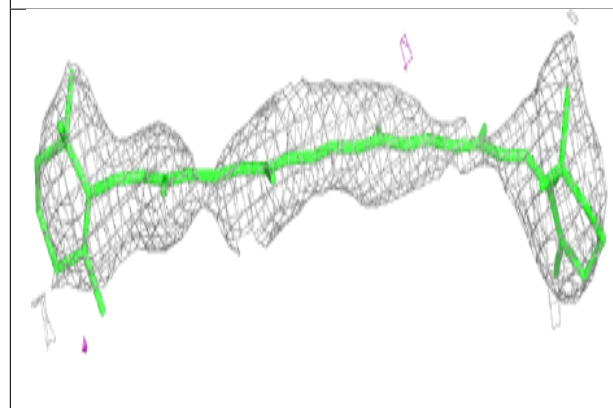
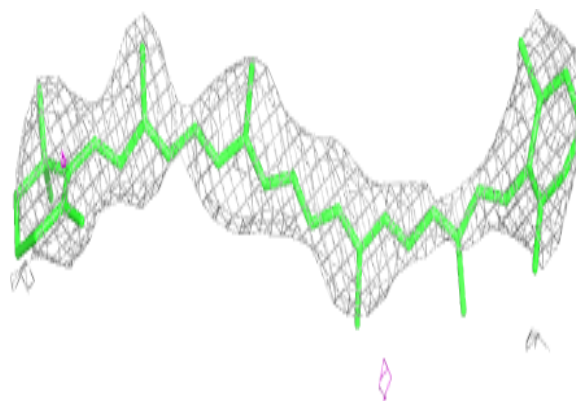
**Electron density around MGE d 5359:**

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

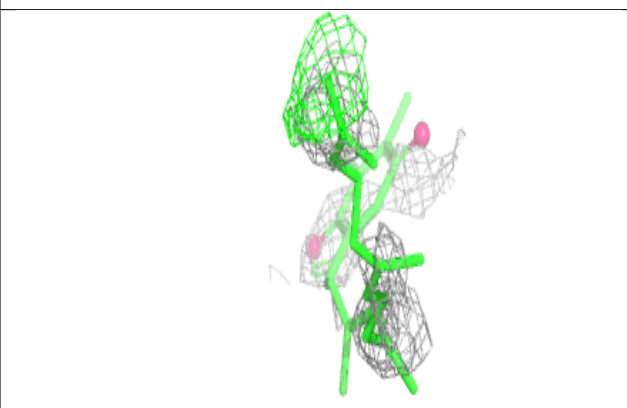
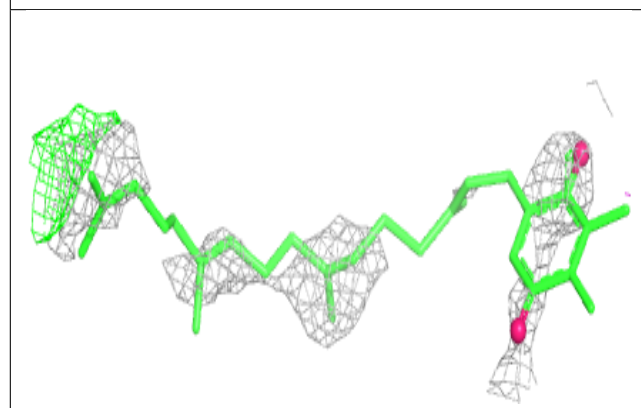
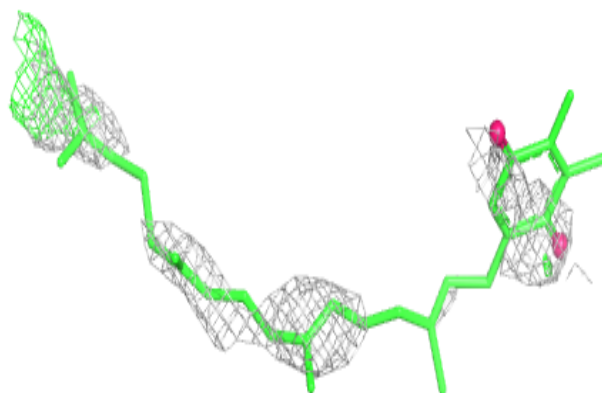


Electron density around BCR c 5506:

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

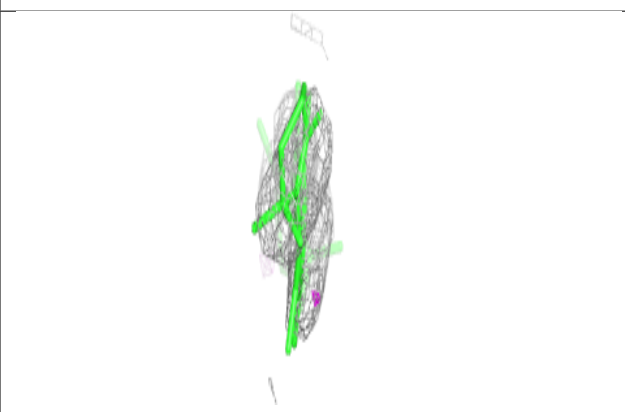
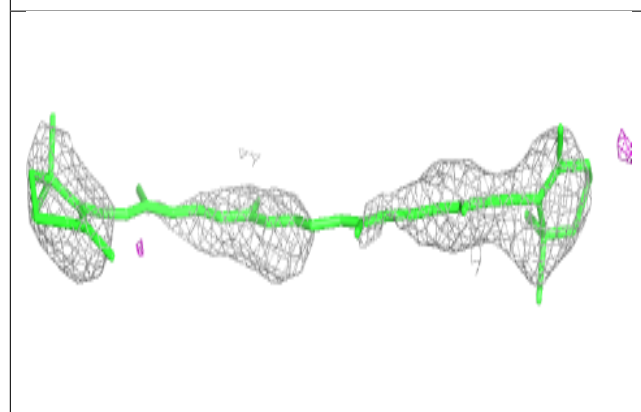
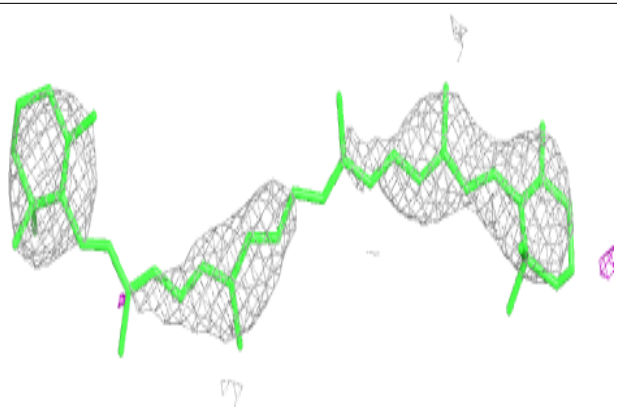
**Electron density around PQ9 A 564:**

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

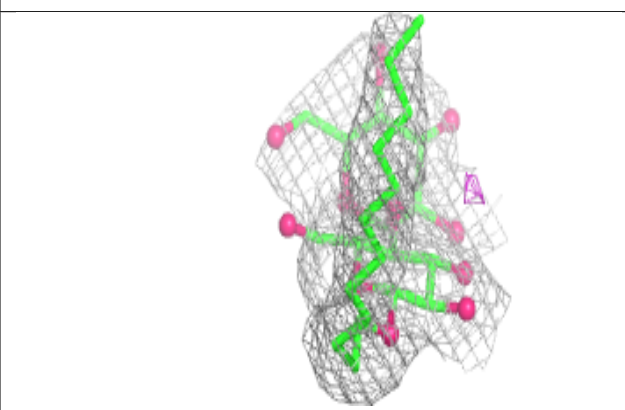
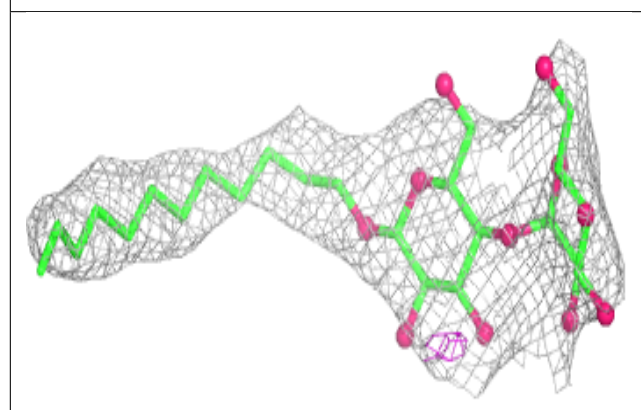
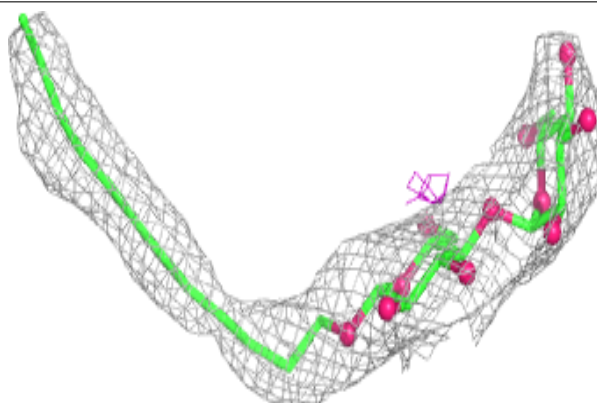


Electron density around BCR x 5130:

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

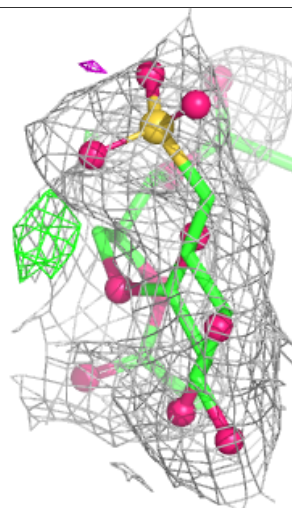
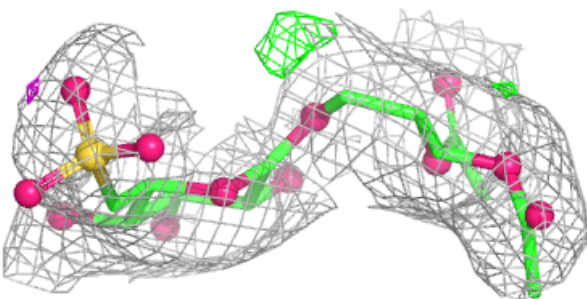
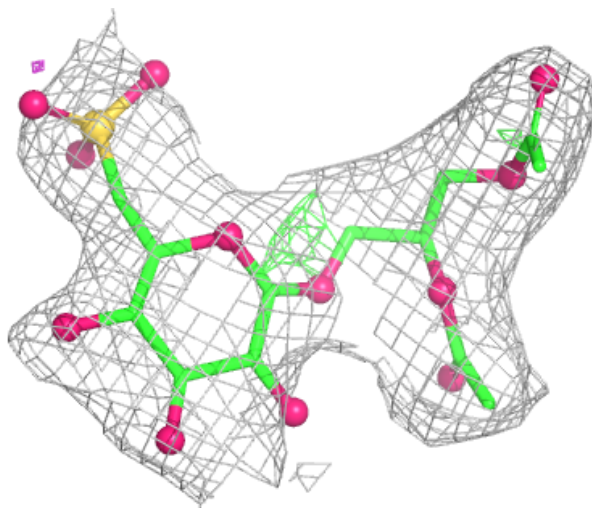
**Electron density around LMT M 5216:**

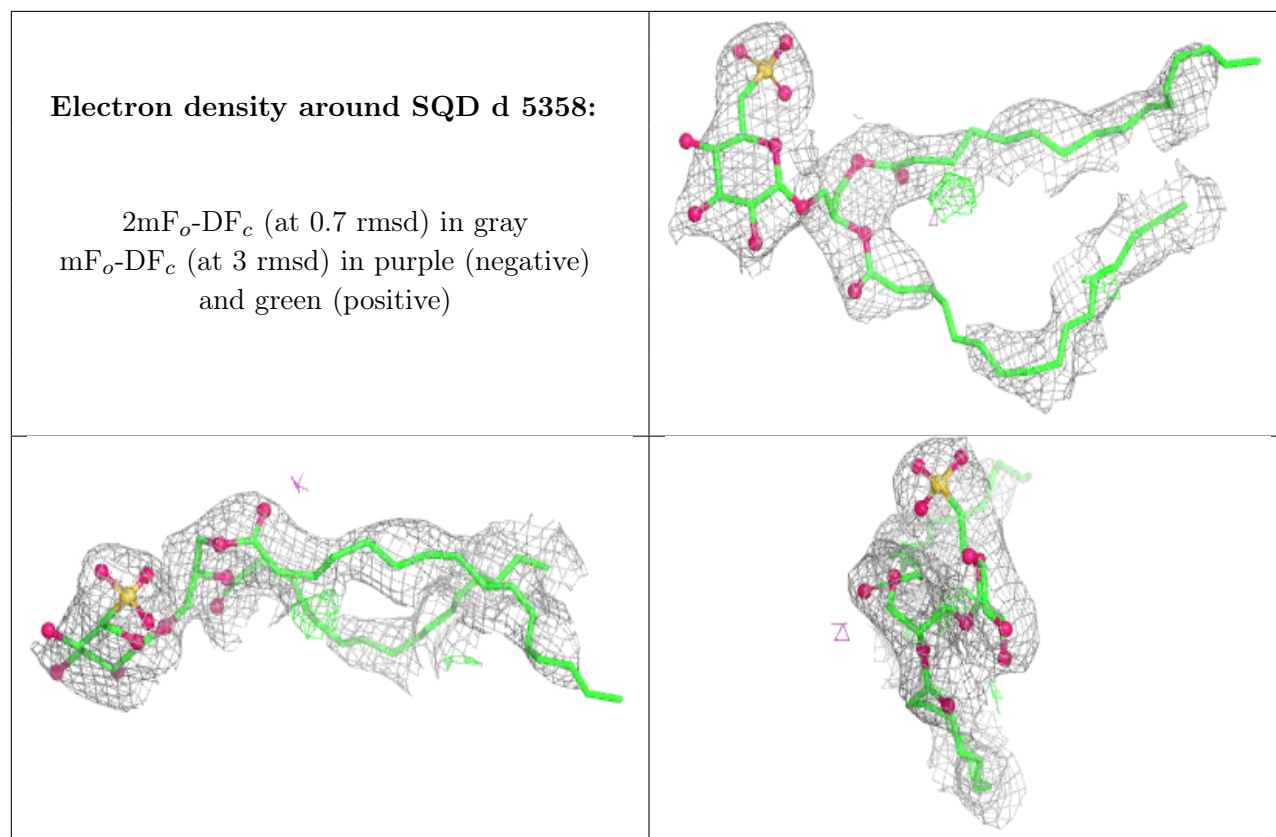
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD a 212:

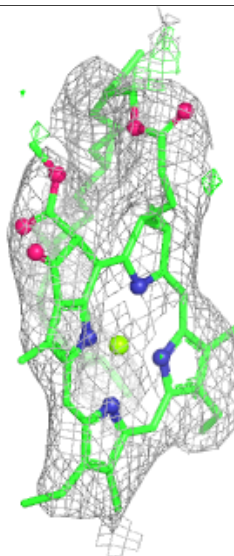
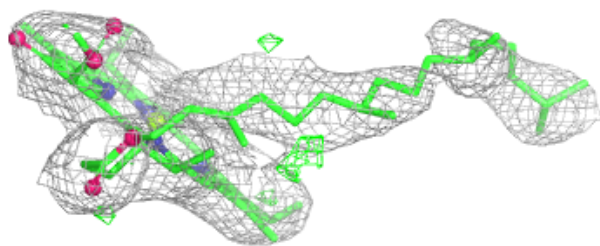
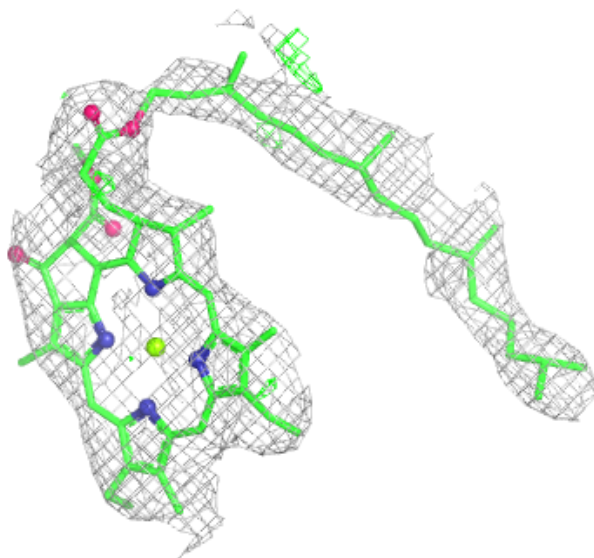
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

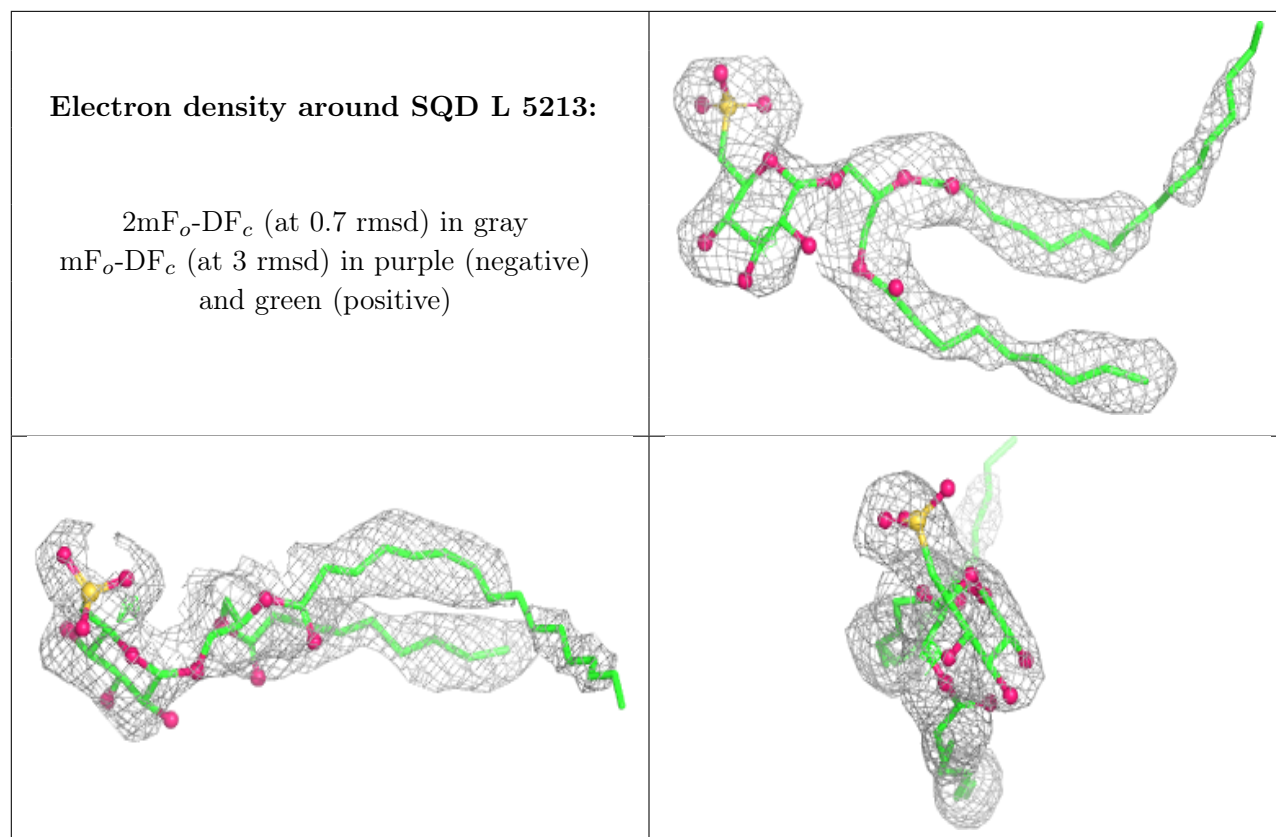




Electron density around CLA b 5526:

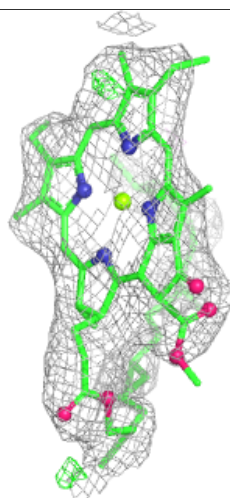
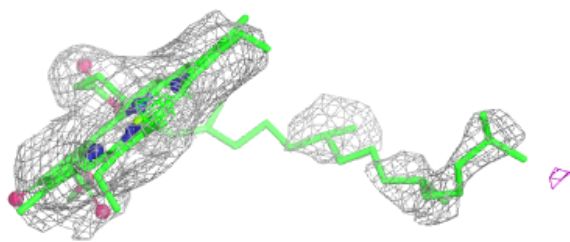
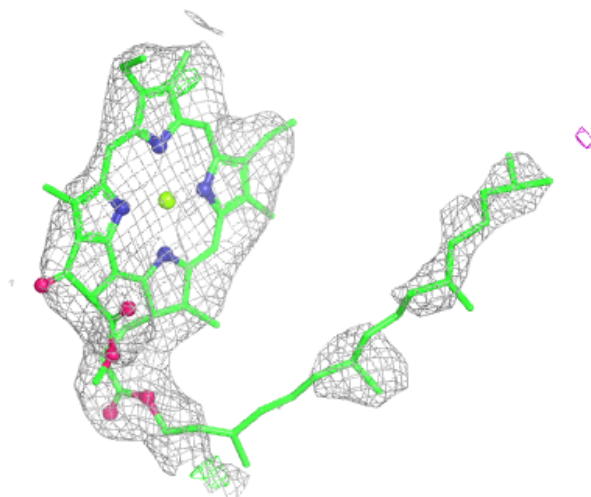
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





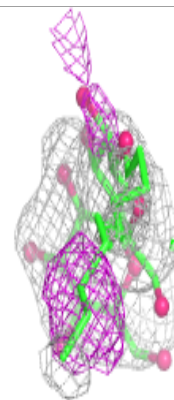
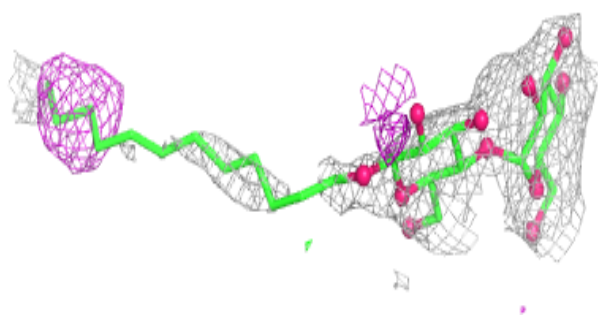
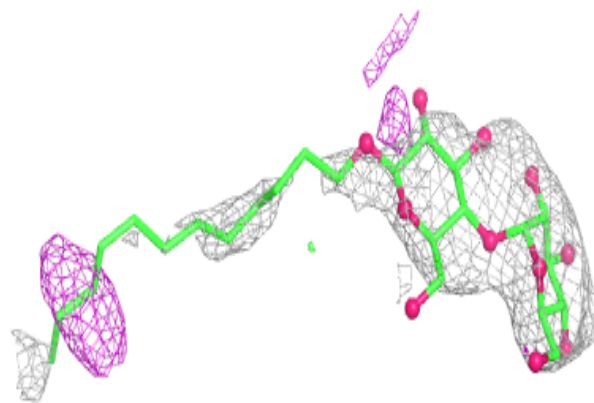
Electron density around CLA B 526:

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

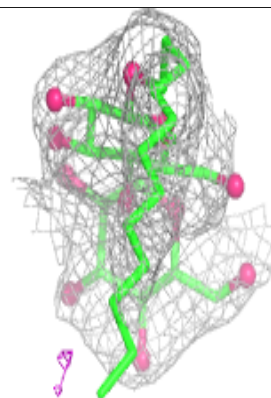
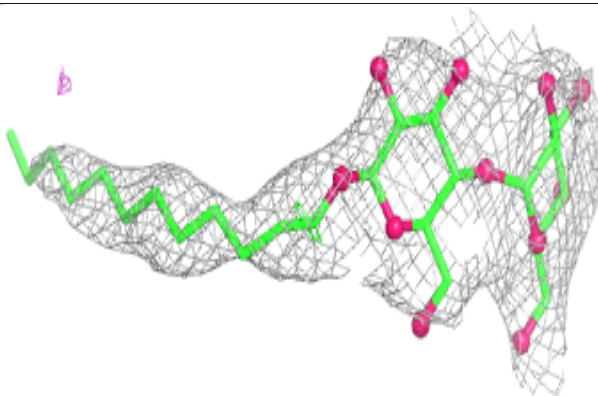
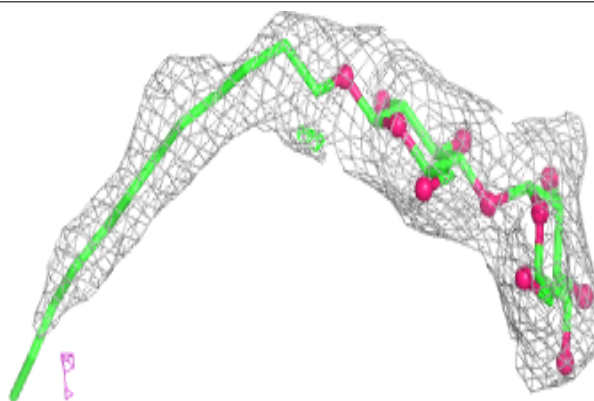


Electron density around LMT a 5568:

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

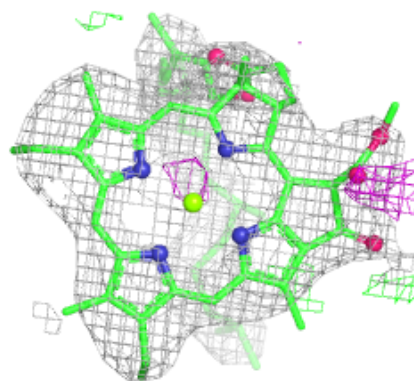
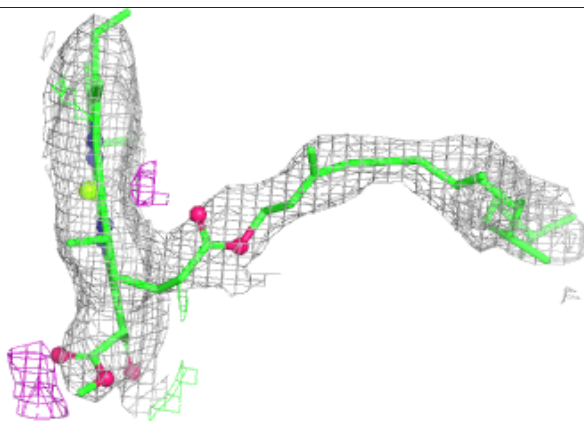
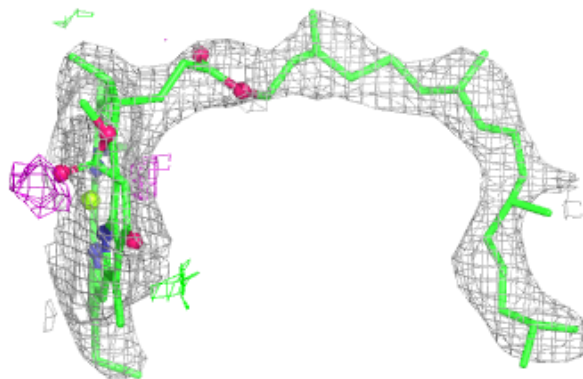
**Electron density around LMT m 216:**

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

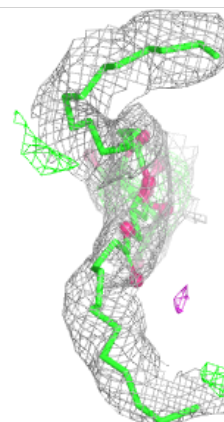
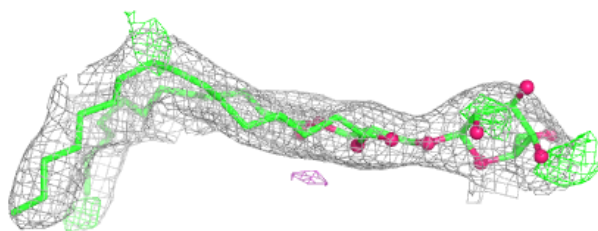
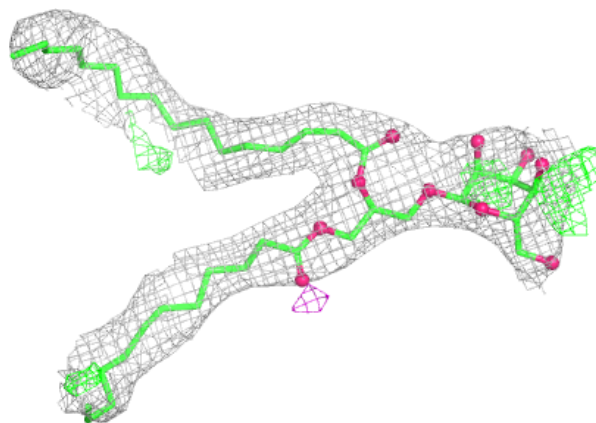


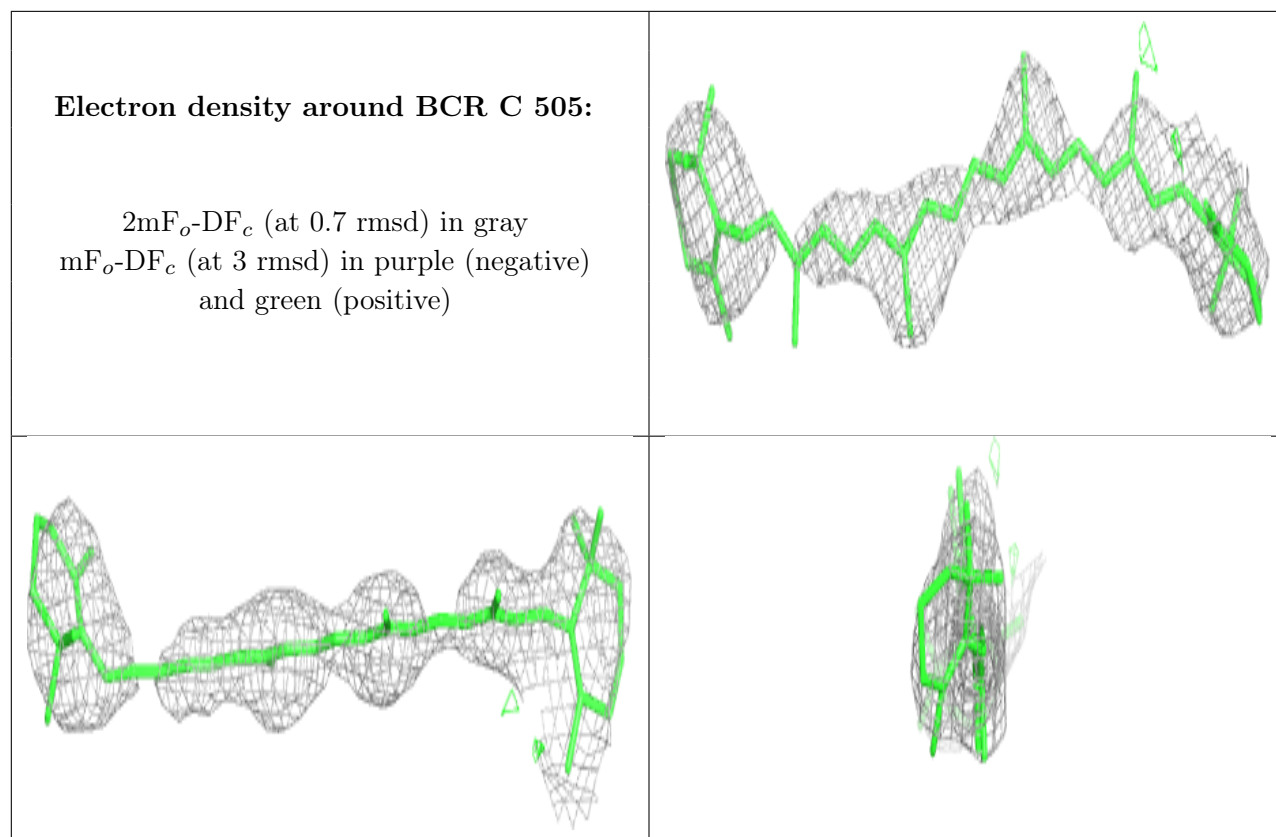
Electron density around CLA b 5516:

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

**Electron density around MGE D 358:**

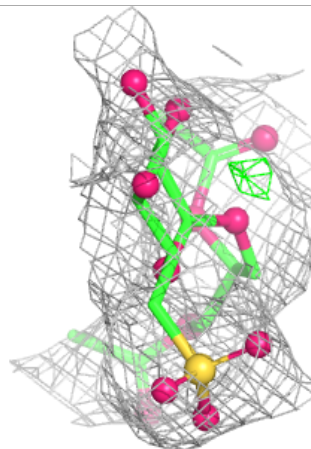
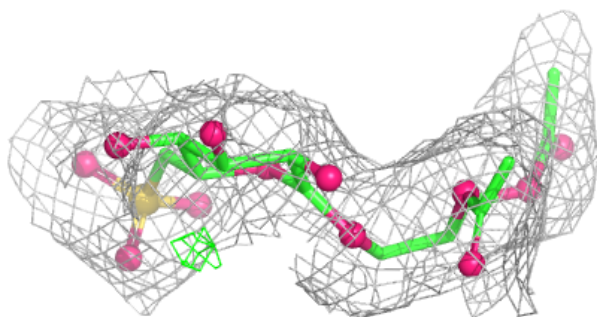
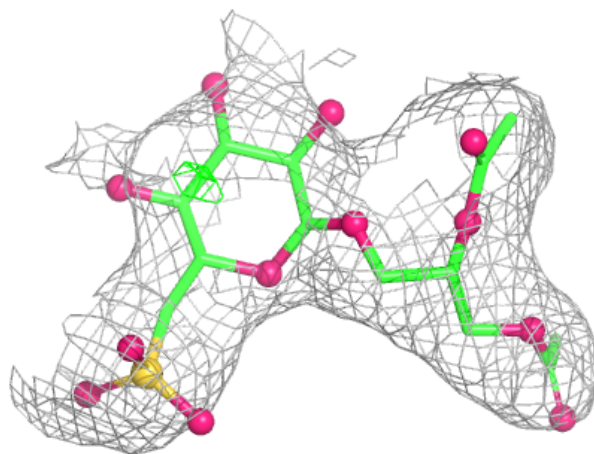
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





