Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 03:28 PM JST

PDB ID	:	5B5N
Title	:	Crystal structure of the Ba-substituted LH1-RC complex from Tch. tepidum
Authors	:	Wang-Otomo, Z.-Y.; Yu, L.-J.
Deposited on	:	2016-05-12
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

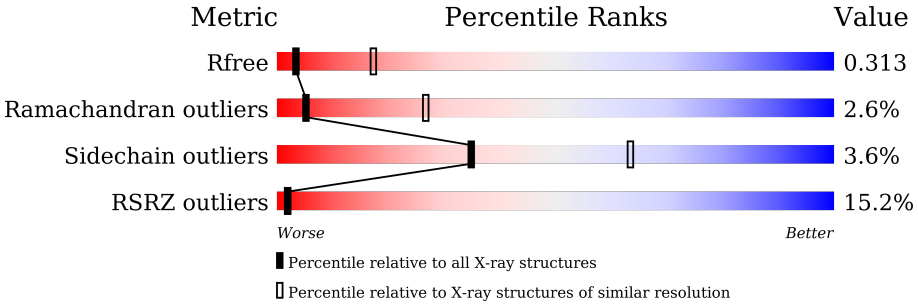
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	C	333	11% 86% 9% 5%
1	o	333	11% 85% 10% • 5%
2	L	281	7% 93% 7%
2	x	281	4% 90% 10%
3	M	319	4% 93% 7%
3	y	319	4% 92% 7%
4	H	259	9% 90% 8% •

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Mol	Chain	Length	Quality of chain
4	t	259	7% 89% 9%
5	1	61	18% 89% 10%
5	3	61	16% 89% 8%
5	5	61	21% 95%
5	7	61	31% 92% 7%
5	9	61	13% 87% 10%
5	A	61	26% 93% 5%
5	AA	61	18% 90% 7%
5	AC	61	26% 89% 10%
5	AE	61	20% 92% 7%
5	AG	61	25% 92% 7%
5	AI	61	26% 95%
5	AK	61	20% 93% 5%
5	D	61	36% 97%
5	F	61	36% 90% 8%
5	I	61	23% 90% 8%
5	K	61	23% 97%
5	O	61	23% 90% 5%
5	Q	61	31% 87% 11%
5	S	61	26% 92% 7%
5	U	61	21% 90% 8%
5	W	61	25% 95%
5	Y	61	20% 92% 7%
5	d	61	18% 95%
5	f	61	21% 90% 8%

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Mol	Chain	Length	Quality of chain
5	h	61	18% 92% 7%
5	j	61	18% 93% 5%
5	l	61	20% 90% 8%
5	m	61	30% 97%
5	p	61	26% 93%
5	r	61	28% 89% 10%
5	u	61	30% 90% 8%
5	w	61	28% 95%
6	0	47	17% 83% 15%
6	2	47	11% 85% 15%
6	4	47	11% 85% 15%
6	6	47	11% 85% 15%
6	8	47	11% 85% 15%
6	AB	47	6% 83% 15%
6	AD	47	21% 85% 15%
6	AF	47	11% 85% 15%
6	AH	47	21% 83% 15%
6	AJ	47	13% 81% 15%
6	AL	47	17% 85% 15%
6	B	47	21% 79% 6% 15%
6	E	47	13% 83% 15%
6	G	47	28% 83% 15%
6	J	47	11% 85% 15%
6	N	47	11% 83% 15%
6	P	47	6% 83% 15%

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Mol	Chain	Length	Quality of chain
6	R	47	23% 85% 15%
6	T	47	6% 83% 15%
6	V	47	2% 85% 15%
6	X	47	13% 79% 6% 15%
6	Z	47	4% 85% 15%
6	c	47	28% 85% 15%
6	e	47	9% 85% 15%
6	g	47	9% 83% 15%
6	i	47	30% 85% 15%
6	k	47	6% 83% 15%
6	n	47	15% 85% 15%
6	q	47	11% 85% 15%
6	s	47	21% 85% 15%
6	v	47	15% 85% 15%
6	z	47	15% 85% 15%

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
12	PEF	A	101	-	-	-	X
12	PEF	H	304	-	-	-	X
14	MQ8	M	404	-	-	-	X
15	CRT	0	101	-	-	-	X
15	CRT	2	101	-	-	-	X
15	CRT	4	101	-	-	-	X
15	CRT	7	101	-	-	-	X
15	CRT	7	103	-	-	-	X
15	CRT	9	101	-	-	-	X
15	CRT	AC	101	-	-	-	X
15	CRT	AD	101	-	-	-	X
15	CRT	AF	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CRT	AH	102	-	-	-	X
15	CRT	AJ	101	-	-	-	X
15	CRT	AL	101	-	-	-	X
15	CRT	E	101	-	-	-	X
15	CRT	G	101	-	-	-	X
15	CRT	I	102	-	-	-	X
15	CRT	M	405	-	-	-	X
15	CRT	O	101	-	-	-	X
15	CRT	P	102	-	-	-	X
15	CRT	R	101	-	-	-	X
15	CRT	T	101	-	-	-	X
15	CRT	V	101	-	-	-	X
15	CRT	e	101	-	-	-	X
15	CRT	g	101	-	-	-	X
15	CRT	i	101	-	-	-	X
15	CRT	k	101	-	-	-	X
15	CRT	m	104	-	-	-	X
15	CRT	n	101	-	-	-	X
15	CRT	q	101	-	-	-	X
15	CRT	v	101	-	-	-	X
15	CRT	z	101	-	-	-	X
16	PO4	H	303	-	-	-	X
7	HEM	o	501	-	-	-	X
9	BCL	AB	102	-	-	-	X
9	BCL	AC	103	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 51893 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	317	2458	1551	430	460	17	0	0	0
1	o	317	2458	1551	430	460	17	0	0	0

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	280	2231	1501	359	361	10	0	0	0
2	x	280	2231	1501	359	361	10	0	0	0

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	318	2546	1710	416	409	11	0	0	0
3	y	318	2546	1710	416	409	11	0	0	0

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	1982	1275	339	363	5	0	0	0
4	t	258	1982	1275	339	363	5	0	0	0

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	60	475	315	77	81	2	0	0	0
5	D	60	475	315	77	81	2	0	0	0
5	F	60	475	315	77	81	2	0	0	0
5	I	60	475	315	77	81	2	0	0	0
5	K	60	475	315	77	81	2	0	0	0
5	O	60	475	315	77	81	2	0	0	0
5	Q	60	475	315	77	81	2	0	0	0
5	S	60	481	318	78	83	2	0	1	0
5	U	60	475	315	77	81	2	0	0	0
5	W	60	475	315	77	81	2	0	0	0
5	Y	60	475	315	77	81	2	0	0	0
5	1	60	475	315	77	81	2	0	0	0
5	3	60	475	315	77	81	2	0	0	0
5	5	60	475	315	77	81	2	0	0	0
5	7	60	475	315	77	81	2	0	0	0
5	9	60	475	315	77	81	2	0	0	0
5	m	60	475	315	77	81	2	0	0	0
5	p	60	475	315	77	81	2	0	0	0
5	r	60	475	315	77	81	2	0	0	0
5	u	60	475	315	77	81	2	0	0	0
5	w	60	475	315	77	81	2	0	0	0
5	AA	60	475	315	77	81	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AC	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	AE	60	481	318	78	83	2	0	1	0
			Total	C	N	O	S			
5	AG	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	AI	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	AK	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	d	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	f	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	h	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	j	60	475	315	77	81	2	0	0	0
			Total	C	N	O	S			
5	l	60	475	315	77	81	2	0	0	0

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	E	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	G	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	J	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	N	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	P	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	R	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	T	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	V	40	337	228	52	55	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	X	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	Z	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	2	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	4	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	6	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	8	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	0	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	n	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	q	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	s	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	v	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	z	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AB	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AD	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AF	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AH	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AJ	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AL	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	e	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	g	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	i	40	337	228	52	55	2	0	0	0

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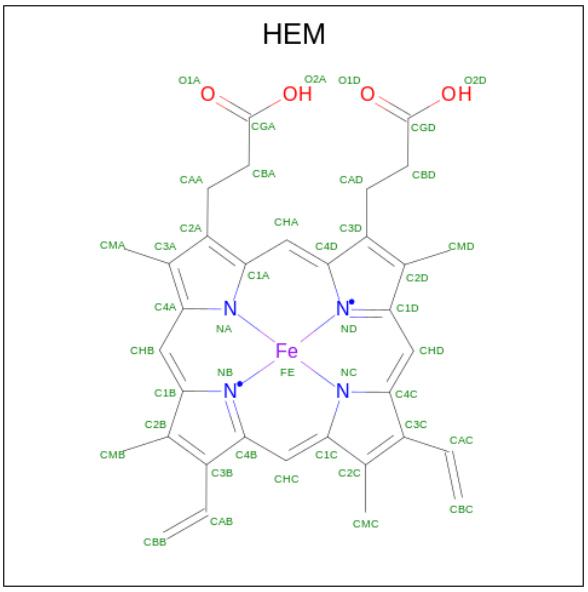
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	k	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	c	40	337	228	52	55	2	0	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
8	C	1	1	1	0	0
8	L	2	2	2	0	0
8	A	2	2	2	0	0
8	D	1	1	1	0	0
8	F	1	1	1	0	0
8	I	1	1	1	0	0
8	K	1	1	1	0	0
8	O	1	1	1	0	0
8	Q	1	1	1	0	0
8	S	1	1	1	0	0
8	U	1	1	1	0	0
8	W	1	1	1	0	0
8	Y	1	1	1	0	0
8	1	1	1	1	0	0
8	3	1	1	1	0	0
8	5	1	1	1	0	0
8	7	1	1	1	0	0
8	o	1	1	1	0	0
8	x	2	2	2	0	0
8	m	2	2	2	0	0
8	p	1	1	1	0	0
8	r	1	1	1	0	0

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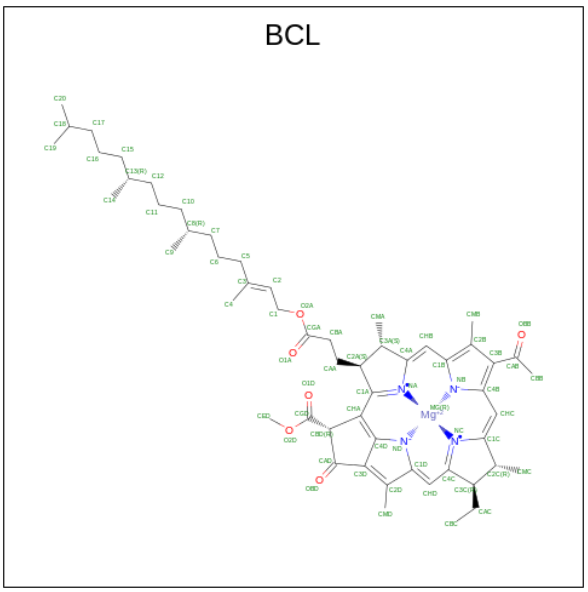
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
8	u	1	1	1	0	0
8	w	1	1	1	0	0
8	AA	1	1	1	0	0
8	AC	1	1	1	0	0
8	AE	1	1	1	0	0
8	AG	1	1	1	0	0
8	AI	1	1	1	0	0
8	AK	1	1	1	0	0
8	d	1	1	1	0	0
8	f	1	1	1	0	0
8	h	1	1	1	0	0
8	j	1	1	1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	D	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	D	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	F	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	G	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	I	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	I	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	K	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	N	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	O	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	P	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	Q	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	R	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	S	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	T	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	U	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	V	1	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	W	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	X	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	Y	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	Z	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	1	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	2	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	3	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	4	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	5	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	6	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	7	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	8	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	9	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	0	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	x	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	x	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	x	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	y	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	m	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	m	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	p	1	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	q	1	66	55	1	4	6	0	0
9	r	1	66	55	1	4	6	0	0
9	s	1	66	55	1	4	6	0	0
9	u	1	66	55	1	4	6	0	0
9	u	1	66	55	1	4	6	0	0
9	w	1	66	55	1	4	6	0	0
9	z	1	66	55	1	4	6	0	0
9	AB	1	66	55	1	4	6	0	0
9	AB	1	66	55	1	4	6	0	0
9	AC	1	66	55	1	4	6	0	0
9	AC	1	66	55	1	4	6	0	0
9	AE	1	66	55	1	4	6	0	0
9	AF	1	66	55	1	4	6	0	0
9	AG	1	66	55	1	4	6	0	0
9	AH	1	66	55	1	4	6	0	0
9	AI	1	66	55	1	4	6	0	0
9	AI	1	66	55	1	4	6	0	0
9	AK	1	66	55	1	4	6	0	0
9	AL	1	66	55	1	4	6	0	0
9	d	1	66	55	1	4	6	0	0
9	e	1	66	55	1	4	6	0	0

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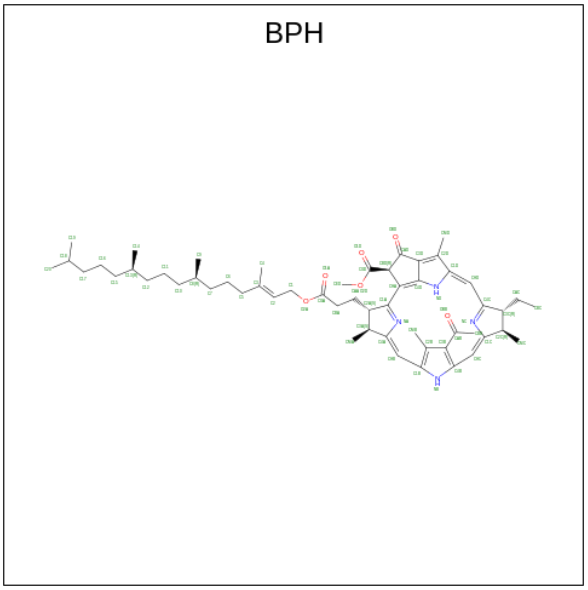
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	f	1	66	55	1	4	6	0	0
9	g	1	66	55	1	4	6	0	0
9	h	1	66	55	1	4	6	0	0
9	i	1	66	55	1	4	6	0	0
9	j	1	66	55	1	4	6	0	0
9	k	1	66	55	1	4	6	0	0
9	l	1	66	55	1	4	6	0	0
9	c	1	66	55	1	4	6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	L	1	65	55	4	6	0	0
10	M	1	65	55	4	6	0	0
10	x	1	65	55	4	6	0	0

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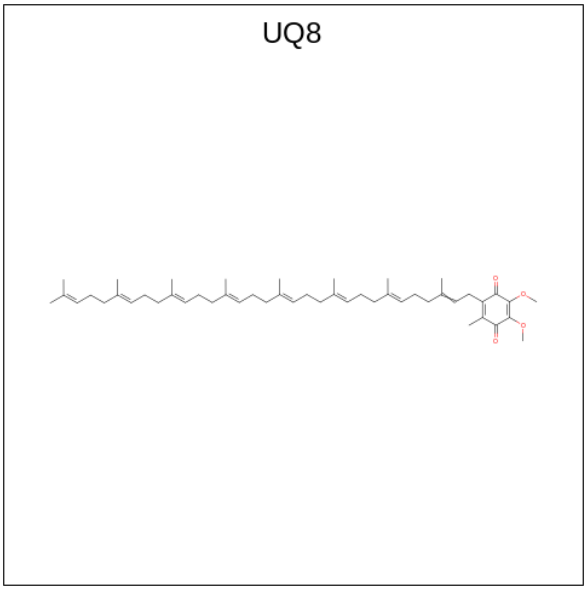
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	y	1	65	55	4	6	0	0

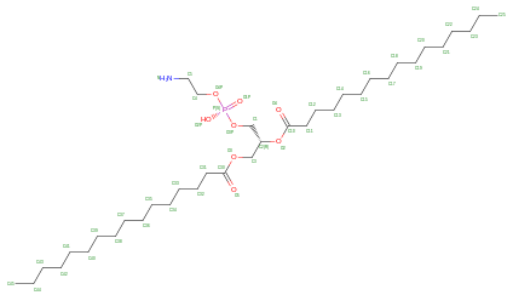
- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	L	1	53	49	4	0	0
			Total	C	O		
11	x	1	53	49	4	0	0

- Molecule 12 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).

PEF



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	L	1	12	5	1	5	1	0	0
			Total	C	N	O	P		
12	M	1	16	7	1	7	1	0	0
			Total	C	N	O	P		
12	M	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	x	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	y	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	y	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	y	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	t	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	t	1	19	9	1	8	1	0	0

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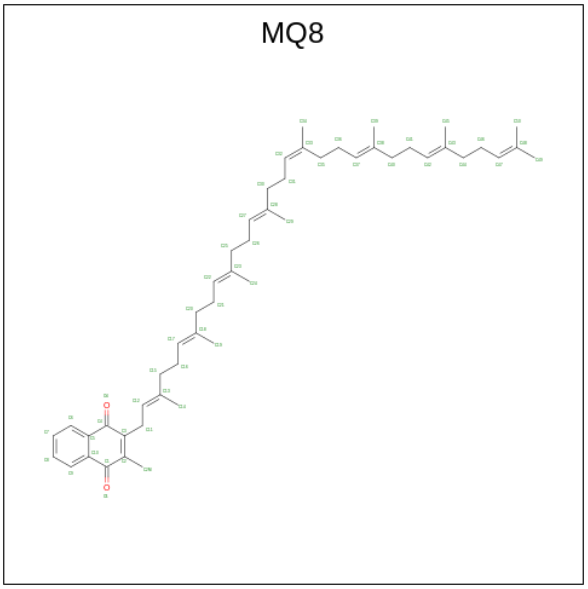
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	m	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
12	p	1	16	7	1	7	1	0	0

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
13	L	1	1	1	0	0
			Total	Fe		
13	x	1	1	1	0	0

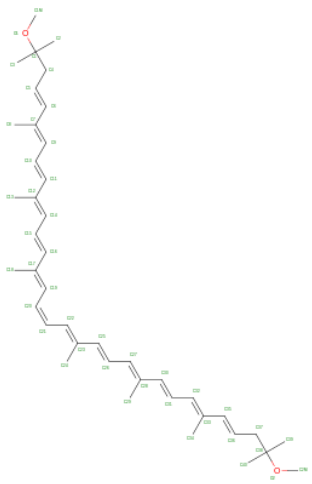
- Molecule 14 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	M	1	53	51	2	0	0
			Total	C	O		
14	y	1	53	51	2	0	0

- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).

CRT



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	M	1	44	42	2	0	0
15	E	1	44	42	2	0	0
15	G	1	44	42	2	0	0
15	I	1	44	42	2	0	0
15	O	1	44	42	2	0	0
15	P	1	44	42	2	0	0
15	R	1	44	42	2	0	0
15	T	1	44	42	2	0	0
15	V	1	44	42	2	0	0
15	X	1	44	42	2	0	0
15	Z	1	44	42	2	0	0
15	2	1	44	42	2	0	0
15	4	1	44	42	2	0	0
15	7	1	44	42	2	0	0

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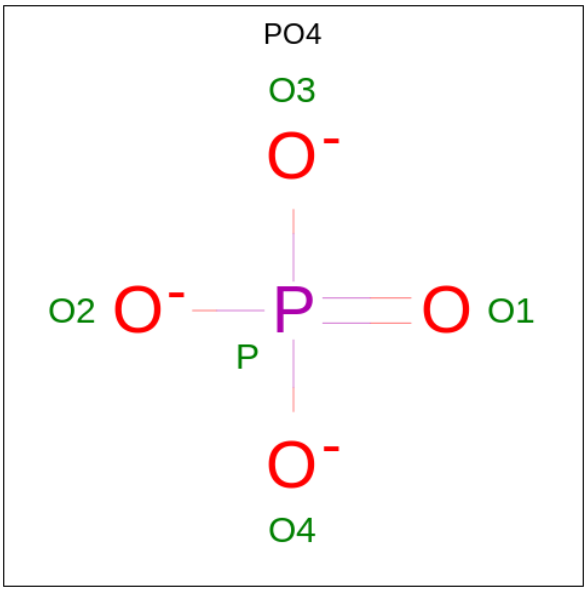
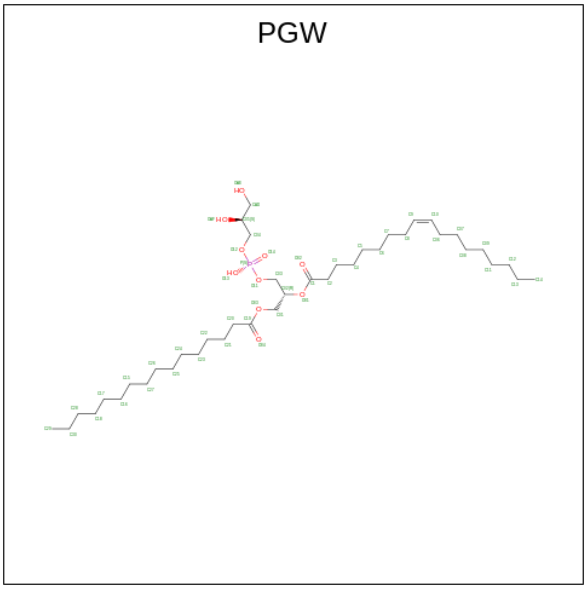
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	7	1	44	42	2	0	0
15	9	1	44	42	2	0	0
15	0	1	44	42	2	0	0
15	y	1	44	42	2	0	0
15	m	1	44	42	2	0	0
15	n	1	44	42	2	0	0
15	q	1	44	42	2	0	0
15	s	1	44	42	2	0	0
15	v	1	44	42	2	0	0
15	z	1	44	42	2	0	0
15	AC	1	44	42	2	0	0
15	AD	1	44	42	2	0	0
15	AF	1	44	42	2	0	0
15	AH	1	44	42	2	0	0
15	AJ	1	44	42	2	0	0
15	AL	1	44	42	2	0	0
15	e	1	44	42	2	0	0
15	g	1	44	42	2	0	0
15	i	1	44	42	2	0	0
15	k	1	44	42	2	0	0

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total O P 5 4 1	0	0
16	H	1	Total O P 5 4 1	0	0
16	y	1	Total O P 5 4 1	0	0
16	t	1	Total O P 5 4 1	0	0

- Molecule 17 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
17	S	1	21	10	10	1	0	0
17	AE	1	21	10	10	1	0	0

- Molecule 18 is water.

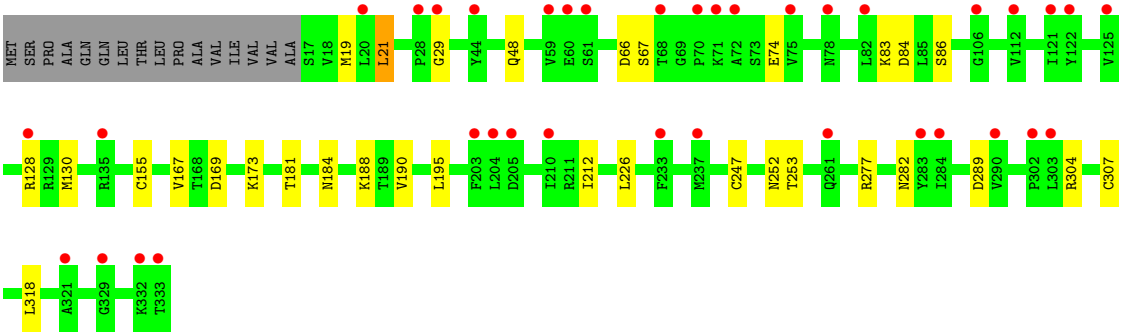
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	L	2	2	2	0	0
18	W	1	1	1	0	0
18	x	2	2	2	0	0
18	AI	1	1	1	0	0

3 Residue-property plots (i)

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

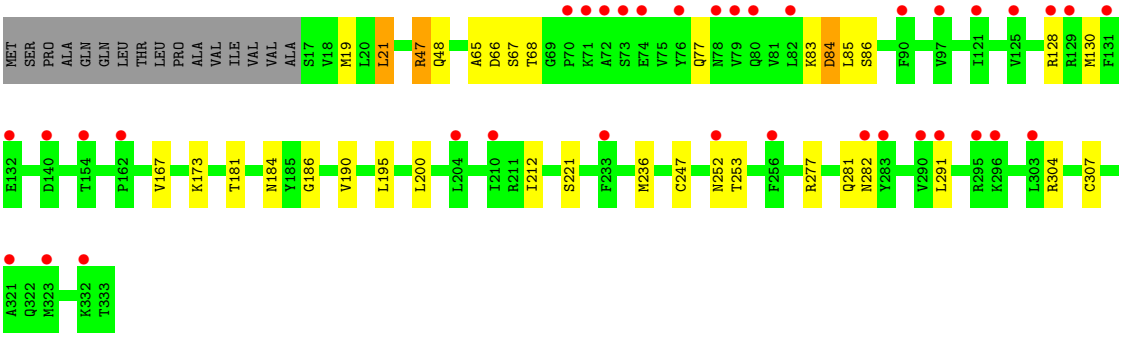
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



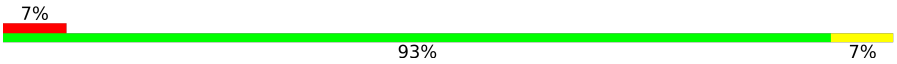
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

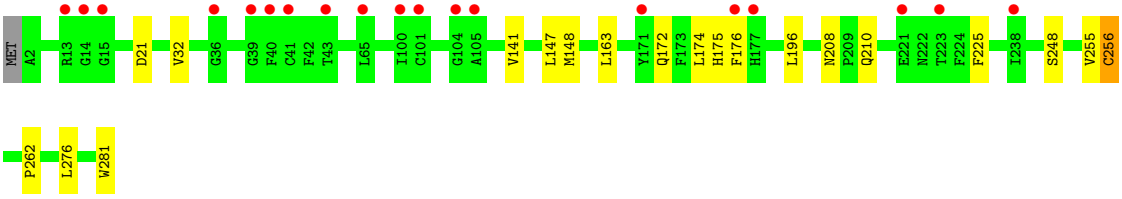
Chain o:



• Molecule 2: Photosynthetic reaction center L subunit

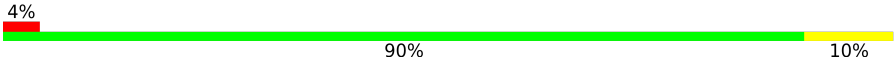
Chain L:

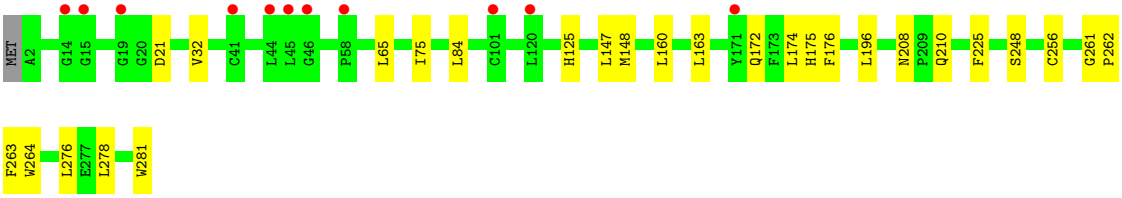




• Molecule 2: Photosynthetic reaction center L subunit

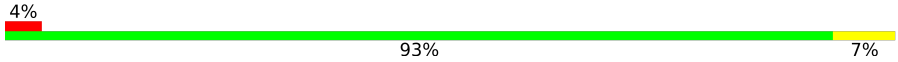
Chain x:

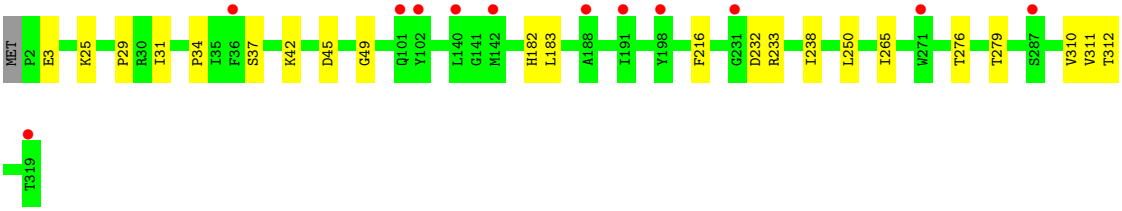




• Molecule 3: Photosynthetic reaction center M subunit

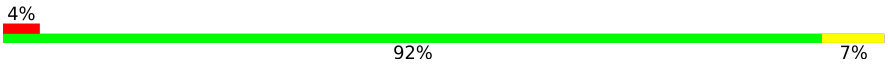
Chain M:

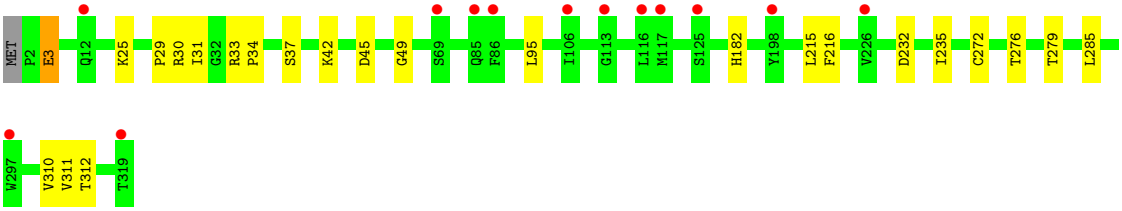




• Molecule 3: Photosynthetic reaction center M subunit

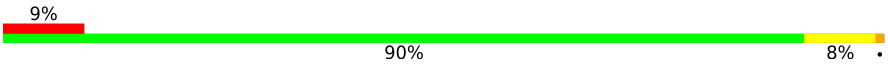
Chain y:

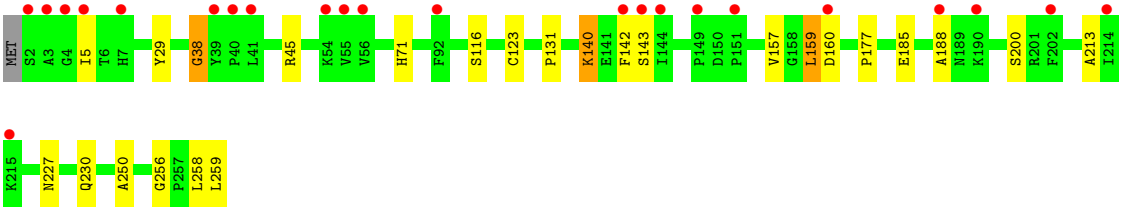




• Molecule 4: Photosynthetic reaction center H subunit

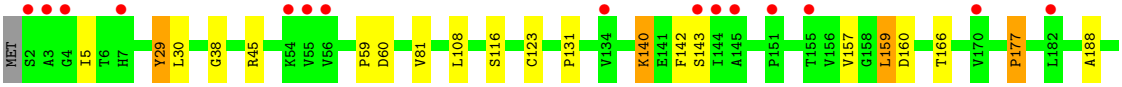
Chain H:

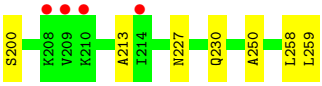




• Molecule 4: Photosynthetic reaction center H subunit

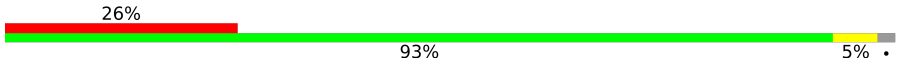
Chain t:

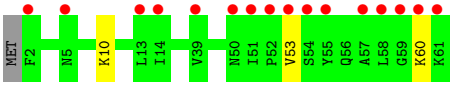




• Molecule 5: LH1 alpha polypeptide

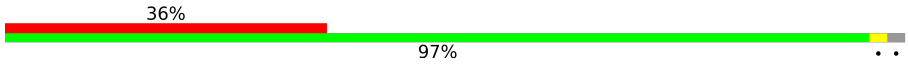
Chain A:

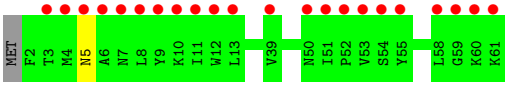




• Molecule 5: LH1 alpha polypeptide

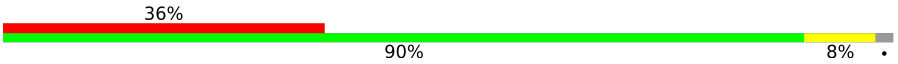
Chain D:

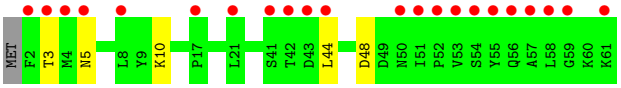




• Molecule 5: LH1 alpha polypeptide

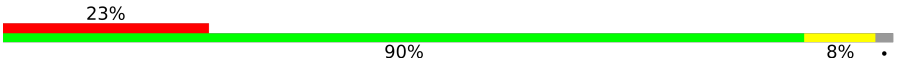
Chain F:

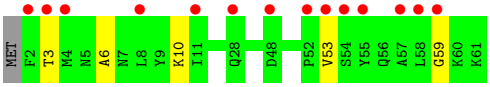




• Molecule 5: LH1 alpha polypeptide

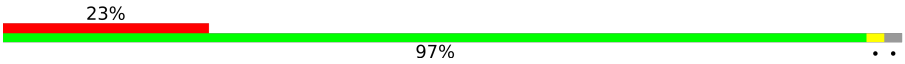
Chain I:

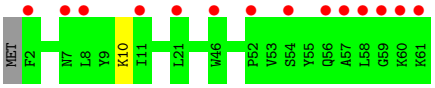




• Molecule 5: LH1 alpha polypeptide

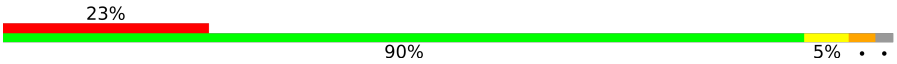
Chain K:

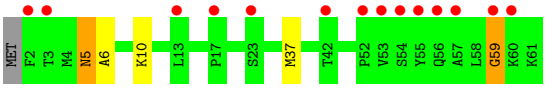




• Molecule 5: LH1 alpha polypeptide

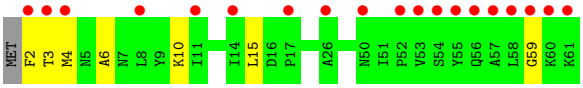
Chain O:





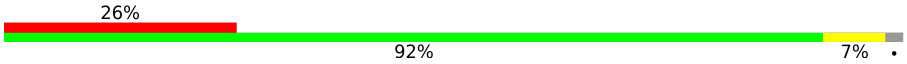
• Molecule 5: LH1 alpha polypeptide

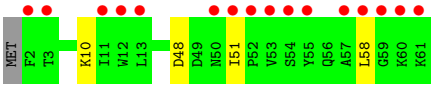
Chain Q:



• Molecule 5: LH1 alpha polypeptide

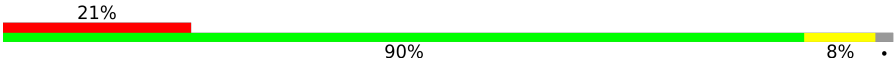
Chain S:

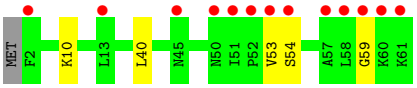




• Molecule 5: LH1 alpha polypeptide

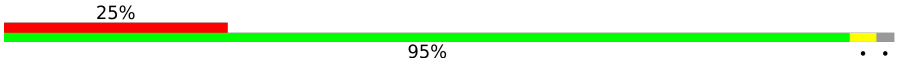
Chain U:

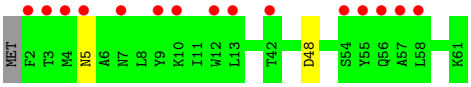




• Molecule 5: LH1 alpha polypeptide

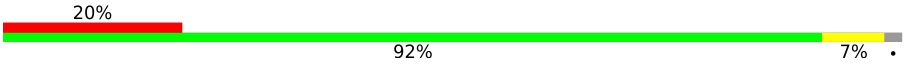
Chain W:

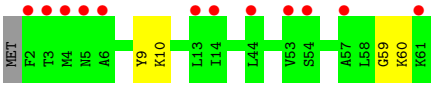




• Molecule 5: LH1 alpha polypeptide

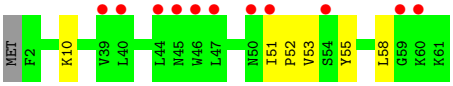
Chain Y:





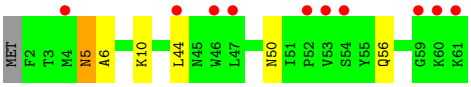
• Molecule 5: LH1 alpha polypeptide

Chain 1:



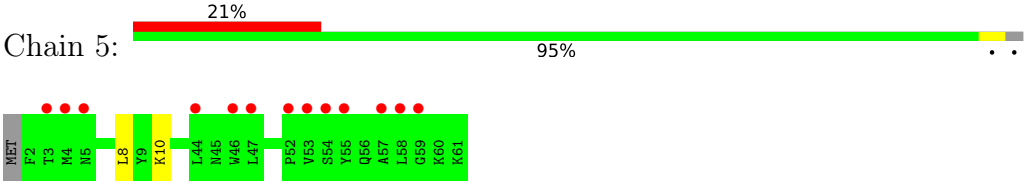
• Molecule 5: LH1 alpha polypeptide

Chain 3:



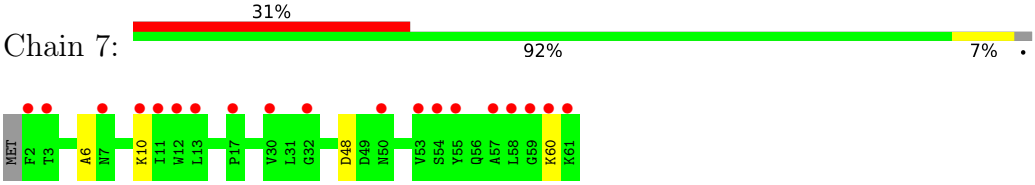
• Molecule 5: LH1 alpha polypeptide

Chain 5:



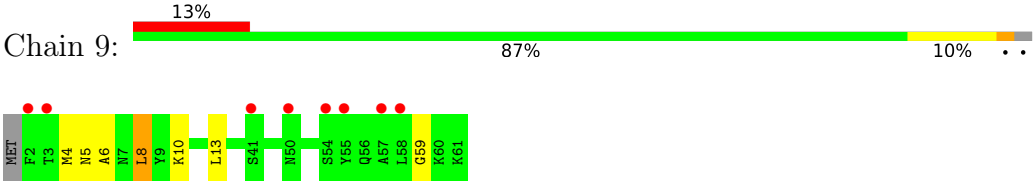
• Molecule 5: LH1 alpha polypeptide

Chain 7:



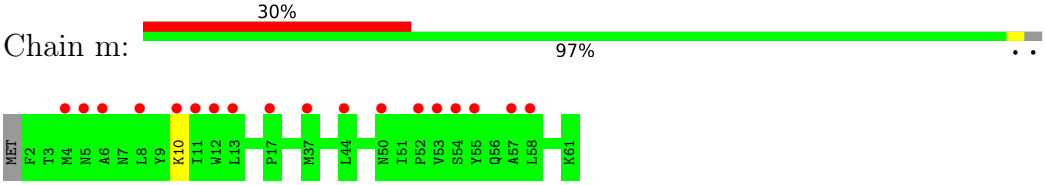
• Molecule 5: LH1 alpha polypeptide

Chain 9:



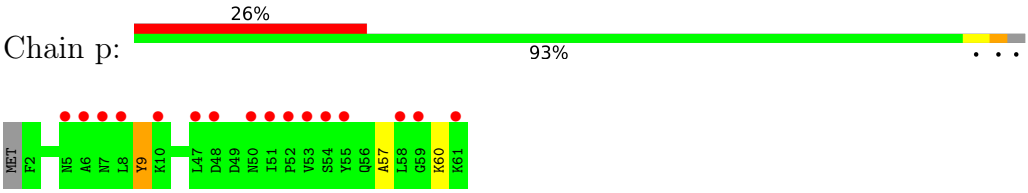
• Molecule 5: LH1 alpha polypeptide

Chain m:



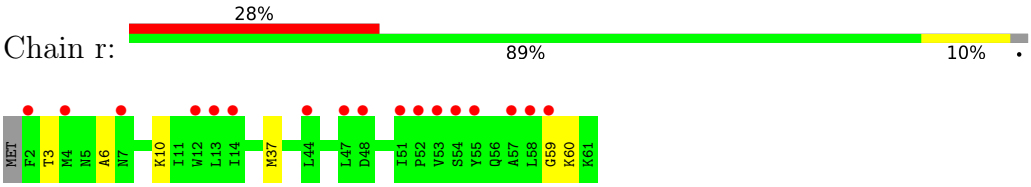
• Molecule 5: LH1 alpha polypeptide

Chain p:



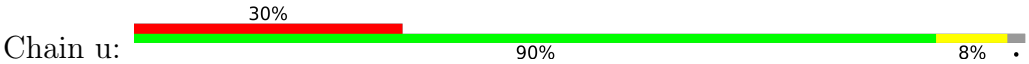
• Molecule 5: LH1 alpha polypeptide

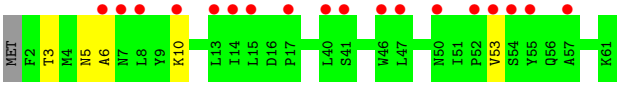
Chain r:



• Molecule 5: LH1 alpha polypeptide

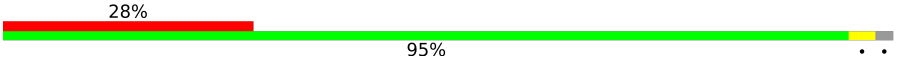
Chain u:

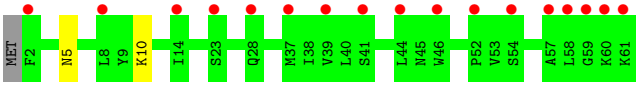




• Molecule 5: LH1 alpha polypeptide

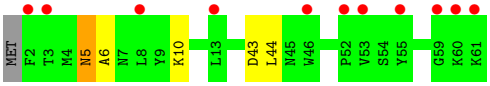
Chain w:





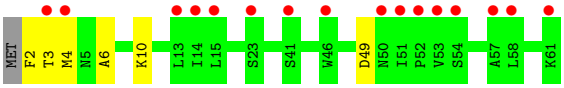
• Molecule 5: LH1 alpha polypeptide

Chain AA:



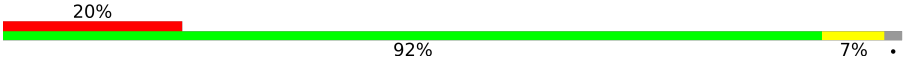
• Molecule 5: LH1 alpha polypeptide

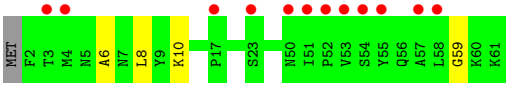
Chain AC:



• Molecule 5: LH1 alpha polypeptide

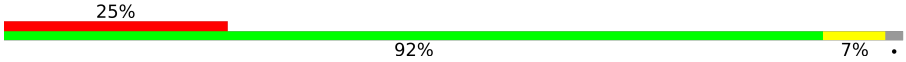
Chain AE:

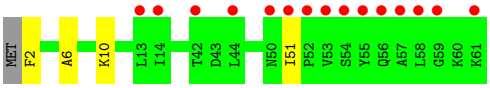




• Molecule 5: LH1 alpha polypeptide

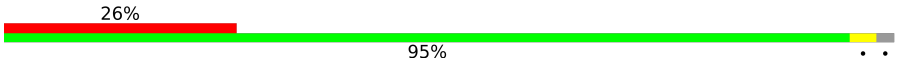
Chain AG:

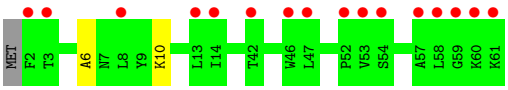




• Molecule 5: LH1 alpha polypeptide

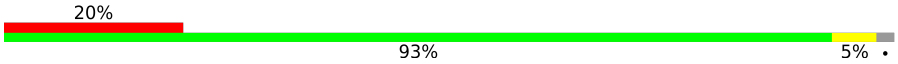
Chain AI:

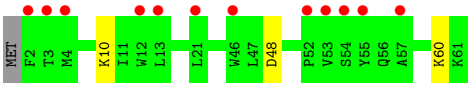




• Molecule 5: LH1 alpha polypeptide

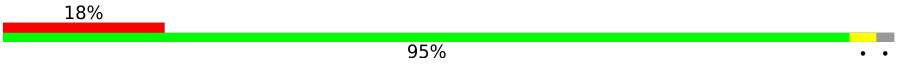
Chain AK:

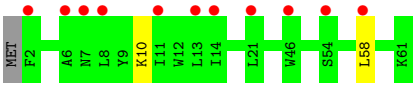




- Molecule 5: LH1 alpha polypeptide

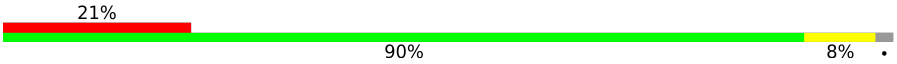
Chain d:

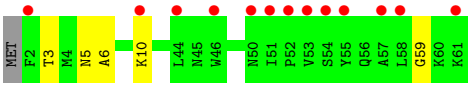




- Molecule 5: LH1 alpha polypeptide

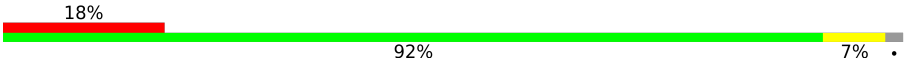
Chain f:

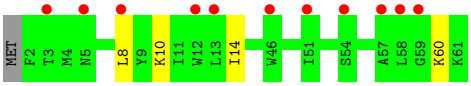




- Molecule 5: LH1 alpha polypeptide

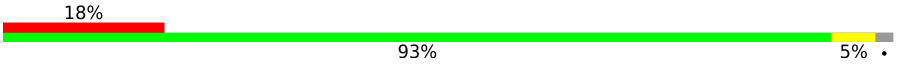
Chain h:

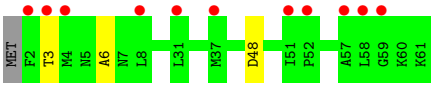




- Molecule 5: LH1 alpha polypeptide

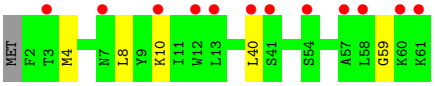
Chain j:





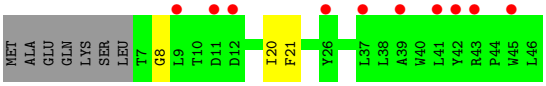
- Molecule 5: LH1 alpha polypeptide

Chain l:



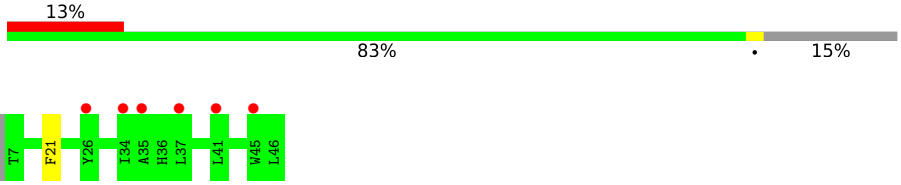
- Molecule 6: LH1 beta polypeptide

Chain B:



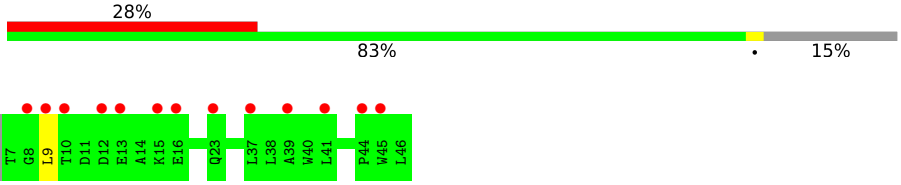
• Molecule 6: LH1 beta polypeptide

Chain E:



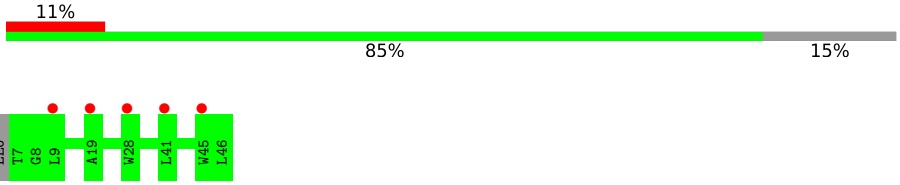
• Molecule 6: LH1 beta polypeptide

Chain G:



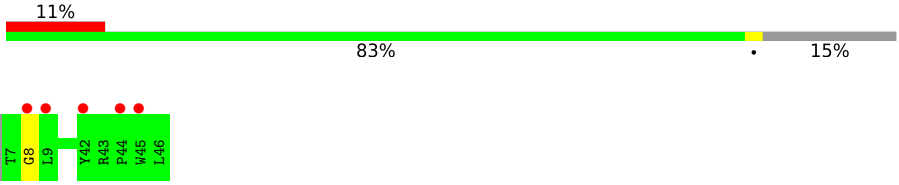
• Molecule 6: LH1 beta polypeptide

Chain J:



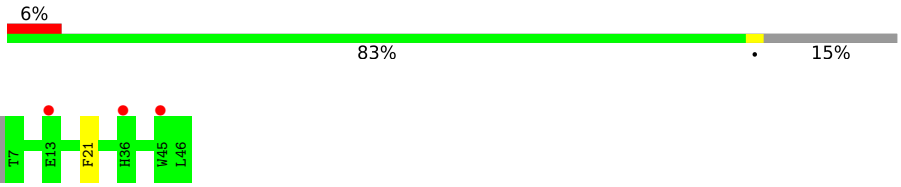
• Molecule 6: LH1 beta polypeptide

Chain N:



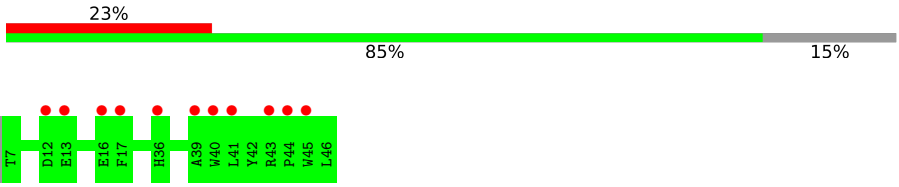
• Molecule 6: LH1 beta polypeptide

Chain P:



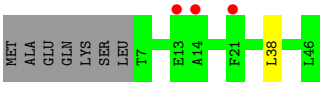
• Molecule 6: LH1 beta polypeptide

Chain R:



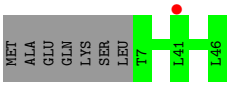
• Molecule 6: LH1 beta polypeptide

Chain T:



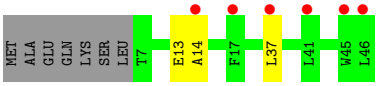
• Molecule 6: LH1 beta polypeptide

Chain V:



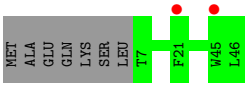
• Molecule 6: LH1 beta polypeptide

Chain X:



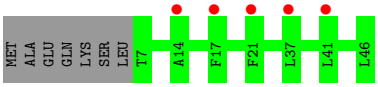
• Molecule 6: LH1 beta polypeptide

Chain Z:



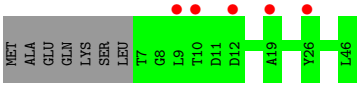
• Molecule 6: LH1 beta polypeptide

Chain 2:



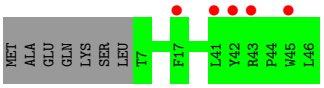
• Molecule 6: LH1 beta polypeptide

Chain 4:



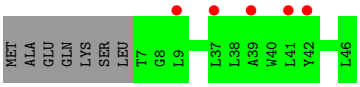
• Molecule 6: LH1 beta polypeptide

Chain 6:



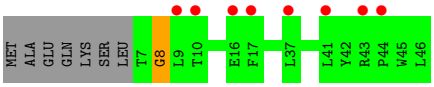
• Molecule 6: LH1 beta polypeptide

Chain 8:



• Molecule 6: LH1 beta polypeptide

Chain 0:

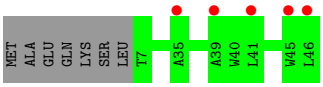


• Molecule 6: LH1 beta polypeptide

Chain n:

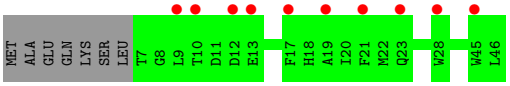
• Molecule 6: LH1 beta polypeptide

Chain q:



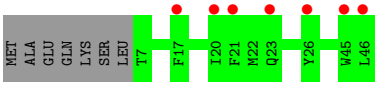
• Molecule 6: LH1 beta polypeptide

Chain s:



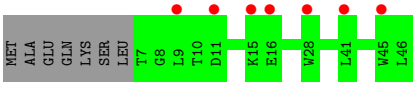
• Molecule 6: LH1 beta polypeptide

Chain v:



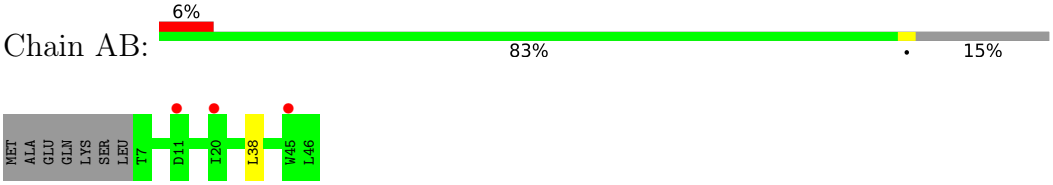
• Molecule 6: LH1 beta polypeptide

Chain z:



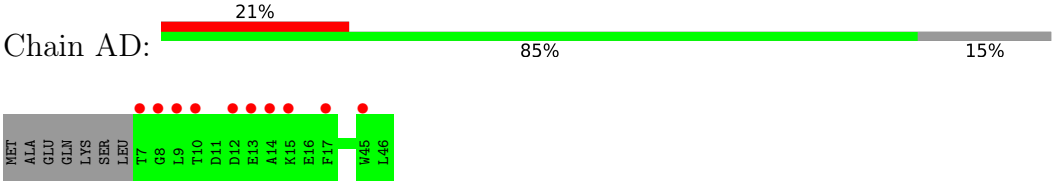
• Molecule 6: LH1 beta polypeptide

Chain AB:



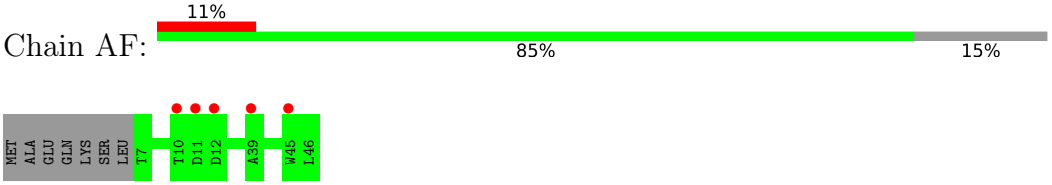
• Molecule 6: LH1 beta polypeptide

Chain AD:



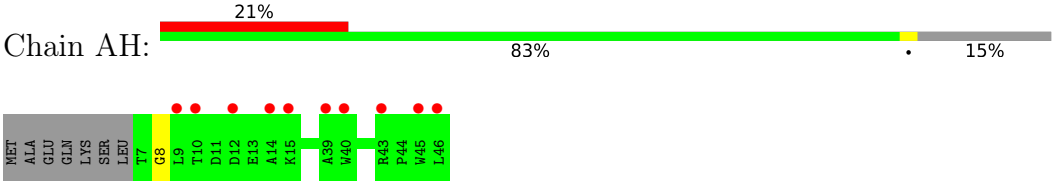
• Molecule 6: LH1 beta polypeptide

Chain AF:



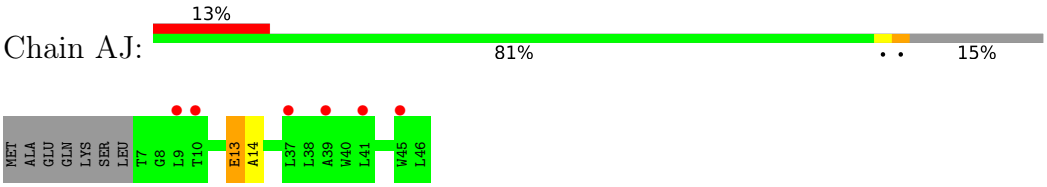
• Molecule 6: LH1 beta polypeptide

Chain AH:



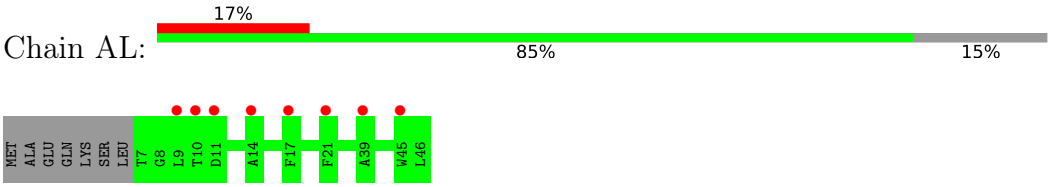
• Molecule 6: LH1 beta polypeptide

Chain AJ:



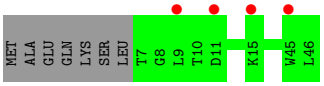
• Molecule 6: LH1 beta polypeptide

Chain AL:



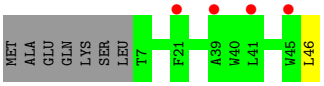
• Molecule 6: LH1 beta polypeptide

Chain e:



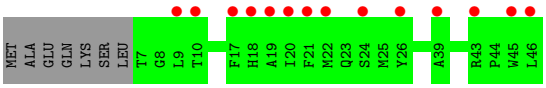
- Molecule 6: LH1 beta polypeptide

Chain g:



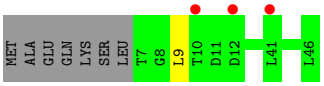
- Molecule 6: LH1 beta polypeptide

Chain i:



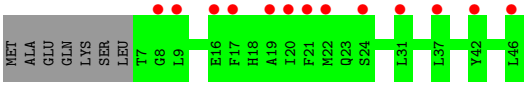
- Molecule 6: LH1 beta polypeptide

Chain k:



- Molecule 6: LH1 beta polypeptide

Chain c:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	163.83Å 148.56Å 210.00Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	49.90 – 3.30 49.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.90-3.30) 92.6 (49.90-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.279 , 0.313 0.280 , 0.313	Depositor DCC
R_{free} test set	6658 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 86.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MQ8, CRT, PO4, BPH, UQ8, BCL, PEF, PGW, HEM, FE, BA

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	C	0.75	1/2528 (0.0%)	1.05	6/3451 (0.2%)
1	o	0.73	1/2528 (0.0%)	1.05	9/3451 (0.3%)
2	L	0.78	1/2318 (0.0%)	1.02	3/3167 (0.1%)
2	x	0.80	1/2318 (0.0%)	1.06	10/3167 (0.3%)
3	M	0.72	0/2646	1.02	5/3621 (0.1%)
3	y	0.71	0/2646	0.98	3/3621 (0.1%)
4	H	0.79	1/2037 (0.0%)	1.08	6/2776 (0.2%)
4	t	0.79	1/2037 (0.0%)	1.07	5/2776 (0.2%)
5	1	0.52	0/485	0.91	0/664
5	3	0.48	0/485	0.76	0/664
5	5	0.47	0/485	0.70	0/664
5	7	0.46	0/485	0.69	0/664
5	9	0.44	0/485	0.77	1/664 (0.2%)
5	A	0.46	0/485	0.78	0/664
5	AA	0.45	0/485	0.78	0/664
5	AC	0.43	0/485	0.72	0/664
5	AE	0.40	0/491	0.70	0/672
5	AG	0.47	0/485	0.76	0/664
5	AI	0.46	0/485	0.77	0/664
5	AK	0.52	0/485	0.76	0/664
5	D	0.47	0/485	0.83	0/664
5	F	0.42	0/485	0.76	1/664 (0.2%)
5	I	0.45	0/485	0.74	0/664
5	K	0.42	0/485	0.76	0/664
5	O	0.45	0/485	0.77	1/664 (0.2%)
5	Q	0.48	0/485	0.80	1/664 (0.2%)
5	S	0.47	0/491	0.74	0/672
5	U	0.51	0/485	0.81	1/664 (0.2%)
5	W	0.54	0/485	0.84	0/664
5	Y	0.55	0/485	0.83	0/664
5	d	0.48	0/485	0.77	0/664
5	f	0.55	0/485	0.84	0/664

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	h	0.50	0/485	0.83	1/664 (0.2%)
5	j	0.46	0/485	0.72	0/664
5	l	0.44	0/485	0.74	0/664
5	m	0.42	0/485	0.75	0/664
5	p	0.49	0/485	0.81	1/664 (0.2%)
5	r	0.47	0/485	0.74	0/664
5	u	0.44	0/485	0.73	0/664
5	w	0.41	0/485	0.77	0/664
6	0	0.42	0/350	0.72	1/476 (0.2%)
6	2	0.52	0/350	0.67	0/476
6	4	0.46	0/350	0.73	0/476
6	6	0.47	0/350	0.71	0/476
6	8	0.43	0/350	0.62	0/476
6	AB	0.43	0/350	0.75	1/476 (0.2%)
6	AD	0.44	0/350	0.61	0/476
6	AF	0.44	0/350	0.60	0/476
6	AH	0.39	0/350	0.62	0/476
6	AJ	0.46	0/350	0.68	0/476
6	AL	0.48	0/350	0.70	0/476
6	B	0.41	0/350	0.75	0/476
6	E	0.43	0/350	0.72	0/476
6	G	0.48	0/350	0.73	1/476 (0.2%)
6	J	0.43	0/350	0.69	0/476
6	N	0.41	0/350	0.63	0/476
6	P	0.44	0/350	0.66	0/476
6	R	0.40	0/350	0.66	0/476
6	T	0.47	0/350	0.70	1/476 (0.2%)
6	V	0.43	0/350	0.64	0/476
6	X	0.47	0/350	0.83	1/476 (0.2%)
6	Z	0.45	0/350	0.65	0/476
6	c	0.43	0/350	0.67	0/476
6	e	0.50	0/350	0.63	0/476
6	g	0.43	0/350	0.67	1/476 (0.2%)
6	i	0.43	0/350	0.66	0/476
6	k	0.42	0/350	0.61	1/476 (0.2%)
6	n	0.51	0/350	0.72	0/476
6	q	0.49	0/350	0.74	0/476
6	s	0.46	0/350	0.69	0/476
6	v	0.44	0/350	0.71	0/476
6	z	0.40	0/350	0.70	0/476
All	All	0.60	6/45790 (0.0%)	0.88	61/62526 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
3	M	0	1
3	y	0	2
4	t	0	1
6	AJ	0	2
6	X	0	1
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	o	247	CYS	CB-SG	-6.19	1.71	1.82
2	L	256	CYS	CB-SG	-6.14	1.71	1.82
4	H	123	CYS	CB-SG	-5.82	1.72	1.81
1	C	155	CYS	CB-SG	-5.78	1.72	1.81
2	x	264	TRP	CB-CG	-5.42	1.40	1.50
4	t	123	CYS	CB-SG	-5.07	1.73	1.81

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	o	247	CYS	CA-CB-SG	-8.94	97.92	114.00
2	L	276	LEU	CB-CG-CD2	-8.58	96.41	111.00
2	x	276	LEU	CB-CG-CD2	-7.94	97.50	111.00
1	C	247	CYS	CA-CB-SG	-7.75	100.06	114.00
1	o	47	ARG	NE-CZ-NH1	7.18	123.89	120.30
6	0	8	GLY	N-CA-C	6.75	129.99	113.10
1	o	252	ASN	N-CA-C	-6.72	92.84	111.00
1	C	318	LEU	CA-CB-CG	6.71	130.73	115.30
4	t	29	TYR	CA-CB-CG	6.52	125.79	113.40
4	t	29	TYR	CB-CG-CD2	-6.51	117.09	121.00
3	M	183	LEU	CB-CG-CD2	-6.46	100.01	111.00
4	H	159	LEU	CB-CG-CD1	6.43	121.92	111.00
4	t	108	LEU	CA-CB-CG	-6.42	100.53	115.30
2	x	174	LEU	CA-CB-CG	6.29	129.77	115.30
2	L	174	LEU	CA-CB-CG	6.09	129.31	115.30
1	o	291	LEU	CA-CB-CG	-5.97	101.57	115.30
1	C	29	GLY	N-CA-C	-5.91	98.31	113.10
2	x	75	ILE	CG1-CB-CG2	-5.86	98.51	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	p	9	TYR	N-CA-C	-5.81	95.30	111.00
2	x	261	GLY	N-CA-C	-5.80	98.59	113.10
4	H	185	GLU	N-CA-C	-5.77	95.42	111.00
1	o	186	GLY	N-CA-C	-5.73	98.77	113.10
6	g	46	LEU	CA-CB-CG	5.73	128.48	115.30
5	h	8	LEU	CA-CB-CG	5.67	128.35	115.30
4	t	159	LEU	CB-CG-CD1	5.67	120.64	111.00
5	U	40	LEU	CA-CB-CG	5.65	128.30	115.30
4	H	71	HIS	N-CA-C	5.65	126.25	111.00
6	AB	38	LEU	CA-CB-CG	5.60	128.18	115.30
3	y	95	LEU	CA-CB-CG	5.58	128.12	115.30
4	H	256	GLY	N-CA-C	-5.56	99.20	113.10
4	H	38	GLY	N-CA-C	5.53	126.92	113.10
6	X	37	LEU	CA-CB-CG	5.51	127.96	115.30
2	x	84	LEU	CA-CB-CG	5.48	127.91	115.30
2	x	278	LEU	CB-CG-CD1	-5.43	101.77	111.00
5	O	59	GLY	N-CA-C	5.43	126.67	113.10
1	o	85	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	C	252	ASN	N-CA-C	-5.39	96.45	111.00
2	L	196	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	C	169	ASP	N-CA-CB	-5.32	101.03	110.60
2	x	196	LEU	CB-CG-CD1	-5.31	101.98	111.00
5	9	8	LEU	CA-CB-CG	5.30	127.49	115.30
4	t	30	LEU	CA-CB-CG	5.28	127.45	115.30
6	k	9	LEU	CA-CB-CG	5.26	127.40	115.30
2	x	263	PHE	CB-CG-CD2	-5.25	117.12	120.80
3	M	238	ILE	CG1-CB-CG2	-5.25	99.86	111.40
2	x	160	LEU	CA-CB-CG	-5.23	103.27	115.30
6	T	38	LEU	CA-CB-CG	5.23	127.32	115.30
1	o	236	MET	CA-CB-CG	-5.23	104.41	113.30
4	H	29	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	o	65	ALA	N-CA-C	-5.22	96.91	111.00
1	o	200	LEU	CB-CG-CD2	-5.21	102.14	111.00
3	M	49	GLY	C-N-CD	-5.15	109.28	120.60
5	F	44	LEU	CA-CB-CG	5.12	127.07	115.30
2	x	65	LEU	CA-CB-CG	5.12	127.07	115.30
6	G	9	LEU	CA-CB-CG	5.09	127.00	115.30
1	C	169	ASP	CB-CG-OD1	5.07	122.86	118.30
5	Q	15	LEU	CA-CB-CG	5.06	126.94	115.30
3	y	49	GLY	C-N-CD	-5.05	109.48	120.60
3	M	250	LEU	CA-CB-CG	5.05	126.91	115.30
3	y	30	ARG	N-CA-C	-5.04	97.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	233	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AJ	13	GLU	Peptide
6	AJ	14	ALA	Peptide
1	C	188	LYS	Mainchain
3	M	265	ILE	Mainchain
6	X	14	ALA	Peptide
4	t	29	TYR	Sidechain
3	y	215	LEU	Mainchain
3	y	272	CYS	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	C	315/333 (95%)	274 (87%)	33 (10%)	8 (2%)	5 27
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	5 27
2	L	278/281 (99%)	248 (89%)	26 (9%)	4 (1%)	11 38
2	x	278/281 (99%)	247 (89%)	28 (10%)	3 (1%)	14 45
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	12 40
3	y	316/319 (99%)	286 (90%)	26 (8%)	4 (1%)	12 40
4	H	256/259 (99%)	216 (84%)	31 (12%)	9 (4%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	t	256/259 (99%)	214 (84%)	32 (12%)	10 (4%)	3	18
5	1	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3	22
5	3	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	8
5	5	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	7	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	9	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1	5
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	AA	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	AC	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	8
5	AE	59/61 (97%)	49 (83%)	7 (12%)	3 (5%)	2	13
5	AG	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	22
5	AI	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	AK	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	D	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
5	F	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	13
5	I	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	K	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	35
5	O	58/61 (95%)	46 (79%)	8 (14%)	4 (7%)	1	8
5	Q	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	8
5	S	59/61 (97%)	49 (83%)	8 (14%)	2 (3%)	3	22
5	U	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	W	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
5	Y	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	13
5	d	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	22
5	f	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	8
5	h	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	22
5	j	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	22
5	l	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	m	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	35
5	p	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	r	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	u	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	w	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
6	0	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	2	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	4	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	6	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	8	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AB	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	37 (97%)	0	1 (3%)	5	27
6	AJ	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AL	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	E	38/47 (81%)	38 (100%)	0	0	100	100
6	G	38/47 (81%)	38 (100%)	0	0	100	100
6	J	38/47 (81%)	38 (100%)	0	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	P	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	Z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	38 (100%)	0	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	s	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	v	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4783 (88%)	483 (9%)	138 (3%)	5	27

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASP
1	C	195	LEU
2	L	262	PRO
4	H	142	PHE
4	H	250	ALA
5	A	10	LYS
5	A	60	LYS
5	F	3	THR
5	F	5	ASN
5	O	5	ASN
5	O	59	GLY
5	Y	60	LYS
5	3	5	ASN
6	0	8	GLY
1	o	21	LEU
1	o	66	ASP
1	o	195	LEU
2	x	262	PRO
4	t	5	ILE
4	t	142	PHE
4	t	250	ALA
5	m	10	LYS
5	p	57	ALA
5	p	60	LYS
5	r	3	THR
5	r	6	ALA
5	r	60	LYS
5	AA	5	ASN
5	AA	6	ALA
5	AC	4	MET
5	AC	49	ASP
5	AK	60	LYS
5	d	58	LEU

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Mol	Chain	Res	Type
5	f	5	ASN
1	C	21	LEU
1	C	83	LYS
1	C	84	ASP
2	L	21	ASP
4	H	5	ILE
4	H	38	GLY
4	H	188	ALA
5	F	10	LYS
5	I	10	LYS
5	K	10	LYS
5	O	6	ALA
5	O	10	LYS
5	Q	6	ALA
5	Q	10	LYS
5	S	10	LYS
5	S	58	LEU
5	U	10	LYS
5	U	54	SER
5	W	5	ASN
5	1	10	LYS
5	1	58	LEU
5	3	6	ALA
5	5	10	LYS
5	7	10	LYS
5	7	60	LYS
5	9	10	LYS
5	9	59	GLY
1	o	83	LYS
1	o	84	ASP
2	x	21	ASP
4	t	38	GLY
4	t	140	LYS
4	t	188	ALA
5	r	10	LYS
5	r	59	GLY
5	u	10	LYS
5	w	10	LYS
5	AA	10	LYS
5	AC	6	ALA
5	AC	10	LYS
5	AE	6	ALA

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Mol	Chain	Res	Type
5	AE	59	GLY
5	AG	6	ALA
5	AG	10	LYS
5	AI	10	LYS
5	AK	10	LYS
5	d	10	LYS
5	f	59	GLY
5	h	10	LYS
5	l	10	LYS
3	M	3	GLU
3	M	29	PRO
4	H	140	LYS
4	H	177	PRO
5	D	5	ASN
5	I	6	ALA
5	Y	59	GLY
5	5	8	LEU
5	9	4	MET
5	9	6	ALA
3	y	3	GLU
3	y	29	PRO
3	y	34	PRO
4	t	177	PRO
5	u	5	ASN
5	AE	10	LYS
5	f	10	LYS
5	j	6	ALA
5	l	4	MET
1	C	67	SER
1	C	253	THR
3	M	34	PRO
3	M	276	THR
5	U	59	GLY
5	3	10	LYS
5	7	6	ALA
5	j	3	THR
1	C	184	ASN
5	I	59	GLY
5	Y	10	LYS
5	3	56	GLN
1	o	67	SER
1	o	184	ASN

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Mol	Chain	Res	Type
1	o	253	THR
3	y	276	THR
5	f	6	ALA
5	h	60	LYS
5	l	59	GLY
4	H	213	ALA
6	B	8	GLY
5	Q	4	MET
5	9	5	ASN
4	t	213	ALA
5	u	6	ALA
5	AI	6	ALA
2	L	32	VAL
2	x	32	VAL
5	Q	59	GLY
4	t	227	ASN
6	AH	8	GLY
2	L	141	VAL
6	N	8	GLY
4	H	227	ASN
4	t	59	PRO

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	C	265/278 (95%)	247 (93%)	18 (7%)	16	44
1	o	265/278 (95%)	245 (92%)	20 (8%)	13	39
2	L	228/229 (100%)	215 (94%)	13 (6%)	20	51
2	x	228/229 (100%)	215 (94%)	13 (6%)	20	51
3	M	256/257 (100%)	244 (95%)	12 (5%)	26	57
3	y	256/257 (100%)	240 (94%)	16 (6%)	18	47
4	H	210/211 (100%)	198 (94%)	12 (6%)	20	51
4	t	210/211 (100%)	194 (92%)	16 (8%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	3	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	5	52/56 (93%)	52 (100%)	0	100	100
5	7	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	9	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	A	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	AA	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	AC	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	AE	53/56 (95%)	52 (98%)	1 (2%)	57	77
5	AG	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	D	52/56 (93%)	52 (100%)	0	100	100
5	F	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	I	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	Q	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	S	53/56 (95%)	51 (96%)	2 (4%)	33	62
5	U	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	W	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	Y	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	d	52/56 (93%)	52 (100%)	0	100	100
5	f	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	h	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	j	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	l	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	m	52/56 (93%)	52 (100%)	0	100	100
5	p	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	r	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	u	52/56 (93%)	50 (96%)	2 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	w	52/56 (93%)	51 (98%)	1 (2%)	57	77
6	0	33/39 (85%)	33 (100%)	0	100	100
6	2	33/39 (85%)	33 (100%)	0	100	100
6	4	33/39 (85%)	33 (100%)	0	100	100
6	6	33/39 (85%)	33 (100%)	0	100	100
6	8	33/39 (85%)	33 (100%)	0	100	100
6	AB	33/39 (85%)	33 (100%)	0	100	100
6	AD	33/39 (85%)	33 (100%)	0	100	100
6	AF	33/39 (85%)	33 (100%)	0	100	100
6	AH	33/39 (85%)	33 (100%)	0	100	100
6	AJ	33/39 (85%)	32 (97%)	1 (3%)	41	68
6	AL	33/39 (85%)	33 (100%)	0	100	100
6	B	33/39 (85%)	31 (94%)	2 (6%)	18	48
6	E	33/39 (85%)	32 (97%)	1 (3%)	41	68
6	G	33/39 (85%)	33 (100%)	0	100	100
6	J	33/39 (85%)	33 (100%)	0	100	100
6	N	33/39 (85%)	33 (100%)	0	100	100
6	P	33/39 (85%)	32 (97%)	1 (3%)	41	68
6	R	33/39 (85%)	33 (100%)	0	100	100
6	T	33/39 (85%)	33 (100%)	0	100	100
6	V	33/39 (85%)	33 (100%)	0	100	100
6	X	33/39 (85%)	32 (97%)	1 (3%)	41	68
6	Z	33/39 (85%)	33 (100%)	0	100	100
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	33 (100%)	0	100	100
6	g	33/39 (85%)	33 (100%)	0	100	100
6	i	33/39 (85%)	33 (100%)	0	100	100
6	k	33/39 (85%)	33 (100%)	0	100	100
6	n	33/39 (85%)	33 (100%)	0	100	100
6	q	33/39 (85%)	33 (100%)	0	100	100
6	s	33/39 (85%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	v	33/39 (85%)	33 (100%)	0	100	100
6	z	33/39 (85%)	33 (100%)	0	100	100
All	All	4640/4990 (93%)	4473 (96%)	167 (4%)	35	63

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

Mol	Chain	Res	Type
1	C	19	MET
1	C	21	LEU
1	C	48	GLN
1	C	74	GLU
1	C	86	SER
1	C	128	ARG
1	C	130	MET
1	C	167	VAL
1	C	173	LYS
1	C	181	THR
1	C	190	VAL
1	C	212	ILE
1	C	226	LEU
1	C	277	ARG
1	C	282	ASN
1	C	289	ASP
1	C	304	ARG
1	C	307	CYS
2	L	147	LEU
2	L	148	MET
2	L	163	LEU
2	L	172	GLN
2	L	175	HIS
2	L	176	PHE
2	L	208	ASN
2	L	210	GLN
2	L	225	PHE
2	L	248	SER
2	L	255	VAL
2	L	256	CYS
2	L	281	TRP
3	M	25	LYS
3	M	31	ILE
3	M	37	SER

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Mol	Chain	Res	Type
3	M	42	LYS
3	M	45	ASP
3	M	182	HIS
3	M	216	PHE
3	M	232	ASP
3	M	279	THR
3	M	310	VAL
3	M	311	VAL
3	M	312	THR
4	H	45	ARG
4	H	116	SER
4	H	131	PRO
4	H	140	LYS
4	H	143	SER
4	H	157	VAL
4	H	159	LEU
4	H	160	ASP
4	H	200	SER
4	H	230	GLN
4	H	258	LEU
4	H	259	LEU
5	A	53	VAL
6	B	20	ILE
6	B	21	PHE
6	E	21	PHE
5	F	48	ASP
5	I	3	THR
5	I	53	VAL
5	O	5	ASN
5	O	37	MET
6	P	21	PHE
5	Q	2	PHE
5	Q	3	THR
5	S	48	ASP
5	S	51	ILE
5	U	53	VAL
5	W	48	ASP
6	X	13	GLU
5	Y	9	TYR
5	1	51	ILE
5	1	53	VAL
5	1	55	TYR

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Mol	Chain	Res	Type
5	3	5	ASN
5	3	44	LEU
5	3	50	ASN
5	7	48	ASP
5	9	8	LEU
5	9	13	LEU
1	o	19	MET
1	o	21	LEU
1	o	47	ARG
1	o	48	GLN
1	o	68	THR
1	o	84	ASP
1	o	86	SER
1	o	128	ARG
1	o	130	MET
1	o	167	VAL
1	o	173	LYS
1	o	181	THR
1	o	190	VAL
1	o	212	ILE
1	o	221	SER
1	o	277	ARG
1	o	281	GLN
1	o	282	ASN
1	o	304	ARG
1	o	307	CYS
2	x	125	HIS
2	x	147	LEU
2	x	148	MET
2	x	163	LEU
2	x	172	GLN
2	x	175	HIS
2	x	176	PHE
2	x	208	ASN
2	x	210	GLN
2	x	225	PHE
2	x	248	SER
2	x	256	CYS
2	x	281	TRP
3	y	3	GLU
3	y	25	LYS
3	y	31	ILE

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Mol	Chain	Res	Type
3	y	33	ARG
3	y	37	SER
3	y	42	LYS
3	y	45	ASP
3	y	182	HIS
3	y	216	PHE
3	y	232	ASP
3	y	235	ILE
3	y	279	THR
3	y	285	LEU
3	y	310	VAL
3	y	311	VAL
3	y	312	THR
4	t	45	ARG
4	t	60	ASP
4	t	81	VAL
4	t	116	SER
4	t	131	PRO
4	t	140	LYS
4	t	143	SER
4	t	157	VAL
4	t	159	LEU
4	t	160	ASP
4	t	166	THR
4	t	177	PRO
4	t	200	SER
4	t	230	GLN
4	t	258	LEU
4	t	259	LEU
5	p	9	TYR
5	r	37	MET
5	u	3	THR
5	u	53	VAL
5	w	5	ASN
5	AA	5	ASN
5	AA	43	ASP
5	AA	44	LEU
5	AC	2	PHE
5	AC	3	THR
5	AE	8	LEU
5	AG	2	PHE
5	AG	51	ILE

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Mol	Chain	Res	Type
6	AJ	13	GLU
5	AK	48	ASP
5	f	3	THR
5	h	14	ILE
5	j	48	ASP
5	l	8	LEU
5	l	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	238	ASN
2	L	208	ASN
3	M	240	HIS
4	H	122	HIS
4	H	189	ASN
4	H	218	HIS
5	A	50	ASN
5	K	56	GLN
5	Y	36	HIS
6	2	23	GLN
1	o	183	GLN
2	x	125	HIS
4	t	221	ASN
5	m	7	ASN
5	m	50	ASN
5	r	56	GLN
5	f	5	ASN
5	f	50	ASN
5	l	56	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 184 ligands modelled in this entry, 40 are monoatomic - leaving 144 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	$\#\|Z\| > 2$
15	CRT	G	101	-	41,43,43	0.71	0	50,54,54	3.76	15 (30%)
14	MQ8	M	404	-	54,54,54	1.01	5 (9%)	66,69,69	1.51	11 (16%)
14	MQ8	y	403	-	54,54,54	1.07	5 (9%)	66,69,69	1.62	17 (25%)
15	CRT	T	101	-	41,43,43	0.72	0	50,54,54	3.90	13 (26%)
12	PEF	M	407	-	15,15,46	1.06	1 (6%)	17,19,51	1.12	1 (5%)
7	HEM	o	502	1	41,50,50	1.90	7 (17%)	45,82,82	2.15	12 (26%)
12	PEF	H	304	-	18,18,46	1.62	2 (11%)	21,23,51	1.56	2 (9%)
12	PEF	x	306	-	18,18,46	1.72	2 (11%)	21,23,51	1.32	3 (14%)
12	PEF	m	101	-	18,18,46	1.53	2 (11%)	21,23,51	1.59	3 (14%)
9	BCL	AH	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.26	24 (30%)
15	CRT	P	102	-	41,43,43	0.70	0	50,54,54	1.77	13 (26%)
15	CRT	AF	102	-	41,43,43	0.74	0	50,54,54	3.67	14 (28%)
15	CRT	AD	101	-	41,43,43	0.82	0	50,54,54	3.60	19 (38%)
9	BCL	x	305	-	64,74,74	1.92	15 (23%)	78,115,115	2.47	28 (35%)
9	BCL	k	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.39	28 (35%)
9	BCL	p	102	-	64,74,74	1.66	13 (20%)	78,115,115	2.34	26 (33%)
9	BCL	I	103	-	64,74,74	1.73	12 (18%)	78,115,115	2.29	25 (32%)
15	CRT	2	101	-	41,43,43	0.80	0	50,54,54	1.66	14 (28%)
15	CRT	9	101	-	41,43,43	0.75	0	50,54,54	3.59	18 (36%)
15	CRT	0	101	-	41,43,43	0.80	0	50,54,54	3.66	22 (44%)
9	BCL	i	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.30	31 (39%)
15	CRT	g	101	-	41,43,43	0.81	0	50,54,54	3.86	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	F	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.27	26 (33%)
9	BCL	G	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.24	24 (30%)
15	CRT	AH	102	-	41,43,43	0.76	0	50,54,54	3.42	14 (28%)
12	PEF	L	305	-	10,11,46	0.74	0	11,14,51	1.21	1 (9%)
9	BCL	3	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.30	24 (30%)
9	BCL	2	102	-	64,74,74	1.73	12 (18%)	78,115,115	2.28	28 (35%)
9	BCL	N	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.32	25 (32%)
7	HEM	o	503	1	41,50,50	1.98	9 (21%)	45,82,82	2.11	16 (35%)
9	BCL	u	101	-	64,74,74	1.66	11 (17%)	78,115,115	2.30	28 (35%)
15	CRT	V	101	-	41,43,43	0.77	0	50,54,54	3.43	16 (32%)
15	CRT	k	101	-	41,43,43	0.76	0	50,54,54	3.71	15 (30%)
9	BCL	O	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.37	31 (39%)
10	BPH	y	402	-	51,70,70	0.76	2 (3%)	52,101,101	1.51	7 (13%)
9	BCL	f	101	-	64,74,74	1.78	12 (18%)	78,115,115	2.35	25 (32%)
11	UQ8	L	304	-	53,53,53	1.50	4 (7%)	64,67,67	1.73	16 (25%)
9	BCL	9	102	-	64,74,74	1.70	12 (18%)	78,115,115	2.19	21 (26%)
9	BCL	I	101	-	64,74,74	1.78	12 (18%)	78,115,115	2.31	29 (37%)
9	BCL	g	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.32	28 (35%)
17	PGW	AE	101	-	20,20,50	0.97	1 (5%)	23,26,56	1.34	2 (8%)
9	BCL	q	102	-	64,74,74	1.70	12 (18%)	78,115,115	2.32	26 (33%)
9	BCL	AI	102	-	64,74,74	1.65	10 (15%)	78,115,115	2.31	25 (32%)
9	BCL	1	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.24	22 (28%)
9	BCL	AC	103	-	64,74,74	1.64	12 (18%)	78,115,115	2.31	27 (34%)
9	BCL	Q	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.26	27 (34%)
16	PO4	t	302	-	4,4,4	0.87	0	6,6,6	1.03	0
11	UQ8	x	304	-	53,53,53	1.54	4 (7%)	64,67,67	1.99	20 (31%)
15	CRT	AL	101	-	41,43,43	0.80	0	50,54,54	1.75	13 (26%)
9	BCL	L	301	-	64,74,74	1.71	13 (20%)	78,115,115	2.41	36 (46%)
9	BCL	AC	102	-	64,74,74	1.76	13 (20%)	78,115,115	2.29	30 (38%)
15	CRT	M	405	-	41,43,43	0.77	0	50,54,54	3.91	14 (28%)
12	PEF	p	101	-	15,15,46	0.92	1 (6%)	17,19,51	0.96	1 (5%)
9	BCL	AE	102	-	64,74,74	1.66	11 (17%)	78,115,115	2.29	28 (35%)
17	PGW	S	101	-	20,20,50	1.02	1 (5%)	23,26,56	1.28	1 (4%)
9	BCL	AB	101	-	64,74,74	1.69	10 (15%)	78,115,115	2.25	26 (33%)
9	BCL	AG	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.38	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	AL	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.21	27 (34%)
15	CRT	q	101	-	41,43,43	0.74	0	50,54,54	3.69	13 (26%)
7	HEM	C	502	1	41,50,50	1.93	8 (19%)	45,82,82	2.26	11 (24%)
9	BCL	j	101	-	64,74,74	1.70	11 (17%)	78,115,115	2.24	25 (32%)
15	CRT	v	101	-	41,43,43	0.76	0	50,54,54	3.75	18 (36%)
9	BCL	A	102	-	64,74,74	1.74	9 (14%)	78,115,115	2.21	24 (30%)
9	BCL	y	401	-	64,74,74	1.73	12 (18%)	78,115,115	2.35	30 (38%)
9	BCL	z	102	-	64,74,74	1.67	10 (15%)	78,115,115	2.24	27 (34%)
12	PEF	H	302	-	18,18,46	1.53	2 (11%)	21,23,51	1.77	2 (9%)
15	CRT	y	404	-	41,43,43	0.87	1 (2%)	50,54,54	3.59	13 (26%)
9	BCL	l	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.35	29 (37%)
7	HEM	C	504	1	41,50,50	1.96	8 (19%)	45,82,82	1.78	10 (22%)
9	BCL	S	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.32	26 (33%)
9	BCL	h	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.23	29 (37%)
15	CRT	E	101	-	41,43,43	0.82	0	50,54,54	3.29	14 (28%)
9	BCL	M	401	-	64,74,74	1.68	12 (18%)	78,115,115	2.42	25 (32%)
9	BCL	6	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.35	29 (37%)
15	CRT	I	102	-	41,43,43	0.76	0	50,54,54	3.67	14 (28%)
9	BCL	w	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.33	30 (38%)
9	BCL	x	301	-	64,74,74	1.72	12 (18%)	78,115,115	2.49	28 (35%)
9	BCL	X	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.37	30 (38%)
12	PEF	t	301	-	18,18,46	1.57	2 (11%)	21,23,51	1.27	2 (9%)
9	BCL	m	102	-	64,74,74	1.76	12 (18%)	78,115,115	2.25	24 (30%)
9	BCL	AB	102	-	64,74,74	1.74	14 (21%)	78,115,115	2.25	30 (38%)
9	BCL	P	101	-	64,74,74	1.74	14 (21%)	78,115,115	2.29	28 (35%)
9	BCL	e	102	-	64,74,74	1.64	11 (17%)	78,115,115	2.25	28 (35%)
15	CRT	n	101	-	41,43,43	0.78	0	50,54,54	3.99	20 (40%)
7	HEM	o	504	1	41,50,50	1.94	8 (19%)	45,82,82	1.84	11 (24%)
12	PEF	y	407	-	18,18,46	1.64	2 (11%)	21,23,51	1.24	3 (14%)
7	HEM	C	501	1	41,50,50	2.07	10 (24%)	45,82,82	2.64	18 (40%)
9	BCL	AI	101	-	64,74,74	1.70	11 (17%)	78,115,115	2.33	28 (35%)
9	BCL	L	303	-	64,74,74	1.71	13 (20%)	78,115,115	2.32	25 (32%)
9	BCL	U	101	-	64,74,74	1.75	12 (18%)	78,115,115	2.25	26 (33%)
7	HEM	C	503	1	41,50,50	1.95	4 (9%)	45,82,82	2.03	14 (31%)
9	BCL	s	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.42	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CRT	R	101	-	41,43,43	0.81	0	50,54,54	3.44	15 (30%)
12	PEF	M	408	-	18,18,46	1.75	2 (11%)	21,23,51	1.58	2 (9%)
15	CRT	m	104	-	41,43,43	0.73	0	50,54,54	3.51	20 (40%)
15	CRT	z	101	-	41,43,43	0.76	0	50,54,54	3.72	19 (38%)
9	BCL	r	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.21	27 (34%)
9	BCL	Z	102	-	64,74,74	1.65	10 (15%)	78,115,115	2.43	30 (38%)
9	BCL	c	101	-	64,74,74	1.65	10 (15%)	78,115,115	2.26	25 (32%)
9	BCL	4	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.39	26 (33%)
9	BCL	m	103	-	64,74,74	1.66	12 (18%)	78,115,115	2.21	28 (35%)
9	BCL	D	102	-	64,74,74	1.66	9 (14%)	78,115,115	2.34	31 (39%)
12	PEF	A	101	-	18,18,46	1.43	2 (11%)	21,23,51	1.91	4 (19%)
15	CRT	7	101	-	41,43,43	0.79	0	50,54,54	3.53	17 (34%)
9	BCL	0	102	-	64,74,74	1.76	13 (20%)	78,115,115	2.26	28 (35%)
15	CRT	e	101	-	41,43,43	0.77	0	50,54,54	1.80	14 (28%)
16	PO4	y	405	-	4,4,4	0.74	0	6,6,6	1.10	0
15	CRT	X	101	-	41,43,43	0.90	0	50,54,54	1.79	11 (22%)
12	PEF	H	301	-	18,18,46	1.43	2 (11%)	21,23,51	1.61	3 (14%)
9	BCL	R	102	-	64,74,74	1.73	15 (23%)	78,115,115	2.42	31 (39%)
9	BCL	M	402	-	64,74,74	1.73	12 (18%)	78,115,115	2.47	31 (39%)
12	PEF	t	303	-	18,18,46	1.43	2 (11%)	21,23,51	2.20	7 (33%)
9	BCL	Y	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.31	26 (33%)
9	BCL	T	102	-	64,74,74	1.71	13 (20%)	78,115,115	2.43	32 (41%)
9	BCL	d	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.28	26 (33%)
7	HEM	o	501	1	41,50,50	2.01	7 (17%)	45,82,82	2.22	16 (35%)
9	BCL	V	102	-	64,74,74	1.71	11 (17%)	78,115,115	2.34	30 (38%)
15	CRT	s	101	-	41,43,43	0.79	0	50,54,54	3.29	17 (34%)
12	PEF	y	408	-	18,18,46	1.70	2 (11%)	21,23,51	2.35	6 (28%)
15	CRT	4	101	-	41,43,43	0.84	0	50,54,54	4.08	21 (42%)
9	BCL	7	102	-	64,74,74	1.62	13 (20%)	78,115,115	2.22	28 (35%)
16	PO4	M	406	-	4,4,4	0.49	0	6,6,6	1.02	0
15	CRT	AJ	101	-	41,43,43	0.78	0	50,54,54	1.97	14 (28%)
15	CRT	Z	101	-	41,43,43	0.86	0	50,54,54	1.92	17 (34%)
9	BCL	A	103	-	64,74,74	1.73	13 (20%)	78,115,115	2.31	29 (37%)
10	BPH	L	302	-	51,70,70	0.40	0	52,101,101	1.92	11 (21%)
9	BCL	K	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.29	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
15	CRT	O	101	-	41,43,43	0.74	0	50,54,54	3.86	17 (34%)
9	BCL	W	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.19	26 (33%)
10	BPH	M	403	-	51,70,70	0.59	0	52,101,101	1.73	7 (13%)
9	BCL	u	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.35	26 (33%)
9	BCL	x	303	-	64,74,74	1.88	14 (21%)	78,115,115	2.29	27 (34%)
15	CRT	AC	101	-	41,43,43	0.80	0	50,54,54	2.04	16 (32%)
12	PEF	H	305	-	18,18,46	1.45	2 (11%)	21,23,51	1.51	3 (14%)
9	BCL	8	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.34	24 (30%)
9	BCL	5	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.30	26 (33%)
9	BCL	AK	101	-	64,74,74	1.68	10 (15%)	78,115,115	2.27	27 (34%)
12	PEF	y	406	-	18,18,46	1.52	2 (11%)	21,23,51	2.04	4 (19%)
9	BCL	D	101	-	64,74,74	1.70	11 (17%)	78,115,115	2.32	24 (30%)
10	BPH	x	302	-	51,70,70	0.63	1 (1%)	52,101,101	1.79	12 (23%)
15	CRT	7	103	-	41,43,43	0.95	1 (2%)	50,54,54	3.62	11 (22%)
9	BCL	AF	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.22	28 (35%)
15	CRT	i	101	-	41,43,43	0.77	0	50,54,54	3.47	16 (32%)
16	PO4	H	303	-	4,4,4	0.62	0	6,6,6	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	G	101	-	-	12/51/51/51	-
14	MQ8	M	404	-	-	20/47/67/67	0/2/2/2
14	MQ8	y	403	-	-	24/47/67/67	0/2/2/2
15	CRT	T	101	-	-	6/51/51/51	-
12	PEF	M	407	-	-	4/16/16/50	-
7	HEM	o	502	1	-	4/12/54/54	-
12	PEF	H	304	-	-	13/20/20/50	-
12	PEF	x	306	-	-	10/20/20/50	-
12	PEF	m	101	-	-	9/20/20/50	-
9	BCL	AH	101	-	-	21/37/137/137	-
15	CRT	P	102	-	-	7/51/51/51	-
15	CRT	AF	102	-	-	5/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AD	101	-	-	8/51/51/51	-
9	BCL	x	305	-	-	13/37/137/137	-
9	BCL	k	102	-	-	21/37/137/137	-
9	BCL	p	102	-	-	12/37/137/137	-
9	BCL	I	103	-	-	13/37/137/137	-
15	CRT	2	101	-	-	4/51/51/51	-
15	CRT	9	101	-	-	12/51/51/51	-
15	CRT	0	101	-	-	9/51/51/51	-
9	BCL	i	102	-	-	19/37/137/137	-
15	CRT	g	101	-	-	5/51/51/51	-
9	BCL	F	101	-	-	18/37/137/137	-
9	BCL	G	102	-	-	16/37/137/137	-
15	CRT	AH	102	-	-	12/51/51/51	-
12	PEF	L	305	-	-	5/11/11/50	-
9	BCL	3	101	-	-	14/37/137/137	-
9	BCL	2	102	-	-	13/37/137/137	-
9	BCL	N	101	-	-	15/37/137/137	-
7	HEM	o	503	1	-	5/12/54/54	-
9	BCL	u	101	-	-	21/37/137/137	-
15	CRT	V	101	-	-	16/51/51/51	-
15	CRT	k	101	-	-	8/51/51/51	-
9	BCL	O	102	-	-	15/37/137/137	-
10	BPH	y	402	-	-	15/37/105/105	0/5/6/6
9	BCL	f	101	-	-	16/37/137/137	-
11	UQ8	L	304	-	-	10/51/75/75	0/1/1/1
9	BCL	9	102	-	-	11/37/137/137	-
9	BCL	I	101	-	-	9/37/137/137	-
9	BCL	g	102	-	-	17/37/137/137	-
17	PGW	AE	101	-	-	12/23/23/55	-
9	BCL	q	102	-	-	18/37/137/137	-
9	BCL	AI	102	-	-	17/37/137/137	-
9	BCL	1	101	-	-	16/37/137/137	-
9	BCL	AC	103	-	-	16/37/137/137	-
9	BCL	Q	101	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	UQ8	x	304	-	-	15/51/75/75	0/1/1/1
15	CRT	AL	101	-	-	10/51/51/51	-
9	BCL	L	301	-	-	11/37/137/137	-
9	BCL	AC	102	-	-	24/37/137/137	-
15	CRT	M	405	-	-	13/51/51/51	-
12	PEF	p	101	-	-	3/16/16/50	-
9	BCL	AE	102	-	-	14/37/137/137	-
17	PGW	S	101	-	-	12/23/23/55	-
9	BCL	AB	101	-	-	14/37/137/137	-
9	BCL	AG	101	-	-	19/37/137/137	-
9	BCL	AL	102	-	-	16/37/137/137	-
15	CRT	q	101	-	-	7/51/51/51	-
7	HEM	C	502	1	-	6/12/54/54	-
9	BCL	j	101	-	-	20/37/137/137	-
15	CRT	v	101	-	-	7/51/51/51	-
9	BCL	A	102	-	-	13/37/137/137	-
9	BCL	y	401	-	-	13/37/137/137	-
9	BCL	z	102	-	-	18/37/137/137	-
12	PEF	H	302	-	-	8/20/20/50	-
15	CRT	y	404	-	-	14/51/51/51	-
9	BCL	l	101	-	-	16/37/137/137	-
7	HEM	C	504	1	-	5/12/54/54	-
9	BCL	S	102	-	-	15/37/137/137	-
9	BCL	h	101	-	-	8/37/137/137	-
15	CRT	E	101	-	-	9/51/51/51	-
9	BCL	M	401	-	-	15/37/137/137	-
9	BCL	6	101	-	-	13/37/137/137	-
15	CRT	I	102	-	-	7/51/51/51	-
9	BCL	w	101	-	-	14/37/137/137	-
9	BCL	x	301	-	-	12/37/137/137	-
9	BCL	X	102	-	-	22/37/137/137	-
12	PEF	t	301	-	-	6/20/20/50	-
9	BCL	m	102	-	-	13/37/137/137	-
9	BCL	AB	102	-	-	16/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	P	101	-	-	13/37/137/137	-
9	BCL	e	102	-	-	15/37/137/137	-
15	CRT	n	101	-	-	14/51/51/51	-
7	HEM	o	504	1	-	3/12/54/54	-
12	PEF	y	407	-	-	6/20/20/50	-
7	HEM	C	501	1	-	6/12/54/54	-
9	BCL	AI	101	-	-	14/37/137/137	-
9	BCL	L	303	-	-	18/37/137/137	-
9	BCL	U	101	-	-	17/37/137/137	-
7	HEM	C	503	1	-	3/12/54/54	-
9	BCL	s	102	-	-	16/37/137/137	-
15	CRT	R	101	-	-	15/51/51/51	-
12	PEF	M	408	-	-	11/20/20/50	-
15	CRT	m	104	-	-	3/51/51/51	-
15	CRT	z	101	-	-	2/51/51/51	-
9	BCL	r	101	-	-	18/37/137/137	-
9	BCL	Z	102	-	-	14/37/137/137	-
9	BCL	c	101	-	-	18/37/137/137	-
9	BCL	4	102	-	-	16/37/137/137	-
9	BCL	m	103	-	-	18/37/137/137	-
9	BCL	D	102	-	-	15/37/137/137	-
12	PEF	A	101	-	-	8/20/20/50	-
15	CRT	7	101	-	-	8/51/51/51	-
9	BCL	0	102	-	-	17/37/137/137	-
15	CRT	e	101	-	-	13/51/51/51	-
15	CRT	X	101	-	-	14/51/51/51	-
12	PEF	H	301	-	-	8/20/20/50	-
9	BCL	R	102	-	-	17/37/137/137	-
9	BCL	M	402	-	-	15/37/137/137	-
12	PEF	t	303	-	-	9/20/20/50	-
9	BCL	Y	101	-	-	14/37/137/137	-
9	BCL	T	102	-	-	17/37/137/137	-
9	BCL	d	101	-	-	12/37/137/137	-
7	HEM	o	501	1	-	7/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	V	102	-	-	15/37/137/137	-
15	CRT	s	101	-	-	9/51/51/51	-
12	PEF	y	408	-	-	7/20/20/50	-
15	CRT	4	101	-	-	17/51/51/51	-
9	BCL	7	102	-	-	19/37/137/137	-
15	CRT	AJ	101	-	-	12/51/51/51	-
15	CRT	Z	101	-	-	9/51/51/51	-
9	BCL	A	103	-	-	12/37/137/137	-
10	BPH	L	302	-	-	18/37/105/105	0/5/6/6
9	BCL	K	101	-	-	13/37/137/137	-
15	CRT	O	101	-	-	8/51/51/51	-
9	BCL	W	101	-	-	20/37/137/137	-
10	BPH	M	403	-	-	16/37/105/105	0/5/6/6
9	BCL	u	102	-	-	10/37/137/137	-
9	BCL	x	303	-	-	17/37/137/137	-
15	CRT	AC	101	-	-	10/51/51/51	-
12	PEF	H	305	-	-	11/20/20/50	-
9	BCL	8	101	-	-	23/37/137/137	-
9	BCL	5	101	-	-	8/37/137/137	-
9	BCL	AK	101	-	-	15/37/137/137	-
12	PEF	y	406	-	-	7/20/20/50	-
9	BCL	D	101	-	-	8/37/137/137	-
10	BPH	x	302	-	-	15/37/105/105	0/5/6/6
15	CRT	7	103	-	-	6/51/51/51	-
9	BCL	AF	101	-	-	13/37/137/137	-
15	CRT	i	101	-	-	8/51/51/51	-

All (971) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	FE-NB	8.57	2.39	1.96
7	o	501	HEM	FE-NB	8.39	2.38	1.96
7	C	503	HEM	FE-NB	8.36	2.38	1.96
7	o	503	HEM	FE-NB	8.30	2.37	1.96
7	C	501	HEM	FE-NB	8.23	2.37	1.96
11	L	304	UQ8	C6-C1	8.18	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	502	HEM	FE-NB	8.18	2.37	1.96
11	x	304	UQ8	C6-C1	8.11	1.50	1.35
7	C	504	HEM	FE-NB	8.09	2.36	1.96
7	C	502	HEM	FE-NB	8.02	2.36	1.96
9	x	303	BCL	MG-ND	-7.44	1.91	2.05
9	f	101	BCL	MG-ND	-6.33	1.93	2.05
9	L	301	BCL	MG-ND	-6.20	1.93	2.05
9	S	102	BCL	MG-ND	-6.19	1.93	2.05
9	0	102	BCL	MG-ND	-6.13	1.93	2.05
9	I	101	BCL	MG-ND	-6.13	1.93	2.05
9	L	303	BCL	MG-ND	-6.11	1.93	2.05
9	M	401	BCL	MG-ND	-6.04	1.93	2.05
9	6	101	BCL	MG-ND	-6.04	1.93	2.05
9	X	102	BCL	MG-ND	-6.03	1.93	2.05
9	w	101	BCL	MG-ND	-6.02	1.93	2.05
9	2	102	BCL	MG-ND	-6.02	1.93	2.05
9	U	101	BCL	MG-ND	-6.00	1.93	2.05
9	e	102	BCL	MG-ND	-6.00	1.93	2.05
9	I	103	BCL	MG-ND	-5.99	1.93	2.05
9	s	102	BCL	MG-ND	-5.99	1.93	2.05
9	A	102	BCL	MG-ND	-5.98	1.93	2.05
9	AI	101	BCL	MG-ND	-5.95	1.94	2.05
9	A	103	BCL	MG-ND	-5.94	1.94	2.05
9	4	102	BCL	MG-ND	-5.93	1.94	2.05
9	x	305	BCL	MG-ND	-5.92	1.94	2.05
9	P	101	BCL	MG-ND	-5.91	1.94	2.05
9	y	401	BCL	MG-ND	-5.89	1.94	2.05
9	K	101	BCL	MG-ND	-5.86	1.94	2.05
9	d	101	BCL	MG-ND	-5.85	1.94	2.05
9	Z	102	BCL	MG-ND	-5.84	1.94	2.05
12	M	408	PEF	O2-C10	5.81	1.48	1.35
9	i	102	BCL	MG-ND	-5.80	1.94	2.05
9	Y	101	BCL	MG-ND	-5.80	1.94	2.05
9	g	102	BCL	MG-ND	-5.80	1.94	2.05
9	Q	101	BCL	MG-ND	-5.79	1.94	2.05
9	r	101	BCL	MG-ND	-5.78	1.94	2.05
9	AL	102	BCL	MG-ND	-5.78	1.94	2.05
9	AF	101	BCL	MG-ND	-5.77	1.94	2.05
9	AC	102	BCL	MG-ND	-5.76	1.94	2.05
9	u	102	BCL	MG-ND	-5.74	1.94	2.05
9	AK	101	BCL	MG-ND	-5.69	1.94	2.05
9	F	101	BCL	MG-ND	-5.68	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	101	BCL	MG-ND	-5.67	1.94	2.05
9	AB	101	BCL	MG-ND	-5.67	1.94	2.05
9	k	102	BCL	MG-ND	-5.65	1.94	2.05
9	O	102	BCL	MG-ND	-5.65	1.94	2.05
9	D	101	BCL	MG-ND	-5.64	1.94	2.05
9	N	101	BCL	MG-ND	-5.64	1.94	2.05
9	q	102	BCL	MG-ND	-5.64	1.94	2.05
9	p	102	BCL	MG-ND	-5.64	1.94	2.05
9	R	102	BCL	MG-ND	-5.64	1.94	2.05
9	m	102	BCL	MG-ND	-5.61	1.94	2.05
9	T	102	BCL	MG-ND	-5.60	1.94	2.05
9	9	102	BCL	MG-ND	-5.60	1.94	2.05
9	G	102	BCL	MG-ND	-5.60	1.94	2.05
9	V	102	BCL	MG-ND	-5.60	1.94	2.05
12	H	302	PEF	O2-C10	5.58	1.47	1.35
9	h	101	BCL	MG-ND	-5.58	1.94	2.05
9	M	402	BCL	MG-ND	-5.57	1.94	2.05
9	AE	102	BCL	MG-ND	-5.57	1.94	2.05
9	x	301	BCL	MG-ND	-5.54	1.94	2.05
9	AI	102	BCL	MG-ND	-5.54	1.94	2.05
12	x	306	PEF	O2-C10	5.53	1.47	1.35
9	z	102	BCL	MG-ND	-5.46	1.95	2.05
9	c	101	BCL	MG-ND	-5.43	1.95	2.05
9	AB	102	BCL	MG-ND	-5.41	1.95	2.05
12	H	304	PEF	O2-C10	5.41	1.47	1.35
9	1	101	BCL	MG-ND	-5.41	1.95	2.05
9	AG	101	BCL	MG-ND	-5.40	1.95	2.05
9	AH	101	BCL	MG-ND	-5.38	1.95	2.05
9	8	101	BCL	MG-ND	-5.35	1.95	2.05
9	l	101	BCL	MG-ND	-5.35	1.95	2.05
9	3	101	BCL	MG-ND	-5.34	1.95	2.05
12	y	408	PEF	O2-C10	5.33	1.47	1.35
9	W	101	BCL	MG-ND	-5.32	1.95	2.05
9	D	102	BCL	MG-ND	-5.31	1.95	2.05
12	y	407	PEF	O2-C10	5.30	1.47	1.35
9	m	103	BCL	MG-ND	-5.29	1.95	2.05
9	u	101	BCL	MG-ND	-5.28	1.95	2.05
12	t	301	PEF	O2-C10	5.27	1.47	1.35
9	j	101	BCL	MG-ND	-5.26	1.95	2.05
9	AC	103	BCL	MG-ND	-5.26	1.95	2.05
9	AF	101	BCL	OBD-CAD	5.22	1.31	1.22
9	Y	101	BCL	OBD-CAD	5.21	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	BCL	OBD-CAD	5.14	1.31	1.22
9	AB	101	BCL	OBD-CAD	5.12	1.31	1.22
9	x	303	BCL	C4D-ND	-5.12	1.30	1.37
9	5	101	BCL	OBD-CAD	5.10	1.31	1.22
9	7	102	BCL	MG-ND	-5.08	1.95	2.05
9	x	305	BCL	C4D-ND	-5.08	1.30	1.37
9	r	101	BCL	OBD-CAD	5.07	1.31	1.22
9	x	305	BCL	OBD-CAD	5.06	1.31	1.22
9	d	101	BCL	OBD-CAD	5.06	1.31	1.22
9	AH	101	BCL	OBD-CAD	5.02	1.31	1.22
9	AB	102	BCL	OBD-CAD	4.99	1.31	1.22
9	L	301	BCL	OBD-CAD	4.99	1.31	1.22
9	1	101	BCL	OBD-CAD	4.98	1.31	1.22
9	z	102	BCL	OBD-CAD	4.98	1.31	1.22
9	7	102	BCL	OBD-CAD	4.97	1.31	1.22
12	m	101	PEF	O2-C10	4.96	1.46	1.35
9	0	102	BCL	OBD-CAD	4.96	1.31	1.22
9	T	102	BCL	OBD-CAD	4.96	1.31	1.22
9	N	101	BCL	OBD-CAD	4.96	1.31	1.22
9	O	102	BCL	OBD-CAD	4.95	1.31	1.22
9	I	103	BCL	OBD-CAD	4.94	1.31	1.22
9	AK	101	BCL	OBD-CAD	4.93	1.31	1.22
9	I	101	BCL	OBD-CAD	4.92	1.31	1.22
9	w	101	BCL	OBD-CAD	4.92	1.31	1.22
9	G	102	BCL	OBD-CAD	4.91	1.30	1.22
9	9	102	BCL	OBD-CAD	4.88	1.30	1.22
9	g	102	BCL	OBD-CAD	4.87	1.30	1.22
9	D	102	BCL	OBD-CAD	4.87	1.30	1.22
9	AG	101	BCL	OBD-CAD	4.86	1.30	1.22
9	u	102	BCL	OBD-CAD	4.86	1.30	1.22
9	AC	102	BCL	OBD-CAD	4.86	1.30	1.22
9	AI	102	BCL	OBD-CAD	4.85	1.30	1.22
9	V	102	BCL	OBD-CAD	4.85	1.30	1.22
9	K	101	BCL	OBD-CAD	4.84	1.30	1.22
9	Q	101	BCL	OBD-CAD	4.84	1.30	1.22
9	A	103	BCL	OBD-CAD	4.84	1.30	1.22
9	3	101	BCL	OBD-CAD	4.83	1.30	1.22
9	y	401	BCL	OBD-CAD	4.83	1.30	1.22
9	AI	101	BCL	OBD-CAD	4.82	1.30	1.22
9	l	101	BCL	OBD-CAD	4.82	1.30	1.22
9	c	101	BCL	OBD-CAD	4.81	1.30	1.22
9	M	401	BCL	OBD-CAD	4.80	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	102	BCL	OBD-CAD	4.80	1.30	1.22
9	P	101	BCL	OBD-CAD	4.80	1.30	1.22
7	C	503	HEM	C3B-C4B	4.79	1.54	1.44
7	o	504	HEM	C1B-NB	-4.79	1.32	1.40
9	h	101	BCL	OBD-CAD	4.77	1.30	1.22
7	C	501	HEM	C4D-ND	-4.77	1.32	1.40
9	u	101	BCL	OBD-CAD	4.76	1.30	1.22
9	x	301	BCL	OBD-CAD	4.76	1.30	1.22
9	m	102	BCL	OBD-CAD	4.75	1.30	1.22
9	6	101	BCL	OBD-CAD	4.74	1.30	1.22
9	j	101	BCL	OBD-CAD	4.73	1.30	1.22
9	U	101	BCL	OBD-CAD	4.73	1.30	1.22
9	f	101	BCL	OBD-CAD	4.73	1.30	1.22
9	R	102	BCL	OBD-CAD	4.72	1.30	1.22
9	M	402	BCL	OBD-CAD	4.72	1.30	1.22
9	A	102	BCL	OBD-CAD	4.71	1.30	1.22
9	S	102	BCL	OBD-CAD	4.70	1.30	1.22
9	k	102	BCL	OBD-CAD	4.69	1.30	1.22
9	R	102	BCL	C4D-ND	-4.67	1.31	1.37
9	s	102	BCL	OBD-CAD	4.66	1.30	1.22
9	q	102	BCL	OBD-CAD	4.66	1.30	1.22
9	e	102	BCL	OBD-CAD	4.63	1.30	1.22
9	x	303	BCL	OBD-CAD	4.63	1.30	1.22
9	m	103	BCL	OBD-CAD	4.62	1.30	1.22
12	y	406	PEF	O2-C10	4.61	1.45	1.35
9	i	102	BCL	OBD-CAD	4.55	1.30	1.22
9	I	101	BCL	C4D-ND	-4.55	1.31	1.37
12	H	301	PEF	O2-C10	4.53	1.45	1.35
9	D	101	BCL	OBD-CAD	4.53	1.30	1.22
9	I	103	BCL	C4D-ND	-4.51	1.31	1.37
9	4	102	BCL	OBD-CAD	4.51	1.30	1.22
9	F	101	BCL	OBD-CAD	4.50	1.30	1.22
12	t	303	PEF	O2-C10	4.49	1.45	1.35
9	AC	103	BCL	OBD-CAD	4.48	1.30	1.22
9	8	101	BCL	OBD-CAD	4.46	1.30	1.22
9	X	102	BCL	OBD-CAD	4.45	1.30	1.22
9	x	305	BCL	O1D-CGD	-4.45	1.10	1.21
9	AE	102	BCL	OBD-CAD	4.44	1.30	1.22
7	C	502	HEM	C1B-NB	-4.43	1.32	1.40
12	H	305	PEF	O2-C10	4.35	1.45	1.35
9	x	301	BCL	O1D-CGD	-4.35	1.10	1.21
9	A	102	BCL	C4D-ND	-4.33	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	102	BCL	O1D-CGD	-4.33	1.10	1.21
7	C	504	HEM	C1B-NB	-4.32	1.32	1.40
7	o	501	HEM	C4D-ND	-4.30	1.32	1.40
9	L	303	BCL	OBD-CAD	4.29	1.29	1.22
9	p	102	BCL	OBD-CAD	4.28	1.29	1.22
9	AB	102	BCL	C4D-ND	-4.27	1.31	1.37
9	3	101	BCL	C4D-ND	-4.26	1.31	1.37
9	2	102	BCL	O1D-CGD	-4.24	1.10	1.21
9	T	102	BCL	O1D-CGD	-4.23	1.10	1.21
7	o	501	HEM	C1B-NB	-4.22	1.33	1.40
12	A	101	PEF	O2-C10	4.21	1.44	1.35
9	Z	102	BCL	OBD-CAD	4.19	1.29	1.22
9	U	101	BCL	C4D-ND	-4.19	1.31	1.37
9	4	102	BCL	O1D-CGD	-4.18	1.10	1.21
9	V	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	AC	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	P	101	BCL	C4D-ND	-4.13	1.32	1.37
9	m	102	BCL	C4D-ND	-4.13	1.32	1.37
9	w	101	BCL	C4D-ND	-4.12	1.32	1.37
9	O	102	BCL	C4D-ND	-4.11	1.32	1.37
9	k	102	BCL	O1D-CGD	-4.11	1.10	1.21
9	h	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	AL	102	BCL	OBD-CAD	4.09	1.29	1.22
7	C	501	HEM	C1B-NB	-4.08	1.33	1.40
9	AG	101	BCL	O1D-CGD	-4.07	1.11	1.21
9	AC	102	BCL	C4D-ND	-4.07	1.32	1.37
9	c	101	BCL	O1D-CGD	-4.06	1.11	1.21
9	h	101	BCL	C4D-ND	-4.06	1.32	1.37
9	X	102	BCL	O1D-CGD	-4.04	1.11	1.21
9	V	102	BCL	C4D-ND	-4.03	1.32	1.37
9	D	102	BCL	O1D-CGD	-4.02	1.11	1.21
9	x	305	BCL	O1A-CGA	-4.02	1.10	1.22
9	f	101	BCL	O1D-CGD	-4.01	1.11	1.21
9	u	102	BCL	C4D-ND	-4.01	1.32	1.37
9	0	102	BCL	O1D-CGD	-4.01	1.11	1.21
9	AE	102	BCL	O1D-CGD	-4.00	1.11	1.21
9	AF	101	BCL	O1D-CGD	-4.00	1.11	1.21
9	j	101	BCL	C4D-ND	-3.99	1.32	1.37
9	u	101	BCL	O1D-CGD	-3.99	1.11	1.21
9	5	101	BCL	O1D-CGD	-3.98	1.11	1.21
9	G	102	BCL	C4D-ND	-3.98	1.32	1.37
9	L	303	BCL	O1D-CGD	-3.97	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	BCL	O1D-CGD	-3.97	1.11	1.21
9	M	402	BCL	C4D-ND	-3.97	1.32	1.37
9	G	102	BCL	O1D-CGD	-3.96	1.11	1.21
9	m	102	BCL	O1D-CGD	-3.96	1.11	1.21
9	p	102	BCL	O1D-CGD	-3.95	1.11	1.21
9	q	102	BCL	O1D-CGD	-3.94	1.11	1.21
9	AI	101	BCL	O1D-CGD	-3.94	1.11	1.21
9	K	101	BCL	C4D-ND	-3.94	1.32	1.37
9	f	101	BCL	C4D-ND	-3.94	1.32	1.37
9	AB	101	BCL	O1D-CGD	-3.94	1.11	1.21
9	6	101	BCL	C4D-ND	-3.94	1.32	1.37
9	AL	102	BCL	O1D-CGD	-3.93	1.11	1.21
9	A	102	BCL	O1D-CGD	-3.93	1.11	1.21
9	P	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	Q	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	U	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	9	102	BCL	C4D-ND	-3.91	1.32	1.37
9	g	102	BCL	O1D-CGD	-3.91	1.11	1.21
9	k	102	BCL	C4D-ND	-3.91	1.32	1.37
9	8	101	BCL	O1D-CGD	-3.91	1.11	1.21
7	o	503	HEM	C4D-ND	-3.90	1.33	1.40
9	9	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	w	101	BCL	O1D-CGD	-3.90	1.11	1.21
9	e	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	AI	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	y	401	BCL	O2D-CED	3.90	1.54	1.45
9	A	103	BCL	O1D-CGD	-3.89	1.11	1.21
9	m	103	BCL	O1D-CGD	-3.88	1.11	1.21
9	D	101	BCL	O1D-CGD	-3.88	1.11	1.21
9	y	401	BCL	C4D-ND	-3.88	1.32	1.37
7	C	502	HEM	C4D-ND	-3.87	1.33	1.40
9	6	101	BCL	O1D-CGD	-3.87	1.11	1.21
9	M	401	BCL	C4D-ND	-3.87	1.32	1.37
9	Z	102	BCL	O1D-CGD	-3.87	1.11	1.21
9	i	102	BCL	O1D-CGD	-3.87	1.11	1.21
9	AH	101	BCL	O1D-CGD	-3.86	1.11	1.21
9	T	102	BCL	C4D-ND	-3.86	1.32	1.37
9	N	101	BCL	C4D-ND	-3.85	1.32	1.37
9	I	101	BCL	O1D-CGD	-3.85	1.11	1.21
9	AK	101	BCL	O1D-CGD	-3.85	1.11	1.21
9	L	303	BCL	C4D-ND	-3.84	1.32	1.37
9	L	301	BCL	C4D-ND	-3.83	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	502	HEM	C1B-NB	-3.83	1.33	1.40
9	AC	103	BCL	O1D-CGD	-3.83	1.11	1.21
9	s	102	BCL	C4D-ND	-3.82	1.32	1.37
9	AF	101	BCL	C4D-ND	-3.82	1.32	1.37
9	M	401	BCL	O1D-CGD	-3.82	1.11	1.21
9	z	102	BCL	O1D-CGD	-3.81	1.11	1.21
7	C	504	HEM	C4D-ND	-3.81	1.33	1.40
9	S	102	BCL	O1D-CGD	-3.81	1.11	1.21
9	x	303	BCL	O1D-CGD	-3.80	1.11	1.21
9	F	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	l	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	AI	101	BCL	C4D-ND	-3.79	1.32	1.37
9	j	101	BCL	O1D-CGD	-3.78	1.11	1.21
9	R	102	BCL	O1D-CGD	-3.78	1.11	1.21
9	4	102	BCL	C4D-ND	-3.78	1.32	1.37
9	M	402	BCL	O2A-CGA	-3.77	1.22	1.33
7	o	503	HEM	C1B-NB	-3.77	1.33	1.40
9	m	103	BCL	O2D-CED	3.74	1.54	1.45
9	d	101	BCL	O2D-CED	3.74	1.54	1.45
9	1	101	BCL	O1D-CGD	-3.74	1.11	1.21
9	AC	103	BCL	C4D-ND	-3.73	1.32	1.37
9	u	102	BCL	O1D-CGD	-3.73	1.11	1.21
9	N	101	BCL	O1D-CGD	-3.73	1.11	1.21
9	S	102	BCL	C4D-ND	-3.73	1.32	1.37
9	L	301	BCL	O1D-CGD	-3.73	1.11	1.21
9	x	301	BCL	O2D-CED	3.73	1.54	1.45
9	AE	102	BCL	C4D-ND	-3.73	1.32	1.37
9	K	101	BCL	O1D-CGD	-3.72	1.11	1.21
9	0	102	BCL	C4D-ND	-3.72	1.32	1.37
9	Q	101	BCL	C4D-ND	-3.71	1.32	1.37
9	M	402	BCL	O2D-CED	3.71	1.54	1.45
9	g	102	BCL	C4D-ND	-3.70	1.32	1.37
9	AK	101	BCL	C4D-ND	-3.70	1.32	1.37
7	o	502	HEM	C4D-ND	-3.69	1.33	1.40
9	x	305	BCL	O2A-CGA	-3.68	1.22	1.33
9	x	305	BCL	O2D-CED	3.68	1.54	1.45
9	F	101	BCL	C4D-ND	-3.67	1.32	1.37
9	i	102	BCL	C4D-ND	-3.67	1.32	1.37
9	Y	101	BCL	O2D-CED	3.67	1.53	1.45
9	I	103	BCL	O1D-CGD	-3.67	1.12	1.21
9	l	101	BCL	C4D-ND	-3.66	1.32	1.37
9	Y	101	BCL	O1D-CGD	-3.66	1.12	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AB	102	BCL	O1D-CGD	-3.66	1.12	1.21
9	8	101	BCL	O2D-CED	3.66	1.53	1.45
9	AB	101	BCL	C4D-ND	-3.65	1.32	1.37
7	C	503	HEM	C1B-NB	-3.63	1.34	1.40
9	u	101	BCL	O2D-CED	3.63	1.53	1.45
9	r	101	BCL	O1D-CGD	-3.62	1.12	1.21
9	AL	102	BCL	O2D-CED	3.62	1.53	1.45
9	1	101	BCL	O2D-CED	3.62	1.53	1.45
9	D	101	BCL	C4D-ND	-3.61	1.32	1.37
9	AI	102	BCL	O2D-CED	3.61	1.53	1.45
9	5	101	BCL	C4D-ND	-3.60	1.32	1.37
9	M	402	BCL	O1D-CGD	-3.60	1.12	1.21
9	x	303	BCL	O2D-CED	3.60	1.53	1.45
9	M	401	BCL	O2D-CED	3.59	1.53	1.45
9	m	102	BCL	O2D-CED	3.58	1.53	1.45
9	AL	102	BCL	C4D-ND	-3.58	1.32	1.37
9	z	102	BCL	C4D-ND	-3.57	1.32	1.37
9	y	401	BCL	O1D-CGD	-3.57	1.12	1.21
9	d	101	BCL	O1D-CGD	-3.56	1.12	1.21
9	x	305	BCL	C1B-NB	3.55	1.38	1.35
9	8	101	BCL	C4D-ND	-3.55	1.32	1.37
9	O	102	BCL	O1D-CGD	-3.54	1.12	1.21
9	f	101	BCL	O2D-CED	3.53	1.53	1.45
9	j	101	BCL	O2D-CED	3.53	1.53	1.45
7	o	501	HEM	C4B-NB	-3.53	1.31	1.38
9	AK	101	BCL	O2D-CED	3.52	1.53	1.45
9	F	101	BCL	O2D-CED	3.52	1.53	1.45
9	G	102	BCL	O2D-CED	3.52	1.53	1.45
9	6	101	BCL	O2D-CED	3.51	1.53	1.45
9	A	103	BCL	C4D-ND	-3.51	1.32	1.37
9	3	101	BCL	O2D-CED	3.49	1.53	1.45
9	l	101	BCL	O2D-CED	3.49	1.53	1.45
9	x	301	BCL	C4D-ND	-3.49	1.32	1.37
9	z	102	BCL	O2D-CED	3.48	1.53	1.45
9	c	101	BCL	O2D-CED	3.48	1.53	1.45
9	r	101	BCL	O2D-CED	3.47	1.53	1.45
9	A	102	BCL	O2D-CED	3.47	1.53	1.45
9	3	101	BCL	O1D-CGD	-3.47	1.12	1.21
9	7	102	BCL	O1D-CGD	-3.46	1.12	1.21
9	p	102	BCL	O2D-CED	3.46	1.53	1.45
9	7	102	BCL	O2D-CED	3.45	1.53	1.45
9	S	102	BCL	O2D-CED	3.45	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AH	101	BCL	C4D-ND	-3.44	1.33	1.37
9	D	102	BCL	O2D-CED	3.44	1.53	1.45
9	9	102	BCL	O2D-CED	3.43	1.53	1.45
9	O	102	BCL	O2D-CED	3.43	1.53	1.45
9	q	102	BCL	C4D-ND	-3.40	1.33	1.37
9	AE	102	BCL	O2D-CED	3.39	1.53	1.45
7	C	501	HEM	C4B-NB	-3.38	1.31	1.38
9	y	401	BCL	O2A-CGA	-3.38	1.23	1.33
9	V	102	BCL	O2D-CED	3.38	1.53	1.45
9	g	102	BCL	O2D-CED	3.37	1.53	1.45
9	0	102	BCL	O2D-CED	3.37	1.53	1.45
9	Y	101	BCL	C4D-ND	-3.36	1.33	1.37
9	W	101	BCL	O2D-CED	3.36	1.53	1.45
9	I	101	BCL	O2D-CED	3.36	1.53	1.45
9	d	101	BCL	C4D-ND	-3.35	1.33	1.37
7	C	503	HEM	C4D-ND	-3.35	1.34	1.40
9	y	401	BCL	O1A-CGA	-3.35	1.12	1.22
9	V	102	BCL	O2D-CGD	-3.35	1.25	1.33
9	U	101	BCL	O2D-CGD	-3.35	1.25	1.33
9	x	301	BCL	C3C-C4C	3.35	1.55	1.51
9	AH	101	BCL	O2D-CED	3.34	1.53	1.45
9	k	102	BCL	O2D-CGD	-3.33	1.25	1.33
9	e	102	BCL	O2D-CED	3.32	1.53	1.45
9	R	102	BCL	O2D-CGD	-3.32	1.25	1.33
9	AC	103	BCL	O2D-CED	3.32	1.53	1.45
9	u	102	BCL	O2D-CED	3.31	1.53	1.45
9	3	101	BCL	O2A-CGA	-3.31	1.23	1.33
9	2	102	BCL	C4D-ND	-3.31	1.33	1.37
9	AB	102	BCL	O2D-CED	3.30	1.53	1.45
9	7	102	BCL	C4D-ND	-3.30	1.33	1.37
9	X	102	BCL	C4D-ND	-3.30	1.33	1.37
9	h	101	BCL	O2D-CED	3.30	1.53	1.45
9	N	101	BCL	O2D-CED	3.30	1.53	1.45
9	A	103	BCL	O2D-CED	3.30	1.53	1.45
9	q	102	BCL	O2D-CED	3.29	1.53	1.45
9	Q	101	BCL	O2D-CGD	-3.29	1.25	1.33
9	p	102	BCL	C4D-ND	-3.28	1.33	1.37
9	A	102	BCL	O2A-CGA	-3.28	1.23	1.33
7	C	502	HEM	C4B-NB	-3.27	1.32	1.38
9	X	102	BCL	O2D-CED	3.27	1.53	1.45
9	j	101	BCL	C4B-NB	3.27	1.38	1.35
9	D	102	BCL	C4D-ND	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	102	BCL	O2D-CED	3.26	1.53	1.45
9	D	101	BCL	O2D-CGD	-3.26	1.25	1.33
9	0	102	BCL	C3C-C4C	3.26	1.55	1.51
9	K	101	BCL	O2D-CED	3.26	1.53	1.45
9	G	102	BCL	O2D-CGD	-3.25	1.25	1.33
9	P	101	BCL	O2D-CED	3.25	1.53	1.45
9	I	103	BCL	O2D-CED	3.24	1.52	1.45
9	q	102	BCL	O1A-CGA	-3.24	1.12	1.22
9	q	102	BCL	O2A-CGA	-3.24	1.23	1.33
9	5	101	BCL	O2D-CED	3.23	1.52	1.45
9	6	101	BCL	O1A-CGA	-3.23	1.12	1.22
7	o	504	HEM	C4D-ND	-3.23	1.34	1.40
9	8	101	BCL	O2A-CGA	-3.22	1.23	1.33
9	2	102	BCL	O2D-CGD	-3.22	1.25	1.33
9	i	102	BCL	O2D-CED	3.22	1.52	1.45
9	w	101	BCL	O2D-CGD	-3.21	1.25	1.33
9	AB	101	BCL	O2D-CED	3.21	1.52	1.45
9	i	102	BCL	O2D-CGD	-3.21	1.25	1.33
9	L	303	BCL	O2D-CED	3.21	1.52	1.45
9	AG	101	BCL	O2D-CED	3.21	1.52	1.45
9	D	101	BCL	O2D-CED	3.20	1.52	1.45
9	Q	101	BCL	O2D-CED	3.20	1.52	1.45
9	AC	102	BCL	O2D-CGD	-3.20	1.25	1.33
9	Z	102	BCL	O2D-CED	3.20	1.52	1.45
9	w	101	BCL	O2D-CED	3.19	1.52	1.45
9	L	303	BCL	O2D-CGD	-3.19	1.25	1.33
9	AI	101	BCL	O2D-CED	3.18	1.52	1.45
7	C	504	HEM	C3B-C4B	3.18	1.51	1.44
9	s	102	BCL	O2D-CGD	-3.17	1.25	1.33
9	AB	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	AI	102	BCL	C4D-ND	-3.16	1.33	1.37
9	c	101	BCL	C4D-ND	-3.16	1.33	1.37
9	g	102	BCL	O2D-CGD	-3.15	1.25	1.33
9	r	101	BCL	C3C-C4C	3.15	1.55	1.51
9	AG	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	T	102	BCL	O2D-CGD	-3.14	1.25	1.33
9	d	101	BCL	C3C-C4C	3.13	1.55	1.51
9	3	101	BCL	O1A-CGA	-3.13	1.13	1.22
12	H	305	PEF	O3-C30	3.13	1.48	1.33
9	D	101	BCL	O2A-CGA	-3.13	1.24	1.33
9	m	102	BCL	O2D-CGD	-3.13	1.25	1.33
12	M	408	PEF	O3-C30	3.13	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AL	102	BCL	C3C-C4C	3.11	1.55	1.51
9	I	103	BCL	O2A-CGA	-3.11	1.24	1.33
9	AF	101	BCL	O2D-CED	3.11	1.52	1.45
9	AC	102	BCL	O2D-CED	3.11	1.52	1.45
9	R	102	BCL	O2D-CED	3.11	1.52	1.45
9	AF	101	BCL	O2D-CGD	-3.11	1.25	1.33
9	I	101	BCL	O2D-CGD	-3.10	1.25	1.33
9	r	101	BCL	C4D-ND	-3.10	1.33	1.37
9	AH	101	BCL	O2D-CGD	-3.10	1.25	1.33
9	P	101	BCL	O2D-CGD	-3.10	1.25	1.33
9	h	101	BCL	O2D-CGD	-3.10	1.25	1.33
9	k	102	BCL	O2D-CED	3.09	1.52	1.45
9	M	402	BCL	O1A-CGA	-3.09	1.13	1.22
9	w	101	BCL	O1A-CGA	-3.09	1.13	1.22
9	x	305	BCL	O2D-CGD	-3.09	1.25	1.33
9	1	101	BCL	C4D-ND	-3.08	1.33	1.37
9	A	103	BCL	O2A-CGA	-3.07	1.24	1.33
9	L	301	BCL	O1A-CGA	-3.07	1.13	1.22
9	X	102	BCL	C1D-C2D	-3.07	1.39	1.45
9	AL	102	BCL	O2A-CGA	-3.05	1.24	1.33
9	Z	102	BCL	C4D-ND	-3.04	1.33	1.37
9	AC	102	BCL	O1A-CGA	-3.04	1.13	1.22
9	x	301	BCL	O2D-CGD	-3.04	1.25	1.33
9	Y	101	BCL	O2D-CGD	-3.03	1.25	1.33
9	I	101	BCL	O2A-CGA	-3.03	1.24	1.33
9	x	303	BCL	C1D-C2D	-3.03	1.39	1.45
9	AG	101	BCL	C4D-ND	-3.01	1.33	1.37
9	AI	102	BCL	O2A-CGA	-3.01	1.24	1.33
9	W	101	BCL	O2D-CGD	-3.01	1.25	1.33
9	T	102	BCL	O2D-CED	3.00	1.52	1.45
9	AG	101	BCL	O1A-CGA	-3.00	1.13	1.22
9	m	103	BCL	O2A-CGA	-3.00	1.24	1.33
9	W	101	BCL	C4D-ND	-3.00	1.33	1.37
9	AH	101	BCL	O1A-CGA	-3.00	1.13	1.22
9	u	101	BCL	C4D-ND	-2.99	1.33	1.37
9	AI	101	BCL	O2D-CGD	-2.99	1.25	1.33
12	y	407	PEF	O3-C30	2.99	1.48	1.33
9	m	102	BCL	C1D-C2D	-2.99	1.39	1.45
7	o	503	HEM	C3B-C4B	2.98	1.50	1.44
9	2	102	BCL	O2D-CED	2.98	1.52	1.45
9	m	102	BCL	O2A-CGA	-2.98	1.24	1.33
9	U	101	BCL	O2A-CGA	-2.97	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	j	101	BCL	O2A-CGA	-2.97	1.24	1.33
12	A	101	PEF	O3-C30	2.96	1.47	1.33
9	x	305	BCL	C1D-C2D	-2.96	1.39	1.45
9	S	102	BCL	O2D-CGD	-2.96	1.26	1.33
9	D	102	BCL	O2D-CGD	-2.95	1.26	1.33
9	u	102	BCL	O2D-CGD	-2.95	1.26	1.33
9	u	102	BCL	C1D-C2D	-2.95	1.39	1.45
9	AC	102	BCL	O2A-CGA	-2.95	1.24	1.33
9	0	102	BCL	O2A-CGA	-2.95	1.24	1.33
9	L	301	BCL	O2D-CGD	-2.94	1.26	1.33
9	I	101	BCL	O1A-CGA	-2.94	1.13	1.22
9	u	102	BCL	O2A-CGA	-2.94	1.24	1.33
9	g	102	BCL	O1A-CGA	-2.94	1.13	1.22
9	I	103	BCL	O1A-CGA	-2.94	1.13	1.22
9	AB	102	BCL	O2D-CGD	-2.93	1.26	1.33
9	j	101	BCL	O2D-CGD	-2.93	1.26	1.33
9	G	102	BCL	O2A-CGA	-2.93	1.24	1.33
9	AE	102	BCL	O2D-CGD	-2.93	1.26	1.33
9	AH	101	BCL	O2A-CGA	-2.93	1.24	1.33
9	s	102	BCL	O2A-CGA	-2.92	1.24	1.33
12	x	306	PEF	O3-C30	2.92	1.47	1.33
9	D	102	BCL	O2A-CGA	-2.92	1.24	1.33
9	X	102	BCL	O1A-CGA	-2.92	1.13	1.22
9	d	101	BCL	C5-C3	2.91	1.57	1.51
7	C	504	HEM	C1D-ND	-2.91	1.32	1.38
9	W	101	BCL	O2A-CGA	-2.91	1.24	1.33
17	S	101	PGW	O01-C1	2.91	1.41	1.35
9	6	101	BCL	O2D-CGD	-2.90	1.26	1.33
9	5	101	BCL	O1A-CGA	-2.90	1.13	1.22
9	R	102	BCL	O2A-CGA	-2.90	1.24	1.33
9	L	301	BCL	O2D-CED	2.89	1.52	1.45
17	AE	101	PGW	O01-C1	2.89	1.41	1.35
9	AG	101	BCL	O2A-CGA	-2.89	1.24	1.33
9	0	102	BCL	O2D-CGD	-2.89	1.26	1.33
9	AK	101	BCL	O2D-CGD	-2.89	1.26	1.33
9	F	101	BCL	O1A-CGA	-2.88	1.14	1.22
12	t	303	PEF	O3-C30	2.88	1.47	1.33
9	8	101	BCL	O2D-CGD	-2.88	1.26	1.33
9	f	101	BCL	C5-C3	2.87	1.57	1.51
9	l	101	BCL	O2A-CGA	-2.87	1.24	1.33
9	z	102	BCL	O2A-CGA	-2.87	1.24	1.33
9	1	101	BCL	O2A-CGA	-2.87	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	102	BCL	C1D-C2D	-2.87	1.39	1.45
7	o	502	HEM	C4B-NB	-2.86	1.32	1.38
9	4	102	BCL	O2A-CGA	-2.86	1.24	1.33
10	y	402	BPH	CHA-CBD	-2.86	1.49	1.52
9	c	101	BCL	O2A-CGA	-2.85	1.25	1.33
9	AB	101	BCL	O2A-CGA	-2.85	1.25	1.33
9	m	103	BCL	O1A-CGA	-2.85	1.14	1.22
9	AF	101	BCL	O2A-CGA	-2.85	1.25	1.33
9	s	102	BCL	O2D-CED	2.85	1.52	1.45
9	8	101	BCL	O1A-CGA	-2.84	1.14	1.22
9	x	303	BCL	O2D-CGD	-2.84	1.26	1.33
9	X	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	9	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	AC	102	BCL	C1B-NB	2.84	1.37	1.35
9	5	101	BCL	O2A-CGA	-2.84	1.25	1.33
9	k	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	p	102	BCL	O2A-CGA	-2.83	1.25	1.33
9	X	102	BCL	O2D-CGD	-2.83	1.26	1.33
9	D	101	BCL	O1A-CGA	-2.83	1.14	1.22
9	F	101	BCL	O2D-CGD	-2.83	1.26	1.33
9	l	101	BCL	O1A-CGA	-2.82	1.14	1.22
9	M	401	BCL	O2D-CGD	-2.82	1.26	1.33
9	s	102	BCL	O1A-CGA	-2.82	1.14	1.22
9	5	101	BCL	O2D-CGD	-2.82	1.26	1.33
9	m	103	BCL	C4D-ND	-2.82	1.33	1.37
9	P	101	BCL	O2A-CGA	-2.82	1.25	1.33
9	F	101	BCL	O2A-CGA	-2.81	1.25	1.33
9	S	102	BCL	C1B-NB	2.81	1.37	1.35
9	j	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	f	101	BCL	O2A-CGA	-2.81	1.25	1.33
9	AB	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	1	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	i	102	BCL	O2A-CGA	-2.80	1.25	1.33
12	t	301	PEF	O3-C30	2.80	1.47	1.33
12	H	304	PEF	O3-C30	2.80	1.47	1.33
9	AI	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	e	102	BCL	C4D-ND	-2.80	1.33	1.37
12	m	101	PEF	O3-C30	2.80	1.47	1.33
9	4	102	BCL	O1A-CGA	-2.79	1.14	1.22
10	x	302	BPH	C2C-C3C	-2.79	1.52	1.54
9	N	101	BCL	O2A-CGA	-2.79	1.25	1.33
9	T	102	BCL	O2A-CGA	-2.79	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	m	103	BCL	C3C-C4C	2.79	1.55	1.51
9	R	102	BCL	C4B-NB	2.79	1.37	1.35
9	AB	102	BCL	O2A-CGA	-2.79	1.25	1.33
9	O	102	BCL	O1A-CGA	-2.79	1.14	1.22
9	V	102	BCL	O2A-CGA	-2.79	1.25	1.33
7	o	504	HEM	C4B-NB	-2.79	1.33	1.38
9	z	102	BCL	O2D-CGD	-2.78	1.26	1.33
9	d	101	BCL	O2D-CGD	-2.78	1.26	1.33
9	u	101	BCL	O2D-CGD	-2.78	1.26	1.33
9	R	102	BCL	O1A-CGA	-2.78	1.14	1.22
9	Z	102	BCL	O1A-CGA	-2.78	1.14	1.22
9	P	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	f	101	BCL	C3C-C4C	2.78	1.55	1.51
9	P	101	BCL	C3C-C4C	2.77	1.55	1.51
9	1	101	BCL	O2D-CGD	-2.77	1.26	1.33
9	AL	102	BCL	O2D-CGD	-2.77	1.26	1.33
9	G	102	BCL	O1A-CGA	-2.77	1.14	1.22
9	A	102	BCL	O1A-CGA	-2.77	1.14	1.22
12	M	407	PEF	O3-C30	2.76	1.47	1.33
9	AB	102	BCL	C1B-NB	2.76	1.37	1.35
9	r	101	BCL	O2A-CGA	-2.75	1.25	1.33
9	AE	102	BCL	O1A-CGA	-2.75	1.14	1.22
9	AE	102	BCL	O2A-CGA	-2.75	1.25	1.33
9	Z	102	BCL	O2D-CGD	-2.75	1.26	1.33
9	AB	102	BCL	C3C-C4C	2.75	1.55	1.51
9	h	101	BCL	O1A-CGA	-2.75	1.14	1.22
9	U	101	BCL	O2D-CED	2.74	1.51	1.45
9	c	101	BCL	O2D-CGD	-2.74	1.26	1.33
9	Z	102	BCL	O2A-CGA	-2.74	1.25	1.33
9	AF	101	BCL	O1A-CGA	-2.74	1.14	1.22
12	y	408	PEF	O3-C30	2.73	1.46	1.33
12	y	406	PEF	O3-C30	2.73	1.46	1.33
9	m	102	BCL	O1A-CGA	-2.73	1.14	1.22
9	x	303	BCL	O2A-CGA	-2.73	1.25	1.33
9	W	101	BCL	O1A-CGA	-2.73	1.14	1.22
9	A	102	BCL	O2D-CGD	-2.73	1.26	1.33
9	x	303	BCL	O1A-CGA	-2.73	1.14	1.22
9	L	303	BCL	O2A-CGA	-2.72	1.25	1.33
9	q	102	BCL	O2D-CGD	-2.72	1.26	1.33
9	2	102	BCL	C1D-C2D	-2.72	1.40	1.45
9	U	101	BCL	O1A-CGA	-2.72	1.14	1.22
12	H	301	PEF	O3-C30	2.71	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	103	BCL	O2D-CGD	-2.71	1.26	1.33
9	p	102	BCL	O1A-CGA	-2.71	1.14	1.22
9	x	301	BCL	C5-C3	2.71	1.56	1.51
9	d	101	BCL	O1A-CGA	-2.71	1.14	1.22
9	u	101	BCL	O1A-CGA	-2.71	1.14	1.22
9	f	101	BCL	O2D-CGD	-2.70	1.26	1.33
9	O	102	BCL	O2A-CGA	-2.70	1.25	1.33
9	f	101	BCL	O1A-CGA	-2.70	1.14	1.22
9	9	102	BCL	O2D-CGD	-2.70	1.26	1.33
9	6	101	BCL	C1D-C2D	-2.70	1.40	1.45
9	A	103	BCL	O1A-CGA	-2.70	1.14	1.22
9	s	102	BCL	C5-C3	2.69	1.56	1.51
9	AH	101	BCL	C4B-NB	2.69	1.37	1.35
9	g	102	BCL	O2A-CGA	-2.69	1.25	1.33
9	x	301	BCL	C3B-CAB	2.69	1.56	1.49
9	W	101	BCL	C3C-C4C	2.69	1.55	1.51
9	N	101	BCL	O2D-CGD	-2.69	1.26	1.33
9	L	303	BCL	C5-C3	2.69	1.56	1.51
9	z	102	BCL	O1A-CGA	-2.69	1.14	1.22
9	AK	101	BCL	O2A-CGA	-2.68	1.25	1.33
9	0	102	BCL	O1A-CGA	-2.68	1.14	1.22
9	4	102	BCL	C3C-C4C	2.68	1.55	1.51
9	u	101	BCL	O2A-CGA	-2.68	1.25	1.33
9	AB	102	BCL	C4B-NB	2.68	1.37	1.35
9	K	101	BCL	O2D-CGD	-2.68	1.26	1.33
9	k	102	BCL	O1A-CGA	-2.67	1.14	1.22
9	K	101	BCL	O1A-CGA	-2.67	1.14	1.22
9	O	102	BCL	O2D-CGD	-2.67	1.26	1.33
9	V	102	BCL	O1A-CGA	-2.66	1.14	1.22
9	I	103	BCL	O2D-CGD	-2.66	1.26	1.33
9	M	401	BCL	O2A-CGA	-2.66	1.25	1.33
9	w	101	BCL	O2A-CGA	-2.65	1.25	1.33
9	AC	103	BCL	O2D-CGD	-2.65	1.26	1.33
9	AC	103	BCL	O2A-CGA	-2.65	1.25	1.33
9	A	102	BCL	C1D-C2D	-2.65	1.40	1.45
9	S	102	BCL	O1A-CGA	-2.65	1.14	1.22
9	q	102	BCL	C3C-C4C	2.65	1.54	1.51
9	f	101	BCL	C1D-C2D	-2.64	1.40	1.45
9	T	102	BCL	O1A-CGA	-2.64	1.14	1.22
9	y	401	BCL	O2D-CGD	-2.63	1.26	1.33
14	y	403	MQ8	C42-C43	2.63	1.39	1.33
9	Q	101	BCL	O1A-CGA	-2.63	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AG	101	BCL	C1D-C2D	-2.63	1.40	1.45
9	9	102	BCL	O1A-CGA	-2.62	1.14	1.22
9	D	102	BCL	O1A-CGA	-2.62	1.14	1.22
7	C	501	HEM	FE-ND	-2.62	1.83	1.96
7	o	501	HEM	C1D-ND	-2.62	1.33	1.38
9	u	102	BCL	O1A-CGA	-2.61	1.14	1.22
9	e	102	BCL	O1A-CGA	-2.61	1.14	1.22
12	p	101	PEF	O3-C30	2.61	1.46	1.33
9	Y	101	BCL	O1A-CGA	-2.61	1.14	1.22
9	AK	101	BCL	C1D-C2D	-2.61	1.40	1.45
9	h	101	BCL	C5-C3	2.60	1.56	1.51
9	Y	101	BCL	O2A-CGA	-2.60	1.25	1.33
9	2	102	BCL	O2A-CGA	-2.60	1.25	1.33
9	L	303	BCL	C3B-C2B	-2.60	1.34	1.39
9	L	303	BCL	O1A-CGA	-2.60	1.14	1.22
7	C	504	HEM	FE-ND	-2.60	1.84	1.96
9	A	103	BCL	C3C-C4C	2.60	1.54	1.51
9	s	102	BCL	C3C-C4C	2.60	1.54	1.51
9	S	102	BCL	O2A-CGA	-2.59	1.25	1.33
9	AK	101	BCL	O1A-CGA	-2.59	1.14	1.22
14	y	403	MQ8	C37-C38	2.59	1.39	1.33
9	0	102	BCL	C1D-C2D	-2.59	1.40	1.45
9	4	102	BCL	O2D-CGD	-2.59	1.26	1.33
9	M	401	BCL	O1A-CGA	-2.59	1.14	1.22
9	D	101	BCL	C1B-NB	2.59	1.37	1.35
9	Y	101	BCL	C3C-C4C	2.58	1.54	1.51
9	AB	102	BCL	O1A-CGA	-2.57	1.14	1.22
9	Q	101	BCL	O2A-CGA	-2.57	1.25	1.33
9	m	102	BCL	C5-C3	2.56	1.56	1.51
9	l	101	BCL	O2D-CGD	-2.56	1.27	1.33
9	r	101	BCL	O1A-CGA	-2.56	1.14	1.22
11	L	304	UQ8	C7-C8	2.56	1.54	1.50
7	o	503	HEM	C4B-NB	-2.56	1.33	1.38
9	AL	102	BCL	O1A-CGA	-2.56	1.15	1.22
9	r	101	BCL	O2D-CGD	-2.55	1.27	1.33
9	K	101	BCL	O2A-CGA	-2.55	1.25	1.33
7	o	501	HEM	FE-ND	-2.54	1.84	1.96
9	h	101	BCL	O2A-CGA	-2.54	1.25	1.33
9	I	103	BCL	C1D-C2D	-2.54	1.40	1.45
9	AI	101	BCL	O2A-CGA	-2.53	1.25	1.33
9	q	102	BCL	C1D-C2D	-2.53	1.40	1.45
9	S	102	BCL	C3C-C4C	2.52	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	504	HEM	C4B-NB	-2.52	1.33	1.38
9	M	401	BCL	C3B-C2B	-2.52	1.34	1.39
9	u	101	BCL	C5-C3	2.51	1.56	1.51
7	C	501	HEM	CAA-C2A	-2.51	1.48	1.52
9	u	101	BCL	C3C-C4C	2.50	1.54	1.51
9	x	305	BCL	C2C-C3C	-2.50	1.47	1.54
9	Y	101	BCL	C3B-CAB	2.50	1.55	1.49
7	o	502	HEM	CHB-C1B	2.50	1.41	1.35
9	AG	101	BCL	C3B-CAB	2.50	1.55	1.49
9	I	101	BCL	C1D-C2D	-2.50	1.40	1.45
9	AH	101	BCL	C3C-C4C	2.49	1.54	1.51
9	i	102	BCL	O1A-CGA	-2.49	1.15	1.22
9	M	402	BCL	C1D-ND	2.49	1.40	1.37
9	e	102	BCL	O2A-CGA	-2.49	1.26	1.33
7	C	501	HEM	CHB-C1B	2.49	1.41	1.35
9	N	101	BCL	O1A-CGA	-2.48	1.15	1.22
9	4	102	BCL	C1D-C2D	-2.47	1.40	1.45
7	o	503	HEM	FE-ND	-2.47	1.84	1.96
9	AI	102	BCL	O1A-CGA	-2.47	1.15	1.22
9	e	102	BCL	O2D-CGD	-2.47	1.27	1.33
9	AC	103	BCL	O1A-CGA	-2.47	1.15	1.22
7	o	503	HEM	C1D-ND	-2.46	1.33	1.38
7	o	501	HEM	CHA-C4D	2.45	1.41	1.35
9	6	101	BCL	C3C-C4C	2.45	1.54	1.51
14	M	404	MQ8	C42-C43	2.45	1.38	1.33
7	o	504	HEM	CHA-C4D	2.45	1.41	1.35
9	q	102	BCL	C3B-C2B	-2.44	1.35	1.39
9	Q	101	BCL	C3B-CAB	2.44	1.55	1.49
9	A	103	BCL	C1D-C2D	-2.44	1.40	1.45
9	F	101	BCL	C1D-C2D	-2.43	1.40	1.45
9	k	102	BCL	C3D-C2D	-2.43	1.32	1.39
9	2	102	BCL	O1A-CGA	-2.42	1.15	1.22
9	N	101	BCL	C4B-NB	2.42	1.37	1.35
9	x	303	BCL	C3D-C2D	-2.41	1.32	1.39
9	6	101	BCL	O2A-CGA	-2.40	1.26	1.33
9	9	102	BCL	C1B-NB	2.40	1.37	1.35
9	T	102	BCL	C1D-C2D	-2.40	1.40	1.45
9	L	301	BCL	O2A-CGA	-2.40	1.26	1.33
9	K	101	BCL	C1D-C2D	-2.40	1.40	1.45
9	G	102	BCL	C3C-C4C	2.39	1.54	1.51
9	T	102	BCL	C5-C3	2.39	1.56	1.51
9	7	102	BCL	O2A-CGA	-2.39	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	101	BCL	C3C-C4C	2.39	1.54	1.51
9	2	102	BCL	C5-C3	2.38	1.56	1.51
9	D	101	BCL	C1D-C2D	-2.38	1.40	1.45
9	R	102	BCL	C1D-C2D	-2.38	1.40	1.45
11	x	304	UQ8	C4-C3	2.38	1.46	1.36
9	s	102	BCL	C1D-C2D	-2.38	1.40	1.45
9	7	102	BCL	O1A-CGA	-2.38	1.15	1.22
9	K	101	BCL	C3B-CAB	2.38	1.55	1.49
9	R	102	BCL	C1B-NB	2.38	1.37	1.35
9	x	305	BCL	C3B-C2B	-2.38	1.35	1.39
9	L	301	BCL	C1D-C2D	-2.37	1.40	1.45
7	o	503	HEM	CHA-C4D	2.37	1.41	1.35
9	U	101	BCL	C5-C3	2.37	1.56	1.51
9	m	103	BCL	O2D-CGD	-2.36	1.27	1.33
9	h	101	BCL	C3B-C2B	-2.36	1.35	1.39
9	p	102	BCL	O2D-CGD	-2.36	1.27	1.33
9	D	102	BCL	C1D-C2D	-2.36	1.40	1.45
9	2	102	BCL	C3C-C4C	2.35	1.54	1.51
9	x	303	BCL	C3D-C4D	-2.35	1.38	1.44
11	x	304	UQ8	C43-C44	2.35	1.39	1.32
9	AC	103	BCL	C1D-C2D	-2.35	1.40	1.45
9	5	101	BCL	C1D-C2D	-2.35	1.40	1.45
9	L	303	BCL	C3D-C2D	-2.35	1.32	1.39
9	G	102	BCL	C1D-C2D	-2.35	1.40	1.45
9	I	101	BCL	C4B-NB	2.35	1.37	1.35
14	M	404	MQ8	C22-C23	2.34	1.38	1.33
9	k	102	BCL	C1B-NB	2.33	1.37	1.35
7	o	504	HEM	C3B-C4B	2.33	1.49	1.44
9	d	101	BCL	O2A-CGA	-2.33	1.26	1.33
9	x	303	BCL	C1A-CHA	-2.33	1.33	1.43
9	L	303	BCL	C3D-C4D	-2.33	1.38	1.44
9	3	101	BCL	C5-C3	2.33	1.56	1.51
9	r	101	BCL	C3B-C2B	-2.32	1.35	1.39
9	d	101	BCL	C1D-C2D	-2.32	1.40	1.45
7	C	501	HEM	CHA-C4D	2.32	1.40	1.35
9	6	101	BCL	C3B-C2B	-2.32	1.35	1.39
9	AC	102	BCL	C3C-C4C	2.32	1.54	1.51
9	c	101	BCL	C3C-C4C	2.32	1.54	1.51
9	AF	101	BCL	C5-C3	2.32	1.56	1.51
9	7	102	BCL	C3B-CAB	2.32	1.55	1.49
9	W	101	BCL	C3D-CAD	2.32	1.53	1.45
9	AI	101	BCL	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	c	101	BCL	O1A-CGA	-2.31	1.15	1.22
9	r	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	L	301	BCL	C3C-C4C	2.31	1.54	1.51
9	p	102	BCL	C3B-CAB	2.31	1.55	1.49
9	AC	102	BCL	C5-C3	2.31	1.56	1.51
9	AE	102	BCL	C4B-NB	2.30	1.37	1.35
9	l	101	BCL	C1D-C2D	-2.30	1.40	1.45
9	u	102	BCL	C4B-NB	2.30	1.37	1.35
9	M	402	BCL	C1B-NB	2.30	1.37	1.35
9	AL	102	BCL	C3D-C4D	-2.29	1.39	1.44
14	y	403	MQ8	C17-C18	2.29	1.38	1.33
7	C	502	HEM	CHA-C4D	2.29	1.40	1.35
14	M	404	MQ8	C17-C18	2.29	1.38	1.33
9	AI	102	BCL	O2D-CGD	-2.28	1.27	1.33
9	I	101	BCL	C5-C3	2.28	1.56	1.51
15	7	103	CRT	C4-C5	2.28	1.53	1.50
9	6	101	BCL	C3B-CAB	2.28	1.55	1.49
9	AC	103	BCL	C3B-CAB	2.28	1.55	1.49
9	y	401	BCL	C2C-C3C	-2.28	1.48	1.54
9	P	101	BCL	C1D-C2D	-2.28	1.40	1.45
7	C	501	HEM	C1B-C2B	-2.27	1.40	1.44
9	x	301	BCL	O2A-CGA	-2.27	1.26	1.33
9	AF	101	BCL	C1D-C2D	-2.26	1.40	1.45
9	3	101	BCL	O2D-CGD	-2.26	1.27	1.33
9	e	102	BCL	C1D-C2D	-2.26	1.40	1.45
9	m	103	BCL	C5-C3	2.26	1.56	1.51
9	T	102	BCL	C1B-NB	2.25	1.37	1.35
9	AH	101	BCL	C3B-CAB	2.25	1.55	1.49
10	y	402	BPH	CBD-CGD	-2.25	1.49	1.52
9	M	401	BCL	C3D-C4D	-2.25	1.39	1.44
9	x	301	BCL	C3D-C4D	-2.24	1.39	1.44
9	w	101	BCL	C3C-C4C	2.24	1.54	1.51
9	U	101	BCL	C1B-NB	2.24	1.37	1.35
9	r	101	BCL	C5-C3	2.24	1.55	1.51
9	AC	102	BCL	C1D-C2D	-2.23	1.40	1.45
9	i	102	BCL	C1D-C2D	-2.23	1.40	1.45
9	k	102	BCL	C5-C3	2.23	1.55	1.51
9	9	102	BCL	C3C-C4C	2.23	1.54	1.51
9	8	101	BCL	C3B-CAB	2.23	1.55	1.49
7	o	503	HEM	CHB-C1B	2.23	1.40	1.35
9	AB	101	BCL	C4B-NB	2.22	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	103	BCL	C3D-C4D	-2.22	1.39	1.44
9	3	101	BCL	C3D-C2D	-2.22	1.33	1.39
9	AE	102	BCL	C1B-NB	2.22	1.37	1.35
9	S	102	BCL	C3B-CAB	2.22	1.55	1.49
9	X	102	BCL	C4B-NB	2.21	1.37	1.35
9	O	102	BCL	C1D-C2D	-2.20	1.41	1.45
9	AI	102	BCL	C5-C3	2.20	1.55	1.51
9	AL	102	BCL	C1D-C2D	-2.20	1.41	1.45
12	H	302	PEF	O3-C30	2.20	1.44	1.33
7	C	504	HEM	CHB-C1B	2.19	1.40	1.35
9	p	102	BCL	C3C-C4C	2.19	1.54	1.51
9	j	101	BCL	C3D-C4D	-2.19	1.39	1.44
9	Q	101	BCL	C4B-NB	2.19	1.37	1.35
9	x	305	BCL	C3D-C4D	-2.19	1.39	1.44
15	y	404	CRT	C32-C33	-2.19	1.32	1.35
7	C	502	HEM	CHB-C1B	2.18	1.40	1.35
9	e	102	BCL	C3C-C4C	2.18	1.54	1.51
9	m	102	BCL	C3B-CAB	2.18	1.54	1.49
9	1	101	BCL	C3C-C4C	2.18	1.54	1.51
9	p	102	BCL	C3D-C4D	-2.18	1.39	1.44
14	M	404	MQ8	C27-C28	2.18	1.38	1.33
9	x	303	BCL	C1B-NB	2.18	1.37	1.35
9	u	101	BCL	C3B-C2B	-2.18	1.35	1.39
9	N	101	BCL	C1D-C2D	-2.18	1.41	1.45
9	m	103	BCL	C1D-C2D	-2.18	1.41	1.45
9	M	402	BCL	O2D-CGD	-2.18	1.27	1.33
9	AF	101	BCL	C3B-CAB	2.18	1.54	1.49
9	L	303	BCL	C2C-C3C	-2.18	1.48	1.54
9	i	102	BCL	C1B-NB	2.17	1.37	1.35
9	V	102	BCL	C5-C3	2.17	1.55	1.51
9	K	101	BCL	C5-C3	2.17	1.55	1.51
9	I	103	BCL	C3C-C4C	2.17	1.54	1.51
9	M	402	BCL	C2C-C3C	-2.17	1.48	1.54
9	9	102	BCL	C1D-C2D	-2.17	1.41	1.45
9	AG	101	BCL	C1B-NB	2.17	1.37	1.35
7	o	502	HEM	CHA-C4D	2.16	1.40	1.35
7	o	504	HEM	CHB-C1B	2.16	1.40	1.35
9	K	101	BCL	C4B-NB	2.16	1.37	1.35
9	x	303	BCL	C2C-C3C	-2.16	1.48	1.54
11	L	304	UQ8	C28-C29	2.16	1.38	1.33
9	X	102	BCL	C3C-C4C	2.16	1.54	1.51
9	m	103	BCL	C3D-CAD	2.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	101	BCL	C2C-C3C	-2.16	1.48	1.54
9	AB	102	BCL	C3D-C2D	-2.15	1.33	1.39
9	Z	102	BCL	C3B-CAB	2.15	1.54	1.49
14	y	403	MQ8	C32-C33	2.15	1.38	1.33
9	Q	101	BCL	C3C-C4C	2.15	1.54	1.51
9	3	101	BCL	C3D-C4D	-2.15	1.39	1.44
9	w	101	BCL	C1D-C2D	-2.15	1.41	1.45
9	AB	102	BCL	C3D-C4D	-2.15	1.39	1.44
9	x	301	BCL	O1A-CGA	-2.15	1.16	1.22
9	w	101	BCL	C3B-CAB	2.14	1.54	1.49
9	i	102	BCL	C3B-C2B	-2.14	1.35	1.39
9	T	102	BCL	C4B-NB	2.14	1.37	1.35
9	S	102	BCL	C1D-C2D	-2.14	1.41	1.45
7	C	502	HEM	FE-ND	-2.14	1.86	1.96
9	7	102	BCL	O2D-CGD	-2.14	1.28	1.33
9	z	102	BCL	C1D-C2D	-2.14	1.41	1.45
9	1	101	BCL	C5-C3	2.13	1.55	1.51
9	s	102	BCL	C3B-CAB	2.13	1.54	1.49
9	7	102	BCL	C3C-C4C	2.13	1.54	1.51
9	M	401	BCL	C4B-NB	2.13	1.37	1.35
9	G	102	BCL	C3B-CAB	2.13	1.54	1.49
9	y	401	BCL	C1D-C2D	-2.13	1.41	1.45
9	1	101	BCL	C1D-C2D	-2.12	1.41	1.45
9	AB	102	BCL	C1D-C2D	-2.12	1.41	1.45
9	c	101	BCL	C1D-C2D	-2.12	1.41	1.45
9	5	101	BCL	C4B-CHC	-2.12	1.35	1.41
9	z	102	BCL	C3B-CAB	2.12	1.54	1.49
9	F	101	BCL	C3D-C4D	-2.12	1.39	1.44
9	0	102	BCL	C1B-NB	2.12	1.37	1.35
9	0	102	BCL	C4B-NB	2.12	1.37	1.35
9	L	301	BCL	C3B-CAB	2.11	1.54	1.49
9	g	102	BCL	C1D-C2D	-2.11	1.41	1.45
9	p	102	BCL	C2C-C3C	-2.11	1.48	1.54
9	U	101	BCL	C1D-C2D	-2.11	1.41	1.45
9	x	305	BCL	C4B-CHC	-2.11	1.35	1.41
9	P	101	BCL	C4B-NB	2.10	1.37	1.35
9	u	102	BCL	C3C-C4C	2.10	1.54	1.51
9	Q	101	BCL	C2C-C3C	-2.10	1.48	1.54
9	h	101	BCL	C3B-CAB	2.10	1.54	1.49
9	8	101	BCL	C3B-C2B	-2.10	1.35	1.39
7	o	502	HEM	FE-ND	-2.10	1.86	1.96
9	P	101	BCL	C5-C3	2.09	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	103	BCL	C3D-C2D	-2.09	1.33	1.39
9	5	101	BCL	C5-C3	2.09	1.55	1.51
9	AB	101	BCL	C5-C3	2.09	1.55	1.51
7	o	504	HEM	FE-ND	-2.08	1.86	1.96
9	AG	101	BCL	C4B-NB	2.08	1.37	1.35
7	C	502	HEM	C1D-ND	-2.08	1.34	1.38
9	P	101	BCL	C1B-NB	2.08	1.37	1.35
9	d	101	BCL	C2C-C3C	-2.08	1.48	1.54
9	k	102	BCL	C3D-C4D	-2.08	1.39	1.44
9	R	102	BCL	C3D-C2D	-2.08	1.33	1.39
14	y	403	MQ8	C12-C13	2.08	1.38	1.33
9	x	305	BCL	C4B-NB	2.08	1.37	1.35
9	l	101	BCL	C3B-CAB	2.07	1.54	1.49
9	V	102	BCL	C1B-NB	2.07	1.37	1.35
9	0	102	BCL	C5-C3	2.07	1.55	1.51
9	e	102	BCL	OBB-CAB	-2.07	1.16	1.22
9	AK	101	BCL	C2C-C3C	-2.07	1.48	1.54
9	R	102	BCL	C5-C3	2.07	1.55	1.51
9	N	101	BCL	C3D-C4D	-2.07	1.39	1.44
9	V	102	BCL	C1D-C2D	-2.07	1.41	1.45
14	M	404	MQ8	C37-C38	2.07	1.37	1.33
9	4	102	BCL	C3D-C4D	-2.06	1.39	1.44
9	y	401	BCL	C3D-C4D	-2.06	1.39	1.44
9	g	102	BCL	C3D-C2D	-2.06	1.33	1.39
9	M	401	BCL	C3D-C2D	-2.06	1.33	1.39
9	8	101	BCL	C5-C3	2.06	1.55	1.51
9	AE	102	BCL	C1D-C2D	-2.06	1.41	1.45
9	L	301	BCL	C3D-C2D	-2.06	1.33	1.39
9	W	101	BCL	C3B-C2B	-2.06	1.35	1.39
9	9	102	BCL	C3B-C2B	-2.06	1.35	1.39
9	AH	101	BCL	C3D-CAD	2.06	1.52	1.45
9	O	102	BCL	C3D-C2D	-2.06	1.33	1.39
11	L	304	UQ8	C4-C3	2.05	1.44	1.36
9	g	102	BCL	C3D-C4D	-2.05	1.39	1.44
9	AC	102	BCL	C4B-CHC	-2.05	1.35	1.41
9	l	101	BCL	C4B-NB	2.05	1.37	1.35
9	2	102	BCL	C3B-C2B	-2.05	1.35	1.39
9	l	101	BCL	C3D-C4D	-2.05	1.39	1.44
7	C	501	HEM	C1D-ND	-2.05	1.34	1.38
9	m	102	BCL	C3C-C4C	2.05	1.54	1.51
9	R	102	BCL	C3D-C4D	-2.04	1.39	1.44
9	R	102	BCL	C3B-CAB	2.04	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	101	BCL	C3B-CAB	2.04	1.54	1.49
9	T	102	BCL	C2C-C3C	-2.04	1.48	1.54
9	AC	103	BCL	C5-C3	2.04	1.55	1.51
9	1	101	BCL	C1B-NB	2.04	1.37	1.35
9	D	101	BCL	C3C-C4C	2.04	1.54	1.51
9	7	102	BCL	C4B-NB	2.04	1.37	1.35
9	k	102	BCL	C4B-NB	2.04	1.37	1.35
9	AC	103	BCL	C3D-C4D	-2.04	1.39	1.44
9	W	101	BCL	C1A-CHA	-2.04	1.34	1.43
9	7	102	BCL	C3D-C4D	-2.03	1.39	1.44
9	O	102	BCL	C4B-NB	2.03	1.37	1.35
9	3	101	BCL	C3B-C2B	-2.03	1.35	1.39
9	M	402	BCL	C4B-NB	2.03	1.37	1.35
9	Y	101	BCL	C2C-C3C	-2.03	1.48	1.54
9	A	103	BCL	C2C-C3C	-2.02	1.48	1.54
9	j	101	BCL	C1D-C2D	-2.02	1.41	1.45
9	d	101	BCL	C3B-CAB	2.02	1.54	1.49
9	P	101	BCL	C3D-C4D	-2.02	1.39	1.44
9	L	301	BCL	C3D-C4D	-2.02	1.39	1.44
9	F	101	BCL	C1B-NB	2.02	1.37	1.35
9	4	102	BCL	C3B-CAB	2.02	1.54	1.49
9	AI	101	BCL	C3B-CAB	2.02	1.54	1.49
9	g	102	BCL	C3B-CAB	2.02	1.54	1.49
9	AH	101	BCL	C1A-CHA	-2.02	1.34	1.43
9	X	102	BCL	C1B-NB	2.02	1.37	1.35
9	7	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	w	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	I	103	BCL	C3D-C4D	-2.01	1.39	1.44
9	u	102	BCL	C5-C3	2.01	1.55	1.51
9	y	401	BCL	C3D-C2D	-2.01	1.33	1.39
9	f	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	h	101	BCL	C4B-NB	2.01	1.37	1.35
9	I	103	BCL	C3D-C2D	-2.01	1.33	1.39
9	AL	102	BCL	C3D-C2D	-2.01	1.33	1.39
11	x	304	UQ8	C26-C24	2.01	1.55	1.51
9	AI	102	BCL	C3B-C2B	-2.00	1.35	1.39
9	I	101	BCL	C3C-C4C	2.00	1.54	1.51
9	p	102	BCL	C4B-CHC	-2.00	1.35	1.41
9	q	102	BCL	C3D-C4D	-2.00	1.39	1.44
9	AI	101	BCL	C5-C3	2.00	1.55	1.51
9	8	101	BCL	C1A-CHA	-2.00	1.34	1.43

