



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:41 AM UTC

PDB ID : 5B5M / pdb_00005b5m
Title : Crystal structure of the Sr-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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

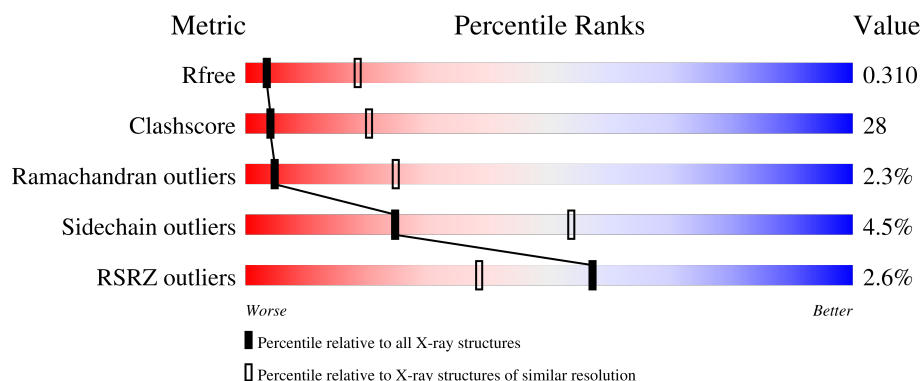
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	C	333	
1	o	333	
2	L	281	
2	x	281	
3	M	319	

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Mol	Chain	Length	Quality of chain
3	y	319	
4	H	259	
4	t	259	
5	1	61	
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	AA	61	
5	AC	61	
5	AE	61	
5	AG	61	
5	AI	61	
5	AK	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	

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Mol	Chain	Length	Quality of chain
5	d	61	
5	f	61	
5	h	61	
5	j	61	
5	l	61	
5	m	61	
5	p	61	
5	r	61	
5	u	61	
5	w	61	
6	0	47	
6	2	47	
6	4	47	
6	6	47	
6	8	47	
6	AB	47	
6	AD	47	
6	AF	47	
6	AH	47	
6	AJ	47	
6	AL	47	
6	B	47	
6	E	47	
6	G	47	
6	J	47	

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Mol	Chain	Length	Quality of chain
6	N	47	
6	P	47	
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	
6	c	47	
6	e	47	
6	g	47	
6	i	47	
6	k	47	
6	n	47	
6	q	47	
6	s	47	
6	v	47	
6	z	47	

2 Entry composition

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
1	C	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			
1	o	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

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

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

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

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

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

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

- Molecule 5 is a protein called LH1 alpha polypeptide.

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

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

- Molecule 6 is a protein called LH1 beta polypeptide.

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

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

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

-
- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring. The structure includes various side chains and a central heme label.

- Molecule 8 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

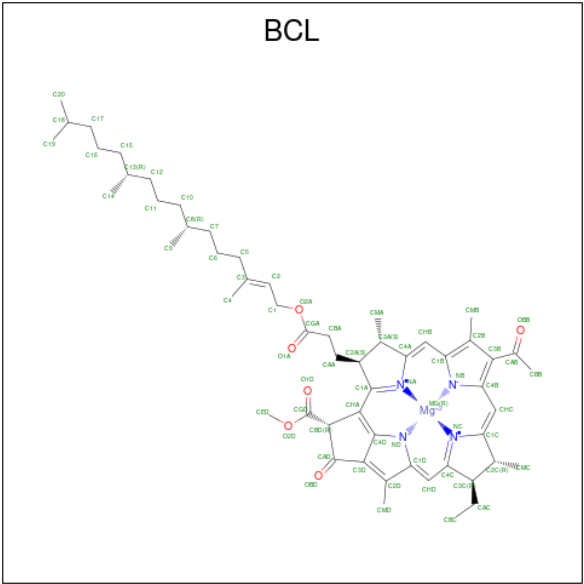
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total 1 Sr 1	0	0
8	L	2	Total 2 Sr 2	0	0
8	A	1	Total 1 Sr 1	0	0
8	D	1	Total 1 Sr 1	0	0
8	F	1	Total 1 Sr 1	0	0
8	I	1	Total 1 Sr 1	0	0
8	K	1	Total 1 Sr 1	0	0
8	O	1	Total 1 Sr 1	0	0
8	Q	1	Total 1 Sr 1	0	0
8	S	1	Total 1 Sr 1	0	0
8	U	1	Total 1 Sr 1	0	0
8	W	1	Total 1 Sr 1	0	0
8	Y	1	Total 1 Sr 1	0	0
8	1	1	Total 1 Sr 1	0	0
8	5	2	Total 2 Sr 2	0	0
8	7	1	Total 1 Sr 1	0	0
8	9	1	Total 1 Sr 1	0	0
8	o	1	Total 1 Sr 1	0	0
8	x	2	Total 2 Sr 2	0	0
8	m	1	Total 1 Sr 1	0	0
8	p	1	Total 1 Sr 1	0	0
8	r	1	Total 1 Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	w	2	Total 2	Sr 2	0	0
8	AA	1	Total 1	Sr 1	0	0
8	AC	1	Total 1	Sr 1	0	0
8	AE	1	Total 1	Sr 1	0	0
8	AI	2	Total 2	Sr 2	0	0
8	AK	1	Total 1	Sr 1	0	0
8	d	1	Total 1	Sr 1	0	0
8	f	1	Total 1	Sr 1	0	0
8	h	1	Total 1	Sr 1	0	0
8	j	1	Total 1	Sr 1	0	0
8	l	1	Total 1	Sr 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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

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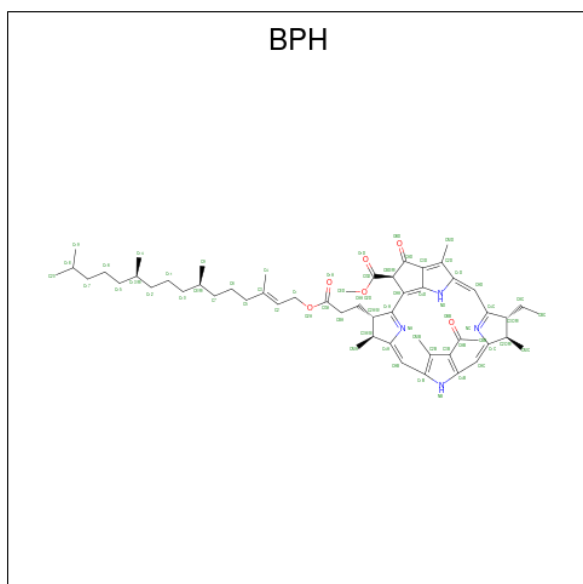
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	p	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	v	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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

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



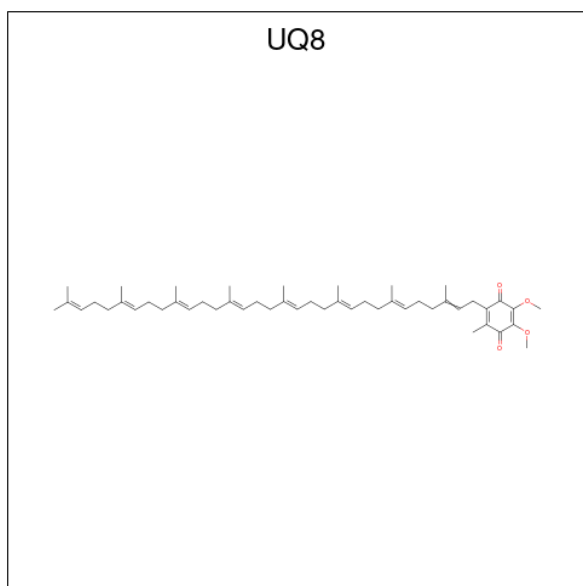
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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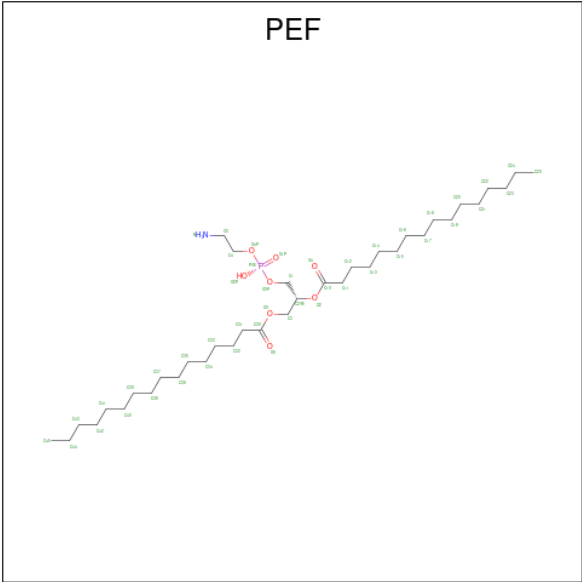
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

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



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

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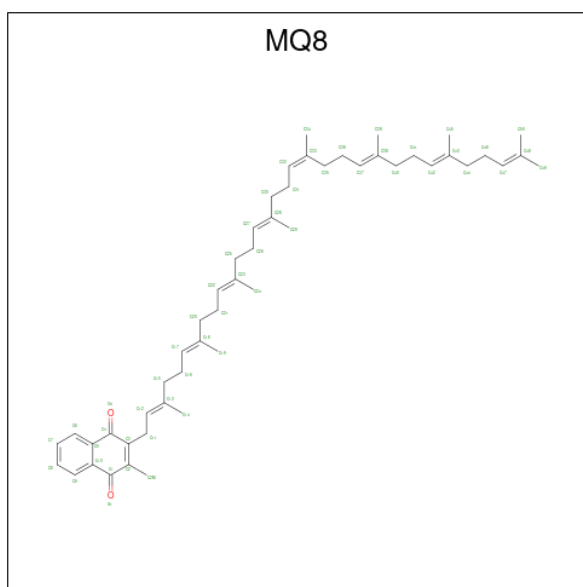
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

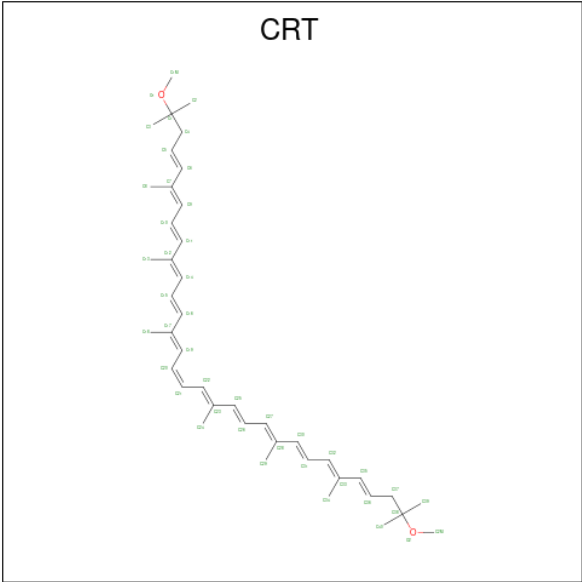
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Fe	0	0
			1	1		
13	x	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



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

- Molecule 15 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



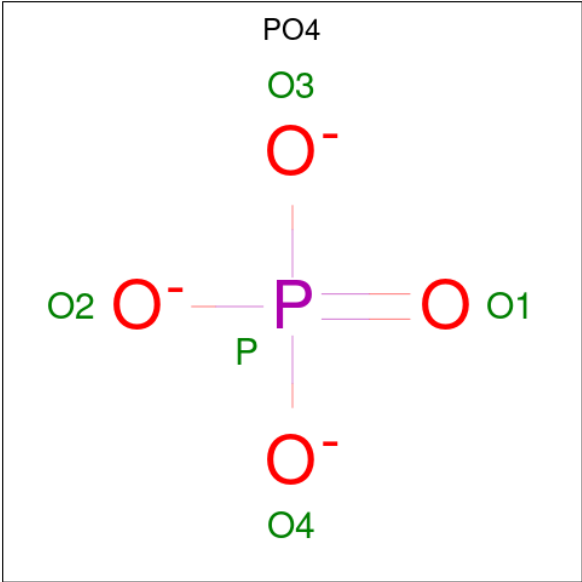
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	J	1	Total	C	O	0	0
			44	42	2		
15	N	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0
			44	42	2		
15	U	1	Total	C	O	0	0
			44	42	2		
15	X	1	Total	C	O	0	0
			44	42	2		
15	Z	1	Total	C	O	0	0
			44	42	2		
15	2	1	Total	C	O	0	0
			44	42	2		
15	4	1	Total	C	O	0	0
			44	42	2		

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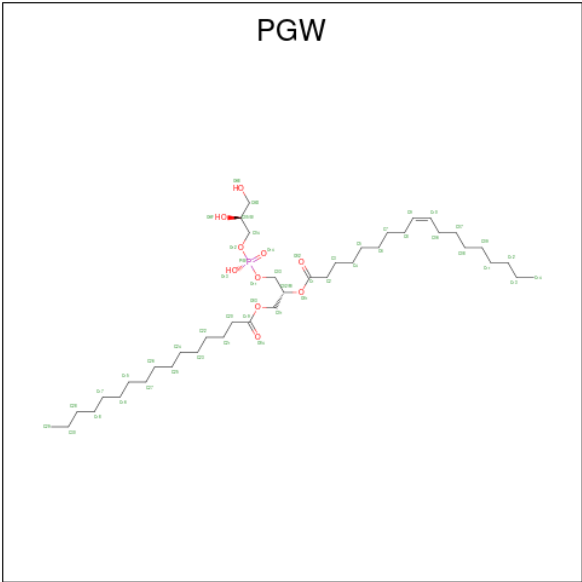
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	6	1	Total	C	O	0	0
			44	42	2		
15	8	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	p	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0
			44	42	2		
15	v	1	Total	C	O	0	0
			44	42	2		
15	z	1	Total	C	O	0	0
			44	42	2		
15	AC	1	Total	C	O	0	0
			44	42	2		
15	AD	1	Total	C	O	0	0
			44	42	2		
15	AE	1	Total	C	O	0	0
			44	42	2		
15	AH	1	Total	C	O	0	0
			44	42	2		
15	AJ	1	Total	C	O	0	0
			44	42	2		
15	AL	1	Total	C	O	0	0
			44	42	2		
15	e	1	Total	C	O	0	0
			44	42	2		
15	f	1	Total	C	O	0	0
			44	42	2		
15	i	1	Total	C	O	0	0
			44	42	2		
15	k	1	Total	C	O	0	0
			44	42	2		
15	c	1	Total	C	O	0	0
			44	42	2		

- Molecule 16 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 17 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



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

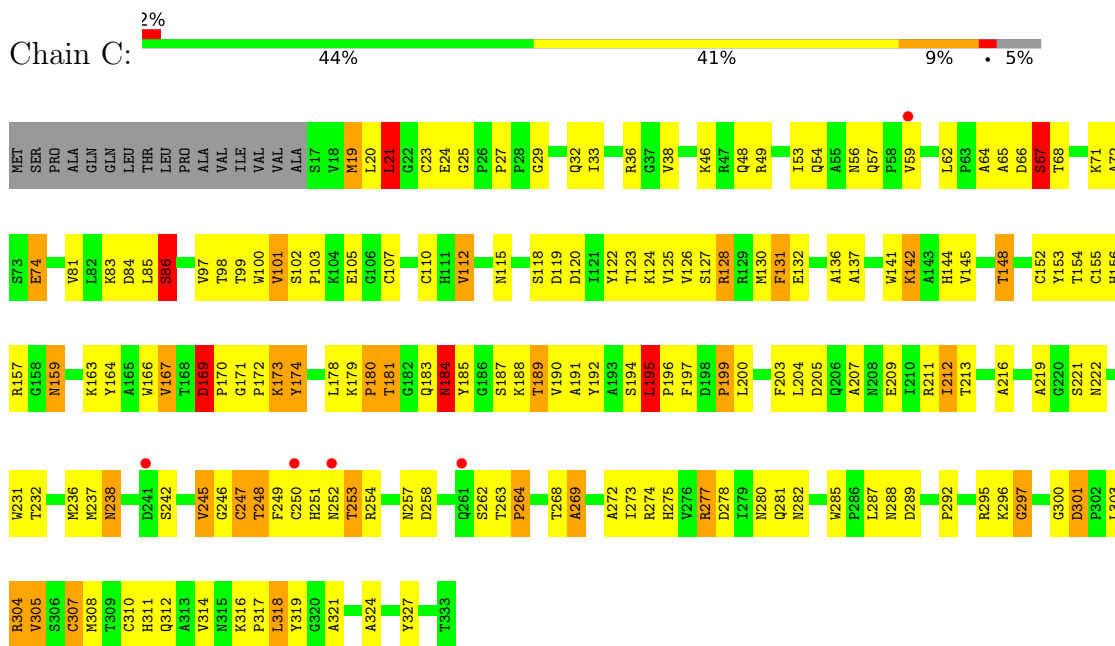
- Molecule 18 is water.

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

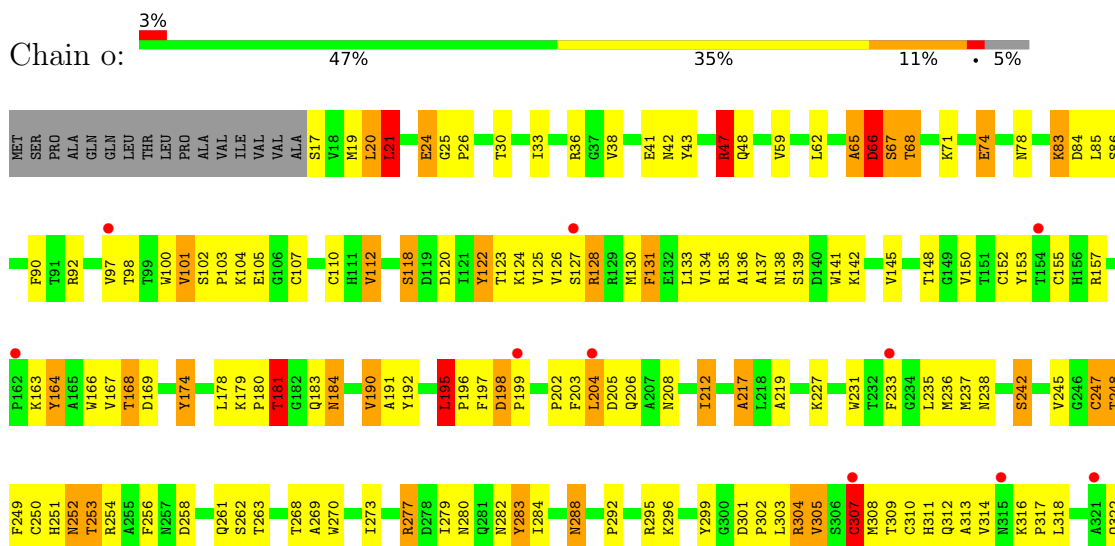
3 Residue-property plots

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

• Molecule 1: Photosynthetic reaction center cytochrome c subunit

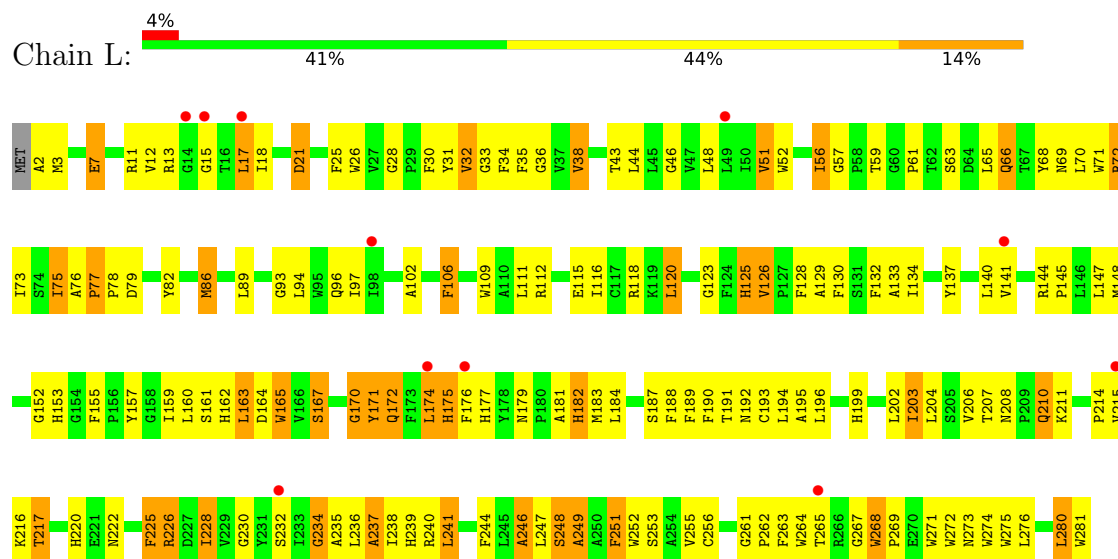


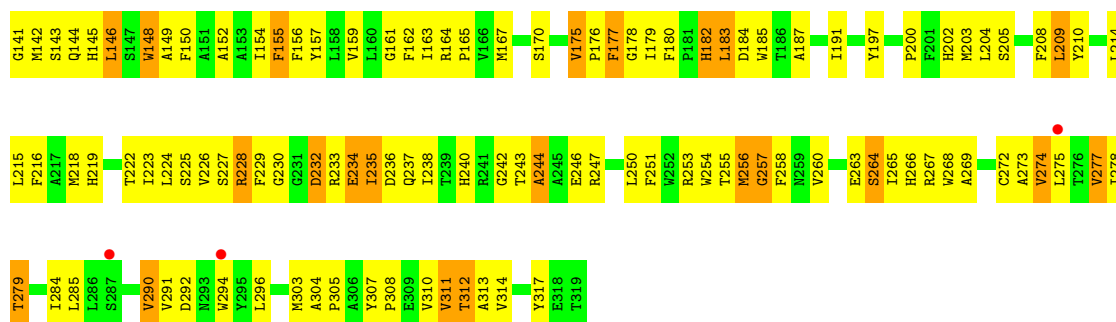
• Molecule 1: Photosynthetic reaction center cytochrome c subunit



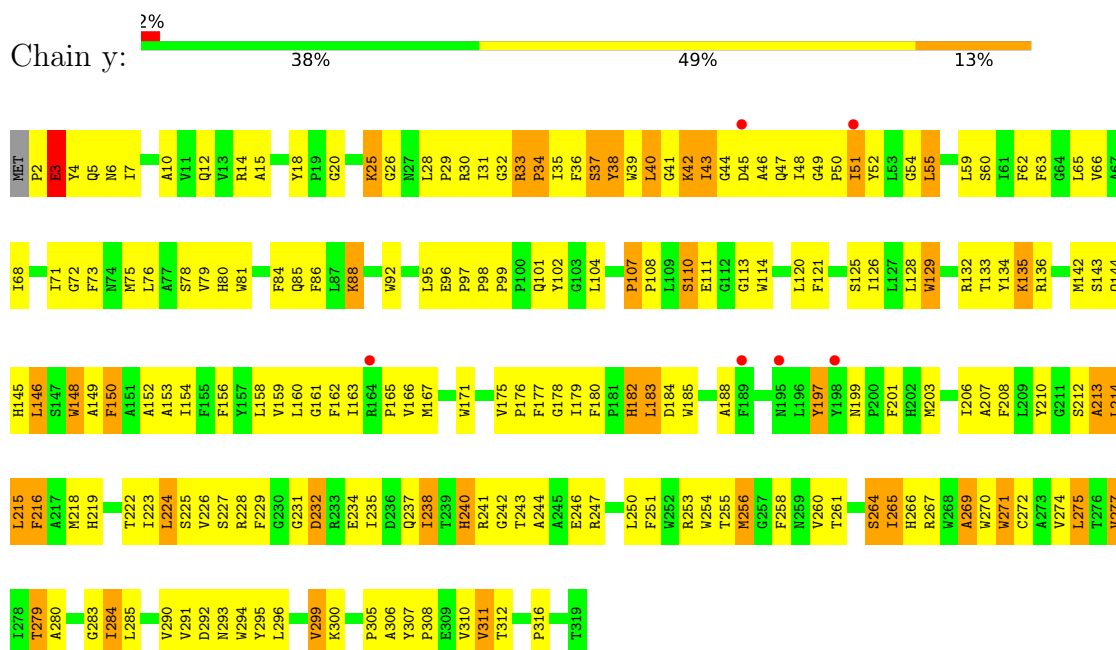


• Molecule 2: Photosynthetic reaction center L subunit

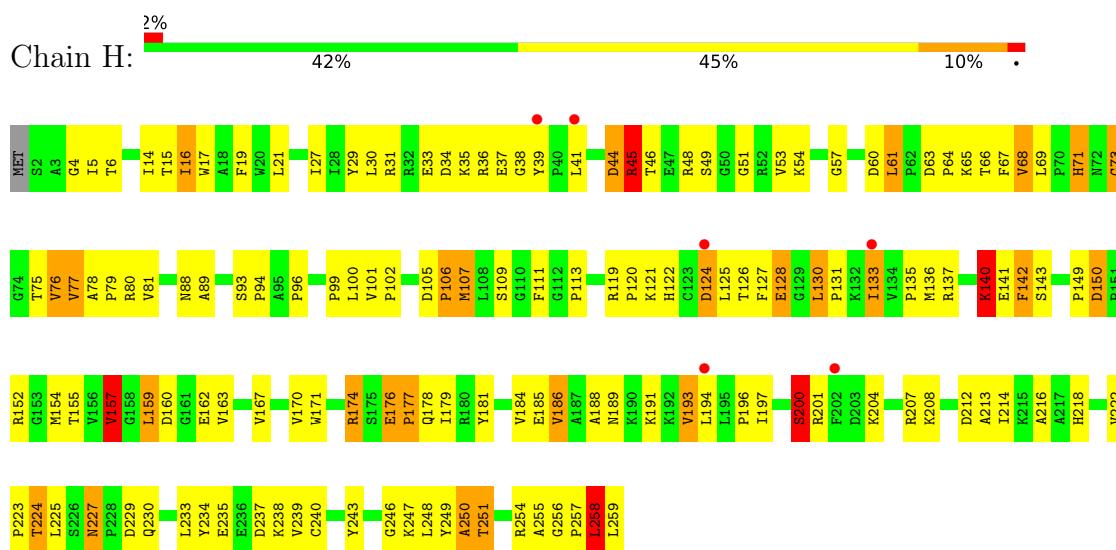




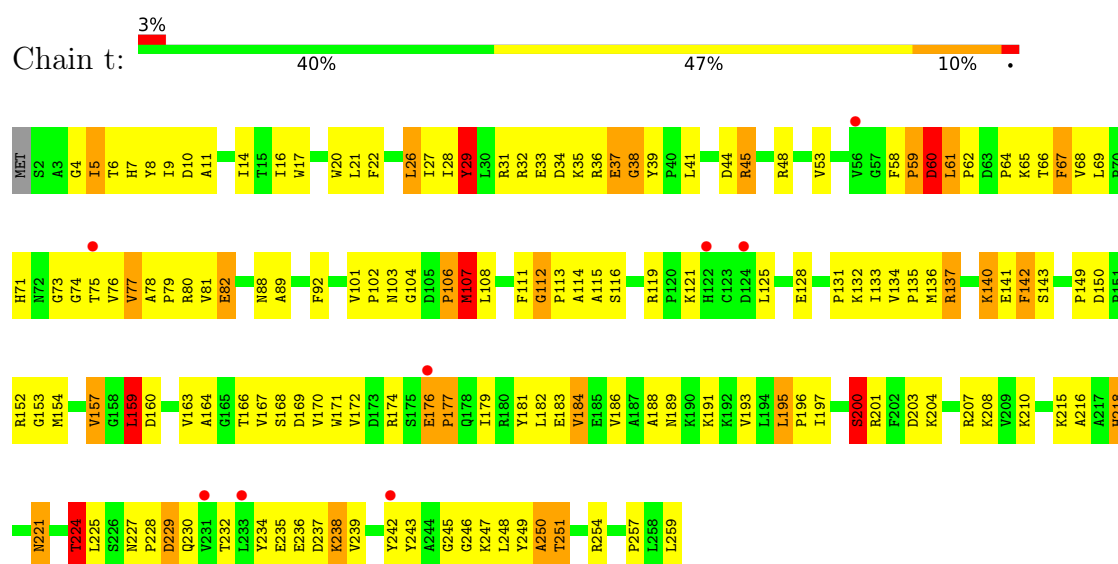
• Molecule 3: Photosynthetic reaction center M subunit



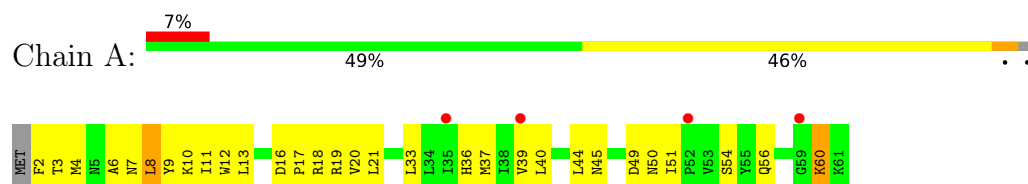
• Molecule 4: Photosynthetic reaction center H subunit



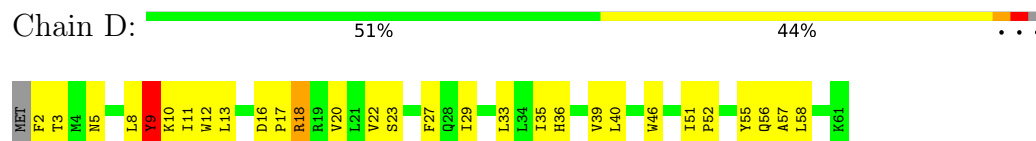
• Molecule 4: Photosynthetic reaction center H subunit



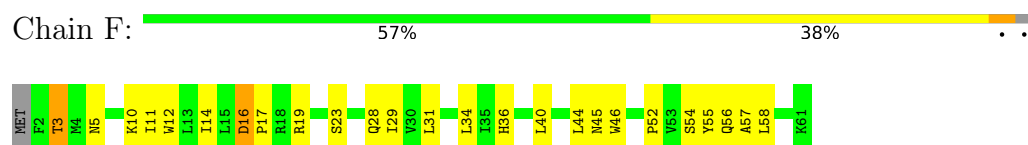
- Molecule 5: LH1 alpha polypeptide



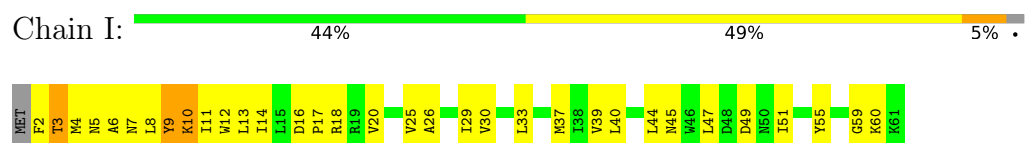
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

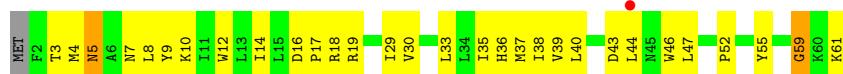


- Molecule 5: LH1 alpha polypeptide

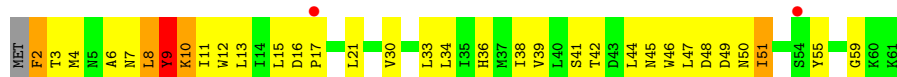
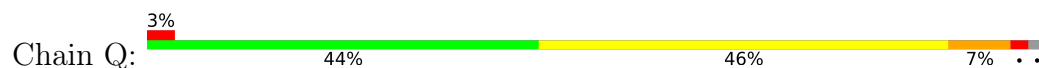




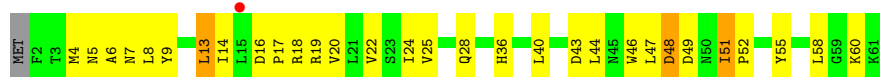
- Molecule 5: LH1 alpha polypeptide



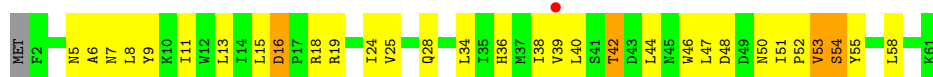
- Molecule 5: LH1 alpha polypeptide



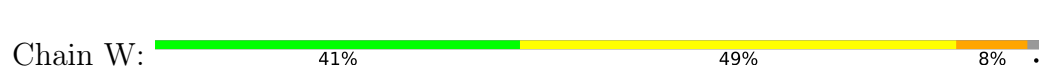
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



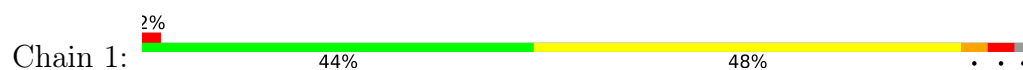
- Molecule 5: LH1 alpha polypeptide



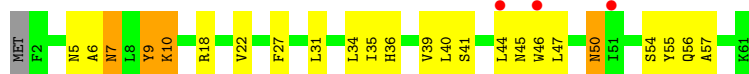
- Molecule 5: LH1 alpha polypeptide



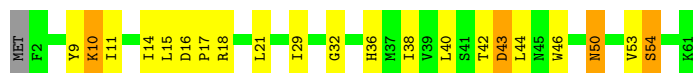
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



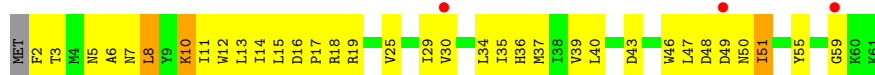
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



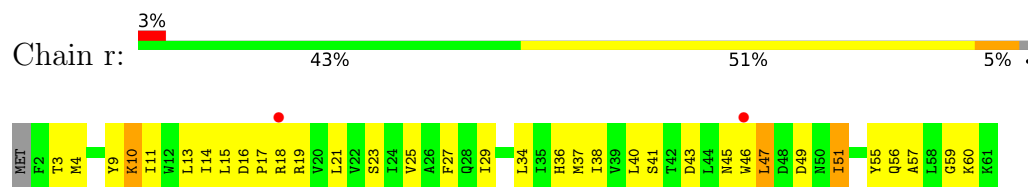
- Molecule 5: LH1 alpha polypeptide



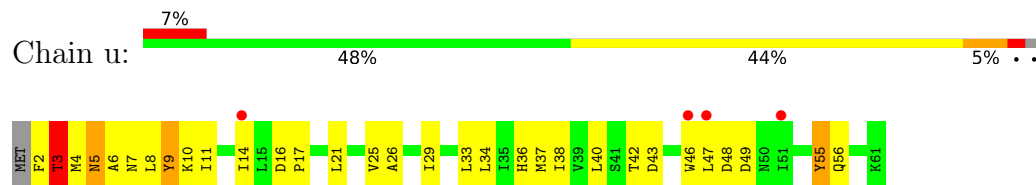
- Molecule 5: LH1 alpha polypeptide



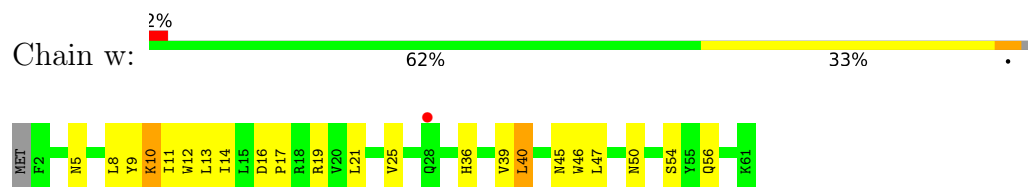
• Molecule 5: LH1 alpha polypeptide



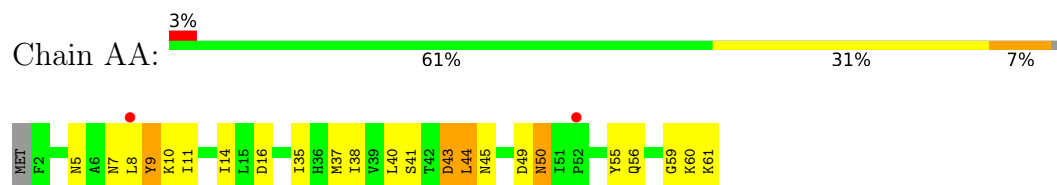
• Molecule 5: LH1 alpha polypeptide



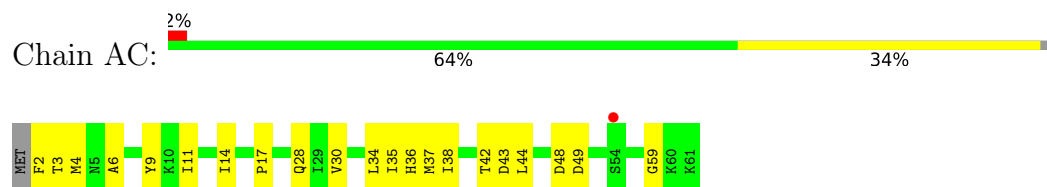
• Molecule 5: LH1 alpha polypeptide



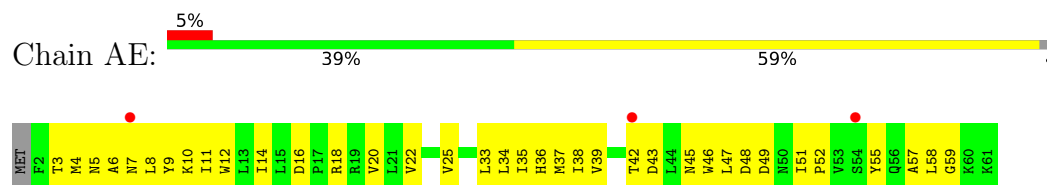
• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide



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- Molecule 5: LH1 alpha polypeptide



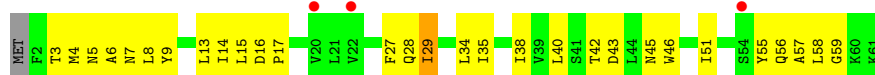
- Molecule 5: LH1 alpha polypeptide



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- Molecule 5: LH1 alpha polypeptide



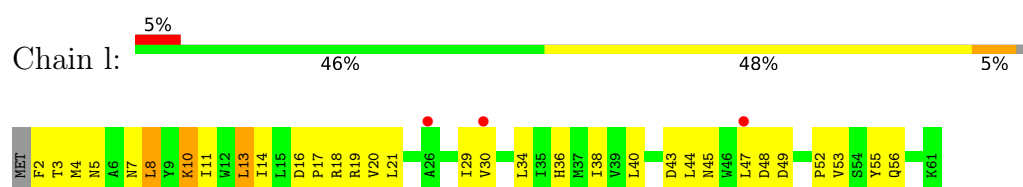
- Molecule 5: LH1 alpha polypeptide



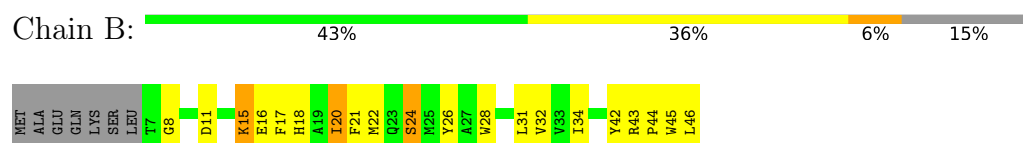
- Molecule 5: LH1 alpha polypeptide



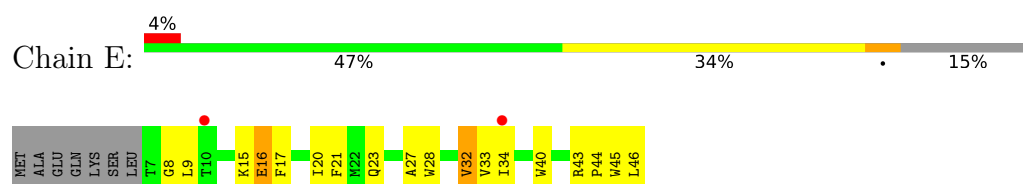
- Molecule 5: LH1 alpha polypeptide



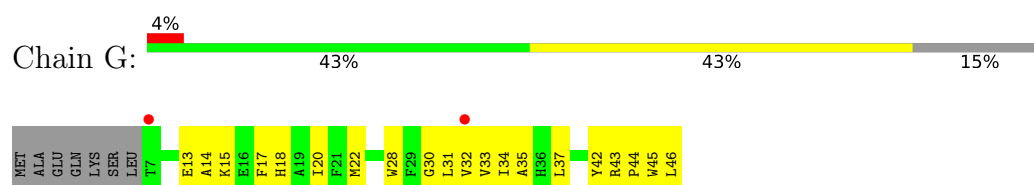
• Molecule 6: LH1 beta polypeptide



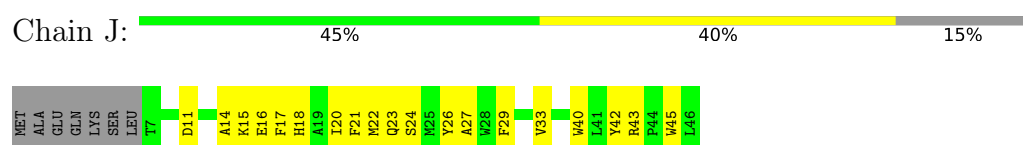
• Molecule 6: LH1 beta polypeptide



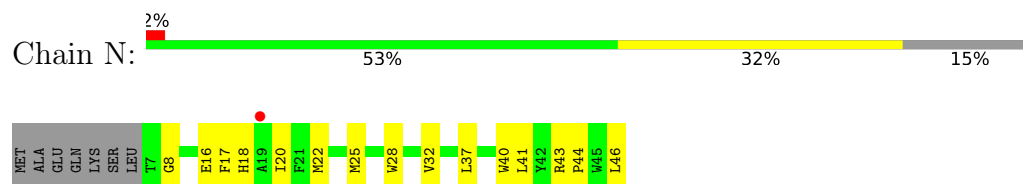
• Molecule 6: LH1 beta polypeptide



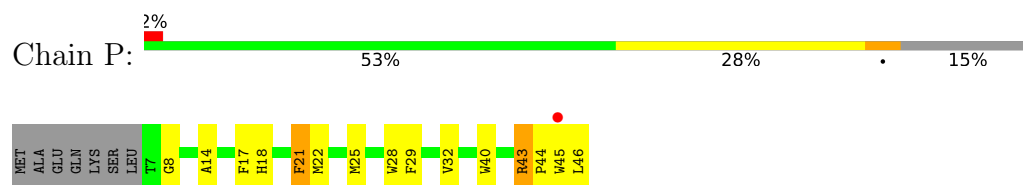
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



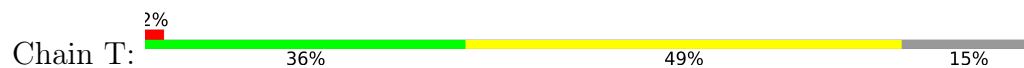
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



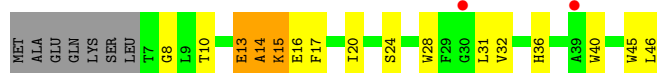
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

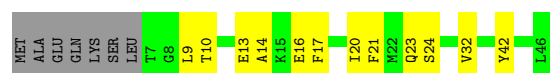


- Molecule 6: LH1 beta polypeptide



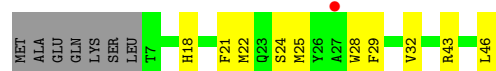
- Molecule 6: LH1 beta polypeptide

Chain 6: 



• Molecule 6: LH1 beta polypeptide

Chain 8: 



• Molecule 6: LH1 beta polypeptide

Chain 0: 



• Molecule 6: LH1 beta polypeptide

Chain n: 



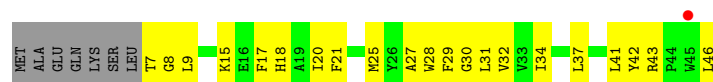
• Molecule 6: LH1 beta polypeptide

Chain q: 



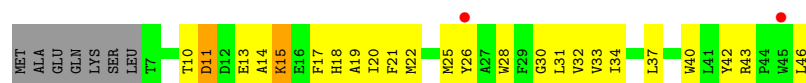
• Molecule 6: LH1 beta polypeptide

Chain s: 



• Molecule 6: LH1 beta polypeptide

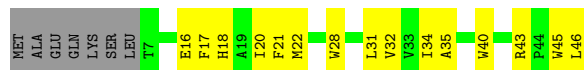
Chain v: 



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



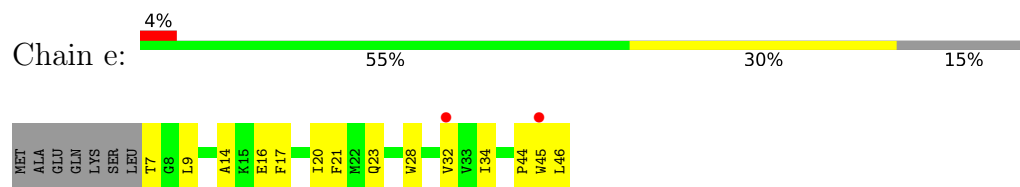
• Molecule 6: LH1 beta polypeptide



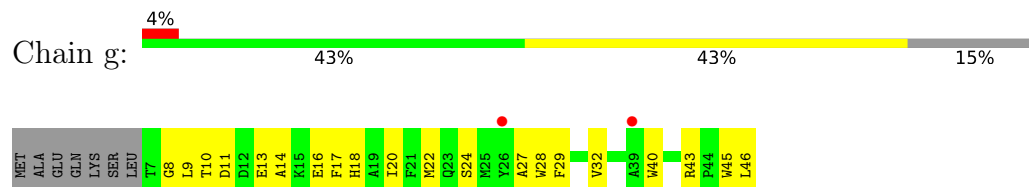
• Molecule 6: LH1 beta polypeptide



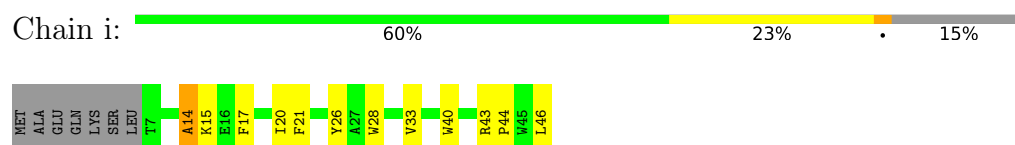
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



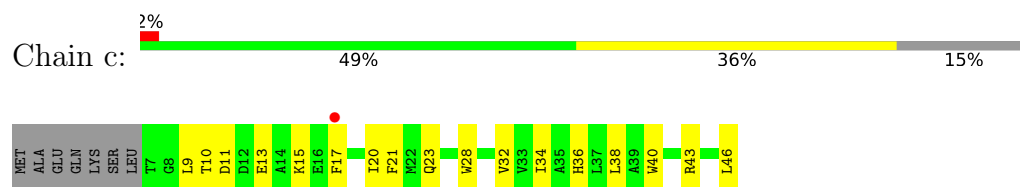
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.89Å 148.95Å 210.23Å 90.00° 108.18° 90.00°	Depositor
Resolution (Å)	48.18 – 3.30 48.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-3.30) 98.3 (48.18-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.271 , 0.309 0.272 , 0.310	Depositor DCC
R_{free} test set	7034 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	107.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 107.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.07	2/2528 (0.1%)	1.72	69/3451 (2.0%)
1	o	1.04	2/2528 (0.1%)	1.59	48/3451 (1.4%)
2	L	1.12	7/2318 (0.3%)	1.61	56/3167 (1.8%)
2	x	1.14	9/2318 (0.4%)	1.55	40/3167 (1.3%)
3	M	1.03	1/2646 (0.0%)	1.59	54/3621 (1.5%)
3	y	1.05	4/2646 (0.2%)	1.50	39/3621 (1.1%)
4	H	1.03	3/2037 (0.1%)	1.61	38/2776 (1.4%)
4	t	1.12	1/2037 (0.0%)	1.67	40/2776 (1.4%)
5	1	0.77	0/485	1.31	4/664 (0.6%)
5	3	0.71	0/485	1.20	2/664 (0.3%)
5	5	0.69	0/485	1.18	4/664 (0.6%)
5	7	0.63	0/485	1.10	3/664 (0.5%)
5	9	0.64	0/485	1.12	3/664 (0.5%)
5	A	0.66	0/485	1.17	3/664 (0.5%)
5	AA	0.60	0/485	1.17	4/664 (0.6%)
5	AC	0.60	0/485	1.02	0/664
5	AE	0.52	0/491	1.07	2/672 (0.3%)
5	AG	0.56	0/485	1.11	2/664 (0.3%)
5	AI	0.71	0/485	1.21	4/664 (0.6%)
5	AK	0.69	0/485	1.18	1/664 (0.2%)
5	D	0.61	0/485	1.19	4/664 (0.6%)
5	F	0.67	0/485	1.19	4/664 (0.6%)
5	I	0.70	0/485	1.21	6/664 (0.9%)
5	K	0.62	0/485	1.14	5/664 (0.8%)
5	O	0.64	0/485	1.25	3/664 (0.5%)
5	Q	0.65	0/485	1.23	6/664 (0.9%)
5	S	0.68	0/491	1.02	2/672 (0.3%)
5	U	0.77	0/485	1.26	4/664 (0.6%)
5	W	0.81	0/485	1.26	3/664 (0.5%)
5	Y	0.86	0/485	1.20	1/664 (0.2%)
5	d	0.63	0/485	1.15	3/664 (0.5%)
5	f	0.71	1/485 (0.2%)	1.19	7/664 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	h	0.71	0/485	1.04	2/664 (0.3%)
5	j	0.61	0/485	1.09	3/664 (0.5%)
5	l	0.64	0/485	1.09	2/664 (0.3%)
5	m	0.65	0/485	1.14	3/664 (0.5%)
5	p	0.66	0/485	1.15	2/664 (0.3%)
5	r	0.79	1/485 (0.2%)	1.11	1/664 (0.2%)
5	u	0.73	0/485	1.22	8/664 (1.2%)
5	w	0.59	0/485	1.09	2/664 (0.3%)
6	0	0.53	0/350	1.07	1/476 (0.2%)
6	2	0.68	0/350	1.17	5/476 (1.1%)
6	4	0.64	0/350	1.01	2/476 (0.4%)
6	6	0.53	0/350	0.89	0/476
6	8	0.54	0/350	0.98	0/476
6	AB	0.53	0/350	0.99	0/476
6	AD	0.47	0/350	0.90	0/476
6	AF	0.50	0/350	0.94	0/476
6	AH	0.56	0/350	1.05	2/476 (0.4%)
6	AJ	0.62	0/350	0.96	0/476
6	AL	0.58	0/350	0.95	0/476
6	B	0.54	0/350	1.01	1/476 (0.2%)
6	E	0.65	0/350	1.18	4/476 (0.8%)
6	G	0.55	0/350	1.00	1/476 (0.2%)
6	J	0.64	0/350	1.05	1/476 (0.2%)
6	N	0.57	0/350	1.08	0/476
6	P	0.57	0/350	1.11	2/476 (0.4%)
6	R	0.56	0/350	1.01	1/476 (0.2%)
6	T	0.55	0/350	1.07	1/476 (0.2%)
6	V	0.59	0/350	0.92	0/476
6	X	0.63	0/350	1.10	2/476 (0.4%)
6	Z	0.62	0/350	0.92	0/476
6	c	0.46	0/350	0.95	0/476
6	e	0.58	0/350	0.88	0/476
6	g	0.57	0/350	0.96	2/476 (0.4%)
6	i	0.58	0/350	0.97	2/476 (0.4%)
6	k	0.45	0/350	0.92	0/476
6	n	0.55	0/350	0.96	0/476
6	q	0.58	0/350	1.11	2/476 (0.4%)
6	s	0.63	0/350	1.07	1/476 (0.2%)
6	v	0.60	0/350	1.06	2/476 (0.4%)
6	z	0.51	0/350	1.07	0/476
All	All	0.85	31/45790 (0.1%)	1.33	519/62526 (0.8%)

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	3
2	x	0	1
3	M	0	2
3	y	0	3
4	t	0	1
5	1	0	2
6	AJ	0	2
6	X	0	1
All	All	0	15

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	241	LEU	CA-C	-7.31	1.43	1.52
2	x	126	VAL	CA-CB	-7.01	1.50	1.54
3	y	261	THR	CA-CB	-6.52	1.42	1.54
3	y	212	SER	CA-C	-6.47	1.43	1.52
2	L	265	THR	CA-CB	-6.47	1.44	1.54
3	M	314	VAL	CA-CB	-6.40	1.47	1.54
2	x	241	LEU	CA-C	-6.38	1.45	1.52
2	x	18	ILE	CA-CB	5.99	1.63	1.54
2	L	195	ALA	CA-CB	-5.88	1.44	1.53
2	x	241	LEU	C-O	-5.75	1.17	1.24
4	H	76	VAL	CA-CB	-5.74	1.46	1.54
2	L	237	ALA	C-O	-5.68	1.17	1.24
2	x	252	TRP	C-O	-5.62	1.16	1.24
2	L	246	ALA	CA-CB	-5.54	1.44	1.53
2	L	251	PHE	CA-C	-5.53	1.46	1.52
2	x	231	TYR	CA-C	-5.50	1.45	1.52
5	f	29	ILE	CA-CB	5.42	1.60	1.54
4	H	127	PHE	CA-C	-5.42	1.45	1.52
1	o	204	LEU	CA-C	5.42	1.60	1.52
3	y	232	ASP	CA-C	-5.42	1.45	1.52
2	x	111	LEU	CA-C	5.36	1.59	1.52
1	C	269	ALA	CA-CB	-5.35	1.44	1.53
4	H	251	THR	CA-CB	5.32	1.62	1.53
4	t	26	LEU	C-O	-5.32	1.18	1.24
3	y	43	ILE	CA-C	5.29	1.58	1.52
2	L	264	TRP	CA-CB	-5.28	1.43	1.53
1	o	284	ILE	CA-CB	-5.16	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	VAL	CA-C	5.15	1.57	1.52
5	r	47	LEU	CA-C	5.14	1.57	1.52
2	x	114	VAL	CA-CB	-5.03	1.48	1.54
2	x	191	THR	CA-C	5.01	1.59	1.52