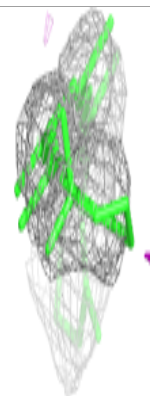
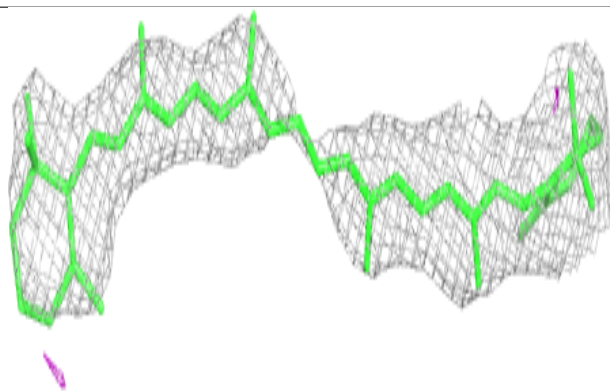
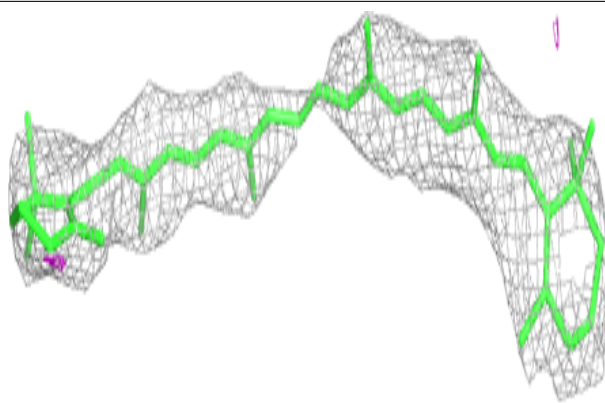
Electron density around SQD A 5212:

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

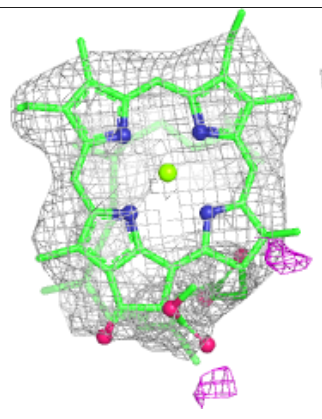
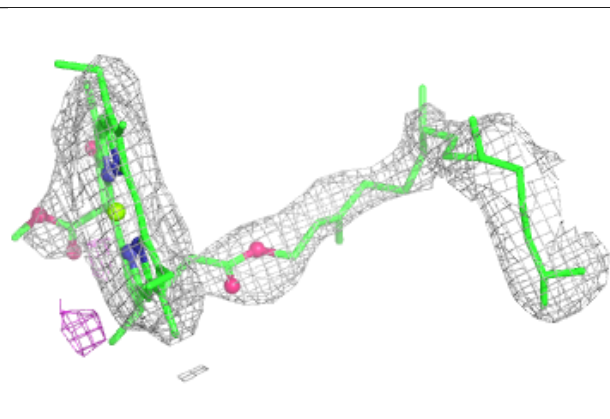
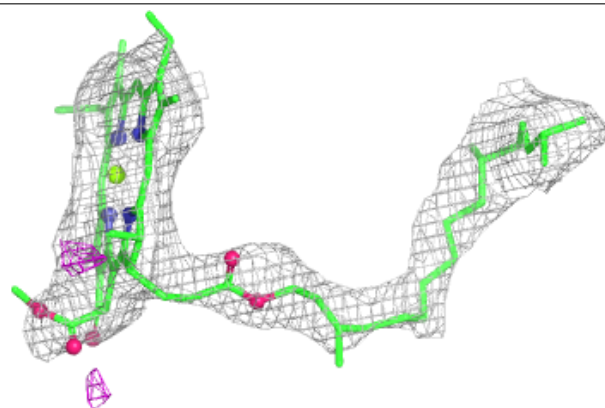


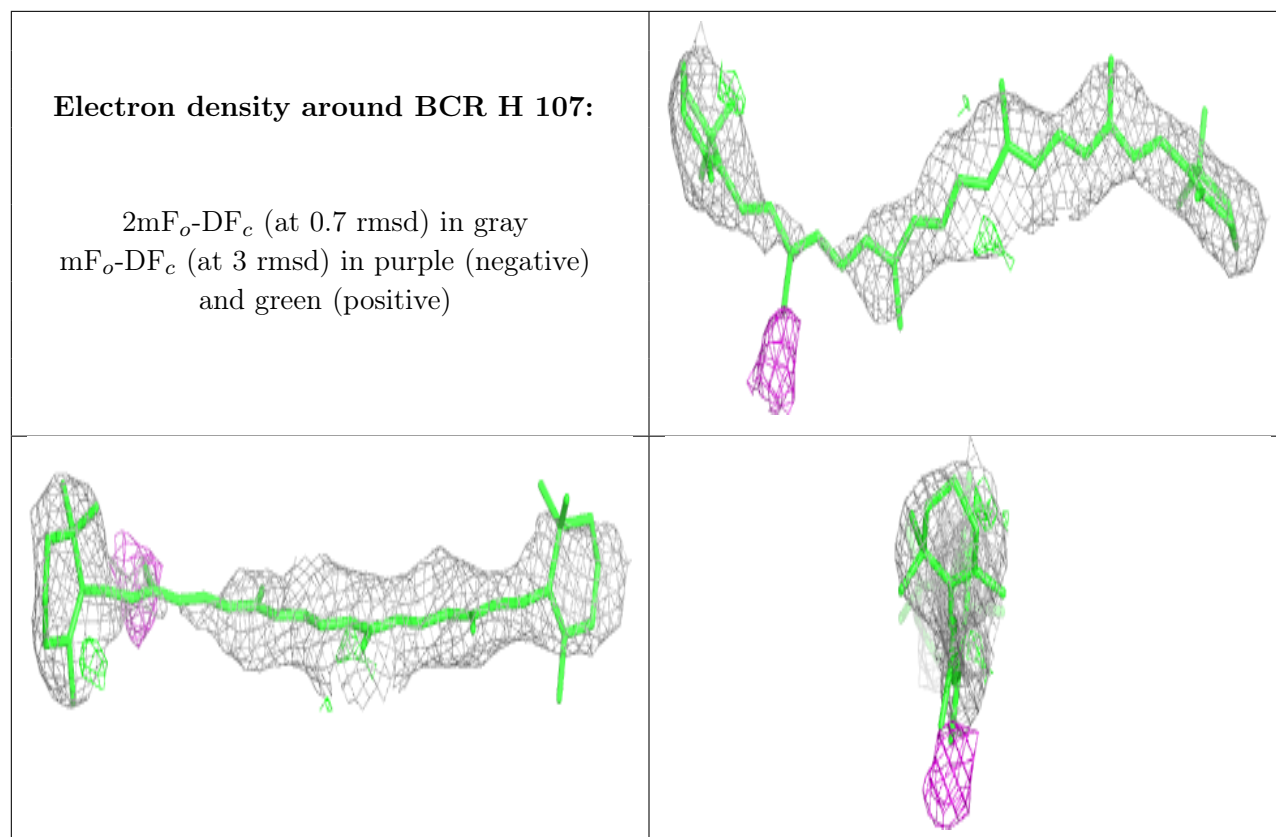
Electron density around BCR d 5357:

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

**Electron density around CLA c 5496:**

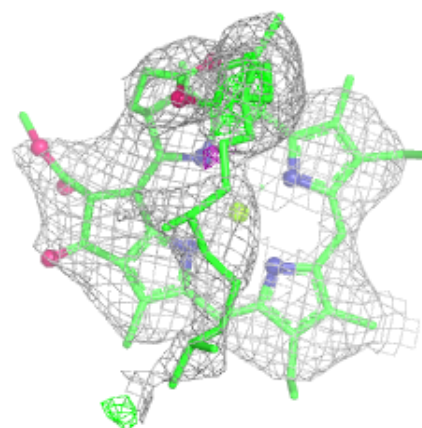
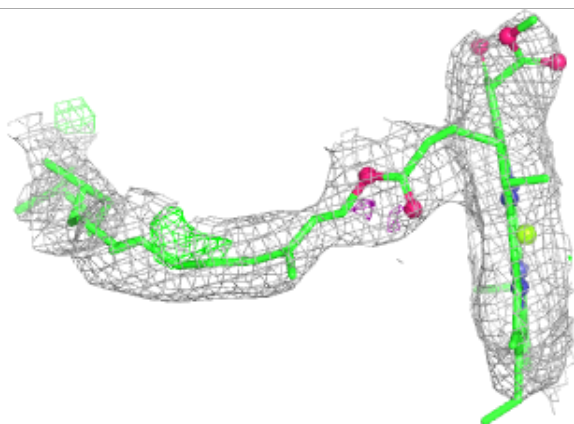
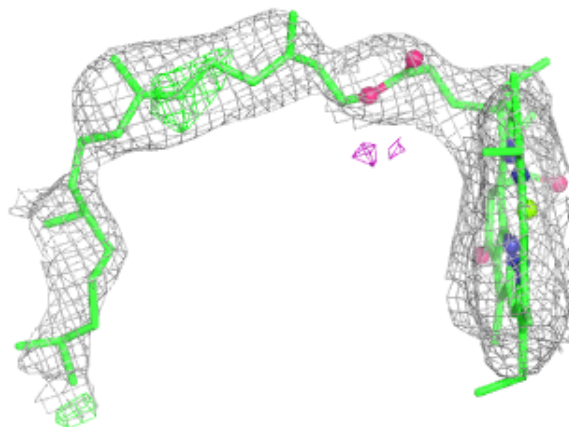
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





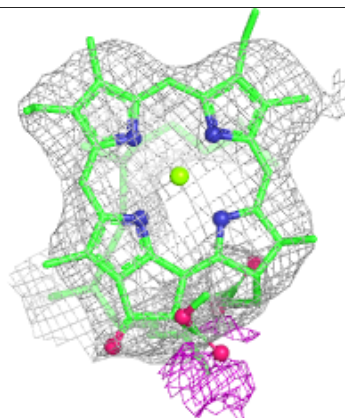
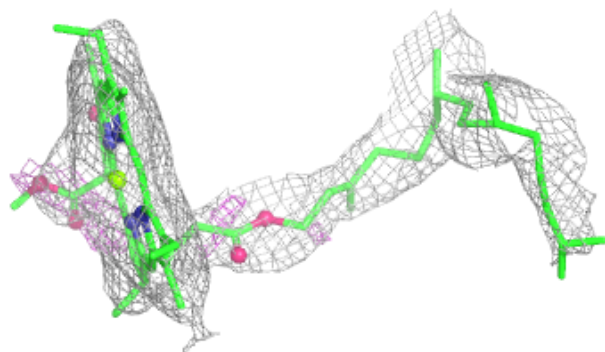
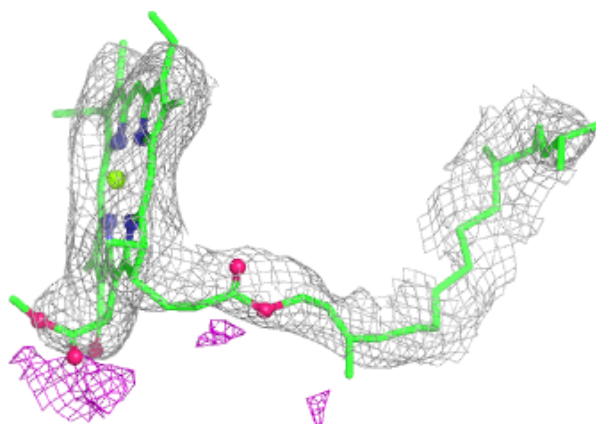
Electron density around CLA B 516:

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

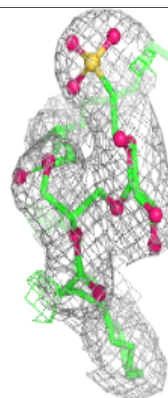
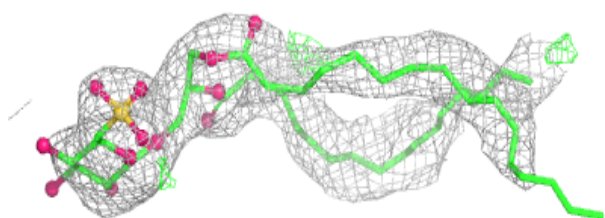
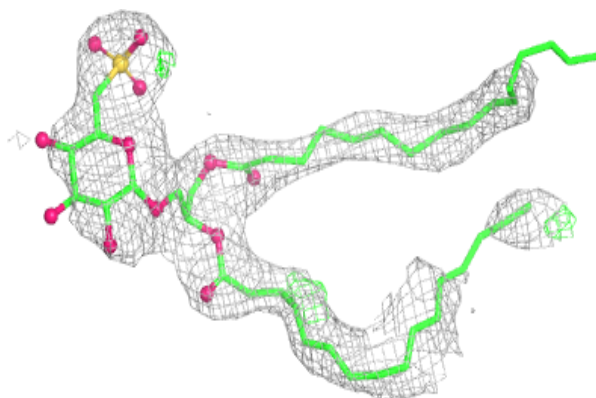


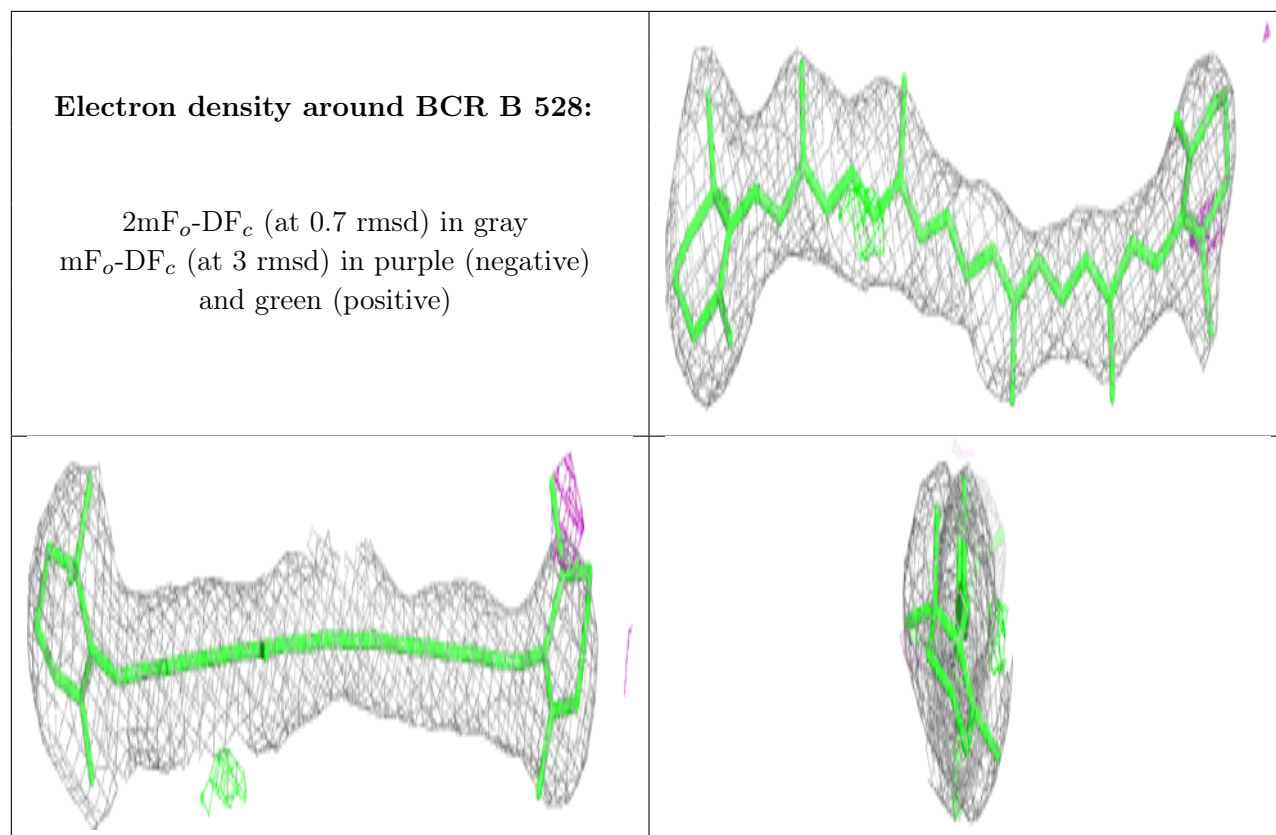
Electron density around CLA C 496:

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

**Electron density around SQD A 568:**

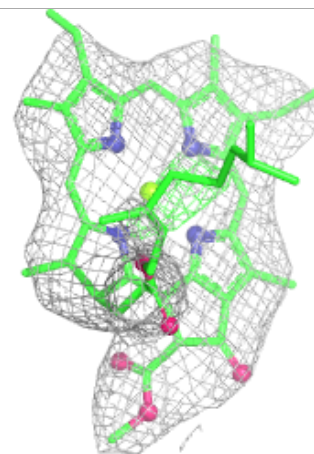
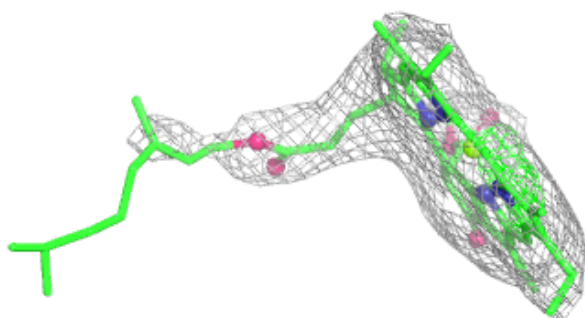
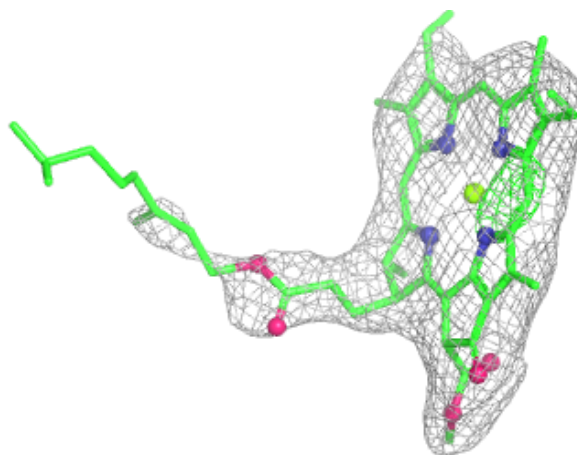
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

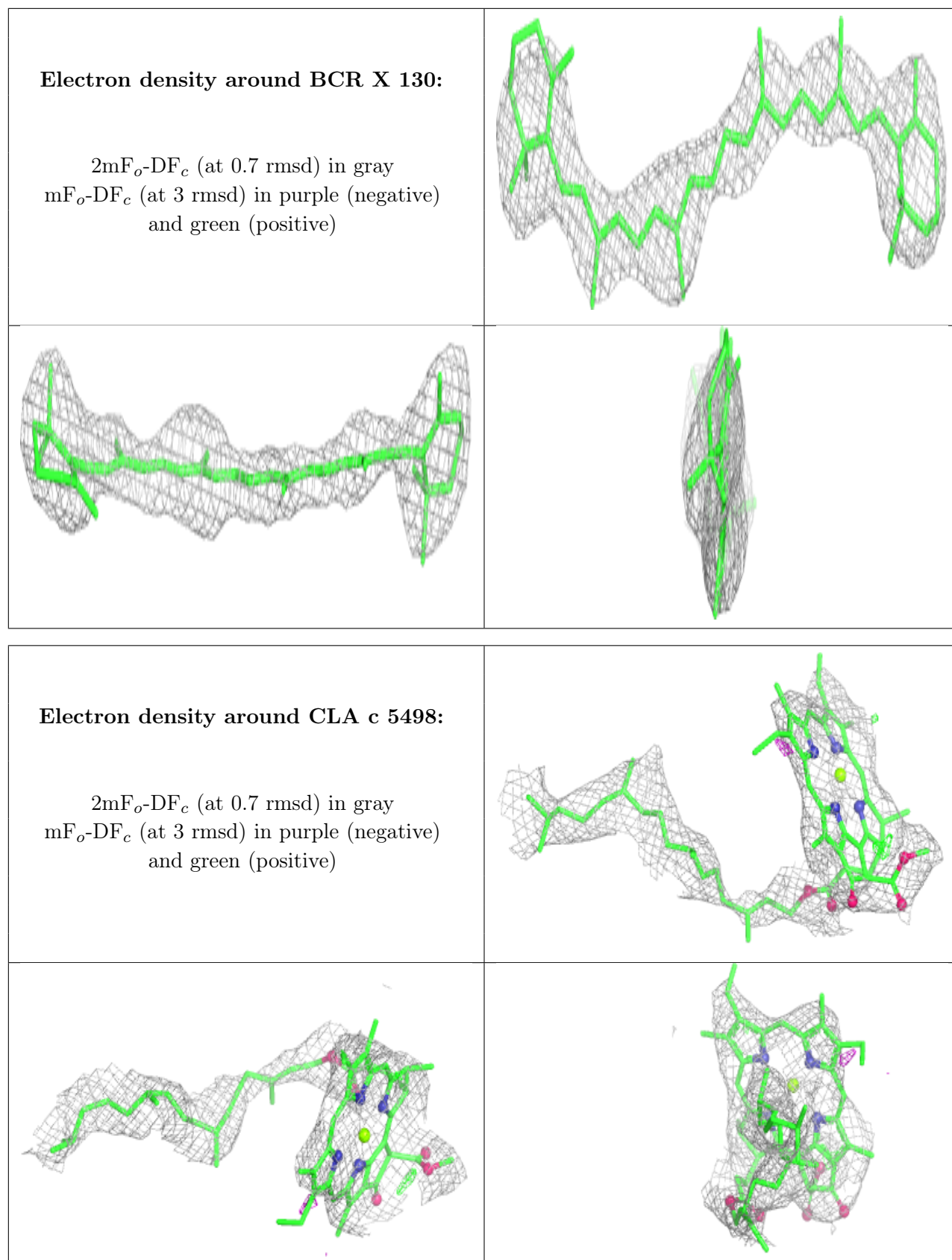


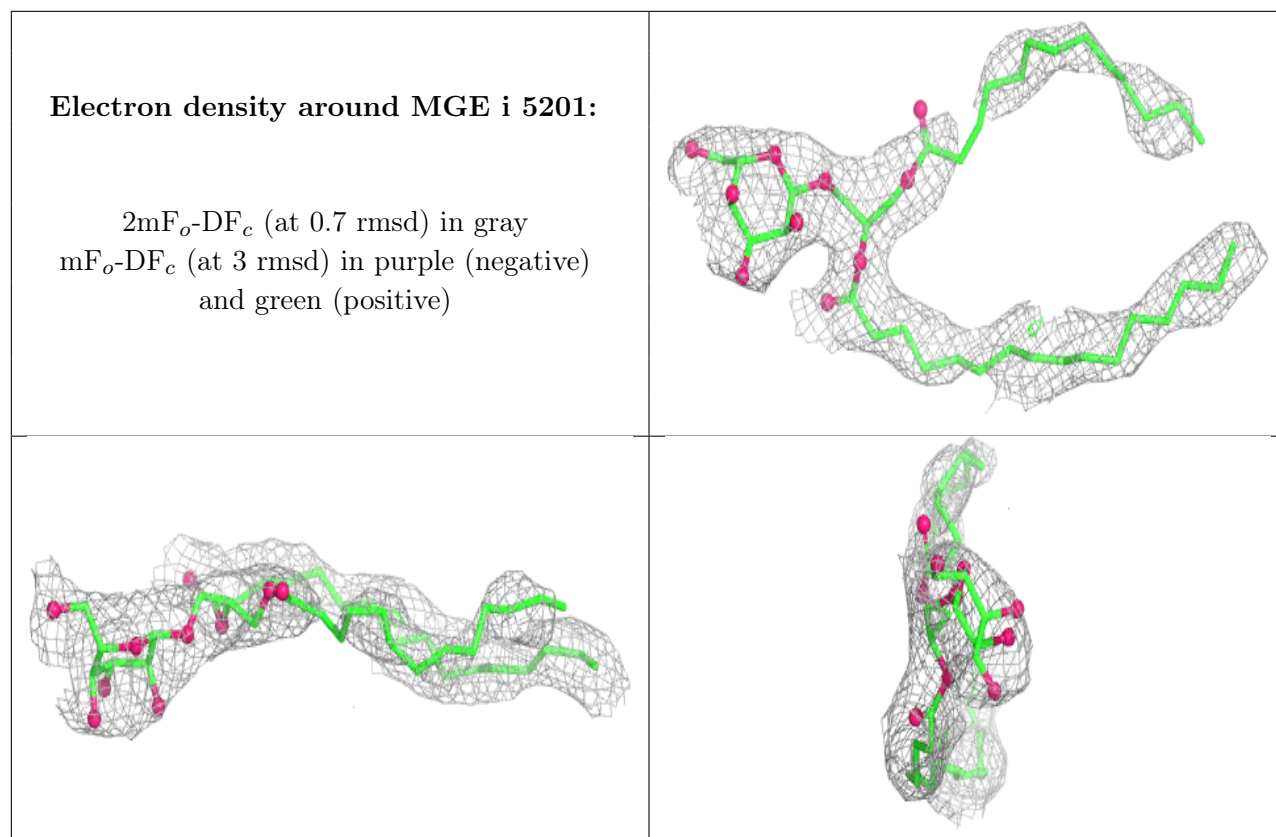


Electron density around CLA a 5563:

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

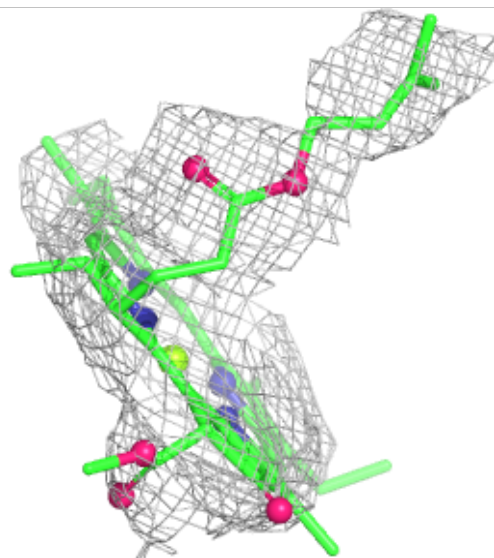
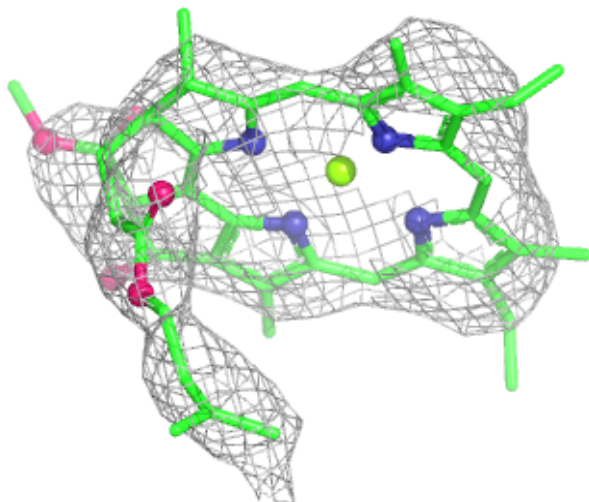
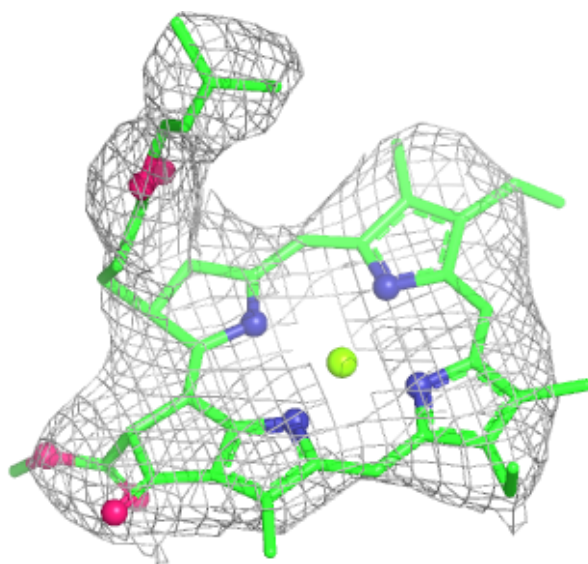


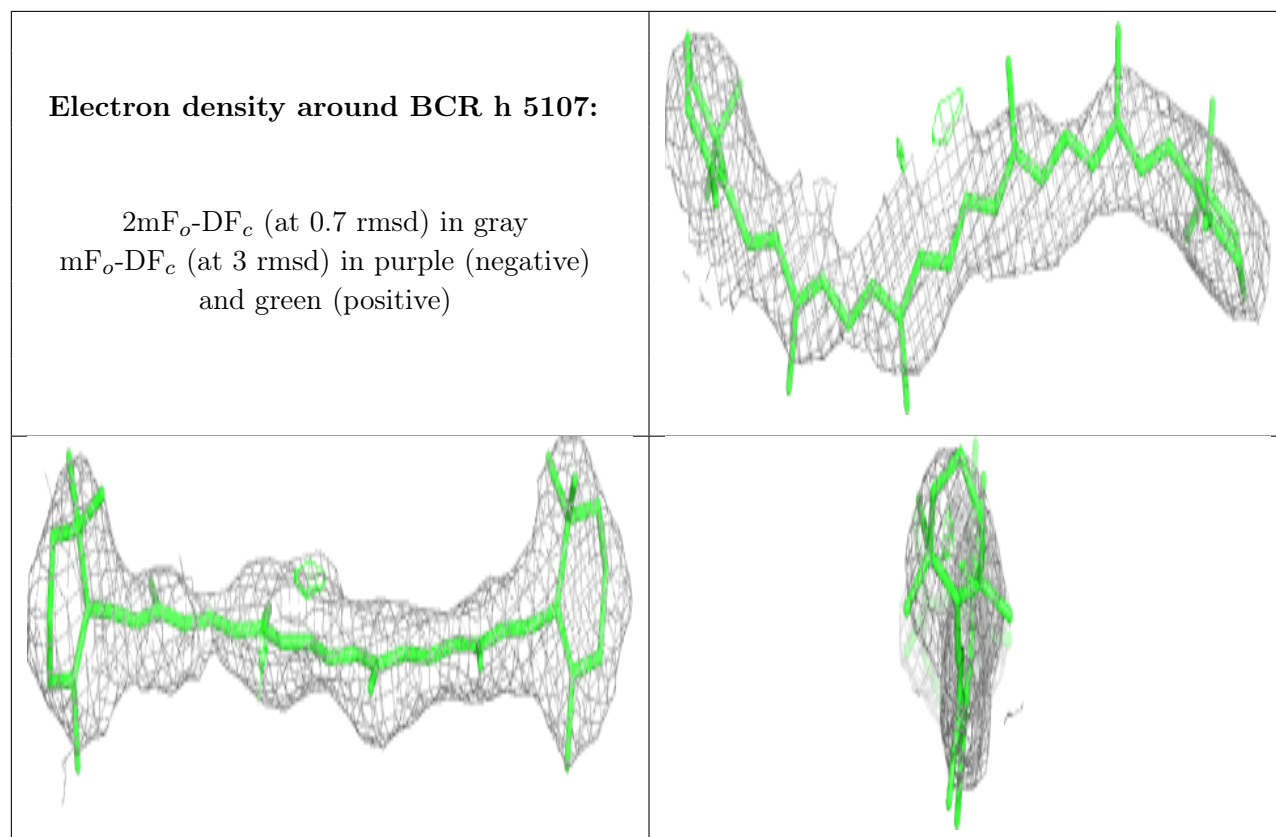




Electron density around CLA c 5503:

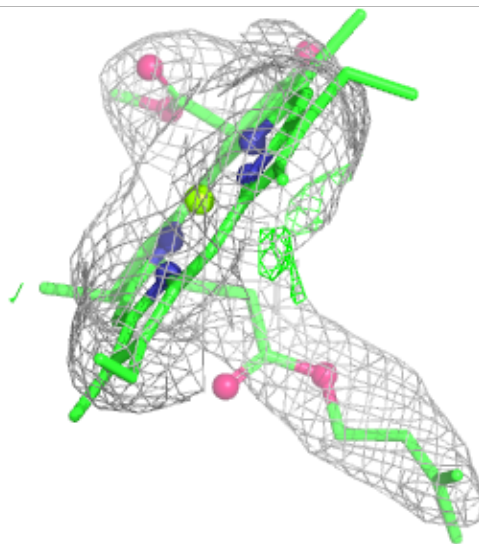
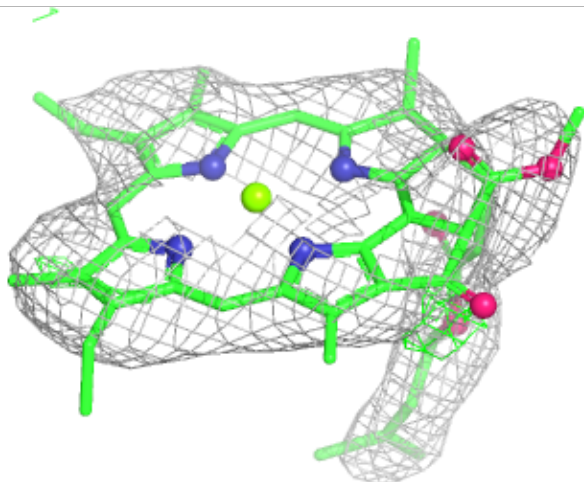
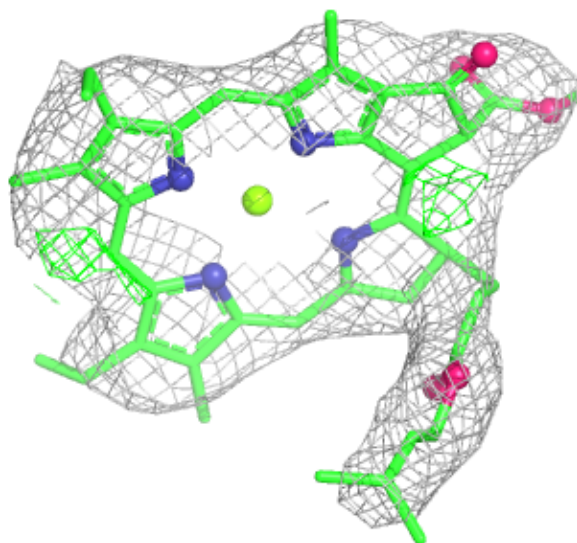
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