All (2759) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	405	CRT	C2-C1-C4	-19.64	80.71	110.86
15	0	101	CRT	C2-C1-C4	-19.23	81.33	110.86
15	T	101	CRT	C3-C1-C4	-18.63	82.26	110.86
15	G	101	CRT	C2-C1-C4	-18.42	82.58	110.86
15	y	404	CRT	C3-C1-C4	-17.75	83.61	110.86
15	4	101	CRT	C3-C1-C4	-17.61	83.82	110.86
15	O	101	CRT	C2-C1-C4	-17.60	83.83	110.86
15	z	101	CRT	C2-C1-C4	-17.56	83.90	110.86
15	n	101	CRT	C2-C1-C4	-17.42	84.12	110.86
15	I	102	CRT	C3-C1-C4	-17.34	84.23	110.86
15	v	101	CRT	C3-C1-C4	-17.28	84.33	110.86
15	k	101	CRT	C2-C1-C4	-16.83	85.02	110.86
15	q	101	CRT	C2-C1-C4	-16.75	85.14	110.86
15	g	101	CRT	C2-C1-C4	-16.71	85.21	110.86
15	AH	102	CRT	C2-C1-C4	-16.46	85.59	110.86
15	V	101	CRT	C2-C1-C4	-16.34	85.78	110.86
15	4	101	CRT	C2-C1-C4	-16.20	85.99	110.86
15	n	101	CRT	C3-C1-C4	-16.15	86.07	110.86
15	q	101	CRT	C3-C1-C4	-15.79	86.62	110.86
15	7	103	CRT	C3-C1-C4	-15.76	86.66	110.86
15	g	101	CRT	C3-C1-C4	-15.72	86.73	110.86
15	7	103	CRT	C2-C1-C4	-15.70	86.76	110.86
15	AF	102	CRT	C3-C1-C4	-15.68	86.79	110.86
15	s	101	CRT	C2-C1-C4	-15.56	86.97	110.86
15	T	101	CRT	C2-C1-C4	-15.44	87.15	110.86
15	m	104	CRT	C2-C1-C4	-15.40	87.22	110.86
15	7	101	CRT	C2-C1-C4	-15.27	87.42	110.86
15	i	101	CRT	C2-C1-C4	-15.27	87.42	110.86
15	9	101	CRT	C2-C1-C4	-15.26	87.43	110.86
15	O	101	CRT	C3-C1-C4	-15.20	87.53	110.86
15	E	101	CRT	C2-C1-C4	-15.18	87.55	110.86
15	AF	102	CRT	C2-C1-C4	-15.10	87.68	110.86
15	R	101	CRT	C2-C1-C4	-14.96	87.89	110.86
15	k	101	CRT	C3-C1-C4	-14.86	88.05	110.86
15	M	405	CRT	C3-C1-C4	-14.71	88.27	110.86
15	AD	101	CRT	C2-C1-C4	-14.43	88.71	110.86
15	G	101	CRT	C3-C1-C4	-14.32	88.87	110.86
15	AD	101	CRT	C3-C1-C4	-14.18	89.09	110.86
15	i	101	CRT	C3-C1-C4	-14.11	89.19	110.86
15	9	101	CRT	C3-C1-C4	-13.91	89.50	110.86
15	y	404	CRT	C2-C1-C4	-13.84	89.61	110.86
15	z	101	CRT	C3-C1-C4	-13.52	90.11	110.86
15	m	104	CRT	C3-C1-C4	-13.51	90.12	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	101	CRT	C3-C1-C4	-12.99	90.91	110.86
15	7	101	CRT	C3-C1-C4	-12.64	91.46	110.86
15	I	102	CRT	C2-C1-C4	-12.47	91.72	110.86
15	E	101	CRT	C3-C1-C4	-12.43	91.77	110.86
15	AH	102	CRT	C3-C1-C4	-11.94	92.52	110.86
15	s	101	CRT	C3-C1-C4	-11.79	92.76	110.86
15	v	101	CRT	C2-C1-C4	-11.57	93.09	110.86
15	V	101	CRT	C3-C1-C4	-10.16	95.26	110.86
15	0	101	CRT	C3-C1-C4	-10.03	95.45	110.86
15	g	101	CRT	C31-C32-C33	-8.99	114.47	127.31
10	L	302	BPH	O2D-CGD-CBD	8.63	121.93	111.00
10	M	403	BPH	O2D-CGD-CBD	8.20	121.39	111.00
9	x	301	BCL	C4A-NA-C1A	7.88	110.25	106.71
9	x	305	BCL	CAC-C3C-C2C	-7.62	95.23	114.26
9	x	301	BCL	O2D-CGD-CBD	7.59	124.76	111.27
7	C	501	HEM	CBA-CAA-C2A	-7.59	99.66	112.62
12	y	408	PEF	C2-O2-C10	-7.51	103.90	117.90
15	AF	102	CRT	C21-C22-C23	-7.50	116.61	127.31
9	R	102	BCL	CMB-C2B-C1B	-7.35	117.17	128.46
9	s	102	BCL	CMB-C2B-C1B	-7.31	117.23	128.46
9	y	401	BCL	CAC-C3C-C2C	-7.17	96.34	114.26
15	M	405	CRT	C3-C1-C2	7.16	123.84	110.37
15	T	101	CRT	C3-C1-C2	7.10	123.72	110.37
9	f	101	BCL	CMB-C2B-C1B	-7.08	117.58	128.46
9	AI	101	BCL	CMB-C2B-C1B	-7.07	117.60	128.46
9	M	401	BCL	C4A-NA-C1A	7.06	109.88	106.71
9	AH	101	BCL	CMB-C2B-C1B	-7.05	117.62	128.46
9	P	101	BCL	CMB-C2B-C1B	-7.02	117.68	128.46
9	q	102	BCL	CAC-C3C-C2C	-6.97	96.84	114.26
12	y	406	PEF	O2-C10-C11	6.97	123.90	111.09
9	AI	102	BCL	CMB-C2B-C1B	-6.92	117.82	128.46
7	C	502	HEM	C1B-NB-C4B	6.87	112.17	105.07
9	3	101	BCL	CMB-C2B-C1B	-6.86	117.92	128.46
9	4	102	BCL	O2D-CGD-CBD	6.86	123.46	111.27
9	D	102	BCL	CMB-C2B-C1B	-6.85	117.94	128.46
9	K	101	BCL	CMB-C2B-C1B	-6.84	117.94	128.46
9	AI	102	BCL	O2D-CGD-CBD	6.83	123.41	111.27
9	O	102	BCL	CMB-C2B-C1B	-6.82	117.98	128.46
9	N	101	BCL	CMB-C2B-C1B	-6.82	117.98	128.46
9	1	101	BCL	CMB-C2B-C1B	-6.78	118.04	128.46
9	7	102	BCL	C1D-ND-C4D	-6.78	101.52	106.33
9	Z	102	BCL	O2D-CGD-CBD	6.77	123.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	102	BCL	CMB-C2B-C1B	-6.75	118.08	128.46
15	n	101	CRT	C3-C1-C2	6.75	123.07	110.37
7	o	502	HEM	C1B-NB-C4B	6.75	112.05	105.07
9	p	102	BCL	CMB-C2B-C1B	-6.75	118.09	128.46
15	I	102	CRT	C3-C1-C2	6.73	123.03	110.37
15	7	101	CRT	C26-C27-C28	-6.72	117.72	127.31
9	M	401	BCL	CAC-C3C-C2C	-6.70	97.51	114.26
9	I	103	BCL	CMB-C2B-C1B	-6.66	118.22	128.46
9	u	102	BCL	CMB-C2B-C1B	-6.66	118.23	128.46
9	c	101	BCL	CMB-C2B-C1B	-6.66	118.23	128.46
15	AD	101	CRT	C3-C1-C2	6.65	122.88	110.37
9	G	102	BCL	CMB-C2B-C1B	-6.62	118.28	128.46
9	F	101	BCL	CMB-C2B-C1B	-6.61	118.30	128.46
15	O	101	CRT	C21-C22-C23	-6.61	117.88	127.31
9	x	303	BCL	CMB-C2B-C1B	-6.60	118.31	128.46
9	AB	102	BCL	CMB-C2B-C1B	-6.58	118.35	128.46
9	e	102	BCL	CMB-C2B-C1B	-6.53	118.43	128.46
10	x	302	BPH	O2D-CGD-CBD	6.52	119.26	111.00
9	j	101	BCL	CMB-C2B-C1B	-6.52	118.44	128.46
9	AF	101	BCL	CMB-C2B-C1B	-6.52	118.45	128.46
9	k	102	BCL	CMB-C2B-C1B	-6.50	118.48	128.46
9	S	102	BCL	CMB-C2B-C1B	-6.49	118.48	128.46
9	g	102	BCL	CMB-C2B-C1B	-6.45	118.54	128.46
9	i	102	BCL	CMB-C2B-C1B	-6.44	118.56	128.46
9	AK	101	BCL	CMB-C2B-C1B	-6.42	118.59	128.46
9	L	303	BCL	CMA-C3A-C4A	-6.42	94.52	111.77
9	A	103	BCL	CMB-C2B-C1B	-6.40	118.62	128.46
9	Z	102	BCL	CMB-C2B-C1B	-6.40	118.63	128.46
9	X	102	BCL	O2D-CGD-CBD	6.40	122.64	111.27
9	d	101	BCL	CMB-C2B-C1B	-6.39	118.64	128.46
9	AG	101	BCL	C1D-ND-C4D	-6.38	101.81	106.33
15	AH	102	CRT	C3-C1-C2	6.37	122.36	110.37
9	6	101	BCL	CAC-C3C-C2C	-6.36	98.37	114.26
9	q	102	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
9	A	102	BCL	CMB-C2B-C1B	-6.33	118.73	128.46
9	l	101	BCL	CMB-C2B-C1B	-6.33	118.74	128.46
10	y	402	BPH	O2D-CGD-CBD	6.33	119.01	111.00
9	j	101	BCL	C1D-ND-C4D	-6.32	101.84	106.33
15	9	101	CRT	C21-C22-C23	-6.32	118.30	127.31
15	V	101	CRT	C21-C22-C23	-6.31	118.30	127.31
9	L	301	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
15	AJ	101	CRT	C10-C9-C7	-6.29	118.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	101	BCL	CMB-C2B-C1B	-6.29	118.79	128.46
9	r	101	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
9	q	102	BCL	O2D-CGD-CBD	6.28	122.43	111.27
9	AE	102	BCL	CMB-C2B-C1B	-6.26	118.83	128.46
15	k	101	CRT	C3-C1-C2	6.26	122.14	110.37
7	C	502	HEM	CHC-C4B-NB	6.26	131.23	124.43
9	Z	102	BCL	O2D-CGD-O1D	-6.26	111.61	123.84
9	x	305	BCL	C4A-NA-C1A	6.24	109.51	106.71
9	5	101	BCL	CAC-C3C-C2C	-6.23	98.68	114.26
9	8	101	BCL	CMB-C2B-C1B	-6.23	118.90	128.46
15	q	101	CRT	C3-C1-C2	6.21	122.05	110.37
9	R	102	BCL	C1D-ND-C4D	-6.20	101.93	106.33
9	w	101	BCL	CMB-C2B-C1B	-6.19	118.95	128.46
9	m	103	BCL	CMB-C2B-C1B	-6.19	118.95	128.46
9	Q	101	BCL	CMB-C2B-C1B	-6.18	118.96	128.46
9	0	102	BCL	CMB-C2B-C1B	-6.18	118.96	128.46
9	p	102	BCL	CAC-C3C-C2C	-6.18	98.82	114.26
9	R	102	BCL	C2D-C1D-ND	6.17	114.65	110.10
9	2	102	BCL	O2D-CGD-CBD	6.16	122.21	111.27
9	A	103	BCL	O2D-CGD-CBD	6.16	122.21	111.27
9	AB	101	BCL	CMB-C2B-C1B	-6.15	119.02	128.46
9	AG	101	BCL	C2D-C1D-ND	6.14	114.63	110.10
9	X	102	BCL	C2D-C1D-ND	6.13	114.62	110.10
9	8	101	BCL	O2D-CGD-CBD	6.13	122.17	111.27
9	AL	102	BCL	CMB-C2B-C1B	-6.09	119.11	128.46
9	8	101	BCL	C1D-ND-C4D	-6.08	102.02	106.33
9	m	102	BCL	CMB-C2B-C1B	-6.05	119.17	128.46
9	D	101	BCL	C2D-C1D-ND	6.04	114.55	110.10
9	m	102	BCL	C2D-C1D-ND	6.04	114.55	110.10
9	u	102	BCL	C2D-C1D-ND	6.02	114.54	110.10
9	I	103	BCL	O2D-CGD-CBD	6.02	121.96	111.27
9	y	401	BCL	C1D-ND-C4D	-6.00	102.07	106.33
9	T	102	BCL	C2D-C1D-ND	6.00	114.53	110.10
9	M	402	BCL	C1D-ND-C4D	-6.00	102.07	106.33
9	M	401	BCL	C1D-ND-C4D	-5.99	102.08	106.33
15	R	101	CRT	C3-C1-C2	5.99	121.63	110.37
9	h	101	BCL	C1D-ND-C4D	-5.97	102.09	106.33
7	o	502	HEM	CHC-C4B-NB	5.95	130.90	124.43
9	e	102	BCL	O2D-CGD-CBD	5.95	121.84	111.27
12	t	303	PEF	C2-O2-C10	-5.95	106.81	117.90
9	s	102	BCL	O2D-CGD-CBD	5.94	121.82	111.27
9	6	101	BCL	CMB-C2B-C1B	-5.93	119.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AC	103	BCL	C1D-ND-C4D	-5.93	102.12	106.33
9	M	402	BCL	O2D-CGD-CBD	5.93	121.80	111.27
15	v	101	CRT	C5-C6-C7	5.92	134.84	125.89
9	L	303	BCL	CMB-C2B-C1B	-5.91	119.38	128.46
9	N	101	BCL	O2D-CGD-CBD	5.91	121.78	111.27
9	T	102	BCL	CMB-C2B-C1B	-5.91	119.38	128.46
9	m	102	BCL	C1D-ND-C4D	-5.90	102.14	106.33
9	x	305	BCL	C2D-C1D-ND	5.89	114.44	110.10
9	k	102	BCL	C1D-ND-C4D	-5.88	102.16	106.33
9	i	102	BCL	C1D-ND-C4D	-5.87	102.16	106.33
15	O	101	CRT	C3-C1-C2	5.83	121.34	110.37
9	u	102	BCL	C1D-ND-C4D	-5.83	102.20	106.33
9	2	102	BCL	CMB-C2B-C1B	-5.82	119.52	128.46
9	s	102	BCL	C2D-C1D-ND	5.82	114.39	110.10
9	9	102	BCL	CMB-C2B-C1B	-5.81	119.53	128.46
9	f	101	BCL	O2D-CGD-CBD	5.81	121.60	111.27
9	M	402	BCL	CMB-C2B-C1B	-5.80	119.54	128.46
9	I	101	BCL	CMB-C2B-C1B	-5.78	119.57	128.46
9	x	301	BCL	CAC-C3C-C2C	-5.78	99.81	114.26
9	z	102	BCL	CMB-C2B-C1B	-5.78	119.58	128.46
9	AG	101	BCL	CMB-C2B-C1B	-5.77	119.59	128.46
9	D	101	BCL	C1D-ND-C4D	-5.76	102.24	106.33
7	C	504	HEM	C1B-NB-C4B	5.75	111.02	105.07
9	Y	101	BCL	CMB-C2B-C1B	-5.75	119.62	128.46
9	Y	101	BCL	CAC-C3C-C2C	-5.74	99.92	114.26
9	AC	103	BCL	C2D-C1D-ND	5.72	114.32	110.10
9	m	103	BCL	O2D-CGD-CBD	5.71	121.42	111.27
9	M	402	BCL	CAC-C3C-C2C	-5.71	99.98	114.26
15	AC	101	CRT	C26-C27-C28	-5.71	119.17	127.31
9	D	102	BCL	C2D-C1D-ND	5.70	114.31	110.10
9	l	101	BCL	C1D-ND-C4D	-5.70	102.29	106.33
12	H	302	PEF	O2-C10-C11	5.69	121.56	111.09
15	v	101	CRT	C3-C1-C2	5.69	121.07	110.37
9	K	101	BCL	C2D-C1D-ND	5.68	114.29	110.10
9	x	303	BCL	C2D-C1D-ND	5.67	114.28	110.10
15	I	102	CRT	C21-C22-C23	-5.66	119.23	127.31
9	4	102	BCL	CMB-C2B-C1B	-5.66	119.77	128.46
9	AC	103	BCL	O2D-CGD-CBD	5.65	121.31	111.27
9	M	402	BCL	O2D-CGD-O1D	-5.65	112.79	123.84
9	Y	101	BCL	CHD-C1D-ND	-5.65	119.26	124.45
15	z	101	CRT	C21-C22-C23	-5.64	119.25	127.31
9	W	101	BCL	CMB-C2B-C1B	-5.64	119.79	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	102	BCL	CAC-C3C-C2C	-5.64	100.16	114.26
9	AC	103	BCL	CMB-C2B-C1B	-5.64	119.79	128.46
9	G	102	BCL	CAC-C3C-C2C	-5.64	100.17	114.26
9	Q	101	BCL	C1D-ND-C4D	-5.64	102.33	106.33
9	4	102	BCL	C1D-ND-C4D	-5.64	102.33	106.33
9	l	101	BCL	O2D-CGD-CBD	5.64	121.28	111.27
9	AI	102	BCL	O2D-CGD-O1D	-5.63	112.82	123.84
9	Z	102	BCL	C2D-C1D-ND	5.63	114.25	110.10
9	X	102	BCL	CMB-C2B-C1B	-5.63	119.81	128.46
9	U	101	BCL	CAC-C3C-C2C	-5.62	100.22	114.26
7	C	503	HEM	C1B-NB-C4B	5.62	110.88	105.07
9	h	101	BCL	CMB-C2B-C1B	-5.62	119.83	128.46
15	7	101	CRT	C3-C1-C2	5.62	120.93	110.37
9	AL	102	BCL	C1D-ND-C4D	-5.61	102.35	106.33
9	u	101	BCL	CMB-C2B-C1B	-5.61	119.85	128.46
9	5	101	BCL	CMB-C2B-C1B	-5.60	119.86	128.46
9	X	102	BCL	O2D-CGD-O1D	-5.59	112.91	123.84
9	T	102	BCL	C1D-ND-C4D	-5.58	102.37	106.33
9	AL	102	BCL	O2D-CGD-CBD	5.58	121.18	111.27
9	X	102	BCL	C1D-ND-C4D	-5.58	102.37	106.33
7	o	501	HEM	CBD-CAD-C3D	-5.58	97.14	112.63
9	A	103	BCL	O2D-CGD-O1D	-5.56	112.96	123.84
9	x	303	BCL	C1D-ND-C4D	-5.56	102.38	106.33
9	d	101	BCL	O2D-CGD-O1D	-5.56	112.97	123.84
9	1	101	BCL	O2D-CGD-CBD	5.56	121.14	111.27
9	3	101	BCL	C1D-ND-C4D	-5.56	102.39	106.33
9	s	102	BCL	C1D-ND-C4D	-5.56	102.39	106.33
15	G	101	CRT	C3-C1-C2	5.55	120.82	110.37
9	5	101	BCL	O2D-CGD-CBD	5.55	121.12	111.27
9	AB	101	BCL	O2D-CGD-CBD	5.55	121.12	111.27
9	L	301	BCL	C1D-ND-C4D	-5.53	102.41	106.33
9	K	101	BCL	C1D-ND-C4D	-5.52	102.41	106.33
15	0	101	CRT	C3-C1-C2	5.52	120.76	110.37
9	O	102	BCL	C1D-ND-C4D	-5.52	102.41	106.33
9	M	401	BCL	CMB-C2B-C1B	-5.52	119.98	128.46
7	o	501	HEM	C4D-ND-C1D	5.48	110.74	105.07
9	9	102	BCL	O2D-CGD-CBD	5.48	121.01	111.27
9	F	101	BCL	O2D-CGD-CBD	5.48	121.00	111.27
9	4	102	BCL	C2D-C1D-ND	5.48	114.14	110.10
15	4	101	CRT	C3-C1-C2	5.48	120.67	110.37
9	9	102	BCL	C1D-ND-C4D	-5.47	102.45	106.33
9	1	101	BCL	O2D-CGD-O1D	-5.44	113.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	102	BCL	O2D-CGD-O1D	-5.44	113.19	123.84
9	AK	101	BCL	O2D-CGD-CBD	5.44	120.94	111.27
9	x	305	BCL	O2D-CGD-CBD	5.44	120.94	111.27
9	p	102	BCL	O2D-CGD-CBD	5.44	120.93	111.27
9	1	101	BCL	C1D-ND-C4D	-5.43	102.48	106.33
9	AK	101	BCL	C2D-C1D-ND	5.42	114.10	110.10
15	v	101	CRT	C6-C7-C9	-5.42	110.63	118.94
9	L	301	BCL	CAC-C3C-C2C	-5.40	100.76	114.26
9	c	101	BCL	O2D-CGD-CBD	5.40	120.86	111.27
9	4	102	BCL	O2D-CGD-O1D	-5.39	113.29	123.84
15	g	101	CRT	C3-C1-C2	5.39	120.51	110.37
9	AG	101	BCL	O2D-CGD-O1D	-5.39	113.30	123.84
9	V	102	BCL	CAC-C3C-C2C	-5.39	100.79	114.26
9	5	101	BCL	C1D-ND-C4D	-5.39	102.51	106.33
9	D	102	BCL	O2D-CGD-CBD	5.39	120.84	111.27
9	Q	101	BCL	C1C-NC-C4C	-5.38	104.29	106.71
9	L	303	BCL	CAC-C3C-C2C	-5.37	100.83	114.26
15	E	101	CRT	C3-C1-C2	5.37	120.48	110.37
9	u	101	BCL	C1D-ND-C4D	-5.36	102.52	106.33
9	8	101	BCL	O2D-CGD-O1D	-5.36	113.35	123.84
9	1	101	BCL	CAC-C3C-C2C	-5.36	100.87	114.26
9	AB	102	BCL	C1D-ND-C4D	-5.35	102.53	106.33
9	AG	101	BCL	O2D-CGD-CBD	5.35	120.77	111.27
9	AC	103	BCL	O2D-CGD-O1D	-5.34	113.39	123.84
7	C	501	HEM	CBD-CAD-C3D	-5.34	97.78	112.63
9	k	102	BCL	C2D-C1D-ND	5.34	114.04	110.10
9	i	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
9	z	102	BCL	C1D-ND-C4D	-5.33	102.55	106.33
9	AC	102	BCL	C1D-ND-C4D	-5.33	102.55	106.33
9	AE	102	BCL	C4D-CHA-C1A	5.32	127.72	121.25
9	w	101	BCL	O2D-CGD-O1D	-5.32	113.44	123.84
9	L	301	BCL	C4A-NA-C1A	5.32	109.10	106.71
9	W	101	BCL	C1D-ND-C4D	-5.31	102.56	106.33
9	AE	102	BCL	C1D-ND-C4D	-5.30	102.57	106.33
9	6	101	BCL	C2D-C1D-ND	5.30	114.01	110.10
9	U	101	BCL	C4D-CHA-C1A	5.30	127.70	121.25
9	I	103	BCL	C1D-ND-C4D	-5.30	102.57	106.33
9	u	101	BCL	CHD-C1D-ND	-5.30	119.59	124.45
9	V	102	BCL	C1D-ND-C4D	-5.30	102.57	106.33
9	O	102	BCL	C2D-C1D-ND	5.29	114.00	110.10
9	d	101	BCL	O2D-CGD-CBD	5.28	120.66	111.27
9	y	401	BCL	CMB-C2B-C1B	-5.27	120.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	101	BCL	O2D-CGD-O1D	-5.25	113.58	123.84
9	AF	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
15	y	404	CRT	C3-C1-C2	5.24	120.22	110.37
9	l	101	BCL	C2D-C1D-ND	5.24	113.96	110.10
9	AL	102	BCL	CAC-C3C-C2C	-5.23	101.18	114.26
9	3	101	BCL	CHD-C1D-ND	-5.23	119.65	124.45
9	0	102	BCL	O2D-CGD-CBD	5.23	120.56	111.27
9	AC	102	BCL	O2D-CGD-CBD	5.23	120.56	111.27
9	AH	101	BCL	C1D-ND-C4D	-5.21	102.63	106.33
9	2	102	BCL	O2D-CGD-O1D	-5.21	113.65	123.84
9	D	102	BCL	C1D-ND-C4D	-5.21	102.63	106.33
9	q	102	BCL	O2D-CGD-O1D	-5.21	113.65	123.84
9	N	101	BCL	C1D-ND-C4D	-5.21	102.63	106.33
9	D	101	BCL	CMB-C2B-C1B	-5.19	120.48	128.46
9	R	102	BCL	CHD-C1D-ND	-5.19	119.68	124.45
9	I	103	BCL	C2D-C1D-ND	5.19	113.93	110.10
9	7	102	BCL	CMB-C2B-C1B	-5.19	120.49	128.46
15	7	103	CRT	C3-C1-C2	5.18	120.12	110.37
9	I	101	BCL	C2D-C1D-ND	5.17	113.92	110.10
12	M	408	PEF	O2-C10-C11	5.17	120.59	111.09
9	AE	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
9	h	101	BCL	O2D-CGD-CBD	5.16	120.44	111.27
9	AC	102	BCL	O2D-CGD-O1D	-5.15	113.77	123.84
9	x	301	BCL	O2D-CGD-O1D	-5.15	113.77	123.84
9	5	101	BCL	O2D-CGD-O1D	-5.15	113.77	123.84
9	I	101	BCL	CAC-C3C-C2C	-5.15	101.40	114.26
9	u	101	BCL	O2D-CGD-CBD	5.14	120.41	111.27
9	AC	102	BCL	CMB-C2B-C1B	-5.14	120.56	128.46
9	S	102	BCL	CHD-C1D-ND	-5.14	119.73	124.45
9	AI	102	BCL	CAC-C3C-C2C	-5.13	101.44	114.26
15	X	101	CRT	C21-C20-C19	5.13	133.97	123.47
9	N	101	BCL	O2D-CGD-O1D	-5.12	113.82	123.84
7	C	501	HEM	C4D-ND-C1D	5.12	110.37	105.07
9	5	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
9	x	305	BCL	C1D-ND-C4D	-5.12	102.70	106.33
9	s	102	BCL	CHD-C1D-ND	-5.11	119.75	124.45
9	AC	103	BCL	CAC-C3C-C2C	-5.11	101.48	114.26
7	C	502	HEM	CAD-CBD-CGD	-5.11	102.61	113.60
9	A	102	BCL	C2D-C1D-ND	5.10	113.87	110.10
9	f	101	BCL	CAC-C3C-C2C	-5.10	101.51	114.26
9	K	101	BCL	O2D-CGD-CBD	5.10	120.33	111.27
9	d	101	BCL	CAC-C3C-C2C	-5.09	101.55	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	c	101	BCL	C1D-ND-C4D	-5.09	102.72	106.33
10	M	403	BPH	O1D-CGD-CBD	-5.09	116.27	124.74
9	A	103	BCL	C1D-ND-C4D	-5.08	102.72	106.33
9	j	101	BCL	O2D-CGD-O1D	-5.08	113.90	123.84
9	u	102	BCL	O2D-CGD-CBD	5.08	120.30	111.27
15	G	101	CRT	C21-C22-C23	-5.08	120.06	127.31
15	AF	102	CRT	C3-C1-C2	5.06	119.88	110.37
9	AI	102	BCL	CHD-C1D-ND	-5.05	119.81	124.45
15	4	101	CRT	C31-C32-C33	-5.05	120.10	127.31
9	F	101	BCL	O2D-CGD-O1D	-5.05	113.97	123.84
9	7	102	BCL	O2D-CGD-CBD	5.05	120.24	111.27
9	u	101	BCL	CAC-C3C-C2C	-5.05	101.65	114.26
9	p	102	BCL	C1D-ND-C4D	-5.04	102.75	106.33
9	w	101	BCL	C1D-ND-C4D	-5.04	102.75	106.33
9	z	102	BCL	O2D-CGD-CBD	5.04	120.22	111.27
9	7	102	BCL	C2D-C1D-ND	5.03	113.81	110.10
9	c	101	BCL	C2D-C1D-ND	5.03	113.81	110.10
7	C	501	HEM	C1B-NB-C4B	5.03	110.27	105.07
9	6	101	BCL	C1D-ND-C4D	-5.03	102.76	106.33
9	P	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
9	AE	102	BCL	O2D-CGD-CBD	5.02	120.19	111.27
7	o	504	HEM	C1B-NB-C4B	5.02	110.25	105.07
9	k	102	BCL	CAC-C3C-C2C	-5.01	101.73	114.26
9	AI	102	BCL	C1D-ND-C4D	-5.01	102.77	106.33
9	g	102	BCL	C1D-ND-C4D	-5.01	102.77	106.33
9	e	102	BCL	CAC-C3C-C2C	-5.01	101.75	114.26
9	AB	101	BCL	O2D-CGD-O1D	-5.00	114.05	123.84
9	V	102	BCL	C4D-CHA-C1A	5.00	127.34	121.25
12	A	101	PEF	O2-C10-C11	5.00	120.29	111.09
15	4	101	CRT	C21-C20-C19	-5.00	113.23	123.47
9	U	101	BCL	O2D-CGD-O1D	-5.00	114.07	123.84
9	8	101	BCL	C2D-C1D-ND	4.99	113.78	110.10
9	i	102	BCL	O2D-CGD-O1D	-4.99	114.08	123.84
9	q	102	BCL	C1D-ND-C4D	-4.99	102.79	106.33
9	z	102	BCL	CHD-C1D-ND	-4.98	119.87	124.45
15	I	102	CRT	C5-C6-C7	4.98	133.42	125.89
9	A	103	BCL	C2D-C1D-ND	4.98	113.77	110.10
9	r	101	BCL	CAC-C3C-C2C	-4.97	101.84	114.26
9	L	303	BCL	C1D-ND-C4D	-4.97	102.81	106.33
15	V	101	CRT	C3-C1-C2	4.97	119.72	110.37
9	9	102	BCL	CAC-C3C-C2C	-4.96	101.85	114.26
9	T	102	BCL	O2D-CGD-CBD	4.95	120.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AD	101	CRT	C21-C22-C23	-4.95	120.24	127.31
9	m	102	BCL	O2D-CGD-CBD	4.95	120.06	111.27
9	A	102	BCL	C1D-ND-C4D	-4.95	102.82	106.33
9	F	101	BCL	C1D-ND-C4D	-4.95	102.82	106.33
9	A	102	BCL	O2D-CGD-CBD	4.95	120.06	111.27
9	AF	101	BCL	C1D-ND-C4D	-4.95	102.82	106.33
9	x	303	BCL	CMB-C2B-C3B	4.94	133.92	124.68
9	9	102	BCL	C2D-C1D-ND	4.94	113.75	110.10
9	j	101	BCL	O2D-CGD-CBD	4.93	120.03	111.27
9	AC	102	BCL	C2D-C1D-ND	4.93	113.74	110.10
15	v	101	CRT	C8-C7-C6	4.93	125.84	118.08
9	6	101	BCL	O2D-CGD-CBD	4.92	120.01	111.27
15	AC	101	CRT	C21-C22-C23	-4.91	120.30	127.31
9	F	101	BCL	C2D-C1D-ND	4.91	113.72	110.10
9	u	102	BCL	C1C-NC-C4C	-4.90	104.50	106.71
9	A	102	BCL	CAC-C3C-C2C	-4.90	102.02	114.26
9	I	101	BCL	C1D-ND-C4D	-4.90	102.86	106.33
9	f	101	BCL	C2D-C1D-ND	4.90	113.71	110.10
9	z	102	BCL	C2D-C1D-ND	4.89	113.71	110.10
9	AH	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
9	k	102	BCL	CHD-C1D-ND	-4.89	119.96	124.45
9	0	102	BCL	C2D-C1D-ND	4.89	113.71	110.10
9	I	101	BCL	O2D-CGD-CBD	4.89	119.95	111.27
9	AC	102	BCL	C4D-CHA-C1A	4.88	127.19	121.25
9	AK	101	BCL	C1D-ND-C4D	-4.88	102.87	106.33
9	m	103	BCL	C2D-C1D-ND	4.88	113.70	110.10
15	7	103	CRT	C20-C19-C17	-4.88	120.35	127.31
9	AC	102	BCL	CAC-C3C-C2C	-4.87	102.08	114.26
9	x	301	BCL	CMB-C2B-C1B	-4.87	120.98	128.46
9	g	102	BCL	CAC-C3C-C2C	-4.87	102.10	114.26
9	m	103	BCL	C1D-ND-C4D	-4.86	102.88	106.33
9	Y	101	BCL	O2D-CGD-O1D	-4.86	114.33	123.84
9	r	101	BCL	C1D-ND-C4D	-4.86	102.89	106.33
9	x	305	BCL	C4D-CHA-C1A	4.85	127.16	121.25
9	AG	101	BCL	CAC-C3C-C2C	-4.85	102.13	114.26
9	Z	102	BCL	C1D-ND-C4D	-4.85	102.89	106.33
9	k	102	BCL	O2D-CGD-CBD	4.85	119.89	111.27
9	w	101	BCL	CHD-C1D-ND	-4.85	120.00	124.45
9	k	102	BCL	O2D-CGD-O1D	-4.85	114.36	123.84
9	h	101	BCL	O2D-CGD-O1D	-4.84	114.37	123.84
9	8	101	BCL	CHD-C1D-ND	-4.84	120.00	124.45
9	N	101	BCL	CAC-C3C-C2C	-4.84	102.17	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	l	101	BCL	O2D-CGD-O1D	-4.84	114.38	123.84
7	o	501	HEM	C1B-NB-C4B	4.83	110.06	105.07
9	w	101	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
15	z	101	CRT	C3-C1-C2	4.82	119.44	110.37
15	s	101	CRT	C3-C1-C2	4.82	119.43	110.37
9	Y	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
9	A	103	BCL	CHD-C1D-ND	-4.81	120.03	124.45
9	M	401	BCL	O2D-CGD-CBD	4.81	119.81	111.27
9	3	101	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
9	8	101	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
15	m	104	CRT	C3-C1-C2	4.81	119.41	110.37
12	H	304	PEF	O2-C10-C11	4.80	119.93	111.09
9	AB	101	BCL	C1D-ND-C4D	-4.80	102.92	106.33
9	x	303	BCL	O2D-CGD-O1D	-4.79	114.46	123.84
9	AH	101	BCL	CAC-C3C-C2C	-4.79	102.28	114.26
15	AD	101	CRT	C5-C6-C7	-4.79	118.66	125.89
9	1	101	BCL	C2D-C1D-ND	4.79	113.63	110.10
9	W	101	BCL	CAC-C3C-C2C	-4.77	102.33	114.26
9	D	102	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
9	x	303	BCL	O2D-CGD-CBD	4.76	119.73	111.27
9	G	102	BCL	C4D-CHA-C1A	4.76	127.04	121.25
9	S	102	BCL	C2D-C1D-ND	4.76	113.61	110.10
9	q	102	BCL	C2D-C1D-ND	4.75	113.61	110.10
9	L	303	BCL	C1-O2A-CGA	4.75	128.91	116.44
9	AH	101	BCL	O2D-CGD-O1D	-4.75	114.56	123.84
9	AK	101	BCL	O2D-CGD-O1D	-4.75	114.56	123.84
9	s	102	BCL	CMB-C2B-C3B	4.74	133.55	124.68
9	L	301	BCL	CMA-C3A-C4A	-4.74	99.03	111.77
9	AI	101	BCL	O2D-CGD-CBD	4.74	119.69	111.27
15	i	101	CRT	C3-C1-C2	4.73	119.28	110.37
15	0	101	CRT	C21-C22-C23	-4.73	120.56	127.31
9	AH	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
9	f	101	BCL	CMB-C2B-C3B	4.73	133.53	124.68
9	G	102	BCL	C2D-C1D-ND	4.73	113.59	110.10
9	d	101	BCL	C1C-NC-C4C	-4.73	104.58	106.71
9	T	102	BCL	CAC-C3C-C2C	-4.72	102.47	114.26
9	R	102	BCL	O2D-CGD-O1D	-4.72	114.61	123.84
9	W	101	BCL	CHD-C1D-ND	-4.71	120.13	124.45
9	m	102	BCL	C4D-CHA-C1A	4.71	126.98	121.25
11	x	304	UQ8	C6-C1-C2	4.71	122.90	119.18
9	AE	102	BCL	O2D-CGD-O1D	-4.70	114.64	123.84
9	4	102	BCL	CHD-C1D-ND	-4.70	120.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	j	101	BCL	C2D-C1D-ND	4.70	113.57	110.10
7	o	502	HEM	CAD-CBD-CGD	-4.70	103.49	113.60
9	R	102	BCL	C4D-CHA-C1A	4.70	126.97	121.25
9	Q	101	BCL	C2D-C1D-ND	4.70	113.57	110.10
9	AL	102	BCL	O2D-CGD-O1D	-4.70	114.66	123.84
9	g	102	BCL	O2D-CGD-CBD	4.69	119.61	111.27
12	m	101	PEF	O2-C10-C11	4.69	119.72	111.09
9	p	102	BCL	O2D-CGD-O1D	-4.69	114.68	123.84
7	o	504	HEM	C4D-ND-C1D	4.68	109.91	105.07
9	AI	101	BCL	CAC-C3C-C2C	-4.68	102.57	114.26
9	M	402	BCL	C2D-C1D-ND	4.68	113.55	110.10
7	C	503	HEM	CHC-C4B-C3B	4.68	131.73	124.57
9	s	102	BCL	CAC-C3C-C2C	-4.67	102.58	114.26
9	V	102	BCL	CHD-C1D-ND	-4.67	120.16	124.45
9	L	303	BCL	C4D-CHA-C1A	4.67	126.93	121.25
9	AB	102	BCL	C4D-CHA-C1A	4.67	126.93	121.25
9	c	101	BCL	O2D-CGD-O1D	-4.67	114.71	123.84
9	P	101	BCL	O2D-CGD-CBD	4.67	119.56	111.27
9	h	101	BCL	C2D-C1D-ND	4.67	113.54	110.10
9	G	102	BCL	C1D-ND-C4D	-4.67	103.02	106.33
15	k	101	CRT	C20-C19-C17	-4.67	120.65	127.31
9	O	102	BCL	O2D-CGD-CBD	4.67	119.56	111.27
9	D	101	BCL	CAC-C3C-C2C	-4.66	102.60	114.26
9	P	101	BCL	CAC-C3C-C2C	-4.66	102.61	114.26
9	V	102	BCL	C2D-C1D-ND	4.66	113.54	110.10
9	2	102	BCL	C1D-ND-C4D	-4.66	103.02	106.33
9	2	102	BCL	C2D-C1D-ND	4.66	113.54	110.10
9	L	303	BCL	CMB-C2B-C3B	4.66	133.40	124.68
9	2	102	BCL	CAC-C3C-C2C	-4.66	102.62	114.26
7	o	501	HEM	CHC-C4B-NB	4.66	129.49	124.43
9	4	102	BCL	CAC-C3C-C2C	-4.65	102.63	114.26
9	AI	101	BCL	O2D-CGD-O1D	-4.65	114.75	123.84
9	e	102	BCL	C2D-C1D-ND	4.65	113.53	110.10
9	P	101	BCL	CHD-C1D-ND	-4.64	120.19	124.45
9	W	101	BCL	C2D-C1D-ND	4.64	113.52	110.10
9	w	101	BCL	O2D-CGD-CBD	4.64	119.51	111.27
9	R	102	BCL	CMB-C2B-C3B	4.64	133.35	124.68
9	r	101	BCL	CHD-C1D-ND	-4.63	120.20	124.45
9	w	101	BCL	C2D-C1D-ND	4.63	113.52	110.10
9	AB	102	BCL	CAC-C3C-C2C	-4.63	102.69	114.26
9	u	102	BCL	O2D-CGD-O1D	-4.63	114.78	123.84
9	y	401	BCL	O2D-CGD-CBD	4.63	119.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	101	BCL	CHD-C1D-ND	-4.63	120.20	124.45
7	o	503	HEM	C1B-NB-C4B	4.63	109.85	105.07
9	P	101	BCL	CMB-C2B-C3B	4.63	133.33	124.68
15	m	104	CRT	C21-C22-C23	-4.62	120.71	127.31
9	O	102	BCL	CAC-C3C-C2C	-4.62	102.72	114.26
9	AL	102	BCL	C2D-C1D-ND	4.62	113.51	110.10
9	D	101	BCL	O2D-CGD-CBD	4.62	119.47	111.27
9	3	101	BCL	CMB-C2B-C3B	4.62	133.31	124.68
9	s	102	BCL	C4D-CHA-C1A	4.61	126.86	121.25
9	AB	102	BCL	O2D-CGD-O1D	-4.61	114.82	123.84
9	I	101	BCL	C4D-CHA-C1A	4.61	126.86	121.25
15	AC	101	CRT	C31-C32-C33	-4.60	120.74	127.31
9	f	101	BCL	O2D-CGD-O1D	-4.60	114.85	123.84
9	s	102	BCL	O2D-CGD-O1D	-4.60	114.85	123.84
9	m	102	BCL	O2D-CGD-O1D	-4.59	114.86	123.84
9	S	102	BCL	O2D-CGD-O1D	-4.59	114.86	123.84
9	M	401	BCL	C2D-C1D-ND	4.59	113.49	110.10
9	u	101	BCL	C2D-C1D-ND	4.59	113.49	110.10
9	AI	102	BCL	CMB-C2B-C3B	4.58	133.25	124.68
9	X	102	BCL	C1C-NC-C4C	-4.58	104.65	106.71
12	H	305	PEF	O2-C10-C11	4.58	119.52	111.09
9	V	102	BCL	CMB-C2B-C3B	4.58	133.24	124.68
9	V	102	BCL	O2D-CGD-CBD	4.58	119.40	111.27
9	u	102	BCL	C4D-CHA-C1A	4.57	126.82	121.25
9	S	102	BCL	O2D-CGD-CBD	4.57	119.38	111.27
9	y	401	BCL	C2D-C1D-ND	4.56	113.46	110.10
12	y	408	PEF	O2-C10-C11	4.55	119.46	111.09
9	T	102	BCL	CHD-C1D-ND	-4.54	120.28	124.45
9	9	102	BCL	CHD-C1D-ND	-4.54	120.28	124.45
9	Q	101	BCL	C4D-CHA-C1A	4.54	126.78	121.25
9	h	101	BCL	CHD-C1D-ND	-4.54	120.29	124.45
9	r	101	BCL	C2D-C1D-ND	4.53	113.44	110.10
9	AI	102	BCL	C2D-C1D-ND	4.53	113.44	110.10
9	y	401	BCL	O2D-CGD-O1D	-4.53	114.98	123.84
9	d	101	BCL	C4A-NA-C1A	4.53	108.74	106.71
15	z	101	CRT	C31-C32-C33	-4.53	120.84	127.31
9	M	402	BCL	O2A-CGA-O1A	-4.53	112.16	123.59
9	D	102	BCL	O2D-CGD-O1D	-4.53	114.98	123.84
9	z	102	BCL	O2D-CGD-O1D	-4.53	114.98	123.84
12	t	303	PEF	O2-C10-C11	4.52	119.41	111.09
9	AB	102	BCL	C2D-C1D-ND	4.52	113.44	110.10
9	AB	101	BCL	C2D-C1D-ND	4.52	113.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	102	BCL	C1D-ND-C4D	-4.51	103.13	106.33
9	P	101	BCL	C2D-C1D-ND	4.51	113.43	110.10
9	0	102	BCL	CAC-C3C-C2C	-4.50	103.00	114.26
9	L	301	BCL	C2D-C1D-ND	4.50	113.42	110.10
9	0	102	BCL	O2D-CGD-O1D	-4.50	115.03	123.84
7	C	501	HEM	CHB-C1B-NB	4.50	129.94	124.38
9	Q	101	BCL	O2D-CGD-CBD	4.50	119.26	111.27
7	o	503	HEM	C4D-ND-C1D	4.50	109.72	105.07
9	D	101	BCL	C4D-CHA-C1A	4.50	126.72	121.25
9	AB	102	BCL	CHD-C1D-ND	-4.49	120.32	124.45
9	G	102	BCL	O2D-CGD-CBD	4.48	119.23	111.27
9	m	102	BCL	CAC-C3C-C2C	-4.48	103.06	114.26
9	2	102	BCL	C4D-CHA-C1A	4.48	126.70	121.25
9	L	303	BCL	CHD-C1D-ND	-4.48	120.34	124.45
9	m	103	BCL	C4D-CHA-C1A	4.47	126.69	121.25
9	Y	101	BCL	C1D-ND-C4D	-4.47	103.16	106.33
9	W	101	BCL	O2D-CGD-CBD	4.47	119.20	111.27
15	T	101	CRT	C21-C22-C23	-4.46	120.94	127.31
9	P	101	BCL	C1D-ND-C4D	-4.46	103.17	106.33
9	x	301	BCL	CHD-C1D-ND	-4.46	120.36	124.45
9	x	305	BCL	O2D-CGD-O1D	-4.46	115.12	123.84
9	m	103	BCL	CHD-C1D-ND	-4.45	120.36	124.45
9	K	101	BCL	CHD-C1D-ND	-4.45	120.36	124.45
9	K	101	BCL	O2D-CGD-O1D	-4.45	115.13	123.84
15	I	102	CRT	C9-C10-C11	-4.45	109.33	123.22
9	A	102	BCL	C4D-CHA-C1A	4.45	126.67	121.25
9	L	301	BCL	O2D-CGD-CBD	4.45	119.17	111.27
9	I	103	BCL	O2D-CGD-O1D	-4.45	115.14	123.84
9	N	101	BCL	C2D-C1D-ND	4.45	113.38	110.10
9	I	103	BCL	CMB-C2B-C3B	4.44	132.99	124.68
9	O	102	BCL	CMB-C2B-C3B	4.44	132.99	124.68
9	z	102	BCL	CAC-C3C-C2C	-4.44	103.16	114.26
9	AI	101	BCL	C1D-ND-C4D	-4.44	103.18	106.33
9	u	102	BCL	CMB-C2B-C3B	4.44	132.99	124.68
9	AI	101	BCL	CMB-C2B-C3B	4.44	132.98	124.68
9	F	101	BCL	CAC-C3C-C2C	-4.43	103.19	114.26
9	P	101	BCL	O2D-CGD-O1D	-4.43	115.18	123.84
9	N	101	BCL	CMB-C2B-C3B	4.43	132.96	124.68
9	3	101	BCL	C2D-C1D-ND	4.43	113.36	110.10
9	u	101	BCL	CMA-C3A-C4A	-4.42	99.88	111.77
12	A	101	PEF	C2-O2-C10	-4.42	109.65	117.90
9	I	101	BCL	CHD-C1D-ND	-4.42	120.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	103	BCL	CAC-C3C-C2C	-4.42	103.22	114.26
9	i	102	BCL	C4D-CHA-C1A	4.41	126.62	121.25
9	c	101	BCL	CAC-C3C-C2C	-4.41	103.24	114.26
9	Z	102	BCL	CAC-C3C-C2C	-4.40	103.26	114.26
9	AH	101	BCL	C4D-CHA-C1A	4.39	126.60	121.25
9	u	102	BCL	CAC-C3C-C2C	-4.38	103.33	114.26
9	3	101	BCL	O2D-CGD-CBD	4.37	119.04	111.27
9	G	102	BCL	CMB-C2B-C3B	4.37	132.86	124.68
9	I	103	BCL	C4D-CHA-C1A	4.37	126.57	121.25
15	7	103	CRT	C25-C23-C22	4.37	125.65	118.94
9	e	102	BCL	C1D-ND-C4D	-4.37	103.23	106.33
11	x	304	UQ8	C15-C14-C16	4.37	122.62	115.27
9	AF	101	BCL	C4A-NA-C1A	4.37	108.67	106.71
9	0	102	BCL	C1C-NC-C4C	-4.36	104.74	106.71
9	AI	101	BCL	C4D-CHA-C1A	4.36	126.56	121.25
9	p	102	BCL	CHD-C1D-ND	-4.36	120.44	124.45
9	g	102	BCL	C4D-CHA-C1A	4.36	126.55	121.25
9	k	102	BCL	O2A-C1-C2	4.35	120.08	108.64
15	s	101	CRT	C26-C27-C28	-4.34	121.11	127.31
9	U	101	BCL	CHA-C1A-NA	-4.34	116.45	126.40
15	9	101	CRT	C15-C14-C12	-4.34	121.11	127.31
9	9	102	BCL	O2D-CGD-O1D	-4.34	115.36	123.84
9	I	103	BCL	CHD-C1D-ND	-4.34	120.47	124.45
9	AH	101	BCL	CMB-C2B-C3B	4.34	132.79	124.68
9	f	101	BCL	CHD-C1D-ND	-4.33	120.48	124.45
9	e	102	BCL	O2D-CGD-O1D	-4.33	115.38	123.84
9	2	102	BCL	CHA-C1A-NA	-4.32	116.50	126.40
9	T	102	BCL	C4D-CHA-C1A	4.31	126.49	121.25
9	AF	101	BCL	CAC-C3C-C2C	-4.31	103.50	114.26
9	A	103	BCL	CAC-C3C-C2C	-4.31	103.50	114.26
7	C	501	HEM	CHC-C4B-NB	4.30	129.11	124.43
7	C	501	HEM	CAD-CBD-CGD	4.30	122.86	113.60
9	x	301	BCL	C1D-ND-C4D	-4.30	103.28	106.33
9	V	102	BCL	O2D-CGD-O1D	-4.30	115.43	123.84
9	g	102	BCL	O2D-CGD-O1D	-4.30	115.44	123.84
9	5	101	BCL	C1C-NC-C4C	-4.30	104.78	106.71
9	e	102	BCL	CMB-C2B-C3B	4.29	132.71	124.68
9	6	101	BCL	C4D-CHA-C1A	4.29	126.47	121.25
9	r	101	BCL	O2D-CGD-CBD	4.28	118.88	111.27
9	D	102	BCL	CMB-C2B-C3B	4.28	132.69	124.68
9	Y	101	BCL	C4B-CHC-C1C	-4.28	121.64	130.12
9	AB	101	BCL	C4D-CHA-C1A	4.28	126.46	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	102	BCL	C1C-NC-C4C	-4.28	104.78	106.71
9	Q	101	BCL	O2D-CGD-O1D	-4.28	115.47	123.84
9	AB	102	BCL	CMB-C2B-C3B	4.27	132.67	124.68
9	G	102	BCL	O2D-CGD-O1D	-4.27	115.49	123.84
9	AH	101	BCL	OBB-CAB-CBB	-4.27	110.57	120.17
15	X	101	CRT	C5-C6-C7	-4.26	119.45	125.89
9	w	101	BCL	C4D-CHA-C1A	4.26	126.43	121.25
9	K	101	BCL	CMB-C2B-C3B	4.26	132.64	124.68
9	AK	101	BCL	CMB-C2B-C3B	4.25	132.64	124.68
9	O	102	BCL	O2D-CGD-O1D	-4.25	115.52	123.84
9	W	101	BCL	O2D-CGD-O1D	-4.25	115.52	123.84
9	l	101	BCL	CAC-C3C-C2C	-4.25	103.64	114.26
9	8	101	BCL	C16-C15-C13	-4.25	102.18	115.92
9	T	102	BCL	CMB-C2B-C3B	4.24	132.61	124.68
9	O	102	BCL	CHD-C1D-ND	-4.24	120.56	124.45
9	M	401	BCL	CAC-C3C-C4C	-4.24	103.18	112.58
9	i	102	BCL	CMB-C2B-C3B	4.22	132.57	124.68
9	i	102	BCL	CAC-C3C-C2C	-4.21	103.73	114.26
9	Z	102	BCL	C1C-NC-C4C	-4.21	104.81	106.71
9	AI	101	BCL	C2D-C1D-ND	4.21	113.21	110.10
9	6	101	BCL	O2D-CGD-O1D	-4.21	115.61	123.84
9	8	101	BCL	O2A-C1-C2	4.20	119.68	108.64
9	R	102	BCL	CAC-C3C-C2C	-4.20	103.77	114.26
9	Y	101	BCL	C2D-C1D-ND	4.19	113.19	110.10
9	5	101	BCL	C4A-NA-C1A	4.19	108.59	106.71
9	M	401	BCL	C4B-CHC-C1C	-4.19	121.81	130.12
9	L	301	BCL	CMB-C2B-C3B	4.19	132.52	124.68
15	AJ	101	CRT	C5-C6-C7	-4.19	119.56	125.89
9	0	102	BCL	C1D-ND-C4D	-4.19	103.36	106.33
9	1	101	BCL	CMB-C2B-C3B	4.18	132.50	124.68
9	F	101	BCL	CMB-C2B-C3B	4.17	132.49	124.68
9	d	101	BCL	C1D-ND-C4D	-4.17	103.37	106.33
7	C	503	HEM	CAB-C3B-C2B	-4.17	114.86	128.60
7	C	501	HEM	CHD-C1D-ND	4.17	128.96	124.43
9	I	101	BCL	O2D-CGD-O1D	-4.17	115.68	123.84
9	k	102	BCL	CMB-C2B-C3B	4.17	132.48	124.68
9	x	303	BCL	C2C-C3C-C4C	-4.17	95.10	101.34
9	p	102	BCL	C4D-CHA-C1A	4.17	126.32	121.25
15	G	101	CRT	C20-C19-C17	-4.16	121.37	127.31
9	x	303	BCL	C16-C15-C13	-4.16	102.46	115.92
17	S	101	PGW	O01-C1-C2	4.16	118.75	111.09
9	c	101	BCL	CMB-C2B-C3B	4.16	132.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	102	BCL	CMB-C2B-C3B	4.16	132.46	124.68
9	d	101	BCL	CMB-C2B-C3B	4.16	132.45	124.68
9	f	101	BCL	C4D-CHA-C1A	4.15	126.30	121.25
9	6	101	BCL	CHA-C1A-NA	-4.14	116.91	126.40
9	g	102	BCL	C2D-C1D-ND	4.14	113.16	110.10
9	7	102	BCL	CHD-C1D-ND	-4.14	120.65	124.45
9	AH	101	BCL	CHA-C1A-NA	-4.14	116.91	126.40
7	C	503	HEM	CHB-C1B-NB	4.14	129.50	124.38
9	l	101	BCL	CMB-C2B-C3B	4.14	132.42	124.68
9	c	101	BCL	CHD-C1D-ND	-4.13	120.66	124.45
9	x	301	BCL	CMA-C3A-C4A	-4.13	100.68	111.77
9	AH	101	BCL	C2D-C1D-ND	4.11	113.14	110.10
9	AG	101	BCL	OBB-CAB-CBB	-4.11	110.91	120.17
15	7	101	CRT	C35-C33-C32	-4.11	112.63	118.94
9	AB	102	BCL	O2D-CGD-CBD	4.11	118.57	111.27
10	x	302	BPH	CMC-C2C-C1C	-4.11	105.38	114.38
9	f	101	BCL	C4B-CHC-C1C	-4.11	121.98	130.12
9	AK	101	BCL	C4D-CHA-C1A	4.11	126.25	121.25
9	U	101	BCL	C1D-ND-C4D	-4.10	103.42	106.33
9	D	101	BCL	C16-C15-C13	-4.10	102.66	115.92
9	e	102	BCL	C4D-CHA-C1A	4.10	126.23	121.25
11	L	304	UQ8	C15-C14-C16	4.09	122.16	115.27
9	U	101	BCL	CMB-C2B-C3B	4.09	132.33	124.68
9	AB	101	BCL	CHD-C1D-ND	-4.09	120.69	124.45
9	AC	103	BCL	CHD-C1D-ND	-4.09	120.70	124.45
9	K	101	BCL	CAC-C3C-C2C	-4.09	104.04	114.26
9	AE	102	BCL	CMB-C2B-C3B	4.09	132.33	124.68
9	9	102	BCL	C4D-CHA-C1A	4.09	126.22	121.25
9	g	102	BCL	CMB-C2B-C3B	4.09	132.32	124.68
9	x	301	BCL	CHA-C1A-NA	-4.08	117.05	126.40
9	y	401	BCL	C1C-NC-C4C	-4.08	104.87	106.71
9	i	102	BCL	O2D-CGD-CBD	4.08	118.52	111.27
9	AL	102	BCL	CMB-C2B-C3B	4.08	132.31	124.68
9	D	102	BCL	C4D-CHA-C1A	4.08	126.21	121.25
9	AB	101	BCL	CAC-C3C-C2C	-4.08	104.07	114.26
14	y	403	MQ8	C34-C33-C35	4.07	122.12	115.27
9	U	101	BCL	CHD-C1D-ND	-4.07	120.71	124.45
12	H	301	PEF	O2-C10-C11	4.06	118.57	111.09
9	3	101	BCL	O2D-CGD-O1D	-4.06	115.89	123.84
12	H	301	PEF	C2-O2-C10	-4.06	110.33	117.90
15	n	101	CRT	C5-C6-C7	-4.06	119.76	125.89
9	AB	101	BCL	CMB-C2B-C3B	4.06	132.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	102	BCL	CMB-C2B-C3B	4.06	132.27	124.68
9	Q	101	BCL	CAC-C3C-C2C	-4.05	104.14	114.26
9	u	101	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
9	N	101	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	0	102	BCL	C4D-CHA-C1A	4.05	126.18	121.25
7	C	502	HEM	C4D-ND-C1D	4.05	109.25	105.07
9	A	103	BCL	CMB-C2B-C3B	4.05	132.25	124.68
9	4	102	BCL	C1C-NC-C4C	-4.05	104.89	106.71
15	k	101	CRT	C25-C23-C22	4.05	125.15	118.94
9	x	301	BCL	CHB-C4A-NA	-4.04	118.92	124.51
9	m	103	BCL	CMB-C2B-C3B	4.04	132.24	124.68
9	r	101	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
9	W	101	BCL	C4D-CHA-C1A	4.04	126.17	121.25
9	S	102	BCL	C4D-CHA-C1A	4.04	126.16	121.25
9	I	101	BCL	C4B-CHC-C1C	-4.03	122.14	130.12
9	p	102	BCL	CMB-C2B-C3B	4.03	132.22	124.68
9	AE	102	BCL	CAC-C3C-C2C	-4.03	104.20	114.26
11	L	304	UQ8	C35-C34-C36	4.02	122.03	115.27
15	e	101	CRT	C15-C14-C12	-4.02	121.58	127.31
9	AE	102	BCL	CHA-C1A-NA	-4.02	117.20	126.40
11	x	304	UQ8	C32-C33-C34	-4.01	118.00	127.66
15	v	101	CRT	C26-C27-C28	-4.01	121.59	127.31
15	4	101	CRT	C27-C26-C25	-4.01	110.71	123.22
15	s	101	CRT	C20-C19-C17	-4.00	121.60	127.31
9	m	103	BCL	O2D-CGD-O1D	-3.99	116.03	123.84
9	AI	101	BCL	CMA-C3A-C4A	-3.99	101.06	111.77
15	AD	101	CRT	C15-C14-C12	-3.98	121.62	127.31
15	7	103	CRT	C24-C23-C22	-3.98	117.35	122.92
9	r	101	BCL	CMB-C2B-C3B	3.98	132.12	124.68
9	4	102	BCL	C4D-CHA-C1A	3.96	126.07	121.25
9	x	305	BCL	O2A-CGA-O1A	-3.96	113.60	123.59
9	x	305	BCL	CHA-C1A-NA	-3.96	117.33	126.40
9	2	102	BCL	C2A-C1A-CHA	3.96	130.78	123.86
9	M	401	BCL	O2D-CGD-O1D	-3.95	116.11	123.84
15	R	101	CRT	C13-C12-C14	-3.95	117.39	122.92
15	k	101	CRT	C24-C23-C22	-3.95	117.39	122.92
15	9	101	CRT	C5-C6-C7	-3.95	119.92	125.89
9	x	305	BCL	C6-C5-C3	-3.95	103.10	113.45
9	j	101	BCL	CHD-C1D-ND	-3.95	120.83	124.45
9	N	101	BCL	C4D-CHA-C1A	3.95	126.05	121.25
9	S	102	BCL	CMB-C2B-C3B	3.94	132.05	124.68
11	L	304	UQ8	C40-C39-C41	3.94	121.90	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	101	BCL	C1C-NC-C4C	-3.93	104.94	106.71
9	f	101	BCL	C1D-ND-C4D	-3.93	103.54	106.33
9	6	101	BCL	OBB-CAB-CBB	-3.93	111.32	120.17
9	Y	101	BCL	C4A-NA-C1A	3.93	108.47	106.71
9	L	303	BCL	CHA-C1A-NA	-3.92	117.41	126.40
9	AE	102	BCL	CHD-C1D-ND	-3.92	120.85	124.45
9	3	101	BCL	C4B-CHC-C1C	-3.92	122.35	130.12
9	AI	101	BCL	C4B-CHC-C1C	-3.91	122.37	130.12
15	AL	101	CRT	C24-C23-C25	3.91	124.24	118.08
9	AB	101	BCL	C4B-CHC-C1C	-3.91	122.38	130.12
15	7	101	CRT	C32-C31-C30	-3.91	111.03	123.22
9	q	102	BCL	CMB-C2B-C3B	3.90	131.98	124.68
9	U	101	BCL	C2D-C1D-ND	3.90	112.98	110.10
9	Z	102	BCL	CHA-C1A-NA	-3.90	117.46	126.40
14	y	403	MQ8	C26-C27-C28	-3.90	118.27	127.66
9	s	102	BCL	CHA-C1A-NA	-3.90	117.47	126.40
15	9	101	CRT	C3-C1-C2	3.90	117.70	110.37
9	x	301	BCL	OBB-CAB-CBB	-3.89	111.41	120.17
15	0	101	CRT	C21-C20-C19	-3.89	115.50	123.47
9	AF	101	BCL	CMB-C2B-C3B	3.89	131.95	124.68
10	L	302	BPH	O1D-CGD-CBD	-3.89	118.26	124.74
15	y	404	CRT	C20-C19-C17	-3.89	121.76	127.31
11	x	304	UQ8	C30-C29-C31	3.89	121.81	115.27
9	q	102	BCL	C4D-CHA-C1A	3.88	125.98	121.25
9	u	101	BCL	CMB-C2B-C3B	3.88	131.94	124.68
9	g	102	BCL	CHA-C1A-NA	-3.88	117.51	126.40
15	R	101	CRT	C15-C14-C12	-3.88	121.77	127.31
9	W	101	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
9	7	102	BCL	C4A-NA-C1A	3.88	108.45	106.71
15	AJ	101	CRT	C15-C14-C12	-3.88	121.78	127.31
9	x	303	BCL	CHA-C1A-NA	-3.88	117.52	126.40
15	2	101	CRT	C26-C27-C28	-3.87	121.78	127.31
15	AC	101	CRT	C29-C28-C30	3.87	124.18	118.08
9	m	103	BCL	CAC-C3C-C2C	-3.87	104.58	114.26
9	w	101	BCL	CMB-C2B-C3B	3.87	131.92	124.68
9	z	102	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
9	M	402	BCL	CMB-C2B-C3B	3.86	131.91	124.68
15	e	101	CRT	C32-C31-C30	-3.86	111.16	123.22
9	z	102	BCL	C4D-CHA-C1A	3.86	125.95	121.25
9	8	101	BCL	OBB-CAB-CBB	-3.86	111.49	120.17
9	S	102	BCL	C4B-CHC-C1C	-3.86	122.48	130.12
15	n	101	CRT	C15-C14-C12	-3.85	121.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	h	101	BCL	CAC-C3C-C2C	-3.85	104.65	114.26
9	AF	101	BCL	C4D-CHA-C1A	3.85	125.93	121.25
9	j	101	BCL	CMB-C2B-C3B	3.84	131.86	124.68
9	U	101	BCL	O2D-CGD-CBD	3.84	118.09	111.27
9	AI	101	BCL	O2A-C1-C2	3.84	118.72	108.64
9	S	102	BCL	CMA-C3A-C4A	-3.84	101.46	111.77
9	p	102	BCL	C2D-C1D-ND	3.83	112.93	110.10
9	c	101	BCL	C4D-CHA-C1A	3.83	125.91	121.25
9	l	101	BCL	C4D-CHA-C1A	3.83	125.90	121.25
9	O	102	BCL	CHA-C1A-NA	-3.82	117.65	126.40
9	I	101	BCL	CHA-C1A-NA	-3.82	117.65	126.40
9	u	102	BCL	CHA-C1A-NA	-3.81	117.66	126.40
9	Z	102	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
9	3	101	BCL	C4D-CHA-C1A	3.81	125.89	121.25
9	AG	101	BCL	C1C-NC-C4C	-3.81	104.99	106.71
9	AF	101	BCL	O2D-CGD-O1D	-3.81	116.39	123.84
9	Q	101	BCL	CHA-C1A-NA	-3.81	117.68	126.40
7	o	503	HEM	CHB-C1B-NB	3.80	129.08	124.38
9	AF	101	BCL	CHD-C1D-ND	-3.80	120.96	124.45
9	M	401	BCL	C11-C10-C8	-3.80	103.64	115.92
9	M	402	BCL	CMA-C3A-C4A	-3.80	101.56	111.77
15	R	101	CRT	C18-C17-C16	3.80	124.06	118.08
15	AF	102	CRT	C10-C9-C7	-3.80	121.89	127.31
15	AH	102	CRT	C26-C27-C28	-3.80	121.89	127.31
9	r	101	BCL	C4B-CHC-C1C	-3.80	122.60	130.12
15	AC	101	CRT	C20-C19-C17	-3.79	121.89	127.31
9	0	102	BCL	CHA-C1A-NA	-3.79	117.73	126.40
9	X	102	BCL	C4D-CHA-C1A	3.79	125.86	121.25
9	8	101	BCL	CMB-C2B-C3B	3.79	131.76	124.68
9	AC	102	BCL	C1C-NC-C4C	-3.78	105.01	106.71
9	d	101	BCL	CHD-C1D-ND	-3.78	120.98	124.45
7	o	501	HEM	CHD-C1D-ND	3.78	128.53	124.43
9	AK	101	BCL	CAC-C3C-C2C	-3.77	104.83	114.26
9	R	102	BCL	CED-O2D-CGD	-3.77	107.41	115.94
15	X	101	CRT	C10-C9-C7	-3.77	121.93	127.31
9	j	101	BCL	C4D-CHA-C1A	3.77	125.83	121.25
9	0	102	BCL	CHD-C1D-ND	-3.76	121.00	124.45
9	X	102	BCL	CAC-C3C-C2C	-3.76	104.87	114.26
15	R	101	CRT	C11-C12-C14	3.75	124.70	118.94
15	P	102	CRT	C20-C19-C17	-3.75	121.96	127.31
15	n	101	CRT	C10-C9-C7	3.75	132.66	127.31
9	4	102	BCL	CHA-C1A-NA	-3.75	117.81	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	102	BCL	CMB-C2B-C3B	3.74	131.68	124.68
9	Q	101	BCL	OBB-CAB-CBB	-3.74	111.75	120.17
9	9	102	BCL	CMB-C2B-C3B	3.74	131.67	124.68
9	q	102	BCL	CHD-C1D-ND	-3.74	121.02	124.45
9	j	101	BCL	CAC-C3C-C2C	-3.73	104.93	114.26
9	7	102	BCL	C4D-CHA-C1A	3.73	125.79	121.25
9	D	102	BCL	CHA-C1A-NA	-3.73	117.85	126.40
9	M	402	BCL	C16-C15-C13	-3.73	103.86	115.92
15	R	101	CRT	C21-C22-C23	-3.73	121.99	127.31
9	F	101	BCL	C4D-CHA-C1A	3.73	125.78	121.25
9	0	102	BCL	OBB-CAB-CBB	-3.72	111.79	120.17
9	e	102	BCL	CHA-C1A-NA	-3.72	117.88	126.40
15	v	101	CRT	C29-C28-C30	3.72	123.94	118.08
7	o	503	HEM	CAB-C3B-C2B	-3.72	116.36	128.60
9	1	101	BCL	CHD-C1D-ND	-3.71	121.04	124.45
9	2	102	BCL	CMB-C2B-C3B	3.71	131.62	124.68
15	AL	101	CRT	C32-C31-C30	-3.70	111.66	123.22
15	i	101	CRT	C21-C22-C23	-3.70	122.02	127.31
15	v	101	CRT	C21-C20-C19	-3.70	115.89	123.47
9	G	102	BCL	CHA-C1A-NA	-3.70	117.92	126.40
9	L	301	BCL	CHA-C1A-NA	-3.70	117.93	126.40
9	AC	103	BCL	OBB-CAB-CBB	-3.70	111.85	120.17
9	m	102	BCL	CHD-C1D-ND	-3.69	121.06	124.45
9	M	402	BCL	CMC-C2C-C3C	-3.69	98.93	113.83
7	C	504	HEM	CHB-C1B-NB	3.69	128.94	124.38
9	1	101	BCL	C11-C10-C8	-3.69	104.00	115.92
9	k	102	BCL	CMD-C2D-C1D	3.69	131.21	124.71
9	u	102	BCL	C11-C10-C8	-3.68	104.01	115.92
15	P	102	CRT	C21-C22-C23	-3.68	122.05	127.31
9	f	101	BCL	CHD-C4C-NC	-3.68	120.99	125.08
9	AB	102	BCL	CHA-C1A-NA	-3.68	117.97	126.40
9	M	401	BCL	CHD-C1D-ND	-3.67	121.08	124.45
11	x	304	UQ8	C7-C8-C9	-3.67	120.68	126.79
9	p	102	BCL	CHA-C1A-NA	-3.67	117.99	126.40
15	v	101	CRT	C9-C10-C11	-3.67	111.77	123.22
9	A	103	BCL	C1C-NC-C4C	-3.67	105.06	106.71
12	y	406	PEF	O2-C10-O4	-3.66	115.69	122.96
9	u	101	BCL	C4D-CHA-C1A	3.66	125.70	121.25
9	L	303	BCL	CGD-CBD-CAD	-3.66	98.88	110.73
9	w	101	BCL	C4B-CHC-C1C	-3.66	122.87	130.12
15	AJ	101	CRT	C21-C20-C19	3.66	130.97	123.47
9	d	101	BCL	C2D-C1D-ND	3.66	112.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AL	102	BCL	CHA-C1A-NA	-3.66	118.03	126.40
9	L	303	BCL	O2D-CGD-O1D	-3.66	116.69	123.84
9	x	303	BCL	O2A-CGA-O1A	-3.66	114.37	123.59
9	l	101	BCL	OBB-CAB-CBB	-3.65	111.94	120.17
15	g	101	CRT	C5-C6-C7	-3.65	120.37	125.89
9	S	102	BCL	OBB-CAB-CBB	-3.65	111.95	120.17
9	S	102	BCL	CHA-C1A-NA	-3.65	118.03	126.40
9	AC	103	BCL	C4D-CHA-C1A	3.65	125.69	121.25
15	7	101	CRT	C34-C33-C35	3.65	123.83	118.08
15	4	101	CRT	C25-C23-C22	-3.65	113.35	118.94
9	X	102	BCL	CHA-C1A-NA	-3.64	118.05	126.40
9	AC	102	BCL	CHA-C1A-NA	-3.64	118.06	126.40
9	z	102	BCL	CHA-C1A-NA	-3.64	118.06	126.40
9	6	101	BCL	C1-O2A-CGA	3.64	125.99	116.44
9	F	101	BCL	CHD-C1D-ND	-3.64	121.11	124.45
9	A	102	BCL	C1C-NC-C4C	-3.64	105.07	106.71
9	W	101	BCL	CMB-C2B-C3B	3.63	131.47	124.68
9	x	303	BCL	CAC-C3C-C2C	-3.63	105.19	114.26
9	r	101	BCL	C4D-CHA-C1A	3.63	125.67	121.25
15	Z	101	CRT	C32-C31-C30	-3.63	111.89	123.22
9	AF	101	BCL	CHA-C1A-NA	-3.63	118.09	126.40
9	I	101	BCL	C7-C6-C5	-3.62	103.52	113.36
9	g	102	BCL	C1C-NC-C4C	-3.62	105.08	106.71
9	AK	101	BCL	CHA-C1A-NA	-3.62	118.11	126.40
9	z	102	BCL	CMB-C2B-C3B	3.62	131.45	124.68
17	AE	101	PGW	O01-C1-C2	3.62	117.75	111.09
9	X	102	BCL	CMB-C2B-C3B	3.62	131.45	124.68
15	Z	101	CRT	C18-C17-C16	3.62	123.77	118.08
9	m	103	BCL	CHA-C1A-NA	-3.61	118.13	126.40
15	AL	101	CRT	C26-C27-C28	-3.61	122.16	127.31
9	1	101	BCL	C1C-NC-C4C	-3.61	105.08	106.71
12	A	101	PEF	C3-O3-C30	3.61	126.17	117.10
9	AC	102	BCL	CHD-C1D-ND	-3.60	121.14	124.45
9	P	101	BCL	CHA-C1A-NA	-3.60	118.15	126.40
15	AH	102	CRT	C21-C22-C23	-3.60	122.18	127.31
9	Y	101	BCL	C1-O2A-CGA	3.60	125.88	116.44
15	R	101	CRT	C5-C6-C7	-3.60	120.46	125.89
9	N	101	BCL	CHA-C1A-NA	-3.60	118.16	126.40
9	A	102	BCL	CHA-C1A-NA	-3.59	118.17	126.40
7	C	502	HEM	CHD-C1D-ND	3.59	128.33	124.43
7	o	502	HEM	CHD-C1D-ND	3.59	128.33	124.43
9	AF	101	BCL	OBB-CAB-CBB	-3.58	112.10	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	102	BCL	C4B-CHC-C1C	-3.58	123.02	130.12
9	AG	101	BCL	C4A-NA-C1A	3.58	108.32	106.71
9	p	102	BCL	OBB-CAB-CBB	-3.58	112.11	120.17
9	h	101	BCL	C4D-CHA-C1A	3.58	125.60	121.25
9	R	102	BCL	CHA-C1A-NA	-3.58	118.21	126.40
9	f	101	BCL	CHA-C1A-NA	-3.58	118.21	126.40
9	s	102	BCL	OBB-CAB-CBB	-3.57	112.13	120.17
9	6	101	BCL	CHD-C1D-ND	-3.57	121.17	124.45
9	O	102	BCL	C4B-CHC-C1C	-3.57	123.04	130.12
9	4	102	BCL	CMB-C2B-C3B	3.57	131.36	124.68
9	u	101	BCL	C11-C12-C13	-3.57	104.38	115.92
9	AF	101	BCL	O2D-CGD-CBD	3.57	117.61	111.27
9	c	101	BCL	C16-C15-C13	-3.57	104.38	115.92
9	Y	101	BCL	CHA-C1A-NA	-3.57	118.23	126.40
15	q	101	CRT	C5-C6-C7	-3.57	120.50	125.89
9	Y	101	BCL	C4D-CHA-C1A	3.56	125.59	121.25
9	h	101	BCL	CMB-C2B-C3B	3.56	131.35	124.68
15	P	102	CRT	C29-C28-C30	3.56	123.69	118.08
9	Q	101	BCL	CMB-C2B-C3B	3.56	131.34	124.68
9	D	102	BCL	OBB-CAB-CBB	-3.56	112.16	120.17
15	i	101	CRT	C14-C15-C16	-3.56	112.12	123.22
9	AC	103	BCL	CHA-C1A-NA	-3.55	118.26	126.40
15	n	101	CRT	C13-C12-C14	-3.55	117.95	122.92
9	T	102	BCL	CHA-C1A-NA	-3.55	118.27	126.40
9	Y	101	BCL	OBB-CAB-CBB	-3.55	112.18	120.17
9	y	401	BCL	CMB-C2B-C3B	3.55	131.31	124.68
9	R	102	BCL	O2D-CGD-CBD	3.55	117.57	111.27
9	Z	102	BCL	C4D-CHA-C1A	3.54	125.56	121.25
9	i	102	BCL	OBB-CAB-CBB	-3.54	112.20	120.17
9	N	101	BCL	C7-C6-C5	-3.54	103.74	113.36
9	k	102	BCL	C4A-NA-C1A	3.54	108.30	106.71
9	N	101	BCL	OBB-CAB-CBB	-3.54	112.20	120.17
15	E	101	CRT	C10-C9-C7	-3.54	122.26	127.31
15	AJ	101	CRT	C32-C31-C30	-3.54	112.17	123.22
9	1	101	BCL	OBB-CAB-CBB	-3.54	112.20	120.17
15	m	104	CRT	C21-C20-C19	-3.54	116.23	123.47
9	AI	101	BCL	OBB-CAB-CBB	-3.54	112.21	120.17
9	7	102	BCL	CAC-C3C-C2C	-3.53	105.43	114.26
9	6	101	BCL	CMB-C2B-C3B	3.53	131.29	124.68
9	AC	102	BCL	C16-C15-C13	-3.53	104.50	115.92
15	9	101	CRT	C21-C20-C19	-3.53	116.24	123.47
15	M	405	CRT	C10-C9-C7	-3.53	122.27	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	m	102	BCL	CMB-C2B-C3B	3.53	131.28	124.68
9	y	401	BCL	CHA-C1A-NA	-3.52	118.33	126.40
9	L	301	BCL	OBB-CAB-CBB	-3.52	112.24	120.17
9	P	101	BCL	C4B-CHC-C1C	-3.52	123.15	130.12
15	P	102	CRT	C32-C31-C30	-3.52	112.24	123.22
15	9	101	CRT	C10-C11-C12	-3.51	116.54	126.42
15	9	101	CRT	C20-C19-C17	-3.51	122.29	127.31
15	Z	101	CRT	C34-C33-C35	3.51	123.61	118.08
9	i	102	BCL	O2A-C1-C2	3.51	117.87	108.64
9	O	102	BCL	C4D-CHA-C1A	3.51	125.52	121.25
9	d	101	BCL	CHB-C4A-NA	-3.51	119.66	124.51
9	K	101	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
9	w	101	BCL	CMA-C3A-C4A	-3.50	102.36	111.77
9	D	101	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
15	AD	101	CRT	C18-C17-C16	3.50	123.59	118.08
12	x	306	PEF	O2-C10-C11	3.50	117.53	111.09
9	5	101	BCL	CHD-C1D-ND	-3.50	121.24	124.45
9	0	102	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
9	p	102	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
9	9	102	BCL	CHA-C1A-NA	-3.49	118.41	126.40
9	AI	101	BCL	CHA-C1A-NA	-3.49	118.41	126.40
15	4	101	CRT	C29-C28-C30	3.49	123.58	118.08
15	Z	101	CRT	C10-C9-C7	-3.49	122.33	127.31
9	M	402	BCL	CHA-C1A-NA	-3.48	118.42	126.40
9	w	101	BCL	CHA-C1A-NA	-3.48	118.42	126.40
7	C	504	HEM	CAD-CBD-CGD	-3.48	106.11	113.60
9	7	102	BCL	OBB-CAB-CBB	-3.48	112.34	120.17
9	L	303	BCL	O2D-CGD-CBD	3.48	117.45	111.27
9	W	101	BCL	CHA-C1A-NA	-3.48	118.43	126.40
9	F	101	BCL	C7-C6-C5	-3.48	103.91	113.36
9	Y	101	BCL	CHD-C4C-NC	-3.48	121.21	125.08
15	q	101	CRT	C21-C20-C19	-3.48	116.35	123.47
9	T	102	BCL	C1C-NC-C4C	-3.48	105.14	106.71
9	X	102	BCL	OBB-CAB-CBB	-3.47	112.35	120.17
9	4	102	BCL	O2A-C1-C2	3.47	117.76	108.64
15	T	101	CRT	C21-C20-C19	-3.47	116.36	123.47
9	A	102	BCL	O2D-CGD-O1D	-3.47	117.05	123.84
9	X	102	BCL	C4B-CHC-C1C	-3.47	123.24	130.12
9	i	102	BCL	CHA-C1A-NA	-3.47	118.45	126.40
15	Z	101	CRT	C16-C17-C19	-3.47	113.62	118.94
11	x	304	UQ8	C35-C34-C33	-3.47	114.79	123.68
7	C	504	HEM	C4D-ND-C1D	3.47	108.65	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	BCL	CHA-C1A-NA	-3.46	118.47	126.40
9	q	102	BCL	OBB-CAB-CBB	-3.46	112.38	120.17
9	V	102	BCL	CHA-C1A-NA	-3.46	118.47	126.40
15	4	101	CRT	C24-C23-C25	3.46	123.53	118.08
9	l	101	BCL	C1C-NC-C4C	-3.46	105.15	106.71
9	d	101	BCL	O2A-C1-C2	3.46	117.73	108.64
9	F	101	BCL	OBB-CAB-CBB	-3.46	112.38	120.17
9	G	102	BCL	C1C-NC-C4C	-3.46	105.15	106.71
9	V	102	BCL	C16-C15-C13	-3.46	104.74	115.92
15	T	101	CRT	C34-C33-C35	3.46	123.52	118.08
9	5	101	BCL	OBB-CAB-CBB	-3.45	112.39	120.17
9	m	102	BCL	CHA-C1A-NA	-3.45	118.49	126.40
9	G	102	BCL	C16-C15-C13	-3.45	104.76	115.92
9	g	102	BCL	OBB-CAB-CBB	-3.45	112.40	120.17
9	g	102	BCL	CHD-C1D-ND	-3.45	121.28	124.45
9	Z	102	BCL	C16-C15-C13	-3.45	104.77	115.92
9	y	401	BCL	C4D-CHA-C1A	3.45	125.45	121.25
9	M	401	BCL	CMA-C3A-C4A	-3.45	102.50	111.77
9	m	102	BCL	OBB-CAB-CBB	-3.45	112.41	120.17
9	l	101	BCL	CHD-C1D-ND	-3.45	121.29	124.45
7	C	504	HEM	CAA-CBA-CGA	-3.44	104.10	113.76
9	k	102	BCL	C4B-CHC-C1C	-3.44	123.30	130.12
15	q	101	CRT	C21-C22-C23	-3.44	122.40	127.31
9	r	101	BCL	OBB-CAB-CBB	-3.44	112.43	120.17
9	N	101	BCL	C16-C15-C13	-3.44	104.81	115.92
9	z	102	BCL	C4B-CHC-C1C	-3.43	123.32	130.12
9	l	101	BCL	CHA-C1A-NA	-3.43	118.54	126.40
9	x	305	BCL	C4B-CHC-C1C	-3.42	123.33	130.12
9	f	101	BCL	O2A-C1-C2	3.42	117.63	108.64
9	G	102	BCL	OBB-CAB-CBB	-3.42	112.47	120.17
9	q	102	BCL	CHA-C1A-NA	-3.42	118.57	126.40
9	R	102	BCL	OBB-CAB-CBB	-3.41	112.49	120.17
9	D	102	BCL	C16-C15-C13	-3.41	104.90	115.92
9	g	102	BCL	C1-O2A-CGA	3.41	125.38	116.44
9	T	102	BCL	CMA-C3A-C4A	-3.40	102.63	111.77
15	e	101	CRT	C34-C33-C35	3.40	123.44	118.08
9	AG	101	BCL	C16-C15-C13	-3.40	104.93	115.92
9	L	301	BCL	O2D-CGD-O1D	-3.40	117.20	123.84
7	o	501	HEM	CAA-CBA-CGA	-3.40	104.24	113.76
9	5	101	BCL	CMB-C2B-C3B	3.39	131.03	124.68
9	M	401	BCL	C6-C5-C3	-3.39	104.55	113.45
9	AC	103	BCL	CMB-C2B-C3B	3.39	131.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	101	BCL	O2A-C1-C2	3.39	117.55	108.64
9	L	303	BCL	O2A-CGA-O1A	-3.39	115.03	123.59
9	AB	102	BCL	OBB-CAB-CBB	-3.39	112.54	120.17
9	d	101	BCL	C4B-CHC-C1C	-3.38	123.42	130.12
15	AJ	101	CRT	C20-C21-C22	-3.38	116.55	123.47
9	w	101	BCL	O2A-C1-C2	3.38	117.52	108.64
9	AB	101	BCL	CHA-C1A-NA	-3.38	118.66	126.40
9	AI	102	BCL	OBB-CAB-CBB	-3.38	112.57	120.17
9	x	305	BCL	C3D-C2D-C1D	-3.38	101.22	105.83
9	M	401	BCL	OBB-CAB-CBB	-3.38	112.57	120.17
9	f	101	BCL	CMA-C3A-C4A	-3.37	102.70	111.77
15	7	101	CRT	C14-C15-C16	-3.37	112.69	123.22
15	s	101	CRT	C34-C33-C35	3.37	123.39	118.08
9	I	101	BCL	CMB-C2B-C3B	3.37	130.99	124.68
9	j	101	BCL	OBB-CAB-CBB	-3.37	112.58	120.17
15	i	101	CRT	C34-C33-C35	3.37	123.39	118.08
9	z	102	BCL	C16-C15-C13	-3.37	105.03	115.92
9	I	101	BCL	CMA-C3A-C4A	-3.37	102.72	111.77
12	y	407	PEF	O2-C10-C11	3.37	117.28	111.09
9	U	101	BCL	O2A-CGA-O1A	-3.37	115.09	123.59
9	T	102	BCL	CMC-C2C-C3C	-3.36	100.26	113.83
9	r	101	BCL	CHA-C1A-NA	-3.36	118.70	126.40
9	AK	101	BCL	C1C-NC-C4C	-3.36	105.20	106.71
11	x	304	UQ8	C8-C7-C6	3.35	121.09	112.05
9	D	101	BCL	CHA-C1A-NA	-3.35	118.72	126.40
9	3	101	BCL	C4A-NA-C1A	3.35	108.21	106.71
15	Z	101	CRT	C13-C12-C11	3.35	123.36	118.08
15	n	101	CRT	C10-C11-C12	-3.35	117.01	126.42
9	A	102	BCL	C4A-NA-C1A	3.35	108.21	106.71
9	h	101	BCL	OBB-CAB-CBB	-3.35	112.64	120.17
15	Z	101	CRT	C21-C20-C19	-3.35	116.62	123.47
15	V	101	CRT	C20-C19-C17	-3.34	122.54	127.31
14	M	404	MQ8	C35-C33-C32	-3.34	114.36	121.12
9	AK	101	BCL	CMC-C2C-C3C	-3.34	100.35	113.83
9	AI	102	BCL	C16-C15-C13	-3.34	105.13	115.92
9	d	101	BCL	OBB-CAB-CBB	-3.34	112.66	120.17
9	N	101	BCL	C11-C10-C8	-3.34	105.13	115.92
9	W	101	BCL	C4B-CHC-C1C	-3.34	123.51	130.12
15	n	101	CRT	C24-C23-C25	3.34	123.33	118.08
9	L	301	BCL	CHD-C1D-ND	-3.33	121.39	124.45
15	P	102	CRT	C26-C25-C23	-3.33	117.05	126.42
9	AE	102	BCL	C4B-CHC-C1C	-3.33	123.52	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	101	BCL	C16-C15-C13	-3.33	105.16	115.92
9	G	102	BCL	CHD-C1D-ND	-3.33	121.40	124.45
9	3	101	BCL	CMD-C2D-C1D	3.32	130.57	124.71
15	m	104	CRT	C18-C17-C16	3.32	123.31	118.08
9	AI	101	BCL	O2A-CGA-O1A	-3.32	115.21	123.59
9	7	102	BCL	O2D-CGD-O1D	-3.32	117.34	123.84
7	o	504	HEM	CHD-C1D-ND	3.32	128.04	124.43
15	AD	101	CRT	C26-C27-C28	-3.32	122.58	127.31
9	AL	102	BCL	C16-C15-C13	-3.32	105.20	115.92
9	M	402	BCL	C2A-C1A-CHA	3.32	129.66	123.86
9	h	101	BCL	CHA-C1A-NA	-3.31	118.81	126.40
9	G	102	BCL	C4B-CHC-C1C	-3.31	123.56	130.12
9	u	102	BCL	OBB-CAB-CBB	-3.31	112.71	120.17
15	4	101	CRT	C16-C17-C19	-3.31	113.86	118.94
15	i	101	CRT	C10-C9-C7	-3.31	122.59	127.31
7	C	502	HEM	CBA-CAA-C2A	-3.31	106.98	112.62
9	y	401	BCL	O2A-CGA-O1A	-3.31	115.25	123.59
9	z	102	BCL	C11-C10-C8	-3.30	105.24	115.92
9	A	103	BCL	O2A-CGA-O1A	-3.30	115.26	123.59
15	AD	101	CRT	C10-C9-C7	-3.30	122.60	127.31
9	AC	103	BCL	C4A-NA-C1A	3.30	108.19	106.71
9	9	102	BCL	C4B-CHC-C1C	-3.30	123.59	130.12
9	A	103	BCL	C4D-CHA-C1A	3.29	125.26	121.25
9	AI	102	BCL	CHA-C1A-NA	-3.29	118.86	126.40
9	D	101	BCL	C7-C6-C5	-3.29	104.41	113.36
15	Z	101	CRT	C24-C23-C25	3.29	123.27	118.08
9	I	101	BCL	O2A-CGA-O1A	-3.29	115.28	123.59
15	I	102	CRT	C15-C14-C12	-3.29	122.61	127.31
9	F	101	BCL	CHA-C1A-NA	-3.29	118.87	126.40
9	K	101	BCL	CHA-C1A-NA	-3.29	118.87	126.40
9	7	102	BCL	C4B-CHC-C1C	-3.29	123.61	130.12
9	AC	102	BCL	CMB-C2B-C3B	3.28	130.82	124.68
9	N	101	BCL	O2A-C1-C2	3.27	117.24	108.64
14	y	403	MQ8	C14-C13-C15	3.27	120.78	115.27
9	k	102	BCL	C3D-C2D-C1D	-3.27	101.37	105.83
9	2	102	BCL	C11-C12-C13	-3.27	105.35	115.92
15	e	101	CRT	C21-C20-C19	-3.27	116.78	123.47
9	e	102	BCL	C1C-NC-C4C	-3.27	105.24	106.71
15	e	101	CRT	C21-C22-C23	-3.27	122.65	127.31
9	I	103	BCL	OBB-CAB-CBB	-3.27	112.82	120.17
15	P	102	CRT	C34-C33-C35	3.27	123.22	118.08
9	m	103	BCL	C4B-CHC-C1C	-3.26	123.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	301	BCL	CMB-C2B-C3B	3.26	130.78	124.68
9	K	101	BCL	OBB-CAB-CBB	-3.26	112.83	120.17
9	k	102	BCL	CHA-C1A-NA	-3.26	118.93	126.40
9	D	101	BCL	CED-O2D-CGD	-3.26	108.57	115.94
9	AK	101	BCL	CMA-C3A-C4A	-3.26	103.02	111.77
9	w	101	BCL	OBB-CAB-CBB	-3.26	112.84	120.17
9	q	102	BCL	CHC-C1C-NC	3.26	129.01	124.51
9	AC	103	BCL	C1C-NC-C4C	-3.25	105.24	106.71
14	M	404	MQ8	C26-C27-C28	-3.25	119.83	127.66
15	i	101	CRT	C32-C31-C30	-3.25	113.07	123.22
9	l	101	BCL	CMA-C3A-C4A	-3.25	103.04	111.77
9	R	102	BCL	C3D-C2D-C1D	-3.25	101.40	105.83
9	AI	102	BCL	C4D-CHA-C1A	3.25	125.20	121.25
9	AE	102	BCL	CMA-C3A-C4A	-3.25	103.05	111.77
15	4	101	CRT	C13-C12-C14	-3.24	118.38	122.92
9	e	102	BCL	CHD-C1D-ND	-3.24	121.47	124.45
9	i	102	BCL	CHD-C1D-ND	-3.24	121.47	124.45
9	4	102	BCL	OBB-CAB-CBB	-3.24	112.87	120.17
9	h	101	BCL	C4B-CHC-C1C	-3.24	123.70	130.12
15	4	101	CRT	C36-C35-C33	-3.24	120.99	125.89
15	O	101	CRT	C21-C20-C19	-3.24	116.84	123.47
9	M	401	BCL	C16-C15-C13	-3.24	105.45	115.92
9	T	102	BCL	C1-C2-C3	-3.24	120.44	126.04
9	A	103	BCL	C4B-CHC-C1C	-3.24	123.71	130.12
15	0	101	CRT	C34-C33-C35	3.23	123.17	118.08
9	1	101	BCL	CHA-C1A-NA	-3.23	118.99	126.40
11	x	304	UQ8	C27-C28-C29	-3.23	119.87	127.66
9	d	101	BCL	CHA-C1A-NA	-3.23	119.00	126.40
9	AI	101	BCL	CHD-C1D-ND	-3.23	121.48	124.45
9	K	101	BCL	C16-C15-C13	-3.23	105.48	115.92
15	i	101	CRT	C35-C33-C32	-3.23	113.99	118.94
9	m	102	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
9	M	401	BCL	CHC-C1C-NC	3.22	128.97	124.51
9	f	101	BCL	C16-C15-C13	-3.22	105.50	115.92
15	4	101	CRT	C29-C28-C27	-3.22	118.41	122.92
9	x	305	BCL	CAC-C3C-C4C	-3.22	105.43	112.58
9	AK	101	BCL	CHB-C4A-NA	-3.22	120.06	124.51
9	u	101	BCL	CHA-C1A-NA	-3.22	119.02	126.40
9	m	103	BCL	OBB-CAB-CBB	-3.22	112.93	120.17
7	o	501	HEM	CMC-C2C-C3C	3.22	130.70	124.68
9	2	102	BCL	CMA-C3A-C4A	-3.22	103.12	111.77
9	e	102	BCL	OBB-CAB-CBB	-3.22	112.93	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	OBB-CAB-CBB	-3.21	112.94	120.17
9	T	102	BCL	C4B-CHC-C1C	-3.21	123.76	130.12
9	Z	102	BCL	C2A-C1A-CHA	3.21	129.47	123.86
15	E	101	CRT	C32-C31-C30	-3.21	113.21	123.22
9	x	301	BCL	C1B-CHB-C4A	-3.20	123.77	130.12
9	I	103	BCL	C11-C10-C8	-3.20	105.56	115.92
9	Y	101	BCL	C7-C6-C5	-3.20	104.66	113.36
9	i	102	BCL	C16-C15-C13	-3.20	105.57	115.92
9	c	101	BCL	OBB-CAB-CBB	-3.20	112.96	120.17
9	AK	101	BCL	C2A-C1A-CHA	3.20	129.46	123.86
9	3	101	BCL	CHA-C1A-NA	-3.20	119.07	126.40
9	AG	101	BCL	CMB-C2B-C3B	3.20	130.67	124.68
9	L	303	BCL	C4B-CHC-C1C	-3.20	123.78	130.12
9	x	303	BCL	CMA-C3A-C4A	-3.20	103.18	111.77
7	C	503	HEM	CAB-C3B-C4B	3.20	139.37	124.47
9	g	102	BCL	C1-C2-C3	-3.20	120.51	126.04
9	x	305	BCL	CHD-C1D-ND	-3.19	121.52	124.45
15	AH	102	CRT	C13-C12-C11	3.19	123.11	118.08
9	p	102	BCL	C7-C6-C5	-3.19	104.68	113.36
9	L	301	BCL	O2A-CGA-O1A	-3.19	115.53	123.59
9	A	102	BCL	C1-O2A-CGA	3.19	124.82	116.44
9	l	101	BCL	C16-C15-C13	-3.19	105.61	115.92
15	O	101	CRT	C15-C14-C12	-3.19	122.76	127.31
15	Z	101	CRT	C26-C27-C28	-3.19	122.76	127.31
9	D	102	BCL	CMA-C3A-C4A	-3.19	103.20	111.77
15	V	101	CRT	C26-C25-C23	-3.19	117.46	126.42
9	Q	101	BCL	C7-C6-C5	-3.19	104.71	113.36
15	k	101	CRT	C15-C14-C12	-3.18	122.77	127.31
17	AE	101	PGW	C02-O01-C1	3.18	123.82	117.90
15	AF	102	CRT	C20-C19-C17	-3.18	122.77	127.31
9	Q	101	BCL	C16-C15-C13	-3.17	105.66	115.92
9	I	101	BCL	OBB-CAB-CBB	-3.17	113.03	120.17
9	s	102	BCL	C4B-CHC-C1C	-3.17	123.83	130.12
9	L	301	BCL	C12-C11-C10	-3.17	98.66	113.24
9	x	305	BCL	CMA-C3A-C4A	-3.17	103.25	111.77
9	j	101	BCL	C4B-CHC-C1C	-3.17	123.84	130.12
9	W	101	BCL	CHB-C4A-NA	-3.17	120.13	124.51
9	e	102	BCL	CHB-C4A-NA	-3.17	120.13	124.51
9	I	101	BCL	C11-C10-C8	-3.17	105.68	115.92
9	AL	102	BCL	CHD-C1D-ND	-3.16	121.55	124.45
9	AF	101	BCL	C7-C6-C5	-3.16	104.77	113.36
7	C	502	HEM	CMC-C2C-C3C	3.16	130.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	z	101	CRT	C21-C20-C19	-3.16	117.00	123.47
9	g	102	BCL	C4B-CHC-C1C	-3.16	123.86	130.12
9	u	102	BCL	CMA-C3A-C4A	-3.16	103.28	111.77
9	D	102	BCL	C1C-NC-C4C	-3.16	105.29	106.71
9	x	301	BCL	C16-C15-C13	-3.16	105.71	115.92
15	V	101	CRT	C24-C23-C22	-3.16	118.50	122.92
9	x	305	BCL	CGD-CBD-CAD	-3.16	100.51	110.73
9	O	102	BCL	C16-C15-C13	-3.16	105.72	115.92
9	x	305	BCL	C16-C15-C13	-3.16	105.72	115.92
9	U	101	BCL	C4B-CHC-C1C	-3.16	123.87	130.12
15	4	101	CRT	C15-C14-C12	-3.15	122.81	127.31
9	D	102	BCL	C11-C12-C13	-3.15	105.73	115.92
9	M	402	BCL	OBD-CAD-C3D	3.15	136.11	128.52
9	AC	102	BCL	OBB-CAB-CBB	-3.15	113.08	120.17
15	V	101	CRT	C34-C33-C35	3.15	123.04	118.08
11	x	304	UQ8	O3-C3-C2	3.15	127.20	116.56
9	AI	102	BCL	C4B-CHC-C1C	-3.15	123.89	130.12
15	q	101	CRT	C24-C23-C25	3.15	123.03	118.08
9	V	102	BCL	C1C-NC-C4C	-3.15	105.29	106.71
9	x	301	BCL	CGD-CBD-CAD	-3.14	100.55	110.73
9	u	101	BCL	C11-C10-C8	-3.14	105.76	115.92
9	c	101	BCL	CHA-C1A-NA	-3.14	119.20	126.40
9	l	101	BCL	C2A-C1A-CHA	3.14	129.35	123.86
9	A	103	BCL	OBB-CAB-CBB	-3.14	113.10	120.17
10	x	302	BPH	CAA-CBA-CGA	-3.14	104.08	113.25
9	U	101	BCL	OBB-CAB-CBB	-3.14	113.11	120.17
9	x	301	BCL	CMD-C2D-C1D	3.14	130.24	124.71
7	o	502	HEM	C4D-ND-C1D	3.13	108.31	105.07
9	W	101	BCL	CHC-C1C-NC	3.13	128.85	124.51
12	A	101	PEF	O2-C10-O4	-3.13	116.74	122.96
9	AI	102	BCL	C3C-C4C-CHD	-3.13	116.70	123.39
9	D	101	BCL	CMB-C2B-C3B	3.13	130.54	124.68
9	1	101	BCL	CHC-C1C-NC	3.13	128.84	124.51
14	M	404	MQ8	C11-C12-C13	-3.13	121.58	126.79
9	c	101	BCL	O2A-C1-C2	3.13	116.86	108.64
7	o	503	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
9	1	101	BCL	C4D-CHA-C1A	3.13	125.06	121.25
7	C	501	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
15	I	102	CRT	C8-C7-C6	3.13	123.01	118.08
9	N	101	BCL	C4B-CHC-C1C	-3.13	123.92	130.12
9	O	102	BCL	C1-O2A-CGA	3.13	124.64	116.44
9	AE	102	BCL	C1C-NC-C4C	-3.13	105.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	X	102	BCL	O2A-C1-C2	3.12	116.85	108.64
9	j	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
9	U	101	BCL	C16-C15-C13	-3.12	105.82	115.92
9	8	101	BCL	C4B-CHC-C1C	-3.12	123.94	130.12
9	AB	101	BCL	OBB-CAB-CBB	-3.12	113.15	120.17
9	m	102	BCL	C1C-NC-C4C	-3.12	105.30	106.71
15	e	101	CRT	C18-C17-C16	3.12	122.99	118.08
9	f	101	BCL	O2A-CGA-O1A	-3.12	115.73	123.59
15	E	101	CRT	C21-C22-C23	-3.11	122.87	127.31
12	L	305	PEF	O3P-C1-C2	3.11	117.59	108.51
9	y	401	BCL	OBB-CAB-CBB	-3.11	113.17	120.17
9	A	102	BCL	CHD-C1D-ND	-3.11	121.60	124.45
9	Z	102	BCL	CHB-C4A-NA	-3.11	120.22	124.51
9	Y	101	BCL	CMB-C2B-C3B	3.11	130.49	124.68
12	H	302	PEF	C2-O2-C10	-3.10	112.11	117.90
15	2	101	CRT	C14-C15-C16	-3.10	113.53	123.22
15	z	101	CRT	C34-C33-C32	-3.10	118.58	122.92
15	V	101	CRT	C32-C31-C30	-3.10	113.55	123.22
9	I	103	BCL	CHA-C1A-NA	-3.10	119.30	126.40
9	3	101	BCL	O2A-CGA-O1A	-3.10	115.78	123.59
9	AL	102	BCL	OBB-CAB-CBB	-3.10	113.20	120.17
9	d	101	BCL	CMA-C3A-C4A	-3.10	103.45	111.77
7	o	503	HEM	CHD-C1D-ND	3.10	127.79	124.43
9	Z	102	BCL	C11-C10-C8	-3.09	105.92	115.92
14	M	404	MQ8	C34-C33-C35	3.09	120.47	115.27
14	M	404	MQ8	C14-C13-C15	3.09	120.47	115.27
9	Y	101	BCL	CMA-C3A-C4A	-3.09	103.46	111.77
15	E	101	CRT	C21-C20-C19	-3.09	117.15	123.47
9	AG	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
11	L	304	UQ8	C45-C44-C43	-3.08	113.75	122.65
9	M	402	BCL	OBB-CAB-CBB	-3.08	113.24	120.17
9	T	102	BCL	C3D-C2D-C1D	-3.08	101.63	105.83
9	3	101	BCL	CMC-C2C-C3C	-3.08	101.41	113.83
15	AJ	101	CRT	C36-C35-C33	3.08	130.54	125.89
7	C	501	HEM	O2D-CGD-CBD	3.08	123.91	114.03
9	M	402	BCL	C4D-CHA-C1A	3.07	124.99	121.25
9	D	101	BCL	C1C-NC-C4C	-3.07	105.32	106.71
9	h	101	BCL	CAA-CBA-CGA	-3.07	104.27	113.25
15	m	104	CRT	C14-C15-C16	-3.07	113.63	123.22
9	K	101	BCL	C2A-C1A-CHA	3.07	129.23	123.86
15	7	101	CRT	C8-C7-C6	3.07	122.92	118.08
7	C	503	HEM	CBD-CAD-C3D	-3.07	104.10	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AL	102	BCL	C2A-C1A-CHA	3.07	129.23	123.86
9	L	303	BCL	C2D-C1D-ND	3.07	112.36	110.10
9	z	102	BCL	C4A-NA-C1A	3.07	108.08	106.71
9	9	102	BCL	OBB-CAB-CBB	-3.06	113.28	120.17
15	P	102	CRT	C26-C27-C28	-3.06	122.94	127.31
15	0	101	CRT	C18-C17-C16	3.06	122.90	118.08
9	AH	101	BCL	C7-C6-C5	-3.06	105.06	113.36
9	X	102	BCL	CHD-C1D-ND	-3.05	121.65	124.45
9	k	102	BCL	C16-C15-C13	-3.05	106.05	115.92
9	D	102	BCL	CHD-C1D-ND	-3.05	121.65	124.45
9	3	101	BCL	C11-C12-C13	-3.05	106.06	115.92
15	m	104	CRT	C26-C27-C28	-3.05	122.96	127.31
9	K	101	BCL	C4D-CHA-C1A	3.05	124.96	121.25
7	o	502	HEM	C4A-C3A-C2A	3.05	109.12	107.00
9	0	102	BCL	C7-C6-C5	-3.05	105.08	113.36
9	k	102	BCL	CGD-CBD-CAD	-3.04	100.87	110.73
9	AB	102	BCL	C11-C10-C8	-3.04	106.08	115.92
11	L	304	UQ8	C20-C19-C21	3.04	120.39	115.27
15	O	101	CRT	C20-C19-C17	-3.04	122.97	127.31
15	AF	102	CRT	C14-C15-C16	-3.04	113.73	123.22
9	u	102	BCL	C2A-C1A-CHA	3.04	129.17	123.86
9	7	102	BCL	C1C-NC-C4C	-3.04	105.34	106.71
9	O	102	BCL	C11-C10-C8	-3.04	106.10	115.92
9	L	303	BCL	CMC-C2C-C3C	-3.04	101.58	113.83
9	k	102	BCL	OBB-CAB-CBB	-3.04	113.34	120.17
9	8	101	BCL	C7-C6-C5	-3.03	105.12	113.36
9	AF	101	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
11	x	304	UQ8	O3-C3-C4	-3.03	112.20	123.64
9	e	102	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
15	O	101	CRT	C9-C10-C11	-3.03	113.76	123.22
9	M	402	BCL	C3C-C4C-CHD	-3.03	116.92	123.39
9	I	103	BCL	C4B-CHC-C1C	-3.03	124.12	130.12
9	M	401	BCL	C11-C12-C13	-3.02	106.15	115.92
15	z	101	CRT	C27-C26-C25	-3.02	113.78	123.22
15	AL	101	CRT	C21-C20-C19	-3.02	117.29	123.47
9	AC	103	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
11	x	304	UQ8	C22-C23-C24	-3.02	120.40	127.66
9	q	102	BCL	O2A-CGA-O1A	-3.02	115.98	123.59
9	AF	101	BCL	CMA-C3A-C4A	-3.02	103.67	111.77
9	c	101	BCL	C7-C6-C5	-3.01	105.17	113.36
15	g	101	CRT	C32-C31-C30	3.01	132.62	123.22
15	AL	101	CRT	C8-C7-C9	-3.01	118.70	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	504	HEM	C4B-C3B-C2B	-3.01	104.72	107.11
9	8	101	BCL	C4D-CHA-C1A	3.01	124.92	121.25
9	u	101	BCL	CGD-CBD-CAD	-3.01	100.98	110.73
7	o	504	HEM	CMC-C2C-C3C	3.01	130.31	124.68
9	9	102	BCL	C11-C10-C8	-3.01	106.19	115.92
9	y	401	BCL	CMC-C2C-C3C	-3.01	101.69	113.83
9	3	101	BCL	C16-C15-C13	-3.01	106.20	115.92
9	3	101	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
9	F	101	BCL	C6-C5-C3	-3.01	105.58	113.45
9	U	101	BCL	C11-C12-C13	-3.00	106.21	115.92
9	h	101	BCL	C1-O2A-CGA	3.00	124.32	116.44
9	AF	101	BCL	C1C-NC-C4C	-3.00	105.36	106.71
9	L	301	BCL	C11-C10-C8	-3.00	106.22	115.92
9	s	102	BCL	O2A-C1-C2	3.00	116.52	108.64
9	5	101	BCL	C4B-CHC-C1C	-3.00	124.18	130.12
9	y	401	BCL	CHD-C1D-ND	-3.00	121.70	124.45
9	l	101	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
9	p	102	BCL	C11-C12-C13	-3.00	106.23	115.92
9	j	101	BCL	O2A-CGA-O1A	-3.00	116.03	123.59
9	AC	103	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
15	m	104	CRT	C27-C26-C25	-2.99	113.87	123.22
9	A	102	BCL	CMA-C3A-C4A	-2.99	103.73	111.77
9	O	102	BCL	C1C-NC-C4C	-2.99	105.36	106.71
9	l	101	BCL	C11-C10-C8	-2.99	106.24	115.92
9	AK	101	BCL	CHD-C1D-ND	-2.99	121.70	124.45
9	O	102	BCL	C3D-C2D-C1D	-2.99	101.75	105.83
9	S	102	BCL	C4A-NA-C1A	2.99	108.05	106.71
9	x	303	BCL	CMC-C2C-C3C	-2.99	101.76	113.83
9	9	102	BCL	CMC-C2C-C3C	-2.99	101.77	113.83
9	r	101	BCL	C16-C15-C13	-2.99	106.26	115.92
11	x	304	UQ8	O4-C4-C3	-2.99	112.38	123.64
9	i	102	BCL	C1C-NC-C4C	-2.99	105.36	106.71
9	q	102	BCL	C4B-CHC-C1C	-2.98	124.21	130.12
9	w	101	BCL	C1-C2-C3	-2.98	120.88	126.04
9	g	102	BCL	O2A-CGA-O1A	-2.98	116.06	123.59
9	AK	101	BCL	CED-O2D-CGD	-2.98	109.19	115.94
9	x	305	BCL	C7-C6-C5	-2.98	105.26	113.36
14	y	403	MQ8	C11-C12-C13	-2.98	121.83	126.79
9	AC	102	BCL	C4B-CHC-C1C	-2.98	124.22	130.12
9	AG	101	BCL	O2A-C1-C2	2.98	116.46	108.64
9	K	101	BCL	C3D-C2D-C1D	-2.98	101.77	105.83
15	V	101	CRT	C35-C33-C32	-2.98	114.38	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302	BPH	CBA-CAA-C2A	-2.98	105.12	113.81
9	y	401	BCL	C2A-C1A-CHA	2.97	129.06	123.86
9	6	101	BCL	C7-C6-C5	-2.97	105.29	113.36
9	AB	101	BCL	C16-C15-C13	-2.97	106.31	115.92
15	X	101	CRT	C15-C14-C12	-2.97	123.07	127.31
9	6	101	BCL	C4B-CHC-C1C	-2.97	124.23	130.12
9	s	102	BCL	CMA-C3A-C4A	-2.97	103.79	111.77
9	9	102	BCL	C7-C6-C5	-2.97	105.29	113.36
15	s	101	CRT	C35-C33-C32	-2.97	114.39	118.94
9	4	102	BCL	C4B-CHC-C1C	-2.97	124.24	130.12
9	g	102	BCL	C7-C6-C5	-2.97	105.30	113.36
15	v	101	CRT	C21-C22-C23	-2.97	123.08	127.31
15	9	101	CRT	C32-C31-C30	-2.97	113.96	123.22
9	r	101	BCL	C7-C6-C5	-2.96	105.31	113.36
9	D	101	BCL	O2A-CGA-O1A	-2.96	116.11	123.59
9	c	101	BCL	C4B-CHC-C1C	-2.96	124.25	130.12
15	7	101	CRT	C20-C21-C22	-2.96	117.41	123.47
14	y	403	MQ8	C31-C32-C33	-2.96	120.53	127.66
9	L	301	BCL	C1-C2-C3	-2.96	120.92	126.04
9	Z	102	BCL	C4A-NA-C1A	2.96	108.04	106.71
9	AL	102	BCL	C1C-NC-C4C	-2.96	105.38	106.71
11	x	304	UQ8	C35-C34-C36	2.96	120.25	115.27
9	m	102	BCL	O2A-CGA-O1A	-2.96	116.13	123.59
9	p	102	BCL	C16-C15-C13	-2.96	106.36	115.92
9	l	101	BCL	CMD-C2D-C1D	2.96	129.92	124.71
9	e	102	BCL	C11-C12-C13	-2.96	106.37	115.92
15	V	101	CRT	C8-C7-C6	2.95	122.73	118.08
9	O	102	BCL	CHC-C1C-NC	2.95	128.60	124.51
9	s	102	BCL	C16-C15-C13	-2.95	106.38	115.92
9	6	101	BCL	CHC-C1C-NC	2.95	128.59	124.51
15	k	101	CRT	C26-C25-C23	-2.95	118.12	126.42
9	z	102	BCL	C7-C6-C5	-2.95	105.34	113.36
9	V	102	BCL	C4B-CHC-C1C	-2.95	124.27	130.12
9	AG	101	BCL	C7-C6-C5	-2.95	105.35	113.36
9	P	101	BCL	C4A-NA-C1A	2.95	108.03	106.71
9	R	102	BCL	C11-C10-C8	-2.95	106.39	115.92
9	h	101	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
7	o	503	HEM	CBD-CAD-C3D	-2.94	104.45	112.63
9	7	102	BCL	CHA-C1A-NA	-2.94	119.66	126.40
9	7	102	BCL	O2A-C1-C2	2.94	116.37	108.64
9	A	103	BCL	CHD-C4C-NC	-2.94	121.81	125.08
15	E	101	CRT	C8-C7-C9	-2.94	118.80	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	101	BCL	OBB-CAB-CBB	-2.94	113.56	120.17
15	0	101	CRT	C16-C17-C19	-2.94	114.43	118.94
15	v	101	CRT	C29-C28-C27	-2.93	118.81	122.92
9	D	101	BCL	C4A-NA-C1A	2.93	108.03	106.71
9	k	102	BCL	C2A-C1A-CHA	2.93	128.99	123.86
15	V	101	CRT	C15-C14-C12	-2.93	123.12	127.31
7	C	501	HEM	CAA-CBA-CGA	-2.93	105.54	113.76
9	AG	101	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
9	Q	101	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
9	T	102	BCL	C1-O2A-CGA	2.93	124.13	116.44
9	AC	103	BCL	C1-C2-C3	-2.93	120.98	126.04
9	P	101	BCL	CHD-C4C-NC	-2.93	121.82	125.08
9	u	101	BCL	OBB-CAB-CBB	-2.93	113.58	120.17
9	A	103	BCL	CMA-C3A-C4A	-2.93	103.90	111.77
14	M	404	MQ8	C19-C18-C20	2.93	120.19	115.27
9	2	102	BCL	C16-C15-C13	-2.92	106.47	115.92
9	O	102	BCL	O2A-CGA-O1A	-2.92	116.22	123.59
9	D	102	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
10	x	302	BPH	CMA-C3A-C4A	-2.92	107.98	114.38
9	u	101	BCL	C2A-C1A-CHA	2.92	128.96	123.86
9	q	102	BCL	C7-C6-C5	-2.92	105.43	113.36
9	X	102	BCL	CMA-C3A-C4A	-2.92	103.93	111.77
15	n	101	CRT	C18-C17-C16	2.92	122.67	118.08
9	AB	101	BCL	CED-O2D-CGD	-2.91	109.35	115.94
9	4	102	BCL	C7-C6-C5	-2.91	105.45	113.36
9	O	102	BCL	O2A-C1-C2	2.91	116.28	108.64
9	7	102	BCL	CMB-C2B-C3B	2.91	130.12	124.68
9	k	102	BCL	C7-C6-C5	-2.91	105.46	113.36
9	g	102	BCL	C12-C11-C10	-2.91	99.88	113.24
15	M	405	CRT	C20-C19-C17	-2.91	123.16	127.31
9	6	101	BCL	CHD-C4C-NC	-2.91	121.85	125.08
15	Z	101	CRT	C25-C23-C22	-2.90	114.48	118.94
9	T	102	BCL	OBB-CAB-CBB	-2.90	113.64	120.17
9	s	102	BCL	C1-C2-C3	-2.90	121.02	126.04
9	M	402	BCL	O2A-CGA-CBA	2.90	121.02	111.91
15	2	101	CRT	C8-C7-C9	-2.90	118.86	122.92
9	S	102	BCL	C11-C10-C8	-2.90	106.54	115.92
11	L	304	UQ8	C46-C44-C45	2.90	121.01	114.60
15	Z	101	CRT	C35-C33-C32	-2.90	114.49	118.94
12	t	303	PEF	C3-O3-C30	2.90	124.39	117.10
15	AH	102	CRT	C32-C31-C30	-2.90	114.17	123.22
15	V	101	CRT	C6-C7-C9	-2.90	114.49	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AC	103	BCL	C16-C15-C13	-2.90	106.56	115.92
9	k	102	BCL	C1C-NC-C4C	-2.90	105.40	106.71
15	2	101	CRT	C10-C9-C7	-2.90	123.18	127.31
15	AH	102	CRT	C5-C6-C7	-2.89	121.52	125.89
9	X	102	BCL	C1-O2A-CGA	2.89	124.04	116.44
9	S	102	BCL	O2A-CGA-O1A	-2.89	116.29	123.59
9	6	101	BCL	C16-C15-C13	-2.89	106.57	115.92
15	y	404	CRT	C32-C31-C30	-2.89	114.19	123.22
9	e	102	BCL	C16-C15-C13	-2.89	106.57	115.92
9	X	102	BCL	C11-C12-C13	-2.89	106.57	115.92
11	x	304	UQ8	O4-C4-C5	2.89	126.34	116.56
9	L	301	BCL	C5-C3-C2	2.89	126.96	121.12
15	AL	101	CRT	C18-C17-C16	2.89	122.62	118.08
9	AB	102	BCL	C4B-CHC-C1C	-2.89	124.40	130.12
9	AE	102	BCL	C3D-C2D-C1D	-2.88	101.89	105.83
15	AC	101	CRT	C34-C33-C35	2.88	122.62	118.08
15	AD	101	CRT	C26-C25-C23	-2.88	118.32	126.42
10	L	302	BPH	C11-C10-C8	-2.88	106.61	115.92
9	T	102	BCL	C3C-C2C-C1C	2.88	106.52	101.87
15	m	104	CRT	C10-C9-C7	-2.88	123.20	127.31
9	p	102	BCL	CMD-C2D-C1D	2.88	129.79	124.71
9	AK	101	BCL	C3D-C2D-C1D	-2.88	101.91	105.83
9	AK	101	BCL	OBB-CAB-CBB	-2.87	113.70	120.17
15	n	101	CRT	C20-C19-C17	-2.87	123.21	127.31
9	O	102	BCL	CMD-C2D-C1D	2.87	129.77	124.71
9	u	101	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
15	n	101	CRT	C26-C27-C28	-2.87	123.22	127.31
9	L	301	BCL	O2A-C1-C2	2.87	116.18	108.64
9	p	102	BCL	CHC-C1C-NC	2.87	128.48	124.51
9	c	101	BCL	CGD-CBD-CAD	-2.87	101.45	110.73
15	v	101	CRT	C31-C32-C33	-2.87	123.22	127.31
9	A	102	BCL	C4B-CHC-C1C	-2.87	124.44	130.12
9	M	401	BCL	CMB-C2B-C3B	2.87	130.04	124.68
15	y	404	CRT	C1-C4-C5	2.86	120.65	113.06
15	n	101	CRT	C9-C10-C11	2.86	132.15	123.22
9	X	102	BCL	C2A-C1A-CHA	2.86	128.86	123.86
9	I	101	BCL	C3D-C2D-C1D	-2.86	101.92	105.83
9	1	101	BCL	C4B-CHC-C1C	-2.86	124.45	130.12
9	D	101	BCL	C3D-C2D-C1D	-2.86	101.93	105.83
7	o	503	HEM	CAA-CBA-CGA	-2.86	105.75	113.76
9	M	402	BCL	CHC-C1C-NC	2.85	128.46	124.51
9	M	402	BCL	CBB-CAB-C3B	2.85	128.81	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	101	BCL	C16-C15-C13	-2.85	106.70	115.92
15	X	101	CRT	C9-C10-C11	2.85	132.11	123.22
9	i	102	BCL	C11-C10-C8	-2.85	106.71	115.92
9	d	101	BCL	C1-O2A-CGA	2.85	123.91	116.44
9	I	103	BCL	CMA-C3A-C4A	-2.84	104.14	111.77
9	AK	101	BCL	C4B-CHC-C1C	-2.84	124.49	130.12
15	AL	101	CRT	C10-C9-C7	-2.84	123.26	127.31
9	AG	101	BCL	C4D-CHA-C1A	2.83	124.70	121.25
9	j	101	BCL	CHC-C1C-NC	2.83	128.43	124.51
9	AK	101	BCL	CHC-C1C-NC	2.83	128.43	124.51
12	t	301	PEF	O2-C10-C11	2.83	116.30	111.09
9	x	303	BCL	C4B-CHC-C1C	-2.83	124.52	130.12
9	P	101	BCL	O2A-CGA-O1A	-2.83	116.46	123.59
7	o	504	HEM	C4A-C3A-C2A	2.83	108.96	107.00
9	M	402	BCL	C4B-CHC-C1C	-2.83	124.52	130.12
15	7	103	CRT	C32-C31-C30	-2.82	114.40	123.22
9	x	303	BCL	CHD-C1D-ND	-2.82	121.86	124.45
9	X	102	BCL	O2A-CGA-O1A	-2.82	116.47	123.59
15	P	102	CRT	C8-C7-C6	2.82	122.52	118.08
15	P	102	CRT	C6-C7-C9	-2.82	114.61	118.94
9	U	101	BCL	CED-O2D-CGD	-2.82	109.56	115.94
11	x	304	UQ8	C12-C13-C14	-2.82	120.87	127.66
7	C	502	HEM	C4A-C3A-C2A	2.82	108.96	107.00
9	AB	101	BCL	C7-C6-C5	-2.82	105.71	113.36
9	K	101	BCL	C3C-C2C-C1C	2.82	106.42	101.87
9	N	101	BCL	CHC-C1C-NC	2.82	128.41	124.51
9	3	101	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
15	z	101	CRT	C18-C17-C16	2.81	122.51	118.08
15	m	104	CRT	C16-C17-C19	-2.81	114.63	118.94
9	y	401	BCL	C4B-CHC-C1C	-2.81	124.55	130.12
9	p	102	BCL	O2A-CGA-O1A	-2.81	116.50	123.59
9	R	102	BCL	C11-C12-C13	-2.81	106.84	115.92
15	V	101	CRT	C9-C10-C11	-2.81	114.45	123.22
9	2	102	BCL	OBB-CAB-CBB	-2.81	113.85	120.17
15	7	103	CRT	C1-C4-C5	2.81	120.49	113.06
15	g	101	CRT	C29-C28-C30	2.80	122.50	118.08
9	l	101	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
9	K	101	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
9	AF	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
9	y	401	BCL	C11-C12-C13	-2.80	106.86	115.92
9	l	101	BCL	CMC-C2C-C3C	-2.80	102.53	113.83
9	x	303	BCL	C1C-NC-C4C	-2.80	105.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	5	101	BCL	C16-C15-C13	-2.80	106.87	115.92
9	M	401	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
15	z	101	CRT	C6-C7-C9	-2.80	114.65	118.94
9	AF	101	BCL	CGD-CBD-CAD	-2.80	101.68	110.73
9	i	102	BCL	C4B-CHC-C1C	-2.79	124.58	130.12
12	H	304	PEF	C3-O3-C30	2.79	124.12	117.10
9	Z	102	BCL	CHC-C1C-NC	2.79	128.37	124.51
15	V	101	CRT	C14-C15-C16	-2.79	114.50	123.22
9	P	101	BCL	CED-O2D-CGD	-2.79	109.62	115.94
10	L	302	BPH	C11-C12-C13	-2.79	106.90	115.92
9	x	301	BCL	C4B-CHC-C1C	-2.79	124.60	130.12
9	s	102	BCL	C2A-C1A-CHA	2.79	128.73	123.86
9	F	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
9	AI	102	BCL	C11-C10-C8	-2.79	106.92	115.92
9	0	102	BCL	CMA-C3A-C4A	-2.78	104.29	111.77
9	A	103	BCL	CMC-C2C-C3C	-2.78	102.59	113.83
9	6	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	D	102	BCL	CGD-CBD-CAD	-2.78	101.72	110.73
9	AL	102	BCL	C4B-CHC-C1C	-2.78	124.60	130.12
9	F	101	BCL	C4B-CHC-C1C	-2.78	124.61	130.12
14	y	403	MQ8	C21-C22-C23	-2.78	120.96	127.66
15	g	101	CRT	C27-C26-C25	-2.78	114.54	123.22
9	x	303	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
9	L	303	BCL	CMD-C2D-C1D	2.78	129.61	124.71
9	X	102	BCL	C11-C10-C8	-2.78	106.93	115.92
15	I	102	CRT	C21-C20-C19	-2.78	117.78	123.47
9	Q	101	BCL	CHC-C1C-NC	2.78	128.36	124.51
15	z	101	CRT	C24-C23-C25	2.78	122.45	118.08
9	AI	101	BCL	O2A-CGA-CBA	2.78	120.63	111.91
12	x	306	PEF	O3P-P-O1P	-2.78	98.21	109.07
9	m	103	BCL	C11-C10-C8	-2.78	106.94	115.92
9	r	101	BCL	CHD-C4C-NC	-2.78	121.99	125.08
9	I	103	BCL	C7-C6-C5	-2.78	105.82	113.36
9	y	401	BCL	C11-C10-C8	-2.78	106.95	115.92
9	4	102	BCL	CED-O2D-CGD	-2.77	109.66	115.94
9	8	101	BCL	CHA-C1A-NA	-2.77	120.05	126.40
9	AL	102	BCL	CHC-C1C-NC	2.77	128.34	124.51
9	u	102	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
9	k	102	BCL	CED-O2D-CGD	-2.77	109.67	115.94
9	A	102	BCL	C3D-C2D-C1D	-2.77	102.06	105.83
9	Q	101	BCL	CMC-C2C-C3C	-2.76	102.67	113.83
9	X	102	BCL	C7-C6-C5	-2.76	105.85	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	s	102	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
9	7	102	BCL	C11-C10-C8	-2.76	106.99	115.92
9	F	101	BCL	C16-C15-C13	-2.76	106.99	115.92
9	V	102	BCL	OBB-CAB-CBB	-2.76	113.95	120.17
9	j	101	BCL	CMD-C2D-C1D	2.76	129.58	124.71
9	j	101	BCL	CED-O2D-CGD	-2.76	109.69	115.94
15	AF	102	CRT	C24-C23-C22	-2.76	119.06	122.92
9	I	103	BCL	O2A-CGA-O1A	-2.76	116.63	123.59
9	AL	102	BCL	C11-C10-C8	-2.76	107.00	115.92
9	P	101	BCL	CMA-C3A-C4A	-2.76	104.36	111.77
9	AH	101	BCL	CMC-C2C-C3C	-2.76	102.70	113.83
9	5	101	BCL	CHA-C1A-NA	-2.76	120.08	126.40
12	y	406	PEF	C2-O2-C10	-2.76	112.76	117.90
9	D	102	BCL	C7-C6-C5	-2.76	105.87	113.36
9	D	102	BCL	O2A-C1-C2	2.76	115.88	108.64
15	M	405	CRT	C5-C6-C7	-2.75	121.73	125.89
15	T	101	CRT	C31-C30-C28	-2.75	118.68	126.42
9	m	103	BCL	CHC-C1C-NC	2.75	128.32	124.51
9	f	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
15	G	101	CRT	C6-C7-C9	-2.75	114.72	118.94
9	P	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
9	4	102	BCL	CAA-CBA-CGA	-2.75	105.23	113.25
9	q	102	BCL	CHD-C4C-NC	-2.75	122.03	125.08
15	9	101	CRT	C34-C33-C35	2.74	122.40	118.08
7	o	504	HEM	CHB-C1B-NB	2.74	127.77	124.38
9	h	101	BCL	C16-C15-C13	-2.74	107.05	115.92
14	y	403	MQ8	C20-C18-C17	-2.74	115.57	121.12
9	AG	101	BCL	CHD-C1D-ND	-2.74	121.93	124.45
9	AH	101	BCL	O2A-CGA-O1A	-2.74	116.67	123.59
12	t	303	PEF	O2-C10-O4	-2.74	117.52	122.96
15	e	101	CRT	C8-C7-C6	2.74	122.39	118.08
15	4	101	CRT	C18-C17-C16	2.74	122.39	118.08
9	M	401	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	i	102	BCL	C3D-C2D-C1D	-2.74	102.10	105.83
15	9	101	CRT	C18-C17-C19	-2.73	119.09	122.92
9	f	101	BCL	C2A-C1A-CHA	2.73	128.64	123.86
9	AK	101	BCL	C4A-NA-C1A	2.73	107.93	106.71
15	7	101	CRT	C8-C7-C9	-2.73	119.10	122.92
9	D	101	BCL	OBB-CAB-CBB	-2.73	114.02	120.17
15	AD	101	CRT	C13-C12-C14	-2.73	119.10	122.92
11	L	304	UQ8	O4-C4-C3	-2.73	113.35	123.64
9	Q	101	BCL	CHD-C1D-ND	-2.73	121.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	C16-C15-C13	-2.73	107.10	115.92
15	AL	101	CRT	C24-C23-C22	-2.73	119.10	122.92
9	8	101	BCL	CMA-C3A-C4A	-2.73	104.44	111.77
9	w	101	BCL	C1C-NC-C4C	-2.73	105.48	106.71
15	AJ	101	CRT	C13-C12-C14	-2.73	119.10	122.92
9	k	102	BCL	CHC-C1C-NC	2.72	128.28	124.51
9	u	102	BCL	C4B-CHC-C1C	-2.72	124.72	130.12
15	e	101	CRT	C27-C26-C25	-2.72	114.72	123.22
9	y	401	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
9	8	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
9	A	102	BCL	C2A-C1A-CHA	2.72	128.62	123.86
9	7	102	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
9	AF	101	BCL	CHB-C4A-NA	-2.72	120.75	124.51
15	AL	101	CRT	C14-C15-C16	-2.72	114.73	123.22
10	y	402	BPH	O2A-CGA-CBA	2.72	120.44	111.91
9	u	101	BCL	CMC-C2C-C3C	-2.72	102.87	113.83
9	AC	103	BCL	C7-C6-C5	-2.72	105.98	113.36
9	N	101	BCL	C1C-NC-C4C	-2.72	105.48	106.71
9	u	102	BCL	O2A-CGA-O1A	-2.72	116.74	123.59
11	L	304	UQ8	O3-C3-C2	2.72	125.75	116.56
7	o	503	HEM	CHA-C4D-ND	2.72	127.74	124.38
9	D	102	BCL	CMC-C2C-C3C	-2.71	102.88	113.83
7	o	503	HEM	CHC-C4B-C3B	2.71	128.72	124.57
9	F	101	BCL	C1C-NC-C4C	-2.71	105.49	106.71
10	x	302	BPH	O1D-CGD-CBD	-2.71	120.22	124.74
11	L	304	UQ8	C37-C36-C34	2.71	121.89	112.98
15	I	102	CRT	C26-C27-C28	-2.71	123.44	127.31
9	T	102	BCL	C7-C6-C5	-2.71	106.00	113.36
9	V	102	BCL	CHB-C4A-NA	-2.71	120.77	124.51
9	M	402	BCL	C11-C10-C8	-2.71	107.17	115.92
9	AG	101	BCL	C11-C10-C8	-2.71	107.17	115.92
9	D	101	BCL	CMA-C3A-C4A	-2.70	104.50	111.77
9	7	102	BCL	C16-C15-C13	-2.70	107.18	115.92
9	Z	102	BCL	C4B-CHC-C1C	-2.70	124.76	130.12
9	r	101	BCL	C2A-C1A-CHA	2.70	128.58	123.86
15	y	404	CRT	C34-C33-C35	2.70	122.33	118.08
9	S	102	BCL	C7-C6-C5	-2.70	106.03	113.36
9	1	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
15	9	101	CRT	C10-C9-C7	2.70	131.16	127.31
9	AL	102	BCL	C4D-CHA-C1A	2.70	124.53	121.25
15	s	101	CRT	C26-C25-C23	-2.70	118.84	126.42
9	D	101	BCL	C11-C12-C13	-2.70	107.20	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	y	401	BCL	O2A-C1-C2	2.70	115.72	108.64
9	F	101	BCL	CMC-C2C-C3C	-2.70	102.95	113.83
9	AK	101	BCL	O2A-CGA-O1A	-2.70	116.79	123.59
15	AF	102	CRT	C8-C7-C9	-2.69	119.15	122.92
9	w	101	BCL	CHD-C4C-NC	-2.69	122.08	125.08
9	A	103	BCL	CMD-C2D-C1D	2.69	129.46	124.71
9	AB	101	BCL	CMA-C3A-C4A	-2.69	104.53	111.77
9	V	102	BCL	CBA-CAA-C2A	2.69	121.81	113.86
9	x	301	BCL	C2D-C1D-ND	2.69	112.09	110.10
9	F	101	BCL	CHC-C1C-NC	2.69	128.23	124.51
9	AL	102	BCL	CMC-C2C-C3C	-2.69	102.97	113.83
15	G	101	CRT	C8-C7-C6	2.69	122.32	118.08
15	AD	101	CRT	C21-C20-C19	-2.69	117.97	123.47
9	O	102	BCL	CMC-C2C-C3C	-2.69	102.98	113.83
9	e	102	BCL	C7-C6-C5	-2.69	106.06	113.36
15	n	101	CRT	C20-C21-C22	-2.69	117.97	123.47
9	4	102	BCL	C3D-C2D-C1D	-2.69	102.17	105.83
9	AB	101	BCL	CMC-C2C-C3C	-2.68	103.00	113.83
9	AI	101	BCL	C11-C10-C8	-2.68	107.25	115.92
9	x	301	BCL	C11-C10-C8	-2.68	107.25	115.92
9	Z	102	BCL	CMA-C3A-C4A	-2.68	104.56	111.77
9	x	305	BCL	CMB-C2B-C1B	-2.68	124.34	128.46
9	g	102	BCL	CMD-C2D-C1D	2.68	129.44	124.71
9	5	101	BCL	C4D-CHA-C1A	2.68	124.51	121.25
9	2	102	BCL	CHC-C1C-NC	2.68	128.22	124.51
9	I	103	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
7	C	503	HEM	C4A-C3A-C2A	2.68	108.86	107.00
7	o	501	HEM	CMA-C3A-C4A	-2.68	124.35	128.46
9	y	401	BCL	CGD-CBD-CAD	-2.67	102.07	110.73
9	0	102	BCL	O2A-CGA-O1A	-2.67	116.84	123.59
12	t	301	PEF	C3-O3-C30	2.67	123.82	117.10
9	D	101	BCL	CMC-C2C-C3C	-2.67	103.05	113.83
9	T	102	BCL	O2A-C1-C2	2.67	115.65	108.64
9	V	102	BCL	CED-O2D-CGD	-2.67	109.90	115.94
9	l	101	BCL	CGD-CBD-CAD	-2.67	102.08	110.73
9	AL	102	BCL	C1-C2-C3	-2.67	121.43	126.04
9	Z	102	BCL	CHD-C1D-ND	-2.67	122.00	124.45
9	AC	102	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
9	7	102	BCL	CMD-C2D-C1D	2.66	129.41	124.71
9	AL	102	BCL	CAA-CBA-CGA	-2.66	105.47	113.25
9	Z	102	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
9	N	101	BCL	CMA-C3A-C4A	-2.66	104.61	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AE	102	BCL	OBB-CAB-CBB	-2.66	114.19	120.17
7	C	504	HEM	CHD-C1D-ND	2.66	127.32	124.43
10	x	302	BPH	O2A-CGA-CBA	2.66	120.24	111.91
9	e	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
15	2	101	CRT	C18-C17-C16	2.65	122.26	118.08
9	G	102	BCL	O2A-C1-C2	2.65	115.61	108.64
15	AC	101	CRT	C18-C17-C16	2.65	122.26	118.08
9	A	103	BCL	C11-C10-C8	-2.65	107.36	115.92
15	q	101	CRT	C14-C15-C16	-2.65	114.95	123.22
15	i	101	CRT	C11-C12-C14	-2.65	114.88	118.94
9	F	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
9	x	301	BCL	C1C-NC-C4C	-2.65	105.52	106.71
15	0	101	CRT	C27-C26-C25	-2.65	114.96	123.22
9	AB	101	BCL	O2A-CGA-O1A	-2.65	116.91	123.59
9	A	102	BCL	OBB-CAB-CBB	-2.65	114.22	120.17
9	AC	102	BCL	O2A-C1-C2	2.65	115.59	108.64
15	M	405	CRT	C9-C10-C11	-2.64	114.97	123.22
9	AC	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
9	AI	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
15	AL	101	CRT	C21-C22-C23	-2.64	123.54	127.31
9	2	102	BCL	C4B-CHC-C1C	-2.64	124.89	130.12
12	m	101	PEF	O3-C3-C2	2.64	116.11	108.43
15	AH	102	CRT	C14-C15-C16	-2.64	114.98	123.22
9	G	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
15	AH	102	CRT	C35-C33-C32	-2.64	114.89	118.94
12	y	408	PEF	C3-C2-C1	2.64	118.02	111.79
9	3	101	BCL	C11-C10-C8	-2.64	107.40	115.92
9	V	102	BCL	CMA-C3A-C4A	-2.63	104.69	111.77
9	AE	102	BCL	C2A-C1A-CHA	2.63	128.47	123.86
9	X	102	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
9	O	102	BCL	OBB-CAB-CBB	-2.63	114.25	120.17
9	A	103	BCL	C16-C15-C13	-2.63	107.41	115.92
9	f	101	BCL	OBB-CAB-CBB	-2.63	114.25	120.17
9	AB	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
9	i	102	BCL	C1-O2A-CGA	2.63	123.35	116.44
9	U	101	BCL	CHD-C4C-NC	-2.63	122.15	125.08
9	O	102	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
15	AC	101	CRT	C14-C15-C16	-2.63	115.01	123.22
9	z	102	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
9	F	101	BCL	O2A-CGA-O1A	-2.63	116.96	123.59
9	K	101	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
15	i	101	CRT	C26-C27-C28	-2.63	123.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	6	101	BCL	C1D-CHD-C4C	-2.63	120.29	126.62
9	y	401	BCL	C16-C15-C13	-2.62	107.44	115.92
9	u	102	BCL	C11-C12-C13	-2.62	107.44	115.92
9	y	401	BCL	C4B-C3B-CAB	-2.62	122.06	127.13
15	4	101	CRT	C5-C6-C7	-2.62	121.93	125.89
9	Y	101	BCL	CED-O2D-CGD	-2.62	110.00	115.94
15	AJ	101	CRT	C13-C12-C11	2.62	122.21	118.08
15	9	101	CRT	C24-C23-C22	-2.62	119.25	122.92
15	R	101	CRT	C32-C31-C30	-2.62	115.03	123.22
9	D	102	BCL	CHC-C1C-NC	2.62	128.14	124.51
9	O	102	BCL	CHB-C4A-NA	-2.62	120.89	124.51
15	R	101	CRT	C15-C16-C17	2.62	133.77	126.42
9	x	305	BCL	C2A-C1A-CHA	2.62	128.44	123.86
9	AB	102	BCL	C3D-C2D-C1D	-2.62	102.26	105.83
9	6	101	BCL	C2A-C1A-CHA	2.62	128.43	123.86
10	L	302	BPH	O2A-CGA-CBA	2.61	120.11	111.91
15	0	101	CRT	C15-C14-C12	-2.61	123.58	127.31
7	o	502	HEM	CAD-C3D-C4D	2.61	129.23	124.66
9	r	101	BCL	C12-C11-C10	-2.61	101.23	113.24
9	K	101	BCL	C7-C6-C5	-2.61	106.27	113.36
9	AE	102	BCL	O2A-CGA-O1A	-2.61	117.00	123.59
9	AI	101	BCL	C16-C15-C13	-2.61	107.48	115.92
15	M	405	CRT	C18-C17-C19	-2.61	119.27	122.92
9	c	101	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
9	Q	101	BCL	C2C-C3C-C4C	-2.61	97.43	101.34
9	s	102	BCL	O2A-CGA-O1A	-2.61	117.01	123.59
9	V	102	BCL	CHC-C1C-NC	2.61	128.12	124.51
9	i	102	BCL	C7-C6-C5	-2.61	106.28	113.36
15	z	101	CRT	C9-C10-C11	-2.61	115.08	123.22
9	AG	101	BCL	CMC-C2C-C3C	-2.60	103.32	113.83
9	l	101	BCL	CHC-C1C-NC	2.60	128.11	124.51
9	L	301	BCL	CMD-C2D-C1D	2.60	129.30	124.71
9	AB	102	BCL	O2A-CGA-O1A	-2.60	117.02	123.59
9	q	102	BCL	C6-C5-C3	-2.60	106.63	113.45
9	k	102	BCL	CMC-C2C-C3C	-2.60	103.33	113.83
9	m	102	BCL	CMC-C2C-C3C	-2.60	103.33	113.83
9	s	102	BCL	CMC-C2C-C3C	-2.60	103.33	113.83
9	w	101	BCL	C3D-C2D-C1D	-2.60	102.28	105.83
9	m	102	BCL	C3D-C2D-C1D	-2.60	102.28	105.83
9	5	101	BCL	O2A-CGA-O1A	-2.60	117.03	123.59
9	K	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	A	102	BCL	CHC-C1C-NC	2.60	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	303	BCL	OBB-CAB-CBB	-2.60	114.33	120.17
9	5	101	BCL	C11-C12-C13	-2.60	107.53	115.92
9	AI	102	BCL	CMC-C2C-C3C	-2.59	103.37	113.83
15	AD	101	CRT	C11-C12-C14	2.59	122.92	118.94
9	S	102	BCL	C3D-C2D-C1D	-2.59	102.29	105.83
7	C	504	HEM	CHC-C4B-NB	2.59	127.25	124.43
9	AC	102	BCL	C11-C12-C13	-2.59	107.54	115.92
9	Z	102	BCL	C7-C6-C5	-2.59	106.32	113.36
9	AI	101	BCL	C1C-NC-C4C	-2.59	105.54	106.71
9	8	101	BCL	CMC-C2C-C3C	-2.59	103.38	113.83
9	K	101	BCL	C1-O2A-CGA	2.59	123.24	116.44
15	0	101	CRT	C35-C33-C32	-2.59	114.97	118.94
9	A	102	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
7	C	501	HEM	O2A-CGA-CBA	2.59	122.34	114.03
9	A	102	BCL	C3C-C2C-C1C	2.59	106.05	101.87
15	2	101	CRT	C32-C31-C30	-2.59	115.15	123.22
15	7	101	CRT	C18-C17-C16	2.58	122.15	118.08
9	T	102	BCL	CED-O2D-CGD	-2.58	110.09	115.94
9	AE	102	BCL	C1-O2A-CGA	2.58	123.22	116.44
9	V	102	BCL	CAA-C2A-C3A	2.58	119.85	112.78
9	AH	101	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
9	p	102	BCL	C2A-C1A-CHA	2.58	128.38	123.86
9	u	101	BCL	CMD-C2D-C1D	2.58	129.26	124.71
9	A	103	BCL	C3D-C2D-C1D	-2.58	102.31	105.83
15	I	102	CRT	C29-C28-C30	2.58	122.14	118.08
9	6	101	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
9	A	102	BCL	C12-C11-C10	-2.58	101.39	113.24
15	X	101	CRT	C40-C38-C37	-2.58	106.90	110.86
9	0	102	BCL	CMC-C2C-C3C	-2.58	103.43	113.83
9	p	102	BCL	C12-C11-C10	-2.58	101.40	113.24
9	F	101	BCL	C2C-C3C-C4C	-2.57	97.48	101.34
9	g	102	BCL	CGD-CBD-CAD	-2.57	102.40	110.73
9	q	102	BCL	C16-C15-C13	-2.57	107.61	115.92
9	h	101	BCL	CMD-C2D-C1D	2.57	129.24	124.71
15	k	101	CRT	C5-C6-C7	-2.57	122.01	125.89
9	D	102	BCL	C2A-C1A-CHA	2.57	128.35	123.86
15	R	101	CRT	C10-C11-C12	-2.57	119.20	126.42
9	V	102	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
9	O	102	BCL	CBA-CAA-C2A	2.57	121.44	113.86
9	L	301	BCL	C2A-C1A-CHA	2.57	128.35	123.86
9	j	101	BCL	CHB-C4A-NA	-2.57	120.96	124.51
9	AB	101	BCL	C3D-C2D-C1D	-2.57	102.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AB	101	BCL	C1-C2-C3	-2.57	121.60	126.04
15	AD	101	CRT	C15-C16-C17	2.57	133.62	126.42
7	o	502	HEM	CMC-C2C-C3C	2.57	129.48	124.68
15	m	104	CRT	C24-C23-C25	2.57	122.12	118.08
9	u	102	BCL	CMC-C2C-C3C	-2.57	103.48	113.83
15	q	101	CRT	C9-C10-C11	-2.56	115.21	123.22
15	7	103	CRT	C26-C25-C23	-2.56	119.21	126.42
7	o	503	HEM	CAB-C3B-C4B	2.56	136.42	124.47
9	AI	102	BCL	C2A-C1A-CHA	2.56	128.34	123.86
15	n	101	CRT	C34-C33-C35	2.56	122.11	118.08
7	o	503	HEM	O2A-CGA-CBA	2.56	122.25	114.03
7	o	502	HEM	CAA-CBA-CGA	-2.56	106.58	113.76
7	C	501	HEM	C3D-C4D-ND	-2.56	107.32	110.17
9	L	303	BCL	C6-C5-C3	2.56	120.16	113.45
15	s	101	CRT	C39-C38-C37	-2.56	106.93	110.86
9	AC	103	BCL	CMC-C2C-C3C	-2.56	103.51	113.83
7	C	501	HEM	CHB-C1B-C2B	-2.56	119.65	126.72
9	Y	101	BCL	CMC-C2C-C1C	-2.56	104.90	111.77
9	P	101	BCL	C1C-NC-C4C	-2.56	105.56	106.71
7	C	501	HEM	CMA-C3A-C2A	2.56	129.76	124.94
9	x	305	BCL	C1D-CHD-C4C	-2.55	120.46	126.62
9	AB	102	BCL	CMD-C2D-C1D	2.55	129.21	124.71
9	L	301	BCL	O2A-CGA-CBA	2.55	119.92	111.91
9	z	102	BCL	C3D-C2D-C1D	-2.55	102.35	105.83
9	9	102	BCL	CHC-C1C-NC	2.55	128.04	124.51
9	AG	101	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
9	S	102	BCL	CMC-C2C-C3C	-2.55	103.54	113.83
9	T	102	BCL	CHB-C4A-NA	-2.55	120.99	124.51
9	T	102	BCL	C16-C15-C13	-2.55	107.68	115.92
9	9	102	BCL	C3D-C2D-C1D	-2.55	102.35	105.83
15	AC	101	CRT	C32-C31-C30	-2.55	115.27	123.22
9	Z	102	BCL	C3C-C4C-CHD	-2.55	117.95	123.39
9	T	102	BCL	CBA-CAA-C2A	2.55	121.38	113.86
9	R	102	BCL	C7-C6-C5	-2.55	106.44	113.36
9	R	102	BCL	C4A-NA-C1A	2.55	107.85	106.71
9	6	101	BCL	CAA-CBA-CGA	-2.55	105.81	113.25
9	AI	102	BCL	CHD-C4C-NC	-2.55	122.25	125.08
9	h	101	BCL	CHC-C1C-NC	2.54	128.03	124.51
9	G	102	BCL	C11-C12-C13	-2.54	107.69	115.92
9	AI	102	BCL	C7-C6-C5	-2.54	106.45	113.36
9	Y	101	BCL	CMD-C2D-C1D	2.54	129.19	124.71
9	r	101	BCL	C1C-NC-C4C	-2.54	105.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AC	101	CRT	C27-C26-C25	-2.54	115.29	123.22
15	X	101	CRT	C20-C21-C22	-2.54	118.28	123.47
9	Q	101	BCL	CBC-CAC-C3C	2.54	119.11	113.47
9	x	303	BCL	CGD-CBD-CAD	-2.54	102.52	110.73
9	I	101	BCL	O2A-C1-C2	2.54	115.30	108.64
9	x	305	BCL	CMC-C2C-C3C	-2.53	103.60	113.83
9	4	102	BCL	C1-O2A-CGA	2.53	123.09	116.44
12	H	305	PEF	O2-C10-O4	-2.53	117.93	122.96
9	x	301	BCL	CHC-C1C-NC	2.53	128.01	124.51
12	y	408	PEF	C3-O3-C30	2.53	123.47	117.10
9	AH	101	BCL	C16-C15-C13	-2.53	107.74	115.92
9	R	102	BCL	CMA-C3A-C2A	-2.53	103.62	113.83
9	W	101	BCL	O2A-CGA-O1A	-2.53	117.21	123.59
10	M	403	BPH	C11-C12-C13	-2.53	107.75	115.92
9	AF	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
15	z	101	CRT	C29-C28-C30	2.53	122.06	118.08
10	x	302	BPH	C4-C3-C5	2.52	119.52	115.27
9	Z	102	BCL	CMC-C2C-C3C	-2.52	103.65	113.83
9	AG	101	BCL	CHC-C1C-NC	2.52	128.00	124.51
15	AH	102	CRT	C34-C33-C35	2.52	122.05	118.08
9	r	101	BCL	CMC-C2C-C3C	-2.52	103.65	113.83
9	e	102	BCL	CBB-CAB-C3B	2.52	127.83	120.34
9	c	101	BCL	C1-O2A-CGA	2.52	123.06	116.44
9	R	102	BCL	CMC-C2C-C3C	-2.52	103.66	113.83
9	U	101	BCL	C3D-C2D-C1D	-2.52	102.39	105.83
7	C	502	HEM	CAD-C3D-C4D	2.52	129.06	124.66
9	c	101	BCL	CHC-C1C-NC	2.52	128.00	124.51
9	m	103	BCL	O2A-CGA-O1A	-2.52	117.23	123.59
9	h	101	BCL	C3D-C2D-C1D	-2.52	102.39	105.83
9	AE	102	BCL	CMC-C2C-C3C	-2.52	103.67	113.83
9	x	303	BCL	C1D-CHD-C4C	-2.52	120.55	126.62
7	o	501	HEM	C3D-C4D-ND	-2.52	107.37	110.17
9	AH	101	BCL	CBB-CAB-C3B	2.52	127.81	120.34
9	AB	102	BCL	CMC-C2C-C3C	-2.51	103.68	113.83
9	7	102	BCL	C1-O2A-CGA	2.51	123.04	116.44
9	AC	103	BCL	C1-O2A-CGA	2.51	123.04	116.44
9	AG	101	BCL	CED-O2D-CGD	-2.51	110.26	115.94
9	AB	102	BCL	C12-C11-C10	-2.51	101.70	113.24
14	y	403	MQ8	C29-C28-C30	2.51	119.49	115.27
9	5	101	BCL	CMC-C2C-C3C	-2.51	103.70	113.83
9	7	102	BCL	CMC-C2C-C3C	-2.51	103.70	113.83
9	M	402	BCL	C3D-C2D-C1D	-2.51	102.41	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BCL	CBC-CAC-C3C	2.51	119.05	113.47
12	p	101	PEF	O3-C30-C31	2.51	123.32	112.38
9	M	402	BCL	C3C-C2C-C1C	2.51	105.92	101.87
10	x	302	BPH	CBC-CAC-C3C	-2.51	108.72	113.77
9	AG	101	BCL	C3D-C2D-C1D	-2.51	102.41	105.83
9	d	101	BCL	C4D-CHA-C1A	2.50	124.30	121.25
9	AL	102	BCL	C3D-C2D-C1D	-2.50	102.42	105.83
10	y	402	BPH	CGD-CBD-CAD	-2.50	102.63	110.73
9	A	102	BCL	O2A-CGA-O1A	-2.50	117.28	123.59
9	M	402	BCL	CHD-C1D-ND	-2.50	122.16	124.45
9	I	101	BCL	CMC-C2C-C3C	-2.50	103.74	113.83
9	AB	101	BCL	CHD-C4C-NC	-2.50	122.30	125.08
9	A	103	BCL	CHB-C4A-NA	-2.50	121.05	124.51
15	O	101	CRT	C13-C12-C11	2.50	122.02	118.08
9	AE	102	BCL	C11-C12-C13	-2.50	107.84	115.92
7	o	504	HEM	O2D-CGD-CBD	2.50	122.05	114.03
9	AB	102	BCL	CHC-C1C-NC	2.50	127.96	124.51
9	L	303	BCL	C6-C7-C8	2.50	123.99	115.92
9	h	101	BCL	C4A-NA-C1A	2.50	107.83	106.71
14	M	404	MQ8	C20-C18-C17	-2.50	116.07	121.12
9	M	402	BCL	C7-C6-C5	-2.49	106.58	113.36
9	N	101	BCL	C3D-C2D-C1D	-2.49	102.43	105.83
9	d	101	BCL	CAA-CBA-CGA	-2.49	105.97	113.25
15	T	101	CRT	C27-C26-C25	-2.49	115.44	123.22
7	o	502	HEM	CHB-C1B-NB	2.49	127.46	124.38
9	L	301	BCL	C1C-NC-C4C	-2.49	105.59	106.71
9	s	102	BCL	CHB-C4A-NA	-2.49	121.07	124.51
9	O	102	BCL	C11-C12-C13	-2.49	107.87	115.92
9	u	101	BCL	C1-C2-C3	-2.49	121.74	126.04
9	O	102	BCL	C4A-NA-C1A	2.49	107.83	106.71
9	p	102	BCL	C1C-NC-C4C	-2.49	105.59	106.71
11	L	304	UQ8	O3-C3-C4	-2.49	114.26	123.64
9	Q	101	BCL	O2A-CGA-O1A	-2.49	117.31	123.59
15	G	101	CRT	C9-C10-C11	-2.49	115.45	123.22
9	m	102	BCL	C11-C10-C8	-2.49	107.88	115.92
7	o	503	HEM	CAD-C3D-C4D	2.49	129.00	124.66
9	A	102	BCL	CMC-C2C-C3C	-2.49	103.80	113.83
9	0	102	BCL	C3D-C2D-C1D	-2.49	102.44	105.83
9	s	102	BCL	C3C-C4C-CHD	-2.49	118.08	123.39
15	2	101	CRT	C13-C12-C11	2.48	121.99	118.08
9	4	102	BCL	C11-C12-C13	-2.48	107.90	115.92
15	9	101	CRT	C18-C17-C16	2.48	121.99	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	102	BCL	C11-C12-C13	-2.48	107.90	115.92
9	Q	101	BCL	CED-O2D-CGD	-2.48	110.33	115.94
9	g	102	BCL	C16-C15-C13	-2.48	107.91	115.92
12	y	408	PEF	O2-C10-O4	-2.48	118.04	122.96
9	m	103	BCL	O2A-C1-C2	2.48	115.14	108.64
15	O	101	CRT	C8-C7-C6	2.48	121.98	118.08
9	l	101	BCL	C4B-CHC-C1C	-2.47	125.22	130.12
9	m	102	BCL	CHC-C1C-NC	2.47	127.93	124.51
15	AF	102	CRT	C8-C7-C6	2.47	121.97	118.08
9	u	102	BCL	CHD-C1D-ND	-2.47	122.18	124.45
9	M	401	BCL	C1D-CHD-C4C	-2.47	120.66	126.62
9	I	103	BCL	C11-C12-C13	-2.47	107.93	115.92
9	P	101	BCL	CMC-C2C-C3C	-2.47	103.86	113.83
9	q	102	BCL	C11-C10-C8	-2.47	107.93	115.92
9	i	102	BCL	CHB-C4A-NA	-2.47	121.10	124.51
9	e	102	BCL	C11-C10-C8	-2.47	107.94	115.92
9	L	301	BCL	C16-C15-C13	-2.47	107.94	115.92
9	j	101	BCL	C3D-C2D-C1D	-2.47	102.46	105.83
9	K	101	BCL	C3C-C4C-CHD	-2.47	118.12	123.39
9	R	102	BCL	C1-O2A-CGA	2.47	122.92	116.44
9	U	101	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
10	y	402	BPH	O2A-CGA-O1A	-2.47	117.37	123.59
10	M	403	BPH	CMC-C2C-C1C	-2.47	108.98	114.38
9	A	103	BCL	O2A-C1-C2	2.46	115.11	108.64
9	6	101	BCL	CMC-C2C-C3C	-2.46	103.89	113.83
9	V	102	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
9	w	101	BCL	C16-C15-C13	-2.46	107.96	115.92
9	g	102	BCL	C3C-C4C-CHD	-2.46	118.13	123.39
15	v	101	CRT	C24-C23-C25	2.46	121.95	118.08
9	L	301	BCL	C1B-CHB-C4A	-2.46	125.25	130.12
9	3	101	BCL	C7-C6-C5	-2.46	106.68	113.36
10	L	302	BPH	C4-C3-C5	2.46	119.41	115.27
9	F	101	BCL	C11-C12-C13	-2.46	107.97	115.92
15	7	101	CRT	C16-C17-C19	-2.46	115.17	118.94
15	e	101	CRT	C20-C19-C17	-2.46	123.80	127.31
15	0	101	CRT	C31-C30-C28	-2.46	119.51	126.42
15	AD	101	CRT	C32-C31-C30	-2.46	115.55	123.22
15	O	101	CRT	C29-C28-C30	2.46	121.95	118.08
15	P	102	CRT	C14-C15-C16	-2.46	115.55	123.22
15	k	101	CRT	C21-C22-C23	-2.46	123.81	127.31
9	X	102	BCL	C3D-C2D-C1D	-2.46	102.48	105.83
9	5	101	BCL	C12-C11-C10	-2.46	101.96	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	101	BCL	CMC-C2C-C3C	-2.45	103.92	113.83
15	4	101	CRT	C10-C9-C7	-2.45	123.81	127.31
9	AC	103	BCL	C11-C10-C8	-2.45	108.00	115.92
9	AC	102	BCL	C11-C10-C8	-2.45	108.00	115.92
9	4	102	BCL	CMC-C2C-C3C	-2.45	103.95	113.83
9	l	101	BCL	C6-C5-C3	-2.45	107.03	113.45
15	g	101	CRT	C18-C17-C16	2.45	121.93	118.08
9	L	301	BCL	CGD-CBD-CAD	-2.45	102.81	110.73
9	AE	102	BCL	C6-C5-C3	-2.45	107.04	113.45
15	g	101	CRT	C21-C20-C19	-2.45	118.46	123.47
12	t	303	PEF	O5-C30-C31	-2.44	115.90	124.81
9	w	101	BCL	CMC-C2C-C3C	-2.44	103.97	113.83
9	I	101	BCL	C4A-NA-C1A	2.44	107.81	106.71
9	7	102	BCL	C3D-C2D-C1D	-2.44	102.50	105.83
9	AH	101	BCL	CMD-C2D-C1D	2.44	129.02	124.71
7	C	501	HEM	CAD-C3D-C2D	-2.44	123.33	127.88
9	S	102	BCL	C16-C15-C13	-2.44	108.04	115.92
9	F	101	BCL	C4A-NA-C1A	2.44	107.80	106.71
14	M	404	MQ8	O1-C1-C2	-2.44	117.09	120.25
12	t	303	PEF	O3-C30-C31	2.44	123.01	112.38
9	X	102	BCL	CBB-CAB-C3B	2.44	127.58	120.34
15	AC	101	CRT	C29-C28-C27	-2.44	119.51	122.92
9	6	101	BCL	C1C-NC-C4C	-2.44	105.61	106.71
9	AH	101	BCL	CED-O2D-CGD	-2.44	110.43	115.94
9	h	101	BCL	CMC-C2C-C3C	-2.43	104.01	113.83
9	9	102	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
9	4	102	BCL	C11-C10-C8	-2.43	108.06	115.92
9	x	303	BCL	C4B-C3B-CAB	-2.43	122.43	127.13
9	i	102	BCL	CBB-CAB-C3B	2.43	127.56	120.34
15	v	101	CRT	C34-C33-C35	2.43	121.91	118.08
9	5	101	BCL	C3D-C2D-C1D	-2.43	102.52	105.83
9	i	102	BCL	CMC-C2C-C3C	-2.43	104.03	113.83
9	e	102	BCL	C3D-C2D-C1D	-2.43	102.52	105.83
9	j	101	BCL	CMC-C2C-C3C	-2.43	104.03	113.83
9	R	102	BCL	O2A-CGA-O1A	-2.43	117.46	123.59
9	AG	101	BCL	C2A-C1A-CHA	2.43	128.11	123.86
9	I	101	BCL	CGD-CBD-CAD	-2.43	102.87	110.73
15	Z	101	CRT	C8-C7-C9	-2.43	119.52	122.92
15	9	101	CRT	C29-C28-C30	2.43	121.90	118.08
15	G	101	CRT	C27-C26-C25	-2.43	115.64	123.22
15	9	101	CRT	C35-C33-C32	-2.43	115.22	118.94
15	AL	101	CRT	C16-C17-C19	-2.43	115.22	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	z	102	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
9	c	101	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
15	E	101	CRT	C26-C27-C28	-2.43	123.85	127.31
9	AI	101	BCL	CMC-C2C-C3C	-2.43	104.04	113.83
7	o	501	HEM	CBA-CAA-C2A	-2.42	108.48	112.62
9	AC	102	BCL	C4A-NA-C1A	2.42	107.80	106.71
9	AE	102	BCL	CBA-CAA-C2A	2.42	121.02	113.86
9	m	103	BCL	C12-C11-C10	-2.42	102.10	113.24
9	O	102	BCL	C7-C6-C5	-2.42	106.78	113.36
9	w	101	BCL	CED-O2D-CGD	-2.42	110.46	115.94
9	W	101	BCL	OBD-CAD-C3D	2.42	134.34	128.52
9	U	101	BCL	CHC-C1C-NC	2.42	127.86	124.51
15	y	404	CRT	C13-C12-C14	-2.42	119.54	122.92
9	T	102	BCL	C4A-NA-C1A	2.42	107.79	106.71
9	z	102	BCL	C11-C12-C13	-2.42	108.11	115.92
9	D	102	BCL	C4B-CHC-C1C	-2.42	125.33	130.12
9	4	102	BCL	C12-C11-C10	-2.42	102.14	113.24
15	2	101	CRT	C21-C20-C19	-2.41	118.53	123.47
9	0	102	BCL	C16-C15-C13	-2.41	108.12	115.92
9	2	102	BCL	O2A-CGA-O1A	-2.41	117.50	123.59
9	AI	102	BCL	C3D-C2D-C1D	-2.41	102.54	105.83
15	q	101	CRT	C24-C23-C22	-2.41	119.55	122.92
10	L	302	BPH	CMC-C2C-C1C	-2.41	109.10	114.38
9	h	101	BCL	O2A-C1-C2	2.41	114.97	108.64
9	g	102	BCL	C3D-C2D-C1D	-2.41	102.54	105.83
9	Y	101	BCL	CMC-C2C-C3C	-2.41	104.11	113.83
10	x	302	BPH	C1-C2-C3	-2.41	121.88	126.04
9	AI	101	BCL	C11-C12-C13	-2.41	108.14	115.92
15	z	101	CRT	C24-C23-C22	-2.41	119.55	122.92
9	M	402	BCL	C5-C3-C2	2.40	125.98	121.12
7	C	503	HEM	C4B-CHC-C1C	2.40	125.73	122.56
15	k	101	CRT	C10-C9-C7	-2.40	123.88	127.31
9	AH	101	BCL	C4B-CHC-C1C	-2.40	125.36	130.12
7	C	501	HEM	CAD-C3D-C4D	2.40	128.86	124.66
9	9	102	BCL	O2A-CGA-O1A	-2.40	117.53	123.59
9	c	101	BCL	C11-C12-C13	-2.40	108.15	115.92
9	l	101	BCL	C4A-NA-C1A	2.40	107.79	106.71
15	i	101	CRT	C20-C19-C17	-2.40	123.88	127.31
9	5	101	BCL	CBB-CAB-C3B	2.40	127.46	120.34
15	AD	101	CRT	C10-C11-C12	-2.40	119.68	126.42
15	AJ	101	CRT	C9-C10-C11	2.40	130.70	123.22
9	y	401	BCL	CMD-C2D-C1D	2.40	128.94	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Y	101	BCL	C16-C15-C13	-2.40	108.18	115.92
9	9	102	BCL	CMD-C2D-C1D	2.40	128.93	124.71
9	K	101	BCL	C11-C10-C8	-2.39	108.18	115.92
9	G	102	BCL	C7-C6-C5	-2.39	106.86	113.36
9	I	103	BCL	C16-C15-C13	-2.39	108.19	115.92
9	D	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
9	AG	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
9	G	102	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
14	M	404	MQ8	C44-C43-C42	-2.39	116.28	121.12
14	y	403	MQ8	C35-C33-C32	-2.39	116.28	121.12
7	C	503	HEM	CAA-CBA-CGA	-2.39	107.06	113.76
15	n	101	CRT	C21-C20-C19	-2.39	118.58	123.47
9	AE	102	BCL	C3C-C2C-C1C	2.39	105.72	101.87
15	O	101	CRT	C26-C27-C28	-2.39	123.90	127.31
9	x	303	BCL	C4D-CHA-C1A	2.39	124.15	121.25
12	x	306	PEF	O3-C30-C31	2.39	122.78	112.38
9	2	102	BCL	CHD-C1D-ND	-2.38	122.26	124.45
9	e	102	BCL	CMC-C2C-C3C	-2.38	104.22	113.83
15	AC	101	CRT	C34-C33-C32	-2.38	119.58	122.92
9	A	103	BCL	C3C-C4C-CHD	-2.38	118.30	123.39
7	o	501	HEM	CHB-C1B-NB	2.38	127.33	124.38
15	7	101	CRT	C21-C20-C19	-2.38	118.60	123.47
15	2	101	CRT	C24-C23-C25	2.38	121.83	118.08
9	Z	102	BCL	CBB-CAB-C3B	2.38	127.40	120.34
9	5	101	BCL	CHC-C1C-NC	2.38	127.80	124.51
9	Q	101	BCL	CAA-CBA-CGA	-2.38	106.30	113.25
9	AB	102	BCL	C1-O2A-CGA	2.38	122.68	116.44
15	V	101	CRT	C18-C17-C16	2.38	121.82	118.08
9	l	101	BCL	C12-C11-C10	-2.38	102.31	113.24
15	AJ	101	CRT	C34-C33-C35	2.38	121.82	118.08
15	Z	101	CRT	C27-C26-C25	-2.38	115.80	123.22
9	AC	103	BCL	C12-C11-C10	-2.38	102.32	113.24
9	T	102	BCL	C11-C12-C13	-2.38	108.24	115.92
15	s	101	CRT	C21-C22-C23	-2.38	123.92	127.31
15	s	101	CRT	C9-C10-C11	-2.37	115.81	123.22
15	m	104	CRT	C36-C35-C33	-2.37	122.31	125.89
9	c	101	BCL	C11-C10-C8	-2.37	108.25	115.92
7	o	503	HEM	CHB-C1B-C2B	-2.37	120.16	126.72
9	m	103	BCL	CBC-CAC-C3C	2.37	118.75	113.47
9	U	101	BCL	CHB-C4A-NA	-2.37	121.23	124.51
9	AF	101	BCL	O2A-CGA-O1A	-2.37	117.61	123.59
9	u	101	BCL	C16-C15-C13	-2.37	108.26	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	101	BCL	C12-C11-C10	-2.37	102.36	113.24
15	X	101	CRT	C32-C31-C30	-2.37	115.83	123.22
15	G	101	CRT	C36-C35-C33	-2.37	122.31	125.89
15	AF	102	CRT	C5-C6-C7	-2.37	122.31	125.89
15	R	101	CRT	C26-C27-C28	-2.37	123.93	127.31
15	y	404	CRT	C39-C38-C37	-2.37	107.22	110.86
15	9	101	CRT	C30-C28-C27	-2.36	115.31	118.94
9	m	102	BCL	C12-C11-C10	-2.36	102.38	113.24
9	W	101	BCL	C7-C6-C5	-2.36	106.94	113.36
9	8	101	BCL	C3C-C2C-C1C	2.36	105.68	101.87
15	AF	102	CRT	C13-C12-C11	2.36	121.80	118.08
9	W	101	BCL	CMC-C2C-C3C	-2.36	104.30	113.83
9	z	102	BCL	C3C-C4C-CHD	-2.36	118.35	123.39
15	Z	101	CRT	C2-C1-C4	-2.36	107.23	110.86
9	l	101	BCL	C11-C12-C13	-2.36	108.29	115.92
9	x	301	BCL	CMC-C2C-C3C	-2.36	104.31	113.83
9	R	102	BCL	CMA-C3A-C4A	-2.36	105.43	111.77
9	AC	102	BCL	CMA-C3A-C4A	-2.36	105.43	111.77
9	R	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
15	T	101	CRT	C36-C35-C33	2.36	129.46	125.89
9	p	102	BCL	C3D-C2D-C1D	-2.36	102.61	105.83
15	z	101	CRT	C14-C15-C16	-2.36	115.86	123.22
9	j	101	BCL	C4A-NA-C1A	2.36	107.77	106.71
15	0	101	CRT	C8-C7-C6	2.36	121.79	118.08
15	I	102	CRT	C32-C31-C30	-2.35	115.87	123.22
9	G	102	BCL	C4A-NA-C1A	2.35	107.76	106.71
15	AF	102	CRT	C9-C10-C11	-2.35	115.88	123.22
9	AI	101	BCL	C4-C3-C5	-2.35	111.32	115.27
9	AH	101	BCL	C11-C10-C8	-2.35	108.32	115.92
9	w	101	BCL	CMD-C2D-C1D	2.35	128.85	124.71
15	y	404	CRT	C8-C7-C9	-2.35	119.63	122.92
9	f	101	BCL	CMC-C2C-C3C	-2.35	104.36	113.83
9	u	101	BCL	O2A-CGA-O1A	-2.35	117.67	123.59
9	e	102	BCL	O2A-C1-C2	2.35	114.80	108.64
9	z	102	BCL	C12-C11-C10	-2.34	102.46	113.24
9	s	102	BCL	C11-C12-C13	-2.34	108.34	115.92
9	u	101	BCL	C3D-C2D-C1D	-2.34	102.63	105.83
11	x	304	UQ8	C25-C24-C26	2.34	119.21	115.27
9	k	102	BCL	CHB-C4A-NA	-2.34	121.27	124.51
7	o	503	HEM	O2D-CGD-CBD	2.34	121.56	114.03
9	u	102	BCL	CBB-CAB-C3B	2.34	127.29	120.34
9	L	301	BCL	C6-C5-C3	-2.34	107.32	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	501	HEM	CAD-C3D-C4D	2.34	128.75	124.66
9	P	101	BCL	C2A-C1A-CHA	2.34	127.95	123.86
9	x	305	BCL	CHC-C1C-NC	2.34	127.74	124.51
9	m	103	BCL	C2A-C1A-CHA	2.34	127.94	123.86
9	AL	102	BCL	CAC-C3C-C4C	2.34	117.77	112.58
9	K	101	BCL	C11-C12-C13	-2.33	108.37	115.92
15	E	101	CRT	C18-C17-C16	2.33	121.75	118.08
9	AH	101	BCL	C1C-NC-C4C	-2.33	105.66	106.71
15	g	101	CRT	C14-C15-C16	-2.33	115.94	123.22
7	C	503	HEM	CHB-C1B-C2B	-2.33	120.27	126.72
9	V	102	BCL	C1-O2A-CGA	2.33	122.56	116.44
15	AH	102	CRT	C9-C10-C11	-2.33	115.95	123.22
9	3	101	BCL	C3C-C2C-C1C	2.33	105.63	101.87
10	L	302	BPH	C1-C2-C3	-2.33	122.01	126.04
9	P	101	BCL	O2A-C1-C2	2.33	114.75	108.64
9	i	102	BCL	CED-O2D-CGD	-2.33	110.67	115.94
9	y	401	BCL	C3C-C4C-CHD	-2.33	118.42	123.39
15	M	405	CRT	C18-C17-C16	2.33	121.74	118.08
9	x	301	BCL	C1-O2A-CGA	2.33	122.55	116.44
9	Q	101	BCL	C2A-C1A-CHA	2.33	127.93	123.86
9	N	101	BCL	C4A-NA-C1A	2.32	107.75	106.71
11	L	304	UQ8	C32-C33-C34	-2.32	122.06	127.66
9	m	102	BCL	CMA-C3A-C4A	-2.32	105.53	111.77
15	m	104	CRT	C20-C19-C17	-2.32	124.00	127.31
9	m	103	BCL	OBD-CAD-C3D	2.32	134.10	128.52
9	k	102	BCL	C11-C10-C8	-2.32	108.42	115.92
9	AK	101	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
9	P	101	BCL	C11-C10-C8	-2.32	108.43	115.92
9	2	102	BCL	O2A-C1-C2	2.32	114.72	108.64
9	L	301	BCL	C4D-CHA-C1A	2.32	124.07	121.25
9	A	103	BCL	C12-C11-C10	-2.32	102.60	113.24
9	I	103	BCL	C3C-C2C-C1C	2.32	105.61	101.87
15	O	101	CRT	C18-C17-C16	2.31	121.72	118.08
9	5	101	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
9	Z	102	BCL	C11-C12-C13	-2.31	108.44	115.92
9	AB	101	BCL	C1C-NC-C4C	-2.31	105.67	106.71
15	i	101	CRT	C8-C7-C6	2.31	121.72	118.08
9	1	101	BCL	CAA-CBA-CGA	-2.31	106.50	113.25
9	h	101	BCL	O2A-CGA-O1A	-2.31	117.76	123.59
15	g	101	CRT	C31-C30-C28	2.31	132.90	126.42
9	T	102	BCL	O2A-CGA-O1A	-2.31	117.77	123.59
9	q	102	BCL	C1C-NC-C4C	-2.31	105.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	101	BCL	CGD-CBD-CAD	-2.31	103.27	110.73
9	j	101	BCL	C7-C6-C5	-2.31	107.10	113.36
9	T	102	BCL	C2A-C1A-CHA	2.30	127.89	123.86
9	I	103	BCL	O2A-C1-C2	2.30	114.69	108.64
9	w	101	BCL	C2A-C1A-CHA	2.30	127.89	123.86
9	W	101	BCL	C11-C10-C8	-2.30	108.48	115.92
9	0	102	BCL	C11-C10-C8	-2.30	108.48	115.92
9	Z	102	BCL	C3C-C2C-C1C	2.30	105.59	101.87
9	r	101	BCL	CMD-C2D-C1D	2.30	128.77	124.71
9	Z	102	BCL	O2A-CGA-O1A	-2.30	117.79	123.59
9	D	102	BCL	CBB-CAB-C3B	2.30	127.16	120.34
15	P	102	CRT	C9-C10-C11	-2.30	116.05	123.22
9	5	101	BCL	C11-C10-C8	-2.30	108.49	115.92
14	y	403	MQ8	C5-C4-C3	2.30	122.63	118.42
15	R	101	CRT	C16-C17-C19	-2.30	115.42	118.94
15	q	101	CRT	C29-C28-C30	2.30	121.70	118.08
9	u	101	BCL	CHC-C1C-NC	2.30	127.69	124.51
15	I	102	CRT	C15-C16-C17	-2.30	119.97	126.42
9	q	102	BCL	C11-C12-C13	-2.30	108.50	115.92
15	M	405	CRT	C26-C27-C28	-2.30	124.03	127.31
9	q	102	BCL	CMC-C2C-C3C	-2.29	104.57	113.83
9	x	303	BCL	C4A-NA-C1A	2.29	107.74	106.71
9	2	102	BCL	C3C-C2C-C1C	2.29	105.57	101.87
14	M	404	MQ8	C39-C38-C37	-2.29	117.80	123.68
9	w	101	BCL	C6-C5-C3	-2.29	107.44	113.45
9	P	101	BCL	CHC-C1C-NC	2.29	127.68	124.51
9	AB	102	BCL	C1-C2-C3	-2.29	122.08	126.04
9	R	102	BCL	C16-C15-C13	-2.29	108.51	115.92
15	k	101	CRT	C13-C12-C11	2.29	121.69	118.08
9	8	101	BCL	CBB-CAB-C3B	2.29	127.14	120.34
15	z	101	CRT	C36-C35-C33	-2.29	122.43	125.89
9	z	102	BCL	C1-O2A-CGA	2.29	122.45	116.44
15	0	101	CRT	C8-C7-C9	-2.29	119.72	122.92
9	u	101	BCL	C12-C11-C10	-2.29	102.72	113.24
9	AC	102	BCL	CMC-C2C-C3C	-2.29	104.59	113.83
15	s	101	CRT	C31-C32-C33	-2.29	124.04	127.31
9	AF	101	BCL	C3C-C2C-C1C	2.29	105.56	101.87
9	G	102	BCL	CED-O2D-CGD	-2.29	110.76	115.94
9	r	101	BCL	C3D-C2D-C1D	-2.29	102.71	105.83
9	h	101	BCL	C7-C6-C5	-2.29	107.15	113.36
9	I	101	BCL	C1C-NC-C4C	-2.28	105.68	106.71
15	M	405	CRT	C32-C31-C30	-2.28	116.09	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	102	BCL	CMC-C2C-C3C	-2.28	104.62	113.83
9	1	101	BCL	CBB-CAB-C3B	2.28	127.11	120.34
9	AL	102	BCL	C11-C12-C13	-2.28	108.55	115.92
9	M	402	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
9	r	101	BCL	O2A-C1-C2	2.28	114.63	108.64
9	V	102	BCL	C11-C10-C8	-2.28	108.55	115.92
9	W	101	BCL	C12-C11-C10	-2.28	102.77	113.24
9	AC	103	BCL	O2A-C1-C2	2.28	114.62	108.64
15	X	101	CRT	C13-C12-C14	-2.28	119.73	122.92
9	6	101	BCL	CBB-CAB-C3B	2.28	127.10	120.34
9	AB	102	BCL	CED-O2D-CGD	-2.28	110.78	115.94
15	X	101	CRT	C8-C7-C9	-2.28	119.73	122.92
9	w	101	BCL	CAA-CBA-CGA	-2.28	106.60	113.25
9	q	102	BCL	CBB-CAB-C3B	2.28	127.10	120.34
9	N	101	BCL	CMC-C2C-C3C	-2.28	104.65	113.83
7	C	503	HEM	C3B-C2B-C1B	2.28	108.17	106.49
15	e	101	CRT	C29-C28-C30	2.28	121.66	118.08
9	AC	103	BCL	C11-C12-C13	-2.28	108.56	115.92
11	L	304	UQ8	C10-C9-C11	2.27	119.10	115.27
9	AG	101	BCL	C12-C11-C10	-2.27	102.79	113.24
9	U	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
10	M	403	BPH	C6-C5-C3	-2.27	107.49	113.45
12	y	407	PEF	C3-O3-C30	2.27	122.81	117.10
9	T	102	BCL	CAA-C2A-C3A	2.27	119.00	112.78
9	x	305	BCL	OBB-CAB-CBB	-2.27	115.06	120.17
9	AG	101	BCL	O2A-CGA-O1A	-2.27	117.86	123.59
15	E	101	CRT	C34-C33-C35	2.27	121.66	118.08
9	x	305	BCL	C1C-NC-C4C	-2.27	105.69	106.71
9	7	102	BCL	CMA-C3A-C2A	-2.27	104.67	113.83
9	AI	101	BCL	C3D-C2D-C1D	-2.27	102.73	105.83
15	O	101	CRT	C15-C16-C17	-2.27	120.04	126.42
9	Y	101	BCL	C3D-C2D-C1D	-2.27	102.73	105.83
10	L	302	BPH	CBC-CAC-C3C	-2.27	109.20	113.77
9	u	102	BCL	C7-C6-C5	-2.27	107.20	113.36
10	M	403	BPH	O2A-CGA-CBA	2.27	119.02	111.91
9	4	102	BCL	O2A-CGA-O1A	-2.27	117.88	123.59
15	Z	101	CRT	C11-C12-C14	-2.27	115.47	118.94
15	AL	101	CRT	C35-C33-C32	-2.27	115.47	118.94
9	L	303	BCL	C1D-CHD-C4C	-2.27	121.16	126.62
9	2	102	BCL	CMD-C2D-C3D	2.26	132.82	127.61
9	m	103	BCL	C1C-NC-C4C	-2.26	105.69	106.71
7	C	503	HEM	CMD-C2D-C1D	2.26	128.49	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AG	101	BCL	CBB-CAB-C3B	2.26	127.06	120.34
11	L	304	UQ8	C35-C34-C33	-2.26	117.87	123.68
9	8	101	BCL	CAA-CBA-CGA	-2.26	106.64	113.25
7	C	503	HEM	O2A-CGA-CBA	2.26	121.30	114.03
9	S	102	BCL	CHD-C4C-NC	-2.26	122.56	125.08
9	AE	102	BCL	CHC-C1C-NC	2.26	127.64	124.51
9	x	305	BCL	C11-C12-C13	-2.26	108.62	115.92
10	x	302	BPH	CBA-CAA-C2A	-2.26	107.21	113.81
9	g	102	BCL	CHC-C1C-NC	2.26	127.64	124.51
9	x	303	BCL	CHC-C1C-NC	2.26	127.64	124.51
15	0	101	CRT	C31-C32-C33	-2.26	124.09	127.31
15	e	101	CRT	C30-C28-C27	-2.26	115.48	118.94
10	y	402	BPH	O2D-CGD-O1D	-2.26	119.43	123.84
9	m	103	BCL	C16-C15-C13	-2.26	108.63	115.92
9	AC	102	BCL	CED-O2D-CGD	-2.25	110.84	115.94
9	9	102	BCL	C3C-C2C-C1C	2.25	105.51	101.87
9	L	303	BCL	OBD-CAD-C3D	2.25	133.94	128.52
9	8	101	BCL	CMD-C2D-C1D	2.25	128.69	124.71
9	w	101	BCL	O2A-CGA-O1A	-2.25	117.90	123.59
11	x	304	UQ8	C30-C29-C28	-2.25	117.90	123.68
9	m	103	BCL	C7-C6-C5	-2.25	107.24	113.36
9	AK	101	BCL	CGD-CBD-CAD	-2.25	103.44	110.73
9	R	102	BCL	O2A-C1-C2	2.25	114.55	108.64
12	M	407	PEF	O2P-P-O1P	2.25	123.37	112.24
9	x	301	BCL	C2A-C1A-CHA	2.25	127.80	123.86
9	7	102	BCL	C11-C12-C13	-2.25	108.64	115.92
15	0	101	CRT	C1-C4-C5	2.25	119.01	113.06
9	AI	102	BCL	CMA-C3A-C4A	-2.25	105.73	111.77
9	m	103	BCL	C3D-C2D-C1D	-2.25	102.77	105.83
9	Z	102	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
9	R	102	BCL	C2C-C3C-C4C	-2.25	97.98	101.34
9	R	102	BCL	C3C-C4C-CHD	-2.25	118.59	123.39
9	i	102	BCL	CMA-C3A-C4A	-2.25	105.74	111.77
15	G	101	CRT	C18-C17-C19	-2.25	119.78	122.92
9	4	102	BCL	C16-C15-C13	-2.25	108.66	115.92
15	4	101	CRT	C31-C30-C28	2.24	132.72	126.42
9	s	102	BCL	CHD-C4C-NC	-2.24	122.58	125.08
9	AC	102	BCL	C1-O2A-CGA	2.24	122.33	116.44
9	AC	102	BCL	C2A-C1A-CHA	2.24	127.78	123.86
9	P	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
9	S	102	BCL	CMA-C3A-C2A	-2.24	104.78	113.83
9	i	102	BCL	C1D-CHD-C4C	-2.24	121.21	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	k	102	BCL	C12-C11-C10	-2.24	102.94	113.24
9	e	102	BCL	CMA-C3A-C4A	-2.24	105.75	111.77
9	AG	101	BCL	C6-C5-C3	-2.24	107.58	113.45
9	V	102	BCL	C7-C6-C5	-2.24	107.27	113.36
15	i	101	CRT	C13-C12-C11	2.24	121.61	118.08
9	6	101	BCL	C10-C8-C7	-2.24	100.35	112.13
15	G	101	CRT	C31-C32-C33	-2.24	124.12	127.31
15	m	104	CRT	C8-C7-C6	2.24	121.60	118.08
15	2	101	CRT	C29-C28-C27	-2.24	119.79	122.92
9	z	102	BCL	C3C-C2C-C1C	2.24	105.48	101.87
15	k	101	CRT	C13-C12-C14	-2.23	119.79	122.92
9	2	102	BCL	C7-C6-C5	-2.23	107.29	113.36
9	X	102	BCL	CMA-C3A-C2A	-2.23	104.82	113.83
9	1	101	BCL	C7-C6-C5	-2.23	107.30	113.36
15	v	101	CRT	C27-C26-C25	-2.23	116.26	123.22
14	y	403	MQ8	C26-C25-C23	-2.23	105.64	112.98
9	m	102	BCL	C7-C6-C5	-2.23	107.31	113.36
15	7	101	CRT	C10-C9-C7	-2.23	124.13	127.31
15	7	101	CRT	C24-C23-C25	2.22	121.58	118.08
9	R	102	BCL	C1C-NC-C4C	-2.22	105.71	106.71
9	c	101	BCL	C4A-NA-C1A	2.22	107.71	106.71
9	x	301	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
9	Q	101	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
9	g	102	BCL	CED-O2D-CGD	-2.22	110.91	115.94
9	X	102	BCL	C3C-C4C-CHD	-2.22	118.65	123.39
9	AE	102	BCL	C7-C6-C5	-2.22	107.33	113.36
7	C	502	HEM	CHB-C1B-NB	2.22	127.12	124.38
9	i	102	BCL	C3C-C2C-C1C	2.22	105.45	101.87
9	Q	101	BCL	C3D-C2D-C1D	-2.22	102.81	105.83
9	d	101	BCL	CMC-C2C-C3C	-2.22	104.89	113.83
9	r	101	BCL	O2A-CGA-O1A	-2.22	118.00	123.59
10	y	402	BPH	C6-C5-C3	-2.22	107.64	113.45
9	x	301	BCL	CBB-CAB-C3B	2.22	126.92	120.34
15	X	101	CRT	C18-C17-C19	-2.22	119.82	122.92
9	y	401	BCL	C7-C6-C5	-2.21	107.34	113.36
15	4	101	CRT	C32-C31-C30	2.21	130.13	123.22
15	z	101	CRT	C20-C19-C17	-2.21	124.15	127.31
9	AK	101	BCL	C2C-C3C-C4C	-2.21	98.02	101.34
9	z	102	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
9	I	101	BCL	C11-C12-C13	-2.21	108.77	115.92
9	AL	102	BCL	CBB-CAB-C3B	2.21	126.91	120.34
9	L	301	BCL	CHC-C1C-NC	2.21	127.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	102	CRT	C34-C33-C35	2.21	121.56	118.08
9	c	101	BCL	CMC-C2C-C3C	-2.21	104.92	113.83
15	s	101	CRT	C13-C12-C11	2.21	121.56	118.08
15	AC	101	CRT	C21-C20-C19	-2.21	118.95	123.47
9	u	102	BCL	C16-C15-C13	-2.20	108.79	115.92
9	M	401	BCL	C1C-NC-C4C	-2.20	105.72	106.71
9	S	102	BCL	O2A-CGA-CBA	2.20	118.82	111.91
9	L	301	BCL	CMC-C2C-C3C	-2.20	104.94	113.83
9	g	102	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
15	E	101	CRT	C13-C12-C11	2.20	121.55	118.08
15	v	101	CRT	C13-C12-C11	2.20	121.55	118.08
9	z	102	BCL	O2A-CGA-O1A	-2.20	118.04	123.59
9	AC	102	BCL	C7-C6-C5	-2.20	107.39	113.36
15	s	101	CRT	C8-C7-C6	2.20	121.54	118.08
9	7	102	BCL	O2A-CGA-O1A	-2.20	118.05	123.59
9	e	102	BCL	O2A-CGA-O1A	-2.20	118.05	123.59
9	K	101	BCL	CMD-C2D-C1D	2.20	128.59	124.71
9	V	102	BCL	O2A-C1-C2	2.20	114.41	108.64
9	f	101	BCL	C1-C2-C3	-2.20	122.25	126.04
9	M	401	BCL	C3D-C2D-C1D	-2.20	102.83	105.83
9	z	102	BCL	CMD-C2D-C1D	2.20	128.58	124.71
9	1	101	BCL	C3D-C2D-C1D	-2.19	102.84	105.83
9	D	102	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
9	j	101	BCL	C16-C15-C13	-2.19	108.83	115.92
7	C	503	HEM	C4D-ND-C1D	2.19	107.34	105.07
9	D	101	BCL	C3C-C4C-CHD	-2.19	118.71	123.39
9	AG	101	BCL	C1-O2A-CGA	2.19	122.20	116.44
15	M	405	CRT	C29-C28-C27	-2.19	119.85	122.92
9	2	102	BCL	CMC-C2C-C3C	-2.19	104.99	113.83
9	8	101	BCL	CHB-C4A-NA	-2.19	121.48	124.51
9	AH	101	BCL	C3D-C2D-C1D	-2.19	102.84	105.83
9	X	102	BCL	CMD-C2D-C3D	2.19	132.65	127.61
9	5	101	BCL	CHB-C4A-NA	-2.19	121.49	124.51
9	l	101	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
9	N	101	BCL	C1-O2A-CGA	2.19	122.18	116.44
9	8	101	BCL	C1-C2-C3	2.19	129.83	126.04
12	H	305	PEF	O3-C3-C2	2.19	114.80	108.43
9	AF	101	BCL	CMC-C2C-C3C	-2.19	105.01	113.83
9	w	101	BCL	C3C-C4C-CHD	-2.19	118.72	123.39
9	AE	102	BCL	C11-C10-C8	-2.19	108.85	115.92
15	7	101	CRT	C31-C32-C33	2.19	130.43	127.31
9	AB	101	BCL	O2A-C1-C2	2.19	114.38	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	102	BCL	CBB-CAB-C3B	2.18	126.82	120.34
15	AC	101	CRT	C8-C7-C6	2.18	121.52	118.08
9	7	102	BCL	CHC-C1C-NC	2.18	127.53	124.51
9	W	101	BCL	C1-O2A-CGA	2.18	122.17	116.44
15	0	101	CRT	C24-C23-C25	2.18	121.52	118.08
15	g	101	CRT	C30-C28-C27	-2.18	115.59	118.94
9	u	102	BCL	CMD-C2D-C3D	2.18	132.63	127.61
9	h	101	BCL	C1C-NC-C4C	-2.18	105.72	106.71
9	0	102	BCL	CHB-C4A-NA	-2.18	121.50	124.51
11	L	304	UQ8	C12-C13-C14	-2.18	122.41	127.66
9	X	102	BCL	C2C-C3C-C4C	-2.18	98.07	101.34
9	d	101	BCL	C2A-C1A-CHA	2.18	127.67	123.86
9	r	101	BCL	C1-O2A-CGA	2.18	122.17	116.44
9	m	102	BCL	C3C-C4C-CHD	-2.18	118.73	123.39
9	p	102	BCL	C4B-C3B-CAB	-2.18	122.92	127.13
15	s	101	CRT	C14-C15-C16	-2.18	116.42	123.22
15	n	101	CRT	C25-C23-C22	-2.18	115.60	118.94
15	n	101	CRT	C21-C22-C23	-2.18	124.20	127.31
9	6	101	BCL	C2A-C3A-C4A	-2.18	98.35	101.87
14	y	403	MQ8	C50-C48-C49	2.18	119.41	114.60
14	y	403	MQ8	C2M-C2-C3	-2.18	120.85	124.40
9	j	101	BCL	CAA-C2A-C3A	2.17	118.73	112.78
15	m	104	CRT	C32-C31-C30	-2.17	116.43	123.22
15	k	101	CRT	C32-C31-C30	-2.17	116.43	123.22
15	n	101	CRT	C11-C12-C14	2.17	122.28	118.94
12	t	303	PEF	O3-C3-C2	2.17	114.76	108.43
9	AF	101	BCL	C11-C10-C8	-2.17	108.89	115.92
15	e	101	CRT	C9-C10-C11	-2.17	116.44	123.22
9	m	102	BCL	CHB-C4A-NA	-2.17	121.51	124.51
9	w	101	BCL	CHC-C1C-NC	2.17	127.52	124.51
9	O	102	BCL	C2A-C1A-CHA	2.17	127.66	123.86
9	AF	101	BCL	CMC-C2C-C1C	-2.17	105.94	111.77
15	2	101	CRT	C35-C33-C32	-2.17	115.61	118.94
15	G	101	CRT	C14-C15-C16	-2.17	116.44	123.22
10	x	302	BPH	C11-C12-C13	-2.17	108.90	115.92
12	y	408	PEF	P-O4P-C4	-2.17	110.91	121.59
9	i	102	BCL	CAA-C2A-C3A	2.17	118.72	112.78
9	D	102	BCL	C4A-NA-C1A	2.17	107.68	106.71
9	r	101	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
9	6	101	BCL	C12-C11-C10	-2.17	103.28	113.24
9	AB	102	BCL	CMA-C3A-C4A	-2.17	105.95	111.77
11	x	304	UQ8	C41-C42-C43	2.17	119.00	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	101	PEF	C3-C2-C1	-2.17	106.67	111.79
15	s	101	CRT	C36-C35-C33	2.16	129.16	125.89
9	Y	101	BCL	C6-C5-C3	-2.16	107.78	113.45
9	AB	101	BCL	C3C-C4C-CHD	-2.16	118.77	123.39
9	I	103	BCL	C2A-C1A-CHA	2.16	127.64	123.86
9	AB	102	BCL	C11-C12-C13	-2.16	108.93	115.92
9	c	101	BCL	CMD-C2D-C1D	2.16	128.52	124.71
9	I	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
9	R	102	BCL	CHB-C4A-NA	-2.16	121.52	124.51
9	2	102	BCL	C11-C10-C8	-2.16	108.93	115.92
15	AL	101	CRT	C20-C21-C22	-2.16	119.05	123.47
9	W	101	BCL	CMA-C3A-C4A	-2.16	105.97	111.77
15	2	101	CRT	C20-C21-C22	-2.16	119.05	123.47
9	y	401	BCL	C3D-C2D-C1D	-2.16	102.89	105.83
9	1	101	BCL	CMC-C2C-C3C	-2.16	105.12	113.83
15	T	101	CRT	C9-C10-C11	-2.16	116.48	123.22
7	C	504	HEM	CAD-C3D-C4D	2.15	128.42	124.66
9	S	102	BCL	C11-C12-C13	-2.15	108.96	115.92
9	W	101	BCL	C2A-C1A-CHA	2.15	127.62	123.86
9	g	102	BCL	CMC-C2C-C3C	-2.15	105.15	113.83
12	y	406	PEF	C3-O3-C30	2.15	122.51	117.10
9	L	303	BCL	C9-C8-C7	2.15	119.08	111.29
9	i	102	BCL	CHC-C1C-NC	2.15	127.49	124.51
15	G	101	CRT	C26-C27-C28	-2.15	124.24	127.31
9	AI	101	BCL	C7-C6-C5	-2.15	107.52	113.36
15	0	101	CRT	O1-C1-C2	2.15	123.75	108.97
9	Q	101	BCL	CHB-C4A-NA	-2.15	121.54	124.51
9	Z	102	BCL	O2A-C1-C2	2.15	114.28	108.64
9	A	103	BCL	CHC-C1C-NC	2.15	127.48	124.51
15	e	101	CRT	C5-C6-C7	-2.15	122.65	125.89
9	F	101	BCL	C3C-C4C-CHD	-2.15	118.81	123.39
9	AI	101	BCL	C6-C5-C3	-2.15	107.83	113.45
15	AC	101	CRT	C6-C7-C9	-2.15	115.65	118.94
9	m	103	BCL	C3C-C4C-CHD	-2.15	118.81	123.39
15	y	404	CRT	O1-C1-C3	2.14	123.71	108.97
15	2	101	CRT	C8-C7-C6	2.14	121.45	118.08
9	r	101	BCL	CGD-CBD-CAD	-2.14	103.79	110.73
9	AB	102	BCL	C1C-NC-C4C	-2.14	105.74	106.71
9	0	102	BCL	O2A-C1-C2	2.14	114.26	108.64
15	y	404	CRT	C14-C15-C16	-2.14	116.54	123.22
9	AB	102	BCL	CBB-CAB-C3B	2.14	126.69	120.34
15	7	103	CRT	C13-C12-C14	-2.14	119.93	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	102	BCL	CBB-CAB-C3B	2.14	126.69	120.34
15	7	103	CRT	C5-C6-C7	-2.14	122.66	125.89
9	K	101	BCL	CED-O2D-CGD	-2.14	111.10	115.94
9	AI	102	BCL	C12-C11-C10	-2.14	103.41	113.24
9	q	102	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
9	d	101	BCL	C11-C10-C8	-2.14	109.01	115.92
14	y	403	MQ8	C24-C23-C25	2.14	118.87	115.27
14	y	403	MQ8	C45-C43-C44	2.14	118.86	115.27
9	x	301	BCL	C12-C11-C10	-2.14	103.42	113.24
9	AI	101	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
9	f	101	BCL	C1C-NC-C4C	-2.14	105.75	106.71
7	o	504	HEM	O2A-CGA-CBA	2.13	120.88	114.03
15	E	101	CRT	C29-C28-C30	2.13	121.44	118.08
15	AD	101	CRT	C18-C17-C19	-2.13	119.94	122.92
11	L	304	UQ8	O4-C4-C5	2.13	123.78	116.56
15	g	101	CRT	C13-C12-C11	2.13	121.44	118.08
15	Z	101	CRT	C20-C21-C22	-2.13	119.11	123.47
9	AC	102	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
15	Z	101	CRT	C14-C15-C16	-2.13	116.56	123.22
9	u	101	BCL	CHD-C4C-NC	-2.13	122.71	125.08
9	Q	101	BCL	C1-O2A-CGA	2.13	122.03	116.44
9	r	101	BCL	CMA-C3A-C4A	-2.13	106.05	111.77
9	D	102	BCL	C11-C10-C8	-2.13	109.04	115.92
9	m	102	BCL	C2A-C1A-CHA	2.13	127.58	123.86
9	N	101	BCL	CMD-C2D-C1D	2.13	128.46	124.71
15	O	101	CRT	C27-C26-C25	-2.13	116.58	123.22
15	M	405	CRT	C36-C35-C33	-2.13	122.68	125.89
9	y	401	BCL	O2A-CGA-CBA	2.13	118.58	111.91
15	2	101	CRT	C34-C33-C35	2.13	121.43	118.08
15	E	101	CRT	C14-C15-C16	-2.12	116.59	123.22
9	5	101	BCL	CMA-C3A-C4A	-2.12	106.06	111.77
9	T	102	BCL	CBB-CAB-C3B	2.12	126.64	120.34
15	AF	102	CRT	C27-C26-C25	-2.12	116.59	123.22
9	AF	101	BCL	C1-O2A-CGA	2.12	122.02	116.44
9	s	102	BCL	C3C-C2C-C1C	2.12	105.30	101.87
9	AB	102	BCL	C6-C5-C3	-2.12	107.89	113.45
9	AB	102	BCL	C16-C15-C13	-2.12	109.06	115.92
15	AJ	101	CRT	C24-C23-C22	-2.12	119.95	122.92
9	x	303	BCL	O2A-CGA-CBA	2.12	118.56	111.91
9	AL	102	BCL	CMD-C2D-C1D	2.12	128.45	124.71
9	AH	101	BCL	C12-C11-C10	-2.12	103.51	113.24
10	x	302	BPH	C11-C10-C8	-2.12	109.08	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	101	BCL	C1C-NC-C4C	-2.12	105.75	106.71
9	P	101	BCL	CBB-CAB-C3B	2.12	126.62	120.34
9	x	305	BCL	C12-C11-C10	-2.11	103.52	113.24
9	O	102	BCL	CAA-C2A-C3A	2.11	118.57	112.78
9	AE	102	BCL	CED-O2D-CGD	-2.11	111.16	115.94
9	F	101	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
9	L	301	BCL	CHB-C4A-NA	-2.11	121.59	124.51
9	4	102	BCL	CMD-C2D-C1D	2.11	128.44	124.71
9	x	305	BCL	C11-C10-C8	-2.11	109.09	115.92
9	m	103	BCL	CMC-C2C-C3C	-2.11	105.31	113.83
9	0	102	BCL	CHD-C4C-NC	-2.11	122.73	125.08
9	L	301	BCL	CBC-CAC-C3C	2.11	118.17	113.47
15	P	102	CRT	C30-C28-C27	-2.11	115.70	118.94
9	d	101	BCL	CBB-CAB-C3B	2.11	126.60	120.34
9	U	101	BCL	C11-C10-C8	-2.11	109.10	115.92
9	f	101	BCL	C3C-C2C-C1C	2.11	105.28	101.87
15	i	101	CRT	C5-C6-C7	-2.11	122.71	125.89
12	y	407	PEF	O2P-P-O1P	2.11	122.66	112.24
9	AK	101	BCL	C16-C15-C13	-2.11	109.11	115.92
9	AB	102	BCL	C7-C6-C5	-2.11	107.64	113.36
9	q	102	BCL	C12-C11-C10	-2.11	103.57	113.24
7	o	502	HEM	C2B-C1B-NB	-2.10	107.34	109.84
15	AD	101	CRT	C14-C15-C16	2.10	129.78	123.22
9	w	101	BCL	C1-O2A-CGA	2.10	121.96	116.44
15	k	101	CRT	C9-C10-C11	-2.10	116.65	123.22
9	u	102	BCL	C2C-C3C-C4C	-2.10	98.19	101.34
11	x	304	UQ8	C25-C24-C23	-2.10	118.28	123.68
7	o	501	HEM	O2D-CGD-CBD	2.10	120.78	114.03
15	0	101	CRT	C10-C9-C7	-2.10	124.31	127.31
15	e	101	CRT	C26-C25-C23	-2.10	120.52	126.42
9	L	301	BCL	C4B-CHC-C1C	-2.10	125.96	130.12
10	y	402	BPH	CMC-C2C-C3C	-2.10	105.54	113.99
9	V	102	BCL	CMD-C2D-C1D	2.10	128.41	124.71
9	L	303	BCL	C11-C10-C8	-2.10	109.14	115.92
9	V	102	BCL	C3C-C4C-CHD	-2.10	118.91	123.39
15	m	104	CRT	C9-C10-C11	-2.10	116.67	123.22
7	C	501	HEM	O2D-CGD-O1D	-2.10	118.07	123.30
9	0	102	BCL	C5-C3-C2	2.10	125.36	121.12
9	0	102	BCL	C1-C2-C3	-2.10	122.42	126.04
9	7	102	BCL	CBB-CAB-C3B	2.10	126.56	120.34
9	AI	102	BCL	C10-C8-C7	-2.09	101.11	112.13
9	u	102	BCL	CHC-C1C-NC	2.09	127.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403	BPH	C6-C7-C8	-2.09	109.15	115.92
9	i	102	BCL	C3C-C4C-CHD	-2.09	118.92	123.39
9	AF	101	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
9	k	102	BCL	C4D-CHA-C1A	2.09	123.79	121.25
9	O	102	BCL	C12-C11-C10	-2.09	103.63	113.24
9	Y	101	BCL	CHC-C1C-NC	2.09	127.40	124.51
9	w	101	BCL	CHB-C4A-NA	-2.09	121.62	124.51
9	k	102	BCL	CMA-C3A-C4A	-2.09	106.16	111.77
9	2	102	BCL	CED-O2D-CGD	-2.09	111.21	115.94
9	AB	101	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
9	1	101	BCL	C1-O2A-CGA	2.09	121.92	116.44
9	0	102	BCL	C4A-NA-C1A	2.09	107.64	106.71
9	M	402	BCL	C12-C11-C10	-2.08	103.66	113.24
9	S	102	BCL	O2A-C1-C2	2.08	114.11	108.64
15	0	101	CRT	C32-C31-C30	-2.08	116.72	123.22
9	T	102	BCL	C11-C10-C8	-2.08	109.19	115.92
7	C	504	HEM	O2D-CGD-CBD	2.08	120.72	114.03
7	o	501	HEM	CHA-C4D-ND	2.08	126.95	124.38
12	H	301	PEF	O2P-P-O1P	2.08	122.53	112.24
10	L	302	BPH	O2D-CGD-O1D	-2.08	119.77	123.84
15	n	101	CRT	C35-C33-C32	-2.08	115.75	118.94
9	K	101	BCL	CHD-C4C-NC	-2.08	122.76	125.08
9	s	102	BCL	C7-C6-C5	-2.08	107.71	113.36
15	q	101	CRT	C18-C17-C16	2.08	121.36	118.08
9	D	102	BCL	O2A-CGA-O1A	-2.08	118.34	123.59
7	o	501	HEM	C4A-C3A-C2A	2.08	108.44	107.00
9	L	301	BCL	CHD-C4C-NC	-2.08	122.77	125.08
9	V	102	BCL	C11-C12-C13	-2.08	109.20	115.92
9	AC	102	BCL	O2A-CGA-O1A	-2.08	118.35	123.59
9	f	101	BCL	C11-C10-C8	-2.08	109.20	115.92
9	AK	101	BCL	C7-C6-C5	-2.08	107.72	113.36
9	p	102	BCL	C11-C10-C8	-2.07	109.21	115.92
15	AC	101	CRT	C26-C25-C23	-2.07	120.59	126.42
9	AC	103	BCL	C3C-C2C-C1C	2.07	105.22	101.87
9	p	102	BCL	O2A-C1-C2	2.07	114.09	108.64
9	i	102	BCL	O2A-CGA-O1A	-2.07	118.36	123.59
9	l	101	BCL	CBB-CAB-C3B	2.07	126.49	120.34
9	m	103	BCL	C2A-C3A-C4A	-2.07	98.52	101.87
9	j	101	BCL	CMA-C3A-C2A	-2.07	105.47	113.83
9	D	102	BCL	CHB-C4A-NA	-2.07	121.65	124.51
9	s	102	BCL	CED-O2D-CGD	-2.07	111.25	115.94
9	d	101	BCL	C2C-C3C-C4C	-2.07	98.24	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	BCL	C7-C6-C5	-2.07	107.74	113.36
9	6	101	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	AI	101	BCL	C4A-NA-C1A	2.07	107.64	106.71
15	R	101	CRT	C35-C33-C32	-2.07	115.77	118.94
7	C	504	HEM	CHB-C1B-C2B	-2.07	121.01	126.72
9	N	101	BCL	CBB-CAB-C3B	2.07	126.47	120.34
15	T	101	CRT	C32-C31-C30	-2.07	116.77	123.22
9	G	102	BCL	O2A-CGA-O1A	-2.06	118.39	123.59
9	A	103	BCL	CED-O2D-CGD	-2.06	111.27	115.94
9	AC	103	BCL	CHC-C1C-NC	2.06	127.36	124.51
7	C	502	HEM	CAD-C3D-C2D	-2.06	124.04	127.88
9	L	301	BCL	C3D-C2D-C1D	-2.06	103.02	105.83
15	AJ	101	CRT	C2-C1-C4	-2.06	107.70	110.86
12	M	408	PEF	C2-O2-C10	-2.06	114.06	117.90
9	L	303	BCL	C14-C13-C12	-2.06	103.84	111.29
15	O	101	CRT	C32-C31-C30	-2.06	116.79	123.22
9	G	102	BCL	C1D-CHD-C4C	-2.06	121.66	126.62
9	d	101	BCL	C14-C13-C12	-2.06	103.84	111.29
15	AH	102	CRT	C15-C14-C12	-2.06	124.37	127.31
9	W	101	BCL	CBB-CAB-C3B	2.06	126.45	120.34
9	M	402	BCL	CGD-CBD-CAD	-2.06	104.07	110.73
15	P	102	CRT	C18-C17-C16	2.06	121.32	118.08
11	x	304	UQ8	C15-C14-C13	-2.06	118.40	123.68
7	o	504	HEM	CHA-C4D-ND	2.06	126.92	124.38
14	M	404	MQ8	C45-C43-C44	2.06	118.73	115.27
9	0	102	BCL	CED-O2D-CGD	-2.05	111.29	115.94
15	AH	102	CRT	C8-C7-C6	2.05	121.31	118.08
9	e	102	BCL	C12-C11-C10	-2.05	103.81	113.24
9	AC	102	BCL	C12-C11-C10	-2.05	103.81	113.24
9	x	303	BCL	CMD-C2D-C1D	2.05	128.33	124.71
15	0	101	CRT	C26-C27-C28	-2.05	124.38	127.31
9	2	102	BCL	CHB-C4A-NA	-2.05	121.67	124.51
9	h	101	BCL	CHB-C4A-NA	-2.05	121.67	124.51
15	i	101	CRT	C8-C7-C9	-2.05	120.05	122.92
9	p	102	BCL	CMA-C3A-C4A	-2.05	106.26	111.77
9	AE	102	BCL	CBB-CAB-C3B	2.05	126.43	120.34
15	M	405	CRT	C21-C20-C19	-2.05	119.28	123.47
9	AB	102	BCL	C3C-C2C-C1C	2.05	105.18	101.87
9	I	103	BCL	CMC-C2C-C3C	-2.05	105.56	113.83
14	y	403	MQ8	O4-C4-C3	-2.05	117.26	120.56
15	4	101	CRT	C13-C12-C11	2.05	121.30	118.08
9	P	101	BCL	C3C-C4C-CHD	-2.05	119.02	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	103	BCL	C12-C11-C10	-2.05	103.83	113.24
9	U	101	BCL	C12-C11-C10	-2.05	103.84	113.24
7	o	502	HEM	CAD-C3D-C2D	-2.05	124.07	127.88
9	g	102	BCL	CBB-CAB-C3B	2.04	126.41	120.34
9	D	102	BCL	C3C-C2C-C1C	2.04	105.17	101.87
9	e	102	BCL	C1D-CHD-C4C	-2.04	121.69	126.62
9	X	102	BCL	C16-C15-C13	-2.04	109.31	115.92
9	AL	102	BCL	C12-C11-C10	-2.04	103.85	113.24
15	O	101	CRT	C34-C33-C35	2.04	121.29	118.08
9	I	101	BCL	C2A-C1A-CHA	2.04	127.43	123.86
15	AD	101	CRT	C29-C28-C30	2.04	121.29	118.08
9	I	101	BCL	O2A-CGA-CBA	2.04	118.31	111.91
15	AJ	101	CRT	C35-C33-C32	-2.04	115.81	118.94
9	M	402	BCL	O2A-C1-C2	2.04	113.99	108.64
15	4	101	CRT	C20-C19-C17	2.04	130.22	127.31
9	u	101	BCL	C1D-CHD-C4C	-2.04	121.71	126.62
9	Y	101	BCL	C11-C12-C13	-2.04	109.34	115.92
15	y	404	CRT	C31-C30-C28	-2.04	120.70	126.42
9	X	102	BCL	C4B-C3B-CAB	-2.03	123.20	127.13
9	D	102	BCL	C1-O2A-CGA	2.03	121.78	116.44
9	AI	102	BCL	CBB-CAB-C3B	2.03	126.38	120.34
7	o	504	HEM	CHC-C4B-NB	2.03	126.64	124.43
7	o	503	HEM	CMD-C2D-C1D	2.03	128.13	125.04
9	I	103	BCL	C3C-C4C-CHD	-2.03	119.05	123.39
9	y	401	BCL	CHD-C4C-NC	-2.03	122.82	125.08
9	AC	103	BCL	CBB-CAB-C3B	2.03	126.37	120.34
9	e	102	BCL	C3C-C2C-C1C	2.03	105.15	101.87
9	x	303	BCL	C2A-C1A-CHA	2.03	127.41	123.86
9	M	401	BCL	C7-C6-C5	-2.03	107.85	113.36
9	m	103	BCL	C11-C12-C13	-2.03	109.36	115.92
9	AG	101	BCL	C10-C8-C7	-2.03	101.46	112.13
11	L	304	UQ8	C6-C1-C2	2.03	120.78	119.18
9	h	101	BCL	C3C-C2C-C1C	2.03	105.14	101.87
9	x	301	BCL	C10-C8-C7	-2.02	101.48	112.13
9	7	102	BCL	C5-C3-C2	2.02	125.21	121.12
15	T	101	CRT	C35-C33-C32	-2.02	115.83	118.94
9	W	101	BCL	C3D-C2D-C1D	-2.02	103.07	105.83
15	z	101	CRT	C30-C28-C27	-2.02	115.84	118.94
9	AC	102	BCL	C4B-C3B-CAB	-2.02	123.22	127.13
9	f	101	BCL	CHC-C1C-NC	2.02	127.31	124.51
15	m	104	CRT	C39-C38-C37	-2.02	107.75	110.86
9	I	101	BCL	C3C-C2C-C1C	2.02	105.14	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	BCL	C11-C12-C13	-2.02	109.39	115.92
15	m	104	CRT	C34-C33-C35	2.02	121.26	118.08
9	AL	102	BCL	C7-C6-C5	-2.02	107.88	113.36
9	s	102	BCL	CBB-CAB-C3B	2.02	126.33	120.34
15	v	101	CRT	C14-C15-C16	-2.02	116.92	123.22
14	y	403	MQ8	C5-C10-C1	-2.02	118.50	120.68
15	s	101	CRT	C13-C12-C14	-2.02	120.10	122.92
9	L	301	BCL	CBB-CAB-C3B	2.02	126.33	120.34
15	q	101	CRT	C16-C17-C19	-2.02	115.85	118.94
15	T	101	CRT	C31-C32-C33	-2.02	124.43	127.31
9	M	401	BCL	CBB-CAB-C3B	2.02	126.32	120.34
15	0	101	CRT	C13-C12-C14	-2.01	120.10	122.92
15	m	104	CRT	C20-C21-C22	-2.01	119.35	123.47
9	2	102	BCL	C3D-C2D-C1D	-2.01	103.09	105.83
9	V	102	BCL	C2A-C1A-CHA	2.01	127.37	123.86
9	u	101	BCL	C3C-C2C-C1C	2.01	105.11	101.87
9	AF	101	BCL	CBB-CAB-C3B	2.01	126.31	120.34
9	S	102	BCL	CED-O2D-CGD	-2.01	111.39	115.94
9	h	101	BCL	O2A-CGA-CBA	2.01	118.21	111.91
7	o	501	HEM	CAD-C3D-C2D	-2.01	124.14	127.88
9	d	101	BCL	O2A-CGA-CBA	2.01	118.21	111.91
9	AI	102	BCL	C11-C12-C13	-2.01	109.43	115.92
9	y	401	BCL	OBD-CAD-C3D	2.01	133.35	128.52
15	z	101	CRT	C15-C14-C12	-2.01	124.45	127.31
9	L	301	BCL	C1-O2A-CGA	2.00	121.70	116.44
15	G	101	CRT	C31-C30-C28	-2.00	120.79	126.42
9	q	102	BCL	C1-O2A-CGA	2.00	121.70	116.44
9	h	101	BCL	C11-C10-C8	-2.00	109.45	115.92