All (519) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	195	LEU	CA-C-N	-12.82	105.65	120.13
1	o	195	LEU	C-N-CA	-12.82	105.65	120.13
2	x	228	ILE	N-CA-C	12.27	122.06	110.53
4	H	71	HIS	N-CA-C	12.10	127.75	111.30
4	H	258	LEU	N-CA-C	-10.96	102.12	114.62
5	p	9	TYR	N-CA-C	-10.77	94.97	110.59
1	C	195	LEU	CA-C-N	-10.65	108.10	120.13
1	C	195	LEU	C-N-CA	-10.65	108.10	120.13
5	O	16	ASP	CA-C-N	10.54	130.75	119.05
5	O	16	ASP	C-N-CA	10.54	130.75	119.05
1	C	112	VAL	N-CA-C	-10.47	97.19	107.76
1	C	222	ASN	CA-C-N	10.30	133.35	120.89
1	C	222	ASN	C-N-CA	10.30	133.35	120.89
3	y	40	LEU	N-CA-C	-10.25	100.11	111.28
3	M	33	ARG	CA-C-N	9.90	132.22	119.84
3	M	33	ARG	C-N-CA	9.90	132.22	119.84
3	M	21	VAL	N-CA-C	-9.88	99.83	109.02
1	C	102	SER	CA-C-N	9.81	129.59	119.19
1	C	102	SER	C-N-CA	9.81	129.59	119.19
1	C	29	GLY	N-CA-C	-9.80	98.65	112.37
4	t	74	GLY	N-CA-C	9.68	122.77	110.38
3	M	55	LEU	N-CA-C	-9.59	100.38	111.03
2	x	33	GLY	N-CA-C	-9.59	100.59	112.68
1	o	332	LYS	N-CA-C	9.48	123.04	110.53
3	y	15	ALA	N-CA-C	-9.44	97.30	108.25
1	C	305	VAL	N-CA-C	9.30	123.39	108.97
2	L	17	LEU	N-CA-C	-9.27	101.75	113.43
1	o	118	SER	N-CA-C	9.27	123.57	110.50
3	M	154	ILE	N-CA-C	-9.26	101.53	110.42
3	M	150	PHE	N-CA-C	-9.26	101.17	111.07
2	L	128	PHE	N-CA-C	-9.21	101.19	111.14
5	W	4	MET	N-CA-C	-9.17	102.22	113.41
6	4	15	LYS	N-CA-C	-9.17	100.67	112.23
3	M	146	LEU	N-CA-C	-9.13	100.89	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	16	ASP	CA-C-N	9.14	129.19	119.05
5	U	16	ASP	C-N-CA	9.14	129.19	119.05
3	M	40	LEU	N-CA-C	-9.12	101.34	111.28
1	C	101	VAL	CA-C-N	-9.10	113.91	122.37
1	C	101	VAL	C-N-CA	-9.10	113.91	122.37
6	X	15	LYS	N-CA-C	-8.99	100.90	112.23
4	t	176	GLU	CA-C-N	8.95	131.03	119.84
4	t	176	GLU	C-N-CA	8.95	131.03	119.84
5	Q	7	ASN	N-CA-C	-8.80	100.50	112.03
4	t	29	TYR	CA-CB-CG	8.77	129.69	113.90
3	y	183	LEU	N-CA-C	-8.73	100.95	111.69
2	L	228	ILE	N-CA-C	8.68	118.69	110.53
5	AG	58	LEU	N-CA-C	-8.61	104.81	114.62
3	M	107	PRO	N-CA-C	8.51	121.08	110.70
4	t	37	GLU	N-CA-C	-8.29	98.01	108.45
1	C	300	GLY	N-CA-C	-8.25	103.94	115.32
1	o	112	VAL	N-CA-C	-8.23	99.45	107.76
5	Q	51	ILE	N-CA-C	8.22	116.85	107.89
1	o	247	CYS	CA-CB-SG	-8.19	95.56	114.40
5	AA	16	ASP	CA-C-N	8.19	128.14	119.05
5	AA	16	ASP	C-N-CA	8.19	128.14	119.05
3	y	146	LEU	N-CA-C	-8.18	101.95	111.03
3	M	264	SER	N-CA-C	8.13	121.06	111.71
1	C	100	TRP	CA-C-N	-8.07	114.83	122.66
1	C	100	TRP	C-N-CA	-8.07	114.83	122.66
2	x	159	ILE	N-CA-C	8.04	118.80	110.36
5	d	49	ASP	N-CA-C	-8.02	103.70	113.97
5	AI	49	ASP	N-CA-C	-7.97	103.77	113.97
4	H	200	SER	N-CA-C	7.92	121.83	109.07
6	AH	15	LYS	N-CA-C	-7.92	101.95	111.69
3	y	33	ARG	CA-C-N	7.92	129.74	119.84
3	y	33	ARG	C-N-CA	7.92	129.74	119.84
4	H	224	THR	N-CA-C	7.90	122.39	110.14
6	q	15	LYS	N-CA-C	-7.87	102.01	111.69
1	C	297	GLY	CA-C-N	7.85	129.65	119.84
1	C	297	GLY	C-N-CA	7.85	129.65	119.84
2	L	228	ILE	CB-CA-C	-7.84	101.75	112.02
4	t	116	SER	CA-C-N	-7.83	110.05	119.84
4	t	116	SER	C-N-CA	-7.83	110.05	119.84
3	y	85	GLN	N-CA-C	-7.81	102.77	111.28
1	o	174	TYR	CA-C-N	-7.81	110.08	119.84
1	o	174	TYR	C-N-CA	-7.81	110.08	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	CYS	N-CA-C	7.80	120.24	108.46
1	o	181	THR	N-CA-C	7.77	121.86	112.38
1	C	64	ALA	CA-C-N	-7.70	111.76	122.93
1	C	64	ALA	C-N-CA	-7.70	111.76	122.93
1	o	252	ASN	N-CA-C	-7.70	91.62	107.70
1	o	199	PRO	N-CA-C	-7.68	105.78	114.92
1	o	327	TYR	CA-C-N	7.67	127.31	119.56
1	o	327	TYR	C-N-CA	7.67	127.31	119.56
4	H	185	GLU	N-CA-C	-7.67	96.79	108.67
3	M	128	LEU	N-CA-C	-7.66	102.87	112.90
5	7	9	TYR	N-CA-C	-7.65	101.82	112.45
4	t	159	LEU	CA-C-N	-7.63	110.44	122.65
4	t	159	LEU	C-N-CA	-7.63	110.44	122.65
6	P	43	ARG	CA-C-N	7.62	127.61	119.76
6	P	43	ARG	C-N-CA	7.62	127.61	119.76
5	m	3	THR	N-CA-C	-7.55	101.98	112.25
2	x	192	ASN	N-CA-C	-7.50	103.04	111.07
1	o	65	ALA	N-CA-C	-7.48	97.54	109.59
2	L	280	LEU	N-CA-C	-7.45	104.69	114.31
5	K	9	TYR	N-CA-C	-7.42	102.14	112.45
3	y	55	LEU	N-CA-C	-7.41	102.81	111.03
4	t	41	LEU	N-CA-C	7.39	119.50	110.41
1	o	136	ALA	N-CA-C	-7.37	103.19	111.07
3	M	25	LYS	N-CA-C	-7.35	100.14	110.50
3	M	290	VAL	N-CA-C	7.34	118.29	112.12
2	L	171	TYR	N-CA-C	7.34	121.81	113.01
2	L	126	VAL	CA-C-N	-7.33	112.15	119.56
2	L	126	VAL	C-N-CA	-7.33	112.15	119.56
4	t	112	GLY	CA-C-N	-7.32	112.65	119.82
4	t	112	GLY	C-N-CA	-7.32	112.65	119.82
3	M	226	VAL	N-CA-C	-7.31	104.13	111.88
4	H	61	LEU	CA-C-N	7.30	127.88	119.99
4	H	61	LEU	C-N-CA	7.30	127.88	119.99
2	L	202	LEU	N-CA-C	7.24	118.82	111.07
1	C	247	CYS	CA-CB-SG	-7.19	97.86	114.40
4	H	15	THR	N-CA-C	-7.18	103.49	112.90
3	y	212	SER	N-CA-C	-7.18	103.18	112.23
1	C	324	ALA	N-CA-C	7.18	120.02	111.33
3	M	7	ILE	N-CA-C	-7.16	104.87	111.67
5	W	58	LEU	N-CA-C	-7.16	104.81	113.97
2	L	159	ILE	N-CA-C	7.14	117.86	110.36
1	C	131	PHE	N-CA-C	-7.11	103.27	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	126	ILE	N-CA-C	-7.11	103.74	110.42
5	F	16	ASP	CA-C-N	7.11	126.94	119.05
5	F	16	ASP	C-N-CA	7.11	126.94	119.05
4	H	237	ASP	N-CA-C	-7.09	103.48	111.07
3	y	10	ALA	N-CA-C	7.05	121.63	112.89
4	t	26	LEU	N-CA-C	-7.04	103.21	111.03
4	H	176	GLU	CA-C-N	7.03	128.63	119.84
4	H	176	GLU	C-N-CA	7.03	128.63	119.84
1	o	101	VAL	CA-C-N	-7.03	115.83	122.37
1	o	101	VAL	C-N-CA	-7.03	115.83	122.37
1	o	305	VAL	N-CA-C	7.03	119.86	108.97
6	2	15	LYS	N-CA-C	-7.02	103.05	111.69
1	C	136	ALA	N-CA-C	-6.99	103.59	111.07
1	C	62	LEU	N-CA-C	-6.98	100.66	110.29
4	t	200	SER	N-CA-C	6.96	120.59	109.24
6	G	15	LYS	N-CA-C	-6.96	103.14	111.69
5	F	56	GLN	N-CA-C	-6.94	104.78	113.18
5	Q	13	LEU	N-CA-C	-6.94	104.82	113.28
5	3	9	TYR	N-CA-C	-6.94	103.16	111.69
5	f	58	LEU	N-CA-C	6.93	121.74	111.96
2	L	33	GLY	N-CA-C	-6.92	103.96	112.68
5	Y	50	ASN	N-CA-C	-6.92	102.65	111.92
1	C	65	ALA	N-CA-C	-6.92	98.46	109.59
1	o	245	VAL	CA-C-N	-6.91	116.32	122.47
1	o	245	VAL	C-N-CA	-6.91	116.32	122.47
2	L	226	ARG	N-CA-C	-6.90	103.53	112.23
6	2	43	ARG	CA-C-N	6.90	126.86	119.76
6	2	43	ARG	C-N-CA	6.90	126.86	119.76
3	y	235	ILE	CB-CA-C	-6.89	103.00	112.02
3	M	21	VAL	CA-C-N	6.88	127.91	120.13
3	M	21	VAL	C-N-CA	6.88	127.91	120.13
6	0	8	GLY	N-CA-C	6.85	129.41	113.18
1	C	301	ASP	CA-C-N	6.84	128.11	120.66
1	C	301	ASP	C-N-CA	6.84	128.11	120.66
4	t	184	VAL	N-CA-C	6.83	117.89	107.77
2	L	261	GLY	CA-C-N	6.82	128.36	119.84
2	L	261	GLY	C-N-CA	6.82	128.36	119.84
1	C	180	PRO	N-CA-C	6.80	121.90	111.15
1	o	25	GLY	CA-C-N	6.77	127.36	120.38
1	o	25	GLY	C-N-CA	6.77	127.36	120.38
2	L	77	PRO	CA-C-N	-6.76	113.83	120.52
2	L	77	PRO	C-N-CA	-6.76	113.83	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	t	224	THR	N-CA-C	6.75	120.61	110.14
3	M	15	ALA	N-CA-C	-6.74	100.44	108.25
5	S	9	TYR	N-CA-C	-6.73	103.09	112.45
5	AI	16	ASP	CA-C-N	6.73	126.52	119.05
5	AI	16	ASP	C-N-CA	6.73	126.52	119.05
6	2	14	ALA	N-CA-C	-6.72	105.12	113.38
2	L	165	TRP	N-CA-C	-6.71	103.90	111.14
2	x	126	VAL	CA-C-N	-6.68	112.81	119.56
2	x	126	VAL	C-N-CA	-6.68	112.81	119.56
1	o	24	GLU	N-CA-C	-6.68	100.33	110.14
5	D	9	TYR	N-CA-C	-6.63	100.98	110.59
5	AK	49	ASP	N-CA-C	-6.62	105.49	113.97
5	u	47	LEU	N-CA-C	-6.61	104.13	112.93
2	L	72	ARG	N-CA-C	6.61	121.34	113.28
1	o	168	THR	N-CA-C	-6.61	100.05	109.96
5	K	16	ASP	CA-C-N	6.61	126.38	119.05
5	K	16	ASP	C-N-CA	6.61	126.38	119.05
1	C	288	ASN	N-CA-C	6.59	119.29	111.71
2	x	70	LEU	N-CA-C	6.59	118.46	111.28
4	H	130	LEU	N-CA-C	-6.58	101.83	110.39
3	y	237	GLN	N-CA-C	-6.58	104.73	112.89
5	AI	51	ILE	N-CA-C	6.58	115.81	108.05
4	H	105	ASP	CA-C-N	6.57	128.05	119.84
4	H	105	ASP	C-N-CA	6.57	128.05	119.84
3	y	216	PHE	N-CA-C	-6.56	104.13	111.28
2	x	261	GLY	N-CA-C	-6.56	98.96	112.34
4	H	41	LEU	N-CA-C	6.55	118.78	110.33
6	J	15	LYS	N-CA-C	-6.54	103.65	111.69
2	L	203	ILE	N-CA-C	-6.53	104.15	110.42
3	M	237	GLN	N-CA-C	-6.52	104.81	112.89
4	H	256	GLY	N-CA-C	-6.52	99.05	112.34
5	I	9	TYR	N-CA-C	-6.51	103.40	112.45
5	K	5	ASN	N-CA-C	6.51	119.64	111.24
4	H	33	GLU	N-CA-C	-6.51	104.27	111.82
1	o	131	PHE	N-CA-C	-6.50	104.04	112.23
2	L	253	SER	N-CA-C	-6.49	104.28	111.36
4	t	82	GLU	N-CA-C	6.49	120.03	109.59
3	y	110	SER	N-CA-C	6.48	120.79	113.01
2	x	182	HIS	N-CA-C	-6.48	104.21	111.28
3	M	88	LYS	N-CA-C	6.45	118.31	111.28
1	C	67	SER	CA-C-N	6.44	133.28	121.70
1	C	67	SER	C-N-CA	6.44	133.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	y	264	SER	N-CA-C	6.43	119.10	111.71
5	D	16	ASP	CA-C-N	6.41	126.17	119.05
5	D	16	ASP	C-N-CA	6.41	126.17	119.05
5	A	3	THR	N-CA-C	-6.41	104.00	112.72
1	o	331	TYR	N-CA-C	-6.40	99.38	109.50
3	M	98	PRO	CA-C-N	-6.40	113.79	120.38
3	M	98	PRO	C-N-CA	-6.40	113.79	120.38
1	o	233	PHE	N-CA-C	-6.38	104.40	111.36
4	H	44	ASP	N-CA-C	-6.38	105.07	112.92
1	C	86	SER	N-CA-C	-6.38	101.94	110.55
5	F	58	LEU	N-CA-C	-6.37	105.38	112.57
3	y	150	PHE	N-CA-C	-6.37	103.47	111.11
5	AA	50	ASN	N-CA-C	-6.36	103.40	111.92
5	I	51	ILE	N-CA-C	6.36	114.98	107.73
4	t	229	ASP	N-CA-C	6.35	121.07	112.88
6	i	15	LYS	N-CA-C	-6.34	103.89	111.69
1	o	62	LEU	N-CA-C	-6.33	101.56	110.29
3	M	148	TRP	N-CA-C	-6.32	105.06	112.89
1	o	125	VAL	N-CA-C	-6.31	103.20	111.09
1	o	242	SER	N-CA-C	6.31	118.23	111.36
5	j	16	ASP	CA-C-N	6.30	126.05	119.05
5	j	16	ASP	C-N-CA	6.30	126.05	119.05
5	7	16	ASP	CA-C-N	6.29	125.52	118.97
5	7	16	ASP	C-N-CA	6.29	125.52	118.97
5	O	9	TYR	N-CA-C	-6.29	104.66	112.90
2	L	217	THR	N-CA-C	6.28	119.42	109.81
2	L	7	GLU	N-CA-C	6.28	121.12	112.90
2	L	76	ALA	CA-C-N	6.28	126.84	120.38
2	L	76	ALA	C-N-CA	6.28	126.84	120.38
4	t	134	VAL	CA-C-N	-6.28	113.49	120.14
4	t	134	VAL	C-N-CA	-6.28	113.49	120.14
3	M	257	GLY	N-CA-C	6.26	123.69	115.36
2	x	165	TRP	N-CA-C	-6.26	104.38	111.14
3	M	49	GLY	C-N-CD	-6.24	106.86	120.60
4	H	71	HIS	CB-CA-C	-6.24	102.59	111.95
3	M	279	THR	N-CA-C	-6.24	104.56	111.36
1	C	122	TYR	N-CA-C	6.22	119.72	111.75
4	H	68	VAL	N-CA-CB	-6.21	105.43	111.89
5	j	58	LEU	N-CA-C	-6.21	105.74	113.38
6	AH	40	TRP	N-CA-C	6.18	118.10	111.36
3	M	119	GLY	N-CA-C	-6.18	105.01	112.49
2	L	181	ALA	N-CA-C	-6.18	104.63	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	PRO	CB-CA-C	-6.17	101.38	111.56
2	x	28	GLY	N-CA-C	-6.17	99.75	112.34
1	o	78	ASN	N-CA-C	6.16	117.98	109.54
3	M	234	GLU	N-CA-C	6.16	119.64	111.75
5	h	5	ASN	N-CA-C	6.14	118.65	109.25
6	q	8	GLY	N-CA-C	-6.14	98.62	113.18
1	o	288	ASN	N-CA-C	6.13	118.76	111.71
2	L	251	PHE	CB-CA-C	-6.13	101.53	110.96
4	H	240	CYS	N-CA-C	6.11	118.44	111.11
5	1	57	ALA	CA-C-N	6.11	132.69	121.70
5	1	57	ALA	C-N-CA	6.11	132.69	121.70
1	C	252	ASN	N-CA-C	-6.10	94.94	107.70
1	C	159	ASN	CA-C-N	6.10	125.99	119.28
1	C	159	ASN	C-N-CA	6.10	125.99	119.28
2	x	169	VAL	N-CA-C	-6.10	104.36	111.00
1	C	112	VAL	CA-C-N	6.08	126.10	119.90
1	C	112	VAL	C-N-CA	6.08	126.10	119.90
2	L	93	GLY	N-CA-C	-6.05	105.16	112.49
3	y	284	ILE	N-CA-C	-6.05	103.33	111.44
5	f	13	LEU	N-CA-C	-6.05	105.90	113.28
2	L	56	ILE	N-CA-C	6.05	119.54	111.44
5	AE	16	ASP	CA-C-N	6.04	126.20	119.32
5	AE	16	ASP	C-N-CA	6.04	126.20	119.32
5	D	18	ARG	N-CA-C	-6.03	103.87	111.11
3	y	43	ILE	N-CA-C	6.01	119.54	113.47
5	u	55	TYR	N-CA-C	-6.01	106.07	113.41
1	C	245	VAL	N-CA-C	6.01	115.86	108.53
1	o	26	PRO	N-CA-C	-6.01	103.37	110.70
2	x	253	SER	N-CA-C	-6.01	104.81	111.36
3	y	197	TYR	N-CA-C	-6.00	104.81	111.71
1	o	164	TYR	N-CA-C	5.99	120.40	112.25
6	s	15	LYS	N-CA-C	-5.99	104.32	111.69
5	A	6	ALA	N-CA-C	5.98	116.49	108.23
3	M	43	ILE	N-CA-C	5.97	119.50	113.47
4	H	125	LEU	N-CA-C	5.97	119.27	109.72
3	y	49	GLY	C-N-CD	-5.96	107.48	120.60
3	M	304	ALA	CA-C-N	5.96	125.92	119.78
3	M	304	ALA	C-N-CA	5.96	125.92	119.78
6	v	11	ASP	N-CA-C	-5.94	105.30	112.54
5	I	8	LEU	N-CA-C	-5.93	106.29	112.93
4	H	124	ASP	N-CA-C	-5.92	102.15	110.50
3	M	134	TYR	N-CA-C	-5.92	104.22	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	248	THR	N-CA-C	-5.92	106.04	113.20
1	o	122	TYR	N-CA-C	5.91	119.31	111.75
3	M	183	LEU	N-CA-C	-5.89	104.45	111.69
2	L	267	GLY	N-CA-C	-5.88	105.01	112.54
5	r	51	ILE	N-CA-C	5.88	114.30	107.89
2	x	280	LEU	N-CA-C	-5.88	107.09	114.56
2	L	123	GLY	CA-C-N	-5.88	113.78	122.83
2	L	123	GLY	C-N-CA	-5.88	113.78	122.83
2	x	236	LEU	CA-C-N	5.88	128.43	120.38
2	x	236	LEU	C-N-CA	5.88	128.43	120.38
4	t	137	ARG	N-CA-C	-5.88	105.94	113.23
5	f	8	LEU	N-CA-C	-5.87	105.97	113.02
4	H	73	GLY	N-CA-C	5.87	122.66	113.86
1	C	174	TYR	CA-C-N	-5.86	112.52	119.84
1	C	174	TYR	C-N-CA	-5.86	112.52	119.84
3	y	240	HIS	N-CA-C	5.86	118.84	107.71
2	L	106	PHE	N-CA-C	-5.83	105.00	111.36
6	4	8	GLY	N-CA-C	5.83	122.00	113.48
1	C	25	GLY	CA-C-N	-5.81	114.39	120.38
1	C	25	GLY	C-N-CA	-5.81	114.39	120.38
5	d	51	ILE	N-CA-C	5.81	114.23	107.89
4	t	8	TYR	CA-C-N	-5.81	115.11	122.37
4	t	8	TYR	C-N-CA	-5.81	115.11	122.37
3	y	88	LYS	N-CA-C	5.79	117.59	111.28
4	t	125	LEU	N-CA-C	5.78	118.96	109.72
5	u	9	TYR	N-CA-C	-5.77	104.43	112.45
1	C	166	TRP	N-CA-C	5.76	117.36	109.18
5	5	16	ASP	CA-C-N	5.76	125.45	119.05
5	5	16	ASP	C-N-CA	5.76	125.45	119.05
5	d	59	GLY	N-CA-C	-5.76	99.53	113.18
3	M	175	VAL	CA-C-N	5.75	126.24	120.14
3	M	175	VAL	C-N-CA	5.75	126.24	120.14
2	L	28	GLY	N-CA-C	-5.75	100.61	112.34
5	p	14	ILE	N-CA-C	-5.75	107.24	111.90
4	t	33	GLU	CA-CB-CG	-5.75	102.61	114.10
5	f	7	ASN	N-CA-C	-5.75	104.50	112.03
2	L	126	VAL	N-CA-C	5.73	119.23	112.35
2	x	230	GLY	N-CA-C	5.73	122.75	114.10
3	M	269	ALA	N-CA-C	-5.72	104.96	111.14
5	W	13	LEU	N-CA-C	-5.72	106.30	113.28
3	y	51	ILE	N-CA-C	5.71	117.64	108.85
1	C	251	HIS	N-CA-C	5.71	118.17	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	90	PHE	N-CA-C	-5.71	104.96	111.07
4	H	157	VAL	N-CA-C	5.71	116.22	107.77
2	x	129	ALA	N-CA-C	-5.70	105.06	111.28
2	x	66	GLN	N-CA-C	-5.70	102.46	110.50
3	y	135	LYS	N-CA-C	-5.70	104.76	110.97
2	L	66	GLN	N-CA-C	-5.70	102.47	110.50
6	g	11	ASP	N-CA-C	-5.70	105.59	112.54
6	E	27	ALA	N-CA-C	-5.69	104.98	111.07
5	U	42	THR	N-CA-C	5.69	118.53	109.65
2	x	228	ILE	CB-CA-C	-5.69	104.57	112.02
3	M	170	SER	N-CA-C	5.68	116.86	107.20
2	x	72	ARG	N-CA-C	5.67	120.20	113.28
2	x	86	MET	N-CA-C	-5.66	100.76	109.76
5	3	7	ASN	N-CA-C	-5.65	104.62	112.03
1	o	198	ASP	CA-C-N	5.65	127.55	121.00
1	o	198	ASP	C-N-CA	5.65	127.55	121.00
1	C	199	PRO	N-CA-C	-5.64	108.21	114.92
2	x	261	GLY	CA-C-N	5.64	126.89	119.84
2	x	261	GLY	C-N-CA	5.64	126.89	119.84
4	H	155	THR	CA-C-N	-5.63	115.10	122.37
4	H	155	THR	C-N-CA	-5.63	115.10	122.37
5	9	13	LEU	N-CA-C	-5.63	106.41	113.28
6	R	14	ALA	N-CA-C	-5.63	106.46	113.38
3	M	177	PHE	N-CA-C	5.62	117.90	108.23
5	u	3	THR	N-CA-C	5.62	120.16	112.68
3	M	20	GLY	N-CA-C	5.62	121.13	112.81
2	x	234	GLY	CA-C-N	5.61	130.10	121.19
2	x	234	GLY	C-N-CA	5.61	130.10	121.19
3	M	106	ILE	N-CA-C	-5.60	102.46	107.56
3	y	214	LEU	N-CA-C	5.60	117.07	110.97
5	I	16	ASP	CA-C-N	5.59	125.70	119.32
5	I	16	ASP	C-N-CA	5.59	125.70	119.32
5	AA	9	TYR	N-CA-C	-5.59	104.68	112.45
6	g	8	GLY	N-CA-C	5.58	126.42	113.18
2	L	234	GLY	CA-C-N	5.57	130.04	121.19
2	L	234	GLY	C-N-CA	5.57	130.04	121.19
3	M	30	ARG	N-CA-C	-5.56	101.06	109.85
5	I	30	VAL	N-CA-C	5.56	115.65	110.42
6	E	15	LYS	N-CA-C	-5.56	104.62	111.40
1	C	115	ASN	N-CA-C	5.55	117.65	108.49
1	C	209	GLU	N-CA-C	5.54	117.74	109.59
2	L	170	GLY	N-CA-C	-5.54	105.78	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	w	40	LEU	N-CA-C	5.54	119.14	112.38
2	x	127	PRO	CA-C-N	5.54	127.97	120.44
2	x	127	PRO	C-N-CA	5.54	127.97	120.44
2	L	51	VAL	N-CA-C	-5.53	105.33	110.53
4	t	38	GLY	N-CA-C	5.53	126.28	113.18
3	y	188	ALA	N-CA-C	-5.53	105.25	111.28
4	H	174	ARG	N-CA-C	-5.53	106.54	113.28
2	x	188	PHE	N-CA-C	-5.52	105.17	111.14
6	X	16	GLU	N-CA-C	5.52	116.97	111.07
6	i	14	ALA	N-CA-C	-5.52	106.22	113.17
1	C	173	LYS	N-CA-C	5.51	117.85	110.35
5	f	57	ALA	N-CA-C	5.50	118.58	109.94
1	C	245	VAL	CA-C-N	-5.50	117.58	122.47
1	C	245	VAL	C-N-CA	-5.50	117.58	122.47
4	H	128	GLU	CA-CB-CG	-5.49	103.11	114.10
6	T	14	ALA	N-CA-C	-5.49	106.58	113.72
3	M	205	SER	N-CA-C	-5.49	105.30	111.28
5	Q	9	TYR	N-CA-C	-5.49	104.82	112.45
5	S	13	LEU	N-CA-C	-5.48	106.59	113.28
3	M	210	TYR	N-CA-C	-5.48	105.39	111.36
2	x	146	LEU	N-CA-C	-5.47	104.19	111.24
3	y	306	ALA	N-CA-C	-5.46	100.51	109.40
5	w	13	LEU	N-CA-C	-5.46	106.62	113.28
4	t	64	PRO	N-CA-C	5.45	119.78	111.11
5	u	3	THR	CA-C-N	5.44	131.50	121.70
5	u	3	THR	C-N-CA	5.44	131.50	121.70
5	l	53	VAL	N-CA-C	5.44	116.50	108.45
1	o	307	CYS	CA-CB-SG	-5.44	101.90	114.40
5	K	13	LEU	N-CA-C	-5.43	106.65	113.28
5	9	51	ILE	N-CA-C	5.43	113.81	107.89
5	Q	16	ASP	CA-C-N	5.43	125.08	119.05
5	Q	16	ASP	C-N-CA	5.43	125.08	119.05
5	l	53	VAL	N-CA-C	-5.42	100.79	108.65
5	u	16	ASP	CA-C-N	5.41	125.06	119.05
5	u	16	ASP	C-N-CA	5.41	125.06	119.05
4	H	128	GLU	CB-CA-C	5.41	120.05	110.85
2	x	256	CYS	N-CA-C	-5.41	105.38	111.28
4	t	61	LEU	CA-C-N	-5.41	114.15	119.99
4	t	61	LEU	C-N-CA	-5.41	114.15	119.99
1	o	20	LEU	CA-C-N	5.41	131.43	121.70
1	o	20	LEU	C-N-CA	5.41	131.43	121.70
1	o	217	ALA	N-CA-C	5.40	116.97	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	t	60	ASP	N-CA-C	-5.39	101.44	109.96
4	H	133	ILE	N-CA-C	5.39	115.34	108.12
2	L	182	HIS	N-CA-C	-5.39	105.41	111.28
1	C	248	THR	N-CA-C	-5.38	106.69	113.20
4	H	93	SER	CA-C-N	-5.37	114.24	120.04
4	H	93	SER	C-N-CA	-5.37	114.24	120.04
2	x	246	ALA	CA-C-N	-5.37	112.66	120.29
2	x	246	ALA	C-N-CA	-5.37	112.66	120.29
6	E	16	GLU	N-CA-C	-5.36	105.35	111.14
2	x	126	VAL	N-CA-C	5.36	118.78	112.35
3	M	155	PHE	N-CA-C	5.35	117.81	111.33
3	y	30	ARG	N-CA-C	-5.35	101.16	109.72
2	L	86	MET	N-CA-C	-5.35	101.26	109.76
1	C	169	ASP	CA-C-N	5.34	127.36	120.89
1	C	169	ASP	C-N-CA	5.34	127.36	120.89
2	L	38	VAL	N-CA-C	-5.34	105.51	110.53
4	H	150	ASP	N-CA-C	-5.34	101.52	109.42
5	f	16	ASP	CA-C-N	5.33	124.51	118.97
5	f	16	ASP	C-N-CA	5.33	124.51	118.97
5	m	13	LEU	N-CA-C	-5.32	106.78	113.28
5	m	58	LEU	N-CA-C	-5.32	105.60	112.68
3	M	61	ILE	N-CA-C	-5.31	105.35	110.72
2	x	172	GLN	N-CA-C	-5.31	106.06	112.54
4	t	195	LEU	CA-C-N	5.31	125.07	119.76
4	t	195	LEU	C-N-CA	5.31	125.07	119.76
4	t	238	LYS	N-CA-C	5.31	117.75	111.33
3	y	269	ALA	N-CA-C	-5.30	105.41	111.14
1	C	197	PHE	N-CA-C	5.30	122.09	110.80
1	C	281	GLN	N-CA-C	5.30	118.21	111.69
5	l	13	LEU	N-CA-C	-5.30	106.81	113.28
1	C	118	SER	N-CA-C	5.29	117.97	110.50
1	C	184	ASN	N-CA-C	5.29	122.07	110.80
2	L	36	GLY	N-CA-C	-5.29	105.92	113.86
3	M	106	ILE	CB-CA-C	-5.29	104.81	110.95
1	C	132	GLU	N-CA-C	-5.29	106.33	112.89
3	y	213	ALA	N-CA-C	-5.29	105.59	111.36
2	L	75	ILE	CG1-CB-CG2	-5.29	94.84	110.70
5	1	25	VAL	N-CA-C	5.28	115.48	110.42
4	t	251	THR	N-CA-CB	5.26	119.72	111.56
5	9	51	ILE	CB-CA-C	-5.26	104.74	110.37
5	h	39	VAL	N-CA-C	5.26	115.47	110.53
2	L	167	SER	N-CA-C	5.25	116.69	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	268	TRP	CA-C-N	-5.25	113.51	119.28
2	L	268	TRP	C-N-CA	-5.25	113.51	119.28
3	M	244	ALA	N-CA-C	-5.25	105.00	111.40
6	2	20	ILE	N-CA-C	5.23	116.00	110.72
2	x	17	LEU	N-CA-C	-5.23	106.84	113.43
5	A	60	LYS	N-CA-C	5.22	121.92	110.80
3	y	299	VAL	N-CA-C	-5.22	105.45	110.72
4	t	203	ASP	N-CA-C	-5.21	97.74	108.53
3	y	265	ILE	CB-CA-C	-5.21	104.08	112.16
4	H	227	ASN	CA-C-N	-5.20	114.34	120.12
4	H	227	ASN	C-N-CA	-5.20	114.34	120.12
3	y	224	LEU	N-CA-C	-5.20	106.77	113.01
3	y	148	TRP	CA-CB-CG	5.20	123.48	113.60
1	C	156	HIS	N-CA-C	5.18	118.07	111.69
1	C	327	TYR	CA-C-N	5.18	124.79	119.56
1	C	327	TYR	C-N-CA	5.18	124.79	119.56
5	5	54	SER	N-CA-C	-5.17	102.73	110.23
6	E	32	VAL	N-CA-C	5.17	115.39	110.53
4	H	121	LYS	N-CA-C	-5.17	104.47	111.55
1	C	301	ASP	N-CA-C	-5.17	102.70	110.24
1	o	330	LEU	N-CA-C	5.16	118.60	112.72
4	t	92	PHE	N-CA-C	-5.14	106.10	112.38
3	y	129	TRP	N-CA-C	-5.14	105.85	111.82
2	L	70	LEU	CA-C-N	-5.13	113.00	120.29
2	L	70	LEU	C-N-CA	-5.13	113.00	120.29
6	B	15	LYS	N-CA-C	-5.13	105.14	111.40
4	t	164	ALA	N-CA-C	-5.13	106.15	112.72
6	v	15	LYS	N-CA-C	-5.13	105.38	111.69
4	t	107	MET	CB-CG-SD	-5.12	97.33	112.70
1	C	254	ARG	N-CA-C	-5.12	106.54	112.89
2	L	159	ILE	CA-C-N	-5.12	113.56	122.36
2	L	159	ILE	C-N-CA	-5.12	113.56	122.36
1	o	197	PHE	N-CA-C	5.12	121.70	110.80
2	L	249	ALA	N-CA-C	-5.12	105.70	111.28
3	M	47	GLN	CA-C-N	-5.12	116.15	123.11
3	M	47	GLN	C-N-CA	-5.12	116.15	123.11
1	C	66	ASP	N-CA-C	5.11	116.54	110.97
1	C	125	VAL	N-CA-C	-5.10	104.71	111.09
2	x	200	GLY	N-CA-C	-5.09	101.12	113.18
2	L	174	LEU	N-CA-C	5.09	121.64	110.80
1	o	283	TYR	CA-C-N	-5.09	116.58	122.63
1	o	283	TYR	C-N-CA	-5.09	116.58	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	y	227	SER	N-CA-C	-5.08	106.59	112.89
3	M	18	TYR	CA-C-N	5.08	125.15	119.87
3	M	18	TYR	C-N-CA	5.08	125.15	119.87
3	M	97	PRO	N-CA-C	5.08	116.90	110.70
3	y	60	SER	N-CA-C	-5.08	105.39	112.45
4	t	17	TRP	CA-CB-CG	5.07	123.23	113.60
5	5	43	ASP	N-CA-C	5.07	117.54	111.71
5	AG	4	MET	N-CA-C	5.07	116.99	109.69
4	H	45	ARG	N-CA-C	-5.06	105.67	111.14
2	L	126	VAL	CB-CA-C	-5.06	107.37	114.00
2	x	226	ARG	N-CA-C	-5.06	106.28	112.90
4	t	67	PHE	N-CA-C	-5.06	101.00	109.24
2	L	115	GLU	N-CA-C	-5.05	105.77	111.28
3	M	209	LEU	N-CA-C	-5.05	105.47	111.69
1	C	296	LYS	N-CA-C	5.05	117.67	109.24
3	y	107	PRO	N-CA-C	5.05	116.86	110.70
1	C	142	LYS	N-CA-C	5.04	117.50	111.71
3	y	307	TYR	CA-CB-CG	5.03	122.95	113.90
2	L	211	LYS	N-CA-C	-5.02	102.95	110.23
2	x	75	ILE	CG1-CB-CG2	-5.02	95.64	110.70
2	x	171	TYR	N-CA-C	5.02	119.03	113.01
1	o	47	ARG	CA-CB-CG	-5.01	104.09	114.10
5	U	48	ASP	N-CA-C	5.00	117.27	108.56

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1	51	ILE	Peptide
5	1	59	GLY	Peptide
6	AJ	13	GLU	Peptide
6	AJ	14	ALA	Peptide
1	C	189	THR	Mainchain
1	C	246	GLY	Mainchain
1	C	57	GLN	Sidechain
3	M	272	CYS	Mainchain
3	M	9	THR	Mainchain
6	X	14	ALA	Peptide
4	t	29	TYR	Sidechain
2	x	268	TRP	Mainchain
3	y	215	LEU	Mainchain
3	y	271	TRP	Mainchain