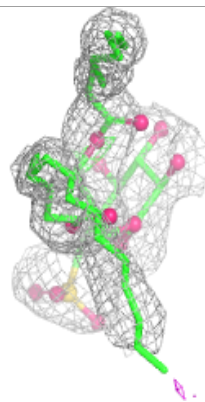
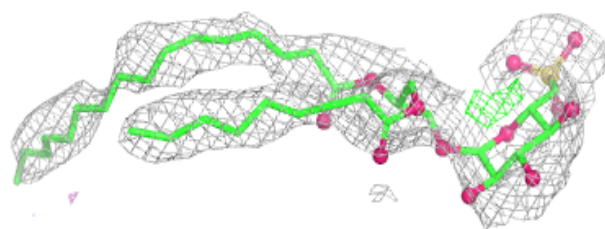
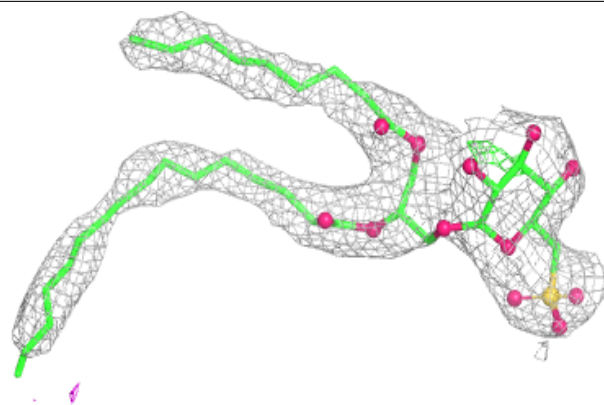
Electron density around CLA C 503:

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

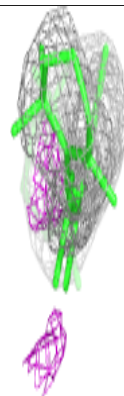
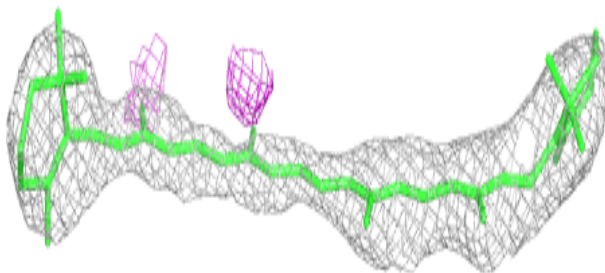
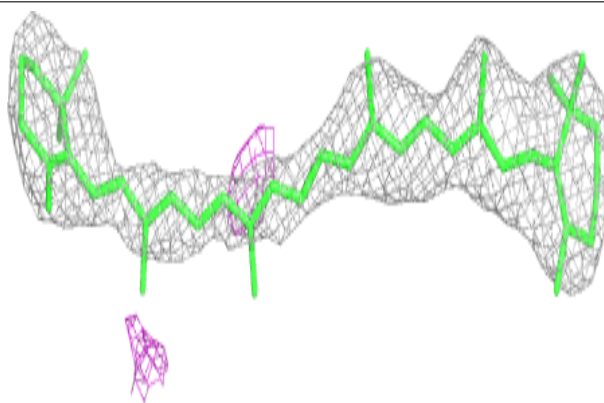


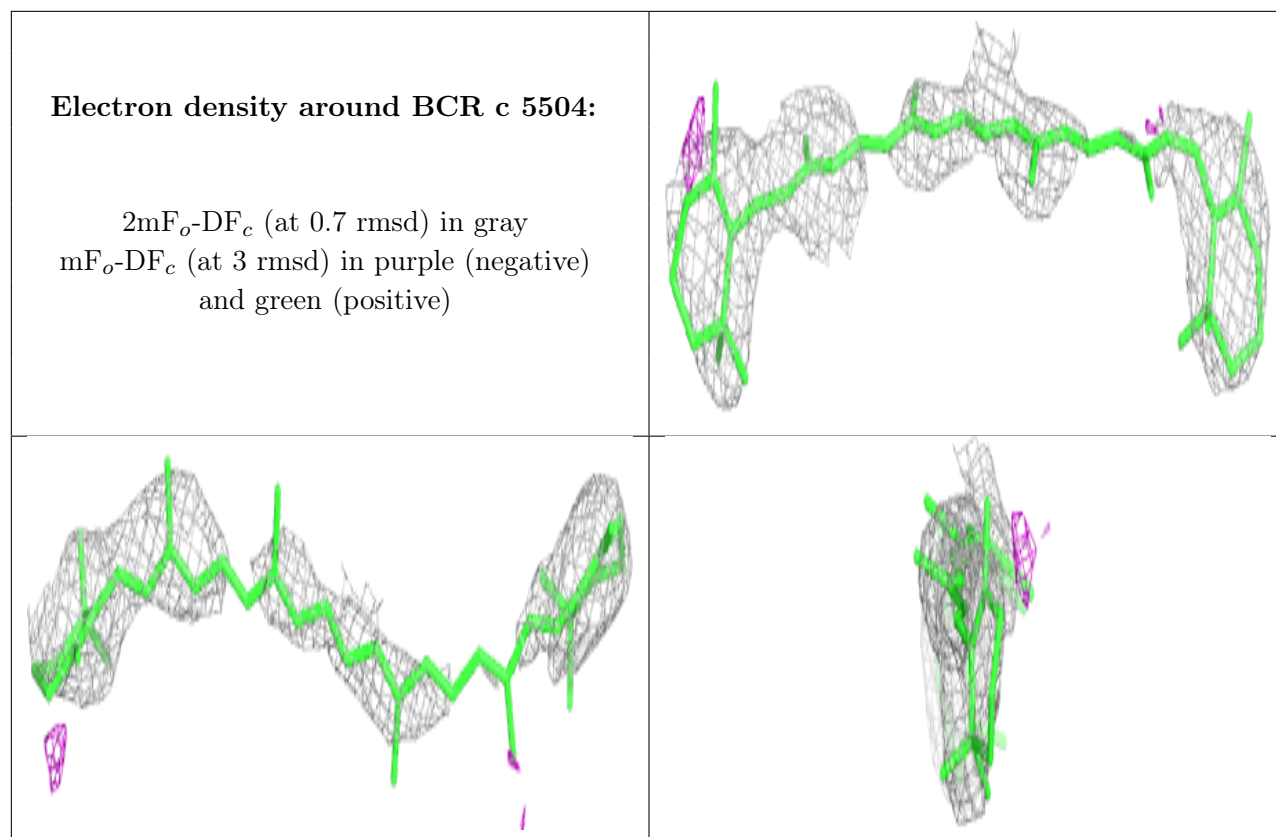
Electron density around SQD t 213:

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

**Electron density around BCR b 5529:**

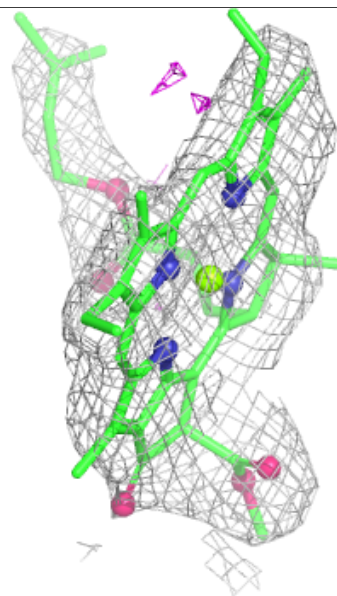
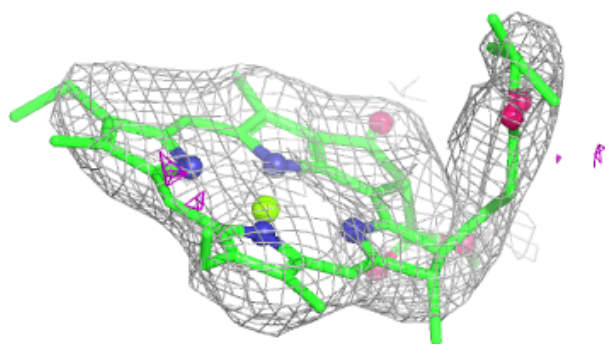
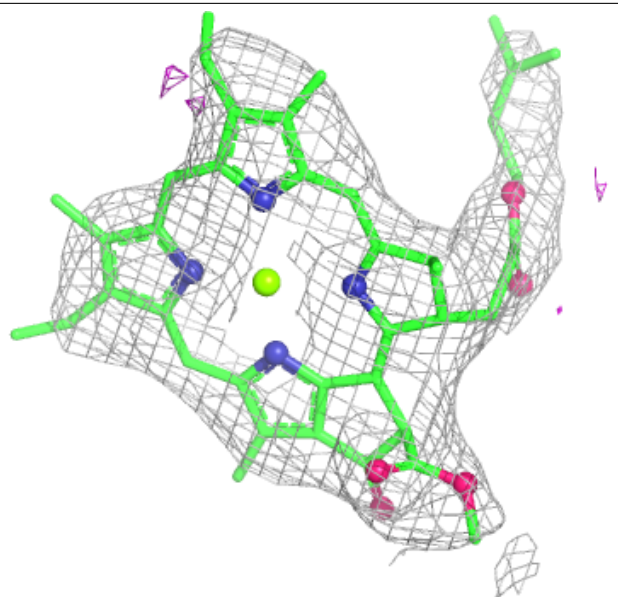
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





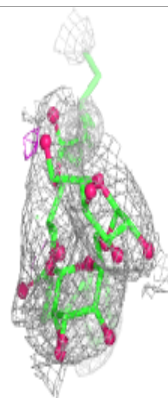
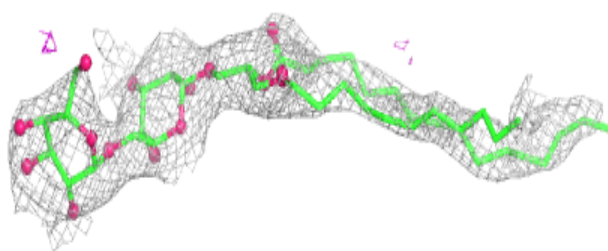
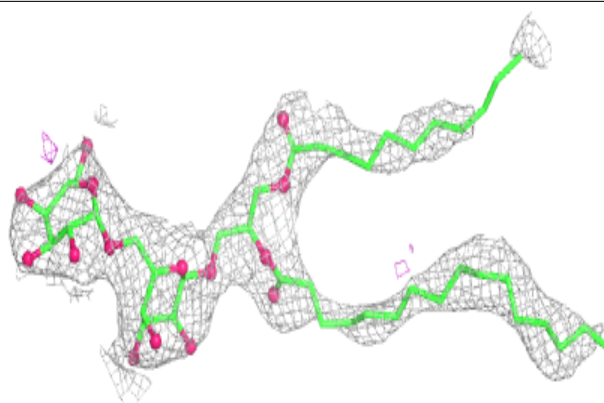
Electron density around CLA d 5355:

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

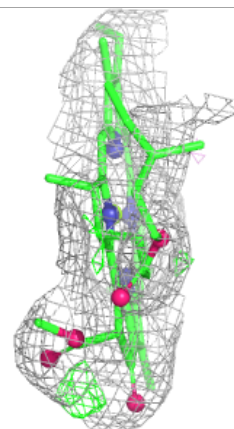
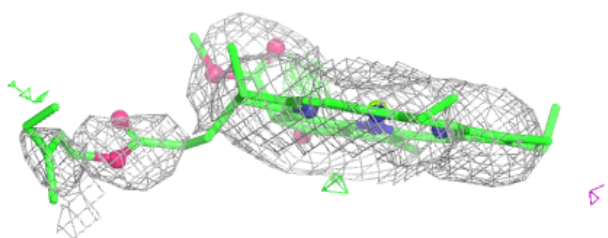
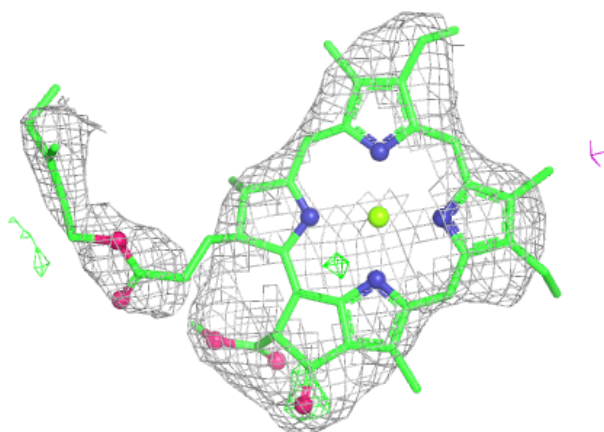


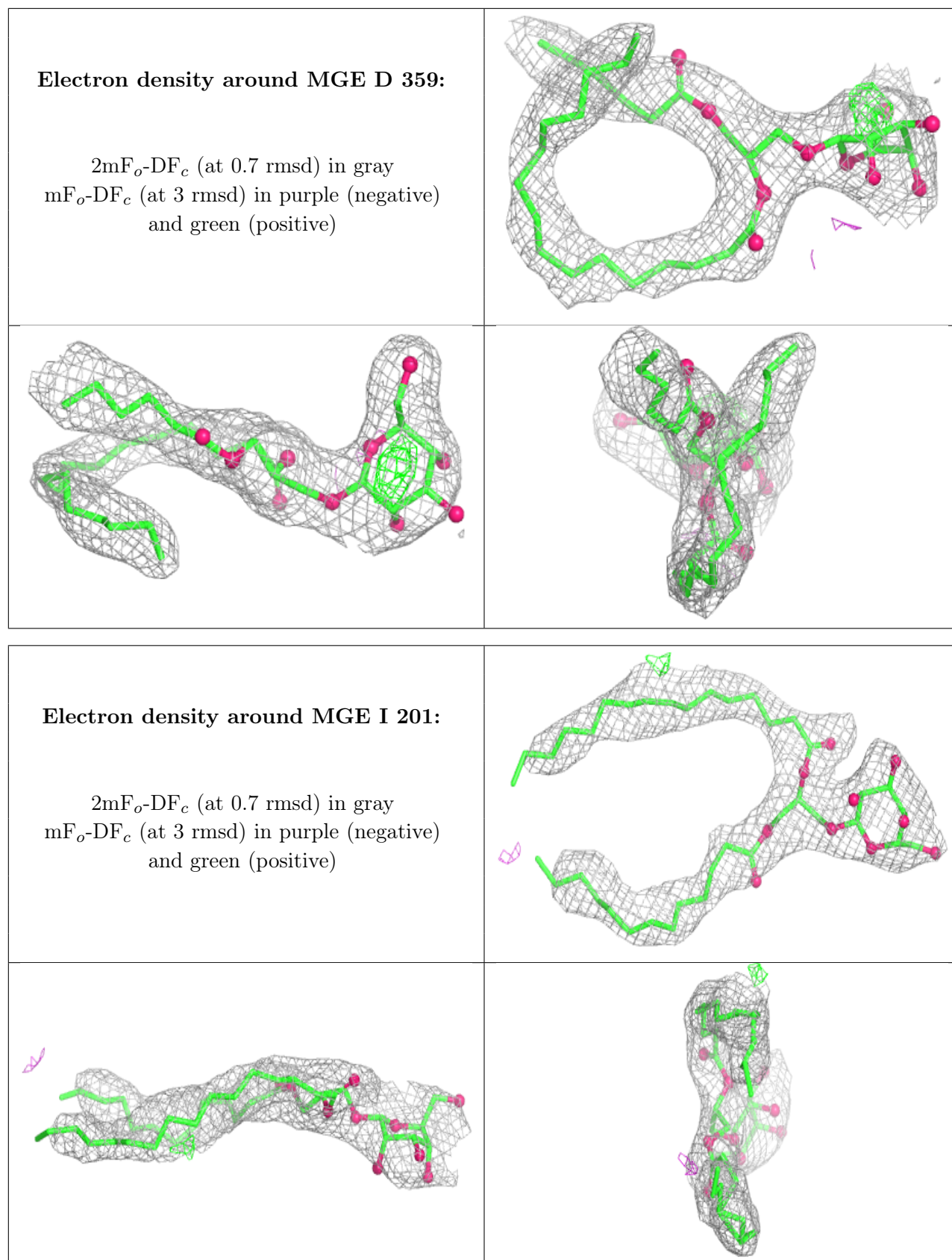
Electron density around DGD c 5509:

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

**Electron density around CLA c 5502:**

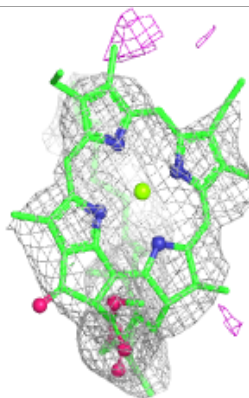
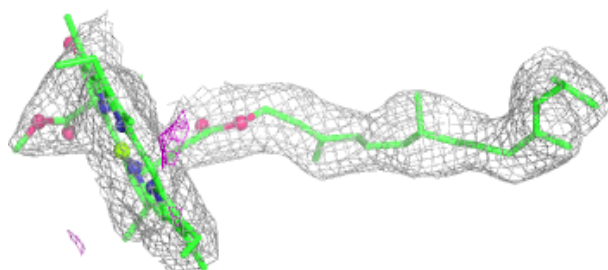
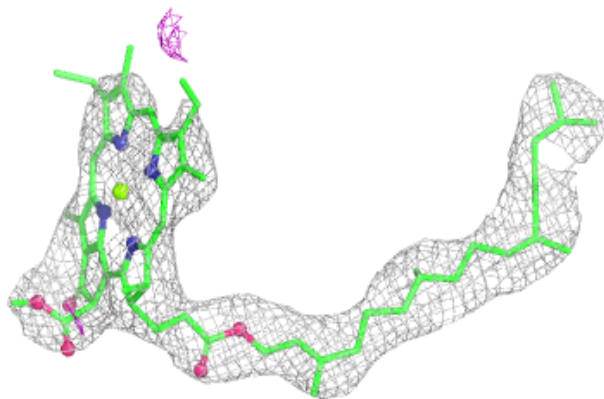
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



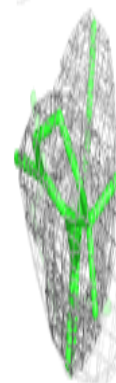
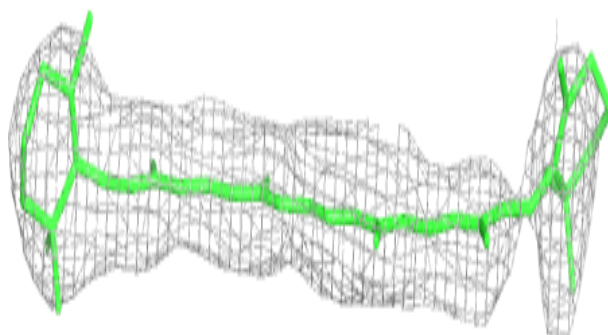
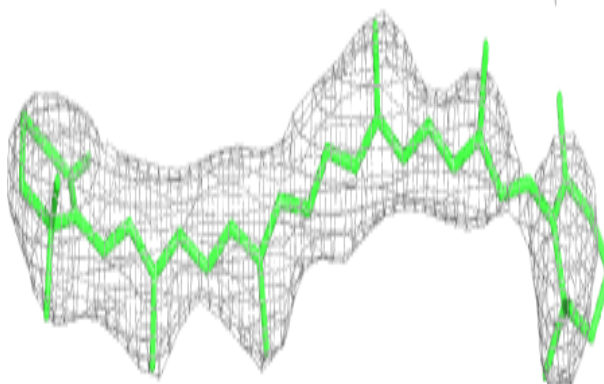


Electron density around CLA B 519:

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

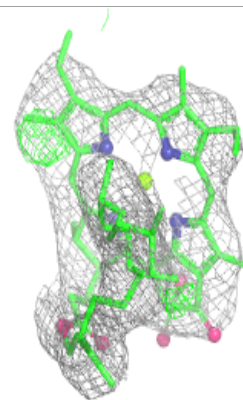
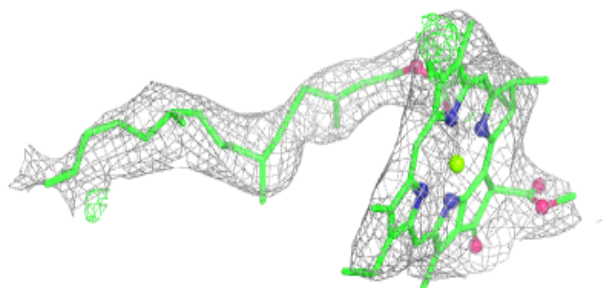
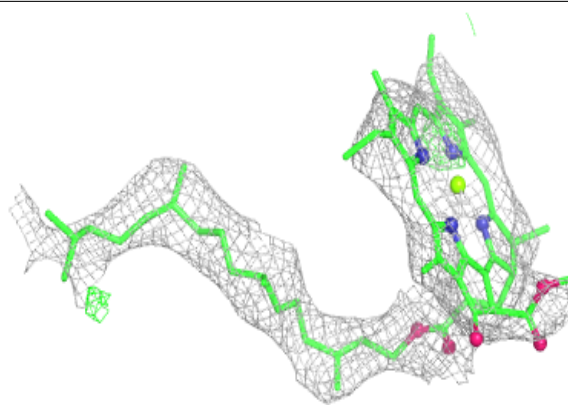
**Electron density around BCR C 506:**

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

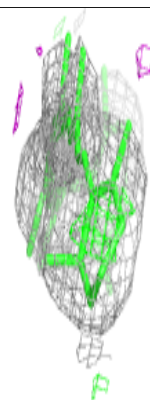
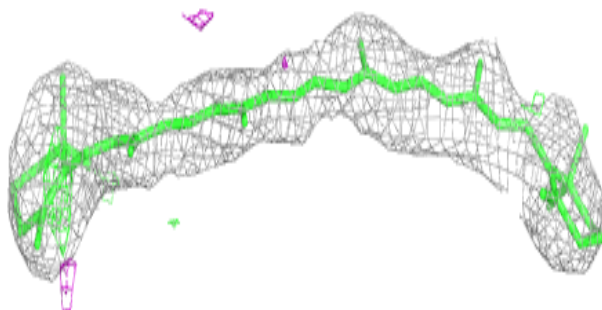
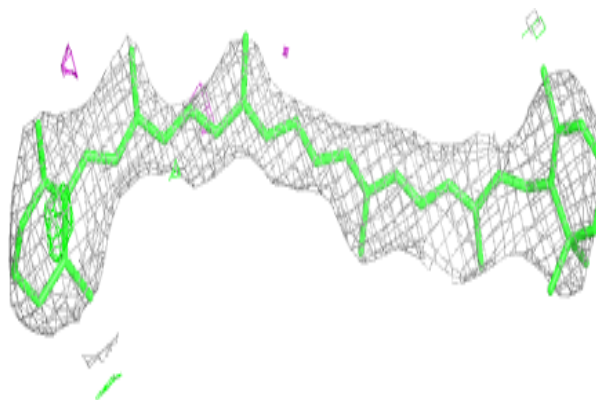


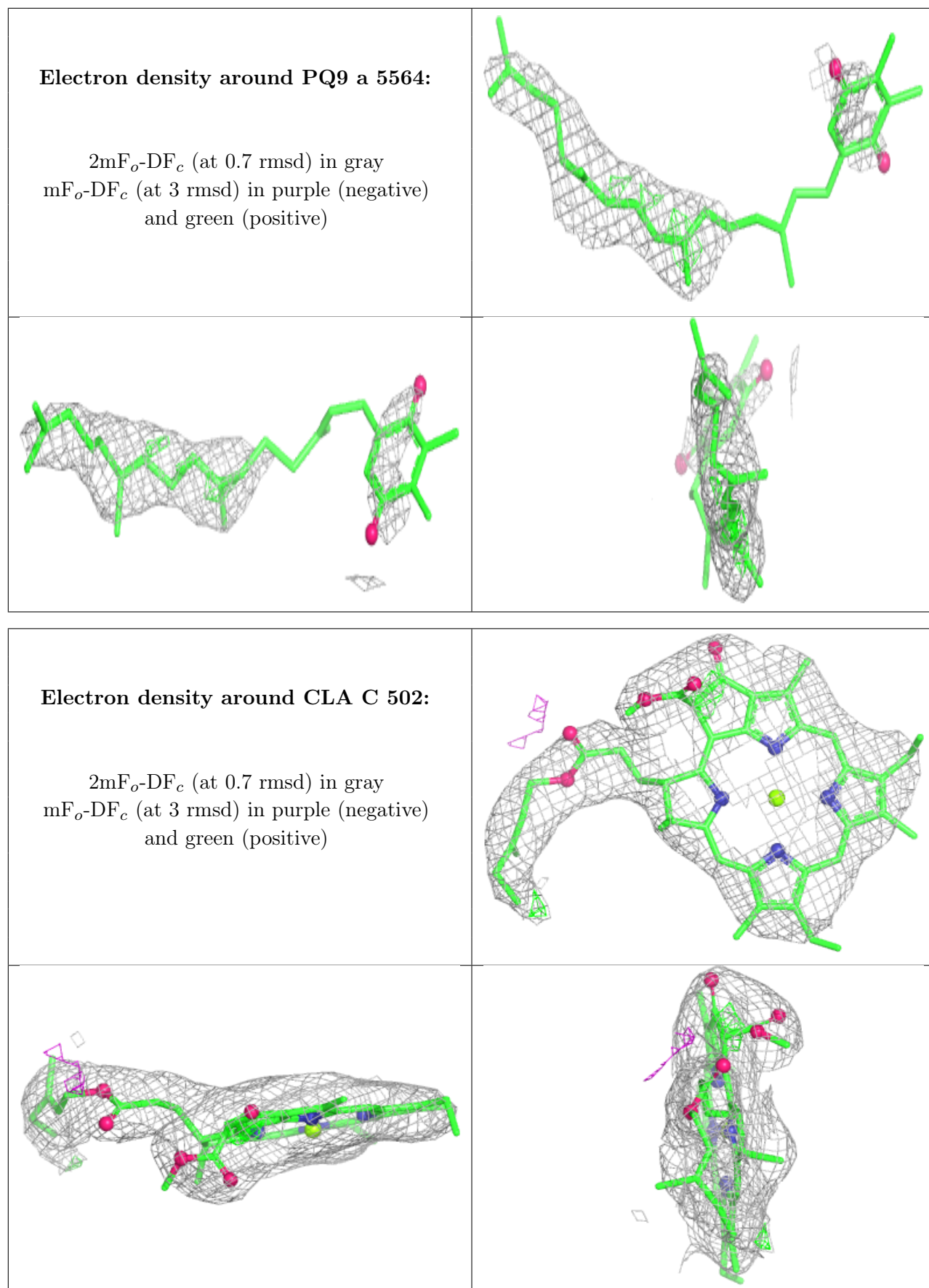
Electron density around CLA C 498:

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

**Electron density around BCR T 5104:**

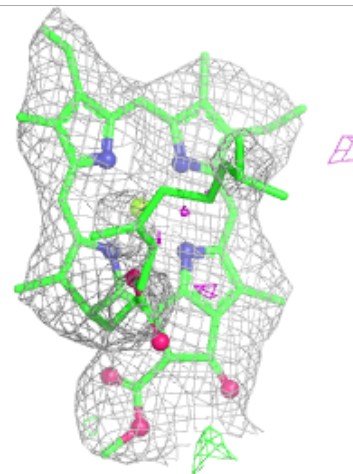
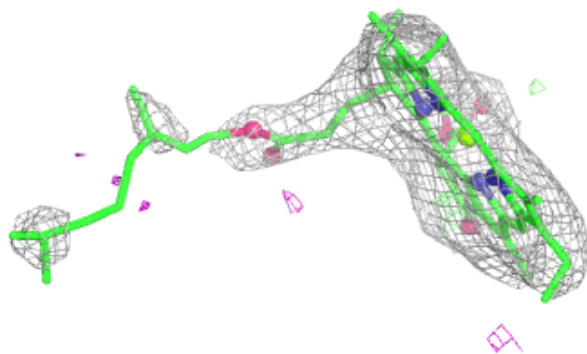
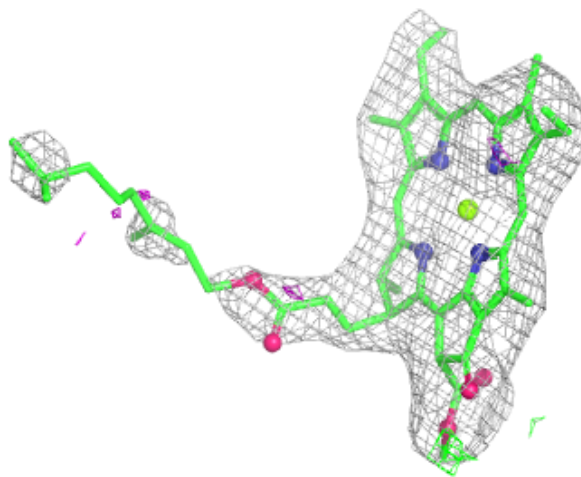
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

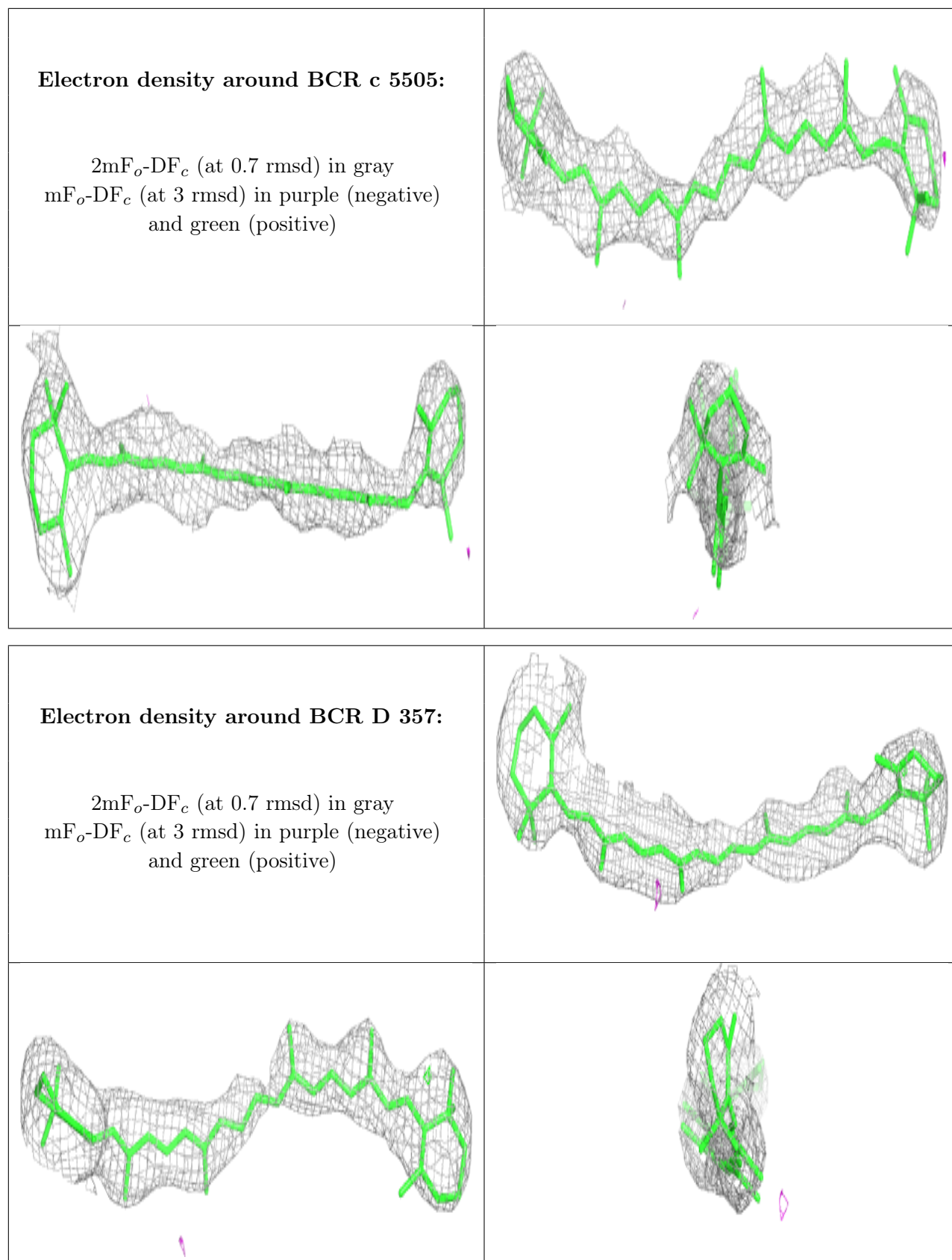


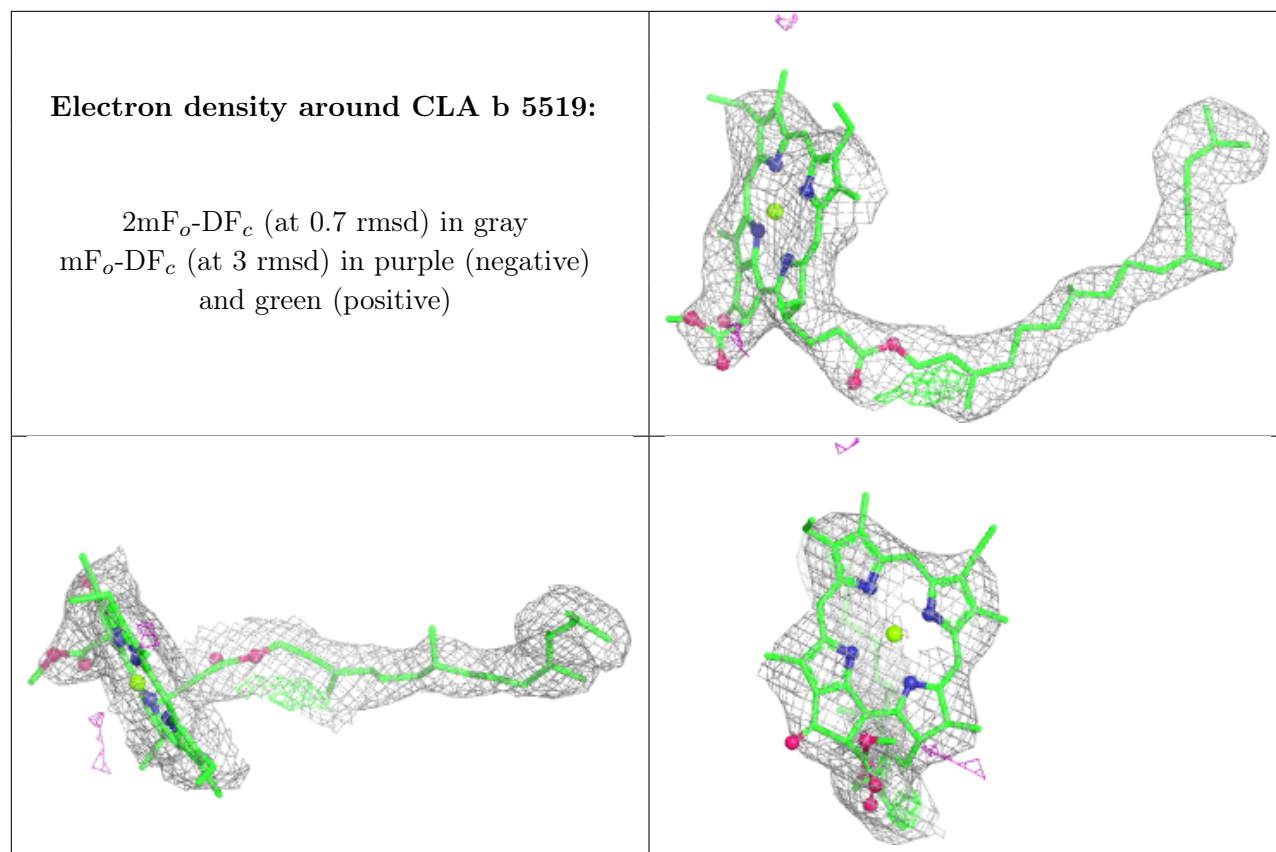


Electron density around CLA A 563:

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

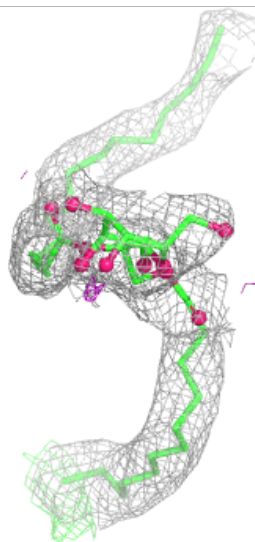
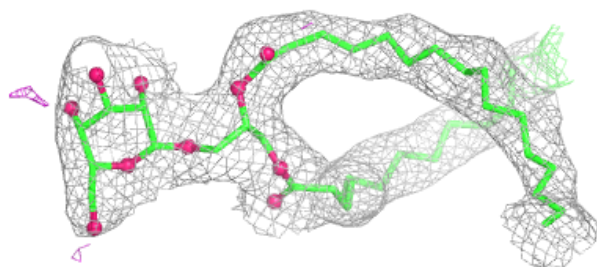
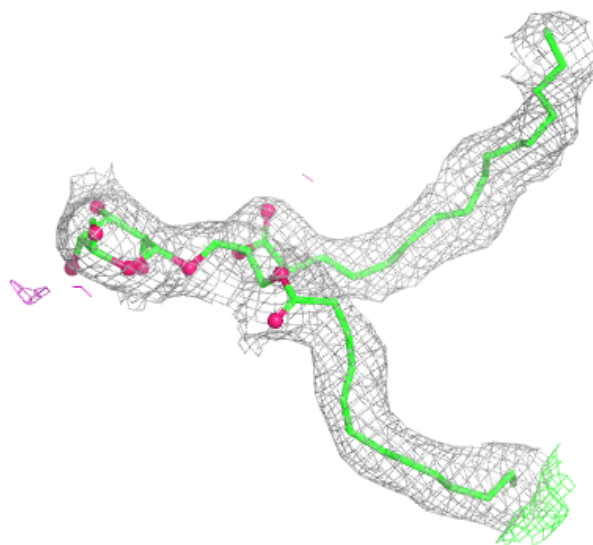






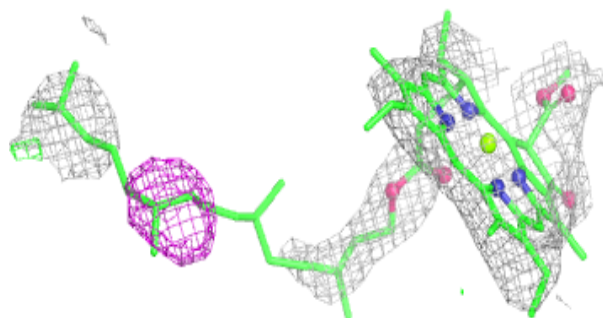
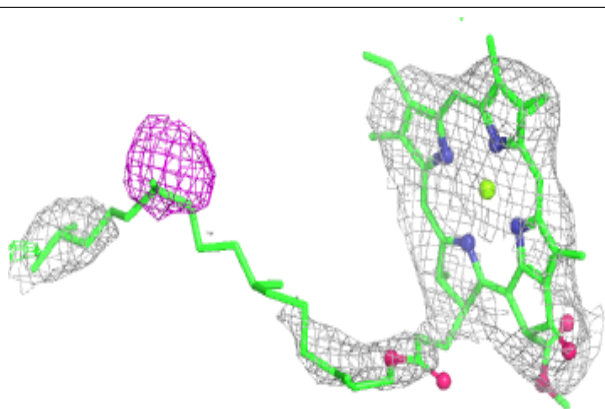
Electron density around MGE B 530:

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

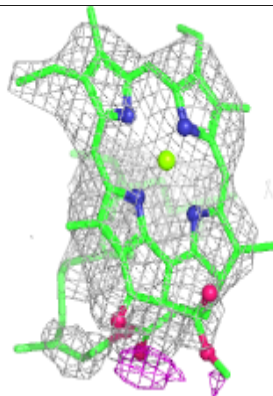
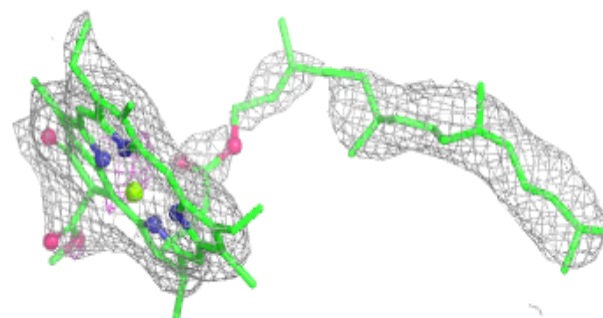
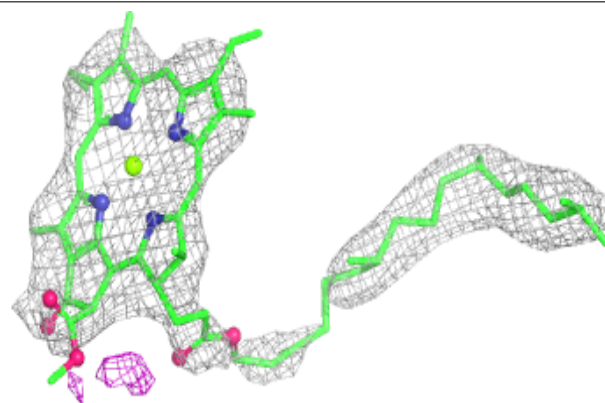


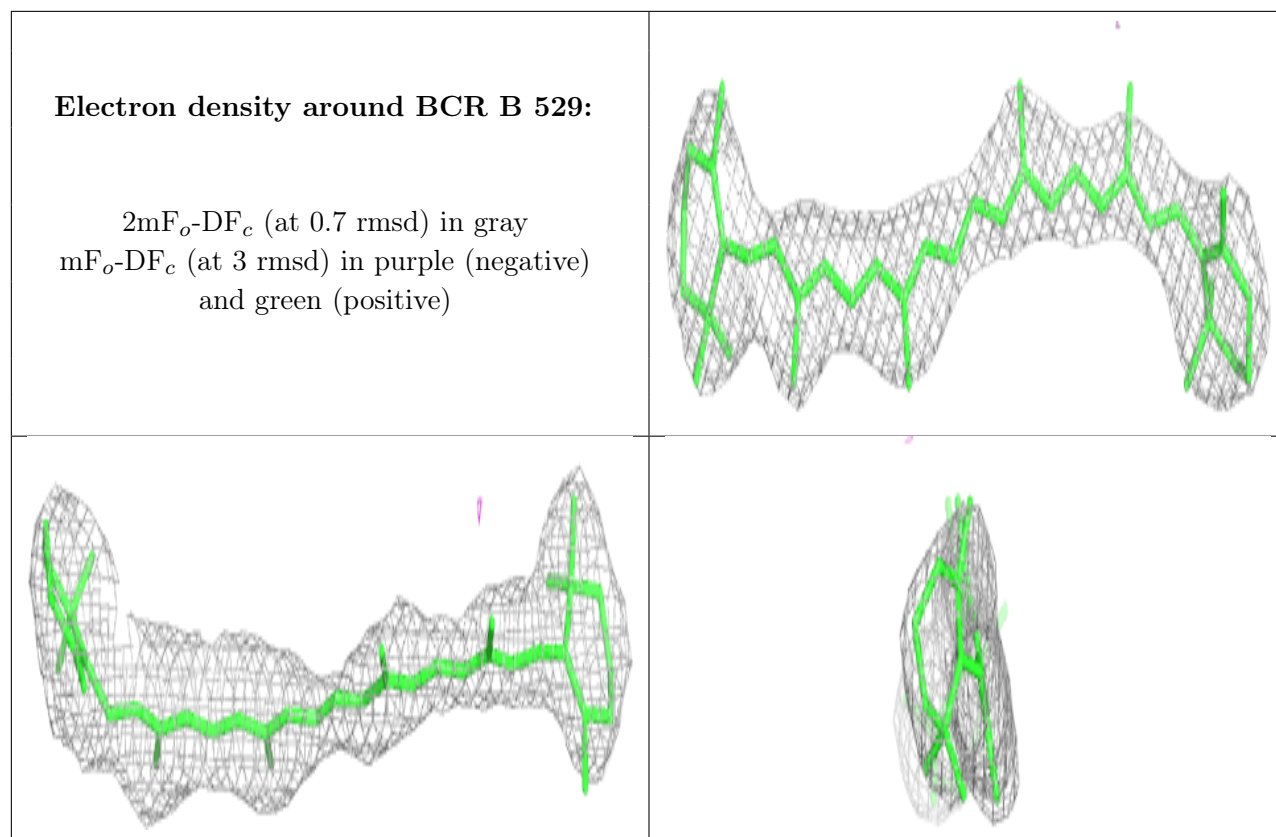
Electron density around CLA c 5501:

$2mF_o-DF_c$ (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:**

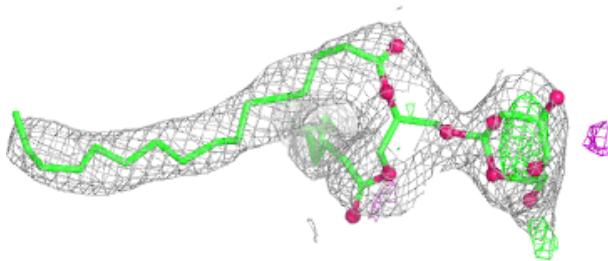
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





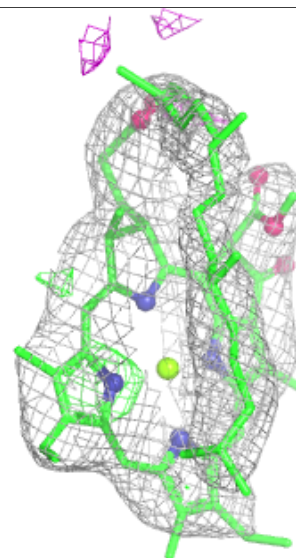
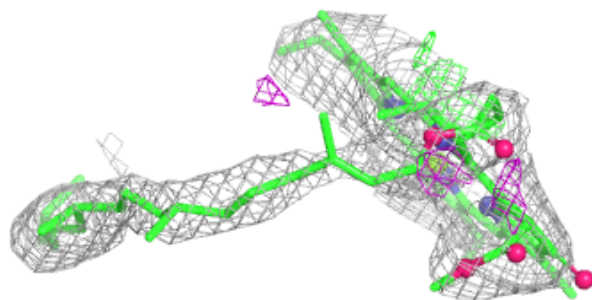
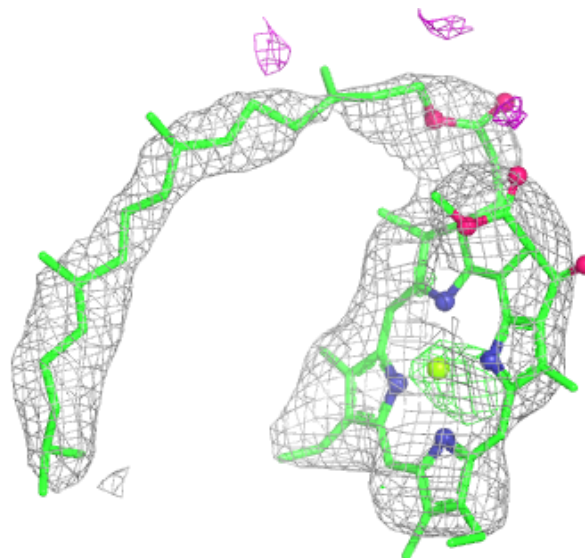
Electron density around MGE L 210:

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



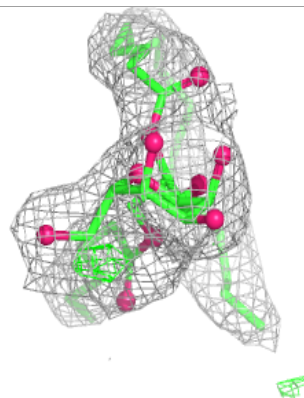
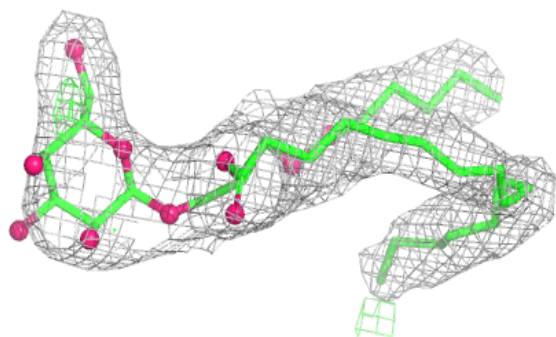
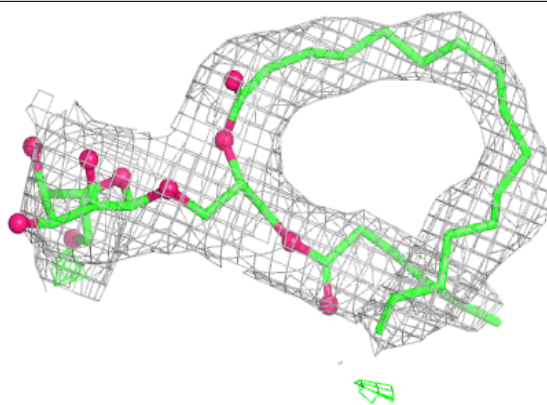
Electron density around CLA C 497:

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

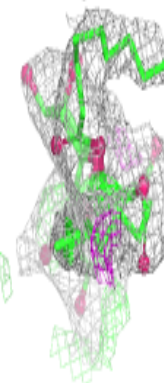
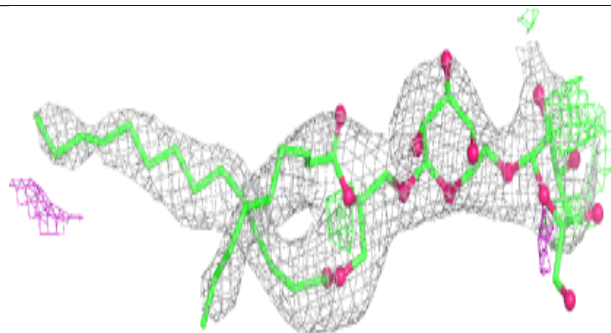
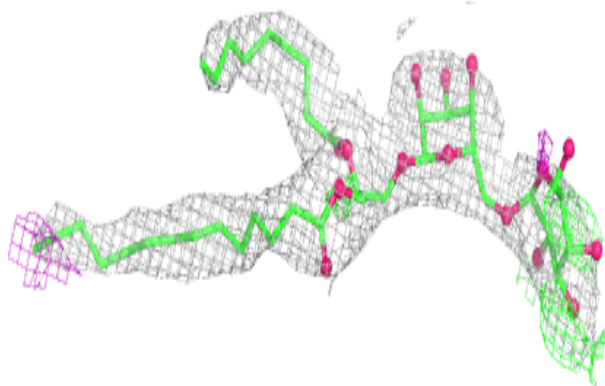


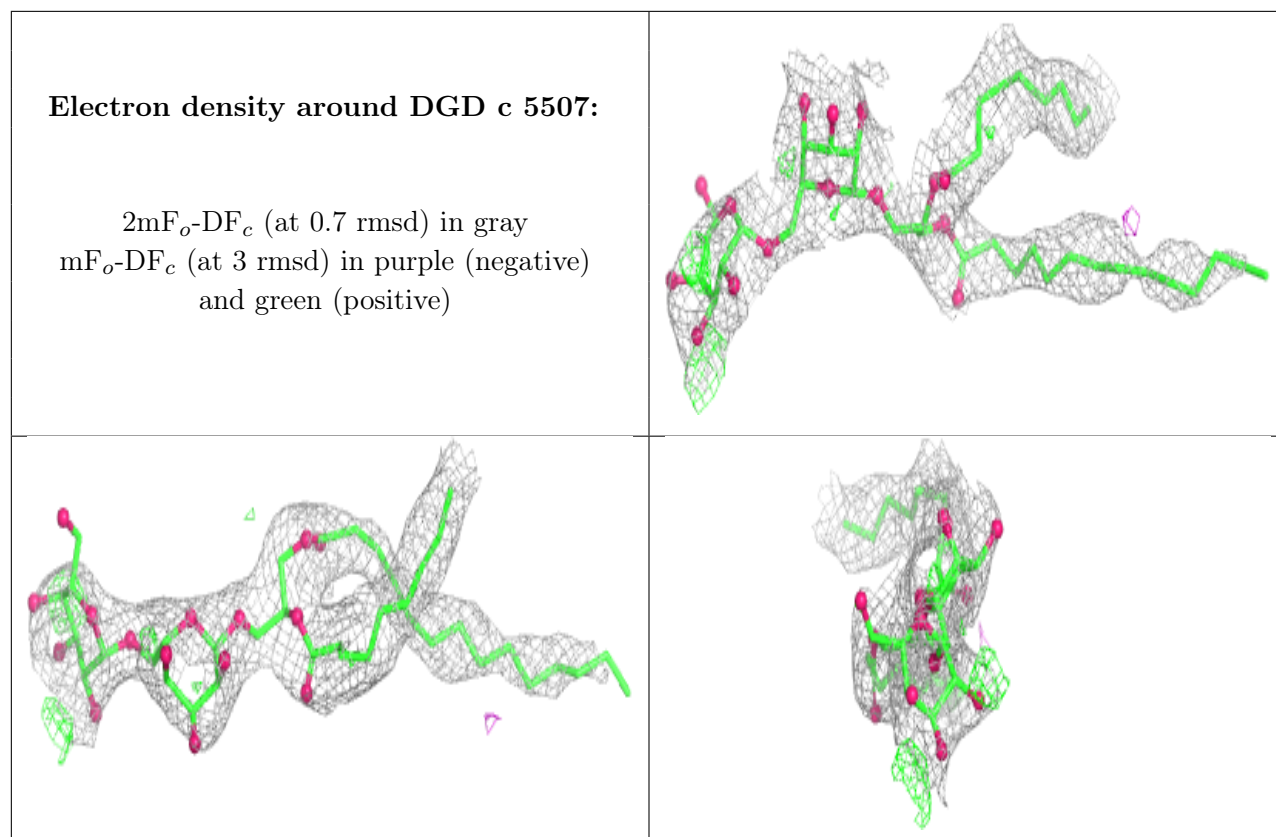
Electron density around MGE d 5360:

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

**Electron density around DGD C 507:**

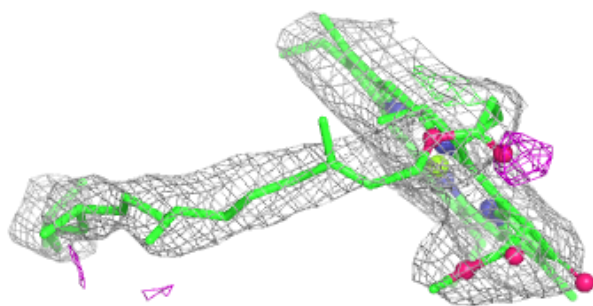
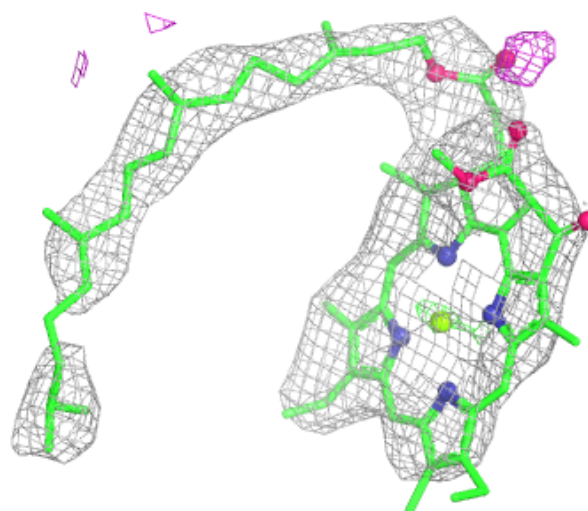
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

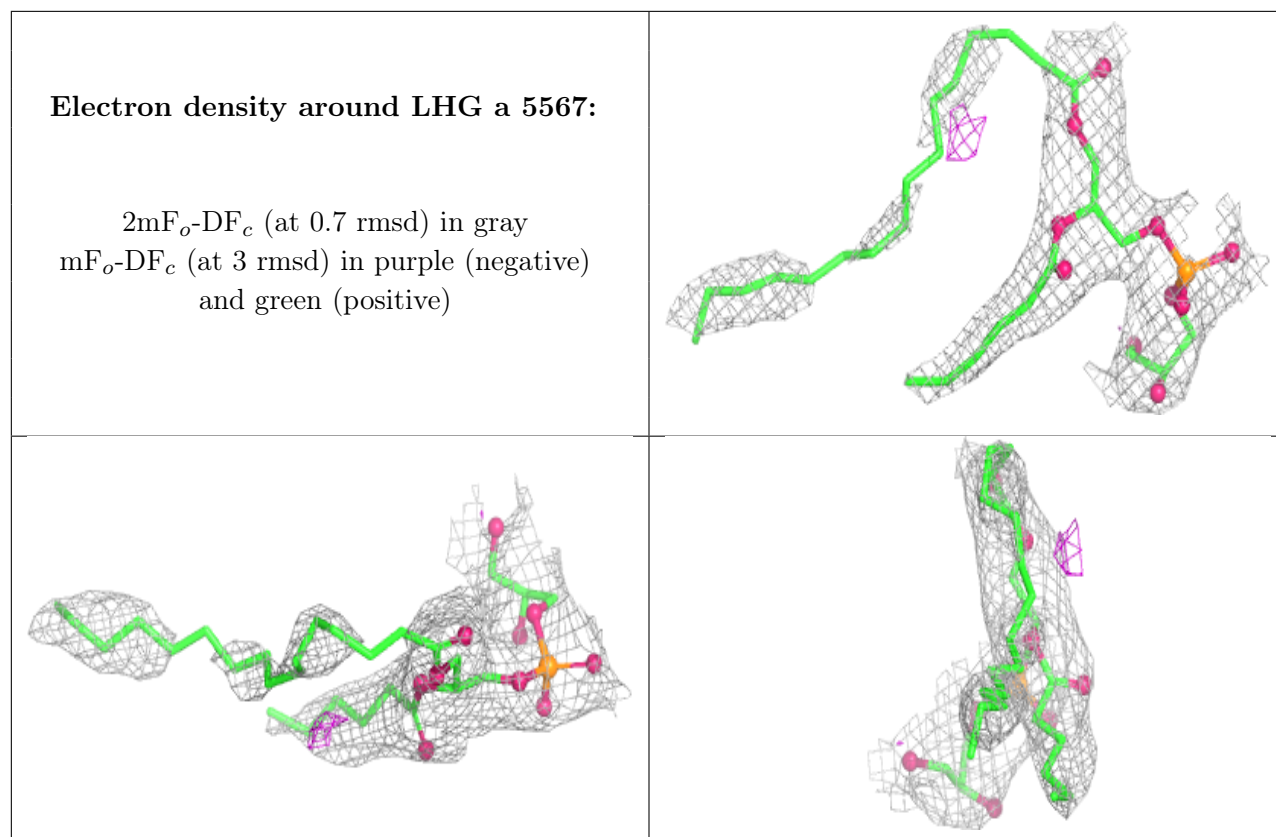




Electron density around CLA c 5497:

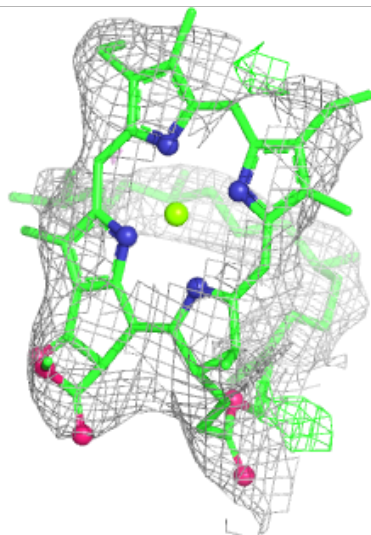
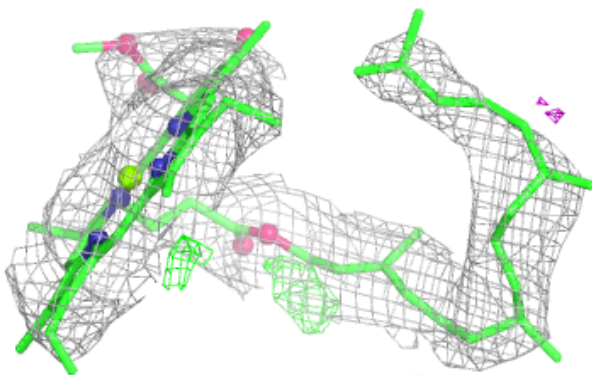
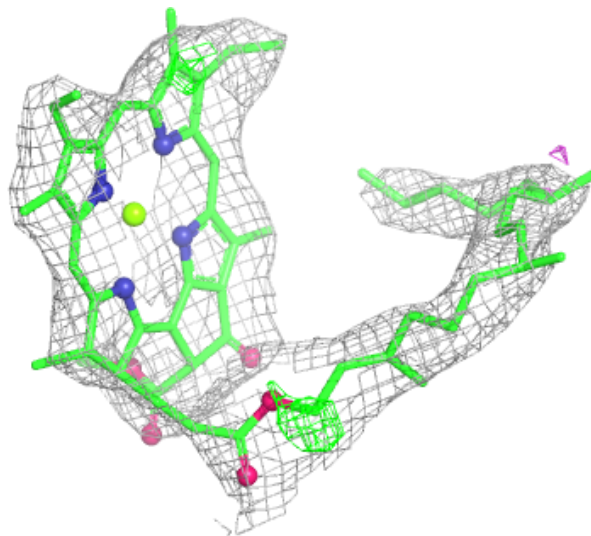
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





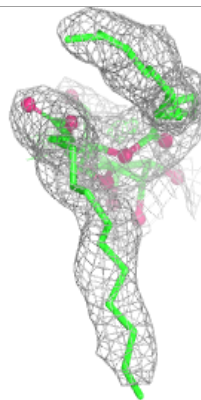
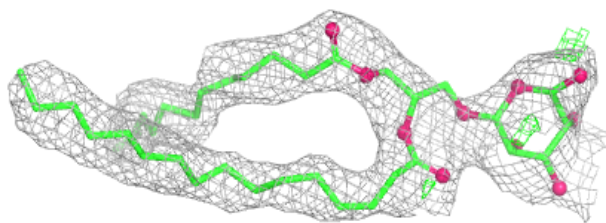
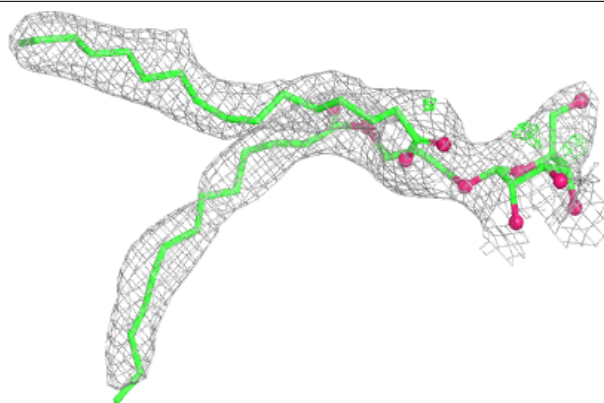
Electron density around CLA c 5493:

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

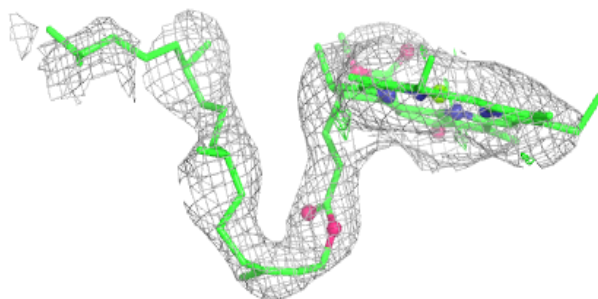
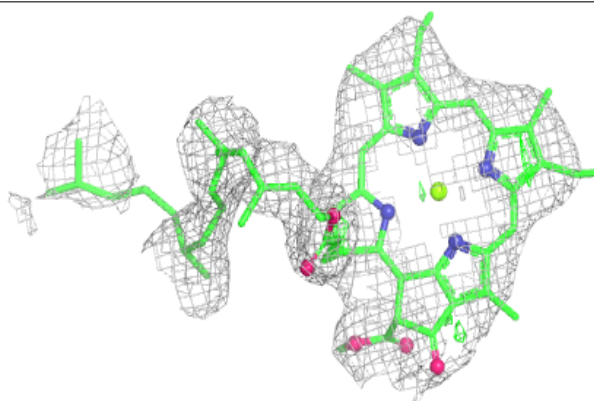


Electron density around MGE d 5361:

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

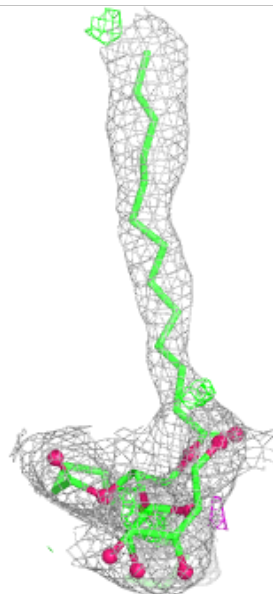
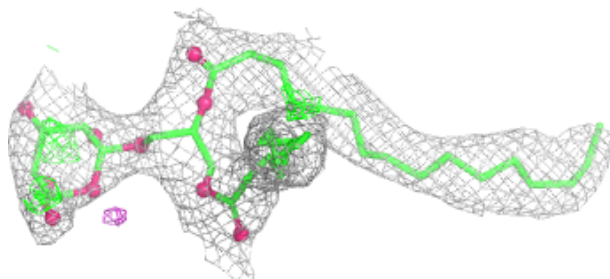
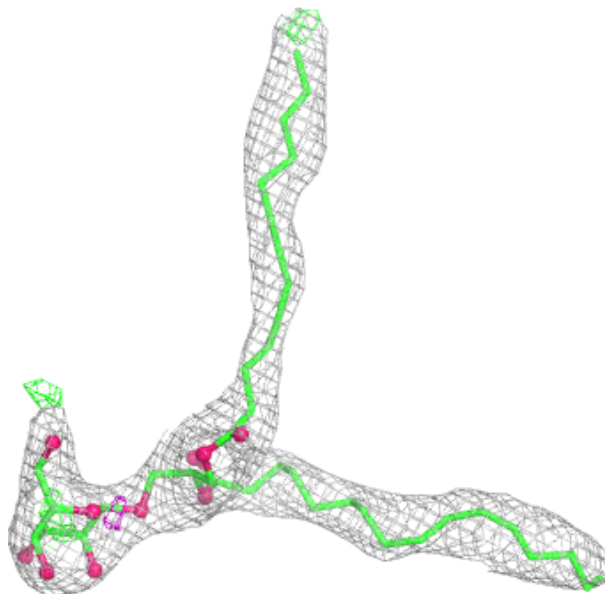
**Electron density around CLA a 5560:**