There are no chirality outliers.

All (1749) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	502	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C3D-CAD-CBD-CGD
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB
7	o	503	HEM	C2B-C3B-CAB-CBB
7	o	503	HEM	C4B-C3B-CAB-CBB
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	301	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	O1D-CGD-O2D-CED
9	L	303	BCL	C3A-C2A-CAA-CBA
9	L	303	BCL	C4C-C3C-CAC-CBC
9	L	303	BCL	CHA-CBD-CGD-O1D
9	L	303	BCL	CHA-CBD-CGD-O2D
9	M	402	BCL	C3A-C2A-CAA-CBA
9	M	402	BCL	C4C-C3C-CAC-CBC
9	A	102	BCL	C1A-C2A-CAA-CBA
9	A	102	BCL	C3A-C2A-CAA-CBA
9	A	103	BCL	C3A-C2A-CAA-CBA
9	A	103	BCL	CBA-CGA-O2A-C1
9	A	103	BCL	O1A-CGA-O2A-C1
9	A	103	BCL	C4C-C3C-CAC-CBC
9	A	103	BCL	O2A-C1-C2-C3
9	D	101	BCL	CBD-CGD-O2D-CED
9	D	102	BCL	C1A-C2A-CAA-CBA
9	D	102	BCL	C3A-C2A-CAA-CBA
9	D	102	BCL	C4C-C3C-CAC-CBC
9	D	102	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CHA-CBD-CGD-O1D
9	F	101	BCL	CHA-CBD-CGD-O2D
9	G	102	BCL	C3A-C2A-CAA-CBA
9	G	102	BCL	C4C-C3C-CAC-CBC
9	G	102	BCL	CBD-CGD-O2D-CED
9	G	102	BCL	C4-C3-C5-C6
9	I	103	BCL	C4C-C3C-CAC-CBC
9	I	103	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	C3A-C2A-CAA-CBA
9	N	101	BCL	CBD-CGD-O2D-CED
9	O	102	BCL	C1A-C2A-CAA-CBA
9	O	102	BCL	C3A-C2A-CAA-CBA
9	O	102	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	CBD-CGD-O2D-CED
9	Q	101	BCL	C2-C1-O2A-CGA
9	Q	101	BCL	C2C-C3C-CAC-CBC
9	Q	101	BCL	CBD-CGD-O2D-CED
9	R	102	BCL	C1A-C2A-CAA-CBA
9	R	102	BCL	C3A-C2A-CAA-CBA
9	R	102	BCL	C4C-C3C-CAC-CBC
9	R	102	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	R	102	BCL	CHA-CBD-CGD-O2D
9	R	102	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	C1A-C2A-CAA-CBA
9	S	102	BCL	C3A-C2A-CAA-CBA
9	S	102	BCL	C4C-C3C-CAC-CBC
9	S	102	BCL	CHA-CBD-CGD-O1D
9	S	102	BCL	CHA-CBD-CGD-O2D
9	S	102	BCL	CBD-CGD-O2D-CED
9	T	102	BCL	C3A-C2A-CAA-CBA
9	T	102	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	C4C-C3C-CAC-CBC
9	V	102	BCL	C1A-C2A-CAA-CBA
9	V	102	BCL	C3A-C2A-CAA-CBA
9	V	102	BCL	CBD-CGD-O2D-CED
9	X	102	BCL	C1A-C2A-CAA-CBA
9	X	102	BCL	C3A-C2A-CAA-CBA
9	X	102	BCL	C2-C1-O2A-CGA
9	X	102	BCL	CBD-CGD-O2D-CED
9	Y	101	BCL	C4C-C3C-CAC-CBC
9	Z	102	BCL	C1A-C2A-CAA-CBA
9	Z	102	BCL	C3A-C2A-CAA-CBA
9	Z	102	BCL	CBD-CGD-O2D-CED
9	Z	102	BCL	C2-C3-C5-C6
9	Z	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C3A-C2A-CAA-CBA
9	2	102	BCL	CBD-CGD-O2D-CED
9	2	102	BCL	C2-C3-C5-C6
9	2	102	BCL	C4-C3-C5-C6
9	3	101	BCL	CBD-CGD-O2D-CED
9	4	102	BCL	C1A-C2A-CAA-CBA
9	4	102	BCL	C3A-C2A-CAA-CBA
9	4	102	BCL	C2C-C3C-CAC-CBC
9	4	102	BCL	C4C-C3C-CAC-CBC
9	4	102	BCL	CBD-CGD-O2D-CED
9	6	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	CBD-CGD-O2D-CED
9	7	102	BCL	C2C-C3C-CAC-CBC
9	7	102	BCL	C4C-C3C-CAC-CBC
9	7	102	BCL	CBD-CGD-O2D-CED
9	8	101	BCL	C1A-C2A-CAA-CBA
9	8	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	CHA-CBD-CGD-O1D
9	8	101	BCL	CHA-CBD-CGD-O2D
9	8	101	BCL	O2A-C1-C2-C3
9	9	102	BCL	C4C-C3C-CAC-CBC
9	0	102	BCL	C1A-C2A-CAA-CBA
9	0	102	BCL	C3A-C2A-CAA-CBA
9	0	102	BCL	C4C-C3C-CAC-CBC
9	x	301	BCL	C4C-C3C-CAC-CBC
9	x	301	BCL	CBD-CGD-O2D-CED
9	x	303	BCL	C3A-C2A-CAA-CBA
9	x	305	BCL	C4C-C3C-CAC-CBC
9	x	305	BCL	CHA-CBD-CGD-O2D
9	x	305	BCL	CBD-CGD-O2D-CED
9	y	401	BCL	C1A-C2A-CAA-CBA
9	y	401	BCL	C3A-C2A-CAA-CBA
9	y	401	BCL	C4C-C3C-CAC-CBC
9	y	401	BCL	CAD-CBD-CGD-O1D
9	y	401	BCL	O2A-C1-C2-C3
9	m	102	BCL	C4C-C3C-CAC-CBC
9	m	103	BCL	C3A-C2A-CAA-CBA
9	m	103	BCL	CBA-CGA-O2A-C1
9	m	103	BCL	O2A-C1-C2-C3
9	p	102	BCL	C1A-C2A-CAA-CBA
9	p	102	BCL	C3A-C2A-CAA-CBA
9	q	102	BCL	C1A-C2A-CAA-CBA
9	q	102	BCL	CBD-CGD-O2D-CED
9	r	101	BCL	C1A-C2A-CAA-CBA
9	r	101	BCL	C3A-C2A-CAA-CBA
9	r	101	BCL	C4C-C3C-CAC-CBC
9	s	102	BCL	C3A-C2A-CAA-CBA
9	s	102	BCL	CBD-CGD-O2D-CED
9	u	101	BCL	C3A-C2A-CAA-CBA
9	u	101	BCL	CBD-CGD-O2D-CED
9	u	102	BCL	C3A-C2A-CAA-CBA
9	u	102	BCL	CBD-CGD-O2D-CED
9	w	101	BCL	C1A-C2A-CAA-CBA
9	w	101	BCL	C3A-C2A-CAA-CBA
9	w	101	BCL	C4C-C3C-CAC-CBC
9	z	102	BCL	C3A-C2A-CAA-CBA
9	z	102	BCL	CBD-CGD-O2D-CED
9	AB	101	BCL	C2-C3-C5-C6
9	AB	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	AB	102	BCL	C3A-C2A-CAA-CBA
9	AB	102	BCL	CBD-CGD-O2D-CED
9	AC	102	BCL	C1A-C2A-CAA-CBA
9	AC	102	BCL	C3A-C2A-CAA-CBA
9	AC	102	BCL	C2A-CAA-CBA-CGA
9	AC	102	BCL	C4C-C3C-CAC-CBC
9	AC	102	BCL	C2-C3-C5-C6
9	AC	102	BCL	C4-C3-C5-C6
9	AC	103	BCL	C3A-C2A-CAA-CBA
9	AC	103	BCL	CBD-CGD-O2D-CED
9	AC	103	BCL	O1D-CGD-O2D-CED
9	AE	102	BCL	C1A-C2A-CAA-CBA
9	AE	102	BCL	C3A-C2A-CAA-CBA
9	AE	102	BCL	CBD-CGD-O2D-CED
9	AG	101	BCL	O2A-C1-C2-C3
9	AH	101	BCL	C1A-C2A-CAA-CBA
9	AH	101	BCL	C3A-C2A-CAA-CBA
9	AH	101	BCL	C2A-CAA-CBA-CGA
9	AI	101	BCL	C1A-C2A-CAA-CBA
9	AI	101	BCL	C3A-C2A-CAA-CBA
9	AI	101	BCL	CHA-CBD-CGD-O1D
9	AI	101	BCL	CHA-CBD-CGD-O2D
9	AI	101	BCL	CBD-CGD-O2D-CED
9	AI	102	BCL	C1A-C2A-CAA-CBA
9	AI	102	BCL	C3A-C2A-CAA-CBA
9	AI	102	BCL	C4C-C3C-CAC-CBC
9	AI	102	BCL	CBD-CGD-O2D-CED
9	AK	101	BCL	C2C-C3C-CAC-CBC
9	AL	102	BCL	C1A-C2A-CAA-CBA
9	AL	102	BCL	C3A-C2A-CAA-CBA
9	AL	102	BCL	C4C-C3C-CAC-CBC
9	AL	102	BCL	CBD-CGD-O2D-CED
9	d	101	BCL	O1A-CGA-O2A-C1
9	e	102	BCL	C1A-C2A-CAA-CBA
9	e	102	BCL	C3A-C2A-CAA-CBA
9	e	102	BCL	CBD-CGD-O2D-CED
9	f	101	BCL	CBD-CGD-O2D-CED
9	g	102	BCL	CBD-CGD-O2D-CED
9	i	102	BCL	C3A-C2A-CAA-CBA
9	i	102	BCL	CBD-CGD-O2D-CED
9	i	102	BCL	C2-C3-C5-C6
9	i	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	j	101	BCL	C2C-C3C-CAC-CBC
9	j	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	CBD-CGD-O2D-CED
9	k	102	BCL	C1A-C2A-CAA-CBA
9	k	102	BCL	C3A-C2A-CAA-CBA
9	k	102	BCL	C2A-CAA-CBA-CGA
9	k	102	BCL	C2C-C3C-CAC-CBC
9	k	102	BCL	C4C-C3C-CAC-CBC
9	k	102	BCL	O2A-C1-C2-C3
9	l	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	CBD-CGD-O2D-CED
9	c	101	BCL	C3A-C2A-CAA-CBA
9	c	101	BCL	C4C-C3C-CAC-CBC
10	M	403	BPH	C4C-C3C-CAC-CBC
10	x	302	BPH	C4C-C3C-CAC-CBC
10	x	302	BPH	C2C-C3C-CAC-CBC
10	y	402	BPH	C4C-C3C-CAC-CBC
10	y	402	BPH	C3A-C2A-CAA-CBA
11	L	304	UQ8	C40-C39-C41-C42
11	L	304	UQ8	C38-C39-C41-C42
11	x	304	UQ8	C39-C41-C42-C43
11	x	304	UQ8	C40-C39-C41-C42
11	x	304	UQ8	C24-C26-C27-C28
12	L	305	PEF	O3P-C1-C2-C3
12	L	305	PEF	O3P-C1-C2-O2
12	L	305	PEF	C4-O4P-P-O3P
12	M	408	PEF	C1-O3P-P-O2P
12	H	301	PEF	C1-O3P-P-O2P
12	H	301	PEF	C4-O4P-P-O1P
12	H	304	PEF	C1-O3P-P-O1P
12	H	305	PEF	C1-O3P-P-O1P
12	H	305	PEF	C1-O3P-P-O2P
12	A	101	PEF	C4-O4P-P-O1P
12	A	101	PEF	C4-O4P-P-O2P
12	A	101	PEF	C4-O4P-P-O3P
12	x	306	PEF	C1-O3P-P-O1P
12	y	406	PEF	O4P-C4-C5-N
12	y	406	PEF	C4-O4P-P-O1P
12	y	407	PEF	O4P-C4-C5-N
12	y	408	PEF	C1-O3P-P-O1P
12	y	408	PEF	C1-O3P-P-O2P
12	y	408	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
12	t	301	PEF	O4P-C4-C5-N
12	t	303	PEF	C1-O3P-P-O1P
12	t	303	PEF	C1-O3P-P-O2P
12	t	303	PEF	C1-O3P-P-O4P
12	t	303	PEF	C4-O4P-P-O2P
12	m	101	PEF	O4P-C4-C5-N
12	m	101	PEF	C5-C4-O4P-P
12	m	101	PEF	C1-O3P-P-O1P
12	m	101	PEF	C1-O3P-P-O2P
12	m	101	PEF	C4-O4P-P-O1P
12	p	101	PEF	C1-O3P-P-O1P
12	p	101	PEF	C1-O3P-P-O2P
14	M	404	MQ8	C14-C13-C15-C16
14	M	404	MQ8	C16-C17-C18-C19
14	M	404	MQ8	C31-C32-C33-C34
14	M	404	MQ8	C31-C32-C33-C35
14	M	404	MQ8	C32-C33-C35-C36
14	M	404	MQ8	C36-C37-C38-C40
14	M	404	MQ8	C43-C44-C46-C47
14	y	403	MQ8	C12-C13-C15-C16
14	y	403	MQ8	C16-C17-C18-C20
14	y	403	MQ8	C36-C37-C38-C39
14	y	403	MQ8	C36-C37-C38-C40
14	y	403	MQ8	C38-C40-C41-C42
14	y	403	MQ8	C41-C42-C43-C44
15	M	405	CRT	C3-C1-C4-C5
15	M	405	CRT	C32-C33-C35-C36
15	M	405	CRT	C34-C33-C35-C36
15	M	405	CRT	C35-C36-C37-C38
15	E	101	CRT	C2-C1-O1-C1M
15	E	101	CRT	C22-C23-C25-C26
15	E	101	CRT	C24-C23-C25-C26
15	G	101	CRT	C5-C6-C7-C8
15	G	101	CRT	C5-C6-C7-C9
15	G	101	CRT	C29-C28-C30-C31
15	G	101	CRT	C32-C33-C35-C36
15	G	101	CRT	C34-C33-C35-C36
15	I	102	CRT	C5-C6-C7-C8
15	I	102	CRT	C5-C6-C7-C9
15	O	101	CRT	C2-C1-O1-C1M
15	O	101	CRT	O1-C1-C4-C5
15	O	101	CRT	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
15	O	101	CRT	C3-C1-C4-C5
15	O	101	CRT	C15-C16-C17-C18
15	O	101	CRT	C15-C16-C17-C19
15	P	102	CRT	C2-C1-C4-C5
15	P	102	CRT	C3-C1-C4-C5
15	P	102	CRT	C22-C23-C25-C26
15	P	102	CRT	C24-C23-C25-C26
15	P	102	CRT	C29-C28-C30-C31
15	R	101	CRT	C5-C6-C7-C8
15	R	101	CRT	C5-C6-C7-C9
15	R	101	CRT	C15-C16-C17-C18
15	R	101	CRT	C15-C16-C17-C19
15	R	101	CRT	C22-C23-C25-C26
15	R	101	CRT	C24-C23-C25-C26
15	R	101	CRT	C27-C28-C30-C31
15	R	101	CRT	C29-C28-C30-C31
15	T	101	CRT	C3-C1-O1-C1M
15	V	101	CRT	C2-C1-C4-C5
15	V	101	CRT	C3-C1-C4-C5
15	V	101	CRT	C10-C11-C12-C13
15	V	101	CRT	C10-C11-C12-C14
15	V	101	CRT	C15-C16-C17-C18
15	V	101	CRT	C15-C16-C17-C19
15	V	101	CRT	C36-C37-C38-C39
15	V	101	CRT	C36-C37-C38-C40
15	V	101	CRT	C36-C37-C38-O2
15	X	101	CRT	O1-C1-C4-C5
15	X	101	CRT	C2-C1-C4-C5
15	X	101	CRT	C3-C1-C4-C5
15	X	101	CRT	C1-C4-C5-C6
15	X	101	CRT	C24-C23-C25-C26
15	Z	101	CRT	C5-C6-C7-C8
15	Z	101	CRT	C5-C6-C7-C9
15	Z	101	CRT	C15-C16-C17-C18
15	Z	101	CRT	C15-C16-C17-C19
15	Z	101	CRT	C27-C28-C30-C31
15	Z	101	CRT	C29-C28-C30-C31
15	Z	101	CRT	C36-C37-C38-C40
15	2	101	CRT	C5-C6-C7-C8
15	2	101	CRT	C5-C6-C7-C9
15	4	101	CRT	C3-C1-C4-C5
15	4	101	CRT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	4	101	CRT	C5-C6-C7-C9
15	4	101	CRT	C10-C11-C12-C13
15	4	101	CRT	C10-C11-C12-C14
15	4	101	CRT	C27-C28-C30-C31
15	4	101	CRT	C29-C28-C30-C31
15	7	101	CRT	C5-C6-C7-C8
15	7	101	CRT	C5-C6-C7-C9
15	7	101	CRT	C22-C23-C25-C26
15	7	101	CRT	C24-C23-C25-C26
15	7	101	CRT	C29-C28-C30-C31
15	7	103	CRT	C2-C1-C4-C5
15	7	103	CRT	C3-C1-C4-C5
15	9	101	CRT	C3-C1-O1-C1M
15	9	101	CRT	C1-C4-C5-C6
15	9	101	CRT	C15-C16-C17-C18
15	9	101	CRT	C15-C16-C17-C19
15	9	101	CRT	C29-C28-C30-C31
15	0	101	CRT	C2-C1-O1-C1M
15	0	101	CRT	C5-C6-C7-C8
15	0	101	CRT	C5-C6-C7-C9
15	y	404	CRT	C32-C33-C35-C36
15	y	404	CRT	C34-C33-C35-C36
15	y	404	CRT	C35-C36-C37-C38
15	n	101	CRT	C2-C1-O1-C1M
15	n	101	CRT	C3-C1-O1-C1M
15	n	101	CRT	C1-C4-C5-C6
15	n	101	CRT	C15-C16-C17-C18
15	n	101	CRT	C15-C16-C17-C19
15	n	101	CRT	C36-C37-C38-C39
15	n	101	CRT	C36-C37-C38-C40
15	n	101	CRT	C36-C37-C38-O2
15	q	101	CRT	C22-C23-C25-C26
15	q	101	CRT	C24-C23-C25-C26
15	s	101	CRT	C5-C6-C7-C8
15	s	101	CRT	C5-C6-C7-C9
15	s	101	CRT	C10-C11-C12-C13
15	s	101	CRT	C10-C11-C12-C14
15	s	101	CRT	C15-C16-C17-C18
15	s	101	CRT	C22-C23-C25-C26
15	s	101	CRT	C24-C23-C25-C26
15	v	101	CRT	C1-C4-C5-C6
15	v	101	CRT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	v	101	CRT	C22-C23-C25-C26
15	v	101	CRT	C24-C23-C25-C26
15	AC	101	CRT	C2-C1-C4-C5
15	AC	101	CRT	C15-C16-C17-C18
15	AD	101	CRT	C3-C1-O1-C1M
15	AF	102	CRT	C27-C28-C30-C31
15	AF	102	CRT	C29-C28-C30-C31
15	AH	102	CRT	C2-C1-O1-C1M
15	AH	102	CRT	C22-C23-C25-C26
15	AH	102	CRT	C24-C23-C25-C26
15	AJ	101	CRT	C27-C28-C30-C31
15	AJ	101	CRT	C29-C28-C30-C31
15	AL	101	CRT	C5-C6-C7-C8
15	AL	101	CRT	C24-C23-C25-C26
15	e	101	CRT	O1-C1-C4-C5
15	e	101	CRT	C2-C1-C4-C5
15	e	101	CRT	C3-C1-C4-C5
15	g	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C10-C11-C12-C13
15	i	101	CRT	C10-C11-C12-C14
15	i	101	CRT	C22-C23-C25-C26
15	i	101	CRT	C24-C23-C25-C26
15	k	101	CRT	C2-C1-C4-C5
15	k	101	CRT	C3-C1-C4-C5
17	AE	101	PGW	C04-C05-CAD-OAE
12	H	304	PEF	C11-C10-O2-C2
12	H	305	PEF	C11-C10-O2-C2
12	H	305	PEF	O4-C10-O2-C2
12	x	306	PEF	C11-C10-O2-C2
17	S	101	PGW	C2-C1-O01-C02
17	AE	101	PGW	C2-C1-O01-C02
9	A	103	BCL	O1D-CGD-O2D-CED
9	D	102	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	O1D-CGD-O2D-CED
9	G	102	BCL	O1D-CGD-O2D-CED
9	I	101	BCL	O1D-CGD-O2D-CED
9	I	103	BCL	O1D-CGD-O2D-CED
9	R	102	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	O1D-CGD-O2D-CED
9	T	102	BCL	O1D-CGD-O2D-CED
9	U	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	X	102	BCL	O1D-CGD-O2D-CED
9	Z	102	BCL	O1D-CGD-O2D-CED
9	2	102	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	O1D-CGD-O2D-CED
9	7	102	BCL	O1D-CGD-O2D-CED
9	9	102	BCL	O1D-CGD-O2D-CED
9	0	102	BCL	O1D-CGD-O2D-CED
9	x	303	BCL	O1D-CGD-O2D-CED
9	p	102	BCL	O1D-CGD-O2D-CED
9	s	102	BCL	O1D-CGD-O2D-CED
9	w	101	BCL	O1D-CGD-O2D-CED
9	z	102	BCL	O1D-CGD-O2D-CED
9	AC	102	BCL	O1D-CGD-O2D-CED
9	AG	101	BCL	O1D-CGD-O2D-CED
9	AI	102	BCL	O1D-CGD-O2D-CED
9	AK	101	BCL	O1D-CGD-O2D-CED
9	AL	102	BCL	O1D-CGD-O2D-CED
9	d	101	BCL	O1D-CGD-O2D-CED
9	e	102	BCL	O1D-CGD-O2D-CED
9	i	102	BCL	O1D-CGD-O2D-CED
9	j	101	BCL	O1D-CGD-O2D-CED
9	k	102	BCL	O1D-CGD-O2D-CED
9	c	101	BCL	O1D-CGD-O2D-CED
12	A	101	PEF	C11-C10-O2-C2
12	x	306	PEF	O4-C10-O2-C2
12	y	407	PEF	C11-C10-O2-C2
12	y	408	PEF	C11-C10-O2-C2
12	t	303	PEF	C11-C10-O2-C2
9	L	303	BCL	O1D-CGD-O2D-CED
9	D	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	O1D-CGD-O2D-CED
9	O	102	BCL	O1D-CGD-O2D-CED
9	P	101	BCL	O1D-CGD-O2D-CED
9	Q	101	BCL	O1D-CGD-O2D-CED
9	V	102	BCL	O1D-CGD-O2D-CED
9	4	102	BCL	O1D-CGD-O2D-CED
9	6	101	BCL	O1D-CGD-O2D-CED
9	x	301	BCL	O1D-CGD-O2D-CED
9	m	103	BCL	O1D-CGD-O2D-CED
9	q	102	BCL	O1D-CGD-O2D-CED
9	u	102	BCL	O1D-CGD-O2D-CED
9	AE	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	AH	101	BCL	O1D-CGD-O2D-CED
9	g	102	BCL	O1D-CGD-O2D-CED
9	l	101	BCL	O1D-CGD-O2D-CED
9	L	303	BCL	CBD-CGD-O2D-CED
9	A	102	BCL	CBD-CGD-O2D-CED
9	A	103	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CBD-CGD-O2D-CED
9	I	101	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	CBD-CGD-O2D-CED
9	W	101	BCL	CBD-CGD-O2D-CED
9	Y	101	BCL	CBD-CGD-O2D-CED
9	1	101	BCL	CBD-CGD-O2D-CED
9	5	101	BCL	CBD-CGD-O2D-CED
9	8	101	BCL	CBD-CGD-O2D-CED
9	9	102	BCL	CBD-CGD-O2D-CED
9	0	102	BCL	CBD-CGD-O2D-CED
9	x	303	BCL	CBD-CGD-O2D-CED
9	m	102	BCL	CBD-CGD-O2D-CED
9	m	103	BCL	CBD-CGD-O2D-CED
9	p	102	BCL	CBD-CGD-O2D-CED
9	r	101	BCL	CBD-CGD-O2D-CED
9	w	101	BCL	CBD-CGD-O2D-CED
9	AB	101	BCL	CBD-CGD-O2D-CED
9	AC	102	BCL	CBD-CGD-O2D-CED
9	AF	101	BCL	CBD-CGD-O2D-CED
9	AG	101	BCL	CBD-CGD-O2D-CED
9	AH	101	BCL	CBD-CGD-O2D-CED
9	AK	101	BCL	CBD-CGD-O2D-CED
9	d	101	BCL	CBD-CGD-O2D-CED
9	h	101	BCL	CBD-CGD-O2D-CED
9	k	102	BCL	CBD-CGD-O2D-CED
9	c	101	BCL	CBD-CGD-O2D-CED
10	L	302	BPH	CBD-CGD-O2D-CED
9	4	102	BCL	O1A-CGA-O2A-C1
9	8	101	BCL	O1A-CGA-O2A-C1
9	m	103	BCL	O1A-CGA-O2A-C1
9	s	102	BCL	O1A-CGA-O2A-C1
9	g	102	BCL	O1A-CGA-O2A-C1
9	k	102	BCL	O1A-CGA-O2A-C1
17	S	101	PGW	O02-C1-O01-C02
17	AE	101	PGW	O02-C1-O01-C02
9	W	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	Y	101	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	O1D-CGD-O2D-CED
9	u	101	BCL	O1D-CGD-O2D-CED
9	AB	101	BCL	O1D-CGD-O2D-CED
9	AF	101	BCL	O1D-CGD-O2D-CED
10	L	302	BPH	O1D-CGD-O2D-CED
9	m	102	BCL	O1D-CGD-O2D-CED
9	AB	102	BCL	O1D-CGD-O2D-CED
9	f	101	BCL	O1D-CGD-O2D-CED
9	h	101	BCL	O1D-CGD-O2D-CED
9	8	101	BCL	CBA-CGA-O2A-C1
9	s	102	BCL	CBA-CGA-O2A-C1
9	g	102	BCL	CBA-CGA-O2A-C1
9	k	102	BCL	CBA-CGA-O2A-C1
14	M	404	MQ8	C46-C47-C48-C49
9	M	401	BCL	CBD-CGD-O2D-CED
10	x	302	BPH	CBD-CGD-O2D-CED
9	G	102	BCL	O1A-CGA-O2A-C1
9	O	102	BCL	O1A-CGA-O2A-C1
9	2	102	BCL	O1A-CGA-O2A-C1
9	6	101	BCL	O1A-CGA-O2A-C1
9	u	102	BCL	O1A-CGA-O2A-C1
9	AB	102	BCL	O1A-CGA-O2A-C1
9	e	102	BCL	O1A-CGA-O2A-C1
9	AI	101	BCL	O1D-CGD-O2D-CED
9	R	102	BCL	C15-C16-C17-C18
9	AC	103	BCL	C15-C16-C17-C18
12	H	304	PEF	O4-C10-O2-C2
9	x	305	BCL	O1D-CGD-O2D-CED
9	K	101	BCL	O1A-CGA-O2A-C1
9	M	401	BCL	C3-C5-C6-C7
9	I	101	BCL	C3-C5-C6-C7
9	I	103	BCL	C3-C5-C6-C7
9	N	101	BCL	C3-C5-C6-C7
9	W	101	BCL	C3-C5-C6-C7
9	6	101	BCL	C3-C5-C6-C7
9	8	101	BCL	C3-C5-C6-C7
9	9	102	BCL	C3-C5-C6-C7
9	u	101	BCL	C3-C5-C6-C7
9	AC	102	BCL	C3-C5-C6-C7
9	AG	101	BCL	C3-C5-C6-C7
9	g	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	k	102	BCL	C3-C5-C6-C7
10	M	403	BPH	C3-C5-C6-C7
9	G	102	BCL	CBA-CGA-O2A-C1
9	O	102	BCL	CBA-CGA-O2A-C1
9	Z	102	BCL	CBA-CGA-O2A-C1
9	4	102	BCL	CBA-CGA-O2A-C1
9	6	101	BCL	CBA-CGA-O2A-C1
9	u	102	BCL	CBA-CGA-O2A-C1
9	d	101	BCL	CBA-CGA-O2A-C1
9	e	102	BCL	CBA-CGA-O2A-C1
9	h	101	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	CBA-CGA-O2A-C1
9	c	101	BCL	CBA-CGA-O2A-C1
12	y	406	PEF	C11-C10-O2-C2
9	8	101	BCL	O1D-CGD-O2D-CED
9	I	103	BCL	O1A-CGA-O2A-C1
9	X	102	BCL	O1A-CGA-O2A-C1
9	q	102	BCL	O1A-CGA-O2A-C1
12	H	304	PEF	C31-C30-O3-C3
9	7	102	BCL	C4-C3-C5-C6
9	s	102	BCL	C4-C3-C5-C6
9	G	102	BCL	C2-C3-C5-C6
9	s	102	BCL	C2-C3-C5-C6
11	x	304	UQ8	C38-C39-C41-C42
14	y	403	MQ8	C42-C43-C44-C46
9	L	303	BCL	C2A-CAA-CBA-CGA
9	V	102	BCL	C2A-CAA-CBA-CGA
9	6	101	BCL	C2A-CAA-CBA-CGA
9	AI	101	BCL	C2A-CAA-CBA-CGA
9	g	102	BCL	C2A-CAA-CBA-CGA
9	7	102	BCL	O1A-CGA-O2A-C1
9	V	102	BCL	C3-C5-C6-C7
9	X	102	BCL	C3-C5-C6-C7
9	z	102	BCL	C3-C5-C6-C7
9	AH	101	BCL	C3-C5-C6-C7
9	i	102	BCL	C3-C5-C6-C7
9	I	103	BCL	CBA-CGA-O2A-C1
9	R	102	BCL	CBA-CGA-O2A-C1
9	2	102	BCL	CBA-CGA-O2A-C1
9	7	102	BCL	CBA-CGA-O2A-C1
9	AB	102	BCL	CBA-CGA-O2A-C1
9	AC	103	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	AE	102	BCL	CBA-CGA-O2A-C1
9	AG	101	BCL	CBA-CGA-O2A-C1
12	t	303	PEF	O4-C10-O2-C2
9	1	101	BCL	O1D-CGD-O2D-CED
14	M	404	MQ8	C46-C47-C48-C50
14	M	404	MQ8	C36-C37-C38-C39
14	y	403	MQ8	C16-C17-C18-C19
14	y	403	MQ8	C41-C42-C43-C45
9	R	102	BCL	O1A-CGA-O2A-C1
9	T	102	BCL	O1A-CGA-O2A-C1
9	Z	102	BCL	O1A-CGA-O2A-C1
9	AC	103	BCL	O1A-CGA-O2A-C1
9	AE	102	BCL	O1A-CGA-O2A-C1
9	AG	101	BCL	O1A-CGA-O2A-C1
9	h	101	BCL	O1A-CGA-O2A-C1
9	i	102	BCL	O1A-CGA-O2A-C1
12	H	305	PEF	C31-C30-O3-C3
15	9	101	CRT	C11-C10-C9-C7
15	n	101	CRT	C11-C10-C9-C7
10	x	302	BPH	O1D-CGD-O2D-CED
9	K	101	BCL	C3-C5-C6-C7
9	L	303	BCL	CBA-CGA-O2A-C1
9	D	102	BCL	CBA-CGA-O2A-C1
9	F	101	BCL	CBA-CGA-O2A-C1
9	K	101	BCL	CBA-CGA-O2A-C1
9	P	101	BCL	CBA-CGA-O2A-C1
9	T	102	BCL	CBA-CGA-O2A-C1
9	X	102	BCL	CBA-CGA-O2A-C1
9	0	102	BCL	CBA-CGA-O2A-C1
9	x	303	BCL	CBA-CGA-O2A-C1
9	q	102	BCL	CBA-CGA-O2A-C1
9	z	102	BCL	CBA-CGA-O2A-C1
9	AB	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	CBA-CGA-O2A-C1
9	i	102	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	O1A-CGA-O2A-C1
9	c	101	BCL	O1A-CGA-O2A-C1
9	A	102	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	C15-C16-C17-C18
9	L	303	BCL	O1A-CGA-O2A-C1
12	A	101	PEF	O4-C10-O2-C2
9	AI	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	y	407	PEF	O5-C30-O3-C3
9	5	101	BCL	O1D-CGD-O2D-CED
12	y	407	PEF	O4-C10-O2-C2
14	y	403	MQ8	C14-C13-C15-C16
14	y	403	MQ8	C34-C33-C35-C36
14	y	403	MQ8	C45-C43-C44-C46
14	M	404	MQ8	C12-C13-C15-C16
14	y	403	MQ8	C32-C33-C35-C36
12	M	408	PEF	O5-C30-O3-C3
12	y	408	PEF	O5-C30-O3-C3
12	y	407	PEF	C31-C30-O3-C3
9	q	102	BCL	C2A-CAA-CBA-CGA
9	w	101	BCL	C2A-CAA-CBA-CGA
12	t	301	PEF	C11-C10-O2-C2
9	0	102	BCL	O1A-CGA-O2A-C1
9	x	303	BCL	O1A-CGA-O2A-C1
9	z	102	BCL	O1A-CGA-O2A-C1
9	AB	101	BCL	O1A-CGA-O2A-C1
9	f	101	BCL	O1A-CGA-O2A-C1
11	L	304	UQ8	C14-C16-C17-C18
14	M	404	MQ8	C38-C40-C41-C42
14	y	403	MQ8	C33-C35-C36-C37
9	N	101	BCL	CBA-CGA-O2A-C1
9	Q	101	BCL	CBA-CGA-O2A-C1
9	W	101	BCL	CBA-CGA-O2A-C1
12	y	408	PEF	C31-C30-O3-C3
12	y	408	PEF	O4-C10-O2-C2
9	D	102	BCL	O1A-CGA-O2A-C1
9	F	101	BCL	O1A-CGA-O2A-C1
14	M	404	MQ8	C15-C16-C17-C18
9	M	401	BCL	O1D-CGD-O2D-CED
12	M	408	PEF	C31-C30-O3-C3
9	N	101	BCL	O1A-CGA-O2A-C1
9	P	101	BCL	O1A-CGA-O2A-C1
9	W	101	BCL	O1A-CGA-O2A-C1
9	D	102	BCL	C3-C5-C6-C7
9	I	101	BCL	CBA-CGA-O2A-C1
9	U	101	BCL	CBA-CGA-O2A-C1
9	V	102	BCL	CBA-CGA-O2A-C1
9	Y	101	BCL	CBA-CGA-O2A-C1
9	1	101	BCL	CBA-CGA-O2A-C1
9	5	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	p	102	BCL	CBA-CGA-O2A-C1
9	AI	102	BCL	CBA-CGA-O2A-C1
9	AL	102	BCL	CBA-CGA-O2A-C1
15	I	102	CRT	C11-C10-C9-C7
9	N	101	BCL	C13-C15-C16-C17
12	H	302	PEF	C11-C10-O2-C2
9	N	101	BCL	C15-C16-C17-C18
9	T	102	BCL	C5-C6-C7-C8
9	AC	102	BCL	C8-C10-C11-C12
9	AG	101	BCL	C13-C15-C16-C17
12	H	304	PEF	O5-C30-O3-C3
9	p	102	BCL	O1A-CGA-O2A-C1
9	AF	101	BCL	C4-C3-C5-C6
9	7	102	BCL	C2-C3-C5-C6
9	M	401	BCL	C6-C7-C8-C9
9	A	102	BCL	C11-C12-C13-C14
9	O	102	BCL	C6-C7-C8-C9
9	6	101	BCL	C6-C7-C8-C9
9	m	103	BCL	C11-C12-C13-C14
9	i	102	BCL	C6-C7-C8-C9
9	c	101	BCL	C6-C7-C8-C9
9	A	102	BCL	C13-C15-C16-C17
9	AB	101	BCL	C5-C6-C7-C8
9	8	101	BCL	C2A-CAA-CBA-CGA
15	T	101	CRT	C29-C28-C30-C31
15	X	101	CRT	C10-C11-C12-C13
15	4	101	CRT	C15-C16-C17-C18
15	9	101	CRT	C5-C6-C7-C8
15	y	404	CRT	C5-C6-C7-C8
15	n	101	CRT	C5-C6-C7-C8
15	AH	102	CRT	C5-C6-C7-C8
15	e	101	CRT	C10-C11-C12-C13
15	e	101	CRT	C15-C16-C17-C18
15	e	101	CRT	C24-C23-C25-C26
15	k	101	CRT	C10-C11-C12-C13
15	G	101	CRT	C27-C28-C30-C31
15	e	101	CRT	C10-C11-C12-C14
17	S	101	PGW	C20-C19-O03-C01
9	U	101	BCL	O1A-CGA-O2A-C1
9	Y	101	BCL	O1A-CGA-O2A-C1
9	AI	102	BCL	O1A-CGA-O2A-C1
9	F	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	C15-C16-C17-C18
9	u	102	BCL	C5-C6-C7-C8
9	AE	102	BCL	C8-C10-C11-C12
9	AI	102	BCL	C8-C10-C11-C12
9	k	102	BCL	C8-C10-C11-C12
9	D	101	BCL	CBA-CGA-O2A-C1
7	o	501	HEM	C2A-CAA-CBA-CGA
9	A	103	BCL	C8-C10-C11-C12
9	I	103	BCL	C5-C6-C7-C8
9	P	101	BCL	C5-C6-C7-C8
9	X	102	BCL	C8-C10-C11-C12
9	3	101	BCL	C5-C6-C7-C8
9	AC	102	BCL	C5-C6-C7-C8
9	AG	101	BCL	C8-C10-C11-C12
9	AH	101	BCL	C10-C11-C12-C13
9	d	101	BCL	C15-C16-C17-C18
9	f	101	BCL	C15-C16-C17-C18
9	h	101	BCL	C10-C11-C12-C13
9	l	101	BCL	C10-C11-C12-C13
10	L	302	BPH	C5-C6-C7-C8
10	L	302	BPH	C8-C10-C11-C12
9	G	102	BCL	C5-C6-C7-C8
9	U	101	BCL	C15-C16-C17-C18
9	W	101	BCL	C10-C11-C12-C13
9	4	102	BCL	C5-C6-C7-C8
9	5	101	BCL	C15-C16-C17-C18
9	7	102	BCL	C8-C10-C11-C12
9	8	101	BCL	C10-C11-C12-C13
9	r	101	BCL	C13-C15-C16-C17
9	z	102	BCL	C5-C6-C7-C8
9	AB	101	BCL	C8-C10-C11-C12
9	AE	102	BCL	C13-C15-C16-C17
9	AK	101	BCL	C13-C15-C16-C17
9	k	102	BCL	C10-C11-C12-C13
9	k	102	BCL	C15-C16-C17-C18
17	AE	101	PGW	OAF-C05-CAD-OAE
9	M	402	BCL	C5-C6-C7-C8
9	F	101	BCL	C15-C16-C17-C18
9	G	102	BCL	C15-C16-C17-C18
9	4	102	BCL	C8-C10-C11-C12
9	AK	101	BCL	CBA-CGA-O2A-C1
12	M	407	PEF	C2-C3-O3-C30

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Mol	Chain	Res	Type	Atoms
12	H	305	PEF	O5-C30-O3-C3
9	i	102	BCL	C2-C1-O2A-CGA
9	Z	102	BCL	C8-C10-C11-C12
9	g	102	BCL	C8-C10-C11-C12
9	h	101	BCL	C15-C16-C17-C18
9	M	401	BCL	C5-C6-C7-C8
9	u	101	BCL	C5-C6-C7-C8
9	7	102	BCL	C11-C10-C8-C7
9	u	101	BCL	C11-C10-C8-C7
9	I	101	BCL	O1A-CGA-O2A-C1
9	V	102	BCL	O1A-CGA-O2A-C1
9	AL	102	BCL	O1A-CGA-O2A-C1
15	AJ	101	CRT	C17-C19-C20-C21
9	I	103	BCL	C2A-CAA-CBA-CGA
9	T	102	BCL	C2A-CAA-CBA-CGA
9	x	303	BCL	C2A-CAA-CBA-CGA
9	F	101	BCL	C5-C6-C7-C8
9	R	102	BCL	C13-C15-C16-C17
9	U	101	BCL	C13-C15-C16-C17
9	V	102	BCL	C8-C10-C11-C12
9	r	101	BCL	C8-C10-C11-C12
9	AI	102	BCL	C15-C16-C17-C18
9	5	101	BCL	O1A-CGA-O2A-C1
9	X	102	BCL	C10-C11-C12-C13
9	AI	101	BCL	C5-C6-C7-C8
11	L	304	UQ8	C29-C31-C32-C33
11	x	304	UQ8	C19-C21-C22-C23
14	M	404	MQ8	C18-C20-C21-C22
14	y	403	MQ8	C28-C30-C31-C32
9	x	303	BCL	C3-C5-C6-C7
9	0	102	BCL	C13-C15-C16-C17
9	s	102	BCL	C5-C6-C7-C8
9	i	102	BCL	C13-C15-C16-C17
9	Q	101	BCL	O1A-CGA-O2A-C1
9	1	101	BCL	O1A-CGA-O2A-C1
9	D	101	BCL	C15-C16-C17-C18
9	S	102	BCL	C8-C10-C11-C12
9	3	101	BCL	C15-C16-C17-C18
9	u	101	BCL	C13-C15-C16-C17
9	z	102	BCL	C15-C16-C17-C18
9	AE	102	BCL	C5-C6-C7-C8
9	e	102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	c	101	BCL	C13-C15-C16-C17
10	M	403	BPH	C13-C15-C16-C17
12	y	406	PEF	O4-C10-O2-C2
9	D	102	BCL	C13-C15-C16-C17
9	G	102	BCL	C8-C10-C11-C12
9	Q	101	BCL	C8-C10-C11-C12
9	x	301	BCL	C15-C16-C17-C18
9	p	102	BCL	C15-C16-C17-C18
9	AB	101	BCL	C13-C15-C16-C17
9	f	101	BCL	C10-C11-C12-C13
10	M	403	BPH	C15-C16-C17-C18
12	M	407	PEF	C1-O3P-P-O4P
12	M	408	PEF	C1-O3P-P-O4P
12	H	301	PEF	C1-O3P-P-O4P
12	H	301	PEF	C4-O4P-P-O3P
12	H	304	PEF	C4-O4P-P-O3P
12	H	305	PEF	C1-O3P-P-O4P
12	A	101	PEF	C1-O3P-P-O4P
12	m	101	PEF	C1-O3P-P-O4P
12	p	101	PEF	C1-O3P-P-O4P
17	S	101	PGW	C04-O12-P-O11
9	x	301	BCL	CBA-CGA-O2A-C1
9	y	401	BCL	CBA-CGA-O2A-C1
9	AC	102	BCL	CBA-CGA-O2A-C1
9	l	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	C5-C6-C7-C8
9	AK	101	BCL	O1A-CGA-O2A-C1
9	W	101	BCL	C4-C3-C5-C6
9	e	102	BCL	C4-C3-C5-C6
9	m	103	BCL	C5-C6-C7-C8
9	r	101	BCL	C5-C6-C7-C8
9	j	101	BCL	C10-C11-C12-C13
9	r	101	BCL	C2A-CAA-CBA-CGA
9	AE	102	BCL	C2A-CAA-CBA-CGA
9	d	101	BCL	C16-C17-C18-C20
9	3	101	BCL	CBA-CGA-O2A-C1
15	y	404	CRT	C25-C26-C27-C28
9	0	102	BCL	C8-C10-C11-C12
9	z	102	BCL	C13-C15-C16-C17
9	D	101	BCL	O1A-CGA-O2A-C1
9	m	103	BCL	C16-C17-C18-C20
9	AC	103	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	AK	101	BCL	C16-C17-C18-C20
9	l	101	BCL	C16-C17-C18-C19
12	x	306	PEF	C1-C2-O2-C10
9	S	102	BCL	C5-C6-C7-C8
9	U	101	BCL	C8-C10-C11-C12
9	x	301	BCL	C5-C6-C7-C8
9	AB	102	BCL	C15-C16-C17-C18
9	Y	101	BCL	C8-C10-C11-C12
9	x	303	BCL	C8-C10-C11-C12
9	AC	102	BCL	O1A-CGA-O2A-C1
9	AC	103	BCL	C16-C17-C18-C19
9	0	102	BCL	C4-C3-C5-C6
9	AF	101	BCL	C2-C3-C5-C6
9	S	102	BCL	C6-C7-C8-C9
9	4	102	BCL	C11-C12-C13-C14
9	m	103	BCL	C6-C7-C8-C9
9	AC	102	BCL	C11-C10-C8-C9
9	AI	102	BCL	C6-C7-C8-C9
10	y	402	BPH	C11-C12-C13-C14
9	Z	102	BCL	C5-C6-C7-C8
9	AI	102	BCL	C13-C15-C16-C17
9	Q	101	BCL	C2A-CAA-CBA-CGA
9	AG	101	BCL	C2A-CAA-CBA-CGA
15	V	101	CRT	C24-C23-C25-C26
15	AF	102	CRT	C5-C6-C7-C8
15	T	101	CRT	C27-C28-C30-C31
15	9	101	CRT	C5-C6-C7-C9
15	9	101	CRT	C27-C28-C30-C31
15	n	101	CRT	C5-C6-C7-C9
15	s	101	CRT	C15-C16-C17-C19
15	AL	101	CRT	C22-C23-C25-C26
9	AK	101	BCL	C3-C5-C6-C7
9	8	101	BCL	C8-C10-C11-C12
12	t	301	PEF	O4-C10-O2-C2
9	W	101	BCL	C16-C17-C18-C19
9	d	101	BCL	C16-C17-C18-C19
9	g	102	BCL	C16-C17-C18-C19
9	g	102	BCL	C16-C17-C18-C20
9	l	101	BCL	C16-C17-C18-C20
9	A	102	BCL	C5-C6-C7-C8
9	D	102	BCL	C15-C16-C17-C18
9	I	103	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	AI	101	BCL	C15-C16-C17-C18
9	1	101	BCL	C13-C15-C16-C17
9	x	301	BCL	O1A-CGA-O2A-C1
9	y	401	BCL	O1A-CGA-O2A-C1
9	u	101	BCL	CBA-CGA-O2A-C1
9	I	103	BCL	C3A-C2A-CAA-CBA
9	q	102	BCL	C3A-C2A-CAA-CBA
9	F	101	BCL	C10-C11-C12-C13
9	AC	103	BCL	C13-C15-C16-C17
9	l	101	BCL	C8-C10-C11-C12
9	l	101	BCL	O1A-CGA-O2A-C1
9	m	103	BCL	C16-C17-C18-C19
9	z	102	BCL	C16-C17-C18-C19
10	M	403	BPH	O2A-C1-C2-C3
9	7	102	BCL	C10-C11-C12-C13
9	U	101	BCL	C4-C3-C5-C6
10	y	402	BPH	C4-C3-C5-C6
9	U	101	BCL	C2-C3-C5-C6
9	0	102	BCL	C2-C3-C5-C6
12	x	306	PEF	C31-C30-O3-C3
9	M	402	BCL	C16-C17-C18-C20
9	W	101	BCL	C16-C17-C18-C20
9	X	102	BCL	C16-C17-C18-C19
9	AE	102	BCL	C16-C17-C18-C20
9	AK	101	BCL	C16-C17-C18-C19
9	AB	101	BCL	C10-C11-C12-C13
9	3	101	BCL	O1A-CGA-O2A-C1
9	AI	101	BCL	C10-C11-C12-C13
9	l	101	BCL	C2-C1-O2A-CGA
9	A	103	BCL	C15-C16-C17-C18
9	R	102	BCL	C10-C11-C12-C13
12	H	302	PEF	O4-C10-O2-C2
9	9	102	BCL	C16-C17-C18-C20
9	S	102	BCL	CBA-CGA-O2A-C1
9	L	301	BCL	C5-C6-C7-C8
9	O	102	BCL	C5-C6-C7-C8
9	x	301	BCL	C13-C15-C16-C17
10	y	402	BPH	C13-C15-C16-C17
7	o	502	HEM	C3D-CAD-CBD-CGD
9	I	101	BCL	C5-C6-C7-C8
9	2	102	BCL	C8-C10-C11-C12
9	AB	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	A	102	BCL	C11-C12-C13-C15
9	I	101	BCL	C2-C3-C5-C6
9	O	102	BCL	C11-C10-C8-C7
9	U	101	BCL	C12-C13-C15-C16
9	4	102	BCL	C11-C12-C13-C15
9	8	101	BCL	C6-C7-C8-C10
9	y	401	BCL	C6-C7-C8-C10
9	m	103	BCL	C11-C12-C13-C15
9	AC	102	BCL	C11-C10-C8-C7
9	AF	101	BCL	C6-C7-C8-C10
9	g	102	BCL	C2-C3-C5-C6
9	i	102	BCL	C11-C12-C13-C15
9	j	101	BCL	C11-C10-C8-C7
10	L	302	BPH	C11-C10-C8-C7
10	y	402	BPH	C11-C12-C13-C15
14	y	403	MQ8	C37-C38-C40-C41
9	u	101	BCL	O1A-CGA-O2A-C1
9	R	102	BCL	C5-C6-C7-C8
9	2	102	BCL	C13-C15-C16-C17
9	AE	102	BCL	C16-C17-C18-C19
10	x	302	BPH	CBA-CGA-O2A-C1
9	y	401	BCL	C5-C6-C7-C8
9	Q	101	BCL	C5-C6-C7-C8
9	W	101	BCL	C5-C6-C7-C8
9	m	102	BCL	C15-C16-C17-C18
9	q	102	BCL	C8-C10-C11-C12
7	o	501	HEM	C2B-C3B-CAB-CBB
14	y	403	MQ8	C21-C22-C23-C24
9	F	101	BCL	C3-C5-C6-C7
9	z	102	BCL	C16-C17-C18-C20
9	L	303	BCL	C5-C6-C7-C8
11	L	304	UQ8	C39-C41-C42-C43
11	L	304	UQ8	C34-C36-C37-C38
7	C	502	HEM	C4B-C3B-CAB-CBB
7	o	501	HEM	C4B-C3B-CAB-CBB
7	o	502	HEM	C4B-C3B-CAB-CBB
9	L	301	BCL	C13-C15-C16-C17
17	S	101	PGW	O04-C19-O03-C01
12	H	305	PEF	O2-C2-C3-O3
9	AI	101	BCL	C16-C17-C18-C20
9	X	102	BCL	C5-C6-C7-C8
9	AL	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	I	101	BCL	C4-C3-C5-C6
9	AK	101	BCL	C4-C3-C5-C6
14	M	404	MQ8	C24-C23-C25-C26
14	y	403	MQ8	C24-C23-C25-C26
9	W	101	BCL	C2-C3-C5-C6
9	e	102	BCL	C2-C3-C5-C6
14	y	403	MQ8	C22-C23-C25-C26
9	L	301	BCL	C11-C12-C13-C14
9	L	303	BCL	C11-C12-C13-C14
9	D	101	BCL	C6-C7-C8-C9
9	F	101	BCL	C11-C12-C13-C14
9	O	102	BCL	C11-C10-C8-C9
9	7	102	BCL	C11-C10-C8-C9
9	8	101	BCL	C6-C7-C8-C9
9	y	401	BCL	C6-C7-C8-C9
9	q	102	BCL	C14-C13-C15-C16
9	r	101	BCL	C11-C12-C13-C14
9	u	101	BCL	C6-C7-C8-C9
9	u	101	BCL	C11-C10-C8-C9
9	AF	101	BCL	C6-C7-C8-C9
9	AL	102	BCL	C6-C7-C8-C9
9	f	101	BCL	C11-C12-C13-C14
9	c	101	BCL	C11-C12-C13-C14
10	L	302	BPH	C11-C10-C8-C9
10	x	302	BPH	O1A-CGA-O2A-C1
10	M	403	BPH	C2C-C3C-CAC-CBC
10	y	402	BPH	C2C-C3C-CAC-CBC
15	V	101	CRT	C22-C23-C25-C26
15	AC	101	CRT	C15-C16-C17-C19
9	L	303	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C1A-C2A-CAA-CBA
9	A	103	BCL	C1A-C2A-CAA-CBA
9	G	102	BCL	C1A-C2A-CAA-CBA
9	I	103	BCL	C1A-C2A-CAA-CBA
9	N	101	BCL	C1A-C2A-CAA-CBA
9	T	102	BCL	C1A-C2A-CAA-CBA
9	2	102	BCL	C1A-C2A-CAA-CBA
9	x	303	BCL	C1A-C2A-CAA-CBA
9	x	305	BCL	C1A-C2A-CAA-CBA
9	m	103	BCL	C1A-C2A-CAA-CBA
9	s	102	BCL	C1A-C2A-CAA-CBA
9	u	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	u	102	BCL	C1A-C2A-CAA-CBA
9	z	102	BCL	C1A-C2A-CAA-CBA
9	AB	102	BCL	C1A-C2A-CAA-CBA
9	AC	103	BCL	C1A-C2A-CAA-CBA
9	i	102	BCL	C1A-C2A-CAA-CBA
9	c	101	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C16-C17-C18-C19
9	8	101	BCL	C16-C17-C18-C20
9	9	102	BCL	C16-C17-C18-C19
9	u	101	BCL	C16-C17-C18-C20
9	AC	102	BCL	C16-C17-C18-C20
9	AI	101	BCL	C16-C17-C18-C19
14	y	403	MQ8	C15-C16-C17-C18
9	M	402	BCL	C15-C16-C17-C18
9	m	102	BCL	C5-C6-C7-C8
9	AB	102	BCL	C10-C11-C12-C13
9	AC	102	BCL	C15-C16-C17-C18
9	c	101	BCL	C3-C5-C6-C7
9	S	102	BCL	O1A-CGA-O2A-C1
9	Q	101	BCL	C10-C11-C12-C13
9	1	101	BCL	C5-C6-C7-C8
17	S	101	PGW	C01-C02-C03-O11
15	M	405	CRT	C1-C4-C5-C6
15	R	101	CRT	C1-C4-C5-C6
9	g	102	BCL	C4-C3-C5-C6
11	x	304	UQ8	C20-C19-C21-C22
9	I	101	BCL	C2C-C3C-CAC-CBC
9	N	101	BCL	C2C-C3C-CAC-CBC
9	m	102	BCL	C2C-C3C-CAC-CBC
9	s	102	BCL	C2C-C3C-CAC-CBC
9	u	101	BCL	C2C-C3C-CAC-CBC
9	z	102	BCL	C2C-C3C-CAC-CBC
9	AG	101	BCL	C2C-C3C-CAC-CBC
9	AI	102	BCL	C2C-C3C-CAC-CBC
9	j	101	BCL	C15-C16-C17-C18
9	M	401	BCL	C16-C17-C18-C19
12	H	304	PEF	C1-C2-C3-O3
9	AF	101	BCL	C5-C6-C7-C8
7	C	504	HEM	C4D-C3D-CAD-CBD
12	H	302	PEF	C31-C30-O3-C3
15	y	404	CRT	C37-C38-O2-C2M
17	S	101	PGW	C02-C01-O03-C19