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Mol	Chain	Res	Type	Group
3	y	272	CYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2458	0	2385	144	0
1	o	2458	0	2385	157	0
2	L	2231	0	2192	181	0
2	x	2231	0	2192	189	0
3	M	2546	0	2521	228	0
3	y	2546	0	2521	221	0
4	H	1982	0	1981	128	0
4	t	1982	0	1981	131	0
5	1	475	0	486	42	0
5	3	475	0	486	23	0
5	5	475	0	486	23	0
5	7	475	0	486	31	0
5	9	475	0	486	41	0
5	A	475	0	486	29	0
5	AA	475	0	486	20	0
5	AC	475	0	486	25	0
5	AE	481	0	490	38	0
5	AG	475	0	486	23	0
5	AI	475	0	486	26	0
5	AK	475	0	486	21	0
5	D	475	0	486	35	0
5	F	475	0	486	27	0
5	I	475	0	486	41	0
5	K	475	0	486	11	0
5	O	475	0	486	31	0
5	Q	475	0	486	35	0
5	S	481	0	490	34	0
5	U	475	0	486	29	0
5	W	475	0	486	39	0
5	Y	475	0	486	38	0
5	d	475	0	486	28	0
5	f	475	0	486	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	h	475	0	486	30	0
5	j	475	0	486	43	0
5	l	475	0	486	40	0
5	m	475	0	486	27	0
5	p	475	0	486	29	0
5	r	475	0	486	32	0
5	u	475	0	486	36	0
5	w	475	0	486	21	0
6	0	337	0	323	22	0
6	2	337	0	323	18	0
6	4	337	0	323	12	0
6	6	337	0	323	11	0
6	8	337	0	323	14	0
6	AB	337	0	323	13	0
6	AD	337	0	323	18	0
6	AF	337	0	323	15	0
6	AH	337	0	323	21	0
6	AJ	337	0	323	21	0
6	AL	337	0	323	17	0
6	B	337	0	323	31	0
6	E	337	0	323	28	0
6	G	337	0	323	25	0
6	J	337	0	323	26	0
6	N	337	0	323	16	0
6	P	337	0	323	21	0
6	R	337	0	323	24	0
6	T	337	0	323	24	0
6	V	337	0	323	16	0
6	X	337	0	323	22	0
6	Z	337	0	323	21	0
6	c	337	0	323	17	0
6	e	337	0	323	19	0
6	g	337	0	323	21	0
6	i	337	0	323	14	0
6	k	337	0	323	18	0
6	n	337	0	323	19	0
6	q	337	0	323	18	0
6	s	337	0	323	23	0
6	v	337	0	323	25	0
6	z	337	0	323	11	0
7	C	172	0	120	33	0
7	o	172	0	120	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1	1	0	0	0	0
8	5	2	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	0	0	0	0
8	AA	1	0	0	0	0
8	AC	1	0	0	0	0
8	AE	1	0	0	0	0
8	AI	2	0	0	0	0
8	AK	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	L	2	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
8	d	1	0	0	0	0
8	f	1	0	0	0	0
8	h	1	0	0	0	0
8	j	1	0	0	0	0
8	l	1	0	0	0	0
8	m	1	0	0	0	0
8	o	1	0	0	0	0
8	p	1	0	0	0	0
8	r	1	0	0	0	0
8	w	2	0	0	0	0
8	x	2	0	0	0	0
9	0	66	0	74	8	0
9	1	132	0	148	14	0
9	3	66	0	74	11	0
9	4	66	0	74	13	0
9	5	132	0	148	14	0
9	7	66	0	74	8	0
9	8	66	0	74	14	0
9	9	66	0	74	10	0
9	A	66	0	74	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AA	66	0	74	8	0
9	AB	66	0	74	10	0
9	AC	66	0	74	8	0
9	AD	66	0	74	12	0
9	AE	132	0	148	13	0
9	AH	132	0	148	22	0
9	AI	66	0	74	11	0
9	AJ	66	0	74	5	0
9	AK	66	0	74	7	0
9	AL	66	0	74	10	0
9	B	66	0	74	9	0
9	D	132	0	148	18	0
9	F	66	0	74	10	0
9	G	66	0	74	7	0
9	I	66	0	74	9	0
9	J	66	0	74	12	0
9	K	66	0	74	5	0
9	L	198	0	222	32	0
9	M	66	0	74	12	0
9	N	66	0	74	5	0
9	O	66	0	74	8	0
9	P	66	0	74	6	0
9	Q	66	0	74	5	0
9	R	66	0	74	6	0
9	S	66	0	74	8	0
9	T	66	0	74	12	0
9	U	66	0	74	10	0
9	V	66	0	74	9	0
9	W	66	0	74	12	0
9	X	66	0	74	12	0
9	Y	66	0	74	13	0
9	Z	66	0	74	9	0
9	c	66	0	74	7	0
9	d	66	0	74	9	0
9	e	66	0	74	11	0
9	f	66	0	74	10	0
9	g	66	0	74	12	0
9	h	66	0	74	10	0
9	i	66	0	74	8	0
9	j	66	0	74	11	0
9	k	66	0	74	12	0
9	l	66	0	74	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	m	132	0	148	13	0
9	p	132	0	148	17	0
9	r	66	0	74	12	0
9	s	66	0	74	4	0
9	u	66	0	74	9	0
9	v	66	0	74	9	0
9	w	66	0	74	12	0
9	x	198	0	222	37	0
9	y	66	0	74	11	0
9	z	66	0	74	6	0
10	L	65	0	76	14	0
10	M	65	0	76	13	0
10	x	65	0	76	12	0
10	y	65	0	76	14	0
11	L	53	0	74	18	0
11	x	53	0	74	20	0
12	A	19	0	11	3	0
12	H	57	0	33	13	0
12	L	12	0	9	1	0
12	M	54	0	33	9	0
12	m	19	0	11	4	0
12	p	16	0	11	5	0
12	t	38	0	22	13	0
12	x	19	0	11	11	0
12	y	57	0	33	8	0
13	L	1	0	0	0	0
13	x	1	0	0	0	0
14	M	53	0	72	9	0
14	y	53	0	72	10	0
15	2	44	0	60	14	0
15	4	44	0	60	10	0
15	6	44	0	60	5	0
15	8	44	0	60	14	0
15	9	44	0	60	14	0
15	A	44	0	60	8	0
15	AC	44	0	60	7	0
15	AD	44	0	60	10	0
15	AE	44	0	60	13	0
15	AH	44	0	60	8	0
15	AJ	44	0	60	10	0
15	AL	44	0	60	11	0
15	E	44	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	G	44	0	60	10	0
15	J	44	0	60	12	0
15	M	44	0	60	11	0
15	N	44	0	60	15	0
15	P	44	0	60	9	0
15	R	44	0	60	8	0
15	T	44	0	60	13	0
15	U	44	0	60	5	0
15	X	44	0	60	12	0
15	Z	44	0	60	9	0
15	c	44	0	60	6	0
15	e	44	0	60	11	0
15	f	44	0	60	12	0
15	i	44	0	60	6	0
15	k	44	0	60	11	0
15	n	44	0	60	15	0
15	p	44	0	60	9	0
15	s	44	0	60	13	0
15	v	44	0	60	7	0
15	y	44	0	60	10	0
15	z	44	0	60	3	0
16	H	5	0	0	0	0
16	M	5	0	0	0	0
16	t	5	0	0	0	0
16	y	5	0	0	1	0
17	AE	21	0	12	1	0
17	S	21	0	12	3	0
18	AI	1	0	0	0	0
18	C	1	0	0	0	0
18	L	1	0	0	0	0
18	W	1	0	0	1	0
18	o	1	0	0	0	0
18	x	1	0	0	0	0
All	All	51893	0	52456	2877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2877) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:45:ASN:O	5:h:49:ASP:OD2	1.56	1.19
5:AA:45:ASN:O	5:AA:49:ASP:OD2	1.63	1.16
1:C:307:CYS:SG	7:C:504:HEM:HAB	1.94	1.07
5:j:45:ASN:O	5:j:49:ASP:OD2	1.74	1.04
5:Y:5:ASN:OD1	6:2:23:GLN:NE2	1.94	1.00
2:x:44:LEU:HD23	5:l:30:VAL:HG11	1.42	0.99
2:L:46:GLY:HA3	10:L:302:BPH:H9C3	1.46	0.98
3:y:65:LEU:HD21	10:y:402:BPH:H102	1.43	0.97
4:H:150:ASP:O	4:H:207:ARG:NH2	1.98	0.97
12:x:306:PEF:H51	4:t:68:VAL:H	1.30	0.97
2:x:188:PHE:CD2	2:x:248:SER:HB3	2.02	0.95
2:L:177:HIS:HB3	3:M:183:LEU:HD13	1.49	0.94
1:C:189:THR:O	1:C:238:ASN:ND2	1.99	0.93
3:y:25:LYS:HD3	3:y:26:GLY:H	1.33	0.93
9:G:102:BCL:H12	9:G:102:BCL:H3A	1.52	0.92
3:y:265:ILE:HD13	14:y:403:MQ8:H121	1.54	0.90
2:L:244:PHE:HD1	11:L:304:UQ8:H43	1.36	0.90
5:9:3:THR:HB	5:9:8:LEU:HB2	1.54	0.89
3:y:267:ARG:NH2	12:t:303:PEF:O2P	2.06	0.89
5:j:10:LYS:HA	5:j:13:LEU:HD13	1.53	0.89
1:o:178:LEU:HA	3:y:110:SER:HB2	1.55	0.89
2:x:176:PHE:HE1	2:x:179:ASN:HD22	1.20	0.89
2:L:239:HIS:CD2	3:M:223:ILE:HG13	2.08	0.88
5:j:35:ILE:HG12	15:k:101:CRT:H403	1.52	0.88
9:y:401:BCL:H2	10:y:402:BPH:HH1	1.54	0.87
5:A:2:PHE:HB3	5:A:4:MET:HB2	1.55	0.87
5:AI:10:LYS:HA	5:AI:13:LEU:HD13	1.55	0.87
1:C:32:GLN:NE2	2:L:79:ASP:OD1	2.08	0.87
5:3:5:ASN:O	5:3:7:ASN:N	2.07	0.87
6:AF:44:PRO:O	5:AG:55:TYR:OH	1.93	0.86
9:R:102:BCL:H3A	9:R:102:BCL:H2	1.55	0.86
9:X:102:BCL:HMA1	9:Y:101:BCL:HMA1	1.57	0.86
12:m:101:PEF:H51	5:l:19:ARG:HH12	1.39	0.85
1:o:107:CYS:SG	7:o:501:HEM:HAB	2.16	0.85
2:L:189:PHE:CD1	2:L:249:ALA:HB1	2.12	0.85
5:j:32:GLY:HA2	9:k:102:BCL:HED2	1.55	0.85
6:T:17:PHE:HA	15:T:101:CRT:H6	1.58	0.85
3:M:18:TYR:CE2	3:M:20:GLY:HA2	2.12	0.85
9:B:101:BCL:H122	5:9:2:PHE:HA	1.55	0.85
2:L:188:PHE:CD2	2:L:248:SER:HB3	2.12	0.85
2:L:176:PHE:HE1	2:L:179:ASN:HD22	1.25	0.84
4:H:137:ARG:NH1	4:H:229:ASP:OD1	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:307:CYS:SG	7:o:504:HEM:HAB	2.17	0.84
6:k:21:PHE:HA	15:k:101:CRT:H11	1.60	0.84
4:H:94:PRO:HG2	6:0:8:GLY:HA2	1.60	0.83
3:M:12:GLN:OE1	3:M:14:ARG:NH2	2.11	0.83
5:A:49:ASP:OD2	6:B:43:ARG:NH1	2.11	0.83
15:k:101:CRT:H243	9:l:101:BCL:H172	1.60	0.83
5:I:11:ILE:HG12	9:K:101:BCL:H161	1.61	0.83
5:5:50:ASN:HB2	5:5:54:SER:HA	1.59	0.83
1:o:152:CYS:SG	7:o:502:HEM:HAB	2.19	0.83
3:y:277:VAL:HG11	10:y:402:BPH:HAC2	1.60	0.83
4:H:113:PRO:HG3	4:H:248:LEU:HB3	1.60	0.81
5:r:51:ILE:HD13	6:s:43:ARG:HH22	1.45	0.81
2:L:44:LEU:HD23	5:9:30:VAL:HG11	1.62	0.81
6:v:32:VAL:HG21	9:v:102:BCL:HBA2	1.62	0.81
3:M:214:LEU:O	3:M:218:MET:HG3	1.80	0.81
4:t:159:LEU:HD22	4:t:254:ARG:NH2	1.95	0.81
1:C:278:ASP:OD1	1:C:282:ASN:ND2	2.14	0.81
6:e:16:GLU:HB3	15:e:101:CRT:H21A	1.63	0.80
3:y:99:PRO:HB2	3:y:101:GLN:HG2	1.62	0.80
6:B:20:ILE:O	6:B:24:SER:OG	1.99	0.80
5:AI:4:MET:O	5:AI:5:ASN:ND2	2.15	0.80
6:J:17:PHE:HA	15:J:101:CRT:H6	1.64	0.80
5:9:11:ILE:HD13	15:9:102:CRT:H10	1.63	0.80
4:t:150:ASP:O	4:t:207:ARG:NH2	2.14	0.79
3:M:99:PRO:HD2	3:M:102:TYR:HD2	1.47	0.79
1:C:20:LEU:HA	1:C:21:LEU:HB2	1.62	0.79
4:t:31:ARG:NH1	4:t:34:ASP:OD2	2.15	0.79
3:M:145:HIS:HA	3:M:148:TRP:CE3	2.17	0.79
4:H:122:HIS:HB3	4:t:121:LYS:HZ2	1.45	0.79
6:P:17:PHE:HA	15:P:102:CRT:H6	1.63	0.79
3:y:179:ILE:O	3:y:182:HIS:ND1	2.15	0.79
5:A:50:ASN:HB3	5:A:54:SER:HA	1.64	0.78
2:x:86:MET:HA	2:x:96:GLN:HE22	1.48	0.78
5:U:5:ASN:OD1	5:U:7:ASN:N	2.15	0.78
2:L:203:ILE:HG13	3:M:266:HIS:CD2	2.19	0.78
2:x:188:PHE:HD2	2:x:248:SER:HB3	1.48	0.78
2:x:86:MET:HG3	5:j:41:SER:HB3	1.65	0.77
5:j:35:ILE:HB	9:k:102:BCL:HED1	1.65	0.77
5:I:40:LEU:O	5:I:45:ASN:ND2	2.17	0.77
3:y:260:VAL:HB	3:y:264:SER:OG	1.85	0.77
6:R:43:ARG:HG3	5:S:55:TYR:CZ	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:189:PHE:CD1	2:x:249:ALA:HB1	2.19	0.77
3:y:253:ARG:HH22	12:t:301:PEF:H52	1.50	0.77
1:C:169:ASP:OD1	1:C:171:GLY:N	2.18	0.77
2:x:125:HIS:NE2	3:y:5:GLN:OE1	2.15	0.77
5:w:50:ASN:HB2	5:w:54:SER:HA	1.67	0.77
1:C:173:LYS:HB2	3:M:80:HIS:HB2	1.66	0.77
2:L:179:ASN:O	2:L:183:MET:HG3	1.85	0.77
5:I:9:TYR:OH	6:J:11:ASP:OD1	2.03	0.77
5:Y:44:LEU:HD23	5:1:55:TYR:HE2	1.48	0.77
2:x:241:LEU:HD21	11:x:304:UQ8:H13	1.66	0.76
2:L:21:ASP:O	5:9:18:ARG:NH2	2.19	0.76
5:AI:49:ASP:O	5:AK:60:LYS:N	2.15	0.76
5:d:49:ASP:HB2	5:d:51:ILE:HG13	1.67	0.76
5:AE:11:ILE:HD12	5:AE:14:ILE:HD12	1.67	0.76
3:M:267:ARG:NH1	12:H:304:PEF:O1P	2.17	0.75
9:4:102:BCL:HMA1	9:5:101:BCL:HMA1	1.66	0.75
6:R:17:PHE:HA	15:R:101:CRT:H6	1.67	0.75
5:Y:51:ILE:HG23	5:Y:52:PRO:HA	1.68	0.75
4:H:37:GLU:O	4:H:39:TYR:N	2.20	0.75
1:o:247:CYS:SG	7:o:503:HEM:CAB	2.74	0.75
5:j:11:ILE:HD13	15:c:101:CRT:H10	1.66	0.75
15:X:101:CRT:H181	15:X:101:CRT:H21	1.69	0.75
15:9:102:CRT:H11	15:9:102:CRT:H81	1.67	0.75
4:t:48:ARG:HG2	6:n:8:GLY:HA3	1.68	0.75
5:r:11:ILE:HD12	5:r:14:ILE:HD11	1.67	0.75
5:r:27:PHE:HB2	9:u:101:BCL:H151	1.69	0.75
12:M:406:PEF:N	4:H:39:TYR:OH	2.20	0.75
6:k:31:LEU:HD23	6:k:34:ILE:HD12	1.67	0.75
6:AL:17:PHE:HA	15:AL:101:CRT:H6	1.69	0.75
4:t:179:ILE:HG22	4:t:197:ILE:HD13	1.69	0.74
5:AA:50:ASN:ND2	5:AC:59:GLY:O	2.19	0.74
6:G:17:PHE:HA	15:G:101:CRT:H6	1.67	0.74
6:n:17:PHE:HD1	15:n:101:CRT:H5	1.52	0.74
5:u:25:VAL:HG13	9:u:101:BCL:H71	1.67	0.74
2:x:203:ILE:HG13	3:y:266:HIS:CD2	2.22	0.74
5:1:57:ALA:H	5:1:58:LEU:C	1.96	0.74
5:AE:43:ASP:HB2	5:AG:48:ASP:HA	1.70	0.74
6:2:17:PHE:HA	15:2:101:CRT:H6	1.68	0.74
3:M:126:ILE:HD13	9:M:401:BCL:H91	1.71	0.73
3:y:219:HIS:ND1	14:y:403:MQ8:O1	2.20	0.73
5:l:10:LYS:HA	5:l:13:LEU:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:40:TRP:HZ3	6:E:46:LEU:H	1.36	0.73
4:H:249:TYR:O	4:H:251:THR:N	2.21	0.73
15:U:102:CRT:H14	6:V:21:PHE:HA	1.69	0.73
2:x:240:ARG:NH1	3:y:7:ILE:O	2.21	0.73
9:f:101:BCL:H121	9:f:101:BCL:H62	1.69	0.73
5:W:11:ILE:HD13	15:Z:101:CRT:H10	1.70	0.73
4:t:44:ASP:HB3	4:t:48:ARG:HH21	1.53	0.73
4:t:249:TYR:O	4:t:251:THR:N	2.22	0.73
2:L:2:ALA:N	12:A:101:PEF:O1P	2.22	0.73
2:L:232:SER:OG	11:L:304:UQ8:O5	2.05	0.73
3:M:65:LEU:HD21	10:M:402:BPH:H102	1.70	0.73
1:o:167:VAL:HG13	1:o:303:LEU:HD23	1.69	0.73
1:C:247:CYS:SG	7:C:503:HEM:CAB	2.76	0.73
6:B:20:ILE:HG23	5:9:5:ASN:HB3	1.71	0.72
6:J:43:ARG:HG3	5:K:55:TYR:CZ	2.24	0.72
1:C:19:MET:O	1:C:21:LEU:HD22	1.89	0.72
6:X:17:PHE:HA	15:X:101:CRT:H6	1.70	0.72
1:o:263:THR:HG22	3:y:311:VAL:HG11	1.71	0.72
6:e:32:VAL:HG21	9:e:102:BCL:HBA2	1.71	0.72
2:L:72:ARG:HD2	3:M:305:PRO:HA	1.70	0.72
3:M:229:PHE:HE2	3:M:247:ARG:HD3	1.51	0.72
2:x:179:ASN:O	2:x:183:MET:HG3	1.88	0.72
4:t:154:MET:HE2	4:t:207:ARG:HA	1.71	0.72
5:7:45:ASN:O	5:7:49:ASP:OD2	2.06	0.72
1:o:20:LEU:HA	1:o:21:LEU:HB2	1.71	0.72
6:AL:21:PHE:HD1	15:AL:101:CRT:H14	1.54	0.72
2:L:118:ARG:NH1	12:L:306:PEF:O1P	2.22	0.72
6:B:17:PHE:HD1	15:9:102:CRT:H5	1.53	0.72
15:i:101:CRT:H36	5:j:33:LEU:HD23	1.72	0.72
3:M:177:PHE:HD1	15:M:404:CRT:H16	1.55	0.72
3:y:241:ARG:NE	3:y:246:GLU:OE1	2.23	0.72
9:M:401:BCL:H61	10:M:402:BPH:C4B	2.19	0.72
2:x:175:HIS:NE2	3:y:184:ASP:OD1	2.23	0.72
5:3:40:LEU:HG	5:3:46:TRP:CH2	2.25	0.72
9:AK:101:BCL:H2	6:AL:28:TRP:CH2	2.25	0.72
1:C:152:CYS:SG	7:C:502:HEM:CAB	2.78	0.71
4:H:154:MET:HE2	4:H:207:ARG:HA	1.72	0.71
2:x:2:ALA:N	12:m:101:PEF:O2P	2.22	0.71
1:C:264:PRO:HD3	3:M:312:THR:O	1.90	0.71
4:H:60:ASP:OD1	4:H:61:LEU:N	2.22	0.71
3:y:145:HIS:HA	3:y:148:TRP:CE3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TYR:CD1	1:C:157:ARG:HA	2.25	0.71
11:x:304:UQ8:H38	11:x:304:UQ8:H35B	1.72	0.71
4:t:45:ARG:HH11	4:t:53:VAL:HG11	1.55	0.71
1:C:263:THR:HG22	3:M:311:VAL:HG11	1.71	0.71
3:M:260:VAL:HB	3:M:264:SER:OG	1.90	0.71
5:r:29:ILE:HG13	9:r:101:BCL:H43	1.70	0.71
5:1:57:ALA:H	5:1:59:GLY:N	1.89	0.71
9:j:101:BCL:H2	6:k:28:TRP:CZ2	2.25	0.71
2:L:206:VAL:CG1	3:M:142:MET:HE3	2.20	0.71
3:M:219:HIS:CE1	3:M:266:HIS:HE1	2.08	0.71
2:x:132:PHE:CZ	11:x:304:UQ8:H40B	2.26	0.71
3:M:37:SER:HG	3:M:40:LEU:H	1.39	0.71
15:s:101:CRT:H372	5:u:36:HIS:CD2	2.25	0.71
2:L:225:PHE:CD2	11:L:304:UQ8:H7A	2.26	0.71
1:C:307:CYS:SG	7:C:504:HEM:CAB	2.77	0.70
10:L:302:BPH:H201	9:L:305:BCL:HMA1	1.72	0.70
6:n:21:PHE:HA	15:n:101:CRT:H14	1.73	0.70
5:r:23:SER:HB3	9:u:101:BCL:H141	1.73	0.70
5:F:34:LEU:HD21	15:G:101:CRT:H2M2	1.72	0.70
6:B:44:PRO:HG2	5:D:52:PRO:HD3	1.73	0.70
15:f:102:CRT:H6	6:g:17:PHE:HA	1.72	0.70
2:L:222:ASN:O	2:L:226:ARG:HG3	1.92	0.70
5:I:11:ILE:HD13	15:N:101:CRT:H10	1.73	0.70
1:C:191:ALA:HB3	1:C:237:MET:HE3	1.72	0.70
15:A:103:CRT:H5	5:7:14:ILE:HD11	1.73	0.70
9:O:101:BCL:HMA1	9:Q:101:BCL:HMA1	1.72	0.70
3:y:62:PHE:HB3	5:AC:30:VAL:HG21	1.74	0.70
9:AK:101:BCL:H2	6:AL:28:TRP:CZ2	2.26	0.70
5:d:5:ASN:HB3	5:d:8:LEU:HB2	1.74	0.70
2:L:183:MET:HE1	3:M:180:PHE:HE1	1.57	0.70
5:Y:39:VAL:HG11	9:Y:101:BCL:HBC1	1.73	0.70
4:t:102:PRO:HB3	4:t:111:PHE:HD2	1.56	0.70
6:AB:45:TRP:CD1	6:AB:46:LEU:HG	2.26	0.70
4:H:122:HIS:HB3	4:t:121:LYS:NZ	2.07	0.70
5:S:44:LEU:HD22	6:T:43:ARG:HD3	1.73	0.70
6:N:32:VAL:HG21	9:N:102:BCL:HBA2	1.74	0.70
15:AJ:101:CRT:H181	15:AJ:101:CRT:H21	1.73	0.70
5:D:33:LEU:HD23	15:9:102:CRT:H36	1.74	0.69
5:U:16:ASP:OD2	5:U:18:ARG:NH2	2.16	0.69
4:H:126:THR:HG23	4:H:130:LEU:O	1.92	0.69
9:D:102:BCL:H92	6:E:33:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:34:PRO:HG3	3:y:50:PRO:HD3	1.73	0.69
3:M:134:TYR:CE1	3:M:144:GLN:HG3	2.26	0.69
2:x:199:HIS:CE1	2:x:239:HIS:CE1	2.80	0.69
3:y:25:LYS:HD3	3:y:26:GLY:N	2.05	0.69
3:y:229:PHE:HB2	3:y:244:ALA:HB2	1.73	0.69
5:h:17:PRO:HB3	6:i:17:PHE:CZ	2.28	0.69
5:h:39:VAL:HG11	9:h:101:BCL:HBC1	1.74	0.69
4:H:14:ILE:HD13	5:I:37:MET:SD	2.32	0.69
5:AG:5:ASN:O	5:AG:7:ASN:N	2.24	0.69
9:Y:101:BCL:H2	6:Z:28:TRP:CZ2	2.27	0.69
6:AB:17:PHE:HA	15:AC:101:CRT:H6	1.75	0.69
3:y:52:TYR:O	3:y:132:ARG:NH2	2.19	0.69
1:C:107:CYS:SG	7:C:501:HEM:HAB	2.32	0.69
1:C:269:ALA:O	1:C:273:ILE:HG13	1.92	0.69
3:M:99:PRO:HD2	3:M:102:TYR:CD2	2.26	0.69
4:t:136:MET:HG3	4:t:170:VAL:O	1.92	0.69
5:f:9:TYR:HB2	6:g:14:ALA:O	1.91	0.69
6:k:32:VAL:HG21	9:k:102:BCL:H11	1.74	0.69
2:L:240:ARG:NH1	3:M:7:ILE:O	2.26	0.69
5:S:51:ILE:HG22	5:S:52:PRO:HA	1.73	0.69
5:U:39:VAL:HG11	9:U:101:BCL:HBC1	1.74	0.69
4:t:37:GLU:O	4:t:39:TYR:N	2.25	0.69
2:x:193:CYS:SG	10:y:402:BPH:HMC3	2.33	0.69
4:t:137:ARG:NH2	4:t:229:ASP:OD1	2.25	0.69
6:G:44:PRO:O	5:I:55:TYR:OH	2.11	0.68
5:9:5:ASN:O	5:9:7:ASN:N	2.20	0.68
5:A:16:ASP:OD2	5:A:19:ARG:HG3	1.93	0.68
15:U:102:CRT:H22A	6:V:17:PHE:HB2	1.76	0.68
9:z:102:BCL:HMA1	9:AA:101:BCL:HMA1	1.74	0.68
6:AB:21:PHE:HA	15:AC:101:CRT:H14	1.75	0.68
6:AD:31:LEU:HD22	9:AD:101:BCL:H191	1.75	0.68
1:o:273:ILE:HG12	7:o:504:HEM:HBB2	1.76	0.68
9:AA:101:BCL:HBD	9:AB:101:BCL:HED3	1.74	0.68
9:AH:101:BCL:HBD	9:AH:101:BCL:HAA1	1.75	0.68
1:C:71:LYS:O	1:C:74:GLU:HG2	1.93	0.68
1:C:292:PRO:HG2	1:C:295:ARG:HG2	1.76	0.68
15:4:101:CRT:H30	9:4:102:BCL:HMA2	1.75	0.68
5:AA:37:MET:HE3	5:AA:41:SER:HB3	1.76	0.68
3:M:175:VAL:HG22	3:M:185:TRP:CE2	2.28	0.68
5:AI:8:LEU:HD11	9:AK:101:BCL:H191	1.76	0.68
4:t:65:LYS:HE2	4:t:67:PHE:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:32:VAL:HG21	9:AB:101:BCL:HBA2	1.76	0.68
3:M:74:ASN:HD21	3:M:114:TRP:CD1	2.12	0.68
3:M:145:HIS:HA	3:M:148:TRP:HE3	1.59	0.68
9:K:101:BCL:HED1	6:N:28:TRP:CZ2	2.29	0.68
5:O:14:ILE:HD11	15:R:101:CRT:H31A	1.75	0.68
1:o:42:ASN:HA	2:x:172:GLN:HE22	1.59	0.68
5:m:4:MET:HE2	5:m:7:ASN:HD22	1.59	0.67
4:H:54:LYS:NZ	12:H:303:PEF:O1P	2.28	0.67
2:x:144:ARG:HB3	2:x:145:PRO:HD3	1.76	0.67
3:y:226:VAL:HG23	3:y:231:GLY:HA3	1.76	0.67
4:H:88:ASN:ND2	4:H:109:SER:O	2.27	0.67
5:d:7:ASN:HB3	5:d:10:LYS:HD2	1.74	0.67
1:o:21:LEU:HD21	2:x:274:TRP:CZ2	2.30	0.67
9:AA:101:BCL:HBA2	9:AB:101:BCL:HED3	1.76	0.67
2:x:204:LEU:HD21	3:y:267:ARG:HG3	1.75	0.67
1:C:112:VAL:HG21	1:C:120:ASP:HB3	1.77	0.67
1:C:310:CYS:SG	7:C:504:HEM:CAC	2.82	0.67
12:x:306:PEF:C5	4:t:68:VAL:H	2.07	0.67
5:p:12:TRP:HB3	5:p:17:PRO:HG3	1.75	0.67
5:AC:28:GLN:HB3	9:AD:101:BCL:H42	1.77	0.67
1:o:148:THR:HA	1:o:322:GLN:HG2	1.77	0.67
15:AL:101:CRT:H35	9:d:101:BCL:HMB1	1.77	0.67
1:o:112:VAL:HG21	1:o:120:ASP:HB3	1.77	0.67
5:AG:5:ASN:OD1	5:AG:7:ASN:HB2	1.95	0.67
2:L:106:PHE:CE1	9:L:301:BCL:H121	2.30	0.66
3:M:208:PHE:CD2	3:M:275:LEU:HB3	2.30	0.66
4:t:234:TYR:O	4:t:238:LYS:HG2	1.95	0.66
1:o:163:LYS:HD2	1:o:164:TYR:CE2	2.29	0.66
4:H:159:LEU:HD22	4:H:254:ARG:NH2	2.10	0.66
5:W:16:ASP:OD2	5:W:19:ARG:HG3	1.95	0.66
5:AC:43:ASP:HB2	5:AE:48:ASP:HA	1.77	0.66
5:AG:5:ASN:C	5:AG:7:ASN:H	2.03	0.66
15:AL:101:CRT:H35	9:d:101:BCL:HHB	1.77	0.66
5:O:5:ASN:OD1	5:O:5:ASN:N	2.29	0.66
4:t:44:ASP:O	4:t:48:ARG:HB2	1.95	0.66
1:C:107:CYS:SG	7:C:501:HEM:CAB	2.83	0.66
5:u:11:ILE:HD12	5:u:14:ILE:HD12	1.77	0.66
1:C:164:TYR:HD2	1:C:312:GLN:HG2	1.59	0.66
3:y:99:PRO:HD2	3:y:102:TYR:CD2	2.31	0.66
2:L:160:LEU:O	2:L:163:LEU:HB2	1.96	0.66
5:S:43:ASP:CG	5:U:50:ASN:HA	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TYR:CE1	1:C:157:ARG:HA	2.30	0.66
3:M:265:ILE:HD13	14:M:403:MQ8:H121	1.78	0.66
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.78	0.66
3:M:229:PHE:CE2	3:M:247:ARG:HD3	2.30	0.65
4:H:65:LYS:HE2	4:H:67:PHE:CE1	2.30	0.65
5:1:51:ILE:HG22	5:1:52:PRO:HA	1.78	0.65
5:AE:22:VAL:HG22	9:AE:102:BCL:H172	1.79	0.65
5:F:31:LEU:HD12	5:F:34:LEU:HD23	1.79	0.65
2:x:132:PHE:HZ	11:x:304:UQ8:H40B	1.59	0.65
3:y:229:PHE:HE2	3:y:247:ARG:HD3	1.61	0.65
4:t:196:PRO:HD3	4:t:243:TYR:CE2	2.31	0.65
6:i:33:VAL:HG22	9:i:102:BCL:H92	1.79	0.65
2:L:225:PHE:HE2	11:L:304:UQ8:H1MA	1.61	0.65
3:M:265:ILE:HG23	3:M:266:HIS:ND1	2.11	0.65
2:L:31:TYR:HB3	2:L:116:ILE:HD11	1.77	0.65
3:y:37:SER:HB2	12:y:406:PEF:H31	1.78	0.65
1:C:137:ALA:HA	1:C:141:TRP:HD1	1.62	0.65
9:e:102:BCL:H12	9:e:102:BCL:H3A	1.79	0.65
1:C:21:LEU:HG	2:L:274:TRP:CD1	2.32	0.65
1:o:19:MET:HB2	1:o:21:LEU:HD13	1.77	0.65
3:y:219:HIS:CE1	3:y:223:ILE:HD11	2.32	0.65
2:L:184:LEU:HD23	2:L:252:TRP:CD2	2.32	0.65
1:C:21:LEU:HD23	2:L:271:TRP:CZ2	2.30	0.65
4:H:31:ARG:NH1	4:H:34:ASP:OD2	2.30	0.65
9:8:102:BCL:H2	9:8:102:BCL:H8	1.78	0.65
4:t:88:ASN:OD1	4:t:103:ASN:HB2	1.96	0.65
5:u:11:ILE:HG12	9:w:101:BCL:H161	1.77	0.65
2:L:188:PHE:CE2	2:L:248:SER:HB3	2.32	0.65
6:G:18:HIS:O	6:G:22:MET:HG2	1.97	0.65
6:G:43:ARG:HG3	5:I:55:TYR:CE1	2.32	0.65
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.32	0.65
6:8:32:VAL:HG21	9:8:102:BCL:HBA2	1.79	0.65
1:o:110:CYS:HA	1:o:123:THR:OG1	1.97	0.65
3:y:208:PHE:CD2	3:y:275:LEU:HB3	2.31	0.65
15:n:101:CRT:H371	9:p:102:BCL:HMB2	1.79	0.65
1:C:194:SER:OG	3:M:184:ASP:OD2	2.13	0.65
1:C:307:CYS:HG	7:C:504:HEM:HAB	1.61	0.65
4:H:246:GLY:HA2	4:H:250:ALA:H	1.61	0.65
2:x:211:LYS:HG2	12:x:306:PEF:C10	2.27	0.65
2:x:242:GLY:HA3	3:y:216:PHE:CE1	2.32	0.65
9:x:303:BCL:H72	10:y:402:BPH:HMA3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:101:BCL:HBC2	9:AJ:102:BCL:HMD1	1.79	0.65
1:o:164:TYR:CD2	1:o:312:GLN:HG2	2.31	0.64
3:y:18:TYR:CE2	3:y:20:GLY:HA2	2.32	0.64
5:j:44:LEU:HD22	6:k:43:ARG:HD3	1.79	0.64
5:S:25:VAL:HG22	9:S:102:BCL:H8	1.80	0.64
6:8:43:ARG:HG3	5:9:55:TYR:CZ	2.32	0.64
6:n:17:PHE:HA	15:n:101:CRT:H83	1.79	0.64
15:AH:102:CRT:H292	9:AI:101:BCL:H43	1.79	0.64
6:B:24:SER:HB3	5:9:2:PHE:C	2.22	0.64
5:K:40:LEU:HG	5:K:46:TRP:CH2	2.33	0.64
14:y:403:MQ8:H242	14:y:403:MQ8:H192	1.78	0.64
4:t:29:TYR:OH	12:t:303:PEF:O4	2.13	0.64
5:m:10:LYS:HB3	15:p:103:CRT:H1M1	1.79	0.64
2:L:239:HIS:CG	3:M:223:ILE:HG21	2.31	0.64
5:F:11:ILE:HD13	15:J:101:CRT:H10	1.79	0.64
5:Q:38:ILE:O	5:Q:42:THR:HG23	1.96	0.64
6:X:24:SER:HB2	15:X:101:CRT:H14	1.77	0.64
1:o:310:CYS:SG	7:o:504:HEM:CAC	2.86	0.64
2:x:84:LEU:HB2	5:h:41:SER:HB2	1.79	0.64
3:y:253:ARG:HH22	12:t:301:PEF:C5	2.09	0.64
6:k:45:TRP:CD1	6:k:46:LEU:HG	2.33	0.64
3:y:160:LEU:HD23	3:y:284:ILE:HG21	1.80	0.64
5:u:7:ASN:HB3	5:u:10:LYS:HD2	1.80	0.64
10:L:302:BPH:H141	9:L:305:BCL:HBB3	1.80	0.64
5:Q:44:LEU:HD12	5:S:47:LEU:HD22	1.79	0.64
1:o:100:TRP:HB3	1:o:152:CYS:HB2	1.79	0.64
2:x:112:ARG:NH2	3:y:255:THR:O	2.28	0.64
1:C:250:CYS:SG	7:C:503:HEM:CAC	2.86	0.64
9:L:303:BCL:H203	9:L:303:BCL:H141	1.80	0.64
6:T:35:ALA:HA	6:T:38:LEU:HD12	1.78	0.64
15:2:101:CRT:H372	5:3:36:HIS:CD2	2.33	0.64
5:7:12:TRP:HB3	5:7:17:PRO:HG3	1.80	0.64
3:M:62:PHE:HB3	5:Q:30:VAL:HG21	1.80	0.64
4:H:150:ASP:OD1	4:H:152:ARG:HB2	1.97	0.64
5:l:36:HIS:HE1	9:l:101:BCL:NB	1.94	0.64
4:H:186:VAL:HG23	4:H:191:LYS:O	1.96	0.64
6:R:32:VAL:HG21	9:R:102:BCL:HBA2	1.80	0.64
15:AL:101:CRT:H372	5:d:36:HIS:CD2	2.33	0.64
1:C:128:ARG:NE	7:C:501:HEM:O2D	2.31	0.63
9:5:102:BCL:HMA1	9:7:101:BCL:HMA1	1.81	0.63
1:o:301:ASP:HB2	1:o:304:ARG:HH12	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:21:LEU:HD11	15:AJ:101:CRT:H133	1.80	0.63
1:C:179:LYS:HD2	3:M:111:GLU:HG3	1.80	0.63
2:L:206:VAL:HG13	3:M:142:MET:HE3	1.80	0.63
4:H:57:GLY:H	12:H:301:PEF:HN2	1.46	0.63
1:o:107:CYS:SG	7:o:501:HEM:CAB	2.85	0.63
3:y:35:ILE:HG13	3:y:48:ILE:HB	1.80	0.63
3:y:277:VAL:CG1	10:y:402:BPH:HAC2	2.27	0.63
4:t:197:ILE:O	4:t:200:SER:OG	2.16	0.63
9:m:103:BCL:H152	6:n:36:HIS:CD2	2.32	0.63
9:r:101:BCL:H2	6:s:28:TRP:CZ2	2.34	0.63
5:AE:38:ILE:O	5:AE:42:THR:HG23	1.98	0.63
2:L:281:TRP:HB2	3:M:88:LYS:HD2	1.78	0.63
6:X:28:TRP:HZ2	9:X:102:BCL:HED1	1.62	0.63
5:p:56:GLN:O	5:p:58:LEU:N	2.27	0.63
5:j:43:ASP:HA	5:l:56:GLN:HE21	1.63	0.63
3:M:34:PRO:HG3	3:M:50:PRO:HD3	1.78	0.63
4:t:29:TYR:CZ	12:t:303:PEF:C30	2.82	0.63
4:H:141:GLU:HG2	4:H:142:PHE:H	1.64	0.63
1:o:203:PHE:CG	1:o:235:LEU:HD22	2.33	0.63
2:x:281:TRP:HB2	3:y:88:LYS:HD2	1.80	0.63
3:y:99:PRO:HD2	3:y:102:TYR:HD2	1.63	0.63
4:t:133:ILE:HA	4:t:172:VAL:O	1.98	0.63
5:l:45:ASN:O	5:l:49:ASP:OD2	2.16	0.63
4:H:234:TYR:O	4:H:238:LYS:HG2	1.99	0.63
1:o:206:GLN:O	1:o:277:ARG:HD2	1.98	0.63
5:w:14:ILE:HD11	15:AC:101:CRT:H21A	1.80	0.63
4:H:45:ARG:HH11	4:H:53:VAL:HG11	1.63	0.63
3:y:197:TYR:CE1	9:y:401:BCL:HMC2	2.34	0.63
6:c:17:PHE:HA	15:c:101:CRT:H6	1.81	0.63
1:C:97:VAL:HG21	1:C:131:PHE:CZ	2.33	0.63
1:C:159:ASN:OD1	1:C:163:LYS:HE3	1.99	0.63
2:L:237:ALA:HA	2:L:240:ARG:HD2	1.81	0.63
3:M:175:VAL:HG13	3:M:185:TRP:CG	2.33	0.63
5:I:39:VAL:HG11	9:I:101:BCL:HAC2	1.81	0.63
9:A:102:BCL:HMA1	9:D:101:BCL:HMA1	1.80	0.63
6:G:45:TRP:CD1	6:G:46:LEU:HG	2.34	0.63
15:G:101:CRT:H32	9:I:101:BCL:H3A	1.80	0.63
5:I:3:THR:HA	6:J:22:MET:HE2	1.81	0.63
9:O:101:BCL:H2	9:O:101:BCL:HBA1	1.81	0.63
6:T:44:PRO:HG2	5:U:52:PRO:HG3	1.80	0.63
2:x:196:LEU:HD11	3:y:269:ALA:HB1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:7:HIS:CE1	5:u:48:ASP:HB3	2.34	0.63
9:AA:101:BCL:H162	9:AA:101:BCL:H101	1.81	0.63
6:AJ:44:PRO:O	5:AK:55:TYR:OH	2.17	0.63
3:M:219:HIS:CE1	3:M:266:HIS:CE1	2.87	0.62
3:y:214:LEU:O	3:y:218:MET:HG3	1.99	0.62
6:AF:45:TRP:HD1	6:AF:46:LEU:HG	1.62	0.62
6:z:32:VAL:HG21	9:z:102:BCL:HBA2	1.80	0.62
5:u:43:ASP:HB3	5:w:50:ASN:HD21	1.64	0.62
3:M:159:VAL:HA	3:M:163:ILE:HB	1.82	0.62
6:0:11:ASP:O	6:0:15:LYS:HG3	2.00	0.62
2:x:211:LYS:HA	12:x:306:PEF:O2	1.98	0.62
9:j:101:BCL:H2	6:k:28:TRP:CH2	2.35	0.62
2:L:68:TYR:HA	2:L:73:ILE:HD11	1.80	0.62
3:M:267:ARG:NH1	12:H:304:PEF:O3	2.33	0.62
5:1:44:LEU:HD23	5:3:55:TYR:CE2	2.34	0.62
15:AJ:101:CRT:H36	5:AK:33:LEU:HD23	1.80	0.62
5:f:42:THR:HG21	5:h:47:LEU:HB3	1.81	0.62
3:M:240:HIS:CE1	4:H:69:LEU:HD11	2.33	0.62
5:5:17:PRO:HB3	6:6:17:PHE:CZ	2.34	0.62
3:y:253:ARG:NH2	12:t:301:PEF:H52	2.14	0.62
3:y:260:VAL:HG12	4:t:34:ASP:OD2	2.00	0.62
5:u:49:ASP:OD2	6:v:43:ARG:NH1	2.33	0.62
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.80	0.62
5:A:45:ASN:O	5:A:49:ASP:OD2	2.17	0.62
6:E:21:PHE:HA	15:E:101:CRT:H11	1.81	0.62
3:y:222:THR:O	3:y:225:SER:OG	2.17	0.62
3:y:253:ARG:HH12	12:t:301:PEF:HN2	1.48	0.62
5:AE:5:ASN:C	5:AE:7:ASN:H	2.06	0.62
3:M:59:LEU:HB3	3:M:128:LEU:HD13	1.82	0.62
5:D:36:HIS:CD2	15:9:102:CRT:H372	2.34	0.62
5:Y:50:ASN:OD1	5:Y:55:TYR:N	2.33	0.62
5:5:14:ILE:HG13	5:5:15:LEU:HG	1.82	0.62
1:o:307:CYS:SG	7:o:504:HEM:CAB	2.87	0.62
3:M:135:LYS:HD3	5:O:19:ARG:HH11	1.64	0.61
6:N:40:TRP:HH2	6:N:46:LEU:OXT	1.83	0.61
2:x:222:ASN:O	2:x:226:ARG:HG3	2.00	0.61
6:z:45:TRP:NE1	9:z:102:BCL:OBB	2.32	0.61
6:AH:28:TRP:CZ2	9:AH:101:BCL:H2	2.34	0.61
1:C:152:CYS:SG	7:C:502:HEM:HAB	2.40	0.61
2:L:69:ASN:OD1	2:L:71:TRP:N	2.30	0.61
1:o:128:ARG:NE	7:o:501:HEM:O2D	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:3:MET:HB3	2:x:7:GLU:HB3	1.82	0.61
9:x:303:BCL:HBC1	9:y:401:BCL:CHA	2.30	0.61
5:p:18:ARG:HD3	12:p:101:PEF:C30	2.29	0.61
5:r:34:LEU:HD21	15:s:101:CRT:H2M2	1.82	0.61
3:M:256:MET:HE2	3:M:258:PHE:CE1	2.35	0.61
5:1:17:PRO:HB3	6:2:17:PHE:CZ	2.36	0.61
3:y:256:MET:HE2	3:y:258:PHE:CE1	2.36	0.61
9:AC:102:BCL:HBA2	6:AD:32:VAL:HG21	1.82	0.61
5:d:8:LEU:HD11	15:f:102:CRT:H133	1.82	0.61
3:M:76:LEU:HG	3:M:81:TRP:HA	1.82	0.61
9:M:401:BCL:C2	10:M:402:BPH:HBB2	2.31	0.61
6:E:43:ARG:HG3	5:F:55:TYR:CZ	2.35	0.61
2:x:202:LEU:HD23	11:x:304:UQ8:H3MA	1.82	0.61
5:p:19:ARG:HH22	12:p:101:PEF:HN2	1.46	0.61
6:AJ:17:PHE:HA	15:AJ:101:CRT:H6	1.82	0.61
6:AJ:32:VAL:HG21	9:AJ:102:BCL:HBA2	1.81	0.61
6:k:32:VAL:HG11	9:k:102:BCL:HBA2	1.82	0.61
4:t:149:PRO:HG3	4:t:204:LYS:HD3	1.82	0.61
6:AF:18:HIS:O	6:AF:22:MET:HG2	2.00	0.61
2:L:196:LEU:HD13	3:M:216:PHE:CG	2.36	0.61
5:w:16:ASP:OD2	5:w:19:ARG:HB2	2.01	0.61
6:AB:18:HIS:O	6:AB:22:MET:HG2	2.00	0.61
3:M:161:GLY:HA3	15:M:404:CRT:H292	1.82	0.61
3:M:6:ASN:HD22	3:M:227:SER:HB2	1.65	0.61
5:A:39:VAL:HG21	9:A:102:BCL:H3C	1.83	0.61
2:x:68:TYR:HA	2:x:73:ILE:HD11	1.81	0.61
5:AK:59:GLY:O	5:AK:61:LYS:N	2.32	0.61
1:C:141:TRP:O	1:C:145:VAL:HG22	2.01	0.61
2:L:175:HIS:NE2	3:M:184:ASP:OD1	2.33	0.61
15:M:404:CRT:H2M3	5:O:38:ILE:HG12	1.81	0.61
5:I:2:PHE:HA	5:I:4:MET:SD	2.41	0.61
5:O:43:ASP:OD2	5:Q:50:ASN:ND2	2.32	0.61
6:Z:43:ARG:HD3	5:1:55:TYR:OH	2.01	0.61
1:C:316:LYS:HG2	7:C:504:HEM:HAD2	1.81	0.61
3:M:146:LEU:O	3:M:149:ALA:N	2.34	0.61
5:A:18:ARG:NH1	12:A:101:PEF:H51	2.16	0.61
5:O:43:ASP:HB2	5:Q:48:ASP:HA	1.83	0.61
3:y:2:PRO:HB2	4:t:201:ARG:CZ	2.31	0.61
3:y:4:TYR:CE1	3:y:6:ASN:HA	2.36	0.61
5:AG:42:THR:HG21	5:AI:47:LEU:HD13	1.83	0.61
10:L:302:BPH:H161	9:L:305:BCL:HMB1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:5:ASN:HB3	5:U:8:LEU:HB2	1.83	0.60
4:t:32:ARG:NH2	4:t:62:PRO:HA	2.16	0.60
5:p:27:PHE:CE1	5:r:29:ILE:HD13	2.36	0.60
5:r:13:LEU:O	6:s:7:THR:N	2.33	0.60
6:z:29:PHE:O	6:z:33:VAL:HG23	2.01	0.60
15:AE:103:CRT:H372	5:AG:36:HIS:CG	2.35	0.60
6:AF:45:TRP:CD1	6:AF:46:LEU:HG	2.35	0.60
5:d:5:ASN:ND2	6:g:20:ILE:HA	2.15	0.60
2:L:77:PRO:HB2	2:L:152:GLY:HA2	1.82	0.60
6:G:13:GLU:HB3	15:G:101:CRT:H21A	1.82	0.60
9:W:101:BCL:HAA2	9:W:101:BCL:HBD	1.83	0.60
9:x:305:BCL:H143	9:x:305:BCL:HMA1	1.81	0.60
3:y:36:PHE:HA	3:y:46:ALA:O	2.00	0.60
4:t:136:MET:HE3	4:t:142:PHE:HB3	1.83	0.60
4:H:60:ASP:CG	4:H:61:LEU:H	2.09	0.60
5:1:10:LYS:HB3	15:4:101:CRT:H22A	1.84	0.60
5:1:36:HIS:CE1	9:1:102:BCL:HMD3	2.35	0.60
5:9:39:VAL:HG11	9:9:103:BCL:HBC1	1.83	0.60
1:o:97:VAL:HG21	1:o:131:PHE:CZ	2.36	0.60
5:f:27:PHE:CE1	5:h:29:ILE:HD13	2.36	0.60
5:j:24:ILE:HG12	9:l:101:BCL:H171	1.84	0.60
9:G:102:BCL:H3A	9:G:102:BCL:C1	2.30	0.60
9:AH:103:BCL:H52	9:AH:103:BCL:H3A	1.83	0.60
3:M:72:GLY:HA3	15:M:404:CRT:C6	2.31	0.60
9:A:102:BCL:HBA2	6:B:32:VAL:HG21	1.84	0.60
9:Y:101:BCL:H2	6:Z:28:TRP:CH2	2.36	0.60
9:x:305:BCL:O1D	3:y:203:MET:HB3	2.00	0.60
6:z:18:HIS:O	6:z:22:MET:HG2	2.01	0.60
1:o:67:SER:HA	1:o:68:THR:HG22	1.83	0.60
9:p:104:BCL:H92	6:q:33:VAL:HG22	1.83	0.60
4:H:235:GLU:O	4:H:239:VAL:HG23	2.02	0.60
6:J:18:HIS:O	6:J:22:MET:HG2	2.00	0.60
1:o:21:LEU:HD21	2:x:274:TRP:CE2	2.36	0.60
9:x:303:BCL:HED1	3:y:179:ILE:HG23	1.83	0.60
5:AA:50:ASN:HB2	5:AC:59:GLY:HA3	1.82	0.60
9:d:101:BCL:H2	6:e:28:TRP:CH2	2.37	0.60
15:AE:103:CRT:H6	6:AF:17:PHE:HA	1.83	0.60
5:j:44:LEU:HD12	5:l:47:LEU:HD22	1.84	0.60
5:l:5:ASN:O	5:l:7:ASN:N	2.27	0.60
4:H:196:PRO:HD3	4:H:243:TYR:CE2	2.37	0.60
9:Z:102:BCL:H52	9:Z:102:BCL:HBA1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1:102:BCL:H102	6:2:36:HIS:CD2	2.37	0.60
5:9:16:ASP:OD2	5:9:19:ARG:HG3	2.01	0.60
9:9:103:BCL:H2	6:0:28:TRP:CZ2	2.36	0.60
5:h:14:ILE:HG22	5:j:18:ARG:HD3	1.82	0.60
3:M:99:PRO:HB2	3:M:101:GLN:HG2	1.82	0.60
5:7:43:ASP:N	5:9:48:ASP:OD1	2.34	0.60
2:x:201:SER:HG	3:y:270:TRP:CD1	2.20	0.60
2:L:125:HIS:CD2	3:M:224:LEU:HB3	2.37	0.59
12:m:101:PEF:H51	5:l:19:ARG:NH1	2.14	0.59
5:AC:14:ILE:HD11	15:AE:103:CRT:H5	1.83	0.59
6:AJ:18:HIS:O	6:AJ:22:MET:HG2	2.01	0.59
5:h:17:PRO:HB3	6:i:17:PHE:CE1	2.36	0.59
2:L:18:ILE:HD12	2:L:35:PHE:HZ	1.67	0.59
2:L:144:ARG:HB3	2:L:145:PRO:HD3	1.84	0.59
6:N:18:HIS:O	6:N:22:MET:HG2	2.02	0.59
6:P:28:TRP:HH2	9:P:101:BCL:HBA1	1.67	0.59
6:4:29:PHE:CE1	9:4:102:BCL:H11	2.37	0.59
6:0:36:HIS:CG	9:0:101:BCL:H91	2.37	0.59
5:AG:54:SER:HB3	5:AG:57:ALA:HB3	1.84	0.59
5:f:15:LEU:HD23	5:h:18:ARG:HG3	1.83	0.59
9:h:101:BCL:H52	9:h:101:BCL:H142	1.84	0.59
1:C:273:ILE:HG12	7:C:504:HEM:HBB2	1.85	0.59
4:H:176:GLU:O	4:H:178:GLN:HG2	2.03	0.59
9:AA:101:BCL:HED2	6:AB:35:ALA:HB2	1.82	0.59
5:f:4:MET:O	5:f:6:ALA:N	2.35	0.59
2:L:191:THR:OG1	9:L:303:BCL:H12	2.02	0.59
3:M:2:PRO:HB2	4:H:201:ARG:CZ	2.32	0.59
2:x:188:PHE:CE2	2:x:248:SER:HB3	2.37	0.59
2:x:209:PRO:HD2	12:x:306:PEF:H12	1.83	0.59
6:E:17:PHE:HA	15:E:101:CRT:H6	1.83	0.59
2:x:273:ASN:O	2:x:276:LEU:N	2.34	0.59
9:m:102:BCL:H41	9:m:102:BCL:H72	1.83	0.59
6:z:45:TRP:CD1	6:z:46:LEU:HG	2.38	0.59
5:D:17:PRO:HB3	6:E:17:PHE:CZ	2.37	0.59
6:Z:17:PHE:HA	15:Z:101:CRT:H6	1.85	0.59
1:o:152:CYS:SG	7:o:502:HEM:CAB	2.90	0.59
2:L:106:PHE:CZ	9:L:301:BCL:H121	2.37	0.59
2:L:167:SER:HA	9:L:301:BCL:HBC1	1.84	0.59
2:L:188:PHE:HD2	2:L:248:SER:HB3	1.66	0.59
4:H:257:PRO:HG3	5:7:19:ARG:NH1	2.17	0.59
5:I:44:LEU:HD13	9:J:102:BCL:HAC1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:45:ASN:O	6:J:43:ARG:NH1	2.34	0.59
2:L:44:LEU:HD23	5:9:30:VAL:CG1	2.32	0.59
10:L:302:BPH:H18	9:L:305:BCL:HMB3	1.85	0.59
5:W:10:LYS:HA	5:W:13:LEU:HD13	1.83	0.59
15:Z:101:CRT:H372	5:1:36:HIS:CD2	2.38	0.59
3:y:243:THR:N	4:t:237:ASP:OD2	2.28	0.59
5:r:45:ASN:O	5:r:49:ASP:OD2	2.21	0.59
5:w:39:VAL:HG11	9:w:101:BCL:HBC1	1.85	0.59
15:AE:103:CRT:H372	5:AG:36:HIS:CD2	2.38	0.59
5:AG:5:ASN:ND2	6:AJ:23:GLN:OE1	2.33	0.59
5:1:56:GLN:HB2	5:1:57:ALA:HA	1.84	0.59
6:AH:43:ARG:HG3	5:AI:55:TYR:CE1	2.37	0.59
15:k:101:CRT:H27	9:k:102:BCL:H41	1.84	0.59
1:C:59:VAL:HG23	1:C:153:TYR:CE2	2.38	0.59
5:I:17:PRO:HB3	6:J:17:PHE:CZ	2.38	0.59
9:U:101:BCL:HED3	6:V:32:VAL:HA	1.85	0.59
1:o:307:CYS:HB3	7:o:504:HEM:C3B	2.38	0.59
5:j:4:MET:HE2	6:c:20:ILE:HG12	1.83	0.59
5:I:3:THR:N	5:I:4:MET:HA	2.18	0.58
6:T:43:ARG:HG3	5:U:55:TYR:OH	2.03	0.58
6:v:11:ASP:O	6:v:15:LYS:HG3	2.03	0.58
5:AC:36:HIS:CD2	15:AC:101:CRT:H372	2.37	0.58
15:k:101:CRT:H372	5:l:36:HIS:ND1	2.17	0.58
1:C:123:THR:O	1:C:127:SER:OG	2.13	0.58
2:L:244:PHE:CD1	11:L:304:UQ8:H43	2.28	0.58
15:A:103:CRT:H371	9:B:101:BCL:HMB2	1.85	0.58
6:Z:21:PHE:HA	15:Z:101:CRT:H11	1.85	0.58
2:x:199:HIS:HE1	2:x:239:HIS:CE1	2.21	0.58
5:AK:14:ILE:HD12	15:e:101:CRT:H82	1.84	0.58
1:o:295:ARG:NH2	7:o:502:HEM:O1A	2.32	0.58
5:m:11:ILE:HD13	15:p:103:CRT:H10	1.84	0.58
6:N:43:ARG:HG3	5:O:55:TYR:OH	2.04	0.58
1:o:103:PRO:HG2	1:o:104:LYS:HD2	1.86	0.58
6:v:17:PHE:CD1	15:v:101:CRT:H6	2.39	0.58
6:G:43:ARG:HG3	5:I:55:TYR:CZ	2.38	0.58
15:8:101:CRT:H27	9:8:102:BCL:H42	1.85	0.58
2:x:43:THR:HG23	10:x:302:BPH:H5C1	1.86	0.58
5:AC:17:PRO:HB3	6:AD:17:PHE:CZ	2.39	0.58
15:AH:102:CRT:H393	5:AI:36:HIS:HB3	1.86	0.58
9:AL:102:BCL:H3A	9:AL:102:BCL:CGA	2.33	0.58
5:d:14:ILE:HG12	15:f:102:CRT:H1M1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:3:THR:HB	5:l:8:LEU:HB2	1.84	0.58
15:A:103:CRT:H14	6:0:21:PHE:HA	1.86	0.58
4:t:246:GLY:HA2	4:t:250:ALA:H	1.67	0.58
15:A:103:CRT:H31A	6:0:17:PHE:HB2	1.84	0.58
6:E:40:TRP:HH2	6:E:46:LEU:HD12	1.67	0.58
6:X:45:TRP:HD1	6:X:46:LEU:HG	1.67	0.58
3:y:3:GLU:OE2	4:t:247:LYS:NZ	2.27	0.58
4:t:4:GLY:O	4:t:6:THR:N	2.36	0.58
5:f:43:ASP:O	5:h:56:GLN:NE2	2.36	0.58
1:C:110:CYS:HA	1:C:123:THR:OG1	2.04	0.58
1:C:164:TYR:CD2	1:C:312:GLN:HG2	2.39	0.58
3:M:3:GLU:OE2	4:H:212:ASP:HB3	2.04	0.58
3:M:96:GLU:HG3	3:M:97:PRO:HD2	1.85	0.58
5:1:5:ASN:OD1	5:1:7:ASN:N	2.37	0.58
1:o:97:VAL:HG21	1:o:131:PHE:HZ	1.69	0.58
12:x:306:PEF:H51	4:t:68:VAL:N	2.10	0.58
5:7:38:ILE:O	5:7:41:SER:OG	2.19	0.58
5:9:49:ASP:HB2	5:9:51:ILE:HG13	1.85	0.58
3:M:7:ILE:HG13	12:M:407:PEF:H11	1.86	0.58
4:H:136:MET:HE3	4:H:142:PHE:HB3	1.86	0.58
5:A:17:PRO:HB3	6:B:17:PHE:CZ	2.39	0.58
6:P:43:ARG:HG3	5:Q:55:TYR:OH	2.04	0.58
5:U:40:LEU:HD11	5:U:47:LEU:HD12	1.86	0.58
5:7:44:LEU:HD12	5:9:47:LEU:HD22	1.85	0.58
1:o:47:ARG:HG2	1:o:47:ARG:HH11	1.68	0.58
2:x:42:PHE:CD2	2:x:104:GLY:HA3	2.39	0.58
5:j:12:TRP:HZ3	5:j:20:VAL:HG21	1.69	0.58
9:F:101:BCL:HBA1	6:G:28:TRP:HH2	1.69	0.57
3:y:201:PHE:HD1	3:y:279:THR:HG22	1.68	0.57
4:H:44:ASP:HB3	4:H:48:ARG:HH21	1.68	0.57
5:U:40:LEU:HD13	5:U:46:TRP:CH2	2.38	0.57
3:y:59:LEU:HB3	3:y:128:LEU:HD13	1.85	0.57
9:g:101:BCL:H12	9:g:101:BCL:H3A	1.86	0.57
15:k:101:CRT:H27	9:k:102:BCL:C4	2.34	0.57
1:C:128:ARG:HH21	7:C:501:HEM:HAD1	1.69	0.57
1:C:232:THR:O	1:C:236:MET:HG2	2.04	0.57
4:t:35:LYS:HG2	4:t:39:TYR:CE1	2.39	0.57
5:d:28:GLN:NE2	9:e:102:BCL:O1A	2.27	0.57
5:d:39:VAL:HG11	9:d:101:BCL:HBC1	1.86	0.57
4:H:45:ARG:HH12	12:H:301:PEF:H21	1.70	0.57
5:F:23:SER:HB3	9:I:101:BCL:H143	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:39:VAL:HG11	9:W:101:BCL:HBC1	1.85	0.57
4:t:29:TYR:CE1	12:t:303:PEF:C30	2.86	0.57
5:w:8:LEU:HD11	15:AC:101:CRT:H133	1.86	0.57
5:j:17:PRO:HB3	6:k:17:PHE:CZ	2.39	0.57
2:L:26:TRP:HZ3	4:H:99:PRO:HB3	1.69	0.57
5:F:12:TRP:HB2	6:G:14:ALA:HB1	1.86	0.57
5:S:17:PRO:HB3	6:T:17:PHE:CZ	2.38	0.57
3:y:229:PHE:CE2	3:y:247:ARG:HD3	2.38	0.57
5:w:40:LEU:O	5:w:45:ASN:ND2	2.37	0.57
10:L:302:BPH:H111	9:L:305:BCL:H192	1.85	0.57
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.86	0.57
3:M:277:VAL:CG1	10:M:402:BPH:HAC2	2.34	0.57
5:F:16:ASP:OD2	5:F:19:ARG:HG3	2.05	0.57
5:S:48:ASP:OD1	5:S:48:ASP:N	2.36	0.57
3:y:271:TRP:CD1	4:t:26:LEU:HD11	2.40	0.57
9:y:401:BCL:H2	10:y:402:BPH:CHC	2.31	0.57
5:AK:14:ILE:HG22	5:d:18:ARG:HG3	1.86	0.57
3:M:178:GLY:O	3:M:182:HIS:HB3	2.05	0.57
6:J:20:ILE:HD12	15:J:101:CRT:C6	2.35	0.57
9:W:101:BCL:H152	9:W:101:BCL:H93	1.87	0.57
6:2:40:TRP:HE3	6:2:45:TRP:CZ3	2.23	0.57
5:7:10:LYS:HA	5:7:13:LEU:HD13	1.86	0.57
9:w:101:BCL:HAA1	9:w:101:BCL:HBD	1.86	0.57
6:AL:32:VAL:HG21	9:AL:102:BCL:HBA2	1.87	0.57
9:g:101:BCL:HMA1	9:h:101:BCL:HMA1	1.87	0.57
4:H:49:SER:O	12:H:303:PEF:N	2.38	0.57
6:0:45:TRP:CD1	6:0:46:LEU:HG	2.40	0.57
5:AA:43:ASP:HB2	5:AC:48:ASP:HA	1.86	0.57
5:AC:43:ASP:HB2	5:AE:48:ASP:OD1	2.05	0.57
1:C:105:GLU:N	1:C:105:GLU:OE2	2.38	0.57
3:M:125:SER:OG	10:M:402:BPH:H2	2.04	0.57
3:M:267:ARG:HD3	12:H:304:PEF:C31	2.34	0.57
5:F:44:LEU:HD23	5:I:55:TYR:CE2	2.40	0.57
6:V:18:HIS:O	6:V:22:MET:HG2	2.03	0.57
2:x:240:ARG:HA	3:y:224:LEU:HD11	1.87	0.57
5:m:33:LEU:HD23	15:c:101:CRT:H36	1.86	0.57
5:m:48:ASP:OD1	5:l:43:ASP:N	2.38	0.57
5:AG:10:LYS:HA	5:AG:13:LEU:HD13	1.86	0.57
5:f:45:ASN:HB3	5:h:56:GLN:HE22	1.70	0.57
3:M:8:PHE:HB2	12:M:407:PEF:H42	1.86	0.57
4:H:157:VAL:HG12	4:H:163:VAL:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:45:TRP:HZ2	9:J:102:BCL:H122	1.70	0.57
5:K:17:PRO:HB3	6:N:17:PHE:CZ	2.39	0.57
5:3:40:LEU:HG	5:3:46:TRP:CZ3	2.39	0.57
15:y:404:CRT:H2M3	5:AA:38:ILE:HA	1.87	0.57
4:t:113:PRO:HG3	4:t:248:LEU:HB3	1.87	0.57
5:p:19:ARG:NH2	12:p:101:PEF:HN2	2.03	0.57
6:B:45:TRP:HD1	6:B:46:LEU:HG	1.71	0.56
5:W:10:LYS:HD3	15:Z:101:CRT:H31A	1.86	0.56
5:W:21:LEU:HD11	15:X:101:CRT:H133	1.87	0.56
6:X:40:TRP:HH2	6:X:46:LEU:OXT	1.87	0.56
5:Y:44:LEU:HD23	5:1:55:TYR:CE2	2.36	0.56
2:x:126:VAL:HG11	3:y:251:PHE:CE2	2.40	0.56
5:w:17:PRO:HB3	6:z:17:PHE:CZ	2.40	0.56
1:C:110:CYS:SG	7:C:501:HEM:CAC	2.93	0.56
2:L:189:PHE:CE1	2:L:249:ALA:HB1	2.40	0.56
9:G:102:BCL:H101	9:G:102:BCL:HBB2	1.88	0.56
5:I:9:TYR:HB2	6:J:14:ALA:O	2.06	0.56
6:R:21:PHE:HA	15:R:101:CRT:H15	1.86	0.56
5:1:57:ALA:N	5:1:58:LEU:C	2.62	0.56
1:o:301:ASP:HB2	1:o:304:ARG:NH1	2.20	0.56
3:y:240:HIS:CE1	4:t:69:LEU:HD11	2.40	0.56
4:t:153:GLY:H	4:t:167:VAL:HB	1.69	0.56
6:s:8:GLY:O	6:s:9:LEU:HD12	2.05	0.56
6:s:21:PHE:HA	15:s:101:CRT:H14	1.86	0.56
5:AK:49:ASP:OD2	6:AL:43:ARG:NH1	2.38	0.56
6:P:21:PHE:CE1	15:P:102:CRT:H16	2.40	0.56
9:U:101:BCL:HAA2	9:U:101:BCL:HBD	1.87	0.56
9:Z:102:BCL:HED2	9:Z:102:BCL:HAA2	1.87	0.56
1:o:152:CYS:CA	7:o:502:HEM:HAB	2.36	0.56
9:AB:101:BCL:H42	9:AD:101:BCL:H172	1.88	0.56
5:AK:45:ASN:OD1	5:AK:47:LEU:N	2.34	0.56
1:C:250:CYS:HA	1:C:263:THR:OG1	2.04	0.56
5:S:5:ASN:C	5:S:7:ASN:H	2.13	0.56
6:s:31:LEU:O	6:s:34:ILE:HB	2.04	0.56
9:u:101:BCL:H12	6:v:28:TRP:CZ2	2.40	0.56
6:e:17:PHE:HB2	15:e:101:CRT:H23	1.88	0.56
1:C:72:ALA:N	1:C:85:LEU:O	2.30	0.56
6:8:21:PHE:HA	15:8:101:CRT:H11	1.88	0.56
5:w:12:TRP:O	6:z:7:THR:OG1	2.22	0.56
5:h:45:ASN:O	5:h:49:ASP:CG	2.43	0.56
5:l:17:PRO:HB3	6:c:17:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:102:ALA:HB2	10:L:302:BPH:H121	1.87	0.56
9:D:102:BCL:HBA2	6:E:32:VAL:HG21	1.88	0.56
1:o:36:ARG:HD2	2:x:77:PRO:O	2.06	0.56
1:o:47:ARG:HH11	1:o:47:ARG:CG	2.19	0.56
10:x:302:BPH:H161	9:x:305:BCL:HMB1	1.87	0.56
4:t:171:TRP:HB2	4:t:181:TYR:HB2	1.86	0.56
5:u:3:THR:HB	5:u:8:LEU:HB3	1.88	0.56
9:w:101:BCL:HAA1	9:w:101:BCL:CBD	2.36	0.56
5:AC:36:HIS:CE1	9:AC:102:BCL:HMD3	2.41	0.56
6:k:44:PRO:O	5:l:52:PRO:HD2	2.06	0.56
9:U:101:BCL:HBC2	9:V:101:BCL:HMD1	1.87	0.56
15:2:101:CRT:C32	9:3:101:BCL:H3A	2.36	0.56
5:5:36:HIS:CE1	9:5:102:BCL:HMD3	2.41	0.56
2:x:177:HIS:HB3	3:y:183:LEU:HD13	1.88	0.56
4:t:189:ASN:OD1	4:t:191:LYS:HB2	2.05	0.56
5:AI:16:ASP:OD2	5:AI:19:ARG:HG3	2.06	0.56
5:h:14:ILE:HD13	15:k:101:CRT:H1M1	1.88	0.56
1:C:242:SER:HA	1:C:308:MET:CE	2.36	0.56
5:F:5:ASN:N	6:J:23:GLN:OE1	2.39	0.56
9:1:102:BCL:HBA2	6:2:32:VAL:HG21	1.87	0.56
5:f:28:GLN:OE1	6:g:28:TRP:NE1	2.32	0.56
5:3:5:ASN:ND2	6:6:23:GLN:OE1	2.39	0.56
1:o:83:LYS:O	1:o:85:LEU:N	2.39	0.56
1:o:127:SER:OG	7:o:501:HEM:HAC	2.05	0.56
1:o:202:PRO:O	1:o:208:ASN:HB2	2.05	0.56
5:u:8:LEU:HD21	9:w:101:BCL:H141	1.88	0.56
5:h:34:LEU:O	5:h:38:ILE:HG13	2.06	0.56
1:C:200:LEU:HD22	1:C:204:LEU:HD12	1.87	0.55
3:M:34:PRO:CG	3:M:50:PRO:HD3	2.36	0.55
3:M:152:ALA:O	3:M:155:PHE:HB3	2.05	0.55
4:H:140:LYS:H	4:H:140:LYS:HD2	1.71	0.55
6:E:16:GLU:O	6:E:20:ILE:HG13	2.07	0.55
5:I:26:ALA:O	5:I:29:ILE:HG22	2.05	0.55
9:T:102:BCL:H3A	9:T:102:BCL:H43	1.88	0.55
5:W:41:SER:O	18:W:201:HOH:O	2.18	0.55
1:o:164:TYR:CB	1:o:309:THR:HA	2.36	0.55
2:x:222:ASN:HD21	4:t:176:GLU:HG3	1.71	0.55
2:x:244:PHE:HE2	11:x:304:UQ8:H21	1.70	0.55
6:AB:45:TRP:HD1	6:AB:46:LEU:HG	1.69	0.55
2:L:129:ALA:HB1	2:L:247:LEU:HD21	1.86	0.55
5:U:16:ASP:OD2	5:U:19:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LYS:HD3	15:8:101:CRT:H22A	1.88	0.55
3:y:150:PHE:O	3:y:154:ILE:HG13	2.06	0.55
4:t:135:PRO:HB3	4:t:171:TRP:CD1	2.41	0.55
15:p:103:CRT:H21A	6:q:13:GLU:HB3	1.86	0.55
6:s:32:VAL:HG21	9:s:102:BCL:HBA2	1.88	0.55
5:d:49:ASP:HB2	5:d:51:ILE:CG1	2.34	0.55
3:M:260:VAL:HG12	4:H:34:ASP:OD2	2.06	0.55
3:M:277:VAL:HG11	10:M:402:BPH:HAC2	1.88	0.55
1:o:71:LYS:O	1:o:74:GLU:HB2	2.06	0.55
1:o:227:LYS:NZ	3:y:96:GLU:OE2	2.39	0.55
5:m:36:HIS:CD2	15:c:101:CRT:H372	2.41	0.55
9:p:102:BCL:HAC1	9:p:104:BCL:HBC2	1.88	0.55
1:C:188:LYS:HB2	1:C:192:TYR:CZ	2.41	0.55
1:C:245:VAL:HG21	1:C:249:PHE:CD2	2.42	0.55
2:L:35:PHE:CD2	2:L:111:LEU:HB3	2.42	0.55
5:A:13:LEU:O	5:D:18:ARG:NH2	2.40	0.55
15:X:101:CRT:H181	15:X:101:CRT:C21	2.33	0.55
6:Z:43:ARG:HD3	5:1:55:TYR:CE1	2.42	0.55
5:r:14:ILE:HG13	5:r:15:LEU:HG	1.89	0.55
5:h:42:THR:HG21	5:j:47:LEU:HD13	1.88	0.55
3:M:102:TYR:OH	3:M:111:GLU:OE1	2.16	0.55
4:H:29:TYR:OH	12:H:304:PEF:C30	2.54	0.55
4:H:44:ASP:O	4:H:48:ARG:HB2	2.06	0.55
5:1:38:ILE:O	5:1:42:THR:HG23	2.06	0.55
3:y:63:PHE:CE1	5:AC:30:VAL:HG22	2.42	0.55
5:r:4:MET:HG3	6:v:19:ALA:HB1	1.89	0.55
6:s:43:ARG:HG3	5:u:55:TYR:CZ	2.42	0.55
15:AL:101:CRT:H27	9:AL:102:BCL:H11	1.89	0.55
5:d:5:ASN:OD1	5:d:7:ASN:N	2.38	0.55
3:M:109:LEU:HD11	5:Q:42:THR:HG22	1.89	0.55
5:5:43:ASP:HB2	5:7:48:ASP:HA	1.88	0.55
15:n:101:CRT:H342	9:p:102:BCL:HBA2	1.88	0.55
5:h:19:ARG:HA	5:h:22:VAL:HG22	1.89	0.55
1:C:20:LEU:HA	1:C:21:LEU:CB	2.34	0.55
1:C:56:ASN:HB3	1:C:318:LEU:HA	1.88	0.55
5:D:12:TRP:HB3	5:D:17:PRO:HG3	1.87	0.55
6:R:40:TRP:CH2	6:R:46:LEU:HB2	2.42	0.55
5:S:25:VAL:HG21	9:S:102:BCL:H121	1.89	0.55
1:o:219:ALA:HB2	3:y:292:ASP:HB2	1.88	0.55
2:x:126:VAL:HG11	3:y:251:PHE:HE2	1.71	0.55
3:y:34:PRO:CG	3:y:50:PRO:HD3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AL:45:TRP:CE2	9:AL:102:BCL:H2C	2.41	0.55
2:L:184:LEU:HD23	2:L:252:TRP:CE2	2.42	0.55
2:L:222:ASN:HB3	2:L:226:ARG:NH1	2.22	0.55
9:F:101:BCL:HAA2	9:F:101:BCL:HBD	1.89	0.55
6:G:46:LEU:HD22	6:J:42:TYR:CE2	2.41	0.55
6:J:21:PHE:HA	15:J:101:CRT:H14	1.87	0.55
15:8:101:CRT:H293	9:9:103:BCL:H202	1.88	0.55
5:9:5:ASN:C	5:9:7:ASN:H	2.12	0.55
5:AA:14:ILE:HD11	15:AD:102:CRT:H31A	1.88	0.55
15:N:101:CRT:H393	5:O:36:HIS:HB3	1.89	0.55
5:U:25:VAL:HG22	9:U:101:BCL:H41	1.89	0.55
15:2:101:CRT:H35	9:3:101:BCL:HMB2	1.89	0.55
5:7:4:MET:HG3	5:7:5:ASN:H	1.72	0.55
3:y:71:ILE:O	3:y:75:MET:HG3	2.06	0.55
6:n:20:ILE:HB	15:n:101:CRT:H82	1.89	0.55
9:l:101:BCL:H101	9:l:101:BCL:H203	1.89	0.55
2:L:71:TRP:CD1	3:M:303:MET:HG2	2.42	0.55
4:H:193:VAL:HB	4:H:222:VAL:HG11	1.89	0.55
5:F:17:PRO:HB3	6:G:17:PHE:CZ	2.42	0.55
5:F:54:SER:HB3	5:F:57:ALA:HB3	1.89	0.55
15:N:101:CRT:H372	5:O:36:HIS:CD2	2.42	0.55
5:S:14:ILE:HD11	15:U:102:CRT:H31A	1.89	0.55
5:Y:51:ILE:CG2	5:Y:52:PRO:HA	2.35	0.55
2:x:96:GLN:O	2:x:100:ILE:HG13	2.07	0.55
10:x:302:BPH:H141	9:x:305:BCL:HBB2	1.89	0.55
4:t:5:ILE:HD12	5:w:56:GLN:O	2.07	0.55
4:t:53:VAL:HG22	12:p:101:PEF:O5	2.07	0.55
9:m:103:BCL:H142	6:n:33:VAL:HG22	1.89	0.55
5:h:44:LEU:HD12	5:j:47:LEU:HD23	1.89	0.55
1:C:124:LYS:HE3	7:C:501:HEM:C3D	2.42	0.54
6:P:43:ARG:HG3	5:Q:55:TYR:CZ	2.42	0.54
1:o:195:LEU:HB3	1:o:196:PRO:CD	2.36	0.54
2:L:203:ILE:HG13	3:M:266:HIS:HD2	1.67	0.54
6:4:20:ILE:HD12	15:4:101:CRT:C6	2.37	0.54
5:9:46:TRP:CD2	9:9:103:BCL:H2C	2.42	0.54
6:0:45:TRP:HD1	6:0:46:LEU:HG	1.71	0.54
1:o:247:CYS:SG	7:o:503:HEM:HAB	2.47	0.54
2:x:219:GLU:HG2	3:y:18:TYR:OH	2.07	0.54
3:y:7:ILE:HB	12:y:407:PEF:O2P	2.07	0.54
3:y:66:VAL:HG11	5:AC:34:LEU:HD13	1.88	0.54
2:x:167:SER:HA	9:x:301:BCL:HBC1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:80:HIS:O	3:y:81:TRP:HB2	2.07	0.54
5:r:45:ASN:OD1	5:r:46:TRP:N	2.41	0.54
6:v:31:LEU:HD23	6:v:34:ILE:HD12	1.89	0.54
5:AA:10:LYS:HB3	15:AD:102:CRT:H33	1.89	0.54
5:AE:3:THR:OG1	5:AE:4:MET:N	2.40	0.54
15:f:102:CRT:H31A	6:g:16:GLU:OE1	2.08	0.54
9:L:303:BCL:H111	9:M:401:BCL:H171	1.89	0.54
3:M:35:ILE:HG13	3:M:48:ILE:HB	1.89	0.54
3:M:39:TRP:O	3:M:40:LEU:C	2.51	0.54
5:S:17:PRO:HB3	6:T:17:PHE:CE1	2.43	0.54
5:3:31:LEU:HD12	5:3:34:LEU:HD23	1.89	0.54
1:o:164:TYR:HB2	1:o:309:THR:HA	1.89	0.54
5:m:8:LEU:HG	6:q:20:ILE:HD13	1.89	0.54
5:m:16:ASP:OD2	5:m:19:ARG:HG3	2.08	0.54
9:AL:102:BCL:CB	9:AL:102:BCL:HAA1	2.37	0.54
1:C:181:THR:C	1:C:183:GLN:H	2.16	0.54
3:M:197:TYR:CE1	9:M:401:BCL:HMC2	2.42	0.54
5:Q:9:TYR:HB2	6:R:14:ALA:O	2.07	0.54
1:o:19:MET:HE3	1:o:21:LEU:CD1	2.38	0.54
3:y:63:PHE:HB2	3:y:125:SER:HB2	1.89	0.54
4:t:224:THR:OG1	4:t:225:LEU:N	2.40	0.54
5:m:17:PRO:HB3	6:n:17:PHE:CZ	2.42	0.54
5:AE:5:ASN:OD1	6:AH:23:GLN:NE2	2.40	0.54
2:L:18:ILE:HD12	2:L:35:PHE:CZ	2.43	0.54
2:L:228:ILE:O	3:M:132:ARG:NH2	2.39	0.54
6:Z:42:TYR:O	6:Z:43:ARG:HG3	2.08	0.54
5:1:44:LEU:HD23	5:3:55:TYR:HE2	1.70	0.54
5:r:55:TYR:C	5:r:57:ALA:H	2.15	0.54
5:AE:34:LEU:HD21	15:AE:103:CRT:H2M2	1.89	0.54
9:AI:101:BCL:HBD	9:AI:101:BCL:HAA1	1.89	0.54
1:C:211:ARG:HD3	3:M:317:TYR:CE2	2.43	0.54
5:A:36:HIS:CD2	15:A:103:CRT:H372	2.43	0.54
6:B:28:TRP:CH2	9:B:101:BCL:H2	2.42	0.54
6:E:46:LEU:HD23	6:G:42:TYR:HE1	1.72	0.54
5:O:17:PRO:HB3	6:P:17:PHE:CZ	2.43	0.54
6:X:36:HIS:CD2	9:X:102:BCL:H8	2.42	0.54
6:0:32:VAL:HG21	9:0:101:BCL:HBA2	1.90	0.54
3:y:37:SER:HB2	12:y:406:PEF:H21	1.89	0.54
5:d:36:HIS:CE1	9:e:102:BCL:HMD3	2.43	0.54
9:e:102:BCL:HBB3	9:f:101:BCL:CHC	2.37	0.54
6:g:32:VAL:HG21	9:g:101:BCL:O1A	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:101:BCL:HBC2	9:c:102:BCL:HMD1	1.90	0.54
1:C:237:MET:SD	2:L:174:LEU:HB3	2.46	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.89	0.54
5:Q:51:ILE:CD1	6:R:43:ARG:HH22	2.21	0.54
1:o:181:THR:HB	1:o:183:GLN:O	2.07	0.54
2:x:203:ILE:HG13	3:y:266:HIS:HD2	1.72	0.54
5:m:40:LEU:HG	5:m:46:TRP:CH2	2.42	0.54
5:u:26:ALA:O	5:u:29:ILE:HG22	2.07	0.54
5:l:17:PRO:HB3	6:c:17:PHE:CE1	2.43	0.54