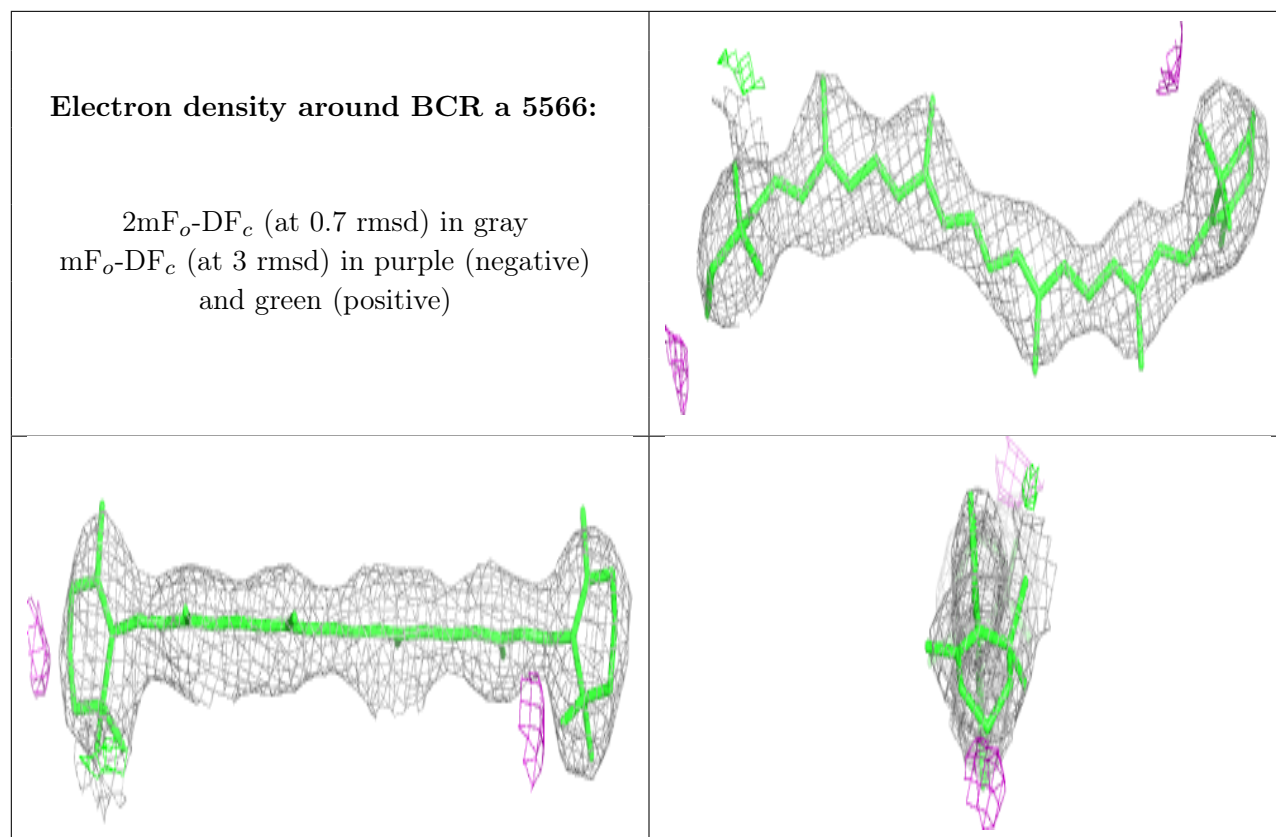
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

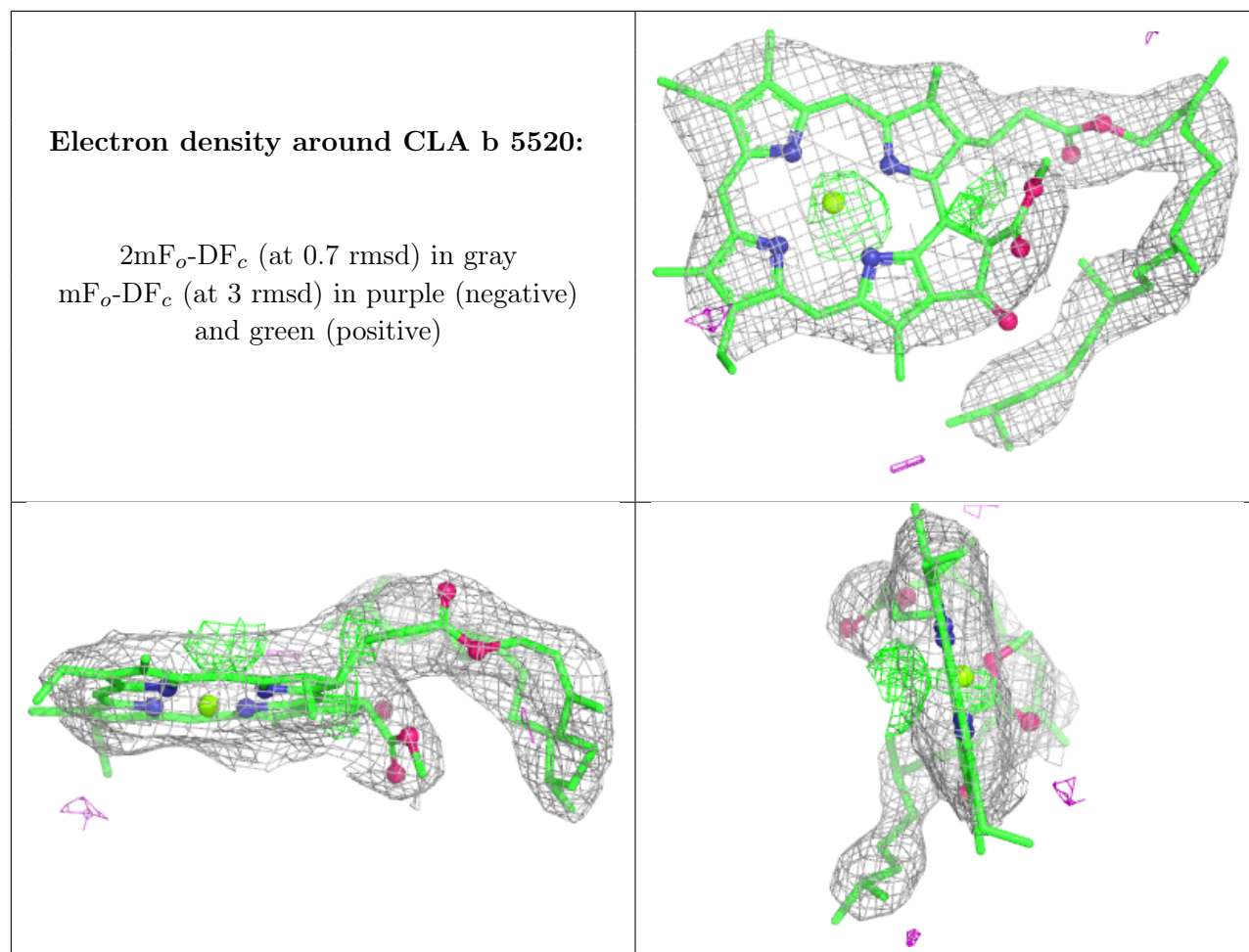


Electron density around MGE 1 5210:

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

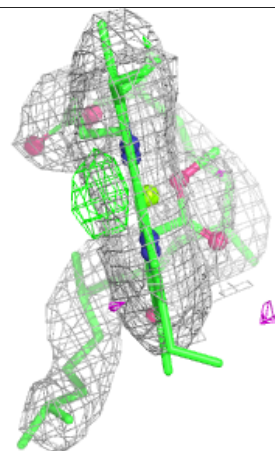
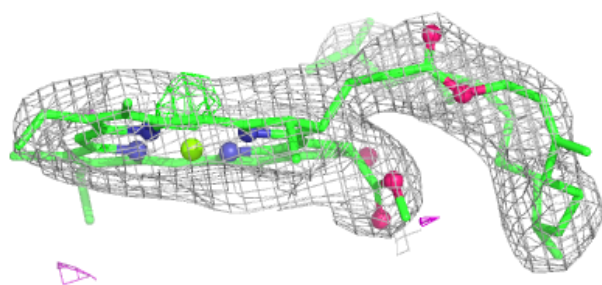
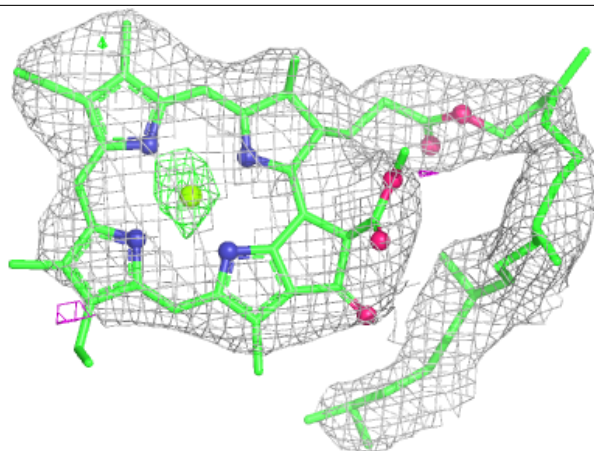




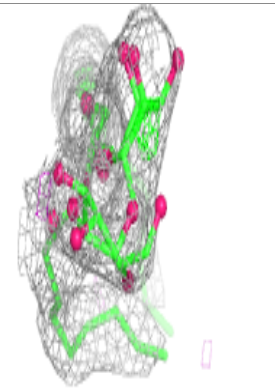
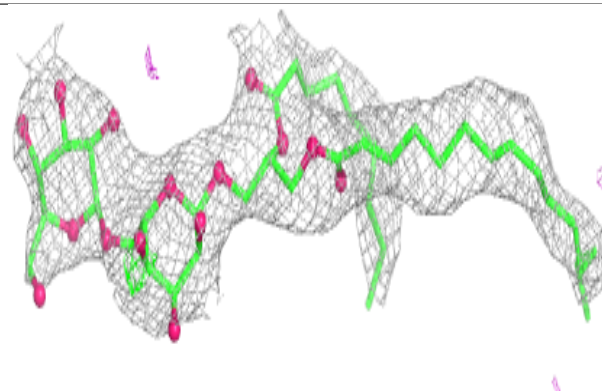
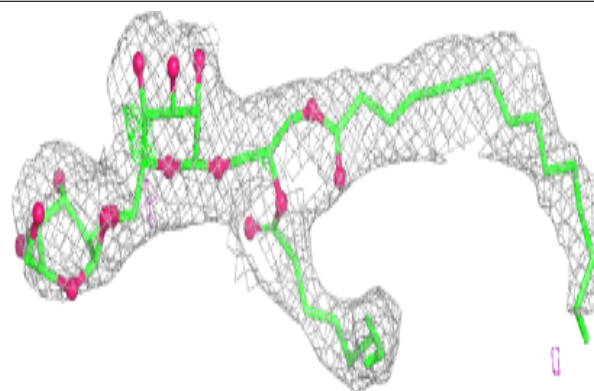


Electron density around CLA B 520:

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

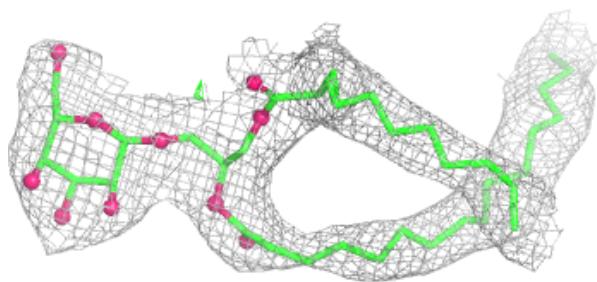
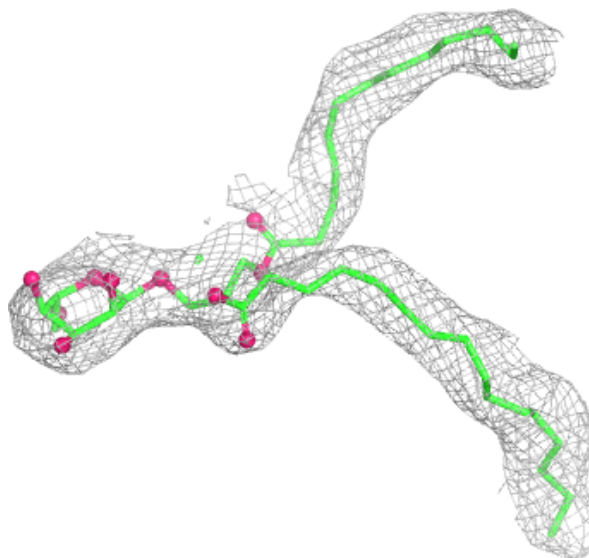
**Electron density around DGD H 208:**

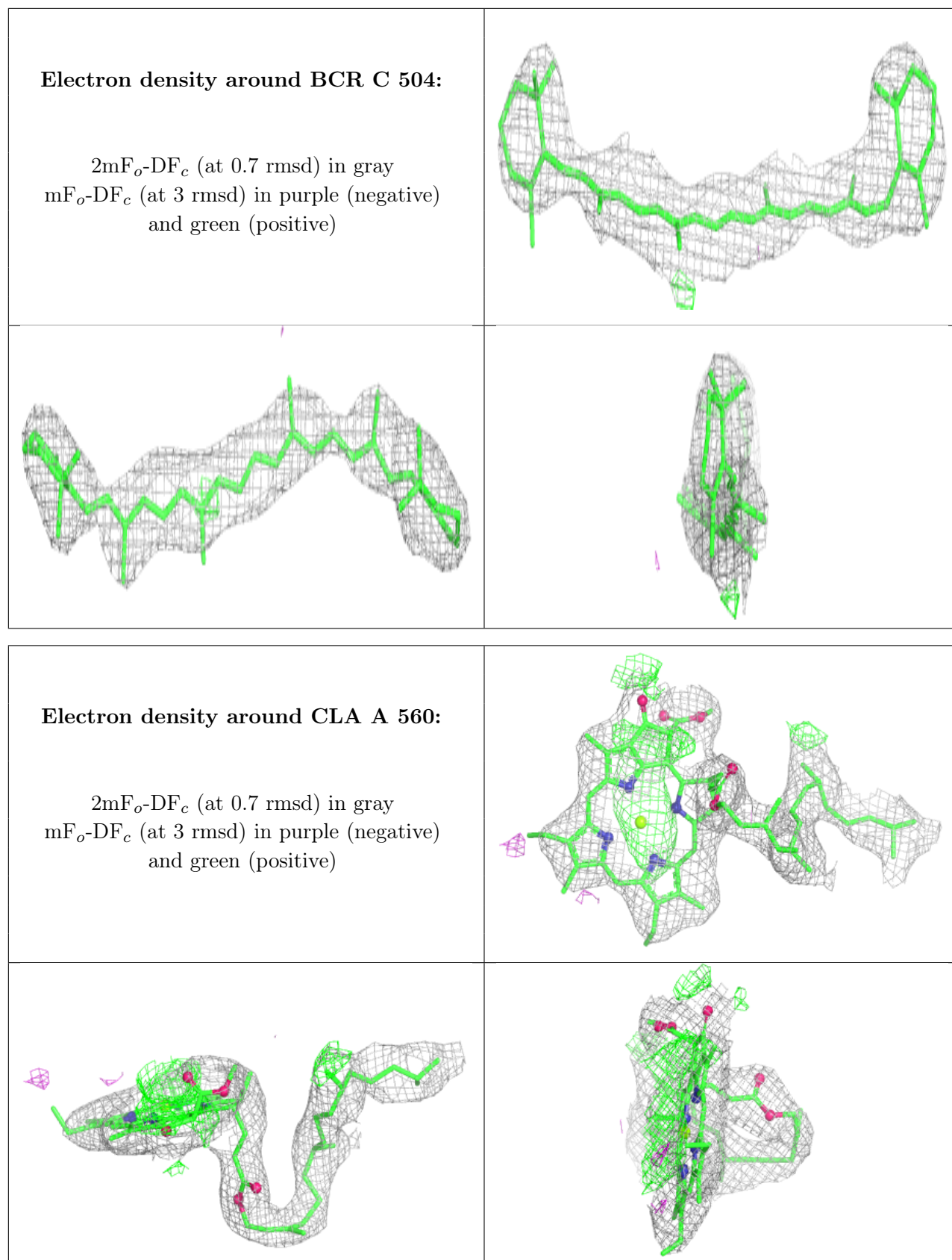
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE b 5530:

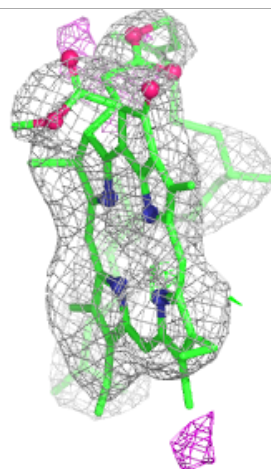
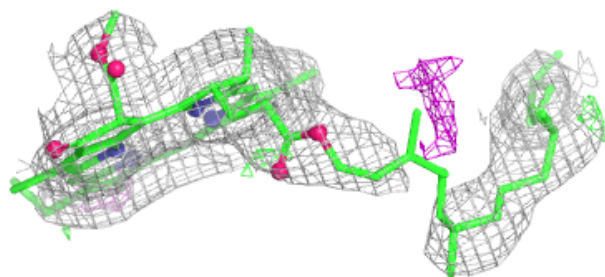
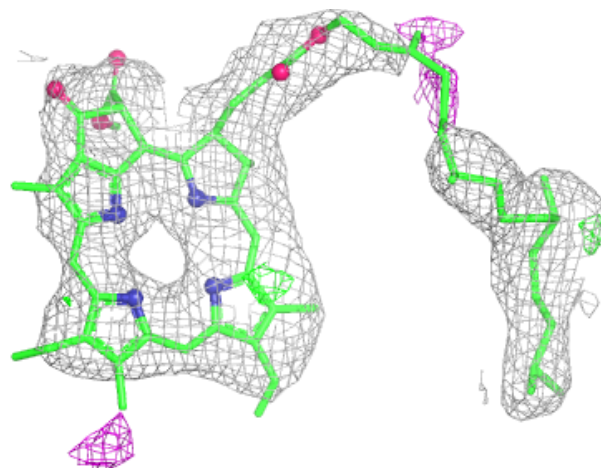
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





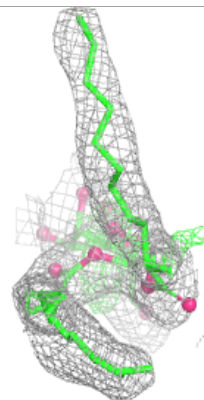
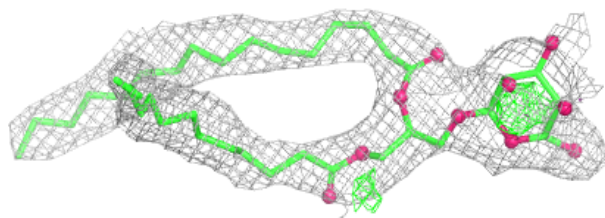
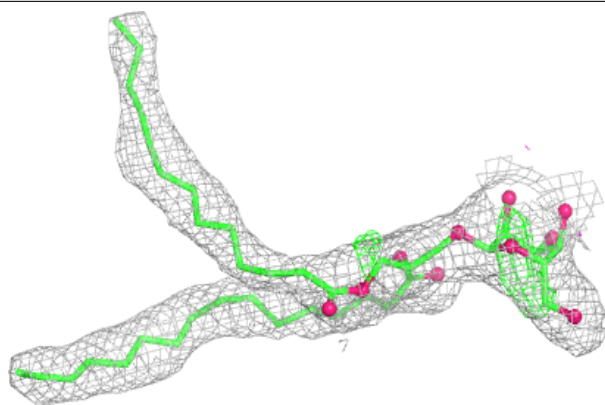
Electron density around PHO a 5562:

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

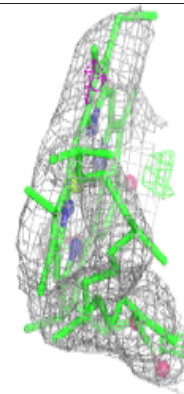
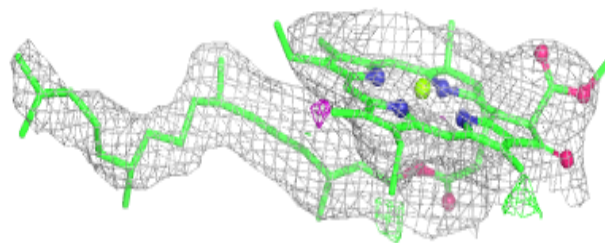
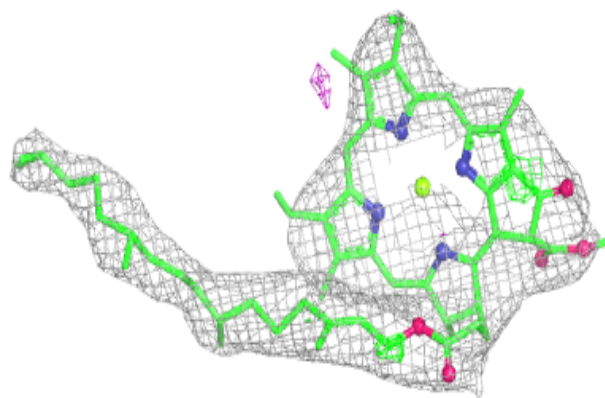


Electron density around MGE D 360:

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

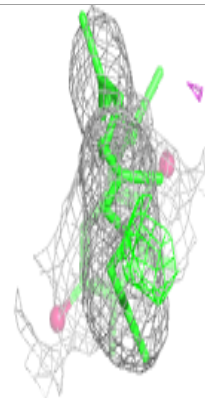
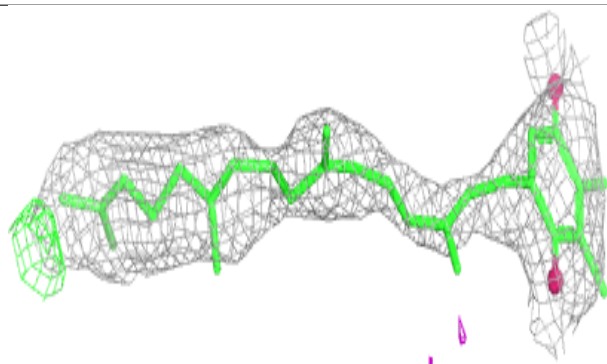
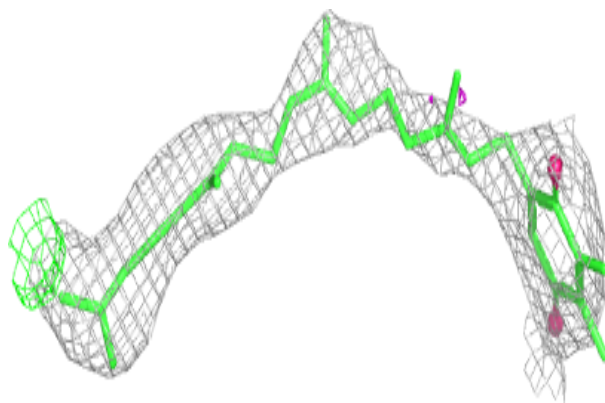
**Electron density around CLA c 5491:**

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

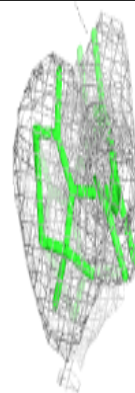
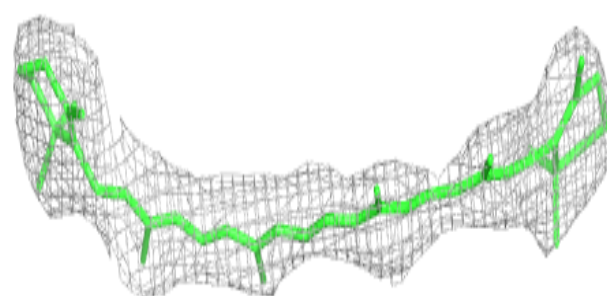
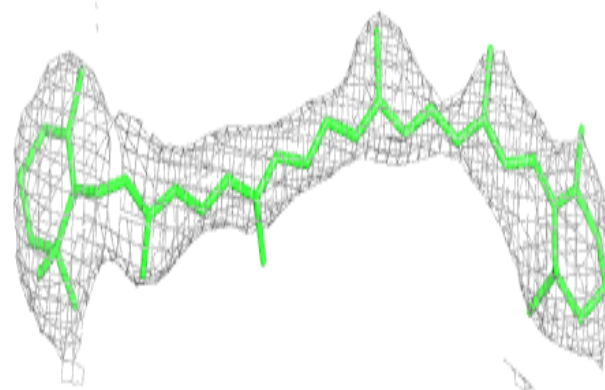


Electron density around PQ9 D 356:

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

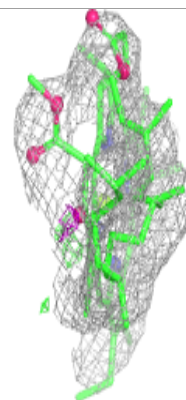
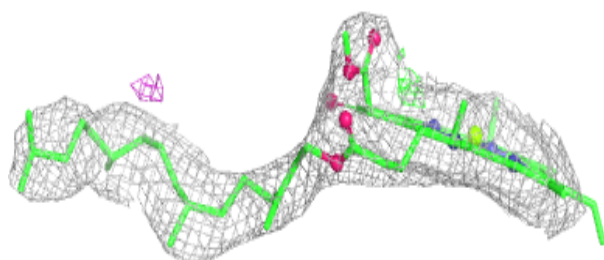
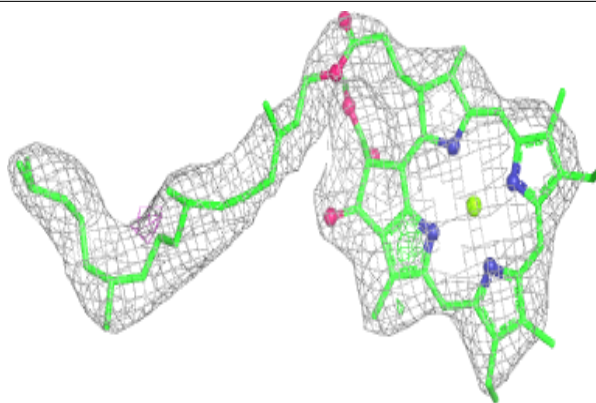
**Electron density around BCR t 104:**

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

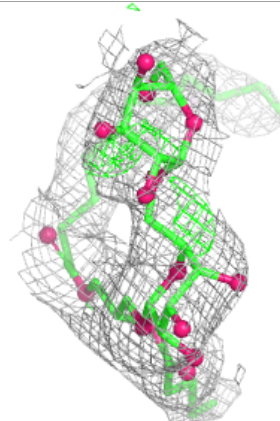
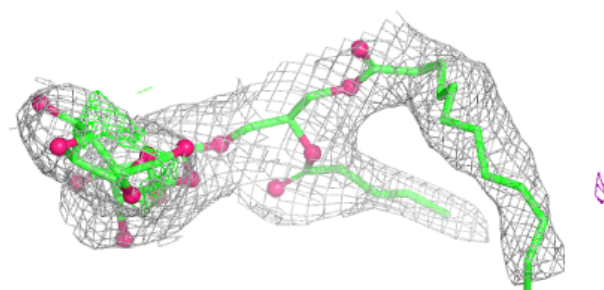
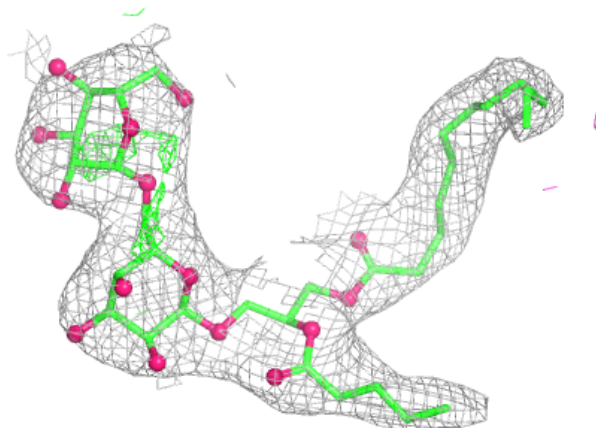


Electron density around CLA B 512:

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

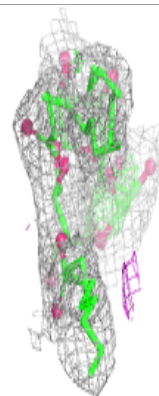
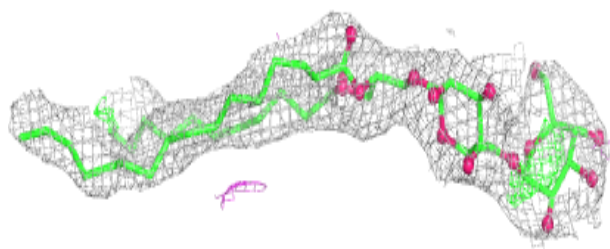
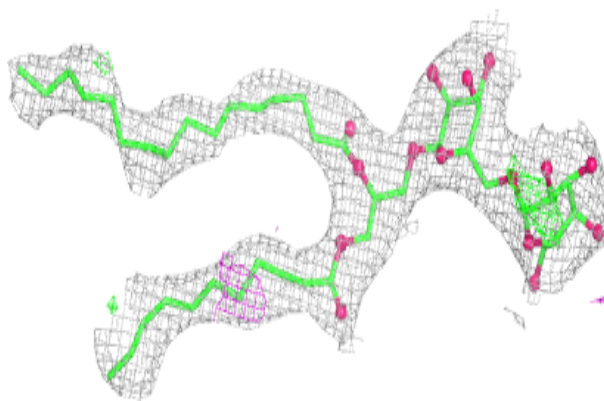
**Electron density around DGD C 508:**

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

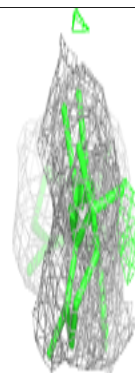
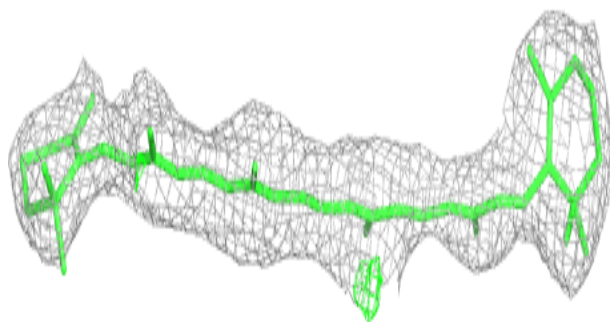
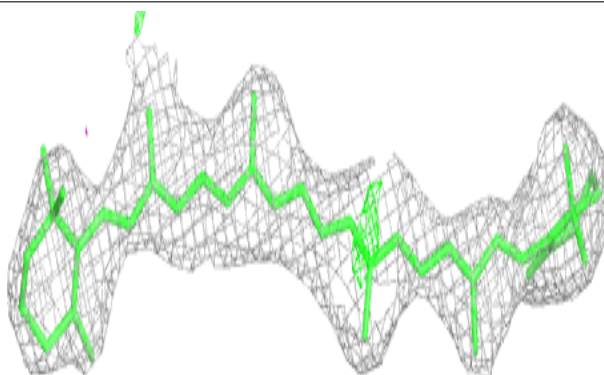


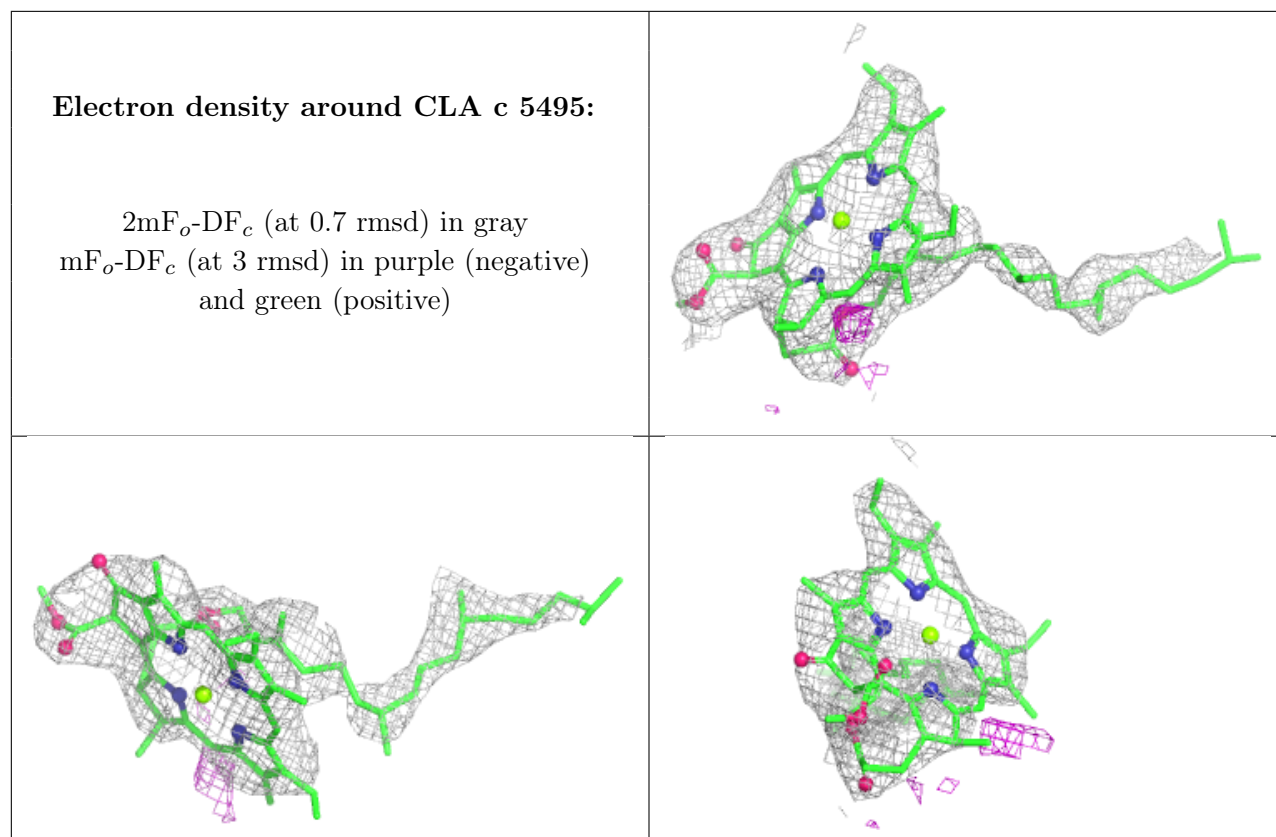
Electron density around DGD C 509:

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

**Electron density around BCR B 527:**

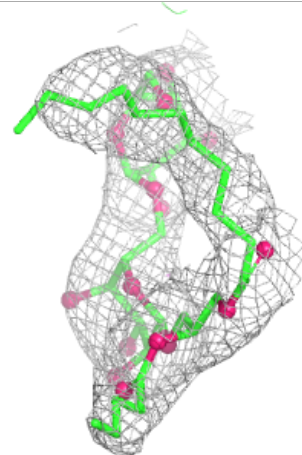
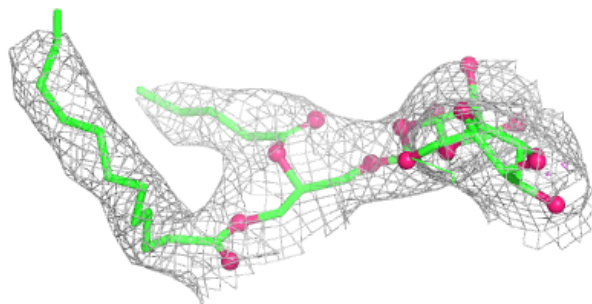
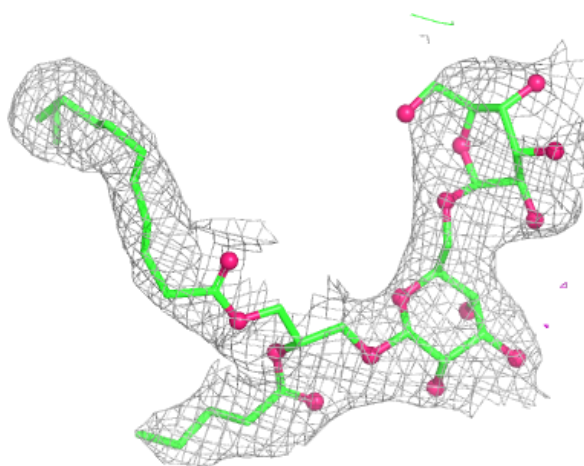
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





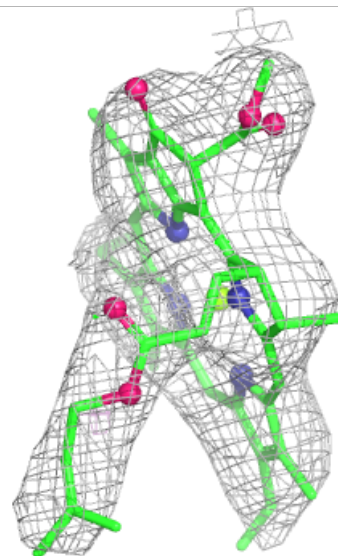
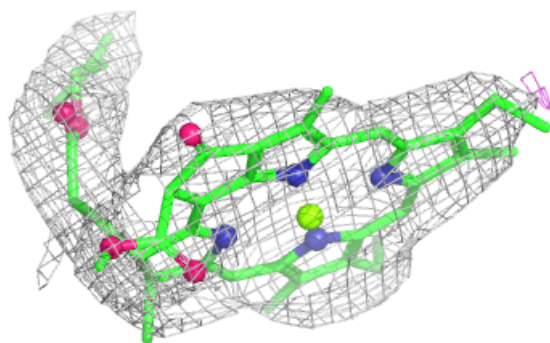
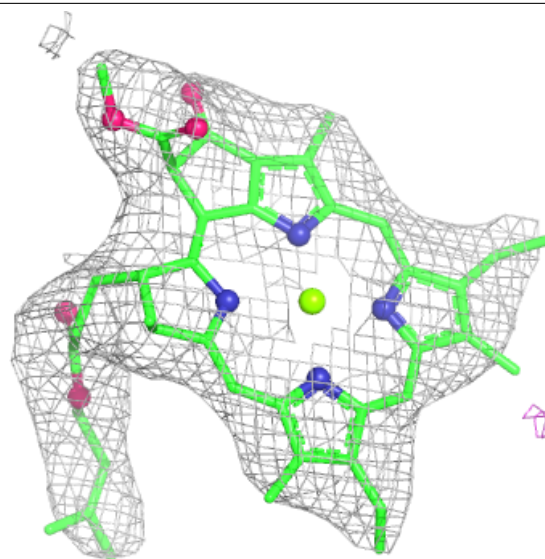
Electron density around DGD c 5508:

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



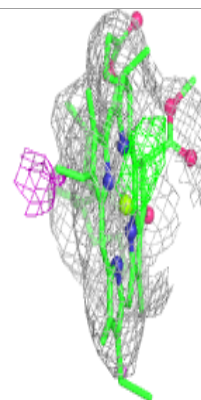
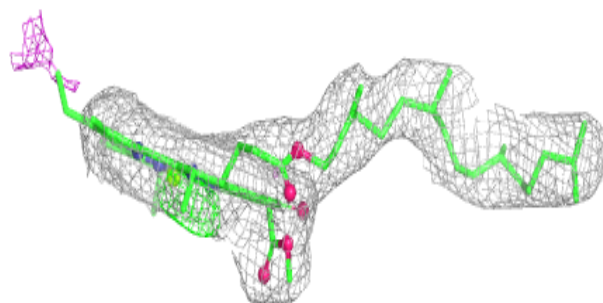
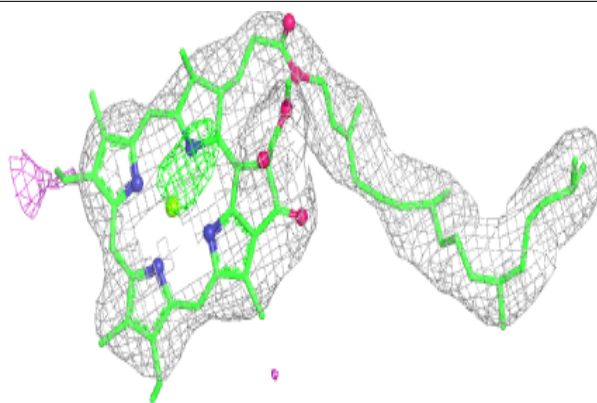
Electron density around CLA D 355:

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

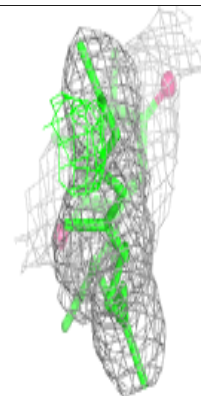
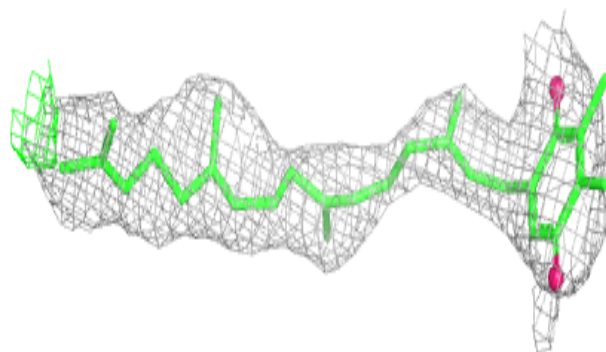
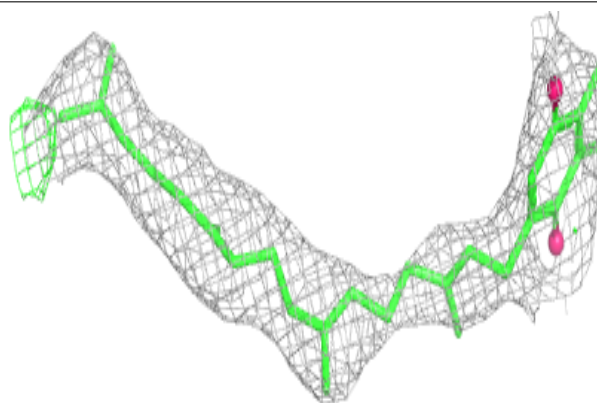


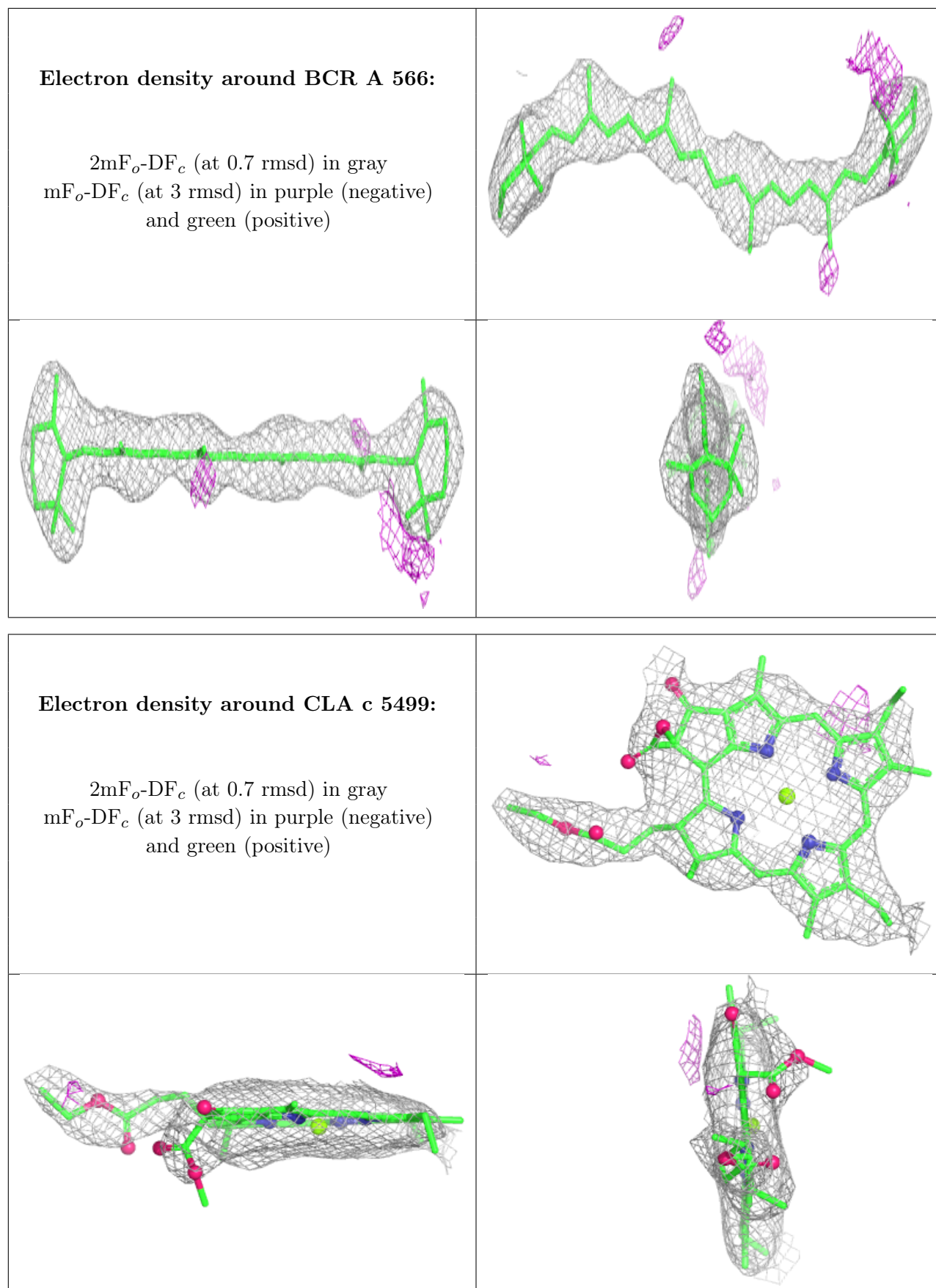
Electron density around CLA b 5512:

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

**Electron density around PQ9 d 5356:**

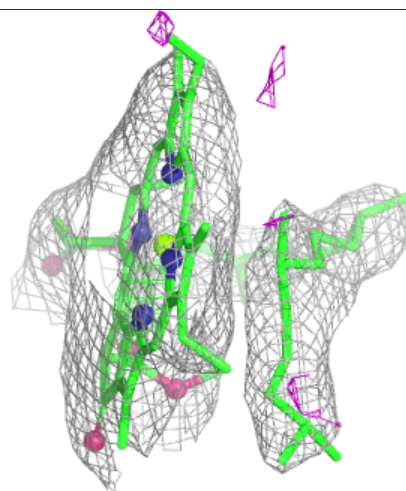
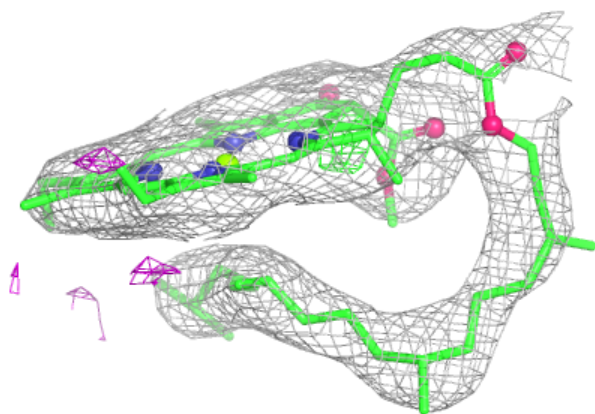
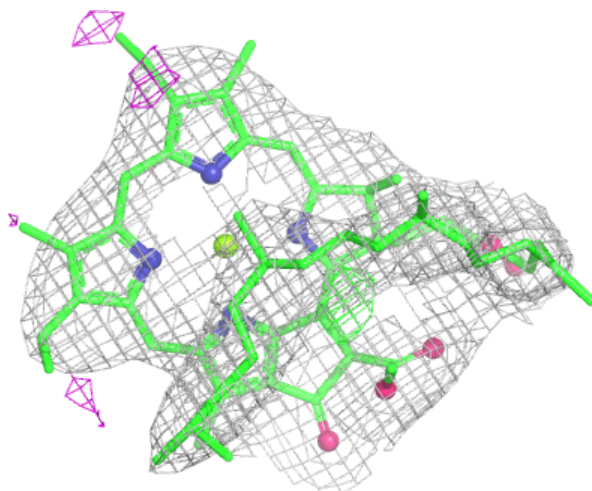
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





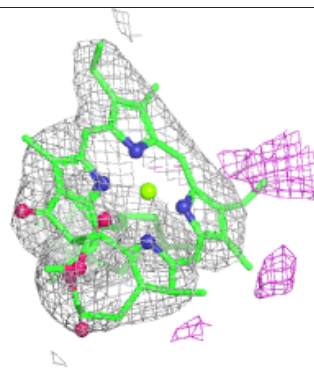
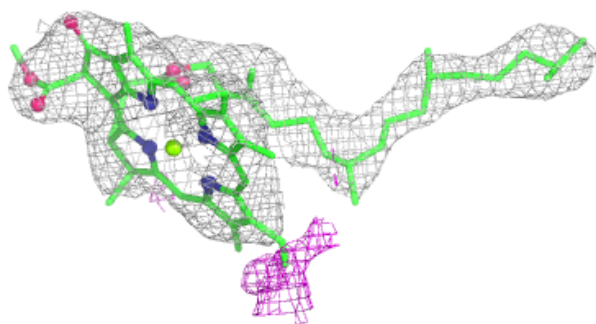
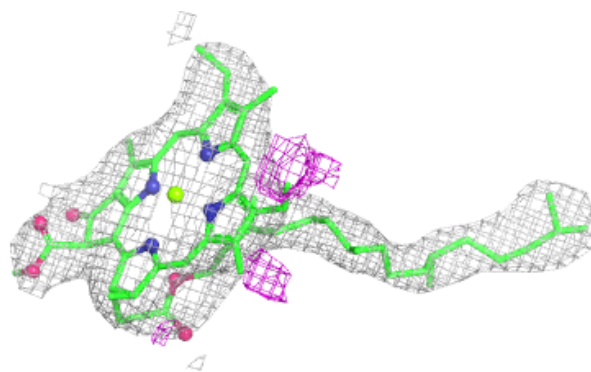
Electron density around CLA c 5500:

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



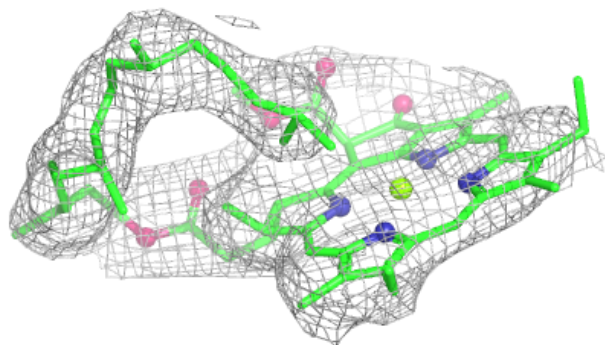
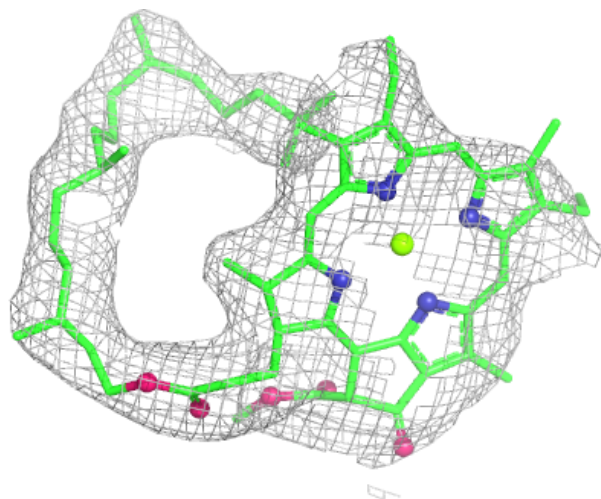
Electron density around CLA C 495:

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



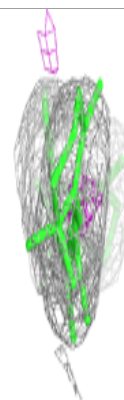
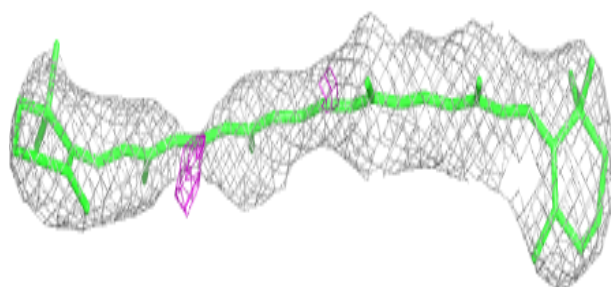
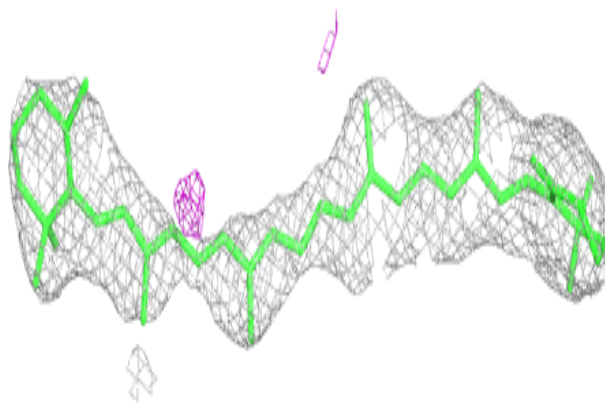
Electron density around CLA b 5525:

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

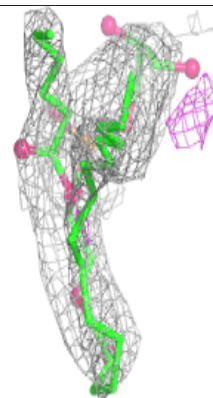
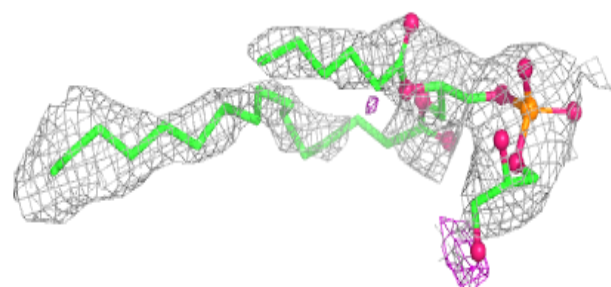
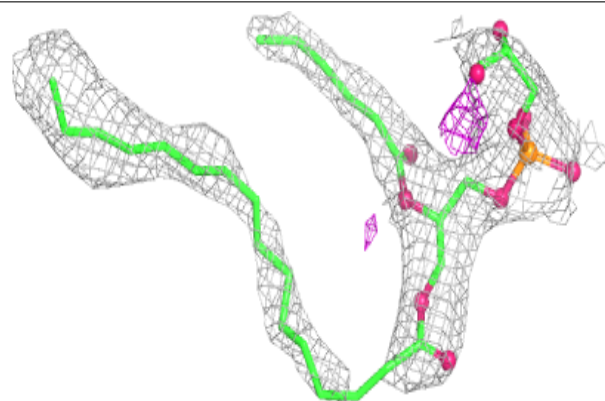


Electron density around BCR b 5527:

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

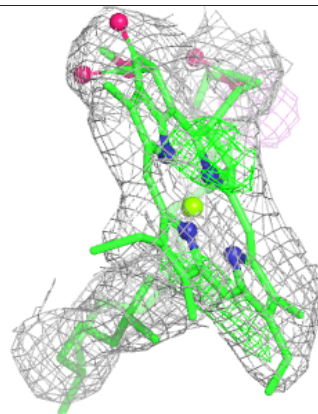
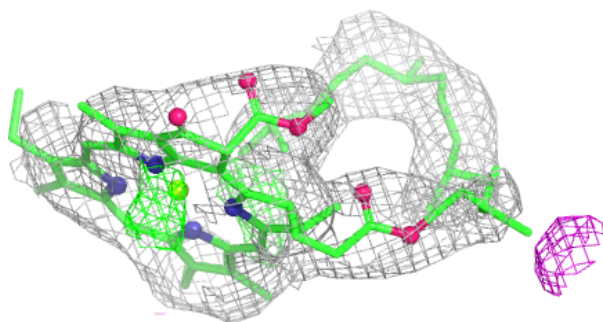
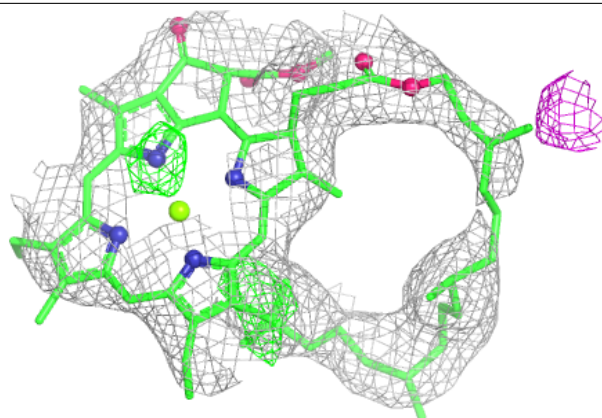
**Electron density around LHG A 567:**

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

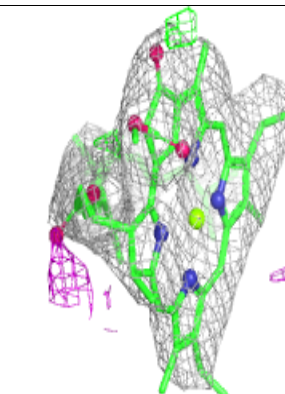
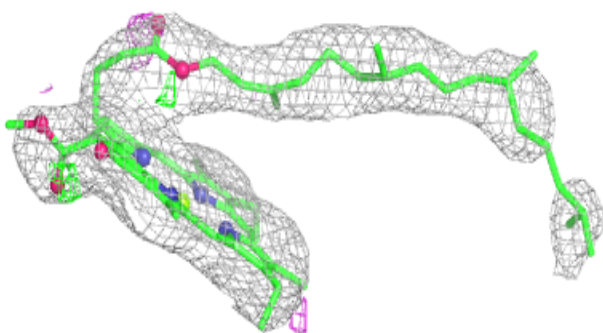
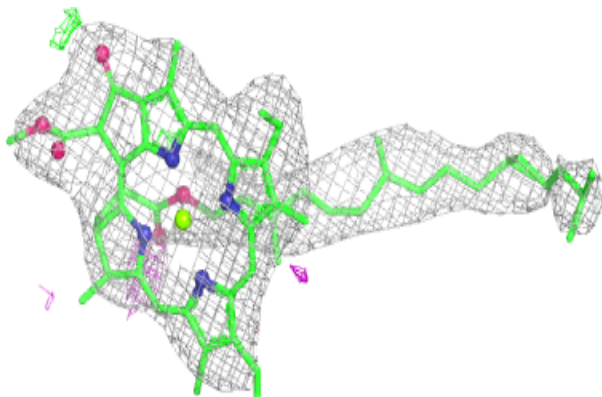


Electron density around CLA B 525:

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

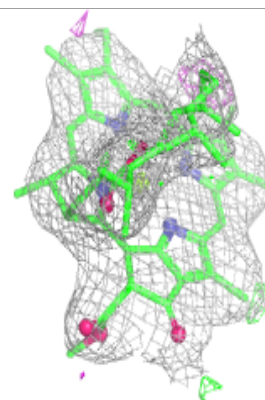
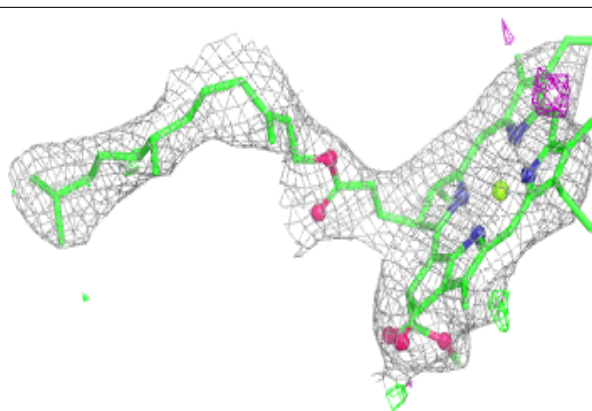
**Electron density around CLA B 518:**

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

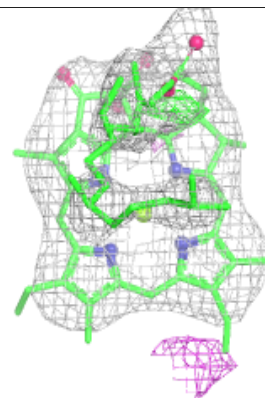
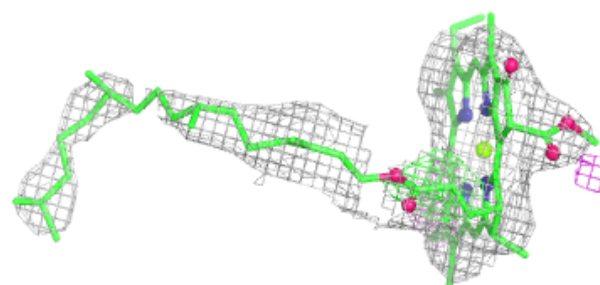
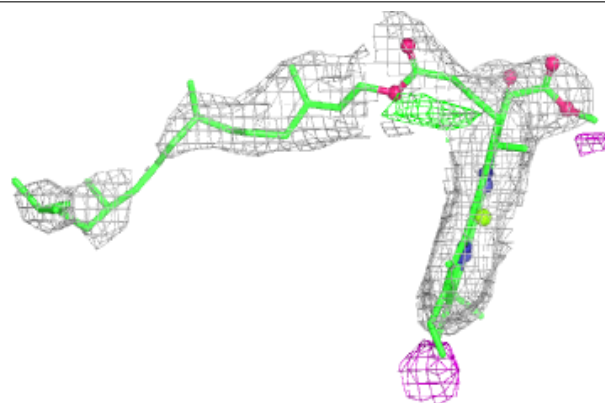


Electron density around CLA c 5492:

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

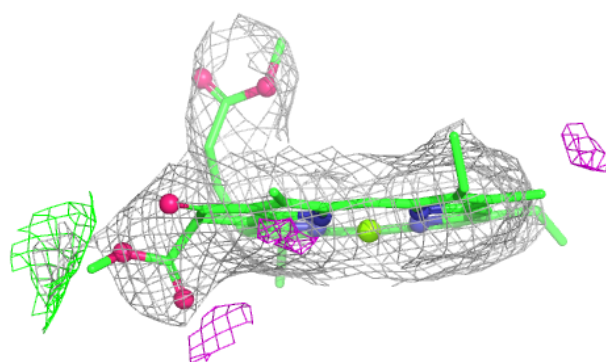
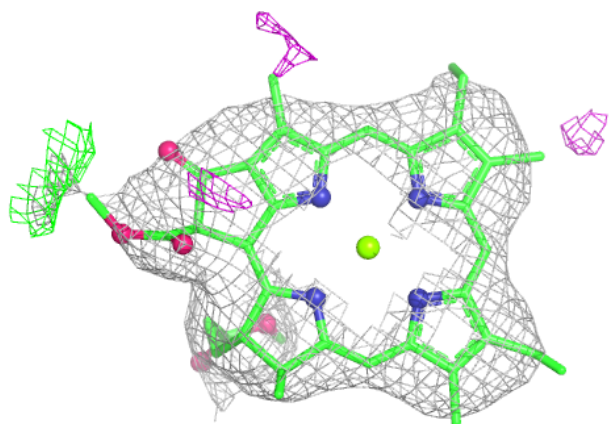
**Electron density around CLA B 515:**

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

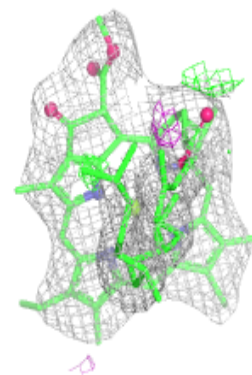
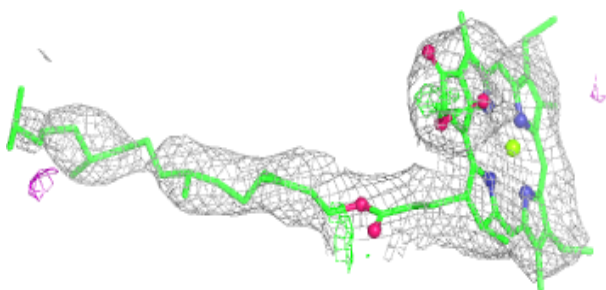
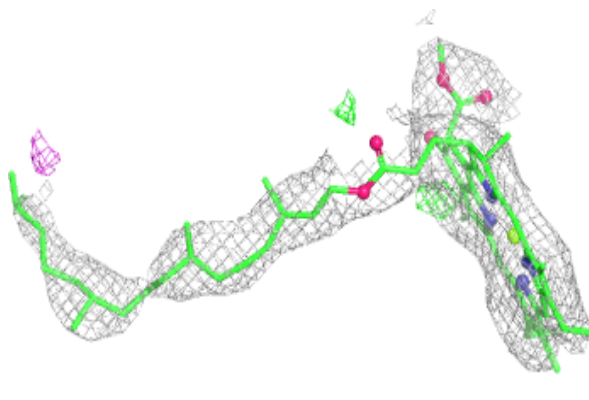


Electron density around CLA c 5494:

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

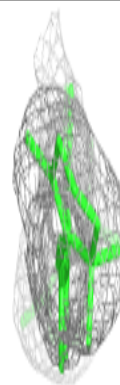
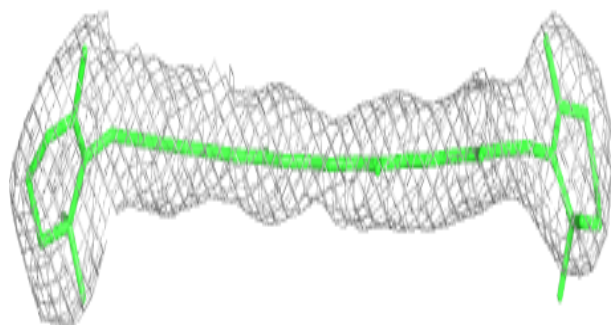
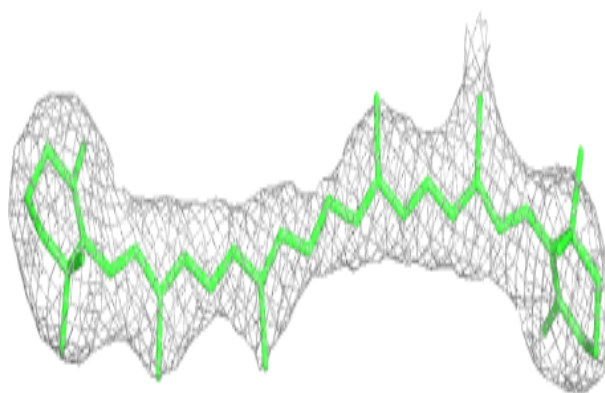
**Electron density around CLA B 514:**

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

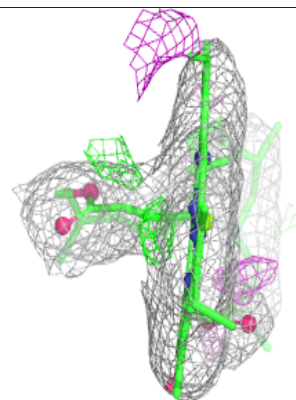
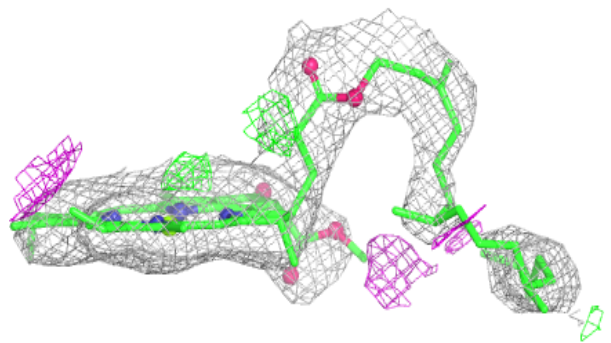
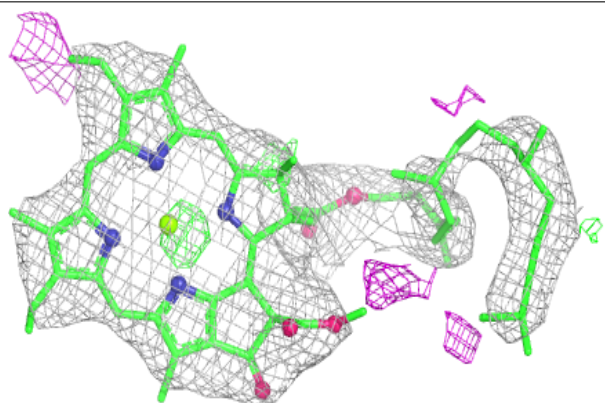