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Mol	Chain	Res	Type	Atoms
9	L	303	BCL	C13-C15-C16-C17
10	x	302	BPH	C4-C3-C5-C6
14	y	403	MQ8	C39-C38-C40-C41
11	x	304	UQ8	C18-C19-C21-C22
14	M	404	MQ8	C22-C23-C25-C26
9	A	102	BCL	C8-C10-C11-C12
9	T	102	BCL	C13-C15-C16-C17
9	f	101	BCL	C8-C10-C11-C12
17	AE	101	PGW	C03-C02-O01-C1
9	S	102	BCL	C2A-CAA-CBA-CGA
9	AL	102	BCL	C13-C15-C16-C17
9	8	101	BCL	C2-C1-O2A-CGA
9	AC	102	BCL	C2-C1-O2A-CGA
9	M	401	BCL	CBA-CGA-O2A-C1
9	L	303	BCL	C16-C17-C18-C19
9	x	303	BCL	C16-C17-C18-C20
9	U	101	BCL	C10-C11-C12-C13
9	0	102	BCL	C15-C16-C17-C18
15	M	405	CRT	C2-C1-O1-C1M
15	G	101	CRT	C2-C1-O1-C1M
15	I	102	CRT	C3-C1-O1-C1M
15	R	101	CRT	C2-C1-O1-C1M
15	T	101	CRT	C2-C1-O1-C1M
15	V	101	CRT	C2-C1-O1-C1M
15	4	101	CRT	C2-C1-O1-C1M
15	7	101	CRT	C3-C1-O1-C1M
15	7	103	CRT	C2-C1-O1-C1M
15	9	101	CRT	C2-C1-O1-C1M
15	y	404	CRT	C3-C1-O1-C1M
15	y	404	CRT	C39-C38-O2-C2M
15	m	104	CRT	C2-C1-O1-C1M
15	q	101	CRT	C3-C1-O1-C1M
15	s	101	CRT	C2-C1-O1-C1M
15	v	101	CRT	C3-C1-O1-C1M
15	z	101	CRT	C2-C1-O1-C1M
15	AC	101	CRT	C2-C1-O1-C1M
15	AF	102	CRT	C2-C1-O1-C1M
15	AH	102	CRT	C39-C38-O2-C2M
15	AH	102	CRT	C40-C38-O2-C2M
15	AJ	101	CRT	C3-C1-O1-C1M
15	e	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C3-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
15	k	101	CRT	C2-C1-O1-C1M
9	M	402	BCL	CAA-CBA-CGA-O2A
9	c	101	BCL	C8-C10-C11-C12
9	R	102	BCL	C16-C17-C18-C20
15	M	405	CRT	C2-C1-C4-C5
15	E	101	CRT	C36-C37-C38-C39
15	E	101	CRT	C36-C37-C38-C40
15	G	101	CRT	C2-C1-C4-C5
15	G	101	CRT	C3-C1-C4-C5
15	G	101	CRT	C36-C37-C38-C39
15	I	102	CRT	C36-C37-C38-C39
15	X	101	CRT	C36-C37-C38-C39
15	X	101	CRT	C36-C37-C38-C40
15	Z	101	CRT	C36-C37-C38-C39
15	2	101	CRT	C2-C1-C4-C5
15	2	101	CRT	C3-C1-C4-C5
15	4	101	CRT	C2-C1-C4-C5
15	0	101	CRT	C2-C1-C4-C5
15	0	101	CRT	C3-C1-C4-C5
15	0	101	CRT	C36-C37-C38-C39
15	n	101	CRT	C2-C1-C4-C5
15	q	101	CRT	C2-C1-C4-C5
15	q	101	CRT	C36-C37-C38-C39
15	q	101	CRT	C36-C37-C38-C40
15	AC	101	CRT	C3-C1-C4-C5
15	AH	102	CRT	C36-C37-C38-C39
15	AH	102	CRT	C36-C37-C38-C40
15	AJ	101	CRT	C36-C37-C38-C39
15	AJ	101	CRT	C36-C37-C38-C40
15	g	101	CRT	C36-C37-C38-C39
9	L	301	BCL	C11-C12-C13-C15
9	L	303	BCL	C11-C12-C13-C15
9	D	101	BCL	C6-C7-C8-C10
9	D	102	BCL	C12-C13-C15-C16
9	F	101	BCL	C11-C12-C13-C15
9	X	102	BCL	C12-C13-C15-C16
9	9	102	BCL	C12-C13-C15-C16
9	q	102	BCL	C12-C13-C15-C16
9	r	101	BCL	C11-C12-C13-C15
9	s	102	BCL	C11-C12-C13-C15
9	AB	102	BCL	C11-C12-C13-C15
9	AH	101	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	AL	102	BCL	C6-C7-C8-C10
9	e	102	BCL	C12-C13-C15-C16
9	f	101	BCL	C11-C12-C13-C15
9	c	101	BCL	C11-C12-C13-C15
10	L	302	BPH	C6-C7-C8-C10
10	L	302	BPH	C11-C12-C13-C15
10	M	403	BPH	C6-C7-C8-C10
10	x	302	BPH	C2-C3-C5-C6
9	M	401	BCL	C11-C10-C8-C9
9	D	102	BCL	C14-C13-C15-C16
9	K	101	BCL	C11-C10-C8-C9
9	1	101	BCL	C11-C10-C8-C9
9	0	102	BCL	C11-C12-C13-C14
9	u	102	BCL	C11-C12-C13-C14
9	AB	102	BCL	C11-C10-C8-C9
9	AH	101	BCL	C11-C12-C13-C14
9	e	102	BCL	C14-C13-C15-C16
9	i	102	BCL	C11-C12-C13-C14
9	j	101	BCL	C11-C10-C8-C9
15	X	101	CRT	C17-C19-C20-C21
9	M	402	BCL	CBA-CGA-O2A-C1
9	W	101	BCL	C8-C10-C11-C12
9	3	101	BCL	C13-C15-C16-C17
9	u	101	BCL	C8-C10-C11-C12
9	l	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C2A-CAA-CBA-CGA
15	M	405	CRT	O1-C1-C4-C5
15	M	405	CRT	C36-C37-C38-O2
15	E	101	CRT	C36-C37-C38-O2
15	G	101	CRT	O1-C1-C4-C5
15	P	102	CRT	O1-C1-C4-C5
15	V	101	CRT	O1-C1-C4-C5
15	X	101	CRT	C36-C37-C38-O2
15	4	101	CRT	O1-C1-C4-C5
15	q	101	CRT	C36-C37-C38-O2
15	AC	101	CRT	O1-C1-C4-C5
15	AH	102	CRT	O1-C1-C4-C5
15	AH	102	CRT	C36-C37-C38-O2
15	E	101	CRT	C5-C6-C7-C8
9	L	303	BCL	C16-C17-C18-C20
9	u	101	BCL	C16-C17-C18-C19
15	P	102	CRT	C27-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
15	AH	102	CRT	C5-C6-C7-C9
9	z	102	BCL	C10-C11-C12-C13
9	AF	101	BCL	CBA-CGA-O2A-C1
10	y	402	BPH	CBA-CGA-O2A-C1
17	AE	101	PGW	C20-C19-O03-C01
9	V	102	BCL	C15-C16-C17-C18
9	x	305	BCL	C13-C15-C16-C17
9	AL	102	BCL	C15-C16-C17-C18
9	1	101	BCL	C15-C16-C17-C18
12	M	407	PEF	O4P-C4-C5-N
12	H	302	PEF	O4P-C4-C5-N
12	A	101	PEF	O4P-C4-C5-N
9	3	101	BCL	C8-C10-C11-C12
9	AH	101	BCL	C5-C6-C7-C8
12	x	306	PEF	O5-C30-O3-C3
9	AH	101	BCL	C4-C3-C5-C6
9	AB	102	BCL	C8-C10-C11-C12
9	Y	101	BCL	C3A-C2A-CAA-CBA
9	m	102	BCL	C3A-C2A-CAA-CBA
9	AG	101	BCL	C3A-C2A-CAA-CBA
9	g	102	BCL	C3A-C2A-CAA-CBA
9	m	102	BCL	C3-C5-C6-C7
9	X	102	BCL	C13-C15-C16-C17
9	6	101	BCL	C5-C6-C7-C8
9	X	102	BCL	C16-C17-C18-C20
10	L	302	BPH	CBA-CGA-O2A-C1
12	M	408	PEF	C1-C2-C3-O3
12	H	305	PEF	C1-C2-C3-O3
9	q	102	BCL	O2A-C1-C2-C3
9	U	101	BCL	C3-C5-C6-C7
9	1	101	BCL	C4-C3-C5-C6
12	H	301	PEF	C31-C30-O3-C3
17	S	101	PGW	O01-C02-C03-O11
9	AH	101	BCL	CBA-CGA-O2A-C1
9	M	401	BCL	O1A-CGA-O2A-C1
9	9	102	BCL	C5-C6-C7-C8
9	AK	101	BCL	C8-C10-C11-C12
9	K	101	BCL	C10-C11-C12-C13
9	O	102	BCL	C15-C16-C17-C18
9	c	101	BCL	C10-C11-C12-C13
9	V	102	BCL	C2-C1-O2A-CGA
9	AH	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	N	101	BCL	C6-C7-C8-C9
9	O	102	BCL	C11-C12-C13-C14
9	U	101	BCL	C14-C13-C15-C16
9	m	102	BCL	C11-C10-C8-C9
9	p	102	BCL	C6-C7-C8-C9
9	AC	103	BCL	C11-C12-C13-C14
9	g	102	BCL	C11-C12-C13-C14
10	L	302	BPH	C11-C12-C13-C14
10	M	403	BPH	C6-C7-C8-C9
10	y	402	BPH	C11-C10-C8-C9
10	y	402	BPH	C1A-C2A-CAA-CBA
12	H	305	PEF	C2-C1-O3P-P
9	x	303	BCL	C16-C17-C18-C19
15	0	101	CRT	C15-C16-C17-C18
9	M	401	BCL	C4C-C3C-CAC-CBC
9	F	101	BCL	C4C-C3C-CAC-CBC
9	P	101	BCL	C4C-C3C-CAC-CBC
9	T	102	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C4C-C3C-CAC-CBC
9	x	303	BCL	C4C-C3C-CAC-CBC
9	AC	103	BCL	C4C-C3C-CAC-CBC
9	AH	101	BCL	C4C-C3C-CAC-CBC
9	AI	101	BCL	C4C-C3C-CAC-CBC
9	h	101	BCL	C4C-C3C-CAC-CBC
9	i	102	BCL	C4C-C3C-CAC-CBC
15	X	101	CRT	C22-C23-C25-C26
15	4	101	CRT	C15-C16-C17-C19
15	7	101	CRT	C27-C28-C30-C31
15	v	101	CRT	C5-C6-C7-C9
15	AL	101	CRT	C5-C6-C7-C9
15	e	101	CRT	C15-C16-C17-C19
15	e	101	CRT	C22-C23-C25-C26
15	k	101	CRT	C10-C11-C12-C14
7	o	503	HEM	C3D-CAD-CBD-CGD
9	P	101	BCL	C16-C17-C18-C20
9	8	101	BCL	C16-C17-C18-C19
7	C	504	HEM	C2D-C3D-CAD-CBD
12	M	408	PEF	O3P-C1-C2-C3
12	H	304	PEF	O3P-C1-C2-C3
17	AE	101	PGW	C01-C02-C03-O11
9	M	401	BCL	C11-C10-C8-C7
9	I	103	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	K	101	BCL	C11-C10-C8-C7
9	O	102	BCL	C11-C12-C13-C15
9	X	102	BCL	C11-C10-C8-C7
9	1	101	BCL	C11-C10-C8-C7
9	8	101	BCL	C11-C12-C13-C15
9	0	102	BCL	C11-C12-C13-C15
9	m	102	BCL	C11-C10-C8-C7
9	p	102	BCL	C6-C7-C8-C10
9	u	102	BCL	C11-C12-C13-C15
9	w	101	BCL	C11-C10-C8-C7
9	AB	102	BCL	C11-C10-C8-C7
9	AC	103	BCL	C11-C12-C13-C15
9	AF	101	BCL	C12-C13-C15-C16
9	g	102	BCL	C11-C12-C13-C15
10	M	403	BPH	C11-C12-C13-C15
10	y	402	BPH	C11-C10-C8-C7
15	AH	102	CRT	C25-C26-C27-C28
15	AJ	101	CRT	C20-C21-C22-C23
9	AK	101	BCL	C15-C16-C17-C18
9	AF	101	BCL	O1A-CGA-O2A-C1
9	AL	102	BCL	C3-C5-C6-C7
9	q	102	BCL	C16-C17-C18-C19
9	0	102	BCL	C10-C11-C12-C13
10	M	403	BPH	CBD-CGD-O2D-CED
9	G	102	BCL	CAD-CBD-CGD-O2D
9	0	102	BCL	CAD-CBD-CGD-O2D
9	y	401	BCL	CAD-CBD-CGD-O2D
9	q	102	BCL	CAD-CBD-CGD-O2D
9	r	101	BCL	CAD-CBD-CGD-O2D
9	u	101	BCL	CAD-CBD-CGD-O2D
9	AF	101	BCL	CAD-CBD-CGD-O2D
9	k	102	BCL	CAD-CBD-CGD-O2D
10	x	302	BPH	CAD-CBD-CGD-O2D
9	x	303	BCL	C10-C11-C12-C13
9	m	103	BCL	C10-C11-C12-C13
9	r	101	BCL	CBA-CGA-O2A-C1
10	M	403	BPH	CBA-CGA-O2A-C1
9	M	401	BCL	C16-C17-C18-C20
12	x	306	PEF	C1-C2-C3-O3
12	m	101	PEF	C1-C2-C3-O3
10	M	403	BPH	O1A-CGA-O2A-C1
10	y	402	BPH	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	AC	102	BCL	C10-C11-C12-C13
9	V	102	BCL	CHA-CBD-CGD-O1D
9	V	102	BCL	CHA-CBD-CGD-O2D
9	W	101	BCL	CHA-CBD-CGD-O1D
9	W	101	BCL	CHA-CBD-CGD-O2D
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D
9	x	303	BCL	CHA-CBD-CGD-O1D
9	x	305	BCL	CHA-CBD-CGD-O1D
9	d	101	BCL	CHA-CBD-CGD-O1D
9	d	101	BCL	CHA-CBD-CGD-O2D
9	M	402	BCL	O1A-CGA-O2A-C1
9	AH	101	BCL	O1A-CGA-O2A-C1
12	M	408	PEF	O2-C2-C3-O3
12	H	304	PEF	O2-C2-C3-O3
12	t	303	PEF	O2-C2-C3-O3
10	L	302	BPH	C4-C3-C5-C6
10	L	302	BPH	O1A-CGA-O2A-C1
10	y	402	BPH	C2-C3-C5-C6
9	X	102	BCL	C11-C10-C8-C9
9	AF	101	BCL	C14-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C9
9	k	102	BCL	C6-C7-C8-C9
9	U	101	BCL	C2A-CAA-CBA-CGA
7	o	504	HEM	C4D-C3D-CAD-CBD
9	e	102	BCL	C5-C6-C7-C8
15	0	101	CRT	C15-C16-C17-C19
9	D	102	BCL	C2-C1-O2A-CGA
15	4	101	CRT	C11-C10-C9-C7
12	x	306	PEF	C1-O3P-P-O4P
12	y	407	PEF	C1-O3P-P-O4P
12	m	101	PEF	C4-O4P-P-O3P
11	x	304	UQ8	C12-C11-C9-C10
10	L	302	BPH	C2-C3-C5-C6
12	M	407	PEF	C1-O3P-P-O1P
12	H	301	PEF	C1-O3P-P-O1P
12	H	301	PEF	C4-O4P-P-O2P
12	H	304	PEF	C4-O4P-P-O2P
12	A	101	PEF	C1-O3P-P-O1P
12	x	306	PEF	C1-O3P-P-O2P
17	S	101	PGW	C03-O11-P-O14
17	S	101	PGW	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
9	W	101	BCL	C13-C15-C16-C17
12	H	305	PEF	O4P-C4-C5-N
9	AC	102	BCL	C16-C17-C18-C19
9	M	402	BCL	CAD-CBD-CGD-O1D
9	x	303	BCL	CAD-CBD-CGD-O1D
9	f	101	BCL	CAD-CBD-CGD-O1D
9	j	101	BCL	C13-C15-C16-C17
15	V	101	CRT	C35-C36-C37-C38
15	AL	101	CRT	C35-C36-C37-C38
7	C	501	HEM	C2A-CAA-CBA-CGA
9	M	401	BCL	C6-C7-C8-C10
9	A	102	BCL	C11-C10-C8-C7
9	N	101	BCL	C11-C10-C8-C7
9	P	101	BCL	C11-C12-C13-C15
9	T	102	BCL	C11-C10-C8-C7
9	5	101	BCL	C2C-C3C-CAC-CBC
9	6	101	BCL	C6-C7-C8-C10
9	7	102	BCL	C11-C12-C13-C15
9	w	101	BCL	C11-C12-C13-C15
9	AB	101	BCL	C11-C12-C13-C15
9	AG	101	BCL	C11-C12-C13-C15
9	AI	102	BCL	C11-C10-C8-C7
9	f	101	BCL	C2C-C3C-CAC-CBC
9	f	101	BCL	C11-C10-C8-C7
9	g	102	BCL	C2C-C3C-CAC-CBC
9	k	102	BCL	C6-C7-C8-C10
12	M	408	PEF	O3P-C1-C2-O2
10	x	302	BPH	C8-C10-C11-C12
9	r	101	BCL	O1A-CGA-O2A-C1
9	R	102	BCL	C16-C17-C18-C19
9	p	102	BCL	C16-C17-C18-C19
9	AH	101	BCL	C16-C17-C18-C20
12	t	301	PEF	O2-C2-C3-O3
9	N	101	BCL	O2A-C1-C2-C3
9	Z	102	BCL	C13-C15-C16-C17
9	AK	101	BCL	C2-C3-C5-C6
9	W	101	BCL	C11-C10-C8-C9
9	9	102	BCL	C14-C13-C15-C16
9	m	103	BCL	C14-C13-C15-C16
9	s	102	BCL	C11-C12-C13-C14
9	z	102	BCL	C6-C7-C8-C9
9	AB	102	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	AE	102	BCL	C6-C7-C8-C9
9	AG	101	BCL	C11-C12-C13-C14
10	L	302	BPH	C6-C7-C8-C9
7	o	504	HEM	C2D-C3D-CAD-CBD
14	y	403	MQ8	C43-C44-C46-C47
15	R	101	CRT	C14-C15-C16-C17
15	X	101	CRT	C9-C10-C11-C12
15	4	101	CRT	C28-C30-C31-C32
15	AD	101	CRT	C14-C15-C16-C17
15	AJ	101	CRT	C9-C10-C11-C12
15	g	101	CRT	C28-C30-C31-C32
14	y	403	MQ8	C46-C47-C48-C50
9	R	102	BCL	C4-C3-C5-C6
11	x	304	UQ8	C15-C14-C16-C17
9	P	101	BCL	C16-C17-C18-C19
9	Q	101	BCL	C16-C17-C18-C20
9	g	102	BCL	C15-C16-C17-C18
9	F	101	BCL	C2A-CAA-CBA-CGA
9	AC	103	BCL	C2A-CAA-CBA-CGA
9	F	101	BCL	C2-C1-O2A-CGA
9	T	102	BCL	C2-C1-O2A-CGA
9	7	102	BCL	C13-C15-C16-C17
15	V	101	CRT	C17-C19-C20-C21
12	H	302	PEF	O3P-C1-C2-O2
17	AE	101	PGW	O01-C02-C03-O11
9	AL	102	BCL	C5-C6-C7-C8
12	M	408	PEF	C2-C3-O3-C30
15	T	101	CRT	C39-C38-O2-C2M
15	V	101	CRT	C39-C38-O2-C2M
15	9	101	CRT	C39-C38-O2-C2M
15	y	404	CRT	C40-C38-O2-C2M
15	AC	101	CRT	C3-C1-O1-C1M
15	AJ	101	CRT	C2-C1-O1-C1M
15	e	101	CRT	C3-C1-O1-C1M
12	H	302	PEF	O5-C30-O3-C3
12	L	305	PEF	C1-O3P-P-O4P
12	H	302	PEF	C1-O3P-P-O4P
12	H	304	PEF	C1-O3P-P-O4P
12	y	406	PEF	C4-O4P-P-O3P
17	AE	101	PGW	C03-O11-P-O12
17	AE	101	PGW	C04-O12-P-O11
15	M	405	CRT	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
15	4	101	CRT	C36-C37-C38-C39
15	y	404	CRT	C2-C1-C4-C5
15	n	101	CRT	C3-C1-C4-C5
15	e	101	CRT	C36-C37-C38-C39
15	i	101	CRT	C2-C1-C4-C5
12	y	406	PEF	C31-C30-O3-C3
9	x	301	BCL	C4-C3-C5-C6
9	D	102	BCL	C11-C12-C13-C15
9	O	102	BCL	C6-C7-C8-C10
9	Y	101	BCL	C11-C12-C13-C15
9	x	305	BCL	C11-C12-C13-C15
9	z	102	BCL	C12-C13-C15-C16
10	x	302	BPH	C11-C10-C8-C7
9	L	303	BCL	C14-C13-C15-C16
9	A	102	BCL	C11-C10-C8-C9
9	P	101	BCL	C11-C12-C13-C14
9	7	102	BCL	C11-C12-C13-C14
9	w	101	BCL	C11-C12-C13-C14
9	AB	101	BCL	C11-C12-C13-C14
9	AI	102	BCL	C11-C10-C8-C9
10	M	403	BPH	C11-C12-C13-C14
9	3	101	BCL	C10-C11-C12-C13
15	0	101	CRT	C25-C26-C27-C28
9	AH	101	BCL	C16-C17-C18-C19
15	y	404	CRT	C36-C37-C38-O2
15	n	101	CRT	O1-C1-C4-C5
15	AJ	101	CRT	C36-C37-C38-O2
15	AC	101	CRT	C10-C11-C12-C13
9	x	305	BCL	C8-C10-C11-C12
9	AG	101	BCL	C16-C17-C18-C19
9	1	101	BCL	C2A-CAA-CBA-CGA
9	c	101	BCL	C2A-CAA-CBA-CGA
7	o	501	HEM	CAA-CBA-CGA-O1A
15	E	101	CRT	C11-C10-C9-C7
15	7	101	CRT	C25-C26-C27-C28
15	AL	101	CRT	C30-C31-C32-C33
12	x	306	PEF	O4P-C4-C5-N
10	L	302	BPH	C13-C15-C16-C17
7	C	501	HEM	C4B-C3B-CAB-CBB
14	M	404	MQ8	C27-C28-C30-C31
9	U	101	BCL	C2-C1-O2A-CGA
9	Z	102	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	x	303	BCL	C2-C1-O2A-CGA
9	m	102	BCL	C2-C1-O2A-CGA
9	s	102	BCL	C2-C1-O2A-CGA
9	AH	101	BCL	C2-C1-O2A-CGA
9	4	102	BCL	C2A-CAA-CBA-CGA
9	M	402	BCL	CAA-CBA-CGA-O1A
15	X	101	CRT	C12-C14-C15-C16
15	m	104	CRT	C11-C10-C9-C7
11	x	304	UQ8	C12-C11-C9-C8
9	7	102	BCL	C5-C6-C7-C8
9	X	102	BCL	C6-C7-C8-C9
9	2	102	BCL	C6-C7-C8-C9
9	w	101	BCL	C6-C7-C8-C9
9	AC	102	BCL	C6-C7-C8-C9
10	x	302	BPH	C11-C10-C8-C9
7	C	501	HEM	CAA-CBA-CGA-O1A
9	M	401	BCL	C13-C15-C16-C17
15	R	101	CRT	C13-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C34
15	7	103	CRT	C21-C22-C23-C24
15	AD	101	CRT	C13-C12-C14-C15
15	g	101	CRT	C31-C32-C33-C34
15	k	101	CRT	C21-C22-C23-C24
9	q	102	BCL	C3-C5-C6-C7
9	x	305	BCL	C2A-CAA-CBA-CGA
10	L	302	BPH	O2A-C1-C2-C3
15	T	101	CRT	C5-C6-C7-C8
15	AD	101	CRT	C5-C6-C7-C8
15	AL	101	CRT	C10-C11-C12-C13
17	AE	101	PGW	O04-C19-O03-C01
9	Y	101	BCL	C1A-C2A-CAA-CBA
9	AG	101	BCL	C1A-C2A-CAA-CBA
9	g	102	BCL	C1A-C2A-CAA-CBA
9	r	101	BCL	C16-C17-C18-C19
9	L	303	BCL	C12-C13-C15-C16
9	1	101	BCL	C2-C3-C5-C6
9	AH	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C11-C10-C8-C7
9	k	102	BCL	C11-C12-C13-C15
9	l	101	BCL	C11-C10-C8-C7
12	H	301	PEF	O5-C30-O3-C3
15	m	104	CRT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
12	t	303	PEF	C4-O4P-P-O3P
9	l	101	BCL	C3-C5-C6-C7
9	AB	101	BCL	C2A-CAA-CBA-CGA
9	AK	101	BCL	C2A-CAA-CBA-CGA
9	W	101	BCL	C15-C16-C17-C18
9	2	102	BCL	C15-C16-C17-C18
12	M	408	PEF	C11-C10-O2-C2
9	F	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C30-C29-C31-C32
11	x	304	UQ8	C13-C14-C16-C17
10	x	302	BPH	C3-C5-C6-C7
15	R	101	CRT	C11-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C35
15	7	103	CRT	C21-C22-C23-C25
15	AD	101	CRT	C11-C12-C14-C15
15	g	101	CRT	C31-C32-C33-C35
15	k	101	CRT	C21-C22-C23-C25
7	o	501	HEM	CAA-CBA-CGA-O2A
7	C	501	HEM	CAD-CBD-CGD-O2D
9	U	101	BCL	C5-C6-C7-C8
15	G	101	CRT	C1-C4-C5-C6
15	O	101	CRT	C1-C4-C5-C6
15	z	101	CRT	C1-C4-C5-C6
11	x	304	UQ8	C29-C31-C32-C33
17	AE	101	PGW	O12-C04-C05-CAD
9	r	101	BCL	C4-C3-C5-C6
9	h	101	BCL	C4-C3-C5-C6
9	c	101	BCL	C4-C3-C5-C6
9	p	102	BCL	C2C-C3C-CAC-CBC
9	q	102	BCL	C2C-C3C-CAC-CBC
14	M	404	MQ8	C42-C43-C44-C46
9	O	102	BCL	C8-C10-C11-C12
7	C	502	HEM	CAA-CBA-CGA-O2A
7	o	501	HEM	CAD-CBD-CGD-O2D
9	L	301	BCL	C14-C13-C15-C16
9	D	102	BCL	C11-C12-C13-C14
9	X	102	BCL	C11-C12-C13-C14
9	x	301	BCL	C6-C7-C8-C9
9	m	102	BCL	C2A-CAA-CBA-CGA
9	AI	102	BCL	C2A-CAA-CBA-CGA
15	M	405	CRT	C25-C26-C27-C28
15	Z	101	CRT	C12-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
15	AJ	101	CRT	C30-C31-C32-C33
15	k	101	CRT	C25-C26-C27-C28
9	l	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C20-C19-C21-C22
15	y	404	CRT	C22-C23-C25-C26
15	AF	102	CRT	C5-C6-C7-C9
9	c	101	BCL	C15-C16-C17-C18
9	R	102	BCL	C2-C3-C5-C6
9	x	301	BCL	C2-C3-C5-C6
7	o	503	HEM	CAA-CBA-CGA-O2A
9	G	102	BCL	C16-C17-C18-C20
9	K	101	BCL	C16-C17-C18-C19
12	H	304	PEF	O3P-C1-C2-O2
7	C	501	HEM	CAD-CBD-CGD-O1D
7	C	502	HEM	CAA-CBA-CGA-O1A
12	H	302	PEF	O3P-C1-C2-C3
9	N	101	BCL	C11-C12-C13-C15
9	T	102	BCL	C11-C12-C13-C15
9	4	102	BCL	C6-C7-C8-C10
9	i	102	BCL	C6-C7-C8-C10
11	L	304	UQ8	C28-C29-C31-C32
9	j	101	BCL	C8-C10-C11-C12
12	H	304	PEF	O4P-C4-C5-N
9	m	103	BCL	C3-C5-C6-C7
15	y	404	CRT	C20-C21-C22-C23
9	AI	101	BCL	CAA-CBA-CGA-O2A
12	m	101	PEF	O2-C2-C3-O3
14	M	404	MQ8	C26-C27-C28-C30
9	7	102	BCL	C3-C5-C6-C7
9	x	301	BCL	C2A-CAA-CBA-CGA
9	P	101	BCL	C13-C15-C16-C17
10	x	302	BPH	C15-C16-C17-C18
9	8	101	BCL	C4-C3-C5-C6
9	AC	103	BCL	C4-C3-C5-C6
9	j	101	BCL	C4-C3-C5-C6
9	k	102	BCL	C4-C3-C5-C6
7	o	501	HEM	CAD-CBD-CGD-O1D
9	F	101	BCL	C2-C3-C5-C6
9	r	101	BCL	C2-C3-C5-C6
9	Y	101	BCL	C16-C17-C18-C19
9	AI	102	BCL	C16-C17-C18-C20
9	I	103	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	N	101	BCL	C11-C10-C8-C9
9	T	102	BCL	C11-C10-C8-C9
9	q	102	BCL	C6-C7-C8-C9
9	u	101	BCL	C14-C13-C15-C16
9	u	102	BCL	C6-C7-C8-C9
9	w	101	BCL	C11-C10-C8-C9
9	z	102	BCL	C14-C13-C15-C16
9	AB	102	BCL	C6-C7-C8-C9
9	AH	101	BCL	C6-C7-C8-C9
9	d	101	BCL	C6-C7-C8-C9
9	l	101	BCL	C6-C7-C8-C9
9	l	101	BCL	C11-C10-C8-C9
9	9	102	BCL	C3A-C2A-CAA-CBA
9	8	101	BCL	C5-C6-C7-C8
9	A	103	BCL	CAD-CBD-CGD-O2D
9	z	102	BCL	CAD-CBD-CGD-O2D
9	AB	101	BCL	CAD-CBD-CGD-O2D
9	AK	101	BCL	CAD-CBD-CGD-O2D
10	y	402	BPH	CAD-CBD-CGD-O2D
15	AJ	101	CRT	C12-C14-C15-C16
15	i	101	CRT	C11-C10-C9-C7
9	K	101	BCL	C4-C3-C5-C6
11	x	304	UQ8	C30-C29-C31-C32
11	x	304	UQ8	C25-C24-C26-C27
14	M	404	MQ8	C37-C38-C40-C41
15	X	101	CRT	C10-C11-C12-C14
15	y	404	CRT	C5-C6-C7-C9
15	v	101	CRT	C15-C16-C17-C19
15	AC	101	CRT	C10-C11-C12-C14
15	AD	101	CRT	C5-C6-C7-C9
11	L	304	UQ8	C19-C21-C22-C23
9	V	102	BCL	O2A-C1-C2-C3
9	AC	102	BCL	O2A-C1-C2-C3
9	i	102	BCL	O2A-C1-C2-C3
10	x	302	BPH	O2A-C1-C2-C3
10	y	402	BPH	O2A-C1-C2-C3
7	o	503	HEM	CAA-CBA-CGA-O1A
9	M	401	BCL	CHA-CBD-CGD-O2D
9	K	101	BCL	CHA-CBD-CGD-O1D
9	K	101	BCL	CHA-CBD-CGD-O2D
9	T	102	BCL	CHA-CBD-CGD-O1D
9	T	102	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	3	101	BCL	CHA-CBD-CGD-O1D
9	3	101	BCL	CHA-CBD-CGD-O2D
9	x	303	BCL	CHA-CBD-CGD-O2D
9	AF	101	BCL	CHA-CBD-CGD-O2D
9	j	101	BCL	CHA-CBD-CGD-O1D
9	j	101	BCL	CHA-CBD-CGD-O2D
9	k	102	BCL	CHA-CBD-CGD-O2D
15	e	101	CRT	C12-C14-C15-C16
9	A	102	BCL	CAA-CBA-CGA-O2A
15	M	405	CRT	C3-C1-O1-C1M
15	7	103	CRT	C40-C38-O2-C2M
15	9	101	CRT	C40-C38-O2-C2M
15	AL	101	CRT	C39-C38-O2-C2M
9	i	102	BCL	CAA-CBA-CGA-O2A
9	w	101	BCL	O1A-CGA-O2A-C1
9	1	101	BCL	CAA-CBA-CGA-O2A
9	q	102	BCL	C16-C17-C18-C20
10	L	302	BPH	CHA-CBD-CGD-O1D
15	M	405	CRT	C36-C37-C38-C39
15	I	102	CRT	C36-C37-C38-C40
15	O	101	CRT	C36-C37-C38-C39
15	AD	101	CRT	C36-C37-C38-C40
15	AL	101	CRT	C2-C1-C4-C5
9	AC	102	BCL	CAA-CBA-CGA-O2A
9	j	101	BCL	CAA-CBA-CGA-O2A
9	M	402	BCL	C6-C7-C8-C10
9	G	102	BCL	C11-C12-C13-C15
9	S	102	BCL	C12-C13-C15-C16
9	X	102	BCL	C11-C12-C13-C15
9	6	101	BCL	C11-C12-C13-C15
9	m	103	BCL	C6-C7-C8-C10
9	q	102	BCL	C6-C7-C8-C10
9	AG	101	BCL	C12-C13-C15-C16
9	j	101	BCL	C2-C3-C5-C6
11	x	304	UQ8	C23-C24-C26-C27
9	M	402	BCL	C6-C7-C8-C9
9	G	102	BCL	C11-C12-C13-C14
9	Q	101	BCL	C14-C13-C15-C16
9	S	102	BCL	C14-C13-C15-C16
9	T	102	BCL	C11-C12-C13-C14
9	4	102	BCL	C6-C7-C8-C9
9	x	305	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	s	102	BCL	C6-C7-C8-C9
9	AG	101	BCL	C14-C13-C15-C16
9	AL	102	BCL	C11-C12-C13-C14
15	AC	101	CRT	C25-C26-C27-C28
9	Q	101	BCL	C16-C17-C18-C19
7	C	501	HEM	CAA-CBA-CGA-O2A
15	I	102	CRT	C36-C37-C38-O2
9	j	101	BCL	C5-C6-C7-C8
15	R	101	CRT	C10-C11-C12-C13
9	w	101	BCL	C10-C11-C12-C13
9	j	101	BCL	C16-C17-C18-C20
9	w	101	BCL	CBA-CGA-O2A-C1
9	0	102	BCL	C3-C5-C6-C7
9	9	102	BCL	C1A-C2A-CAA-CBA
9	m	102	BCL	C1A-C2A-CAA-CBA
14	y	403	MQ8	C25-C26-C27-C28
9	Z	102	BCL	C10-C11-C12-C13
12	y	406	PEF	O5-C30-O3-C3
9	e	102	BCL	C2A-CAA-CBA-CGA
17	S	101	PGW	C03-O11-P-O12
9	AB	102	BCL	C16-C17-C18-C20
9	p	102	BCL	C10-C11-C12-C13
9	A	102	BCL	CAA-CBA-CGA-O1A
12	L	305	PEF	C1-O3P-P-O1P
12	M	408	PEF	C4-O4P-P-O1P
12	t	303	PEF	C4-O4P-P-O1P
9	y	401	BCL	C16-C17-C18-C20
9	AC	102	BCL	CAA-CBA-CGA-O1A
10	M	403	BPH	O1D-CGD-O2D-CED
9	D	101	BCL	C5-C6-C7-C8
7	C	504	HEM	CAA-CBA-CGA-O1A
7	o	504	HEM	CAA-CBA-CGA-O2A
9	7	102	BCL	C16-C17-C18-C20
9	k	102	BCL	C5-C6-C7-C8
9	4	102	BCL	CAA-CBA-CGA-O2A
9	i	102	BCL	CAA-CBA-CGA-O1A
9	8	101	BCL	C2-C3-C5-C6
9	AC	103	BCL	C2-C3-C5-C6
9	5	101	BCL	C8-C10-C11-C12
9	Z	102	BCL	C16-C17-C18-C19
7	C	504	HEM	CAD-CBD-CGD-O1D
7	C	504	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	CAD-CBD-CGD-O1D
9	X	102	BCL	CAD-CBD-CGD-O1D
9	Y	101	BCL	CAD-CBD-CGD-O1D
9	2	102	BCL	CAD-CBD-CGD-O1D
9	x	305	BCL	CAD-CBD-CGD-O1D
9	s	102	BCL	CAD-CBD-CGD-O1D
9	AE	102	BCL	CAD-CBD-CGD-O1D
9	AH	101	BCL	CAD-CBD-CGD-O1D
12	t	301	PEF	C1-C2-O2-C10
12	t	301	PEF	C3-C2-O2-C10
17	S	101	PGW	C03-C02-O01-C1
9	5	101	BCL	CAA-CBA-CGA-O2A
9	L	301	BCL	C11-C10-C8-C9
9	Q	101	BCL	C11-C10-C8-C9
9	W	101	BCL	C11-C12-C13-C14
9	X	102	BCL	C14-C13-C15-C16
9	3	101	BCL	C11-C10-C8-C9
9	6	101	BCL	C11-C12-C13-C14
9	AG	101	BCL	C11-C10-C8-C9
9	d	101	BCL	C11-C10-C8-C9
9	e	102	BCL	C11-C12-C13-C14
10	L	302	BPH	C14-C13-C15-C16
10	M	403	BPH	C11-C10-C8-C9
7	C	503	HEM	CAA-CBA-CGA-O2A
9	1	101	BCL	CAA-CBA-CGA-O1A
9	Y	101	BCL	CAA-CBA-CGA-O2A
9	7	102	BCL	CAA-CBA-CGA-O2A
9	f	101	BCL	CAA-CBA-CGA-O2A
15	AD	101	CRT	C35-C36-C37-C38
9	AG	101	BCL	CAA-CBA-CGA-O2A
9	f	101	BCL	CAA-CBA-CGA-O1A
9	u	101	BCL	C4-C3-C5-C6
9	Y	101	BCL	C15-C16-C17-C18
9	L	301	BCL	C2C-C3C-CAC-CBC
9	A	103	BCL	C11-C10-C8-C7
9	Q	101	BCL	C12-C13-C15-C16
9	3	101	BCL	C11-C10-C8-C7
9	m	103	BCL	C12-C13-C15-C16
9	s	102	BCL	C6-C7-C8-C10
9	u	101	BCL	C6-C7-C8-C10
9	u	101	BCL	C12-C13-C15-C16
9	AL	102	BCL	C11-C12-C13-C15

Continued on next page...

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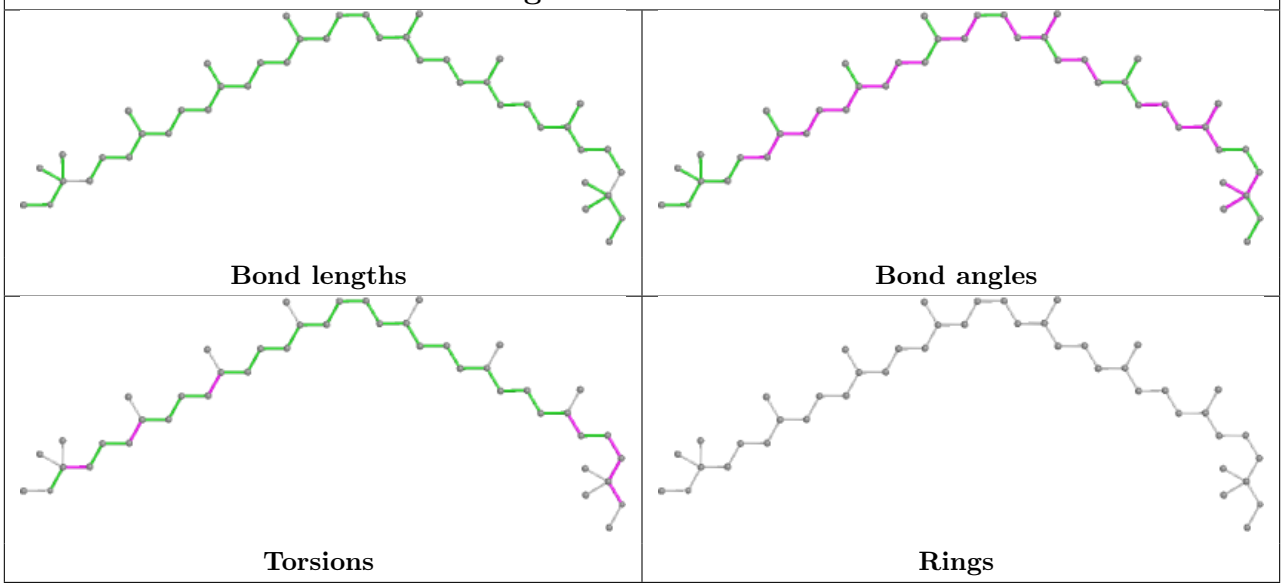
Mol	Chain	Res	Type	Atoms
9	e	102	BCL	C11-C12-C13-C15
9	c	101	BCL	C6-C7-C8-C10
10	M	403	BPH	C11-C10-C8-C7
7	C	502	HEM	CAD-CBD-CGD-O2D
9	P	101	BCL	CAA-CBA-CGA-O2A
9	W	101	BCL	CAA-CBA-CGA-O2A
9	x	305	BCL	C15-C16-C17-C18
15	E	101	CRT	C5-C6-C7-C9
15	R	101	CRT	C10-C11-C12-C14
15	AL	101	CRT	C10-C11-C12-C14
9	Y	101	BCL	CAA-CBA-CGA-O1A
9	j	101	BCL	CAA-CBA-CGA-O1A
9	y	401	BCL	CAA-CBA-CGA-O2A
9	M	402	BCL	C13-C15-C16-C17
9	K	101	BCL	C13-C15-C16-C17
7	o	502	HEM	CAA-CBA-CGA-O1A
9	P	101	BCL	C4-C3-C5-C6
9	V	102	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

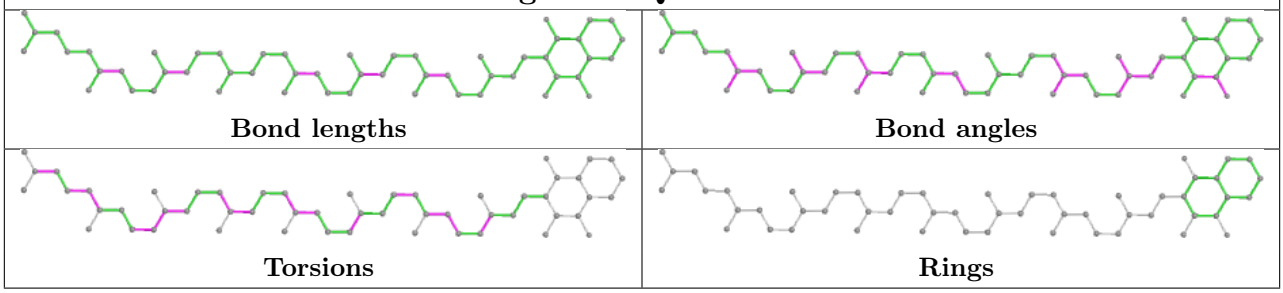
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

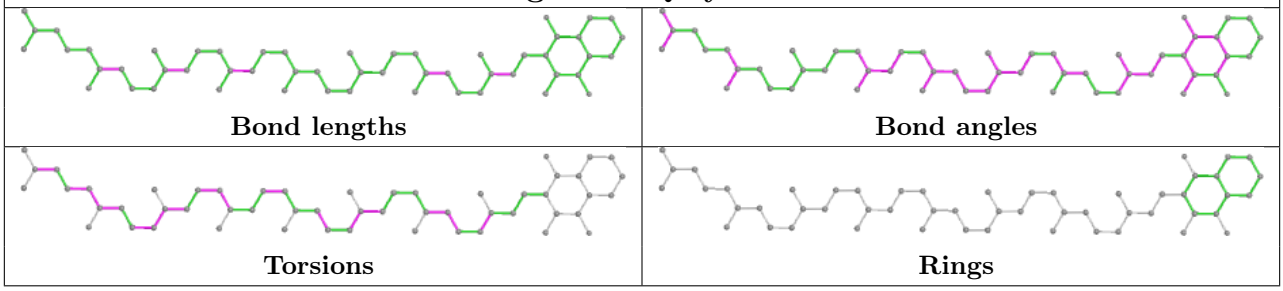
Ligand CRT G 101



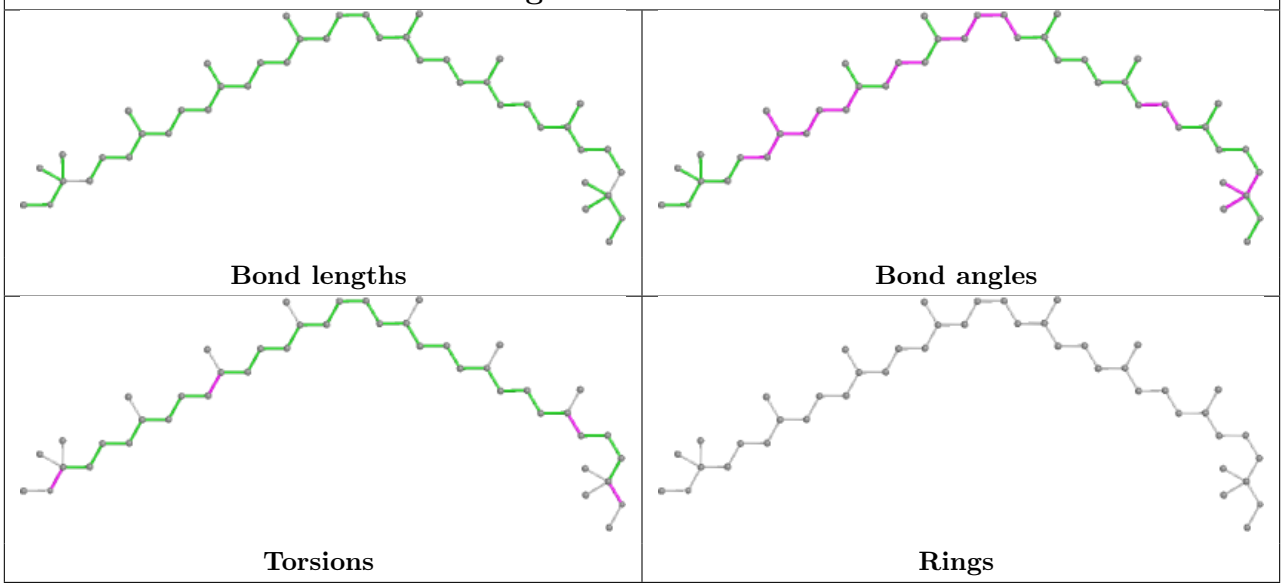
Ligand MQ8 M 404



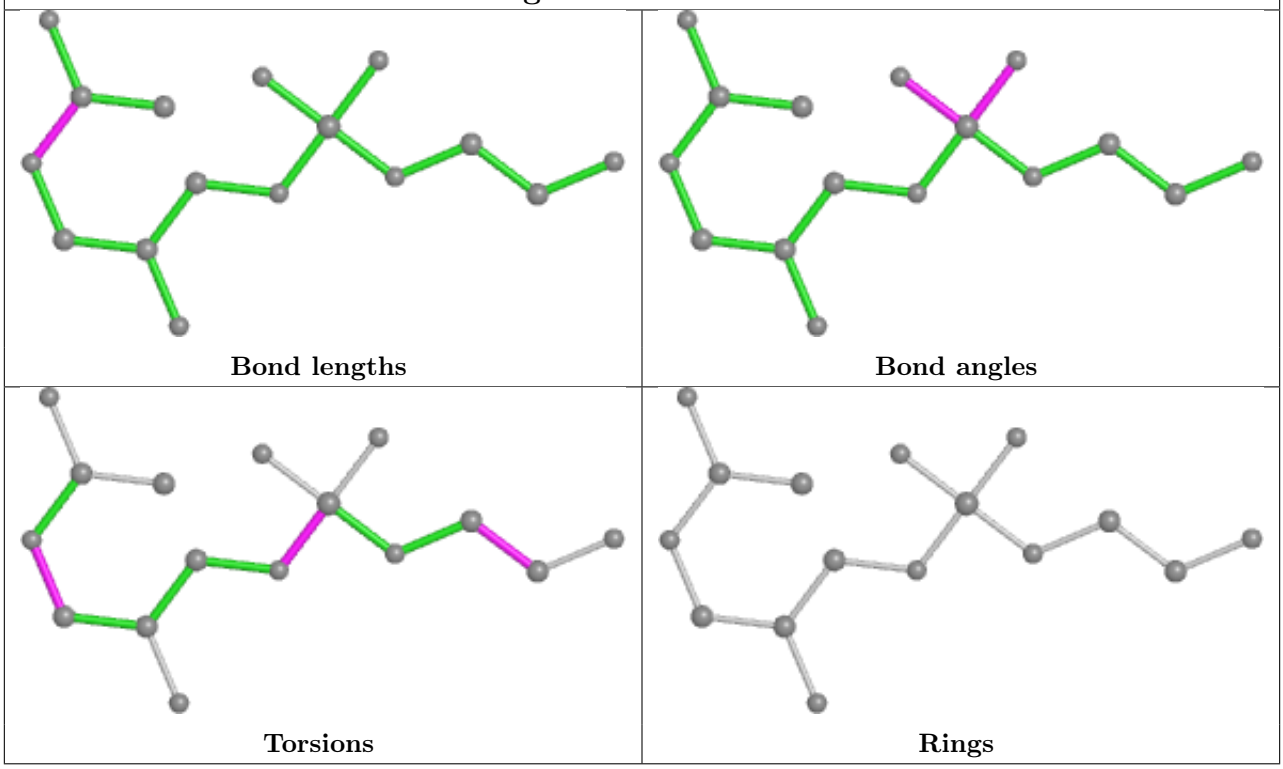
Ligand MQ8 y 403



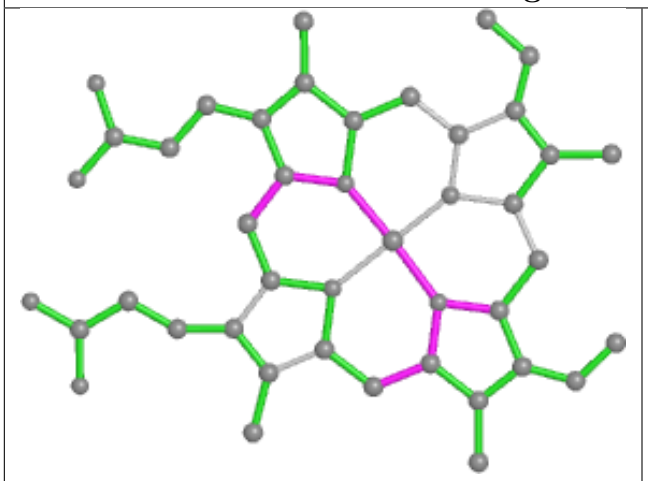
Ligand CRT T 101



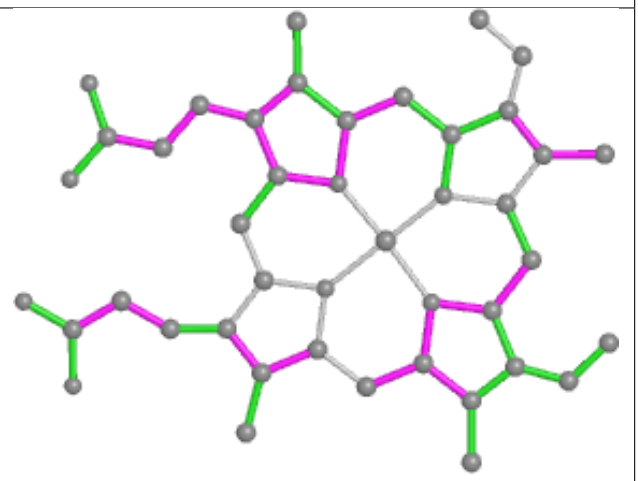
Ligand PEF M 407



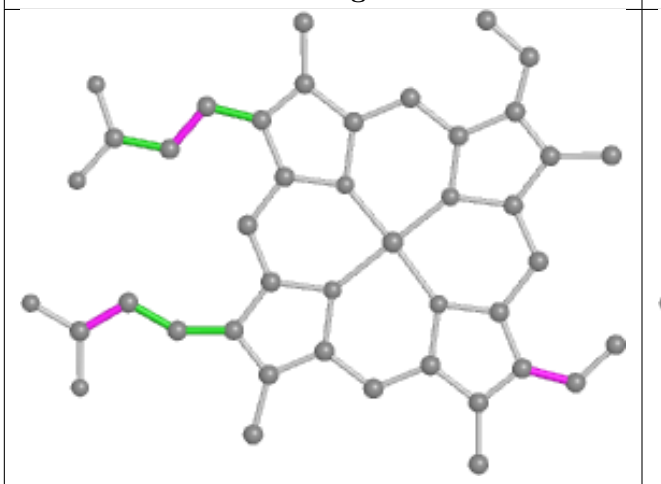
Ligand HEM o 502



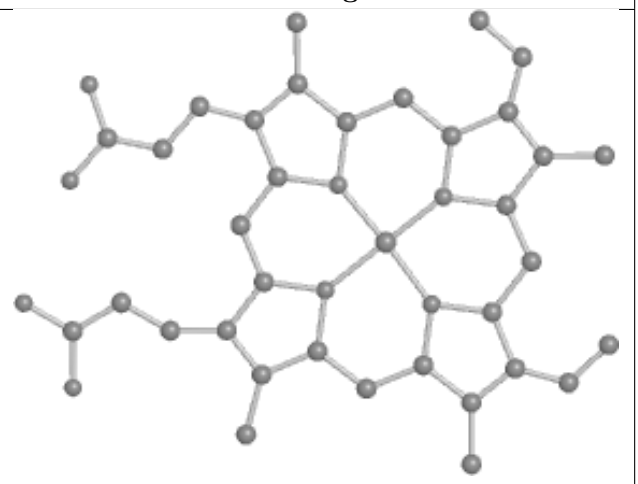
Bond lengths



Bond angles

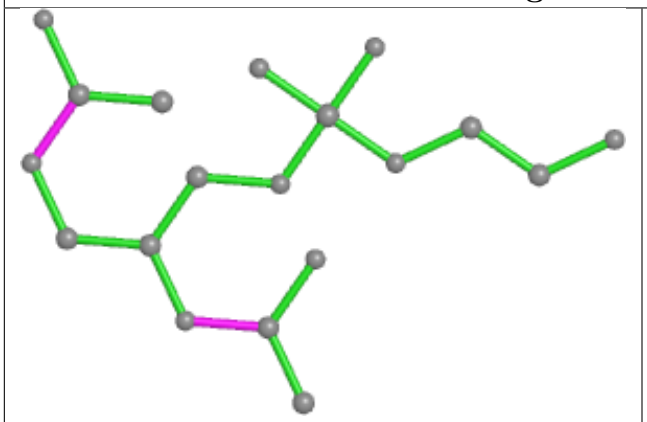


Torsions



Rings

Ligand PEF H 304



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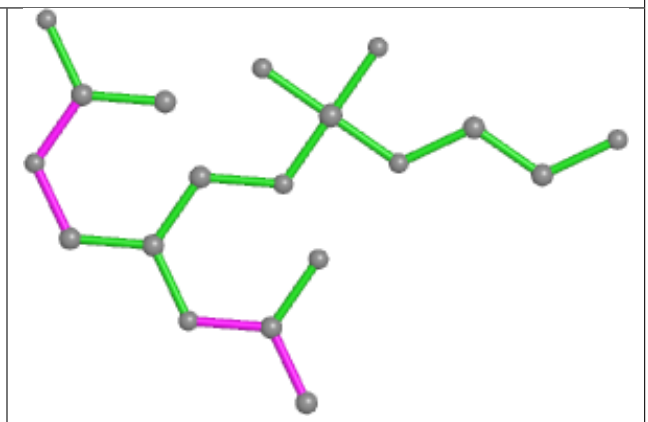

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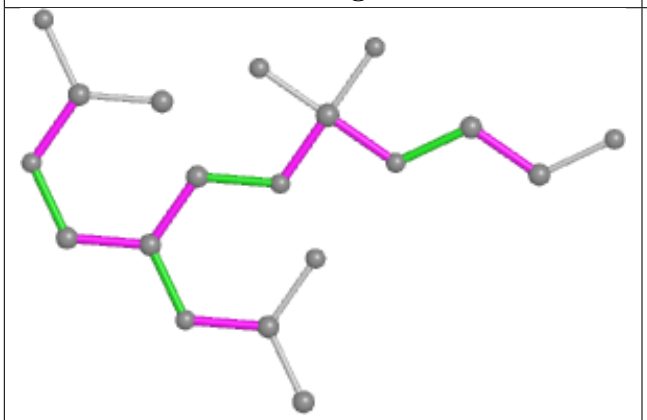

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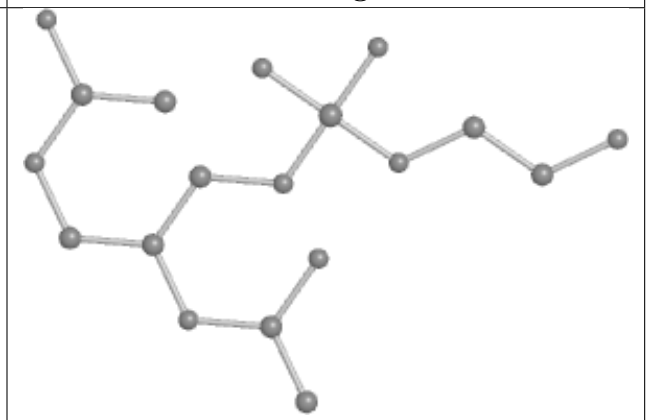
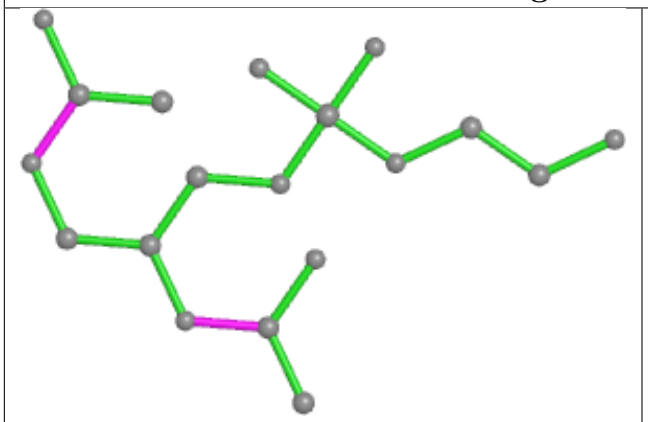


Rings

Ligand PEF x 306



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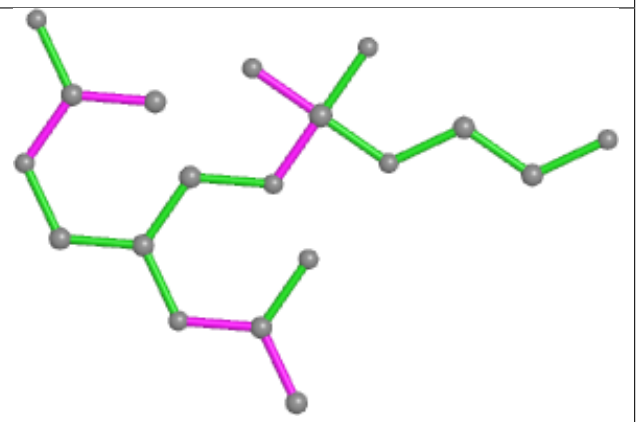

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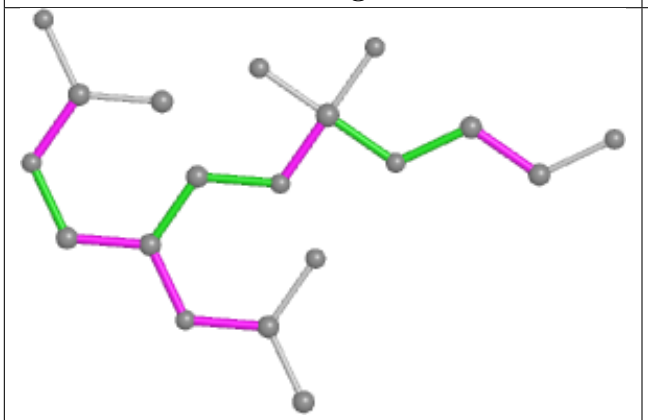

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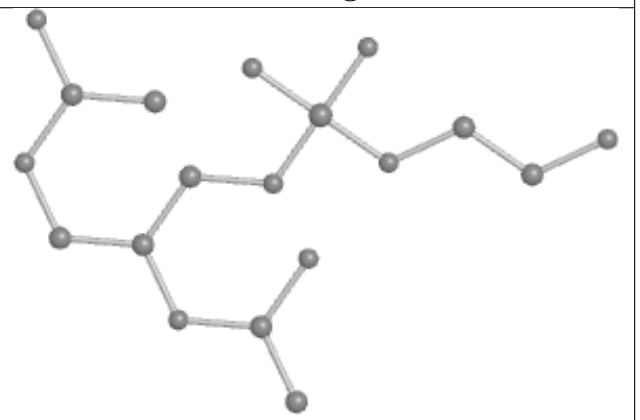
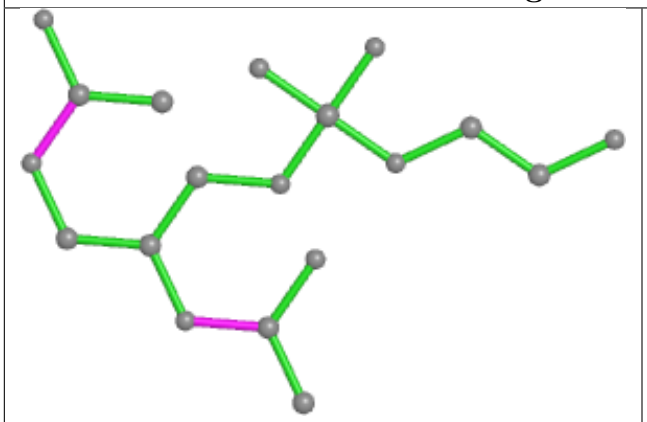


Rings

Ligand PEF m 101



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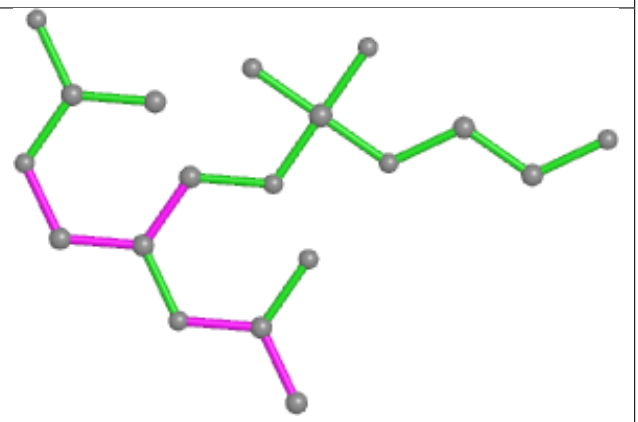

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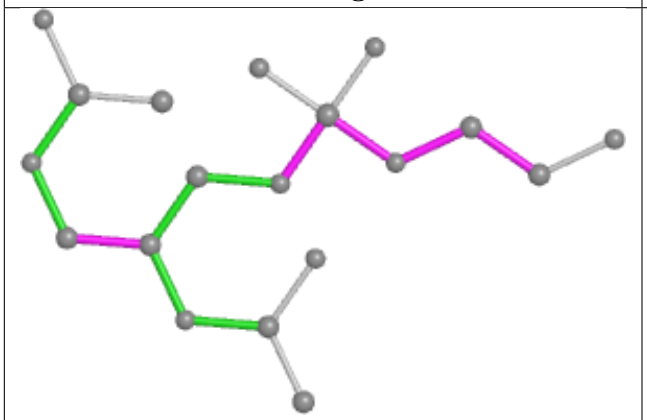

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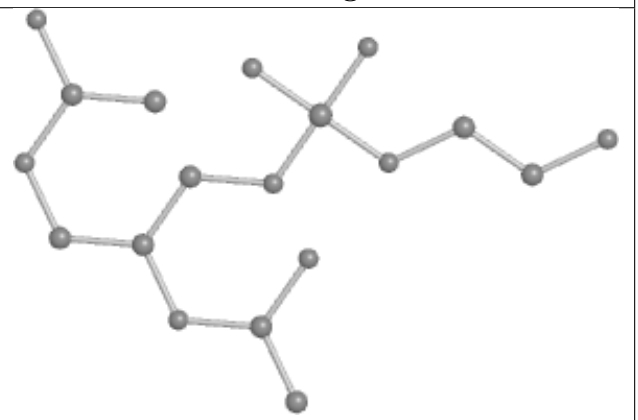
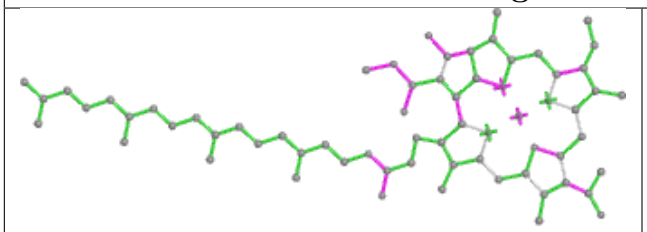


Rings

Ligand BCL AH 101



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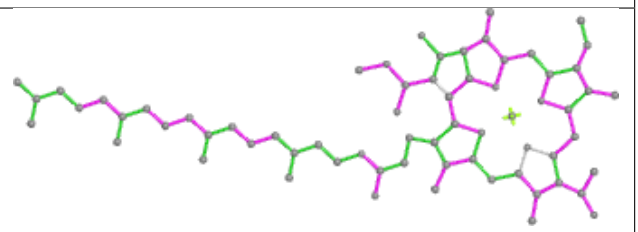

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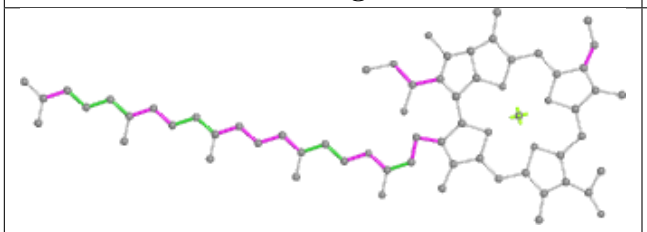

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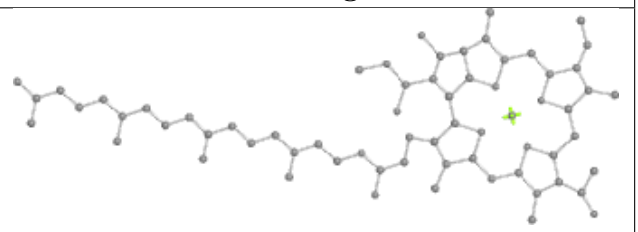

Rings

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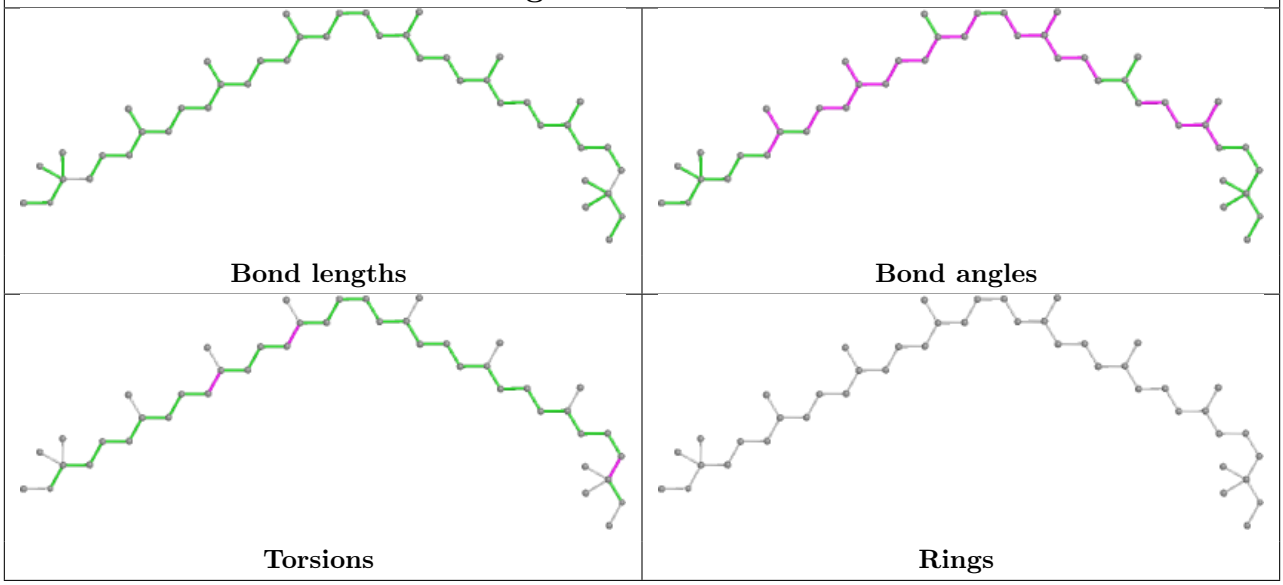
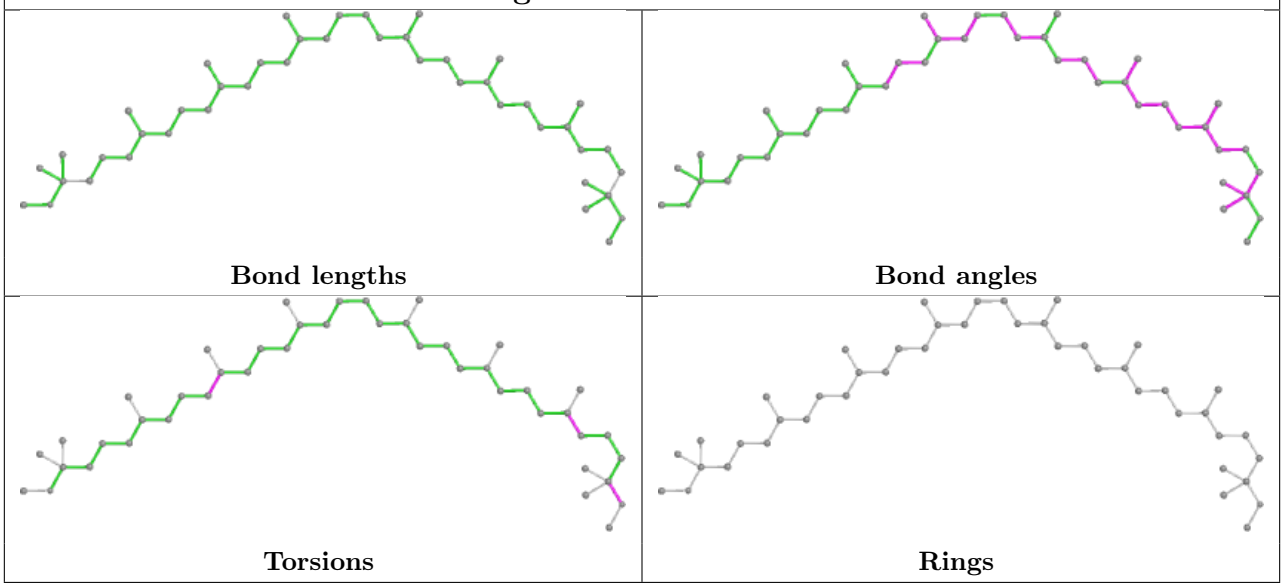


Ligand CRT AF 102



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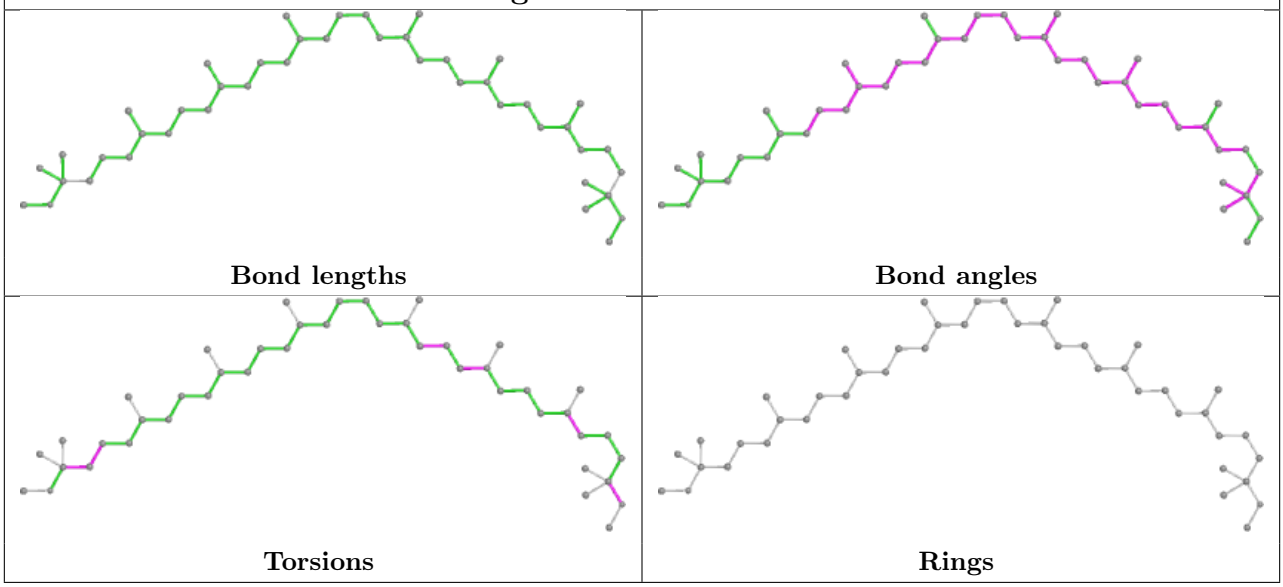
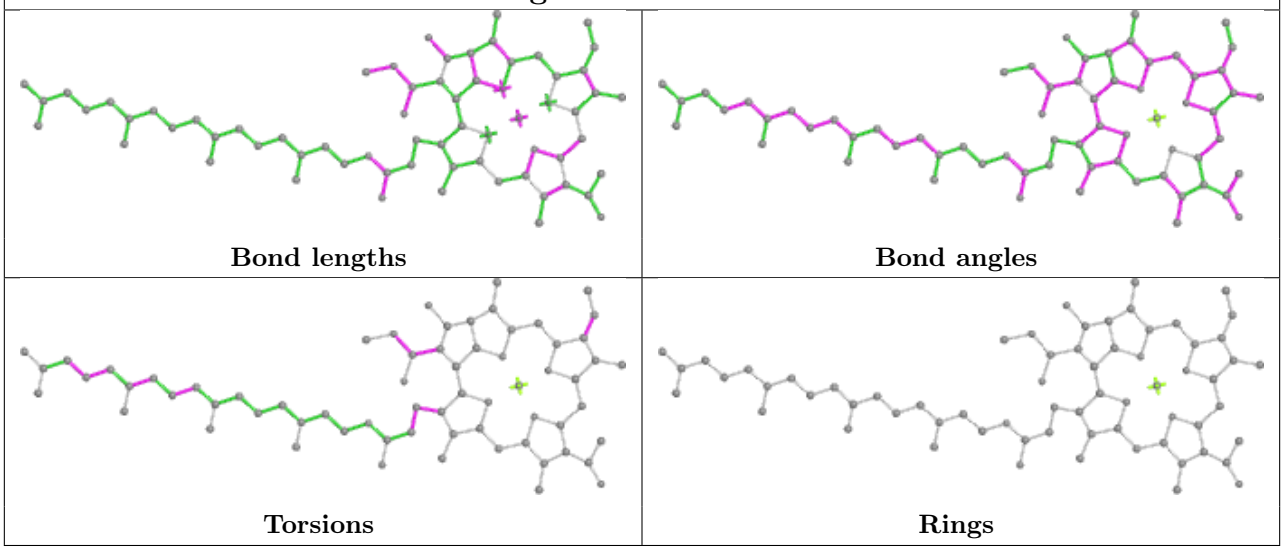


Ligand BCL x 305



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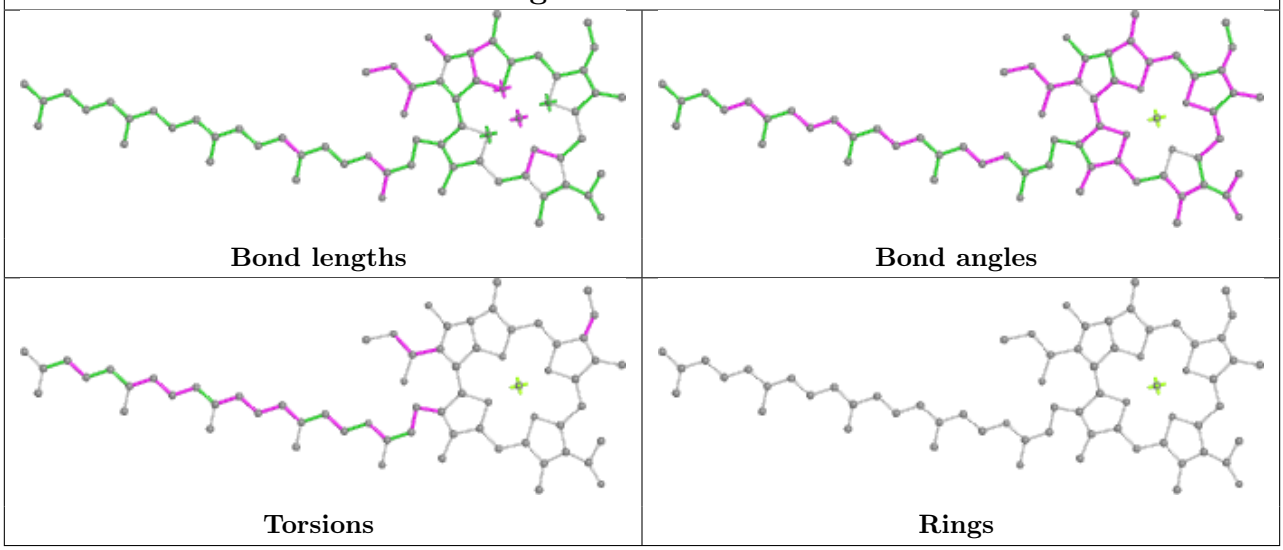

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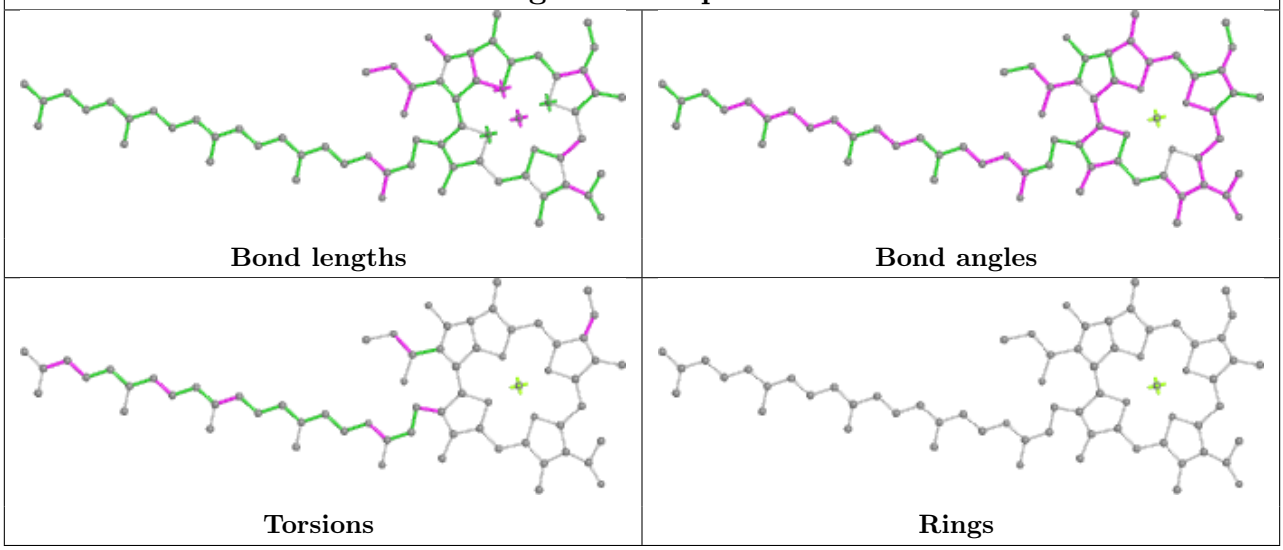

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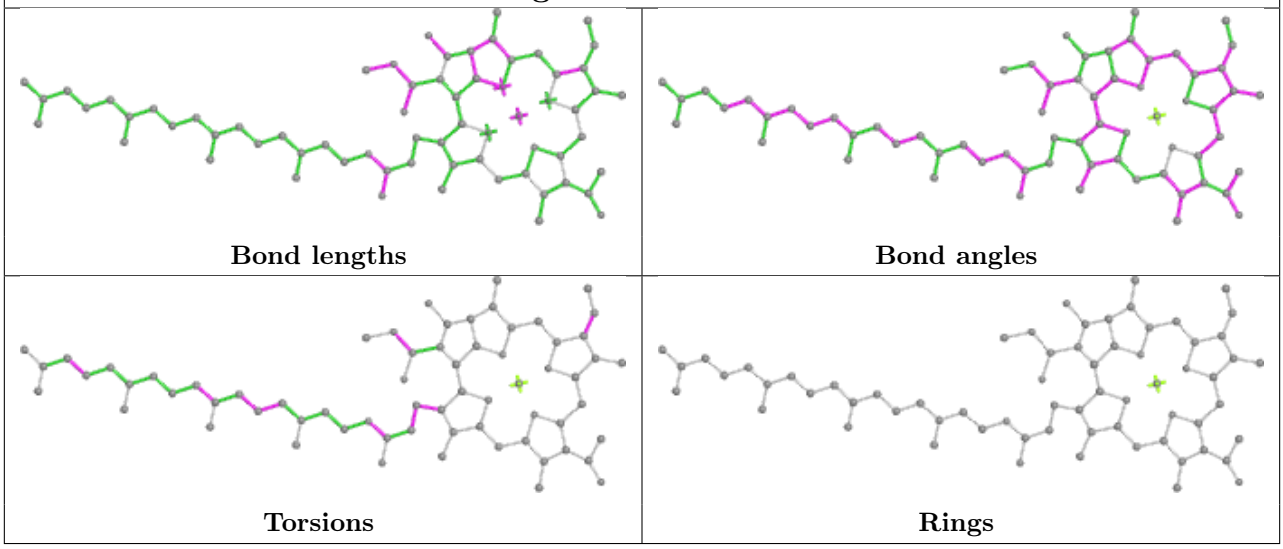

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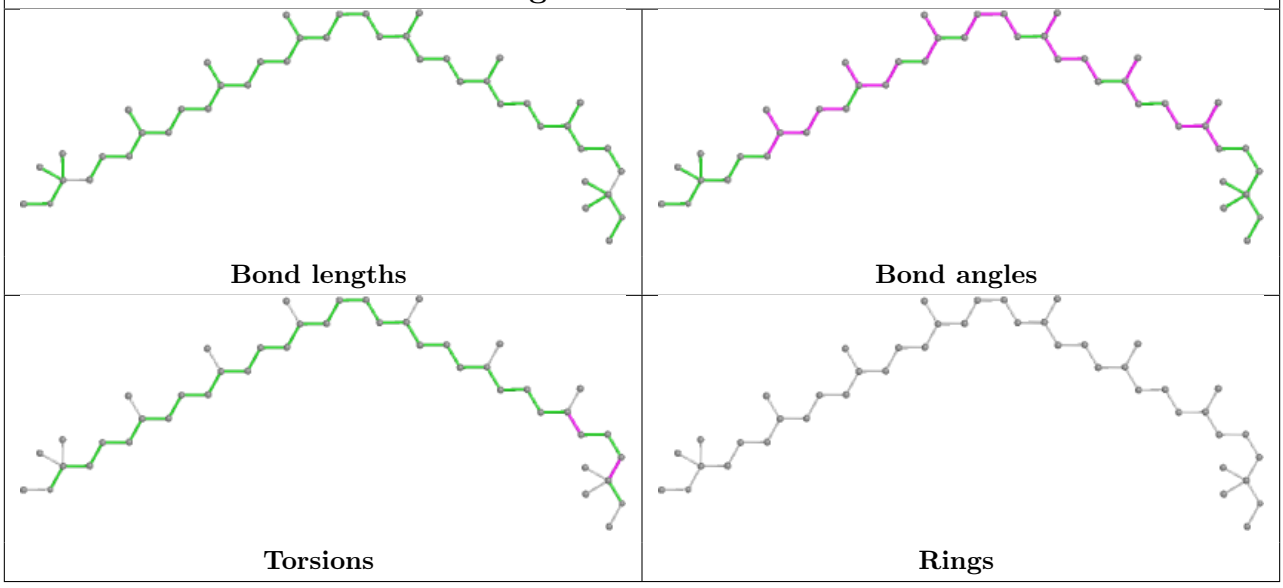

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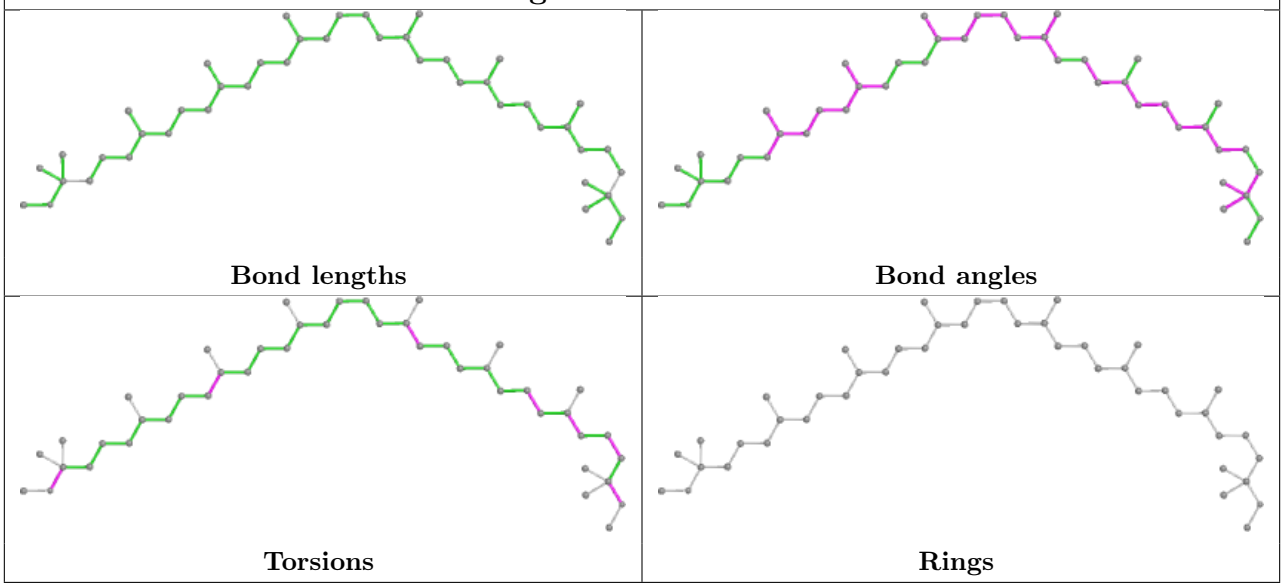

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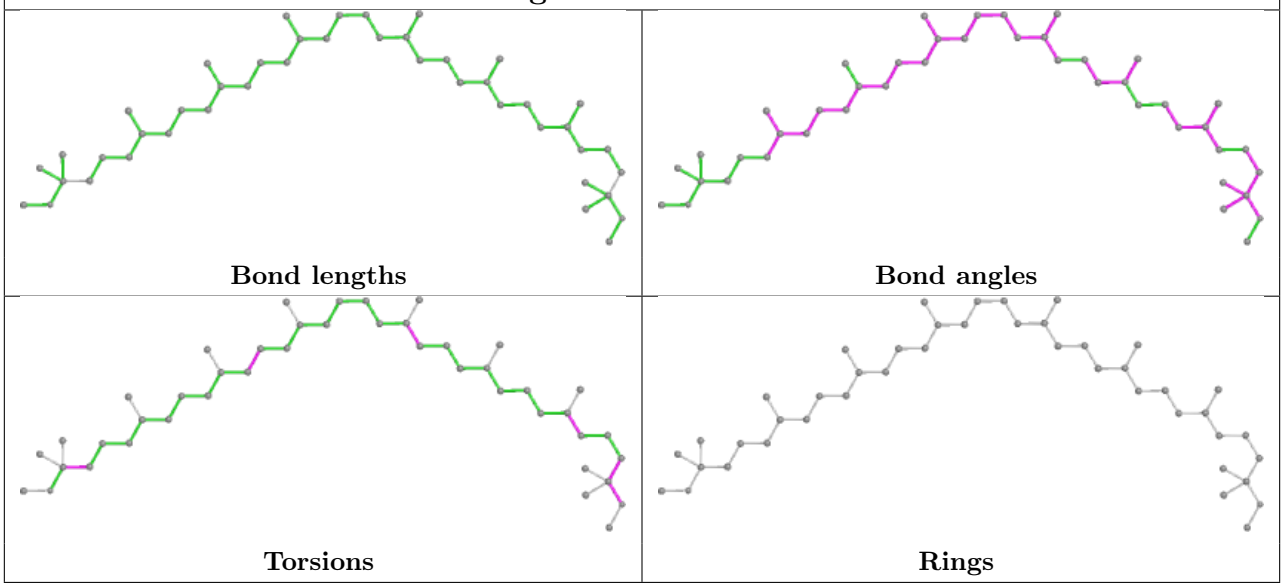

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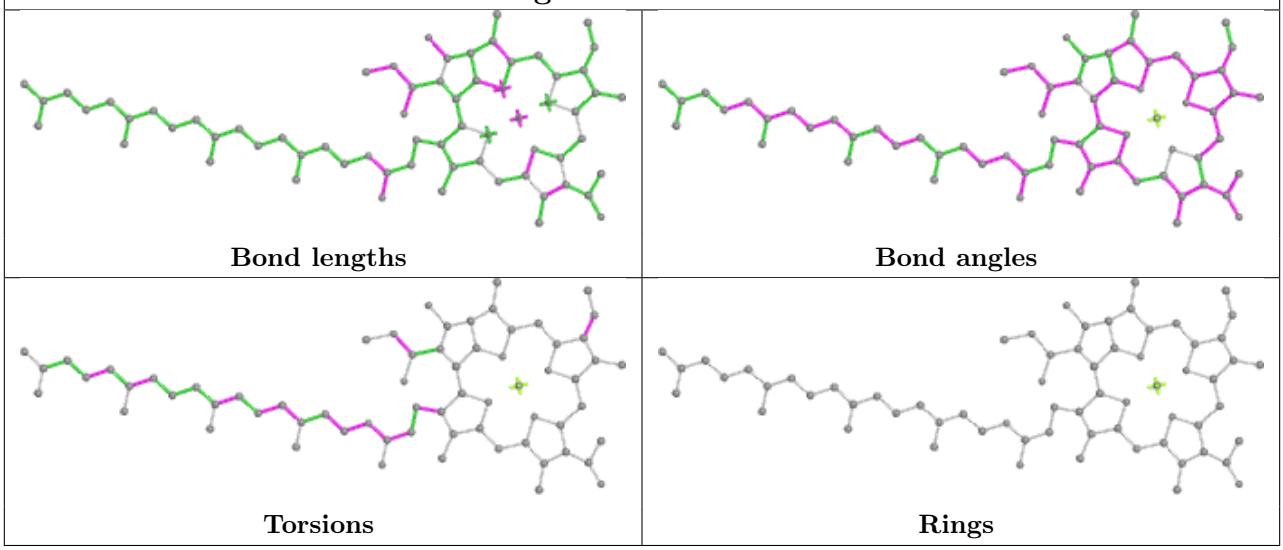

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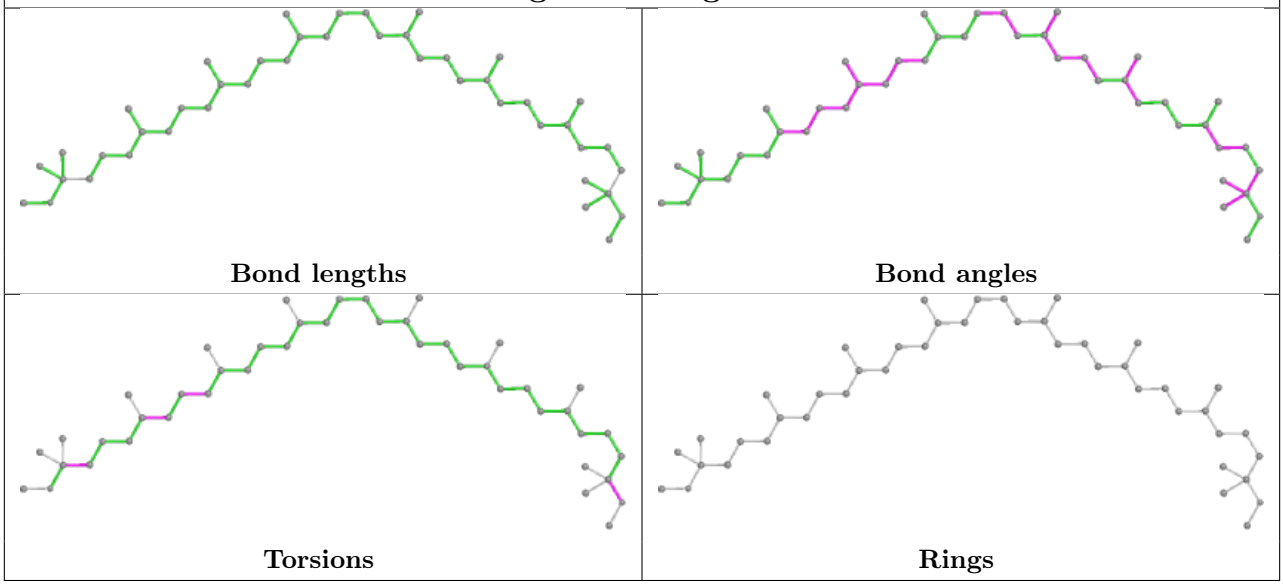
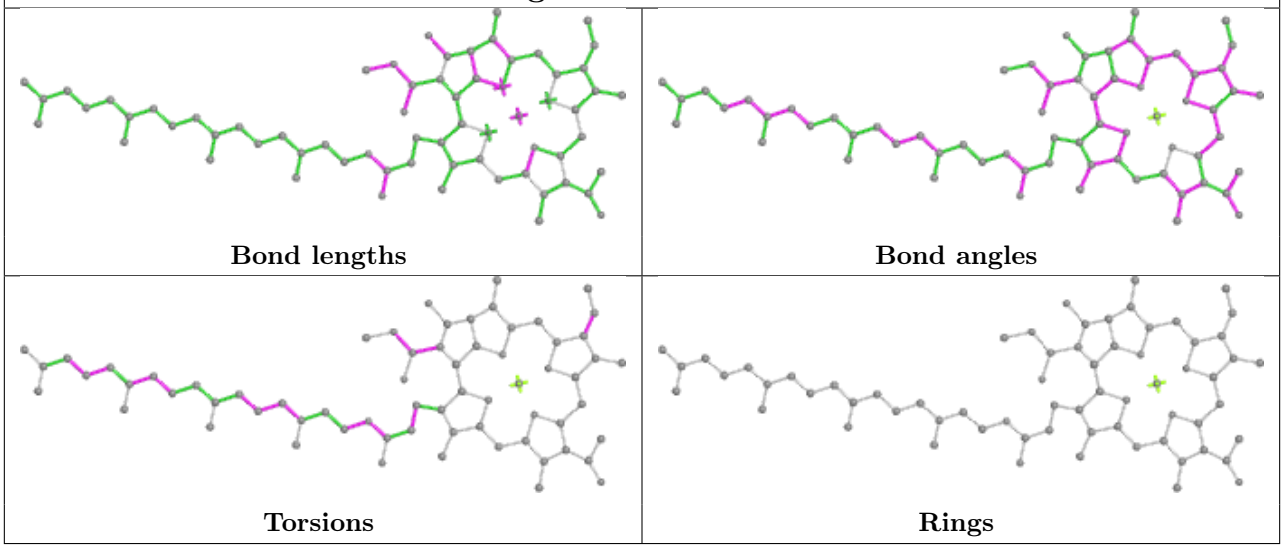
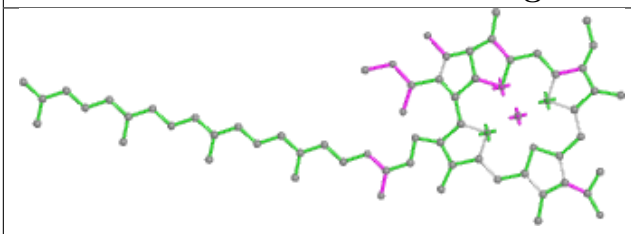
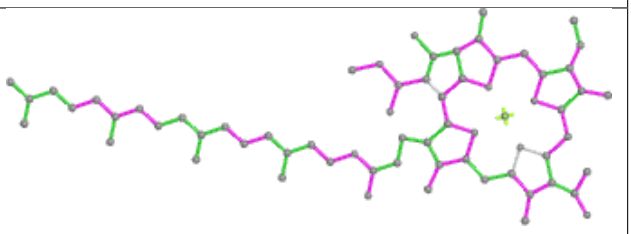
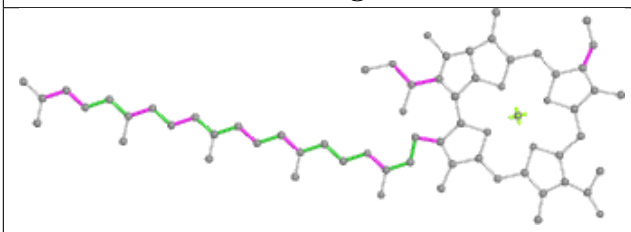
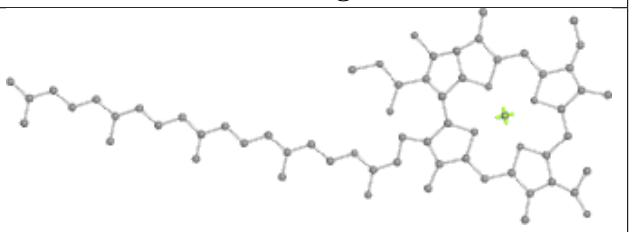
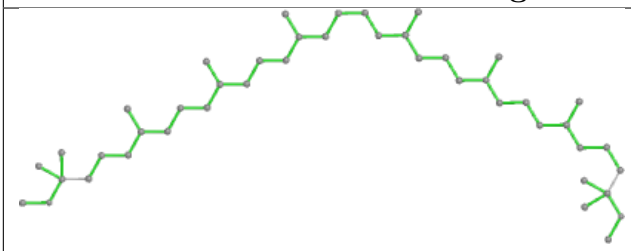
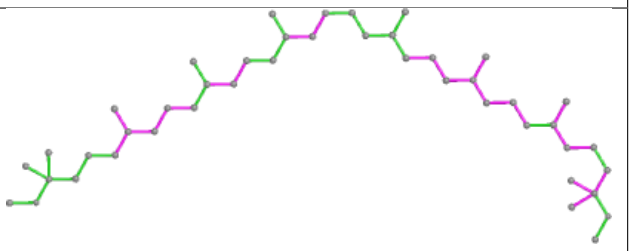
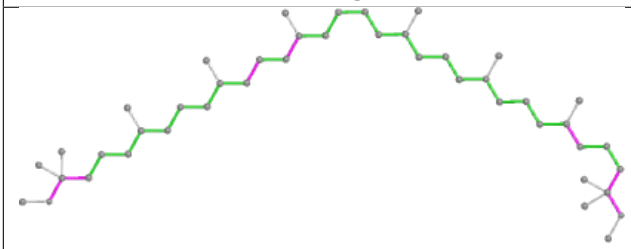
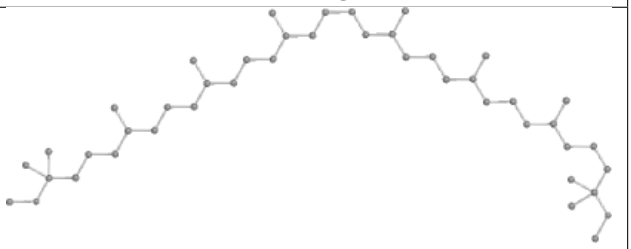


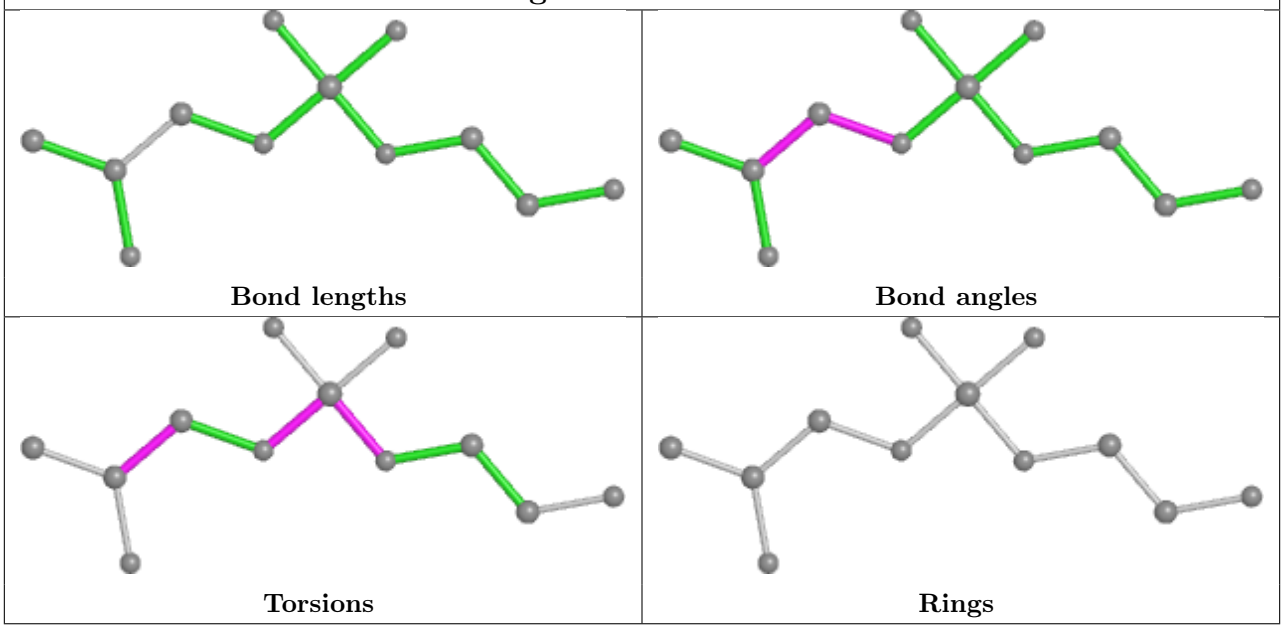
Ligand BCL F 101



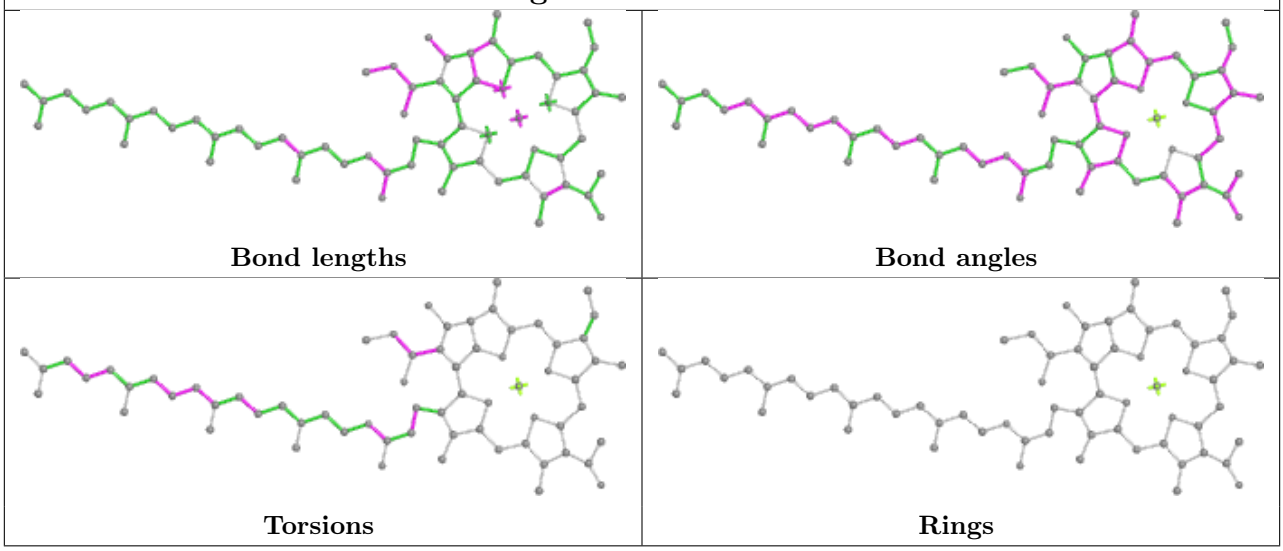
Ligand BCL G 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CRT AH 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF L 305



Ligand BCL 3 101



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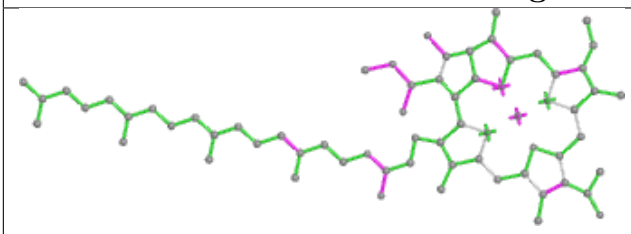
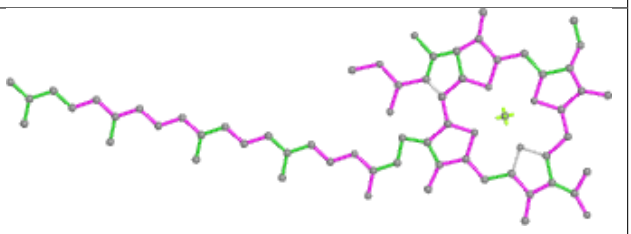
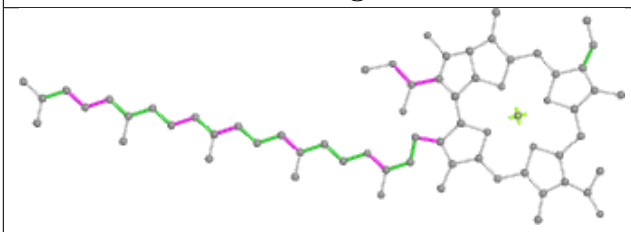
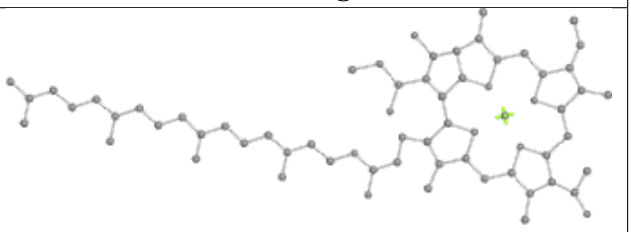
 Bond lengths	 Bond angles
 Torsions	 Rings

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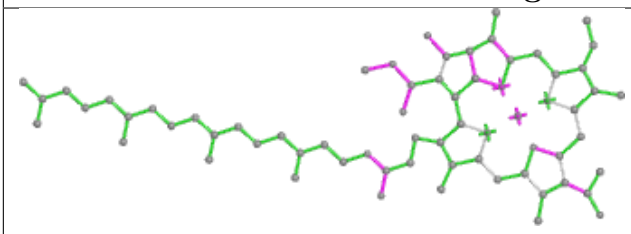
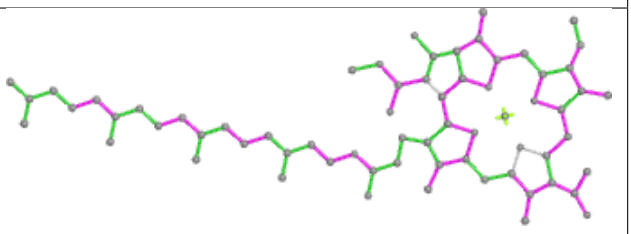
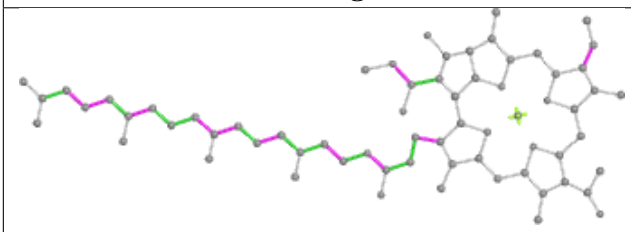
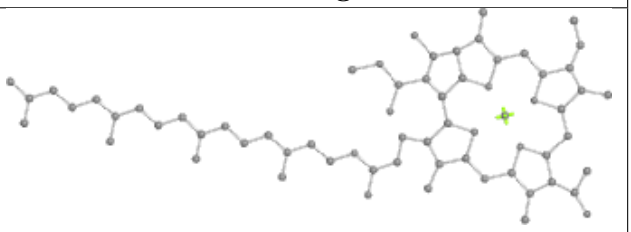
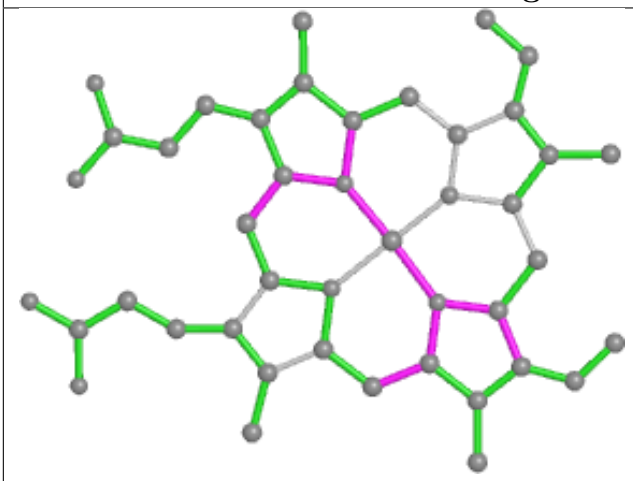
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM o 503



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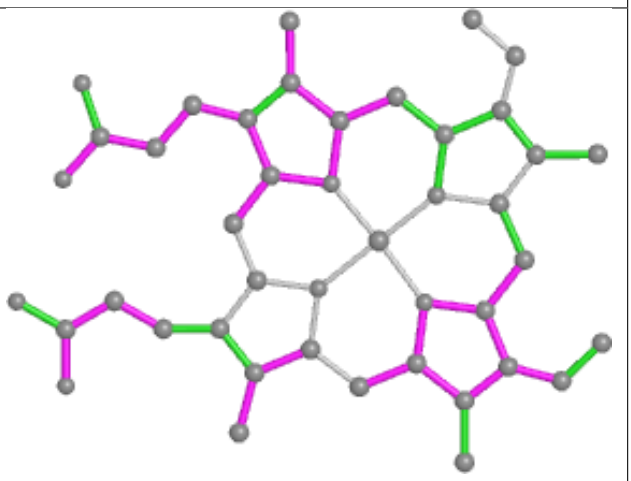

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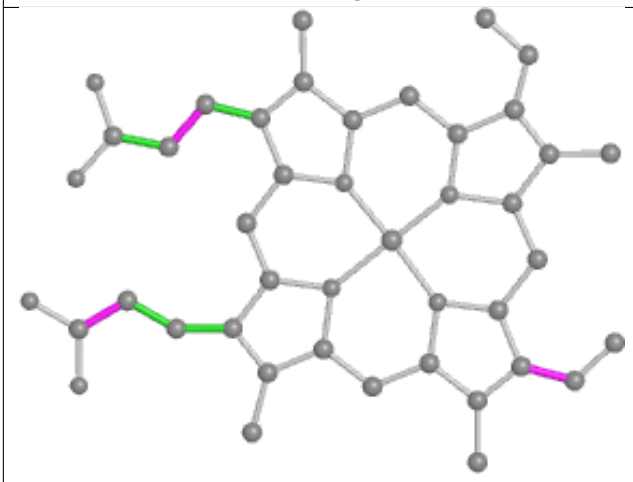

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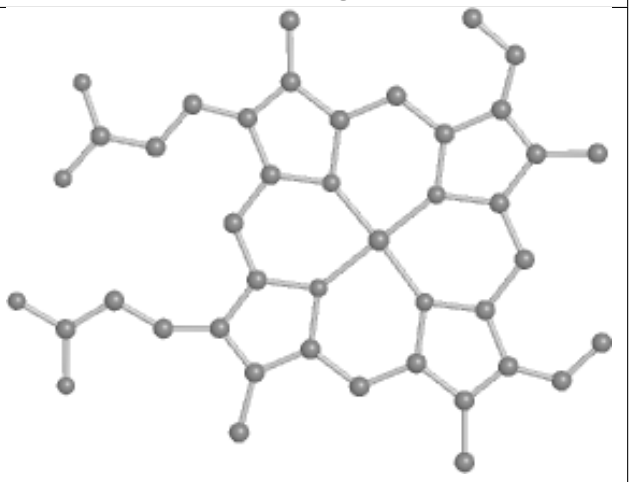
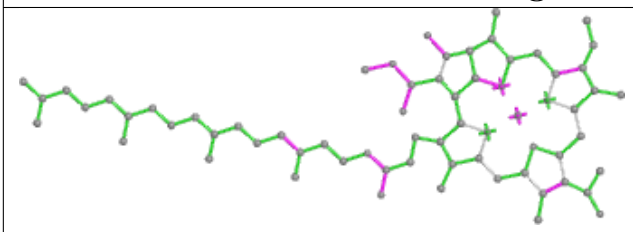


Rings

Ligand BCL u 101



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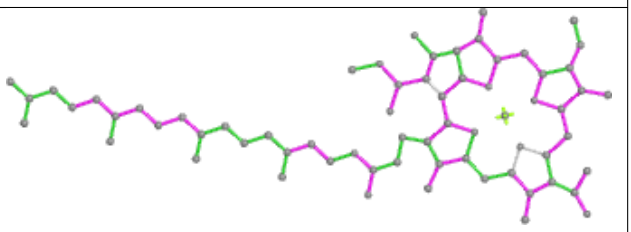

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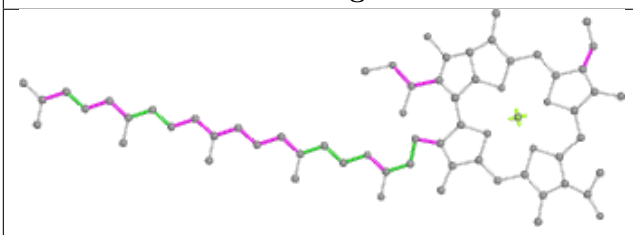

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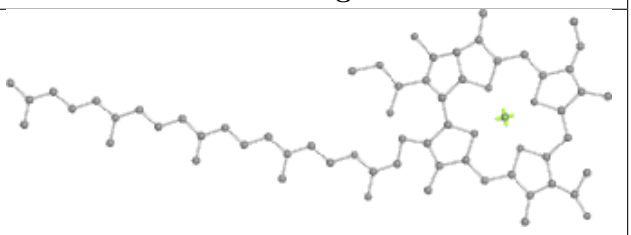
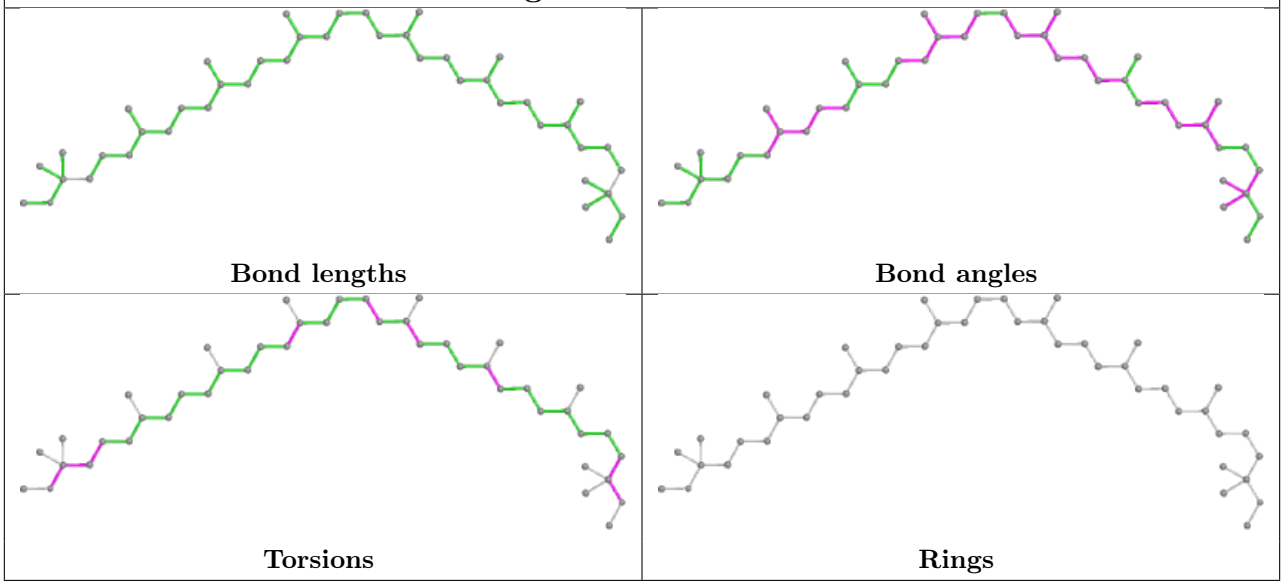


Rings

Ligand CRT V 101



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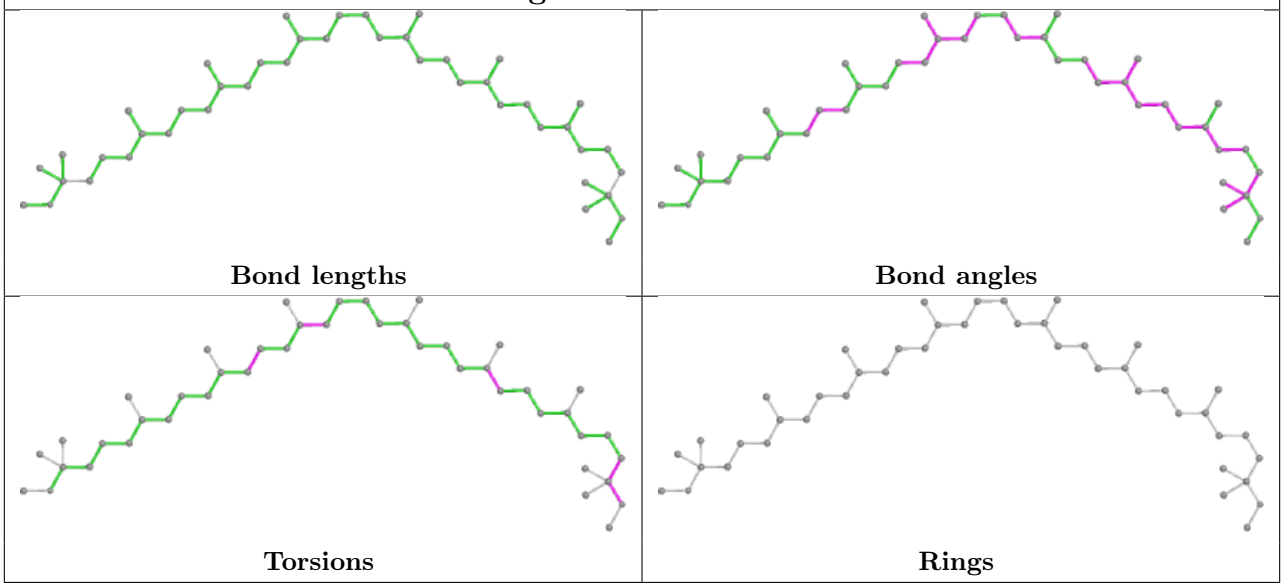

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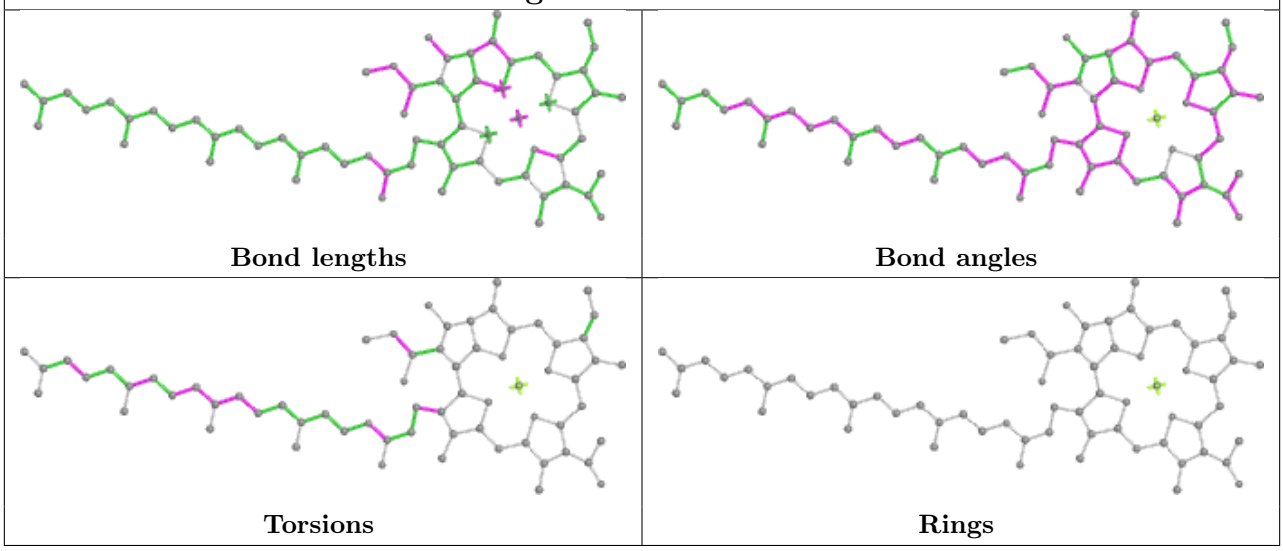

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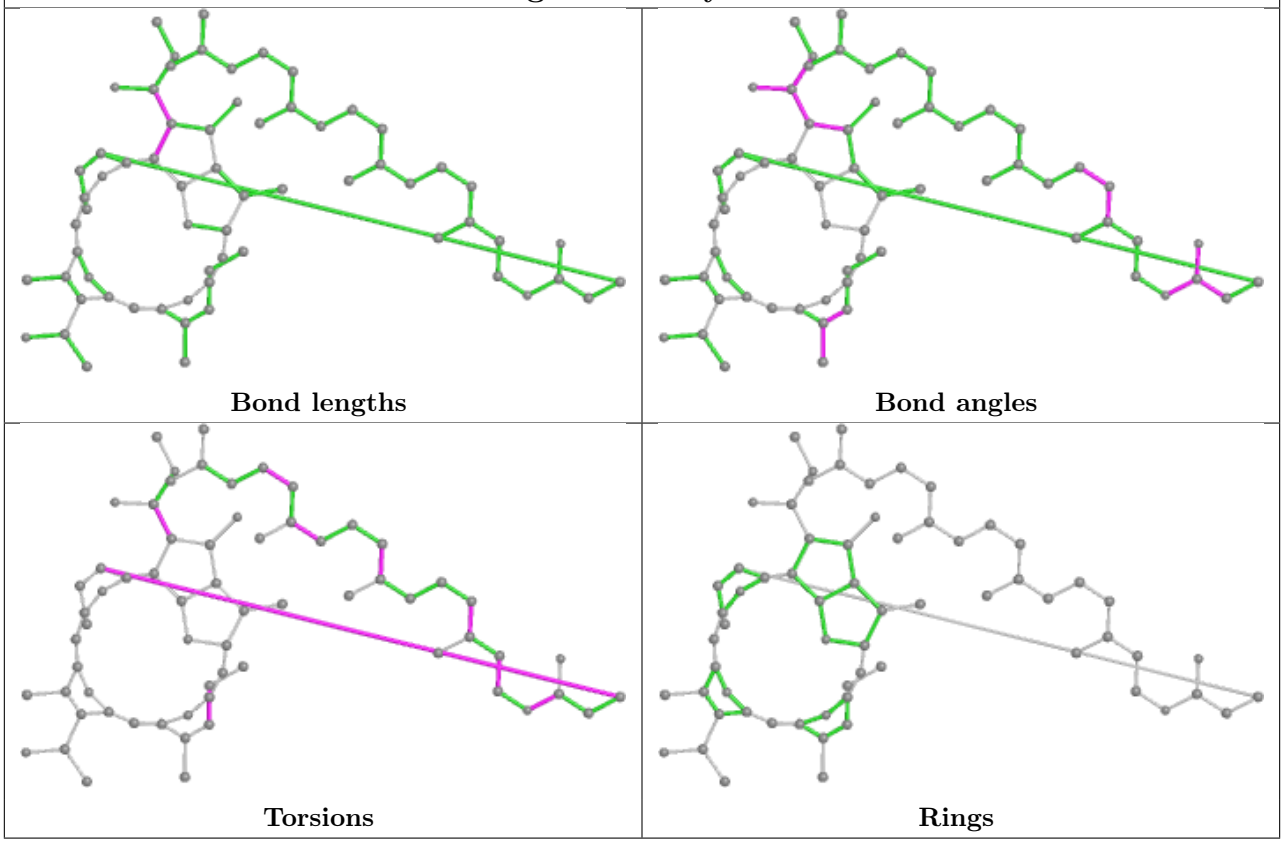

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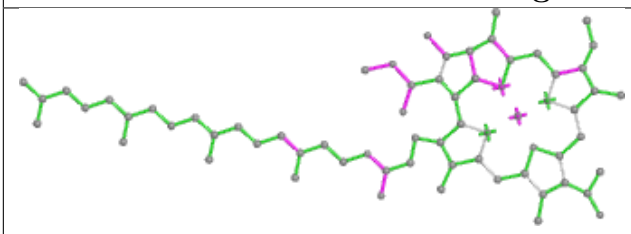
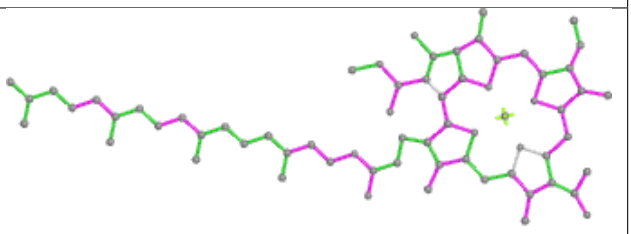
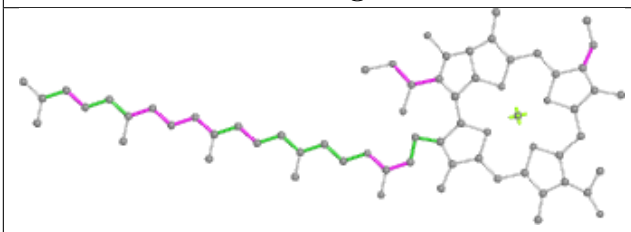
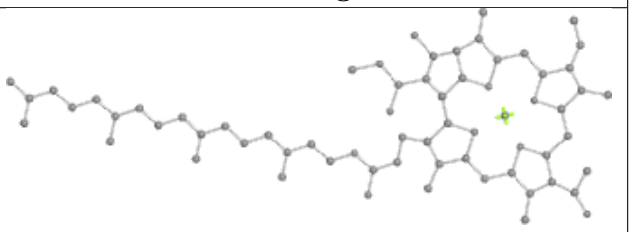
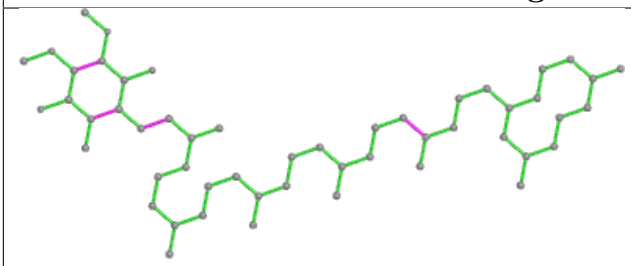
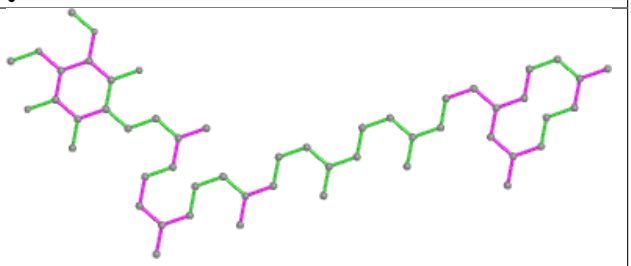
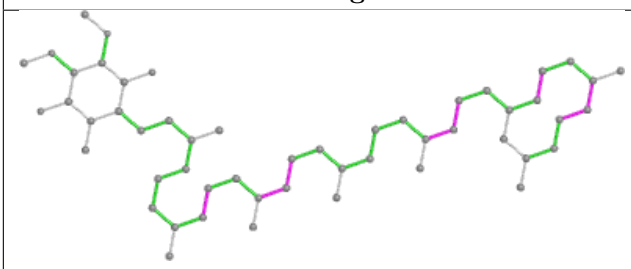
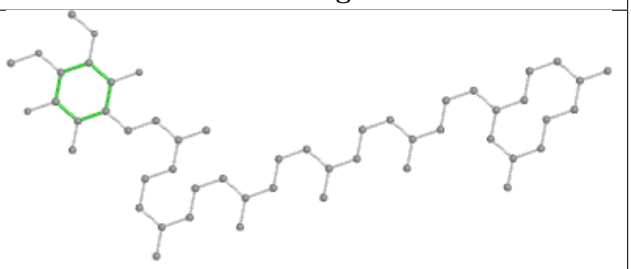
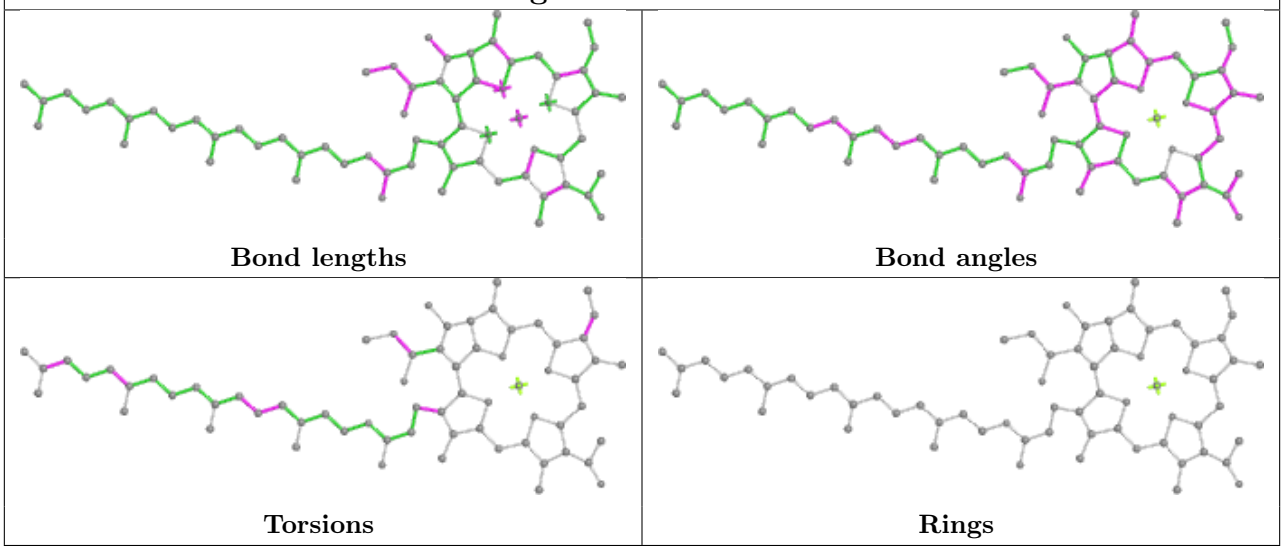
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 L 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 9 102



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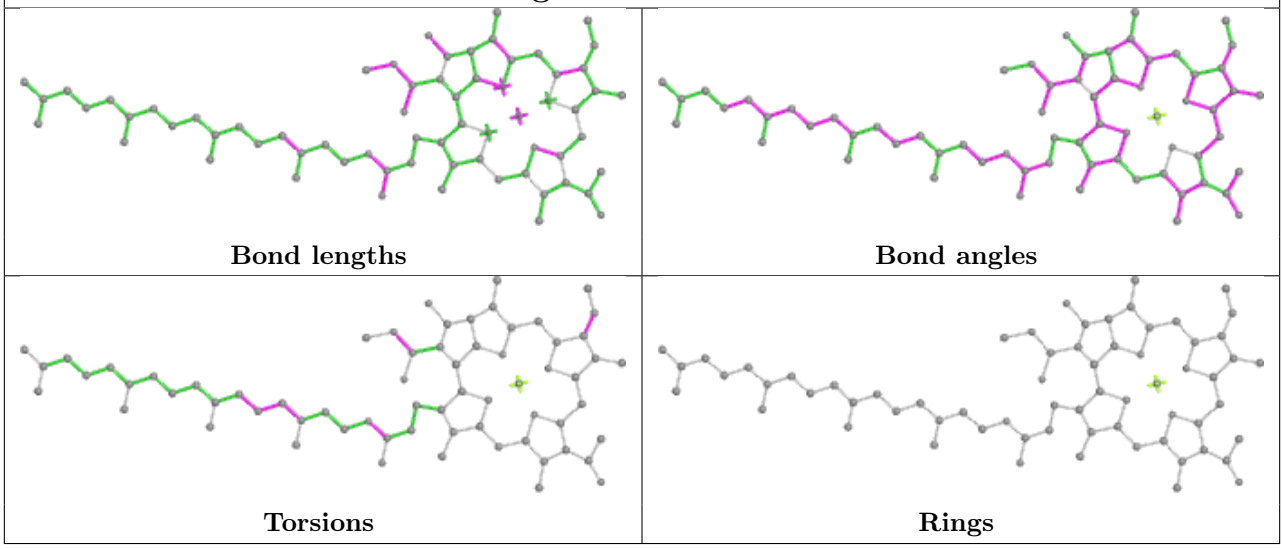

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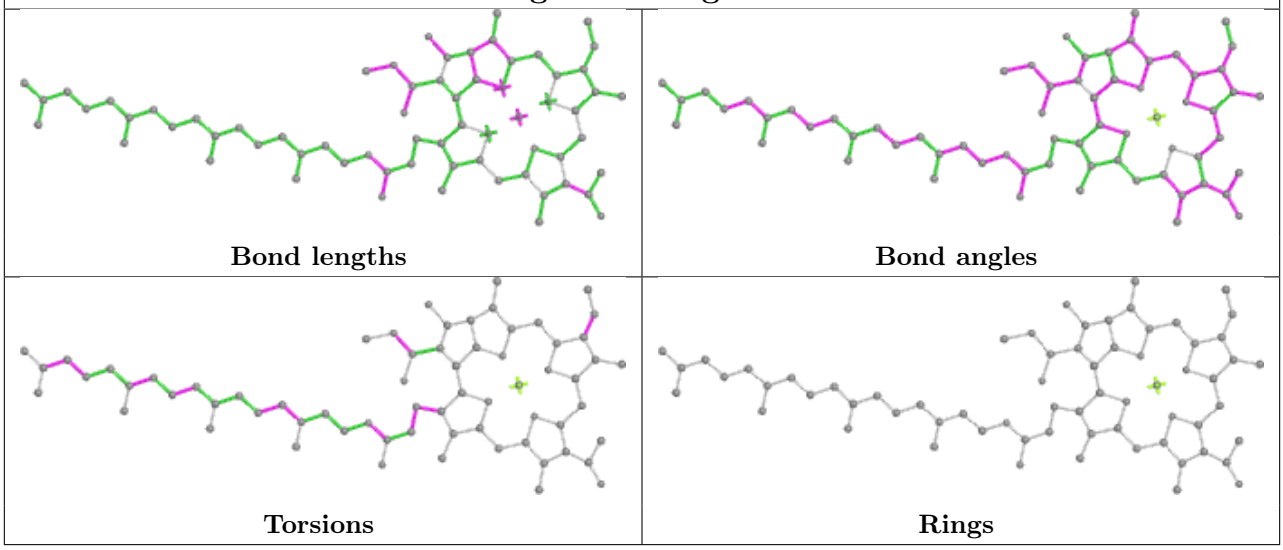
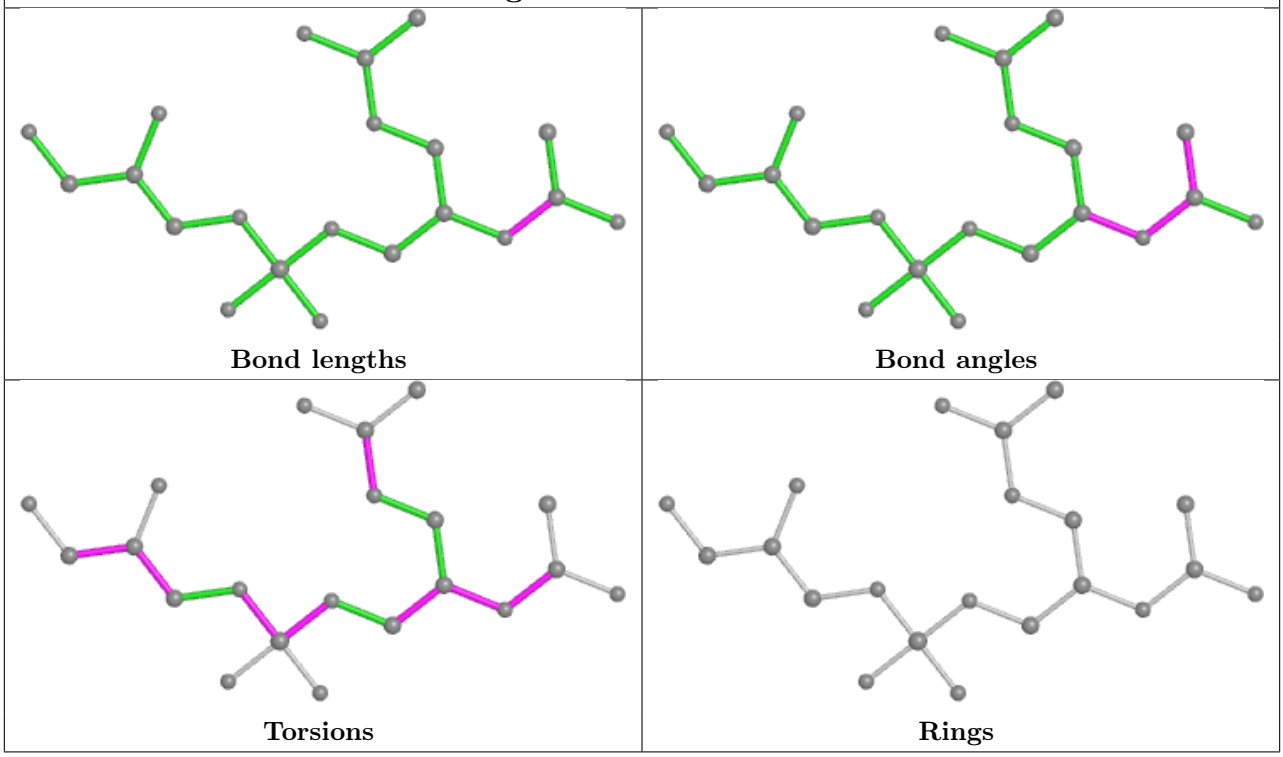


Ligand PGW AE 101



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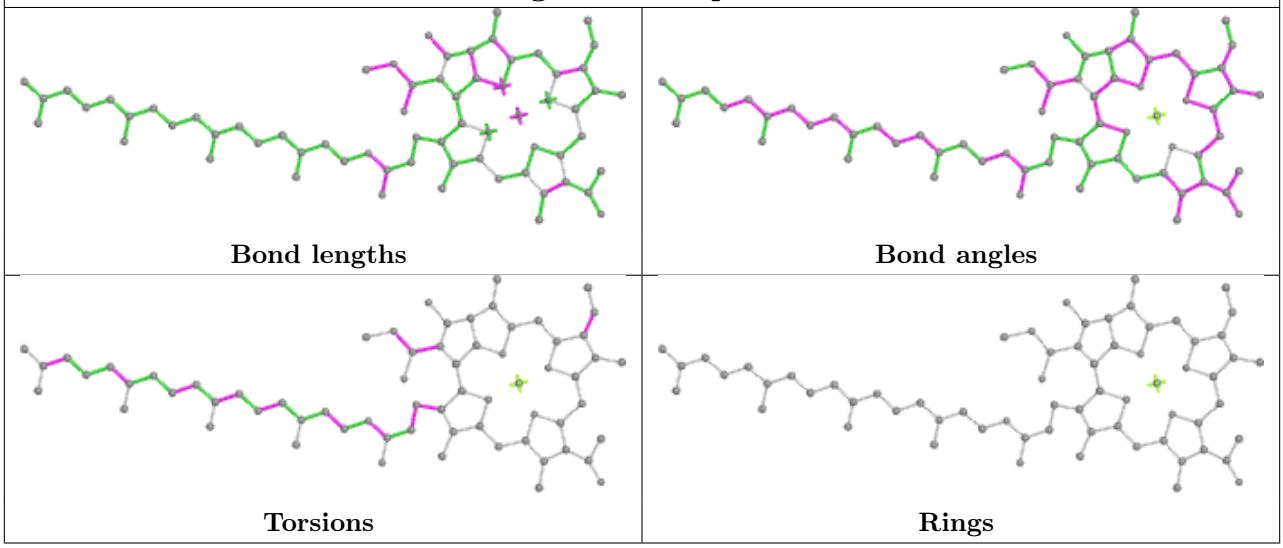

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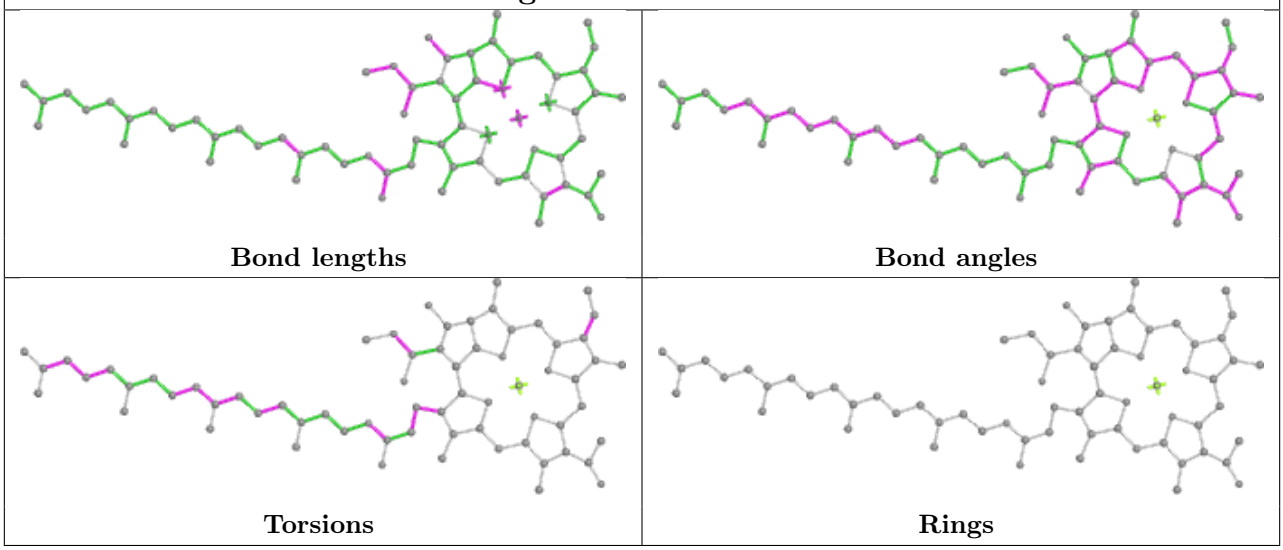

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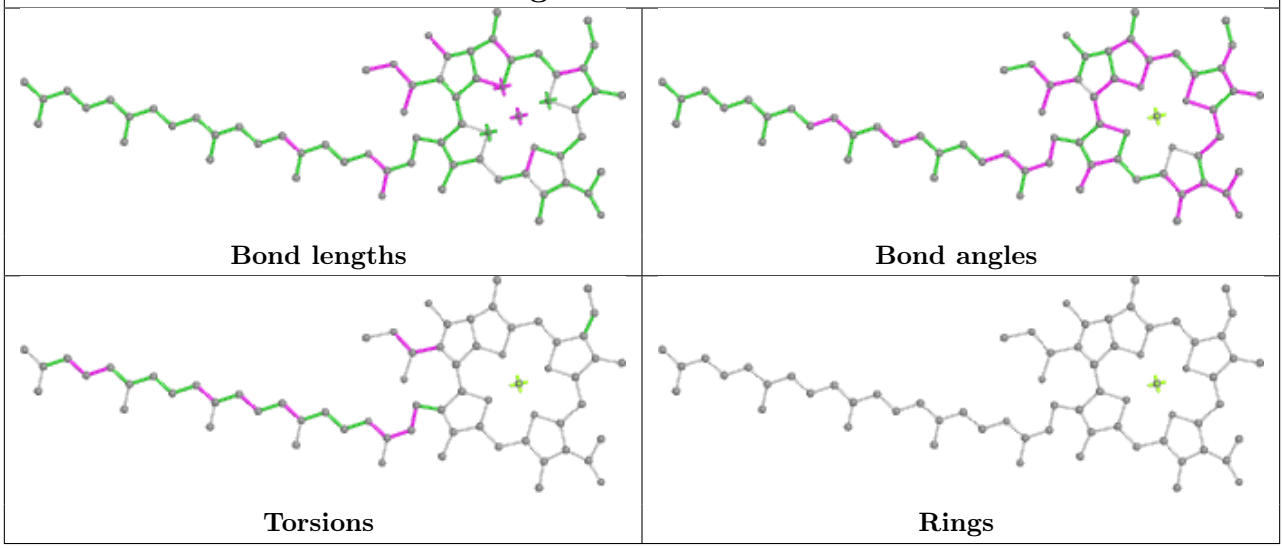