4:H:247:LYS:HA	4:H:254:ARG:HH11	1.72	0.54
5:W:9:TYR:CE1	5:W:10:LYS:HG3	2.43	0.54
5:W:43:ASP:OD2	5:Y:55:TYR:HB2	2.08	0.54
9:X:102:BCL:CHB	9:X:102:BCL:H71	2.38	0.54
9:1:101:BCL:H2	6:2:28:TRP:CH2	2.42	0.54
5:r:16:ASP:OD1	5:r:18:ARG:N	2.41	0.54
5:j:43:ASP:HB2	5:l:48:ASP:HA	1.89	0.54
6:c:36:HIS:ND1	9:c:102:BCL:H111	2.23	0.54
1:C:19:MET:C	1:C:21:LEU:HD13	2.33	0.54
9:B:101:BCL:H61	5:9:2:PHE:CE1	2.43	0.54
5:I:45:ASN:O	5:I:49:ASP:OD2	2.25	0.54
9:Q:101:BCL:H191	6:R:31:LEU:HD22	1.90	0.54
6:T:43:ARG:HG3	5:U:55:TYR:CZ	2.43	0.54
5:Y:46:TRP:CD2	9:Y:101:BCL:H2C	2.43	0.54
5:7:40:LEU:HG	5:7:46:TRP:CH2	2.42	0.54
1:o:152:CYS:HA	7:o:502:HEM:HAB	1.90	0.54
3:y:260:VAL:HG12	4:t:34:ASP:CG	2.32	0.54
5:u:34:LEU:O	5:u:38:ILE:HG13	2.08	0.54
5:f:17:PRO:HG2	6:g:9:LEU:HD21	1.89	0.54
5:j:27:PHE:CE1	5:l:29:ILE:HD13	2.42	0.54
1:o:41:GLU:OE2	2:x:80:LEU:HD11	2.08	0.53
1:o:269:ALA:O	1:o:273:ILE:HG13	2.07	0.53
6:AJ:43:ARG:HG3	5:AK:55:TYR:CE1	2.43	0.53
5:h:42:THR:HG21	5:j:47:LEU:HB3	1.89	0.53
1:C:21:LEU:HD11	2:L:274:TRP:CD2	2.42	0.53
3:M:163:ILE:O	3:M:167:MET:HG3	2.07	0.53
4:H:96:PRO:HD3	6:0:7:THR:HA	1.90	0.53
4:H:141:GLU:HG2	4:H:142:PHE:HD1	1.73	0.53
5:U:51:ILE:HG23	5:U:52:PRO:HA	1.91	0.53
5:W:36:HIS:NE2	9:W:101:BCL:NB	2.56	0.53
5:7:35:ILE:HG12	15:8:101:CRT:H403	1.89	0.53
2:x:238:ILE:HG12	11:x:304:UQ8:C2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:106:PHE:CD2	9:L:301:BCL:H91	2.43	0.53
3:M:175:VAL:CG1	3:M:176:PRO:HD2	2.38	0.53
3:M:265:ILE:CD1	14:M:403:MQ8:H121	2.38	0.53
5:A:33:LEU:HD23	15:A:103:CRT:H36	1.90	0.53
1:o:181:THR:C	1:o:183:GLN:H	2.15	0.53
2:x:196:LEU:HD13	3:y:216:PHE:HB2	1.90	0.53
3:y:12:GLN:OE1	3:y:14:ARG:NH2	2.34	0.53
15:y:404:CRT:C6	15:y:404:CRT:H33	2.36	0.53
5:AI:3:THR:HG22	6:AJ:18:HIS:NE2	2.24	0.53
5:D:2:PHE:O	5:D:3:THR:OG1	2.26	0.53
5:W:40:LEU:HG	5:W:46:TRP:CH2	2.43	0.53
1:o:19:MET:C	1:o:21:LEU:HD22	2.33	0.53
1:o:110:CYS:O	1:o:124:LYS:HB2	2.09	0.53
3:y:126:ILE:HD13	9:y:401:BCL:H91	1.89	0.53
5:AI:50:ASN:HB3	5:AI:54:SER:HA	1.89	0.53
5:AK:17:PRO:HG2	6:AL:9:LEU:HD11	1.91	0.53
4:H:36:ARG:C	4:H:37:GLU:HG2	2.33	0.53
4:H:57:GLY:H	12:H:301:PEF:C5	2.20	0.53
5:U:5:ASN:OD1	5:U:6:ALA:N	2.41	0.53
9:U:101:BCL:H2	6:V:28:TRP:CZ2	2.42	0.53
5:Y:5:ASN:HA	6:2:23:GLN:HE22	1.72	0.53
5:Y:23:SER:HB3	9:1:101:BCL:H151	1.90	0.53
6:i:40:TRP:CE3	6:i:44:PRO:HA	2.43	0.53
1:C:311:HIS:HA	1:C:317:PRO:HG3	1.90	0.53
3:M:202:HIS:HE1	9:M:401:BCL:ND	2.07	0.53
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.91	0.53
4:H:189:ASN:ND2	4:H:191:LYS:HB2	2.24	0.53
5:A:18:ARG:HH12	12:A:101:PEF:H51	1.74	0.53
9:B:101:BCL:H193	9:B:101:BCL:H8	1.91	0.53
6:J:29:PHE:O	6:J:33:VAL:HG23	2.08	0.53
5:O:35:ILE:HG12	5:O:38:ILE:HD12	1.91	0.53
5:Q:10:LYS:HB3	15:T:101:CRT:H22A	1.90	0.53
5:S:16:ASP:OD1	5:S:18:ARG:N	2.41	0.53
6:T:34:ILE:O	6:T:38:LEU:HG	2.08	0.53
5:5:43:ASP:OD2	5:7:50:ASN:HA	2.09	0.53
2:x:17:LEU:HD11	2:x:114:VAL:HG11	1.90	0.53
2:x:190:PHE:CE1	9:y:401:BCL:HBA2	2.44	0.53
9:x:303:BCL:CED	3:y:179:ILE:HG23	2.38	0.53
3:y:215:LEU:HD21	14:y:403:MQ8:C18	2.38	0.53
5:j:32:GLY:HA2	9:k:102:BCL:CED	2.34	0.53
5:7:28:GLN:OE1	6:8:28:TRP:NE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:65:LEU:HD13	3:y:308:PRO:HG3	1.90	0.53
2:x:206:VAL:CG1	3:y:142:MET:HE3	2.38	0.53
5:p:9:TYR:CZ	5:p:10:LYS:HE2	2.43	0.53
6:c:11:ASP:O	6:c:15:LYS:HG3	2.09	0.53
2:L:3:MET:HB3	2:L:7:GLU:HB3	1.91	0.53
9:M:401:BCL:H61	10:M:402:BPH:CHC	2.39	0.53
9:T:102:BCL:HMA1	9:U:101:BCL:HMA1	1.89	0.53
5:U:9:TYR:HB2	6:V:14:ALA:O	2.09	0.53
5:5:18:ARG:O	5:5:21:LEU:HB2	2.09	0.53
1:o:118:SER:O	1:o:124:LYS:HD3	2.09	0.53
2:x:250:ALA:HB2	10:x:302:BPH:HAC2	1.91	0.53
5:p:11:ILE:HD12	5:p:14:ILE:HD12	1.91	0.53
6:q:46:LEU:HB3	6:s:42:TYR:OH	2.08	0.53
6:AH:17:PHE:HA	15:AH:102:CRT:H6	1.90	0.53
6:AH:45:TRP:CD1	6:AH:46:LEU:HG	2.43	0.53
6:i:17:PHE:HA	15:i:101:CRT:H6	1.91	0.53
5:l:44:LEU:HD22	6:c:43:ARG:HD3	1.91	0.53
5:A:51:ILE:HG21	6:0:46:LEU:HA	1.90	0.53
5:K:35:ILE:HD11	15:N:101:CRT:H403	1.89	0.53
5:5:46:TRP:CH2	9:5:101:BCL:H2C	2.43	0.53
9:AH:103:BCL:HAA2	9:AH:103:BCL:HED3	1.90	0.53
2:L:179:ASN:HB3	2:L:182:HIS:HB2	1.91	0.53
4:H:124:ASP:HB2	4:H:233:LEU:HD21	1.91	0.53
6:B:17:PHE:HA	15:9:102:CRT:H83	1.91	0.53
1:o:85:LEU:HD21	1:o:329:GLY:HA3	1.91	0.53
1:o:250:CYS:O	1:o:262:SER:HB3	2.09	0.53
2:x:199:HIS:HA	11:x:304:UQ8:O2	2.09	0.53
5:p:3:THR:HG22	6:s:27:ALA:HA	1.91	0.53
5:p:4:MET:O	5:p:5:ASN:HB2	2.09	0.53
3:M:18:TYR:CD2	3:M:20:GLY:HA2	2.44	0.52
3:M:63:PHE:CD1	5:Q:30:VAL:HG22	2.45	0.52
3:M:208:PHE:CE2	3:M:275:LEU:HB3	2.44	0.52
4:H:64:PRO:HA	4:H:78:ALA:O	2.08	0.52
5:A:56:GLN:HG2	5:9:43:ASP:CG	2.34	0.52
6:E:44:PRO:O	5:F:55:TYR:OH	2.24	0.52
5:K:40:LEU:HD21	5:K:47:LEU:HD12	1.91	0.52
5:Q:12:TRP:CH2	6:R:17:PHE:HE2	2.26	0.52
5:Q:42:THR:HG21	5:S:47:LEU:HD13	1.91	0.52
6:4:21:PHE:CD1	15:4:101:CRT:H14	2.44	0.52
1:o:67:SER:HA	1:o:68:THR:CG2	2.39	0.52
2:x:148:MET:HG2	2:x:262:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:154:MET:O	4:t:167:VAL:HG23	2.09	0.52
6:n:20:ILE:HD12	15:n:101:CRT:H82	1.91	0.52
5:AG:25:VAL:HG13	9:AH:101:BCL:H192	1.91	0.52
5:d:9:TYR:HB2	6:e:14:ALA:O	2.09	0.52
5:j:44:LEU:HD13	9:k:102:BCL:HBC2	1.90	0.52
5:l:16:ASP:OD2	5:l:19:ARG:HG3	2.09	0.52
1:C:21:LEU:HD21	2:L:274:TRP:CZ2	2.44	0.52
2:L:71:TRP:CD2	3:M:303:MET:HE3	2.43	0.52
3:M:64:GLY:HA3	10:M:402:BPH:H5C2	1.91	0.52
6:N:37:LEU:O	6:N:41:LEU:HG	2.09	0.52
5:O:29:ILE:O	5:O:33:LEU:HG	2.09	0.52
6:R:18:HIS:O	6:R:22:MET:HG2	2.08	0.52
5:5:40:LEU:HG	5:5:46:TRP:CH2	2.44	0.52
2:x:10:TYR:O	2:x:12:VAL:N	2.38	0.52
2:x:26:TRP:HE1	3:y:254:TRP:CG	2.27	0.52
3:y:97:PRO:HD3	3:y:176:PRO:HB3	1.90	0.52
5:p:18:ARG:HB3	12:p:101:PEF:O3	2.08	0.52
6:v:17:PHE:HD1	15:v:101:CRT:H6	1.75	0.52
2:L:15:GLY:N	4:H:255:ALA:O	2.33	0.52
2:L:196:LEU:HD13	3:M:216:PHE:CD2	2.44	0.52
4:H:247:LYS:O	4:H:254:ARG:HD3	2.09	0.52
5:Y:46:TRP:CE3	9:Y:101:BCL:HAC1	2.45	0.52
3:y:96:GLU:HG3	3:y:97:PRO:HD2	1.92	0.52
4:t:29:TYR:CE1	12:t:303:PEF:O5	2.62	0.52
15:AE:103:CRT:C14	6:AF:21:PHE:HA	2.40	0.52
5:d:24:ILE:HD11	9:f:101:BCL:H152	1.91	0.52
15:k:101:CRT:H372	5:l:36:HIS:CE1	2.44	0.52
9:c:102:BCL:H2	9:c:102:BCL:H3A	1.92	0.52
3:M:4:TYR:HE1	3:M:6:ASN:OD1	1.92	0.52
4:H:45:ARG:NH1	4:H:53:VAL:HG21	2.25	0.52
6:B:16:GLU:O	6:B:20:ILE:HG13	2.09	0.52
6:P:29:PHE:O	6:P:32:VAL:HB	2.10	0.52
5:Q:51:ILE:HD11	6:R:43:ARG:HH22	1.75	0.52
5:W:17:PRO:HB3	6:X:17:PHE:CZ	2.44	0.52
5:9:14:ILE:HD11	15:9:102:CRT:C5	2.39	0.52
3:y:134:TYR:CE2	3:y:144:GLN:HG3	2.43	0.52
6:s:17:PHE:HB2	15:s:101:CRT:H31A	1.92	0.52
6:AD:28:TRP:O	6:AD:32:VAL:HG23	2.09	0.52
1:C:167:VAL:HG12	1:C:301:ASP:OD2	2.10	0.52
1:C:263:THR:C	3:M:313:ALA:HB2	2.34	0.52
1:C:301:ASP:HB2	1:C:304:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:199:HIS:HA	11:L:304:UQ8:O2	2.10	0.52
3:M:36:PHE:HA	3:M:46:ALA:O	2.09	0.52
6:B:31:LEU:HD23	6:B:34:ILE:HD12	1.91	0.52
6:R:40:TRP:CZ3	6:R:46:LEU:HB2	2.44	0.52
5:S:16:ASP:OD2	5:S:19:ARG:HG3	2.09	0.52
5:3:9:TYR:HB2	6:4:14:ALA:O	2.10	0.52
6:4:40:TRP:CG	9:4:102:BCL:H18	2.44	0.52
2:x:236:LEU:O	2:x:239:HIS:HB2	2.09	0.52
2:x:241:LEU:O	2:x:244:PHE:HB3	2.09	0.52
5:u:46:TRP:CD1	9:u:101:BCL:HMC2	2.45	0.52
6:AH:29:PHE:CD1	9:AH:103:BCL:H2	2.45	0.52
9:V:101:BCL:HBD	9:V:101:BCL:HAA1	1.90	0.52
6:2:7:THR:HG23	6:2:9:LEU:H	1.73	0.52
9:7:101:BCL:H111	9:7:101:BCL:H41	1.91	0.52
3:y:107:PRO:HG2	3:y:113:GLY:N	2.25	0.52
5:p:10:LYS:NZ	6:q:11:ASP:OD2	2.40	0.52
5:r:27:PHE:CZ	5:u:29:ILE:HD11	2.45	0.52
15:v:101:CRT:H372	5:w:36:HIS:CD2	2.45	0.52
5:d:13:LEU:HA	6:e:7:THR:HG21	1.92	0.52
9:L:301:BCL:NA	9:M:401:BCL:HBB2	2.25	0.52
15:T:101:CRT:H27	9:T:102:BCL:O1A	2.10	0.52
2:x:34:PHE:O	2:x:38:VAL:HG23	2.09	0.52
2:x:273:ASN:O	2:x:275:TRP:N	2.43	0.52
9:x:305:BCL:H11	3:y:210:TYR:HB3	1.92	0.52
3:y:161:GLY:HA3	15:y:404:CRT:H292	1.91	0.52
5:AE:5:ASN:O	5:AE:7:ASN:N	2.42	0.52
2:L:59:THR:OG1	2:L:63:SER:OG	2.09	0.52
6:N:17:PHE:CD1	15:N:101:CRT:H9	2.44	0.52
5:U:54:SER:O	5:U:58:LEU:N	2.43	0.52
5:w:40:LEU:HG	5:w:46:TRP:CH2	2.45	0.52
5:AC:34:LEU:O	5:AC:38:ILE:HG13	2.09	0.52
9:AC:102:BCL:HMD1	9:AD:101:BCL:HBC2	1.90	0.52
5:j:24:ILE:HD11	9:l:101:BCL:H151	1.91	0.52
1:C:219:ALA:HB2	3:M:292:ASP:HB2	1.92	0.52
5:S:13:LEU:HD21	6:T:11:ASP:HA	1.91	0.52
6:8:29:PHE:CD1	9:8:102:BCL:H12	2.45	0.52
6:8:32:VAL:HG21	9:8:102:BCL:H11	1.92	0.52
3:y:219:HIS:HB2	14:y:403:MQ8:H2M1	1.91	0.52
5:AK:3:THR:O	6:e:23:GLN:NE2	2.43	0.52
9:k:102:BCL:HMA1	9:l:101:BCL:HMA1	1.92	0.52
5:D:56:GLN:C	5:D:58:LEU:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:43:ASP:OD2	5:1:50:ASN:HA	2.10	0.52
5:1:49:ASP:O	5:1:51:ILE:HG13	2.10	0.52
1:o:33:ILE:HG21	1:o:248:THR:O	2.10	0.52
1:o:236:MET:HB3	7:o:503:HEM:C4B	2.45	0.52
2:x:137:TYR:CE1	9:x:305:BCL:HBB1	2.45	0.52
2:x:206:VAL:HG13	3:y:142:MET:HE3	1.91	0.52
3:y:219:HIS:CE1	3:y:266:HIS:HE1	2.28	0.52
6:n:31:LEU:HD23	6:n:34:ILE:HD12	1.92	0.52
6:AF:32:VAL:O	6:AF:36:HIS:ND1	2.41	0.52
2:L:125:HIS:CE1	3:M:5:GLN:OE1	2.63	0.51
2:L:275:TRP:NE1	3:M:88:LYS:O	2.42	0.51
3:M:177:PHE:CD1	15:M:404:CRT:H16	2.41	0.51
5:1:24:ILE:HD13	9:3:101:BCL:H18	1.91	0.51
5:5:43:ASP:O	5:7:55:TYR:HB2	2.10	0.51
6:0:12:ASP:O	6:0:15:LYS:HB2	2.10	0.51
6:0:40:TRP:CZ2	9:0:101:BCL:H191	2.44	0.51
1:o:250:CYS:HA	1:o:263:THR:OG1	2.10	0.51
9:x:301:BCL:H171	9:x:305:BCL:H162	1.92	0.51
3:y:63:PHE:CD1	5:AC:30:VAL:HG22	2.45	0.51
1:C:268:THR:HG21	7:C:504:HEM:C2A	2.45	0.51
3:M:187:ALA:HA	9:M:401:BCL:HBC2	1.91	0.51
3:M:240:HIS:NE2	4:H:69:LEU:HD11	2.26	0.51
1:o:43:TYR:CZ	2:x:148:MET:HE1	2.45	0.51
2:x:189:PHE:CE1	2:x:249:ALA:HB1	2.45	0.51
2:x:226:ARG:HH21	3:y:47:GLN:HB3	1.74	0.51
2:x:233:ILE:HG12	2:x:237:ALA:CB	2.41	0.51
3:y:219:HIS:O	3:y:223:ILE:HG12	2.10	0.51
12:y:407:PEF:H52	12:y:408:PEF:O1P	2.10	0.51
5:j:9:TYR:HD1	5:j:9:TYR:H	1.58	0.51
4:H:135:PRO:HA	4:H:171:TRP:HA	1.92	0.51
6:E:17:PHE:HB2	15:E:101:CRT:H31A	1.91	0.51
6:E:44:PRO:O	5:F:52:PRO:HD2	2.10	0.51
6:J:40:TRP:CE2	9:J:102:BCL:H202	2.45	0.51
15:T:101:CRT:H372	5:U:36:HIS:CD2	2.45	0.51
1:o:227:LYS:HZ1	3:y:97:PRO:HD2	1.74	0.51
2:x:17:LEU:HD11	2:x:114:VAL:CG1	2.40	0.51
2:x:130:PHE:CD2	2:x:134:ILE:HD11	2.46	0.51
6:n:43:ARG:HG3	5:p:55:TYR:CZ	2.45	0.51
5:r:51:ILE:HD13	6:s:43:ARG:NH2	2.20	0.51
6:AH:32:VAL:HG21	9:AH:103:BCL:HBA2	1.93	0.51
1:C:203:PHE:O	1:C:277:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:136:MET:HG3	4:H:170:VAL:O	2.09	0.51
6:B:44:PRO:O	5:D:55:TYR:OH	2.29	0.51
6:R:43:ARG:HG3	5:S:55:TYR:CE1	2.44	0.51
9:S:102:BCL:H41	9:S:102:BCL:H92	1.93	0.51
5:Y:11:ILE:HD13	15:2:101:CRT:H10	1.92	0.51
1:o:190:VAL:HG12	1:o:237:MET:HB2	1.92	0.51
2:x:209:PRO:HD2	12:x:306:PEF:H41	1.91	0.51
9:y:401:BCL:C2	10:y:402:BPH:HH2	2.33	0.51
9:AJ:102:BCL:CGA	9:AJ:102:BCL:H3A	2.41	0.51
1:o:74:GLU:HA	1:o:74:GLU:OE2	2.11	0.51
1:o:252:ASN:OD1	1:o:254:ARG:HG2	2.11	0.51
3:y:71:ILE:HA	3:y:95:LEU:HD22	1.93	0.51
3:y:73:PHE:N	15:y:404:CRT:H32A	2.25	0.51
5:AE:9:TYR:HB2	6:AF:14:ALA:O	2.10	0.51
5:AI:36:HIS:CE1	9:AJ:102:BCL:HMD3	2.45	0.51
5:f:34:LEU:O	5:f:38:ILE:HG13	2.10	0.51
6:i:40:TRP:HH2	6:i:46:LEU:OXT	1.94	0.51
2:L:225:PHE:CE2	11:L:304:UQ8:H1MA	2.42	0.51
3:M:274:VAL:O	3:M:278:ILE:HG12	2.11	0.51
4:H:130:LEU:HB3	4:H:174:ARG:NH2	2.26	0.51
6:P:18:HIS:O	6:P:22:MET:HG2	2.11	0.51
5:S:19:ARG:NH1	17:S:101:PGW:H01	2.26	0.51
6:O:40:TRP:HZ3	6:O:45:TRP:H	1.57	0.51
4:t:45:ARG:HH21	5:m:16:ASP:N	2.07	0.51
5:m:2:PHE:C	5:m:4:MET:H	2.18	0.51
15:n:101:CRT:H10	5:l:11:ILE:HD13	1.93	0.51
6:N:44:PRO:O	5:O:52:PRO:HD3	2.11	0.51
5:u:11:ILE:HD13	15:z:101:CRT:H10	1.92	0.51
10:L:302:BPH:H141	9:L:305:BCL:CBB	2.40	0.51
6:P:45:TRP:HD1	6:P:46:LEU:HG	1.76	0.51
5:Y:10:LYS:HB3	15:2:101:CRT:H5	1.92	0.51
5:1:17:PRO:HA	5:1:20:VAL:HG22	1.92	0.51
5:5:43:ASP:OD1	5:7:56:GLN:HG2	2.10	0.51
3:y:267:ARG:NH1	12:t:303:PEF:H31	2.25	0.51
5:m:56:GLN:NE2	5:l:43:ASP:O	2.44	0.51
5:r:9:TYR:OH	5:r:10:LYS:HE2	2.11	0.51
5:u:9:TYR:HB2	6:v:14:ALA:O	2.10	0.51
5:AE:25:VAL:HG21	9:AE:102:BCL:C15	2.41	0.51
5:f:28:GLN:HE22	9:g:101:BCL:HBA1	1.76	0.51
9:i:102:BCL:H52	9:i:102:BCL:HBA1	1.93	0.51
1:C:242:SER:HA	1:C:308:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:243:THR:O	3:M:247:ARG:HD2	2.10	0.51
6:B:20:ILE:CG2	5:9:5:ASN:HB3	2.41	0.51
9:J:102:BCL:H2	9:J:102:BCL:HBA1	1.93	0.51
1:o:98:THR:HA	7:o:501:HEM:HMC3	1.93	0.51
1:o:105:GLU:N	1:o:105:GLU:OE2	2.44	0.51
1:o:174:TYR:OH	3:y:78:SER:HB2	2.11	0.51
3:y:159:VAL:HA	3:y:163:ILE:HB	1.93	0.51
4:t:107:MET:HE2	4:t:218:HIS:HD2	1.76	0.51
2:L:155:PHE:HA	2:L:165:TRP:CD1	2.46	0.51
2:L:170:GLY:HA2	2:L:176:PHE:CD2	2.46	0.51
3:M:6:ASN:HD22	3:M:227:SER:CB	2.24	0.51
6:B:44:PRO:HG2	5:D:52:PRO:CD	2.39	0.51
5:p:9:TYR:OH	5:p:10:LYS:HE2	2.11	0.51
9:g:101:BCL:HMA1	9:g:101:BCL:H43	1.93	0.51
5:j:11:ILE:HD12	5:j:14:ILE:HD12	1.93	0.51
12:M:407:PEF:H51	12:M:408:PEF:O2P	2.11	0.50
5:I:11:ILE:HD12	5:I:14:ILE:HD12	1.92	0.50
6:R:29:PHE:O	6:R:33:VAL:HG23	2.12	0.50
1:o:65:ALA:HB2	1:o:92:ARG:HB2	1.93	0.50
1:o:302:PRO:O	1:o:304:ARG:HG2	2.11	0.50
3:y:104:LEU:HD11	3:y:166:VAL:HA	1.93	0.50
9:AA:101:BCL:HBD	9:AA:101:BCL:HBA2	1.91	0.50
6:AH:33:VAL:HG22	9:AH:103:BCL:H92	1.93	0.50
5:AI:20:VAL:O	5:AI:24:ILE:HG12	2.11	0.50
2:L:179:ASN:HB3	2:L:182:HIS:CB	2.41	0.50
5:D:56:GLN:O	5:D:58:LEU:N	2.44	0.50
15:P:102:CRT:H372	5:Q:36:HIS:CD2	2.45	0.50
5:f:51:ILE:HD13	6:g:43:ARG:HH22	1.76	0.50
5:h:40:LEU:HG	5:h:46:TRP:CH2	2.47	0.50
2:L:133:ALA:HB1	9:L:301:BCL:H62	1.94	0.50
5:I:25:VAL:HG13	9:I:101:BCL:H62	1.92	0.50
15:X:101:CRT:H372	5:Y:36:HIS:CD2	2.46	0.50
5:1:42:THR:HG21	5:3:47:LEU:HD13	1.91	0.50
9:1:102:BCL:H2	6:2:29:PHE:CE1	2.46	0.50
5:f:43:ASP:OD1	5:h:56:GLN:HG2	2.12	0.50
9:h:101:BCL:HAA2	9:h:101:BCL:HBD	1.93	0.50
3:M:121:PHE:HZ	5:Q:34:LEU:HA	1.77	0.50
3:M:219:HIS:CE1	3:M:223:ILE:HD11	2.46	0.50
5:Y:40:LEU:HG	5:Y:46:TRP:CH2	2.47	0.50
1:o:191:ALA:O	1:o:192:TYR:HB2	2.12	0.50
2:x:2:ALA:HB2	12:m:101:PEF:H12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:35:LYS:NZ	12:t:301:PEF:O2P	2.30	0.50
5:r:25:VAL:HG13	9:r:101:BCL:H41	1.94	0.50
6:e:46:LEU:HD21	5:f:46:TRP:HB2	1.92	0.50
5:f:9:TYR:O	6:g:14:ALA:HB1	2.11	0.50
5:j:46:TRP:NE1	9:j:101:BCL:OBB	2.41	0.50
1:C:67:SER:OG	1:C:86:SER:OG	2.24	0.50
2:L:206:VAL:HG12	3:M:142:MET:HE3	1.90	0.50
4:H:141:GLU:HG2	4:H:142:PHE:N	2.26	0.50
5:D:9:TYR:C	5:D:11:ILE:H	2.19	0.50
5:O:59:GLY:C	5:O:61:LYS:HA	2.36	0.50
1:o:155:CYS:SG	7:o:502:HEM:CAC	2.99	0.50
1:o:316:LYS:HE3	7:o:504:HEM:O1A	2.10	0.50
2:x:206:VAL:HB	2:x:216:LYS:HB2	1.94	0.50
3:y:177:PHE:CD1	15:y:404:CRT:H19	2.47	0.50
3:y:208:PHE:CE2	3:y:275:LEU:HB3	2.46	0.50
15:p:103:CRT:H9	6:q:17:PHE:CE1	2.46	0.50
5:AE:51:ILE:O	5:AE:55:TYR:HE2	1.95	0.50
2:L:120:LEU:HD11	3:M:250:LEU:HB2	1.94	0.50
9:L:303:BCL:HED1	3:M:179:ILE:HG23	1.94	0.50
6:G:32:VAL:HG21	9:G:102:BCL:HBA2	1.93	0.50
6:P:21:PHE:HA	15:P:102:CRT:H14	1.92	0.50
6:X:20:ILE:HD12	15:X:101:CRT:C5	2.42	0.50
1:o:66:ASP:O	1:o:67:SER:OG	2.20	0.50
1:o:152:CYS:CB	7:o:502:HEM:HAB	2.41	0.50
2:x:209:PRO:CD	12:x:306:PEF:H41	2.41	0.50
6:e:46:LEU:HA	5:f:51:ILE:HG22	1.93	0.50
6:g:10:THR:HG23	6:g:13:GLU:CD	2.37	0.50
1:C:19:MET:HB2	1:C:21:LEU:HD13	1.93	0.50
1:C:216:ALA:C	3:M:296:LEU:HD12	2.36	0.50
3:M:63:PHE:CE1	5:Q:30:VAL:HG22	2.46	0.50
5:A:7:ASN:ND2	6:E:23:GLN:OE1	2.45	0.50
9:D:102:BCL:HED1	6:E:28:TRP:HZ2	1.76	0.50
6:6:21:PHE:HA	15:6:101:CRT:H14	1.94	0.50
9:9:103:BCL:HED1	6:0:28:TRP:CZ3	2.47	0.50
10:x:302:BPH:H18	9:x:305:BCL:C2B	2.42	0.50
3:y:39:TRP:O	3:y:40:LEU:C	2.54	0.50
3:y:300:LYS:HE2	4:t:10:ASP:OD1	2.11	0.50
4:t:45:ARG:HE	5:m:16:ASP:HB2	1.76	0.50
6:e:45:TRP:CD1	6:e:46:LEU:HG	2.47	0.50
1:C:183:GLN:O	1:C:184:ASN:HB2	2.12	0.50
1:C:236:MET:HB3	7:C:503:HEM:C4B	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:244:PHE:HB2	11:L:304:UQ8:H45	1.94	0.50
5:Q:10:LYS:HD3	15:T:101:CRT:H21A	1.93	0.50
5:S:43:ASP:HB3	5:U:47:LEU:O	2.12	0.50
9:T:102:BCL:H3A	9:T:102:BCL:CGA	2.42	0.50
5:U:44:LEU:HD13	9:V:101:BCL:HAC1	1.94	0.50
1:o:141:TRP:O	1:o:145:VAL:HG22	2.11	0.50
3:y:73:PHE:CZ	3:y:81:TRP:HH2	2.30	0.50
3:y:146:LEU:O	3:y:149:ALA:N	2.44	0.50
2:L:65:LEU:HD13	3:M:308:PRO:HG3	1.94	0.50
2:L:271:TRP:HZ3	2:L:272:TRP:CH2	2.30	0.50
4:H:251:THR:OG1	4:H:254:ARG:HG3	2.12	0.50
5:D:40:LEU:HG	5:D:46:TRP:CH2	2.47	0.50
5:3:39:VAL:HG11	9:3:101:BCL:HBC1	1.93	0.50
6:4:40:TRP:CD2	9:4:102:BCL:H18	2.47	0.50
6:6:10:THR:HG23	6:6:13:GLU:CD	2.36	0.50
1:o:204:LEU:CD2	7:o:504:HEM:HBB1	2.42	0.50
9:r:101:BCL:HAA1	9:r:101:BCL:HBD	1.93	0.50
5:AE:14:ILE:HD11	15:AH:102:CRT:C5	2.42	0.50
1:C:24:GLU:O	2:L:263:PHE:HA	2.11	0.49
1:C:124:LYS:HG3	7:C:501:HEM:HMD3	1.94	0.49
2:L:61:PRO:HA	2:L:66:GLN:HG3	1.92	0.49
2:L:228:ILE:HD13	3:M:133:THR:HG22	1.94	0.49
3:M:219:HIS:ND1	14:M:403:MQ8:O1	2.41	0.49
6:V:29:PHE:O	6:V:32:VAL:HB	2.12	0.49
5:Y:46:TRP:NE1	9:Y:101:BCL:OBB	2.43	0.49
2:x:7:GLU:HB2	3:y:250:LEU:HD21	1.94	0.49
4:t:36:ARG:O	4:t:37:GLU:HG2	2.12	0.49
5:AG:11:ILE:HD13	15:AJ:101:CRT:C10	2.42	0.49
5:j:51:ILE:HD11	5:l:55:TYR:O	2.12	0.49
5:l:29:ILE:HD11	9:l:101:BCL:H201	1.94	0.49
1:C:316:LYS:HE3	7:C:504:HEM:CGA	2.42	0.49
2:L:78:PRO:HB2	2:L:82:TYR:CD2	2.47	0.49
2:L:162:HIS:CE1	2:L:163:LEU:HD23	2.47	0.49
4:H:257:PRO:HG3	5:7:19:ARG:CZ	2.42	0.49
5:F:44:LEU:HD12	5:I:47:LEU:HD22	1.93	0.49
5:S:4:MET:HE1	5:S:8:LEU:HD23	1.94	0.49
6:X:24:SER:CB	15:X:101:CRT:H14	2.41	0.49
15:2:101:CRT:H291	9:3:101:BCL:H11	1.94	0.49
9:5:102:BCL:H12	6:6:32:VAL:HG11	1.94	0.49
1:o:178:LEU:HA	3:y:110:SER:CB	2.36	0.49
1:o:250:CYS:SG	7:o:503:HEM:CAC	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:x:302:BPH:HMB1	10:x:302:BPH:HBB3	1.95	0.49
3:y:4:TYR:HE1	3:y:6:ASN:OD1	1.95	0.49
6:AJ:14:ALA:CB	6:AJ:17:PHE:HB3	2.42	0.49
5:d:27:PHE:CD2	9:f:101:BCL:H191	2.47	0.49
2:L:217:THR:HG23	2:L:220:HIS:CE1	2.47	0.49
5:W:5:ASN:OD1	5:W:6:ALA:N	2.45	0.49
9:1:102:BCL:HMA1	9:3:101:BCL:HMA1	1.94	0.49
5:9:17:PRO:HB3	6:0:17:PHE:CE1	2.47	0.49
6:AH:32:VAL:HG11	9:AH:103:BCL:HBA1	1.95	0.49
3:M:80:HIS:O	3:M:81:TRP:HB2	2.13	0.49
4:H:46:THR:HG23	4:H:51:GLY:HA2	1.95	0.49
5:O:40:LEU:HG	5:O:46:TRP:CH2	2.47	0.49
5:S:49:ASP:HB3	5:S:51:ILE:HG13	1.93	0.49
5:W:44:LEU:HD12	5:Y:47:LEU:HD22	1.94	0.49
2:x:199:HIS:NE2	3:y:266:HIS:NE2	2.60	0.49
3:y:247:ARG:NH2	4:t:113:PRO:O	2.37	0.49
4:t:36:ARG:C	4:t:37:GLU:HG2	2.37	0.49
4:t:65:LYS:HE2	4:t:67:PHE:CZ	2.47	0.49
5:AA:8:LEU:HD11	15:AD:102:CRT:H133	1.93	0.49
5:AC:11:ILE:HD13	15:AE:103:CRT:H10	1.94	0.49
6:AH:29:PHE:CE1	9:AH:103:BCL:H2	2.47	0.49
6:AJ:20:ILE:HD12	15:AJ:101:CRT:C5	2.43	0.49
6:AJ:45:TRP:HD1	6:AJ:46:LEU:HG	1.78	0.49
15:f:102:CRT:H292	9:h:101:BCL:H51	1.95	0.49
6:g:40:TRP:NE1	9:g:101:BCL:H201	2.27	0.49
1:C:99:THR:HA	1:C:103:PRO:HB3	1.94	0.49
3:M:114:TRP:HA	3:M:114:TRP:CE3	2.47	0.49
4:H:77:VAL:O	4:H:80:ARG:NE	2.43	0.49
6:B:17:PHE:CD1	15:9:102:CRT:H5	2.41	0.49
1:o:17:SER:OG	1:o:19:MET:HG2	2.12	0.49
2:x:32:VAL:HG12	2:x:33:GLY:O	2.12	0.49
4:t:107:MET:SD	4:t:249:TYR:HB2	2.53	0.49
15:f:102:CRT:C6	6:g:20:ILE:HD12	2.42	0.49
1:C:98:THR:HA	7:C:501:HEM:HMC3	1.93	0.49
1:C:155:CYS:SG	1:C:310:CYS:SG	3.10	0.49
2:L:137:TYR:CE1	9:L:305:BCL:HBB1	2.48	0.49
11:L:304:UQ8:H4MB	11:L:304:UQ8:H3MA	1.95	0.49
3:M:162:PHE:C	3:M:165:PRO:HD2	2.36	0.49
3:M:260:VAL:HG22	14:M:403:MQ8:C4	2.43	0.49
6:V:29:PHE:CD1	9:V:101:BCL:H2	2.48	0.49
6:Z:43:ARG:HD3	5:1:55:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:20:ILE:O	6:6:24:SER:OG	2.19	0.49
2:x:261:GLY:O	2:x:264:TRP:N	2.39	0.49
5:m:17:PRO:HB3	6:n:17:PHE:CE2	2.48	0.49
6:AH:21:PHE:CD2	15:AH:102:CRT:H14	2.47	0.49
9:d:101:BCL:H2A	9:d:101:BCL:O2D	2.13	0.49
5:l:34:LEU:O	5:l:38:ILE:HG13	2.12	0.49
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.12	0.49
2:L:86:MET:HA	2:L:96:GLN:HE22	1.77	0.49
2:L:237:ALA:O	2:L:240:ARG:N	2.46	0.49
6:B:16:GLU:OE2	5:9:10:LYS:HE3	2.13	0.49
6:T:16:GLU:HB3	15:T:101:CRT:H33	1.94	0.49
15:U:102:CRT:H36	5:W:33:LEU:HD23	1.94	0.49
6:V:40:TRP:CH2	6:V:46:LEU:HB2	2.48	0.49
9:8:102:BCL:HED2	9:8:102:BCL:O1A	2.12	0.49
3:y:197:TYR:CZ	9:y:401:BCL:HMC2	2.48	0.49
6:v:10:THR:OG1	6:v:13:GLU:N	2.40	0.49
5:AK:49:ASP:HB3	5:AK:51:ILE:HG22	1.94	0.49
1:C:137:ALA:HA	1:C:141:TRP:CD1	2.46	0.49
2:L:239:HIS:NE2	3:M:223:ILE:HG13	2.27	0.49
3:M:60:SER:HB2	3:M:128:LEU:HB3	1.95	0.49
5:A:18:ARG:HG3	5:9:15:LEU:HD23	1.95	0.49
9:B:101:BCL:H121	9:B:101:BCL:H91	1.93	0.49
5:F:3:THR:HG22	5:I:2:PHE:CE2	2.48	0.49
5:I:12:TRP:HB3	5:I:17:PRO:HG3	1.95	0.49
1:o:219:ALA:CB	3:y:292:ASP:HB2	2.43	0.49
4:t:29:TYR:OH	12:t:303:PEF:H21	2.13	0.49
5:m:56:GLN:HG2	5:l:43:ASP:CG	2.38	0.49
6:AJ:25:MET:HG2	6:AJ:29:PHE:CZ	2.48	0.49
1:C:126:VAL:HG13	1:C:287:LEU:HD13	1.94	0.49
9:1:102:BCL:H3A	9:1:102:BCL:H12	1.94	0.49
6:0:40:TRP:HH2	6:0:46:LEU:OXT	1.94	0.49
1:o:101:VAL:HG21	7:o:502:HEM:CMB	2.43	0.49
1:o:253:THR:HG22	1:o:256:PHE:CE1	2.48	0.49
2:x:71:TRP:HB3	2:x:160:LEU:HD12	1.94	0.49
2:x:129:ALA:HB1	2:x:247:LEU:HD21	1.94	0.49
5:f:35:ILE:HA	5:f:38:ILE:HD12	1.95	0.49
5:l:5:ASN:C	5:l:7:ASN:H	2.19	0.49
6:c:40:TRP:HH2	6:c:46:LEU:HB2	1.76	0.49
3:y:98:PRO:HG3	3:y:107:PRO:HG3	1.95	0.49
9:AA:101:BCL:HBC2	9:AB:101:BCL:HMD1	1.94	0.49
6:AD:28:TRP:CZ2	9:AD:101:BCL:H43	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:46:LEU:O	6:AJ:42:TYR:OH	2.26	0.49
5:AI:5:ASN:HB3	6:AL:23:GLN:OE1	2.13	0.49
3:M:71:ILE:O	3:M:75:MET:HG3	2.13	0.48
5:3:36:HIS:CE1	9:4:102:BCL:HMD3	2.48	0.48
4:t:135:PRO:HB3	4:t:171:TRP:NE1	2.28	0.48
9:p:104:BCL:H42	6:q:32:VAL:HG11	1.93	0.48
5:AE:34:LEU:O	5:AE:38:ILE:HG13	2.12	0.48
1:C:263:THR:HG22	3:M:311:VAL:CG1	2.41	0.48
2:L:206:VAL:HB	2:L:216:LYS:HB2	1.95	0.48
3:M:253:ARG:HH12	12:M:406:PEF:HN2	1.58	0.48
3:M:260:VAL:HG12	4:H:34:ASP:CG	2.38	0.48
5:S:40:LEU:HD13	5:S:46:TRP:CH2	2.48	0.48
1:o:20:LEU:CA	1:o:21:LEU:HB2	2.41	0.48
1:o:135:ARG:NH1	1:o:332:LYS:HA	2.27	0.48
1:o:153:TYR:CD1	1:o:157:ARG:HA	2.48	0.48
1:o:166:TRP:HE1	1:o:305:VAL:C	2.20	0.48
9:p:102:BCL:H2	6:q:28:TRP:CH2	2.48	0.48
15:AD:102:CRT:H26	15:AD:102:CRT:H241	1.66	0.48
5:AE:12:TRP:CZ3	5:AE:20:VAL:HG11	2.48	0.48
2:L:30:PHE:CE1	3:M:257:GLY:HA3	2.49	0.48
4:H:113:PRO:HG2	4:H:249:TYR:CE2	2.48	0.48
5:A:49:ASP:HB2	5:A:51:ILE:HG13	1.95	0.48
5:I:44:LEU:HD13	9:J:102:BCL:CAC	2.42	0.48
6:N:17:PHE:CE1	15:N:101:CRT:H9	2.48	0.48
5:9:40:LEU:HD21	5:9:47:LEU:HD12	1.95	0.48
1:o:312:GLN:O	1:o:313:ALA:HB3	2.11	0.48
3:y:234:GLU:OE1	3:y:266:HIS:NE2	2.40	0.48
15:AH:102:CRT:H342	9:AI:101:BCL:O1A	2.14	0.48
9:AL:102:BCL:HAA1	9:AL:102:BCL:HBD	1.94	0.48
1:C:67:SER:HA	1:C:68:THR:OG1	2.14	0.48
5:Q:8:LEU:HD11	15:T:101:CRT:H133	1.95	0.48
6:6:17:PHE:HA	15:6:101:CRT:H6	1.94	0.48
3:y:41:GLY:HA2	3:y:44:GLY:O	2.13	0.48
4:t:9:ILE:HG12	5:r:41:SER:HB3	1.95	0.48
15:AD:102:CRT:H372	5:AE:36:HIS:CD2	2.49	0.48
5:AG:44:LEU:HD23	5:AI:55:TYR:CD2	2.48	0.48
6:e:44:PRO:O	5:f:55:TYR:OH	2.27	0.48
5:Y:43:ASP:C	5:Y:45:ASN:H	2.20	0.48
9:1:102:BCL:H3A	9:1:102:BCL:HBA1	1.51	0.48
5:5:32:GLY:HA2	9:5:102:BCL:O1D	2.13	0.48
3:y:72:GLY:HA3	15:y:404:CRT:C6	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:84:PHE:HE1	5:AI:37:MET:HE2	1.78	0.48
3:y:265:ILE:HG23	3:y:266:HIS:ND1	2.28	0.48
4:t:14:ILE:HD13	5:u:37:MET:SD	2.53	0.48
5:d:44:LEU:HD11	6:e:45:TRP:HB2	1.96	0.48
2:L:34:PHE:O	2:L:38:VAL:HG23	2.13	0.48
2:L:48:LEU:HB3	5:9:34:LEU:HD13	1.95	0.48
5:3:5:ASN:C	5:3:7:ASN:H	2.14	0.48
1:o:242:SER:HA	1:o:308:MET:CE	2.42	0.48
5:u:25:VAL:CG1	9:u:101:BCL:H71	2.41	0.48
1:C:21:LEU:HD21	2:L:274:TRP:CE2	2.49	0.48
3:M:256:MET:HE3	14:M:403:MQ8:H293	1.96	0.48
9:D:101:BCL:H91	9:D:101:BCL:H142	1.96	0.48
6:E:8:GLY:C	6:E:9:LEU:HD12	2.39	0.48
6:T:12:ASP:O	6:T:15:LYS:HB2	2.13	0.48
15:T:101:CRT:H22A	15:T:101:CRT:H5	1.69	0.48
5:3:10:LYS:HE3	6:6:16:GLU:OE2	2.13	0.48
5:5:46:TRP:CZ3	9:5:101:BCL:HAC2	2.49	0.48
2:x:9:LYS:HD2	4:t:115:ALA:HB1	1.96	0.48
3:y:102:TYR:HE2	3:y:111:GLU:HB3	1.78	0.48
3:y:163:ILE:O	3:y:167:MET:HG3	2.13	0.48
5:u:42:THR:HG21	5:w:47:LEU:HD13	1.96	0.48
5:AC:38:ILE:O	5:AC:42:THR:HG23	2.14	0.48
5:AI:6:ALA:HB2	6:AL:23:GLN:OE1	2.13	0.48
9:j:101:BCL:H61	6:k:28:TRP:CZ3	2.47	0.48
1:C:97:VAL:HG21	1:C:131:PHE:HZ	1.74	0.48
2:L:241:LEU:HD21	11:L:304:UQ8:H13	1.94	0.48
10:L:302:BPH:H18	9:L:305:BCL:CMB	2.43	0.48
3:M:65:LEU:HD21	10:M:402:BPH:H7C2	1.95	0.48
3:M:215:LEU:HD23	3:M:215:LEU:HA	1.64	0.48
3:M:225:SER:O	3:M:228:ARG:HD2	2.13	0.48
3:M:233:ARG:NH2	4:H:124:ASP:OD2	2.47	0.48
4:H:214:ILE:HB	4:H:218:HIS:HB2	1.96	0.48
6:G:45:TRP:HD1	6:G:46:LEU:HG	1.75	0.48
9:W:101:BCL:HBA1	6:X:28:TRP:HH2	1.79	0.48
5:5:9:TYR:HD1	5:5:9:TYR:H	1.62	0.48
1:o:19:MET:HB2	1:o:21:LEU:HD22	1.95	0.48
1:o:153:TYR:CE1	1:o:157:ARG:HA	2.48	0.48
1:o:270:TRP:CG	3:y:316:PRO:HG2	2.48	0.48
2:x:160:LEU:O	2:x:163:LEU:HB2	2.14	0.48
3:y:3:GLU:CD	4:t:247:LYS:HZ3	2.18	0.48
3:y:219:HIS:CE1	3:y:265:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:32:VAL:HG21	9:c:102:BCL:HBA2	1.96	0.48
3:M:65:LEU:HD11	10:M:402:BPH:H122	1.95	0.48
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.96	0.48
1:o:212:ILE:HD13	1:o:212:ILE:N	2.29	0.48
3:y:162:PHE:C	3:y:165:PRO:HD2	2.39	0.48
4:t:159:LEU:HD21	4:t:251:THR:HG23	1.95	0.48
4:t:163:VAL:O	4:t:216:ALA:HB1	2.14	0.48
5:d:28:GLN:NE2	6:e:28:TRP:HE1	2.11	0.48
9:e:102:BCL:H12	9:e:102:BCL:HBA1	1.57	0.48
1:C:141:TRP:C	1:C:145:VAL:HG22	2.39	0.48
2:L:194:LEU:HD11	10:M:402:BPH:ND	2.29	0.48
9:R:102:BCL:H142	9:R:102:BCL:H112	1.71	0.48
2:x:191:THR:OG1	9:x:303:BCL:H12	2.14	0.48
5:p:11:ILE:HD13	15:s:101:CRT:H10	1.94	0.48
6:s:46:LEU:HD22	6:v:42:TYR:CE2	2.49	0.48
9:z:102:BCL:HBA1	9:z:102:BCL:H3A	1.60	0.48
6:AH:40:TRP:HH2	6:AH:46:LEU:OXT	1.97	0.48
5:f:14:ILE:HD12	15:i:101:CRT:H82	1.95	0.48
2:L:43:THR:HA	10:L:302:BPH:H7C1	1.96	0.47
6:B:20:ILE:HB	15:9:102:CRT:H82	1.95	0.47
5:F:45:ASN:OD1	5:F:46:TRP:N	2.47	0.47
9:F:101:BCL:H2	6:G:28:TRP:CH2	2.49	0.47
5:U:15:LEU:HD23	5:W:18:ARG:HG3	1.95	0.47
5:U:34:LEU:O	5:U:38:ILE:HG13	2.14	0.47
5:W:51:ILE:HD11	5:Y:58:LEU:CB	2.44	0.47
6:8:18:HIS:O	6:8:22:MET:HG2	2.13	0.47
11:x:304:UQ8:H35	11:x:304:UQ8:H32	1.63	0.47
6:v:20:ILE:HD12	15:v:101:CRT:C6	2.44	0.47
9:w:101:BCL:H102	9:w:101:BCL:H171	1.96	0.47
6:AJ:14:ALA:HB1	6:AJ:17:PHE:HB3	1.95	0.47
5:d:12:TRP:HZ3	5:d:20:VAL:HG21	1.78	0.47
9:G:102:BCL:H62	9:G:102:BCL:H41	1.61	0.47
9:I:101:BCL:HAA2	9:I:101:BCL:HBD	1.96	0.47
9:U:101:BCL:HBA1	6:V:28:TRP:HH2	1.80	0.47
5:1:33:LEU:O	5:1:37:MET:HG3	2.13	0.47
15:8:101:CRT:H26	15:8:101:CRT:H241	1.75	0.47
3:y:37:SER:C	3:y:39:TRP:N	2.72	0.47
4:t:238:LYS:HD3	4:t:238:LYS:HA	1.72	0.47
9:m:102:BCL:H203	5:l:20:VAL:HG13	1.96	0.47
5:p:2:PHE:O	5:p:3:THR:OG1	2.28	0.47
5:p:9:TYR:O	5:p:10:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASP:OD1	1:C:169:ASP:C	2.56	0.47
4:H:64:PRO:HA	4:H:79:PRO:HD2	1.96	0.47
6:B:21:PHE:HA	15:9:102:CRT:H14	1.95	0.47
5:D:22:VAL:HG13	9:D:101:BCL:H191	1.94	0.47
5:Y:44:LEU:HA	5:1:55:TYR:CE2	2.49	0.47
5:9:11:ILE:HG23	5:9:12:TRP:CD2	2.48	0.47
1:o:204:LEU:HD22	7:o:504:HEM:HBB1	1.96	0.47
10:x:302:BPH:H141	9:x:305:BCL:CBB	2.45	0.47
5:p:46:TRP:CD2	9:p:102:BCL:H2C	2.49	0.47
6:v:21:PHE:CD2	15:v:101:CRT:H16	2.49	0.47
2:L:193:CYS:SG	10:M:402:BPH:HMC3	2.54	0.47
3:M:177:PHE:CD1	15:M:404:CRT:H19	2.47	0.47
4:H:35:LYS:HG2	4:H:39:TYR:CE1	2.49	0.47
4:H:60:ASP:CG	4:H:61:LEU:N	2.70	0.47
6:G:20:ILE:HD12	15:G:101:CRT:C6	2.44	0.47
6:P:40:TRP:HH2	6:P:46:LEU:OXT	1.97	0.47
5:7:36:HIS:CE1	9:8:102:BCL:HMD3	2.49	0.47
2:x:253:SER:O	9:x:301:BCL:HED2	2.14	0.47
3:y:76:LEU:HG	3:y:81:TRP:HA	1.95	0.47
9:m:103:BCL:C2	9:m:103:BCL:H102	2.45	0.47
9:m:103:BCL:HAA1	9:m:103:BCL:HBD	1.96	0.47
9:s:102:BCL:HBA1	9:s:102:BCL:H12	1.70	0.47
5:AA:11:ILE:HD13	15:AD:102:CRT:H132	1.96	0.47
5:d:28:GLN:HE21	6:e:28:TRP:HE1	1.61	0.47
2:L:112:ARG:NH2	3:M:255:THR:O	2.28	0.47
3:M:268:TRP:CD2	4:H:30:LEU:HD13	2.48	0.47
12:H:301:PEF:O4	5:D:18:ARG:HD3	2.14	0.47
6:B:17:PHE:HE1	5:9:14:ILE:HD13	1.80	0.47
6:X:45:TRP:CD1	6:X:46:LEU:HG	2.49	0.47
5:Y:50:ASN:C	5:Y:51:ILE:HD12	2.40	0.47
6:Z:32:VAL:HG21	9:Z:102:BCL:HBA2	1.96	0.47
9:4:102:BCL:H121	9:4:102:BCL:HBB2	1.96	0.47
11:x:304:UQ8:H38	11:x:304:UQ8:C35	2.44	0.47
3:y:219:HIS:CE1	3:y:266:HIS:CE1	3.02	0.47
5:w:10:LYS:HE3	6:AB:16:GLU:OE2	2.13	0.47
15:e:101:CRT:C31	9:f:101:BCL:HBA2	2.44	0.47
9:i:102:BCL:H61	9:i:102:BCL:H41	1.63	0.47
5:j:45:ASN:HB3	5:l:56:GLN:HE22	1.80	0.47
4:H:29:TYR:HH	12:H:304:PEF:C10	2.26	0.47
2:x:184:LEU:HD12	2:x:184:LEU:HA	1.63	0.47
2:x:216:LYS:HD3	2:x:220:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:37:SER:HB2	12:y:406:PEF:C2	2.44	0.47
3:y:42:LYS:NZ	12:y:408:PEF:H52	2.29	0.47
3:y:143:SER:HB2	3:y:145:HIS:ND1	2.30	0.47
4:t:137:ARG:NH2	4:t:228:PRO:O	2.48	0.47
9:l:101:BCL:HBC3	9:l:101:BCL:H2C	1.64	0.47
7:C:503:HEM:CMC	7:C:503:HEM:HBC2	2.45	0.47
2:L:52:TRP:O	2:L:56:ILE:HG23	2.14	0.47
2:L:235:ALA:N	11:L:304:UQ8:O4	2.48	0.47
3:M:222:THR:O	3:M:225:SER:N	2.48	0.47
4:H:36:ARG:O	4:H:37:GLU:HG2	2.14	0.47
5:A:2:PHE:HE2	6:E:23:GLN:HE21	1.58	0.47
5:S:43:ASP:OD2	5:U:50:ASN:HA	2.15	0.47
5:U:24:ILE:HD11	9:W:101:BCL:H202	1.96	0.47
6:X:14:ALA:HB1	6:X:17:PHE:HB3	1.97	0.47
5:Y:16:ASP:OD2	5:Y:19:ARG:HB2	2.14	0.47
5:Y:51:ILE:HG12	5:1:59:GLY:HA3	1.95	0.47
15:8:101:CRT:H342	9:9:103:BCL:HBA2	1.97	0.47
3:y:37:SER:HB2	12:y:406:PEF:C3	2.42	0.47
3:y:114:TRP:CZ2	5:AE:37:MET:HE1	2.50	0.47
4:t:60:ASP:OD1	4:t:60:ASP:N	2.47	0.47
5:m:4:MET:CE	5:m:7:ASN:HD22	2.26	0.47
5:m:56:GLN:OE1	5:m:56:GLN:HA	2.14	0.47
9:r:101:BCL:H8	6:s:28:TRP:CZ3	2.50	0.47
5:AC:35:ILE:HA	5:AC:38:ILE:HD12	1.97	0.47
15:AE:103:CRT:H14	6:AF:21:PHE:CD2	2.49	0.47
5:AG:5:ASN:C	5:AG:7:ASN:N	2.68	0.47
6:AH:45:TRP:HD1	6:AH:46:LEU:HG	1.79	0.47
5:AI:11:ILE:HD13	15:AL:101:CRT:H10	1.95	0.47
5:AI:39:VAL:HG11	9:AI:101:BCL:HBC1	1.97	0.47
5:f:40:LEU:HG	5:f:46:TRP:CH2	2.49	0.47
5:f:45:ASN:HB3	5:h:56:GLN:NE2	2.29	0.47
15:f:102:CRT:H292	9:h:101:BCL:H71	1.96	0.47
6:i:20:ILE:HD12	15:i:101:CRT:C6	2.45	0.47
1:C:174:TYR:CZ	1:C:180:PRO:HA	2.49	0.47
2:L:17:LEU:O	4:H:258:LEU:HB2	2.15	0.47
2:L:239:HIS:CD2	3:M:223:ILE:HG21	2.49	0.47
12:H:303:PEF:C11	6:E:8:GLY:HA3	2.45	0.47
5:K:38:ILE:O	5:K:42:THR:HG23	2.15	0.47
5:1:40:LEU:HG	5:1:46:TRP:CH2	2.50	0.47
6:2:13:GLU:HB3	15:2:101:CRT:H23	1.96	0.47
1:o:164:TYR:HD2	1:o:312:GLN:HG2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:196:PRO:HG2	1:o:231:TRP:CG	2.50	0.47
2:x:130:PHE:O	2:x:134:ILE:HG13	2.14	0.47
14:y:403:MQ8:H421	14:y:403:MQ8:H361	1.97	0.47
6:AD:21:PHE:HA	15:AD:102:CRT:H15	1.96	0.47
5:AE:14:ILE:HD13	6:AH:17:PHE:CE1	2.49	0.47
9:c:102:BCL:H3A	9:c:102:BCL:HBA1	1.42	0.47
4:H:63:ASP:OD2	5:F:19:ARG:NH2	2.47	0.47
5:A:9:TYR:HB3	6:B:18:HIS:CG	2.50	0.47
15:J:101:CRT:H27	9:J:102:BCL:O1A	2.15	0.47
5:K:39:VAL:HG11	9:K:101:BCL:HBC1	1.97	0.47
9:O:101:BCL:H12	9:O:101:BCL:H3A	1.97	0.47
6:X:20:ILE:HB	15:X:101:CRT:C9	2.44	0.47
2:x:225:PHE:HD1	2:x:225:PHE:HA	1.60	0.47
9:x:301:BCL:HBC3	3:y:197:TYR:OH	2.15	0.47
6:n:17:PHE:CD1	15:n:101:CRT:H5	2.41	0.47
5:p:43:ASP:OD1	5:r:56:GLN:HG2	2.15	0.47
15:AE:103:CRT:C32	9:AH:101:BCL:H3A	2.45	0.47
5:AG:21:LEU:HA	5:AG:21:LEU:HD23	1.67	0.47
5:h:42:THR:O	5:h:45:ASN:HB2	2.15	0.47
6:k:33:VAL:O	6:k:37:LEU:HG	2.15	0.47
1:C:200:LEU:HD21	1:C:238:ASN:OD1	2.15	0.47
2:L:72:ARG:HH11	3:M:305:PRO:HA	1.80	0.47
2:L:170:GLY:HA2	2:L:176:PHE:HD2	1.79	0.47
15:A:103:CRT:C14	6:0:21:PHE:HA	2.44	0.47
6:G:30:GLY:O	6:G:34:ILE:HG12	2.15	0.47
5:I:3:THR:OG1	5:I:5:ASN:N	2.48	0.47
9:I:101:BCL:H91	9:I:101:BCL:H112	1.60	0.47
5:Y:10:LYS:HB3	15:2:101:CRT:H31A	1.96	0.47
5:3:35:ILE:HD11	9:5:101:BCL:HMB3	1.97	0.47
6:4:46:LEU:HD22	6:6:42:TYR:CE2	2.50	0.47
5:5:38:ILE:O	5:5:42:THR:HG23	2.15	0.47
5:9:10:LYS:HB3	15:9:102:CRT:H41	1.96	0.47
1:o:280:ASN:OD1	1:o:304:ARG:HB2	2.14	0.47
2:x:65:LEU:CD1	3:y:308:PRO:HG3	2.45	0.47
2:x:167:SER:HA	9:x:301:BCL:CBC	2.45	0.47
3:y:28:LEU:O	3:y:52:TYR:HE1	1.98	0.47
3:y:98:PRO:HB2	3:y:171:TRP:HB2	1.97	0.47
3:y:175:VAL:HG22	3:y:185:TRP:CE2	2.50	0.47
4:t:80:ARG:HG3	4:t:82:GLU:HG3	1.96	0.47
4:t:108:LEU:HA	4:t:108:LEU:HD23	1.61	0.47
4:t:257:PRO:HG2	5:j:19:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:49:ASP:O	5:AE:57:ALA:HB3	2.14	0.47
9:AK:101:BCL:HED3	6:AL:28:TRP:CH2	2.50	0.47
9:e:102:BCL:H3A	9:e:102:BCL:HBA1	1.60	0.47
2:L:57:GLY:HA3	2:L:66:GLN:HA	1.97	0.46
15:G:101:CRT:C32	9:I:101:BCL:H3A	2.45	0.46
9:V:101:BCL:HAA1	9:V:101:BCL:CB D	2.44	0.46
9:1:101:BCL:O2D	9:1:101:BCL:H2A	2.15	0.46
5:3:27:PHE:CE1	5:5:29:ILE:HD13	2.49	0.46
5:p:40:LEU:HG	5:p:46:TRP:CH2	2.50	0.46
6:q:26:TYR:HD1	6:q:29:PHE:HD2	1.63	0.46
5:AE:14:ILE:HD13	6:AH:17:PHE:HE1	1.81	0.46
9:AE:102:BCL:H72	9:AE:102:BCL:H112	1.50	0.46
9:f:101:BCL:H92	15:f:102:CRT:H15	1.96	0.46
5:h:40:LEU:HG	5:h:46:TRP:CZ3	2.50	0.46
7:C:503:HEM:HBC2	7:C:503:HEM:HMC2	1.97	0.46
2:L:210:GLN:HB2	3:M:141:GLY:O	2.15	0.46
3:M:13:VAL:HG22	4:H:178:GLN:HA	1.98	0.46
4:H:106:PRO:HB3	4:H:249:TYR:CD1	2.50	0.46
4:H:141:GLU:HG2	4:H:142:PHE:CD1	2.50	0.46
9:B:101:BCL:HMA1	9:0:101:BCL:HMA1	1.98	0.46
6:E:46:LEU:HD23	6:G:42:TYR:CE1	2.50	0.46
5:Q:45:ASN:O	5:Q:49:ASP:OD2	2.33	0.46
9:R:102:BCL:HMB2	9:S:102:BCL:HMA3	1.97	0.46
9:X:102:BCL:HED2	9:X:102:BCL:HBD	1.60	0.46
9:1:102:BCL:H12	9:1:102:BCL:HBA1	1.56	0.46
1:o:107:CYS:CB	7:o:501:HEM:HAB	2.45	0.46
11:x:304:UQ8:H30	11:x:304:UQ8:H27A	1.55	0.46
3:y:102:TYR:CZ	3:y:108:PRO:HD2	2.51	0.46
4:t:135:PRO:HD3	4:t:171:TRP:CH2	2.50	0.46
15:p:103:CRT:H9	6:q:17:PHE:CD1	2.51	0.46
9:g:101:BCL:H12	9:g:101:BCL:HBA2	1.50	0.46
5:h:9:TYR:HB2	6:i:14:ALA:O	2.15	0.46
1:C:183:GLN:HA	1:C:196:PRO:HA	1.96	0.46
3:M:4:TYR:CE1	3:M:6:ASN:HA	2.50	0.46
3:M:155:PHE:O	3:M:159:VAL:HG23	2.15	0.46
4:H:149:PRO:HG3	4:H:204:LYS:HD3	1.97	0.46
9:F:101:BCL:HED3	6:G:35:ALA:HB2	1.97	0.46
5:S:22:VAL:HG22	9:S:102:BCL:H18	1.96	0.46
6:V:32:VAL:HG21	9:V:101:BCL:HBA2	1.96	0.46
1:o:59:VAL:HG21	1:o:100:TRP:HE1	1.80	0.46
3:y:42:LYS:HZ1	12:y:408:PEF:H52	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:10:LYS:HB3	15:AH:102:CRT:H33	1.97	0.46
5:AK:44:LEU:HD11	6:AL:45:TRP:HB2	1.97	0.46
9:l:101:BCL:H121	9:l:101:BCL:H161	1.64	0.46
1:C:205:ASP:CG	1:C:285:TRP:HE1	2.23	0.46
2:L:132:PHE:CD2	2:L:247:LEU:HB3	2.49	0.46
5:A:44:LEU:HD23	5:D:55:TYR:CE2	2.50	0.46
15:A:103:CRT:H403	5:9:35:ILE:HG12	1.97	0.46
5:D:12:TRP:CZ3	5:D:20:VAL:HG11	2.51	0.46
5:D:39:VAL:HG12	5:D:46:TRP:HZ3	1.81	0.46
5:I:3:THR:HB	6:J:18:HIS:NE2	2.30	0.46
6:J:24:SER:O	6:J:27:ALA:HB3	2.16	0.46
15:8:101:CRT:H371	9:9:103:BCL:HMB2	1.97	0.46
9:8:102:BCL:H3A	9:8:102:BCL:HBA1	1.45	0.46
1:o:134:VAL:HG13	1:o:150:VAL:HG23	1.97	0.46
7:o:504:HEM:HHA	7:o:504:HEM:HBD1	1.98	0.46
2:x:261:GLY:O	2:x:263:PHE:N	2.48	0.46
3:y:135:LYS:HB3	3:y:136:ARG:HH21	1.80	0.46
3:y:156:PHE:CZ	3:y:280:ALA:HB1	2.51	0.46
4:t:225:LEU:HA	4:t:235:GLU:OE1	2.15	0.46
9:z:102:BCL:H111	9:z:102:BCL:H143	1.59	0.46
5:AG:28:GLN:HB3	9:AH:101:BCL:H12	1.97	0.46
9:e:102:BCL:H112	9:e:102:BCL:H71	1.81	0.46
9:j:101:BCL:H51	9:j:101:BCL:H8	1.42	0.46
3:M:65:LEU:CD2	10:M:402:BPH:H7C2	2.45	0.46
3:M:126:ILE:HD11	9:M:401:BCL:H142	1.97	0.46
3:M:204:LEU:HD13	4:H:19:PHE:CE2	2.50	0.46
5:I:10:LYS:HD3	15:N:101:CRT:H22A	1.97	0.46
6:J:17:PHE:CD1	15:J:101:CRT:H9	2.50	0.46
6:J:21:PHE:CD2	15:J:101:CRT:H14	2.51	0.46
5:O:43:ASP:HB2	5:Q:48:ASP:OD1	2.15	0.46
6:P:21:PHE:C	6:P:21:PHE:CD1	2.93	0.46
6:P:21:PHE:C	6:P:21:PHE:HD1	2.23	0.46
5:W:25:VAL:HG11	9:W:101:BCL:H192	1.97	0.46
1:o:19:MET:HE3	1:o:21:LEU:HD11	1.97	0.46
7:o:501:HEM:HMC2	7:o:501:HEM:HBC2	1.97	0.46
2:x:179:ASN:HB3	2:x:182:HIS:CB	2.46	0.46
3:y:28:LEU:HD12	3:y:54:GLY:HA2	1.98	0.46
5:m:49:ASP:HB3	5:m:51:ILE:HG13	1.98	0.46
6:z:20:ILE:HD12	15:z:101:CRT:C6	2.45	0.46
5:AK:40:LEU:HG	5:AK:46:TRP:CH2	2.50	0.46
1:C:178:LEU:HA	3:M:110:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:VAL:HG22	7:C:502:HEM:HAC	1.97	0.46
3:M:242:GLY:O	3:M:246:GLU:HG3	2.15	0.46
9:A:102:BCL:HBD	9:B:101:BCL:HBD	1.98	0.46
6:B:46:LEU:C	5:D:51:ILE:HG21	2.41	0.46
5:D:46:TRP:CD2	9:D:101:BCL:H2C	2.51	0.46
5:S:19:ARG:NH2	17:S:101:PGW:H04A	2.31	0.46
5:Y:21:LEU:HD23	5:Y:21:LEU:HA	1.83	0.46
5:3:45:ASN:OD1	5:3:46:TRP:N	2.49	0.46
5:7:27:PHE:CZ	5:7:31:LEU:HD22	2.51	0.46
2:x:52:TRP:CH2	5:l:38:ILE:HG23	2.51	0.46
2:x:194:LEU:HD11	10:y:402:BPH:ND	2.31	0.46
6:s:25:MET:HG3	15:s:101:CRT:C20	2.46	0.46
9:l:101:BCL:H2	6:c:28:TRP:CZ2	2.50	0.46
2:L:240:ARG:NE	3:M:6:ASN:O	2.49	0.46
3:M:228:ARG:H	3:M:228:ARG:HG3	1.40	0.46
5:D:46:TRP:CE2	9:D:101:BCL:H2C	2.51	0.46
2:x:86:MET:HG2	5:j:37:MET:O	2.16	0.46
2:x:219:GLU:HG2	3:y:18:TYR:CZ	2.51	0.46
2:x:240:ARG:NH1	3:y:43:ILE:HA	2.31	0.46
4:t:168:SER:OG	4:t:183:GLU:HB3	2.16	0.46
15:n:101:CRT:H372	5:p:36:HIS:CD2	2.51	0.46
9:p:102:BCL:H142	9:p:102:BCL:H91	1.98	0.46
15:s:101:CRT:H36	5:u:33:LEU:HD23	1.97	0.46
5:h:46:TRP:CD2	9:h:101:BCL:H2C	2.50	0.46
1:C:36:ARG:HD2	2:L:77:PRO:O	2.15	0.46
2:L:126:VAL:HG11	3:M:251:PHE:CE2	2.50	0.46
4:H:16:ILE:HD12	4:H:16:ILE:HA	1.78	0.46
6:X:24:SER:HB2	15:X:101:CRT:C14	2.45	0.46
5:Y:46:TRP:CE3	9:Y:101:BCL:H2C	2.50	0.46
4:t:36:ARG:NE	4:t:65:LYS:HD2	2.31	0.46
5:j:17:PRO:HB3	6:k:17:PHE:CE2	2.51	0.46
3:M:59:LEU:HB3	3:M:128:LEU:CD1	2.45	0.46
3:M:126:ILE:HD13	9:M:401:BCL:C9	2.44	0.46
3:M:233:ARG:NH1	4:H:133:ILE:HD11	2.31	0.46
5:D:10:LYS:HG2	5:D:13:LEU:HD12	1.98	0.46
5:F:31:LEU:O	5:F:34:LEU:HB3	2.16	0.46
6:X:36:HIS:CD2	9:X:102:BCL:H112	2.51	0.46
5:1:5:ASN:HB3	5:1:8:LEU:HB2	1.97	0.46
1:o:263:THR:HA	3:y:311:VAL:HG13	1.98	0.46
1:o:311:HIS:NE2	7:o:504:HEM:NC	2.63	0.46
2:x:138:LEU:O	2:x:142:PHE:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:138:LEU:HD23	2:x:138:LEU:HA	1.79	0.46
2:x:232:SER:OG	11:x:304:UQ8:O5	2.31	0.46
4:t:29:TYR:OH	12:t:303:PEF:C2	2.64	0.46
15:n:101:CRT:H20	15:n:101:CRT:H181	1.81	0.46
5:AC:17:PRO:HB3	6:AD:17:PHE:CE1	2.51	0.46
6:AJ:12:ASP:C	6:AJ:15:LYS:H	2.23	0.46
1:C:119:ASP:OD1	1:C:124:LYS:HE2	2.16	0.46
3:M:5:GLN:HG2	12:M:407:PEF:O1P	2.15	0.46
3:M:232:ASP:C	3:M:234:GLU:H	2.24	0.46
5:A:21:LEU:HA	5:A:21:LEU:HD23	1.62	0.46
6:B:22:MET:HE3	6:B:26:TYR:CZ	2.51	0.46
5:D:29:ILE:HD11	9:D:101:BCL:H101	1.98	0.46
15:G:101:CRT:H20	15:G:101:CRT:H181	1.78	0.46
5:K:17:PRO:HB3	6:N:17:PHE:CE2	2.49	0.46
5:O:7:ASN:HB3	5:O:10:LYS:HD2	1.98	0.46
9:T:102:BCL:HBB3	9:U:101:BCL:CHC	2.46	0.46
5:W:10:LYS:HB3	15:Z:101:CRT:C3	2.45	0.46
2:x:224:PHE:CE1	2:x:228:ILE:HD11	2.50	0.46
9:x:305:BCL:H11	3:y:210:TYR:CB	2.46	0.46
3:y:177:PHE:HD1	15:y:404:CRT:H19	1.80	0.46
4:t:32:ARG:HG3	4:t:59:PRO:HG2	1.97	0.46
4:t:78:ALA:HA	4:t:79:PRO:C	2.40	0.46
9:AB:101:BCL:H93	9:AB:101:BCL:H61	1.79	0.46
5:AI:34:LEU:HA	5:AI:37:MET:HE3	1.97	0.46
9:i:102:BCL:HAA2	9:i:102:BCL:O2D	2.16	0.46
9:i:102:BCL:HBC3	9:i:102:BCL:H2C	1.66	0.46
1:C:148:THR:HG23	1:C:321:ALA:O	2.17	0.45
2:L:140:LEU:HD11	9:L:301:BCL:HED2	1.97	0.45
2:L:239:HIS:CE1	3:M:234:GLU:CD	2.94	0.45
5:O:5:ASN:HB2	5:O:8:LEU:HB2	1.97	0.45
5:Y:23:SER:CB	9:1:101:BCL:H151	2.46	0.45
2:x:26:TRP:HE1	3:y:254:TRP:CD1	2.34	0.45
2:x:48:LEU:HD13	5:l:34:LEU:HD22	1.97	0.45
2:x:125:HIS:CD2	2:x:125:HIS:N	2.83	0.45
11:x:304:UQ8:C35	11:x:304:UQ8:H30B	2.46	0.45
6:n:20:ILE:HB	15:n:101:CRT:C8	2.46	0.45
9:r:101:BCL:H122	9:r:101:BCL:H172	1.98	0.45
9:u:101:BCL:HBA1	9:u:101:BCL:HED2	1.98	0.45
2:L:52:TRP:CZ3	5:A:40:LEU:HD13	2.50	0.45
4:H:120:PRO:HB3	4:H:122:HIS:CD2	2.51	0.45
4:H:249:TYR:C	4:H:251:THR:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:101:BCL:H61	6:G:28:TRP:CZ3	2.51	0.45
6:T:45:TRP:CD1	6:T:46:LEU:HG	2.50	0.45
5:W:39:VAL:HG12	5:W:46:TRP:HZ3	1.80	0.45
1:o:30:THR:O	1:o:30:THR:OG1	2.32	0.45
2:x:77:PRO:HB2	2:x:152:GLY:HA2	1.96	0.45
2:x:274:TRP:CH2	2:x:275:TRP:HE3	2.34	0.45
12:x:306:PEF:H32	12:x:306:PEF:H52	1.98	0.45
3:y:153:ALA:HB2	10:y:402:BPH:HAC1	1.98	0.45
15:s:101:CRT:H372	5:u:36:HIS:CG	2.51	0.45
9:u:101:BCL:H142	9:u:101:BCL:H112	1.62	0.45
6:AD:18:HIS:O	6:AD:22:MET:HG2	2.16	0.45
4:H:171:TRP:CE2	4:H:194:LEU:HD21	2.51	0.45
9:A:102:BCL:H62	9:A:102:BCL:H102	1.51	0.45
6:E:21:PHE:C	6:E:21:PHE:CD1	2.94	0.45
5:S:16:ASP:OD1	5:S:16:ASP:C	2.59	0.45
2:x:192:ASN:ND2	3:y:213:ALA:HA	2.31	0.45
2:x:224:PHE:O	2:x:228:ILE:HG13	2.16	0.45
3:y:135:LYS:HB3	3:y:136:ARG:NH2	2.31	0.45
5:r:55:TYR:C	5:r:57:ALA:N	2.74	0.45
6:s:30:GLY:O	6:s:34:ILE:HG12	2.16	0.45
6:v:25:MET:HE3	6:v:26:TYR:CE1	2.51	0.45
9:AC:102:BCL:HBA2	6:AD:32:VAL:CG2	2.46	0.45
5:d:24:ILE:HD13	5:d:24:ILE:HA	1.70	0.45
9:i:102:BCL:HMA1	9:j:101:BCL:HMA3	1.97	0.45
1:C:155:CYS:SG	7:C:502:HEM:CAC	3.05	0.45
6:B:11:ASP:O	6:B:15:LYS:HG3	2.17	0.45
6:E:17:PHE:HA	15:E:101:CRT:H42	1.99	0.45
15:N:101:CRT:H27	9:N:102:BCL:H12	1.98	0.45
15:N:101:CRT:H342	9:P:101:BCL:O1A	2.17	0.45
6:P:40:TRP:CE3	6:P:44:PRO:HA	2.52	0.45
6:P:45:TRP:CD1	6:P:46:LEU:HG	2.51	0.45
9:S:102:BCL:H92	9:S:102:BCL:H61	1.71	0.45
9:X:102:BCL:C1C	9:Y:101:BCL:HBB3	2.46	0.45
6:Z:40:TRP:CE2	9:Z:102:BCL:H202	2.52	0.45
5:1:57:ALA:H	5:1:59:GLY:CA	2.30	0.45
9:7:101:BCL:H122	9:7:101:BCL:H162	1.57	0.45
2:x:233:ILE:HG21	2:x:238:ILE:HD13	1.98	0.45
3:y:38:TYR:CD1	3:y:38:TYR:C	2.93	0.45
5:m:12:TRP:HB3	5:m:17:PRO:HG3	1.99	0.45
6:AD:31:LEU:HB3	9:AD:101:BCL:HED3	1.97	0.45
15:AE:103:CRT:H342	9:AH:101:BCL:O1A	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:109:TRP:CZ2	14:M:403:MQ8:H291	2.51	0.45
2:L:199:HIS:CE1	2:L:239:HIS:CE1	3.05	0.45
11:L:304:UQ8:H37A	11:L:304:UQ8:H40	1.61	0.45
5:O:4:MET:N	6:R:23:GLN:OE1	2.50	0.45
5:U:11:ILE:HG12	9:W:101:BCL:H142	1.98	0.45
5:3:35:ILE:HG21	9:4:102:BCL:C1D	2.47	0.45
9:5:101:BCL:H112	9:5:101:BCL:H72	1.33	0.45
5:7:4:MET:HB2	6:0:23:GLN:OE1	2.16	0.45
1:o:183:GLN:O	1:o:184:ASN:HB2	2.16	0.45
4:t:132:LYS:O	4:t:174:ARG:HG3	2.16	0.45
6:AD:28:TRP:CE3	9:AD:101:BCL:H101	2.51	0.45
5:AE:36:HIS:CE1	9:AE:104:BCL:HMD3	2.51	0.45
9:AK:101:BCL:HBC2	9:AK:101:BCL:H2C	1.79	0.45
6:AL:43:ARG:HG2	5:d:55:TYR:CZ	2.52	0.45
3:M:128:LEU:HD23	3:M:128:LEU:HA	1.61	0.45
4:H:89:ALA:HB1	4:H:101:VAL:O	2.17	0.45
4:H:122:HIS:CB	4:t:121:LYS:HZ2	2.25	0.45
4:H:149:PRO:HG3	4:H:204:LYS:HB3	1.98	0.45
9:A:102:BCL:HBA1	9:A:102:BCL:H3A	1.78	0.45
9:A:102:BCL:HMB2	9:A:102:BCL:H122	1.99	0.45
6:G:33:VAL:O	6:G:37:LEU:HG	2.17	0.45
6:N:20:ILE:HD12	15:N:101:CRT:C6	2.46	0.45
5:O:44:LEU:HD12	5:Q:47:LEU:HD22	1.99	0.45
9:Q:101:BCL:C12	9:Q:101:BCL:H51	2.46	0.45
5:S:5:ASN:C	5:S:7:ASN:N	2.75	0.45
6:V:28:TRP:O	6:V:32:VAL:HG23	2.17	0.45
5:Y:46:TRP:O	5:Y:47:LEU:HD23	2.17	0.45
2:x:35:PHE:CD2	2:x:111:LEU:HB3	2.51	0.45
2:x:177:HIS:NE2	9:x:301:BCL:HMC2	2.31	0.45
4:t:141:GLU:HG2	4:t:142:PHE:H	1.81	0.45
4:t:215:LYS:HB2	4:t:218:HIS:CE1	2.52	0.45
5:d:17:PRO:HG2	6:e:9:LEU:HD21	1.98	0.45
6:e:20:ILE:HB	15:e:101:CRT:H9	1.99	0.45
6:e:21:PHE:HA	15:e:101:CRT:H14	1.98	0.45
6:g:18:HIS:O	6:g:22:MET:HG2	2.17	0.45
9:j:101:BCL:H112	9:j:101:BCL:H41	1.98	0.45
1:C:46:LYS:O	1:C:49:ARG:HB3	2.17	0.45
1:C:212:ILE:HD11	7:C:503:HEM:HMA3	1.98	0.45
2:L:35:PHE:CE2	2:L:111:LEU:HB3	2.51	0.45
2:L:177:HIS:NE2	9:L:301:BCL:HMC2	2.32	0.45
2:L:184:LEU:O	2:L:187:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:252:TRP:HE1	11:L:304:UQ8:H35A	1.81	0.45
3:M:268:TRP:NE1	4:H:30:LEU:HB3	2.32	0.45
5:K:14:ILE:HG22	5:O:18:ARG:HG2	1.97	0.45
9:O:101:BCL:H141	9:O:101:BCL:H193	1.99	0.45
5:Q:2:PHE:HD1	6:R:26:TYR:HE2	1.64	0.45
15:2:101:CRT:C29	9:3:101:BCL:H11	2.47	0.45
9:x:303:BCL:HHD	9:x:303:BCL:HBC2	1.97	0.45
3:y:201:PHE:CD1	3:y:279:THR:HG22	2.50	0.45
15:y:404:CRT:C2M	5:AA:38:ILE:HG12	2.47	0.45
5:p:56:GLN:C	5:p:58:LEU:H	2.22	0.45
9:AH:101:BCL:H102	9:AH:101:BCL:H203	1.99	0.45
5:d:55:TYR:HD1	5:d:61:LYS:O	2.00	0.45
5:j:12:TRP:CZ3	5:j:20:VAL:HG21	2.49	0.45
1:C:127:SER:OG	7:C:501:HEM:HAC	2.17	0.45
1:C:191:ALA:O	1:C:192:TYR:HB2	2.17	0.45
3:M:6:ASN:ND2	3:M:227:SER:HB2	2.31	0.45
4:H:45:ARG:NH1	4:H:53:VAL:HG11	2.31	0.45
4:H:154:MET:HB3	4:H:207:ARG:O	2.16	0.45
5:A:8:LEU:HB2	6:E:20:ILE:HD13	1.98	0.45
5:D:8:LEU:HD23	5:D:8:LEU:HA	1.75	0.45
6:E:17:PHE:HD1	15:E:101:CRT:H33	1.82	0.45
5:Q:9:TYR:HD1	5:Q:9:TYR:H	1.64	0.45
9:Y:101:BCL:HHC	9:Y:101:BCL:HMC2	1.62	0.45
2:x:233:ILE:HG12	2:x:237:ALA:HB3	1.98	0.45
3:y:79:VAL:HG21	3:y:86:PHE:HB2	1.97	0.45
4:t:20:TRP:HA	4:t:20:TRP:CE3	2.52	0.45
15:s:101:CRT:H20	15:s:101:CRT:H181	1.81	0.45
9:w:101:BCL:H61	9:w:101:BCL:H41	1.58	0.45
9:g:101:BCL:H42	9:h:101:BCL:H92	1.98	0.45
5:l:3:THR:O	5:l:5:ASN:N	2.50	0.45
2:L:65:LEU:CD1	3:M:308:PRO:HG3	2.46	0.45
3:M:33:ARG:HA	3:M:34:PRO:HD3	1.66	0.45
6:B:43:ARG:HG3	5:D:55:TYR:CE1	2.52	0.45
1:o:68:THR:HG23	1:o:68:THR:O	2.17	0.45
2:x:17:LEU:HA	2:x:17:LEU:HD23	1.66	0.45
2:x:120:LEU:HD11	3:y:250:LEU:HB2	1.98	0.45
2:x:211:LYS:HG2	12:x:306:PEF:C11	2.47	0.45
2:x:270:GLU:O	2:x:271:TRP:C	2.60	0.45
11:x:304:UQ8:H35	11:x:304:UQ8:H30B	1.99	0.45
4:t:135:PRO:HB2	4:t:169:ASP:OD2	2.17	0.45
5:m:43:ASP:OD1	5:p:56:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:101:BCL:H3A	9:AI:101:BCL:HBA1	1.78	0.45
6:g:40:TRP:CG	9:g:101:BCL:H191	2.52	0.45
1:C:27:PRO:HD3	5:3:41:SER:HB2	1.99	0.45
1:C:207:ALA:HB1	1:C:277:ARG:HH21	1.82	0.45
2:L:3:MET:HB3	2:L:7:GLU:CD	2.42	0.45
2:L:192:ASN:OD1	2:L:246:ALA:HB2	2.16	0.45