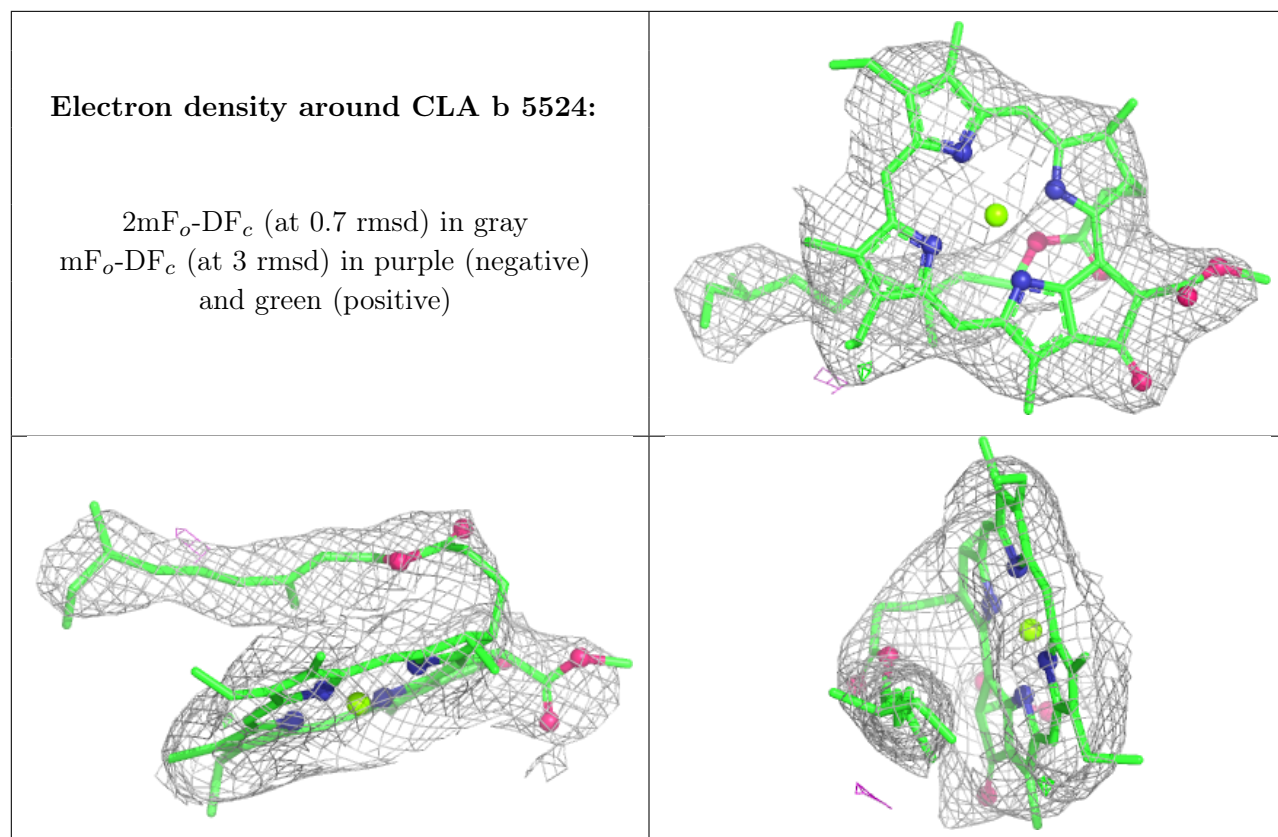
Electron density around BCR b 5528:

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

**Electron density around CLA B 522:**

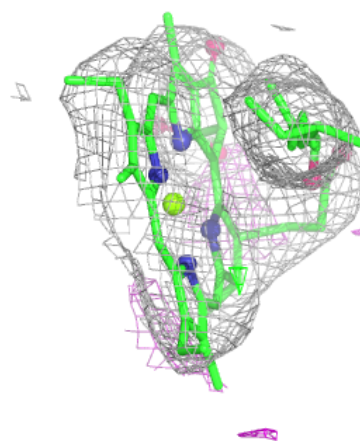
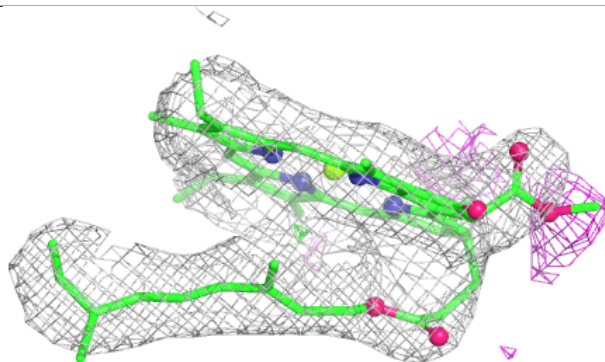
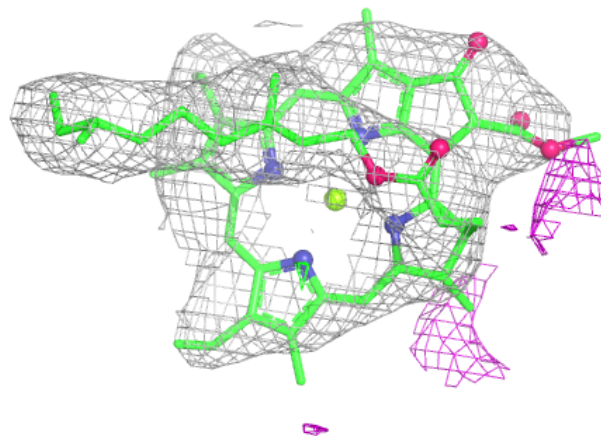
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





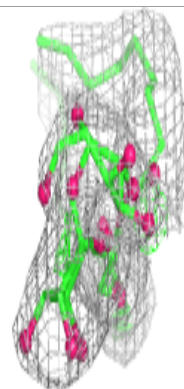
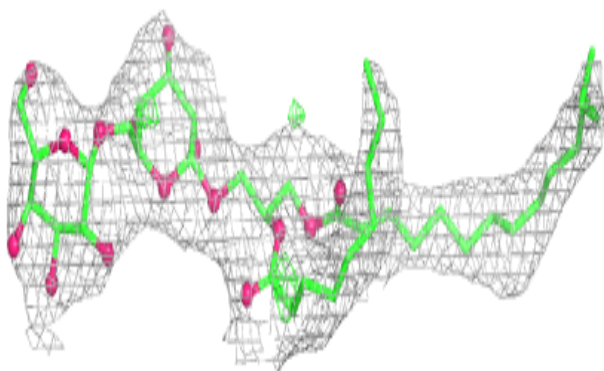
Electron density around CLA B 524:

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

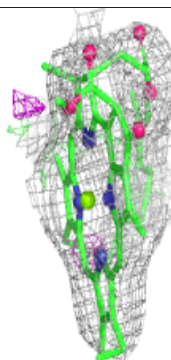
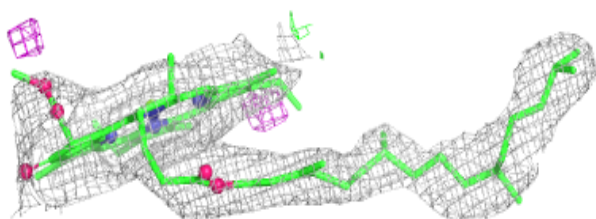
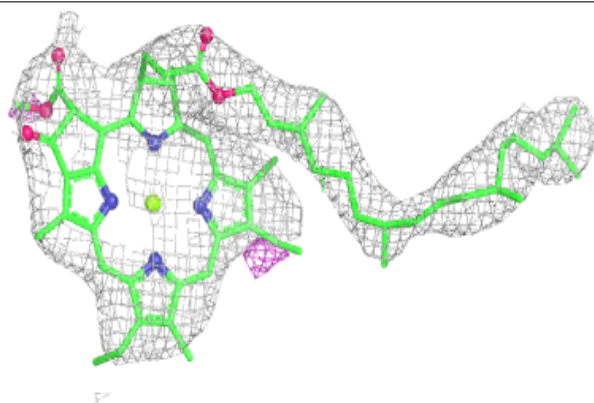


Electron density around DGD h 5208:

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

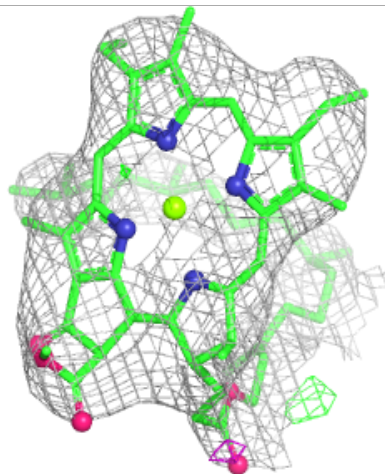
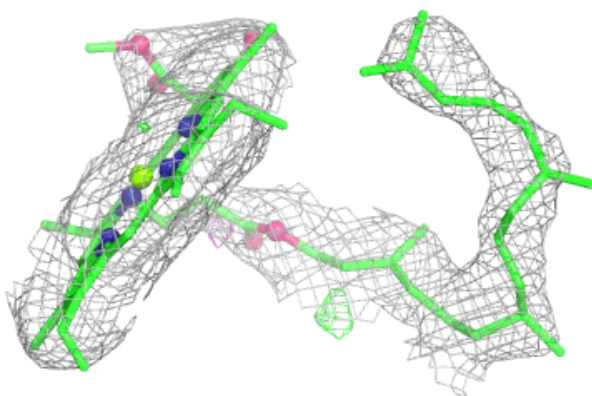
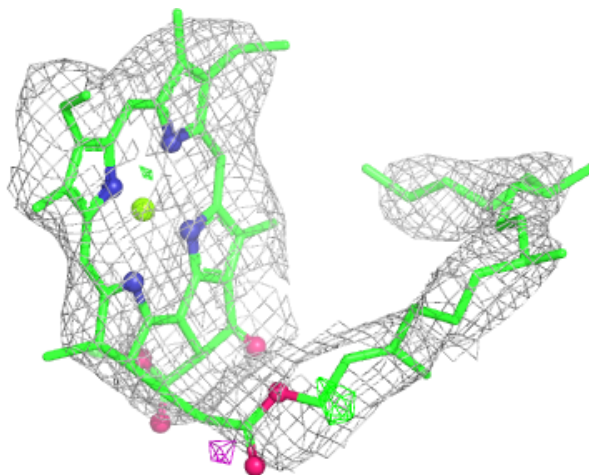
**Electron density around CLA B 513:**

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



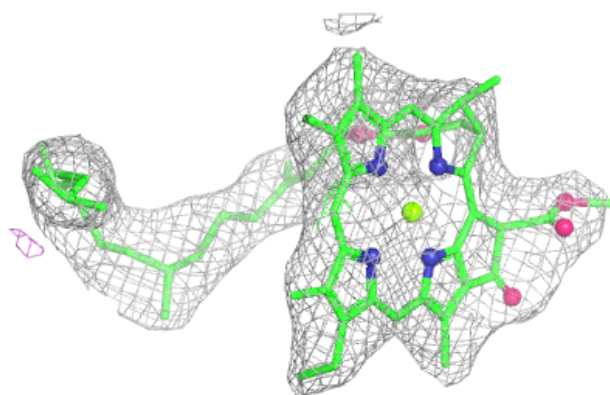
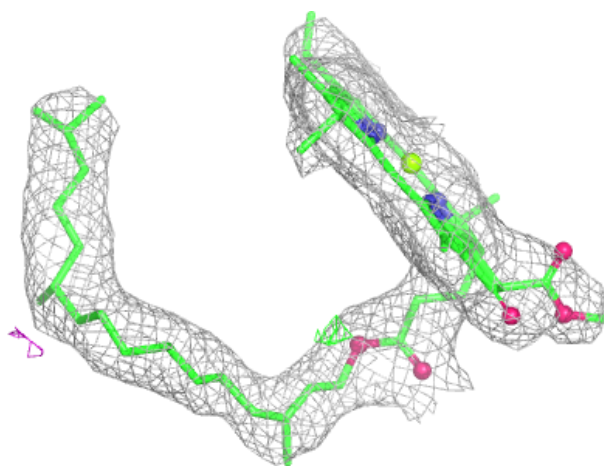
Electron density around CLA C 493:

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



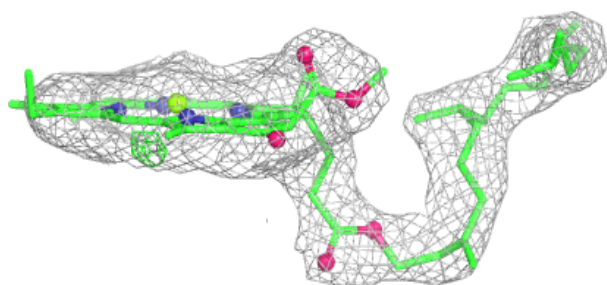
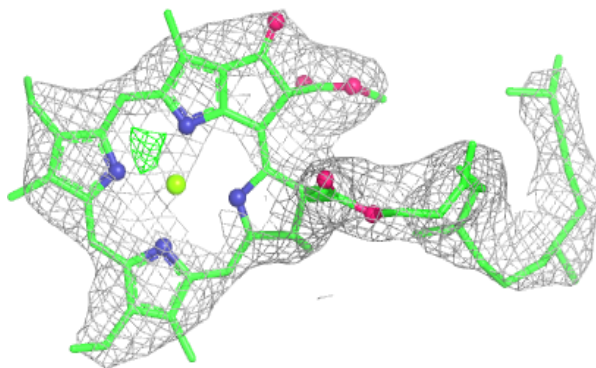
Electron density around CLA b 5521:

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

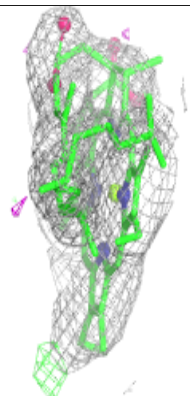
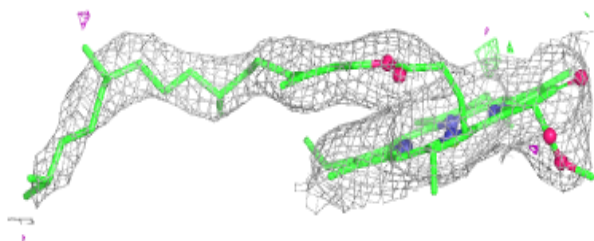
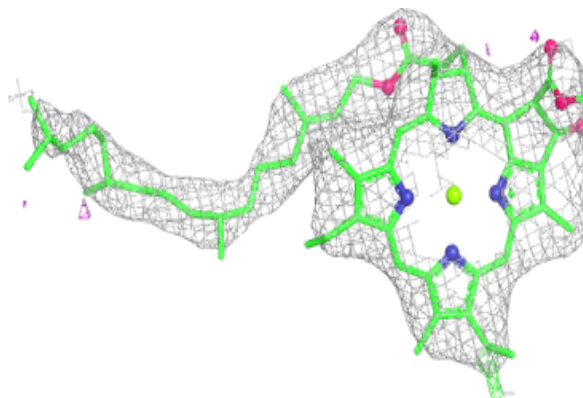


Electron density around CLA b 5522:

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

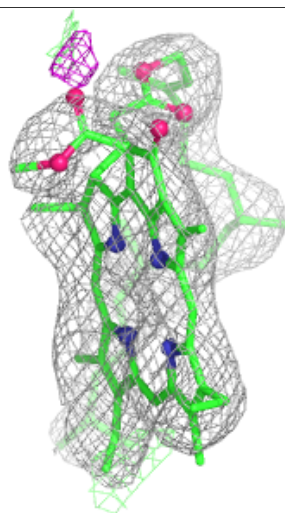
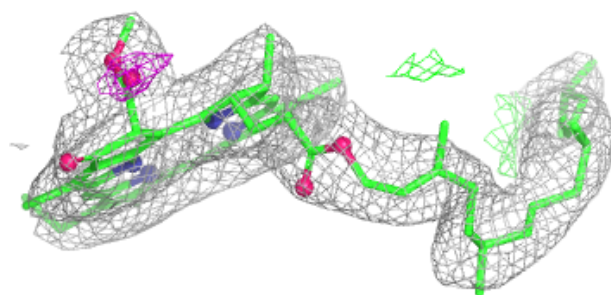
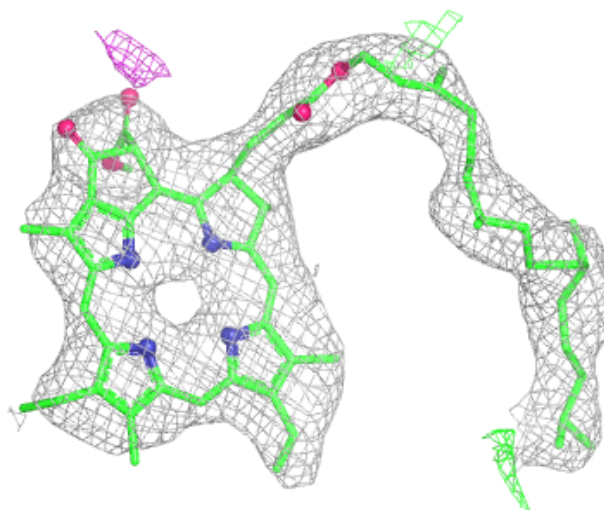
**Electron density around CLA b 5513:**

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



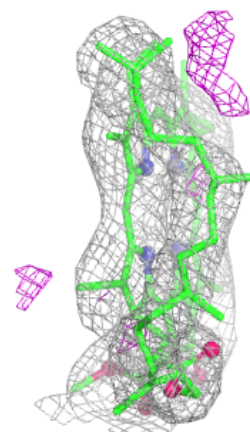
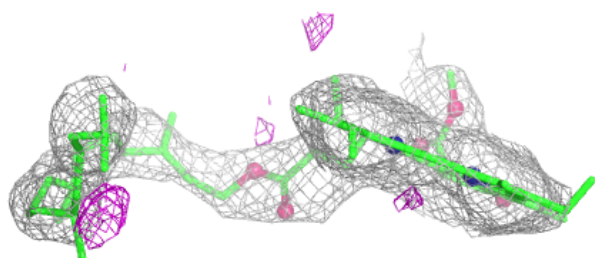
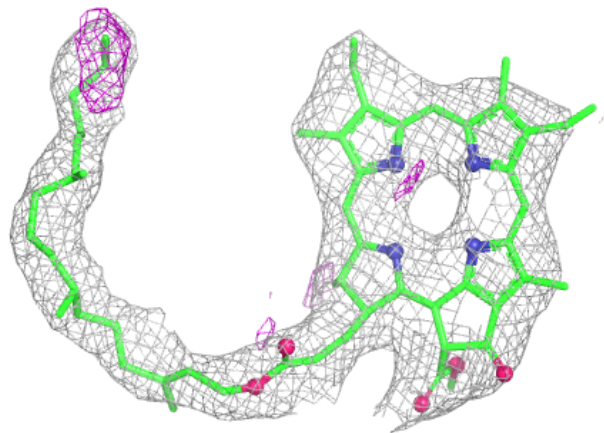
Electron density around PHO A 562:

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



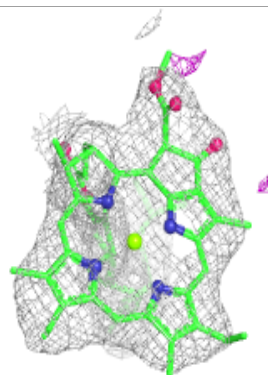
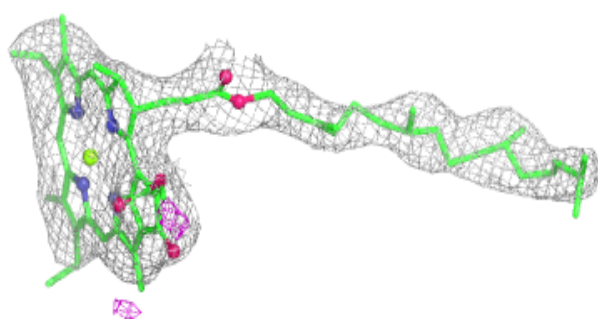
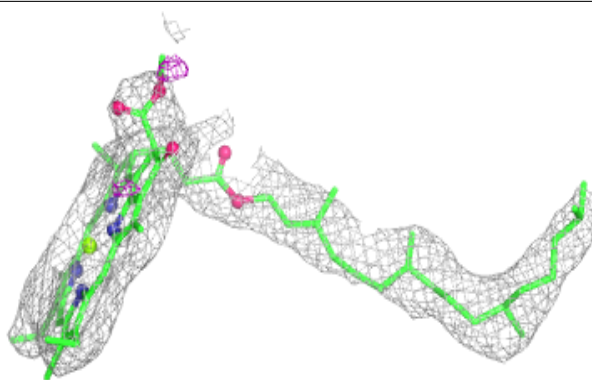
Electron density around PHO a 5561:

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

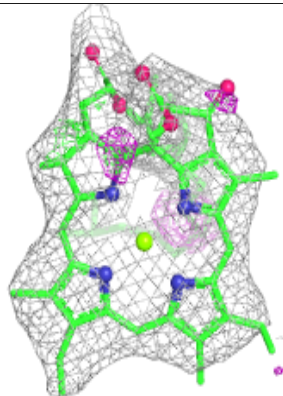
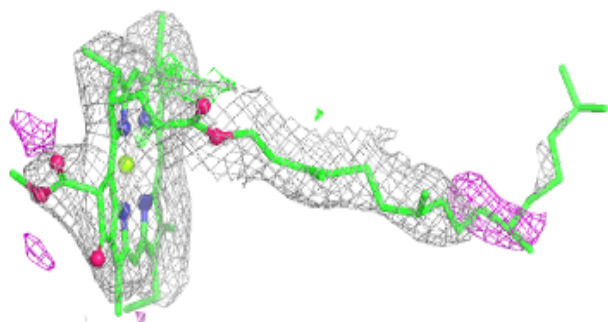
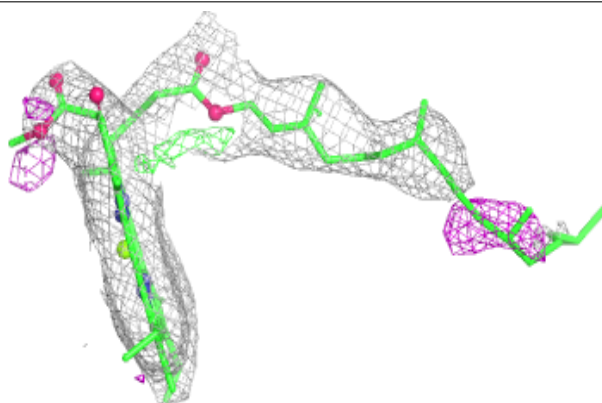


Electron density around CLA b 5514:

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

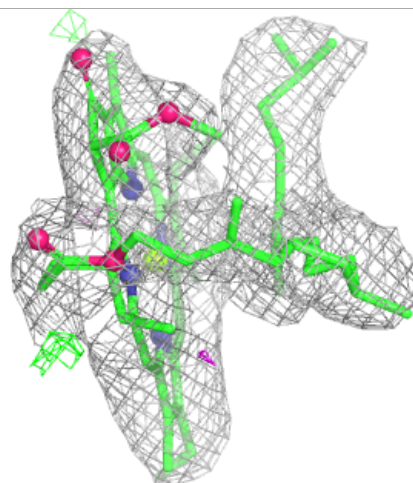
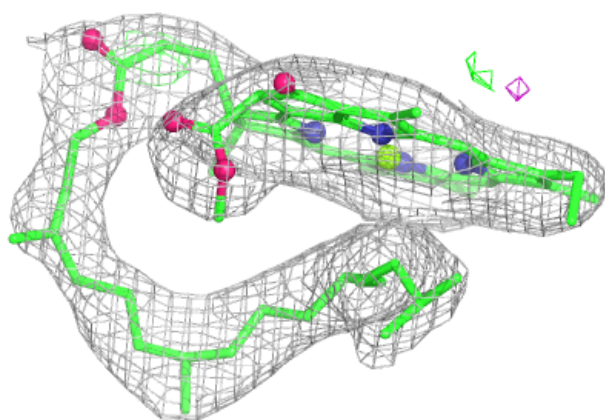
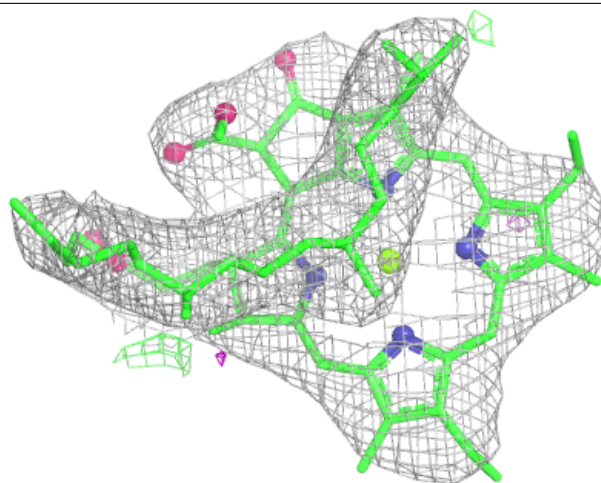
**Electron density around CLA b 5515:**

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



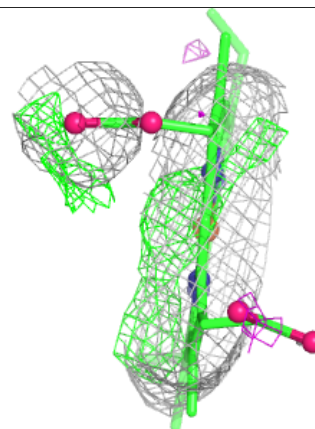
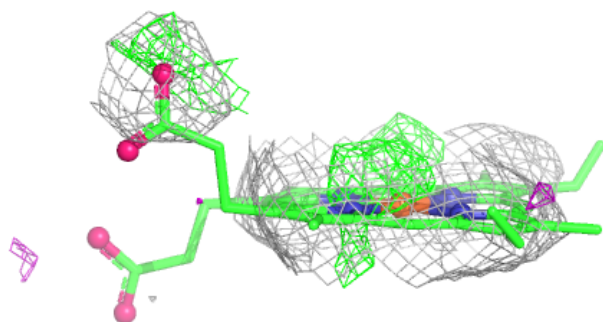
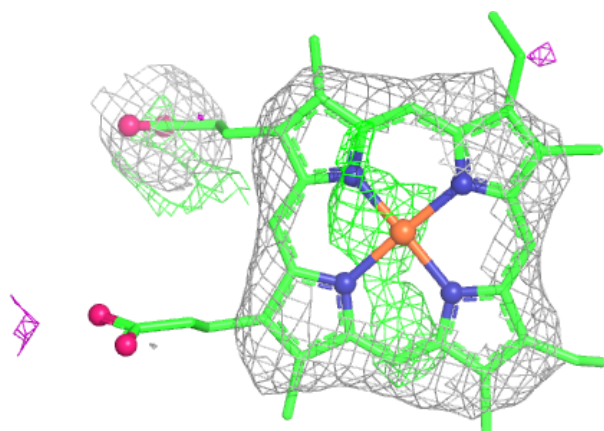
Electron density around CLA C 500:

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

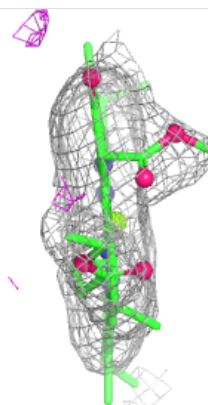
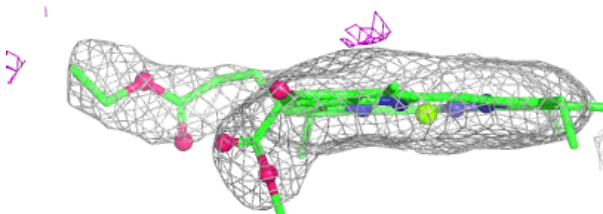
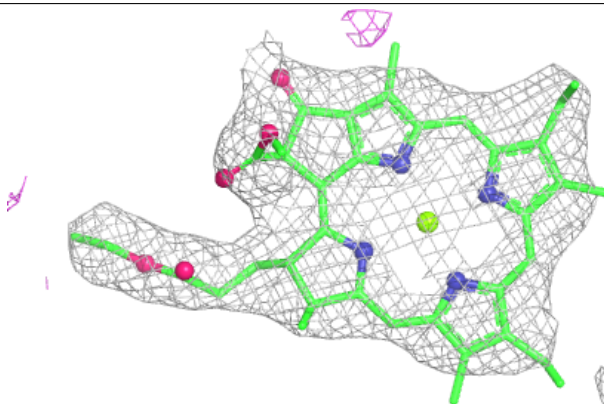


Electron density around HEM f 5051:

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

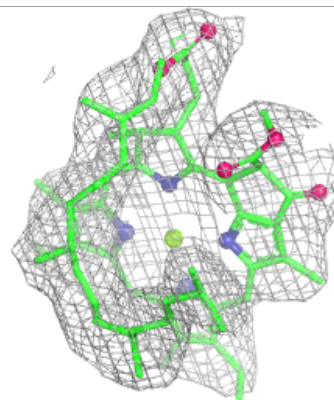
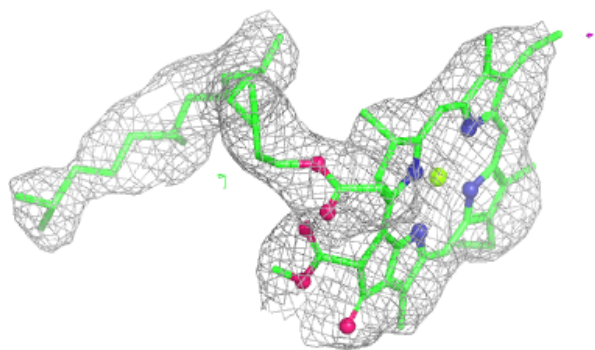
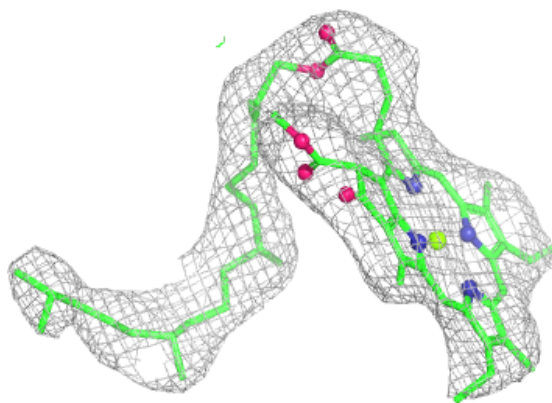
**Electron density around CLA C 499:**

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

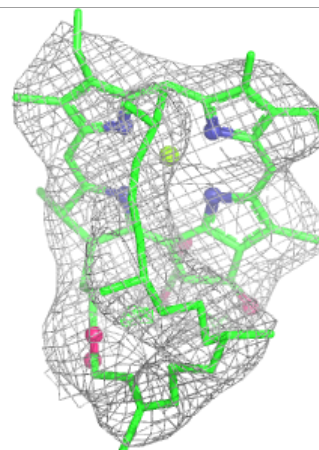
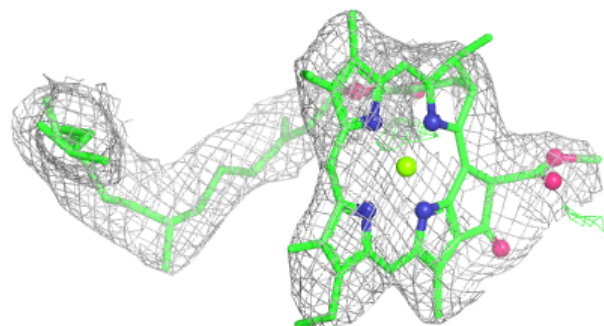
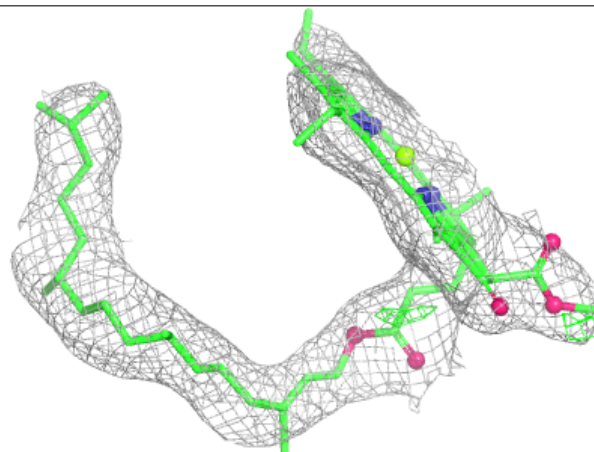


Electron density around CLA b 5523:

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

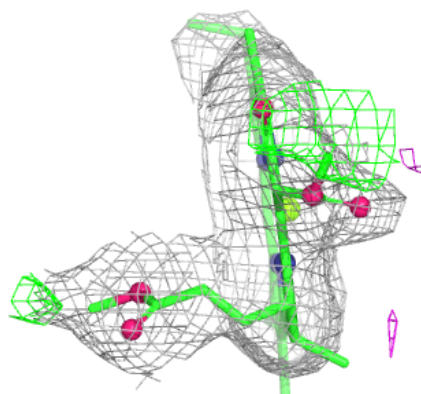
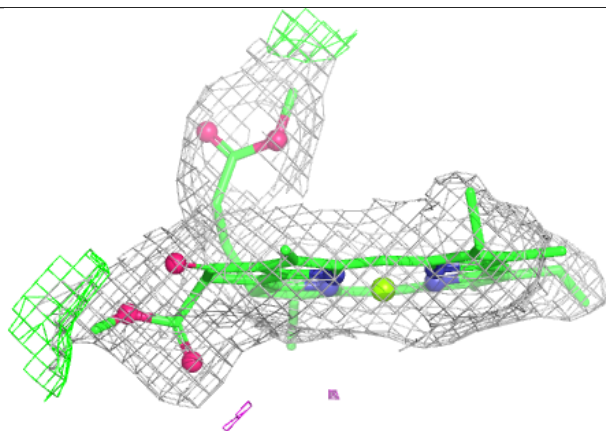
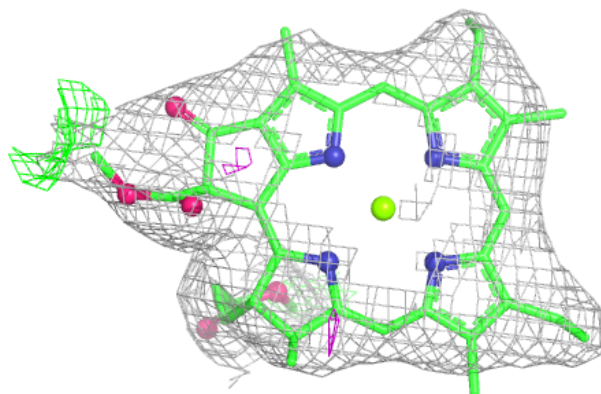
**Electron density around CLA B 521:**

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

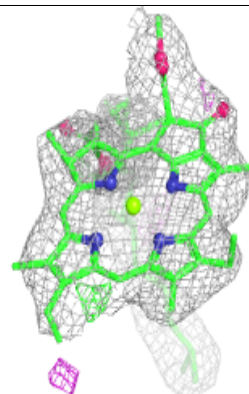
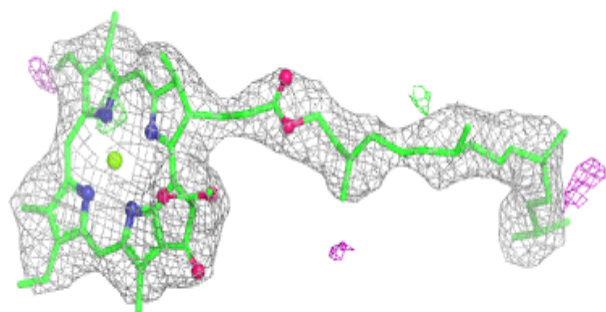
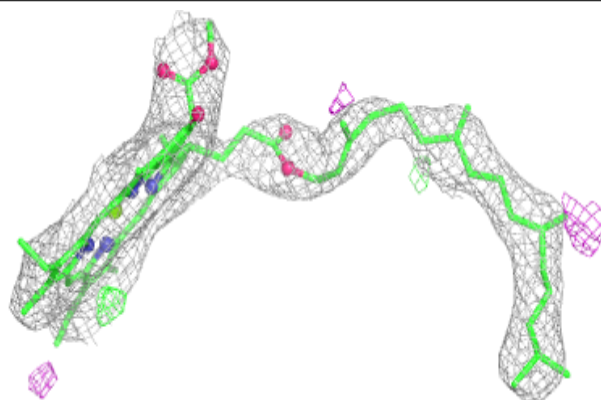


Electron density around CLA C 494:

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

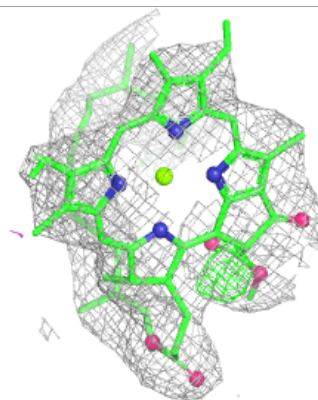
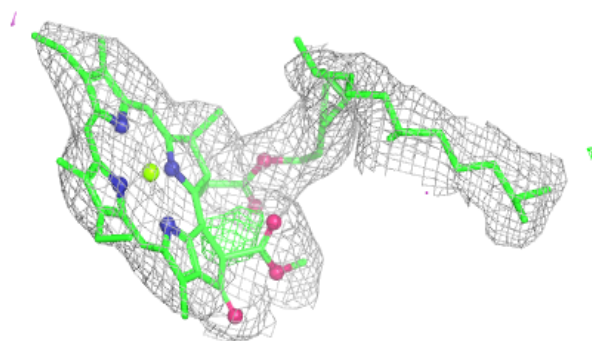
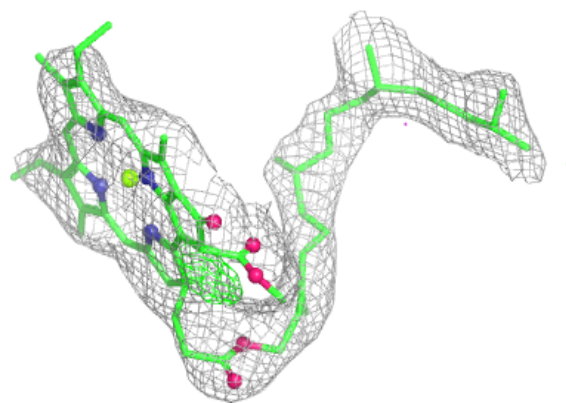
**Electron density around CLA d 5354:**

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

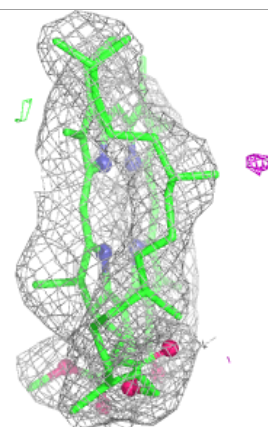
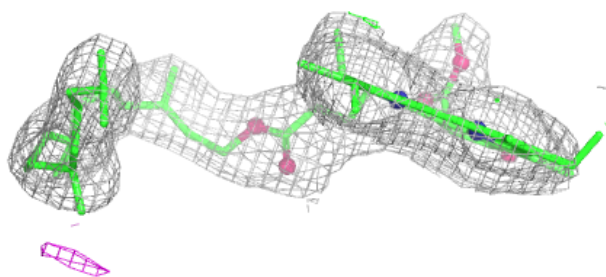
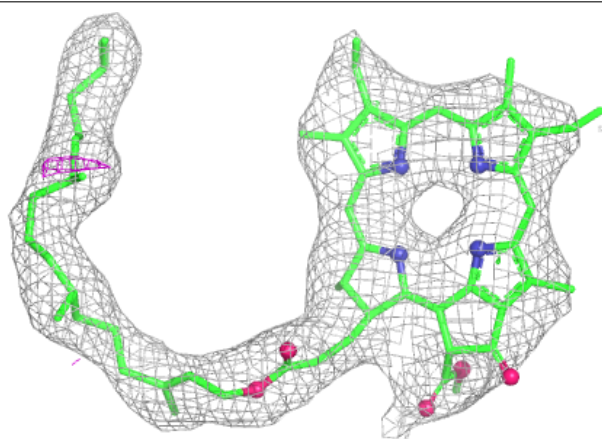


Electron density around CLA B 523:

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

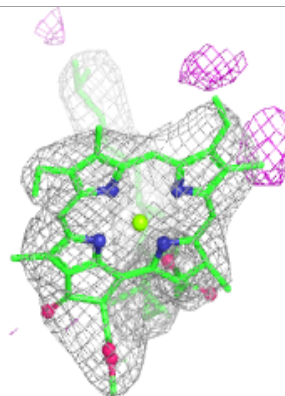
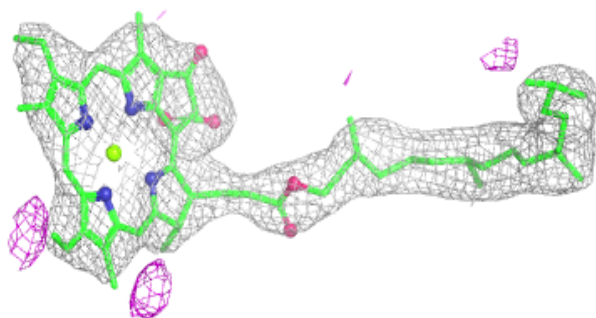
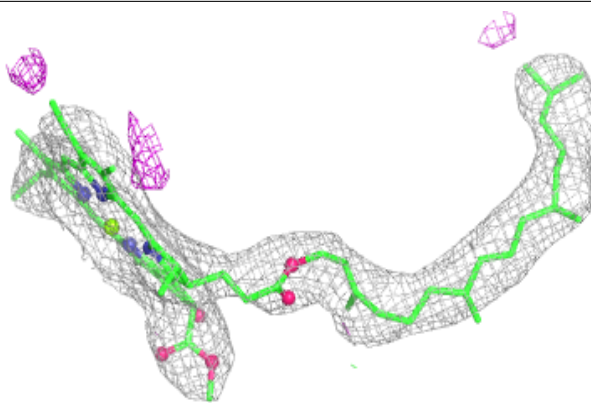
**Electron density around PHO A 561:**

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

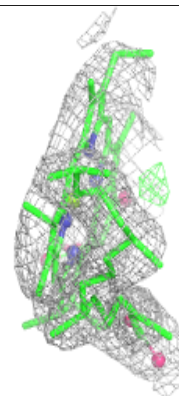
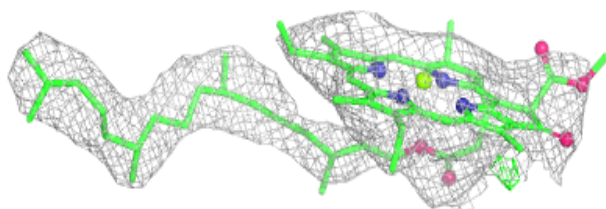
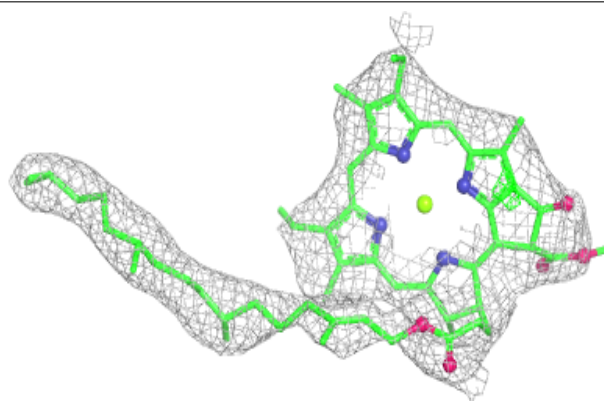


Electron density around CLA D 354:

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

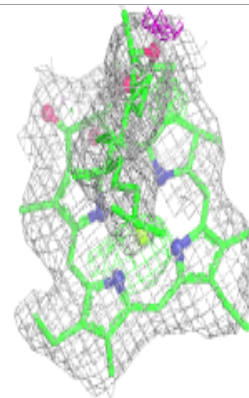
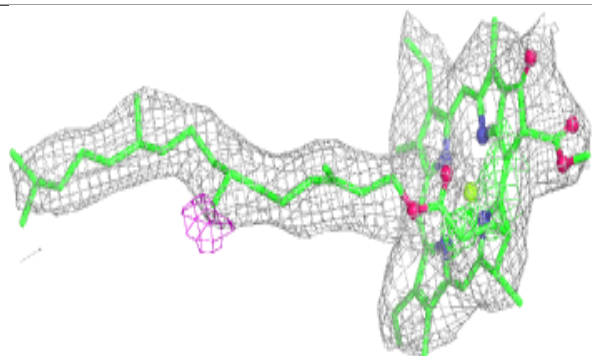
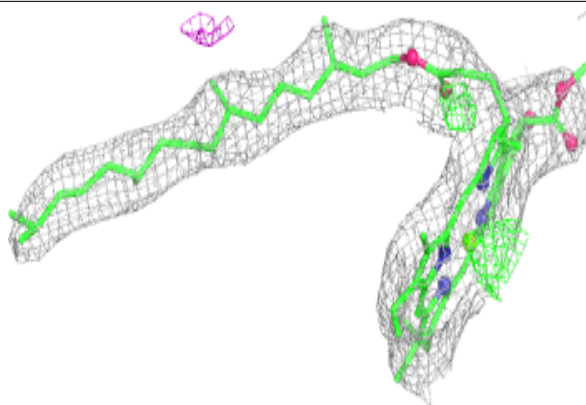
**Electron density around CLA C 491:**

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

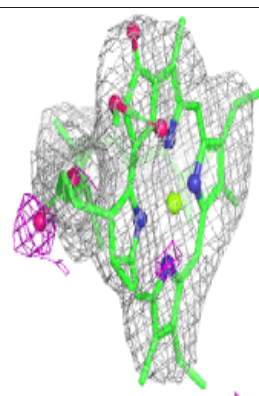
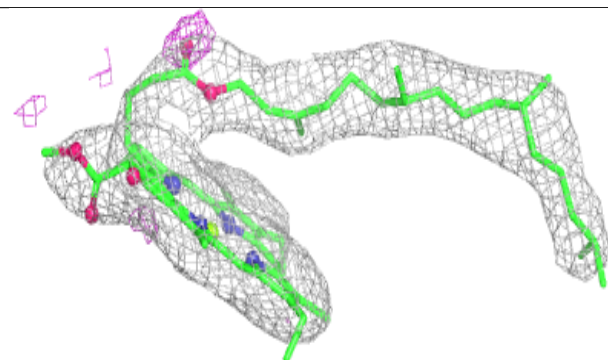
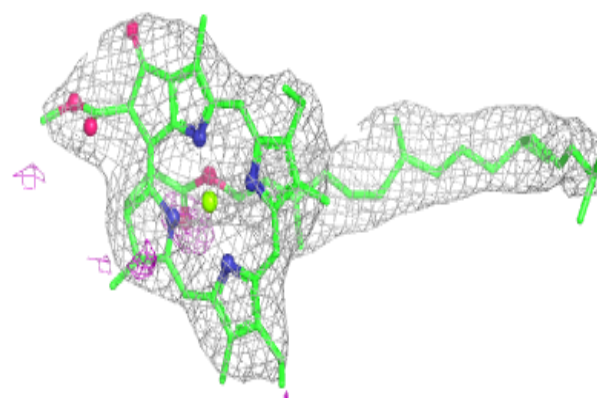


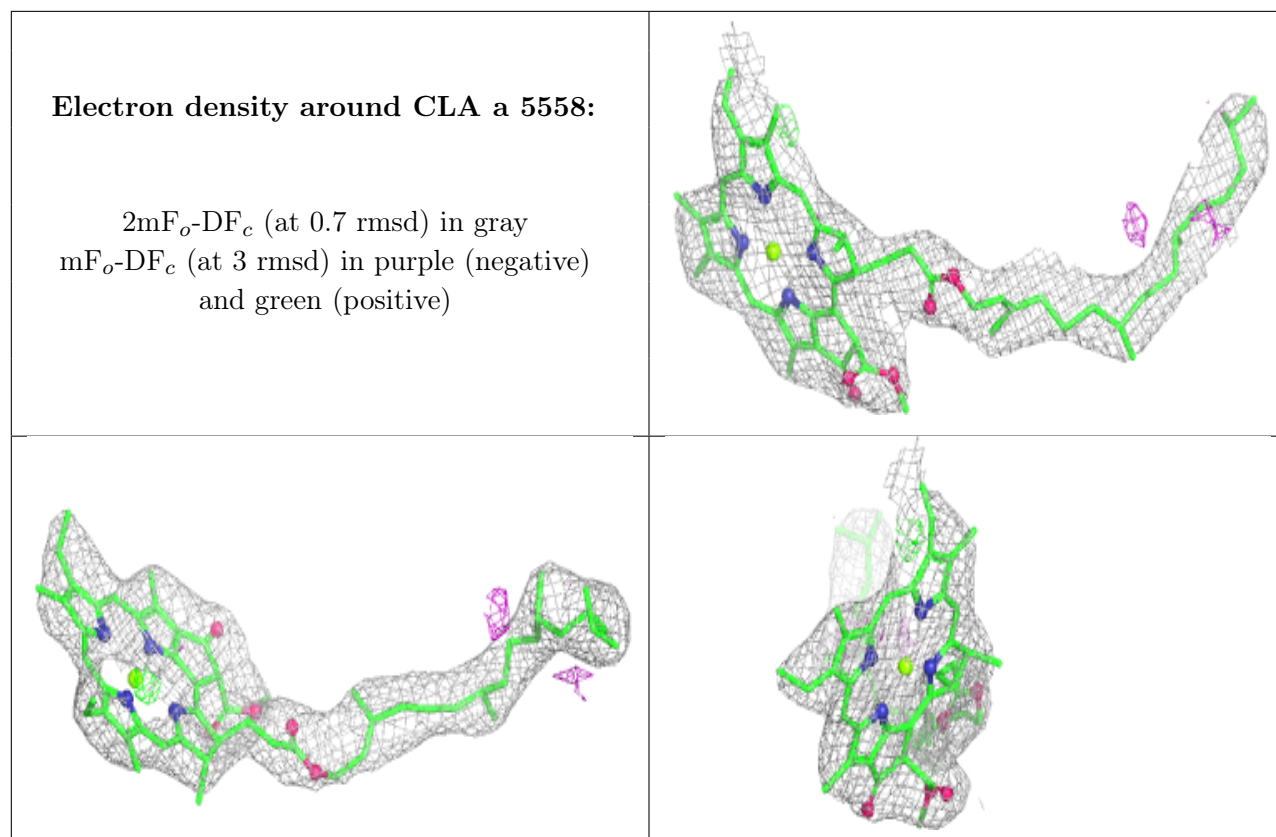
Electron density around CLA b 5517:

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

**Electron density around CLA b 5518:**

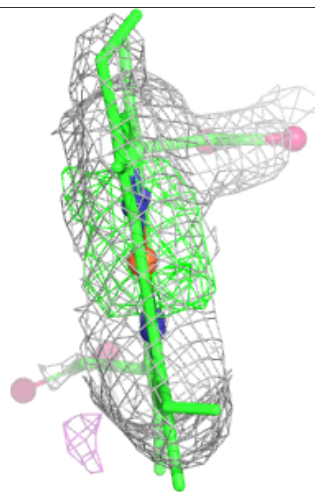
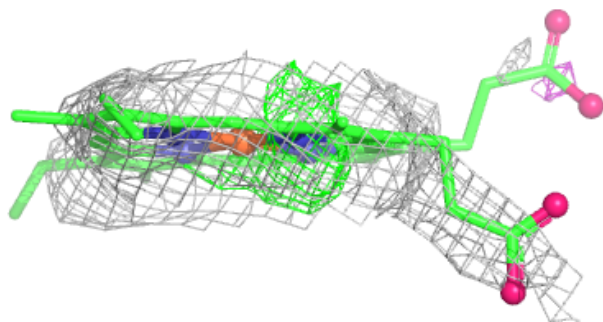
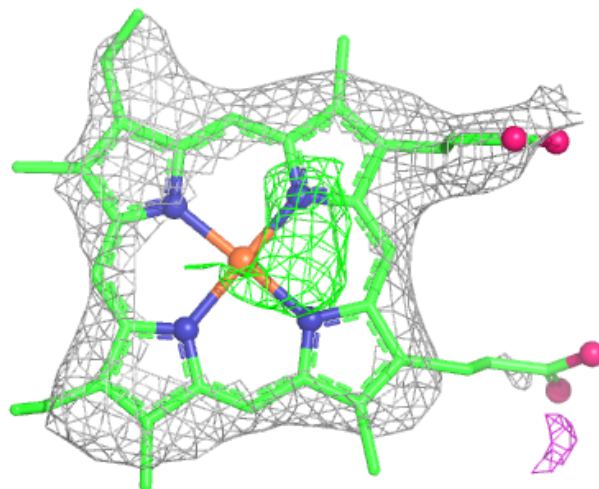
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





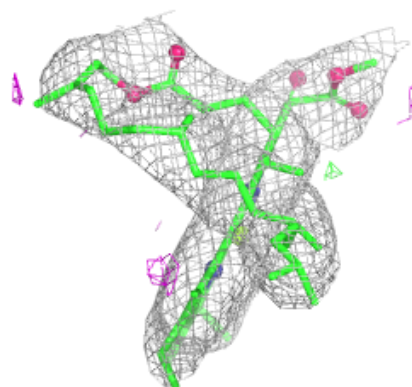
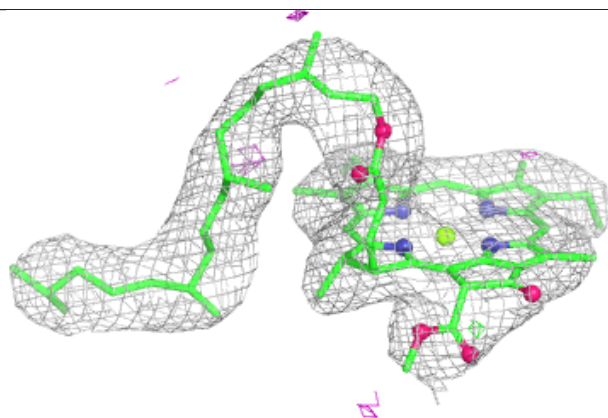
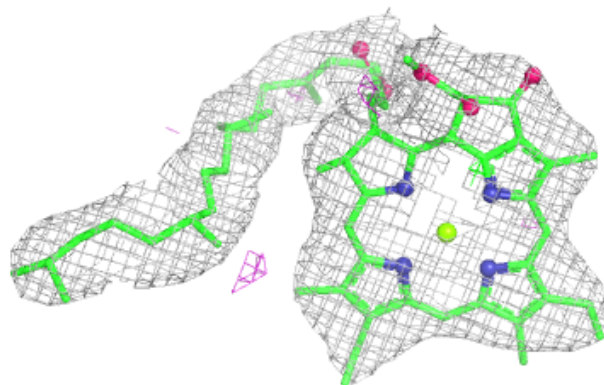
Electron density around HEM F 51:

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

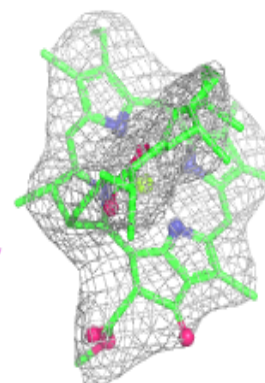
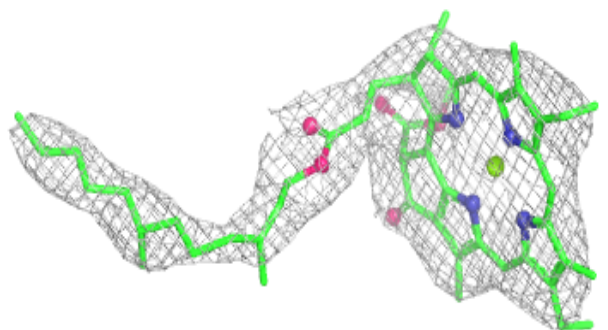
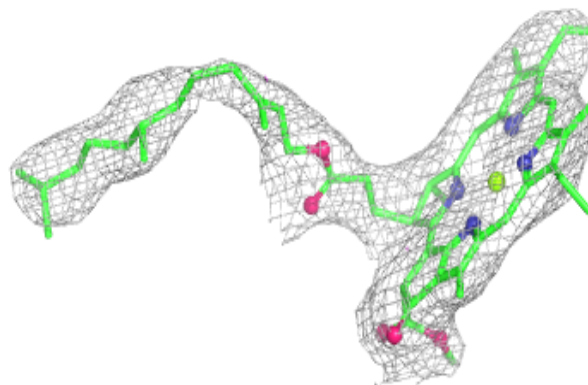


Electron density around CLA a 5559:

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

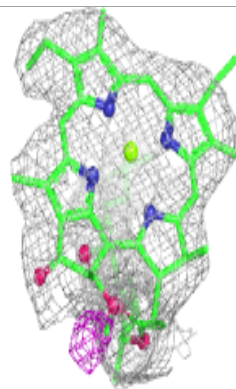
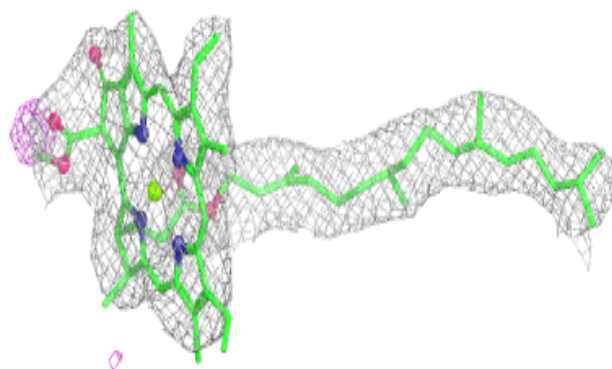
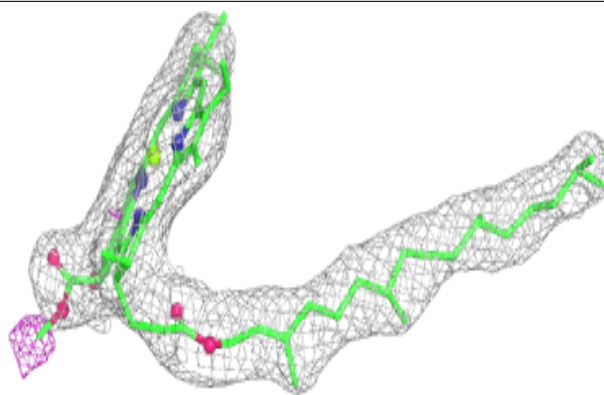
**Electron density around CLA C 492:**

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

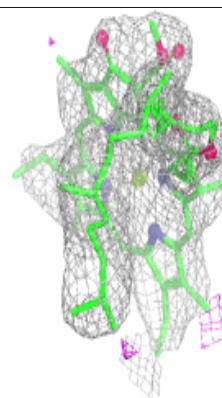
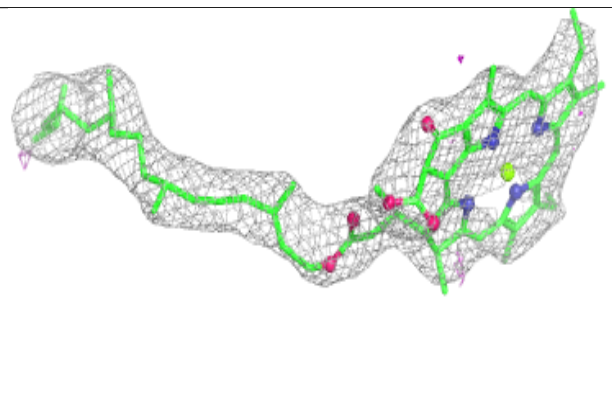
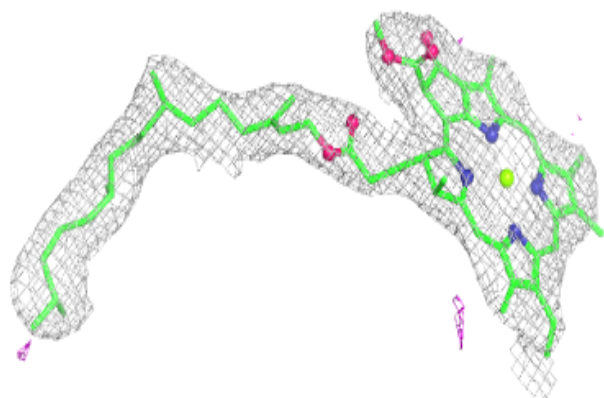


Electron density around CLA B 517:

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

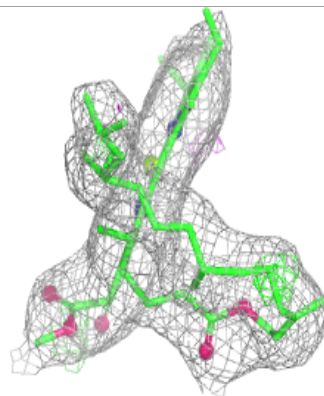
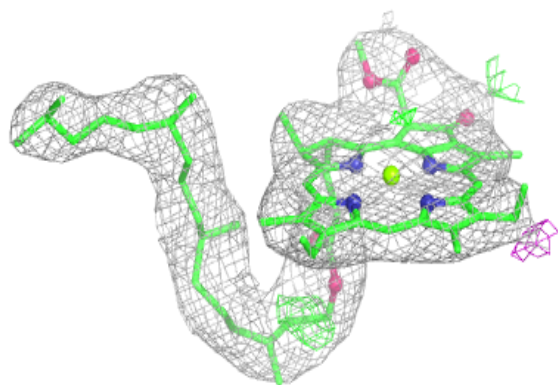
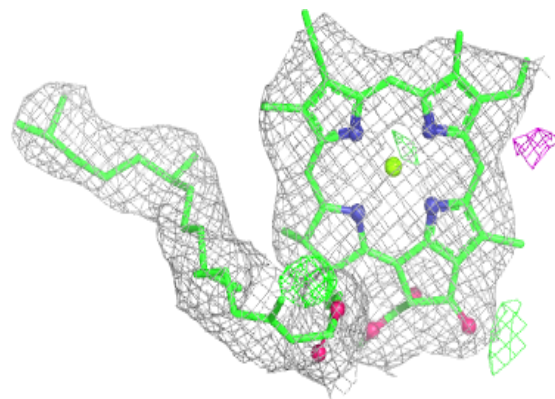
**Electron density around CLA A 558:**

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

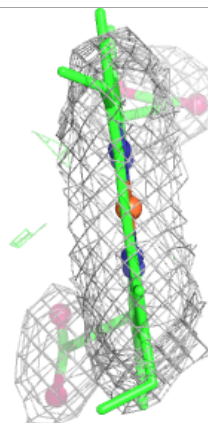
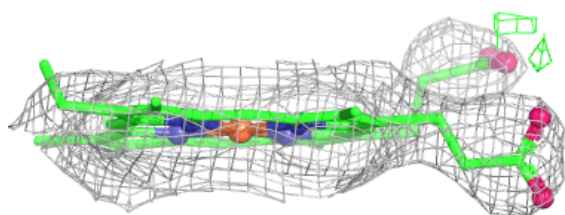
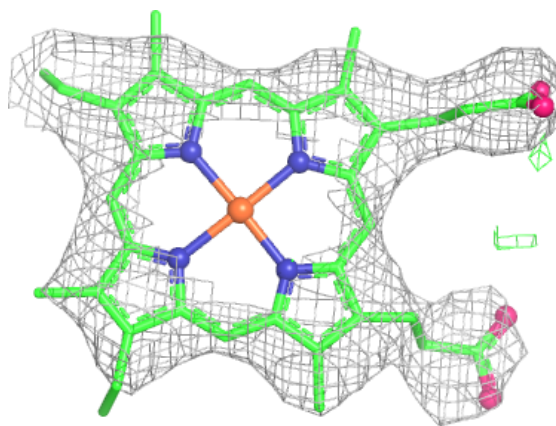


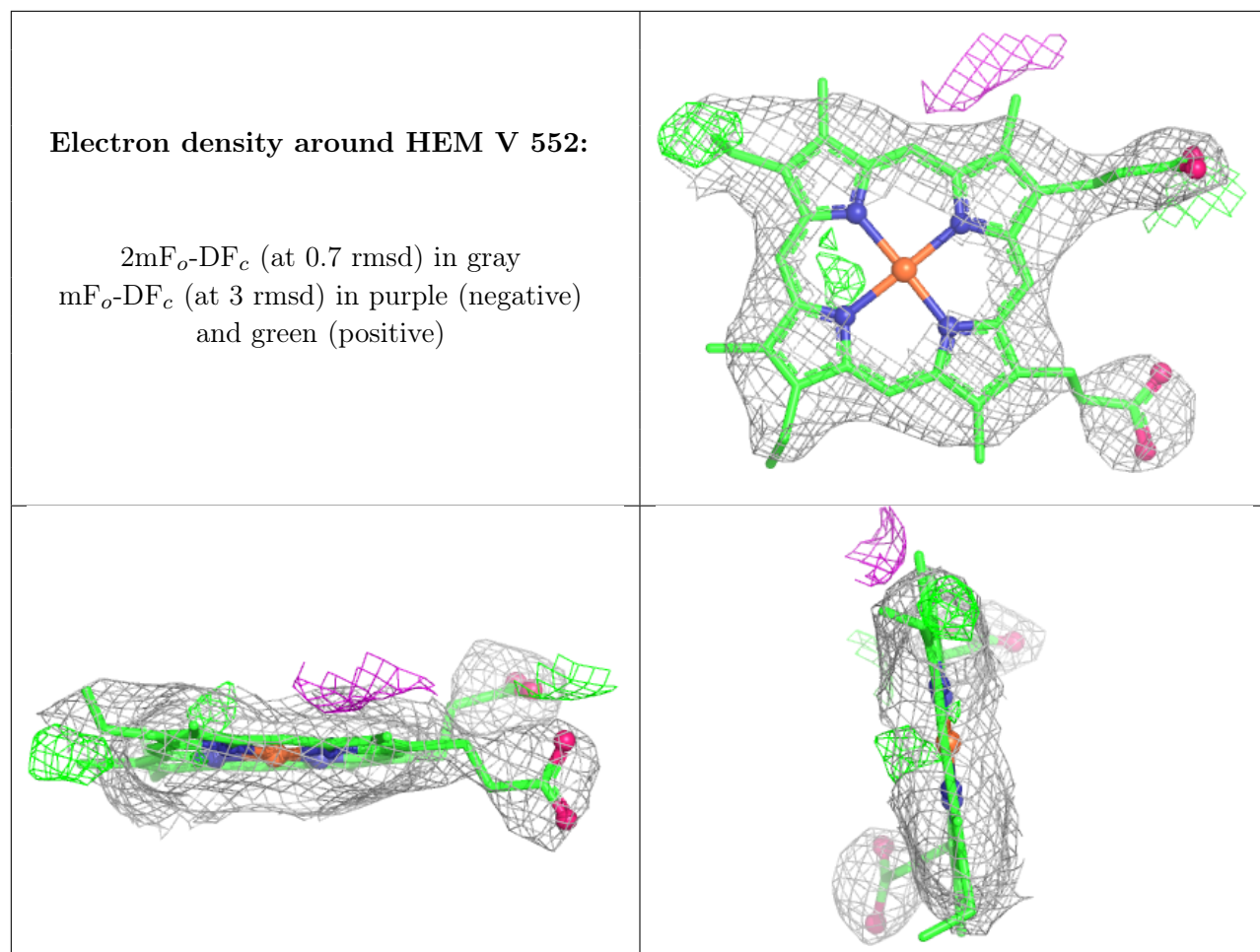
Electron density around CLA A 559:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.