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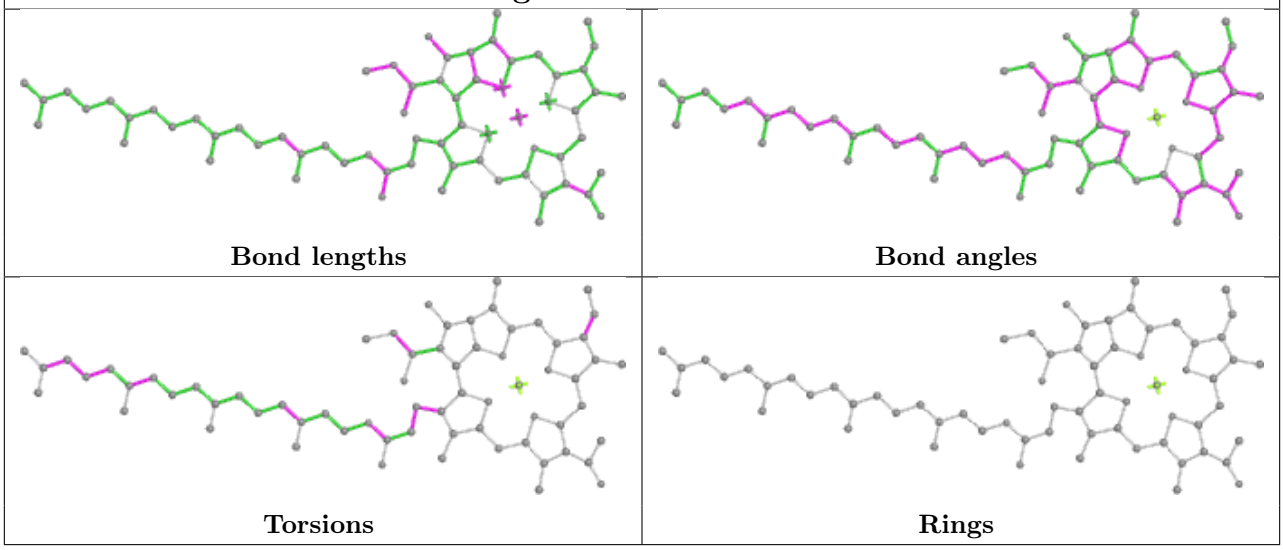

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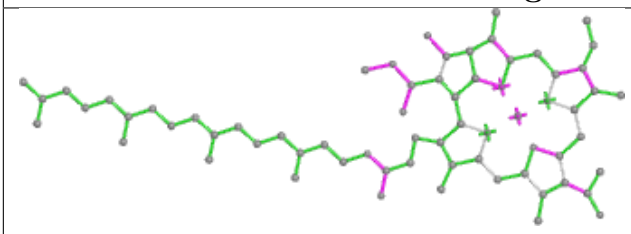
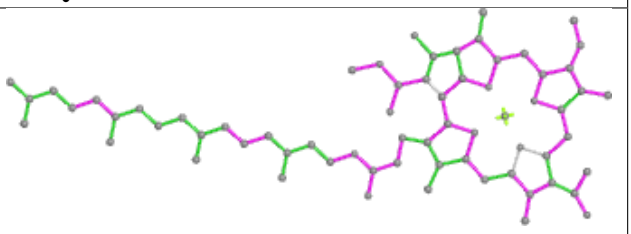
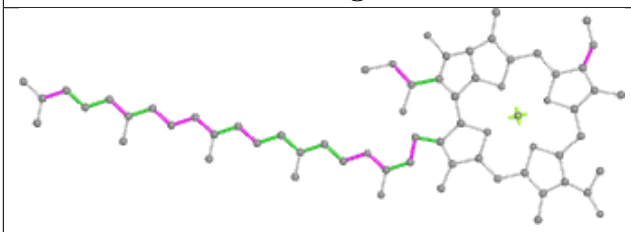
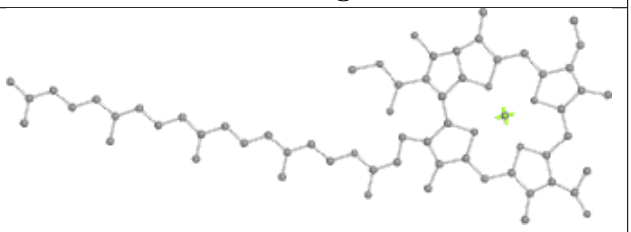
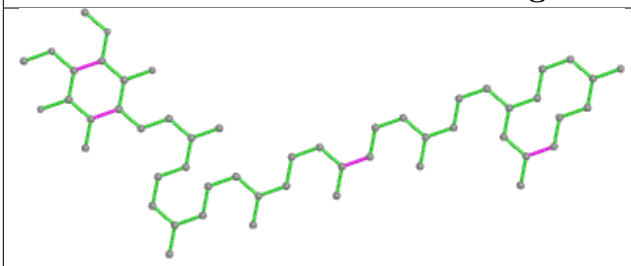
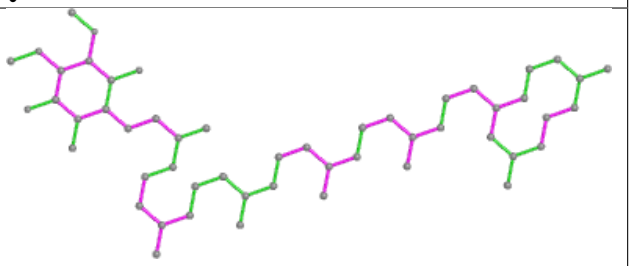
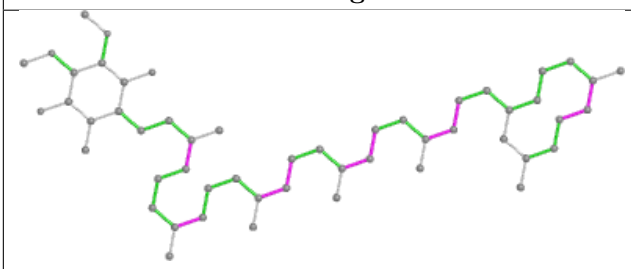
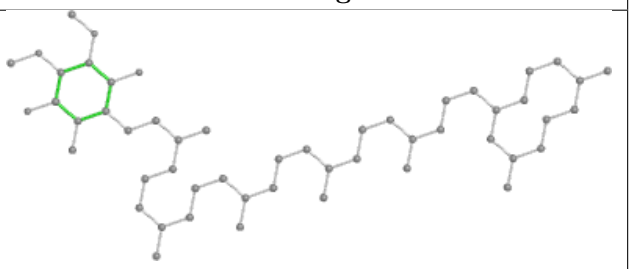
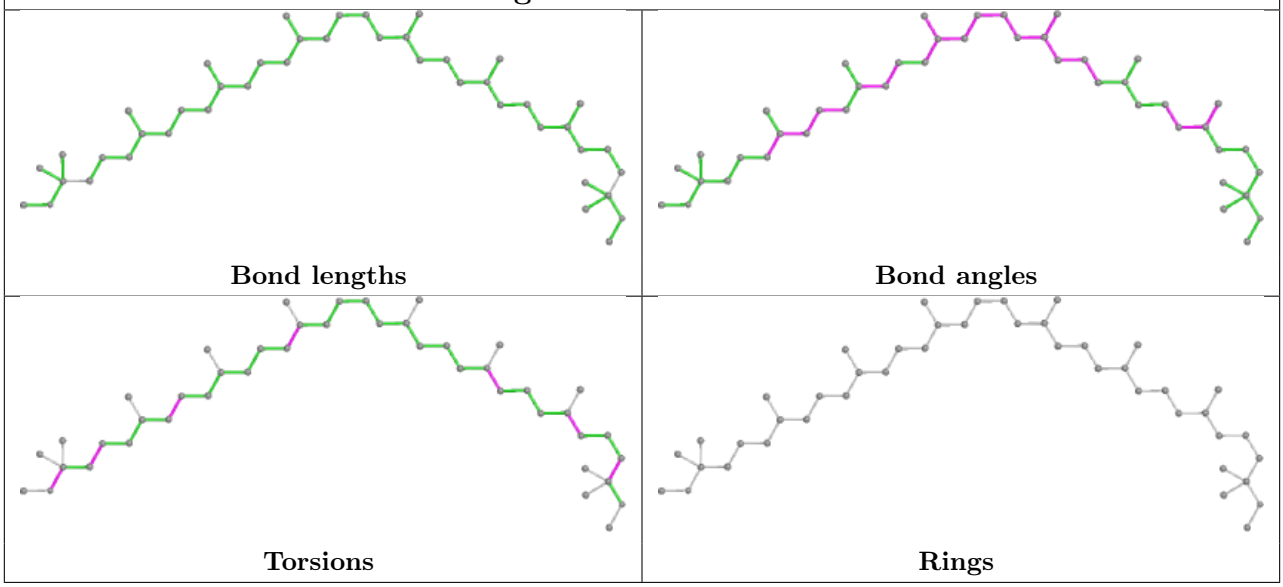
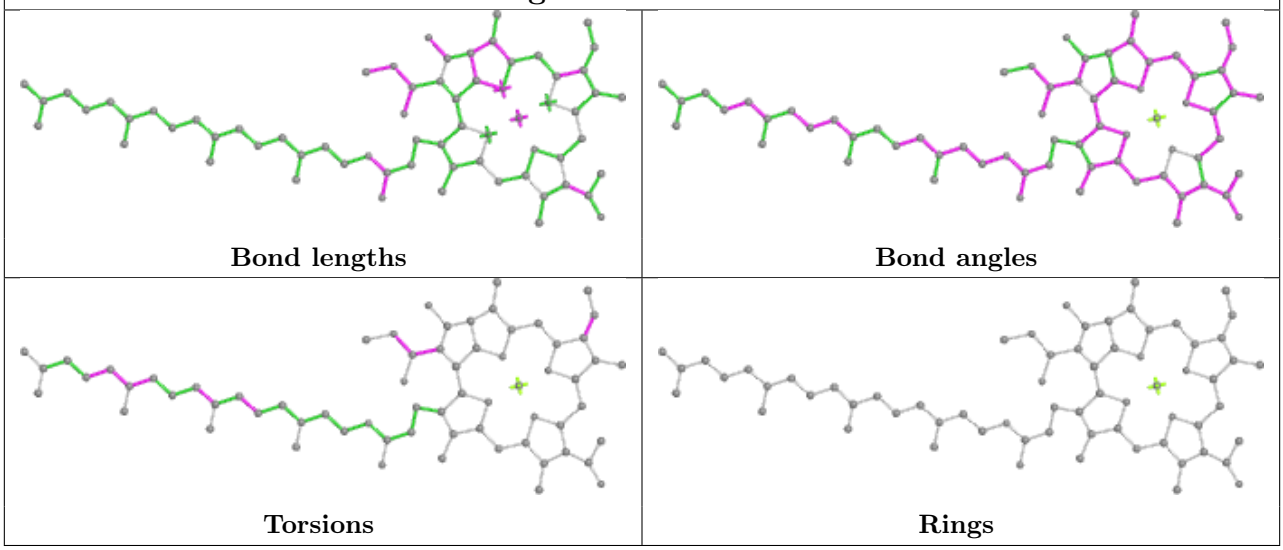
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 x 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

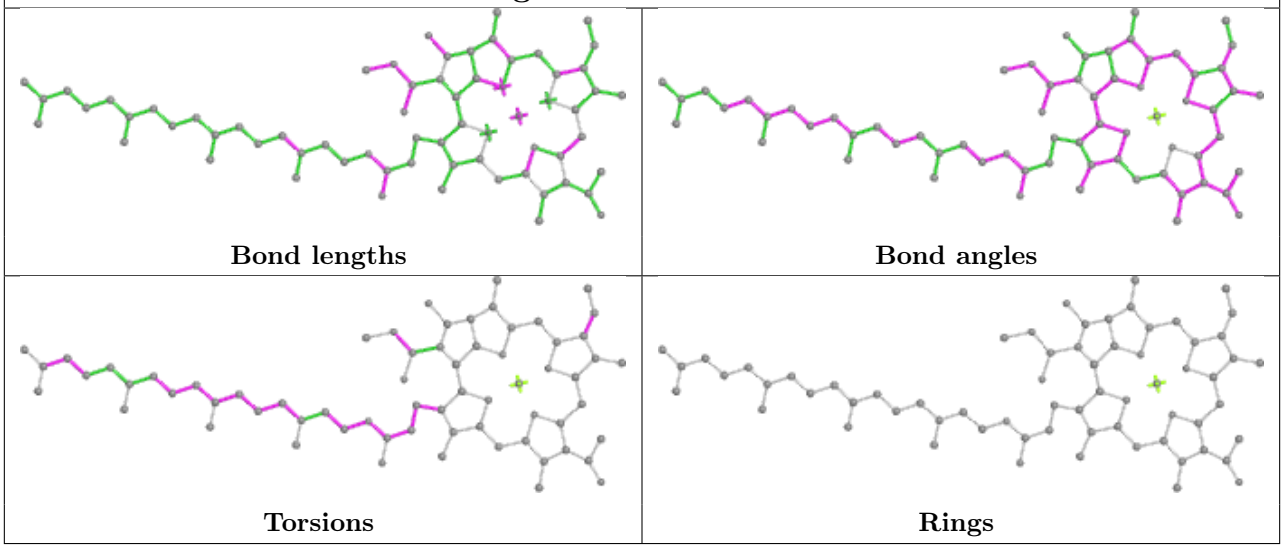
Ligand CRT AL 101



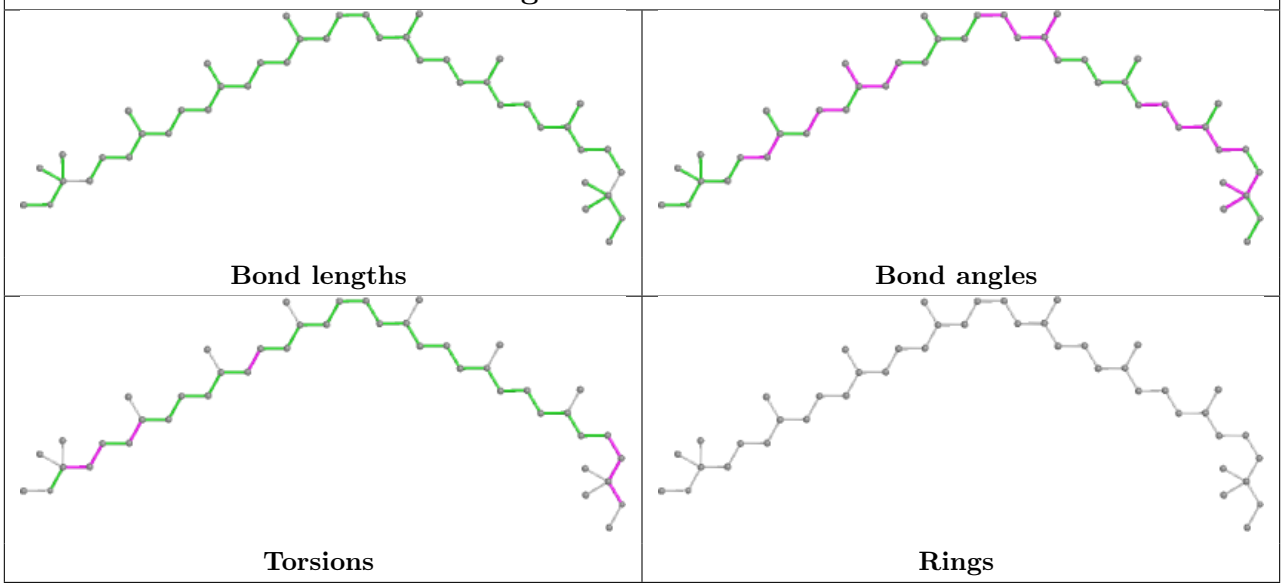
Ligand BCL L 301



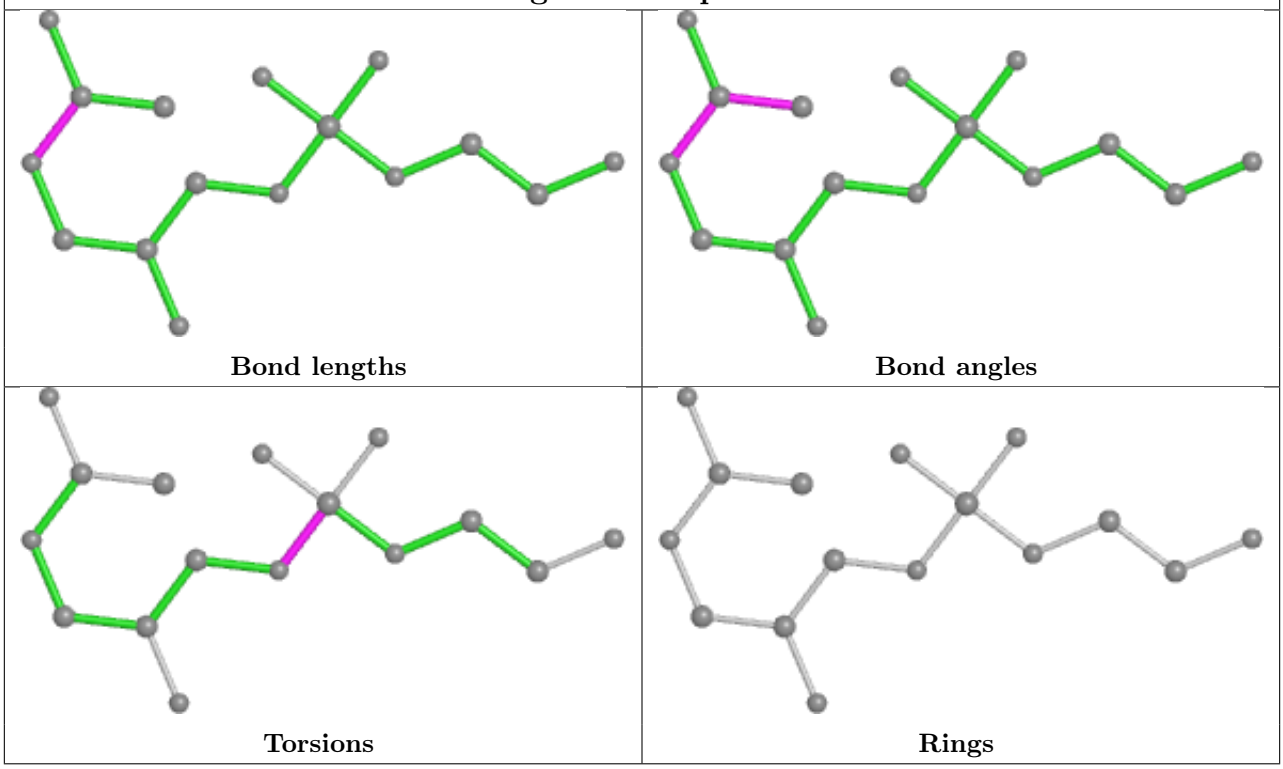
Ligand BCL AC 102



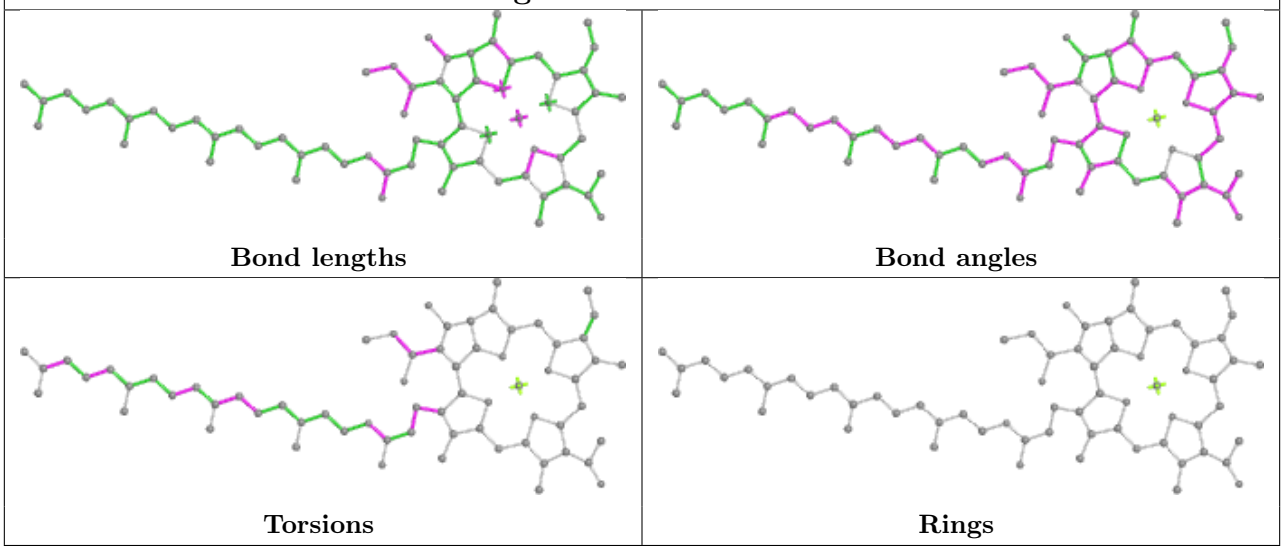
Ligand CRT M 405



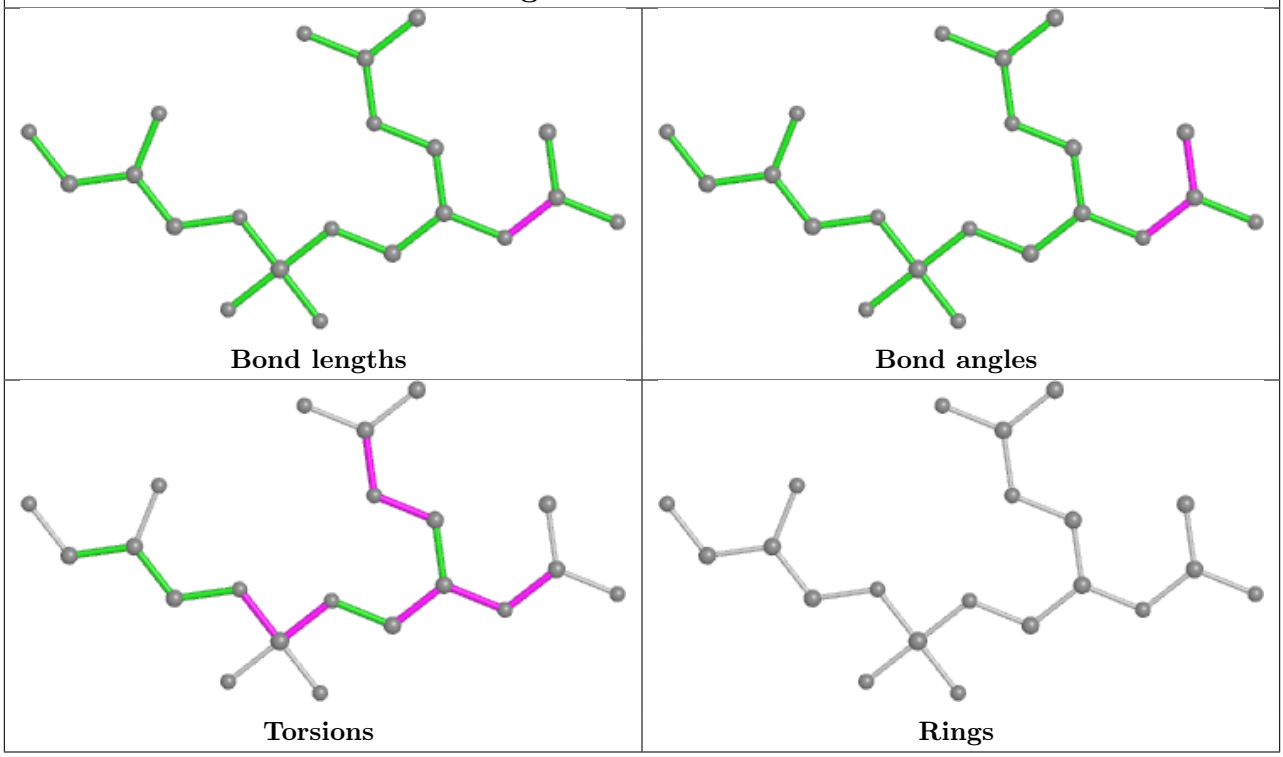
Ligand PEF p 101



Ligand BCL AE 102



Ligand PGW S 101



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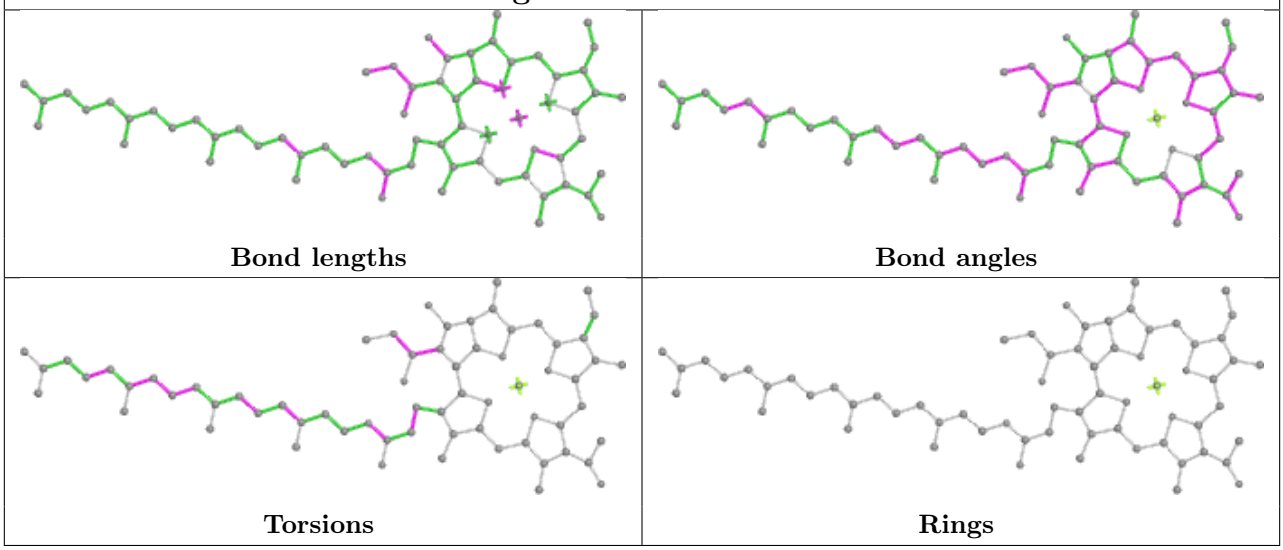

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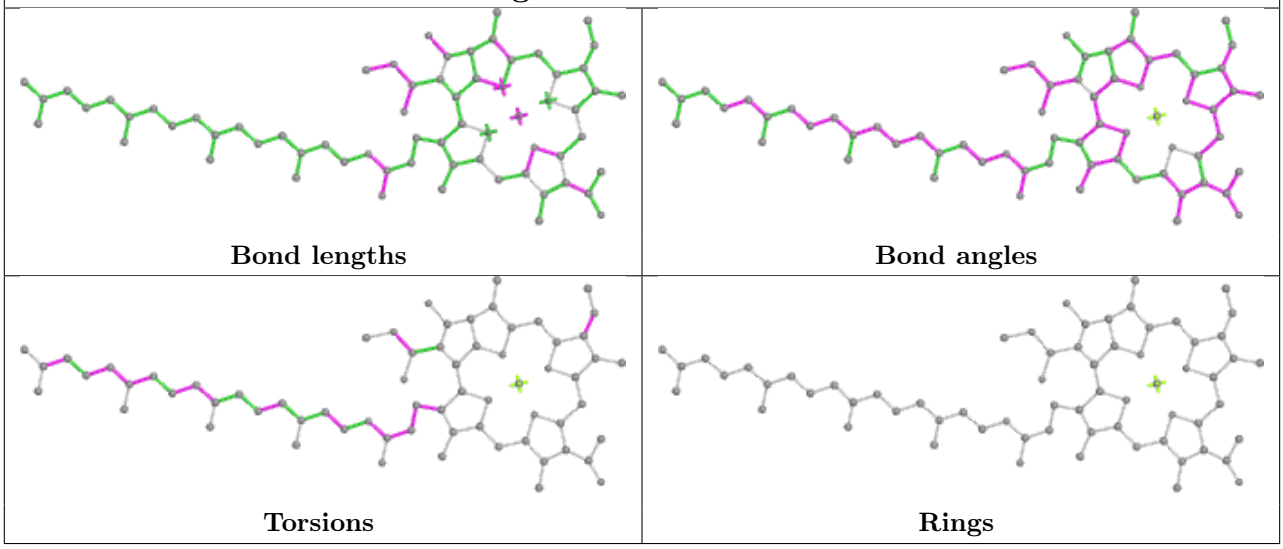

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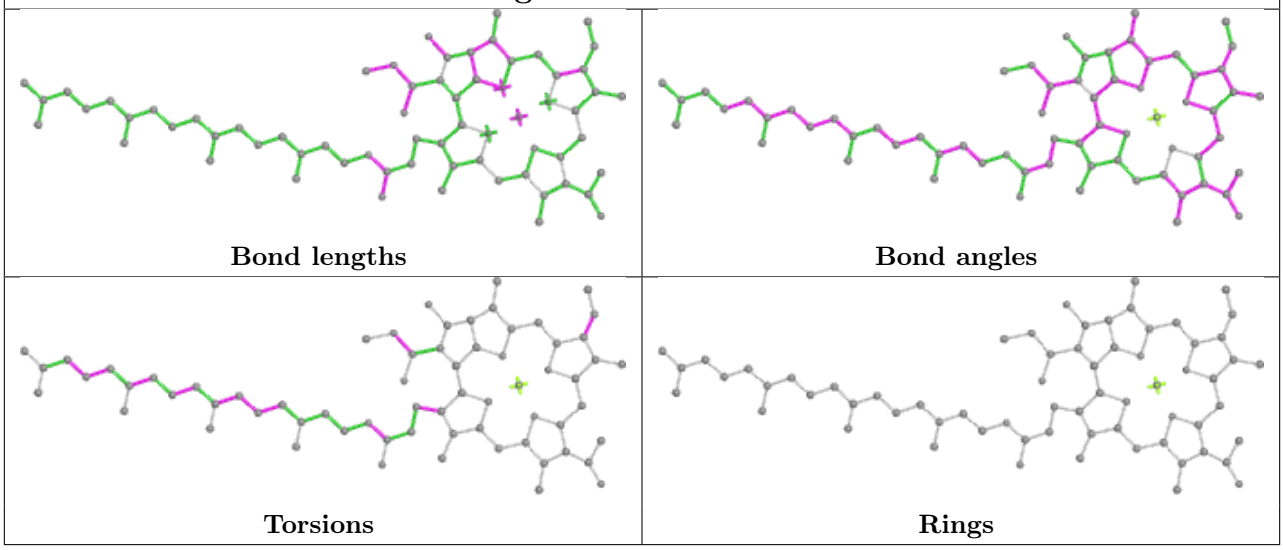
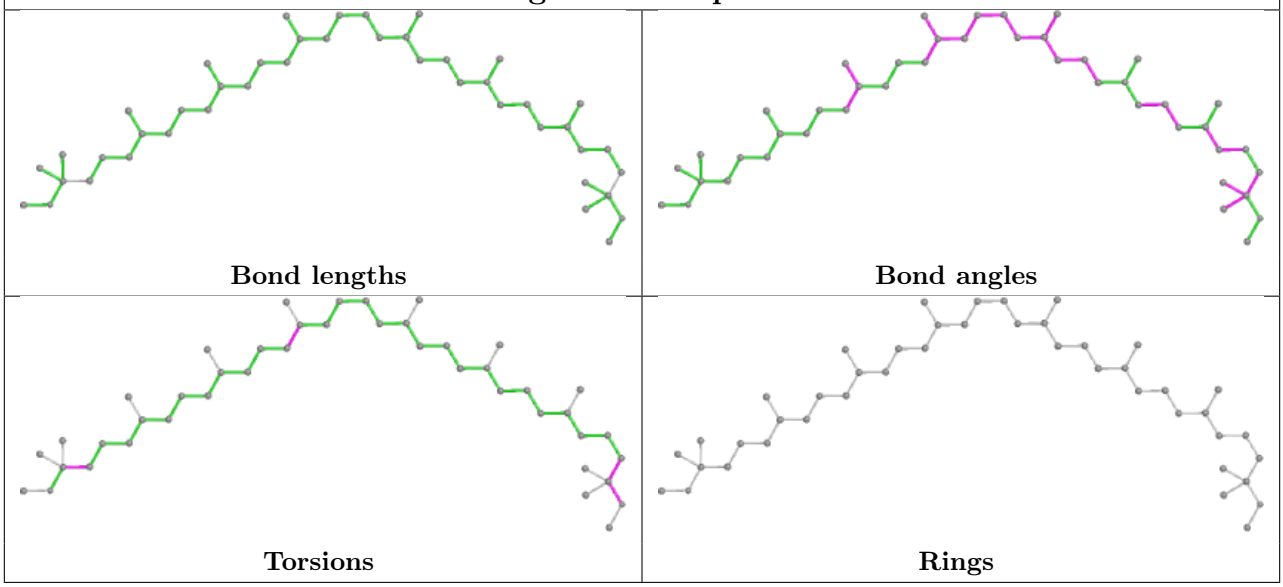
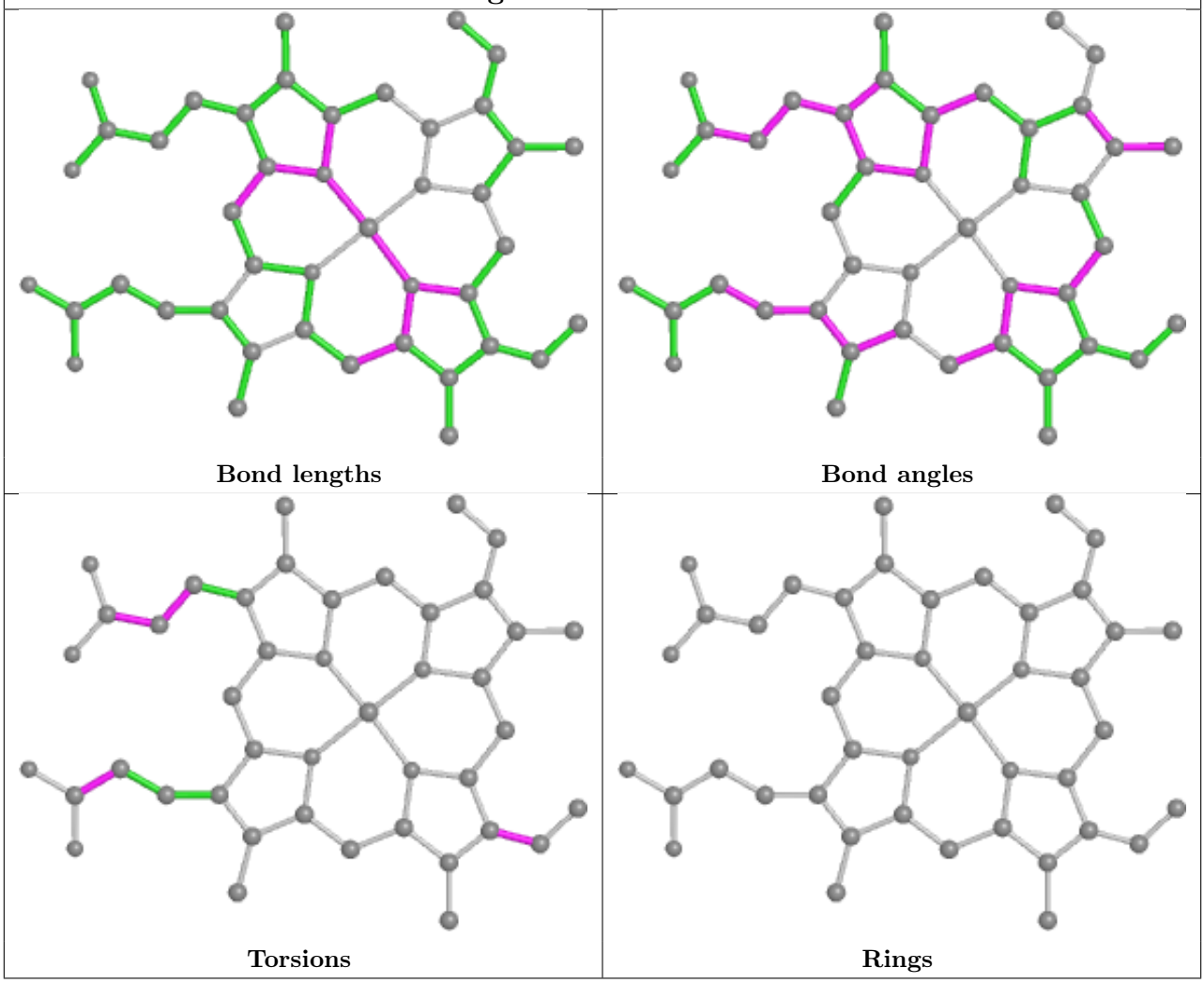


Ligand CRT q 101



Ligand HEM C 502



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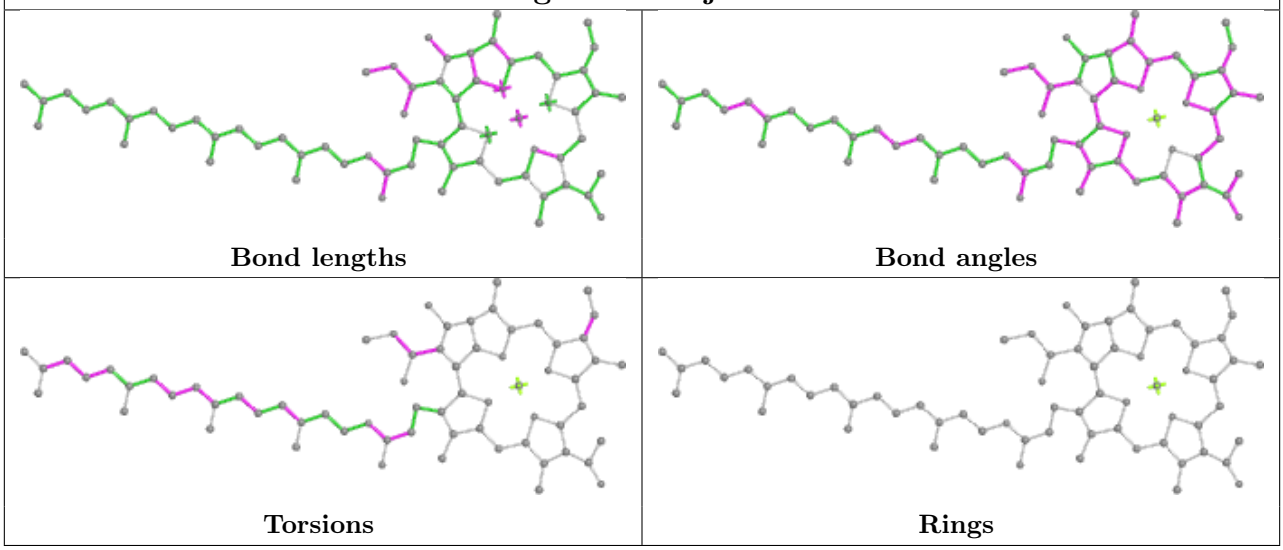

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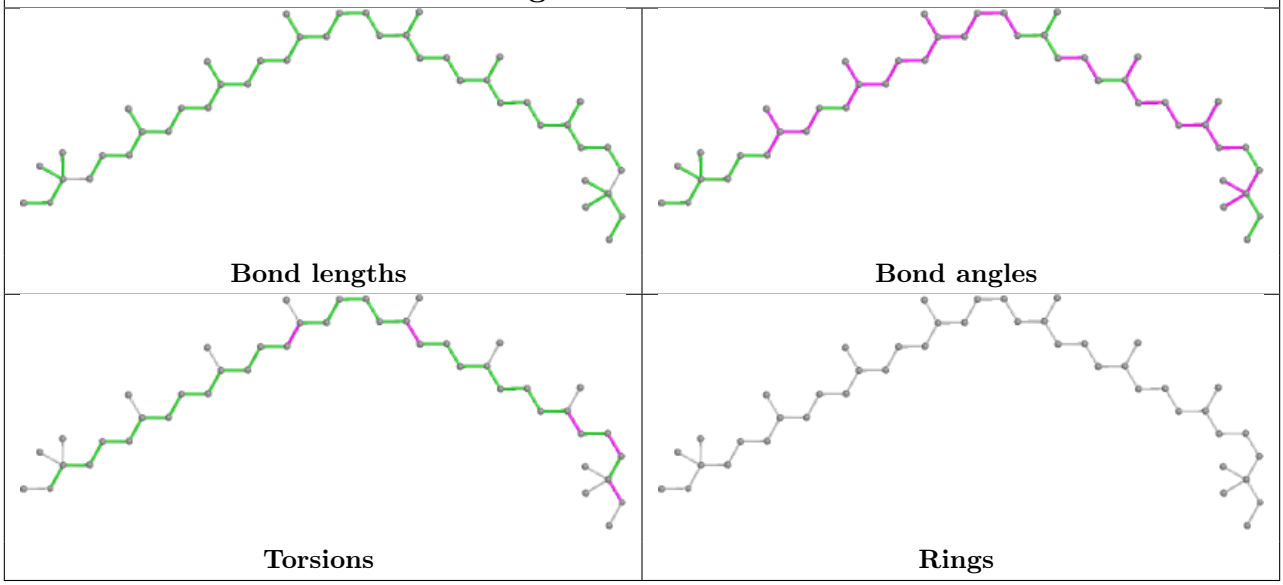

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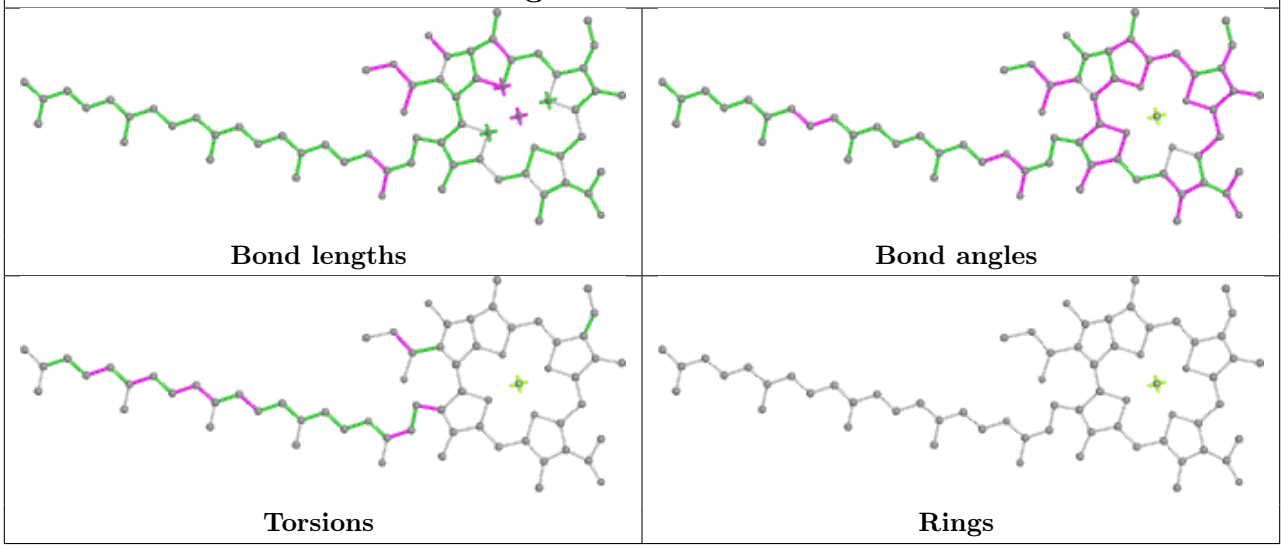

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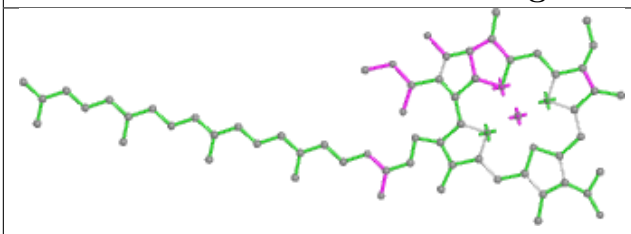
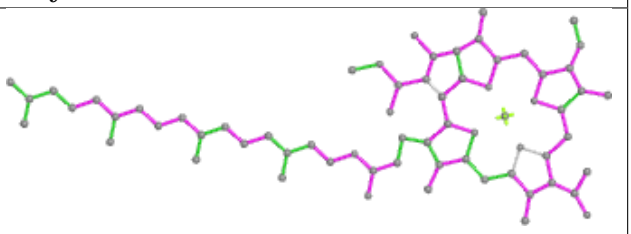
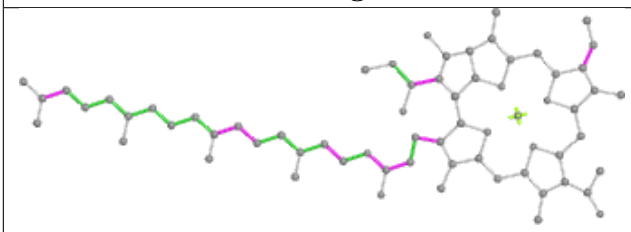
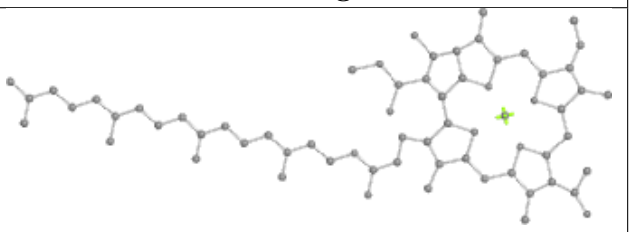
 Bond lengths	 Bond angles
 Torsions	 Rings

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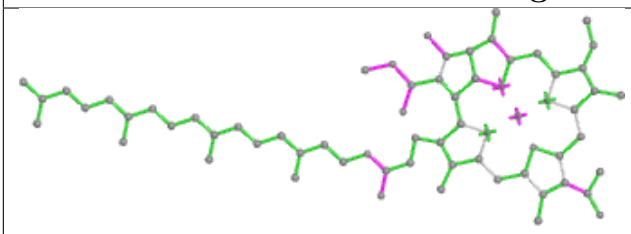
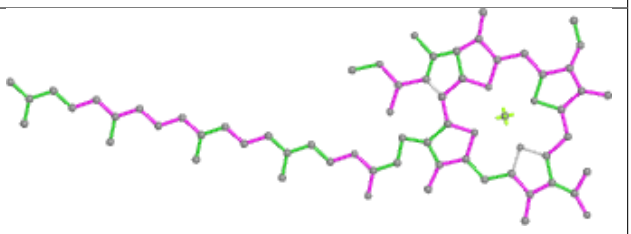
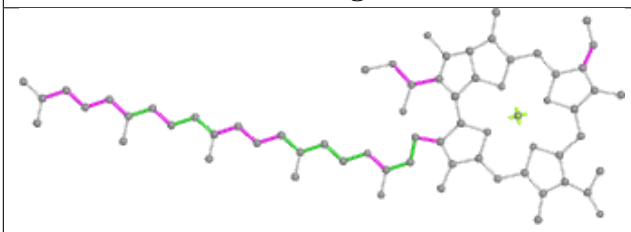
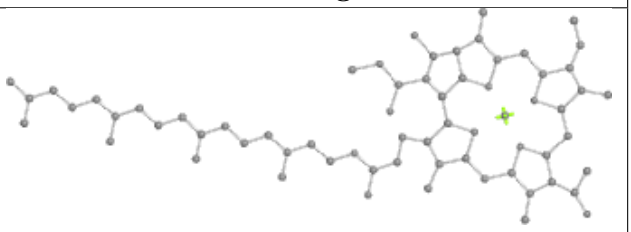
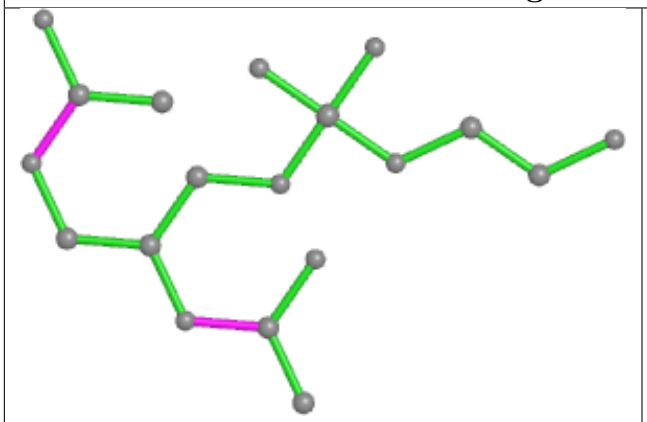
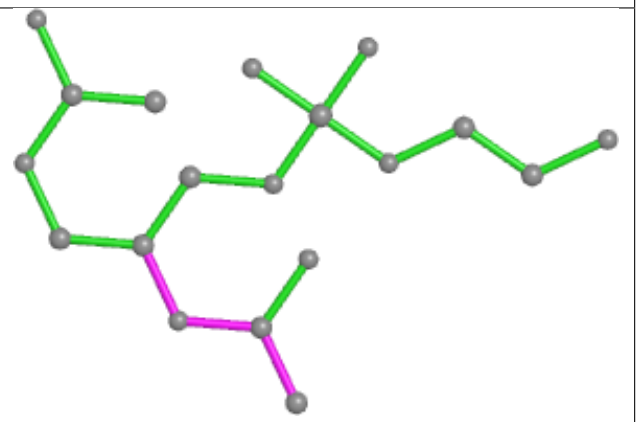
 Bond lengths	 Bond angles
 Torsions	 Rings

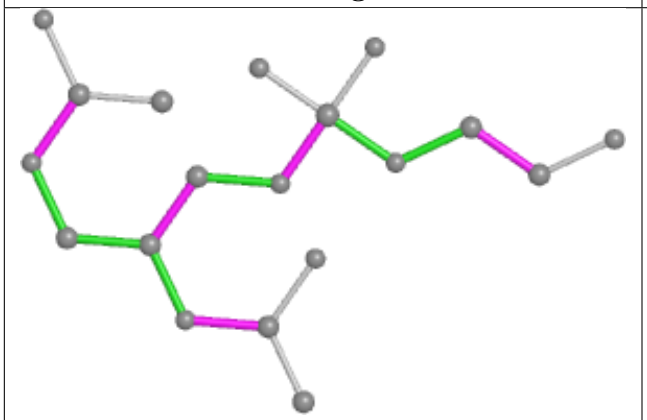
Ligand PEF H 302



Bond lengths



Bond angles



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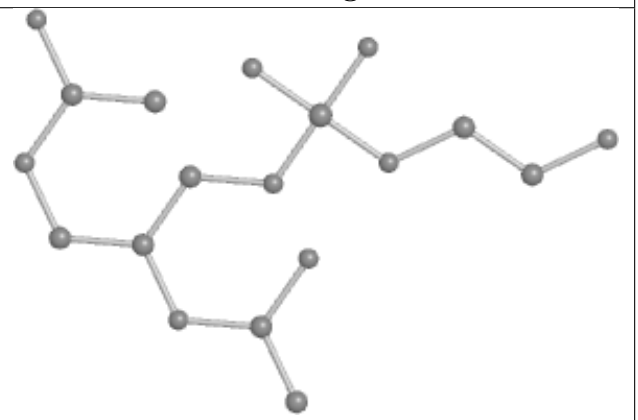
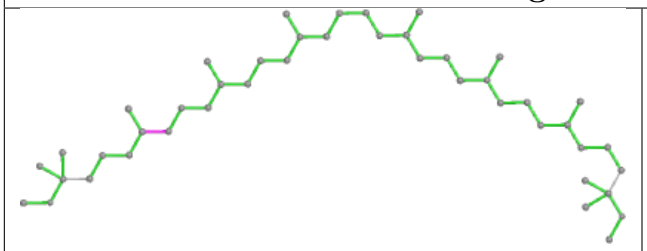
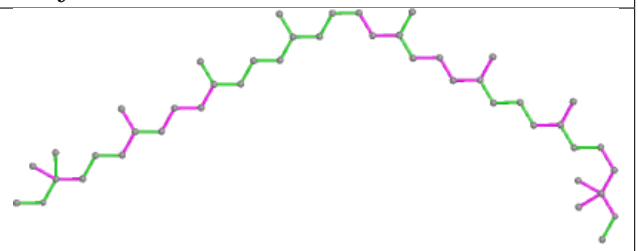


Rings

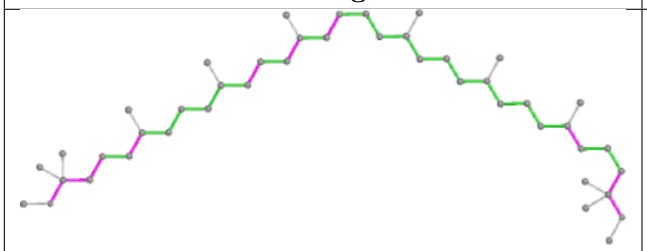
Ligand CRT y 404



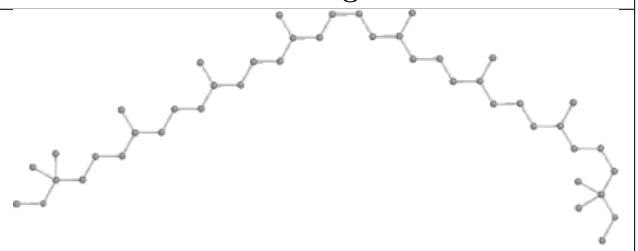
Bond lengths



Bond angles

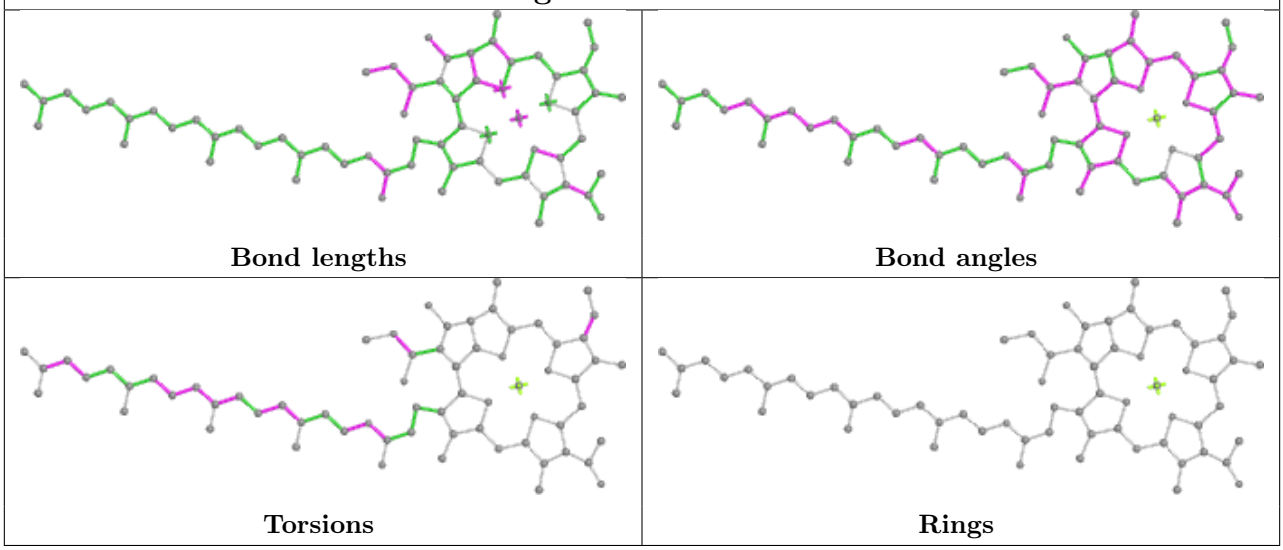


Torsions

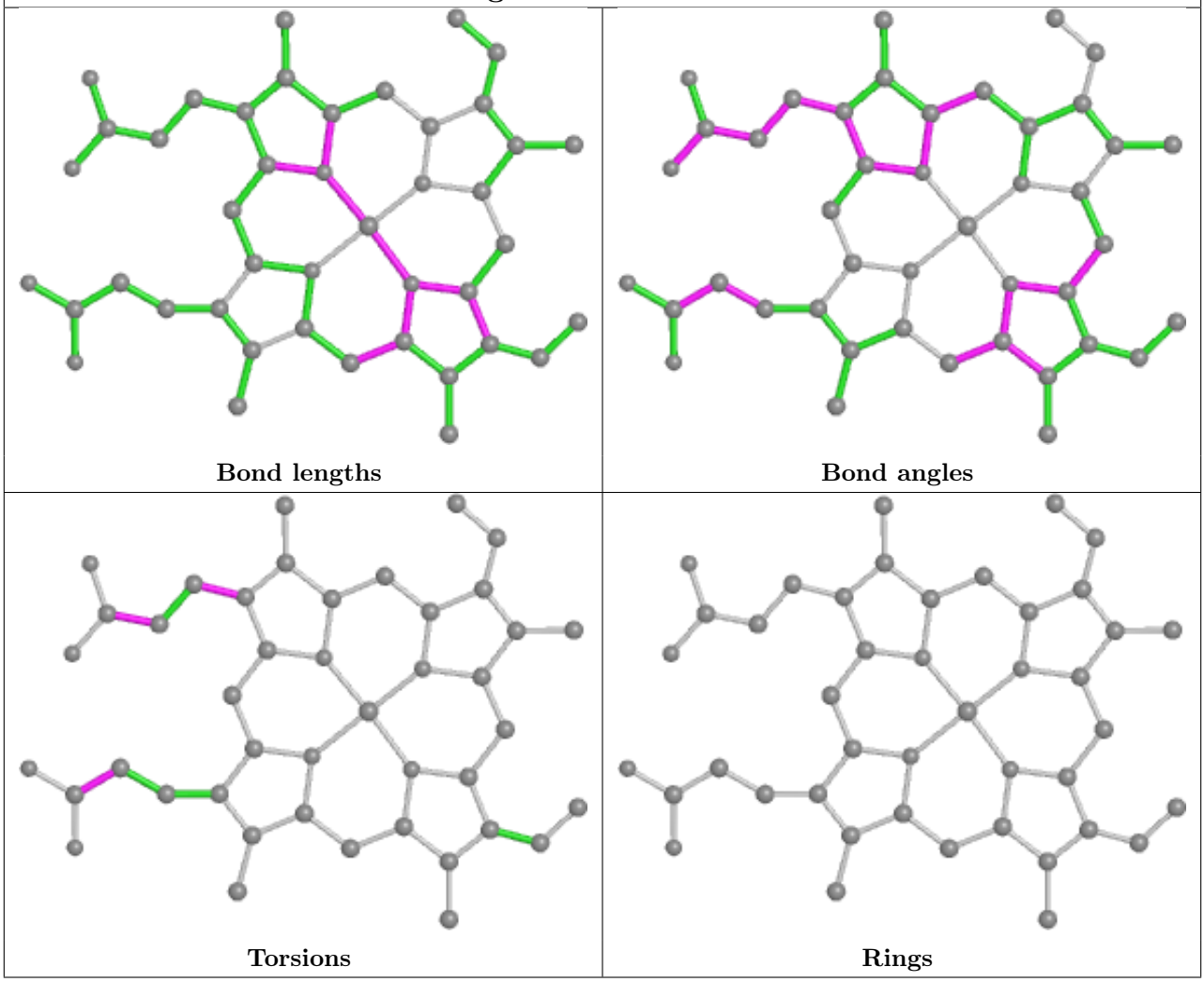


Rings

Ligand BCL l 101



Ligand HEM C 504



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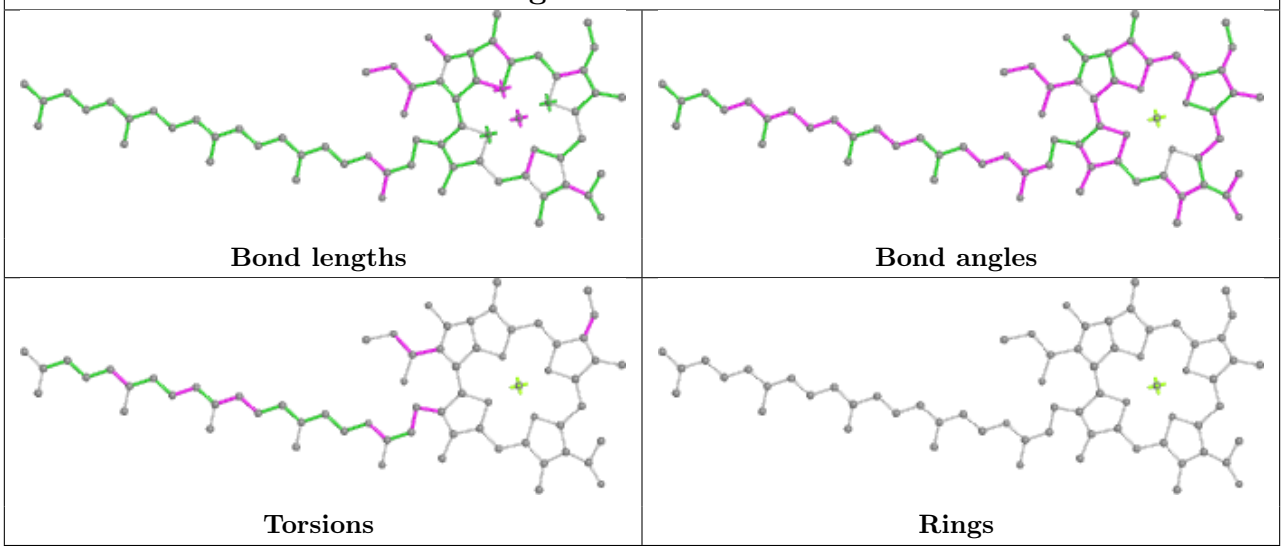

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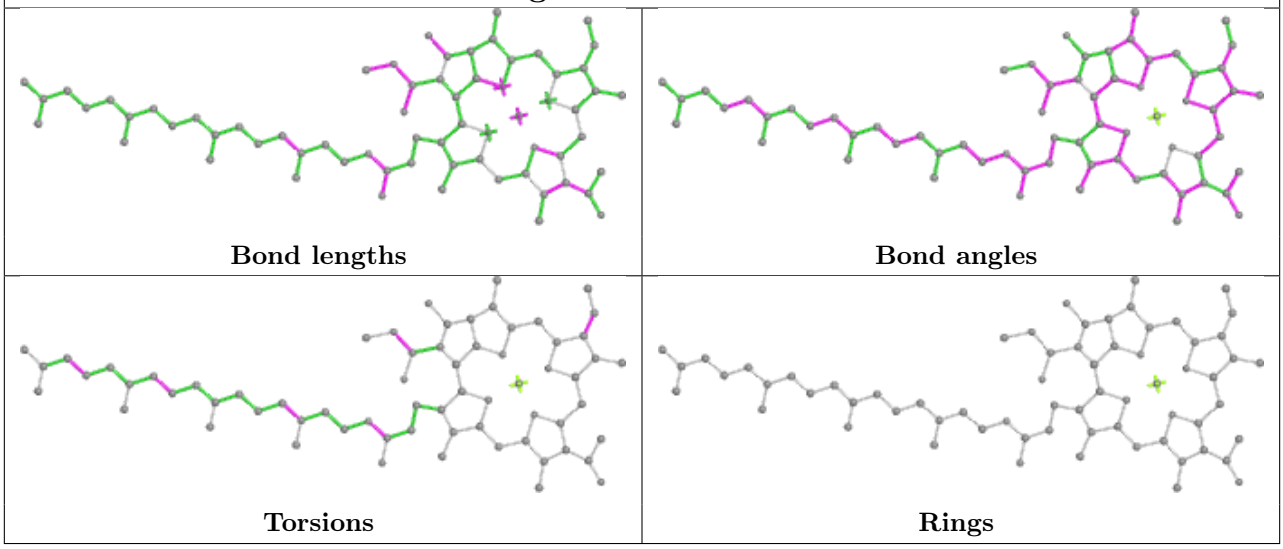
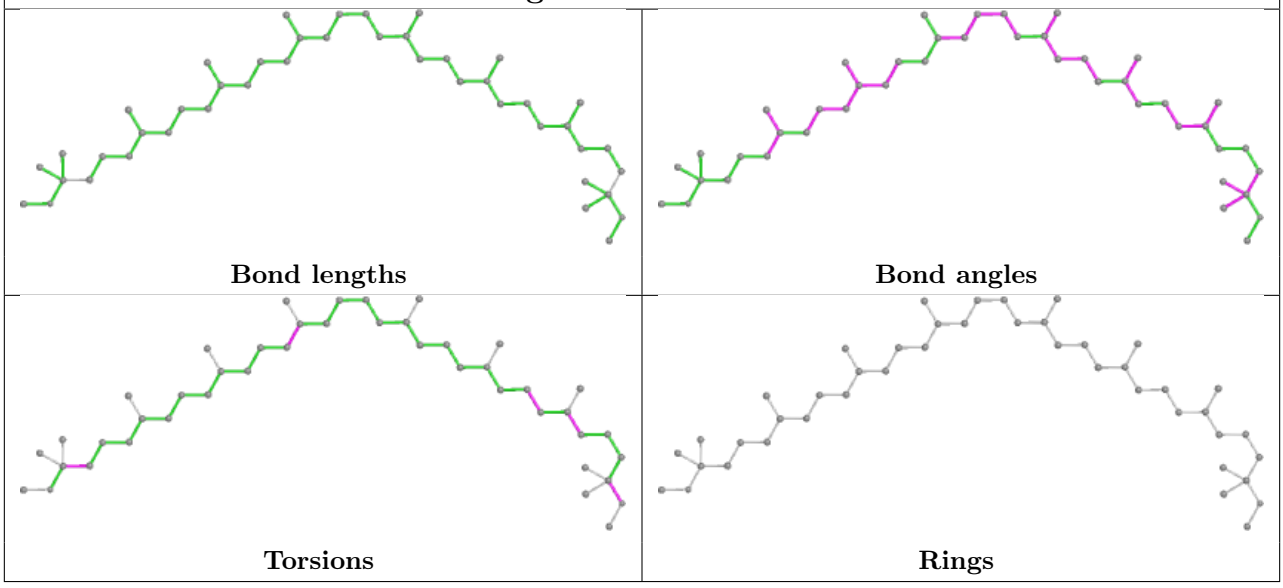


Ligand CRT E 101



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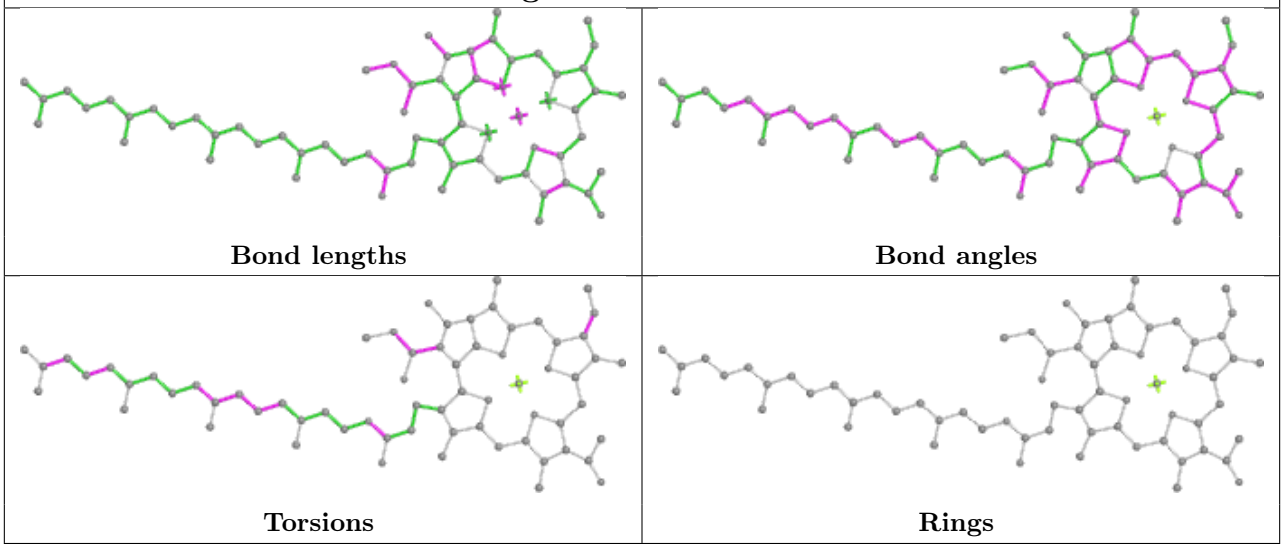
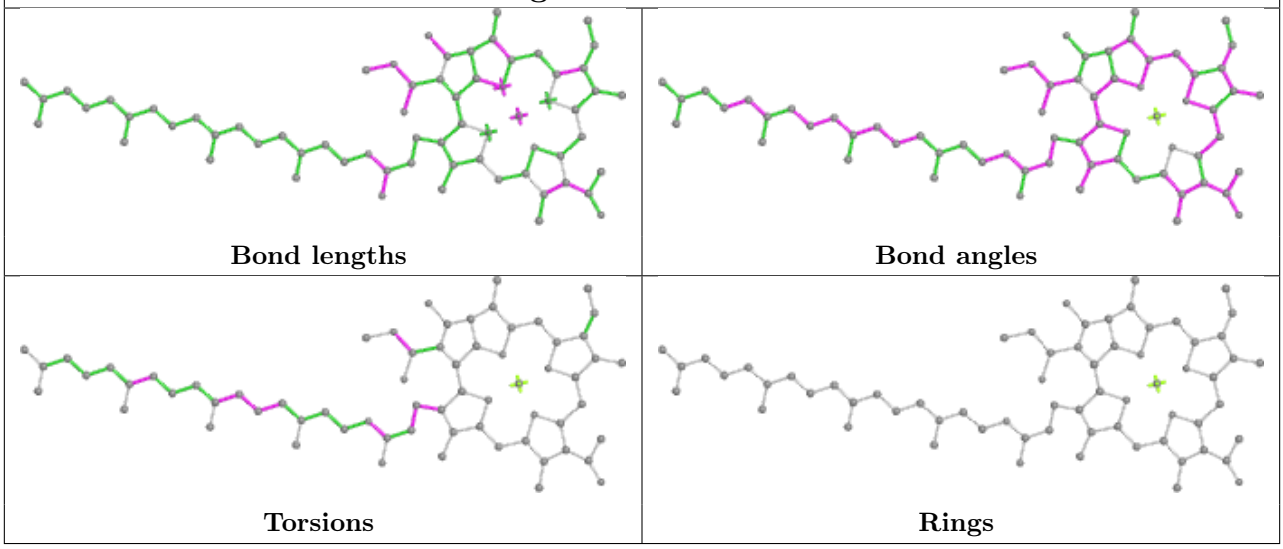
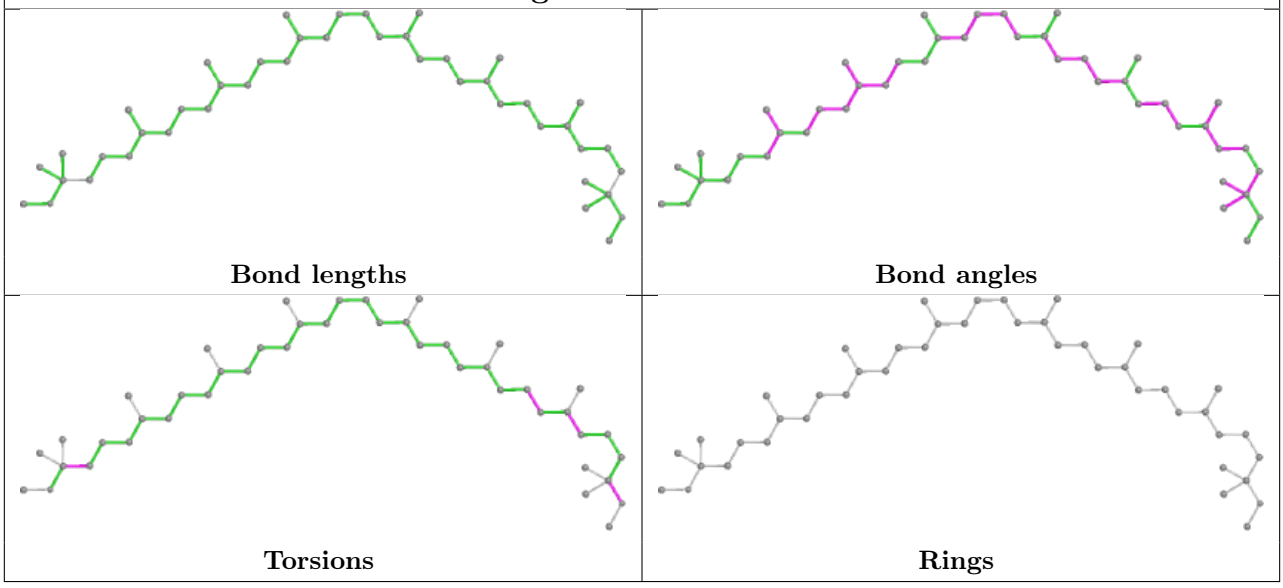


Ligand BCL 6 101



Ligand CRT I 102



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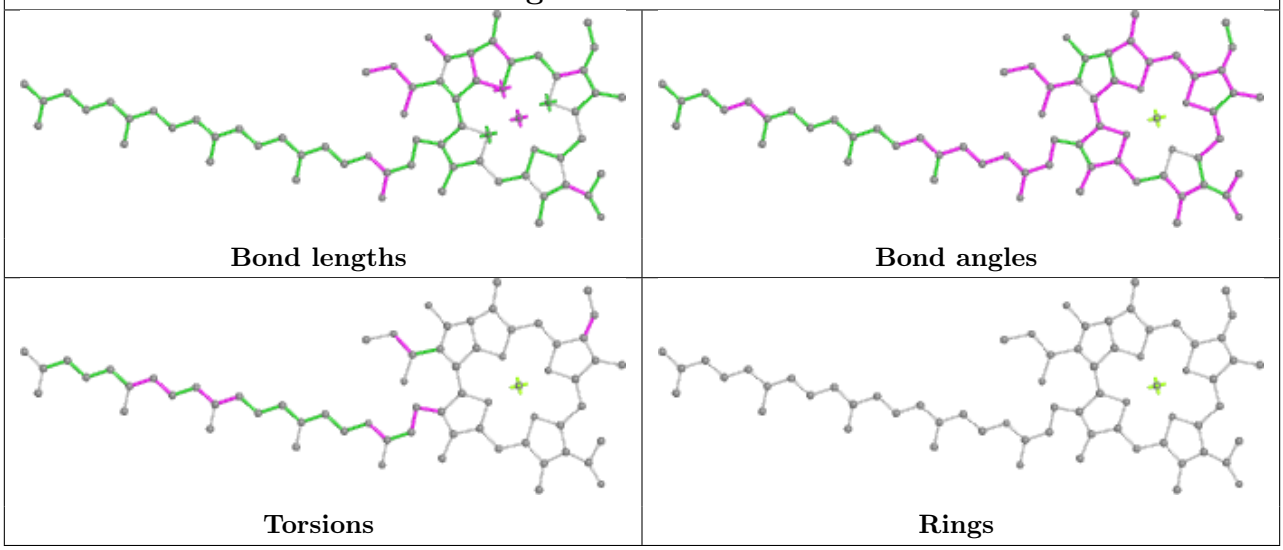
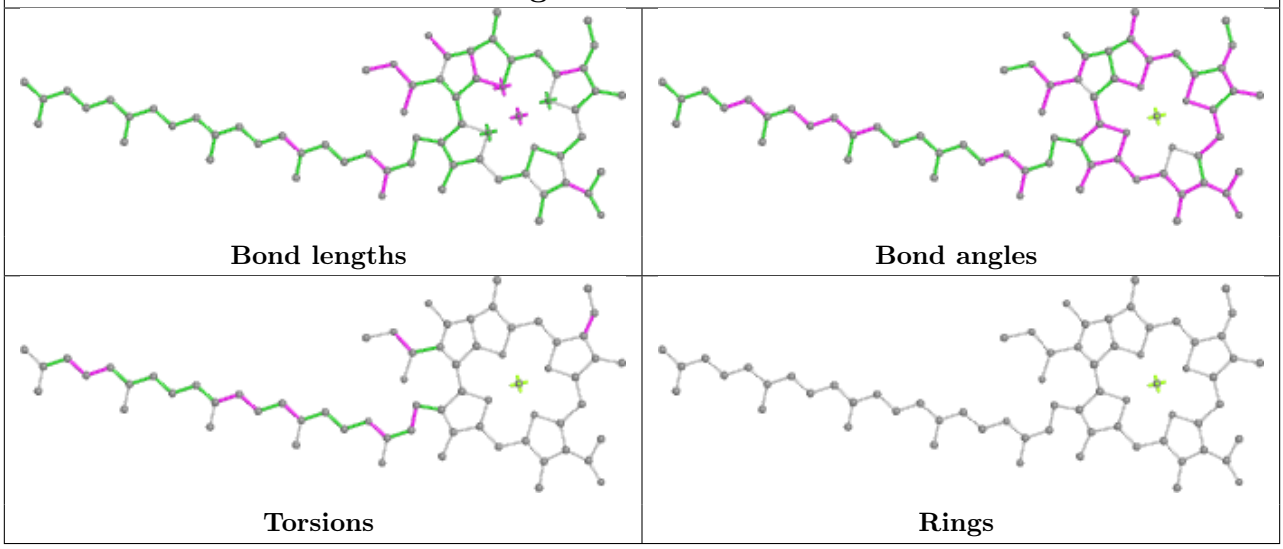


Ligand BCL x 301



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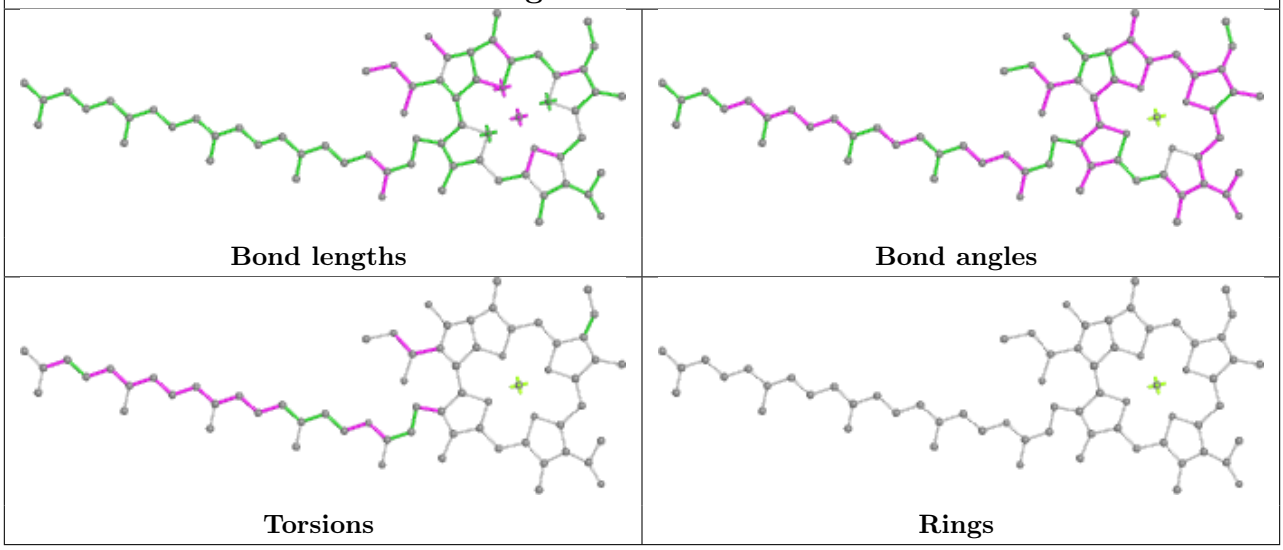
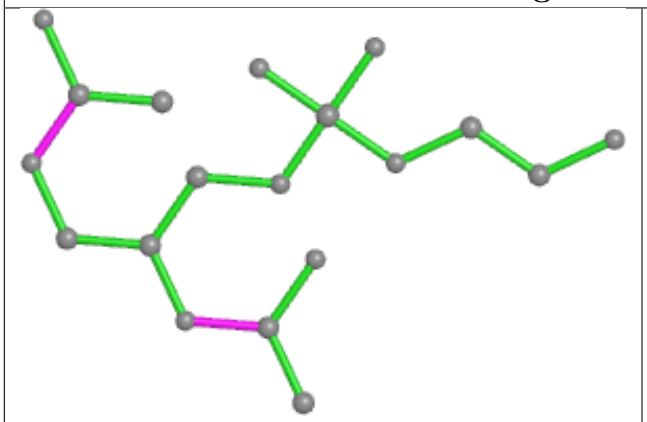
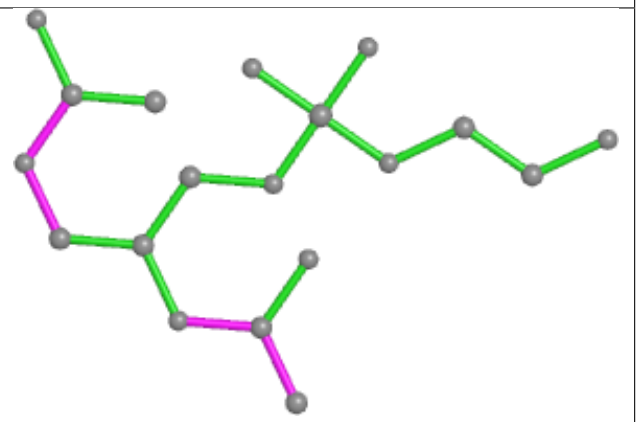


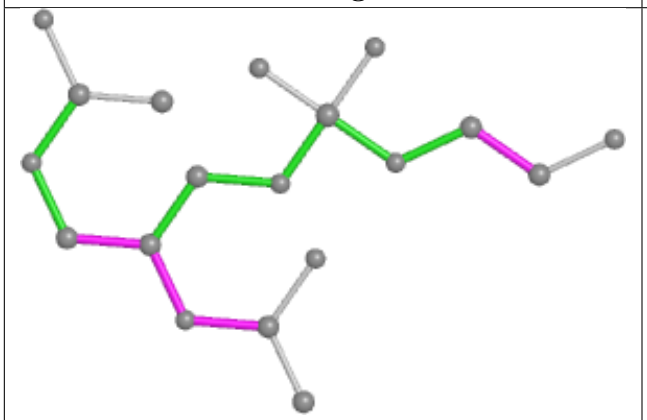
Ligand PEF t 301



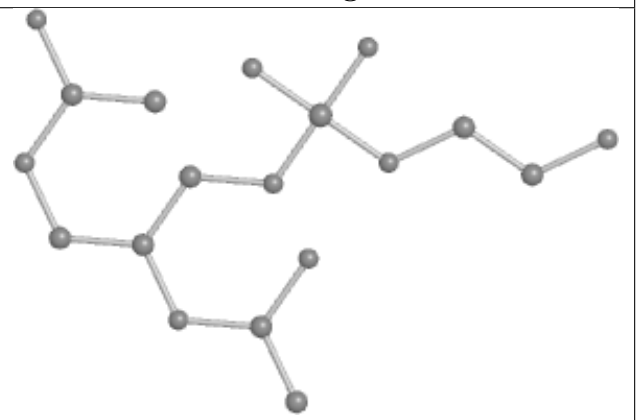
Bond lengths



Bond angles

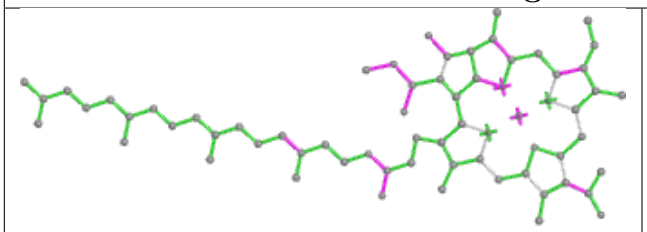


Torsions



Rings

Ligand BCL m 102



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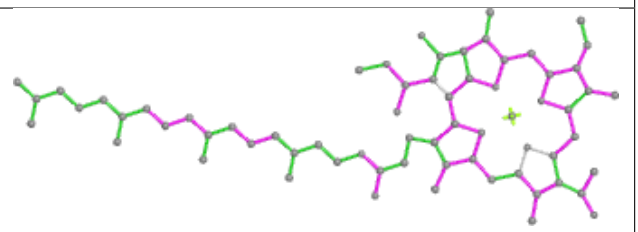
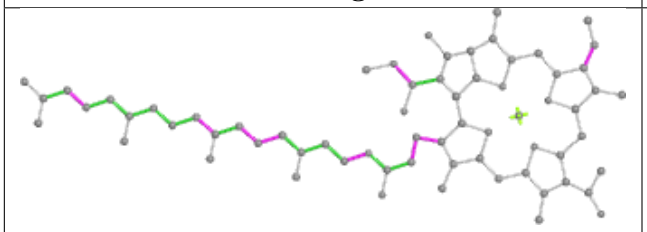


Bond angles



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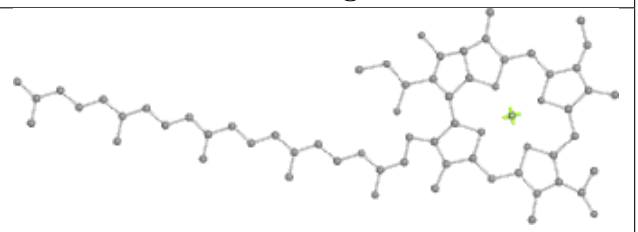
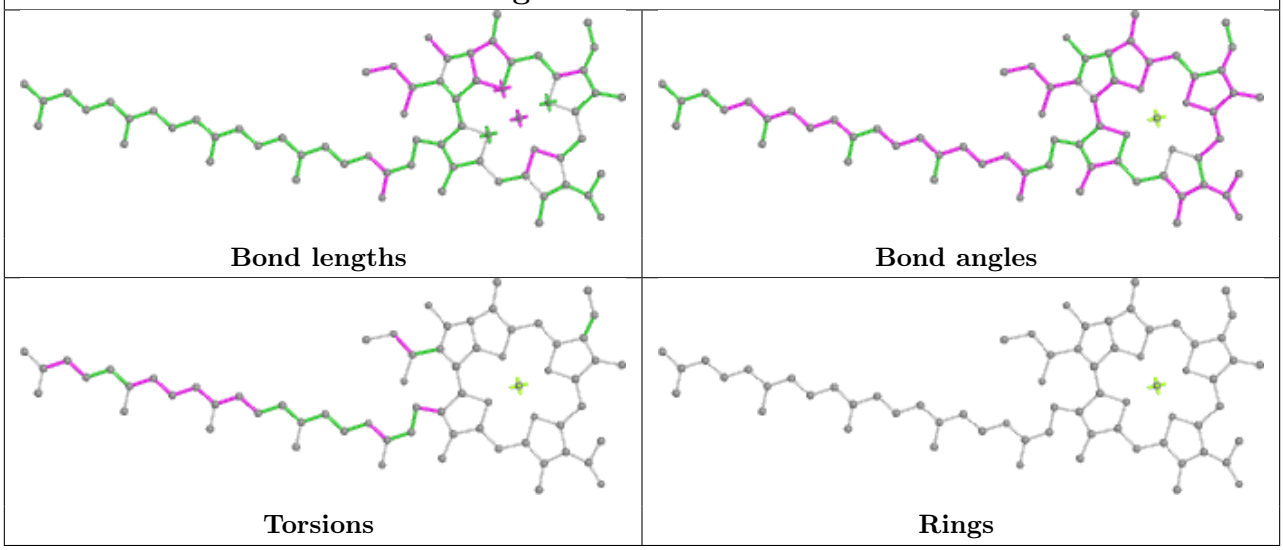
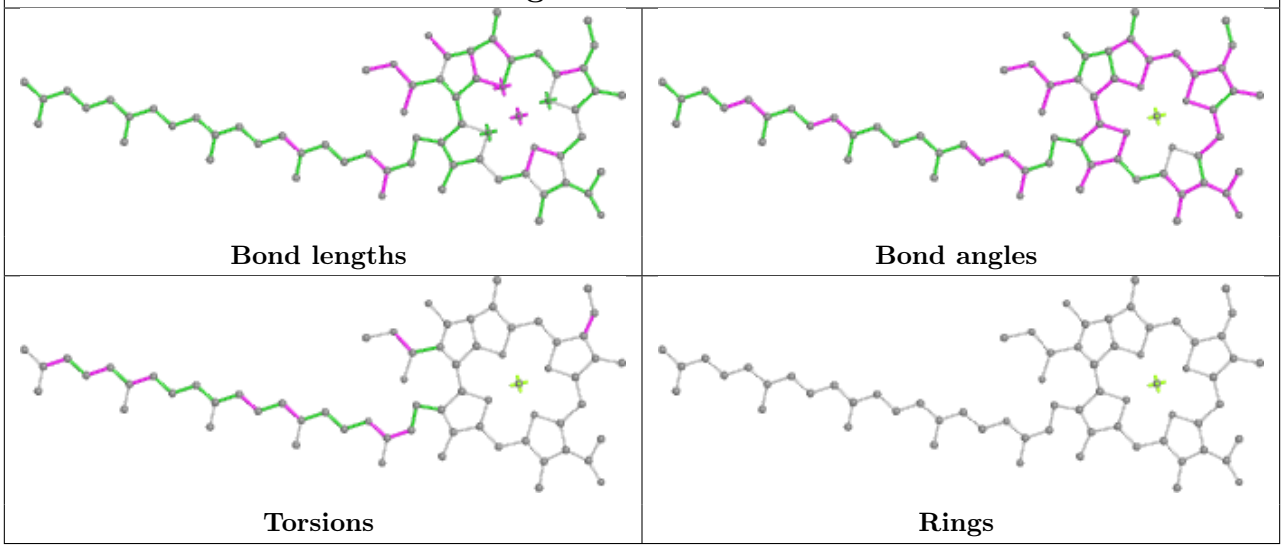


Rings

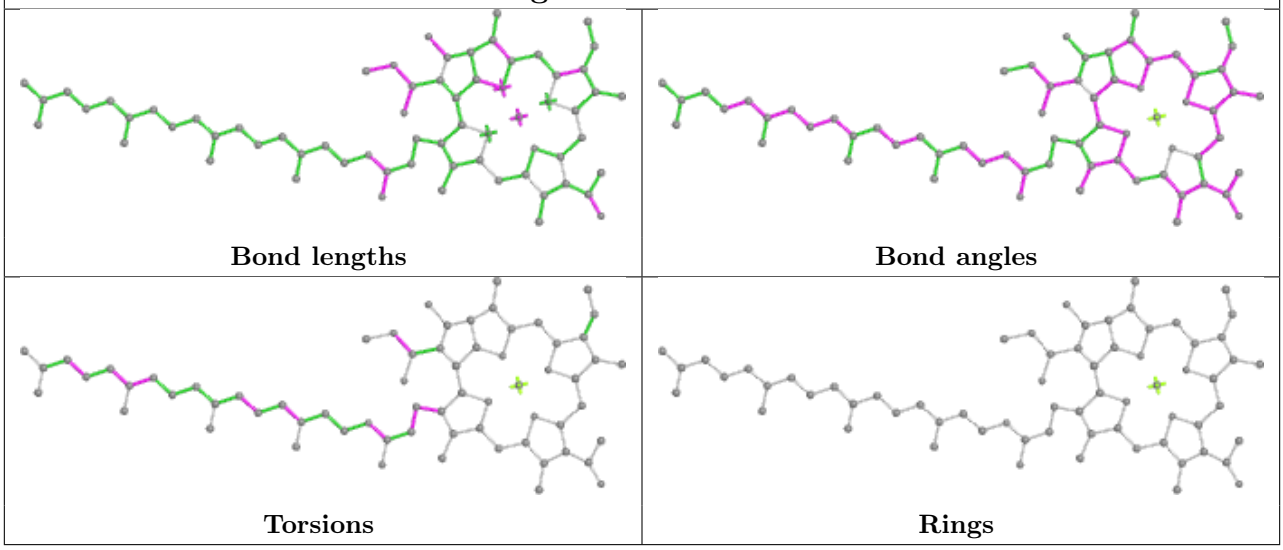
Ligand BCL AB 102



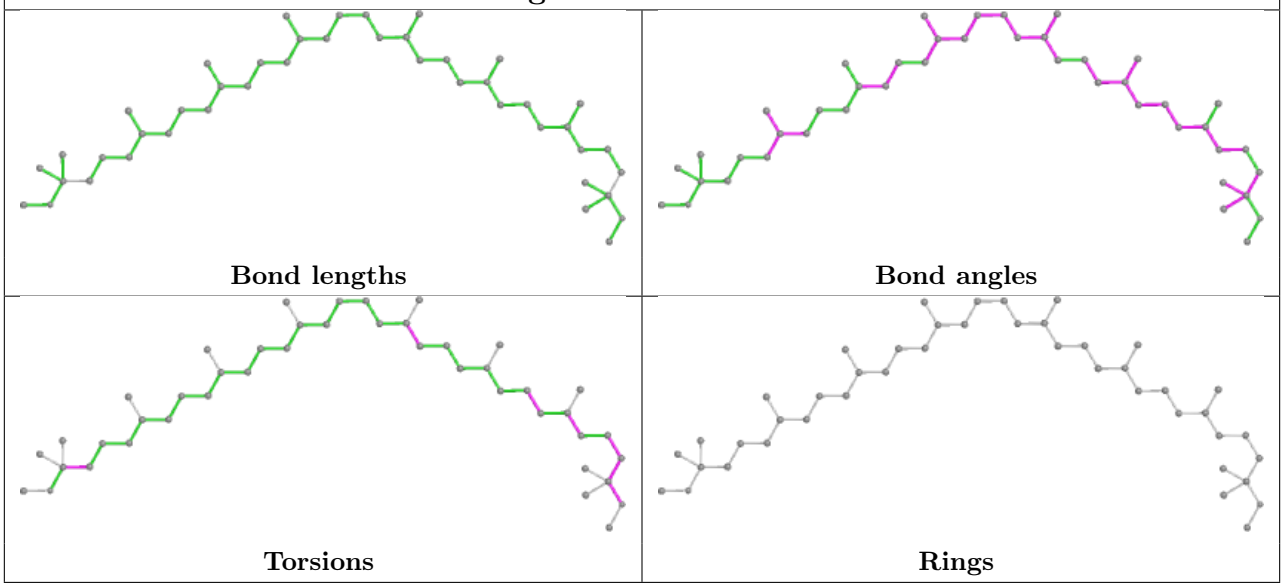
Ligand BCL P 101



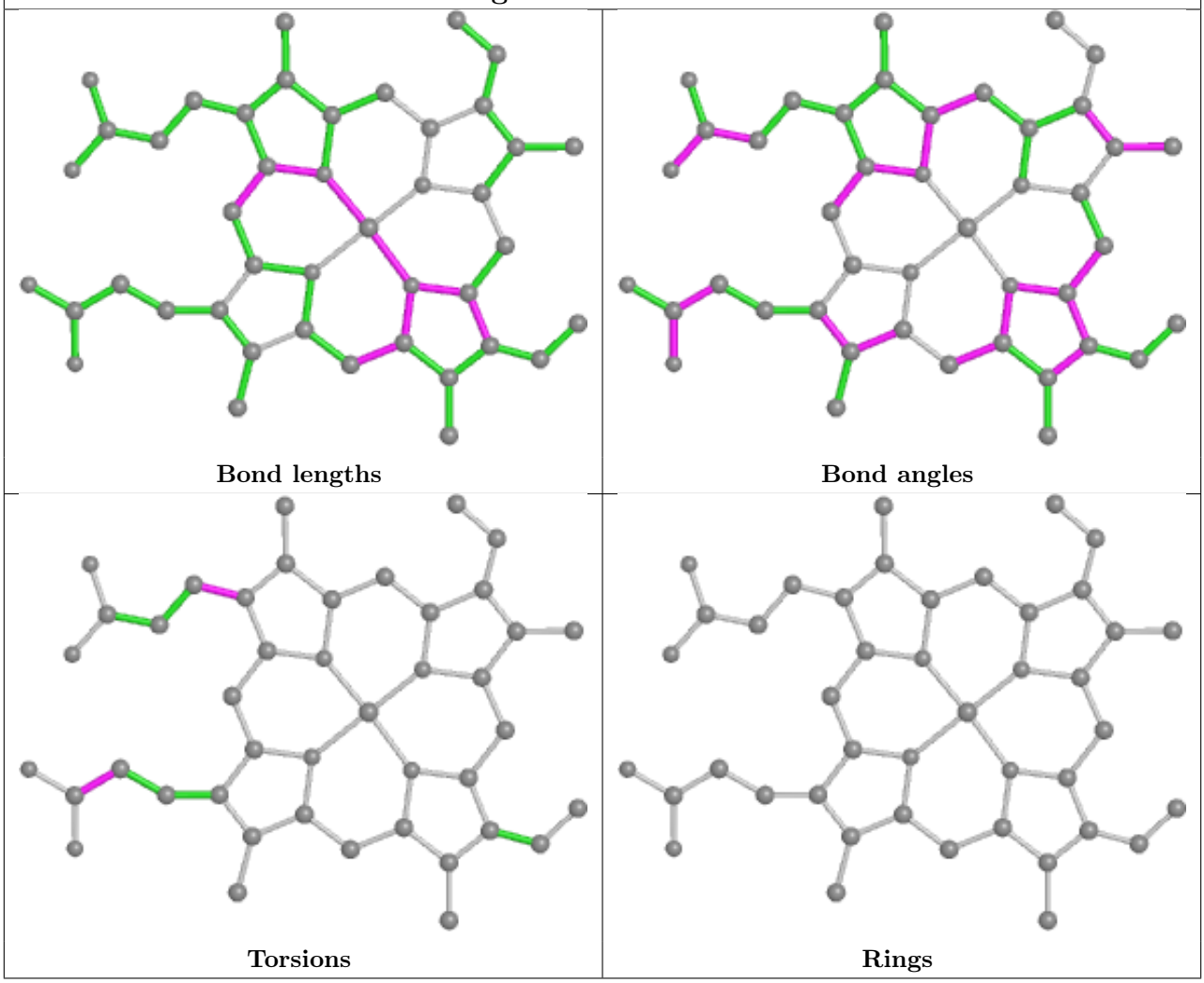
Ligand BCL e 102



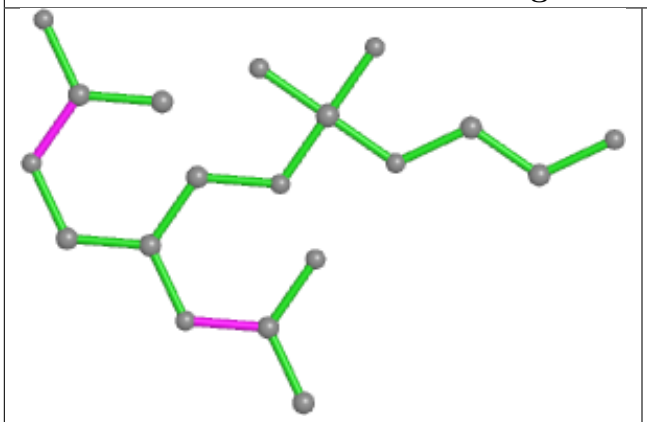
Ligand CRT n 101



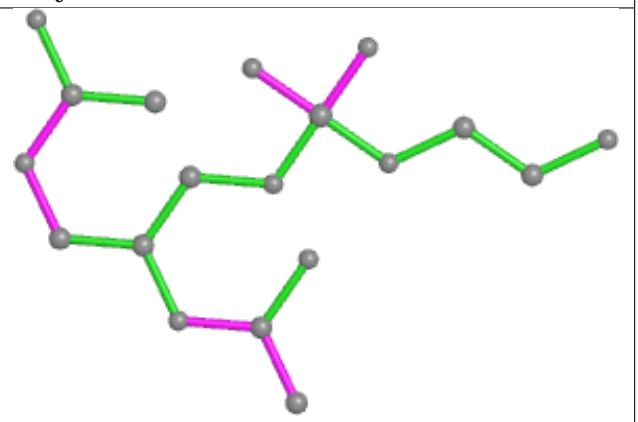
Ligand HEM o 504



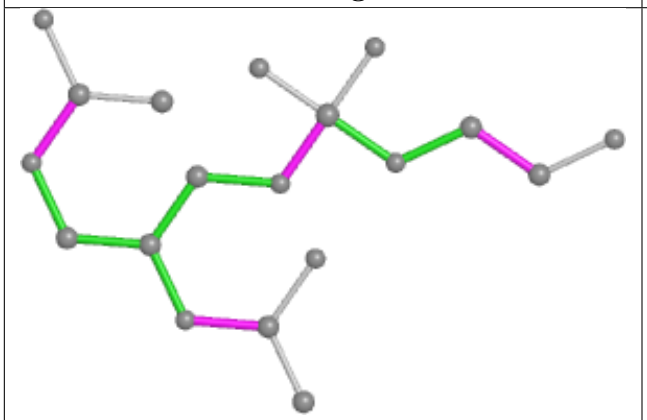
Ligand PEF y 407



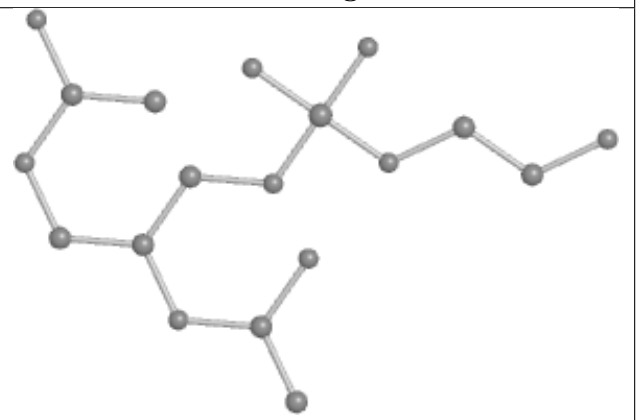
Bond lengths



Bond angles

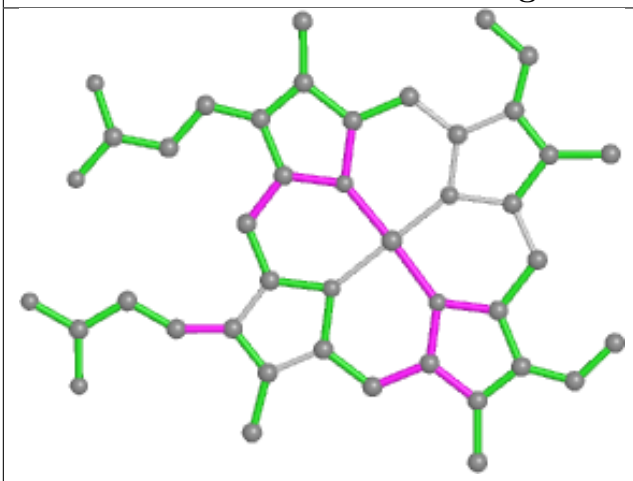


Torsions

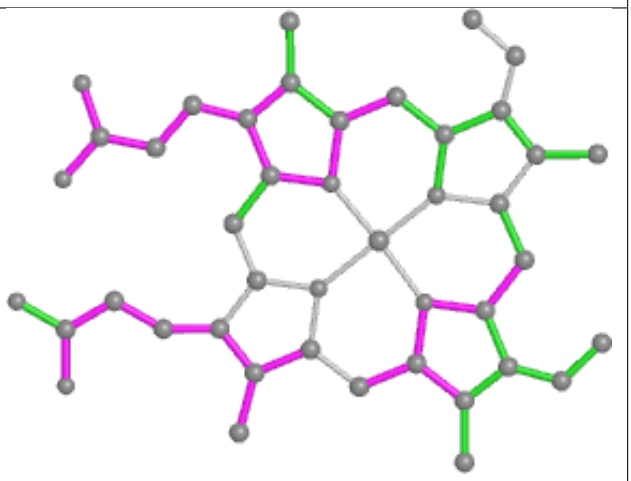


Rings

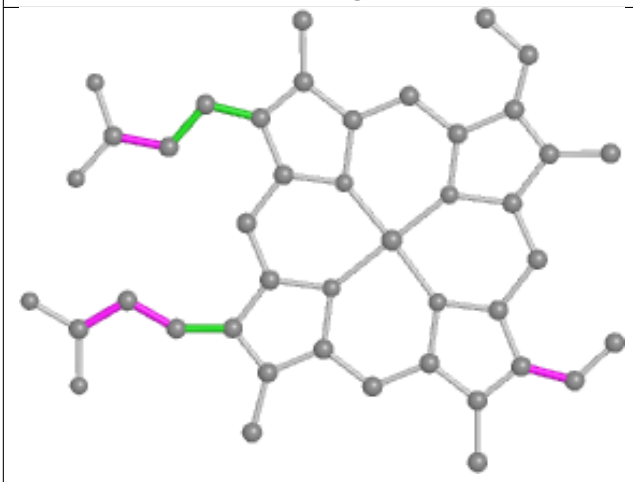
Ligand HEM C 501



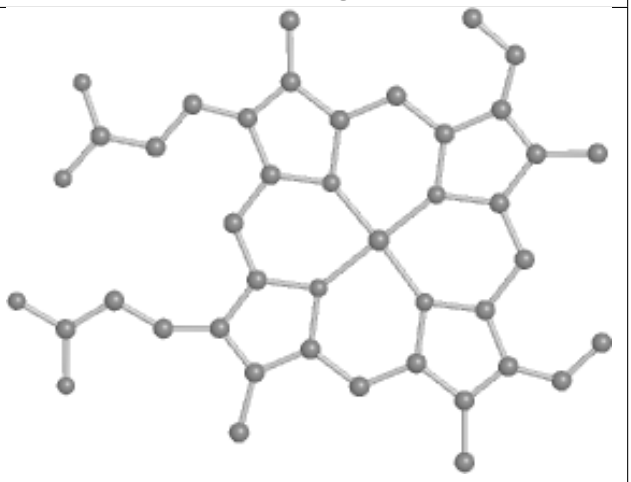
Bond lengths



Bond angles

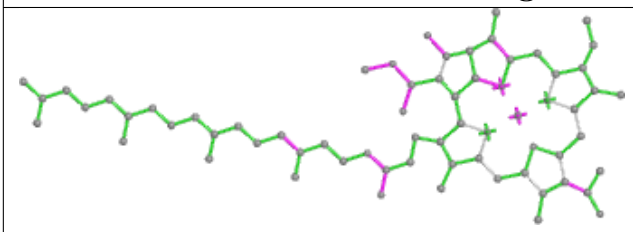


Torsions



Rings

Ligand BCL AI 101



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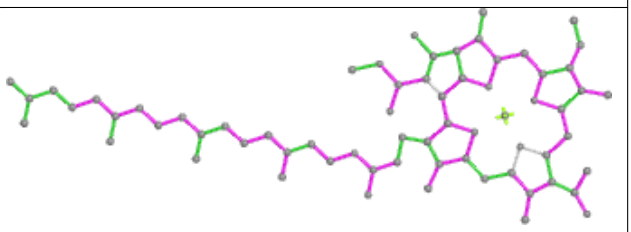
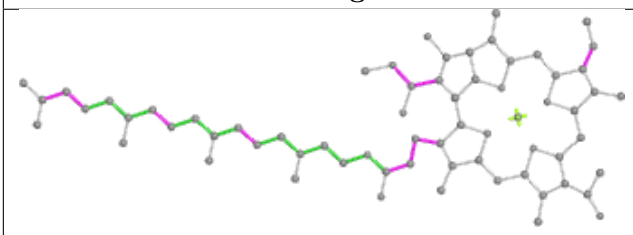
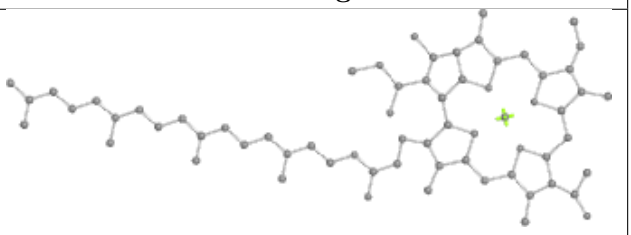


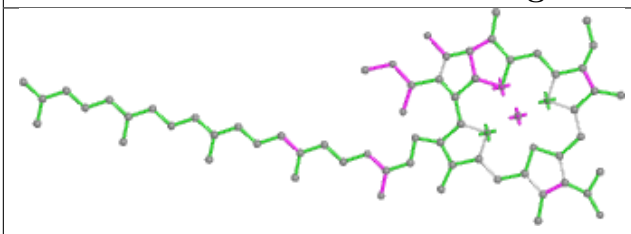
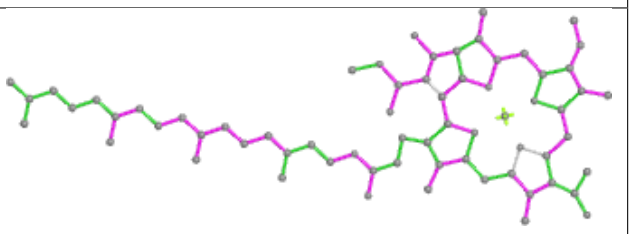
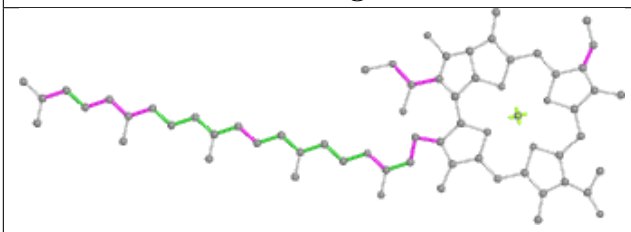
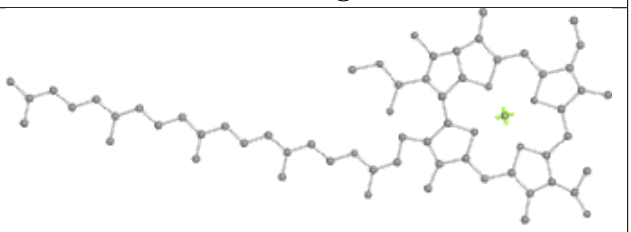
Bond angles

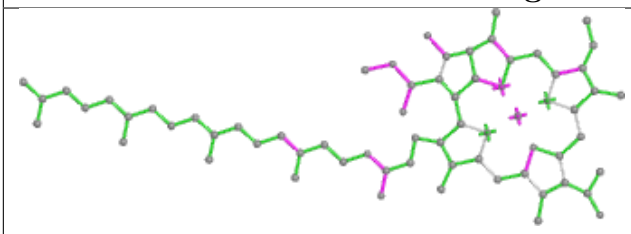
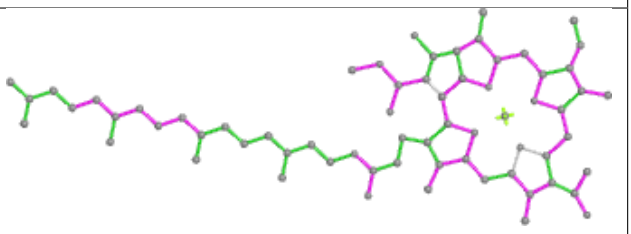
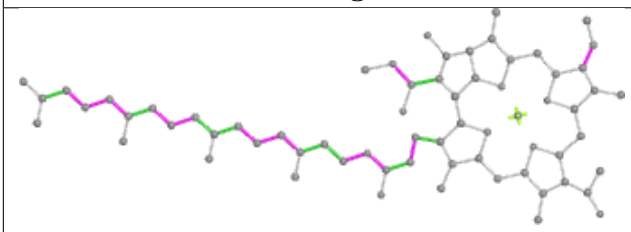
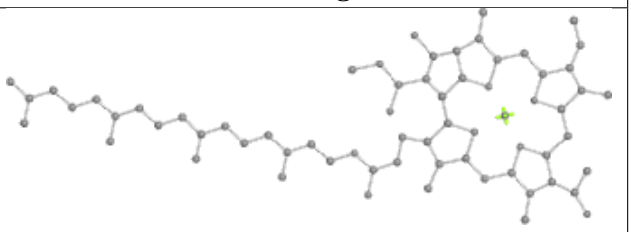


Torsions

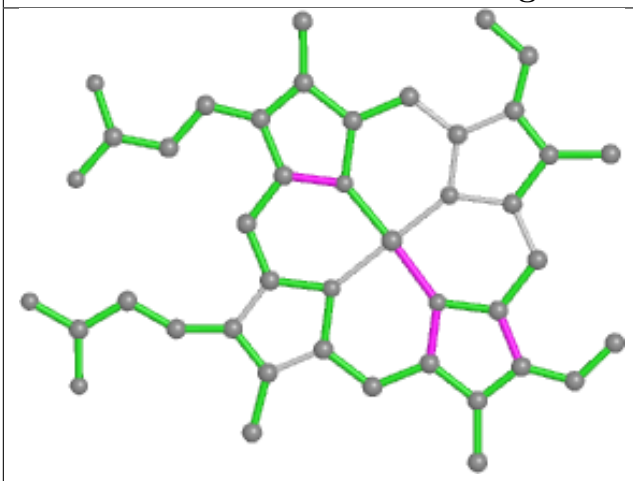


Rings

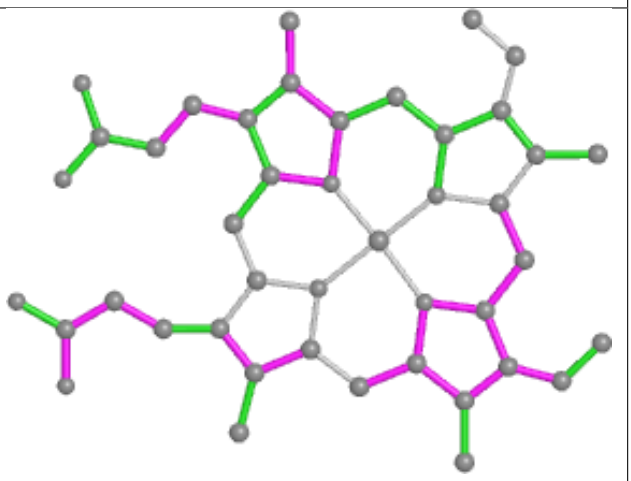
Ligand BCL L 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

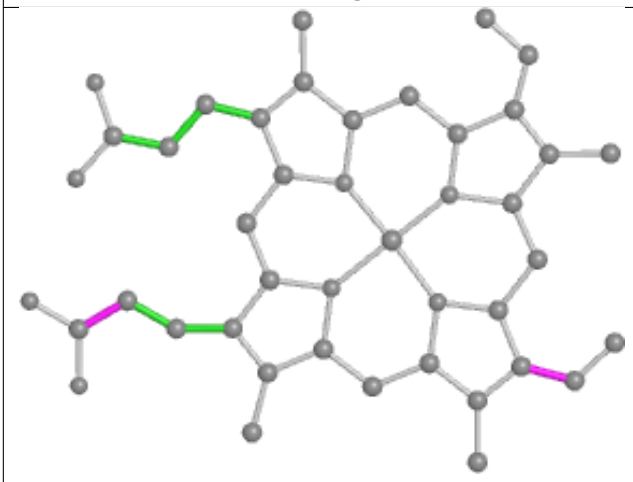
Ligand HEM C 503



Bond lengths



Bond angles



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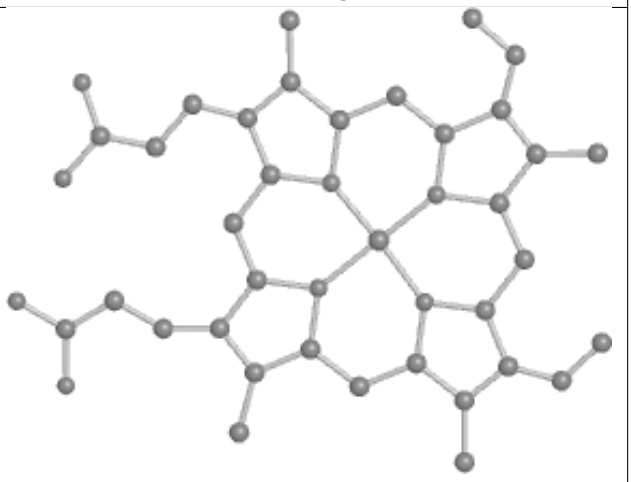
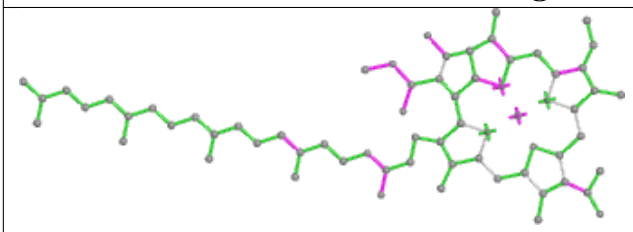


Rings

Ligand BCL s 102



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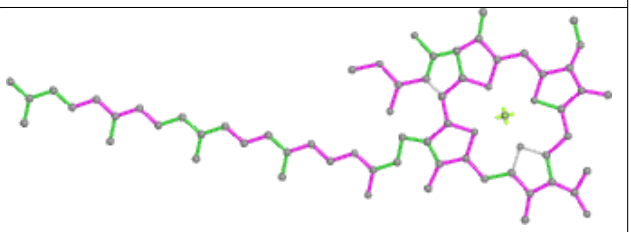
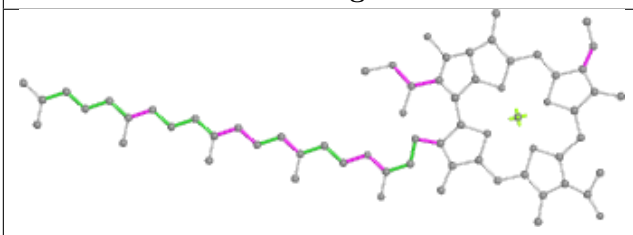


Bond angles



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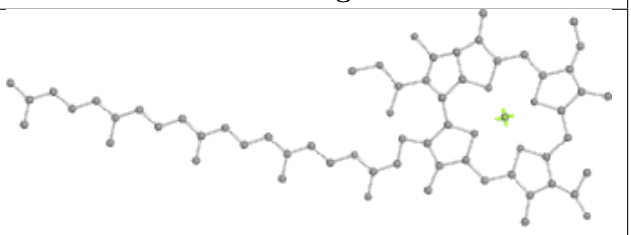
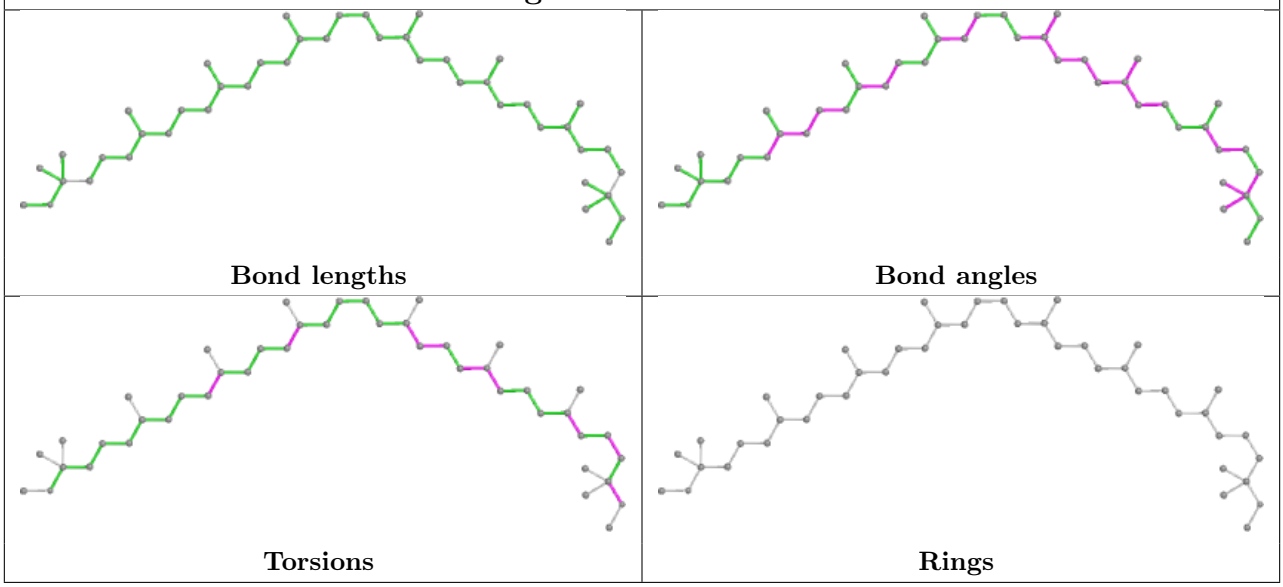
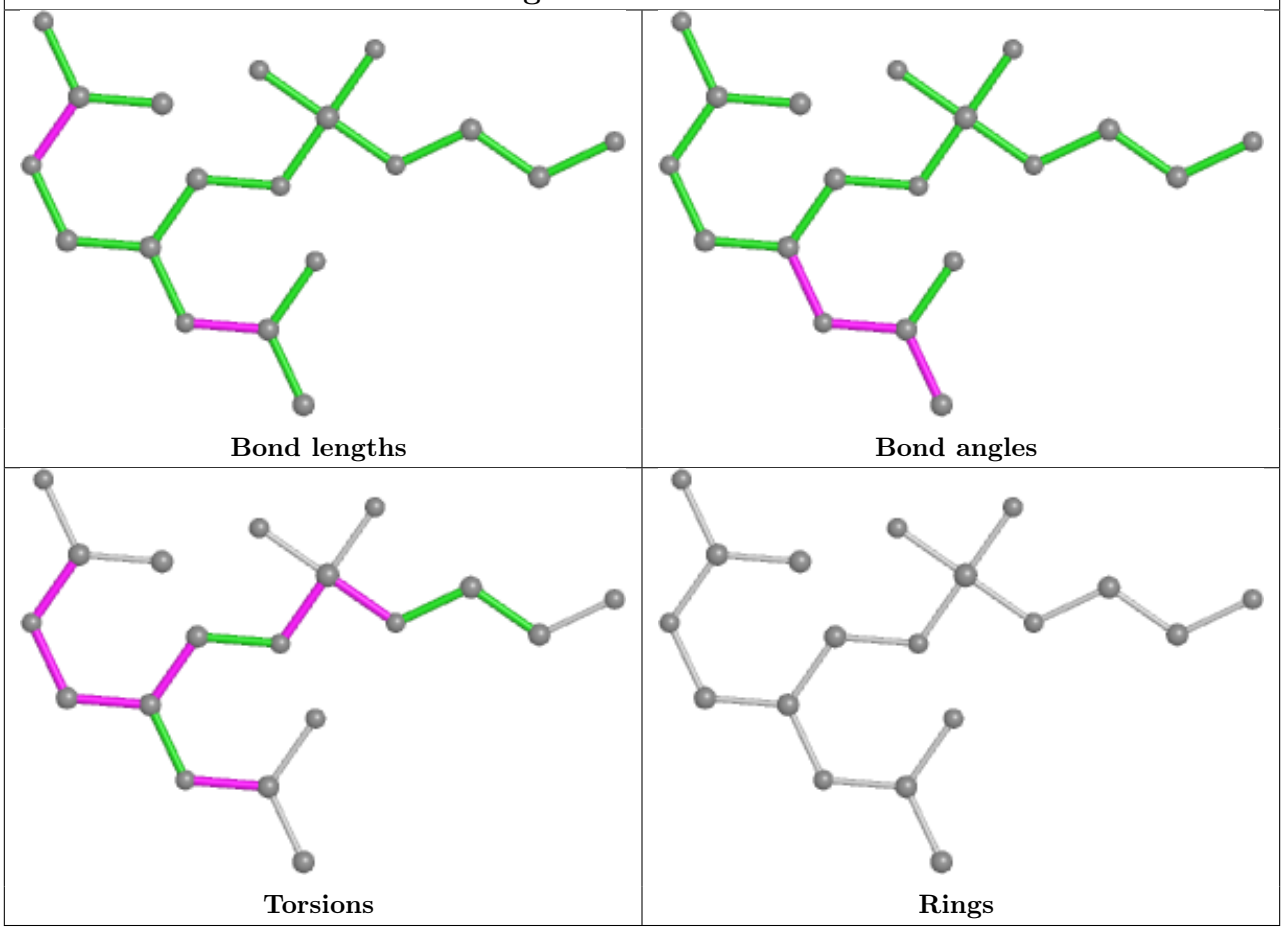


Rings

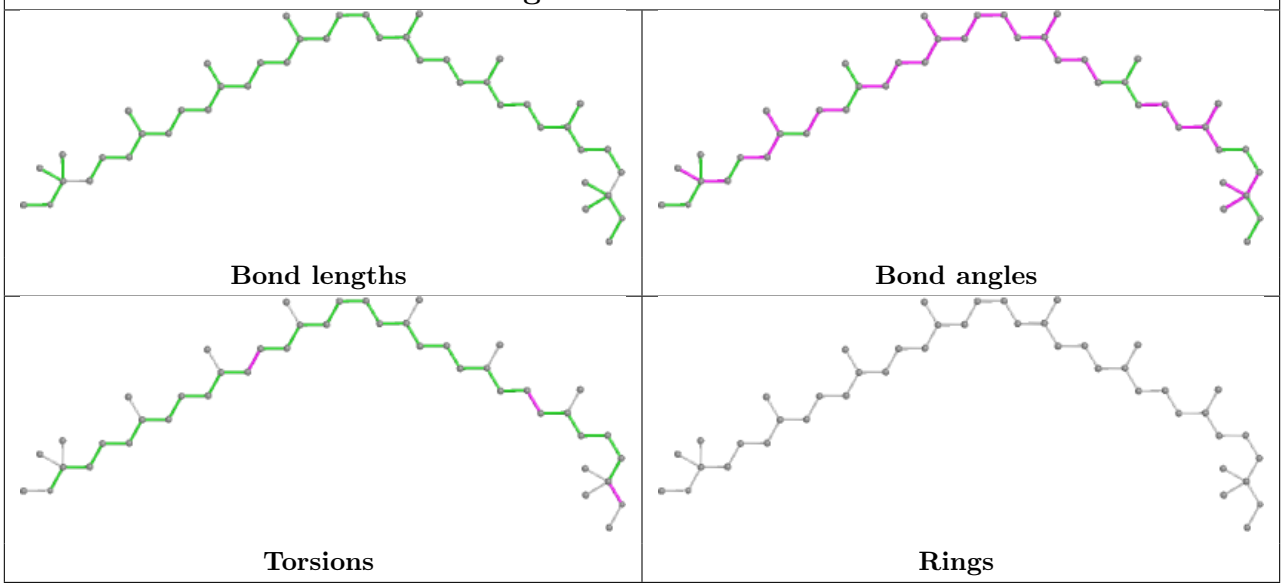
Ligand CRT R 101



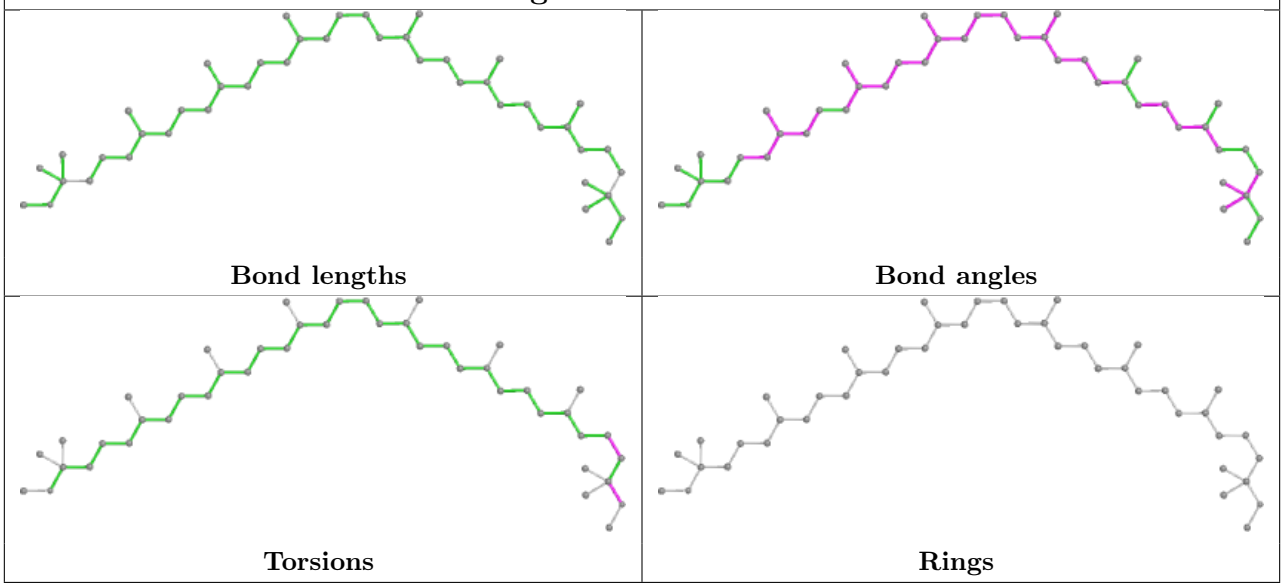
Ligand PEF M 408



Ligand CRT m 104



Ligand CRT z 101



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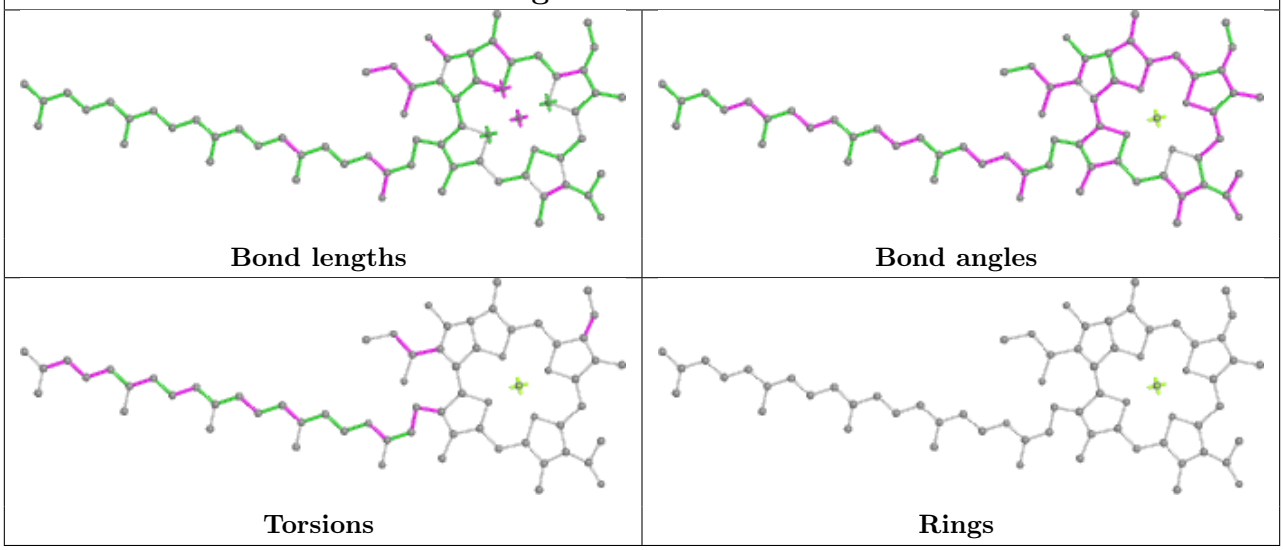

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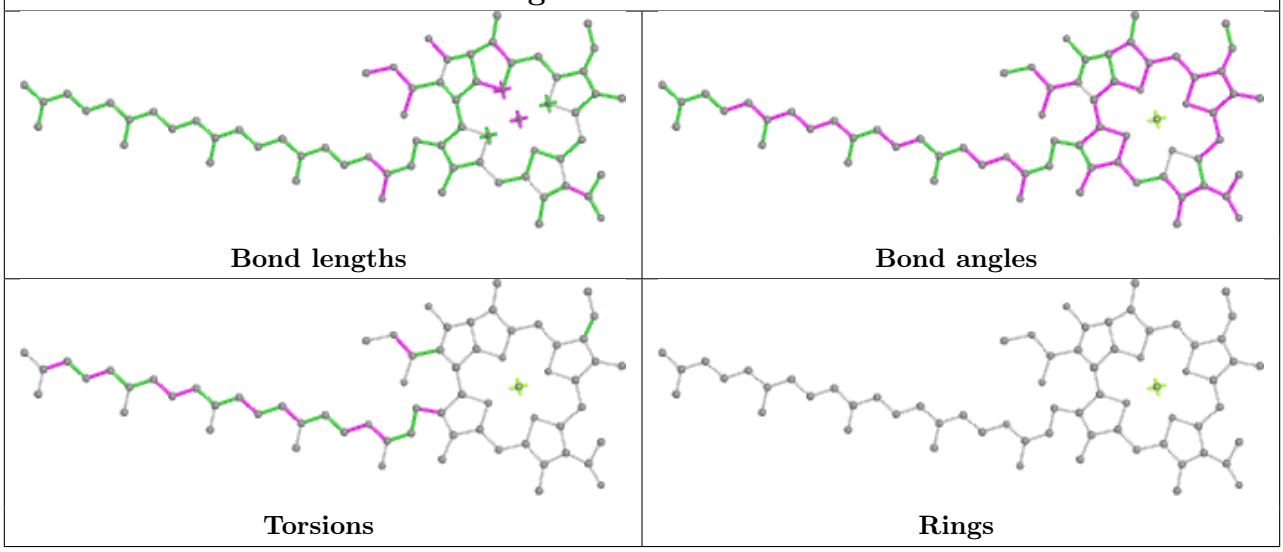
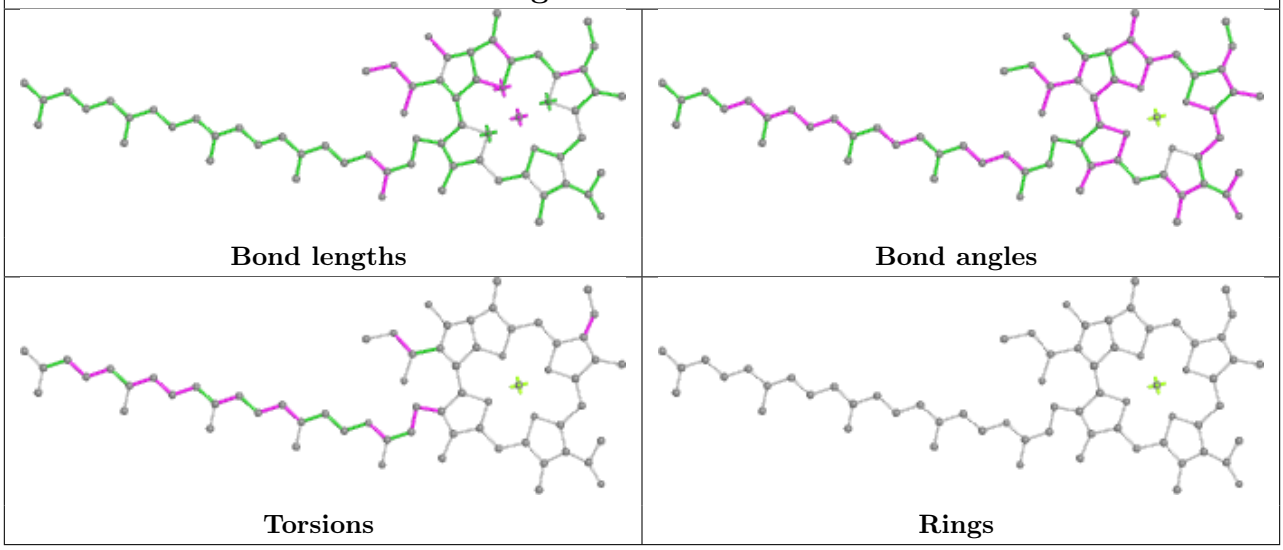
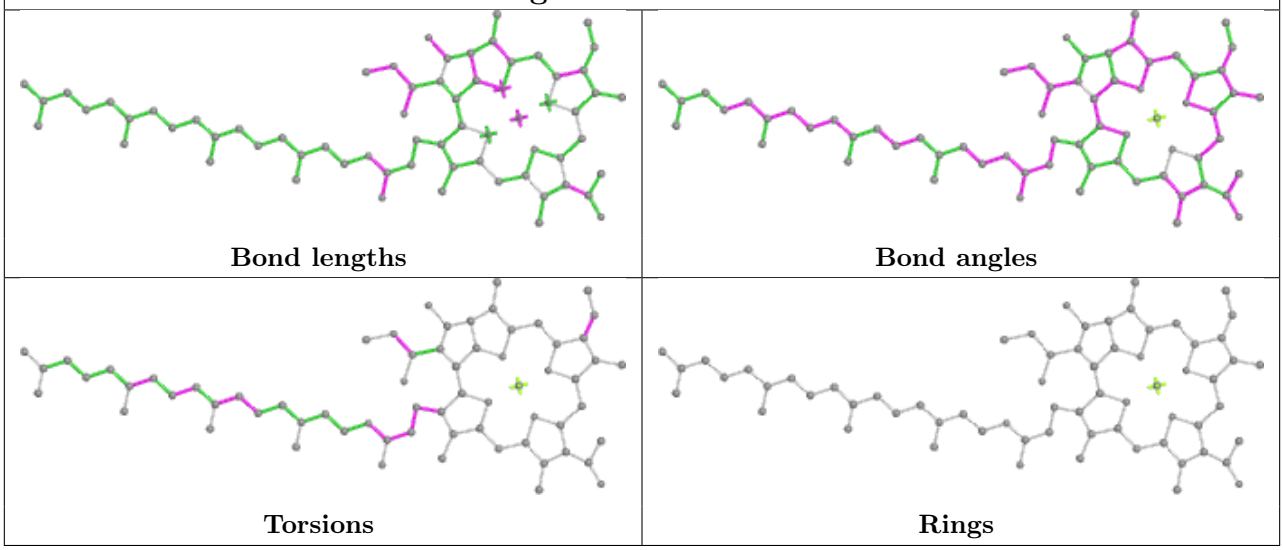


Ligand BCL c 101



Ligand BCL 4 102



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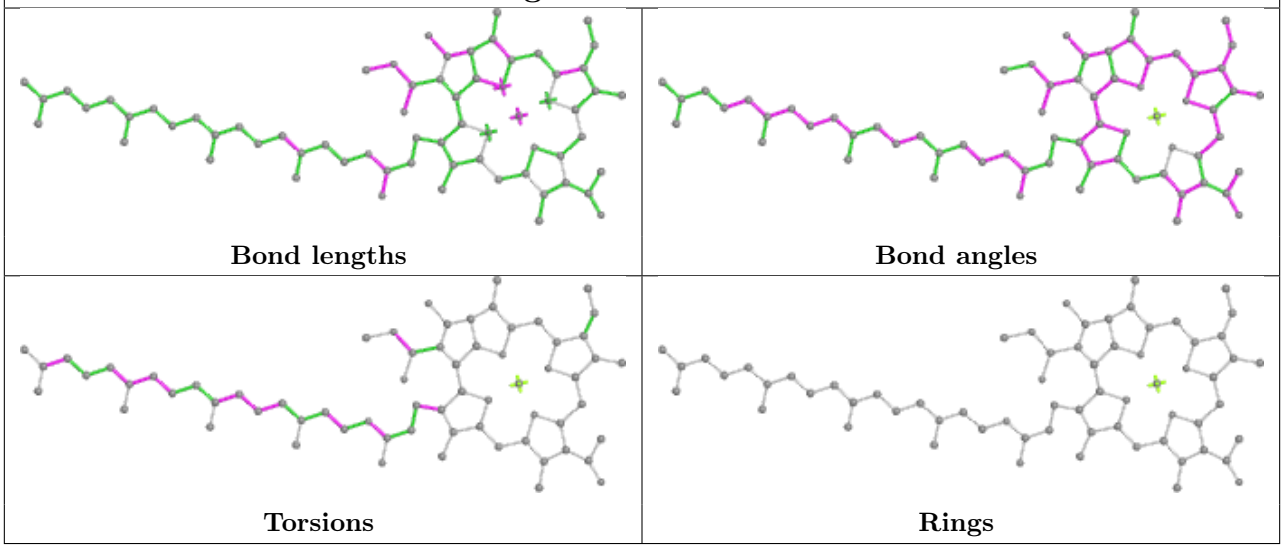
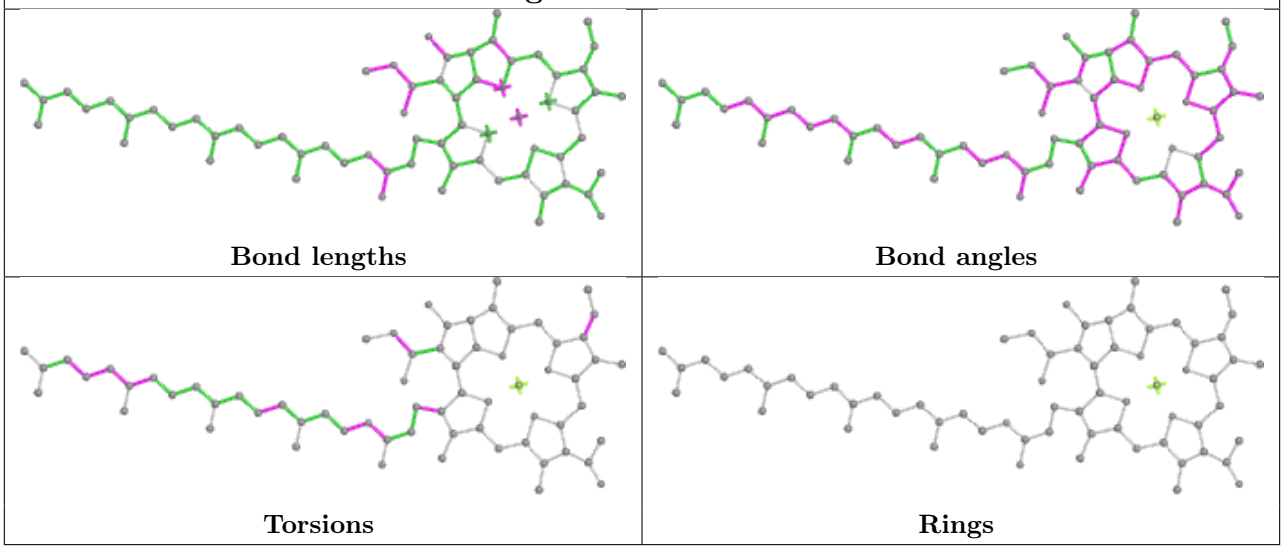
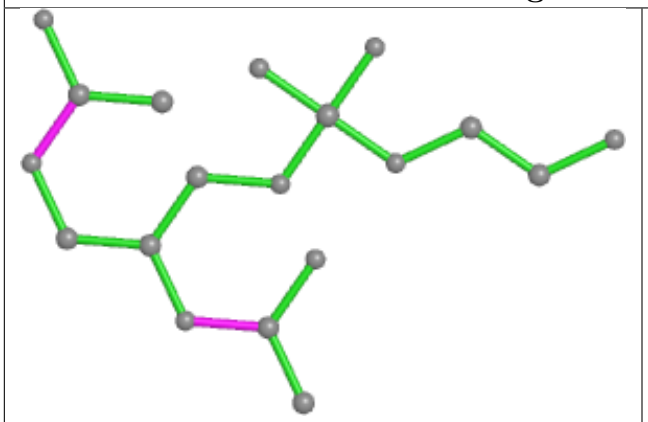


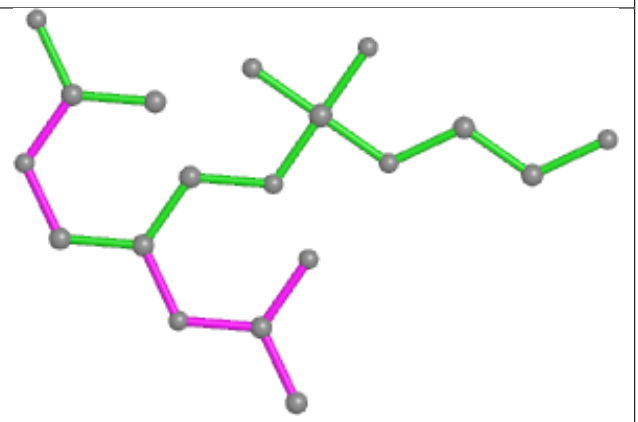
Ligand BCL D 102



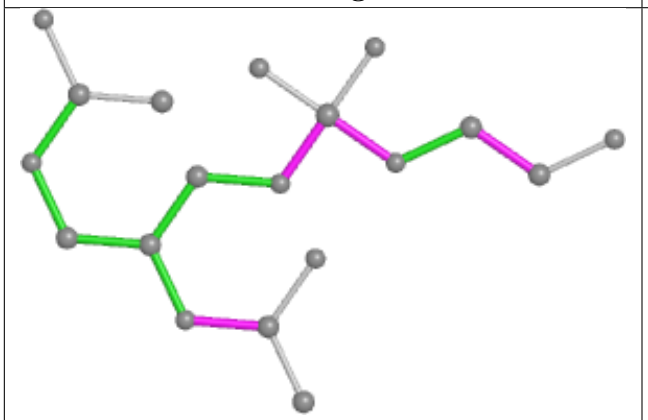
Ligand PEF A 101



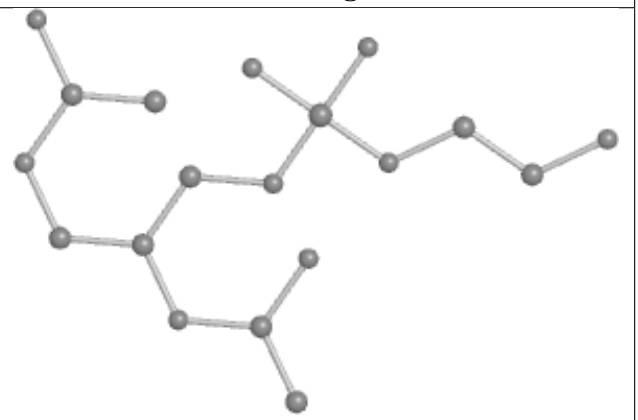
Bond lengths



Bond angles

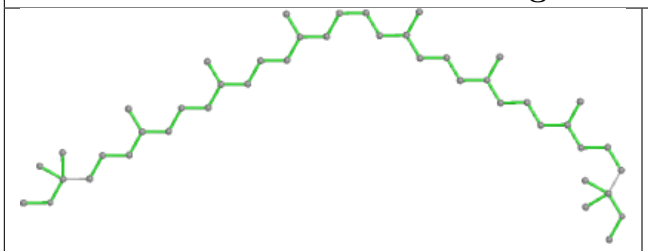


Torsions



Rings

Ligand CRT 7 101



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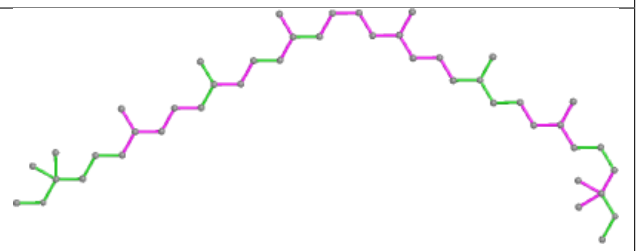
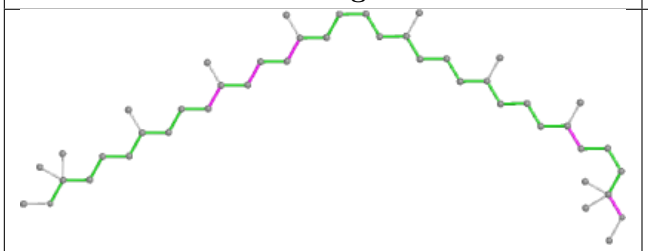