2:L:236:LEU:O	2:L:239:HIS:HB2	2.17	0.45
5:D:12:TRP:HZ3	5:D:20:VAL:HG11	1.82	0.45
5:F:11:ILE:CD1	15:J:101:CRT:H10	2.47	0.45
5:O:12:TRP:HB2	6:P:14:ALA:HB1	1.99	0.45
6:R:17:PHE:HB2	15:R:101:CRT:H22A	1.98	0.45
9:W:101:BCL:HBC3	9:W:101:BCL:H2C	1.77	0.45
5:Y:36:HIS:CE1	9:Z:102:BCL:HMD3	2.52	0.45
15:6:101:CRT:H393	5:7:36:HIS:CD2	2.52	0.45
5:7:18:ARG:H	5:7:18:ARG:HG2	1.54	0.45
5:9:46:TRP:CZ3	9:9:103:BCL:HBC3	2.53	0.45
1:o:256:PHE:HZ	2:x:171:TYR:CE2	2.35	0.45
1:o:288:ASN:OD1	1:o:296:LYS:HE2	2.18	0.45
2:x:116:ILE:HG22	3:y:251:PHE:HD1	1.82	0.45
2:x:183:MET:HE1	3:y:180:PHE:HE1	1.80	0.45
10:x:302:BPH:HHC	10:x:302:BPH:OBB	2.17	0.45
9:x:305:BCL:H12	3:y:207:ALA:O	2.16	0.45
3:y:63:PHE:CB	3:y:125:SER:HB2	2.47	0.45
3:y:271:TRP:HB3	4:t:26:LEU:HD21	1.99	0.45
4:t:31:ARG:HA	4:t:31:ARG:HD2	1.72	0.45
4:t:181:TYR:OH	4:t:236:GLU:OE1	2.20	0.45
5:u:3:THR:OG1	5:u:5:ASN:N	2.50	0.45
5:AC:44:LEU:HD12	5:AE:47:LEU:HD22	1.99	0.45
15:AH:102:CRT:H33	15:AH:102:CRT:H5	1.66	0.45
6:g:45:TRP:HD1	6:g:46:LEU:HG	1.81	0.45
1:C:199:PRO:O	1:C:203:PHE:HD2	1.99	0.44
3:M:42:LYS:NZ	12:M:408:PEF:H52	2.32	0.44
9:A:102:BCL:HAA2	9:A:102:BCL:HED3	1.99	0.44
5:D:20:VAL:O	5:D:23:SER:HB2	2.17	0.44
15:G:101:CRT:H36	5:I:33:LEU:HD23	1.98	0.44
5:I:7:ASN:OD1	5:I:9:TYR:HE2	2.00	0.44
6:T:45:TRP:CZ2	9:T:102:BCL:H143	2.52	0.44
2:x:186:ILE:HD11	9:x:301:BCL:C2B	2.46	0.44
2:x:225:PHE:CD2	11:x:304:UQ8:C7	3.00	0.44
3:y:242:GLY:O	3:y:246:GLU:HG3	2.17	0.44
6:z:43:ARG:HG3	5:AA:55:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:102:BCL:H43	6:AF:28:TRP:CH2	2.52	0.44
1:C:128:ARG:HH21	7:C:501:HEM:CAD	2.29	0.44
2:L:130:PHE:CE2	2:L:134:ILE:HD11	2.52	0.44
2:L:273:ASN:C	2:L:275:TRP:N	2.74	0.44
3:M:273:ALA:O	3:M:274:VAL:C	2.58	0.44
6:J:26:TYR:HD1	6:J:29:PHE:CD2	2.36	0.44
5:Y:13:LEU:O	6:Z:7:THR:HG23	2.16	0.44
5:7:35:ILE:CG1	15:8:101:CRT:H403	2.47	0.44
1:o:133:LEU:HA	1:o:283:TYR:CE2	2.52	0.44
1:o:168:THR:HA	1:o:198:ASP:OD2	2.17	0.44
6:AH:18:HIS:O	6:AH:22:MET:HG2	2.17	0.44
6:AL:20:ILE:HD12	15:AL:101:CRT:C6	2.46	0.44
2:L:196:LEU:HB2	3:M:216:PHE:CD2	2.52	0.44
9:D:101:BCL:H93	9:D:101:BCL:H111	1.85	0.44
6:T:11:ASP:O	6:T:15:LYS:HG3	2.18	0.44
1:o:212:ILE:HD13	1:o:212:ILE:H	1.83	0.44
4:t:249:TYR:C	4:t:251:THR:H	2.25	0.44
5:r:43:ASP:OD1	5:u:56:GLN:HG2	2.17	0.44
5:u:2:PHE:O	6:v:22:MET:HE2	2.17	0.44
9:AH:103:BCL:H151	9:AH:103:BCL:H18	1.60	0.44
6:k:30:GLY:O	6:k:34:ILE:HG13	2.16	0.44
1:C:54:GLN:OE1	1:C:54:GLN:HA	2.16	0.44
2:L:132:PHE:CE2	11:L:304:UQ8:H40B	2.53	0.44
2:L:234:GLY:C	11:L:304:UQ8:O4	2.60	0.44
9:L:303:BCL:H151	15:M:404:CRT:H133	1.99	0.44
3:M:23:LEU:HD22	3:M:139:ALA:HB1	1.99	0.44
3:M:37:SER:O	3:M:37:SER:OG	2.30	0.44
3:M:42:LYS:HE3	12:M:408:PEF:O2P	2.17	0.44
3:M:81:TRP:CD1	5:U:40:LEU:HG	2.52	0.44
4:H:107:MET:HE3	4:H:107:MET:HB3	1.57	0.44
5:A:11:ILE:HG23	5:A:12:TRP:CD2	2.53	0.44
9:F:101:BCL:HBA1	6:G:28:TRP:CH2	2.51	0.44
9:x:305:BCL:H92	9:x:305:BCL:H62	1.68	0.44
9:x:305:BCL:HMD2	9:y:401:BCL:HBB3	1.99	0.44
3:y:158:LEU:HD23	3:y:158:LEU:HA	1.74	0.44
9:m:103:BCL:HBA2	6:n:32:VAL:HG21	1.99	0.44
15:s:101:CRT:H241	15:s:101:CRT:H26	1.66	0.44
5:d:11:ILE:HD13	15:f:102:CRT:H10	1.99	0.44
5:j:4:MET:HB2	6:c:23:GLN:CD	2.43	0.44
9:D:101:BCL:HAA2	9:D:101:BCL:HBD	1.99	0.44
9:F:101:BCL:H161	9:F:101:BCL:H192	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:31:LEU:O	6:G:34:ILE:HB	2.17	0.44
9:G:102:BCL:H3A	9:G:102:BCL:CGA	2.47	0.44
6:X:10:THR:OG1	6:X:13:GLU:HG3	2.18	0.44
5:1:44:LEU:HA	5:3:55:TYR:CD2	2.52	0.44
6:8:21:PHE:HA	15:8:101:CRT:H14	1.99	0.44
2:x:157:TYR:CG	10:x:302:BPH:H151	2.52	0.44
2:x:211:LYS:HB3	2:x:211:LYS:HE2	1.83	0.44
2:x:231:TYR:CE1	2:x:233:ILE:HA	2.52	0.44
3:y:199:ASN:HD21	3:y:283:GLY:CA	2.31	0.44
3:y:216:PHE:HD1	3:y:216:PHE:O	2.01	0.44
6:s:37:LEU:O	6:s:41:LEU:HG	2.17	0.44
5:u:5:ASN:HA	5:u:6:ALA:HA	1.78	0.44
5:AC:42:THR:HG21	5:AE:47:LEU:HD13	1.99	0.44
5:AE:12:TRP:HZ3	5:AE:20:VAL:HG11	1.82	0.44
5:AE:43:ASP:OD2	5:AG:55:TYR:HD2	2.00	0.44
2:L:7:GLU:OE1	2:L:11:ARG:NE	2.42	0.44
2:L:214:PRO:O	2:L:215:VAL:C	2.61	0.44
3:M:215:LEU:HD21	14:M:403:MQ8:C19	2.48	0.44
9:A:102:BCL:HBA1	9:A:102:BCL:H11	1.67	0.44
5:Q:45:ASN:OD1	5:Q:46:TRP:N	2.51	0.44
5:3:50:ASN:HB3	5:3:54:SER:HA	1.99	0.44
9:4:102:BCL:H93	9:4:102:BCL:H111	1.65	0.44
1:o:122:TYR:O	1:o:126:VAL:HG23	2.17	0.44
3:y:114:TRP:HA	3:y:114:TRP:CE3	2.53	0.44
4:t:104:GLY:O	4:t:106:PRO:HD3	2.16	0.44
9:AD:101:BCL:H62	9:AD:101:BCL:H41	1.30	0.44
9:d:101:BCL:H62	9:d:101:BCL:H41	1.81	0.44
6:k:32:VAL:HG13	6:k:36:HIS:CE1	2.53	0.44
1:C:172:PRO:HG3	1:C:185:TYR:CE1	2.53	0.44
1:C:213:THR:HG21	1:C:257:ASN:CG	2.43	0.44
2:L:167:SER:HA	9:L:301:BCL:CB	2.47	0.44
3:M:8:PHE:HB2	12:M:407:PEF:C4	2.48	0.44
5:S:19:ARG:HH22	17:S:101:PGW:H04A	1.82	0.44
5:S:40:LEU:HD11	5:S:47:LEU:HD12	1.99	0.44
6:V:32:VAL:CG2	9:V:101:BCL:HBA2	2.48	0.44
5:5:9:TYR:HB2	6:6:14:ALA:O	2.18	0.44
5:5:46:TRP:CZ3	9:5:101:BCL:H2C	2.53	0.44
1:o:133:LEU:HB2	1:o:283:TYR:CD2	2.53	0.44
3:y:108:PRO:HG2	3:y:111:GLU:HB2	1.99	0.44
4:t:71:HIS:C	4:t:73:GLY:N	2.74	0.44
15:p:103:CRT:C6	6:q:20:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:r:16:ASP:OD1	5:r:16:ASP:C	2.61	0.44
6:s:17:PHE:HD1	15:s:101:CRT:H33	1.83	0.44
15:e:101:CRT:H20	15:e:101:CRT:H181	1.84	0.44
1:C:33:ILE:HG21	1:C:248:THR:O	2.17	0.44
2:L:75:ILE:N	2:L:75:ILE:HD12	2.33	0.44
3:M:156:PHE:CD2	9:M:401:BCL:H43	2.53	0.44
4:H:68:VAL:O	4:H:68:VAL:HG12	2.18	0.44
6:J:26:TYR:HD1	6:J:29:PHE:HD2	1.66	0.44
5:S:25:VAL:HG21	9:S:102:BCL:H152	1.99	0.44
9:Y:101:BCL:H111	9:Y:101:BCL:H151	1.42	0.44
6:Z:40:TRP:CH2	6:Z:46:LEU:HB2	2.53	0.44
9:3:101:BCL:H2	6:4:28:TRP:CH2	2.53	0.44
9:4:102:BCL:H192	9:4:102:BCL:H162	1.75	0.44
1:o:155:CYS:HG	7:o:502:HEM:CAC	2.31	0.44
4:t:184:VAL:HB	4:t:193:VAL:HG22	1.99	0.44
4:t:197:ILE:HD12	4:t:197:ILE:HA	1.85	0.44
4:t:235:GLU:O	4:t:239:VAL:HG23	2.18	0.44
15:p:103:CRT:H6	6:q:17:PHE:HD1	1.83	0.44
15:p:103:CRT:H393	5:r:36:HIS:HB3	2.00	0.44
9:f:101:BCL:H192	9:f:101:BCL:H161	1.60	0.44
1:C:53:ILE:HA	1:C:319:TYR:CE1	2.52	0.44
9:L:301:BCL:HBC3	3:M:197:TYR:OH	2.18	0.44
3:M:182:HIS:CD2	15:M:404:CRT:H20	2.53	0.44
4:H:162:GLU:HB2	4:H:216:ALA:CB	2.48	0.44
6:B:42:TYR:OH	6:B:43:ARG:NH2	2.51	0.44
9:J:102:BCL:H192	9:J:102:BCL:H161	1.83	0.44
9:T:102:BCL:CHB	9:T:102:BCL:H62	2.47	0.44
6:V:45:TRP:HA	5:W:55:TYR:OH	2.17	0.44
5:1:20:VAL:O	5:1:23:SER:HB2	2.18	0.44
15:6:101:CRT:H36	5:7:33:LEU:HD23	1.99	0.44
1:o:102:SER:HB2	1:o:105:GLU:HB2	1.99	0.44
2:x:137:TYR:O	2:x:141:VAL:HG22	2.18	0.44
2:x:237:ALA:HA	2:x:240:ARG:HG3	1.99	0.44
3:y:120:LEU:HD22	5:AC:37:MET:HE2	1.99	0.44
9:m:103:BCL:H71	9:m:103:BCL:H111	1.77	0.44
6:v:28:TRP:HZ2	9:v:102:BCL:HED1	1.82	0.44
5:AA:7:ASN:HB3	5:AA:10:LYS:HD2	1.99	0.44
9:AE:102:BCL:H43	6:AF:28:TRP:CZ2	2.53	0.44
5:l:17:PRO:O	5:l:21:LEU:HG	2.18	0.44
2:L:12:VAL:HG22	2:L:13:ARG:N	2.33	0.43
3:M:63:PHE:CE2	3:M:124:LEU:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:404:CRT:H26	15:M:404:CRT:H241	1.85	0.43
6:N:43:ARG:HG3	5:O:55:TYR:CZ	2.53	0.43
15:P:102:CRT:H10	15:P:102:CRT:H81	1.90	0.43
5:W:4:MET:O	5:W:5:ASN:HB2	2.17	0.43
5:W:31:LEU:HD12	5:W:34:LEU:HD23	2.00	0.43
5:Y:35:ILE:HG12	15:Z:101:CRT:H392	2.00	0.43
5:5:14:ILE:HG21	15:8:101:CRT:H1M1	2.00	0.43
9:7:101:BCL:HED2	6:8:32:VAL:HG22	1.99	0.43
15:8:101:CRT:H30	9:8:102:BCL:H41	1.99	0.43
2:x:242:GLY:HA3	3:y:216:PHE:CZ	2.53	0.43
2:x:274:TRP:CZ3	2:x:278:LEU:HD21	2.53	0.43
5:r:40:LEU:O	5:r:45:ASN:ND2	2.50	0.43
5:u:21:LEU:HD21	15:v:101:CRT:C14	2.48	0.43
5:AE:45:ASN:O	5:AE:49:ASP:OD2	2.36	0.43
5:AG:16:ASP:OD2	5:AG:19:ARG:HG3	2.18	0.43
1:C:71:LYS:HB2	1:C:74:GLU:OE2	2.17	0.43
1:C:152:CYS:HA	7:C:502:HEM:HAB	2.00	0.43
2:L:48:LEU:HD13	5:9:34:LEU:HD22	1.99	0.43
2:L:225:PHE:HD1	2:L:225:PHE:HA	1.56	0.43
3:M:117:MET:HE2	5:Q:41:SER:OG	2.19	0.43
3:M:242:GLY:CA	4:H:119:ARG:HD2	2.48	0.43
5:D:39:VAL:HG21	9:D:102:BCL:H3C	1.99	0.43
9:T:102:BCL:H2C	9:T:102:BCL:HBC3	1.62	0.43
9:X:102:BCL:H122	9:X:102:BCL:H161	1.60	0.43
9:4:102:BCL:H162	9:4:102:BCL:H122	1.87	0.43
9:7:101:BCL:HMC2	9:7:101:BCL:HHC	1.78	0.43
2:x:29:PRO:O	3:y:254:TRP:HA	2.18	0.43
10:x:302:BPH:HBA2	10:x:302:BPH:H3A	1.61	0.43
9:x:303:BCL:H161	9:x:303:BCL:H141	1.49	0.43
3:y:104:LEU:HA	3:y:171:TRP:CD1	2.53	0.43
4:t:159:LEU:HD22	4:t:254:ARG:CZ	2.46	0.43
4:t:221:ASN:HD22	4:t:221:ASN:N	2.16	0.43
9:p:102:BCL:H162	9:p:102:BCL:H141	1.63	0.43
5:u:3:THR:HG23	5:u:5:ASN:H	1.82	0.43
5:u:4:MET:O	5:u:5:ASN:HB2	2.18	0.43
9:AH:101:BCL:HBC3	9:AH:101:BCL:H2C	1.72	0.43
15:AJ:101:CRT:H15	15:AJ:101:CRT:H131	1.88	0.43
6:i:43:ARG:HA	6:i:44:PRO:HD2	1.91	0.43
5:j:43:ASP:CB	5:l:48:ASP:HA	2.48	0.43
1:C:167:VAL:HG11	1:C:297:GLY:HA3	2.00	0.43
1:C:274:ARG:N	1:C:274:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:184:VAL:HB	4:H:193:VAL:HG22	2.00	0.43
5:O:14:ILE:HD11	15:R:101:CRT:H21A	1.98	0.43
9:O:101:BCL:HHB	9:O:101:BCL:HMB1	1.80	0.43
6:P:46:LEU:O	6:R:42:TYR:OH	2.22	0.43
15:P:102:CRT:H36	5:Q:33:LEU:HD23	2.00	0.43
6:T:40:TRP:HH2	6:T:46:LEU:OXT	2.02	0.43
6:X:14:ALA:CB	6:X:17:PHE:HB3	2.48	0.43
5:1:12:TRP:HZ3	5:1:20:VAL:HG21	1.83	0.43
5:1:24:ILE:CD1	9:3:101:BCL:H18	2.48	0.43
2:L:26:TRP:CZ3	4:H:99:PRO:HB3	2.51	0.43
2:L:184:LEU:HD12	2:L:184:LEU:HA	1.74	0.43
3:M:21:VAL:HA	3:M:22:PRO:HD3	1.73	0.43
9:K:101:BCL:H162	9:K:101:BCL:H122	1.79	0.43
5:9:8:LEU:HG	6:0:18:HIS:NE2	2.34	0.43
6:v:18:HIS:O	6:v:22:MET:HG2	2.19	0.43
6:AH:44:PRO:O	5:AI:52:PRO:HD2	2.18	0.43
6:AH:44:PRO:O	5:AI:55:TYR:OH	2.34	0.43
9:AI:101:BCL:HBA2	9:AJ:102:BCL:O2D	2.17	0.43
5:AK:23:SER:OG	9:d:101:BCL:H152	2.18	0.43
6:AL:21:PHE:CD1	15:AL:101:CRT:H14	2.43	0.43
9:AL:102:BCL:H111	9:AL:102:BCL:H93	1.55	0.43
5:j:13:LEU:HD22	15:c:101:CRT:H1M1	2.00	0.43
2:L:188:PHE:HB3	2:L:249:ALA:HB2	2.00	0.43
3:M:39:TRP:O	3:M:42:LYS:N	2.50	0.43
3:M:63:PHE:CD2	3:M:124:LEU:HB3	2.54	0.43
5:Q:12:TRP:O	6:R:9:LEU:HD12	2.18	0.43
5:W:15:LEU:O	5:W:17:PRO:HD3	2.18	0.43
6:X:31:LEU:HD23	6:X:31:LEU:HA	1.74	0.43
15:6:101:CRT:H10	15:6:101:CRT:H81	1.85	0.43
5:7:46:TRP:CE3	9:7:101:BCL:HBC3	2.53	0.43
1:o:258:ASP:O	1:o:262:SER:OG	2.34	0.43
3:y:149:ALA:O	3:y:152:ALA:N	2.49	0.43
6:q:26:TYR:CD1	6:q:29:PHE:HD2	2.35	0.43
6:AB:20:ILE:HD12	15:AC:101:CRT:C5	2.49	0.43
9:AE:104:BCL:H111	9:AE:104:BCL:H91	1.71	0.43
9:AH:101:BCL:H122	9:AH:101:BCL:H162	1.64	0.43
6:k:36:HIS:CG	9:k:102:BCL:H13	2.53	0.43
2:L:172:GLN:O	2:L:172:GLN:HG3	2.11	0.43
5:A:36:HIS:NE2	9:B:101:BCL:NB	2.66	0.43
6:R:17:PHE:HD1	15:R:101:CRT:H22A	1.83	0.43
9:W:101:BCL:H143	9:W:101:BCL:H112	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:17:PRO:HB3	6:Z:17:PHE:CZ	2.53	0.43
15:4:101:CRT:H293	9:5:101:BCL:H11	2.01	0.43
5:9:10:LYS:HB3	15:9:102:CRT:C4	2.49	0.43
1:o:251:HIS:ND1	1:o:256:PHE:O	2.48	0.43
2:x:86:MET:HA	2:x:96:GLN:NE2	2.25	0.43
2:x:198:MET:HE3	10:y:402:BPH:HED1	2.01	0.43
9:x:301:BCL:H143	10:x:302:BPH:H6C1	2.01	0.43
3:y:293:ASN:OD1	3:y:293:ASN:C	2.61	0.43
10:y:402:BPH:H6C2	10:y:402:BPH:H4C1	1.50	0.43
4:t:113:PRO:HB2	4:t:245:GLY:HA2	2.00	0.43
4:t:251:THR:OG1	4:t:254:ARG:HG3	2.18	0.43
6:n:24:SER:OG	5:l:3:THR:HA	2.18	0.43
5:r:9:TYR:HA	6:s:18:HIS:CG	2.54	0.43
5:r:21:LEU:HD23	5:r:21:LEU:HA	1.81	0.43
15:v:101:CRT:H32	9:w:101:BCL:HMA1	2.00	0.43
6:AB:40:TRP:HH2	6:AB:46:LEU:OXT	2.01	0.43
9:AB:101:BCL:H61	9:AB:101:BCL:H41	1.72	0.43
9:AH:103:BCL:HBC3	9:AH:103:BCL:H2C	1.79	0.43
6:c:10:THR:OG1	6:c:13:GLU:HG3	2.18	0.43
1:C:189:THR:HG23	1:C:238:ASN:HD21	1.83	0.43
2:L:160:LEU:HD11	3:M:303:MET:HE2	2.00	0.43
2:L:276:LEU:O	3:M:88:LYS:HE3	2.19	0.43
9:L:303:BCL:HBC2	9:L:303:BCL:H2C	1.73	0.43
3:M:98:PRO:HG3	3:M:107:PRO:HG3	2.01	0.43
3:M:235:ILE:CG2	3:M:236:ASP:N	2.82	0.43
4:H:63:ASP:CG	5:F:19:ARG:HH22	2.27	0.43
6:N:25:MET:HG3	15:N:101:CRT:C20	2.48	0.43
6:P:28:TRP:CH2	9:P:101:BCL:HBA1	2.52	0.43
6:V:16:GLU:O	6:V:20:ILE:HG13	2.18	0.43
2:x:172:GLN:O	2:x:172:GLN:HG3	2.06	0.43
2:x:201:SER:HG	3:y:270:TRP:HD1	1.64	0.43
9:x:303:BCL:HBA2	9:x:303:BCL:H3A	1.74	0.43
9:AD:101:BCL:HBA1	9:AD:101:BCL:H3A	1.68	0.43
9:AI:101:BCL:H121	9:AI:101:BCL:H161	1.38	0.43
6:g:10:THR:OG1	6:g:13:GLU:HG3	2.18	0.43
2:L:97:ILE:HG21	5:9:37:MET:HE1	1.99	0.43
2:L:230:GLY:HA3	3:M:51:ILE:HD12	2.01	0.43
9:L:305:BCL:O1D	3:M:203:MET:HB3	2.19	0.43
3:M:18:TYR:HA	3:M:19:PRO:HD2	1.87	0.43
3:M:37:SER:HG	3:M:40:LEU:N	2.11	0.43
3:M:91:PHE:N	3:M:91:PHE:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:263:GLU:OE1	3:M:267:ARG:NH2	2.49	0.43
4:H:100:LEU:HB2	4:H:111:PHE:CZ	2.53	0.43
4:H:136:MET:HE3	4:H:142:PHE:CB	2.46	0.43
5:A:20:VAL:HG22	9:D:101:BCL:H162	1.99	0.43
6:B:17:PHE:CD1	15:9:102:CRT:H83	2.53	0.43
9:K:101:BCL:H171	9:K:101:BCL:H13	1.83	0.43
9:R:102:BCL:HAA2	9:R:102:BCL:CED	2.49	0.43
5:W:9:TYR:HD1	5:W:9:TYR:H	1.67	0.43
2:x:52:TRP:HZ3	5:m:40:LEU:HD13	1.84	0.43
2:x:106:PHE:CE1	9:x:301:BCL:H121	2.53	0.43
2:x:188:PHE:O	2:x:189:PHE:C	2.62	0.43
3:y:129:TRP:O	3:y:133:THR:HG23	2.17	0.43
4:t:89:ALA:HB1	4:t:101:VAL:O	2.18	0.43
4:t:113:PRO:HG2	4:t:249:TYR:CE2	2.54	0.43
6:AB:31:LEU:O	6:AB:34:ILE:HB	2.18	0.43
9:AB:101:BCL:HMA1	9:AD:101:BCL:HMA1	2.00	0.43
6:AD:33:VAL:O	6:AD:37:LEU:HG	2.19	0.43
6:AJ:40:TRP:CE3	6:AJ:44:PRO:HA	2.53	0.43
9:AL:102:BCL:H162	9:AL:102:BCL:H141	1.76	0.43
6:c:21:PHE:HA	15:c:101:CRT:H14	1.99	0.43
2:L:130:PHE:CD1	10:L:302:BPH:C4D	3.01	0.43
3:M:149:ALA:O	3:M:152:ALA:N	2.46	0.43
15:J:101:CRT:H15	15:J:101:CRT:H131	1.82	0.43
5:Q:21:LEU:HD23	5:Q:21:LEU:HA	1.87	0.43
5:Q:39:VAL:HG12	5:Q:46:TRP:HZ3	1.83	0.43
1:o:127:SER:CB	7:o:501:HEM:HAC	2.48	0.43
1:o:307:CYS:O	1:o:311:HIS:HD2	2.02	0.43
9:x:301:BCL:HHB	9:y:401:BCL:HMB2	2.00	0.43
3:y:277:VAL:O	3:y:280:ALA:HB3	2.19	0.43
14:y:403:MQ8:H462	14:y:403:MQ8:H451	1.51	0.43
5:p:9:TYR:C	5:p:11:ILE:H	2.27	0.43
15:AD:102:CRT:H36	5:AE:33:LEU:HD23	2.01	0.43
5:h:46:TRP:CE2	9:h:101:BCL:H2C	2.53	0.43
2:L:116:ILE:HD13	3:M:254:TRP:CB	2.49	0.43
14:M:403:MQ8:H262	14:M:403:MQ8:H221	1.74	0.43
4:H:76:VAL:HG12	4:H:77:VAL:N	2.33	0.43
5:D:46:TRP:NE1	9:D:101:BCL:HHC	2.33	0.43
15:E:101:CRT:H372	5:F:36:HIS:CD2	2.54	0.43
15:N:101:CRT:H372	5:O:36:HIS:CG	2.53	0.43
6:R:43:ARG:HG3	5:S:55:TYR:OH	2.19	0.43
6:X:13:GLU:HA	6:X:14:ALA:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:101:BCL:H143	9:Y:101:BCL:H162	1.91	0.43
6:0:32:VAL:HG11	9:0:101:BCL:HBA1	2.00	0.43
1:o:83:LYS:C	1:o:85:LEU:H	2.26	0.43
2:x:184:LEU:HD23	2:x:252:TRP:CD2	2.54	0.43
2:x:207:THR:HG21	3:y:238:ILE:HG21	2.01	0.43
2:x:273:ASN:C	2:x:275:TRP:N	2.76	0.43
11:x:304:UQ8:H17	11:x:304:UQ8:H20	1.90	0.43
9:x:305:BCL:H62	9:x:305:BCL:H41	1.63	0.43
3:y:183:LEU:HD23	3:y:183:LEU:HA	1.75	0.43
6:n:31:LEU:HD23	6:n:31:LEU:HA	1.79	0.43
9:AC:102:BCL:H3A	9:AC:102:BCL:HBA1	1.40	0.43
5:AI:12:TRP:HE1	6:AJ:18:HIS:HB2	1.83	0.43
9:e:102:BCL:HBC2	9:e:102:BCL:H2C	1.73	0.43
15:f:102:CRT:H30	9:g:101:BCL:HMA2	2.00	0.43
1:C:81:VAL:HG11	1:C:131:PHE:HB3	2.00	0.42
9:L:305:BCL:CHD	9:L:305:BCL:HBC2	2.49	0.42
3:M:18:TYR:CE2	3:M:20:GLY:CA	2.95	0.42
3:M:63:PHE:HB2	3:M:125:SER:HB2	2.01	0.42
6:E:34:ILE:HD13	6:E:34:ILE:HA	1.88	0.42
5:F:40:LEU:HG	5:F:46:TRP:CH2	2.54	0.42
6:P:25:MET:HG2	6:P:29:PHE:CE2	2.54	0.42
9:R:102:BCL:H3A	9:R:102:BCL:C2	2.39	0.42
15:U:102:CRT:H393	5:W:36:HIS:CD2	2.54	0.42
5:W:43:ASP:O	5:Y:56:GLN:NE2	2.52	0.42
6:4:32:VAL:HG21	9:4:102:BCL:HBA2	2.00	0.42
9:7:101:BCL:H41	9:7:101:BCL:H62	1.78	0.42
1:o:212:ILE:N	7:o:503:HEM:O1A	2.41	0.42
1:o:311:HIS:NE2	7:o:504:HEM:NB	2.67	0.42
2:x:273:ASN:OD1	2:x:277:GLU:HG2	2.18	0.42
3:y:175:VAL:HG13	3:y:185:TRP:CG	2.54	0.42
3:y:242:GLY:HA2	4:t:119:ARG:HD2	2.00	0.42
4:t:234:TYR:CE1	4:t:238:LYS:HG3	2.54	0.42
6:n:24:SER:O	6:n:27:ALA:HB3	2.19	0.42
6:g:24:SER:O	6:g:27:ALA:HB3	2.19	0.42
6:i:21:PHE:CZ	9:j:101:BCL:H172	2.54	0.42
5:j:4:MET:CE	6:c:20:ILE:HG12	2.48	0.42
5:l:17:PRO:HG2	6:c:9:LEU:HD11	1.99	0.42
1:C:253:THR:HG21	2:L:171:TYR:CB	2.49	0.42
2:L:17:LEU:HD23	2:L:17:LEU:HA	1.78	0.42
2:L:196:LEU:HB2	3:M:216:PHE:HD2	1.83	0.42
2:L:248:SER:O	2:L:251:PHE:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:37:SER:C	3:M:39:TRP:N	2.76	0.42
9:D:102:BCL:C9	6:E:33:VAL:HG22	2.45	0.42
9:N:102:BCL:HBA1	9:N:102:BCL:H3A	1.78	0.42
9:O:101:BCL:HBA1	9:O:101:BCL:C2	2.48	0.42
5:S:36:HIS:O	5:S:40:LEU:HB2	2.19	0.42
6:T:45:TRP:CZ2	9:T:102:BCL:H151	2.54	0.42
6:4:21:PHE:HA	15:4:101:CRT:H14	2.00	0.42
1:o:42:ASN:HA	2:x:172:GLN:NE2	2.29	0.42
1:o:292:PRO:HD2	1:o:295:ARG:HG2	2.01	0.42
2:x:48:LEU:HD11	5:m:33:LEU:HD13	2.02	0.42
2:x:120:LEU:HD21	3:y:254:TRP:CH2	2.54	0.42
2:x:172:GLN:HE21	2:x:172:GLN:HB2	1.44	0.42
3:y:121:PHE:N	3:y:121:PHE:CD1	2.86	0.42
3:y:178:GLY:O	3:y:182:HIS:HB3	2.18	0.42
3:y:179:ILE:O	3:y:183:LEU:HG	2.19	0.42
4:t:113:PRO:HD2	4:t:249:TYR:OH	2.18	0.42
9:p:104:BCL:H13	9:p:104:BCL:HBB2	2.01	0.42
5:r:17:PRO:HB3	6:s:17:PHE:CZ	2.54	0.42
5:u:43:ASP:CB	5:w:50:ASN:HD21	2.30	0.42
5:AA:45:ASN:C	5:AA:49:ASP:OD2	2.52	0.42
6:AH:32:VAL:HA	9:AH:101:BCL:HED2	2.00	0.42
5:AI:9:TYR:CE1	5:AI:10:LYS:HG3	2.54	0.42
6:AJ:25:MET:HG3	15:AJ:101:CRT:C21	2.49	0.42
6:AJ:40:TRP:HH2	6:AJ:46:LEU:OXT	2.02	0.42
9:AK:101:BCL:H41	9:AK:101:BCL:H61	1.65	0.42
1:C:153:TYR:O	1:C:154:THR:C	2.62	0.42
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.76	0.42
1:C:275:HIS:C	1:C:275:HIS:CD2	2.96	0.42
2:L:179:ASN:O	2:L:182:HIS:HB3	2.18	0.42
9:L:301:BCL:H111	10:L:302:BPH:HHB	2.01	0.42
3:M:122:LEU:HA	3:M:122:LEU:HD12	1.67	0.42
6:E:40:TRP:HZ3	6:E:45:TRP:H	1.67	0.42
5:I:4:MET:O	5:I:5:ASN:HB2	2.19	0.42
6:N:32:VAL:HG12	9:N:102:BCL:H92	2.00	0.42
6:T:18:HIS:O	6:T:22:MET:HG2	2.18	0.42
9:T:102:BCL:H93	9:T:102:BCL:H61	1.76	0.42
5:W:2:PHE:O	5:W:3:THR:HG23	2.18	0.42
9:X:102:BCL:H41	9:X:102:BCL:H61	1.71	0.42
9:Z:102:BCL:HBA1	9:Z:102:BCL:H3A	1.71	0.42
5:1:5:ASN:OD1	5:1:6:ALA:N	2.52	0.42
5:1:57:ALA:HB3	5:1:58:LEU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:101:CRT:C31	9:3:101:BCL:H3A	2.49	0.42
9:0:101:BCL:H91	9:0:101:BCL:H111	1.78	0.42
1:o:139:SER:HA	1:o:142:LYS:HE3	2.02	0.42
2:x:52:TRP:CZ3	5:m:40:LEU:HD13	2.54	0.42
2:x:117:CYS:HB2	2:x:124:PHE:CE1	2.55	0.42
3:y:128:LEU:HD23	3:y:128:LEU:HA	1.69	0.42
9:p:102:BCL:H2	6:q:28:TRP:CZ2	2.55	0.42
9:r:101:BCL:H143	9:r:101:BCL:H162	1.72	0.42
6:s:17:PHE:HA	15:s:101:CRT:H6	2.00	0.42
6:s:20:ILE:HD12	15:s:101:CRT:C6	2.49	0.42
9:AE:104:BCL:HMB3	9:AE:104:BCL:HHB	1.83	0.42
9:AE:104:BCL:H192	6:AF:40:TRP:NE1	2.34	0.42
5:AI:10:LYS:O	5:AI:13:LEU:HB2	2.19	0.42
5:d:43:ASP:OD1	5:f:56:GLN:HG2	2.20	0.42
9:e:102:BCL:H93	9:e:102:BCL:H111	1.85	0.42
9:i:102:BCL:H3A	9:i:102:BCL:O2A	2.19	0.42
5:j:16:ASP:HA	5:j:17:PRO:HD3	1.90	0.42
15:k:101:CRT:H243	9:l:101:BCL:H152	2.00	0.42
2:L:237:ALA:HA	2:L:240:ARG:CG	2.50	0.42
15:J:101:CRT:H21A	15:J:101:CRT:H5	1.68	0.42
15:T:101:CRT:H10	15:T:101:CRT:H81	1.85	0.42
5:1:39:VAL:HG12	5:1:46:TRP:HZ3	1.84	0.42
6:6:9:LEU:HD23	6:6:13:GLU:O	2.19	0.42
2:x:59:THR:OG1	2:x:65:LEU:HD12	2.18	0.42
2:x:160:LEU:HD23	2:x:160:LEU:HA	1.93	0.42
2:x:196:LEU:HD12	2:x:196:LEU:HA	1.66	0.42
9:m:102:BCL:H61	9:m:102:BCL:H102	1.85	0.42
9:p:102:BCL:H142	9:p:102:BCL:H111	1.75	0.42
5:r:45:ASN:OD1	5:r:47:LEU:N	2.36	0.42
9:r:101:BCL:H112	9:r:101:BCL:H72	1.34	0.42
6:AD:31:LEU:HD23	6:AD:31:LEU:HA	1.91	0.42
5:AG:40:LEU:HD12	5:AG:40:LEU:HA	1.73	0.42
9:AI:101:BCL:HBC3	9:AI:101:BCL:H2C	1.82	0.42
9:d:101:BCL:HBC3	9:d:101:BCL:H2C	1.55	0.42
9:e:102:BCL:H61	9:e:102:BCL:H41	1.68	0.42
9:L:303:BCL:HAC2	9:L:303:BCL:HHD	1.19	0.42
3:M:63:PHE:CB	3:M:125:SER:HB2	2.50	0.42
3:M:200:PRO:HD2	3:M:294:TRP:CZ3	2.55	0.42
4:H:71:HIS:C	4:H:73:GLY:N	2.77	0.42
4:H:159:LEU:C	4:H:159:LEU:HD12	2.45	0.42
5:W:45:ASN:HB3	5:Y:56:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:10:THR:OG1	6:Z:13:GLU:HG3	2.20	0.42
5:1:9:TYR:HB2	6:2:14:ALA:O	2.20	0.42
9:1:101:BCL:H61	9:1:101:BCL:H41	1.91	0.42
6:4:21:PHE:HA	15:4:101:CRT:H11	2.00	0.42
1:o:181:THR:HG21	1:o:184:ASN:HD22	1.84	0.42
2:x:162:HIS:CE1	2:x:163:LEU:HD23	2.55	0.42
3:y:73:PHE:CZ	3:y:81:TRP:CH2	3.07	0.42
4:t:232:THR:O	4:t:236:GLU:HG3	2.19	0.42
5:u:37:MET:HE1	5:u:40:LEU:HD12	2.00	0.42
9:v:102:BCL:HMA1	9:w:101:BCL:HMB3	2.01	0.42
5:AA:44:LEU:HD13	6:AB:43:ARG:HD3	2.01	0.42
5:AC:28:GLN:OE1	6:AD:28:TRP:NE1	2.49	0.42
15:AJ:101:CRT:H2M1	5:AK:37:MET:HG3	2.02	0.42
6:AL:40:TRP:CH2	9:AL:102:BCL:H193	2.54	0.42
6:c:34:ILE:O	6:c:38:LEU:HG	2.19	0.42
1:C:169:ASP:HA	1:C:170:PRO:HD3	1.89	0.42
2:L:157:TYR:CG	10:L:302:BPH:H151	2.55	0.42
2:L:281:TRP:CB	3:M:88:LYS:HD2	2.49	0.42
3:M:230:GLY:O	3:M:233:ARG:HB2	2.20	0.42
6:B:31:LEU:HD23	6:B:31:LEU:HA	1.86	0.42
9:D:101:BCL:H162	9:D:101:BCL:H141	1.52	0.42
5:Q:11:ILE:O	5:Q:15:LEU:N	2.43	0.42
2:x:179:ASN:HB3	2:x:182:HIS:HB3	2.01	0.42
2:x:227:ASP:O	3:y:51:ILE:HG13	2.20	0.42
3:y:290:VAL:HG11	4:t:11:ALA:HB3	2.02	0.42
6:s:29:PHE:HB3	9:s:102:BCL:H42	2.01	0.42
5:AI:12:TRP:HE1	6:AJ:18:HIS:HD1	1.67	0.42
5:h:38:ILE:O	5:h:42:THR:HG23	2.20	0.42
1:C:258:ASP:O	1:C:262:SER:OG	2.33	0.42
2:L:125:HIS:HE1	3:M:5:GLN:OE1	2.03	0.42
4:H:66:THR:HG22	4:H:77:VAL:CG2	2.50	0.42
5:D:39:VAL:HG12	5:D:46:TRP:CZ3	2.55	0.42
9:O:101:BCL:H172	9:O:101:BCL:H13	1.57	0.42
15:P:102:CRT:H342	9:Q:101:BCL:H11	2.01	0.42
15:X:101:CRT:H81	15:X:101:CRT:H10	1.62	0.42
6:Z:40:TRP:HZ3	6:Z:46:LEU:H	1.67	0.42
5:7:49:ASP:O	5:7:50:ASN:HB2	2.18	0.42
1:o:134:VAL:O	1:o:137:ALA:HB3	2.20	0.42
1:o:205:ASP:OD1	1:o:304:ARG:NE	2.51	0.42
1:o:279:ILE:O	1:o:283:TYR:HB2	2.20	0.42
2:x:132:PHE:CE2	11:x:304:UQ8:H40B	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:194:LEU:HD12	10:y:402:BPH:C4C	2.49	0.42
2:x:273:ASN:O	2:x:274:TRP:C	2.63	0.42
15:y:404:CRT:H10	15:y:404:CRT:H81	1.90	0.42
4:t:112:GLY:C	4:t:114:ALA:N	2.78	0.42
5:p:31:LEU:HD21	9:p:104:BCL:HMA2	2.00	0.42
9:r:101:BCL:H151	9:r:101:BCL:H18	1.49	0.42
9:v:102:BCL:H91	9:v:102:BCL:H112	1.83	0.42
5:AG:11:ILE:HG23	5:AG:12:TRP:CD2	2.55	0.42
15:k:101:CRT:H15	15:k:101:CRT:H131	1.85	0.42
6:c:32:VAL:CG2	9:c:102:BCL:HBA2	2.49	0.42
1:C:179:LYS:HA	1:C:180:PRO:HD3	1.92	0.42
2:L:153:HIS:O	2:L:165:TRP:HZ2	2.03	0.42
2:L:183:MET:HB3	9:L:303:BCL:O1D	2.20	0.42
4:H:4:GLY:O	4:H:6:THR:N	2.53	0.42
4:H:136:MET:SD	4:H:152:ARG:NH2	2.93	0.42
4:H:224:THR:OG1	4:H:225:LEU:N	2.52	0.42
9:D:102:BCL:H111	9:D:102:BCL:H93	1.72	0.42
6:E:40:TRP:CH2	6:E:46:LEU:HD12	2.50	0.42
5:F:28:GLN:HB3	9:F:101:BCL:H12	2.02	0.42
5:I:3:THR:H	5:I:4:MET:HA	1.85	0.42
6:P:21:PHE:CD1	15:P:102:CRT:H16	2.55	0.42
6:P:32:VAL:HG22	9:P:101:BCL:HED2	2.02	0.42
5:3:31:LEU:O	5:3:34:LEU:HB3	2.20	0.42
9:5:102:BCL:H111	9:5:102:BCL:H93	1.72	0.42
2:x:84:LEU:HB2	5:h:41:SER:CB	2.48	0.42
2:x:175:HIS:CD2	2:x:178:TYR:CE1	3.08	0.42
3:y:18:TYR:CD2	3:y:20:GLY:HA2	2.55	0.42
3:y:121:PHE:N	3:y:121:PHE:HD1	2.18	0.42
9:m:103:BCL:H11	9:m:103:BCL:H3A	2.01	0.42
6:q:26:TYR:HD1	6:q:29:PHE:CD2	2.37	0.42
5:u:21:LEU:HD23	5:u:21:LEU:HA	1.86	0.42
9:u:101:BCL:H62	9:u:101:BCL:H102	1.79	0.42
9:v:102:BCL:HBC3	9:v:102:BCL:H2C	1.65	0.42
9:AE:104:BCL:H71	6:AF:36:HIS:CG	2.55	0.42
15:AL:101:CRT:H32	9:d:101:BCL:HHB	2.02	0.42
6:k:32:VAL:O	6:k:36:HIS:ND1	2.46	0.42
2:L:25:PHE:CE1	2:L:32:VAL:HG21	2.54	0.42
4:H:197:ILE:O	4:H:200:SER:OG	2.34	0.42
5:A:49:ASP:O	5:A:50:ASN:HB2	2.19	0.42
5:I:13:LEU:HB2	15:N:101:CRT:H1M1	2.01	0.42
15:N:101:CRT:H26	15:N:101:CRT:H241	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:101:CRT:H81	15:R:101:CRT:H10	1.78	0.42
6:T:21:PHE:HA	15:T:101:CRT:H14	2.02	0.42
6:Z:29:PHE:O	6:Z:32:VAL:HB	2.20	0.42
15:Z:101:CRT:C27	9:Z:102:BCL:H11	2.50	0.42
5:5:9:TYR:C	5:5:11:ILE:N	2.78	0.42
3:y:32:GLY:O	3:y:50:PRO:HB3	2.20	0.42
4:t:66:THR:HG22	4:t:77:VAL:CG2	2.49	0.42
4:t:119:ARG:HD2	4:t:237:ASP:CG	2.45	0.42
4:t:135:PRO:HD3	4:t:171:TRP:CZ2	2.55	0.42
5:r:16:ASP:OD2	5:r:19:ARG:HG3	2.19	0.42
5:r:56:GLN:OE1	5:r:56:GLN:HA	2.20	0.42
9:r:101:BCL:HBC3	9:r:101:BCL:H2C	1.86	0.42
6:v:30:GLY:O	6:v:34:ILE:HG13	2.20	0.42
15:AD:102:CRT:H372	5:AE:36:HIS:CG	2.54	0.42
5:AE:18:ARG:NH1	17:AE:101:PGW:OAE	2.53	0.42
9:k:102:BCL:H151	9:k:102:BCL:H111	1.68	0.42
1:C:189:THR:CG2	1:C:238:ASN:HD21	2.33	0.42
1:C:263:THR:O	3:M:313:ALA:HB2	2.20	0.42
1:C:275:HIS:O	1:C:275:HIS:HD2	2.03	0.42
2:L:196:LEU:HD13	3:M:216:PHE:CB	2.50	0.42
4:H:66:THR:HG22	4:H:77:VAL:HG23	2.02	0.42
4:H:135:PRO:C	4:H:137:ARG:H	2.28	0.42
5:I:33:LEU:O	5:I:37:MET:HG2	2.19	0.42
5:O:30:VAL:HA	5:O:33:LEU:HD12	2.02	0.42
5:O:35:ILE:HA	5:O:38:ILE:HD12	2.02	0.42
5:Q:17:PRO:HB3	6:R:17:PHE:CE2	2.54	0.42
5:U:38:ILE:O	5:U:42:THR:HG23	2.19	0.42
9:3:101:BCL:HMB3	9:3:101:BCL:HHB	1.84	0.42
15:4:101:CRT:H10	15:4:101:CRT:H81	1.86	0.42
9:4:102:BCL:CHB	9:5:101:BCL:HMB2	2.50	0.42
5:7:21:LEU:HD23	5:7:21:LEU:HA	1.83	0.42
5:7:31:LEU:HD23	9:8:102:BCL:HED1	2.01	0.42
2:x:125:HIS:HE1	3:y:5:GLN:O	2.03	0.42
2:x:186:ILE:HG21	2:x:186:ILE:HD13	1.76	0.42
2:x:196:LEU:HD13	3:y:216:PHE:CG	2.55	0.42
9:x:305:BCL:H18	9:x:305:BCL:H151	1.50	0.42
3:y:219:HIS:NE2	3:y:266:HIS:CE1	2.88	0.42
15:y:404:CRT:H15	15:y:404:CRT:H131	1.80	0.42
15:n:101:CRT:H31	15:n:101:CRT:H291	1.89	0.42
6:v:40:TRP:CD2	9:v:102:BCL:H193	2.54	0.42
5:AA:40:LEU:HD23	5:AA:40:LEU:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AB:101:BCL:HED2	9:AB:101:BCL:HBD	1.69	0.42
5:AE:35:ILE:HD11	9:AH:101:BCL:HMB3	2.00	0.42
9:AI:101:BCL:H62	9:AI:101:BCL:H201	2.01	0.42
9:f:101:BCL:H2	6:g:28:TRP:CZ2	2.55	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.41
4:H:154:MET:O	4:H:167:VAL:HG23	2.20	0.41
4:H:223:PRO:HG2	4:H:238:LYS:O	2.19	0.41
6:B:20:ILE:CG2	5:9:3:THR:HG22	2.50	0.41
9:T:102:BCL:HAA1	9:T:102:BCL:HBD	2.02	0.41
5:3:18:ARG:O	5:3:22:VAL:HG22	2.20	0.41
5:7:12:TRP:HZ3	5:7:20:VAL:HG11	1.85	0.41
1:o:196:PRO:HG2	1:o:231:TRP:HA	2.02	0.41
1:o:268:THR:HG21	7:o:504:HEM:CAA	2.50	0.41
2:x:78:PRO:HB3	2:x:92:GLY:HA3	2.02	0.41
2:x:173:PHE:CZ	2:x:260:SER:HB3	2.55	0.41
9:x:305:BCL:H61	14:y:403:MQ8:H243	2.02	0.41
4:t:27:ILE:HG23	4:t:27:ILE:HD12	1.81	0.41
9:w:101:BCL:H171	9:w:101:BCL:H13	1.75	0.41
5:AA:35:ILE:HG12	15:AC:101:CRT:H403	2.02	0.41
5:j:29:ILE:HG13	9:j:101:BCL:H43	2.02	0.41
1:C:316:LYS:O	1:C:317:PRO:C	2.60	0.41
2:L:68:TYR:CA	2:L:73:ILE:HD11	2.49	0.41
2:L:235:ALA:O	2:L:238:ILE:HG22	2.19	0.41
2:L:271:TRP:O	2:L:273:ASN:N	2.53	0.41
3:M:31:ILE:HD11	3:M:53:LEU:HB2	2.02	0.41
15:M:404:CRT:H31	15:M:404:CRT:H291	1.89	0.41
4:H:31:ARG:HD2	4:H:31:ARG:HA	1.86	0.41
15:E:101:CRT:H393	5:F:36:HIS:HB3	2.01	0.41
9:J:102:BCL:HED2	9:J:102:BCL:HBD	1.90	0.41
5:O:3:THR:O	5:O:4:MET:HG2	2.19	0.41
9:Q:101:BCL:H51	9:Q:101:BCL:H122	2.02	0.41
9:S:102:BCL:H2A	9:S:102:BCL:O2D	2.20	0.41
15:T:101:CRT:H26	15:T:101:CRT:H241	1.88	0.41
5:U:13:LEU:C	6:V:7:THR:HG23	2.45	0.41
6:X:36:HIS:CG	9:X:102:BCL:H8	2.56	0.41
15:X:101:CRT:H393	5:Y:36:HIS:HB3	2.02	0.41
6:Z:46:LEU:HD23	6:Z:46:LEU:HA	1.96	0.41
1:o:138:ASN:ND2	1:o:330:LEU:O	2.52	0.41
9:r:101:BCL:HBC1	9:s:102:BCL:HBC3	2.02	0.41
5:AA:7:ASN:OD1	5:AA:9:TYR:HE1	2.03	0.41
15:AE:103:CRT:H14	6:AF:21:PHE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AK:40:LEU:HD21	5:AK:47:LEU:HD12	2.01	0.41
15:k:101:CRT:H20	15:k:101:CRT:H181	1.76	0.41
1:C:21:LEU:HD11	2:L:274:TRP:CE3	2.55	0.41
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.69	0.41
2:L:161:SER:O	2:L:164:ASP:HB2	2.20	0.41
2:L:177:HIS:HB3	3:M:183:LEU:HD22	2.02	0.41
3:M:143:SER:HB2	3:M:145:HIS:CE1	2.55	0.41
3:M:242:GLY:HA2	4:H:119:ARG:HD2	2.02	0.41
14:M:403:MQ8:H401	14:M:403:MQ8:H361	1.79	0.41
4:H:45:ARG:HD3	4:H:45:ARG:HA	1.83	0.41
9:D:102:BCL:HBA1	9:D:102:BCL:H3A	1.77	0.41
9:N:102:BCL:H192	9:N:102:BCL:H161	1.64	0.41
5:W:21:LEU:HA	5:W:21:LEU:HD23	1.81	0.41
5:W:24:ILE:HD13	5:W:24:ILE:HA	1.83	0.41
9:Z:102:BCL:H62	9:Z:102:BCL:H41	1.54	0.41
6:4:17:PHE:HA	15:4:101:CRT:H6	2.02	0.41
6:8:32:VAL:HG12	9:8:102:BCL:H121	2.01	0.41
15:9:102:CRT:H20	15:9:102:CRT:H181	1.89	0.41
1:o:38:VAL:O	1:o:38:VAL:HG12	2.20	0.41
1:o:59:VAL:HG21	1:o:100:TRP:NE1	2.34	0.41
1:o:314:VAL:HG12	1:o:316:LYS:H	1.85	0.41
1:o:316:LYS:O	1:o:317:PRO:C	2.61	0.41
2:x:112:ARG:O	2:x:116:ILE:HG13	2.20	0.41
2:x:268:TRP:O	2:x:269:PRO:C	2.62	0.41
9:x:305:BCL:O1A	9:x:305:BCL:H43	2.21	0.41
9:v:102:BCL:H161	9:v:102:BCL:H122	1.78	0.41
9:AE:104:BCL:HED2	9:AE:104:BCL:HBD	1.80	0.41
5:AK:35:ILE:HG12	15:AL:101:CRT:H403	2.02	0.41
2:L:189:PHE:HB3	3:M:209:LEU:HD21	2.01	0.41
3:M:159:VAL:HG13	3:M:285:LEU:HG	2.01	0.41
6:J:40:TRP:CZ2	9:J:102:BCL:H202	2.55	0.41
15:J:101:CRT:H241	15:J:101:CRT:H26	1.83	0.41
15:R:101:CRT:H31A	15:R:101:CRT:H5	1.82	0.41
9:T:102:BCL:HBD	9:T:102:BCL:HED2	1.77	0.41
5:W:49:ASP:HB3	5:W:51:ILE:HG13	2.01	0.41
6:X:32:VAL:HG21	9:X:102:BCL:HBA2	2.03	0.41
6:Z:29:PHE:CZ	9:Z:102:BCL:H2	2.55	0.41
5:9:36:HIS:CE1	9:0:101:BCL:HMD3	2.56	0.41
9:9:103:BCL:H112	9:9:103:BCL:H152	1.48	0.41
1:o:299:TYR:HB2	1:o:301:ASP:OD1	2.21	0.41
2:x:31:TYR:CZ	2:x:119:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:136:MET:HE2	4:t:136:MET:HB3	1.78	0.41
5:m:8:LEU:HG	6:q:20:ILE:CD1	2.50	0.41
15:p:103:CRT:H83	6:q:20:ILE:HD13	2.02	0.41
5:u:9:TYR:HA	6:v:18:HIS:CG	2.56	0.41
5:AC:9:TYR:C	5:AC:11:ILE:H	2.28	0.41
9:AD:101:BCL:HAA1	9:AD:101:BCL:HBD	2.01	0.41
5:AE:35:ILE:CD1	9:AH:101:BCL:HMB3	2.50	0.41
6:AJ:25:MET:HB2	15:AJ:101:CRT:H182	2.01	0.41
5:AK:14:ILE:CD1	15:e:101:CRT:H82	2.50	0.41
6:e:17:PHE:N	15:e:101:CRT:H23	2.35	0.41
6:i:21:PHE:HA	15:i:101:CRT:H14	2.02	0.41
5:j:17:PRO:HB3	6:k:17:PHE:CE1	2.54	0.41
9:j:101:BCL:HMB1	9:j:101:BCL:HHB	1.81	0.41
2:L:155:PHE:HA	2:L:165:TRP:NE1	2.35	0.41
4:H:102:PRO:HB3	4:H:111:PHE:HD2	1.86	0.41
9:F:101:BCL:H2	6:G:28:TRP:CZ2	2.55	0.41
5:I:17:PRO:HB3	6:J:17:PHE:CE1	2.55	0.41
5:I:17:PRO:HB3	6:J:17:PHE:CE2	2.55	0.41
9:8:102:BCL:H172	9:8:102:BCL:CAB	2.51	0.41
1:o:24:GLU:OE2	2:x:265:THR:OG1	2.29	0.41
1:o:249:PHE:O	1:o:263:THR:OG1	2.24	0.41
2:x:190:PHE:HB2	9:x:303:BCL:O1A	2.21	0.41
2:x:196:LEU:HD13	3:y:216:PHE:CD2	2.55	0.41
12:x:306:PEF:O4	12:x:306:PEF:H11	2.19	0.41
3:y:37:SER:HG	3:y:40:LEU:H	1.63	0.41
3:y:76:LEU:HA	3:y:76:LEU:HD12	1.72	0.41
3:y:291:VAL:HG11	3:y:294:TRP:CE3	2.56	0.41
4:t:22:PHE:CD2	4:t:22:PHE:C	2.99	0.41
4:t:157:VAL:HG23	4:t:210:LYS:HA	2.02	0.41
4:t:159:LEU:C	4:t:159:LEU:HD12	2.46	0.41
9:v:102:BCL:HHD	9:v:102:BCL:HAC2	1.83	0.41
5:AK:11:ILE:HD13	15:e:101:CRT:H132	2.03	0.41
5:d:40:LEU:HD23	5:d:40:LEU:HA	1.81	0.41
6:g:45:TRP:CD1	6:g:46:LEU:HG	2.55	0.41
2:L:26:TRP:HZ2	3:M:254:TRP:CZ3	2.37	0.41
2:L:268:TRP:O	2:L:269:PRO:C	2.60	0.41
10:L:302:BPH:H3A	10:L:302:BPH:HBA2	1.86	0.41
9:L:303:BCL:H13	9:L:303:BCL:H172	1.91	0.41
3:M:96:GLU:HA	3:M:97:PRO:HD3	1.89	0.41
4:H:14:ILE:HA	4:H:17:TRP:CD1	2.56	0.41
4:H:21:LEU:HA	4:H:21:LEU:HD23	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:ARG:O	4:H:34:ASP:HB2	2.21	0.41
15:E:101:CRT:H20	15:E:101:CRT:H181	1.94	0.41
5:O:10:LYS:HE3	6:R:16:GLU:OE2	2.20	0.41
9:V:101:BCL:HBB3	9:W:101:BCL:CHC	2.51	0.41
6:Z:28:TRP:O	6:Z:32:VAL:HG23	2.21	0.41
15:4:101:CRT:H342	9:5:101:BCL:HBA1	2.03	0.41
1:o:128:ARG:HH21	7:o:501:HEM:HAD1	1.86	0.41
10:y:402:BPH:HBA2	10:y:402:BPH:H3A	1.69	0.41
4:t:107:MET:HB3	4:t:107:MET:HE3	1.32	0.41
9:r:101:BCL:H3A	9:r:101:BCL:HBA1	1.63	0.41
5:u:17:PRO:HB3	6:v:17:PHE:CZ	2.56	0.41
6:v:33:VAL:O	6:v:37:LEU:HG	2.21	0.41
6:AD:28:TRP:HH2	9:AD:101:BCL:HAA2	1.85	0.41
15:f:102:CRT:H10	15:f:102:CRT:H81	1.83	0.41
1:C:21:LEU:HD23	2:L:271:TRP:CH2	2.56	0.41
1:C:183:GLN:HB2	1:C:195:LEU:C	2.45	0.41
2:L:15:GLY:O	2:L:118:ARG:NE	2.47	0.41
2:L:204:LEU:HD11	3:M:266:HIS:O	2.21	0.41
3:M:159:VAL:CG1	3:M:285:LEU:HG	2.51	0.41
4:H:247:LYS:HA	4:H:254:ARG:NH1	2.34	0.41
6:E:8:GLY:O	6:E:9:LEU:HD12	2.20	0.41
9:I:101:BCL:H61	9:I:101:BCL:H2	1.84	0.41
9:O:101:BCL:HMB3	9:O:101:BCL:H93	2.01	0.41
5:W:9:TYR:CD2	6:X:15:LYS:HG2	2.55	0.41
5:W:36:HIS:CE1	9:X:102:BCL:HMD3	2.55	0.41
9:Y:101:BCL:HED1	6:Z:31:LEU:HB3	2.02	0.41
5:1:56:GLN:O	5:1:59:GLY:HA2	2.21	0.41
6:2:31:LEU:HD23	6:2:31:LEU:HA	1.83	0.41
5:9:8:LEU:HG	6:0:18:HIS:CE1	2.55	0.41
5:9:40:LEU:HD12	5:9:40:LEU:HA	1.75	0.41
1:o:133:LEU:HD23	1:o:133:LEU:C	2.46	0.41
2:x:56:ILE:O	2:x:60:GLY:C	2.64	0.41
2:x:202:LEU:HA	2:x:202:LEU:HD12	1.54	0.41
2:x:266:ARG:HD3	2:x:270:GLU:OE1	2.21	0.41
2:x:275:TRP:HA	2:x:278:LEU:HG	2.02	0.41
3:y:179:ILE:HG22	3:y:180:PHE:N	2.35	0.41
5:m:2:PHE:HB3	5:m:4:MET:HB2	2.02	0.41
15:n:101:CRT:H10	15:n:101:CRT:H132	1.97	0.41
15:n:101:CRT:H393	5:p:36:HIS:CD2	2.55	0.41
5:w:11:ILE:HG23	5:w:12:TRP:CD2	2.56	0.41
5:AA:60:LYS:HA	5:AA:61:LYS:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AD:41:LEU:HD23	6:AD:41:LEU:HA	1.84	0.41
5:AG:39:VAL:HG11	9:AH:101:BCL:HBC1	2.03	0.41
9:g:101:BCL:H111	9:g:101:BCL:H93	1.61	0.41
5:h:28:GLN:OE1	6:i:28:TRP:NE1	2.53	0.41
9:l:101:BCL:HAA2	9:l:101:BCL:HBD	2.03	0.41
1:C:38:VAL:HG22	3:M:307:TYR:CD2	2.55	0.41
1:C:101:VAL:HG22	1:C:152:CYS:HB3	2.03	0.41
1:C:142:LYS:C	1:C:144:HIS:N	2.78	0.41
1:C:187:SER:C	1:C:189:THR:H	2.29	0.41
3:M:157:TYR:CZ	15:M:404:CRT:H293	2.56	0.41
6:B:46:LEU:HA	5:D:51:ILE:HD13	2.03	0.41
5:S:20:VAL:O	5:S:24:ILE:HG13	2.21	0.41
5:S:28:GLN:OE1	6:T:28:TRP:NE1	2.38	0.41
6:T:16:GLU:HB3	15:T:101:CRT:C3	2.50	0.41
6:T:28:TRP:O	6:T:32:VAL:HG23	2.20	0.41
5:Y:10:LYS:CB	15:2:101:CRT:H5	2.50	0.41
1:o:203:PHE:O	1:o:277:ARG:NH1	2.40	0.41
1:o:258:ASP:OD2	1:o:261:GLN:HG3	2.20	0.41
11:x:304:UQ8:H7	11:x:304:UQ8:H10	1.91	0.41
3:y:206:ILE:HD13	3:y:206:ILE:HG21	1.72	0.41
3:y:226:VAL:HB	3:y:244:ALA:HB1	2.02	0.41
3:y:265:ILE:CD1	14:y:403:MQ8:H121	2.39	0.41
4:t:69:LEU:HD21	4:t:76:VAL:HG23	2.03	0.41
4:t:150:ASP:OD1	4:t:152:ARG:HB2	2.20	0.41
4:t:195:LEU:HA	4:t:196:PRO:HD3	1.76	0.41
9:m:102:BCL:H151	9:m:102:BCL:H111	1.67	0.41
6:AJ:8:GLY:C	6:AJ:9:LEU:HD12	2.46	0.41
9:f:101:BCL:H2	6:g:28:TRP:CH2	2.56	0.41
6:i:26:TYR:HD1	6:i:26:TYR:HA	1.73	0.41
9:i:102:BCL:H3A	9:i:102:BCL:C5	2.51	0.41
1:C:167:VAL:HG22	1:C:303:LEU:HD23	2.03	0.41
1:C:196:PRO:HB2	1:C:231:TRP:CZ3	2.55	0.41
1:C:269:ALA:HB2	7:C:504:HEM:HMA1	2.02	0.41
1:C:272:ALA:HB1	7:C:504:HEM:C4B	2.55	0.41
2:L:239:HIS:CD2	3:M:223:ILE:CG1	2.95	0.41
9:L:303:BCL:H142	9:L:303:BCL:CMA	2.50	0.41
3:M:84:PHE:CD1	5:W:37:MET:HG3	2.56	0.41
5:A:44:LEU:HD23	5:D:55:TYR:HE2	1.86	0.41
5:D:27:PHE:CE1	5:F:29:ILE:HG21	2.56	0.41
5:D:35:ILE:HG12	15:E:101:CRT:H403	2.02	0.41
5:I:12:TRP:CZ3	5:I:20:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:18:ARG:HE	5:I:18:ARG:HB2	1.73	0.41
9:J:102:BCL:HAA2	9:J:102:BCL:O2D	2.21	0.41
5:K:42:THR:HG21	5:O:47:LEU:HB3	2.03	0.41
5:U:53:VAL:HG13	5:U:55:TYR:CZ	2.55	0.41
9:V:101:BCL:HBC3	9:V:101:BCL:H2C	1.60	0.41
5:1:29:ILE:O	5:1:33:LEU:HG	2.20	0.41
9:1:102:BCL:HMA2	15:2:101:CRT:H30	2.02	0.41
6:2:41:LEU:HD23	6:2:41:LEU:HA	1.80	0.41
9:8:102:BCL:HMB1	9:8:102:BCL:HHB	1.89	0.41
2:x:176:PHE:O	2:x:178:TYR:N	2.54	0.41
2:x:182:HIS:CE1	9:x:301:BCL:NA	2.89	0.41
2:x:237:ALA:HA	2:x:240:ARG:HD2	2.03	0.41
10:x:302:BPH:H162	10:x:302:BPH:H192	1.76	0.41
3:y:240:HIS:O	3:y:241:ARG:C	2.64	0.41
4:t:21:LEU:HD23	4:t:21:LEU:HA	1.89	0.41
4:t:221:ASN:HB2	4:t:242:TYR:OH	2.21	0.41
9:m:103:BCL:H3A	9:m:103:BCL:C1	2.51	0.41
6:n:24:SER:HB3	5:l:2:PHE:C	2.46	0.41
5:p:36:HIS:CE1	9:p:104:BCL:HMD3	2.56	0.41
5:r:34:LEU:O	5:r:38:ILE:HG13	2.21	0.41
9:w:101:BCL:H203	15:z:101:CRT:H131	2.03	0.41
9:AB:101:BCL:HBA1	9:AB:101:BCL:H3A	1.73	0.41
6:AD:25:MET:HG3	15:AD:102:CRT:C21	2.51	0.41
9:AI:101:BCL:HHC	9:AI:101:BCL:HMC2	1.82	0.41
6:AL:32:VAL:CG2	9:AL:102:BCL:HBA2	2.49	0.41
6:e:20:ILE:HD12	15:e:101:CRT:C6	2.51	0.41
5:j:18:ARG:H	5:j:18:ARG:HG2	1.55	0.41
5:l:18:ARG:O	5:l:21:LEU:HB2	2.21	0.41
9:c:102:BCL:H141	9:c:102:BCL:H161	1.78	0.41
1:C:142:LYS:C	1:C:144:HIS:H	2.29	0.41
2:L:207:THR:HG21	3:M:238:ILE:HD13	2.03	0.41
3:M:121:PHE:N	3:M:121:PHE:CD1	2.89	0.41
4:H:179:ILE:HG22	4:H:197:ILE:HD13	2.03	0.41
9:J:102:BCL:H3A	9:J:102:BCL:H12	2.03	0.41
6:N:16:GLU:O	6:N:20:ILE:HG13	2.20	0.41
9:P:101:BCL:H62	9:P:101:BCL:H41	1.70	0.41
5:W:4:MET:HG2	5:W:8:LEU:HD22	2.03	0.41
5:W:34:LEU:O	5:W:38:ILE:HG13	2.21	0.41
5:1:20:VAL:O	5:1:24:ILE:HG12	2.20	0.41
5:5:44:LEU:HD23	5:7:55:TYR:CD2	2.55	0.41
6:8:46:LEU:HD23	6:8:46:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:102:BCL:HBA2	9:8:102:BCL:H11	1.62	0.41
1:o:179:LYS:HA	1:o:180:PRO:HD3	1.93	0.41
2:x:133:ALA:HB1	9:x:301:BCL:H62	2.03	0.41
3:y:218:MET:HG3	3:y:218:MET:H	1.52	0.41
3:y:256:MET:HE2	3:y:258:PHE:CZ	2.56	0.41
3:y:295:TYR:O	3:y:299:VAL:HG23	2.21	0.41
14:y:403:MQ8:H221	14:y:403:MQ8:H262	1.83	0.41
9:p:102:BCL:H111	9:p:102:BCL:H93	1.68	0.41
6:v:40:TRP:CZ3	6:v:46:LEU:HB2	2.56	0.41
5:w:9:TYR:HB2	6:z:14:ALA:O	2.21	0.41
5:w:21:LEU:O	5:w:25:VAL:HG23	2.20	0.41
9:z:102:BCL:HMC2	9:z:102:BCL:HHC	1.89	0.41
5:AK:46:TRP:CD1	9:AK:101:BCL:HMC2	2.56	0.41
5:j:44:LEU:HD12	5:l:47:LEU:CD2	2.51	0.41
2:L:225:PHE:CD2	11:L:304:UQ8:C7	3.00	0.40
11:L:304:UQ8:H27A	11:L:304:UQ8:H30	1.90	0.40
4:H:246:GLY:O	4:H:250:ALA:HB3	2.21	0.40
6:T:20:ILE:HD12	15:T:101:CRT:C6	2.50	0.40
6:2:17:PHE:CD1	15:2:101:CRT:H6	2.56	0.40
6:8:25:MET:HG3	15:8:101:CRT:C20	2.51	0.40
1:o:21:LEU:HD11	2:x:274:TRP:CD2	2.56	0.40
1:o:192:TYR:O	3:y:92:TRP:NE1	2.50	0.40
1:o:217:ALA:HB2	3:y:296:LEU:HB3	2.02	0.40
1:o:327:TYR:HA	1:o:328:PRO:HD2	1.88	0.40
2:x:3:MET:HG2	2:x:11:ARG:NH2	2.36	0.40
4:t:58:PHE:CG	4:t:59:PRO:HA	2.55	0.40
4:t:170:VAL:HG22	4:t:182:LEU:CD2	2.51	0.40
5:m:18:ARG:HG3	5:l:14:ILE:HG22	2.03	0.40
5:w:45:ASN:HB3	5:AA:56:GLN:OE1	2.21	0.40
6:z:32:VAL:HG13	6:z:36:HIS:CE1	2.56	0.40
9:AC:102:BCL:H61	9:AC:102:BCL:HHB	2.02	0.40
5:AE:51:ILE:HA	5:AE:52:PRO:HA	1.84	0.40
5:AG:9:TYR:HA	6:AH:18:HIS:CG	2.56	0.40
15:f:102:CRT:H2M1	5:h:36:HIS:HB3	2.03	0.40
5:j:35:ILE:HD12	9:k:102:BCL:HED1	2.03	0.40
3:M:3:GLU:OE2	4:H:247:LYS:NZ	2.28	0.40
3:M:138:GLU:C	3:M:140:LEU:N	2.78	0.40
3:M:275:LEU:HA	3:M:275:LEU:HD23	1.53	0.40
5:D:27:PHE:HE1	5:F:29:ILE:HG21	1.87	0.40
5:F:44:LEU:HD23	5:I:55:TYR:CD2	2.56	0.40
15:P:102:CRT:H372	5:Q:36:HIS:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:10:LYS:HB3	15:Z:101:CRT:H31A	2.02	0.40
6:2:12:ASP:O	6:2:15:LYS:HB2	2.21	0.40
6:2:45:TRP:CD1	6:2:46:LEU:HG	2.56	0.40
1:o:174:TYR:CZ	3:y:78:SER:HA	2.56	0.40
2:x:217:THR:HG23	2:x:220:HIS:CE1	2.56	0.40
2:x:225:PHE:CD2	11:x:304:UQ8:H7A	2.56	0.40
11:x:304:UQ8:H37A	11:x:304:UQ8:H40	1.85	0.40
5:w:46:TRP:CH2	9:w:101:BCL:H2C	2.56	0.40
9:AC:102:BCL:H91	6:AD:36:HIS:CD2	2.57	0.40
5:AE:39:VAL:HG12	5:AE:46:TRP:HZ3	1.86	0.40
15:AE:103:CRT:H26	15:AE:103:CRT:H241	1.89	0.40
1:C:311:HIS:HB3	1:C:314:VAL:O	2.21	0.40
2:L:236:LEU:HD21	3:M:6:ASN:CG	2.47	0.40
9:L:303:BCL:HED3	9:L:303:BCL:CHA	2.51	0.40
3:M:37:SER:O	3:M:38:TYR:C	2.65	0.40
3:M:68:ILE:HG21	3:M:68:ILE:HD13	1.91	0.40
3:M:164:ARG:HD3	3:M:284:ILE:HG22	2.01	0.40
4:H:29:TYR:CZ	12:H:304:PEF:C30	3.04	0.40
15:G:101:CRT:H36	5:I:33:LEU:CD2	2.52	0.40
15:G:101:CRT:H2M1	5:I:33:LEU:HD22	2.03	0.40
6:J:16:GLU:O	6:J:20:ILE:HG13	2.20	0.40
5:O:39:VAL:HG11	9:P:101:BCL:CBC	2.51	0.40
6:T:24:SER:O	6:T:27:ALA:HB3	2.21	0.40
5:U:28:GLN:HB3	9:U:101:BCL:C1	2.51	0.40
5:5:53:VAL:HG22	5:5:54:SER:O	2.22	0.40
1:o:152:CYS:HG	7:o:502:HEM:HAB	1.86	0.40
2:x:120:LEU:HD13	3:y:247:ARG:HA	2.02	0.40
2:x:124:PHE:O	2:x:127:PRO:HD2	2.21	0.40
2:x:167:SER:HB2	3:y:197:TYR:CE2	2.56	0.40
3:y:75:MET:O	3:y:79:VAL:HG22	2.21	0.40
9:y:401:BCL:HHC	9:y:401:BCL:OBB	2.20	0.40
4:t:102:PRO:HB3	4:t:111:PHE:CD2	2.46	0.40
5:u:3:THR:HB	5:u:8:LEU:CB	2.51	0.40
5:u:17:PRO:HB3	6:v:17:PHE:CE1	2.55	0.40
9:v:102:BCL:H152	9:v:102:BCL:H18	1.83	0.40
5:AE:25:VAL:HG21	9:AE:102:BCL:H152	2.01	0.40
5:f:29:ILE:HD13	9:f:101:BCL:H193	2.04	0.40
9:h:101:BCL:H112	9:h:101:BCL:H72	1.72	0.40
7:C:504:HEM:HHA	7:C:504:HEM:HBD1	2.04	0.40
9:F:101:BCL:HAA2	9:F:101:BCL:CBD	2.51	0.40
9:I:101:BCL:C1D	9:J:102:BCL:CMD	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:10:LYS:O	5:K:13:LEU:HB2	2.22	0.40
5:W:40:LEU:HG	5:W:46:TRP:CZ3	2.56	0.40
9:W:101:BCL:HAA2	9:W:101:BCL:CB D	2.47	0.40
5:1:40:LEU:HD23	5:1:40:LEU:HA	1.93	0.40
5:7:36:HIS:NE2	9:7:101:BCL:NB	2.69	0.40
6:8:24:SER:HB2	15:8:101:CRT:C14	2.51	0.40
6:8:43:ARG:HG3	5:9:55:TYR:CE1	2.56	0.40
5:9:25:VAL:O	5:9:29:ILE:HG13	2.22	0.40
1:o:47:ARG:CG	1:o:47:ARG:NH1	2.83	0.40
1:o:163:LYS:HD2	1:o:164:TYR:CZ	2.55	0.40
1:o:254:ARG:NH1	3:y:305:PRO:O	2.44	0.40
3:y:54:GLY:HA3	16:y:405:PO4:O4	2.20	0.40
4:t:61:LEU:HD12	4:t:61:LEU:N	2.36	0.40
4:t:201:ARG:NH1	4:t:210:LYS:HD3	2.37	0.40
9:m:103:BCL:HBC2	9:m:103:BCL:H2C	1.79	0.40
5:p:13:LEU:HD23	5:p:13:LEU:HA	1.83	0.40
5:p:46:TRP:CE2	9:p:102:BCL:H2C	2.56	0.40
6:v:40:TRP:HZ3	6:v:46:LEU:HB2	1.86	0.40
9:AA:101:BCL:H51	6:AB:28:TRP:CZ3	2.57	0.40
5:AE:52:PRO:HD2	5:AE:55:TYR:OH	2.22	0.40
15:AE:103:CRT:H5	15:AE:103:CRT:H22A	1.65	0.40
6:g:29:PHE:CE1	9:g:101:BCL:H11	2.56	0.40
9:j:101:BCL:H122	9:j:101:BCL:H162	1.91	0.40
1:C:212:ILE:HD11	7:C:503:HEM:CMA	2.52	0.40
2:L:51:VAL:CG1	5:A:37:MET:HG3	2.51	0.40
2:L:190:PHE:HD1	2:L:190:PHE:HA	1.70	0.40
2:L:271:TRP:HZ3	2:L:272:TRP:CZ3	2.40	0.40
11:L:304:UQ8:H15	11:L:304:UQ8:H12A	1.79	0.40
3:M:140:LEU:HD23	3:M:140:LEU:HA	1.94	0.40
4:H:27:ILE:HG23	4:H:27:ILE:HD12	1.83	0.40
4:H:46:THR:OG1	4:H:53:VAL:O	2.29	0.40
6:G:46:LEU:HD12	9:G:102:BCL:H141	2.03	0.40
6:J:21:PHE:CD2	15:J:101:CRT:H16	2.56	0.40
15:N:101:CRT:H20	15:N:101:CRT:H181	1.87	0.40
6:Z:41:LEU:HD23	6:Z:41:LEU:HA	1.75	0.40
5:1:12:TRP:HB2	6:2:14:ALA:HB1	2.04	0.40
9:9:103:BCL:H112	9:9:103:BCL:H91	1.84	0.40
9:0:101:BCL:HBA1	9:0:101:BCL:H3A	1.69	0.40
1:o:242:SER:HA	1:o:308:MET:HE2	2.03	0.40
3:y:102:TYR:CD2	3:y:107:PRO:HB3	2.57	0.40
3:y:175:VAL:HA	3:y:185:TRP:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:58:PHE:HA	4:t:59:PRO:O	2.22	0.40
9:p:102:BCL:OBD	6:q:36:HIS:CE1	2.74	0.40
5:w:9:TYR:C	5:w:11:ILE:H	2.29	0.40
9:AC:102:BCL:H91	9:AC:102:BCL:H112	1.84	0.40
9:AE:104:BCL:H121	6:AF:45:TRP:HZ2	1.86	0.40
6:i:17:PHE:HD1	15:i:101:CRT:H33	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	315/333 (95%)	276 (88%)	32 (10%)	7 (2%)	5	26
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	4	23
2	L	278/281 (99%)	247 (89%)	27 (10%)	4 (1%)	9	33
2	x	278/281 (99%)	248 (89%)	27 (10%)	3 (1%)	11	39
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	9	35
3	y	316/319 (99%)	284 (90%)	28 (9%)	4 (1%)	9	35
4	H	256/259 (99%)	213 (83%)	34 (13%)	9 (4%)	3	18
4	t	256/259 (99%)	214 (84%)	33 (13%)	9 (4%)	3	18
5	1	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	3	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	7
5	5	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	7	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18
5	9	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1	7
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	AA	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AC	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	AE	59/61 (97%)	50 (85%)	6 (10%)	3 (5%)	1	11
5	AG	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
5	AI	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
5	AK	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
5	D	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
5	F	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18
5	I	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	7
5	K	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
5	O	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
5	Q	58/61 (95%)	47 (81%)	6 (10%)	5 (9%)	0	4
5	S	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	1	11
5	U	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	30
5	W	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	Y	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18
5	d	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	f	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	18
5	h	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	11
5	j	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	30
5	l	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	18
5	m	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	18
5	p	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	0	4
5	r	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	7
5	u	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	7	30
5	w	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
6	0	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
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%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36 (95%)	2 (5%)	0	100	100
6	AJ	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AL	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
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%)	37 (97%)	1 (3%)	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	P	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	Z	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	37 (97%)	1 (3%)	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
6	s	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	v	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4736 (88%)	543 (10%)	125 (2%)	5	25