Bond angles



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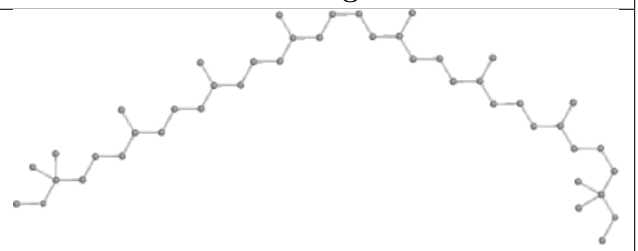
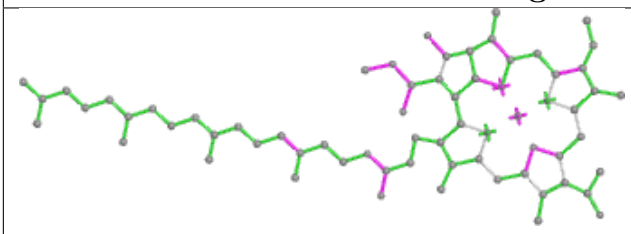
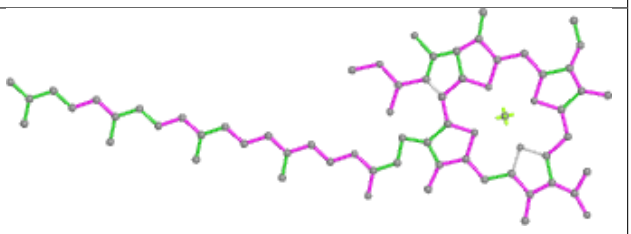
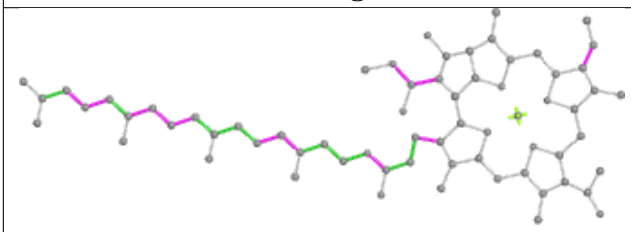
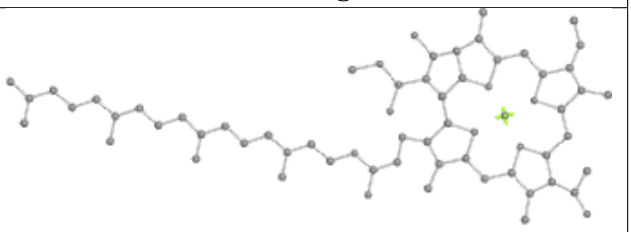
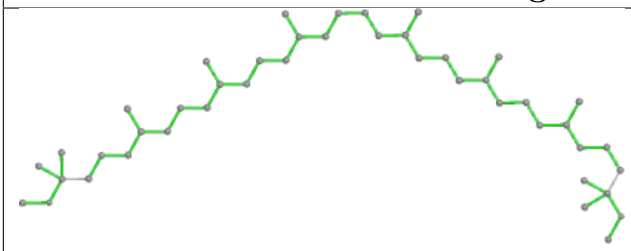
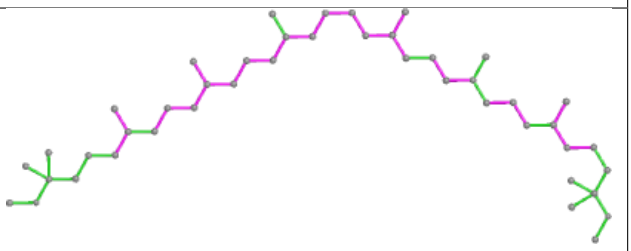
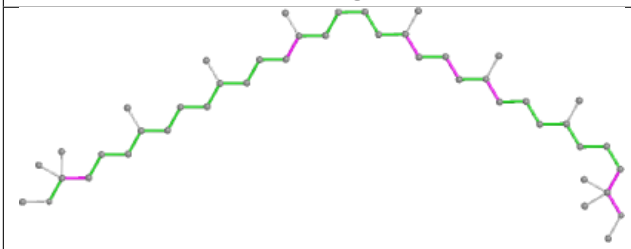
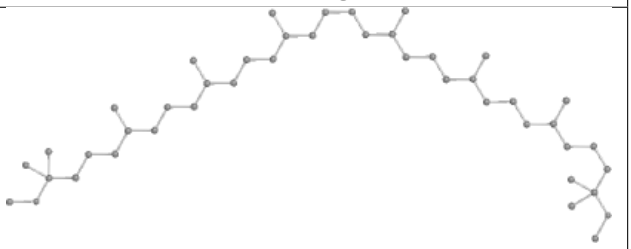
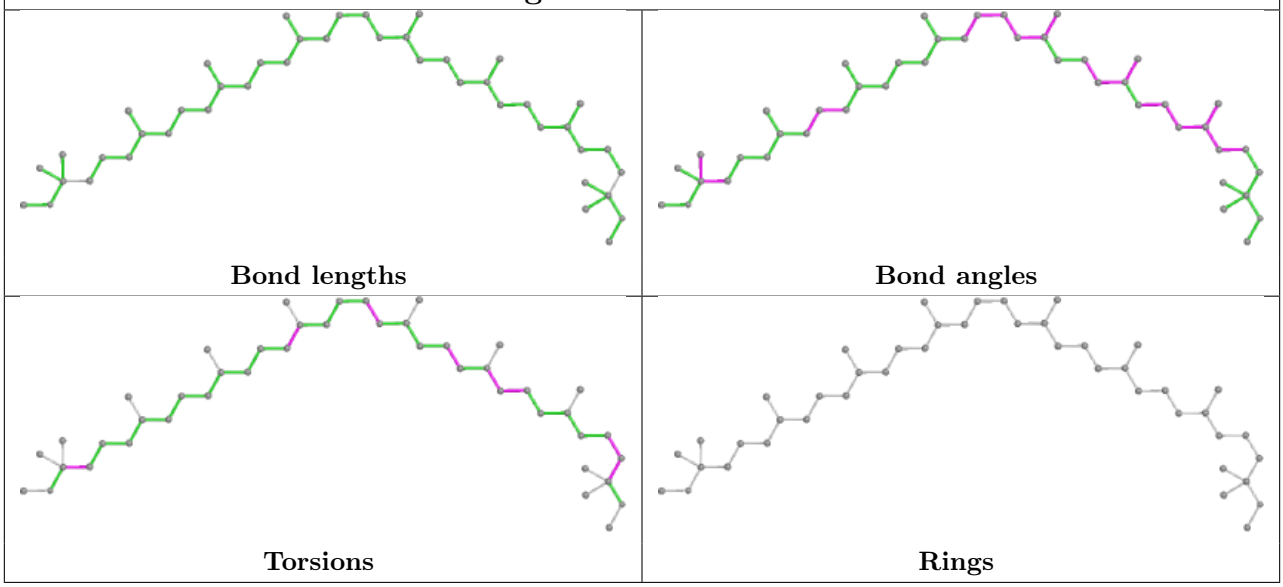


Rings

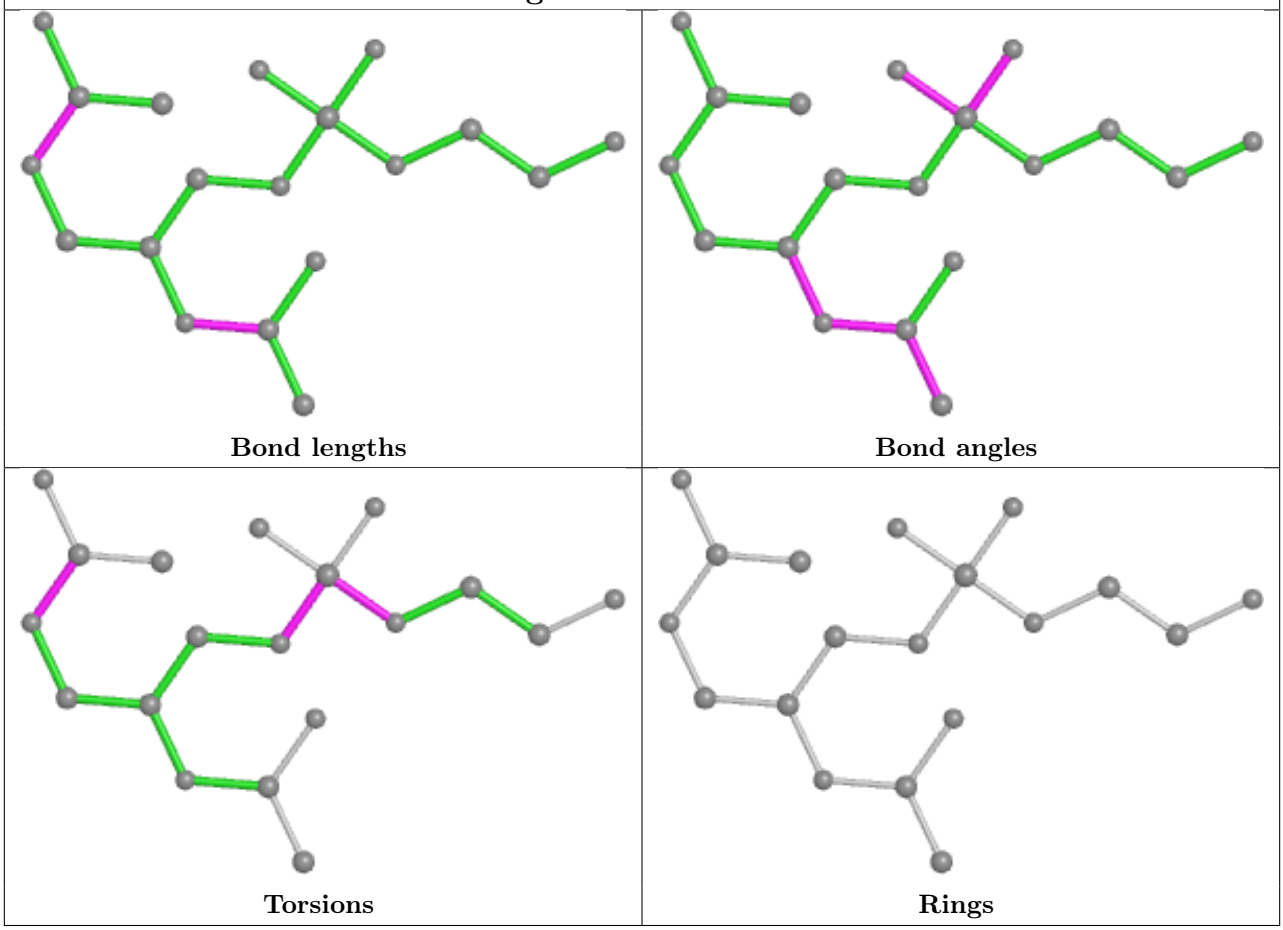
Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

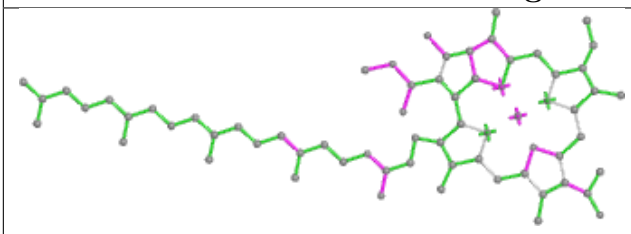
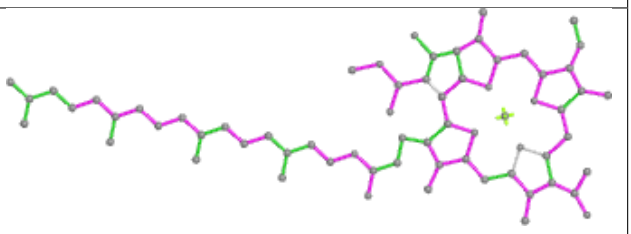
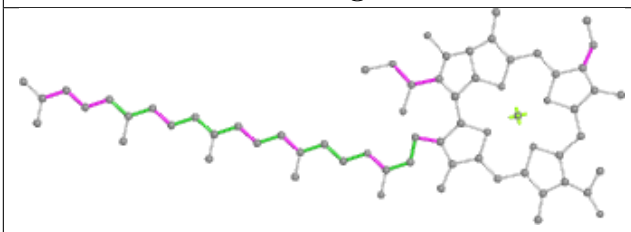
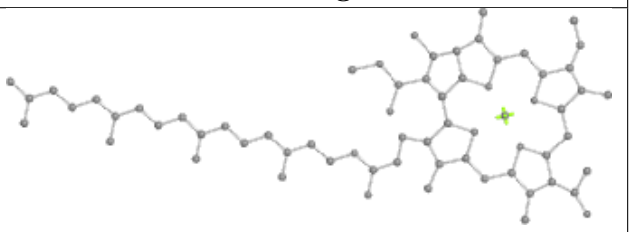
Ligand CRT e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CRT X 101



Ligand PEF H 301



Ligand BCL R 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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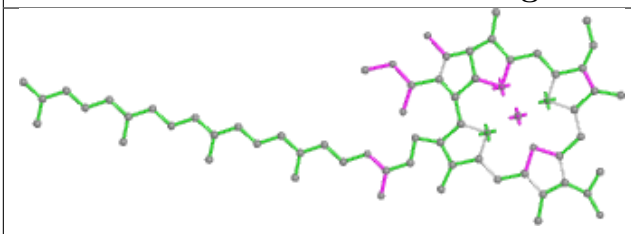
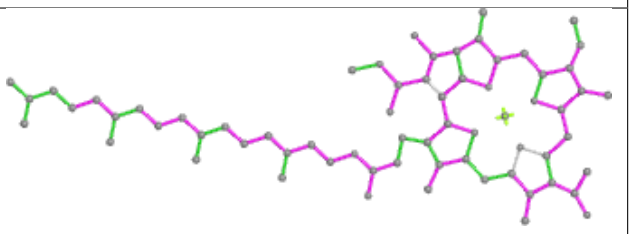
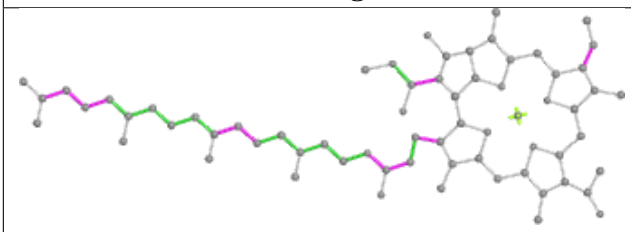
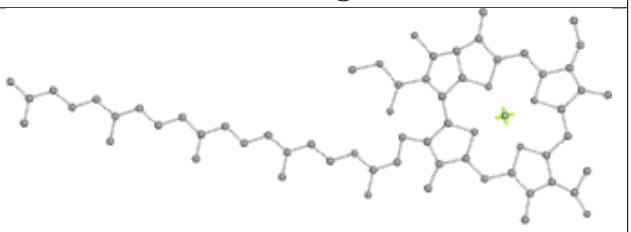
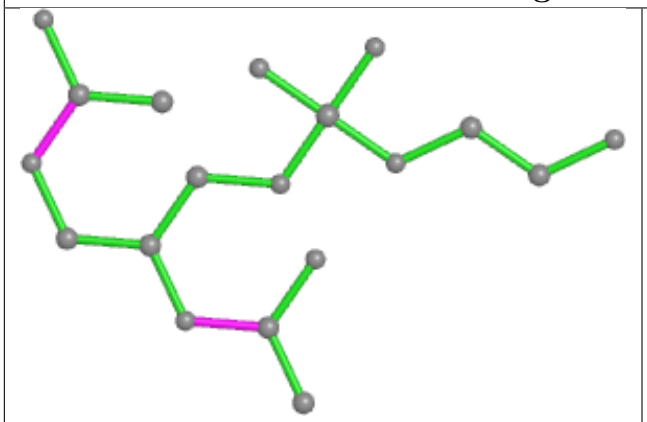
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF t 303



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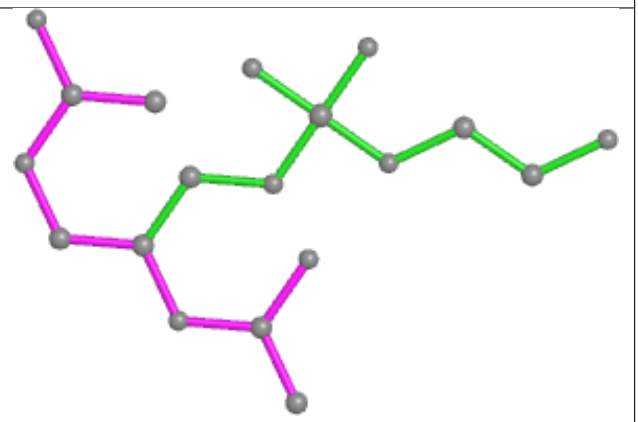

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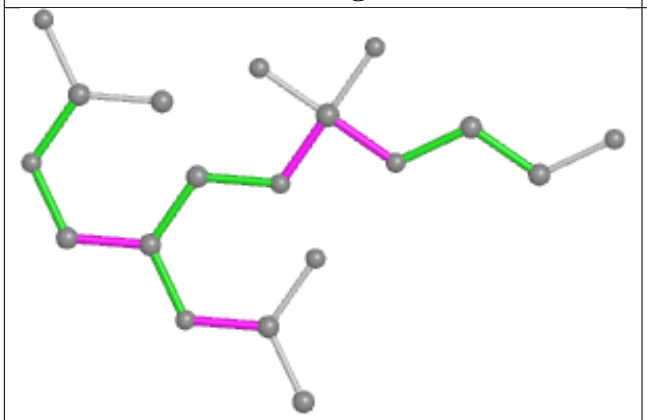

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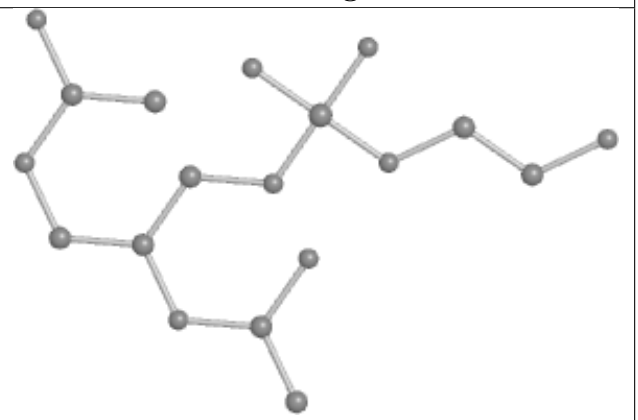
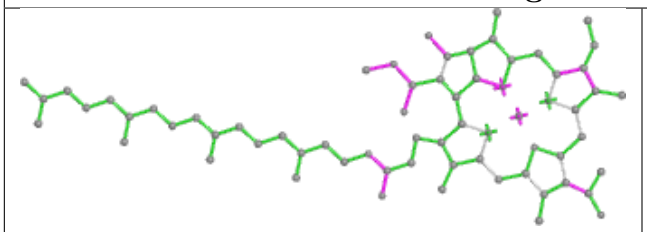


Rings

Ligand BCL Y 101



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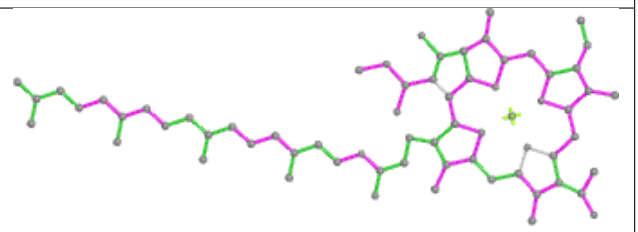

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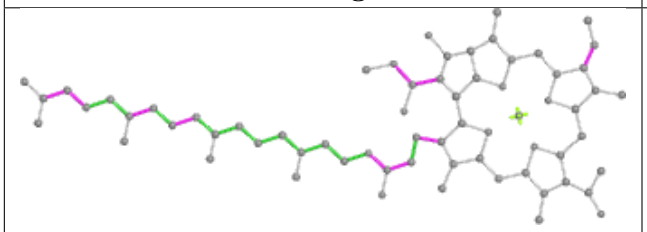

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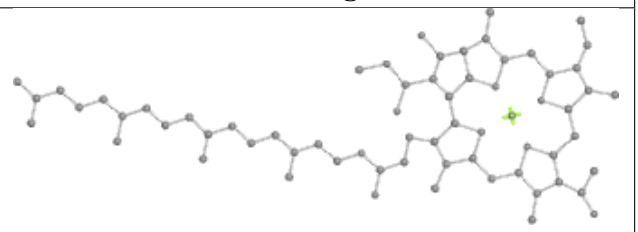

Rings

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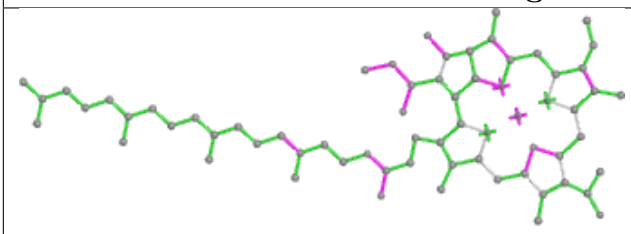
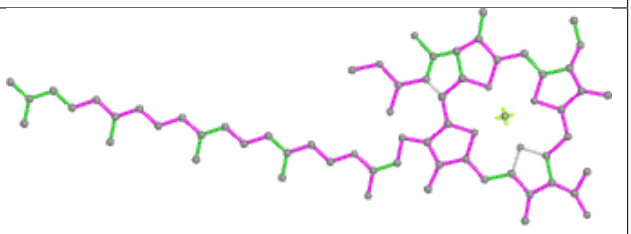
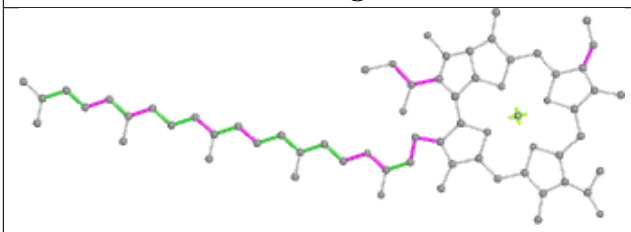
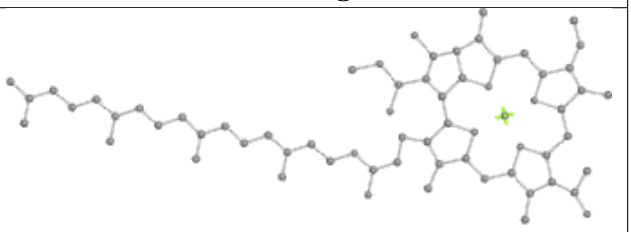
 Bond lengths	 Bond angles
 Torsions	 Rings

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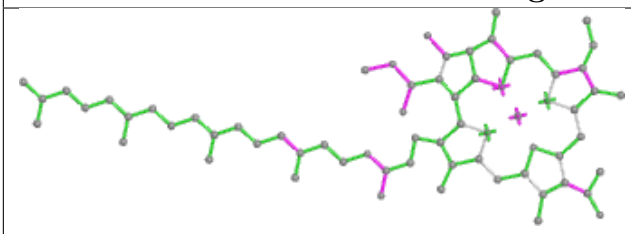
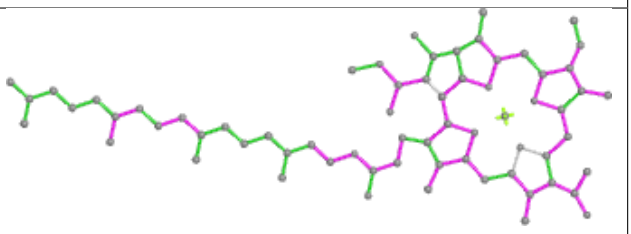
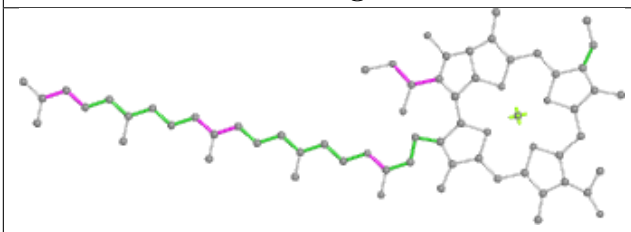
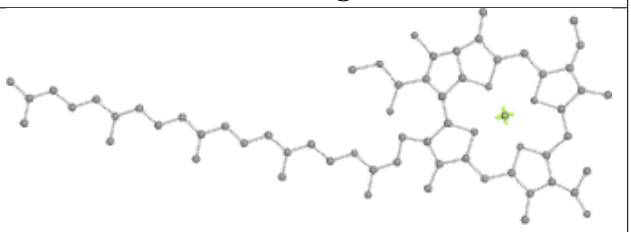
 Bond lengths	 Bond angles
 Torsions	 Rings

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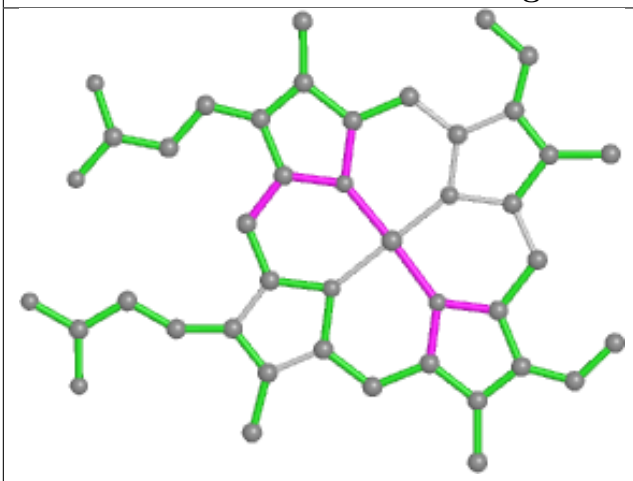

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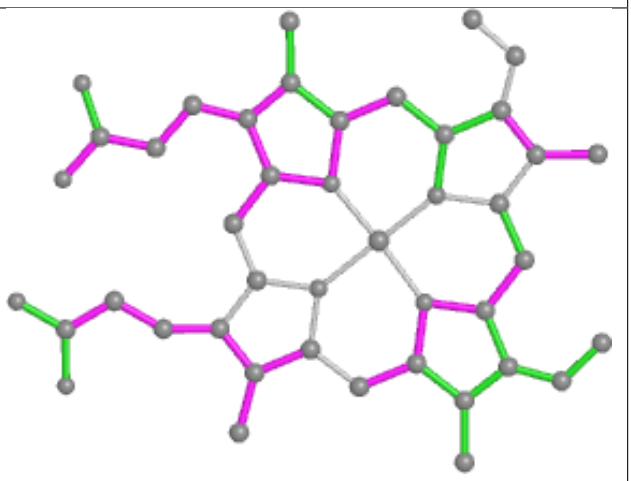
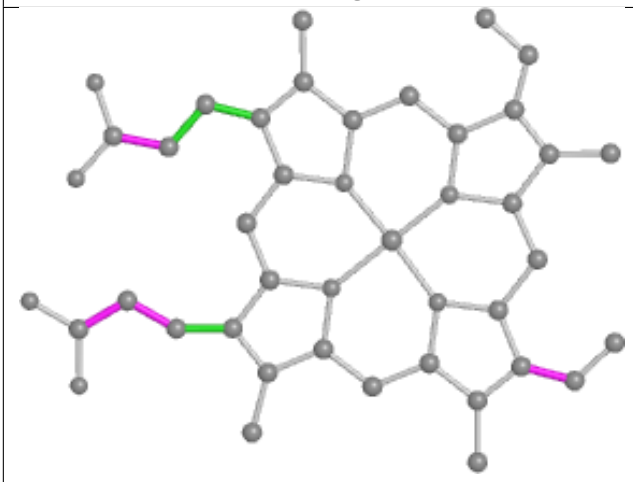


Bond angles



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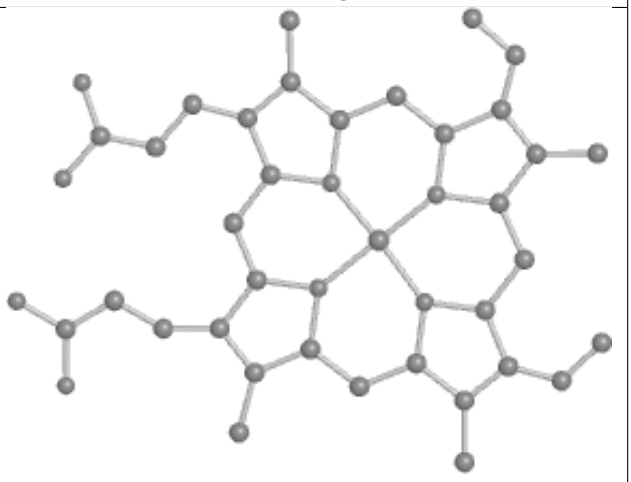

Rings

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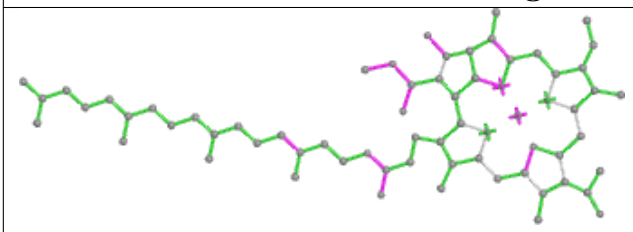

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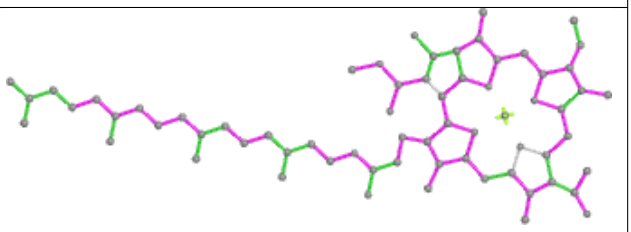

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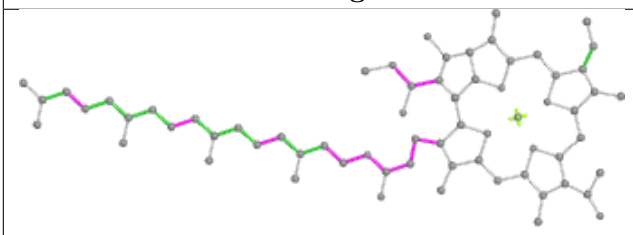

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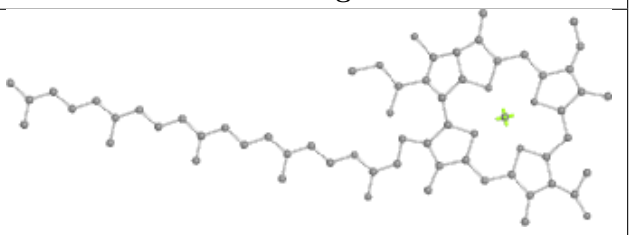
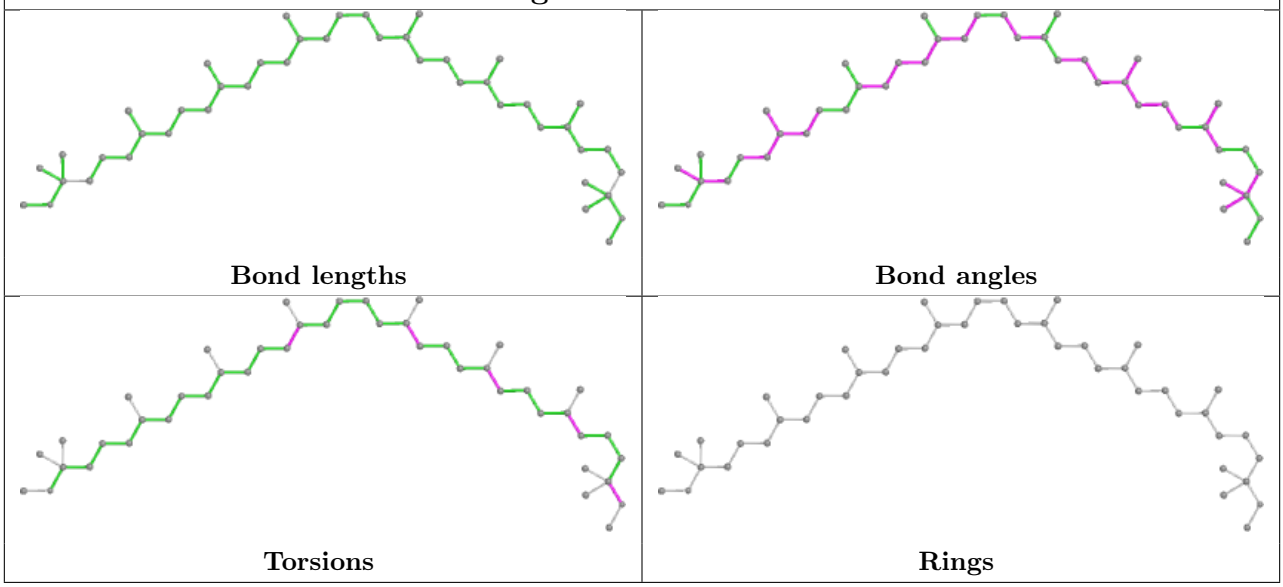
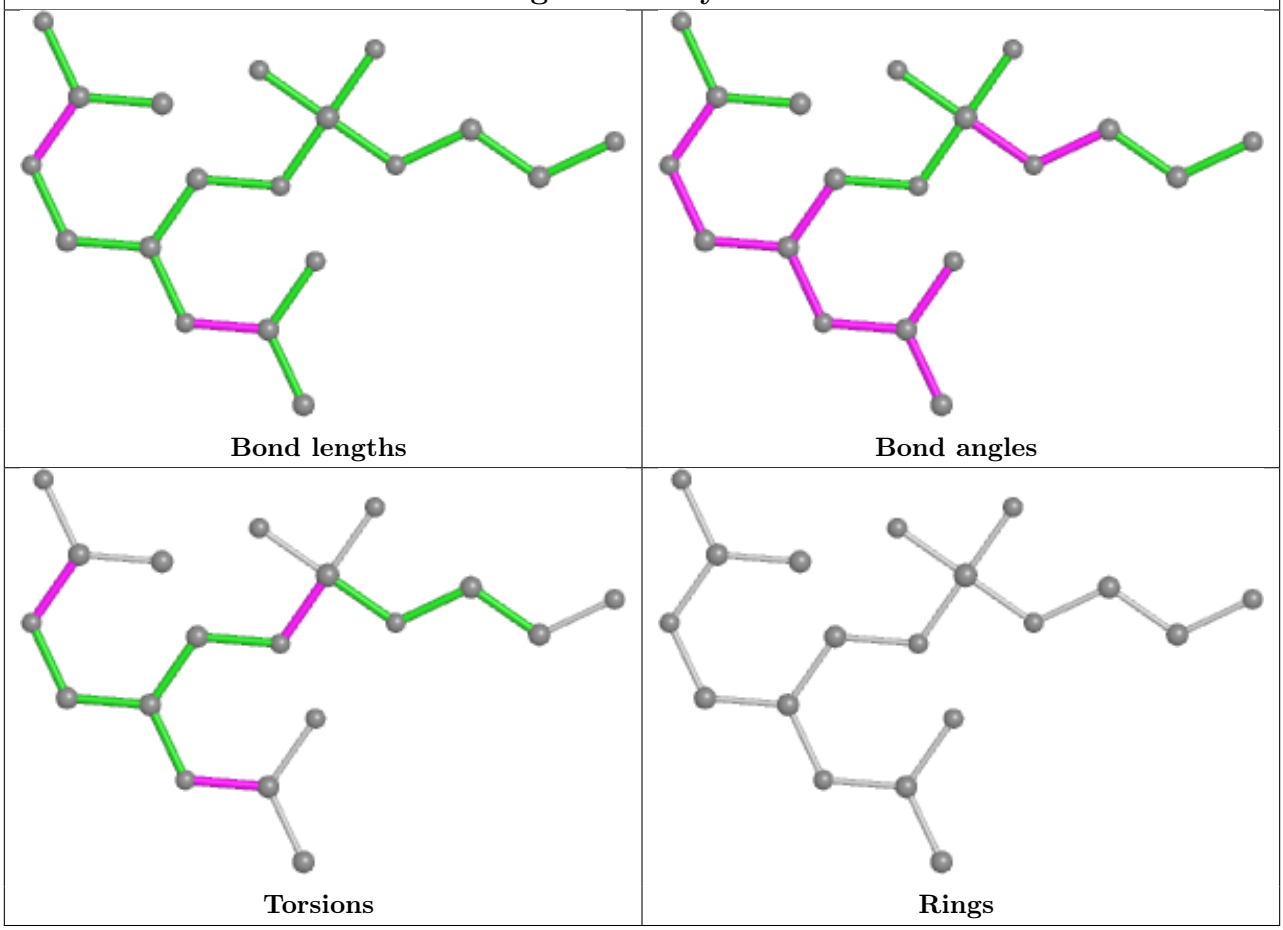


Rings

Ligand CRT s 101



Ligand PEF y 408



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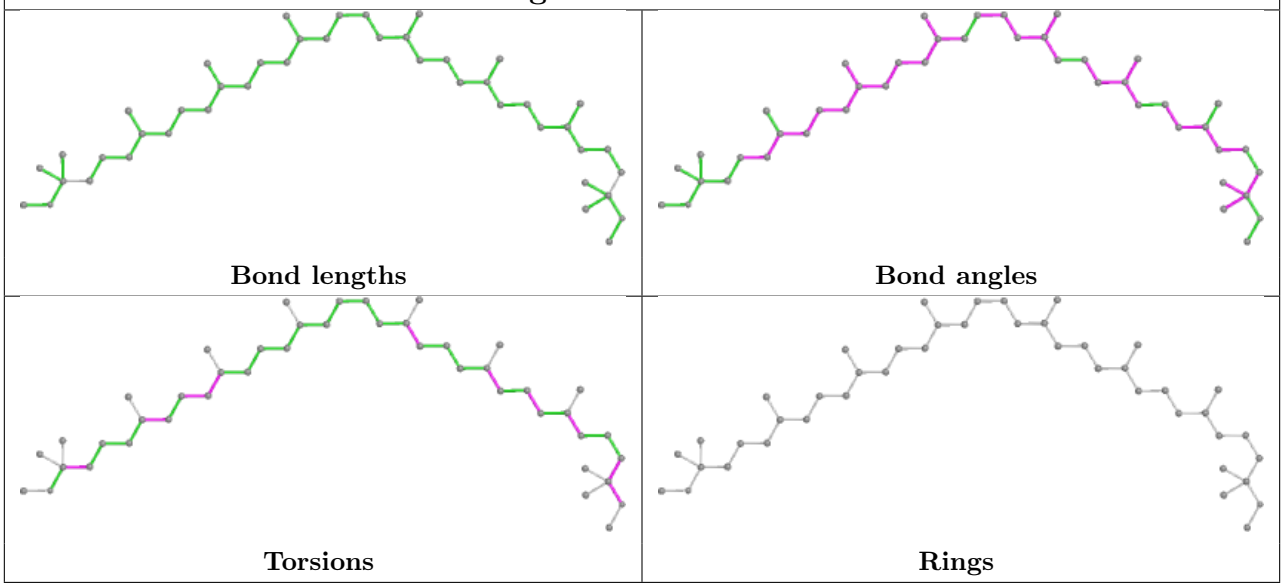

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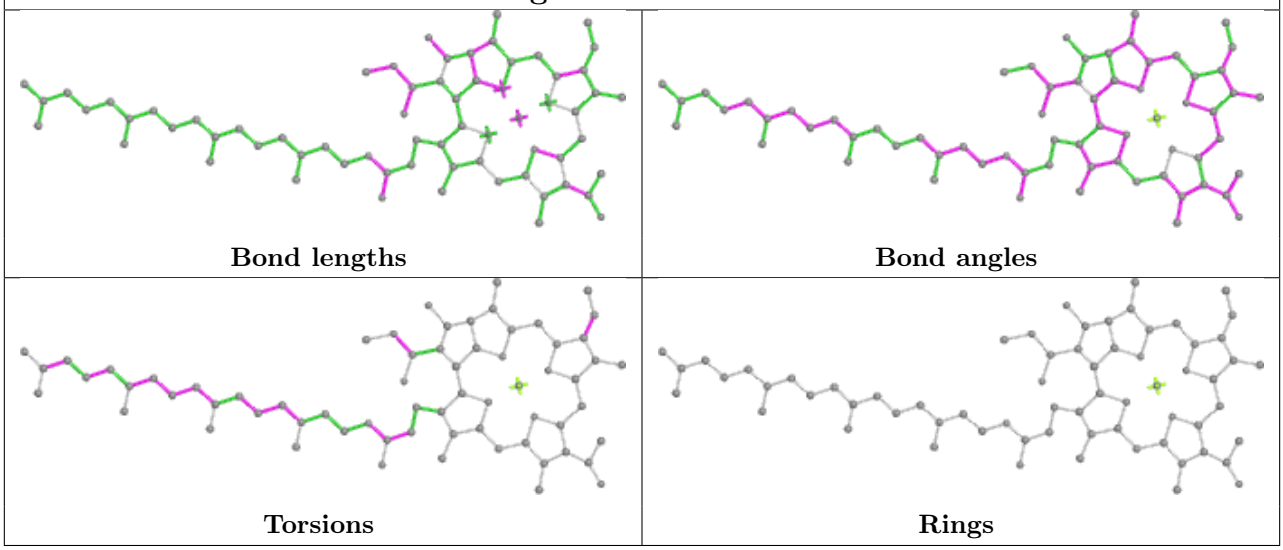

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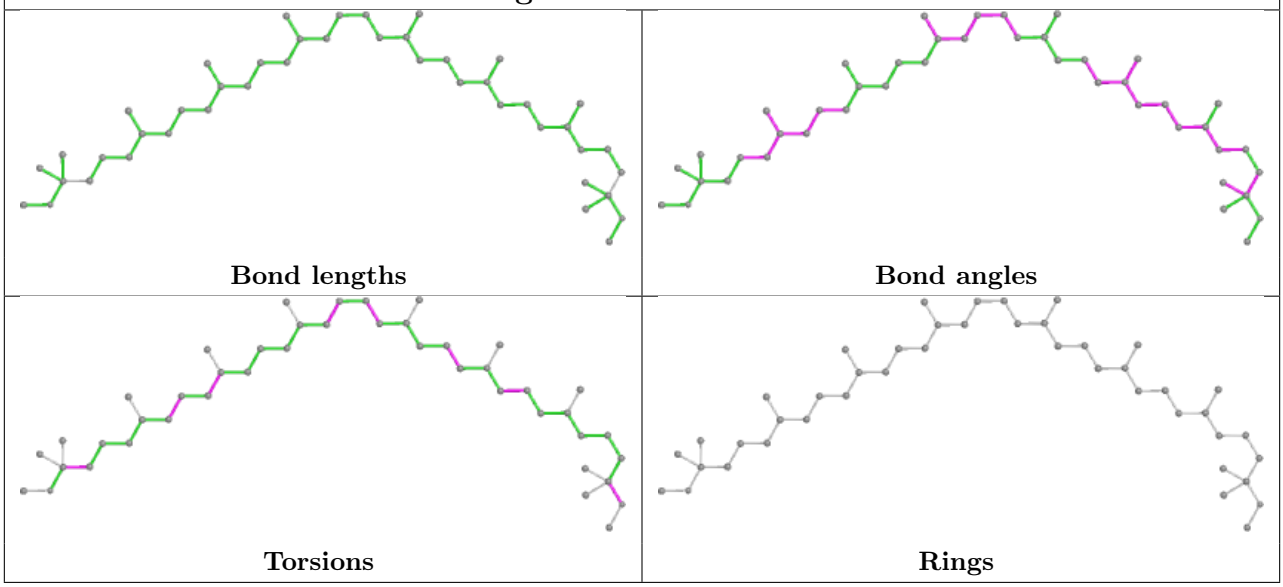

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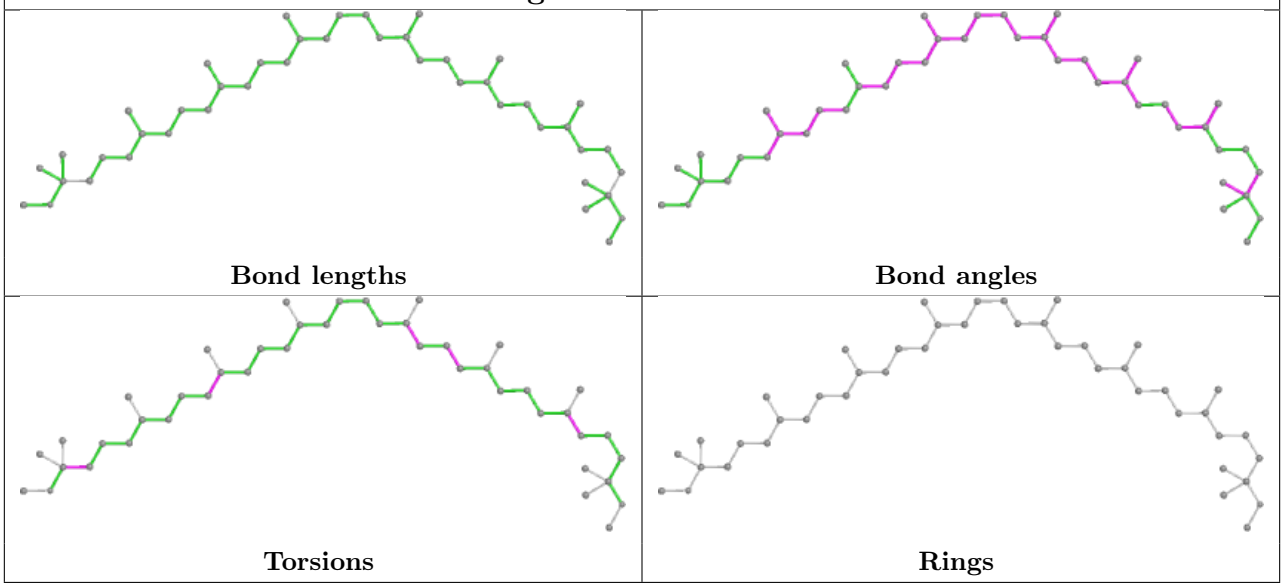

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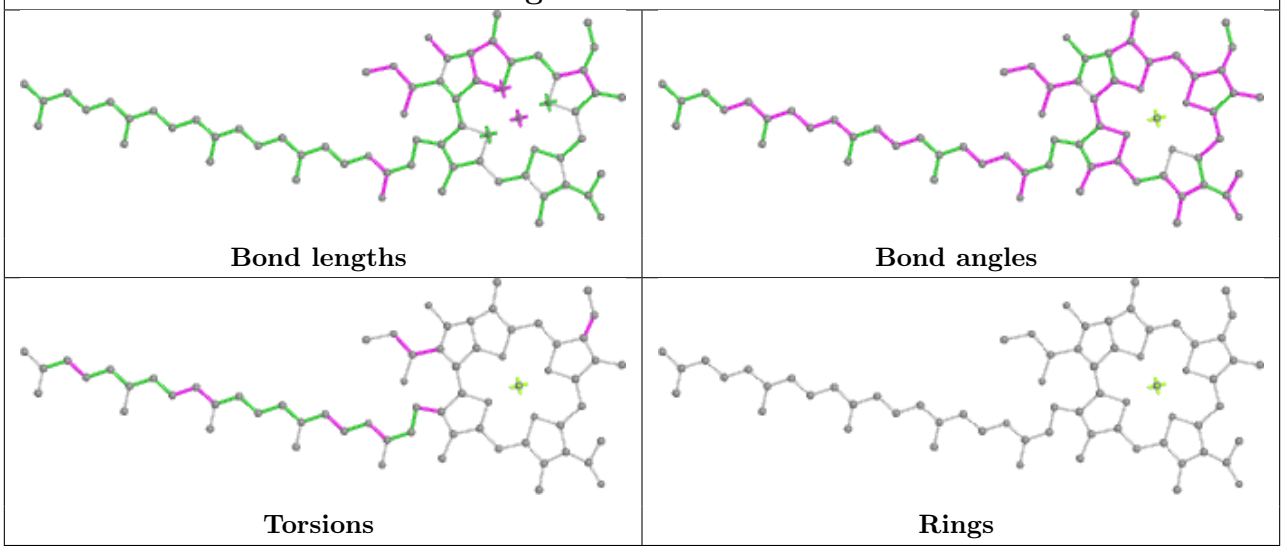

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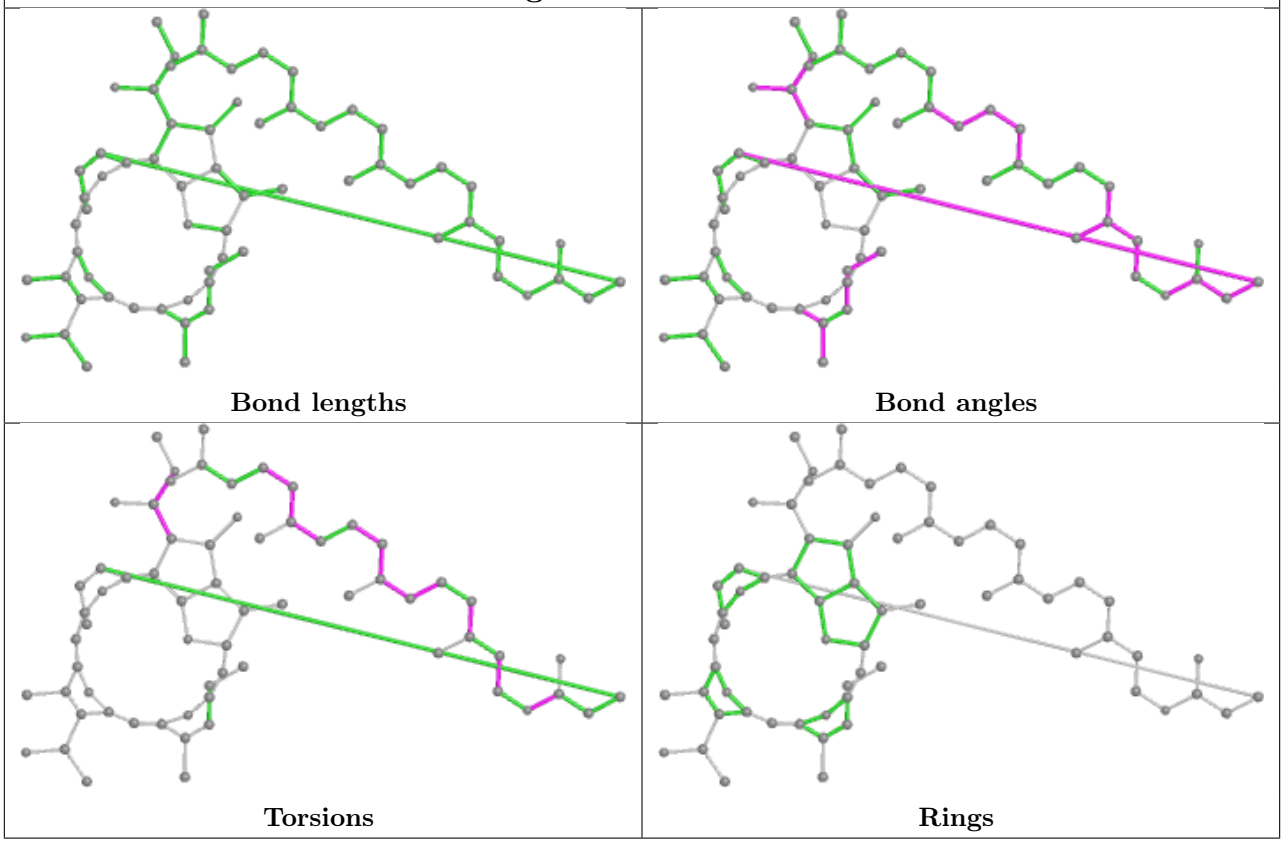

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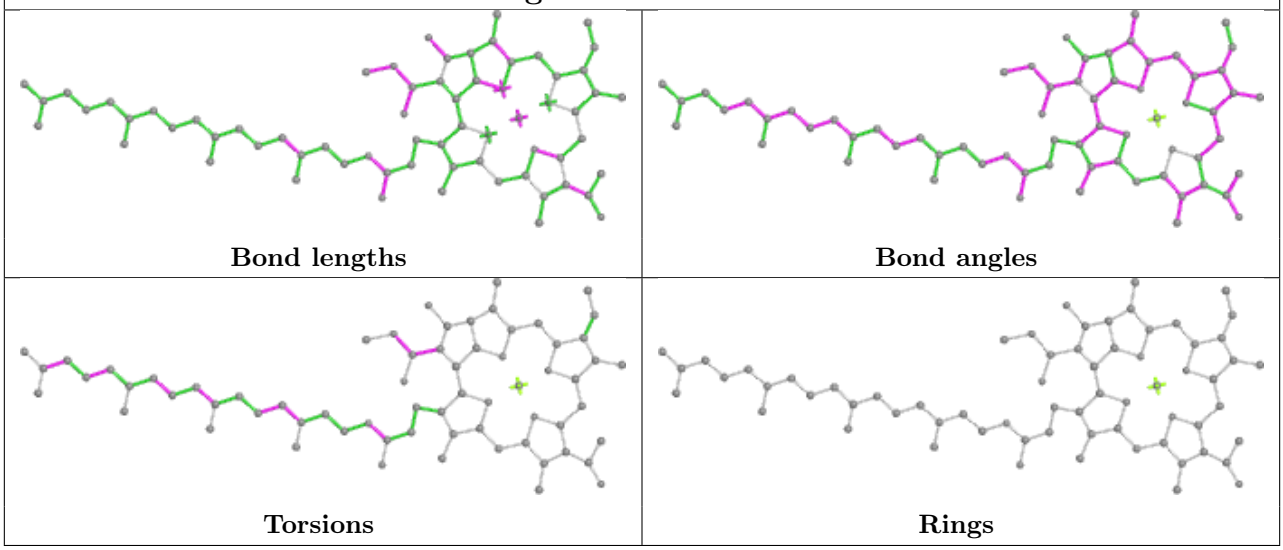

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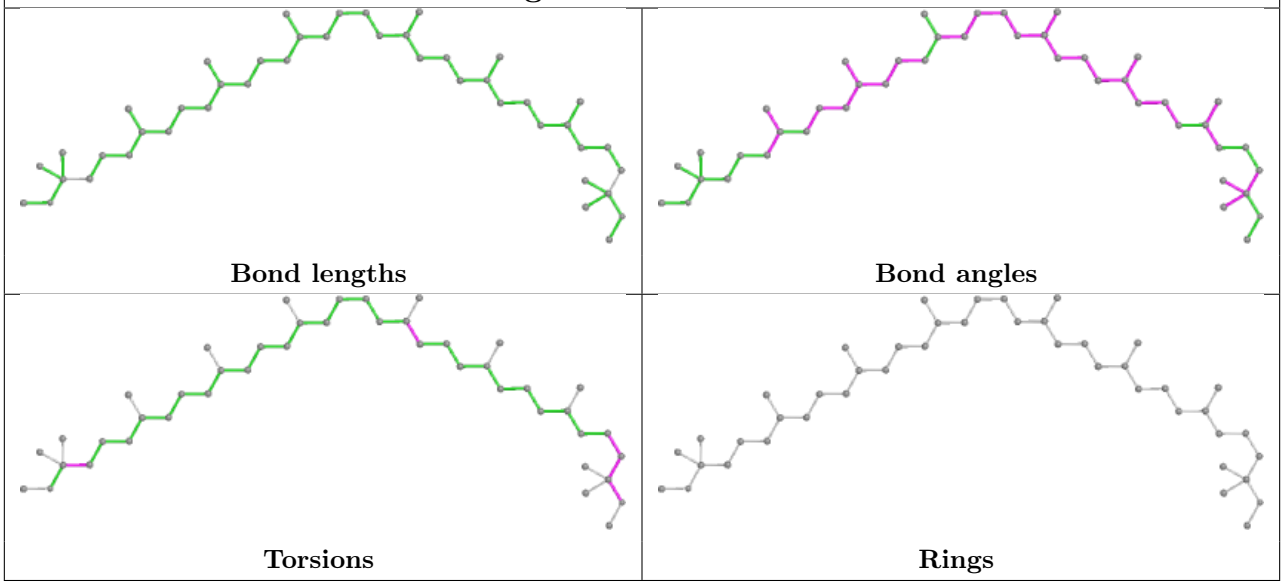

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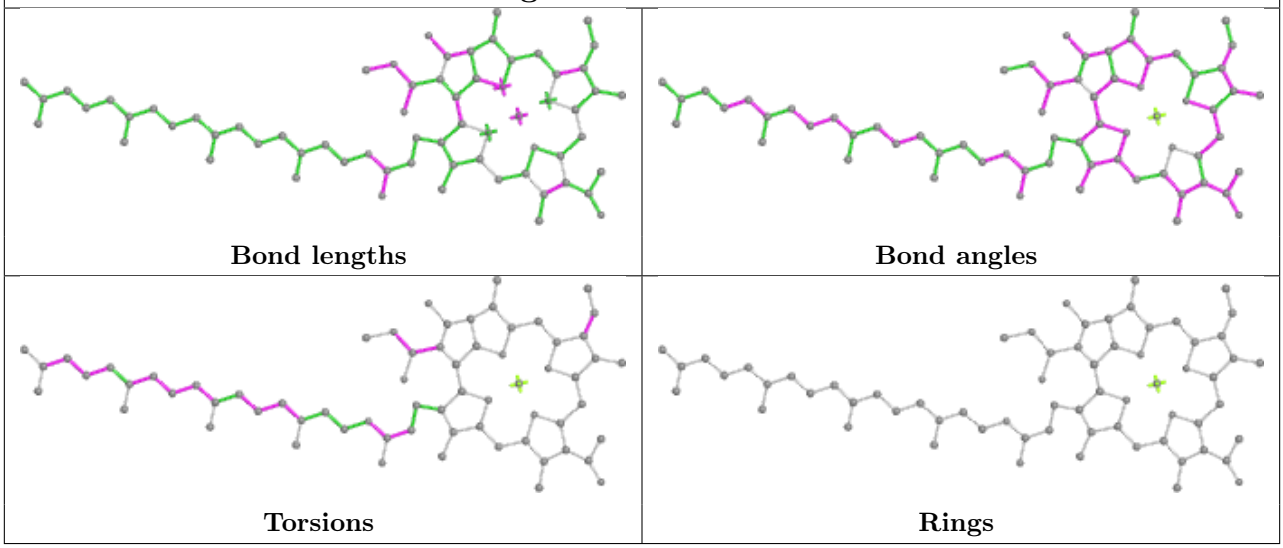

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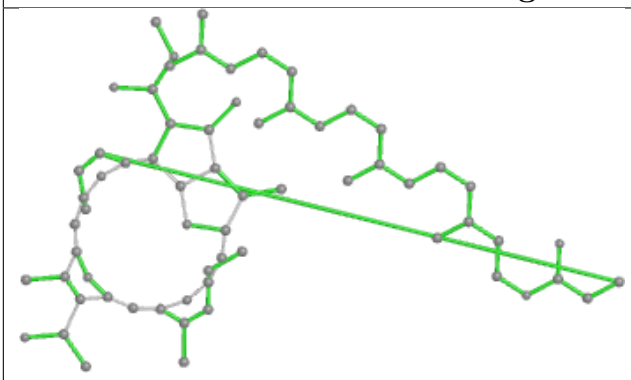
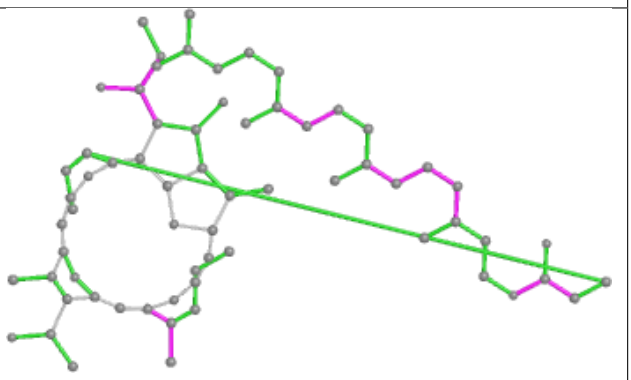
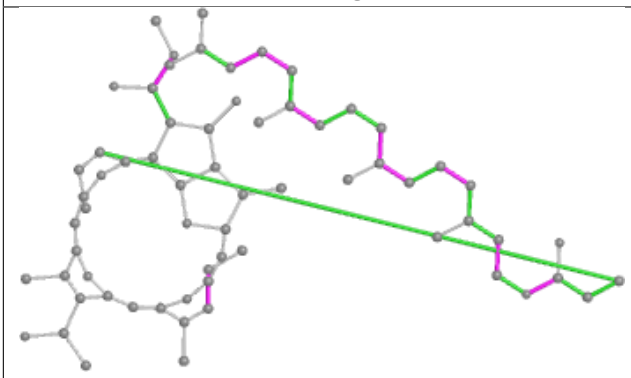


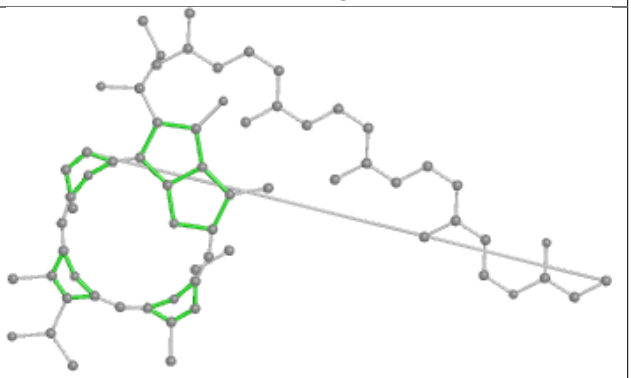
Bond lengths



Bond angles

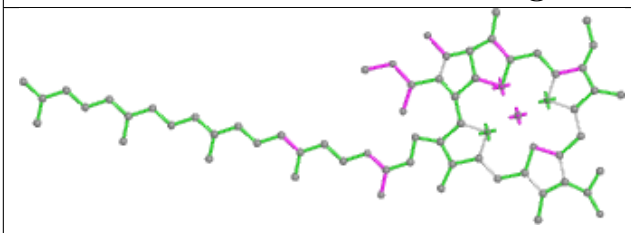


Torsions



Rings

Ligand BCL u 102



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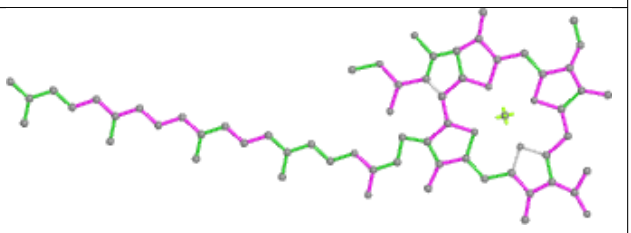
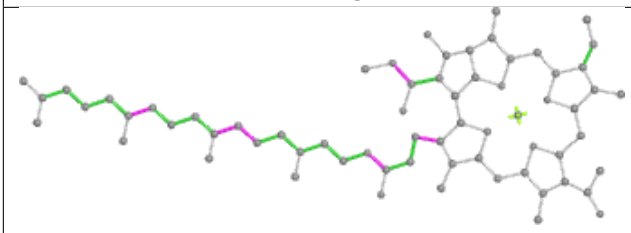


Bond angles



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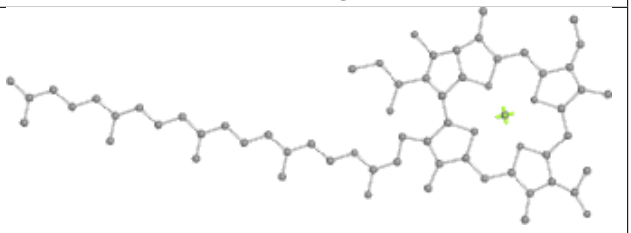

Rings

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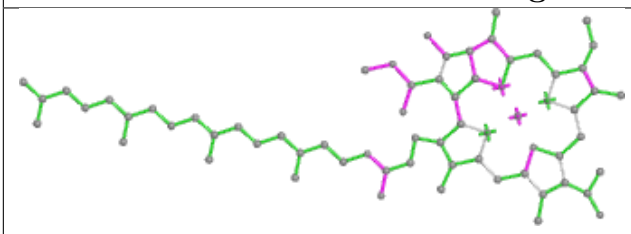
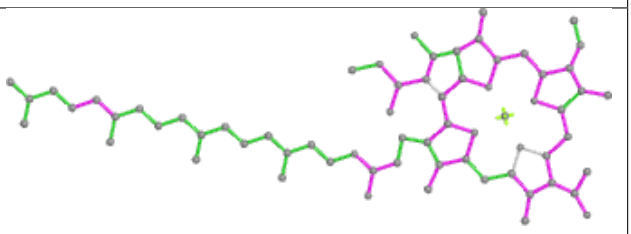
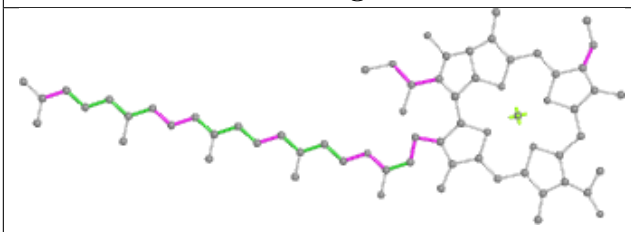
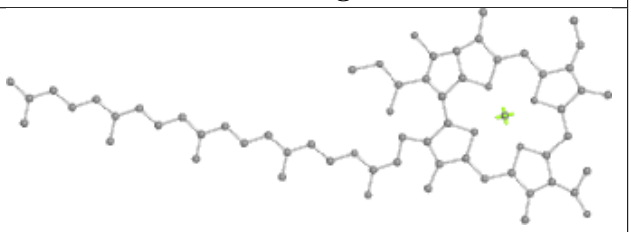
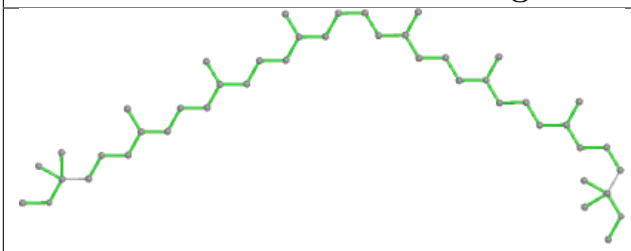
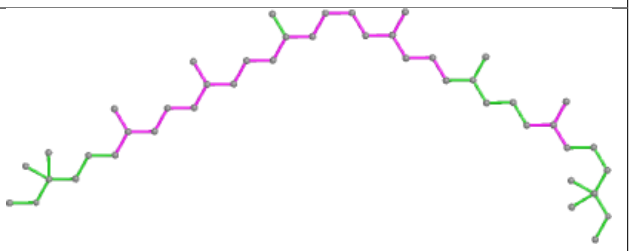
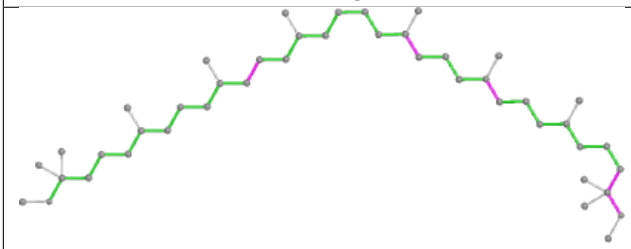
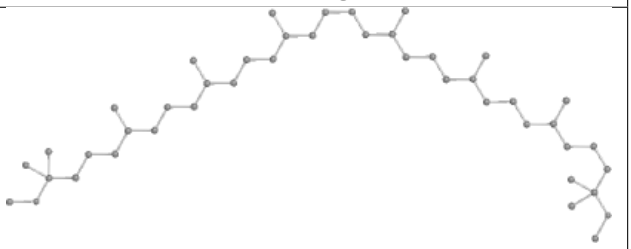
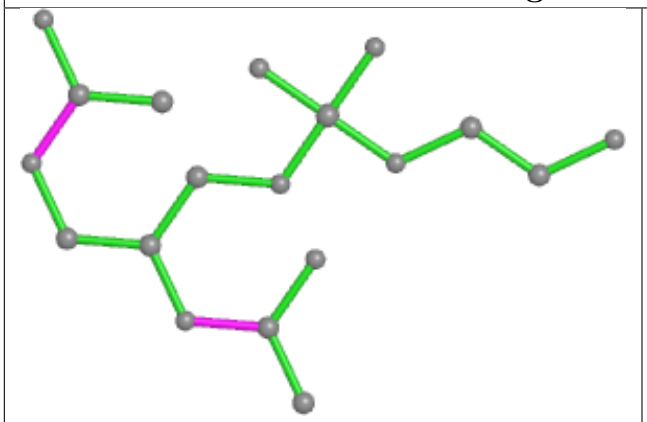
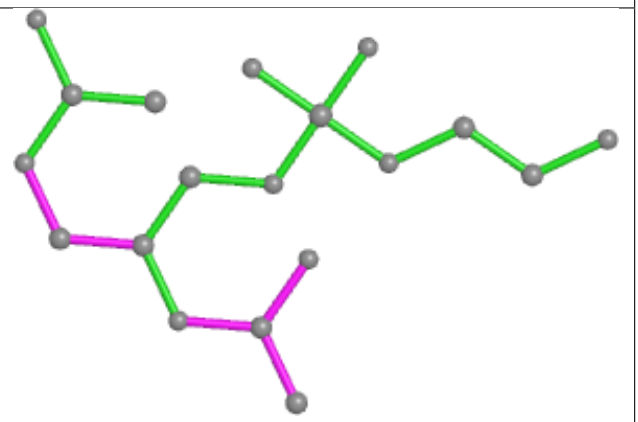
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CRT AC 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF H 305



Bond lengths



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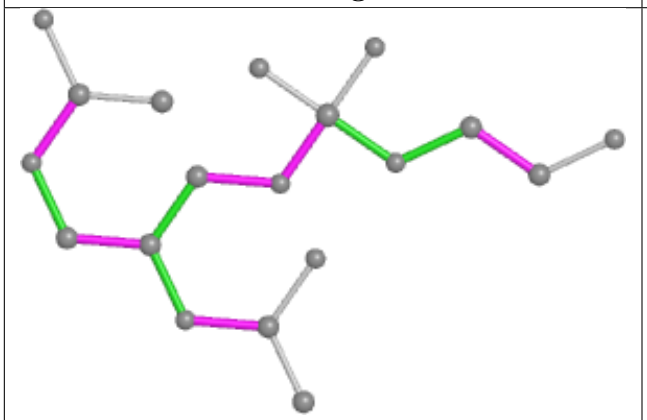
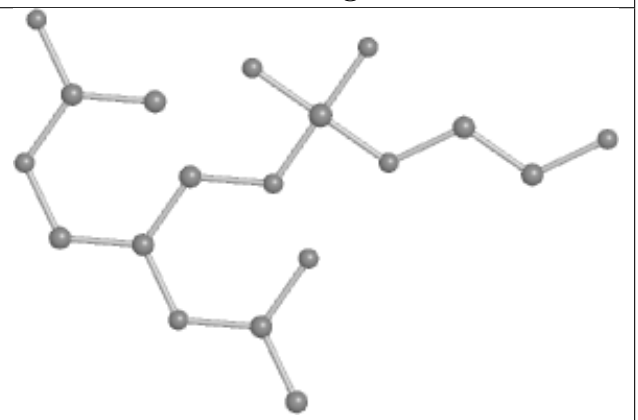
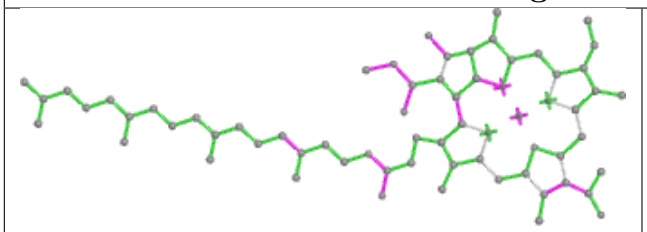


Torsions

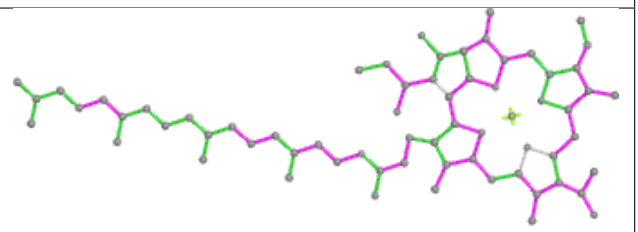


Rings

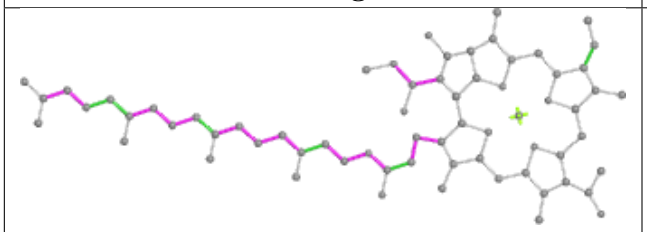
Ligand BCL 8 101



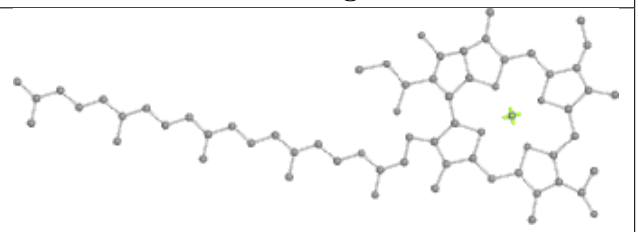
Bond lengths



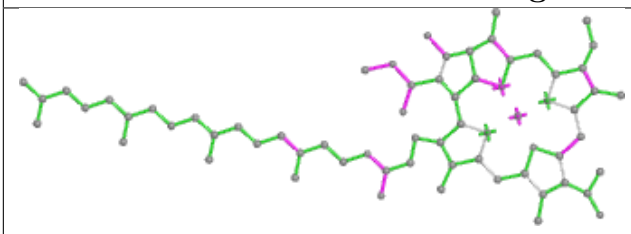
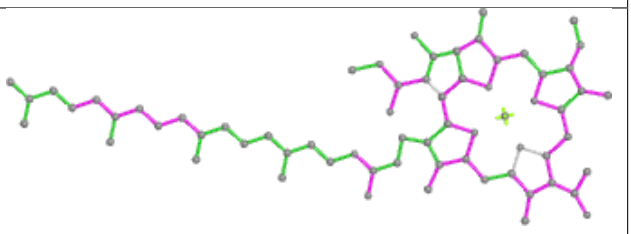
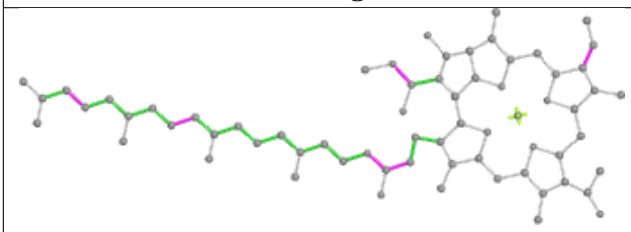
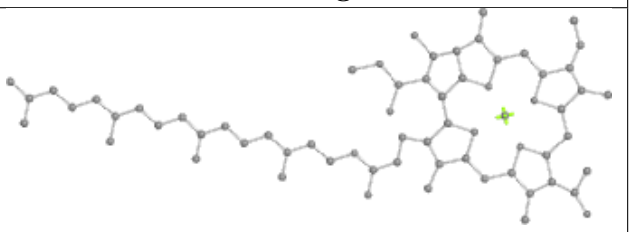
Bond angles



Torsions



Rings

Ligand BCL 5 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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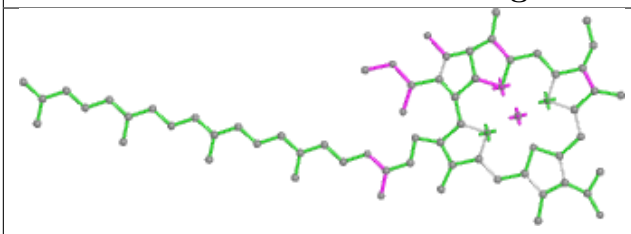
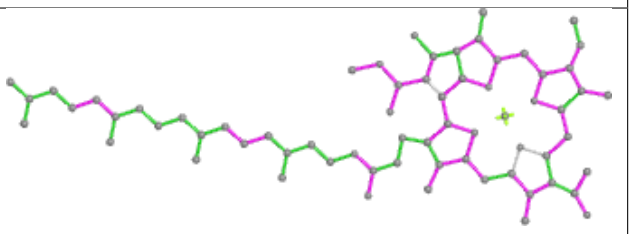
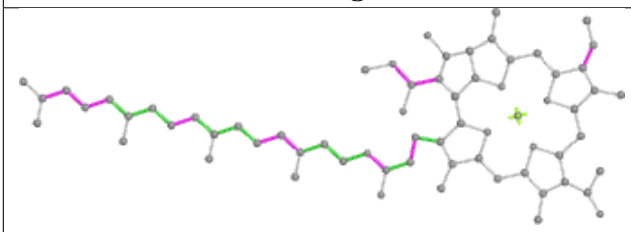
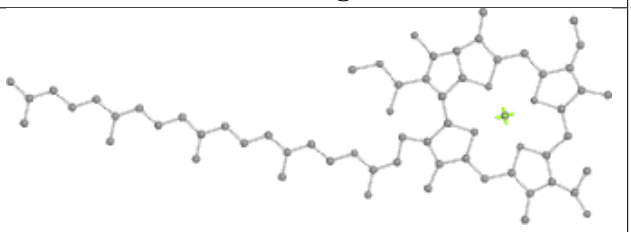
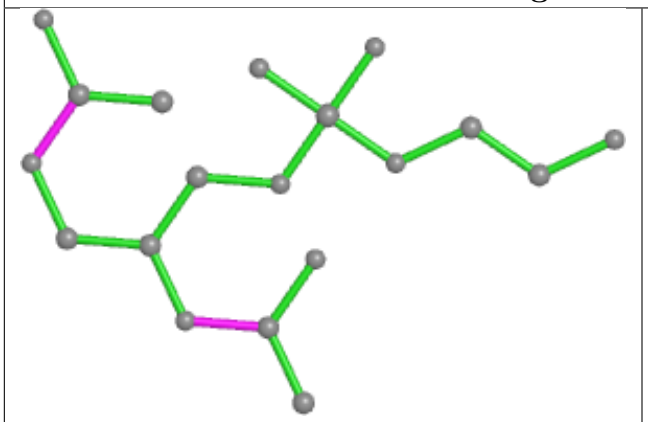
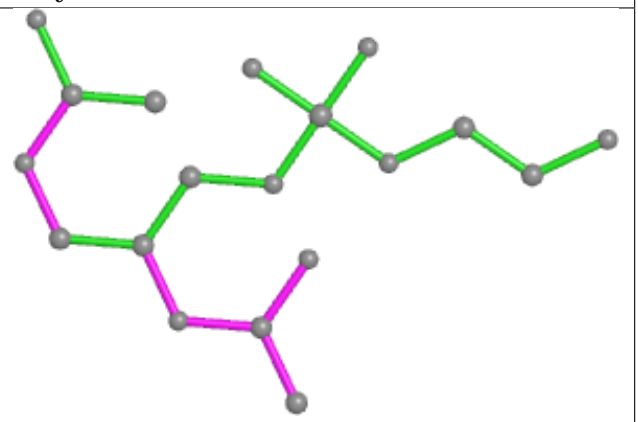
 Bond lengths	 Bond angles
 Torsions	 Rings

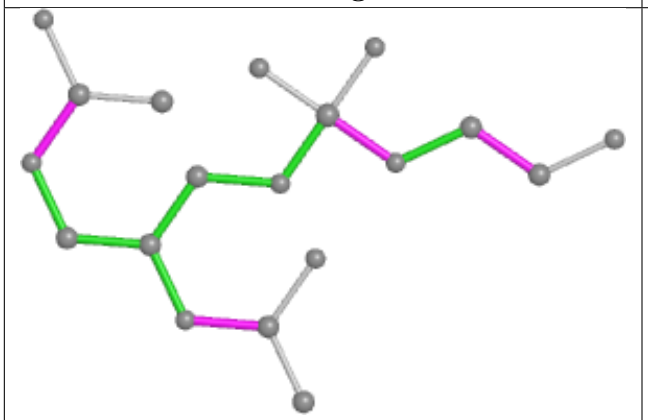
Ligand PEF y 406



Bond lengths



Bond angles



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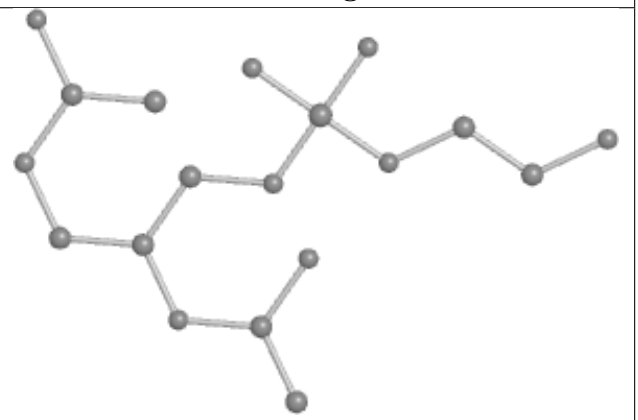
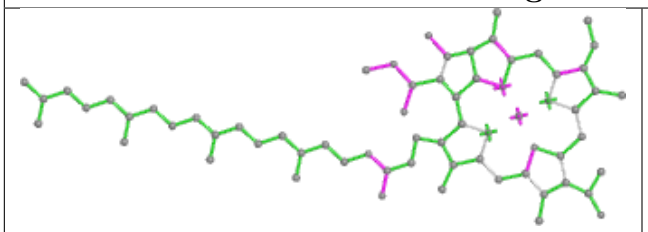


Rings

Ligand BCL D 101



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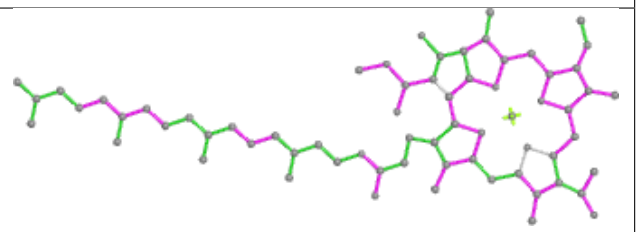
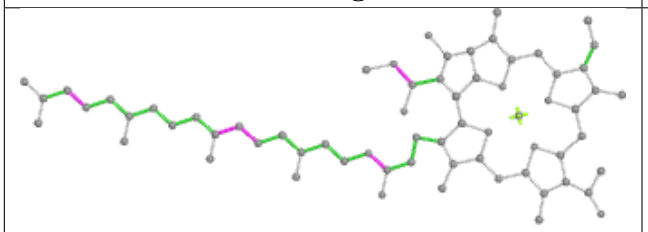


Bond angles



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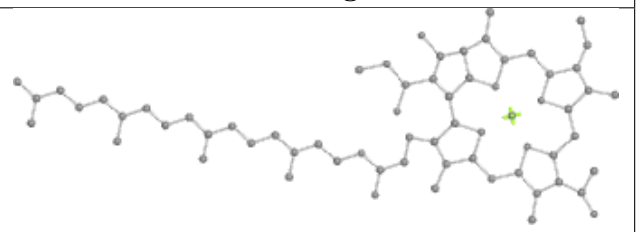
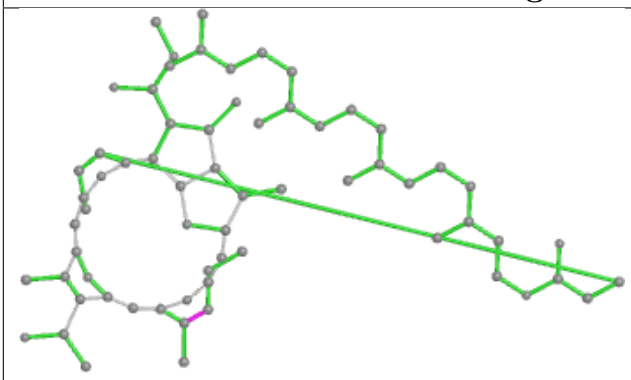
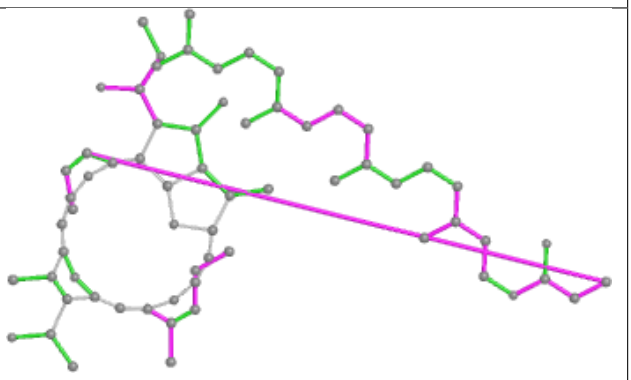


Rings

Ligand BPH x 302



Bond lengths



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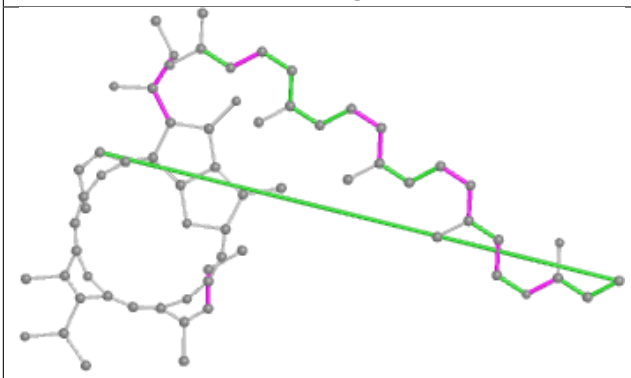

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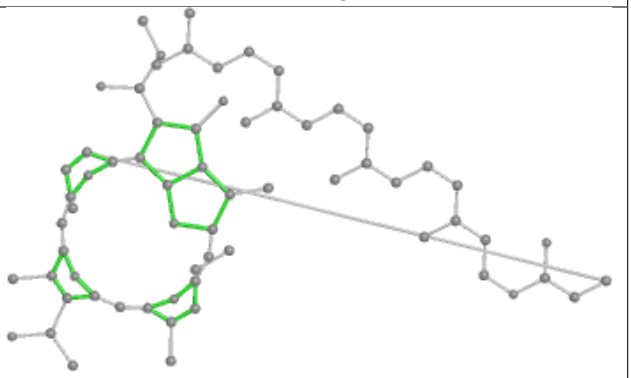
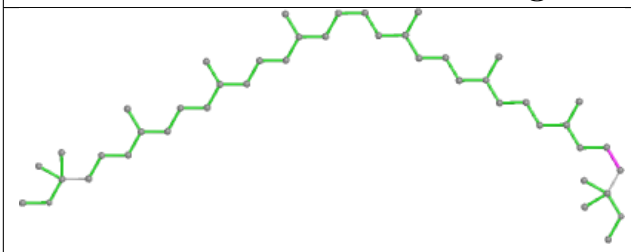
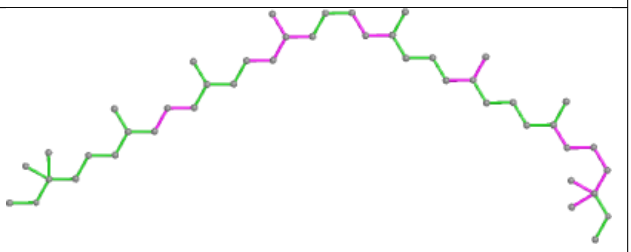


Rings

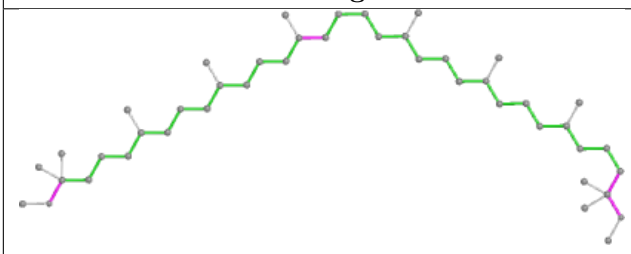
Ligand CRT 7 103



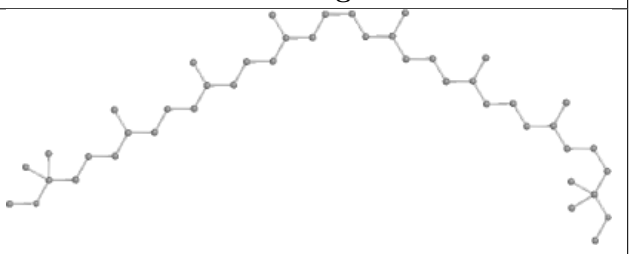
Bond lengths



Bond angles

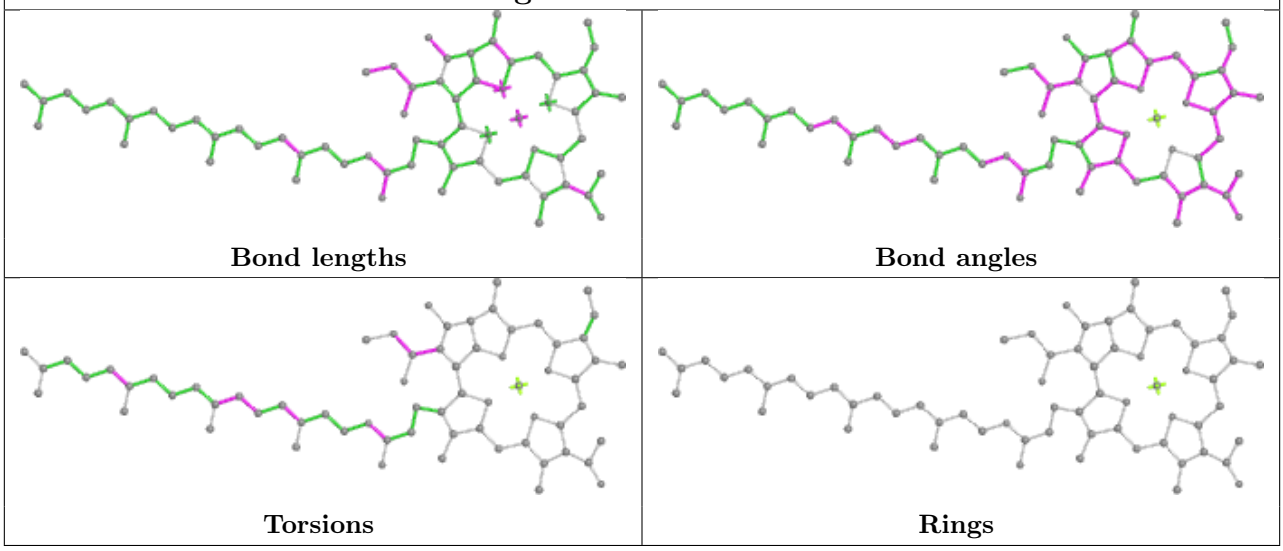


Torsions

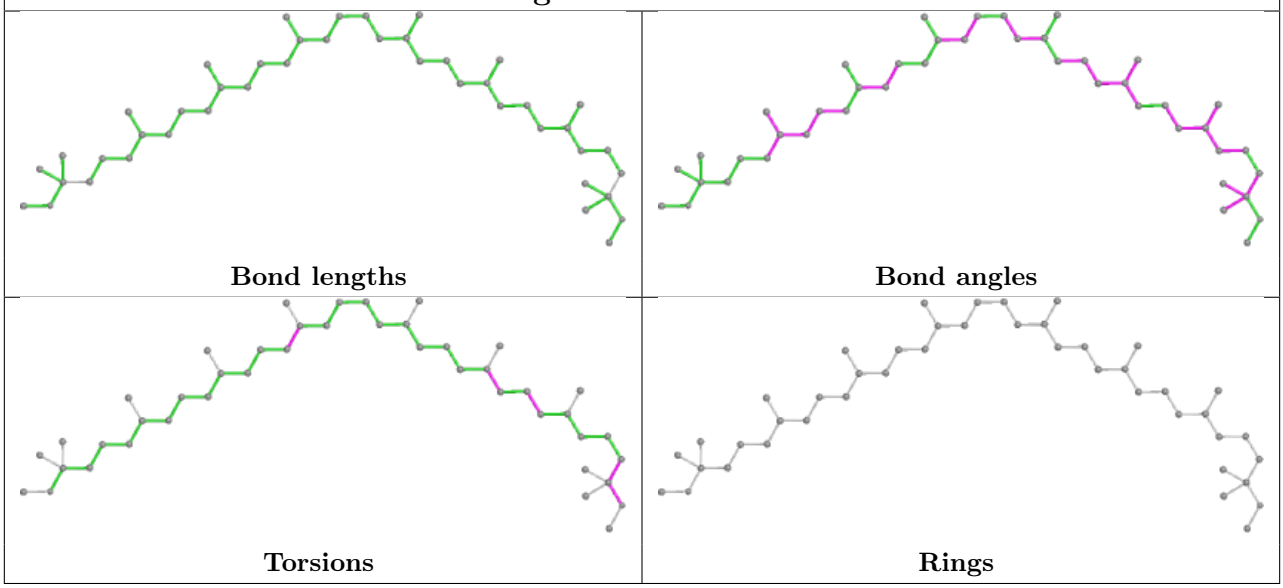


Rings

Ligand BCL AF 101



Ligand CRT i 101



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	C	317/333 (95%)	0.55	37 (11%)	4	4	89, 118, 143, 160	0
1	o	317/333 (95%)	0.53	36 (11%)	5	4	97, 126, 153, 166	0
2	L	280/281 (99%)	0.25	19 (6%)	17	17	73, 99, 149, 173	0
2	x	280/281 (99%)	0.19	11 (3%)	39	37	75, 98, 145, 174	0
3	M	318/319 (99%)	0.18	12 (3%)	40	37	73, 105, 141, 160	0
3	y	318/319 (99%)	0.24	13 (4%)	37	35	73, 110, 148, 173	0
4	H	258/259 (99%)	0.50	23 (8%)	9	10	78, 105, 162, 245	0
4	t	258/259 (99%)	0.40	19 (7%)	14	14	84, 107, 140, 240	0
5	1	60/61 (98%)	0.79	11 (18%)	1	1	134, 157, 202, 223	0
5	3	60/61 (98%)	1.26	10 (16%)	1	1	137, 157, 204, 216	0
5	5	60/61 (98%)	1.14	13 (21%)	0	1	142, 169, 243, 251	0
5	7	60/61 (98%)	1.99	19 (31%)	0	0	155, 180, 257, 271	0
5	9	60/61 (98%)	1.02	8 (13%)	3	3	156, 191, 228, 241	0
5	A	60/61 (98%)	2.02	16 (26%)	0	0	165, 198, 248, 252	0
5	AA	60/61 (98%)	1.55	11 (18%)	1	1	157, 202, 261, 269	0
5	AC	60/61 (98%)	1.52	16 (26%)	0	0	161, 205, 258, 265	0
5	AE	60/61 (98%)	1.33	12 (20%)	1	1	169, 207, 255, 264	0
5	AG	60/61 (98%)	1.51	15 (25%)	0	0	161, 192, 245, 246	0
5	AI	60/61 (98%)	1.35	16 (26%)	0	0	145, 177, 226, 231	0
5	AK	60/61 (98%)	0.62	12 (20%)	1	1	139, 163, 219, 236	0
5	D	60/61 (98%)	1.86	22 (36%)	0	0	161, 206, 256, 265	0
5	F	60/61 (98%)	1.90	22 (36%)	0	0	169, 210, 255, 258	0
5	I	60/61 (98%)	1.45	14 (23%)	0	1	178, 209, 255, 264	0
5	K	60/61 (98%)	1.97	14 (23%)	0	1	162, 203, 269, 278	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
5	O	60/61 (98%)	1.35	14 (23%)	0	1	140, 193, 265, 272	0
5	Q	60/61 (98%)	1.81	19 (31%)	0	0	142, 180, 254, 258	0
5	S	60/61 (98%)	1.85	16 (26%)	0	0	154, 189, 247, 254	0
5	U	60/61 (98%)	1.47	13 (21%)	0	1	145, 178, 238, 244	0
5	W	60/61 (98%)	1.01	15 (25%)	0	0	131, 159, 215, 220	0
5	Y	60/61 (98%)	1.13	12 (20%)	1	1	128, 156, 220, 249	0
5	d	60/61 (98%)	0.86	11 (18%)	1	1	134, 165, 216, 223	0
5	f	60/61 (98%)	1.20	13 (21%)	0	1	143, 161, 217, 229	0
5	h	60/61 (98%)	0.76	11 (18%)	1	1	140, 170, 234, 249	0
5	j	60/61 (98%)	0.80	11 (18%)	1	1	149, 179, 230, 245	0
5	l	60/61 (98%)	0.97	12 (20%)	1	1	141, 174, 222, 231	0
5	m	60/61 (98%)	1.32	18 (30%)	0	0	142, 178, 239, 244	0
5	p	60/61 (98%)	1.80	16 (26%)	0	0	136, 182, 239, 240	0
5	r	60/61 (98%)	1.63	17 (28%)	0	0	143, 184, 248, 251	0
5	u	60/61 (98%)	1.40	18 (30%)	0	0	162, 195, 251, 260	0
5	w	60/61 (98%)	1.52	17 (28%)	0	0	165, 204, 259, 265	0
6	0	40/47 (85%)	0.82	8 (20%)	1	1	166, 222, 247, 250	0
6	2	40/47 (85%)	0.61	5 (12%)	3	3	164, 179, 206, 212	0
6	4	40/47 (85%)	0.11	5 (12%)	3	3	162, 176, 195, 200	0
6	6	40/47 (85%)	0.47	5 (12%)	3	3	174, 192, 206, 209	0
6	8	40/47 (85%)	0.63	5 (12%)	3	3	186, 217, 229, 232	0
6	AB	40/47 (85%)	0.53	3 (7%)	14	13	177, 217, 249, 252	0
6	AD	40/47 (85%)	0.89	10 (25%)	0	0	196, 226, 250, 256	0
6	AF	40/47 (85%)	0.57	5 (12%)	3	3	211, 233, 245, 251	0
6	AH	40/47 (85%)	0.71	10 (25%)	0	0	201, 219, 238, 242	0
6	AJ	40/47 (85%)	0.66	6 (15%)	2	2	180, 200, 220, 224	0
6	AL	40/47 (85%)	0.69	8 (20%)	1	1	169, 183, 204, 214	0
6	B	40/47 (85%)	1.32	10 (25%)	0	0	180, 225, 250, 252	0
6	E	40/47 (85%)	0.66	6 (15%)	2	2	186, 222, 253, 255	0
6	G	40/47 (85%)	1.19	13 (32%)	0	0	182, 227, 257, 259	0
6	J	40/47 (85%)	0.64	5 (12%)	3	3	187, 227, 259, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
6	N	40/47 (85%)	0.53	5 (12%)	3	3	167, 212, 250, 252	0
6	P	40/47 (85%)	0.28	3 (7%)	14	13	166, 212, 248, 255	0
6	R	40/47 (85%)	1.20	11 (27%)	0	0	164, 208, 240, 243	0
6	T	40/47 (85%)	0.06	3 (7%)	14	13	178, 211, 230, 241	0
6	V	40/47 (85%)	0.03	1 (2%)	57	54	172, 198, 213, 222	0
6	X	40/47 (85%)	0.29	6 (15%)	2	2	162, 182, 195, 198	0
6	Z	40/47 (85%)	0.04	2 (5%)	28	27	161, 175, 196, 201	0
6	c	40/47 (85%)	1.68	13 (32%)	0	0	151, 202, 239, 250	0
6	e	40/47 (85%)	0.30	4 (10%)	7	7	172, 185, 215, 220	0
6	g	40/47 (85%)	0.20	4 (10%)	7	7	180, 190, 212, 218	0
6	i	40/47 (85%)	1.37	14 (35%)	0	0	182, 201, 214, 214	0
6	k	40/47 (85%)	0.54	3 (7%)	14	13	175, 212, 229, 243	0
6	n	40/47 (85%)	0.87	7 (17%)	1	1	146, 196, 239, 246	0
6	q	40/47 (85%)	0.60	5 (12%)	3	3	152, 190, 235, 243	0
6	s	40/47 (85%)	0.88	10 (25%)	0	0	156, 194, 238, 243	0
6	v	40/47 (85%)	0.31	7 (17%)	1	1	175, 201, 247, 250	0
6	z	40/47 (85%)	0.87	7 (17%)	1	1	176, 210, 255, 256	0
All	All	5546/5840 (94%)	0.78	843 (15%)	2	2	73, 162, 243, 278	0

All (843) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	p	54	SER	25.9
5	A	52	PRO	17.7
5	K	57	ALA	17.0
5	A	53	VAL	16.7
5	AE	54	SER	16.2
5	AA	3	THR	16.1
5	K	60	LYS	15.7
5	AC	54	SER	15.7
5	U	58	LEU	15.1
4	t	3	ALA	14.2
5	f	54	SER	14.0
5	A	61	LYS	13.9
5	AA	52	PRO	13.9
5	F	53	VAL	13.7

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Mol	Chain	Res	Type	RSRZ
5	S	58	LEU	13.4
5	K	59	GLY	13.0
5	I	53	VAL	12.6
5	Q	61	LYS	12.4
5	AA	2	PHE	11.8
5	S	59	GLY	11.6
5	Q	57	ALA	11.5
5	Q	54	SER	11.4
5	Y	3	THR	11.4
4	H	2	SER	11.4
5	r	54	SER	11.0
5	7	2	PHE	10.9
5	O	52	PRO	10.5
5	3	61	LYS	10.5
5	K	61	LYS	10.4
5	p	53	VAL	9.7
5	AI	57	ALA	9.6
5	w	59	GLY	9.5
5	AE	53	VAL	9.5
5	D	5	ASN	9.5
5	K	58	LEU	9.3
5	d	13	LEU	9.3
5	S	57	ALA	9.2
5	f	53	VAL	9.2
5	7	60	LYS	9.1
5	p	5	ASN	9.0
5	D	7	ASN	9.0
5	r	13	LEU	8.9
5	7	61	LYS	8.8
5	7	3	THR	8.7
5	r	53	VAL	8.7
5	I	52	PRO	8.5
5	AG	58	LEU	8.5
5	U	59	GLY	8.4
6	c	17	PHE	8.4
5	u	53	VAL	8.4
5	AA	53	VAL	8.4
5	F	54	SER	8.3
5	m	54	SER	8.3
5	U	53	VAL	8.3
6	n	17	PHE	8.1
4	t	2	SER	8.1

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Mol	Chain	Res	Type	RSRZ
5	3	46	TRP	8.1
5	p	55	TYR	8.0
5	A	60	LYS	7.9
5	7	58	LEU	7.9
5	AG	55	TYR	7.8
5	w	60	LYS	7.7
5	K	52	PRO	7.7
5	S	52	PRO	7.7
5	3	53	VAL	7.6
5	AA	60	LYS	7.5
5	5	3	THR	7.5
6	AJ	9	LEU	7.5
5	U	54	SER	7.4
5	Y	2	PHE	7.3
5	m	6	ALA	7.2
5	AG	57	ALA	7.2
4	H	4	GLY	7.2
6	R	45	TRP	7.1
5	S	55	TYR	7.1
5	5	58	LEU	7.1
6	R	44	PRO	7.1
6	s	45	TRP	7.1
5	7	54	SER	7.1
5	7	13	LEU	7.1
5	AG	51	ILE	7.0
5	A	54	SER	7.0
5	A	59	GLY	7.0
5	F	57	ALA	7.0
5	AG	61	LYS	7.0
5	D	6	ALA	7.0
6	AL	45	TRP	7.0
5	f	2	PHE	7.0
4	t	4	GLY	6.9
5	3	52	PRO	6.9
1	o	76	TYR	6.8
5	F	4	MET	6.8
5	AI	52	PRO	6.8
4	H	5	ILE	6.8
5	m	5	ASN	6.8
5	S	53	VAL	6.8
5	h	57	ALA	6.8
5	A	55	TYR	6.7

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Mol	Chain	Res	Type	RSRZ
6	e	45	TRP	6.7
5	p	58	LEU	6.6
5	AG	54	SER	6.6
6	N	8	GLY	6.5
6	v	45	TRP	6.5
6	AF	11	ASP	6.5
6	c	21	PHE	6.5
5	5	57	ALA	6.4
6	q	45	TRP	6.4
6	q	41	LEU	6.4
5	K	8	LEU	6.4
6	G	9	LEU	6.4
6	i	21	PHE	6.3
6	B	9	LEU	6.3
5	O	54	SER	6.2
5	Y	61	LYS	6.2
6	R	17	PHE	6.2
5	F	3	THR	6.2
5	AK	54	SER	6.2
5	AG	13	LEU	6.2
5	u	50	ASN	6.1
6	AD	45	TRP	6.1
5	U	61	LYS	6.1
5	AC	52	PRO	6.1
5	7	57	ALA	6.1
5	AI	53	VAL	6.0
1	o	73	SER	6.0
2	L	14	GLY	6.0
5	AE	52	PRO	5.9
5	Q	60	LYS	5.9
6	AH	45	TRP	5.9
6	8	41	LEU	5.9
6	G	45	TRP	5.9
5	3	54	SER	5.9
5	Q	59	GLY	5.9
5	W	7	ASN	5.8
5	h	12	TRP	5.8
5	F	56	GLN	5.8
5	Y	4	MET	5.8
5	I	55	TYR	5.8
5	U	51	ILE	5.8
5	D	59	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
5	Q	3	THR	5.8
5	AK	3	THR	5.8
1	C	70	PRO	5.7
5	m	53	VAL	5.7
6	6	43	ARG	5.7
5	Q	58	LEU	5.7
6	J	45	TRP	5.7
6	s	9	LEU	5.7
5	9	3	THR	5.6
5	U	57	ALA	5.6
5	5	52	PRO	5.6
5	D	52	PRO	5.6
5	I	48	ASP	5.6
5	O	42	THR	5.6
4	H	54	LYS	5.6
5	D	55	TYR	5.6
5	O	2	PHE	5.5
5	U	50	ASN	5.5
5	I	54	SER	5.5
5	S	51	ILE	5.5
5	W	13	LEU	5.5
1	C	121	ILE	5.5
5	w	58	LEU	5.5
5	f	10	LYS	5.4
1	o	72	ALA	5.4
5	D	54	SER	5.4
6	q	46	LEU	5.4
5	r	57	ALA	5.3
5	j	3	THR	5.3
5	AC	3	THR	5.3
1	C	72	ALA	5.3
5	r	2	PHE	5.3
5	Q	53	VAL	5.3
1	o	233	PHE	5.3
5	AI	2	PHE	5.3
5	w	46	TRP	5.3
5	F	50	ASN	5.2
5	S	60	LYS	5.2
5	1	44	LEU	5.2
5	I	59	GLY	5.2
5	w	57	ALA	5.2
6	AJ	45	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
6	E	41	LEU	5.2
5	O	53	VAL	5.2
5	7	59	GLY	5.2
5	u	54	SER	5.2
4	t	7	HIS	5.2
6	G	12	ASP	5.2
5	5	53	VAL	5.2
5	K	46	TRP	5.1
5	r	14	ILE	5.1
6	AB	45	TRP	5.1
5	j	2	PHE	5.1
1	o	321	ALA	5.1
6	AD	9	LEU	5.1
5	D	3	THR	5.1
5	d	6	ALA	5.1
6	R	43	ARG	5.1
5	W	57	ALA	5.1
5	w	61	LYS	5.0
5	AG	52	PRO	5.0
6	c	8	GLY	5.0
5	1	50	ASN	5.0
5	1	46	TRP	5.0
5	p	50	ASN	5.0
5	9	57	ALA	5.0
6	k	41	LEU	5.0
4	H	40	PRO	5.0
5	w	52	PRO	4.9
5	l	54	SER	4.9
5	r	55	TYR	4.9
5	u	46	TRP	4.9
5	5	5	ASN	4.9
5	f	58	LEU	4.9
6	4	10	THR	4.9
6	AD	14	ALA	4.9
5	O	57	ALA	4.9
5	AI	46	TRP	4.9
5	3	59	GLY	4.9
6	AF	10	THR	4.9
5	F	51	ILE	4.8
5	Y	57	ALA	4.8
1	C	332	LYS	4.8
5	AI	58	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
5	S	3	THR	4.8
5	p	8	LEU	4.8
6	i	10	THR	4.8
5	A	57	ALA	4.8
5	h	5	ASN	4.7
6	B	37	LEU	4.7
4	H	149	PRO	4.7
5	S	54	SER	4.7
5	Y	54	SER	4.7
5	r	52	PRO	4.7
6	i	17	PHE	4.7
5	5	54	SER	4.7
5	l	10	LYS	4.7
6	N	9	LEU	4.6
5	u	7	ASN	4.6
5	m	10	LYS	4.6
5	u	14	ILE	4.6
6	AD	13	GLU	4.6
1	o	125	VAL	4.6
5	u	47	LEU	4.6
5	9	50	ASN	4.6
6	P	45	TRP	4.5
6	n	42	TYR	4.5
5	3	44	LEU	4.5
5	Q	4	MET	4.5
5	9	54	SER	4.5
5	AK	53	VAL	4.5
5	U	13	LEU	4.5
5	AK	2	PHE	4.5
4	t	56	VAL	4.5
6	6	45	TRP	4.5
5	F	52	PRO	4.5
5	9	55	TYR	4.5
4	t	145	ALA	4.5
5	AC	13	LEU	4.4
5	p	10	LYS	4.4
5	AC	53	VAL	4.4
6	0	41	LEU	4.4
4	H	202	PHE	4.4
5	Q	55	TYR	4.4
1	o	162	PRO	4.4
5	AG	50	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
5	r	48	ASP	4.4
4	H	55	VAL	4.3
5	AI	13	LEU	4.3
6	i	46	LEU	4.3
6	B	41	LEU	4.3
6	i	45	TRP	4.3
5	O	56	GLN	4.3
6	B	45	TRP	4.3
5	p	7	ASN	4.3
6	G	41	LEU	4.2
6	c	9	LEU	4.2
5	u	55	TYR	4.2
6	AL	9	LEU	4.2
6	z	45	TRP	4.2
3	y	198	TYR	4.2
4	t	214	ILE	4.2
6	N	45	TRP	4.2
5	AI	54	SER	4.2
6	E	45	TRP	4.2
6	R	40	TRP	4.2
5	W	54	SER	4.2
5	p	47	LEU	4.2
5	7	53	VAL	4.2
5	5	44	LEU	4.2
5	AK	13	LEU	4.2
2	L	15	GLY	4.2
6	0	17	PHE	4.2
5	D	60	LYS	4.1
5	S	13	LEU	4.1
1	o	121	ILE	4.1
5	7	12	TRP	4.1
5	j	52	PRO	4.1
6	i	43	ARG	4.1
6	s	23	GLN	4.1
5	f	55	TYR	4.1
5	D	53	VAL	4.1
4	t	209	VAL	4.1
5	K	54	SER	4.0
5	u	6	ALA	4.0
6	P	36	HIS	4.0
6	AD	8	GLY	4.0
1	C	61	SER	4.0

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Mol	Chain	Res	Type	RSRZ
5	Y	13	LEU	4.0
5	5	4	MET	4.0
5	AI	60	LYS	4.0
5	A	39	VAL	4.0
6	AF	45	TRP	4.0
5	3	60	LYS	4.0
3	y	117	MET	3.9
5	m	55	TYR	3.9
1	o	128	ARG	3.9
5	I	57	ALA	3.9
5	d	2	PHE	3.9
5	AC	57	ALA	3.9
4	H	39	TYR	3.9
3	M	101	GLN	3.9
5	O	55	TYR	3.9
5	I	58	LEU	3.9
6	c	20	ILE	3.9
6	n	41	LEU	3.8
5	Y	5	ASN	3.8
5	1	47	LEU	3.8
5	u	8	LEU	3.8
6	AL	10	THR	3.8
5	A	58	LEU	3.8
6	i	18	HIS	3.8
3	M	198	TYR	3.8
5	F	61	LYS	3.8
5	W	4	MET	3.8
5	AE	3	THR	3.8
6	0	16	GLU	3.8
5	m	13	LEU	3.8
4	H	92	PHE	3.8
5	l	7	ASN	3.8
6	n	43	ARG	3.8
1	C	303	LEU	3.8
5	AA	61	LYS	3.7
5	m	37	MET	3.7
6	i	19	ALA	3.7
5	m	58	LEU	3.7
1	o	290	VAL	3.7
5	AI	59	GLY	3.7
1	o	154	THR	3.7
1	o	82	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
5	AG	53	VAL	3.7
5	l	12	TRP	3.7
5	j	58	LEU	3.7
6	AL	21	PHE	3.7
5	l	57	ALA	3.7
5	K	56	GLN	3.7
5	AA	59	GLY	3.7
5	F	44	LEU	3.7
5	AC	58	LEU	3.7
1	C	284	ILE	3.6
6	G	23	GLN	3.6
5	l	61	LYS	3.6
5	AC	4	MET	3.6
5	AG	14	ILE	3.6
6	z	16	GLU	3.6
5	r	4	MET	3.6
1	o	323	MET	3.6
5	F	42	THR	3.6
6	AH	9	LEU	3.6
5	r	47	LEU	3.6
6	c	42	TYR	3.6
5	D	61	LYS	3.6
6	R	13	GLU	3.6
6	G	8	GLY	3.6
6	0	44	PRO	3.6
5	S	61	LYS	3.5
6	q	39	ALA	3.5
5	F	2	PHE	3.5
6	B	11	ASP	3.5
4	H	144	ILE	3.5
5	F	59	GLY	3.5
5	AG	44	LEU	3.5
6	X	41	LEU	3.5
5	D	50	ASN	3.5
5	Q	2	PHE	3.5
1	o	71	LYS	3.5
6	AF	12	ASP	3.5
5	AK	57	ALA	3.5
5	r	51	ILE	3.4
5	f	51	ILE	3.4
6	s	21	PHE	3.4
5	F	55	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
6	v	23	GLN	3.4
5	9	58	LEU	3.4
5	W	2	PHE	3.4
6	0	37	LEU	3.4
6	AB	11	ASP	3.4
5	m	57	ALA	3.4
1	o	74	GLU	3.4
5	D	11	ILE	3.4
4	t	55	VAL	3.4
5	3	4	MET	3.4
6	G	16	GLU	3.4
6	c	46	LEU	3.4
5	m	52	PRO	3.4
5	u	52	PRO	3.4
5	D	4	MET	3.4
5	F	8	LEU	3.4
6	J	41	LEU	3.4
6	8	37	LEU	3.3
4	H	214	ILE	3.3
6	2	21	PHE	3.3
5	u	13	LEU	3.3
6	4	12	ASP	3.3
6	B	43	ARG	3.3
6	z	41	LEU	3.3
5	I	11	ILE	3.3
5	D	8	LEU	3.3
3	M	191	ILE	3.3
6	B	39	ALA	3.3
5	D	58	LEU	3.3
5	j	8	LEU	3.3
1	C	125	VAL	3.3
1	C	321	ALA	3.3
2	L	41	CYS	3.3
6	J	19	ALA	3.3
6	AD	7	THR	3.3
6	g	41	LEU	3.3
5	f	50	ASN	3.3
5	S	2	PHE	3.3
5	I	8	LEU	3.3
6	c	31	LEU	3.3
1	C	28	PRO	3.3
5	AC	50	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
5	F	58	LEU	3.2
6	i	9	LEU	3.2
6	6	41	LEU	3.2
6	AD	10	THR	3.2
1	o	132	GLU	3.2
5	AE	50	ASN	3.2
5	9	41	SER	3.2
6	B	42	TYR	3.2
5	w	37	MET	3.2
5	9	2	PHE	3.2
5	h	54	SER	3.2
5	AK	52	PRO	3.2
2	L	43	THR	3.2
6	B	26	TYR	3.2
6	8	42	TYR	3.2
6	v	26	TYR	3.2
1	C	210	ILE	3.1
5	AC	51	ILE	3.1
5	w	41	SER	3.1
6	2	41	LEU	3.1
5	5	46	TRP	3.1
5	h	58	LEU	3.1
5	A	51	ILE	3.1
3	M	319	THR	3.1
5	W	10	LYS	3.1
5	h	3	THR	3.1
3	y	85	GLN	3.1
6	B	12	ASP	3.1
6	i	24	SER	3.1
5	1	60	LYS	3.1
5	m	44	LEU	3.1
6	E	34	ILE	3.1
5	U	52	PRO	3.1
1	C	329	GLY	3.1
5	U	60	LYS	3.1
5	O	13	LEU	3.1
6	4	9	LEU	3.1
6	8	39	ALA	3.1
3	M	36	PHE	3.0
4	H	7	HIS	3.0
5	1	51	ILE	3.0
1	C	290	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	o	129	ARG	3.0
5	d	58	LEU	3.0
5	AC	46	TRP	3.0
5	AI	47	LEU	3.0
5	d	7	ASN	3.0
5	A	13	LEU	3.0
6	AH	46	LEU	3.0
6	G	15	LYS	3.0
5	AE	57	ALA	3.0
5	h	59	GLY	3.0
6	z	9	LEU	3.0
2	x	15	GLY	3.0
5	1	59	GLY	3.0
5	7	55	TYR	3.0
1	o	79	VAL	3.0
5	AA	13	LEU	3.0
6	s	12	ASP	3.0
6	e	11	ASP	3.0
1	C	237	MET	3.0
5	D	10	LYS	3.0
4	H	143	SER	3.0
1	C	333	THR	3.0
2	x	14	GLY	2.9
6	i	26	TYR	2.9
6	AL	39	ALA	2.9
6	6	17	PHE	2.9
2	L	13	ARG	2.9
5	I	28	GLN	2.9
1	o	210	ILE	2.9
5	Y	14	ILE	2.9
6	AH	39	ALA	2.9
5	I	3	THR	2.9
6	E	37	LEU	2.9
6	c	37	LEU	2.9
5	AC	41	SER	2.9
4	H	215	LYS	2.9
5	W	42	THR	2.9
6	X	45	TRP	2.9
5	O	59	GLY	2.9
5	AK	4	MET	2.9
5	7	30	VAL	2.9
6	2	37	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	K	7	ASN	2.9
5	AG	42	THR	2.9
5	l	3	THR	2.9
6	E	35	ALA	2.9
5	A	50	ASN	2.9
5	5	55	TYR	2.9
5	u	15	LEU	2.9
5	AI	61	LYS	2.8
6	6	42	TYR	2.8
6	AL	14	ALA	2.8
5	r	12	TRP	2.8
5	W	56	GLN	2.8
1	C	302	PRO	2.8
6	X	17	PHE	2.8
4	t	143	SER	2.8
5	AK	46	TRP	2.8
5	j	57	ALA	2.8
3	y	319	THR	2.8
2	x	101	CYS	2.8
1	o	131	PHE	2.8
5	m	4	MET	2.8
5	AC	23	SER	2.8
1	C	233	PHE	2.8
4	H	56	VAL	2.8
5	O	3	THR	2.8
5	AE	4	MET	2.8
1	C	20	LEU	2.8
2	x	171	TYR	2.8
6	g	21	PHE	2.8
5	p	52	PRO	2.8
2	x	120	LEU	2.8
6	c	19	ALA	2.8
5	w	28	GLN	2.8
3	M	287	SER	2.8
6	k	12	ASP	2.8
1	C	59	VAL	2.8
5	f	61	LYS	2.8
6	E	26	TYR	2.8
5	Q	56	GLN	2.7
3	y	12	GLN	2.7
5	AG	59	GLY	2.7
5	Q	52	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
5	r	58	LEU	2.7
5	w	44	LEU	2.7
5	F	41	SER	2.7
6	N	44	PRO	2.7
6	AJ	41	LEU	2.7
2	L	101	CYS	2.7
3	y	125	SER	2.7
2	L	105	ALA	2.7
5	AI	14	ILE	2.7
6	X	46	LEU	2.7
2	x	41	CYS	2.7
6	s	13	GLU	2.7
5	d	14	ILE	2.7
6	n	26	TYR	2.7
1	C	44	TYR	2.7
5	AC	14	ILE	2.7
5	l	41	SER	2.7
1	C	106	GLY	2.7
2	L	40	PHE	2.6
1	o	332	LYS	2.6
5	D	51	ILE	2.6
5	7	17	PRO	2.6
6	Z	45	TRP	2.6
6	g	45	TRP	2.6
5	U	45	ASN	2.6
4	H	151	PRO	2.6
1	o	80	GLN	2.6
5	K	11	ILE	2.6
5	h	51	ILE	2.6
5	u	41	SER	2.6
5	AI	3	THR	2.6
3	y	106	ILE	2.6
6	4	26	TYR	2.6
6	AB	20	ILE	2.6
5	d	46	TRP	2.6
5	w	8	LEU	2.6
1	C	135	ARG	2.6
6	T	13	GLU	2.6
4	H	41	LEU	2.6
5	j	4	MET	2.6
3	M	102	TYR	2.6
1	C	75	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	128	ARG	2.6
3	y	116	LEU	2.6
6	i	22	MET	2.6
2	L	171	TYR	2.6
5	A	5	ASN	2.6
2	L	238	ILE	2.6
5	A	2	PHE	2.5
2	x	19	GLY	2.5
5	AI	8	LEU	2.5
6	V	41	LEU	2.5
5	W	3	THR	2.5
5	W	55	TYR	2.5
6	N	42	TYR	2.5
1	C	78	ASN	2.5
6	J	9	LEU	2.5
1	C	203	PHE	2.5
1	C	71	LYS	2.5
5	1	54	SER	2.5
5	f	52	PRO	2.5
2	L	36	GLY	2.5
6	Z	21	PHE	2.5
6	i	20	ILE	2.5
5	1	39	VAL	2.5
5	S	50	ASN	2.5
5	1	45	ASN	2.5
5	AK	12	TRP	2.5
1	C	283	TYR	2.5
5	3	47	LEU	2.5
5	r	7	ASN	2.5
6	AH	15	LYS	2.5
1	C	261	GLN	2.5
5	7	50	ASN	2.5
2	L	65	LEU	2.5
5	AE	23	SER	2.5
4	t	144	ILE	2.5
5	p	51	ILE	2.5
6	s	10	THR	2.5
5	W	58	LEU	2.5
5	AE	58	LEU	2.5
6	AD	12	ASP	2.5
6	G	13	GLU	2.5
6	R	36	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
6	X	14	ALA	2.4
2	L	39	GLY	2.4
3	M	231	GLY	2.4
5	p	61	LYS	2.4
5	p	59	GLY	2.4
5	r	59	GLY	2.4
5	AA	8	LEU	2.4
5	AC	15	LEU	2.4
5	j	59	GLY	2.4
6	8	9	LEU	2.4
1	o	204	LEU	2.4
5	F	43	ASP	2.4
6	0	43	ARG	2.4
5	U	2	PHE	2.4
5	m	50	ASN	2.4
5	u	10	LYS	2.4
6	G	10	THR	2.4
1	C	29	GLY	2.4
5	Q	8	LEU	2.4
5	j	31	LEU	2.4
4	H	142	PHE	2.4
6	k	10	THR	2.4
5	5	59	GLY	2.4
6	AL	11	ASP	2.4
2	x	44	LEU	2.4
5	Q	17	PRO	2.4
5	Q	50	ASN	2.4
5	D	12	TRP	2.4
6	AL	17	PHE	2.4
5	S	11	ILE	2.4
6	X	37	LEU	2.4
5	W	5	ASN	2.4
5	W	12	TRP	2.4
5	w	2	PHE	2.4
4	t	170	VAL	2.3
1	o	70	PRO	2.3
5	u	57	ALA	2.3
2	L	177	HIS	2.3
6	v	46	LEU	2.3
6	AJ	10	THR	2.3
3	y	69	SER	2.3
5	K	21	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	d	11	ILE	2.3
5	j	51	ILE	2.3
2	x	45	LEU	2.3
5	AE	51	ILE	2.3
6	AD	17	PHE	2.3
1	C	60	GLU	2.3
5	7	7	ASN	2.3
5	f	46	TRP	2.3
1	o	291	LEU	2.3
5	Y	44	LEU	2.3
5	AA	55	TYR	2.3
6	J	28	TRP	2.3
5	A	14	ILE	2.3
6	AH	14	ALA	2.3
6	g	39	ALA	2.3
5	Q	11	ILE	2.3
5	AA	46	TRP	2.3
1	C	205	ASP	2.3
5	AI	42	THR	2.3
5	O	23	SER	2.3
6	c	24	SER	2.3
5	Q	14	ILE	2.3
3	M	188	ALA	2.3
4	t	134	VAL	2.3
5	W	9	TYR	2.3
6	z	15	LYS	2.3
3	M	142	MET	2.3
1	C	82	LEU	2.3
5	w	14	ILE	2.3
5	D	9	TYR	2.3
5	w	39	VAL	2.3
1	o	78	ASN	2.3
5	l	13	LEU	2.3
1	o	97	VAL	2.3
5	Q	26	ALA	2.3
6	R	39	ALA	2.3
2	L	223	THR	2.2
5	p	48	ASP	2.2
5	l	58	LEU	2.2
1	o	296	LYS	2.2
5	7	32	GLY	2.2
5	w	23	SER	2.2

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Mol	Chain	Res	Type	RSRZ
5	d	54	SER	2.2
6	s	19	ALA	2.2
6	AF	39	ALA	2.2
6	R	12	ASP	2.2
6	2	17	PHE	2.2
5	5	47	LEU	2.2
5	r	44	LEU	2.2
5	K	2	PHE	2.2
2	x	58	PRO	2.2
1	C	122	TYR	2.2
2	L	221	GLU	2.2
6	AH	43	ARG	2.2
4	t	210	LYS	2.2
5	7	11	ILE	2.2
4	t	155	THR	2.2
5	AE	55	TYR	2.2
5	F	21	LEU	2.2
5	f	57	ALA	2.2
6	AJ	39	ALA	2.2
3	y	297	TRP	2.2
4	H	160	ASP	2.2
6	R	41	LEU	2.2
3	M	271	TRP	2.2
6	P	13	GLU	2.2
5	O	17	PRO	2.2
5	m	8	LEU	2.2
5	Y	53	VAL	2.2
4	t	182	LEU	2.2
5	1	40	LEU	2.2
4	H	190	LYS	2.2
1	C	204	LEU	2.2
1	o	303	LEU	2.2
5	w	54	SER	2.2
5	d	8	LEU	2.2
1	o	90	PHE	2.2
6	T	21	PHE	2.2
6	z	11	ASP	2.2
6	c	16	GLU	2.2
5	S	12	TRP	2.2
6	q	35	ALA	2.2
6	AH	12	ASP	2.2
6	0	10	THR	2.2

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Mol	Chain	Res	Type	RSRZ
6	0	9	LEU	2.1
3	y	113	GLY	2.1
1	o	252	ASN	2.1
5	F	5	ASN	2.1
6	e	9	LEU	2.1
5	Y	6	ALA	2.1
6	4	19	ALA	2.1
6	n	13	GLU	2.1
1	C	68	THR	2.1
1	o	282	ASN	2.1
6	z	28	TRP	2.1
5	h	8	LEU	2.1
6	T	14	ALA	2.1
6	AH	10	THR	2.1
2	L	104	GLY	2.1
1	o	283	TYR	2.1
1	o	295	ARG	2.1
5	h	46	TRP	2.1
6	G	39	ALA	2.1
6	s	28	TRP	2.1
2	L	100	ILE	2.1
4	t	54	LYS	2.1
5	u	17	PRO	2.1
6	e	15	LYS	2.1
5	I	2	PHE	2.1
6	n	28	TRP	2.1
5	AG	56	GLN	2.1
3	M	140	LEU	2.1
5	7	10	LYS	2.1
6	AD	15	LYS	2.1
5	AK	55	TYR	2.1
5	O	60	LYS	2.1
5	m	12	TRP	2.1
6	v	17	PHE	2.1
5	m	11	ILE	2.1
6	v	20	ILE	2.1
6	v	21	PHE	2.1
4	H	3	ALA	2.1
5	F	17	PRO	2.1
5	m	17	PRO	2.1
6	i	39	ALA	2.1
1	o	140	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	j	37	MET	2.1
6	c	22	MET	2.1
1	C	112	VAL	2.1
4	t	151	PRO	2.1
5	AE	17	PRO	2.1
6	2	14	ALA	2.1
5	u	40	LEU	2.1
5	d	21	LEU	2.0
4	H	188	ALA	2.0
5	l	40	LEU	2.0
5	AC	61	LYS	2.0
3	y	86	PHE	2.0
6	R	16	GLU	2.0
6	AH	40	TRP	2.0
6	G	37	LEU	2.0
5	D	39	VAL	2.0
5	D	13	LEU	2.0
5	f	44	LEU	2.0
5	h	13	LEU	2.0
2	x	46	GLY	2.0
1	o	256	PHE	2.0
6	G	44	PRO	2.0
6	s	17	PHE	2.0
5	p	6	ALA	2.0
2	L	176	PHE	2.0
5	I	4	MET	2.0
4	t	208	LYS	2.0
5	l	60	LYS	2.0
3	y	226	VAL	2.0
5	AK	21	LEU	2.0
6	AJ	37	LEU	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
15	CRT	n	101	44/44	0.34	0.98	166,179,185,189	0
15	CRT	v	101	44/44	0.34	1.10	170,189,194,196	0
15	CRT	R	101	44/44	0.39	0.87	159,181,189,191	0
15	CRT	0	101	44/44	0.39	0.77	175,197,206,206	0
15	CRT	I	102	44/44	0.40	1.06	194,205,211,214	0
15	CRT	i	101	44/44	0.42	0.91	156,180,197,201	0
15	CRT	z	101	44/44	0.43	0.74	176,193,197,198	0
15	CRT	g	101	44/44	0.45	0.79	145,172,198,202	0
15	CRT	q	101	44/44	0.46	0.92	159,174,179,182	0
15	CRT	m	104	44/44	0.48	1.01	171,183,189,191	0
15	CRT	O	101	44/44	0.50	0.75	179,194,202,205	0
15	CRT	7	101	44/44	0.56	0.81	155,177,191,193	0
15	CRT	9	101	44/44	0.56	0.83	181,205,211,215	0
15	CRT	AC	101	44/44	0.58	0.94	180,197,200,202	0
15	CRT	P	102	44/44	0.59	0.75	170,186,189,190	0
15	CRT	7	103	44/44	0.60	0.63	171,193,205,208	0
12	PEF	p	101	16/47	0.62	0.30	131,142,148,151	0
15	CRT	AF	102	44/44	0.65	0.72	170,212,229,231	0
8	BA	w	102	1/1	0.67	0.09	271,271,271,271	0
15	CRT	T	101	44/44	0.69	0.83	154,186,198,199	0
14	MQ8	M	404	53/53	0.69	0.48	82,100,144,151	0
15	CRT	AD	101	44/44	0.70	0.49	175,204,211,213	0
15	CRT	E	101	44/44	0.70	0.58	179,205,211,213	0
16	PO4	H	303	5/5	0.70	0.55	158,160,164,166	0
16	PO4	t	302	5/5	0.71	0.33	142,142,144,149	0
9	BCL	AC	103	66/66	0.73	0.49	188,211,257,265	0
12	PEF	A	101	19/47	0.73	0.46	142,147,157,161	0
12	PEF	H	304	19/47	0.74	0.57	160,166,175,180	0
15	CRT	G	101	44/44	0.75	0.91	187,209,215,218	0
15	CRT	M	405	44/44	0.76	0.41	90,108,139,148	0
15	CRT	AH	102	44/44	0.76	0.60	155,198,229,231	0
7	HEM	o	501	43/43	0.77	0.47	129,137,145,148	0
15	CRT	AL	101	44/44	0.77	1.06	130,168,200,203	0
15	CRT	e	101	44/44	0.78	0.87	140,173,206,210	0
15	CRT	V	101	44/44	0.78	0.69	140,179,197,198	0
15	CRT	4	101	44/44	0.78	0.52	141,166,185,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	AB	102	66/66	0.78	0.53	187,214,258,267	0
9	BCL	AG	101	66/66	0.78	0.34	179,190,215,226	0
15	CRT	y	404	44/44	0.79	0.38	99,115,146,154	0
15	CRT	k	101	44/44	0.79	0.60	166,186,199,202	0
8	BA	u	103	1/1	0.79	0.23	264,264,264,264	0
15	CRT	AJ	101	44/44	0.79	0.88	139,182,214,217	0
15	CRT	Z	101	44/44	0.80	1.06	127,160,186,189	0
15	CRT	2	101	44/44	0.80	1.04	136,165,190,194	0
9	BCL	D	101	66/66	0.80	0.36	153,209,226,231	0
9	BCL	AE	102	66/66	0.80	0.35	188,207,244,262	0
15	CRT	X	101	44/44	0.80	0.90	129,166,188,191	0
8	BA	K	102	1/1	0.81	0.08	265,265,265,265	0
9	BCL	K	101	66/66	0.81	0.51	183,209,225,229	0
12	PEF	y	406	19/47	0.81	0.24	116,122,128,131	0
11	UQ8	L	304	53/53	0.81	0.60	81,86,88,89	0
12	PEF	L	305	12/47	0.81	0.29	113,118,123,123	0
12	PEF	H	302	19/47	0.82	0.24	139,156,167,170	0
10	BPH	y	402	65/65	0.82	0.33	87,95,132,142	0
8	BA	AG	102	1/1	0.82	0.08	225,225,225,225	0
15	CRT	s	101	44/44	0.82	0.90	163,178,182,183	0
9	BCL	6	101	66/66	0.82	0.44	154,174,210,221	0
12	PEF	m	101	19/47	0.82	0.34	119,125,133,136	0
9	BCL	m	102	66/66	0.83	0.43	157,190,207,214	0
9	BCL	AC	102	66/66	0.83	0.38	181,205,218,228	0
9	BCL	z	102	66/66	0.83	0.39	183,211,253,269	0
17	PGW	S	101	21/51	0.83	0.23	122,133,142,147	0
12	PEF	y	407	19/47	0.84	0.23	97,101,106,108	0
9	BCL	d	101	66/66	0.84	0.35	131,157,168,173	0
11	UQ8	x	304	53/53	0.84	0.55	80,87,90,91	0
8	BA	p	103	1/1	0.84	0.07	257,257,257,257	0
14	MQ8	y	403	53/53	0.84	0.38	79,93,131,138	0
12	PEF	M	408	19/47	0.84	0.28	95,99,103,105	0
17	PGW	AE	101	21/51	0.84	0.37	141,155,167,171	0
9	BCL	I	103	66/66	0.85	0.37	200,223,264,273	0
9	BCL	g	102	66/66	0.86	0.38	153,171,206,215	0
9	BCL	j	101	66/66	0.86	0.33	166,183,198,203	0
9	BCL	0	102	66/66	0.86	0.40	183,208,254,257	0
9	BCL	N	101	66/66	0.86	0.37	189,213,255,262	0
9	BCL	D	102	66/66	0.86	0.48	194,218,258,259	0
9	BCL	f	101	66/66	0.86	0.49	144,163,174,180	0
12	PEF	x	306	19/47	0.87	0.25	97,102,107,107	0
9	BCL	7	102	66/66	0.87	0.34	163,180,195,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	p	102	66/66	0.87	0.34	128,189,203,208	0
8	BA	W	102	1/1	0.87	0.11	209,209,209,209	0
9	BCL	y	401	66/66	0.87	0.40	86,93,102,106	0
9	BCL	O	102	66/66	0.88	0.38	179,206,250,251	0
12	PEF	y	408	19/47	0.88	0.37	102,108,116,118	0
9	BCL	F	101	66/66	0.88	0.43	183,211,226,232	0
8	BA	AE	103	1/1	0.88	0.08	248,248,248,248	0
12	PEF	H	301	19/47	0.89	0.28	108,115,119,121	0
9	BCL	i	102	66/66	0.89	0.33	161,181,218,232	0
9	BCL	AF	101	66/66	0.89	0.34	161,205,215,225	0
9	BCL	k	102	66/66	0.89	0.33	171,195,223,234	0
10	BPH	M	403	65/65	0.89	0.28	84,88,117,126	0
9	BCL	A	102	66/66	0.89	0.29	182,205,221,225	0
9	BCL	AH	101	66/66	0.89	0.35	182,196,206,212	0
9	BCL	x	301	66/66	0.89	0.35	81,86,92,97	0
9	BCL	u	101	66/66	0.89	0.34	133,196,212,216	0
9	BCL	R	102	66/66	0.89	0.36	170,194,236,245	0
9	BCL	P	101	66/66	0.90	0.35	173,201,216,221	0
10	BPH	L	302	65/65	0.90	0.24	79,88,109,114	0
12	PEF	t	303	19/47	0.90	0.19	94,97,104,104	0
9	BCL	G	102	66/66	0.90	0.34	197,220,264,265	0
9	BCL	V	102	66/66	0.90	0.34	162,177,208,223	0
9	BCL	3	101	66/66	0.90	0.42	138,153,165,168	0
9	BCL	m	103	66/66	0.90	0.29	173,198,219,230	0
9	BCL	I	101	66/66	0.90	0.36	149,216,231,234	0
9	BCL	AI	102	66/66	0.90	0.28	163,172,197,203	0
8	BA	F	102	1/1	0.90	0.09	271,271,271,271	0
9	BCL	e	102	66/66	0.90	0.44	152,164,191,197	0
9	BCL	u	102	66/66	0.90	0.37	181,205,248,268	0
9	BCL	w	101	66/66	0.90	0.39	176,199,217,222	0
9	BCL	8	101	66/66	0.90	0.32	173,196,221,230	0
9	BCL	9	102	66/66	0.90	0.29	165,191,211,216	0
9	BCL	A	103	66/66	0.91	0.34	190,213,242,251	0
12	PEF	H	305	19/47	0.91	0.21	93,97,104,105	0
9	BCL	AB	101	66/66	0.91	0.29	176,202,220,226	0
9	BCL	h	101	66/66	0.91	0.29	155,171,185,187	0
9	BCL	q	102	66/66	0.91	0.40	170,194,226,241	0
9	BCL	1	101	66/66	0.91	0.33	123,149,159,163	0
12	PEF	M	407	16/47	0.91	0.16	86,89,91,92	0
7	HEM	C	501	43/43	0.91	0.33	118,126,133,136	0
9	BCL	c	101	66/66	0.91	0.34	173,199,243,258	0
9	BCL	T	102	66/66	0.91	0.34	166,185,223,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	l	101	66/66	0.92	0.34	157,189,205,210	0
9	BCL	AI	101	66/66	0.92	0.35	167,179,190,196	0
9	BCL	5	101	66/66	0.92	0.32	147,166,178,183	0
8	BA	3	102	1/1	0.92	0.14	191,191,191,191	0
10	BPH	x	302	65/65	0.92	0.27	78,84,104,106	0
8	BA	x	308	1/1	0.92	0.16	175,175,175,175	0
9	BCL	U	101	66/66	0.92	0.27	153,176,186,191	0
8	BA	m	106	1/1	0.92	0.05	242,242,242,242	0
12	PEF	t	301	19/47	0.92	0.24	100,104,107,108	0
9	BCL	r	101	66/66	0.92	0.41	160,190,204,208	0
8	BA	L	306	1/1	0.92	0.22	185,185,185,185	0
9	BCL	Q	101	66/66	0.92	0.33	166,193,205,211	0
9	BCL	x	303	66/66	0.92	0.33	82,89,97,98	0
9	BCL	M	401	66/66	0.93	0.29	86,94,107,114	0
8	BA	D	103	1/1	0.93	0.17	252,252,252,252	0
9	BCL	W	101	66/66	0.93	0.33	152,165,171,179	0
7	HEM	C	502	43/43	0.93	0.36	108,114,120,121	0
9	BCL	2	102	66/66	0.93	0.34	145,156,185,195	0
7	HEM	o	503	43/43	0.93	0.38	98,109,122,124	0
9	BCL	4	102	66/66	0.93	0.29	144,159,189,198	0
7	HEM	C	504	43/43	0.93	0.35	105,106,110,111	0
8	BA	AK	102	1/1	0.93	0.03	186,186,186,186	0
9	BCL	s	102	66/66	0.93	0.47	174,198,247,260	0
9	BCL	L	301	66/66	0.93	0.29	79,84,98,103	0
9	BCL	AL	102	66/66	0.93	0.34	152,161,183,190	0
9	BCL	S	102	66/66	0.93	0.34	136,186,197,205	0
9	BCL	L	303	66/66	0.93	0.32	79,86,91,96	0
8	BA	d	102	1/1	0.94	0.05	174,174,174,174	0
8	BA	f	102	1/1	0.94	0.05	205,205,205,205	0
8	BA	j	102	1/1	0.94	0.03	228,228,228,228	0
7	HEM	o	504	43/43	0.94	0.32	111,114,119,122	0
8	BA	O	103	1/1	0.94	0.10	244,244,244,244	0
9	BCL	X	102	66/66	0.94	0.36	148,159,180,192	0
9	BCL	Y	101	66/66	0.94	0.35	142,152,162,174	0
9	BCL	Z	102	66/66	0.94	0.32	143,151,174,182	0
7	HEM	o	502	43/43	0.94	0.42	119,124,128,129	0
9	BCL	M	402	66/66	0.94	0.36	83,90,96,99	0
9	BCL	AK	101	66/66	0.94	0.34	152,162,177,193	0
9	BCL	x	305	66/66	0.94	0.29	83,90,98,105	0
7	HEM	C	503	43/43	0.95	0.37	96,107,121,123	0
8	BA	5	102	1/1	0.95	0.09	212,212,212,212	0
8	BA	AA	101	1/1	0.95	0.02	260,260,260,260	0

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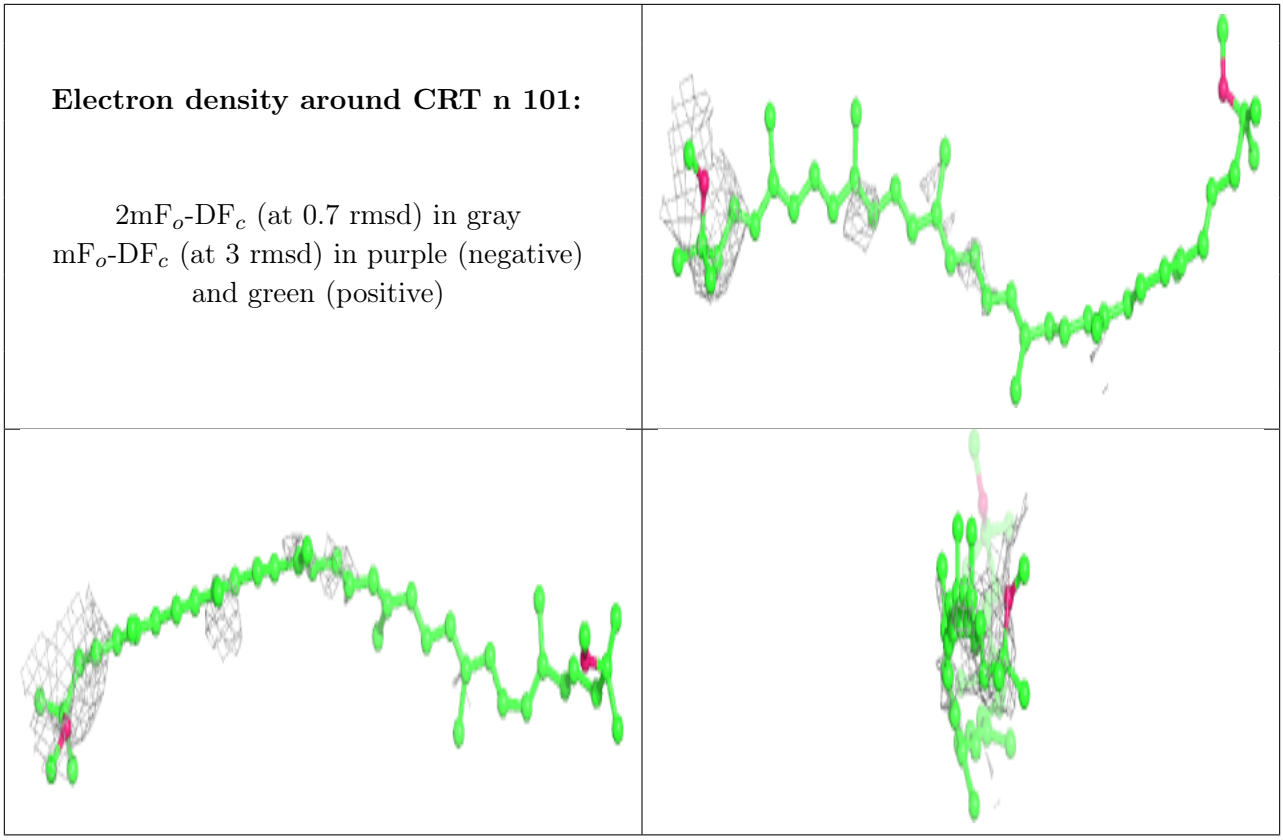
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BA	7	104	1/1	0.95	0.19	215,215,215,215	0
16	PO4	M	406	5/5	0.95	0.11	121,126,127,128	0
8	BA	L	307	1/1	0.95	0.24	160,160,160,160	0
8	BA	AI	103	1/1	0.95	0.11	210,210,210,210	0
8	BA	Q	102	1/1	0.95	0.03	245,245,245,245	0
8	BA	I	104	1/1	0.95	0.09	276,276,276,276	0
8	BA	AC	104	1/1	0.96	0.11	257,257,257,257	0
8	BA	A	105	1/1	0.96	0.15	243,243,243,243	0
16	PO4	y	405	5/5	0.96	0.18	134,136,141,141	0
8	BA	A	104	1/1	0.96	0.08	247,247,247,247	0
8	BA	h	102	1/1	0.96	0.04	210,210,210,210	0
8	BA	1	102	1/1	0.96	0.02	177,177,177,177	0
8	BA	U	102	1/1	0.97	0.18	224,224,224,224	0
8	BA	r	102	1/1	0.97	0.06	250,250,250,250	0
8	BA	x	307	1/1	0.97	0.21	186,186,186,186	0
8	BA	S	103	1/1	0.97	0.02	227,227,227,227	0
8	BA	m	105	1/1	0.97	0.03	226,226,226,226	0
8	BA	Y	102	1/1	0.97	0.05	181,181,181,181	0
13	FE	L	308	1/1	0.98	0.15	76,76,76,76	0
13	FE	x	309	1/1	0.98	0.17	76,76,76,76	0
8	BA	C	505	1/1	0.99	0.24	93,93,93,93	0
8	BA	o	505	1/1	1.00	0.25	100,100,100,100	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.