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	SER
1	C	84	ASP

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Mol	Chain	Res	Type
1	C	195	LEU
4	H	38	GLY
4	H	142	PHE
4	H	250	ALA
5	A	60	LYS
5	F	3	THR
5	O	59	GLY
5	Y	60	LYS
5	3	6	ALA
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	38	GLY
4	t	142	PHE
4	t	250	ALA
5	m	60	LYS
5	p	57	ALA
5	r	3	THR
5	AC	4	MET
5	AE	6	ALA
5	AG	6	ALA
5	AK	60	LYS
5	d	58	LEU
5	f	5	ASN
1	C	21	LEU
2	L	21	ASP
2	L	262	PRO
4	H	5	ILE
4	H	140	LYS
4	H	188	ALA
5	F	10	LYS
5	I	59	GLY
5	Q	6	ALA
5	S	6	ALA
5	S	58	LEU
5	U	54	SER
5	W	5	ASN
6	X	8	GLY
5	Y	59	GLY

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Mol	Chain	Res	Type
5	1	3	THR
5	3	56	GLN
1	o	83	LYS
1	o	84	ASP
2	x	21	ASP
4	t	140	LYS
4	t	188	ALA
5	m	10	LYS
5	p	6	ALA
5	p	56	GLN
5	p	60	LYS
5	r	59	GLY
5	AE	59	GLY
5	l	4	MET
1	C	83	LYS
1	C	184	ASN
3	M	3	GLU
3	M	29	PRO
3	M	34	PRO
4	H	177	PRO
5	A	10	LYS
5	D	5	ASN
5	Q	10	LYS
5	S	60	LYS
5	3	57	ALA
5	5	10	LYS
5	7	6	ALA
5	7	10	LYS
5	9	6	ALA
5	9	59	GLY
1	o	67	SER
3	y	3	GLU
3	y	29	PRO
3	y	34	PRO
4	t	177	PRO
5	AC	6	ALA
5	AE	58	LEU
5	AI	10	LYS
5	f	59	GLY
5	h	6	ALA
5	j	6	ALA
5	l	10	LYS

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Mol	Chain	Res	Type
1	C	253	THR
5	I	10	LYS
5	I	60	LYS
6	N	8	GLY
6	P	8	GLY
5	W	6	ALA
5	3	10	LYS
5	5	50	ASN
1	o	253	THR
5	p	5	ASN
5	w	10	LYS
5	d	10	LYS
5	h	8	LEU
3	M	38	TYR
5	D	57	ALA
5	I	6	ALA
5	Q	8	LEU
1	o	184	ASN
3	y	38	TYR
5	r	60	LYS
5	u	5	ASN
5	AK	10	LYS
5	h	10	LYS
4	H	213	ALA
5	Q	4	MET
5	Q	59	GLY
5	9	10	LYS
5	9	50	ASN
5	r	10	LYS
2	L	32	VAL
6	B	8	GLY
2	x	32	VAL
6	T	8	GLY
5	1	59	GLY
4	t	227	ASN
5	AA	59	GLY
2	L	141	VAL
4	H	227	ASN
4	t	59	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/278 (95%)	245 (92%)	20 (8%)	12	38
1	o	265/278 (95%)	246 (93%)	19 (7%)	13	40
2	L	228/229 (100%)	212 (93%)	16 (7%)	14	41
2	x	228/229 (100%)	212 (93%)	16 (7%)	14	41
3	M	256/257 (100%)	233 (91%)	23 (9%)	9	31
3	y	256/257 (100%)	234 (91%)	22 (9%)	10	33
4	H	210/211 (100%)	188 (90%)	22 (10%)	6	25
4	t	210/211 (100%)	184 (88%)	26 (12%)	4	19
5	1	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	3	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	5	52/56 (93%)	52 (100%)	0	100	100
5	7	52/56 (93%)	52 (100%)	0	100	100
5	9	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	A	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	AA	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	AC	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	AE	53/56 (95%)	52 (98%)	1 (2%)	50	68
5	AG	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	52 (100%)	0	100	100
5	D	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	F	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	I	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	K	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	O	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	Q	52/56 (93%)	49 (94%)	3 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	53/56 (95%)	51 (96%)	2 (4%)	29	57
5	U	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	W	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	Y	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	d	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	f	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	h	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	j	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	l	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	m	52/56 (93%)	52 (100%)	0	100	100
5	p	52/56 (93%)	52 (100%)	0	100	100
5	r	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	u	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	w	52/56 (93%)	51 (98%)	1 (2%)	50	68
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%)	36	61
6	AL	33/39 (85%)	33 (100%)	0	100	100
6	B	33/39 (85%)	31 (94%)	2 (6%)	17	45
6	E	33/39 (85%)	33 (100%)	0	100	100
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%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	36	61
6	Z	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	32 (97%)	1 (3%)	36	61
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
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%)	4431 (96%)	209 (4%)	24	53

All (209) 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	148	THR
1	C	167	VAL
1	C	169	ASP
1	C	181	THR
1	C	190	VAL
1	C	212	ILE
1	C	221	SER
1	C	238	ASN
1	C	277	ARG
1	C	289	ASP

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Mol	Chain	Res	Type
1	C	304	ARG
1	C	307	CYS
1	C	318	LEU
2	L	89	LEU
2	L	94	LEU
2	L	120	LEU
2	L	125	HIS
2	L	147	LEU
2	L	148	MET
2	L	163	LEU
2	L	172	GLN
2	L	175	HIS
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	280	LEU
3	M	3	GLU
3	M	25	LYS
3	M	31	ILE
3	M	33	ARG
3	M	35	ILE
3	M	37	SER
3	M	42	LYS
3	M	45	ASP
3	M	68	ILE
3	M	79	VAL
3	M	106	ILE
3	M	182	HIS
3	M	191	ILE
3	M	228	ARG
3	M	232	ASP
3	M	235	ILE
3	M	256	MET
3	M	274	VAL
3	M	277	VAL
3	M	279	THR
3	M	310	VAL
3	M	311	VAL
3	M	312	THR

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Mol	Chain	Res	Type
4	H	16	ILE
4	H	45	ARG
4	H	75	THR
4	H	77	VAL
4	H	81	VAL
4	H	106	PRO
4	H	107	MET
4	H	128	GLU
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	177	PRO
4	H	186	VAL
4	H	193	VAL
4	H	200	SER
4	H	208	LYS
4	H	230	GLN
4	H	258	LEU
4	H	259	LEU
5	A	8	LEU
6	B	20	ILE
6	B	24	SER
5	D	9	TYR
5	F	14	ILE
5	I	3	THR
5	K	43	ASP
5	O	5	ASN
5	O	37	MET
6	P	21	PHE
5	Q	2	PHE
5	Q	3	THR
5	Q	9	TYR
5	S	48	ASP
5	S	51	ILE
5	U	53	VAL
5	W	9	TYR
6	X	13	GLU
5	Y	51	ILE
6	Z	34	ILE

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Mol	Chain	Res	Type
5	1	51	ILE
5	1	55	TYR
5	3	44	LEU
5	3	50	ASN
5	9	8	LEU
1	o	21	LEU
1	o	47	ARG
1	o	48	GLN
1	o	66	ASP
1	o	68	THR
1	o	74	GLU
1	o	86	SER
1	o	128	ARG
1	o	130	MET
1	o	169	ASP
1	o	181	THR
1	o	190	VAL
1	o	212	ILE
1	o	238	ASN
1	o	277	ARG
1	o	282	ASN
1	o	304	ARG
1	o	307	CYS
1	o	318	LEU
2	x	59	THR
2	x	89	LEU
2	x	94	LEU
2	x	128	PHE
2	x	147	LEU
2	x	148	MET
2	x	163	LEU
2	x	172	GLN
2	x	175	HIS
2	x	208	ASN
2	x	210	GLN
2	x	225	PHE
2	x	238	ILE
2	x	248	SER
2	x	255	VAL
2	x	256	CYS
3	y	3	GLU
3	y	25	LYS

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Mol	Chain	Res	Type
3	y	31	ILE
3	y	33	ARG
3	y	37	SER
3	y	42	LYS
3	y	45	ASP
3	y	55	LEU
3	y	68	ILE
3	y	182	HIS
3	y	228	ARG
3	y	232	ASP
3	y	238	ILE
3	y	256	MET
3	y	274	VAL
3	y	275	LEU
3	y	277	VAL
3	y	279	THR
3	y	285	LEU
3	y	310	VAL
3	y	311	VAL
3	y	312	THR
4	t	16	ILE
4	t	28	ILE
4	t	45	ARG
4	t	60	ASP
4	t	75	THR
4	t	77	VAL
4	t	81	VAL
4	t	106	PRO
4	t	107	MET
4	t	128	GLU
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	186	VAL
4	t	200	SER
4	t	208	LYS
4	t	218	HIS

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Mol	Chain	Res	Type
4	t	221	ASN
4	t	224	THR
4	t	230	GLN
4	t	259	LEU
5	r	37	MET
5	u	3	THR
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
6	AJ	13	GLU
5	d	24	ILE
6	e	34	ILE
5	f	3	THR
5	h	14	ILE
5	j	9	TYR
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 (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	ASN
1	C	238	ASN
2	L	96	GLN
2	L	125	HIS
2	L	153	HIS
2	L	192	ASN
2	L	222	ASN
3	M	6	ASN
3	M	27	ASN
4	H	122	HIS
4	H	189	ASN
5	A	50	ASN
5	D	5	ASN
5	Q	5	ASN

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Mol	Chain	Res	Type
5	Q	56	GLN
5	S	7	ASN
6	V	23	GLN
6	X	23	GLN
6	X	36	HIS
5	Y	36	HIS
5	Y	56	GLN
5	1	36	HIS
6	2	18	HIS
5	3	36	HIS
5	7	36	HIS
6	8	36	HIS
1	o	42	ASN
1	o	54	GLN
2	x	172	GLN
2	x	273	ASN
3	y	27	ASN
3	y	101	GLN
3	y	240	HIS
3	y	259	ASN
3	y	301	HIS
5	m	7	ASN
5	m	50	ASN
5	u	50	ASN
5	w	50	ASN
5	w	56	GLN
6	AD	23	GLN
5	d	28	GLN
6	e	23	GLN
6	k	23	GLN
5	l	56	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
14	MQ8	M	403	-	54,54,54	1.12	5 (9%)	67,69,69	1.59	15 (22%)
9	BCL	k	102	-	69,74,74	1.73	12 (17%)	79,115,115	2.25	30 (37%)
9	BCL	3	101	-	69,74,74	1.81	15 (21%)	79,115,115	2.08	29 (36%)
7	HEM	o	504	1	50,50,50	2.63	12 (24%)	67,82,82	1.99	20 (29%)
9	BCL	p	104	-	69,74,74	1.82	14 (20%)	79,115,115	2.17	29 (36%)
12	PEF	L	306	-	11,11,46	0.79	0	13,14,51	1.36	1 (7%)
9	BCL	5	101	-	69,74,74	1.79	14 (20%)	79,115,115	2.19	27 (34%)
15	CRT	G	101	-	43,43,43	0.69	0	48,54,54	2.36	16 (33%)
9	BCL	j	101	-	69,74,74	1.72	11 (15%)	79,115,115	2.16	28 (35%)
15	CRT	A	103	-	43,43,43	0.81	0	48,54,54	2.22	17 (35%)
15	CRT	AC	101	-	43,43,43	0.66	0	48,54,54	2.18	13 (27%)
12	PEF	M	406	-	18,18,46	1.47	2 (11%)	21,23,51	2.32	4 (19%)
7	HEM	C	504	1	50,50,50	2.62	10 (20%)	67,82,82	2.15	19 (28%)
12	PEF	t	303	-	18,18,46	1.52	2 (11%)	21,23,51	2.47	9 (42%)
9	BCL	A	102	-	69,74,74	1.77	12 (17%)	79,115,115	2.11	28 (35%)
15	CRT	M	404	-	43,43,43	0.84	0	48,54,54	2.18	11 (22%)
12	PEF	y	406	-	18,18,46	1.59	2 (11%)	21,23,51	1.78	3 (14%)
12	PEF	y	408	-	18,18,46	1.78	3 (16%)	21,23,51	2.07	5 (23%)
9	BCL	m	102	-	69,74,74	1.76	14 (20%)	79,115,115	2.11	24 (30%)
9	BCL	u	101	-	69,74,74	1.80	16 (23%)	79,115,115	2.03	27 (34%)
9	BCL	x	305	-	69,74,74	1.77	13 (18%)	79,115,115	2.40	31 (39%)
9	BCL	AE	104	-	69,74,74	1.71	13 (18%)	79,115,115	2.17	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	AJ	102	-	69,74,74	1.77	15 (21%)	79,115,115	2.02	23 (29%)
9	BCL	c	102	-	69,74,74	1.71	12 (17%)	79,115,115	2.14	28 (35%)
15	CRT	9	102	-	43,43,43	0.76	0	48,54,54	2.33	15 (31%)
12	PEF	x	306	-	18,18,46	1.75	2 (11%)	21,23,51	1.45	3 (14%)
9	BCL	v	102	-	69,74,74	1.75	14 (20%)	79,115,115	2.20	28 (35%)
15	CRT	AJ	101	-	43,43,43	0.74	0	48,54,54	2.38	16 (33%)
15	CRT	4	101	-	43,43,43	0.71	0	48,54,54	2.36	20 (41%)
16	PO4	H	302	-	4,4,4	0.80	0	6,6,6	0.57	0
10	BPH	x	302	-	59,70,70	0.91	1 (1%)	59,101,101	1.75	8 (13%)
9	BCL	G	102	-	69,74,74	1.77	13 (18%)	79,115,115	2.16	31 (39%)
10	BPH	y	402	-	59,70,70	0.85	3 (5%)	59,101,101	1.36	8 (13%)
15	CRT	z	101	-	43,43,43	0.68	0	48,54,54	2.19	14 (29%)
7	HEM	o	503	1	50,50,50	2.57	9 (18%)	67,82,82	1.94	22 (32%)
9	BCL	f	101	-	69,74,74	1.80	15 (21%)	79,115,115	2.03	24 (30%)
9	BCL	P	101	-	69,74,74	1.79	15 (21%)	79,115,115	2.18	33 (41%)
9	BCL	l	101	-	69,74,74	1.71	13 (18%)	79,115,115	2.19	31 (39%)
9	BCL	R	102	-	69,74,74	1.66	11 (15%)	79,115,115	2.16	28 (35%)
15	CRT	p	103	-	43,43,43	0.67	0	48,54,54	2.43	16 (33%)
9	BCL	AK	101	-	69,74,74	1.75	12 (17%)	79,115,115	2.22	31 (39%)
9	BCL	AB	101	-	69,74,74	1.77	15 (21%)	79,115,115	2.10	28 (35%)
7	HEM	C	503	1	50,50,50	2.59	12 (24%)	67,82,82	2.26	22 (32%)
9	BCL	8	102	-	69,74,74	1.74	13 (18%)	79,115,115	2.08	27 (34%)
7	HEM	C	501	1	50,50,50	2.57	8 (16%)	67,82,82	2.08	18 (26%)
9	BCL	0	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.04	28 (35%)
9	BCL	F	101	-	69,74,74	1.74	16 (23%)	79,115,115	2.11	32 (40%)
9	BCL	y	401	-	69,74,74	1.86	15 (21%)	79,115,115	2.22	33 (41%)
9	BCL	g	101	-	69,74,74	1.72	13 (18%)	79,115,115	2.15	32 (40%)
15	CRT	Z	101	-	43,43,43	0.81	0	48,54,54	2.07	15 (31%)
9	BCL	B	101	-	69,74,74	1.71	14 (20%)	79,115,115	2.07	26 (32%)
9	BCL	s	102	-	69,74,74	1.84	14 (20%)	79,115,115	2.18	25 (31%)
9	BCL	Z	102	-	69,74,74	1.81	14 (20%)	79,115,115	2.26	30 (37%)
9	BCL	AC	102	-	69,74,74	1.69	14 (20%)	79,115,115	2.07	28 (35%)
12	PEF	H	301	-	18,18,46	1.61	2 (11%)	21,23,51	1.78	3 (14%)
15	CRT	6	101	-	43,43,43	0.77	0	48,54,54	2.39	19 (39%)
17	PGW	AE	101	-	20,20,50	1.07	2 (10%)	23,26,56	1.41	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	AH	103	-	69,74,74	1.74	12 (17%)	79,115,115	2.17	29 (36%)
12	PEF	M	407	-	15,15,46	1.08	1 (6%)	17,19,51	1.34	2 (11%)
12	PEF	y	407	-	18,18,46	1.85	2 (11%)	21,23,51	1.62	3 (14%)
16	PO4	M	405	-	4,4,4	0.64	0	6,6,6	1.10	0
15	CRT	AE	103	-	43,43,43	0.70	0	48,54,54	2.20	16 (33%)
15	CRT	e	101	-	43,43,43	0.72	0	48,54,54	2.01	15 (31%)
9	BCL	D	101	-	69,74,74	1.79	13 (18%)	79,115,115	2.15	24 (30%)
9	BCL	AD	101	-	69,74,74	1.73	11 (15%)	79,115,115	2.04	29 (36%)
9	BCL	e	102	-	69,74,74	1.78	13 (18%)	79,115,115	2.14	27 (34%)
15	CRT	AL	101	-	43,43,43	0.74	0	48,54,54	1.85	14 (29%)
9	BCL	m	103	-	69,74,74	1.75	15 (21%)	79,115,115	2.14	28 (35%)
12	PEF	M	408	-	18,18,46	1.69	2 (11%)	21,23,51	2.03	4 (19%)
9	BCL	r	101	-	69,74,74	1.78	15 (21%)	79,115,115	1.96	26 (32%)
9	BCL	O	101	-	69,74,74	1.73	13 (18%)	79,115,115	2.22	30 (37%)
9	BCL	i	102	-	69,74,74	1.75	12 (17%)	79,115,115	2.09	24 (30%)
9	BCL	AL	102	-	69,74,74	1.82	16 (23%)	79,115,115	2.18	25 (31%)
9	BCL	J	102	-	69,74,74	1.76	15 (21%)	79,115,115	2.17	31 (39%)
12	PEF	H	304	-	18,18,46	1.61	2 (11%)	21,23,51	1.85	5 (23%)
9	BCL	z	102	-	69,74,74	1.72	13 (18%)	79,115,115	2.12	29 (36%)
15	CRT	N	101	-	43,43,43	0.76	0	48,54,54	2.76	19 (39%)
7	HEM	o	501	1	50,50,50	2.47	7 (14%)	67,82,82	1.77	12 (17%)
15	CRT	8	101	-	43,43,43	0.87	1 (2%)	48,54,54	1.70	9 (18%)
14	MQ8	y	403	-	54,54,54	1.22	6 (11%)	67,69,69	1.67	14 (20%)
9	BCL	S	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.13	31 (39%)
9	BCL	7	101	-	69,74,74	1.73	14 (20%)	79,115,115	2.07	29 (36%)
9	BCL	x	301	-	69,74,74	1.84	18 (26%)	79,115,115	2.42	24 (30%)
9	BCL	L	305	-	69,74,74	1.74	11 (15%)	79,115,115	2.14	27 (34%)
15	CRT	c	101	-	43,43,43	0.75	0	48,54,54	2.24	17 (35%)
9	BCL	X	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.01	28 (35%)
15	CRT	v	101	-	43,43,43	0.69	0	48,54,54	2.88	19 (39%)
9	BCL	AE	102	-	69,74,74	1.71	12 (17%)	79,115,115	2.08	27 (34%)
17	PGW	S	101	-	20,20,50	1.07	1 (5%)	23,26,56	1.28	3 (13%)
9	BCL	Y	101	-	69,74,74	1.85	13 (18%)	79,115,115	2.05	25 (31%)
15	CRT	k	101	-	43,43,43	0.80	1 (2%)	48,54,54	2.13	17 (35%)
9	BCL	1	101	-	69,74,74	1.75	12 (17%)	79,115,115	2.06	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEM	o	502	1	50,50,50	2.47	9 (18%)	67,82,82	2.20	24 (35%)
12	PEF	A	101	-	18,18,46	1.57	2 (11%)	21,23,51	1.80	3 (14%)
9	BCL	h	101	-	69,74,74	1.79	16 (23%)	79,115,115	2.02	28 (35%)
9	BCL	T	102	-	69,74,74	1.73	14 (20%)	79,115,115	2.19	28 (35%)
9	BCL	p	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.12	29 (36%)
15	CRT	U	102	-	43,43,43	0.70	0	48,54,54	2.40	19 (39%)
9	BCL	5	102	-	69,74,74	1.85	15 (21%)	79,115,115	2.22	31 (39%)
12	PEF	m	101	-	18,18,46	1.67	2 (11%)	21,23,51	1.61	3 (14%)
9	BCL	Q	101	-	69,74,74	1.76	13 (18%)	79,115,115	2.20	27 (34%)
15	CRT	n	101	-	43,43,43	0.79	0	48,54,54	2.33	15 (31%)
15	CRT	X	101	-	43,43,43	0.87	0	48,54,54	1.97	10 (20%)
9	BCL	D	102	-	69,74,74	1.72	12 (17%)	79,115,115	2.22	31 (39%)
15	CRT	y	404	-	43,43,43	0.96	2 (4%)	48,54,54	2.29	16 (33%)
9	BCL	d	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.11	25 (31%)
9	BCL	I	101	-	69,74,74	1.78	14 (20%)	79,115,115	2.14	28 (35%)
15	CRT	AD	102	-	43,43,43	0.80	0	48,54,54	2.27	15 (31%)
15	CRT	i	101	-	43,43,43	0.78	0	48,54,54	1.97	14 (29%)
15	CRT	T	101	-	43,43,43	0.73	0	48,54,54	2.64	22 (45%)
9	BCL	AI	101	-	69,74,74	1.75	14 (20%)	79,115,115	2.09	26 (32%)
10	BPH	M	402	-	59,70,70	0.86	4 (6%)	59,101,101	1.71	10 (16%)
7	HEM	C	502	1	50,50,50	2.47	9 (18%)	67,82,82	2.23	20 (29%)
9	BCL	AA	101	-	69,74,74	1.75	12 (17%)	79,115,115	2.07	25 (31%)
12	PEF	p	101	-	15,15,46	0.95	1 (6%)	17,19,51	0.86	1 (5%)
15	CRT	E	101	-	43,43,43	0.76	0	48,54,54	2.15	16 (33%)
15	CRT	f	102	-	43,43,43	0.91	1 (2%)	48,54,54	2.47	21 (43%)
9	BCL	W	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.05	25 (31%)
9	BCL	4	102	-	69,74,74	1.79	14 (20%)	79,115,115	2.19	29 (36%)
9	BCL	w	101	-	69,74,74	1.78	15 (21%)	79,115,115	2.13	28 (35%)
9	BCL	l	102	-	69,74,74	1.79	14 (20%)	79,115,115	2.03	20 (25%)
9	BCL	AH	101	-	69,74,74	1.74	12 (17%)	79,115,115	2.14	28 (35%)
12	PEF	H	303	-	18,18,46	1.54	2 (11%)	21,23,51	1.37	2 (9%)
9	BCL	U	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.06	23 (29%)
16	PO4	y	405	-	4,4,4	0.86	0	6,6,6	0.55	0
15	CRT	s	101	-	43,43,43	0.69	0	48,54,54	2.37	17 (35%)
16	PO4	t	302	-	4,4,4	0.54	0	6,6,6	2.03	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CRT	2	101	-	43,43,43	0.70	0	48,54,54	1.97	18 (37%)
9	BCL	9	103	-	69,74,74	1.74	16 (23%)	79,115,115	2.10	29 (36%)
15	CRT	J	101	-	43,43,43	0.71	0	48,54,54	2.68	18 (37%)
9	BCL	M	401	-	69,74,74	1.91	17 (24%)	79,115,115	2.33	30 (37%)
12	PEF	t	301	-	18,18,46	1.53	2 (11%)	21,23,51	1.35	4 (19%)
15	CRT	R	101	-	43,43,43	0.75	0	48,54,54	2.35	15 (31%)
9	BCL	L	303	-	69,74,74	1.75	16 (23%)	79,115,115	2.40	27 (34%)
15	CRT	P	102	-	43,43,43	0.67	0	48,54,54	2.20	16 (33%)
9	BCL	x	303	-	69,74,74	2.00	16 (23%)	79,115,115	2.22	28 (35%)
11	UQ8	L	304	-	53,53,53	1.53	6 (11%)	66,67,67	1.78	18 (27%)
9	BCL	L	301	-	69,74,74	1.87	17 (24%)	79,115,115	2.16	25 (31%)
11	UQ8	x	304	-	53,53,53	1.55	3 (5%)	66,67,67	2.19	24 (36%)
9	BCL	N	102	-	69,74,74	1.72	14 (20%)	79,115,115	2.14	27 (34%)
9	BCL	K	101	-	69,74,74	1.73	16 (23%)	79,115,115	2.15	30 (37%)
9	BCL	V	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.11	26 (32%)
10	BPH	L	302	-	59,70,70	0.69	1 (1%)	59,101,101	1.51	11 (18%)
15	CRT	AH	102	-	43,43,43	0.75	0	48,54,54	2.17	16 (33%)

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
14	MQ8	M	403	-	-	22/47/67/67	0/2/2/2
9	BCL	k	102	-	-	21/41/137/137	-
9	BCL	3	101	-	-	11/41/137/137	-
7	HEM	o	504	1	-	2/14/54/54	-
9	BCL	p	104	-	-	15/41/137/137	-
12	PEF	L	306	-	-	7/11/11/50	-
9	BCL	5	101	-	-	16/41/137/137	-
15	CRT	G	101	-	-	6/51/51/51	-
9	BCL	j	101	-	-	18/41/137/137	-
15	CRT	A	103	-	-	7/51/51/51	-
15	CRT	AC	101	-	-	5/51/51/51	-
12	PEF	M	406	-	-	11/20/20/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	C	504	1	-	6/14/54/54	-
12	PEF	t	303	-	-	7/20/20/50	-
9	BCL	A	102	-	-	10/41/137/137	-
15	CRT	M	404	-	-	11/51/51/51	-
12	PEF	y	406	-	-	1/20/20/50	-
12	PEF	y	408	-	-	9/20/20/50	-
9	BCL	m	102	-	-	16/41/137/137	-
9	BCL	u	101	-	-	15/41/137/137	-
9	BCL	x	305	-	-	19/41/137/137	-
9	BCL	AE	104	-	-	11/41/137/137	-
9	BCL	AJ	102	-	-	16/41/137/137	-
9	BCL	c	102	-	-	17/41/137/137	-
15	CRT	9	102	-	-	9/51/51/51	-
12	PEF	x	306	-	-	14/20/20/50	-
9	BCL	v	102	-	-	12/41/137/137	-
15	CRT	AJ	101	-	-	7/51/51/51	-
15	CRT	4	101	-	-	12/51/51/51	-
10	BPH	x	302	-	-	13/37/105/105	0/5/6/6
9	BCL	G	102	-	-	16/41/137/137	-
10	BPH	y	402	-	-	12/37/105/105	0/5/6/6
15	CRT	z	101	-	-	2/51/51/51	-
7	HEM	o	503	1	-	4/14/54/54	-
9	BCL	f	101	-	-	17/41/137/137	-
9	BCL	P	101	-	-	17/41/137/137	-
9	BCL	l	101	-	-	15/41/137/137	-
9	BCL	R	102	-	-	15/41/137/137	-
15	CRT	p	103	-	-	9/51/51/51	-
9	BCL	AK	101	-	-	14/41/137/137	-
9	BCL	AB	101	-	-	20/41/137/137	-
7	HEM	C	503	1	-	4/14/54/54	-
9	BCL	8	102	-	-	26/41/137/137	-
7	HEM	C	501	1	-	6/14/54/54	-
9	BCL	0	101	-	-	12/41/137/137	-
9	BCL	F	101	-	-	20/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	y	401	-	-	14/41/137/137	-
9	BCL	g	101	-	-	19/41/137/137	-
15	CRT	Z	101	-	-	11/51/51/51	-
9	BCL	B	101	-	-	13/41/137/137	-
9	BCL	s	102	-	-	16/41/137/137	-
9	BCL	Z	102	-	-	16/41/137/137	-
9	BCL	AC	102	-	-	15/41/137/137	-
12	PEF	H	301	-	-	6/20/20/50	-
15	CRT	6	101	-	-	8/51/51/51	-
17	PGW	AE	101	-	-	11/23/23/55	-
9	BCL	AH	103	-	-	22/41/137/137	-
12	PEF	M	407	-	-	8/16/16/50	-
12	PEF	y	407	-	-	6/20/20/50	-
15	CRT	AE	103	-	-	4/51/51/51	-
15	CRT	e	101	-	-	7/51/51/51	-
9	BCL	D	101	-	-	11/41/137/137	-
9	BCL	AD	101	-	-	20/41/137/137	-
9	BCL	e	102	-	-	18/41/137/137	-
15	CRT	AL	101	-	-	9/51/51/51	-
9	BCL	m	103	-	-	17/41/137/137	-
12	PEF	M	408	-	-	12/20/20/50	-
9	BCL	r	101	-	-	18/41/137/137	-
9	BCL	O	101	-	-	16/41/137/137	-
9	BCL	i	102	-	-	17/41/137/137	-
9	BCL	AL	102	-	-	15/41/137/137	-
9	BCL	J	102	-	-	11/41/137/137	-
12	PEF	H	304	-	-	11/20/20/50	-
9	BCL	z	102	-	-	17/41/137/137	-
15	CRT	N	101	-	-	10/51/51/51	-
7	HEM	o	501	1	-	5/14/54/54	-
15	CRT	8	101	-	-	6/51/51/51	-
14	MQ8	y	403	-	-	26/47/67/67	0/2/2/2
9	BCL	S	102	-	-	14/41/137/137	-
9	BCL	7	101	-	-	17/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	x	301	-	-	10/41/137/137	-
9	BCL	L	305	-	-	15/41/137/137	-
15	CRT	c	101	-	-	9/51/51/51	-
9	BCL	X	102	-	-	23/41/137/137	-
15	CRT	v	101	-	-	9/51/51/51	-
9	BCL	AE	102	-	-	12/41/137/137	-
17	PGW	S	101	-	-	13/23/23/55	-
9	BCL	Y	101	-	-	20/41/137/137	-
15	CRT	k	101	-	-	6/51/51/51	-
9	BCL	l	101	-	-	19/41/137/137	-
7	HEM	o	502	1	-	5/14/54/54	-
12	PEF	A	101	-	-	9/20/20/50	-
9	BCL	h	101	-	-	9/41/137/137	-
9	BCL	T	102	-	-	15/41/137/137	-
9	BCL	p	102	-	-	17/41/137/137	-
15	CRT	U	102	-	-	10/51/51/51	-
9	BCL	5	102	-	-	17/41/137/137	-
12	PEF	m	101	-	-	5/20/20/50	-
9	BCL	Q	101	-	-	22/41/137/137	-
15	CRT	n	101	-	-	19/51/51/51	-
15	CRT	X	101	-	-	14/51/51/51	-
9	BCL	D	102	-	-	12/41/137/137	-
15	CRT	y	404	-	-	9/51/51/51	-
9	BCL	d	101	-	-	17/41/137/137	-
9	BCL	I	101	-	-	11/41/137/137	-
15	CRT	AD	102	-	-	11/51/51/51	-
15	CRT	i	101	-	-	12/51/51/51	-
15	CRT	T	101	-	-	7/51/51/51	-
9	BCL	AI	101	-	-	18/41/137/137	-
10	BPH	M	402	-	-	22/37/105/105	0/5/6/6
7	HEM	C	502	1	-	5/14/54/54	-
9	BCL	AA	101	-	-	15/41/137/137	-
12	PEF	p	101	-	-	4/16/16/50	-
15	CRT	E	101	-	-	7/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	f	102	-	-	9/51/51/51	-
9	BCL	W	101	-	-	19/41/137/137	-
9	BCL	4	102	-	-	13/41/137/137	-
9	BCL	w	101	-	-	15/41/137/137	-
9	BCL	1	102	-	-	14/41/137/137	-
9	BCL	AH	101	-	-	21/41/137/137	-
12	PEF	H	303	-	-	11/20/20/50	-
9	BCL	U	101	-	-	15/41/137/137	-
15	CRT	s	101	-	-	8/51/51/51	-
15	CRT	2	101	-	-	9/51/51/51	-
9	BCL	9	103	-	-	14/41/137/137	-
15	CRT	J	101	-	-	11/51/51/51	-
9	BCL	M	401	-	-	9/41/137/137	-
12	PEF	t	301	-	-	5/20/20/50	-
15	CRT	R	101	-	-	12/51/51/51	-
9	BCL	L	303	-	-	19/41/137/137	-
15	CRT	P	102	-	-	7/51/51/51	-
9	BCL	x	303	-	-	14/41/137/137	-
11	UQ8	L	304	-	-	10/51/75/75	0/1/1/1
9	BCL	L	301	-	-	10/41/137/137	-
11	UQ8	x	304	-	-	7/51/75/75	0/1/1/1
9	BCL	N	102	-	-	17/41/137/137	-
9	BCL	K	101	-	-	11/41/137/137	-
9	BCL	V	101	-	-	13/41/137/137	-
10	BPH	L	302	-	-	14/37/105/105	0/5/6/6
15	CRT	AH	102	-	-	13/51/51/51	-

All (1136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	FE-NB	14.50	2.39	1.94
7	o	503	HEM	FE-NB	14.35	2.39	1.94
7	C	503	HEM	FE-NB	14.22	2.38	1.94
7	C	504	HEM	FE-NB	13.81	2.37	1.94
7	o	502	HEM	FE-NB	13.58	2.36	1.94
7	o	501	HEM	FE-NB	13.55	2.36	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	501	HEM	FE-NB	13.33	2.35	1.94
7	C	502	HEM	FE-NB	12.85	2.34	1.94
11	x	304	UQ8	C6-C1	8.07	1.49	1.35
11	L	304	UQ8	C6-C1	7.99	1.49	1.35
9	x	303	BCL	MG-ND	-7.89	1.90	2.05
9	x	303	BCL	MG-NB	-6.45	1.93	2.05
9	L	305	BCL	MG-ND	-6.44	1.93	2.05
9	f	101	BCL	MG-ND	-6.41	1.93	2.05
9	v	102	BCL	MG-ND	-6.32	1.93	2.05
9	I	101	BCL	MG-ND	-6.29	1.93	2.05
9	5	102	BCL	MG-ND	-6.28	1.93	2.05
9	AJ	102	BCL	MG-ND	-6.24	1.93	2.05
9	L	301	BCL	OBD-CAD	6.23	1.33	1.22
9	s	102	BCL	MG-ND	-6.23	1.93	2.05
9	AL	102	BCL	MG-ND	-6.22	1.93	2.05
9	S	102	BCL	MG-ND	-6.22	1.93	2.05
9	y	401	BCL	MG-ND	-6.21	1.93	2.05
9	AB	101	BCL	MG-ND	-6.14	1.93	2.05
9	9	103	BCL	MG-ND	-6.13	1.93	2.05
9	K	101	BCL	MG-ND	-6.11	1.93	2.05
9	Y	101	BCL	MG-ND	-6.09	1.93	2.05
9	Q	101	BCL	MG-ND	-6.09	1.93	2.05
9	1	102	BCL	MG-ND	-6.09	1.93	2.05
9	w	101	BCL	MG-ND	-6.06	1.93	2.05
9	e	102	BCL	MG-ND	-6.06	1.93	2.05
9	5	101	BCL	MG-ND	-6.06	1.93	2.05
9	D	101	BCL	MG-ND	-6.05	1.93	2.05
9	O	101	BCL	MG-ND	-6.05	1.93	2.05
9	4	102	BCL	MG-ND	-6.05	1.93	2.05
9	0	101	BCL	MG-ND	-6.03	1.93	2.05
9	A	102	BCL	MG-ND	-6.01	1.93	2.05
9	P	101	BCL	MG-ND	-5.99	1.93	2.05
9	AK	101	BCL	MG-ND	-5.98	1.93	2.05
9	3	101	BCL	MG-ND	-5.98	1.93	2.05
9	d	101	BCL	MG-ND	-5.97	1.93	2.05
9	AA	101	BCL	MG-ND	-5.97	1.94	2.05
9	AH	101	BCL	MG-ND	-5.96	1.94	2.05
12	x	306	PEF	O2-C10	5.94	1.48	1.35
9	h	101	BCL	MG-ND	-5.94	1.94	2.05
9	AI	101	BCL	MG-ND	-5.93	1.94	2.05
9	L	301	BCL	MG-ND	-5.93	1.94	2.05
9	G	102	BCL	MG-ND	-5.92	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCL	MG-ND	-5.92	1.94	2.05
9	p	102	BCL	MG-ND	-5.90	1.94	2.05
9	J	102	BCL	MG-ND	-5.89	1.94	2.05
12	H	301	PEF	O2-C10	5.87	1.48	1.35
9	z	102	BCL	MG-ND	-5.86	1.94	2.05
9	AD	101	BCL	MG-ND	-5.85	1.94	2.05
9	F	101	BCL	MG-ND	-5.84	1.94	2.05
9	s	102	BCL	MG-NB	-5.83	1.94	2.05
9	p	104	BCL	MG-ND	-5.82	1.94	2.05
9	M	401	BCL	MG-ND	-5.82	1.94	2.05
12	y	407	PEF	O2-C10	5.82	1.48	1.35
9	k	102	BCL	MG-ND	-5.79	1.94	2.05
9	X	102	BCL	MG-ND	-5.79	1.94	2.05
9	x	301	BCL	MG-ND	-5.75	1.94	2.05
9	7	101	BCL	MG-ND	-5.74	1.94	2.05
9	g	101	BCL	MG-ND	-5.72	1.94	2.05
9	i	102	BCL	MG-ND	-5.72	1.94	2.05
9	N	102	BCL	MG-ND	-5.71	1.94	2.05
9	u	101	BCL	MG-ND	-5.68	1.94	2.05
9	x	305	BCL	MG-ND	-5.68	1.94	2.05
9	3	101	BCL	MG-NB	-5.68	1.94	2.05
9	p	104	BCL	MG-NB	-5.68	1.94	2.05
9	B	101	BCL	MG-ND	-5.67	1.94	2.05
9	5	101	BCL	MG-NB	-5.67	1.94	2.05
9	y	401	BCL	MG-NB	-5.66	1.94	2.05
9	AE	104	BCL	MG-ND	-5.65	1.94	2.05
9	W	101	BCL	MG-ND	-5.65	1.94	2.05
9	V	101	BCL	MG-ND	-5.65	1.94	2.05
9	T	102	BCL	MG-ND	-5.62	1.94	2.05
12	M	408	PEF	O2-C10	5.62	1.47	1.35
9	U	101	BCL	MG-ND	-5.62	1.94	2.05
9	J	102	BCL	MG-NB	-5.59	1.94	2.05
9	Z	102	BCL	MG-ND	-5.58	1.94	2.05
9	G	102	BCL	MG-NB	-5.57	1.94	2.05
9	5	102	BCL	MG-NB	-5.57	1.94	2.05
9	e	102	BCL	MG-NB	-5.56	1.94	2.05
9	I	101	BCL	MG-NB	-5.55	1.94	2.05
9	j	101	BCL	MG-ND	-5.54	1.94	2.05
9	l	101	BCL	MG-ND	-5.52	1.94	2.05
9	f	101	BCL	MG-NB	-5.50	1.94	2.05
12	y	408	PEF	O2-C10	5.49	1.47	1.35
9	D	101	BCL	MG-NB	-5.49	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	102	BCL	MG-NB	-5.48	1.94	2.05
9	u	101	BCL	MG-NB	-5.46	1.95	2.05
12	m	101	PEF	O2-C10	5.44	1.47	1.35
9	L	303	BCL	MG-ND	-5.43	1.95	2.05
9	Y	101	BCL	MG-NB	-5.43	1.95	2.05
7	C	501	HEM	FE-NC	5.41	2.13	1.95
9	AH	103	BCL	MG-ND	-5.41	1.95	2.05
9	P	101	BCL	MG-NB	-5.40	1.95	2.05
9	c	102	BCL	MG-ND	-5.38	1.95	2.05
9	D	102	BCL	MG-ND	-5.37	1.95	2.05
9	l	102	BCL	MG-NB	-5.37	1.95	2.05
7	C	504	HEM	C3C-C4C	-5.36	1.36	1.46
9	O	101	BCL	MG-NB	-5.36	1.95	2.05
9	T	102	BCL	OBD-CAD	5.36	1.31	1.22
9	AE	102	BCL	MG-ND	-5.36	1.95	2.05
7	C	501	HEM	C4D-ND	-5.36	1.31	1.40
9	A	102	BCL	MG-NB	-5.35	1.95	2.05
9	8	102	BCL	MG-ND	-5.35	1.95	2.05
9	m	102	BCL	MG-ND	-5.34	1.95	2.05
9	B	101	BCL	MG-NB	-5.34	1.95	2.05
9	r	101	BCL	MG-NB	-5.33	1.95	2.05
9	M	401	BCL	OBD-CAD	5.33	1.31	1.22
9	AC	102	BCL	MG-ND	-5.32	1.95	2.05
9	AJ	102	BCL	MG-NB	-5.32	1.95	2.05
9	j	101	BCL	MG-NB	-5.31	1.95	2.05
9	Z	102	BCL	MG-NB	-5.27	1.95	2.05
12	H	303	PEF	O2-C10	5.25	1.46	1.35
12	H	304	PEF	O2-C10	5.22	1.46	1.35
9	M	401	BCL	MG-NB	-5.20	1.95	2.05
9	AB	101	BCL	OBD-CAD	5.19	1.31	1.22
9	4	102	BCL	MG-NB	-5.18	1.95	2.05
9	R	102	BCL	MG-ND	-5.18	1.95	2.05
9	AH	103	BCL	OBD-CAD	5.18	1.31	1.22
9	i	102	BCL	MG-NB	-5.18	1.95	2.05
9	AI	101	BCL	MG-NB	-5.18	1.95	2.05
9	AA	101	BCL	MG-NB	-5.17	1.95	2.05
9	AE	102	BCL	MG-NB	-5.16	1.95	2.05
9	0	101	BCL	MG-NB	-5.16	1.95	2.05
9	8	102	BCL	MG-NB	-5.15	1.95	2.05
9	AL	102	BCL	MG-NB	-5.15	1.95	2.05
9	Q	101	BCL	MG-NB	-5.12	1.95	2.05
9	k	102	BCL	MG-NB	-5.11	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	BCL	MG-NB	-5.11	1.95	2.05
9	9	103	BCL	MG-NB	-5.09	1.95	2.05
9	Q	101	BCL	OBD-CAD	5.08	1.31	1.22
9	p	104	BCL	OBD-CAD	5.07	1.31	1.22
9	w	101	BCL	OBD-CAD	5.06	1.31	1.22
9	Y	101	BCL	OBD-CAD	5.06	1.31	1.22
9	D	102	BCL	MG-NB	-5.04	1.95	2.05
9	W	101	BCL	OBD-CAD	5.03	1.31	1.22
9	m	103	BCL	MG-ND	-5.03	1.95	2.05
9	v	102	BCL	MG-NB	-5.03	1.95	2.05
9	AK	101	BCL	MG-NB	-5.02	1.95	2.05
9	x	305	BCL	OBD-CAD	5.01	1.31	1.22
9	AD	101	BCL	MG-NB	-5.00	1.95	2.05
9	AE	104	BCL	MG-NB	-4.99	1.95	2.05
9	z	102	BCL	MG-NB	-4.99	1.95	2.05
9	m	103	BCL	OBD-CAD	4.98	1.31	1.22
9	L	305	BCL	MG-NB	-4.97	1.95	2.05
9	AC	102	BCL	MG-NB	-4.97	1.95	2.05
9	K	101	BCL	MG-NB	-4.97	1.95	2.05
9	5	102	BCL	OBD-CAD	4.97	1.31	1.22
9	m	102	BCL	MG-NB	-4.97	1.95	2.05
9	N	102	BCL	OBD-CAD	4.97	1.31	1.22
9	AH	101	BCL	OBD-CAD	4.95	1.31	1.22
12	y	406	PEF	O2-C10	4.94	1.46	1.35
9	D	101	BCL	OBD-CAD	4.94	1.31	1.22
9	g	101	BCL	MG-NB	-4.94	1.96	2.05
9	r	101	BCL	OBD-CAD	4.93	1.31	1.22
9	S	102	BCL	MG-NB	-4.93	1.96	2.05
9	d	101	BCL	MG-NB	-4.93	1.96	2.05
9	AD	101	BCL	OBD-CAD	4.93	1.31	1.22
9	1	101	BCL	MG-ND	-4.92	1.96	2.05
9	V	101	BCL	OBD-CAD	4.91	1.30	1.22
9	l	101	BCL	MG-NB	-4.91	1.96	2.05
9	X	102	BCL	MG-NB	-4.91	1.96	2.05
9	7	101	BCL	MG-NB	-4.91	1.96	2.05
9	i	102	BCL	OBD-CAD	4.91	1.30	1.22
9	R	102	BCL	OBD-CAD	4.90	1.30	1.22
12	t	303	PEF	O2-C10	4.90	1.46	1.35
9	AE	104	BCL	OBD-CAD	4.89	1.30	1.22
9	c	102	BCL	MG-NB	-4.89	1.96	2.05
9	1	101	BCL	MG-NB	-4.89	1.96	2.05
9	1	101	BCL	OBD-CAD	4.88	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	w	101	BCL	MG-NB	-4.88	1.96	2.05
9	AA	101	BCL	OBD-CAD	4.85	1.30	1.22
9	c	102	BCL	OBD-CAD	4.85	1.30	1.22
7	C	501	HEM	C1B-NB	-4.85	1.31	1.40
9	m	103	BCL	MG-NB	-4.84	1.96	2.05
9	k	102	BCL	OBD-CAD	4.84	1.30	1.22
9	5	101	BCL	OBD-CAD	4.84	1.30	1.22
9	AH	101	BCL	MG-NB	-4.84	1.96	2.05
9	l	101	BCL	OBD-CAD	4.84	1.30	1.22
7	C	503	HEM	C3B-C4B	4.83	1.54	1.44
9	AE	102	BCL	OBD-CAD	4.83	1.30	1.22
12	t	301	PEF	O2-C10	4.83	1.45	1.35
9	V	101	BCL	MG-NB	-4.82	1.96	2.05
9	AB	101	BCL	MG-NB	-4.82	1.96	2.05
9	N	102	BCL	MG-NB	-4.81	1.96	2.05
9	AK	101	BCL	OBD-CAD	4.81	1.30	1.22
9	d	101	BCL	OBD-CAD	4.80	1.30	1.22
9	7	101	BCL	OBD-CAD	4.79	1.30	1.22
9	U	101	BCL	OBD-CAD	4.78	1.30	1.22
9	m	102	BCL	OBD-CAD	4.78	1.30	1.22
9	j	101	BCL	OBD-CAD	4.78	1.30	1.22
9	X	102	BCL	OBD-CAD	4.75	1.30	1.22
9	O	101	BCL	OBD-CAD	4.75	1.30	1.22
9	D	102	BCL	OBD-CAD	4.75	1.30	1.22
9	G	102	BCL	OBD-CAD	4.75	1.30	1.22
7	o	501	HEM	FE-NC	4.74	2.10	1.95
9	T	102	BCL	MG-NB	-4.74	1.96	2.05
12	A	101	PEF	O2-C10	4.74	1.45	1.35
9	W	101	BCL	MG-NB	-4.74	1.96	2.05
9	Z	102	BCL	OBD-CAD	4.73	1.30	1.22
9	g	101	BCL	OBD-CAD	4.73	1.30	1.22
9	A	102	BCL	OBD-CAD	4.73	1.30	1.22
9	u	101	BCL	OBD-CAD	4.72	1.30	1.22
9	L	305	BCL	OBD-CAD	4.72	1.30	1.22
9	h	101	BCL	OBD-CAD	4.72	1.30	1.22
9	AI	101	BCL	OBD-CAD	4.71	1.30	1.22
7	C	502	HEM	FE-NC	4.71	2.10	1.95
9	R	102	BCL	MG-NB	-4.70	1.96	2.05
9	U	101	BCL	MG-NB	-4.70	1.96	2.05
9	P	101	BCL	OBD-CAD	4.69	1.30	1.22
12	M	406	PEF	O2-C10	4.69	1.45	1.35
9	I	101	BCL	OBD-CAD	4.68	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	102	BCL	OBD-CAD	4.67	1.30	1.22
9	J	102	BCL	OBD-CAD	4.66	1.30	1.22
9	x	301	BCL	C3C-C4C	4.64	1.57	1.51
9	AH	103	BCL	MG-NB	-4.64	1.96	2.05
9	3	101	BCL	OBD-CAD	4.61	1.30	1.22
9	K	101	BCL	OBD-CAD	4.61	1.30	1.22
9	B	101	BCL	OBD-CAD	4.60	1.30	1.22
9	AJ	102	BCL	OBD-CAD	4.60	1.30	1.22
9	y	401	BCL	OBD-CAD	4.60	1.30	1.22
7	C	502	HEM	C1B-NB	-4.59	1.32	1.40
9	v	102	BCL	OBD-CAD	4.58	1.30	1.22
9	h	101	BCL	MG-NB	-4.57	1.96	2.05
9	F	101	BCL	OBD-CAD	4.57	1.30	1.22
9	AC	102	BCL	OBD-CAD	4.56	1.30	1.22
7	o	503	HEM	C3B-C4B	4.54	1.53	1.44
9	0	101	BCL	OBD-CAD	4.54	1.30	1.22
9	z	102	BCL	OBD-CAD	4.52	1.30	1.22
9	4	102	BCL	OBD-CAD	4.51	1.30	1.22
9	8	102	BCL	OBD-CAD	4.51	1.30	1.22
9	1	102	BCL	OBD-CAD	4.50	1.30	1.22
9	s	102	BCL	OBD-CAD	4.49	1.30	1.22
9	x	305	BCL	MG-NB	-4.48	1.96	2.05
9	x	303	BCL	OBD-CAD	4.48	1.30	1.22
9	L	301	BCL	MG-NB	-4.48	1.96	2.05
9	AL	102	BCL	OBD-CAD	4.47	1.30	1.22
9	x	301	BCL	OBD-CAD	4.46	1.30	1.22
7	o	502	HEM	FE-NC	4.45	2.09	1.95
7	C	501	HEM	FE-ND	-4.42	1.81	1.94
9	e	102	BCL	OBD-CAD	4.41	1.30	1.22
9	x	305	BCL	O1D-CGD	-4.41	1.10	1.21
9	L	303	BCL	OBD-CAD	4.40	1.30	1.22
9	f	101	BCL	OBD-CAD	4.39	1.30	1.22
10	x	302	BPH	C2C-C3C	-4.36	1.50	1.54
9	9	103	BCL	OBD-CAD	4.34	1.29	1.22
9	L	303	BCL	O1D-CGD	-4.33	1.10	1.21
9	4	102	BCL	O1D-CGD	-4.30	1.10	1.21
9	s	102	BCL	O1D-CGD	-4.26	1.10	1.21
9	L	303	BCL	MG-NB	-4.25	1.97	2.05
7	o	501	HEM	C1B-NB	-4.25	1.32	1.40
9	p	104	BCL	O1D-CGD	-4.23	1.10	1.21
9	g	101	BCL	O1D-CGD	-4.20	1.10	1.21
9	h	101	BCL	O1D-CGD	-4.20	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	101	BCL	O1D-CGD	-4.18	1.10	1.21
9	G	102	BCL	O1D-CGD	-4.17	1.10	1.21
9	AK	101	BCL	O1D-CGD	-4.17	1.10	1.21
9	m	102	BCL	O1D-CGD	-4.16	1.10	1.21
7	o	504	HEM	FE-NC	4.16	2.08	1.95
9	V	101	BCL	O1D-CGD	-4.15	1.10	1.21
7	o	504	HEM	C1B-NB	-4.15	1.33	1.40
7	C	504	HEM	C1B-NB	-4.14	1.33	1.40
9	y	401	BCL	O2D-CED	4.10	1.54	1.45
9	Y	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	Y	101	BCL	C3C-C4C	4.10	1.56	1.51
9	AI	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	M	401	BCL	O2A-CGA	-4.10	1.21	1.33
9	AL	102	BCL	O1D-CGD	-4.09	1.11	1.21
9	x	301	BCL	O1D-CGD	-4.07	1.11	1.21
9	5	101	BCL	O1D-CGD	-4.06	1.11	1.21
9	f	101	BCL	O1D-CGD	-4.05	1.11	1.21
9	x	301	BCL	O2D-CED	4.05	1.54	1.45
9	M	401	BCL	C3C-C4C	4.04	1.56	1.51
9	p	102	BCL	OBD-CAD	4.03	1.29	1.22
7	o	501	HEM	C4B-NB	-4.03	1.30	1.38
9	U	101	BCL	O1D-CGD	-4.03	1.11	1.21
9	P	101	BCL	O1D-CGD	-4.02	1.11	1.21
9	u	101	BCL	O1D-CGD	-4.02	1.11	1.21
9	9	103	BCL	O1D-CGD	-4.00	1.11	1.21
9	c	102	BCL	O1D-CGD	-3.99	1.11	1.21
9	T	102	BCL	O1D-CGD	-3.99	1.11	1.21
9	D	102	BCL	O1D-CGD	-3.99	1.11	1.21
9	k	102	BCL	O1D-CGD	-3.98	1.11	1.21
9	l	102	BCL	O1D-CGD	-3.97	1.11	1.21
9	v	102	BCL	O1D-CGD	-3.97	1.11	1.21
9	M	401	BCL	O1D-CGD	-3.97	1.11	1.21
9	AB	101	BCL	O1D-CGD	-3.96	1.11	1.21
9	O	101	BCL	O2D-CED	3.95	1.54	1.45
9	l	101	BCL	O2D-CED	3.95	1.54	1.45
9	8	102	BCL	O2D-CED	3.95	1.54	1.45
9	m	103	BCL	O1D-CGD	-3.94	1.11	1.21
9	x	301	BCL	MG-NB	-3.94	1.98	2.05
9	x	305	BCL	O2D-CED	3.94	1.54	1.45
9	AH	103	BCL	O1D-CGD	-3.94	1.11	1.21
9	AH	101	BCL	O1D-CGD	-3.92	1.11	1.21
7	o	504	HEM	C3C-C4C	-3.92	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	101	BCL	O2D-CED	3.91	1.54	1.45
9	y	401	BCL	O1D-CGD	-3.91	1.11	1.21
9	AA	101	BCL	O1D-CGD	-3.91	1.11	1.21
9	W	101	BCL	O1D-CGD	-3.90	1.11	1.21
9	j	101	BCL	O1D-CGD	-3.89	1.11	1.21
9	3	101	BCL	O2D-CED	3.89	1.53	1.45
7	C	502	HEM	C4B-NB	-3.88	1.31	1.38
9	5	102	BCL	O1D-CGD	-3.88	1.11	1.21
9	I	101	BCL	O1D-CGD	-3.88	1.11	1.21
9	AE	102	BCL	O1D-CGD	-3.88	1.11	1.21
9	Z	102	BCL	O1D-CGD	-3.87	1.11	1.21
9	8	102	BCL	O1D-CGD	-3.85	1.11	1.21
9	A	102	BCL	O1D-CGD	-3.85	1.11	1.21
9	p	102	BCL	O1D-CGD	-3.85	1.11	1.21
9	l	101	BCL	O1D-CGD	-3.85	1.11	1.21
9	Q	101	BCL	O1D-CGD	-3.84	1.11	1.21
9	K	101	BCL	O1D-CGD	-3.82	1.11	1.21
7	C	501	HEM	C4B-NB	-3.82	1.31	1.38
9	e	102	BCL	O1D-CGD	-3.82	1.11	1.21
9	i	102	BCL	O1D-CGD	-3.82	1.11	1.21
9	c	102	BCL	O2D-CED	3.81	1.53	1.45
7	o	501	HEM	C4D-ND	-3.81	1.33	1.40
9	x	303	BCL	O1D-CGD	-3.81	1.11	1.21
9	W	101	BCL	O2D-CED	3.81	1.53	1.45
9	m	103	BCL	O2D-CED	3.81	1.53	1.45
9	z	102	BCL	O1D-CGD	-3.80	1.11	1.21
9	w	101	BCL	O1D-CGD	-3.80	1.11	1.21
9	U	101	BCL	O2D-CGD	-3.79	1.23	1.33
9	m	102	BCL	O2D-CED	3.79	1.53	1.45
9	S	102	BCL	O1D-CGD	-3.79	1.11	1.21
9	AC	102	BCL	O1D-CGD	-3.79	1.11	1.21
9	B	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	3	101	BCL	O1D-CGD	-3.78	1.11	1.21
9	9	103	BCL	O2D-CED	3.78	1.53	1.45
9	AD	101	BCL	O1D-CGD	-3.76	1.11	1.21
9	M	401	BCL	O2D-CED	3.76	1.53	1.45
9	F	101	BCL	O1D-CGD	-3.75	1.11	1.21
9	N	102	BCL	O2D-CED	3.74	1.53	1.45
9	0	101	BCL	O1D-CGD	-3.74	1.11	1.21
9	0	101	BCL	O2D-CED	3.74	1.53	1.45
9	f	101	BCL	O2D-CED	3.73	1.53	1.45
12	y	407	PEF	O3-C30	3.73	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	x	305	BCL	C1D-C2D	-3.72	1.38	1.45
9	R	102	BCL	O2D-CED	3.72	1.53	1.45
9	y	401	BCL	C3C-C4C	3.72	1.56	1.51
9	AE	102	BCL	O2D-CED	3.71	1.53	1.45
9	F	101	BCL	O2D-CED	3.71	1.53	1.45
9	1	101	BCL	O1D-CGD	-3.70	1.11	1.21
9	AJ	102	BCL	O1D-CGD	-3.70	1.11	1.21
9	r	101	BCL	O2D-CED	3.70	1.53	1.45
9	7	101	BCL	O2D-CED	3.70	1.53	1.45
9	u	101	BCL	O2D-CED	3.69	1.53	1.45
9	AJ	102	BCL	O2D-CED	3.69	1.53	1.45
7	o	502	HEM	C1B-NB	-3.68	1.33	1.40
9	l	101	BCL	O2D-CED	3.68	1.53	1.45
9	AE	104	BCL	O1D-CGD	-3.68	1.12	1.21
9	AE	104	BCL	O2D-CED	3.68	1.53	1.45
9	X	102	BCL	O1D-CGD	-3.67	1.12	1.21
9	5	101	BCL	O2D-CED	3.67	1.53	1.45
9	N	102	BCL	O1D-CGD	-3.66	1.12	1.21
9	7	101	BCL	O1D-CGD	-3.66	1.12	1.21
9	i	102	BCL	O2D-CED	3.66	1.53	1.45
9	5	102	BCL	O2D-CED	3.66	1.53	1.45
9	U	101	BCL	O2A-CGA	-3.65	1.22	1.33
9	S	102	BCL	O2D-CED	3.64	1.53	1.45
9	p	102	BCL	O2D-CED	3.63	1.53	1.45
9	L	305	BCL	O1D-CGD	-3.61	1.12	1.21
9	p	104	BCL	O2D-CED	3.61	1.53	1.45
7	o	501	HEM	FE-ND	-3.61	1.83	1.94
7	C	504	HEM	C4D-ND	-3.61	1.34	1.40
9	J	102	BCL	O2D-CED	3.60	1.53	1.45
9	V	101	BCL	O2D-CED	3.60	1.53	1.45
9	d	101	BCL	O2D-CED	3.60	1.53	1.45
9	e	102	BCL	O2D-CED	3.60	1.53	1.45
9	j	101	BCL	O2D-CED	3.59	1.53	1.45
7	C	504	HEM	FE-NC	3.59	2.07	1.95
7	o	503	HEM	FE-NC	3.59	2.07	1.95
9	AL	102	BCL	O2D-CED	3.59	1.53	1.45
9	h	101	BCL	O2D-CED	3.59	1.53	1.45
7	o	504	HEM	C3B-C4B	3.58	1.51	1.44
9	1	102	BCL	O2D-CED	3.57	1.53	1.45
9	x	303	BCL	O2D-CGD	-3.57	1.24	1.33
9	I	101	BCL	O2D-CED	3.57	1.53	1.45
9	G	102	BCL	O2D-CED	3.56	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	102	BCL	O2D-CED	3.54	1.53	1.45
9	AA	101	BCL	O2D-CED	3.54	1.53	1.45
9	J	102	BCL	O1D-CGD	-3.53	1.12	1.21
9	O	101	BCL	O1D-CGD	-3.53	1.12	1.21
9	d	101	BCL	O1D-CGD	-3.53	1.12	1.21
9	A	102	BCL	O2D-CED	3.52	1.53	1.45
9	r	101	BCL	O1D-CGD	-3.51	1.12	1.21
7	o	502	HEM	C4D-ND	-3.51	1.34	1.40
9	4	102	BCL	C3C-C4C	3.51	1.56	1.51
9	R	102	BCL	O1D-CGD	-3.50	1.12	1.21
9	g	101	BCL	O2D-CED	3.50	1.53	1.45
9	X	102	BCL	O2D-CED	3.49	1.53	1.45
9	D	102	BCL	O2D-CED	3.48	1.53	1.45
9	u	101	BCL	C5-C3	3.47	1.58	1.51
9	4	102	BCL	O2D-CED	3.47	1.53	1.45
9	B	101	BCL	O2D-CED	3.46	1.53	1.45
7	C	503	HEM	C3C-C4C	-3.46	1.40	1.46
9	L	301	BCL	O1D-CGD	-3.46	1.12	1.21
9	AB	101	BCL	O2D-CED	3.45	1.53	1.45
9	L	301	BCL	O2D-CED	3.45	1.53	1.45
7	C	502	HEM	C1A-C2A	-3.45	1.37	1.44
9	L	305	BCL	O2D-CED	3.45	1.53	1.45
9	v	102	BCL	O2D-CED	3.45	1.52	1.45
9	L	303	BCL	O2D-CED	3.44	1.52	1.45
9	AI	101	BCL	O2D-CED	3.42	1.52	1.45
9	AD	101	BCL	O2D-CED	3.41	1.52	1.45
9	Z	102	BCL	O2D-CED	3.40	1.52	1.45
9	AH	101	BCL	O2D-CGD	-3.40	1.24	1.33
9	L	301	BCL	C3C-C4C	3.39	1.55	1.51
9	AH	103	BCL	O2D-CED	3.38	1.52	1.45
9	T	102	BCL	O2D-CED	3.38	1.52	1.45
9	x	305	BCL	O1A-CGA	-3.37	1.12	1.22
7	o	504	HEM	C4D-ND	-3.37	1.34	1.40
9	5	102	BCL	C1D-C2D	-3.37	1.38	1.45
9	h	101	BCL	O2D-CGD	-3.36	1.25	1.33
7	o	503	HEM	C3C-C4C	-3.36	1.40	1.46
9	D	101	BCL	O2D-CGD	-3.36	1.25	1.33
9	w	101	BCL	O2D-CGD	-3.35	1.25	1.33
11	x	304	UQ8	C4-C3	3.33	1.48	1.36
9	Q	101	BCL	O2D-CED	3.32	1.52	1.45
9	AK	101	BCL	O2D-CGD	-3.31	1.25	1.33
9	AL	102	BCL	O2A-CGA	-3.31	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	101	BCL	O2D-CED	3.31	1.52	1.45
9	AC	102	BCL	O2D-CED	3.31	1.52	1.45
9	x	303	BCL	C1D-C2D	-3.30	1.38	1.45
9	Q	101	BCL	O2D-CGD	-3.30	1.25	1.33
9	V	101	BCL	O2A-CGA	-3.29	1.23	1.33
7	C	504	HEM	C3B-C4B	3.28	1.51	1.44
9	v	102	BCL	O2D-CGD	-3.28	1.25	1.33
9	x	301	BCL	C3B-CAB	3.27	1.56	1.46
7	C	504	HEM	FE-ND	-3.27	1.84	1.94
9	P	101	BCL	C3C-C4C	3.26	1.55	1.51
9	AK	101	BCL	O2D-CED	3.26	1.52	1.45
7	C	503	HEM	C4D-ND	-3.25	1.34	1.40
9	m	102	BCL	O2D-CGD	-3.25	1.25	1.33
7	o	502	HEM	C4B-NB	-3.24	1.32	1.38
9	K	101	BCL	O2D-CED	3.24	1.52	1.45
7	C	504	HEM	C1D-ND	-3.24	1.32	1.38
9	AH	101	BCL	O2D-CED	3.23	1.52	1.45
7	C	502	HEM	C4D-ND	-3.22	1.34	1.40
9	s	102	BCL	C5-C3	3.22	1.57	1.51
9	M	401	BCL	OBB-CAB	-3.22	1.15	1.23
9	AH	103	BCL	O2D-CGD	-3.22	1.25	1.33
9	x	303	BCL	O2D-CED	3.22	1.52	1.45
9	D	101	BCL	O2A-CGA	-3.22	1.24	1.33
9	p	104	BCL	O2D-CGD	-3.21	1.25	1.33
9	D	101	BCL	O2D-CED	3.20	1.52	1.45
9	k	102	BCL	O2D-CED	3.19	1.52	1.45
9	w	101	BCL	O2D-CED	3.19	1.52	1.45
9	I	101	BCL	O2D-CGD	-3.18	1.25	1.33
9	T	102	BCL	O2D-CGD	-3.18	1.25	1.33
9	L	303	BCL	O2D-CGD	-3.17	1.25	1.33
9	x	301	BCL	C5-C3	3.17	1.57	1.51
9	M	401	BCL	O1A-CGA	-3.15	1.13	1.22
9	r	101	BCL	C3C-C4C	3.15	1.55	1.51
9	AA	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	D	102	BCL	O2A-CGA	-3.14	1.24	1.33
9	V	101	BCL	O2D-CGD	-3.14	1.25	1.33
12	A	101	PEF	O3-C30	3.14	1.48	1.33
9	k	102	BCL	O2D-CGD	-3.14	1.25	1.33
7	o	503	HEM	C4D-ND	-3.13	1.34	1.40
9	p	104	BCL	O1A-CGA	-3.13	1.13	1.22
9	G	102	BCL	O2D-CGD	-3.13	1.25	1.33
9	y	401	BCL	O1A-CGA	-3.12	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	304	PEF	O3-C30	3.12	1.48	1.33
9	h	101	BCL	C3C-C4C	3.11	1.55	1.51
9	AD	101	BCL	O2D-CGD	-3.11	1.25	1.33
17	AE	101	PGW	O01-C1	3.11	1.42	1.35
9	Z	102	BCL	C1D-C2D	-3.10	1.39	1.45
9	G	102	BCL	O2A-CGA	-3.09	1.24	1.33
9	AJ	102	BCL	O2A-CGA	-3.09	1.24	1.33
7	C	502	HEM	C3C-C2C	3.09	1.43	1.37
9	l	101	BCL	OBB-CAB	-3.08	1.16	1.23
9	P	101	BCL	O2D-CGD	-3.07	1.25	1.33
9	m	102	BCL	C3B-CAB	3.06	1.56	1.46
9	8	102	BCL	O2A-CGA	-3.06	1.24	1.33
9	d	101	BCL	C5-C3	3.06	1.57	1.51
7	o	501	HEM	C1D-ND	-3.06	1.32	1.38
14	y	403	MQ8	C37-C38	3.06	1.40	1.33
9	Z	102	BCL	O1A-CGA	-3.05	1.13	1.22
9	x	303	BCL	O2A-CGA	-3.05	1.24	1.33
9	AB	101	BCL	O2D-CGD	-3.05	1.25	1.33
9	u	101	BCL	O2D-CGD	-3.05	1.25	1.33
7	o	502	HEM	C3C-C2C	3.05	1.43	1.37
9	U	101	BCL	O1A-CGA	-3.04	1.13	1.22
10	L	302	BPH	CBD-CGD	-3.04	1.48	1.52
9	y	401	BCL	O2D-CGD	-3.03	1.25	1.33
9	s	102	BCL	O2D-CGD	-3.03	1.25	1.33
9	j	101	BCL	O2D-CGD	-3.03	1.25	1.33
9	N	102	BCL	O2A-CGA	-3.03	1.24	1.33
9	AI	101	BCL	O2D-CGD	-3.03	1.25	1.33
9	p	104	BCL	O2A-CGA	-3.02	1.24	1.33
7	o	503	HEM	FE-ND	-3.02	1.85	1.94
9	L	301	BCL	O1A-CGA	-3.01	1.13	1.22
9	Z	102	BCL	O2A-CGA	-3.01	1.24	1.33
12	M	407	PEF	O3-C30	3.01	1.47	1.33
9	X	102	BCL	O2A-CGA	-3.01	1.24	1.33
9	O	101	BCL	O2A-CGA	-3.00	1.24	1.33
12	M	406	PEF	O3-C30	3.00	1.47	1.33
9	3	101	BCL	O1A-CGA	-2.99	1.13	1.22
12	t	301	PEF	O3-C30	2.98	1.47	1.33
9	AH	103	BCL	O2A-CGA	-2.98	1.24	1.33
9	U	101	BCL	O2D-CED	2.98	1.51	1.45
7	o	502	HEM	FE-ND	-2.98	1.85	1.94
9	m	103	BCL	O2A-CGA	-2.98	1.24	1.33
9	L	303	BCL	C5-C3	2.97	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	BCL	O2D-CGD	-2.97	1.25	1.33
12	y	408	PEF	O3-C30	2.97	1.47	1.33
9	AC	102	BCL	O2A-CGA	-2.96	1.24	1.33
9	1	102	BCL	C1D-C2D	-2.96	1.39	1.45
9	p	102	BCL	O2A-CGA	-2.96	1.24	1.33
9	T	102	BCL	O2A-CGA	-2.95	1.24	1.33
9	S	102	BCL	O1A-CGA	-2.94	1.13	1.22
9	5	101	BCL	OBb-CAB	-2.94	1.16	1.23
9	X	102	BCL	O1A-CGA	-2.94	1.13	1.22
9	s	102	BCL	O2A-CGA	-2.94	1.24	1.33
9	f	101	BCL	C5-C3	2.94	1.57	1.51
9	K	101	BCL	O2D-CGD	-2.94	1.26	1.33
12	M	408	PEF	O3-C30	2.94	1.47	1.33
9	l	101	BCL	O2A-CGA	-2.94	1.24	1.33
9	W	101	BCL	C3C-C4C	2.93	1.55	1.51
9	A	102	BCL	O2D-CGD	-2.93	1.26	1.33
9	y	401	BCL	O2A-CGA	-2.93	1.24	1.33
9	w	101	BCL	O1A-CGA	-2.93	1.13	1.22
9	g	101	BCL	O2D-CGD	-2.92	1.26	1.33
9	AA	101	BCL	O2A-CGA	-2.92	1.24	1.33
12	t	303	PEF	O3-C30	2.92	1.47	1.33
9	4	102	BCL	O1A-CGA	-2.92	1.13	1.22
9	l	101	BCL	C3B-CAB	2.91	1.55	1.46
7	o	503	HEM	C1B-NB	-2.91	1.35	1.40
9	Z	102	BCL	O2D-CGD	-2.91	1.26	1.33
9	L	305	BCL	O2D-CGD	-2.91	1.26	1.33
9	L	305	BCL	C3B-CAB	2.90	1.55	1.46
9	g	101	BCL	O2A-CGA	-2.90	1.24	1.33
9	p	102	BCL	O2D-CGD	-2.90	1.26	1.33
9	s	102	BCL	C1D-C2D	-2.90	1.39	1.45
9	y	401	BCL	OBb-CAB	-2.90	1.16	1.23
7	C	503	HEM	C1B-NB	-2.89	1.35	1.40
9	e	102	BCL	OBb-CAB	-2.89	1.16	1.23
9	g	101	BCL	O1A-CGA	-2.89	1.13	1.22
9	1	101	BCL	C5-C3	2.89	1.57	1.51
9	T	102	BCL	O1A-CGA	-2.89	1.13	1.22
7	C	503	HEM	FE-NC	2.89	2.04	1.95
9	J	102	BCL	O2A-CGA	-2.89	1.25	1.33
9	AC	102	BCL	O2D-CGD	-2.88	1.26	1.33
9	AH	101	BCL	O2A-CGA	-2.88	1.25	1.33
9	A	102	BCL	O2A-CGA	-2.88	1.25	1.33
9	m	103	BCL	O1A-CGA	-2.88	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	102	BCL	O2D-CED	2.88	1.51	1.45
9	x	303	BCL	O1A-CGA	-2.88	1.13	1.22
9	r	101	BCL	O1A-CGA	-2.87	1.13	1.22
9	5	102	BCL	C3C-C4C	2.87	1.55	1.51
9	3	101	BCL	O2A-CGA	-2.87	1.25	1.33
9	AK	101	BCL	C1D-C2D	-2.87	1.39	1.45
9	X	102	BCL	C3C-C4C	2.86	1.55	1.51
9	x	303	BCL	C3D-C4D	-2.86	1.37	1.44
9	X	102	BCL	O2D-CGD	-2.85	1.26	1.33
9	AB	101	BCL	O2A-CGA	-2.85	1.25	1.33
9	8	102	BCL	O1A-CGA	-2.85	1.14	1.22
9	5	101	BCL	O2D-CGD	-2.85	1.26	1.33
9	e	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	m	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	L	305	BCL	O2A-CGA	-2.84	1.25	1.33
9	AD	101	BCL	O2A-CGA	-2.84	1.25	1.33
7	o	503	HEM	C1D-ND	-2.84	1.33	1.38
9	S	102	BCL	O2A-CGA	-2.84	1.25	1.33
9	c	102	BCL	O2A-CGA	-2.83	1.25	1.33
9	r	101	BCL	O2A-CGA	-2.83	1.25	1.33
9	W	101	BCL	O2D-CGD	-2.83	1.26	1.33
9	x	303	BCL	C3D-C2D	-2.83	1.31	1.39
9	v	102	BCL	C1D-C2D	-2.83	1.39	1.45
9	AH	103	BCL	O1A-CGA	-2.82	1.14	1.22
9	AJ	102	BCL	O1A-CGA	-2.82	1.14	1.22
9	c	102	BCL	O2D-CGD	-2.82	1.26	1.33
9	z	102	BCL	O2A-CGA	-2.82	1.25	1.33
9	p	104	BCL	C1B-C2B	-2.82	1.36	1.43
9	J	102	BCL	C3B-CAB	2.82	1.55	1.46
9	4	102	BCL	OBB-CAB	-2.82	1.16	1.23
12	m	101	PEF	O3-C30	2.82	1.46	1.33
9	L	301	BCL	O2D-CGD	-2.81	1.26	1.33
11	L	304	UQ8	C4-C3	2.81	1.46	1.36
9	d	101	BCL	O2D-CGD	-2.81	1.26	1.33
9	I	101	BCL	O1A-CGA	-2.81	1.14	1.22
9	0	101	BCL	O2A-CGA	-2.81	1.25	1.33
17	S	101	PGW	O01-C1	2.80	1.41	1.35
9	m	103	BCL	O2D-CGD	-2.80	1.26	1.33
9	0	101	BCL	C1D-C2D	-2.80	1.39	1.45
9	5	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	s	102	BCL	O1A-CGA	-2.80	1.14	1.22
9	5	102	BCL	C3B-CAB	2.80	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AI	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	v	102	BCL	O2A-CGA	-2.79	1.25	1.33
9	O	101	BCL	O1A-CGA	-2.79	1.14	1.22
14	y	403	MQ8	C9-C10	2.79	1.44	1.39
9	5	101	BCL	O2A-CGA	-2.79	1.25	1.33
9	L	303	BCL	C3D-C2D	-2.79	1.31	1.39
9	B	101	BCL	C1D-C2D	-2.79	1.39	1.45
9	4	102	BCL	O2A-CGA	-2.78	1.25	1.33
9	1	101	BCL	O2D-CGD	-2.78	1.26	1.33
9	5	102	BCL	O2A-CGA	-2.78	1.25	1.33
9	K	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	AD	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	e	102	BCL	C1D-C2D	-2.77	1.39	1.45
9	G	102	BCL	O1A-CGA	-2.77	1.14	1.22
9	AB	101	BCL	C1D-C2D	-2.77	1.39	1.45
9	D	101	BCL	O1A-CGA	-2.77	1.14	1.22
9	AH	103	BCL	C3B-CAB	2.77	1.55	1.46
9	S	102	BCL	O2D-CGD	-2.77	1.26	1.33
12	y	406	PEF	O3-C30	2.77	1.46	1.33
9	L	301	BCL	OBB-CAB	-2.77	1.17	1.23
9	AE	102	BCL	O1A-CGA	-2.77	1.14	1.22
9	0	101	BCL	O1A-CGA	-2.76	1.14	1.22
9	AE	102	BCL	O2A-CGA	-2.76	1.25	1.33
7	C	503	HEM	FE-ND	-2.76	1.86	1.94
9	AL	102	BCL	O2D-CGD	-2.76	1.26	1.33
9	Y	101	BCL	O2A-CGA	-2.76	1.25	1.33
9	P	101	BCL	O2A-CGA	-2.76	1.25	1.33
9	AA	101	BCL	O1A-CGA	-2.76	1.14	1.22
9	1	101	BCL	O2A-CGA	-2.75	1.25	1.33
9	Y	101	BCL	O2D-CGD	-2.75	1.26	1.33
9	m	102	BCL	C5-C3	2.75	1.57	1.51
9	AE	102	BCL	O2D-CGD	-2.74	1.26	1.33
9	I	101	BCL	O2A-CGA	-2.74	1.25	1.33
9	I	101	BCL	C1D-C2D	-2.74	1.39	1.45
9	R	102	BCL	O2A-CGA	-2.74	1.25	1.33
9	4	102	BCL	O2D-CGD	-2.73	1.26	1.33
9	AB	101	BCL	O1A-CGA	-2.73	1.14	1.22
9	L	301	BCL	C3B-CAB	2.73	1.55	1.46
9	AC	102	BCL	O1A-CGA	-2.73	1.14	1.22
9	Y	101	BCL	O1A-CGA	-2.72	1.14	1.22
9	D	102	BCL	O2D-CGD	-2.72	1.26	1.33
9	L	301	BCL	C1D-C2D	-2.72	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	102	BCL	O2A-CGA	-2.72	1.25	1.33
9	AK	101	BCL	O2A-CGA	-2.72	1.25	1.33
9	N	102	BCL	O1A-CGA	-2.72	1.14	1.22
10	y	402	BPH	OBD-CAD	-2.72	1.18	1.22
9	L	305	BCL	O1A-CGA	-2.71	1.14	1.22
12	x	306	PEF	O3-C30	2.71	1.46	1.33
9	3	101	BCL	C1B-C2B	-2.71	1.36	1.43
9	P	101	BCL	O1A-CGA	-2.71	1.14	1.22
9	j	101	BCL	O2A-CGA	-2.71	1.25	1.33
9	e	102	BCL	O2D-CGD	-2.71	1.26	1.33
9	w	101	BCL	C5-C3	2.71	1.56	1.51
9	9	103	BCL	OBB-CAB	-2.70	1.17	1.23
10	y	402	BPH	CBD-CGD	-2.70	1.49	1.52
9	0	101	BCL	O2D-CGD	-2.70	1.26	1.33
9	AE	104	BCL	O1A-CGA	-2.70	1.14	1.22
9	D	102	BCL	O1A-CGA	-2.69	1.14	1.22
9	J	102	BCL	O1A-CGA	-2.69	1.14	1.22
9	J	102	BCL	C3D-C2D	-2.68	1.31	1.39
9	V	101	BCL	O1A-CGA	-2.68	1.14	1.22
9	L	301	BCL	C5-C3	2.67	1.56	1.51
9	Y	101	BCL	C3B-CAB	2.67	1.55	1.46
9	AE	104	BCL	O2A-CGA	-2.67	1.25	1.33
9	K	101	BCL	C1D-C2D	-2.67	1.40	1.45
9	z	102	BCL	C3B-CAB	2.67	1.55	1.46
9	m	103	BCL	C3C-C4C	2.67	1.55	1.51
9	e	102	BCL	O1A-CGA	-2.67	1.14	1.22
9	Z	102	BCL	OBB-CAB	-2.67	1.17	1.23
9	f	101	BCL	OBB-CAB	-2.67	1.17	1.23
7	C	503	HEM	CHC-C1C	2.66	1.43	1.38
9	i	102	BCL	C1D-C2D	-2.66	1.40	1.45
9	l	101	BCL	O1A-CGA	-2.66	1.14	1.22
9	i	102	BCL	O2D-CGD	-2.66	1.26	1.33
9	u	101	BCL	C1B-C2B	-2.65	1.36	1.43
9	k	102	BCL	O2A-CGA	-2.65	1.25	1.33
9	l	101	BCL	O2D-CGD	-2.65	1.26	1.33
14	y	403	MQ8	C32-C33	2.65	1.39	1.33
9	F	101	BCL	C3C-C4C	2.65	1.54	1.51
9	J	102	BCL	C1D-C2D	-2.65	1.40	1.45
9	l	101	BCL	O1A-CGA	-2.65	1.14	1.22
7	o	502	HEM	C1A-C2A	-2.65	1.39	1.44
9	h	101	BCL	O2A-CGA	-2.64	1.25	1.33
9	p	102	BCL	O1A-CGA	-2.64	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AE	102	BCL	C3B-CAB	2.64	1.55	1.46
9	A	102	BCL	C1D-C2D	-2.64	1.40	1.45
9	R	102	BCL	O1A-CGA	-2.63	1.14	1.22
9	F	101	BCL	O1A-CGA	-2.63	1.14	1.22
9	K	101	BCL	O2A-CGA	-2.63	1.25	1.33
9	F	101	BCL	OBB-CAB	-2.63	1.17	1.23
9	3	101	BCL	OBB-CAB	-2.62	1.17	1.23
7	o	504	HEM	C4A-NA	-2.62	1.34	1.39
9	s	102	BCL	C3B-CAB	2.62	1.54	1.46
9	F	101	BCL	O2D-CGD	-2.62	1.26	1.33
9	U	101	BCL	OBB-CAB	-2.62	1.17	1.23
9	7	101	BCL	O2A-CGA	-2.62	1.25	1.33
9	B	101	BCL	OBB-CAB	-2.62	1.17	1.23
9	AL	102	BCL	C1D-C2D	-2.62	1.40	1.45
9	X	102	BCL	C1D-C2D	-2.62	1.40	1.45
9	k	102	BCL	O1A-CGA	-2.62	1.14	1.22
9	AI	101	BCL	C1D-C2D	-2.62	1.40	1.45
9	O	101	BCL	OBB-CAB	-2.62	1.17	1.23
9	U	101	BCL	C5-C3	2.61	1.56	1.51
9	A	102	BCL	O1A-CGA	-2.61	1.14	1.22
9	8	102	BCL	OBB-CAB	-2.61	1.17	1.23
9	g	101	BCL	C1D-C2D	-2.61	1.40	1.45
9	B	101	BCL	O1A-CGA	-2.61	1.14	1.22
9	AH	101	BCL	C3B-CAB	2.61	1.54	1.46
9	X	102	BCL	OBB-CAB	-2.61	1.17	1.23
9	9	103	BCL	O2D-CGD	-2.60	1.26	1.33
9	N	102	BCL	O2D-CGD	-2.60	1.26	1.33
9	c	102	BCL	O1A-CGA	-2.60	1.14	1.22
12	p	101	PEF	O3-C30	2.60	1.45	1.33
9	5	102	BCL	O1A-CGA	-2.60	1.14	1.22
9	j	101	BCL	O1A-CGA	-2.60	1.14	1.22
9	9	103	BCL	O1A-CGA	-2.60	1.14	1.22
9	1	102	BCL	O2A-CGA	-2.60	1.25	1.33
9	P	101	BCL	C1B-C2B	-2.59	1.37	1.43
9	9	103	BCL	O2A-CGA	-2.59	1.25	1.33
9	h	101	BCL	C5-C3	2.59	1.56	1.51
9	AH	101	BCL	C1B-C2B	-2.59	1.37	1.43
9	K	101	BCL	C3B-CAB	2.59	1.54	1.46
9	R	102	BCL	OBB-CAB	-2.59	1.17	1.23
9	V	101	BCL	C3B-CAB	2.59	1.54	1.46
9	1	102	BCL	O1A-CGA	-2.59	1.14	1.22
9	R	102	BCL	O2D-CGD	-2.59	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCL	O2D-CGD	-2.59	1.26	1.33
9	W	101	BCL	O1A-CGA	-2.59	1.14	1.22
9	Q	101	BCL	C3B-CAB	2.58	1.54	1.46
9	f	101	BCL	O1A-CGA	-2.58	1.14	1.22
9	z	102	BCL	O2D-CGD	-2.58	1.26	1.33
9	9	103	BCL	C3C-C4C	2.58	1.54	1.51
9	d	101	BCL	C3C-C4C	2.58	1.54	1.51
9	i	102	BCL	C3B-CAB	2.58	1.54	1.46
9	L	301	BCL	O2A-CGA	-2.58	1.25	1.33
9	W	101	BCL	C3B-CAB	2.57	1.54	1.46
9	z	102	BCL	O1A-CGA	-2.57	1.14	1.22
9	m	102	BCL	O1A-CGA	-2.57	1.14	1.22
9	u	101	BCL	C3C-C4C	2.57	1.54	1.51
9	x	303	BCL	C1B-C2B	-2.57	1.37	1.43
9	AH	101	BCL	O1A-CGA	-2.56	1.14	1.22
9	L	303	BCL	OBB-CAB	-2.56	1.17	1.23
9	8	102	BCL	O2D-CGD	-2.56	1.26	1.33
9	AL	102	BCL	OBB-CAB	-2.56	1.17	1.23
9	S	102	BCL	C3B-CAB	2.56	1.54	1.46
9	M	401	BCL	O2D-CGD	-2.55	1.26	1.33
9	3	101	BCL	C5-C3	2.55	1.56	1.51
9	B	101	BCL	O2A-CGA	-2.55	1.25	1.33
9	e	102	BCL	C1B-C2B	-2.55	1.37	1.43
9	N	102	BCL	C3B-CAB	2.55	1.54	1.46
10	M	402	BPH	C2C-C3C	2.54	1.56	1.54
9	D	102	BCL	C1B-C2B	-2.54	1.37	1.43
9	i	102	BCL	O1A-CGA	-2.54	1.14	1.22
9	AI	101	BCL	OBB-CAB	-2.54	1.17	1.23
9	AK	101	BCL	O1A-CGA	-2.54	1.14	1.22
9	B	101	BCL	C1B-C2B	-2.53	1.37	1.43
9	W	101	BCL	O2A-CGA	-2.53	1.26	1.33
9	AL	102	BCL	C3D-C2D	-2.53	1.32	1.39
7	C	504	HEM	C4B-NB	-2.53	1.33	1.38
9	z	102	BCL	C1D-C2D	-2.53	1.40	1.45
14	M	403	MQ8	C42-C43	2.53	1.38	1.33
9	B	101	BCL	O2D-CGD	-2.53	1.27	1.33
9	AH	101	BCL	OBB-CAB	-2.53	1.17	1.23
9	D	102	BCL	C1D-C2D	-2.53	1.40	1.45
9	h	101	BCL	O1A-CGA	-2.52	1.15	1.22
9	p	104	BCL	C1D-C2D	-2.52	1.40	1.45
9	R	102	BCL	C3B-CAB	2.52	1.54	1.46
9	w	101	BCL	O2A-CGA	-2.52	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	m	103	BCL	C3D-CAD	2.52	1.53	1.45
9	O	101	BCL	C1D-C2D	-2.52	1.40	1.45
9	AJ	102	BCL	C1D-C2D	-2.51	1.40	1.45
12	H	303	PEF	O3-C30	2.51	1.45	1.33
9	k	102	BCL	OBB-CAB	-2.51	1.17	1.23
9	m	102	BCL	C3C-C4C	2.51	1.54	1.51
9	7	101	BCL	O1A-CGA	-2.51	1.15	1.22
9	v	102	BCL	C3B-CAB	2.51	1.54	1.46
9	T	102	BCL	OBB-CAB	-2.50	1.17	1.23
9	O	101	BCL	C1B-C2B	-2.50	1.37	1.43
9	h	101	BCL	OBB-CAB	-2.50	1.17	1.23
9	1	102	BCL	C1B-C2B	-2.50	1.37	1.43
9	Q	101	BCL	C3C-C4C	2.50	1.54	1.51
9	x	303	BCL	C4B-NB	-2.50	1.34	1.37
9	AK	101	BCL	C1B-C2B	-2.49	1.37	1.43
9	p	104	BCL	OBB-CAB	-2.49	1.17	1.23
9	Q	101	BCL	O1A-CGA	-2.48	1.15	1.22
9	x	305	BCL	C3D-C4D	-2.48	1.38	1.44
9	W	101	BCL	C1D-C2D	-2.48	1.40	1.45
9	1	102	BCL	C3C-C4C	2.48	1.54	1.51
9	AL	102	BCL	O1A-CGA	-2.47	1.15	1.22
9	v	102	BCL	O1A-CGA	-2.47	1.15	1.22
9	u	101	BCL	O2A-CGA	-2.47	1.26	1.33
9	1	102	BCL	O2D-CGD	-2.47	1.27	1.33
9	AE	104	BCL	C1B-C2B	-2.47	1.37	1.43
9	D	101	BCL	C1B-C2B	-2.47	1.37	1.43
9	x	301	BCL	C3B-C4B	2.46	1.46	1.41
9	L	303	BCL	C3B-C2B	-2.46	1.34	1.42
9	Q	101	BCL	C1D-C2D	-2.46	1.40	1.45
9	F	101	BCL	C1B-C2B	-2.46	1.37	1.43
9	AI	101	BCL	O2A-CGA	-2.46	1.26	1.33
9	d	101	BCL	C3B-CAB	2.46	1.54	1.46
9	G	102	BCL	C1D-C2D	-2.46	1.40	1.45
9	7	101	BCL	C1D-C2D	-2.46	1.40	1.45
9	AB	101	BCL	OBB-CAB	-2.45	1.17	1.23
9	U	101	BCL	C3B-CAB	2.44	1.54	1.46
9	j	101	BCL	C3B-CAB	2.44	1.54	1.46
9	x	305	BCL	O2A-CGA	-2.44	1.26	1.33
9	s	102	BCL	C3C-C4C	2.44	1.54	1.51
9	m	103	BCL	OBB-CAB	-2.44	1.17	1.23
9	m	103	BCL	C3B-CAB	2.44	1.54	1.46
9	P	101	BCL	OBB-CAB	-2.44	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	101	BCL	C1B-C2B	-2.44	1.37	1.43
9	AK	101	BCL	OBB-CAB	-2.43	1.17	1.23
9	AE	104	BCL	O2D-CGD	-2.43	1.27	1.33
9	x	303	BCL	C2C-C3C	-2.43	1.47	1.54
9	D	101	BCL	C1D-C2D	-2.43	1.40	1.45
9	D	102	BCL	OBB-CAB	-2.43	1.17	1.23
9	j	101	BCL	OBB-CAB	-2.43	1.17	1.23
9	x	305	BCL	O2D-CGD	-2.43	1.27	1.33
9	r	101	BCL	C1B-C2B	-2.43	1.37	1.43
9	Z	102	BCL	C3B-C2B	-2.42	1.34	1.42
9	S	102	BCL	C3C-C4C	2.42	1.54	1.51
9	f	101	BCL	O2A-CGA	-2.42	1.26	1.33
9	0	101	BCL	OBB-CAB	-2.42	1.17	1.23
7	o	504	HEM	C1D-ND	-2.42	1.34	1.38
9	Q	101	BCL	O2A-CGA	-2.41	1.26	1.33
9	8	102	BCL	C1B-C2B	-2.41	1.37	1.43
9	7	101	BCL	C3C-C4C	2.41	1.54	1.51
9	f	101	BCL	C3C-C4C	2.41	1.54	1.51
9	w	101	BCL	C1B-C2B	-2.41	1.37	1.43
9	l	101	BCL	C1B-C2B	-2.41	1.37	1.43
9	c	102	BCL	C1D-C2D	-2.40	1.40	1.45
9	G	102	BCL	C3B-CAB	2.40	1.54	1.46
7	o	503	HEM	CHC-C1C	2.40	1.43	1.38
9	w	101	BCL	C3B-CAB	2.40	1.54	1.46
9	AH	103	BCL	C3C-C4C	2.40	1.54	1.51
9	AL	102	BCL	C5-C3	2.40	1.56	1.51
9	j	101	BCL	C1B-C2B	-2.40	1.37	1.43
9	AJ	102	BCL	C3B-CAB	2.40	1.54	1.46
9	J	102	BCL	C3D-C4D	-2.40	1.38	1.44
9	d	101	BCL	O1A-CGA	-2.39	1.15	1.22
9	M	401	BCL	C1D-ND	2.39	1.41	1.37
9	AB	101	BCL	C1B-C2B	-2.39	1.37	1.43
9	L	303	BCL	C1B-C2B	-2.39	1.37	1.43
9	G	102	BCL	C1B-C2B	-2.39	1.37	1.43
9	Z	102	BCL	C3B-CAB	2.39	1.54	1.46
9	I	101	BCL	OBB-CAB	-2.39	1.17	1.23
9	l	101	BCL	OBB-CAB	-2.38	1.17	1.23
9	i	102	BCL	C5-C3	2.38	1.56	1.51
11	L	304	UQ8	C23-C24	2.38	1.38	1.33
9	AJ	102	BCL	C1B-C2B	-2.38	1.37	1.43
9	k	102	BCL	C3B-CAB	2.38	1.54	1.46
9	A	102	BCL	C3B-CAB	2.38	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	101	BCL	C3B-CAB	2.38	1.54	1.46
9	s	102	BCL	C1B-C2B	-2.38	1.37	1.43
9	1	102	BCL	OBB-CAB	-2.38	1.17	1.23
9	x	305	BCL	C3B-CAB	2.37	1.54	1.46
9	I	101	BCL	C3B-CAB	2.37	1.54	1.46
9	7	101	BCL	C3B-CAB	2.37	1.54	1.46
9	0	101	BCL	C5-C3	2.37	1.56	1.51
9	z	102	BCL	OBB-CAB	-2.37	1.17	1.23
9	AL	102	BCL	C1B-C2B	-2.37	1.37	1.43
9	0	101	BCL	C3B-CAB	2.37	1.54	1.46
9	Z	102	BCL	C1B-C2B	-2.37	1.37	1.43
9	F	101	BCL	O2A-CGA	-2.37	1.26	1.33
9	AA	101	BCL	C3B-CAB	2.37	1.54	1.46
10	M	402	BPH	C4A-C3A	2.36	1.56	1.51
9	p	102	BCL	OBB-CAB	-2.36	1.17	1.23
15	k	101	CRT	C4-C5	2.36	1.53	1.50
9	AI	101	BCL	C3B-CAB	2.36	1.54	1.46
9	AL	102	BCL	C3B-CAB	2.36	1.54	1.46
9	N	102	BCL	OBB-CAB	-2.36	1.17	1.23
9	AD	101	BCL	C3B-CAB	2.36	1.54	1.46
9	u	101	BCL	O1A-CGA	-2.35	1.15	1.22
9	3	101	BCL	C2C-C3C	-2.35	1.48	1.54
9	P	101	BCL	C1D-C2D	-2.35	1.40	1.45
9	O	101	BCL	O2D-CGD	-2.35	1.27	1.33
9	x	301	BCL	C1B-C2B	-2.35	1.37	1.43
9	AE	104	BCL	OBB-CAB	-2.35	1.17	1.23
9	s	102	BCL	OBB-CAB	-2.35	1.17	1.23
9	Z	102	BCL	C5-C3	2.34	1.56	1.51
9	x	301	BCL	O2A-CGA	-2.34	1.26	1.33
9	V	101	BCL	C1D-C2D	-2.34	1.40	1.45
7	C	501	HEM	C1D-ND	-2.34	1.34	1.38
9	N	102	BCL	C3D-C2D	-2.34	1.32	1.39
7	o	504	HEM	FE-ND	-2.34	1.87	1.94
10	M	402	BPH	O2D-CGD	2.34	1.39	1.33
9	c	102	BCL	OBB-CAB	-2.34	1.17	1.23
9	3	101	BCL	O2D-CGD	-2.33	1.27	1.33
9	x	301	BCL	CHC-C1C	2.33	1.43	1.37
9	5	101	BCL	C1D-C2D	-2.33	1.40	1.45
9	y	401	BCL	C1B-C2B	-2.33	1.37	1.43
7	C	503	HEM	C1C-NC	-2.33	1.35	1.39
9	I	101	BCL	C5-C3	2.33	1.56	1.51
9	AE	104	BCL	C1D-C2D	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	101	BCL	C3B-CAB	2.33	1.54	1.46
9	V	101	BCL	OBB-CAB	-2.32	1.18	1.23
9	d	101	BCL	OBB-CAB	-2.32	1.18	1.23
9	w	101	BCL	C1D-C2D	-2.32	1.40	1.45
9	7	101	BCL	OBB-CAB	-2.32	1.18	1.23
7	C	502	HEM	FE-ND	-2.32	1.87	1.94
9	7	101	BCL	O2D-CGD	-2.32	1.27	1.33
9	V	101	BCL	C5-C3	2.32	1.56	1.51
9	p	104	BCL	C3C-C4C	2.31	1.54	1.51
9	m	102	BCL	C1D-C2D	-2.31	1.40	1.45
7	C	501	HEM	C1C-C2C	-2.31	1.40	1.45
9	V	101	BCL	C1B-C2B	-2.31	1.37	1.43
9	D	101	BCL	OBB-CAB	-2.31	1.18	1.23
9	AE	104	BCL	C3B-CAB	2.31	1.54	1.46
9	AD	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	m	103	BCL	C5-C3	2.30	1.56	1.51
9	AC	102	BCL	C1B-C2B	-2.30	1.37	1.43
9	x	301	BCL	C3D-C2D	-2.30	1.32	1.39
9	AC	102	BCL	C5-C3	2.29	1.56	1.51
9	4	102	BCL	C1D-C2D	-2.29	1.40	1.45
9	AI	101	BCL	C1B-C2B	-2.29	1.37	1.43
9	T	102	BCL	C1D-C2D	-2.29	1.40	1.45
9	0	101	BCL	C3C-C4C	2.29	1.54	1.51
9	AH	103	BCL	C1D-C2D	-2.29	1.40	1.45
9	M	401	BCL	C5-C3	2.29	1.56	1.51
9	AJ	102	BCL	O2D-CGD	-2.29	1.27	1.33
9	c	102	BCL	C3B-CAB	2.29	1.53	1.46
9	J	102	BCL	C3C-C4C	2.29	1.54	1.51
9	d	101	BCL	C1D-C2D	-2.29	1.40	1.45
9	g	101	BCL	OBB-CAB	-2.29	1.18	1.23
9	AH	103	BCL	OBB-CAB	-2.28	1.18	1.23
9	L	305	BCL	C1D-C2D	-2.28	1.40	1.45
9	F	101	BCL	C1D-C2D	-2.28	1.40	1.45
9	AC	102	BCL	OBB-CAB	-2.28	1.18	1.23
9	M	401	BCL	C2A-C1A	2.28	1.57	1.52
9	x	305	BCL	C3B-C2B	-2.28	1.34	1.42
9	w	101	BCL	C3C-C4C	2.28	1.54	1.51
7	o	504	HEM	C4B-NB	-2.27	1.34	1.38
9	S	102	BCL	C1D-C2D	-2.27	1.40	1.45
9	AD	101	BCL	OBB-CAB	-2.27	1.18	1.23
9	K	101	BCL	C5-C3	2.27	1.56	1.51
9	X	102	BCL	C3B-CAB	2.27	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	102	BCL	C3B-CAB	2.27	1.53	1.46
9	x	301	BCL	O1A-CGA	-2.27	1.15	1.22
9	x	305	BCL	C2C-C3C	-2.27	1.48	1.54
9	r	101	BCL	C3B-CAB	2.26	1.53	1.46
9	L	303	BCL	C3D-C4D	-2.26	1.39	1.44
9	N	102	BCL	C1D-C2D	-2.26	1.40	1.45
9	D	101	BCL	C3B-C2B	-2.26	1.34	1.42
9	AA	101	BCL	C5-C3	2.26	1.55	1.51
9	5	101	BCL	C2C-C3C	-2.26	1.48	1.54
9	AB	101	BCL	C3B-CAB	2.25	1.53	1.46
9	x	301	BCL	C3B-C2B	-2.25	1.34	1.42
9	Q	101	BCL	OBB-CAB	-2.25	1.18	1.23
9	AL	102	BCL	C3D-C4D	-2.25	1.39	1.44
9	L	301	BCL	C3A-C2A	2.25	1.60	1.54
9	f	101	BCL	C3D-C4D	-2.25	1.39	1.44
9	AL	102	BCL	C3B-C2B	-2.24	1.34	1.42
9	u	101	BCL	C3B-C2B	-2.24	1.34	1.42
9	0	101	BCL	C1B-C2B	-2.24	1.37	1.43
9	1	102	BCL	C5-C3	2.24	1.55	1.51
9	r	101	BCL	C5-C3	2.24	1.55	1.51
9	F	101	BCL	C3B-CAB	2.24	1.53	1.46
9	AK	101	BCL	C3B-CAB	2.24	1.53	1.46
9	M	401	BCL	C1B-C2B	-2.24	1.37	1.43
9	5	101	BCL	C1B-C2B	-2.24	1.37	1.43
9	7	101	BCL	C3B-C2B	-2.24	1.34	1.42
9	AC	102	BCL	C3B-CAB	2.23	1.53	1.46
9	e	102	BCL	C5-C3	2.23	1.55	1.51
11	L	304	UQ8	C42-C43	2.23	1.57	1.50
9	AJ	102	BCL	C5-C3	2.23	1.55	1.51
9	R	102	BCL	C1B-C2B	-2.23	1.37	1.43
9	Y	101	BCL	C1B-NB	-2.23	1.34	1.37
14	y	403	MQ8	C42-C43	2.23	1.38	1.33
9	y	401	BCL	C4B-NB	-2.23	1.34	1.37
9	AA	101	BCL	OBB-CAB	-2.23	1.18	1.23
9	p	102	BCL	C3B-CAB	2.22	1.53	1.46
9	1	102	BCL	C3B-C2B	-2.22	1.35	1.42
7	o	504	HEM	C1C-C2C	-2.22	1.40	1.45
9	k	102	BCL	C1D-C2D	-2.22	1.40	1.45
9	N	102	BCL	C1B-C2B	-2.22	1.37	1.43
9	P	101	BCL	C3B-CAB	2.22	1.53	1.46
9	p	102	BCL	C3D-C4D	-2.22	1.39	1.44
9	5	102	BCL	C2A-C1A	2.21	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AC	102	BCL	C1D-C2D	-2.21	1.41	1.45
9	9	103	BCL	C3D-C2D	-2.21	1.33	1.39
9	u	101	BCL	C1D-C2D	-2.21	1.41	1.45
9	c	102	BCL	C1B-C2B	-2.21	1.37	1.43
9	3	101	BCL	C3C-C4C	2.21	1.54	1.51
9	U	101	BCL	C1D-C2D	-2.20	1.41	1.45
9	V	101	BCL	C3C-C4C	2.20	1.54	1.51
9	AA	101	BCL	C1D-C2D	-2.20	1.41	1.45
9	h	101	BCL	C3B-C2B	-2.20	1.35	1.42
9	7	101	BCL	C1B-C2B	-2.20	1.38	1.43
9	z	102	BCL	C3D-C4D	-2.20	1.39	1.44
9	z	102	BCL	C3D-C2D	-2.19	1.33	1.39
9	8	102	BCL	C3B-C2B	-2.19	1.35	1.42
9	AE	102	BCL	OBB-CAB	-2.19	1.18	1.23
9	p	102	BCL	C1B-C2B	-2.19	1.38	1.43
14	y	403	MQ8	C17-C18	2.19	1.38	1.33
9	D	102	BCL	C3B-CAB	2.18	1.53	1.46
9	x	301	BCL	C3D-C4D	-2.18	1.39	1.44
9	8	102	BCL	C3B-CAB	2.18	1.53	1.46
9	AI	101	BCL	C5-C3	2.18	1.55	1.51
9	AE	102	BCL	C1D-C2D	-2.18	1.41	1.45
9	AE	104	BCL	C2C-C3C	-2.18	1.48	1.54
9	P	101	BCL	C5-C3	2.18	1.55	1.51
9	5	102	BCL	C1B-C2B	-2.17	1.38	1.43
9	AJ	102	BCL	OBB-CAB	-2.17	1.18	1.23
9	O	101	BCL	C3B-CAB	2.17	1.53	1.46
14	M	403	MQ8	C17-C18	2.17	1.38	1.33
9	p	104	BCL	C3B-C2B	-2.16	1.35	1.42
12	H	301	PEF	O3-C30	2.16	1.43	1.33
9	I	101	BCL	C1B-C2B	-2.16	1.38	1.43
9	N	102	BCL	C3D-C4D	-2.16	1.39	1.44
9	u	101	BCL	C3B-CAB	2.16	1.53	1.46
9	P	101	BCL	C3D-C4D	-2.16	1.39	1.44
7	C	502	HEM	C1C-C2C	-2.16	1.41	1.45
9	A	102	BCL	OBB-CAB	-2.16	1.18	1.23
7	C	504	HEM	C1A-C2A	-2.16	1.40	1.44
9	9	103	BCL	C3D-C4D	-2.16	1.39	1.44
9	g	101	BCL	C5-C3	2.16	1.55	1.51
9	v	102	BCL	C1B-C2B	-2.15	1.38	1.43
9	G	102	BCL	OBB-CAB	-2.15	1.18	1.23
9	S	102	BCL	C3D-C4D	-2.15	1.39	1.44
9	x	301	BCL	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	301	BCL	C1B-C2B	-2.15	1.38	1.43
9	g	101	BCL	C1B-C2B	-2.15	1.38	1.43
9	x	303	BCL	OBB-CAB	-2.15	1.18	1.23
9	3	101	BCL	C3D-C4D	-2.15	1.39	1.44
9	8	102	BCL	C1D-C2D	-2.15	1.41	1.45
9	AJ	102	BCL	C3D-C4D	-2.14	1.39	1.44
9	v	102	BCL	OBB-CAB	-2.14	1.18	1.23
9	T	102	BCL	C5-C3	2.14	1.55	1.51
9	h	101	BCL	C1D-C2D	-2.14	1.41	1.45
9	w	101	BCL	OBB-CAB	-2.14	1.18	1.23
9	9	103	BCL	C1B-C2B	-2.13	1.38	1.43
9	4	102	BCL	C3D-C4D	-2.13	1.39	1.44
9	y	401	BCL	C3B-C2B	-2.13	1.35	1.42
15	f	102	CRT	C4-C5	2.13	1.53	1.50
9	5	102	BCL	C3B-C2B	-2.13	1.35	1.42
9	S	102	BCL	C1B-C2B	-2.13	1.38	1.43
9	y	401	BCL	C2C-C3C	-2.13	1.48	1.54
9	4	102	BCL	C3B-C2B	-2.13	1.35	1.42
14	M	403	MQ8	C27-C28	2.13	1.38	1.33
11	L	304	UQ8	O5-C5	2.13	1.28	1.23
9	x	303	BCL	C3B-CAB	2.13	1.53	1.46
7	C	503	HEM	C1D-ND	-2.13	1.34	1.38
9	L	303	BCL	C1D-C2D	-2.13	1.41	1.45
10	M	402	BPH	C3B-C4B	2.13	1.44	1.41
9	M	401	BCL	C4B-NB	-2.12	1.35	1.37
9	Y	101	BCL	C1B-C2B	-2.12	1.38	1.43
14	M	403	MQ8	C37-C38	2.12	1.37	1.33
9	U	101	BCL	C1B-C2B	-2.12	1.38	1.43
9	m	103	BCL	C1D-C2D	-2.12	1.41	1.45
9	W	101	BCL	C3B-C2B	-2.12	1.35	1.42
15	8	101	CRT	C4-C5	2.12	1.53	1.50
9	k	102	BCL	C5-C3	2.12	1.55	1.51
9	F	101	BCL	C3D-C4D	-2.11	1.39	1.44
9	1	101	BCL	C3B-C2B	-2.11	1.35	1.42
9	x	301	BCL	C3A-C2A	2.11	1.60	1.54
14	M	403	MQ8	C32-C33	2.10	1.37	1.33
9	T	102	BCL	C1B-C2B	-2.10	1.38	1.43
9	4	102	BCL	CHC-C4B	-2.10	1.34	1.39
9	AB	101	BCL	C5-C3	2.10	1.55	1.51
9	K	101	BCL	OBB-CAB	-2.10	1.18	1.23
9	L	301	BCL	C3D-C2D	-2.09	1.33	1.39
9	l	101	BCL	C2C-C3C	-2.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCL	C3B-C2B	-2.09	1.35	1.42
9	w	101	BCL	C3D-C2D	-2.09	1.33	1.39
10	y	402	BPH	C3D-CAD	-2.09	1.43	1.47
7	C	503	HEM	C2A-C3A	-2.09	1.33	1.38
9	L	301	BCL	C3B-C2B	-2.09	1.35	1.42
9	L	303	BCL	O1A-CGA	-2.08	1.16	1.22
9	L	305	BCL	C1B-C2B	-2.08	1.38	1.43
9	I	101	BCL	C3D-C4D	-2.08	1.39	1.44
9	J	102	BCL	C5-C3	2.08	1.55	1.51
9	f	101	BCL	C1-C2	2.08	1.55	1.49
9	i	102	BCL	OBB-CAB	-2.08	1.18	1.23
9	9	103	BCL	C3B-C2B	-2.08	1.35	1.42
9	T	102	BCL	C2C-C3C	-2.08	1.48	1.54
9	F	101	BCL	C5-C3	2.08	1.55	1.51
9	m	103	BCL	C1B-C2B	-2.07	1.38	1.43
9	3	101	BCL	C3B-C2B	-2.07	1.35	1.42
15	y	404	CRT	C25-C23	2.07	1.50	1.46
9	F	101	BCL	C3B-C2B	-2.07	1.35	1.42
9	AJ	102	BCL	C2C-C3C	-2.07	1.48	1.54
9	v	102	BCL	C5-C3	2.07	1.55	1.51
9	v	102	BCL	C3C-C4C	2.07	1.54	1.51
7	o	504	HEM	C4D-C3D	2.07	1.48	1.45
7	o	502	HEM	C4D-C3D	2.07	1.48	1.45
9	l	101	BCL	C1D-C2D	-2.07	1.41	1.45
9	h	101	BCL	C3B-CAB	2.06	1.53	1.46
9	9	103	BCL	C1D-C2D	-2.06	1.41	1.45
9	M	401	BCL	C3B-C2B	-2.06	1.35	1.42
9	L	303	BCL	C6-C5	2.06	1.59	1.52
9	Y	101	BCL	C3B-C2B	-2.06	1.35	1.42
9	d	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	r	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	m	102	BCL	C2C-C3C	-2.06	1.48	1.54
9	K	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	l	101	BCL	C3D-C2D	-2.05	1.33	1.39
9	Q	101	BCL	C1B-C2B	-2.05	1.38	1.43
15	y	404	CRT	C4-C1	2.05	1.56	1.52
12	y	408	PEF	C1-C2	2.05	1.57	1.50
9	f	101	BCL	C1A-CHA	-2.04	1.34	1.43
9	J	102	BCL	O2D-CGD	-2.04	1.28	1.33
9	9	103	BCL	C2C-C3C	-2.04	1.49	1.54
9	AB	101	BCL	C3C-C4C	2.03	1.54	1.51
9	T	102	BCL	C3B-CAB	2.03	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	h	101	BCL	C2C-C3C	-2.03	1.49	1.54
11	L	304	UQ8	C43-C44	2.03	1.38	1.32
9	AI	101	BCL	C2C-C3C	-2.03	1.49	1.54
14	y	403	MQ8	C6-C5	2.03	1.43	1.39
9	5	102	BCL	O2D-CGD	-2.03	1.28	1.33
9	W	101	BCL	OBB-CAB	-2.03	1.18	1.23
9	G	102	BCL	C5-C3	2.03	1.55	1.51
9	h	101	BCL	CHB-C1B	2.03	1.44	1.39
9	D	101	BCL	C3B-CAB	2.02	1.53	1.46
9	p	104	BCL	C3B-CAB	2.02	1.53	1.46
9	A	102	BCL	C2C-C3C	-2.02	1.49	1.54
9	X	102	BCL	C1B-C2B	-2.02	1.38	1.43
7	C	503	HEM	C4B-NB	-2.02	1.34	1.38
9	B	101	BCL	C3D-C2D	-2.02	1.33	1.39
9	r	101	BCL	OBB-CAB	-2.02	1.18	1.23
9	K	101	BCL	C3C-C4C	2.02	1.54	1.51
9	B	101	BCL	C3B-CAB	2.02	1.53	1.46
9	L	303	BCL	O2A-C1	2.01	1.51	1.46
9	K	101	BCL	C3D-C2D	-2.01	1.33	1.39
9	K	101	BCL	C1B-C2B	-2.01	1.38	1.43
9	u	101	BCL	OBB-CAB	-2.01	1.18	1.23
11	x	304	UQ8	C43-C44	2.01	1.38	1.32
9	AH	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	y	401	BCL	C2A-C1A	2.01	1.56	1.52
9	m	102	BCL	OBB-CAB	-2.01	1.18	1.23
9	O	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	p	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	J	102	BCL	C1B-C2B	-2.01	1.38	1.43
9	5	101	BCL	C5-C3	2.01	1.55	1.51
9	U	101	BCL	C3B-C2B	-2.00	1.35	1.42
9	AB	101	BCL	C2C-C3C	-2.00	1.49	1.54
9	AE	102	BCL	C5-C3	2.00	1.55	1.51
9	AC	102	BCL	C2C-C3C	-2.00	1.49	1.54
9	5	102	BCL	C3D-C4D	-2.00	1.39	1.44
9	M	401	BCL	C3D-CAD	2.00	1.52	1.45
9	B	101	BCL	C3D-C4D	-2.00	1.39	1.44
9	u	101	BCL	C2C-C3C	-2.00	1.49	1.54
17	AE	101	PGW	O03-C19	2.00	1.43	1.33