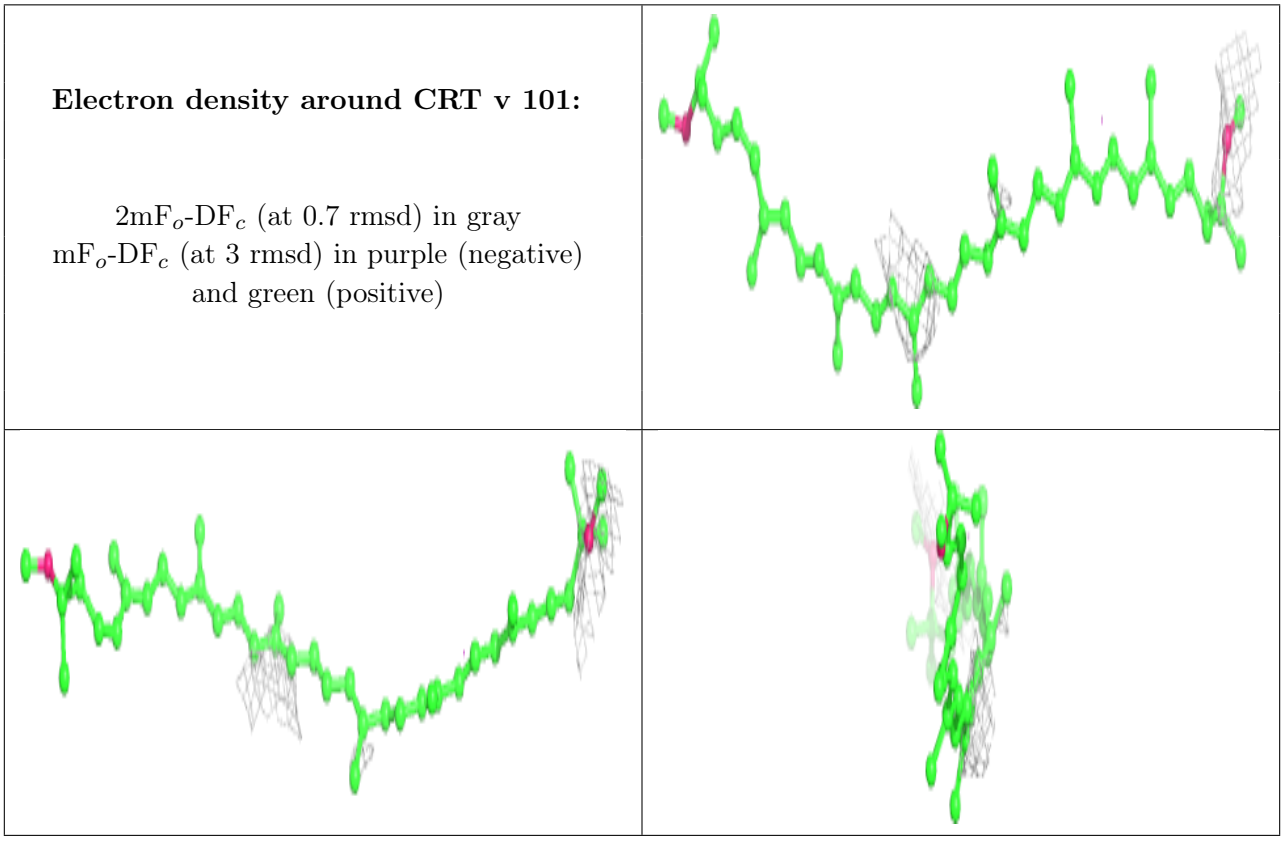
Electron density around CRT n 101:

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



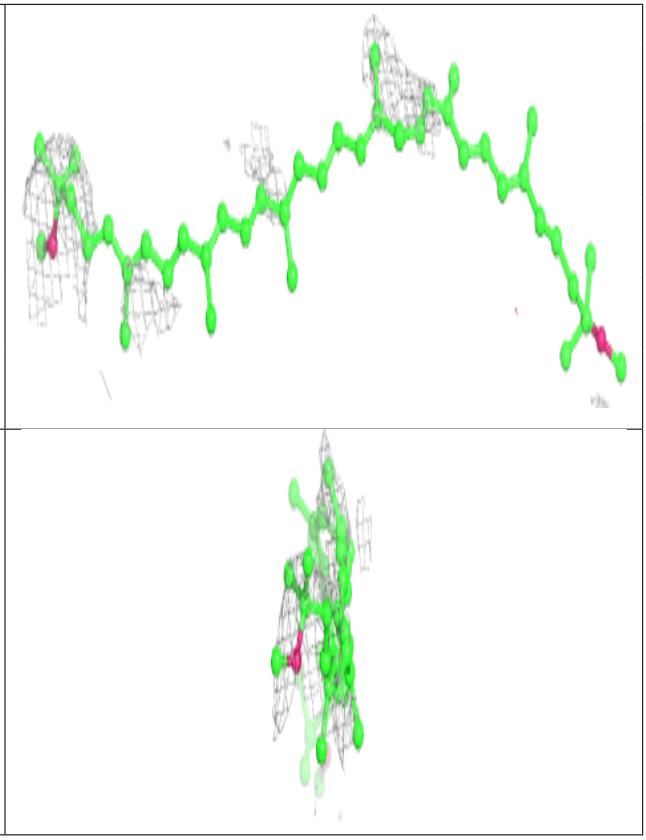
Electron density around CRT v 101:

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



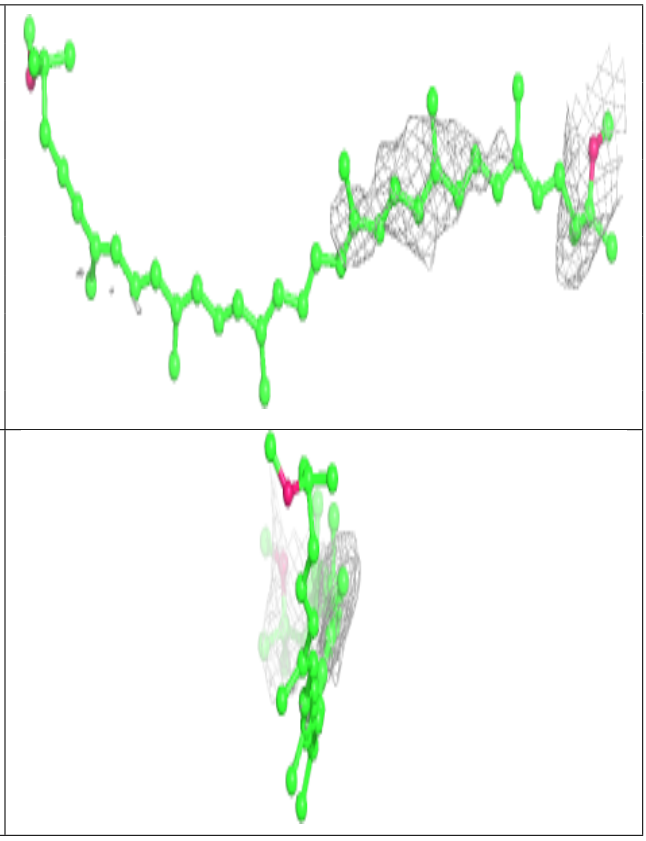
Electron density around CRT R 101:

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



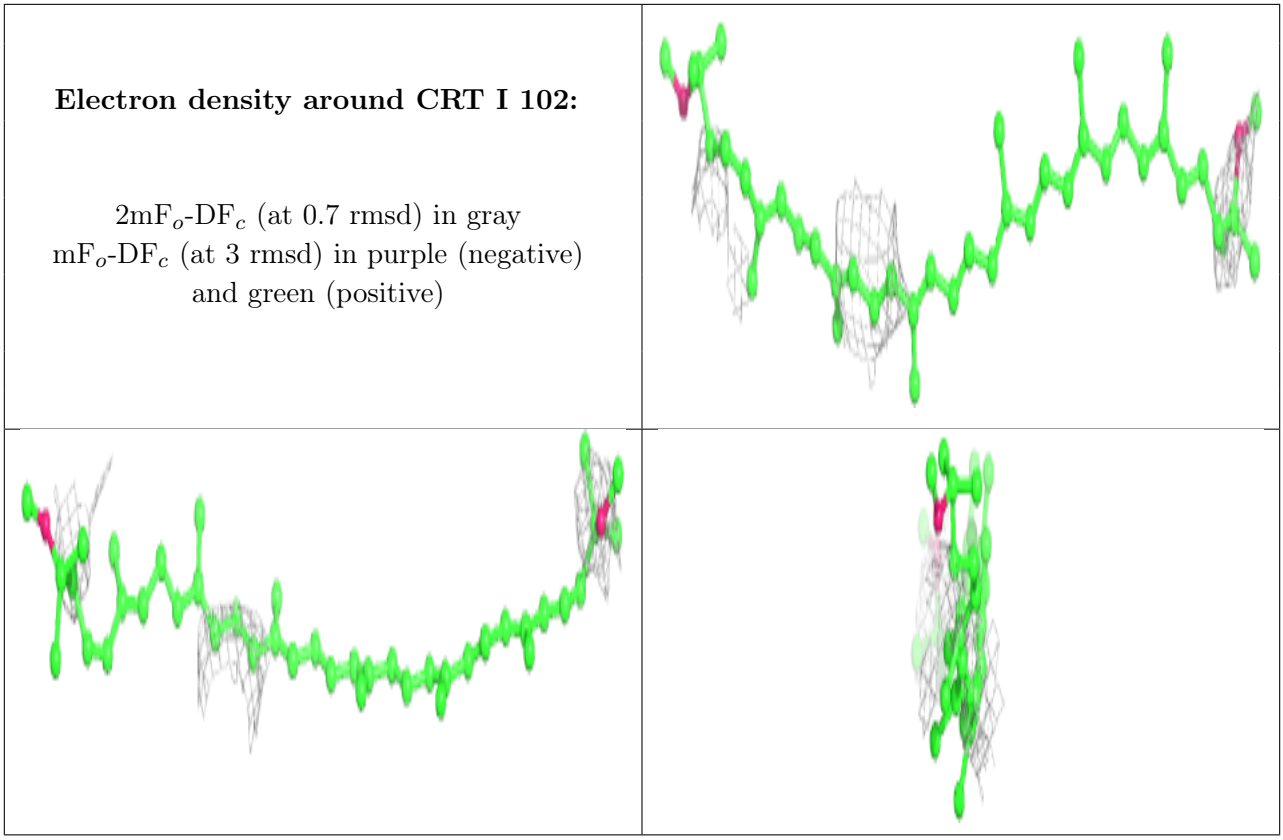
Electron density around CRT 0 101:

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



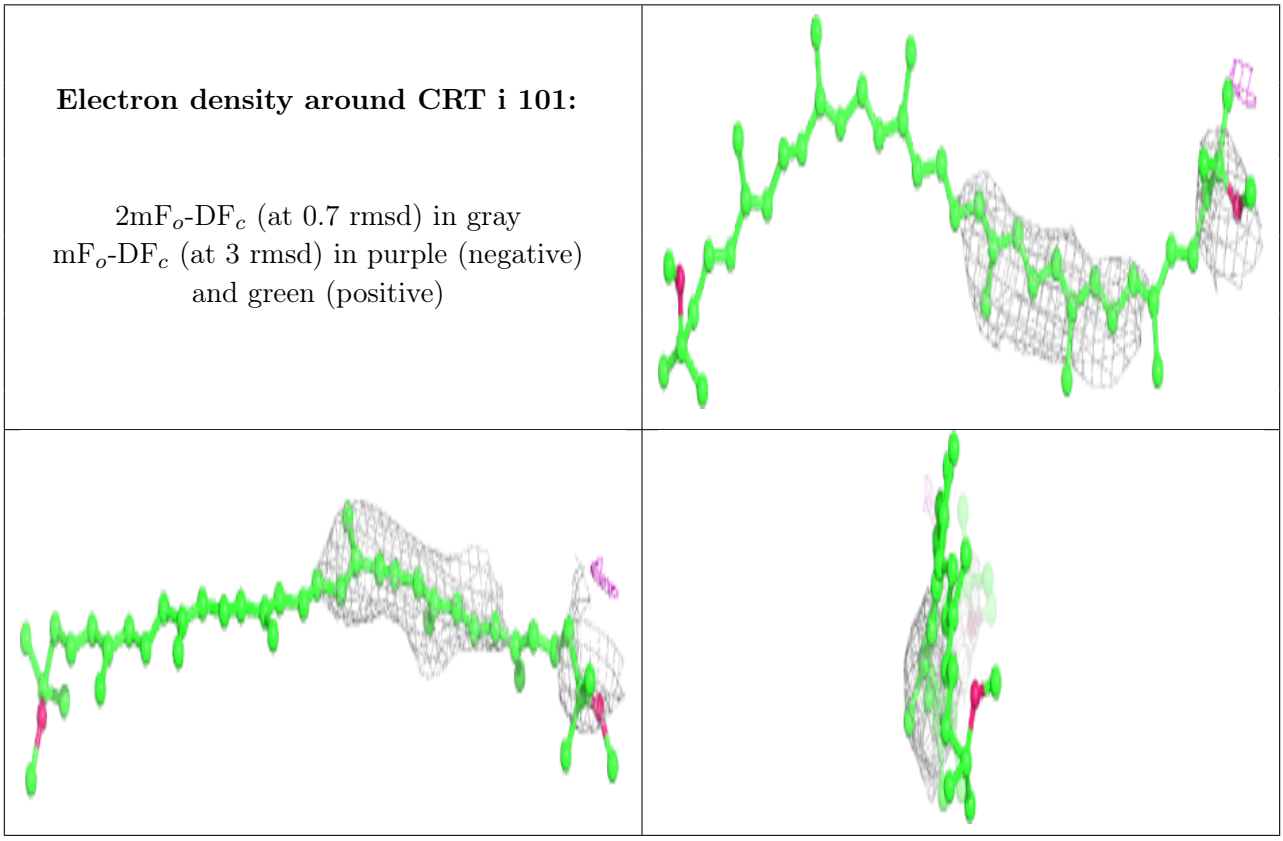
Electron density around CRT I 102:

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



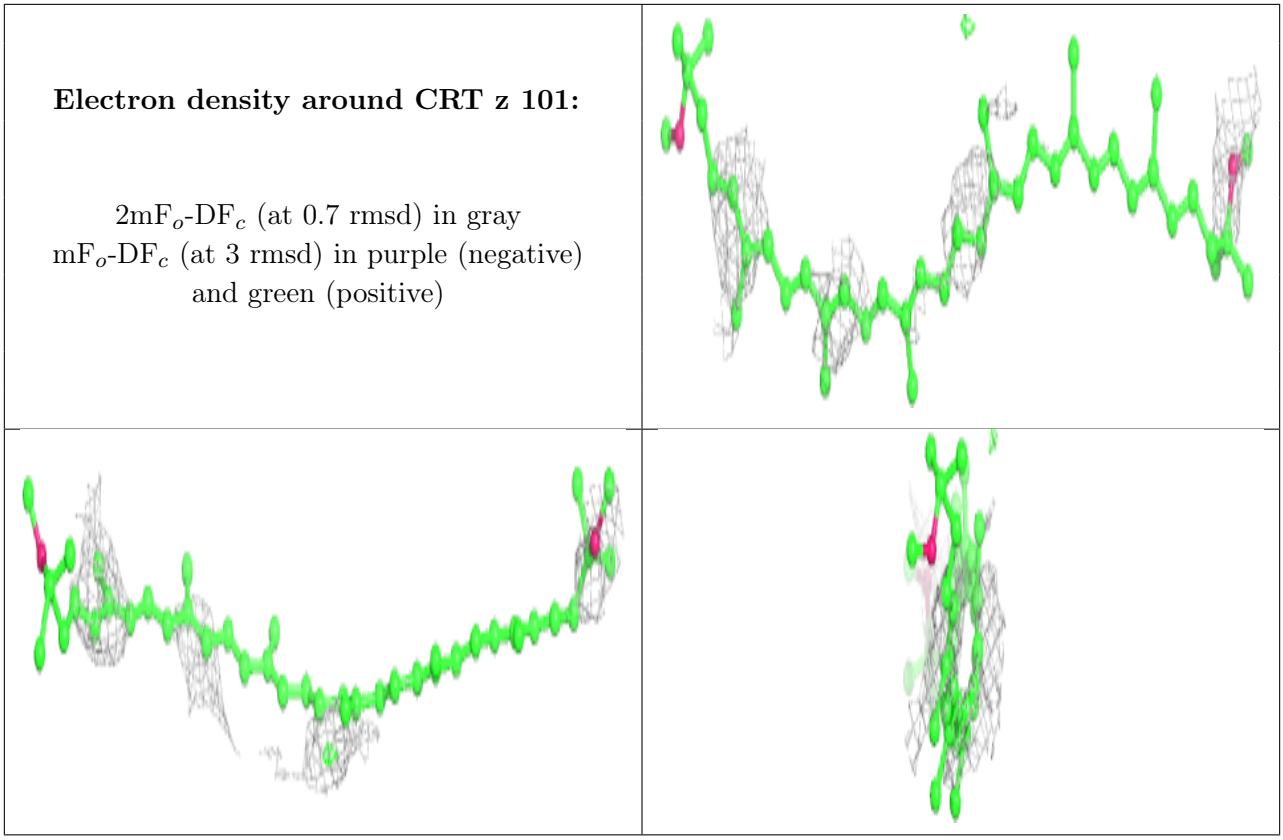
Electron density around CRT i 101:

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



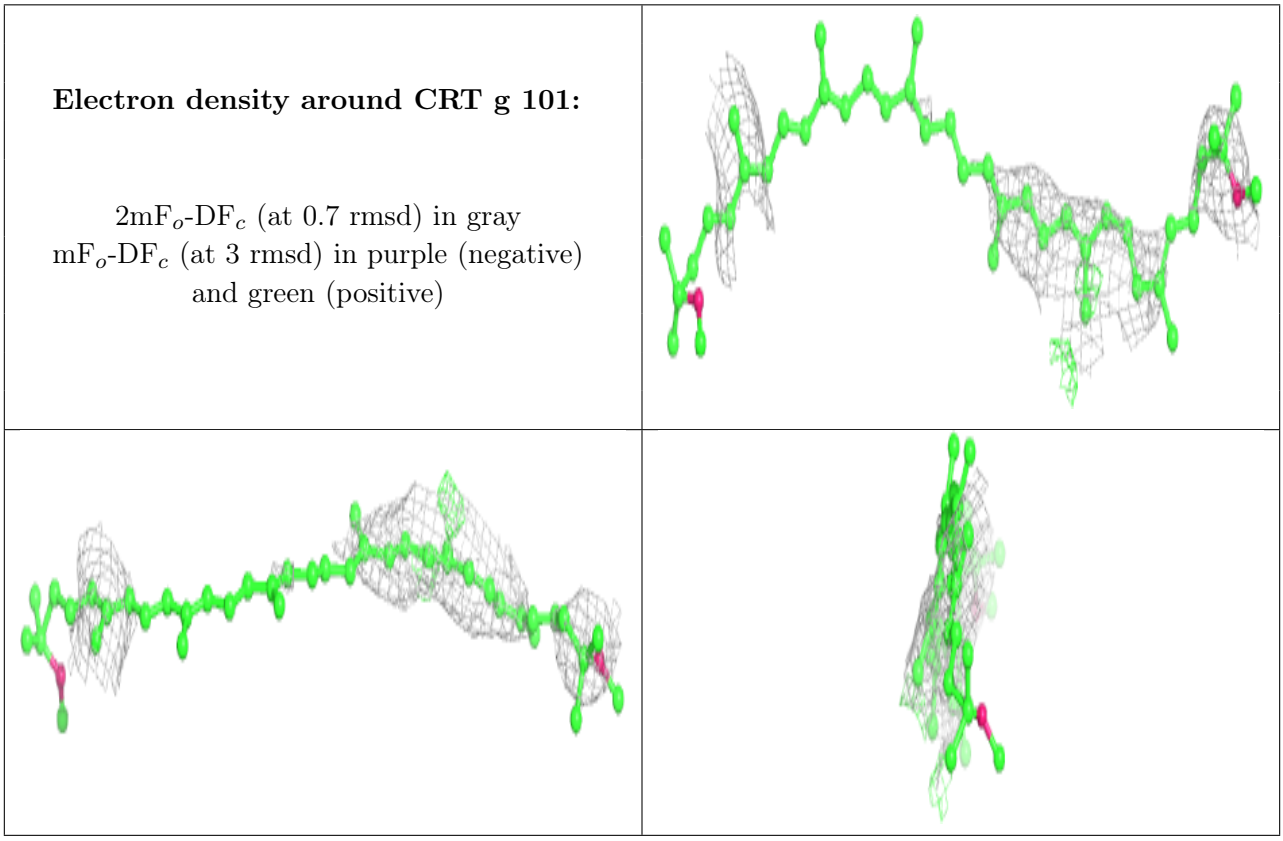
Electron density around CRT z 101:

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



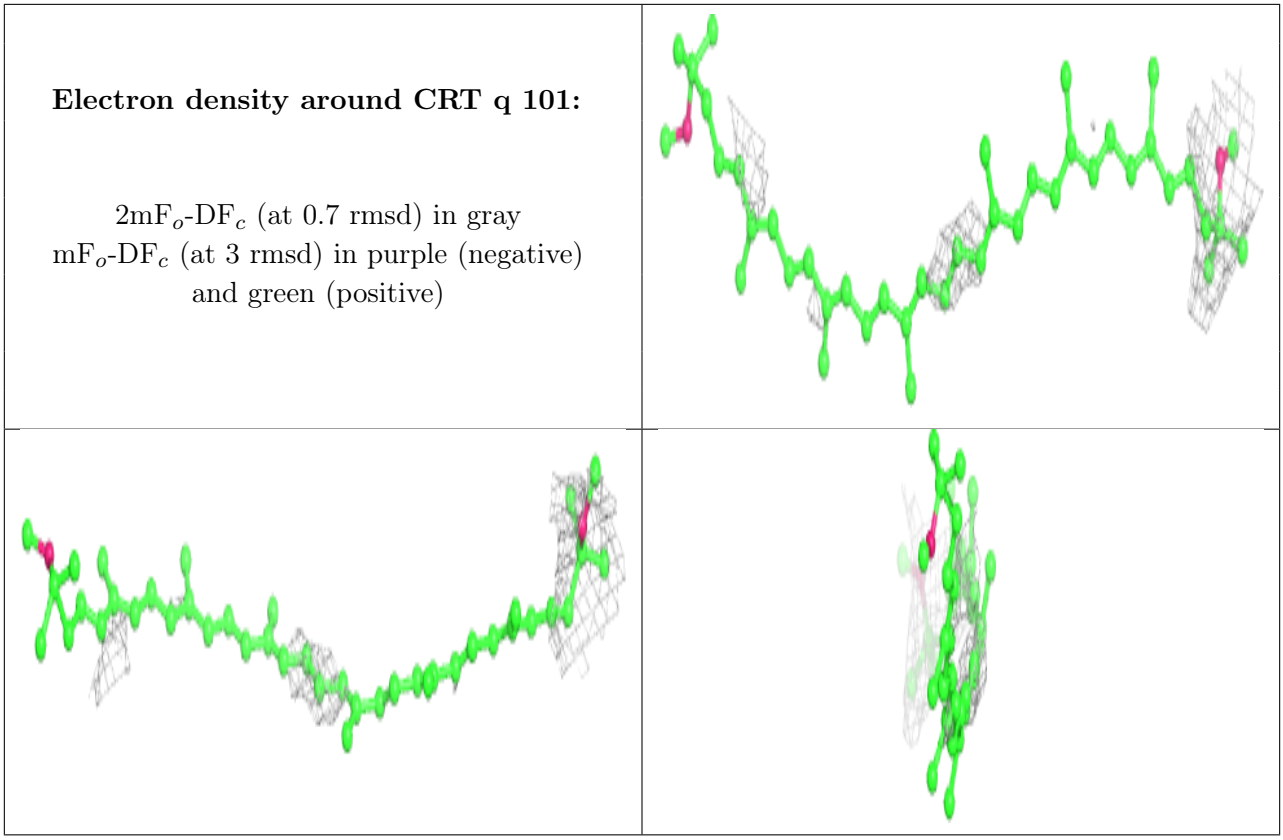
Electron density around CRT g 101:

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



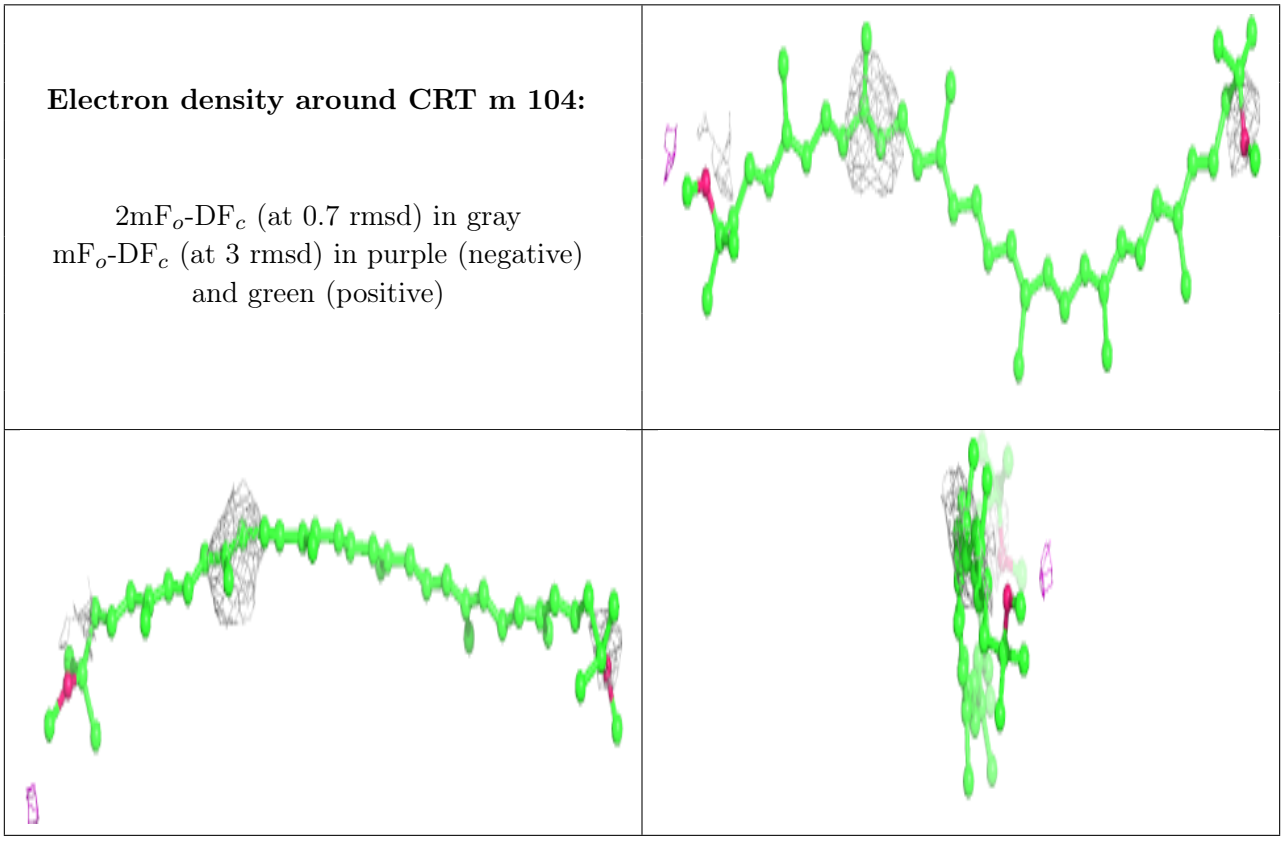
Electron density around CRT q 101:

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



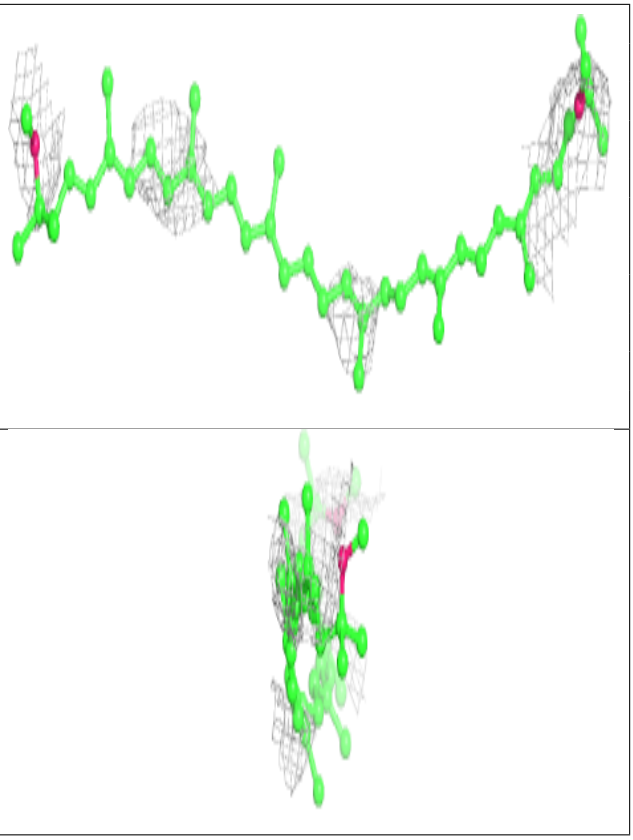
Electron density around CRT m 104:

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



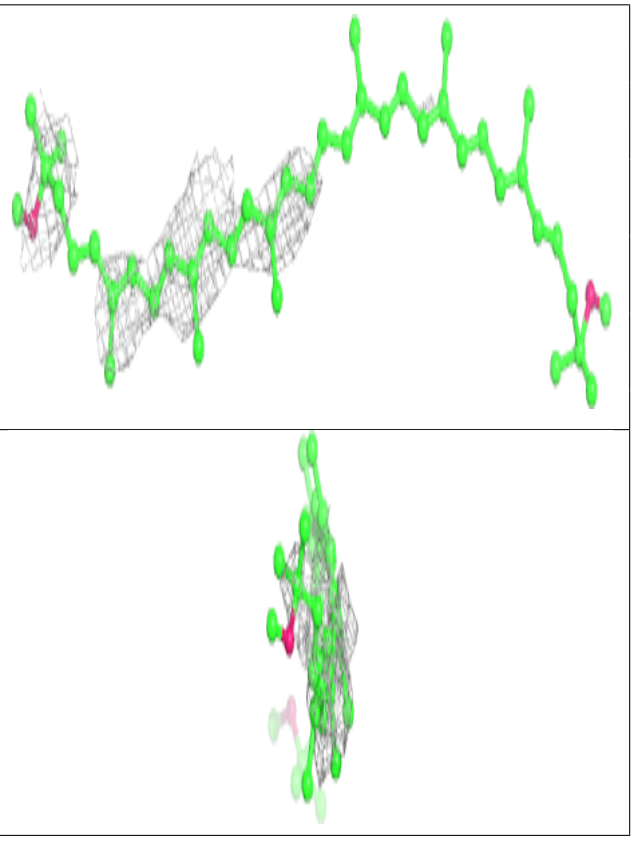
Electron density around CRT O 101:

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



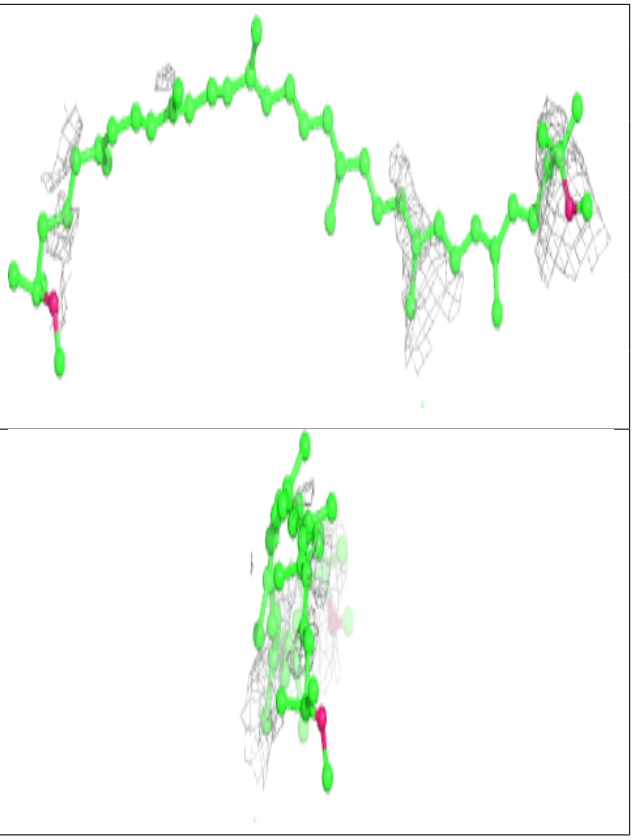
Electron density around CRT 7 101:

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



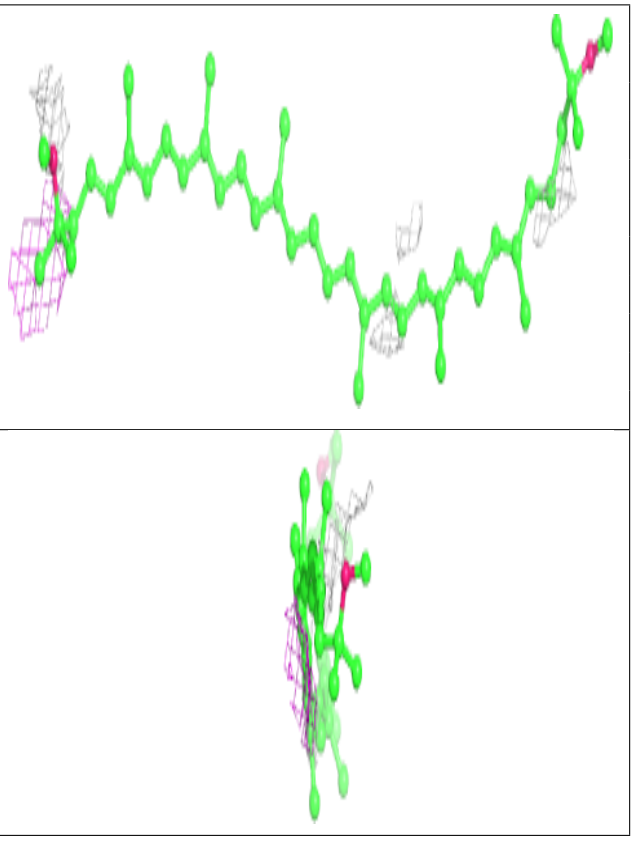
Electron density around CRT 9 101:

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



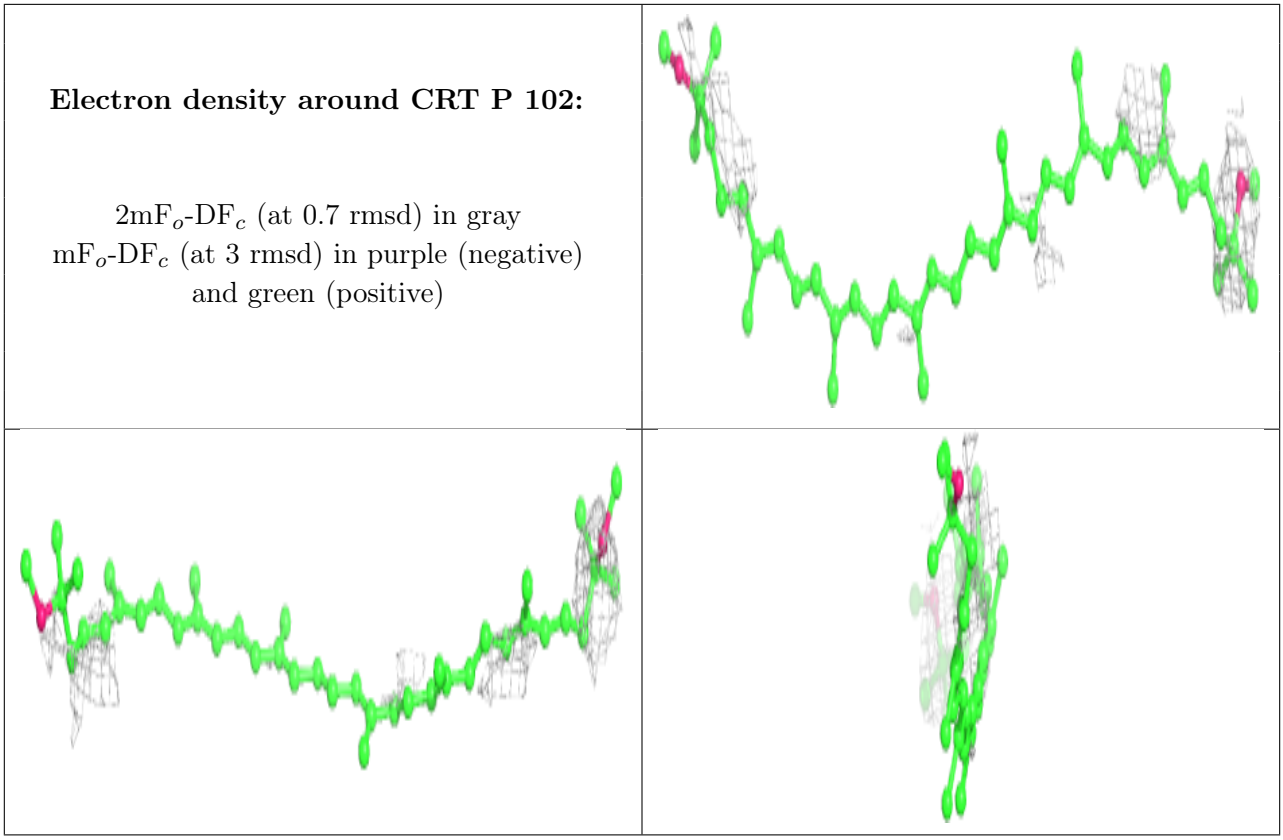
Electron density around CRT AC 101:

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



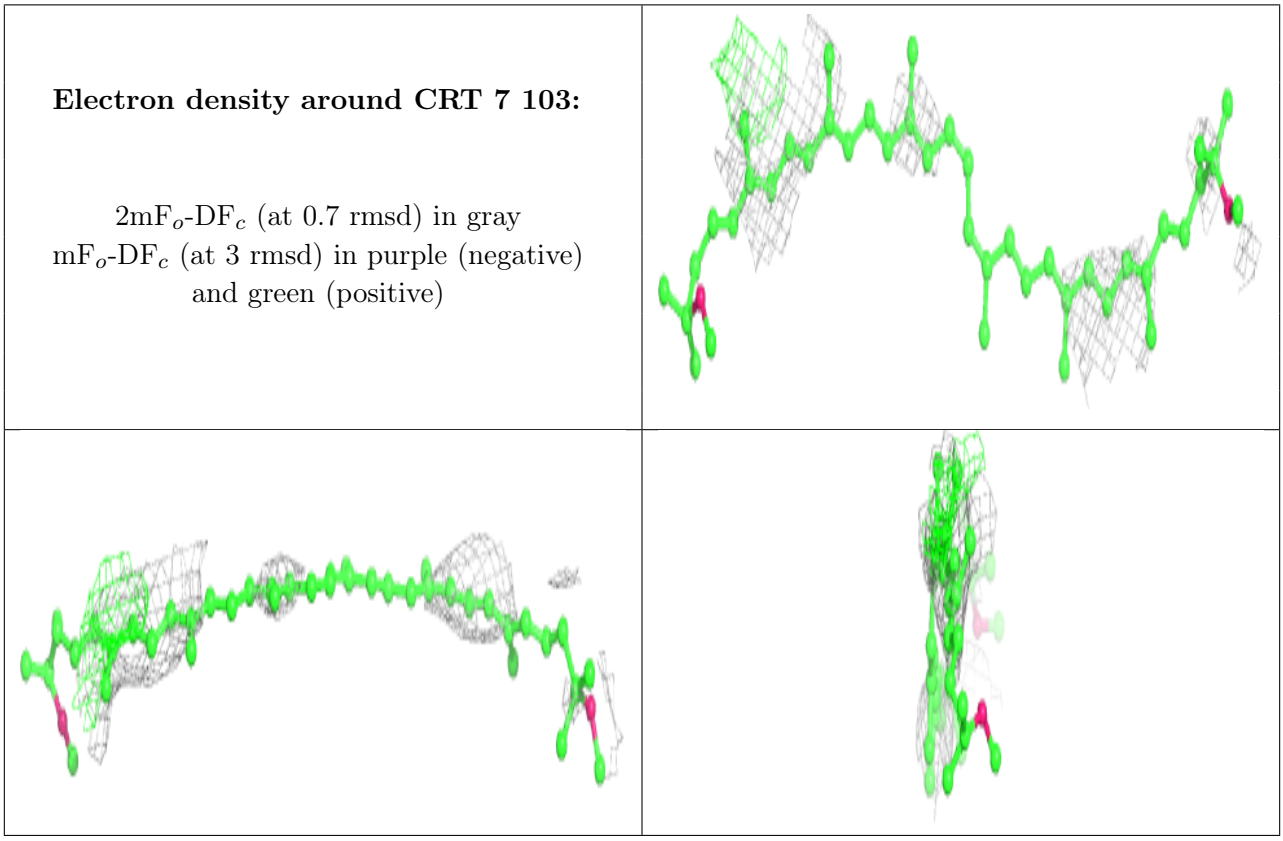
Electron density around CRT P 102:

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



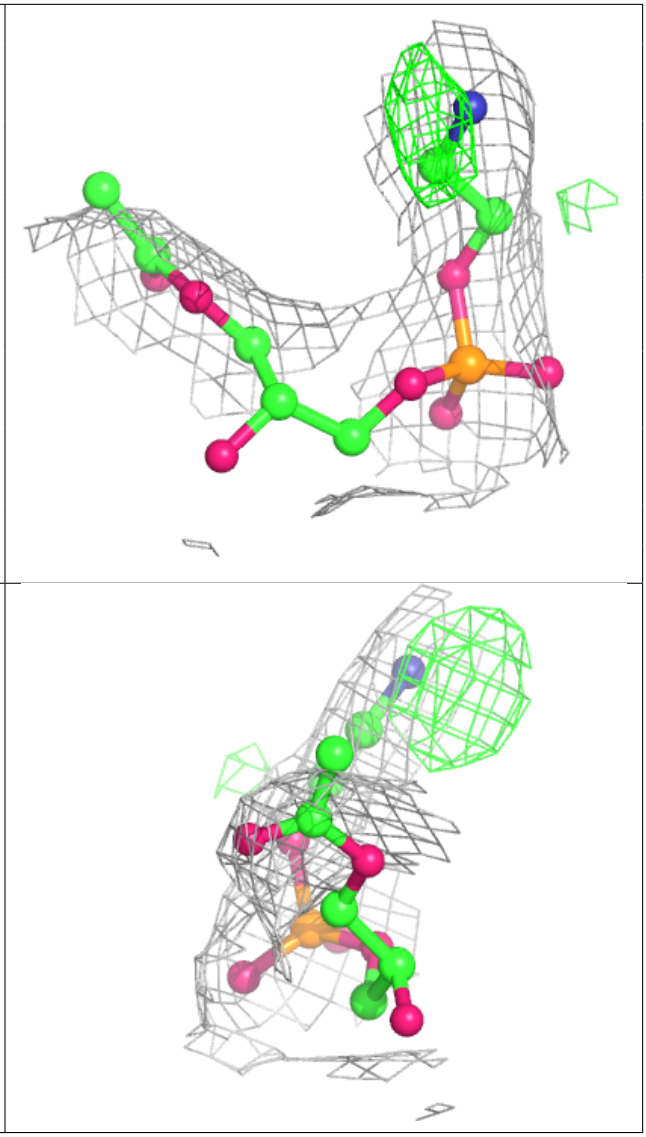
Electron density around CRT 7 103:

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



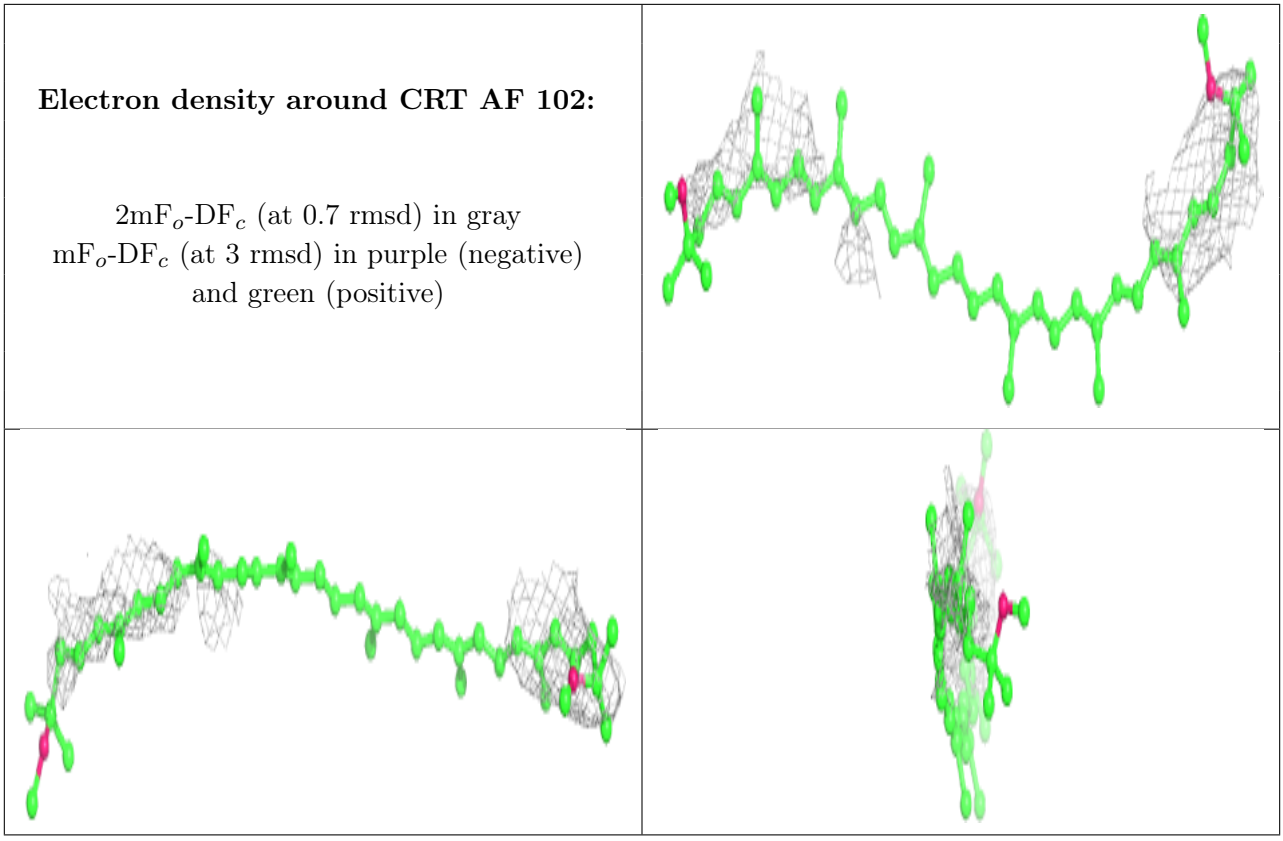
Electron density around PEF p 101:

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



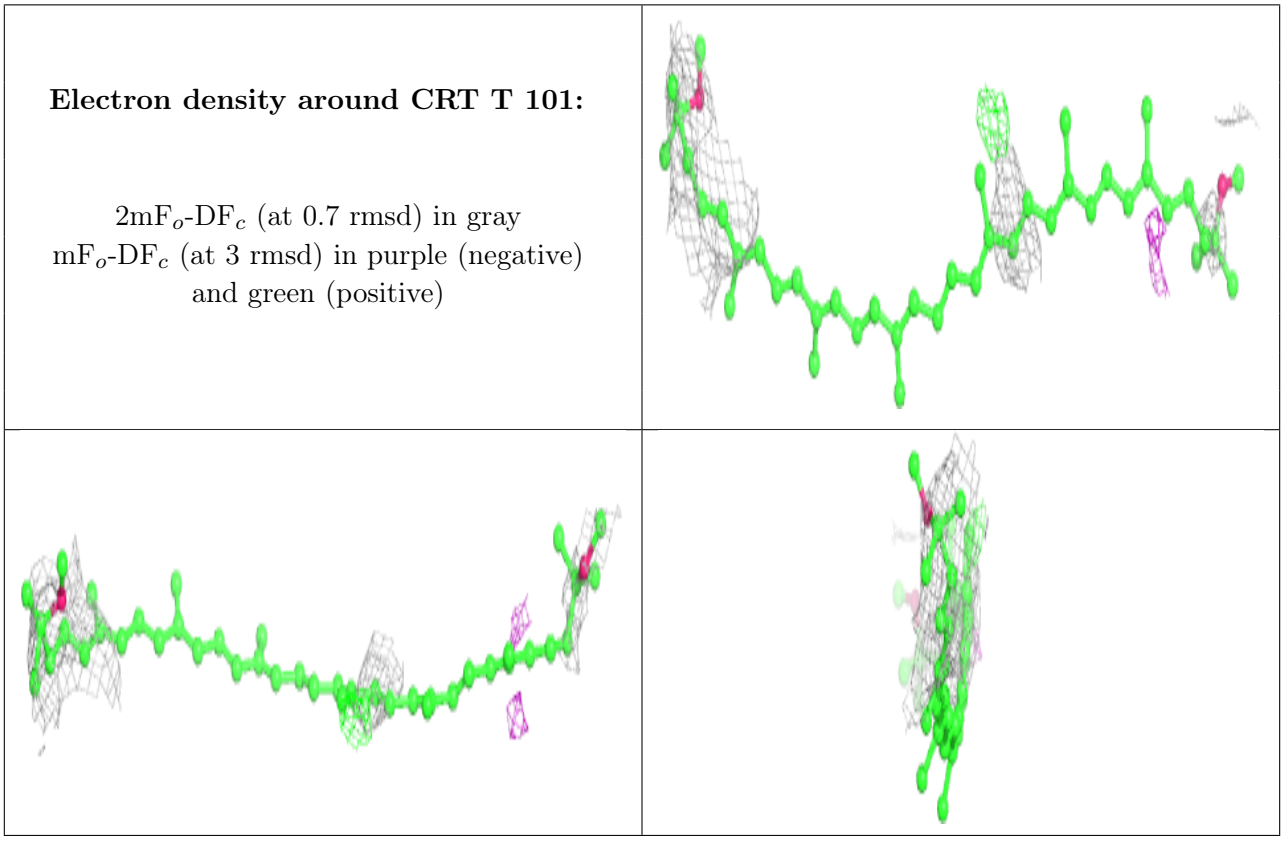
Electron density around CRT AF 102:

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



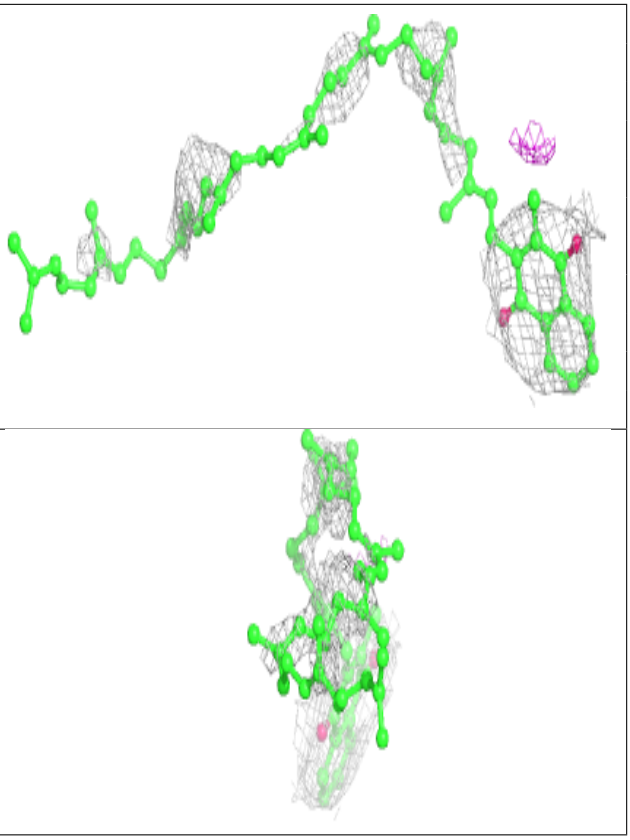
Electron density around CRT T 101:

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



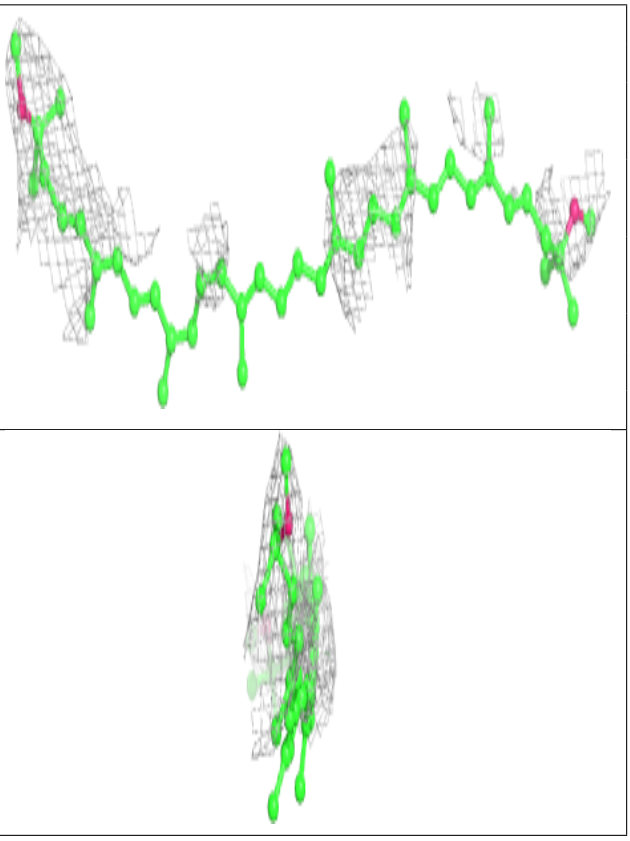
Electron density around MQ8 M 404:

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



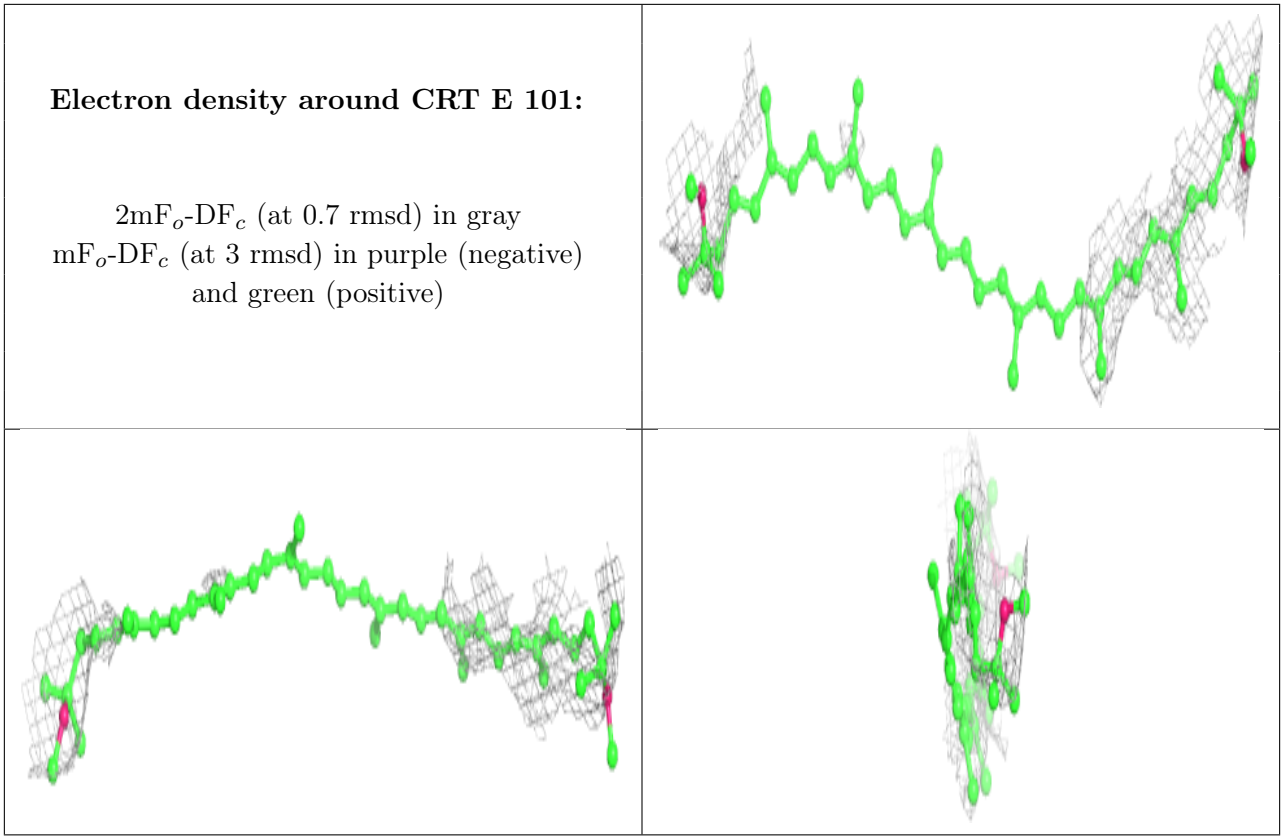
Electron density around CRT AD 101:

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



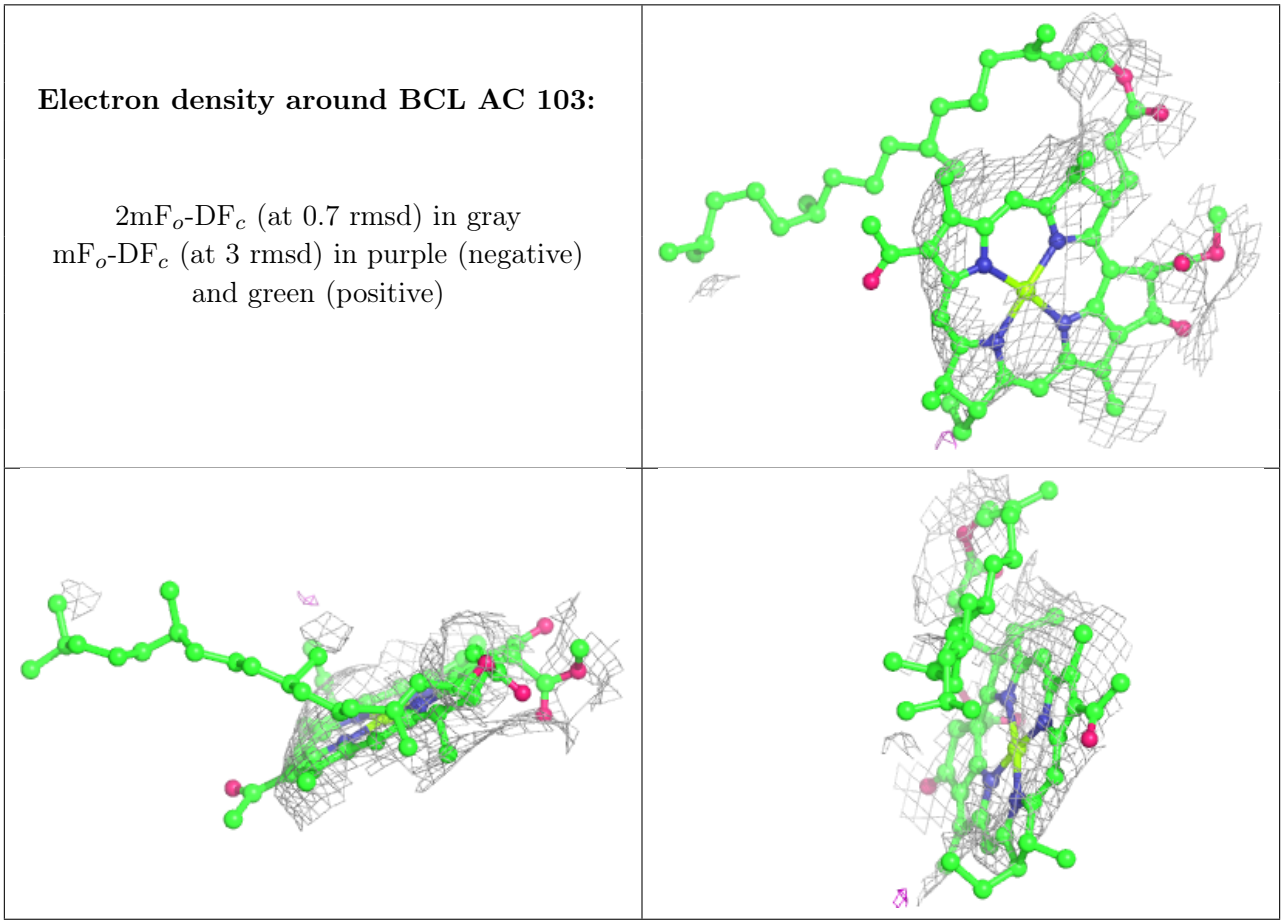
Electron density around CRT E 101:

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



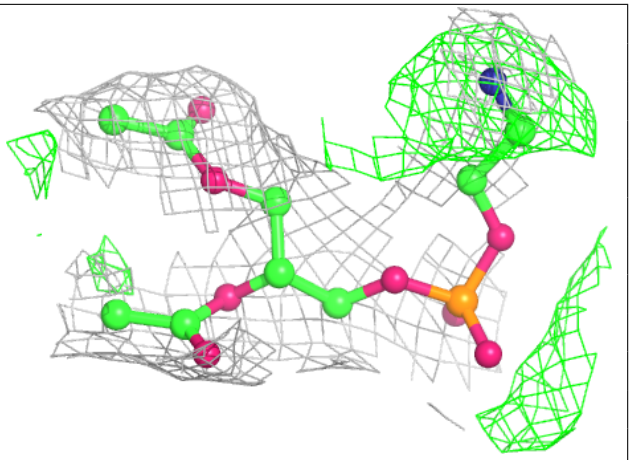
Electron density around BCL AC 103:

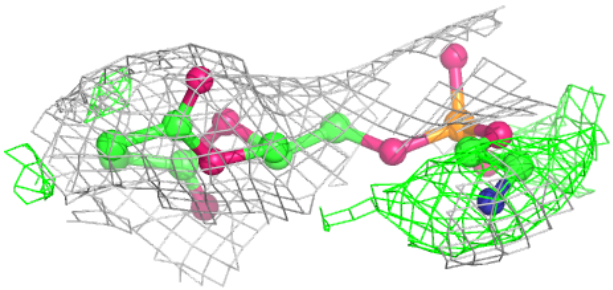
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

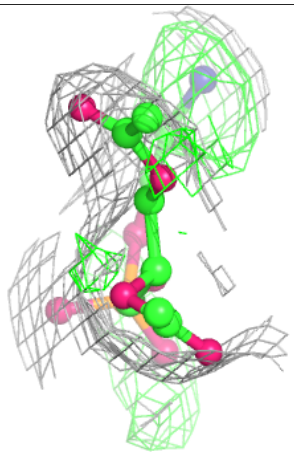


Electron density around PEF A 101:

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

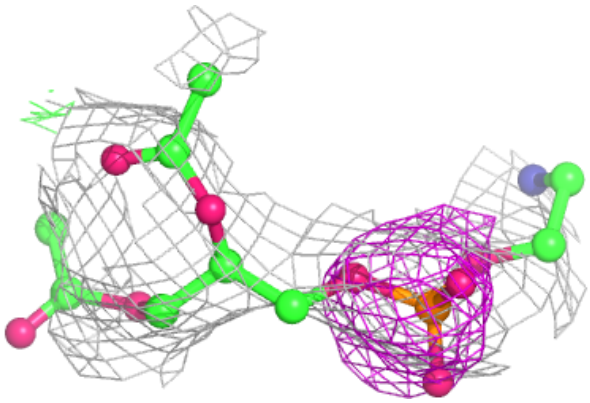


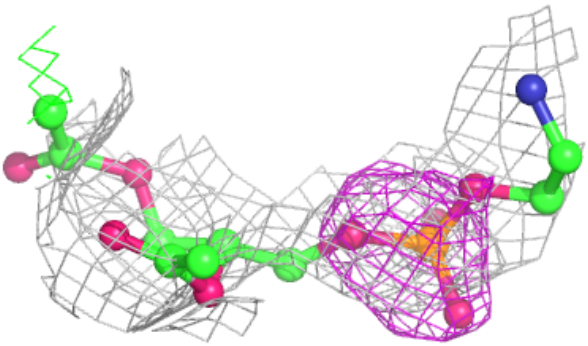


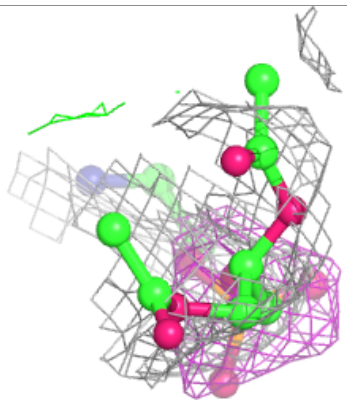


Electron density around PEF H 304:

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

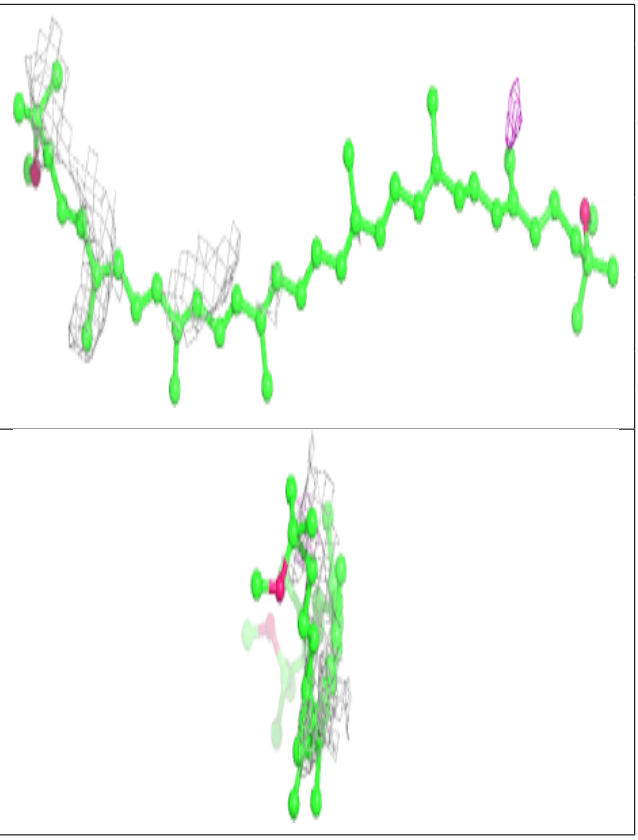






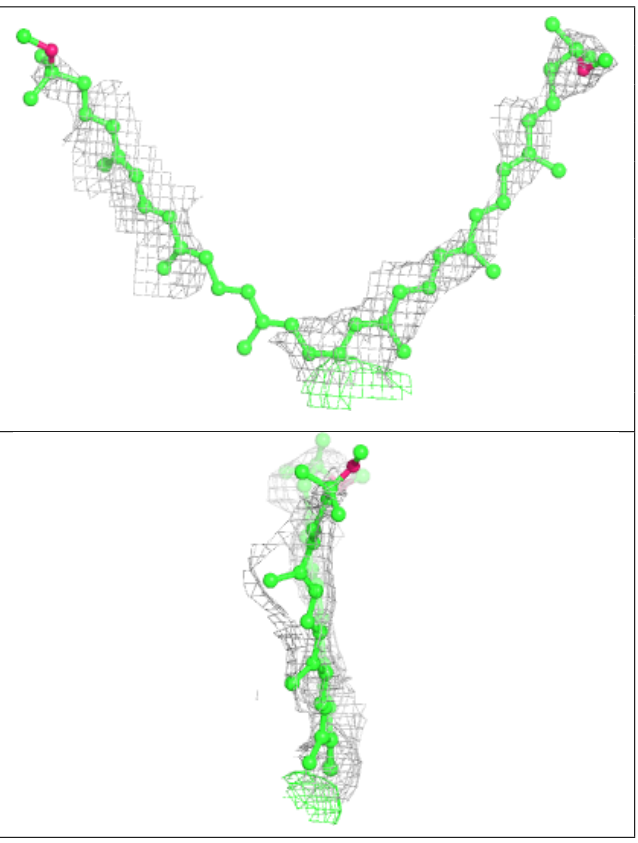
Electron density around CRT G 101:

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



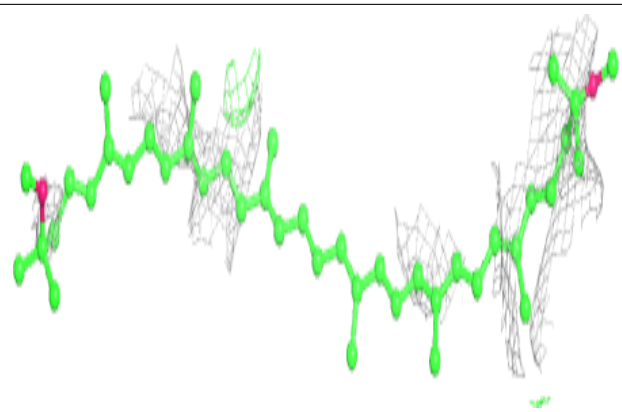
Electron density around CRT M 405:

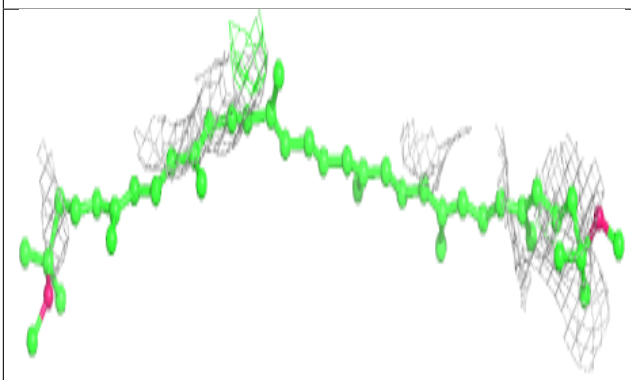
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

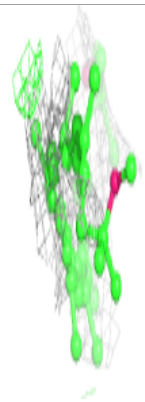


Electron density around CRT AH 102:

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

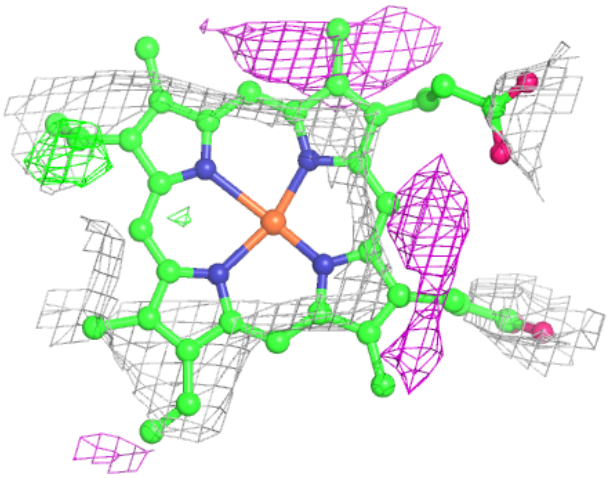


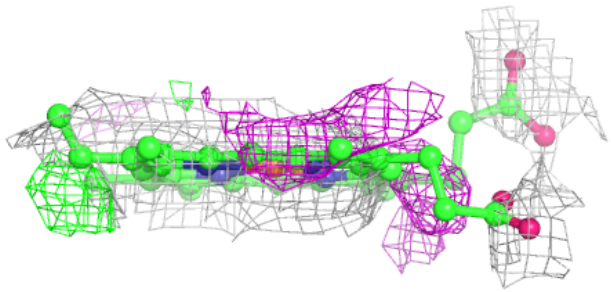


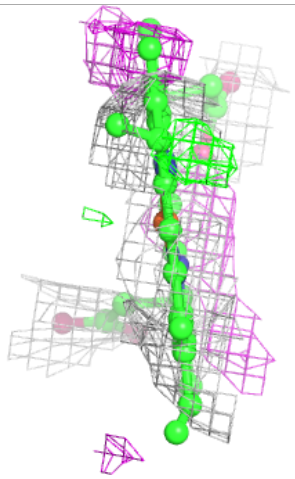


Electron density around HEM o 501:

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

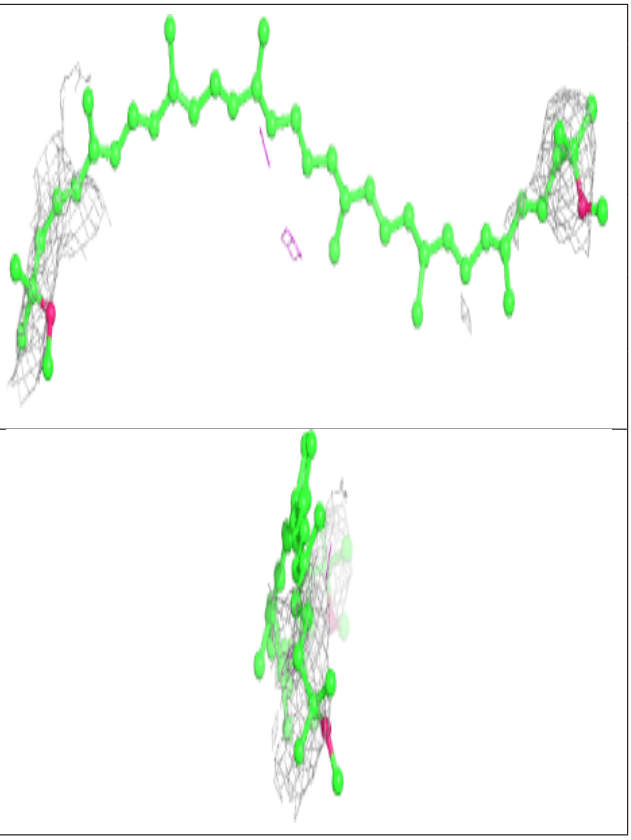


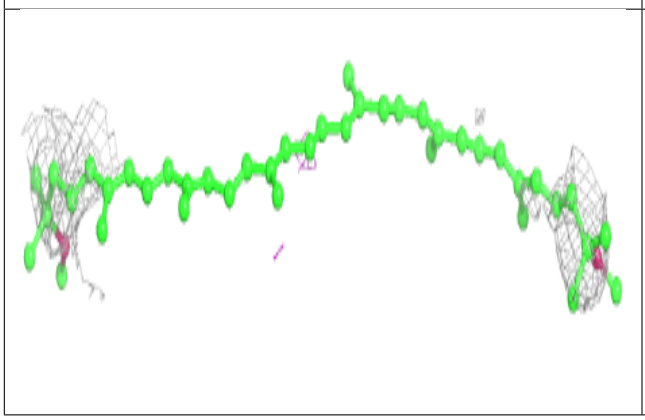




Electron density around CRT AL 101:

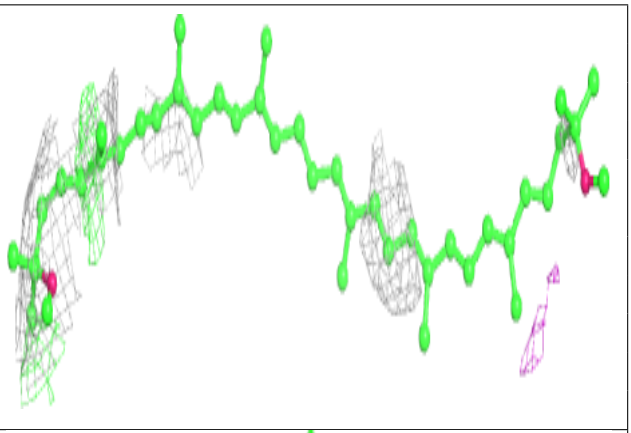
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

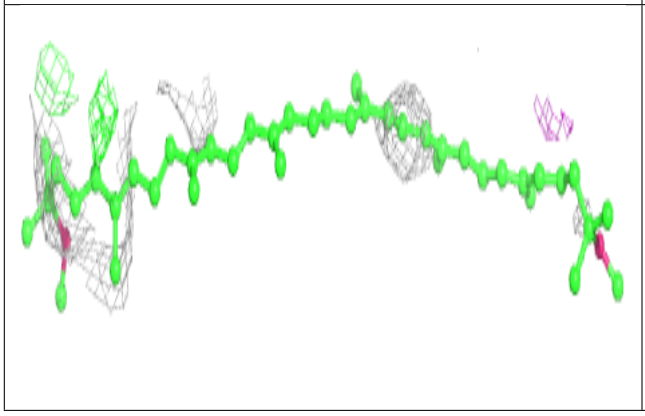




Electron density around CRT e 101:

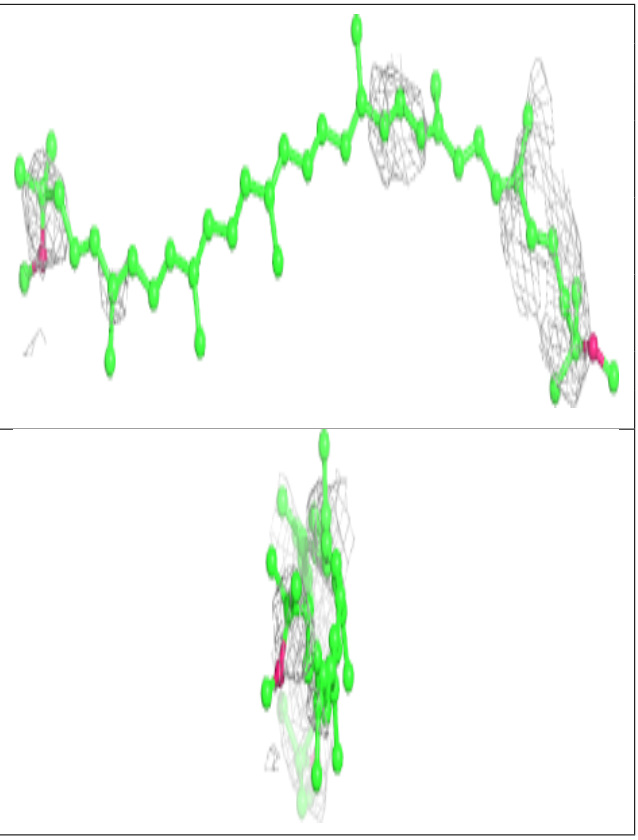
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





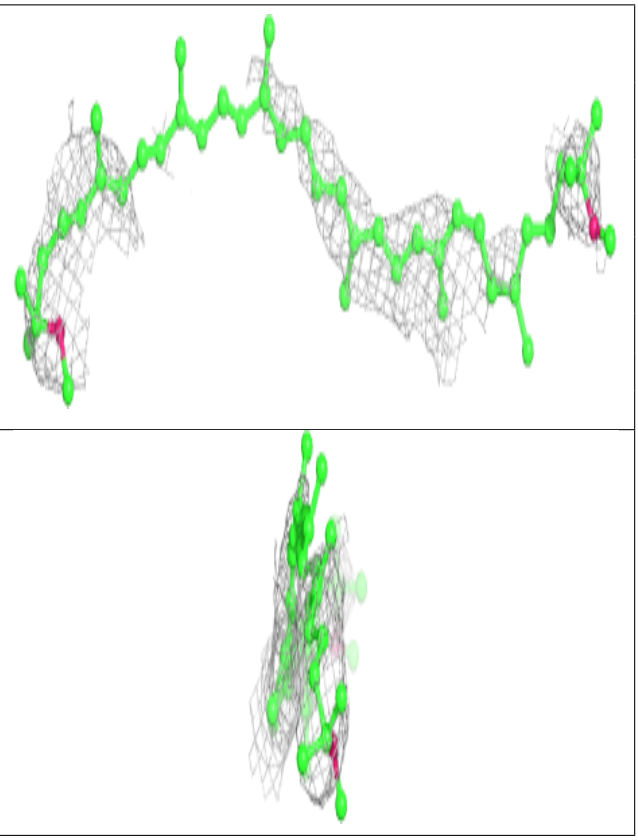
Electron density around CRT V 101:

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



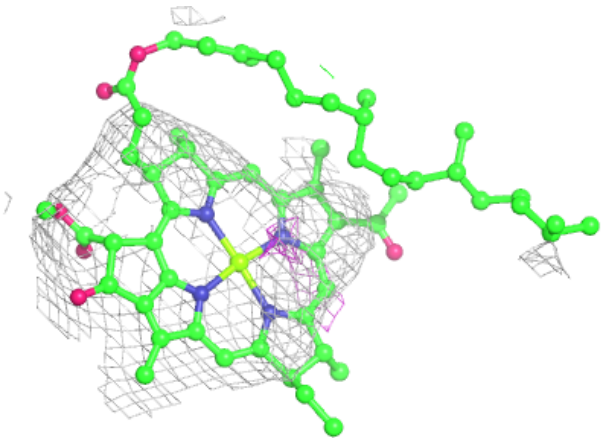
Electron density around CRT 4 101:

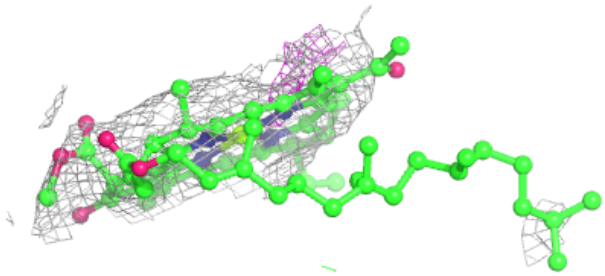
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

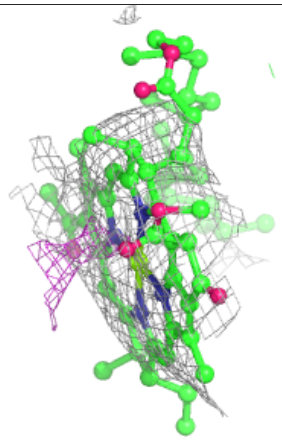


Electron density around BCL AB 102:

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

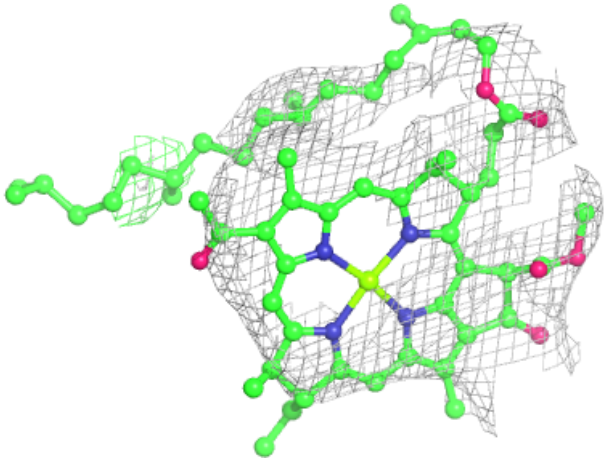


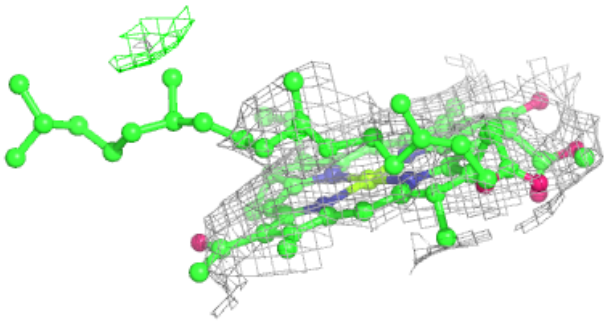


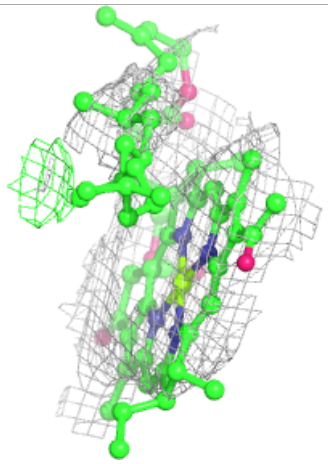


Electron density around BCL AG 101:

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

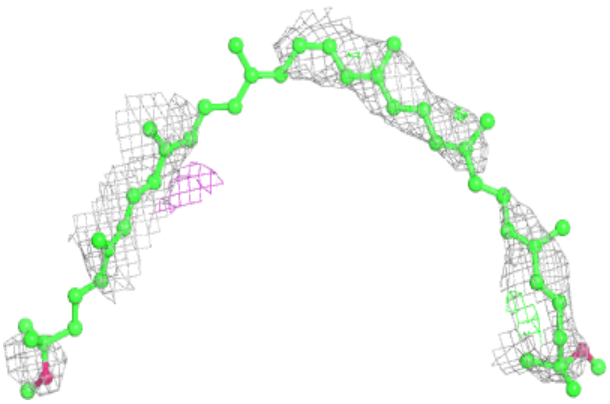


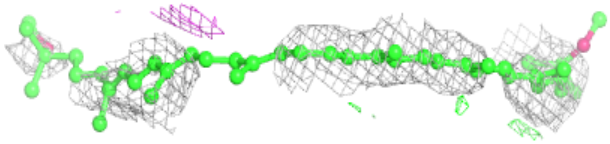


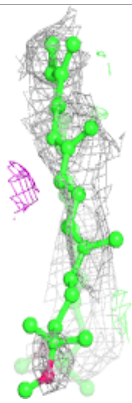


Electron density around CRT y 404:

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

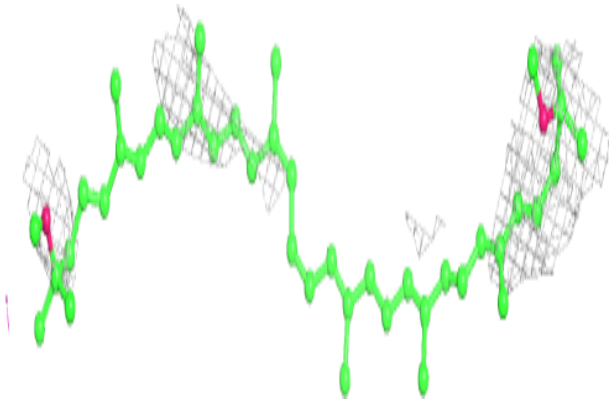


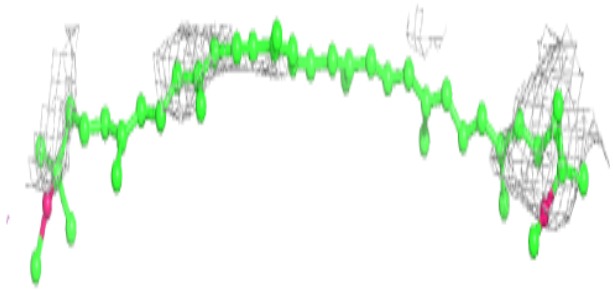


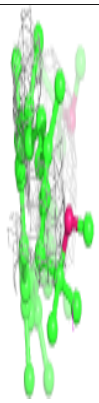


Electron density around CRT k 101:

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

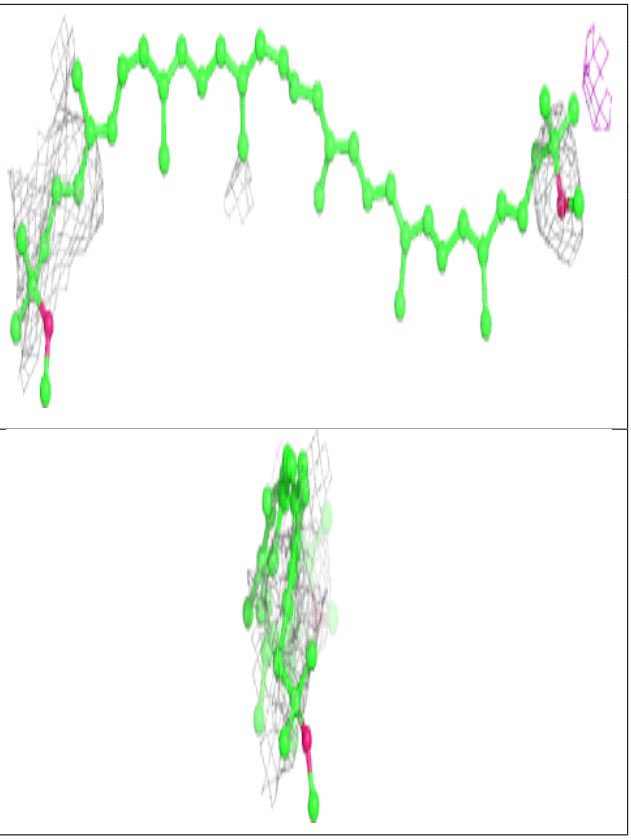






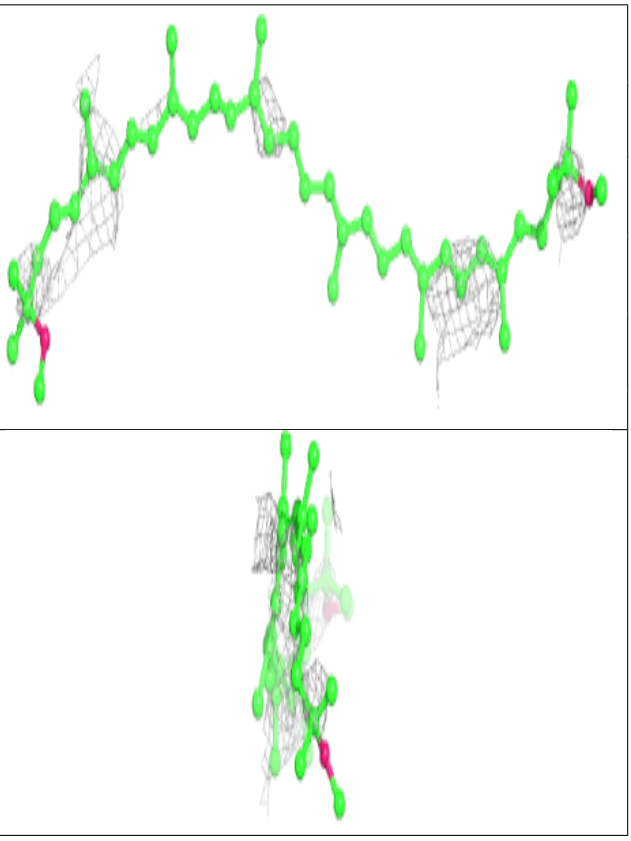
Electron density around CRT AJ 101:

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



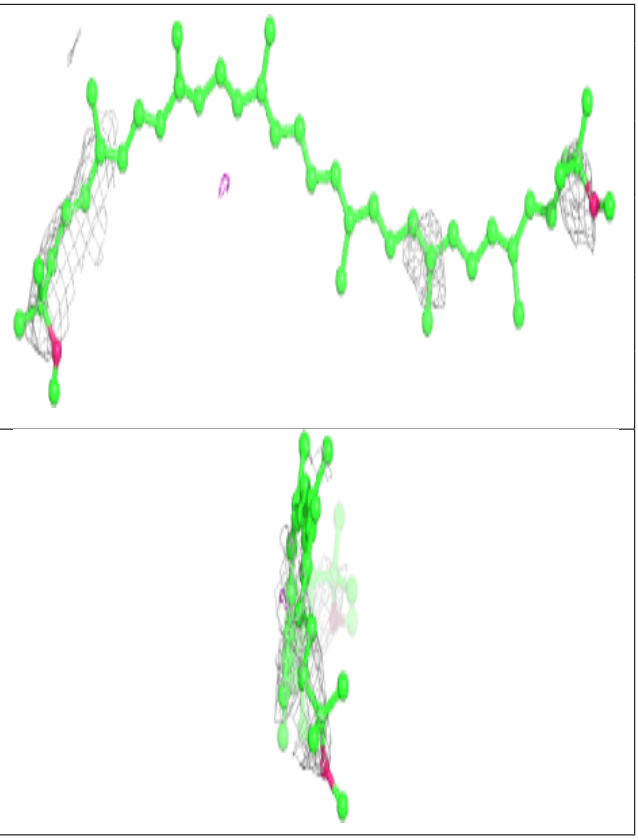
Electron density around CRT Z 101:

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



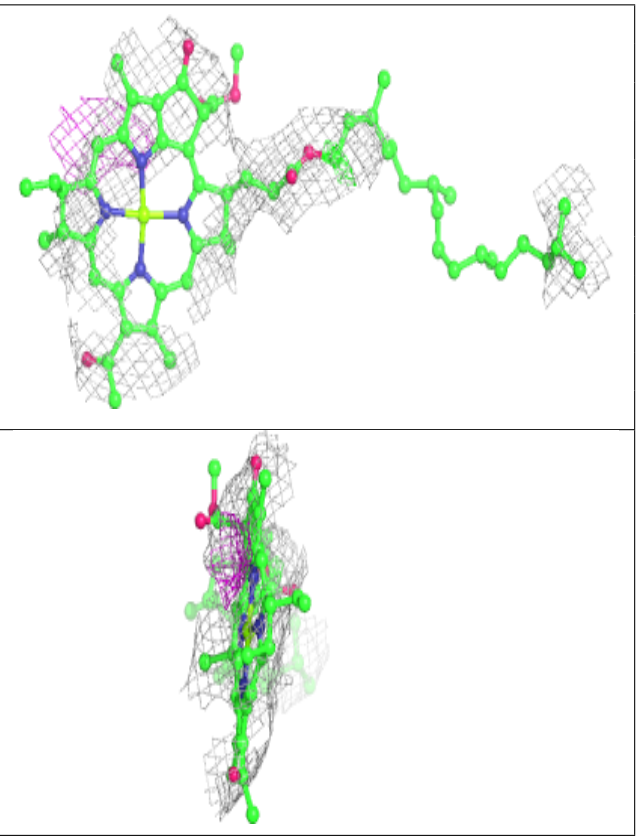
Electron density around CRT 2 101:

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



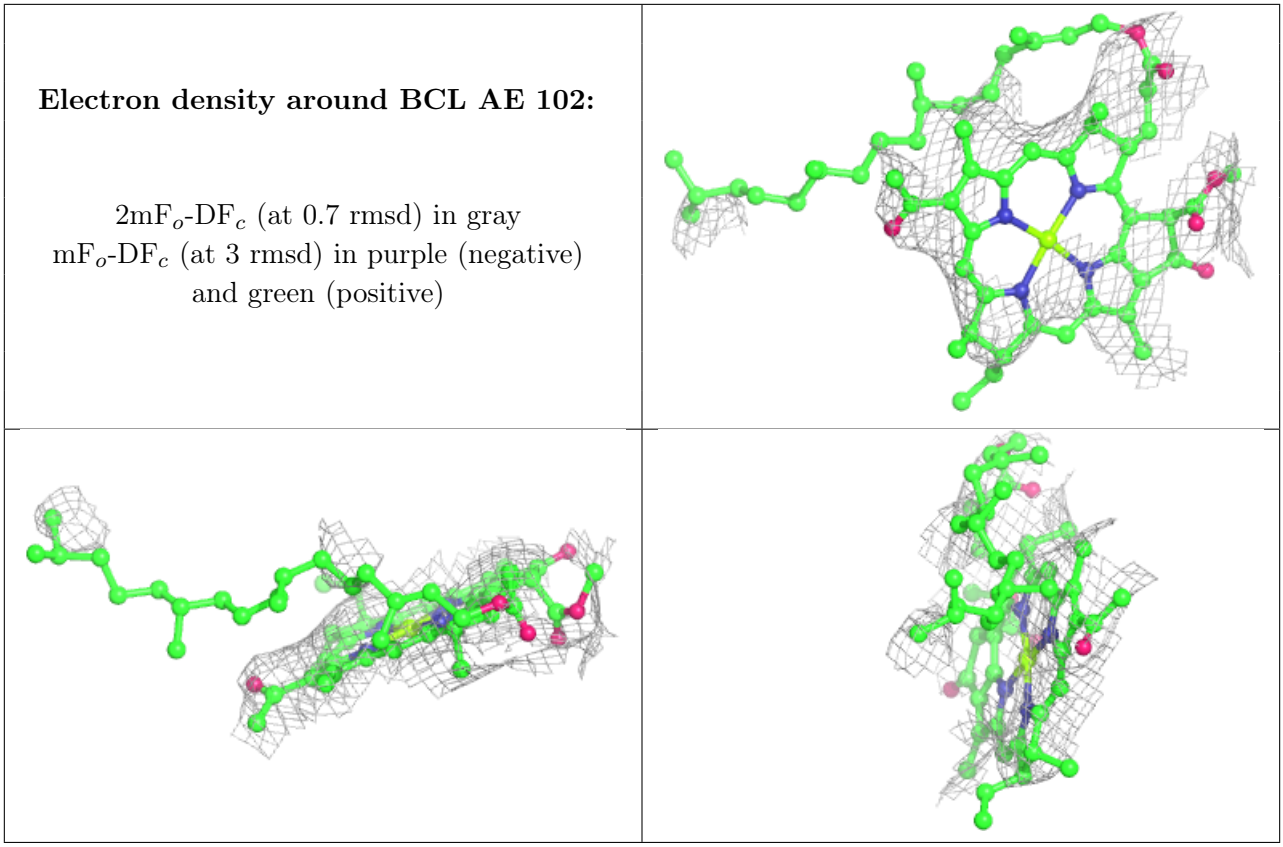
Electron density around BCL D 101:

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



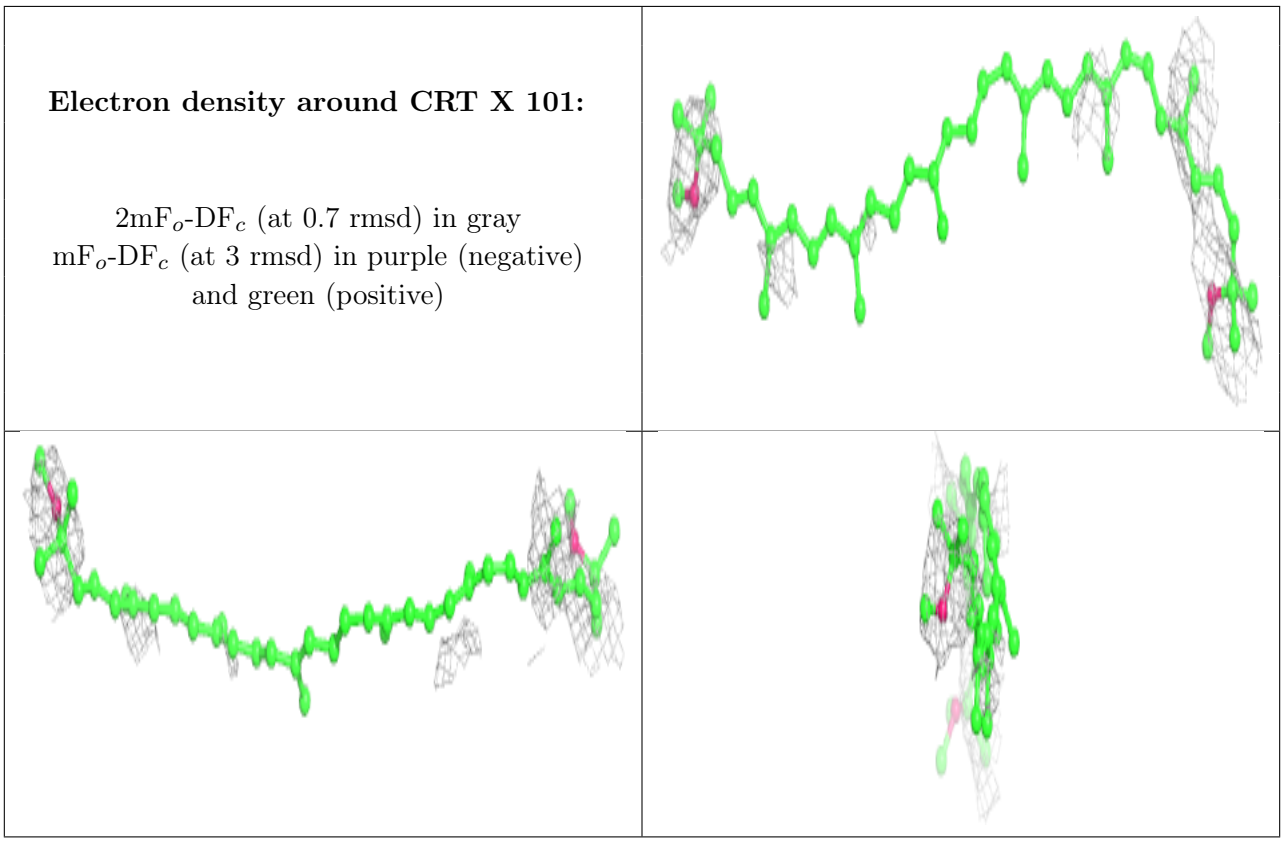
Electron density around BCL AE 102:

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



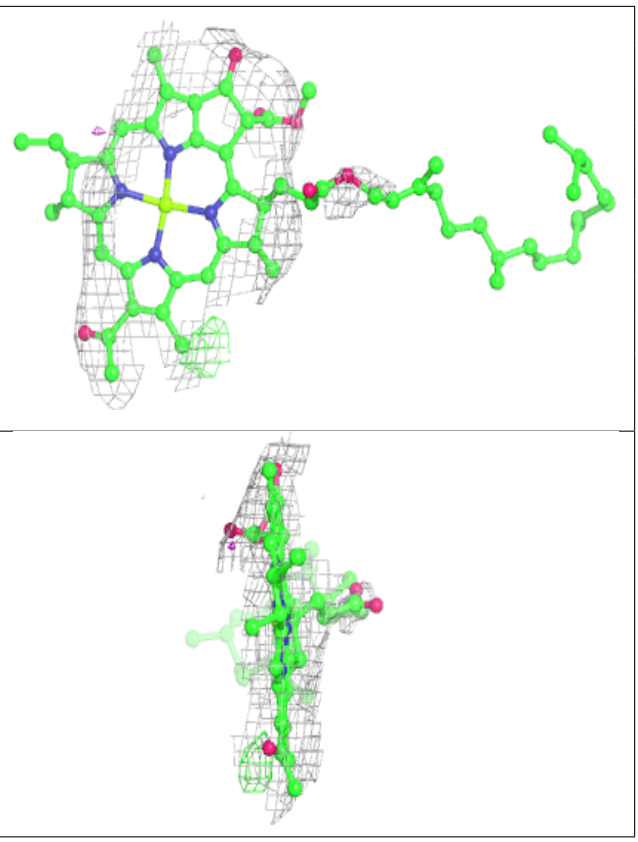
Electron density around CRT X 101:

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



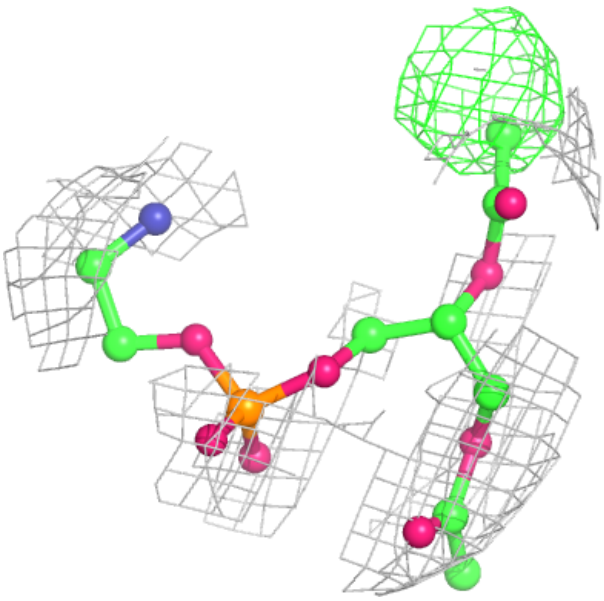
Electron density around BCL K 101:

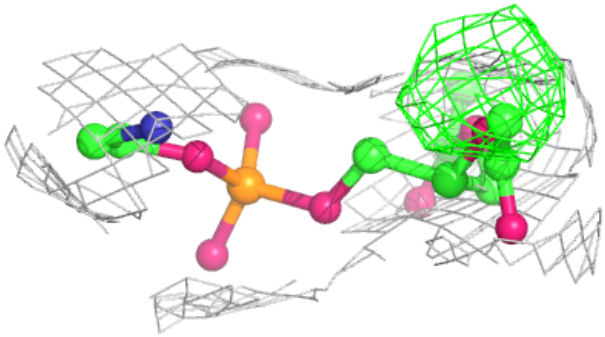
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

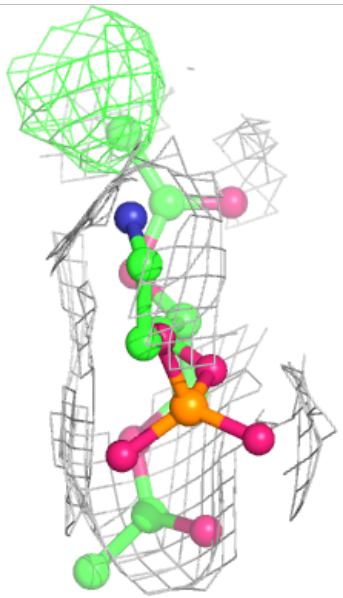


Electron density around PEF y 406:

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

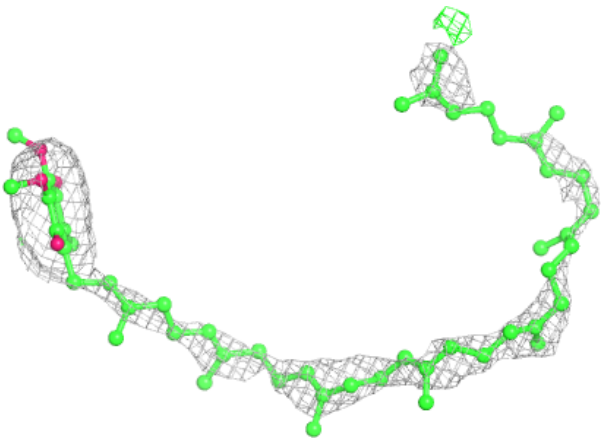


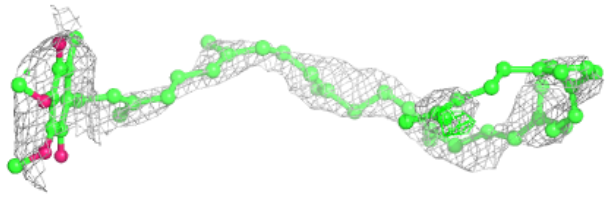


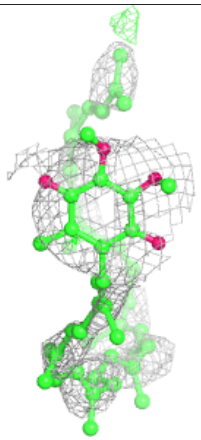


Electron density around UQ8 L 304:

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

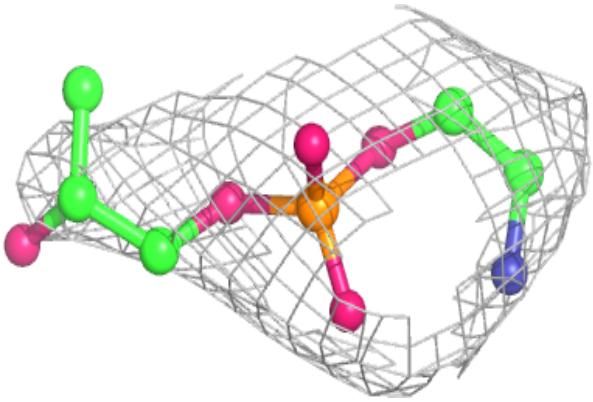


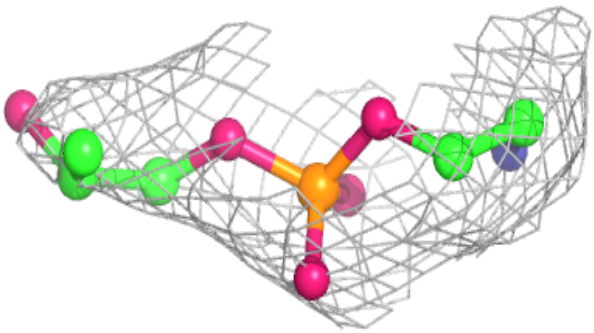


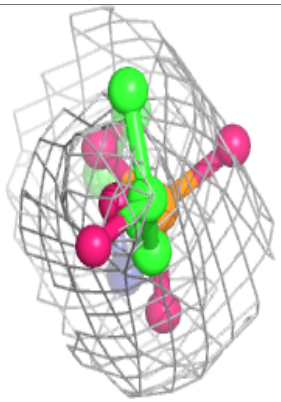


Electron density around PEF L 305:

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

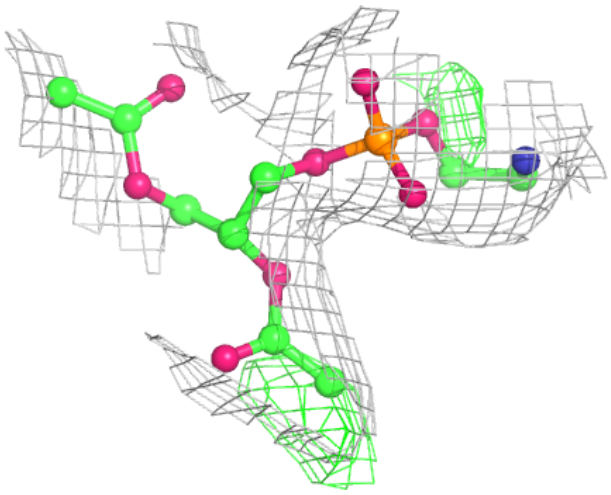


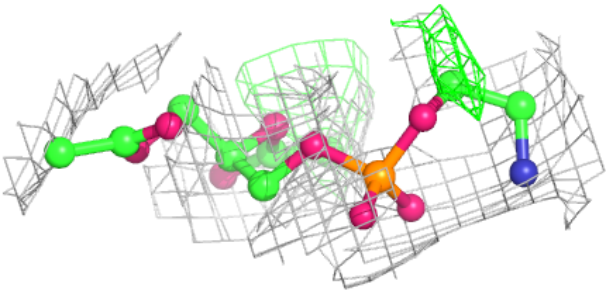


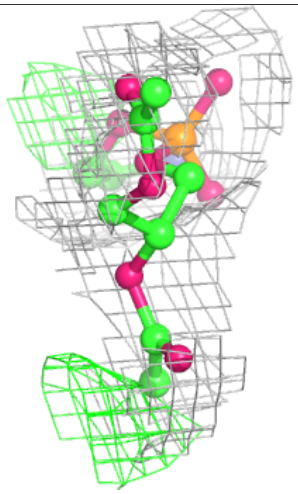


Electron density around PEF H 302:

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

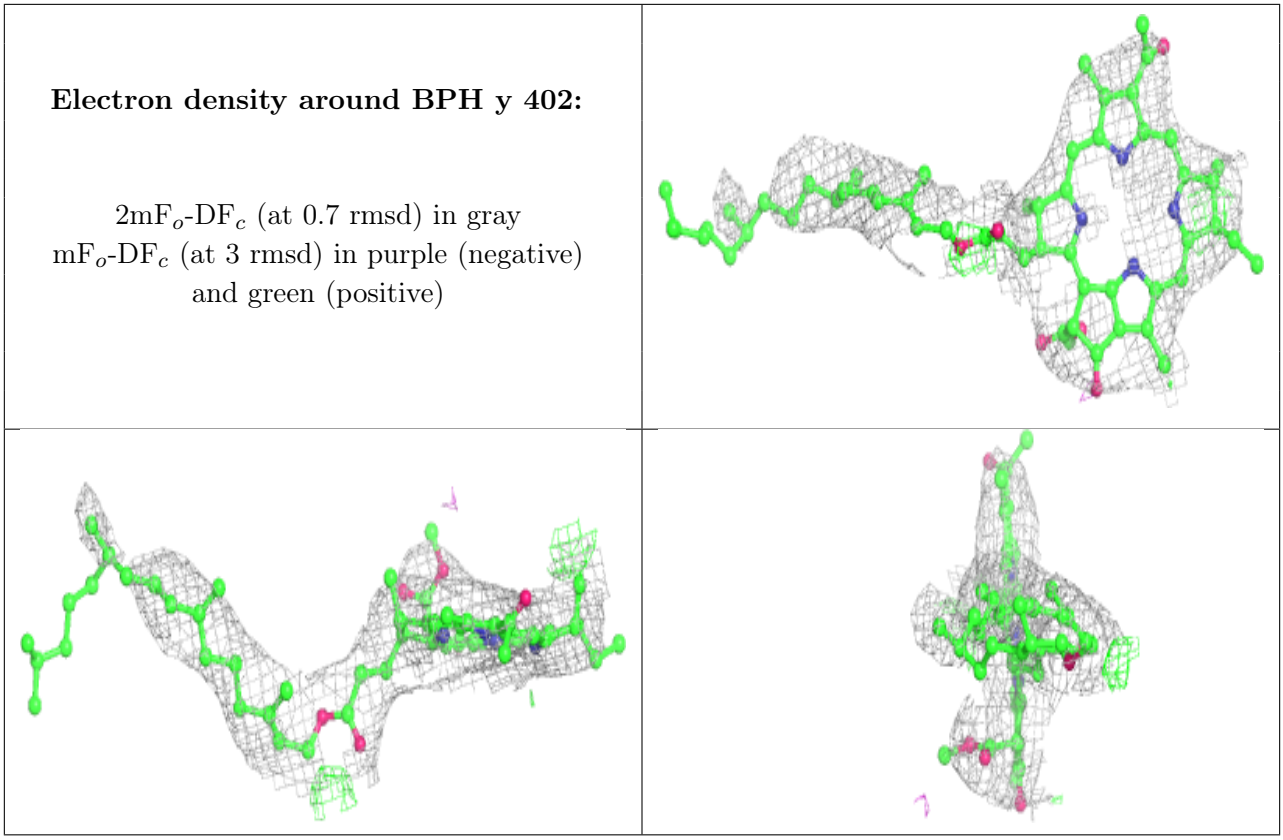






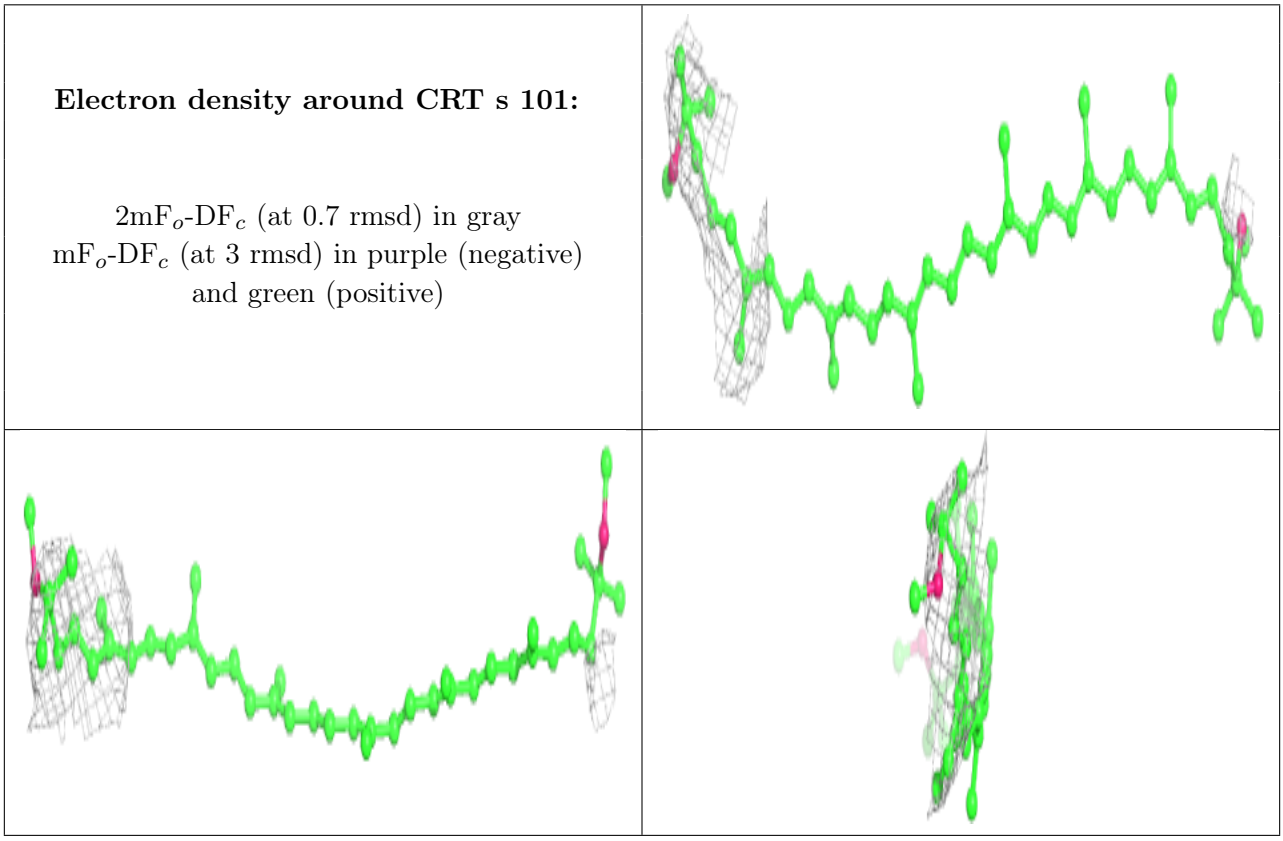
Electron density around BPH y 402:

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



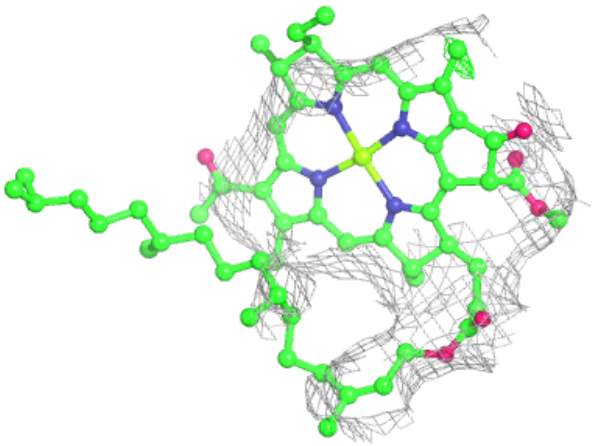
Electron density around CRT s 101:

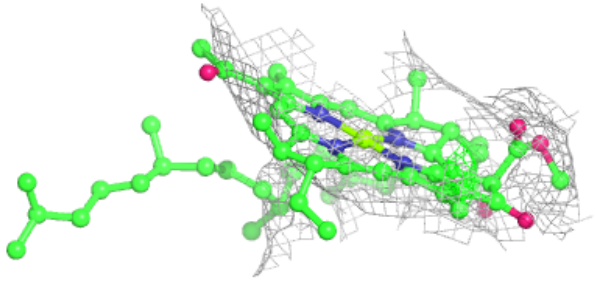
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

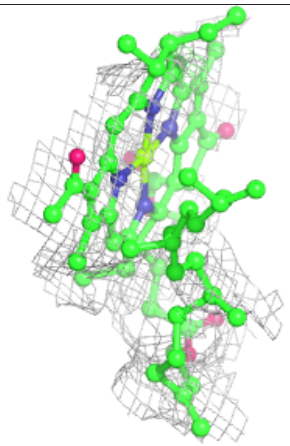


Electron density around BCL 6 101:

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

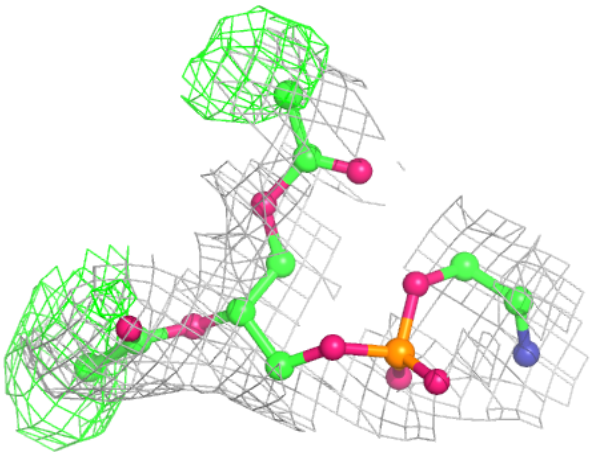


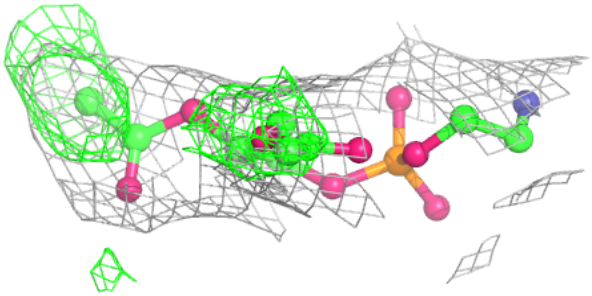


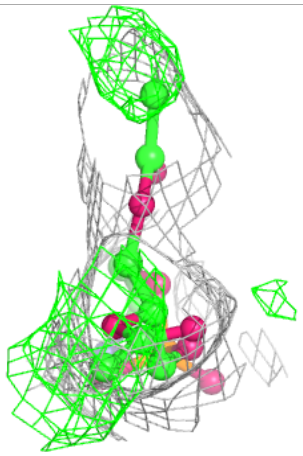


Electron density around PEF m 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

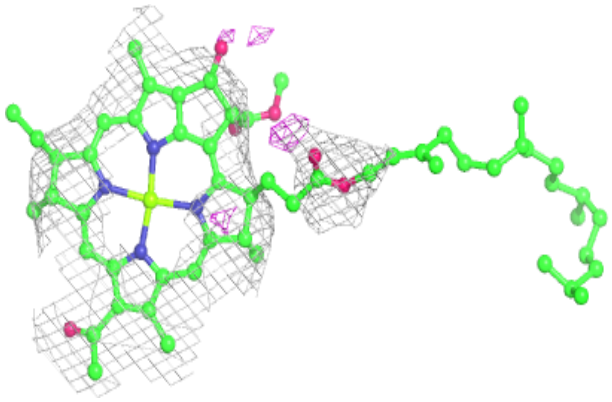


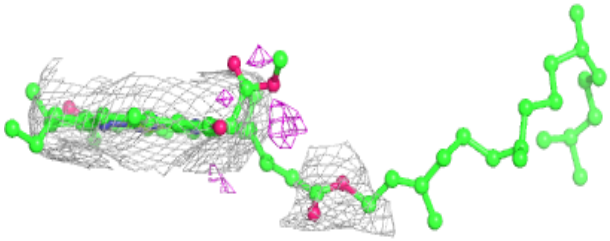


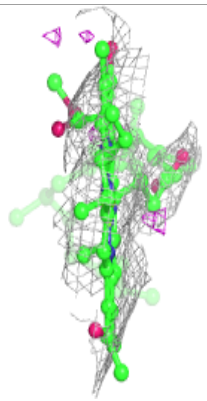


Electron density around BCL m 102:

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

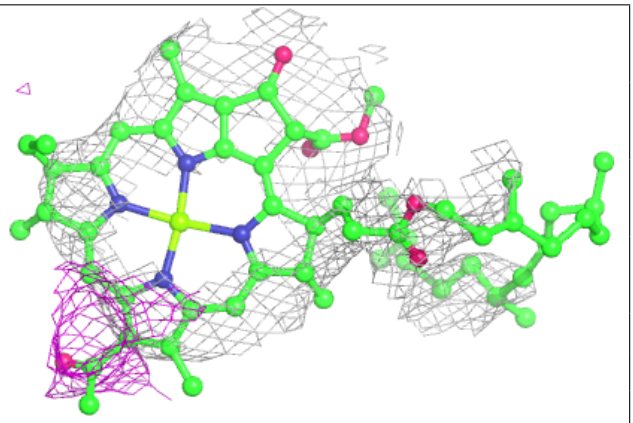


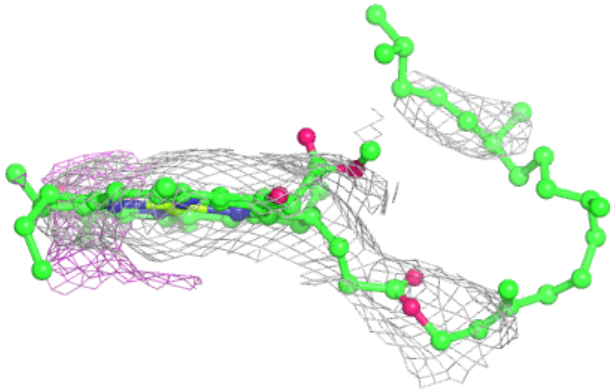


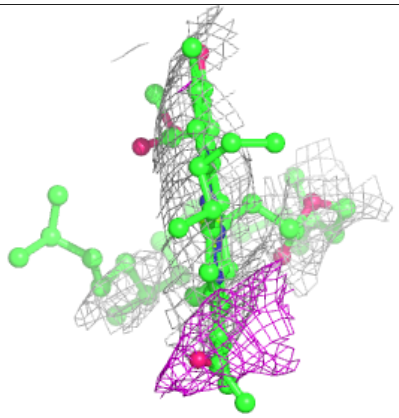


Electron density around BCL AC 102:

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

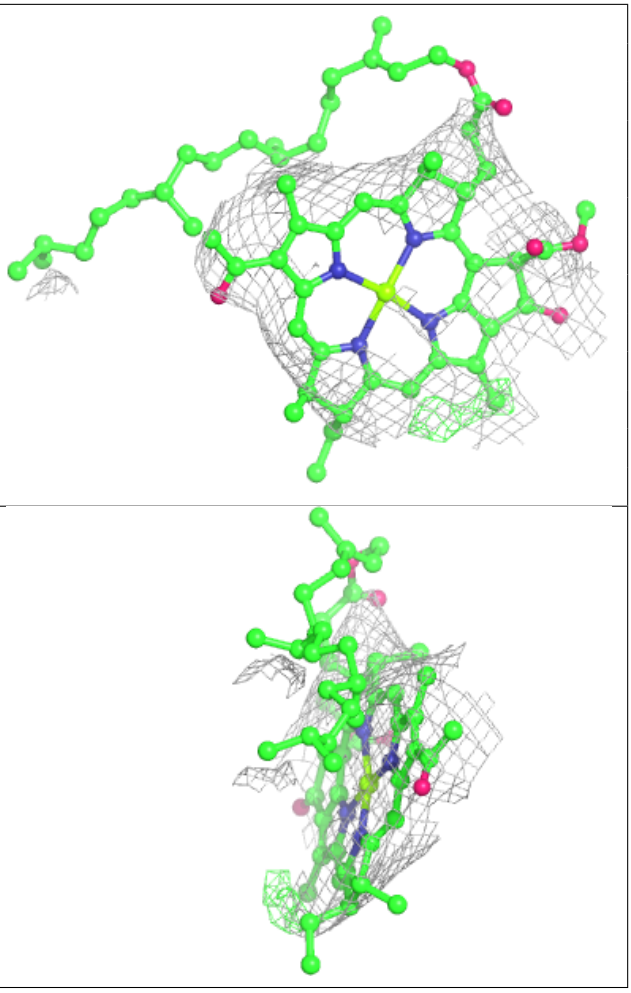






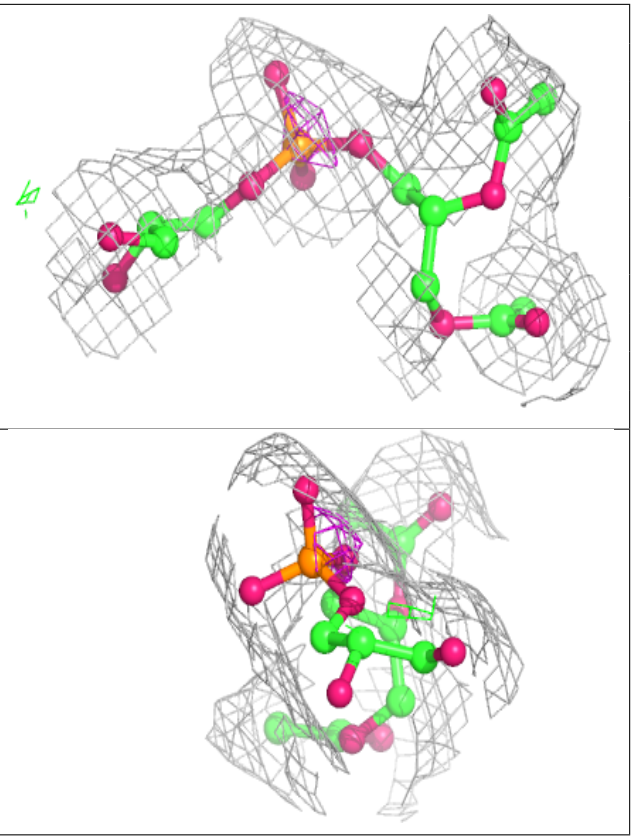
Electron density around BCL z 102:

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



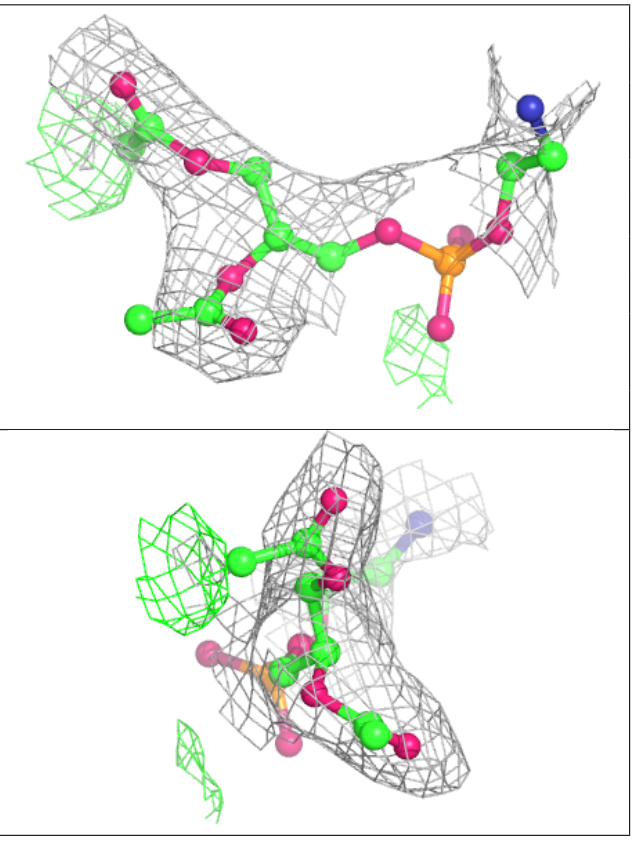
Electron density around PGW S 101:

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



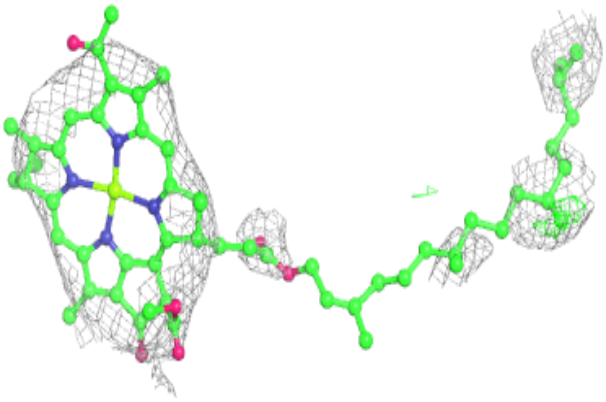
Electron density around PEF y 407:

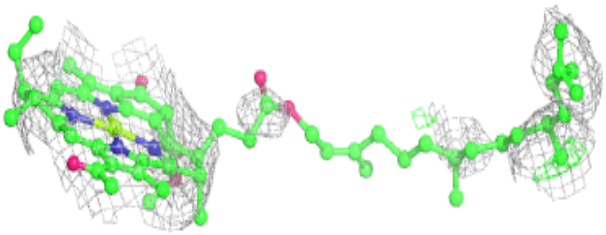
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

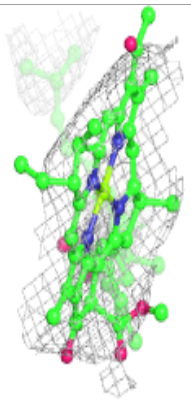


Electron density around BCL d 101:

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

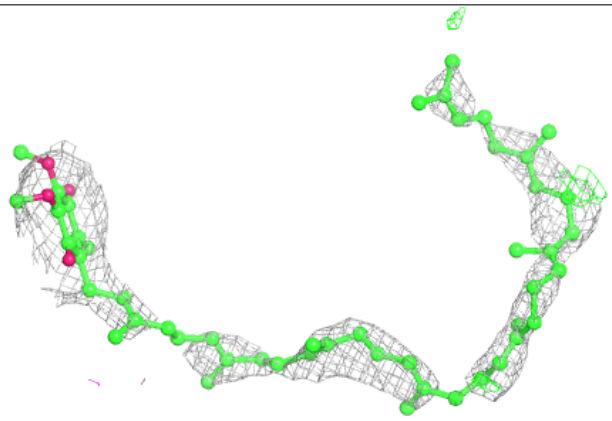


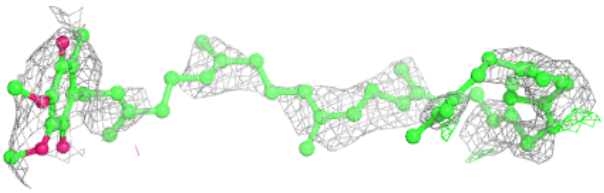


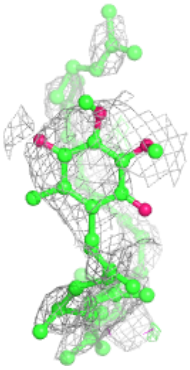


Electron density around UQ8 x 304:

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

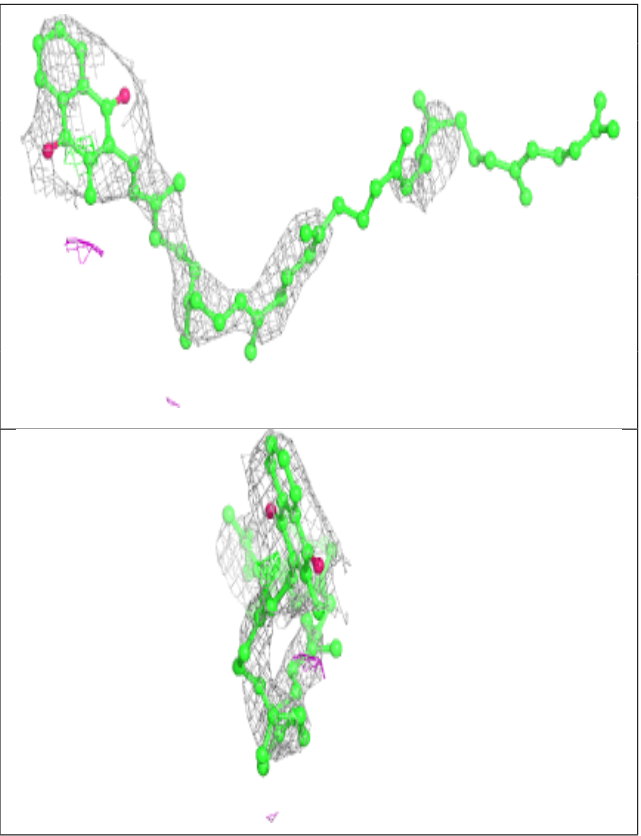


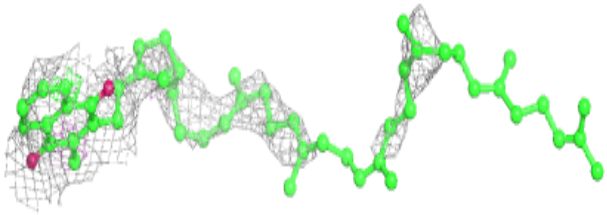




Electron density around MQ8 y 403:

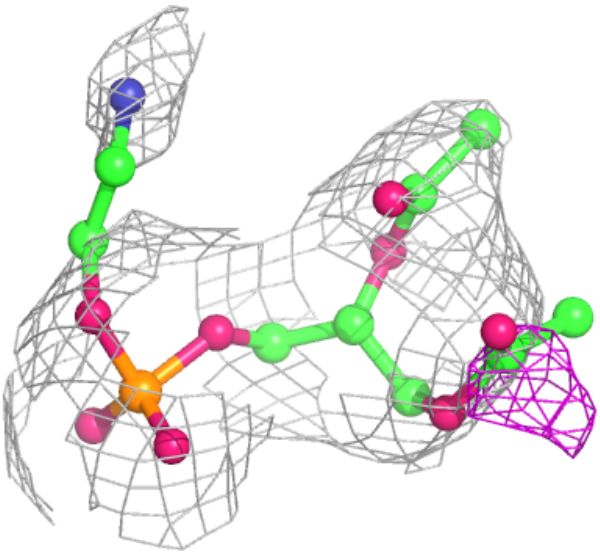
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

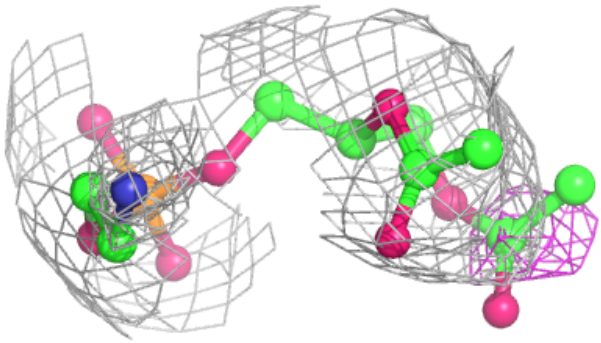


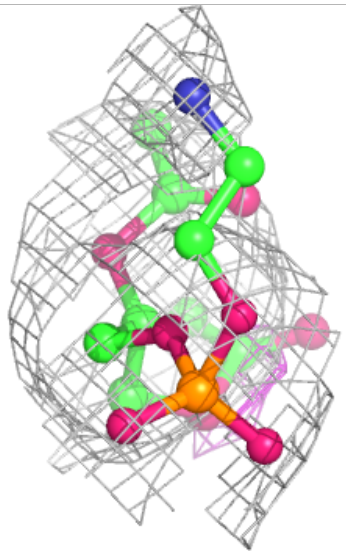


Electron density around PEF M 408:

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

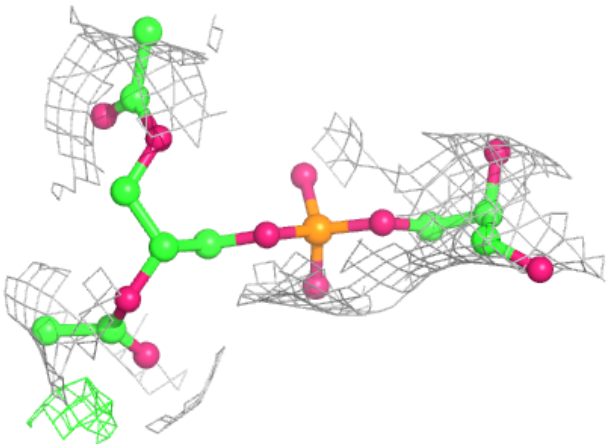


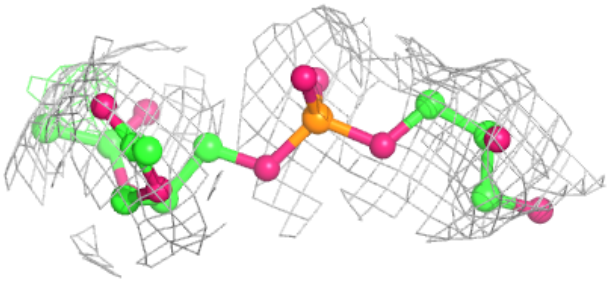


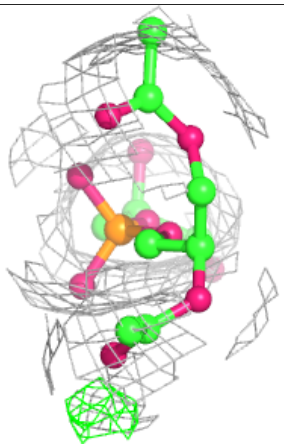


Electron density around PGW AE 101:

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

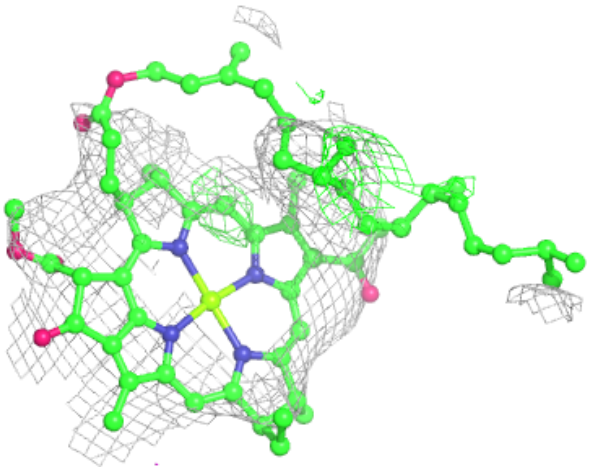


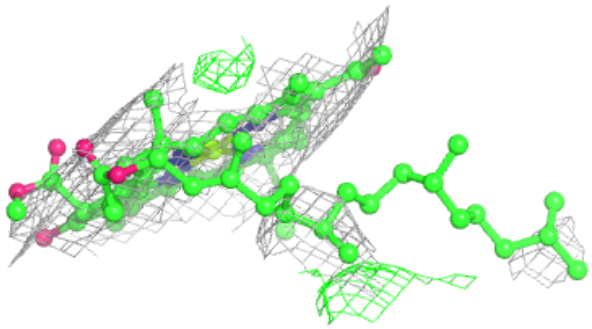


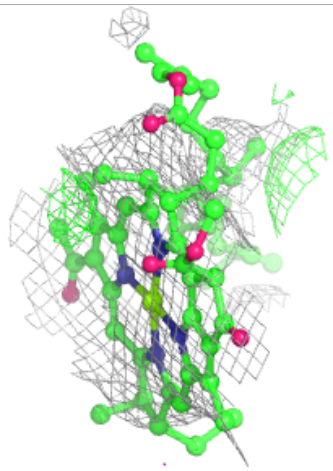


Electron density around BCL I 103:

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

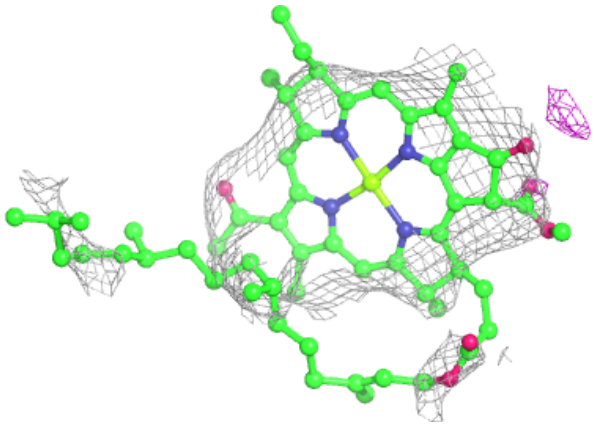


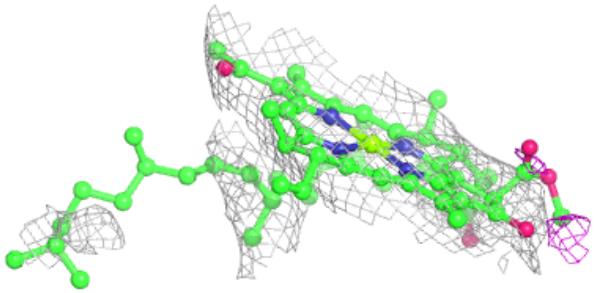


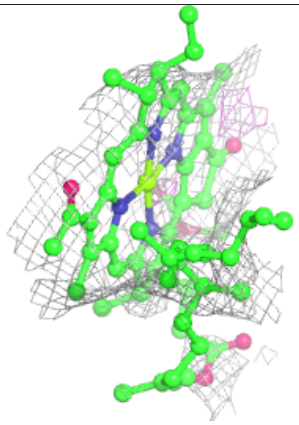


Electron density around BCL g 102:

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

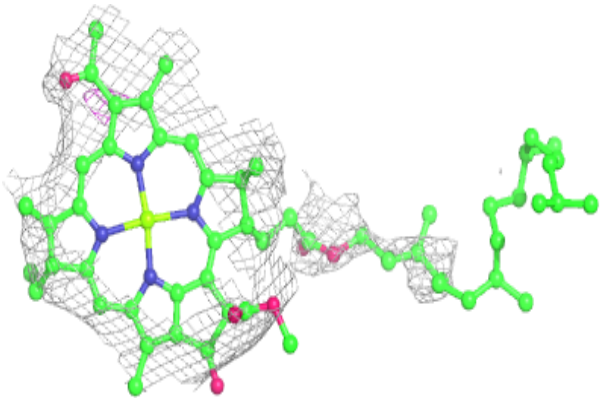


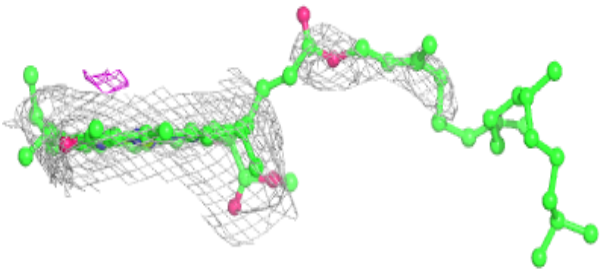


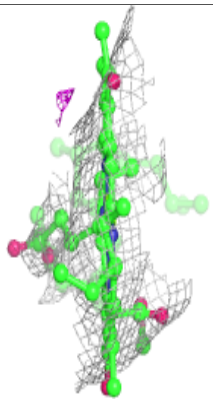


Electron density around BCL j 101:

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

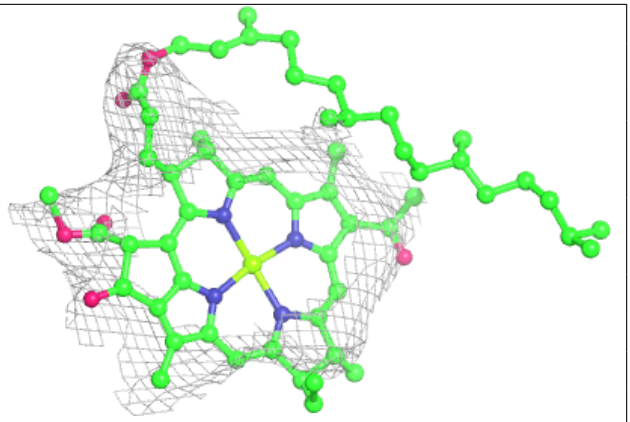


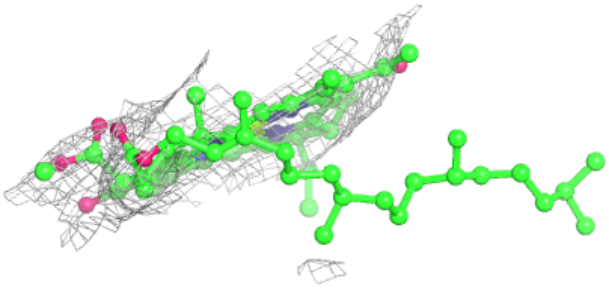


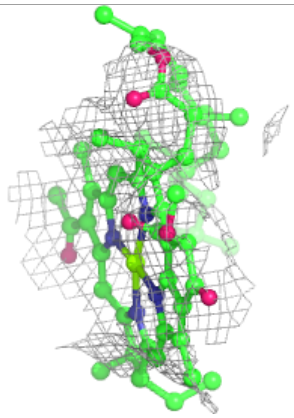


Electron density around BCL 0 102:

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

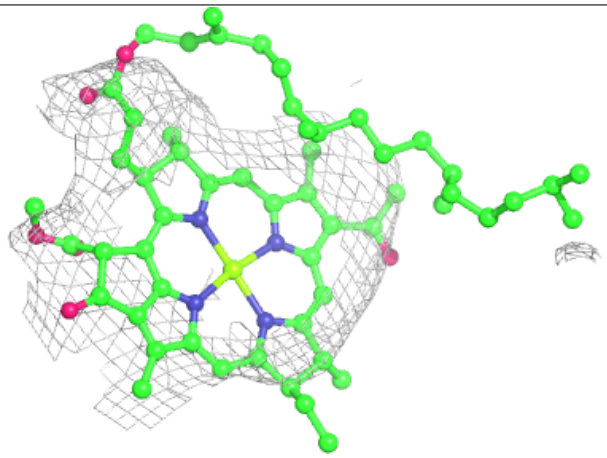


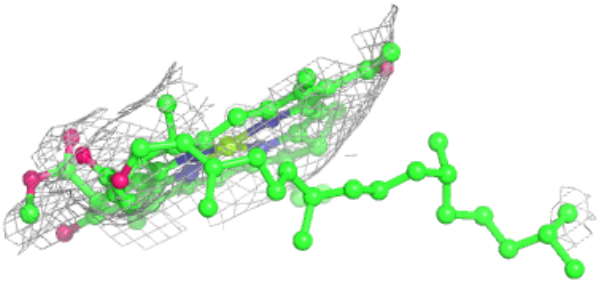


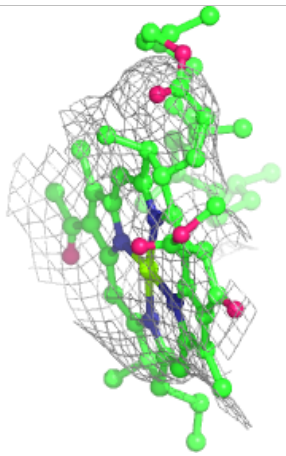


Electron density around BCL N 101:

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

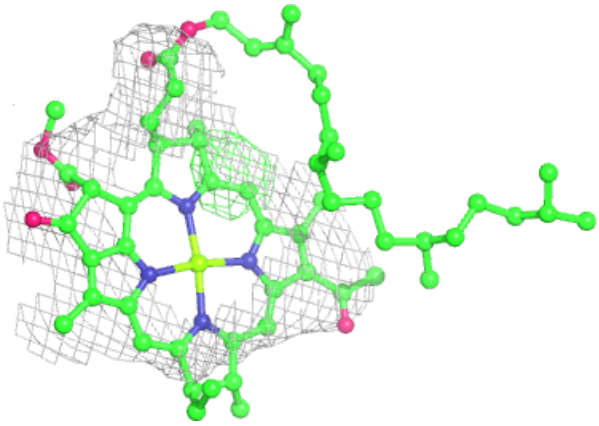


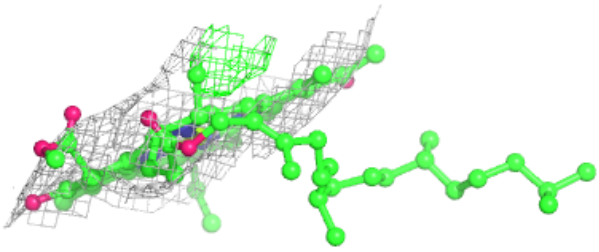


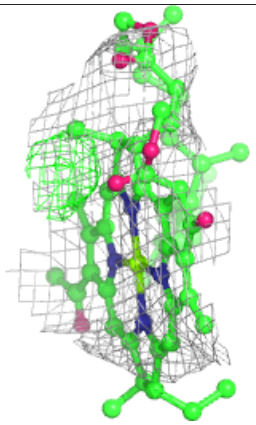


Electron density around BCL D 102:

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

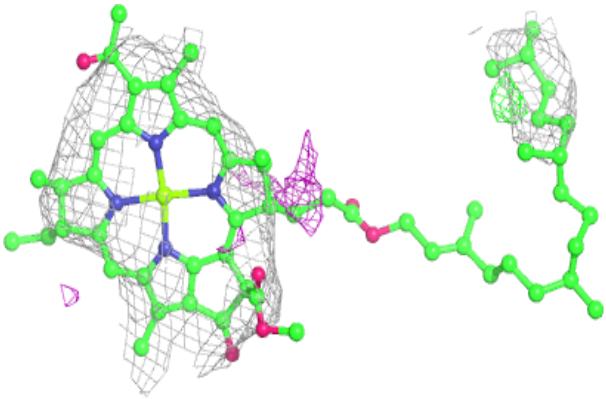


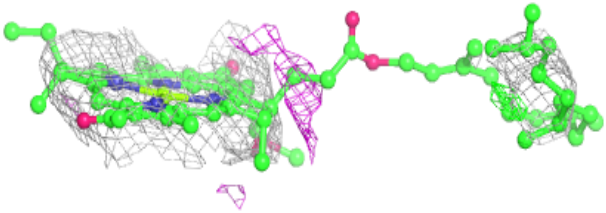


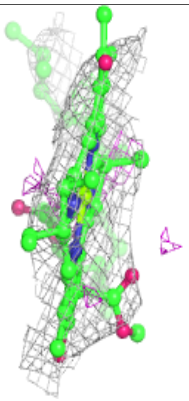


Electron density around BCL f 101:

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

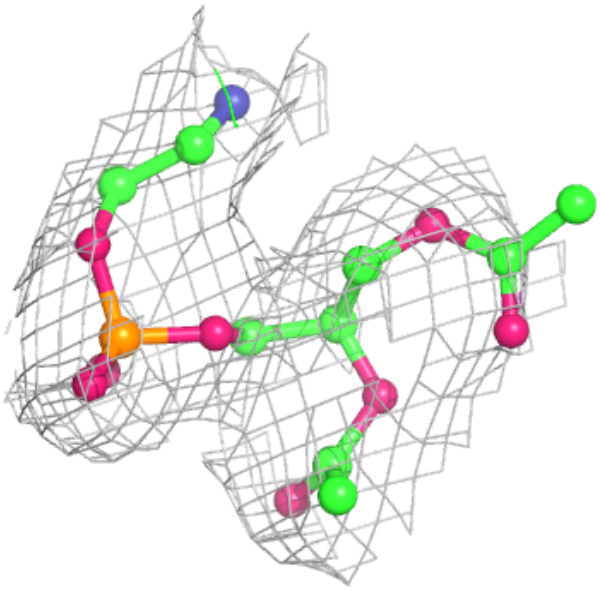


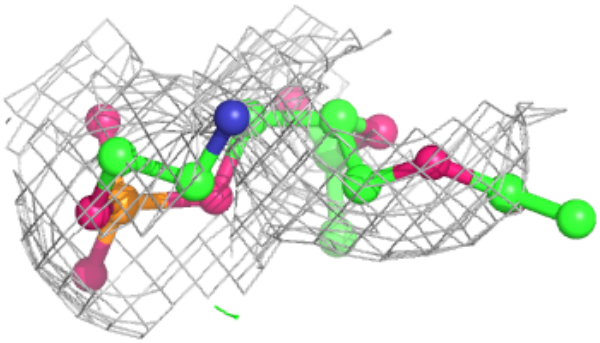


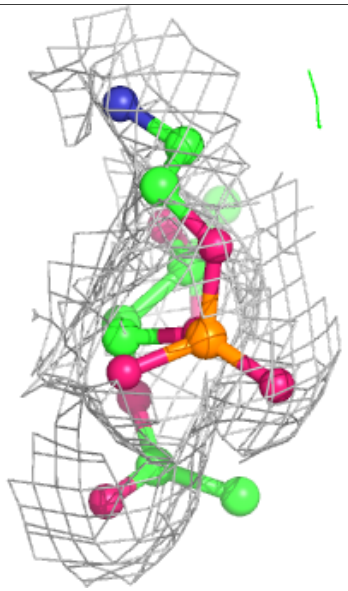


Electron density around PEF x 306:

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

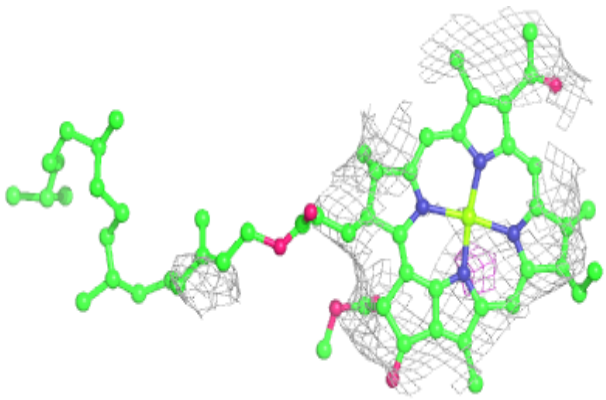


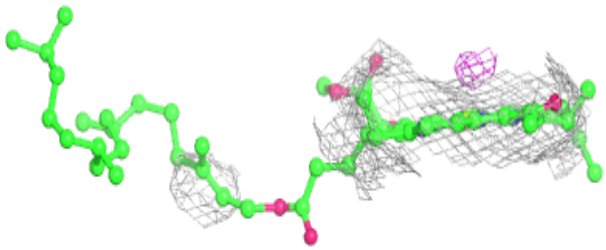


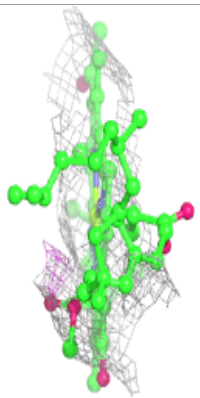


Electron density around BCL 7 102:

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

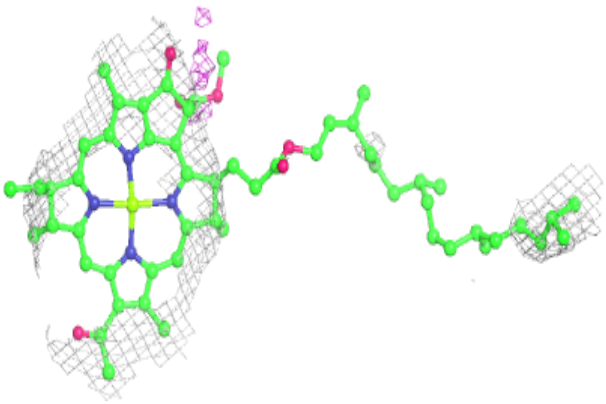


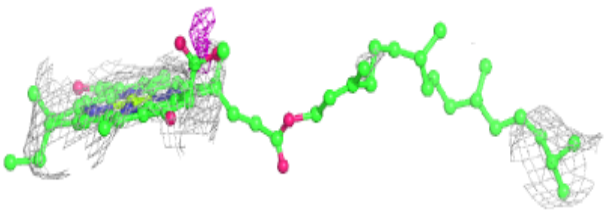


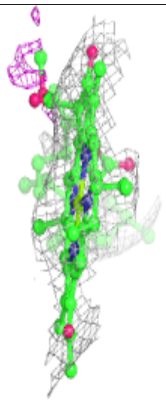


Electron density around BCL p 102:

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

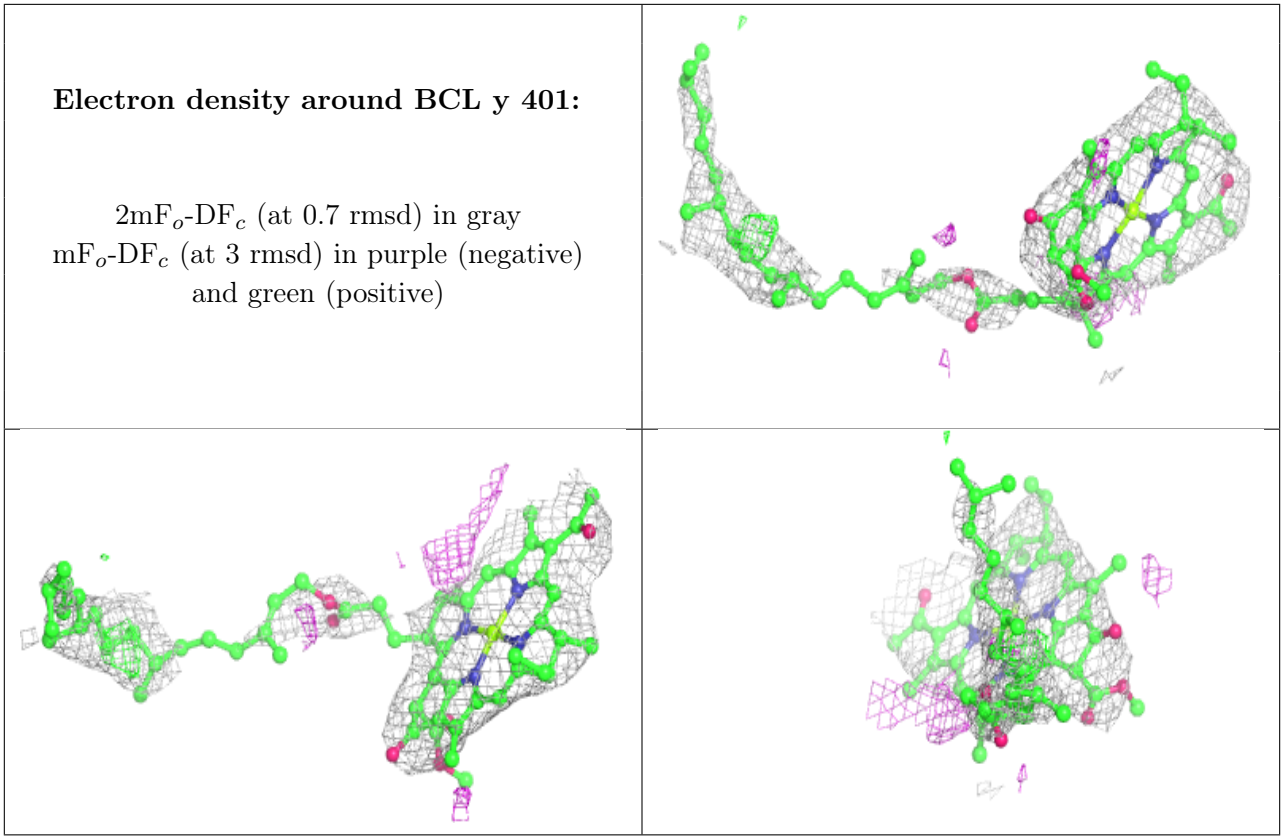






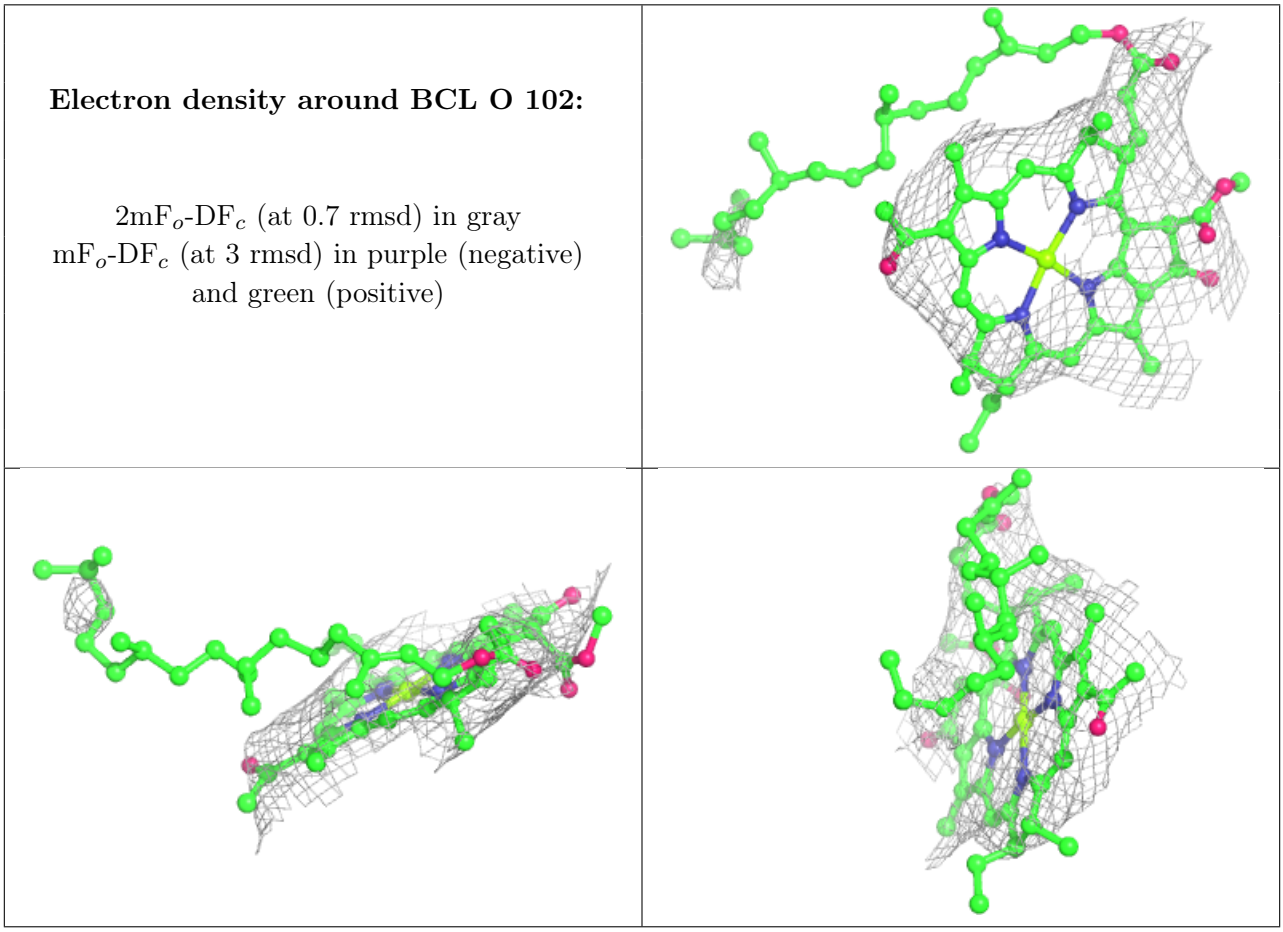
Electron density around BCL y 401:

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



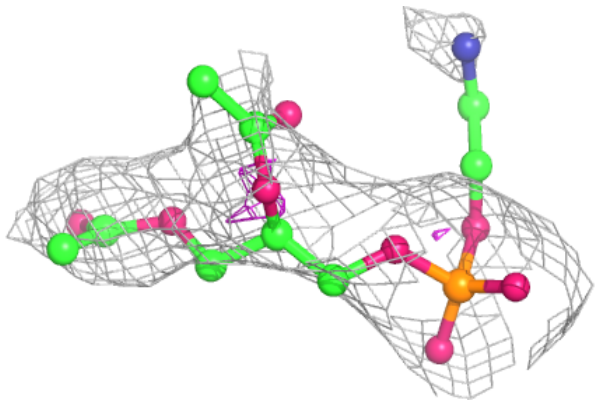
Electron density around BCL O 102:

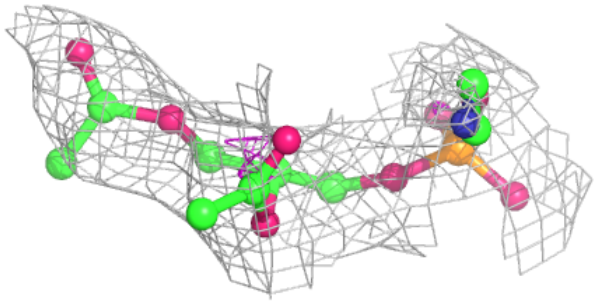
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

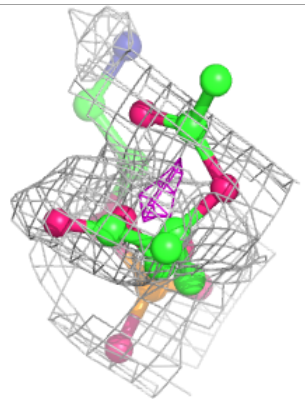


Electron density around PEF y 408:

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

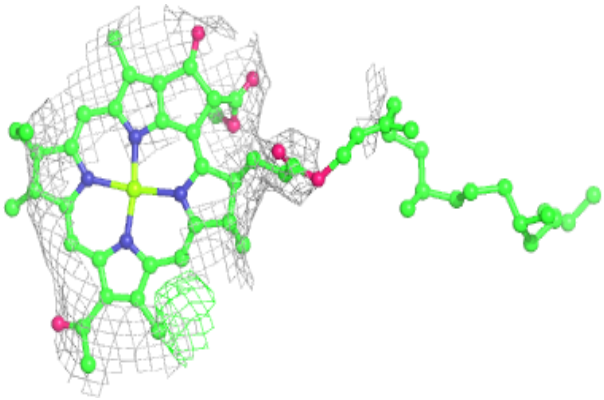


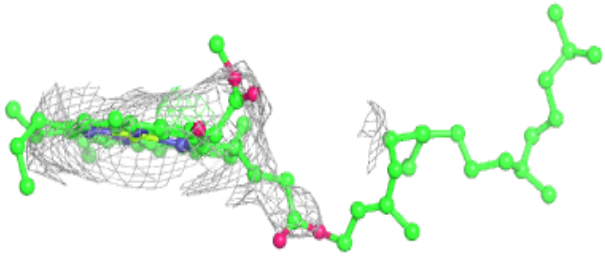


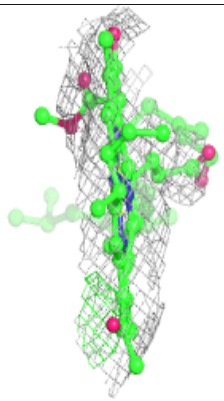


Electron density around BCL F 101:

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

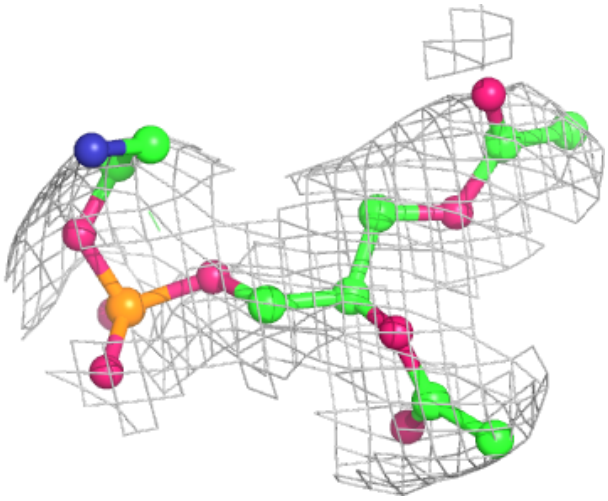


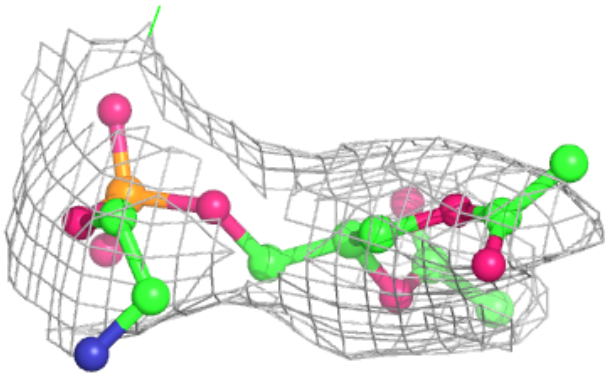


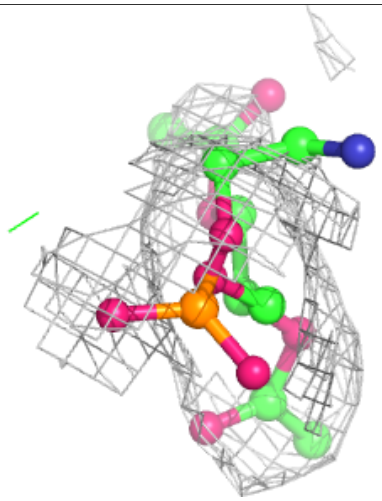


Electron density around PEF H 301:

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

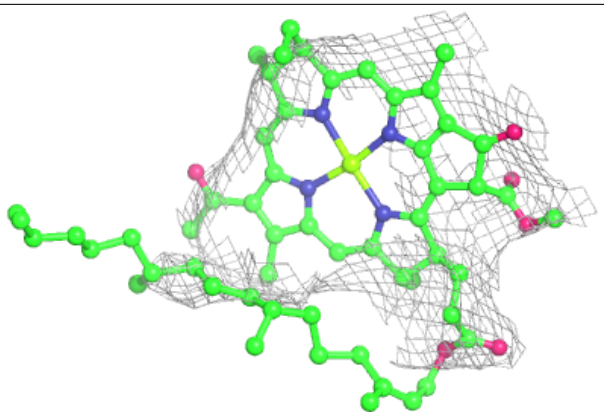


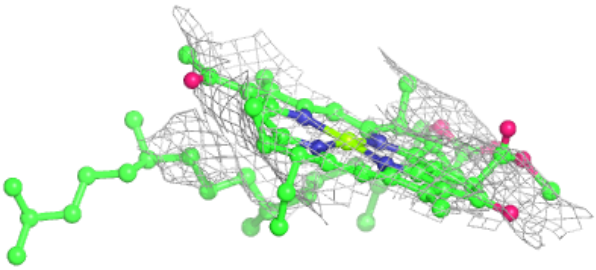


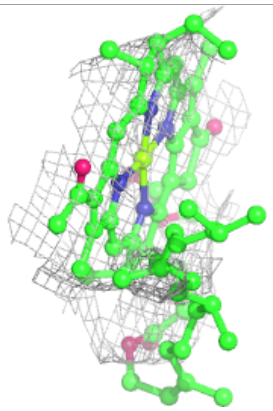


Electron density around BCL i 102:

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

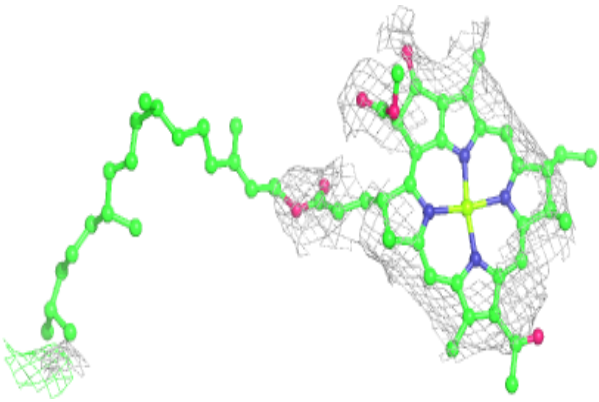


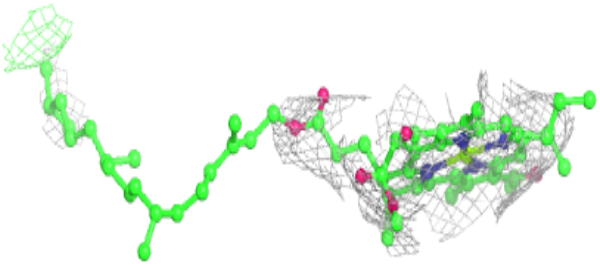


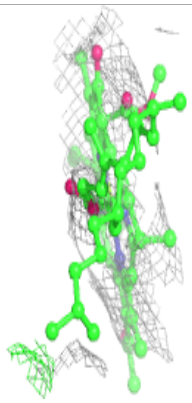


Electron density around BCL AF 101:

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

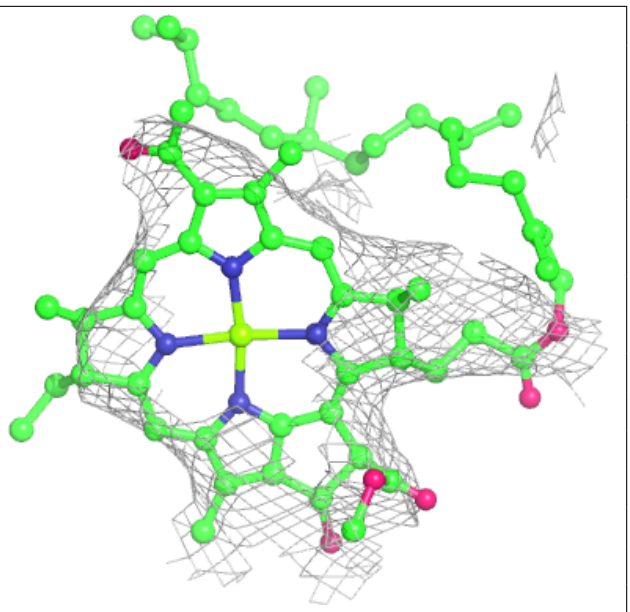


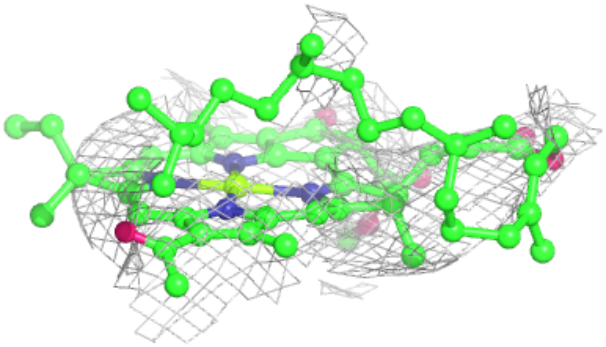


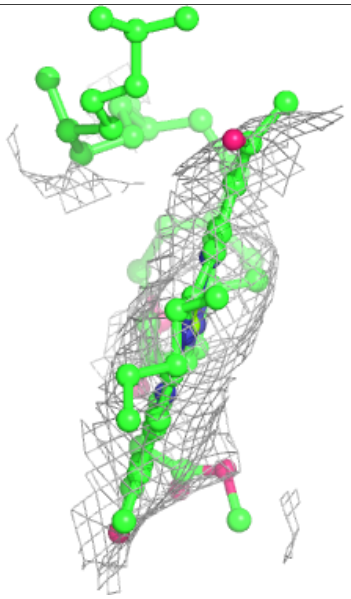


Electron density around BCL k 102:

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

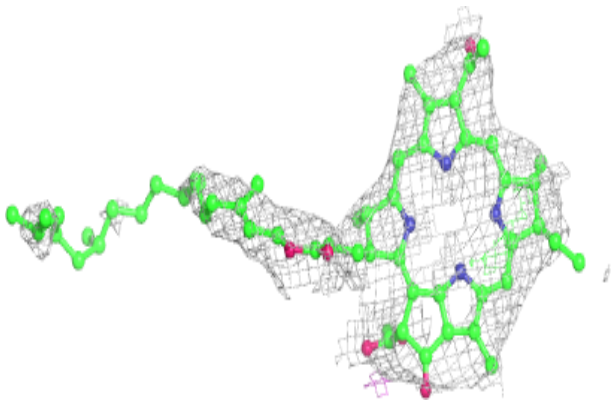


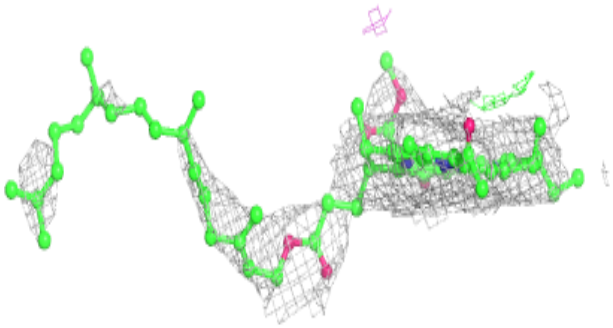


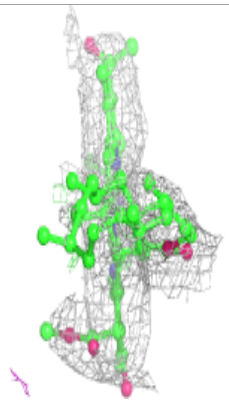


Electron density around BPH M 403:

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

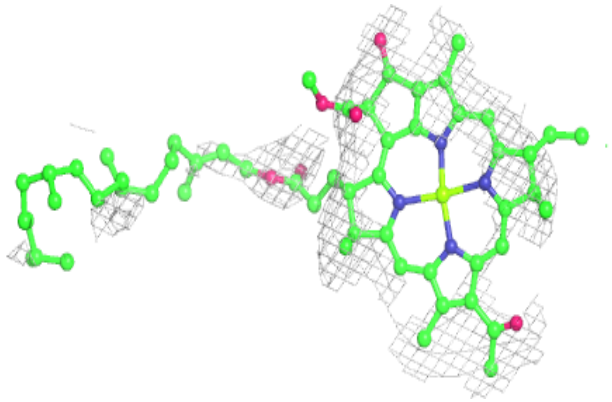


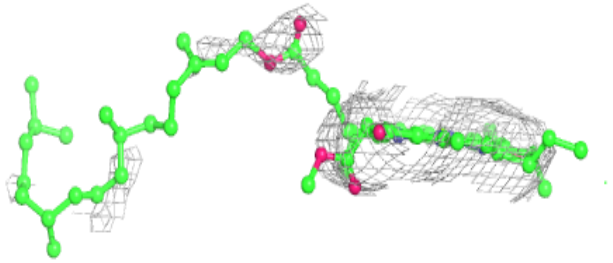


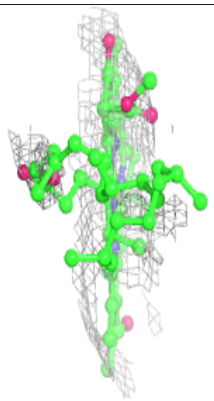


Electron density around BCL A 102:

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

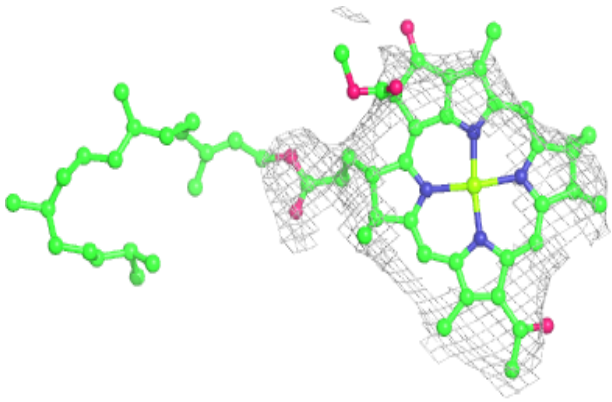


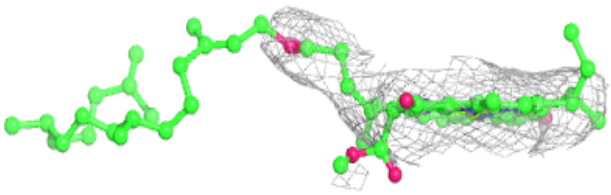




Electron density around BCL AH 101:

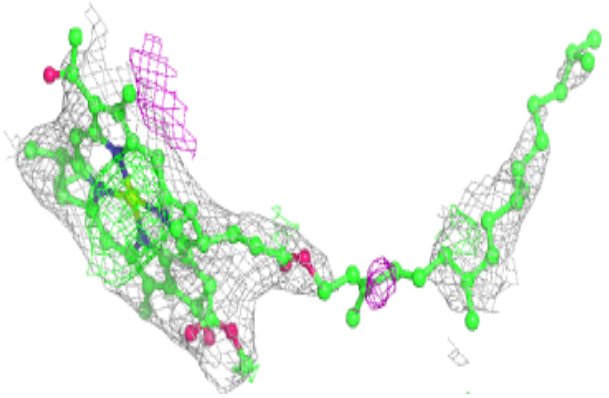
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

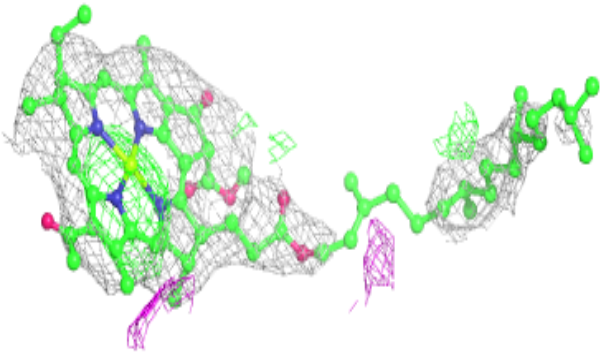


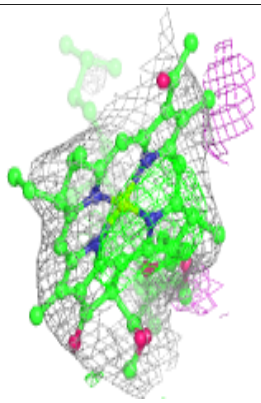


Electron density around BCL x 301:

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

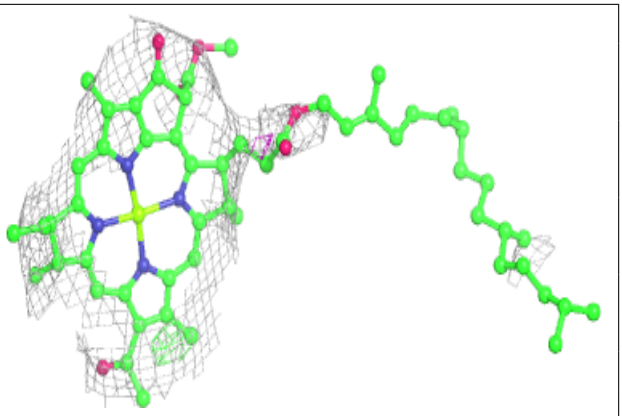


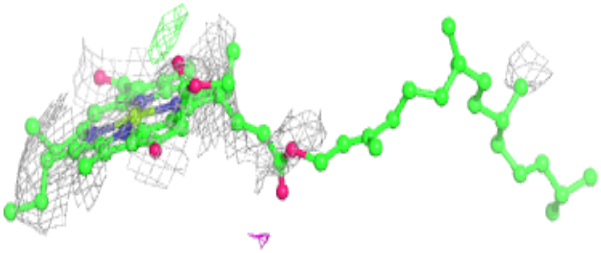


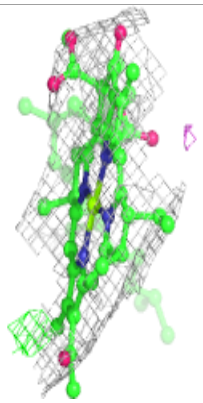


Electron density around BCL u 101:

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

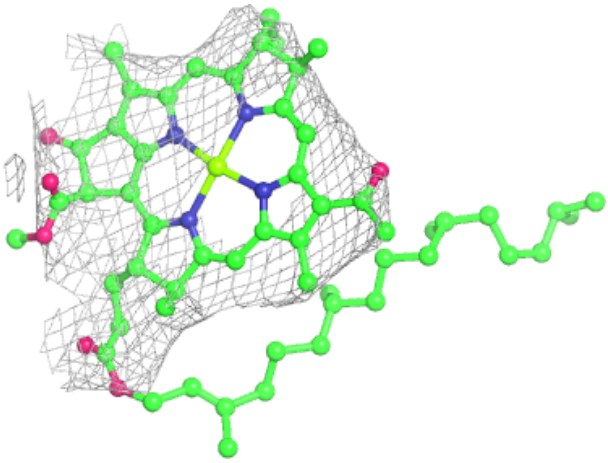


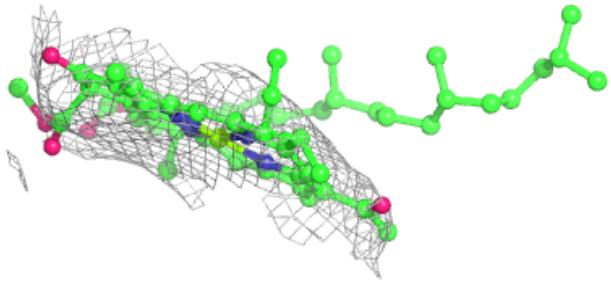


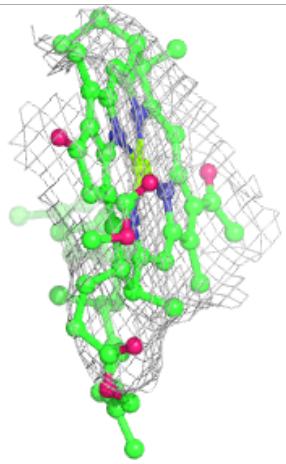


Electron density around BCL R 102:

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

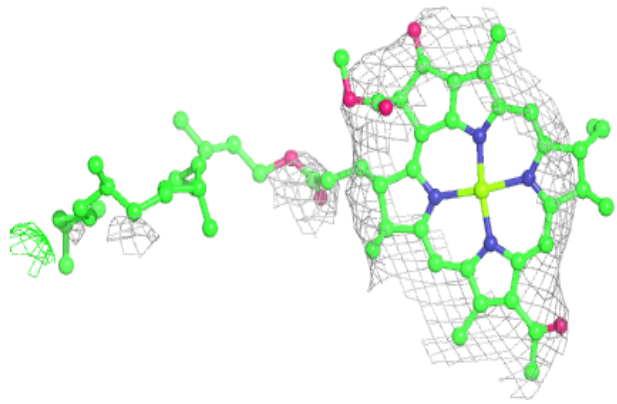


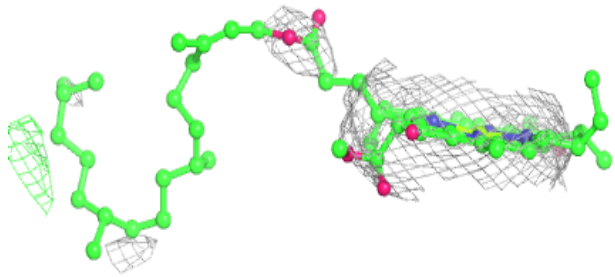


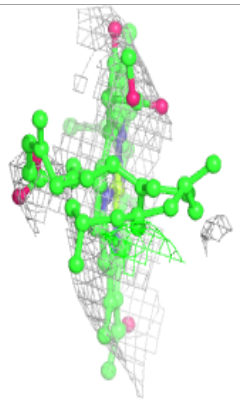


Electron density around BCL P 101:

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

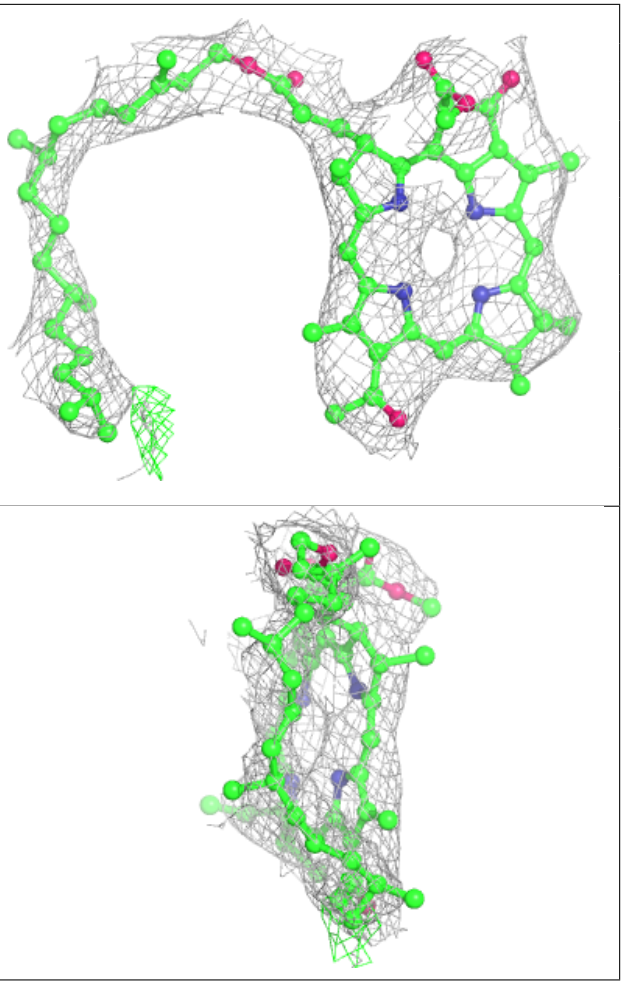






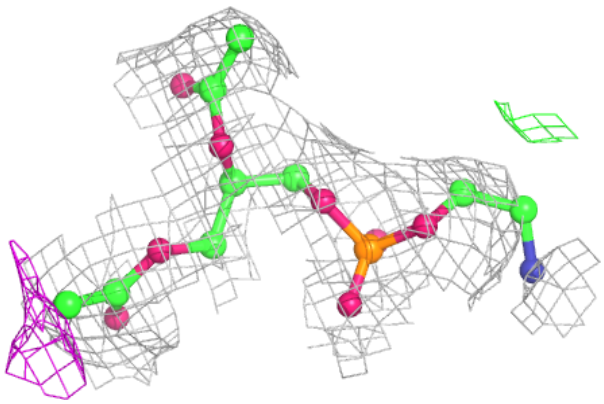
Electron density around BPH L 302:

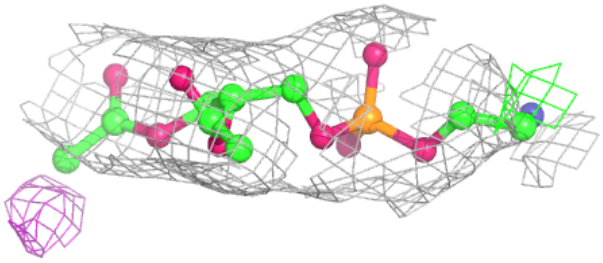
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

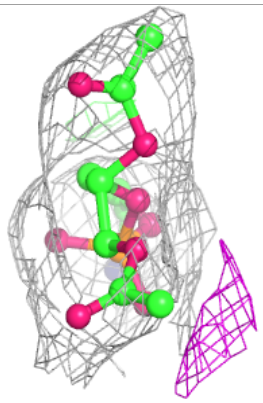


Electron density around PEF t 303:

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

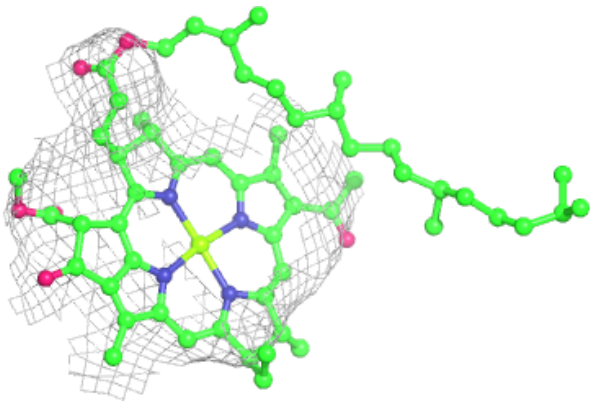


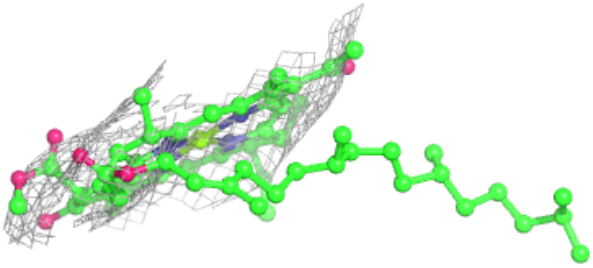


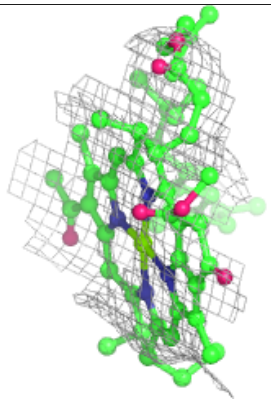


Electron density around BCL G 102:

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

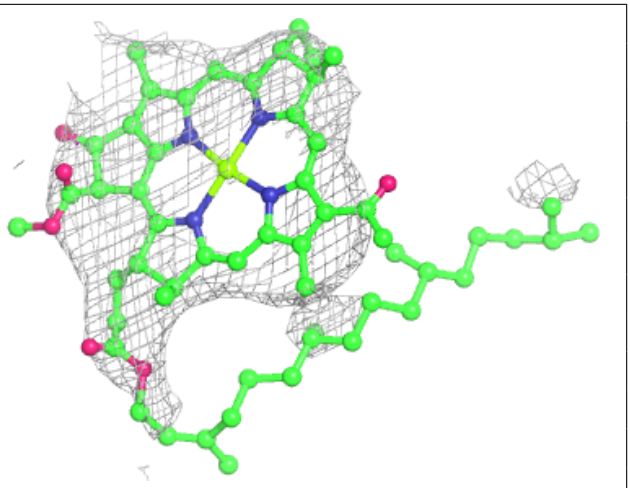


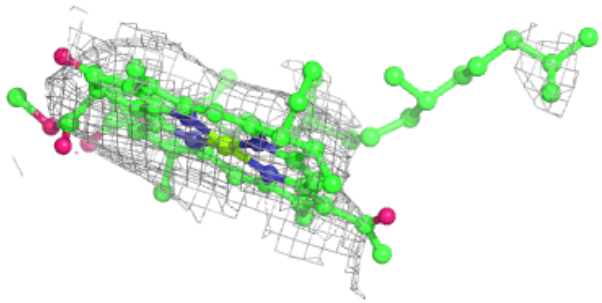


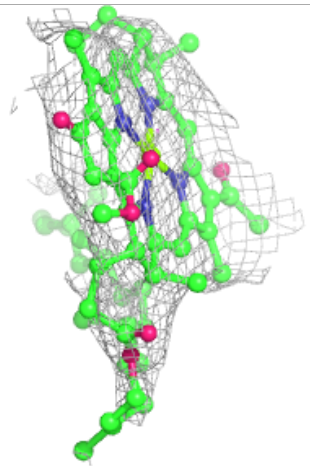


Electron density around BCL V 102:

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

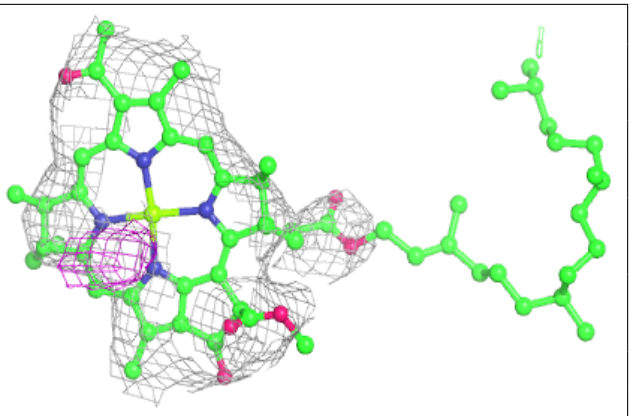


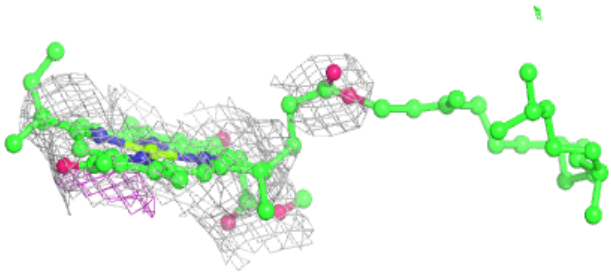


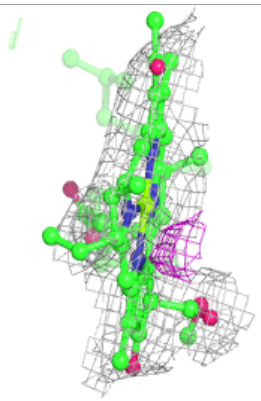


Electron density around BCL 3 101:

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

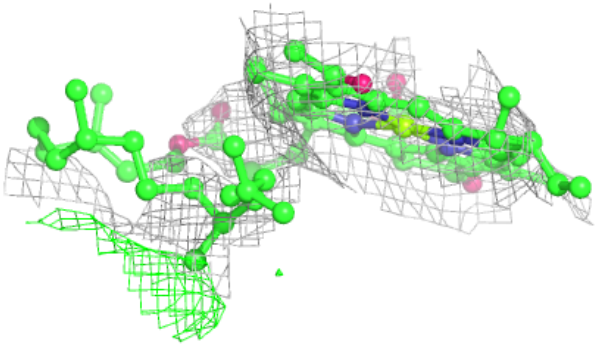


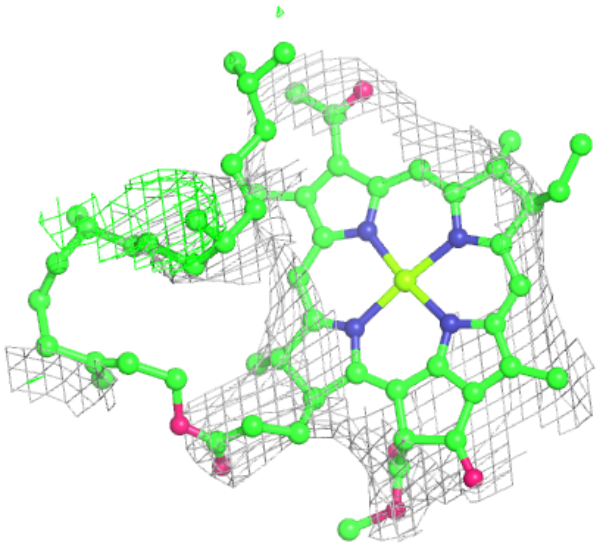


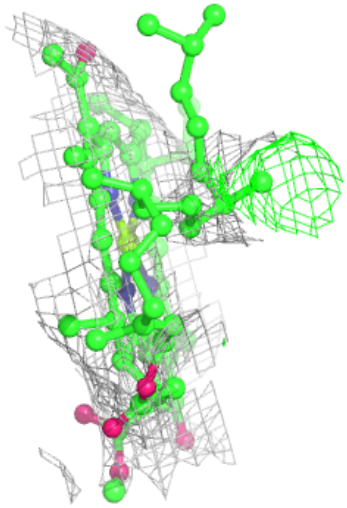


Electron density around BCL m 103:

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

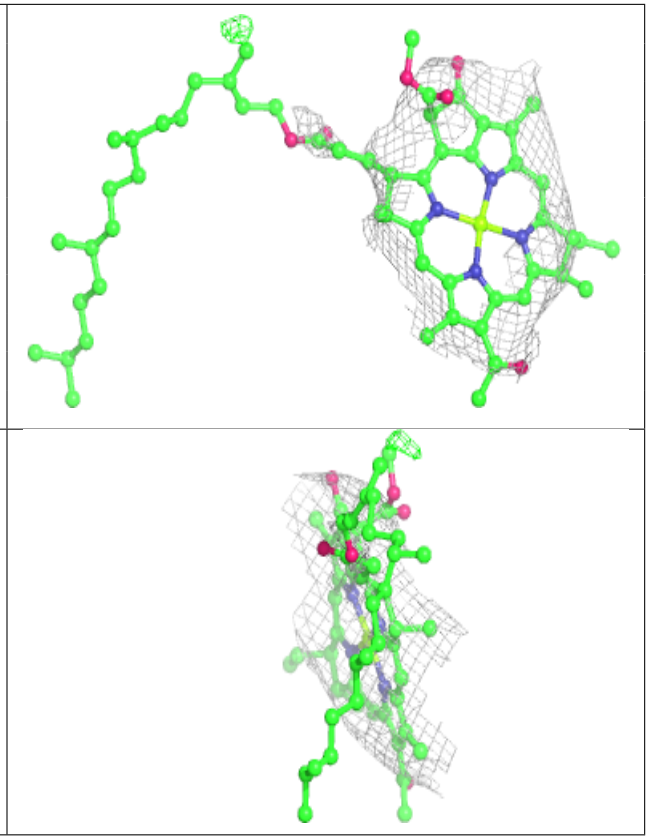






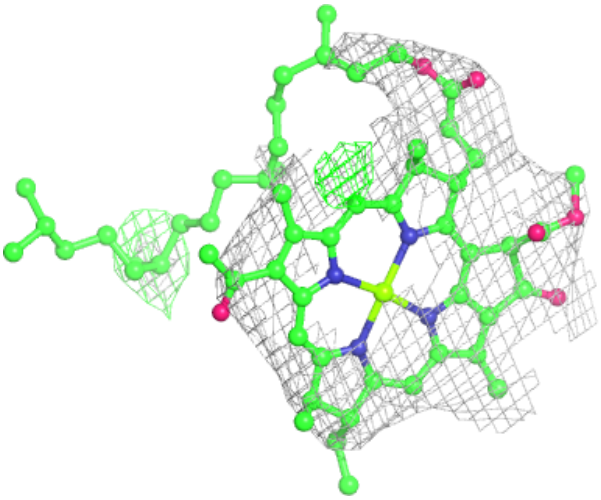
Electron density around BCL I 101:

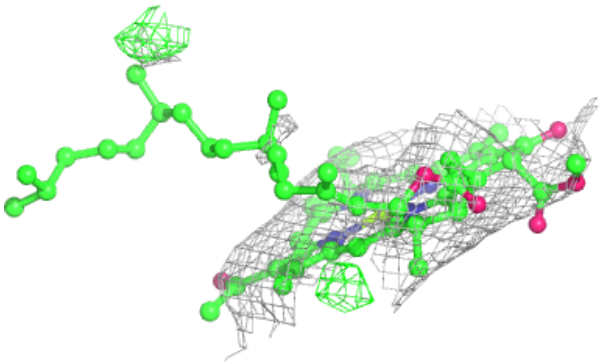
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

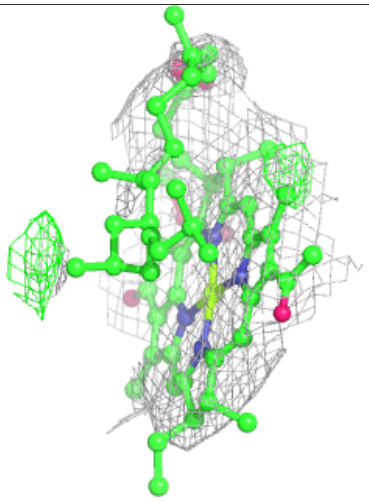


Electron density around BCL AI 102:

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

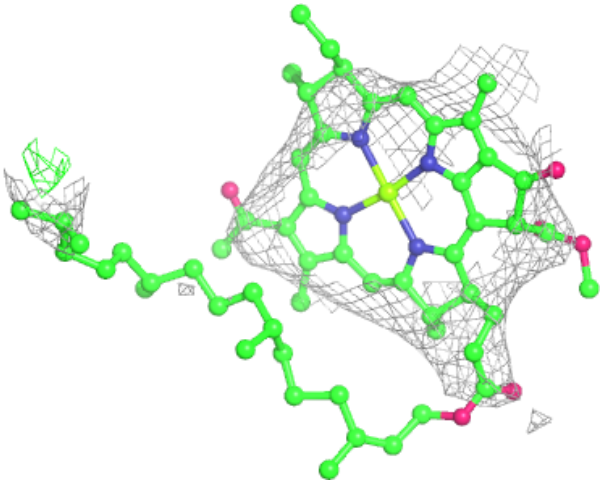


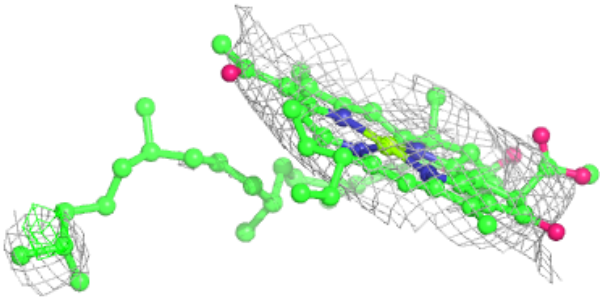


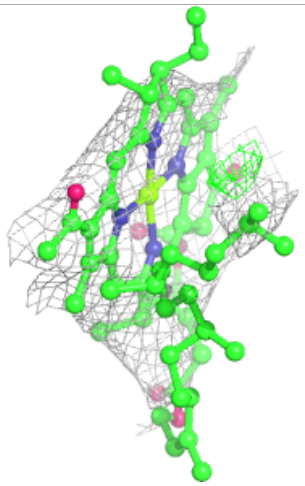


Electron density around BCL e 102:

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

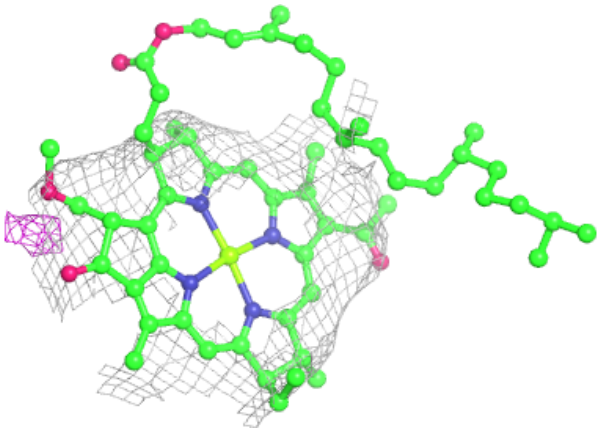


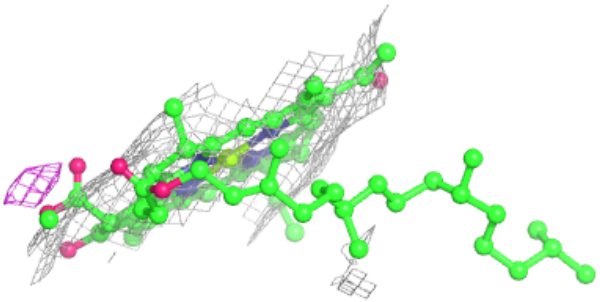


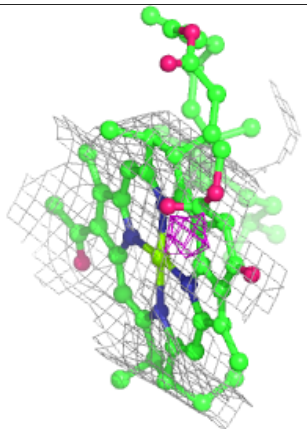


Electron density around BCL u 102:

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

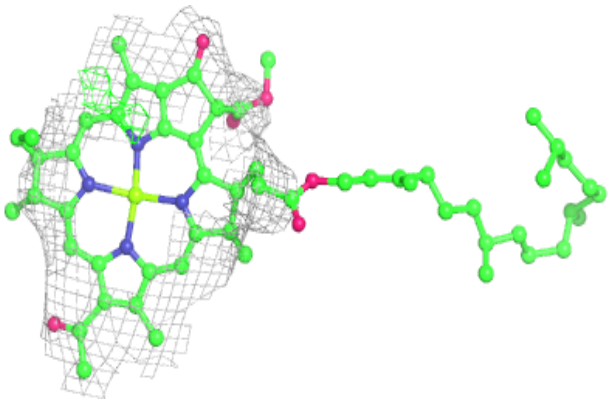


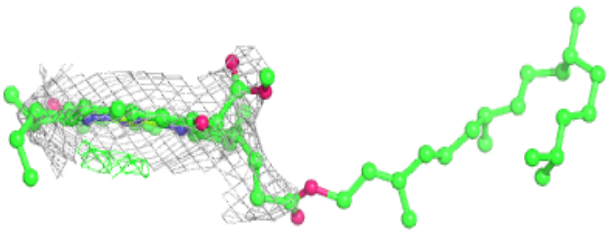


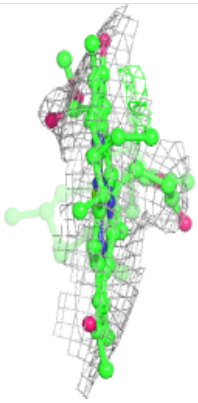


Electron density around BCL w 101:

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

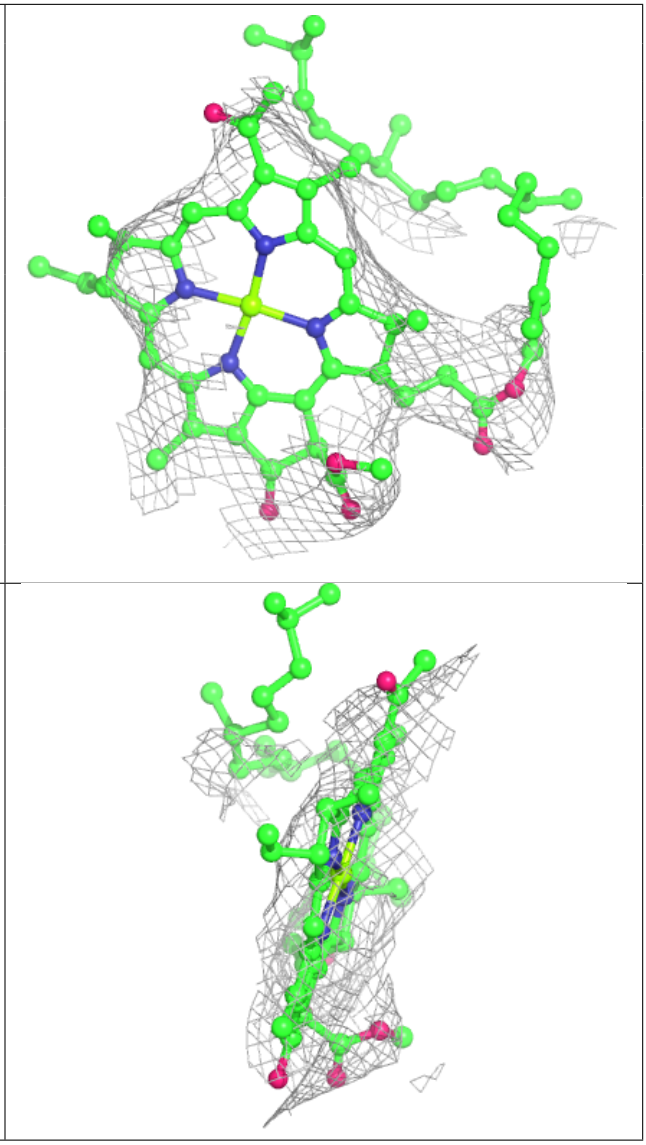






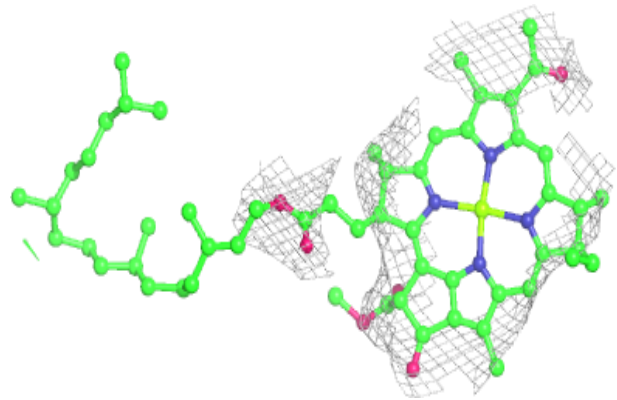
Electron density around BCL 8 101:

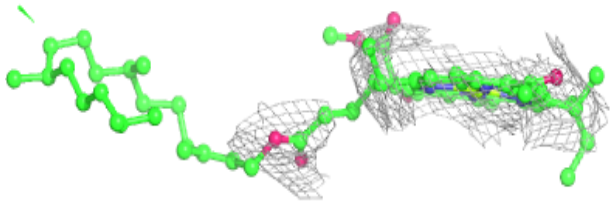
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

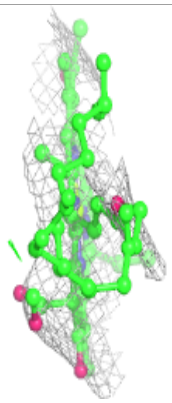


Electron density around BCL 9 102:

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

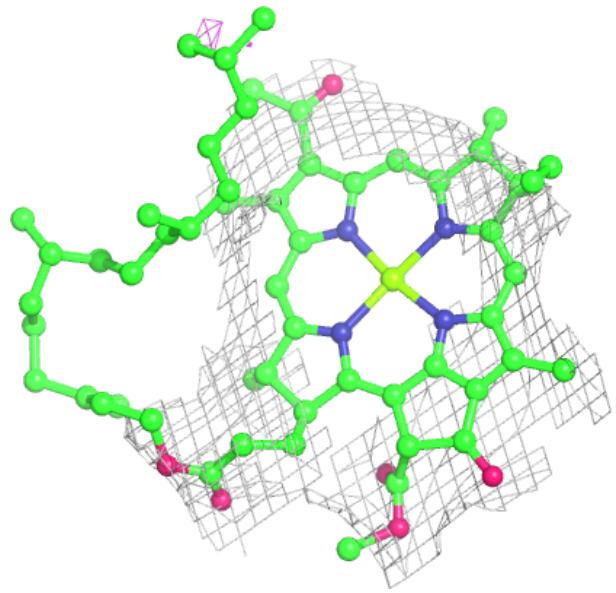


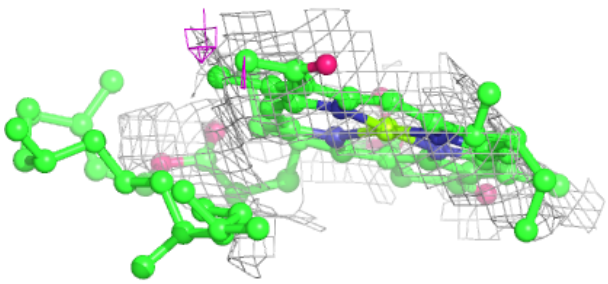


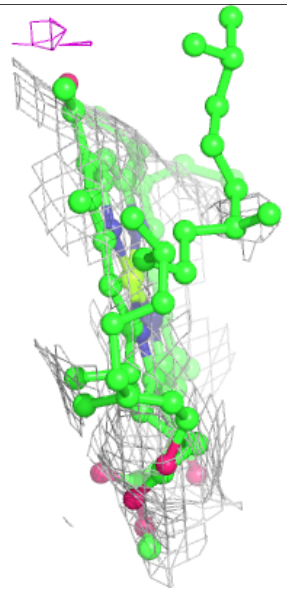


Electron density around BCL A 103:

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

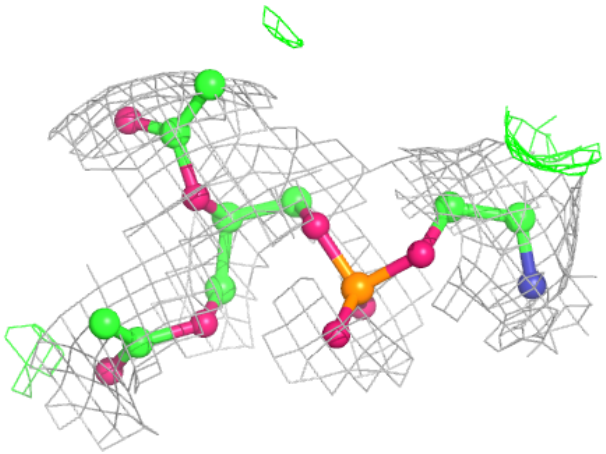


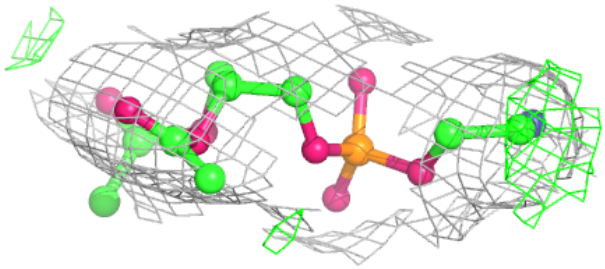


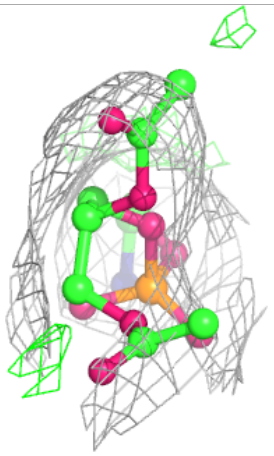


Electron density around PEF H 305:

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

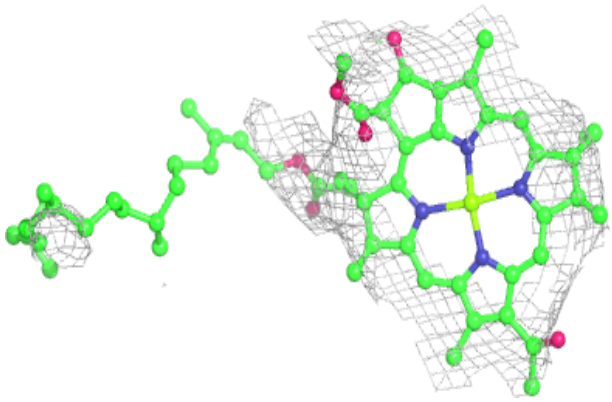


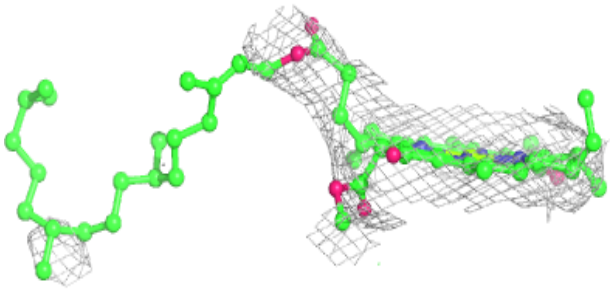


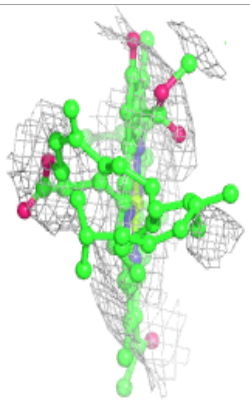


Electron density around BCL AB 101:

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

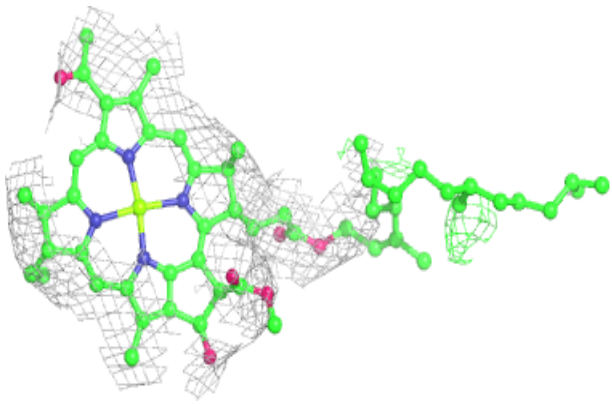


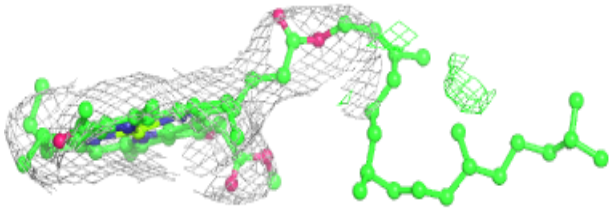


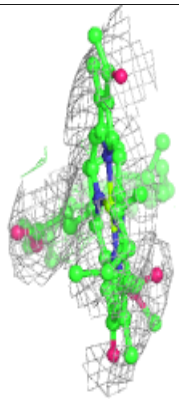


Electron density around BCL h 101:

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

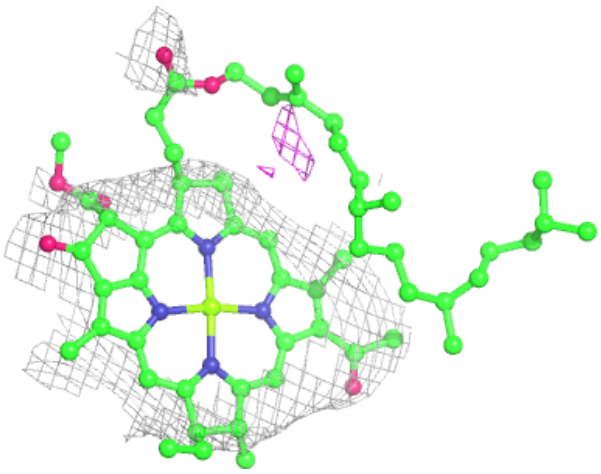


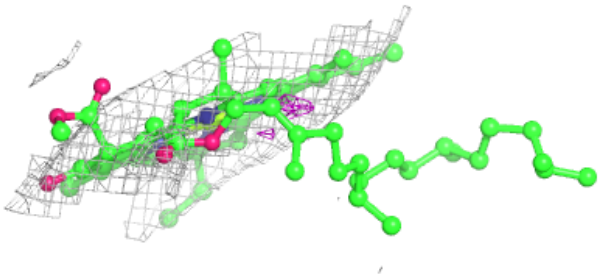


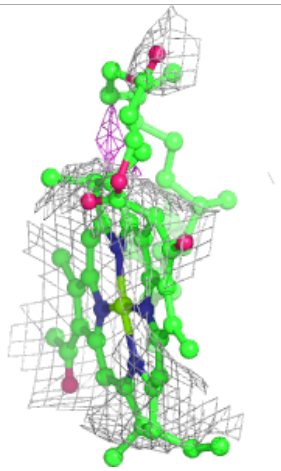


Electron density around BCL q 102:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

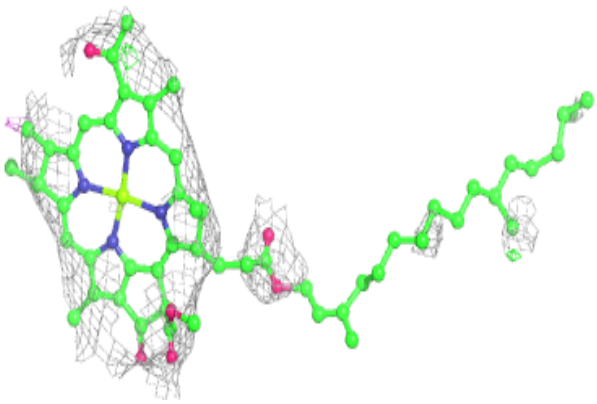


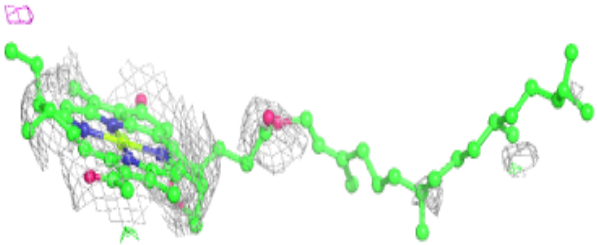


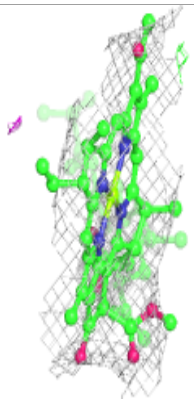


Electron density around BCL 1 101:

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

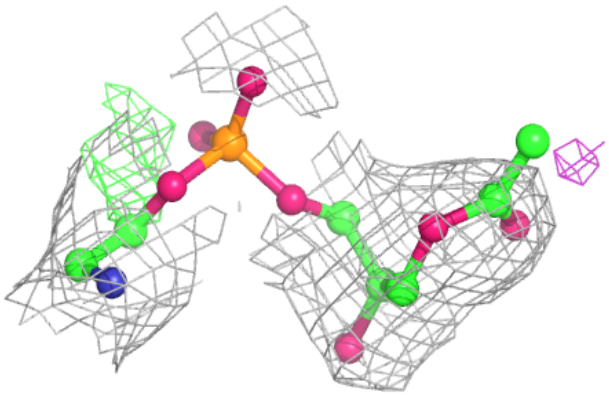


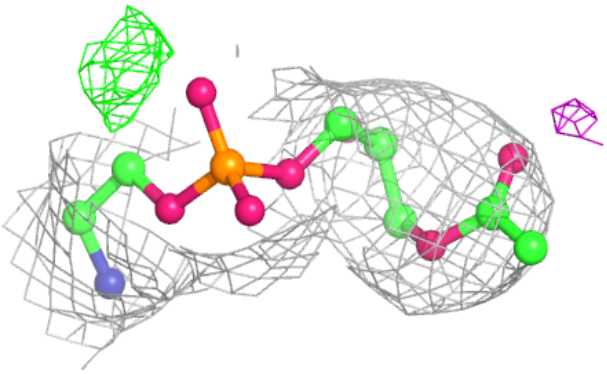


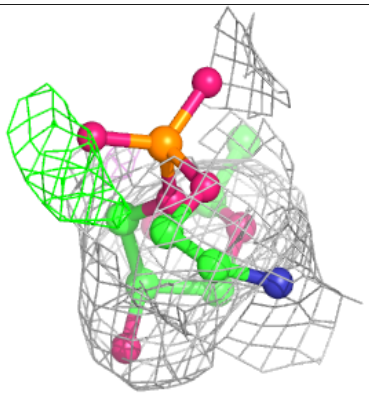


Electron density around PEF M 407:

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

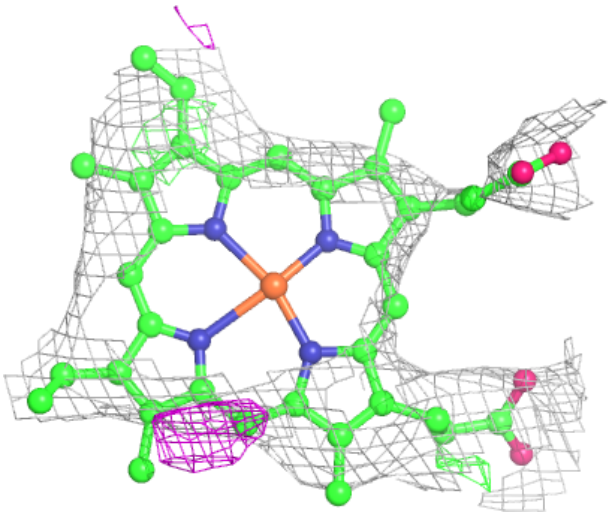


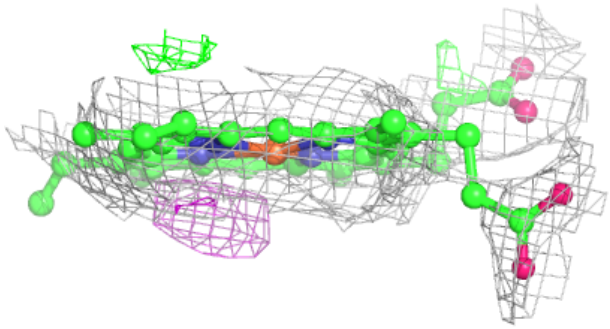


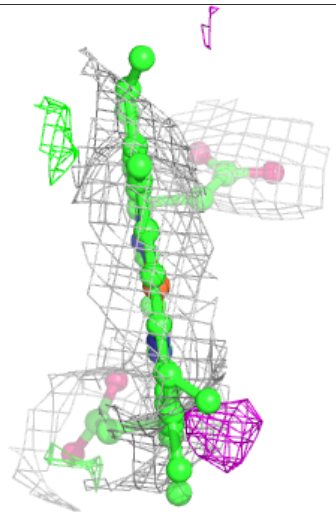


Electron density around HEM C 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

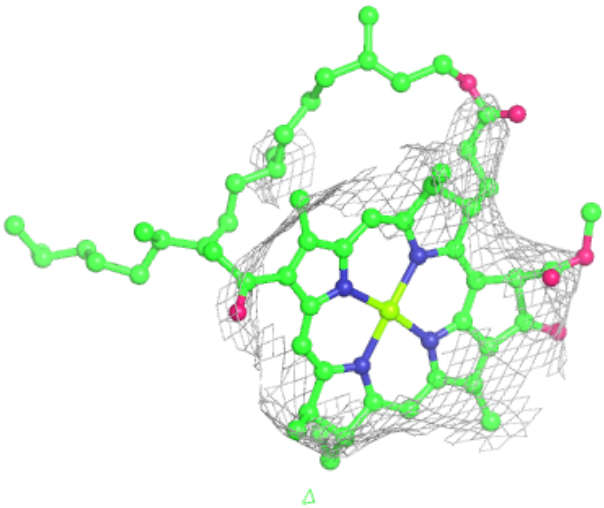


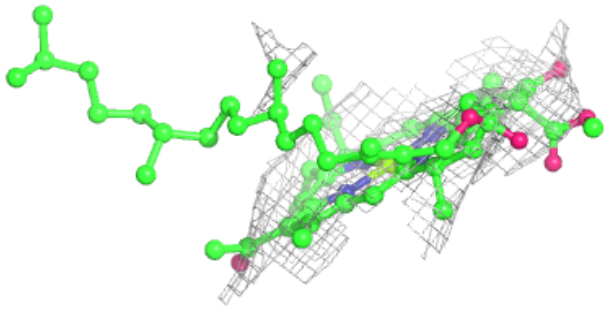


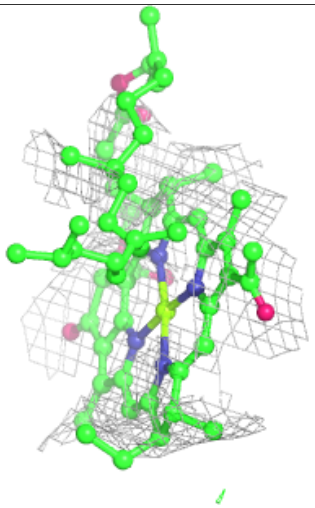


Electron density around BCL c 101:

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

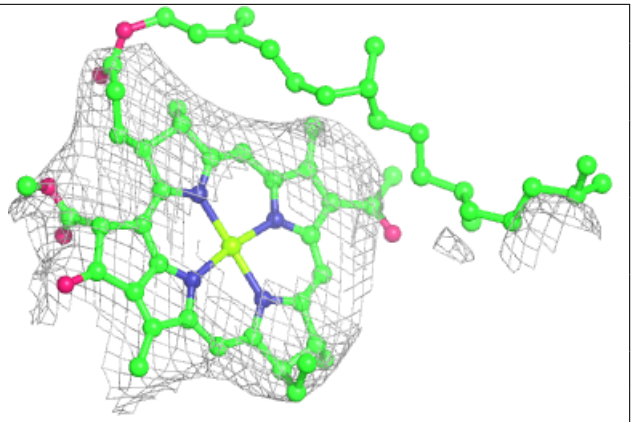


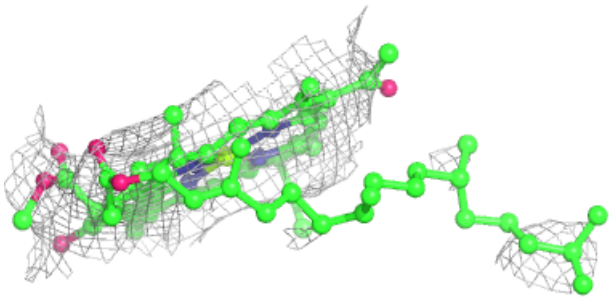


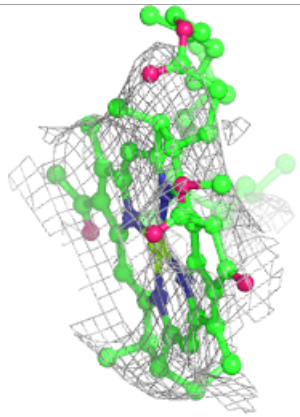


Electron density around BCL T 102:

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

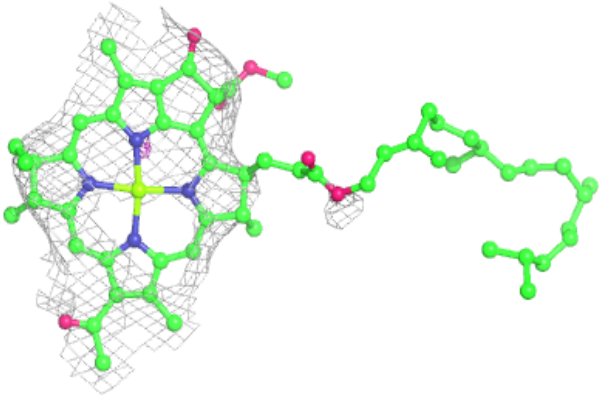


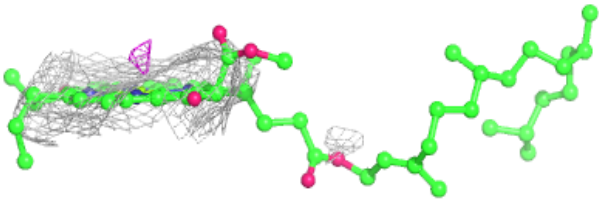


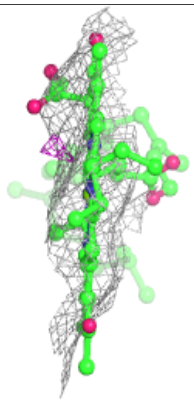


Electron density around BCL l 101:

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

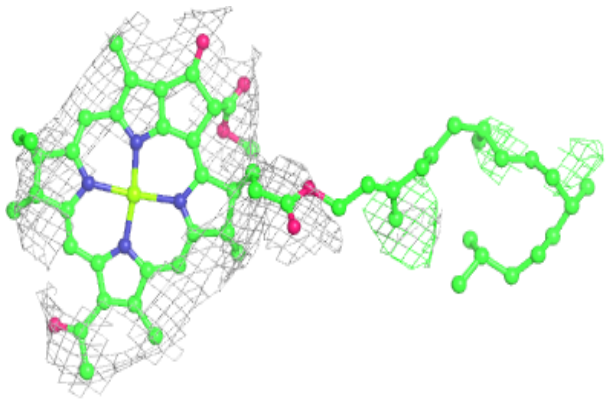


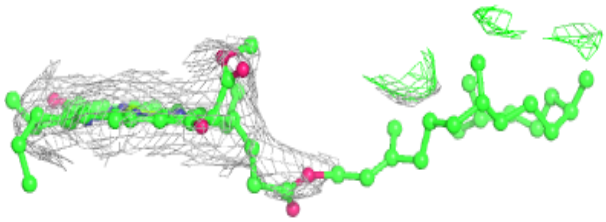


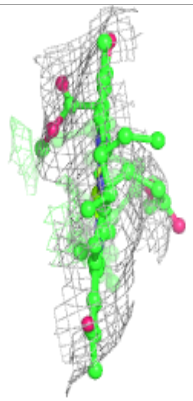


Electron density around BCL AI 101:

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

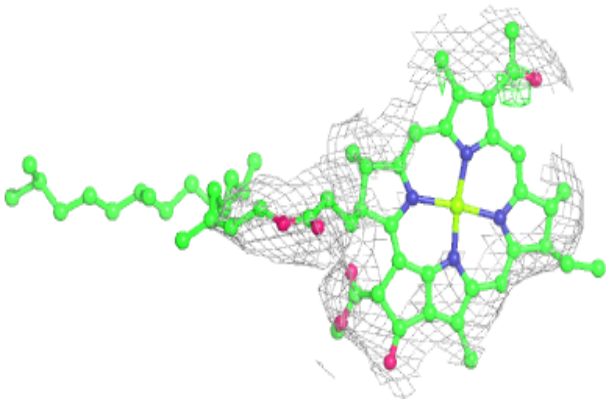


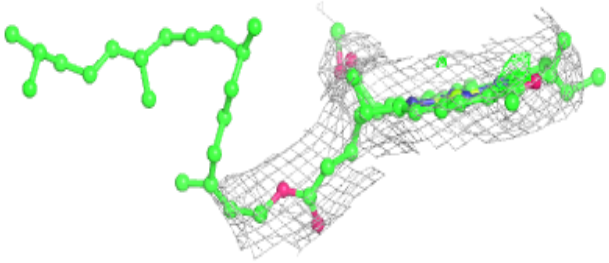


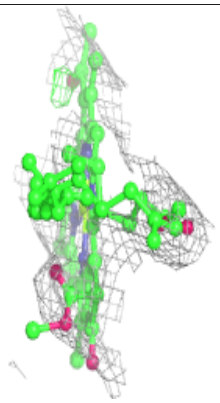


Electron density around BCL 5 101:

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

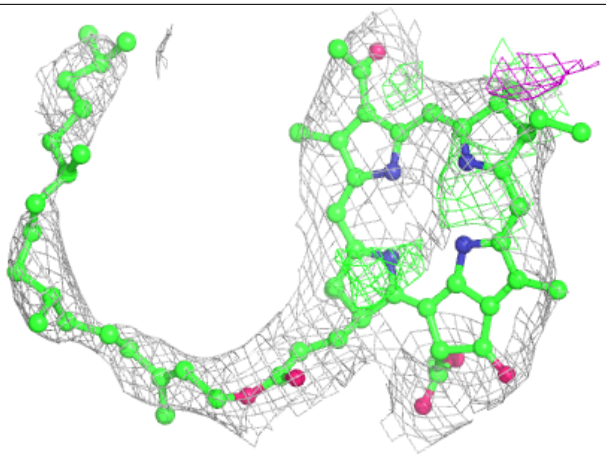


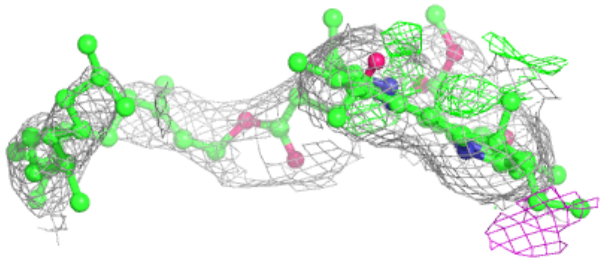


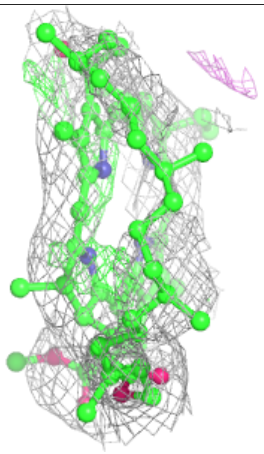


Electron density around BPH x 302:

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

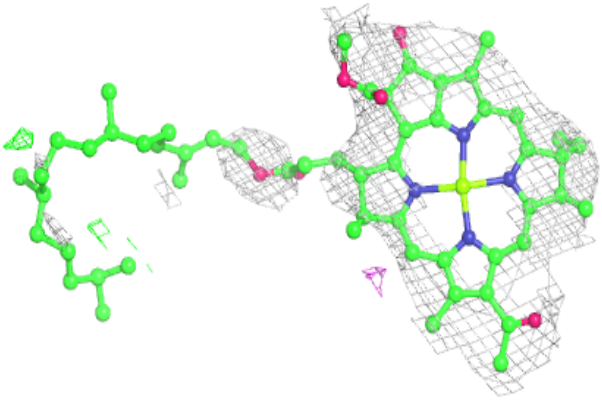


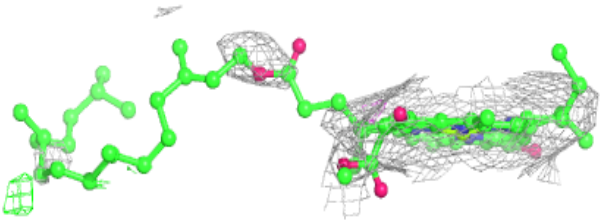


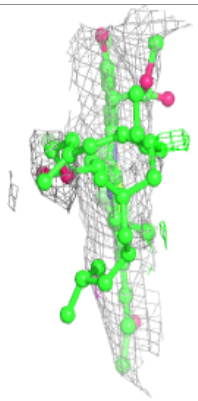


Electron density around BCL U 101:

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

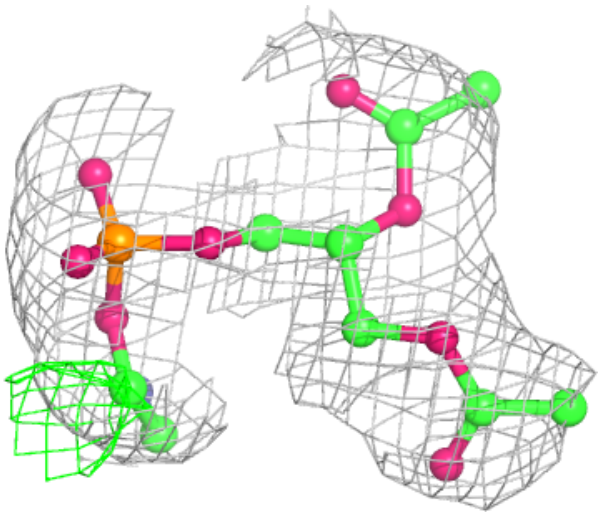


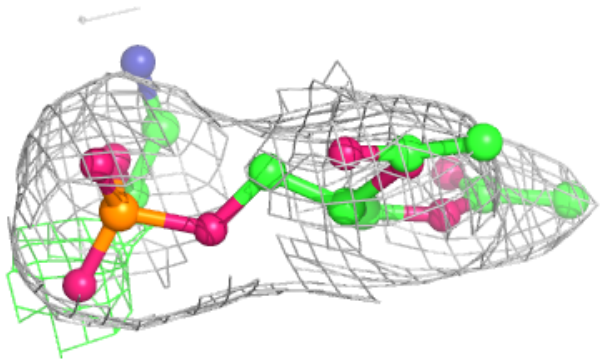


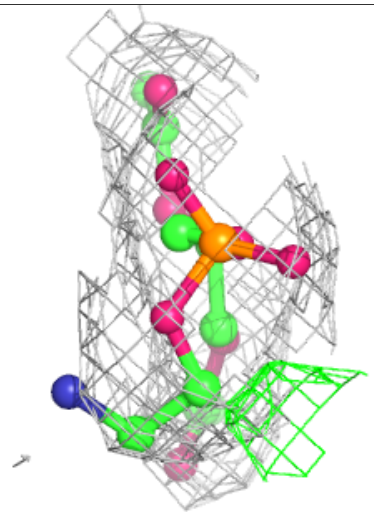


Electron density around PEF t 301:

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

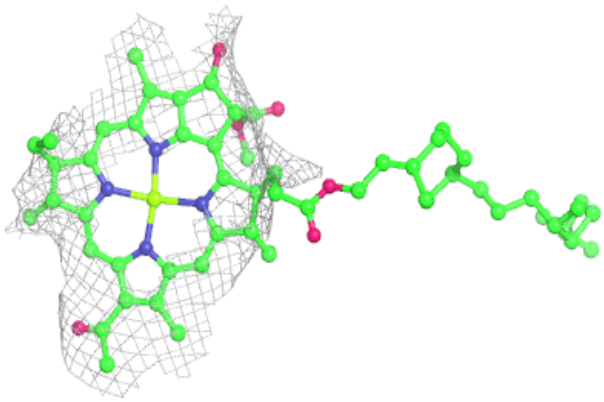


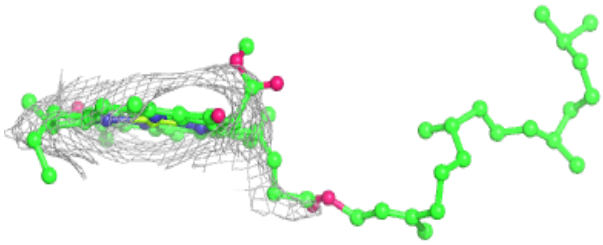


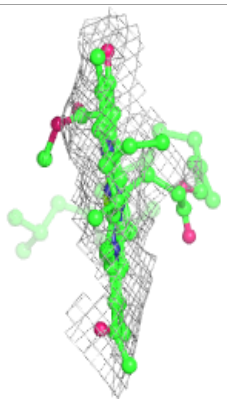


Electron density around BCL r 101:

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

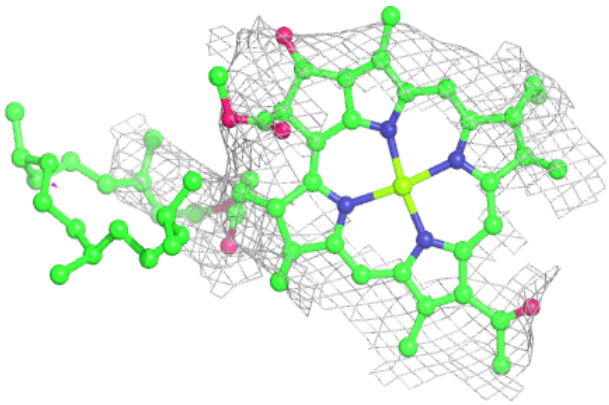


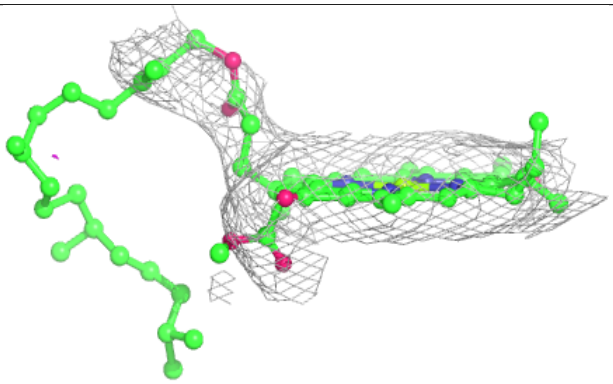


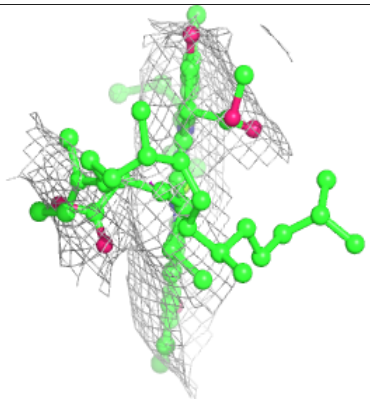


Electron density around BCL Q 101:

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

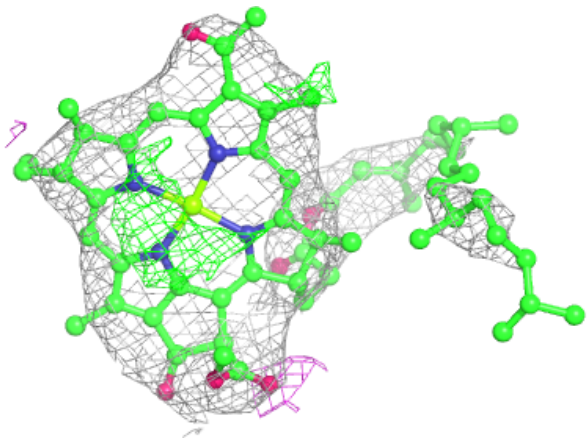


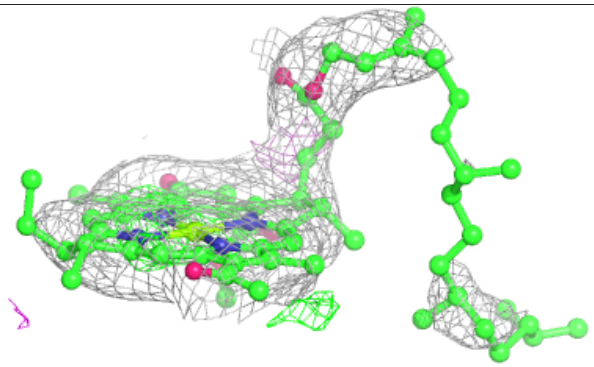


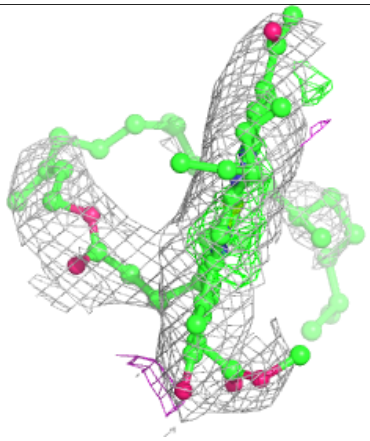


Electron density around BCL x 303:

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

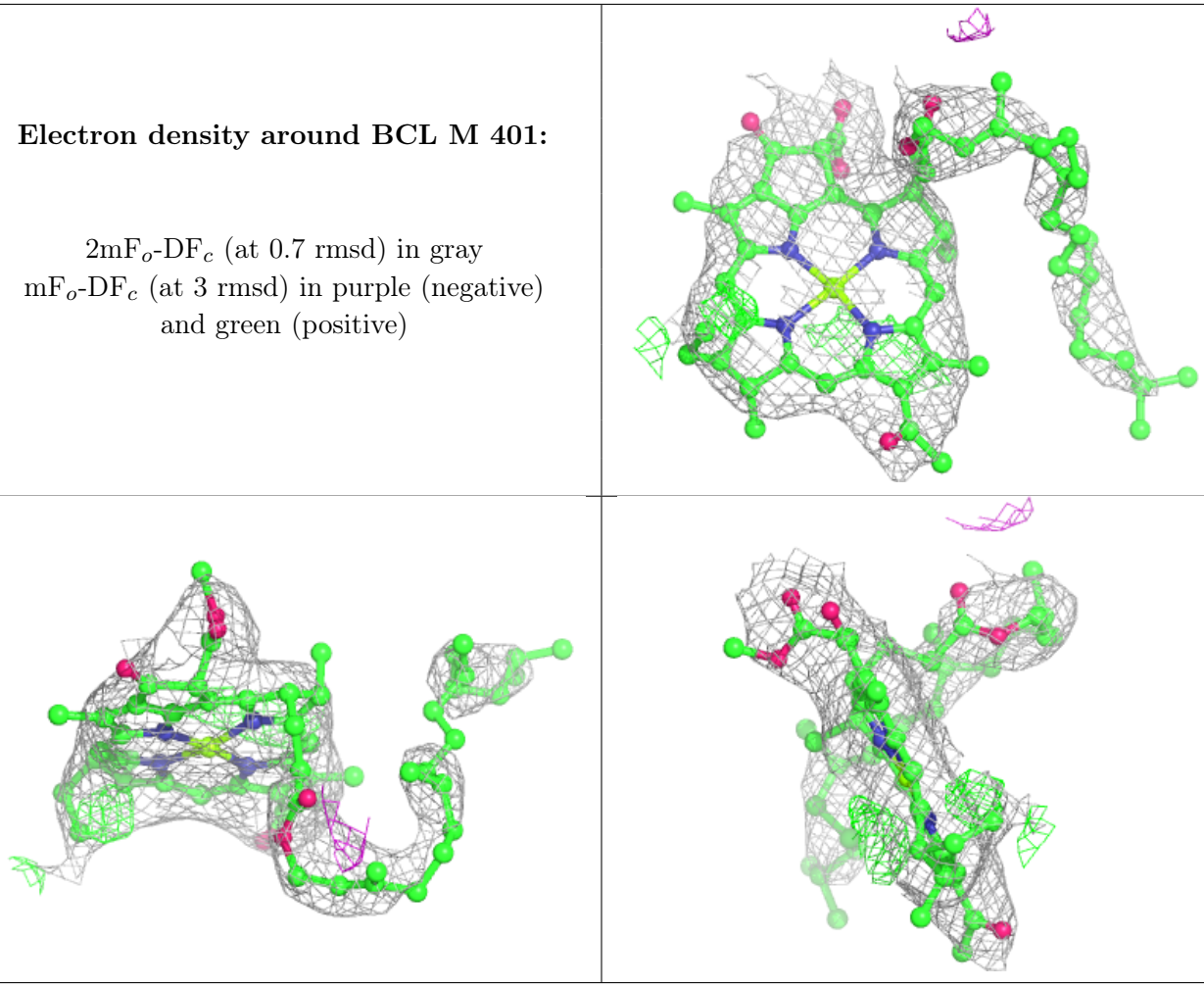






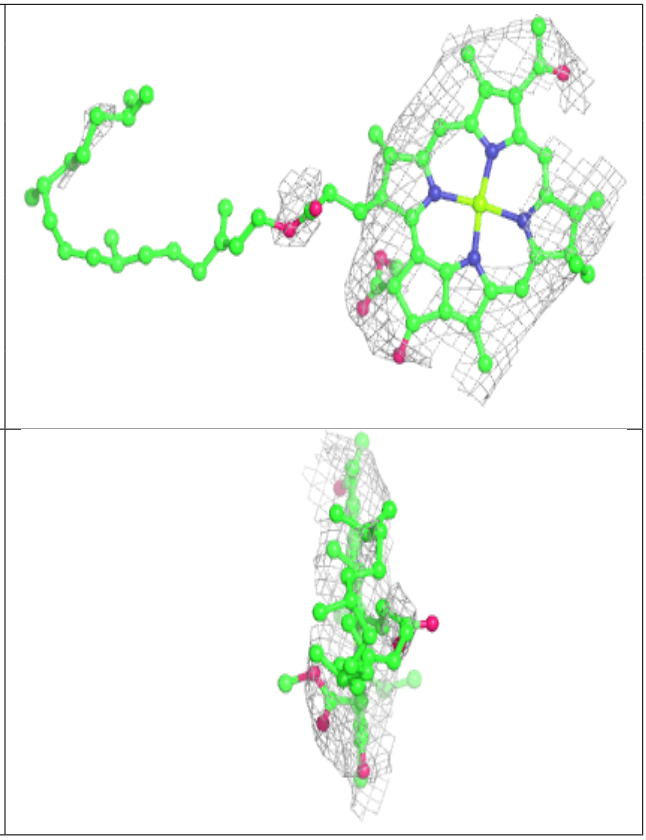
Electron density around BCL M 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



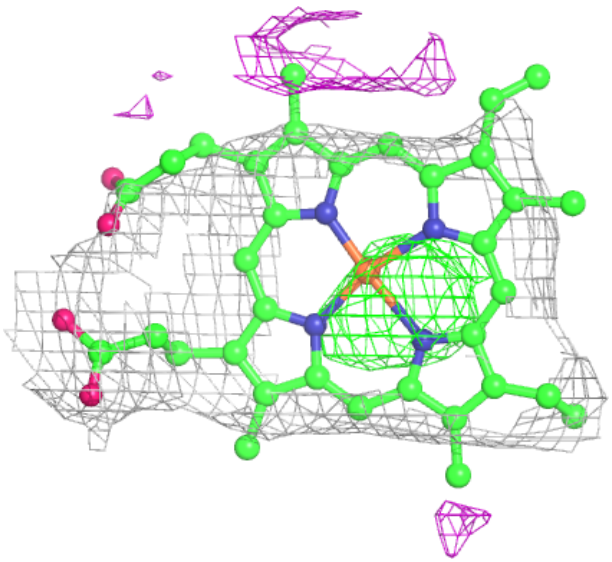
Electron density around BCL W 101:

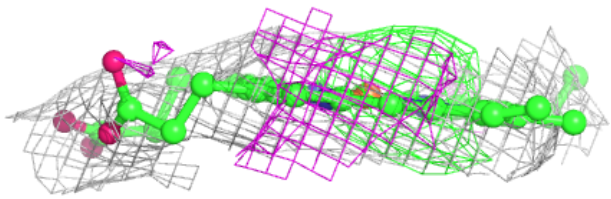
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

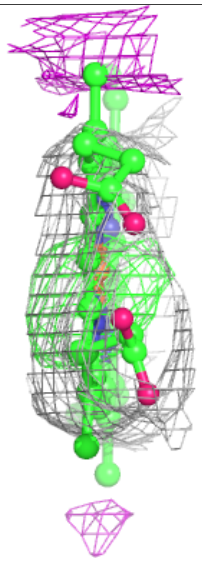


Electron density around HEM C 502:

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

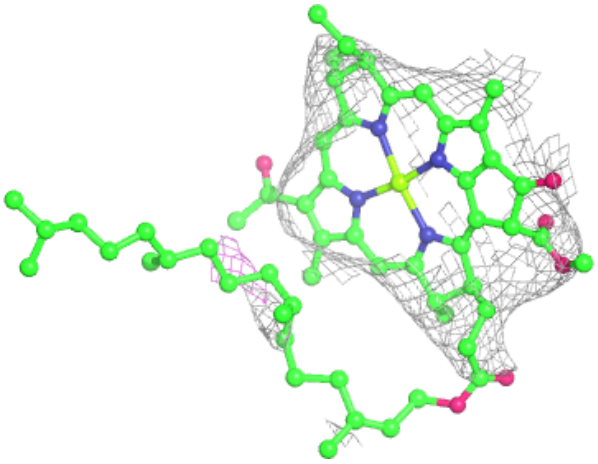


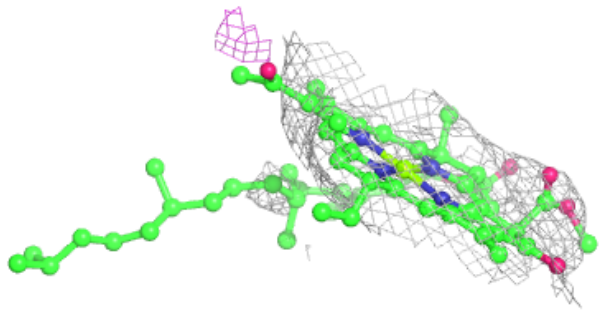


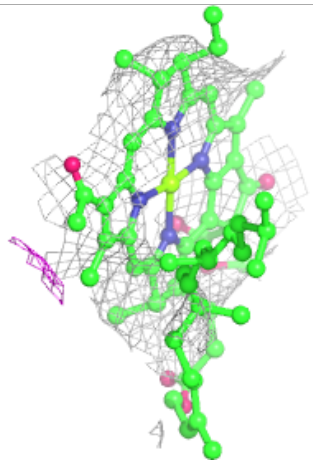


Electron density around BCL 2 102:

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

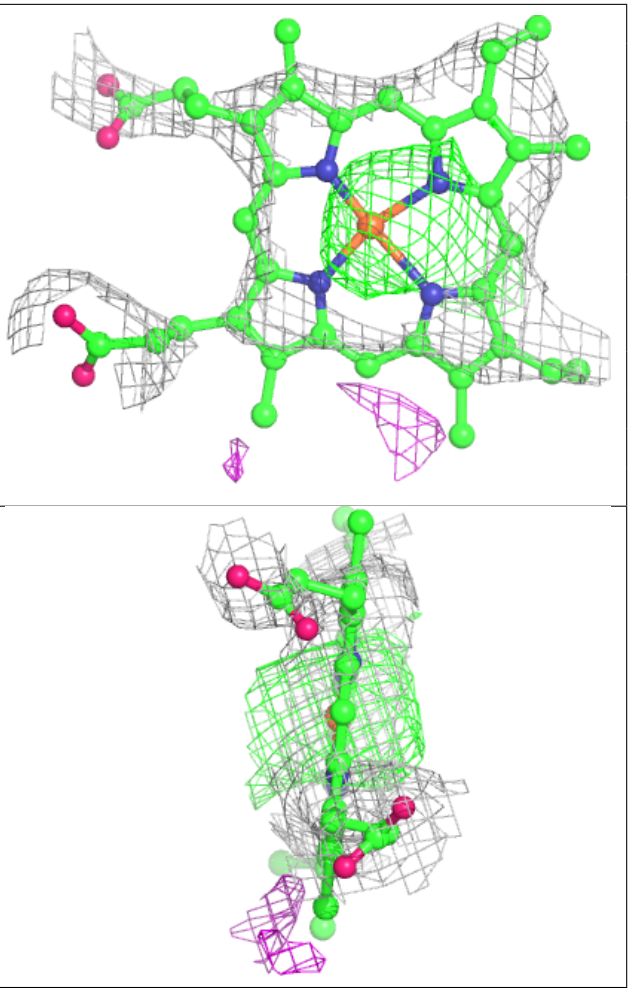






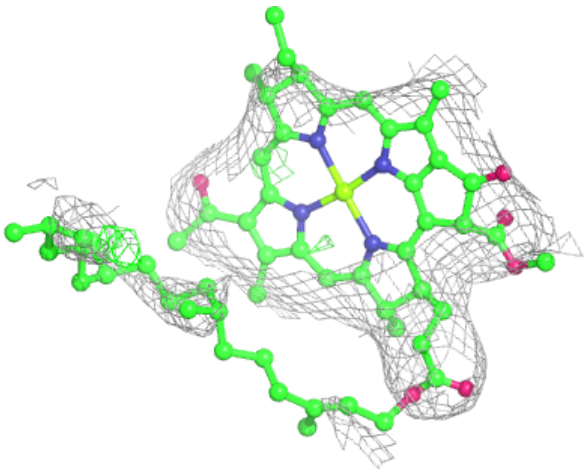
Electron density around HEM o 503:

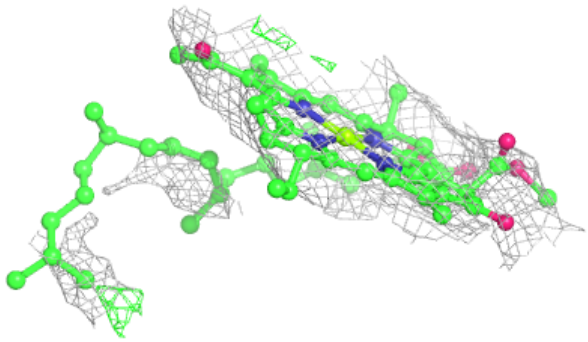
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

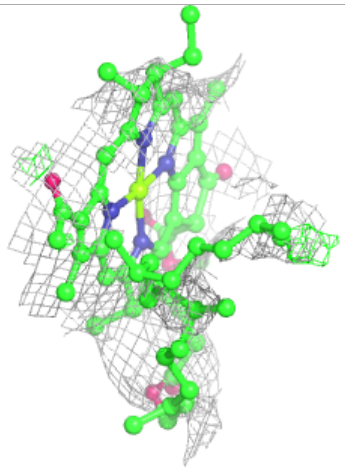


Electron density around BCL 4 102:

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

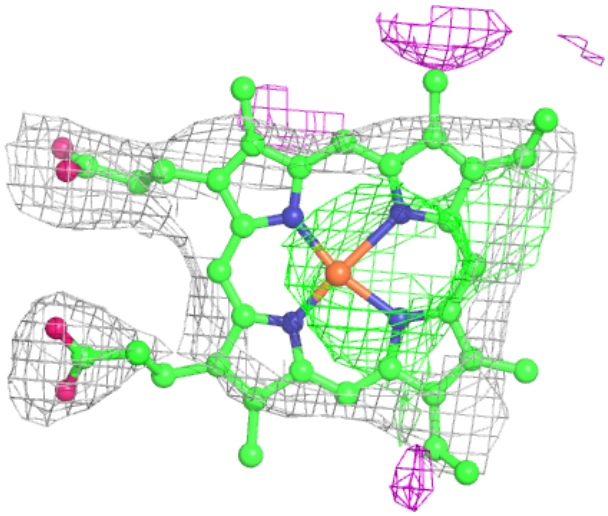


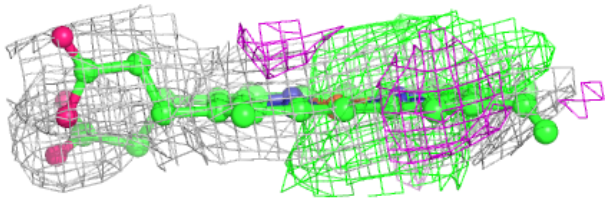


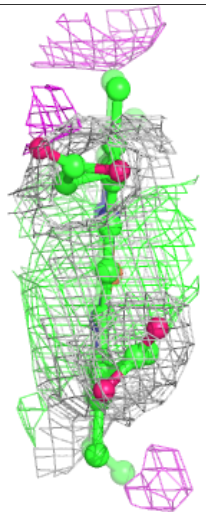


Electron density around HEM C 504:

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

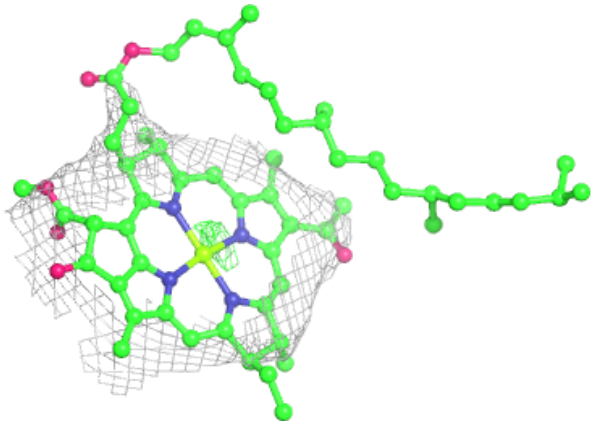


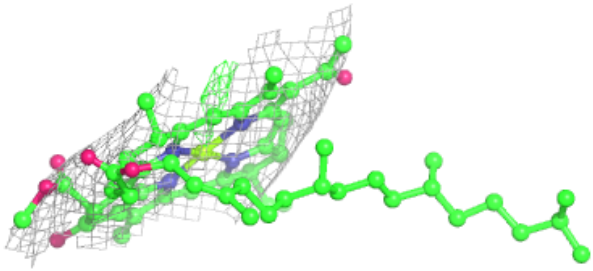


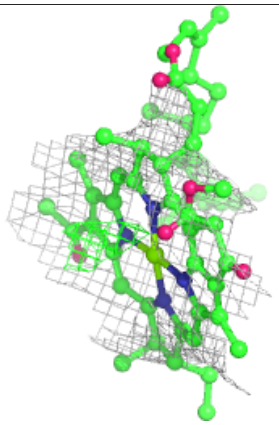


Electron density around BCL s 102:

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

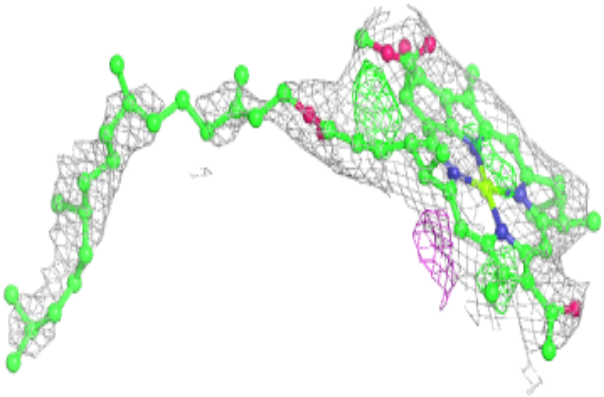


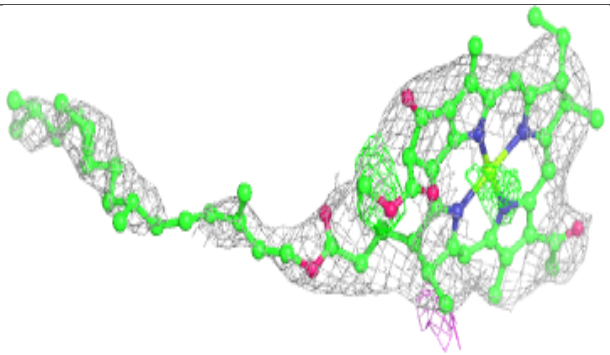


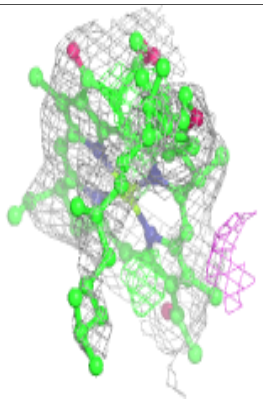


Electron density around BCL L 301:

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

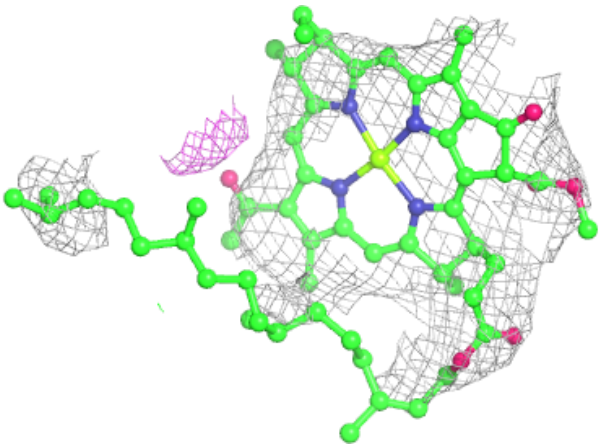


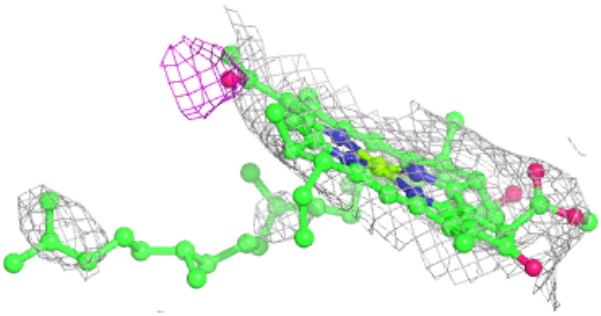


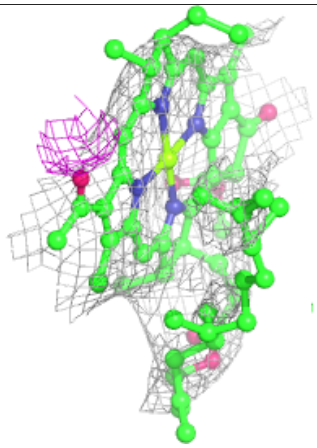


Electron density around BCL AL 102:

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

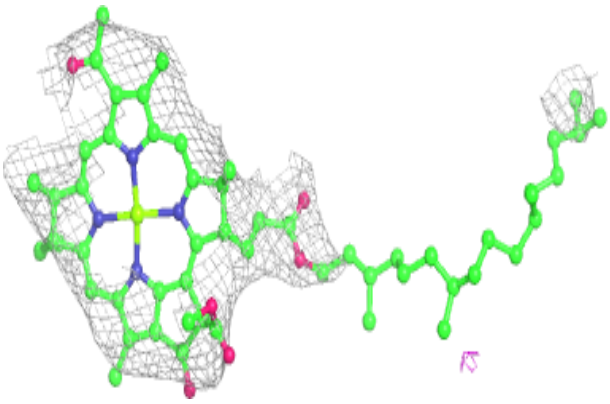


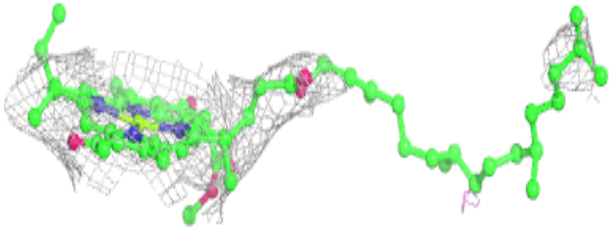


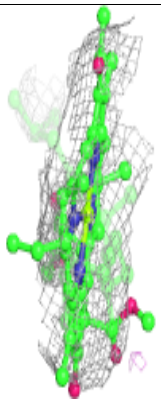


Electron density around BCL S 102:

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

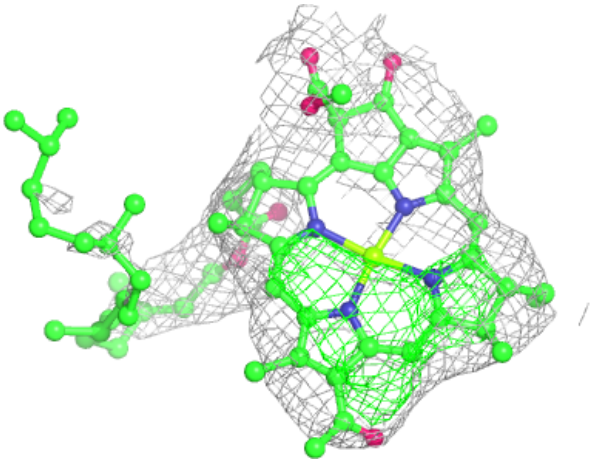


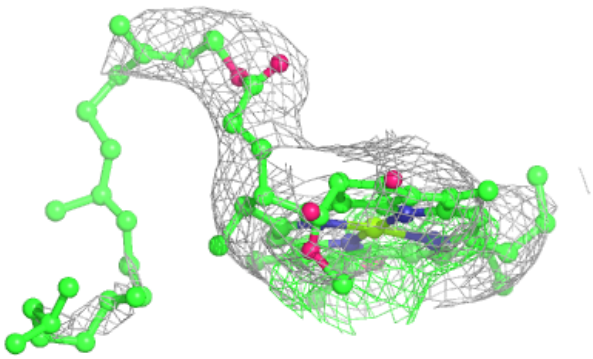


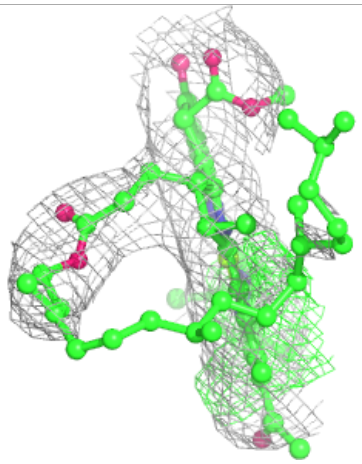


Electron density around BCL L 303:

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

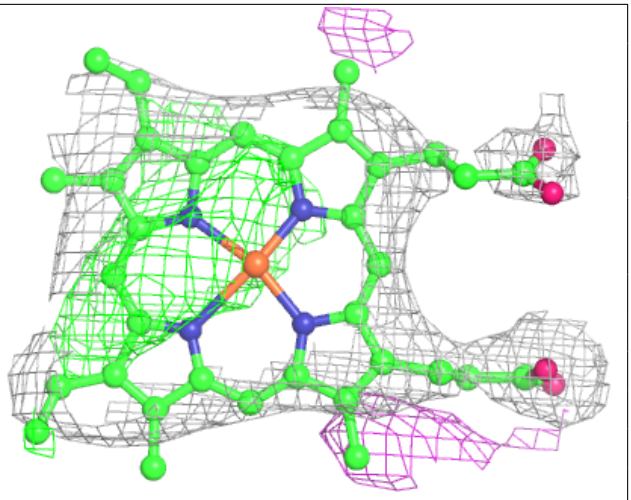


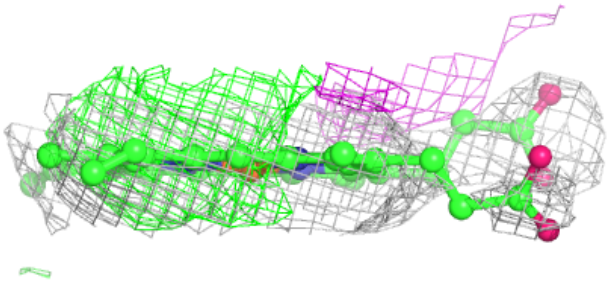


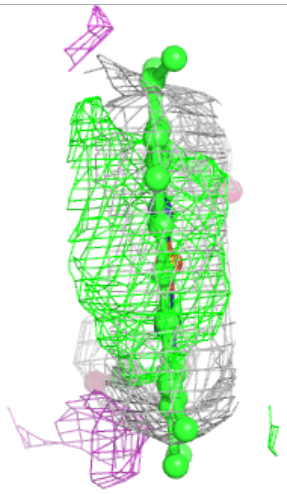


Electron density around HEM o 504:

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

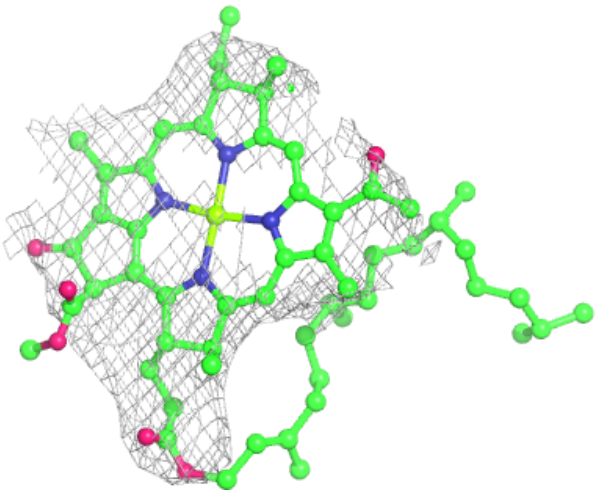


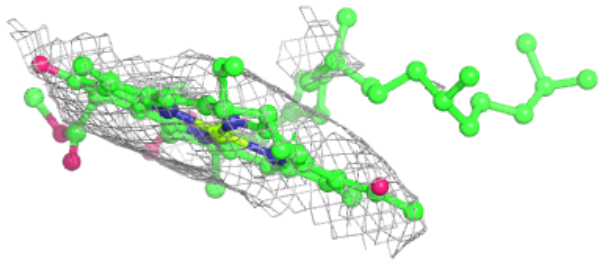


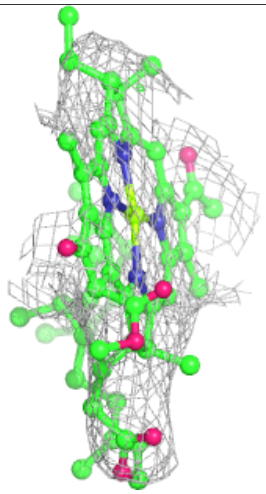


Electron density around BCL X 102:

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

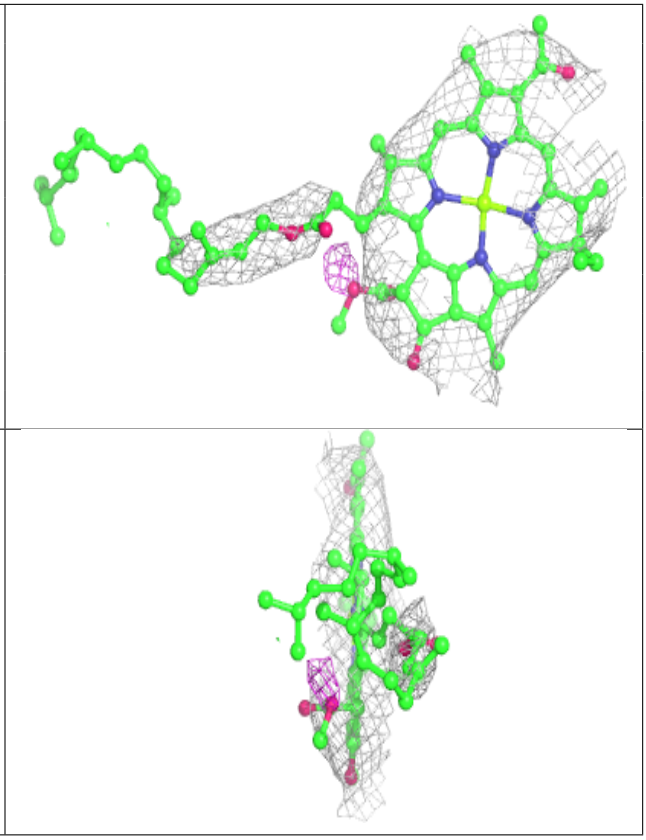






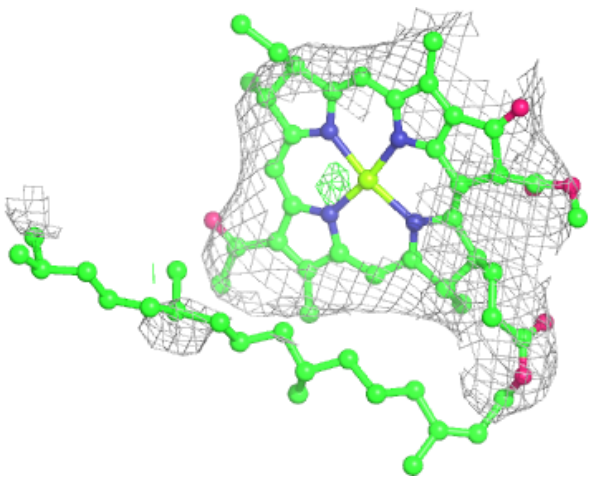
Electron density around BCL Y 101:

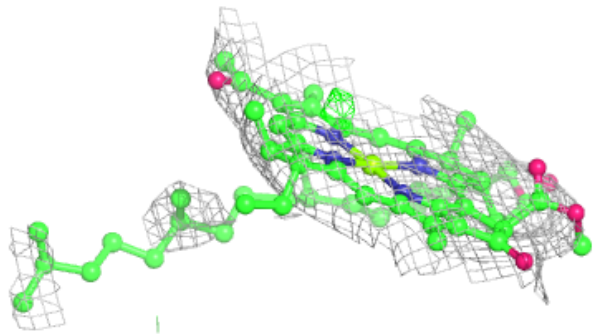
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

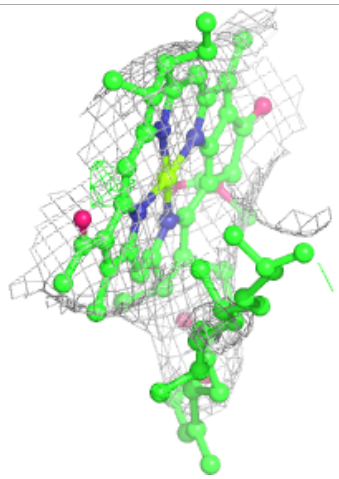


Electron density around BCL Z 102:

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

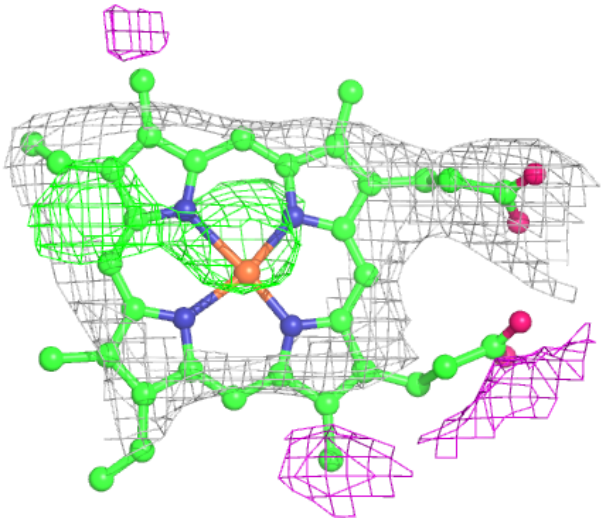


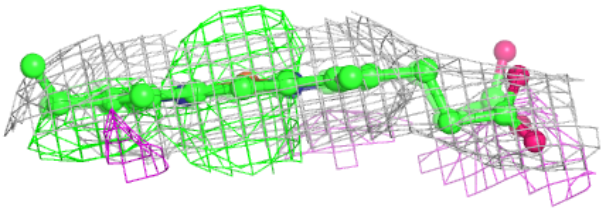


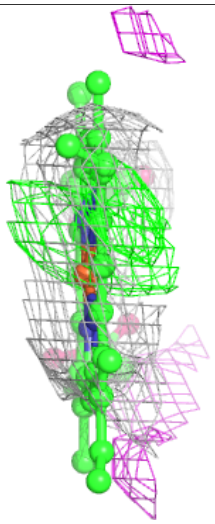


Electron density around HEM o 502:

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

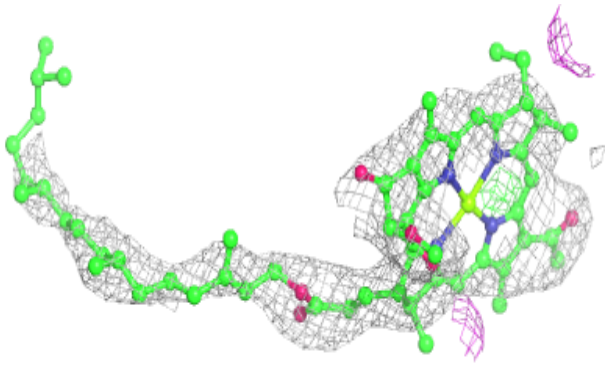


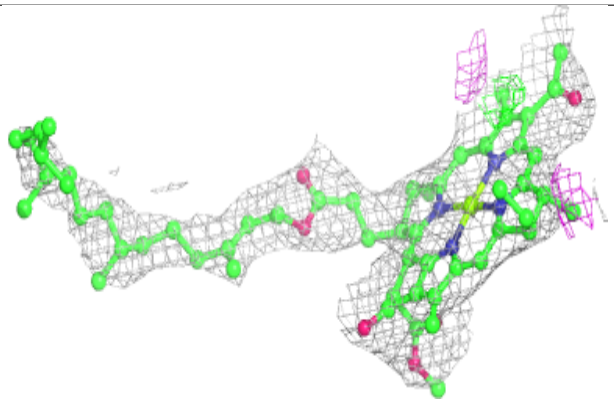


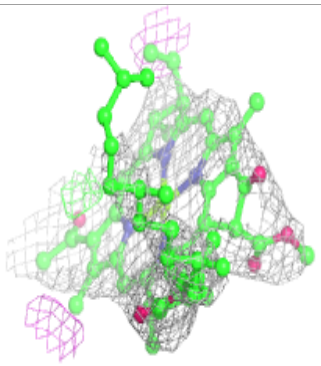


Electron density around BCL M 402:

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

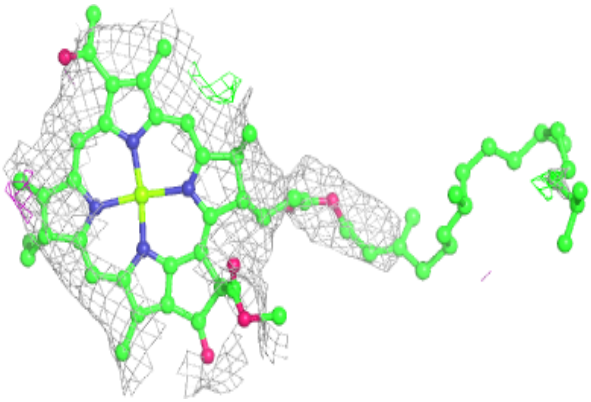


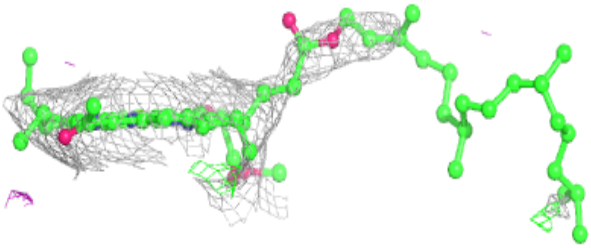


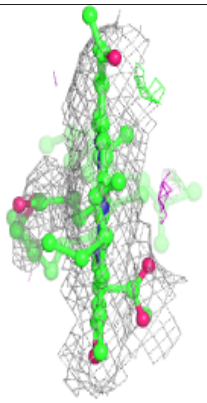


Electron density around BCL AK 101:

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

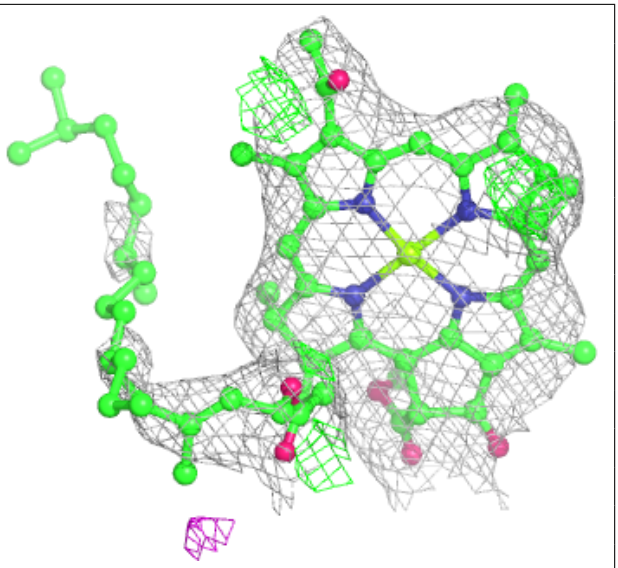


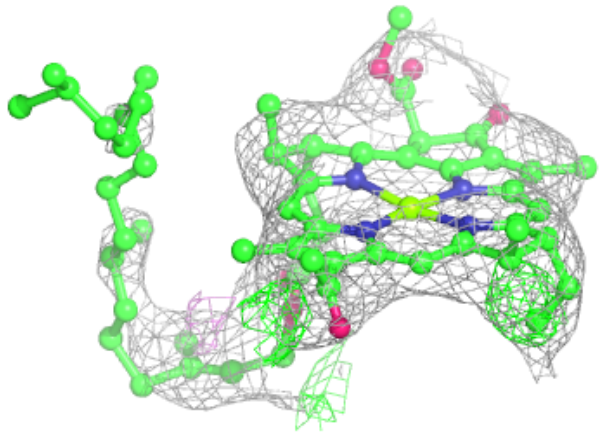


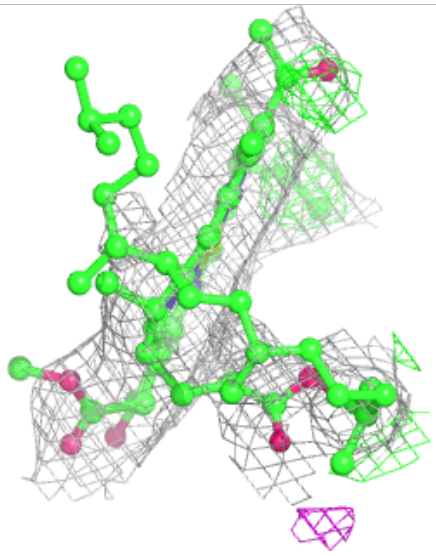


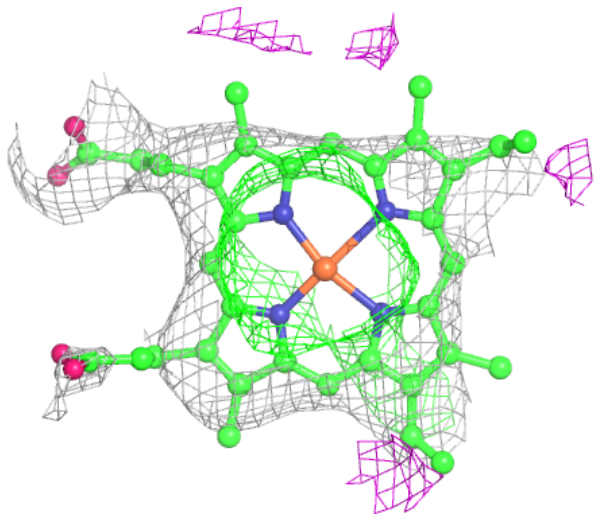
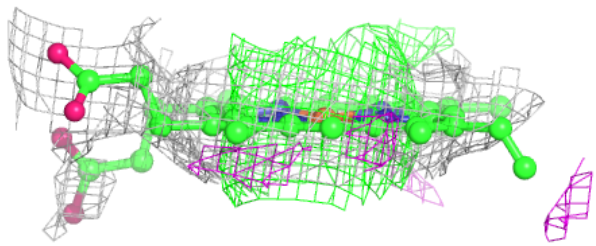
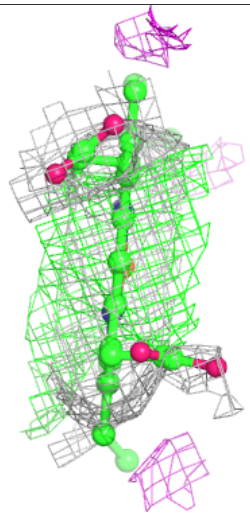
Electron density around BCL x 305:

$2mF_o$-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 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.