All (2870) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	x	301	BCL	C4A-NA-C1A	10.75	111.58	106.68
15	s	101	CRT	C37-C36-C35	-9.29	111.87	124.91
15	f	102	CRT	C31-C32-C33	-9.15	114.45	127.28
15	AJ	101	CRT	C37-C36-C35	-8.68	112.72	124.91
15	y	404	CRT	C37-C36-C35	-8.43	113.07	124.91
7	C	504	HEM	CHD-C4C-NC	8.41	133.61	124.45
15	J	101	CRT	C37-C36-C35	-8.29	113.28	124.91
15	N	101	CRT	C37-C36-C35	-7.90	113.82	124.91
15	p	103	CRT	C37-C36-C35	-7.89	113.84	124.91
15	T	101	CRT	C3-C1-C2	7.85	124.78	110.43
7	o	504	HEM	CHD-C4C-NC	7.74	132.88	124.45
10	x	302	BPH	O2D-CGD-CBD	7.72	119.42	110.95
9	5	102	BCL	O2D-CGD-CBD	7.46	124.27	111.23
7	C	502	HEM	CHC-C4B-NB	7.44	132.43	124.42
15	v	101	CRT	C21-C22-C23	-7.37	116.95	127.28
15	G	101	CRT	C37-C36-C35	-7.05	115.01	124.91
7	C	503	HEM	C3B-C4B-NB	-7.00	104.44	109.47
15	N	101	CRT	C21-C22-C23	-6.96	117.52	127.28
15	N	101	CRT	C4-C5-C6	-6.78	115.39	124.91
15	J	101	CRT	C21-C22-C23	-6.77	117.78	127.28
15	A	103	CRT	C37-C36-C35	-6.72	115.48	124.91
9	4	102	BCL	O2D-CGD-CBD	6.68	122.91	111.23
9	AJ	102	BCL	O2D-CGD-CBD	6.66	122.87	111.23
9	L	303	BCL	C1-O2A-CGA	6.63	132.70	116.65
10	M	402	BPH	O2D-CGD-CBD	6.63	118.23	110.95
9	x	305	BCL	C4D-CHA-C1A	6.58	129.10	121.24
15	T	101	CRT	C37-C36-C35	-6.56	115.70	124.91
15	AE	103	CRT	C37-C36-C35	-6.56	115.70	124.91
15	AC	101	CRT	C37-C36-C35	-6.54	115.72	124.91
9	s	102	BCL	O2D-CGD-CBD	6.52	122.63	111.23
15	N	101	CRT	C3-C1-C2	6.50	122.31	110.43
15	U	102	CRT	C4-C5-C6	-6.50	115.79	124.91
15	J	101	CRT	C3-C1-C2	6.48	122.27	110.43
12	M	408	PEF	C2-O2-C10	-6.45	106.46	117.85
7	o	502	HEM	CHC-C4B-NB	6.44	131.36	124.42
15	AH	102	CRT	C3-C1-C2	6.44	122.20	110.43
15	v	101	CRT	C3-C1-C2	6.43	122.18	110.43
7	C	502	HEM	C1B-NB-C4B	6.41	112.80	105.21
15	AD	102	CRT	C3-C1-C2	6.41	122.14	110.43
15	9	102	CRT	C21-C22-C23	-6.40	118.31	127.28
12	M	406	PEF	O2-C10-C11	6.40	122.50	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	U	102	CRT	C37-C36-C35	-6.34	116.00	124.91
15	X	101	CRT	C10-C9-C7	-6.34	118.38	127.28
15	M	404	CRT	C4-C5-C6	-6.31	116.05	124.91
9	M	401	BCL	O2D-CGD-CBD	6.29	122.23	111.23
9	R	102	BCL	C1D-ND-C4D	-6.28	101.90	106.31
15	R	101	CRT	C37-C36-C35	-6.27	116.10	124.91
15	v	101	CRT	C5-C6-C7	6.26	135.36	125.89
9	v	102	BCL	C1C-NC-C4C	-6.26	103.82	106.68
9	AE	102	BCL	C1D-ND-C4D	-6.26	101.92	106.31
9	AL	102	BCL	C1D-ND-C4D	-6.23	101.94	106.31
7	C	503	HEM	CHD-C4C-NC	6.22	131.23	124.45
9	AH	103	BCL	C1D-ND-C4D	-6.21	101.96	106.31
9	v	102	BCL	C4A-NA-C1A	6.21	109.51	106.68
15	f	102	CRT	C3-C1-C2	6.20	121.76	110.43
15	AE	103	CRT	C21-C22-C23	-6.19	118.59	127.28
9	x	301	BCL	O2D-CGD-CBD	6.16	122.00	111.23
9	Z	102	BCL	O2D-CGD-O1D	-6.14	111.89	123.85
9	f	101	BCL	O2D-CGD-CBD	6.14	121.97	111.23
9	g	101	BCL	O2D-CGD-CBD	6.14	121.96	111.23
9	x	303	BCL	C2C-C3C-C4C	-6.12	92.17	101.34
15	c	101	CRT	C37-C36-C35	-6.12	116.32	124.91
7	C	501	HEM	CHC-C4B-NB	6.12	131.01	124.42
9	J	102	BCL	C1D-ND-C4D	-6.12	102.02	106.31
15	AH	102	CRT	C37-C36-C35	-6.10	116.35	124.91
15	p	103	CRT	C3-C1-C2	6.10	121.57	110.43
15	4	101	CRT	C3-C1-C2	6.09	121.56	110.43
9	B	101	BCL	C1D-ND-C4D	-6.08	102.04	106.31
9	i	102	BCL	C1D-ND-C4D	-6.06	102.06	106.31
9	AL	102	BCL	O2D-CGD-CBD	6.06	121.82	111.23
9	x	305	BCL	O2D-CGD-CBD	6.05	121.81	111.23
15	G	101	CRT	C21-C22-C23	-6.04	118.80	127.28
15	A	103	CRT	C3-C1-C2	6.03	121.46	110.43
9	1	101	BCL	O2D-CGD-CBD	6.02	121.75	111.23
9	L	303	BCL	CMA-C3A-C4A	-6.01	95.62	111.77
9	T	102	BCL	C1D-ND-C4D	-6.00	102.10	106.31
15	9	102	CRT	C37-C36-C35	-6.00	116.49	124.91
15	n	101	CRT	C3-C1-C2	5.98	121.36	110.43
9	AE	104	BCL	O2D-CGD-CBD	5.94	121.62	111.23
9	Z	102	BCL	O2D-CGD-CBD	5.93	121.59	111.23
9	m	102	BCL	C1D-ND-C4D	-5.92	102.16	106.31
9	Q	101	BCL	C1C-NC-C4C	-5.92	103.98	106.68
15	v	101	CRT	C37-C36-C35	-5.91	116.61	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BCL	C1D-ND-C4D	-5.90	102.17	106.31
9	D	102	BCL	O2D-CGD-CBD	5.90	121.55	111.23
9	L	305	BCL	O2D-CGD-CBD	5.89	121.52	111.23
9	z	102	BCL	O2D-CGD-CBD	5.89	121.52	111.23
15	M	404	CRT	C10-C9-C7	-5.89	119.02	127.28
7	C	501	HEM	CHD-C1D-ND	5.88	130.75	124.42
9	AC	102	BCL	C1D-ND-C4D	-5.87	102.19	106.31
12	y	406	PEF	O2-C10-C11	5.87	121.56	111.09
15	8	101	CRT	C3-C1-C2	5.87	121.15	110.43
15	4	101	CRT	C36-C35-C33	-5.85	117.06	125.89
9	A	102	BCL	C1D-ND-C4D	-5.84	102.21	106.31
9	AJ	102	BCL	O2D-CGD-O1D	-5.84	112.48	123.85
9	9	103	BCL	O2D-CGD-CBD	5.84	121.43	111.23
15	Z	101	CRT	C37-C36-C35	-5.83	116.73	124.91
15	y	404	CRT	C3-C1-C2	5.82	121.07	110.43
9	d	101	BCL	O2D-CGD-CBD	5.82	121.40	111.23
9	7	101	BCL	C1D-ND-C4D	-5.80	102.24	106.31
9	A	102	BCL	O2D-CGD-CBD	5.80	121.37	111.23
9	S	102	BCL	O2D-CGD-CBD	5.80	121.37	111.23
15	E	101	CRT	C37-C36-C35	-5.80	116.77	124.91
9	5	102	BCL	O2D-CGD-O1D	-5.79	112.57	123.85
9	h	101	BCL	O2D-CGD-CBD	5.79	121.36	111.23
9	L	301	BCL	C4A-NA-C1A	5.79	109.32	106.68
9	i	102	BCL	O2D-CGD-CBD	5.78	121.33	111.23
9	O	101	BCL	CMB-C2B-C1B	-5.78	116.62	125.42
9	J	102	BCL	O2D-CGD-CBD	5.77	121.31	111.23
9	Y	101	BCL	O2D-CGD-CBD	5.76	121.31	111.23
9	G	102	BCL	C4A-NA-C1A	5.76	109.31	106.68
12	t	303	PEF	O2-C10-C11	5.75	121.35	111.09
9	M	401	BCL	O2D-CGD-O1D	-5.75	112.66	123.85
12	H	304	PEF	O2-C10-C11	5.73	121.32	111.09
9	8	102	BCL	O2D-CGD-CBD	5.72	121.23	111.23
9	1	102	BCL	O2D-CGD-CBD	5.72	121.22	111.23
15	6	101	CRT	C37-C36-C35	-5.72	116.89	124.91
9	I	101	BCL	C4D-CHA-C1A	5.70	128.05	121.24
15	k	101	CRT	C3-C1-C2	5.70	120.85	110.43
15	P	102	CRT	C37-C36-C35	-5.70	116.91	124.91
9	AH	101	BCL	CMB-C2B-C1B	-5.70	116.74	125.42
7	o	502	HEM	C1B-NB-C4B	5.66	111.91	105.21
9	N	102	BCL	C1D-ND-C4D	-5.66	102.34	106.31
9	j	101	BCL	C1D-ND-C4D	-5.65	102.35	106.31
9	l	101	BCL	C1D-ND-C4D	-5.64	102.35	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	102	BCL	C1D-ND-C4D	-5.63	102.36	106.31
9	u	101	BCL	C1D-ND-C4D	-5.62	102.37	106.31
15	M	404	CRT	C37-C36-C35	-5.61	117.03	124.91
9	1	101	BCL	C1D-ND-C4D	-5.61	102.38	106.31
15	6	101	CRT	C26-C27-C28	-5.61	119.41	127.28
12	y	408	PEF	C3-O3-C30	5.57	130.82	117.08
9	d	101	BCL	O2D-CGD-O1D	-5.57	113.01	123.85
15	M	404	CRT	C3-C1-C2	5.57	120.60	110.43
9	j	101	BCL	CMB-C2B-C1B	-5.56	116.96	125.42
9	y	401	BCL	O2D-CGD-CBD	5.55	120.94	111.23
9	D	101	BCL	C1D-ND-C4D	-5.55	102.42	106.31
15	AC	101	CRT	C4-C5-C6	-5.55	117.12	124.91
9	k	102	BCL	C4A-NA-C1A	5.55	109.21	106.68
9	z	102	BCL	C1D-ND-C4D	-5.52	102.44	106.31
12	H	301	PEF	O2-C10-C11	5.52	120.94	111.09
9	p	104	BCL	C1D-ND-C4D	-5.52	102.44	106.31
9	s	102	BCL	O2D-CGD-O1D	-5.51	113.12	123.85
15	z	101	CRT	C3-C1-C2	5.50	120.48	110.43
7	o	501	HEM	CHC-C4B-NB	5.50	130.34	124.42
9	V	101	BCL	O2D-CGD-CBD	5.50	120.84	111.23
10	M	402	BPH	O1D-CGD-CBD	-5.49	116.40	124.72
15	AD	102	CRT	C37-C36-C35	-5.48	117.21	124.91
9	D	101	BCL	O2D-CGD-O1D	-5.48	113.17	123.85
15	G	101	CRT	C3-C1-C2	5.47	120.43	110.43
15	AD	102	CRT	C5-C6-C7	-5.47	117.62	125.89
9	AE	104	BCL	C1D-ND-C4D	-5.47	102.47	106.31
9	5	101	BCL	O2D-CGD-CBD	5.47	120.79	111.23
9	1	102	BCL	O2D-CGD-O1D	-5.47	113.21	123.85
9	Z	102	BCL	C1D-ND-C4D	-5.45	102.49	106.31
15	AJ	101	CRT	C10-C9-C7	-5.45	119.64	127.28
15	6	101	CRT	C3-C1-C2	5.45	120.38	110.43
9	x	301	BCL	O2D-CGD-O1D	-5.44	113.26	123.85
9	AB	101	BCL	CMB-C2B-C1B	-5.43	117.15	125.42
15	E	101	CRT	C3-C1-C2	5.43	120.34	110.43
9	m	103	BCL	O2D-CGD-CBD	5.42	120.71	111.23
9	l	101	BCL	O2D-CGD-CBD	5.42	120.70	111.23
9	k	102	BCL	C1D-ND-C4D	-5.42	102.51	106.31
9	5	101	BCL	C1C-NC-C4C	-5.42	104.21	106.68
9	X	102	BCL	C1D-ND-C4D	-5.41	102.52	106.31
9	c	102	BCL	O2D-CGD-CBD	5.40	120.67	111.23
9	D	102	BCL	CMB-C2B-C1B	-5.40	117.20	125.42
9	P	101	BCL	O2D-CGD-CBD	5.39	120.65	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	102	BCL	O2D-CGD-O1D	-5.38	113.37	123.85
15	AJ	101	CRT	C5-C6-C7	-5.38	117.76	125.89
9	V	101	BCL	O2D-CGD-O1D	-5.37	113.39	123.85
9	p	102	BCL	C4D-CHA-C1A	5.37	127.64	121.24
9	e	102	BCL	O2D-CGD-CBD	5.37	120.61	111.23
9	AH	103	BCL	O2D-CGD-O1D	-5.36	113.41	123.85
9	8	102	BCL	C1D-ND-C4D	-5.36	102.55	106.31
15	AL	101	CRT	C4-C5-C6	-5.36	117.39	124.91
9	j	101	BCL	O2D-CGD-CBD	5.36	120.60	111.23
9	D	101	BCL	O2D-CGD-CBD	5.36	120.59	111.23
12	t	303	PEF	C2-O2-C10	-5.35	108.39	117.85
11	x	304	UQ8	C27-C28-C29	-5.35	115.39	127.62
9	d	101	BCL	C1C-NC-C4C	-5.34	104.24	106.68
9	U	101	BCL	C4D-CHA-C1A	5.34	127.62	121.24
15	AE	103	CRT	C3-C1-C2	5.33	120.17	110.43
9	s	102	BCL	C1D-ND-C4D	-5.31	102.58	106.31
15	z	101	CRT	C4-C5-C6	-5.31	117.45	124.91
15	n	101	CRT	C37-C36-C35	-5.31	117.46	124.91
9	4	102	BCL	O2D-CGD-O1D	-5.31	113.52	123.85
9	F	101	BCL	O2D-CGD-CBD	5.30	120.50	111.23
9	7	101	BCL	O2D-CGD-CBD	5.29	120.48	111.23
9	3	101	BCL	O2D-CGD-CBD	5.29	120.48	111.23
9	W	101	BCL	O2D-CGD-CBD	5.28	120.46	111.23
9	p	102	BCL	C1D-ND-C4D	-5.28	102.61	106.31
12	M	406	PEF	C2-O2-C10	-5.28	108.52	117.85
9	G	102	BCL	C1D-ND-C4D	-5.27	102.61	106.31
9	w	101	BCL	C1D-ND-C4D	-5.27	102.61	106.31
15	k	101	CRT	C37-C36-C35	-5.27	117.52	124.91
9	x	305	BCL	C4A-NA-C1A	5.27	109.08	106.68
15	R	101	CRT	C3-C1-C2	5.26	120.05	110.43
9	T	102	BCL	O2D-CGD-O1D	-5.26	113.62	123.85
9	l	101	BCL	CMB-C2B-C1B	-5.26	117.42	125.42
11	x	304	UQ8	C6-C1-C2	5.25	123.31	119.17
12	y	407	PEF	O2-C10-C11	5.24	120.44	111.09
9	x	303	BCL	O2D-CGD-O1D	-5.24	113.64	123.85
9	AD	101	BCL	C1D-ND-C4D	-5.23	102.64	106.31
9	N	102	BCL	O2D-CGD-CBD	5.21	120.34	111.23
9	AJ	102	BCL	C4A-NA-C1A	5.21	109.05	106.68
9	AH	103	BCL	O2D-CGD-CBD	5.20	120.32	111.23
9	i	102	BCL	O2D-CGD-O1D	-5.19	113.74	123.85
9	e	102	BCL	O2D-CGD-O1D	-5.19	113.74	123.85
7	o	503	HEM	CHD-C4C-NC	5.19	130.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	101	BCL	O2D-CGD-O1D	-5.19	113.75	123.85
15	P	102	CRT	C21-C22-C23	-5.18	120.02	127.28
9	m	103	BCL	C1D-ND-C4D	-5.17	102.68	106.31
7	C	501	HEM	CBD-CAD-C3D	-5.17	98.25	112.53
15	G	101	CRT	C31-C32-C33	-5.16	120.04	127.28
9	B	101	BCL	O2D-CGD-CBD	5.15	120.22	111.23
9	P	101	BCL	CMB-C2B-C1B	-5.14	117.58	125.42
9	r	101	BCL	O2D-CGD-CBD	5.14	120.22	111.23
9	V	101	BCL	C1D-ND-C4D	-5.14	102.70	106.31
9	g	101	BCL	C1D-ND-C4D	-5.14	102.70	106.31
9	AA	101	BCL	C4D-CHA-C1A	5.14	127.38	121.24
7	C	501	HEM	C4D-ND-C1D	5.13	111.29	105.21
9	I	101	BCL	C1D-ND-C4D	-5.13	102.71	106.31
15	R	101	CRT	C15-C14-C12	-5.13	120.08	127.28
15	i	101	CRT	C37-C36-C35	-5.13	117.71	124.91
9	A	102	BCL	O2D-CGD-O1D	-5.13	113.87	123.85
15	v	101	CRT	C8-C7-C6	5.13	125.92	118.09
7	o	503	HEM	C3B-C4B-NB	-5.13	105.79	109.47
10	x	302	BPH	CMC-C2C-C1C	-5.12	103.58	114.61
9	AL	102	BCL	C4A-NA-C1A	5.10	109.01	106.68
9	f	101	BCL	O2D-CGD-O1D	-5.10	113.92	123.85
9	N	102	BCL	O2D-CGD-O1D	-5.10	113.93	123.85
9	u	101	BCL	O2D-CGD-CBD	5.10	120.14	111.23
9	AK	101	BCL	O2D-CGD-CBD	5.09	120.13	111.23
15	9	102	CRT	C5-C6-C7	-5.09	118.20	125.89
9	D	102	BCL	C1D-ND-C4D	-5.09	102.74	106.31
9	x	301	BCL	C1D-ND-C4D	-5.09	102.74	106.31
9	p	102	BCL	O2D-CGD-CBD	5.09	120.12	111.23
7	C	504	HEM	C3B-C4B-NB	-5.09	105.81	109.47
9	L	303	BCL	C4A-NA-C1A	5.08	109.00	106.68
9	O	101	BCL	C1D-ND-C4D	-5.08	102.75	106.31
7	C	504	HEM	C1B-NB-C4B	5.08	111.22	105.21
9	f	101	BCL	CMB-C2B-C1B	-5.08	117.69	125.42
9	p	104	BCL	O2D-CGD-CBD	5.06	120.08	111.23
9	Q	101	BCL	C4D-CHA-C1A	5.06	127.28	121.24
9	AC	102	BCL	O2D-CGD-O1D	-5.06	114.00	123.85
9	Y	101	BCL	O2D-CGD-O1D	-5.06	114.00	123.85
9	v	102	BCL	O2D-CGD-O1D	-5.06	114.00	123.85
9	K	101	BCL	C1D-ND-C4D	-5.05	102.77	106.31
9	Q	101	BCL	C1D-ND-C4D	-5.05	102.77	106.31
9	AA	101	BCL	O2D-CGD-CBD	5.04	120.03	111.23
9	AC	102	BCL	O2D-CGD-CBD	5.03	120.03	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	101	BCL	O2D-CGD-O1D	-5.03	114.06	123.85
15	T	101	CRT	C4-C5-C6	-5.03	117.85	124.91
9	AH	101	BCL	O2D-CGD-O1D	-5.03	114.06	123.85
7	o	502	HEM	CHD-C4C-NC	5.02	129.92	124.45
9	m	102	BCL	O2D-CGD-CBD	5.02	120.01	111.23
9	4	102	BCL	C1D-ND-C4D	-5.02	102.79	106.31
9	x	301	BCL	CHB-C4A-NA	-5.02	117.16	124.40
15	9	102	CRT	C3-C1-C2	5.02	119.59	110.43
9	h	101	BCL	C1D-ND-C4D	-5.02	102.79	106.31
7	o	502	HEM	C3B-C4B-NB	-5.01	105.87	109.47
9	D	102	BCL	O2D-CGD-O1D	-5.01	114.10	123.85
9	R	102	BCL	O2D-CGD-CBD	5.01	119.99	111.23
9	h	101	BCL	O2D-CGD-O1D	-5.00	114.11	123.85
9	U	101	BCL	C1D-ND-C4D	-5.00	102.80	106.31
9	T	102	BCL	O2D-CGD-CBD	4.99	119.95	111.23
15	AH	102	CRT	C26-C27-C28	-4.98	120.29	127.28
9	0	101	BCL	O2D-CGD-CBD	4.98	119.94	111.23
9	x	305	BCL	C1D-ND-C4D	-4.98	102.82	106.31
15	i	101	CRT	C3-C1-C2	4.98	119.53	110.43
9	AI	101	BCL	O2D-CGD-CBD	4.98	119.94	111.23
15	p	103	CRT	C4-C5-C6	-4.98	117.92	124.91
9	9	103	BCL	C1D-ND-C4D	-4.97	102.82	106.31
9	Q	101	BCL	C7-C6-C5	-4.97	100.01	113.26
9	AE	104	BCL	CMB-C2B-C1B	-4.97	117.85	125.42
15	R	101	CRT	C21-C22-C23	-4.97	120.31	127.28
9	y	401	BCL	O2D-CGD-O1D	-4.97	114.18	123.85
9	AE	104	BCL	O2D-CGD-O1D	-4.96	114.20	123.85
9	p	104	BCL	CMB-C2B-C1B	-4.95	117.88	125.42
15	s	101	CRT	C3-C1-C2	4.95	119.48	110.43
9	Q	101	BCL	O2D-CGD-O1D	-4.94	114.23	123.85
9	4	102	BCL	CMA-C3A-C4A	-4.93	98.53	111.77
9	1	102	BCL	C1C-NC-C4C	-4.92	104.43	106.68
9	L	305	BCL	O2D-CGD-O1D	-4.92	114.27	123.85
7	C	502	HEM	C3B-C4B-NB	-4.92	105.93	109.47
15	v	101	CRT	C6-C7-C9	-4.92	111.27	119.01
9	AK	101	BCL	O2D-CGD-O1D	-4.92	114.28	123.85
9	N	102	BCL	CMB-C2B-C1B	-4.91	117.94	125.42
9	3	101	BCL	CMB-C2B-C1B	-4.90	117.95	125.42
9	M	401	BCL	CMA-C3A-C4A	-4.90	98.60	111.77
9	AH	101	BCL	C4D-CHA-C1A	4.90	127.09	121.24
9	w	101	BCL	O2D-CGD-O1D	-4.89	114.33	123.85
9	p	104	BCL	O2D-CGD-O1D	-4.89	114.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AB	101	BCL	O2D-CGD-CBD	4.88	119.76	111.23
9	AD	101	BCL	O2D-CGD-O1D	-4.87	114.37	123.85
15	n	101	CRT	C10-C9-C7	4.86	134.10	127.28
9	X	102	BCL	O2D-CGD-O1D	-4.86	114.39	123.85
15	c	101	CRT	C3-C1-C2	4.86	119.30	110.43
9	z	102	BCL	O2D-CGD-O1D	-4.85	114.40	123.85
9	Z	102	BCL	C2D-C1D-ND	4.85	114.93	110.13
9	3	101	BCL	O2D-CGD-O1D	-4.85	114.40	123.85
9	S	102	BCL	C4D-CHA-C1A	4.84	127.02	121.24
9	AK	101	BCL	C1D-ND-C4D	-4.84	102.92	106.31
9	U	101	BCL	O2D-CGD-O1D	-4.83	114.45	123.85
15	U	102	CRT	C3-C1-C2	4.82	119.24	110.43
7	C	503	HEM	C1B-NB-C4B	4.82	110.91	105.21
9	5	101	BCL	CMB-C2B-C1B	-4.82	118.09	125.42
9	O	101	BCL	O2D-CGD-CBD	4.81	119.63	111.23
9	G	102	BCL	O2D-CGD-CBD	4.80	119.63	111.23
9	m	103	BCL	O2D-CGD-O1D	-4.79	114.52	123.85
9	L	301	BCL	OBB-CAB-CBB	-4.79	109.03	119.77
9	AB	101	BCL	O2D-CGD-O1D	-4.79	114.53	123.85
12	M	408	PEF	O2-C10-C11	4.78	119.61	111.09
9	x	303	BCL	C1D-ND-C4D	-4.77	102.96	106.31
9	w	101	BCL	CMA-C3A-C4A	-4.77	98.96	111.77
15	P	102	CRT	C20-C19-C17	-4.76	120.60	127.28
15	s	101	CRT	C4-C5-C6	-4.75	118.24	124.91
15	e	101	CRT	C32-C31-C30	-4.75	109.44	123.20
9	I	101	BCL	O2D-CGD-CBD	4.75	119.53	111.23
9	m	102	BCL	CMB-C2B-C1B	-4.75	118.19	125.42
9	L	305	BCL	C4A-NA-C1A	4.74	108.84	106.68
9	AA	101	BCL	C1D-ND-C4D	-4.73	103.00	106.31
9	AE	102	BCL	O2D-CGD-CBD	4.73	119.49	111.23
7	o	501	HEM	C1B-NB-C4B	4.73	110.80	105.21
9	k	102	BCL	O2D-CGD-CBD	4.72	119.47	111.23
9	e	102	BCL	CMB-C2B-C1B	-4.71	118.25	125.42
9	5	101	BCL	O2D-CGD-O1D	-4.70	114.69	123.85
11	x	304	UQ8	C15-C14-C16	4.70	123.38	115.23
9	5	101	BCL	C1D-ND-C4D	-4.68	103.03	106.31
9	L	305	BCL	C1D-ND-C4D	-4.67	103.03	106.31
9	K	101	BCL	O2D-CGD-CBD	4.66	119.38	111.23
15	X	101	CRT	C5-C6-C7	-4.66	118.85	125.89
12	m	101	PEF	O2-C10-C11	4.66	119.39	111.09
15	c	101	CRT	C31-C32-C33	-4.66	120.75	127.28
9	AI	101	BCL	O2D-CGD-O1D	-4.64	114.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	CRT	C26-C27-C28	-4.64	120.78	127.28
9	v	102	BCL	O2D-CGD-CBD	4.63	119.33	111.23
7	o	504	HEM	CHC-C1C-NC	4.63	129.49	124.45
9	u	101	BCL	O2D-CGD-O1D	-4.62	114.85	123.85
9	S	102	BCL	CMB-C2B-C1B	-4.62	118.38	125.42
9	s	102	BCL	CMB-C2B-C1B	-4.62	118.38	125.42
15	z	101	CRT	C37-C36-C35	-4.62	118.42	124.91
9	AI	101	BCL	C1D-ND-C4D	-4.62	103.07	106.31
9	L	303	BCL	CHD-C1D-ND	-4.62	118.31	124.80
14	y	403	MQ8	C11-C3-C4	-4.61	113.72	118.58
9	v	102	BCL	C1D-ND-C4D	-4.61	103.08	106.31
9	m	102	BCL	C4D-CHA-C1A	4.61	126.74	121.24
9	D	101	BCL	C4D-CHA-C1A	4.61	126.74	121.24
9	I	101	BCL	CMB-C2B-C1B	-4.60	118.41	125.42
9	F	101	BCL	O2D-CGD-O1D	-4.60	114.89	123.85
9	V	101	BCL	C1C-NC-C4C	-4.60	104.58	106.68
15	8	101	CRT	C37-C36-C35	-4.58	118.48	124.91
9	B	101	BCL	C4D-CHA-C1A	4.58	126.71	121.24
9	8	102	BCL	O2D-CGD-O1D	-4.57	114.95	123.85
9	F	101	BCL	C1D-ND-C4D	-4.57	103.11	106.31
9	P	101	BCL	O2D-CGD-O1D	-4.57	114.96	123.85
9	AH	101	BCL	CHA-C1A-NA	-4.56	116.06	126.39
7	o	504	HEM	C1B-NB-C4B	4.56	110.61	105.21
9	e	102	BCL	C1D-ND-C4D	-4.56	103.12	106.31
9	5	102	BCL	CHA-C1A-NA	-4.55	116.08	126.39
11	x	304	UQ8	C30-C29-C31	4.55	123.13	115.23
9	AL	102	BCL	O2D-CGD-O1D	-4.55	114.99	123.85
9	R	102	BCL	CMB-C2B-C1B	-4.55	118.50	125.42
9	L	303	BCL	O2D-CGD-CBD	4.55	119.18	111.23
9	x	305	BCL	C2D-C1D-ND	4.55	114.63	110.13
9	m	102	BCL	O2D-CGD-O1D	-4.55	115.00	123.85
9	AA	101	BCL	C1C-NC-C4C	-4.54	104.61	106.68
9	p	102	BCL	O2D-CGD-O1D	-4.54	115.02	123.85
9	B	101	BCL	CMB-C2B-C1B	-4.53	118.52	125.42
9	AE	104	BCL	C4D-CHA-C1A	4.53	126.65	121.24
9	d	101	BCL	C1-O2A-CGA	4.53	127.61	116.65
15	P	102	CRT	C4-C5-C6	-4.53	118.56	124.91
15	X	101	CRT	C21-C20-C19	4.52	132.78	123.52
15	J	101	CRT	C5-C6-C7	4.52	132.72	125.89
9	AI	101	BCL	CMB-C2B-C1B	-4.52	118.54	125.42
9	A	102	BCL	C2D-C1D-ND	4.51	114.59	110.13
9	V	101	BCL	CMB-C2B-C1B	-4.50	118.56	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	x	301	BCL	OBB-CAB-CBB	-4.50	109.69	119.77
9	M	401	BCL	O2A-CGA-O1A	-4.50	112.38	123.63
9	AH	101	BCL	O2D-CGD-CBD	4.49	119.09	111.23
9	V	101	BCL	C4D-CHA-C1A	4.49	126.60	121.24
9	9	103	BCL	O2D-CGD-O1D	-4.49	115.11	123.85
9	AH	103	BCL	C2D-C1D-ND	4.48	114.56	110.13
9	K	101	BCL	O2D-CGD-O1D	-4.48	115.13	123.85
7	C	502	HEM	CHD-C1D-ND	4.48	129.24	124.42
15	4	101	CRT	C4-C5-C6	-4.45	118.66	124.91
9	g	101	BCL	C4D-CHA-C1A	4.45	126.55	121.24
9	L	303	BCL	CAC-C3C-C4C	-4.45	102.71	112.58
15	AD	102	CRT	C15-C14-C12	-4.44	121.05	127.28
9	AD	101	BCL	O2D-CGD-CBD	4.44	119.00	111.23
12	A	101	PEF	O2-C10-C11	4.44	119.01	111.09
9	D	101	BCL	C2D-C1D-ND	4.44	114.52	110.13
9	R	102	BCL	C4D-CHA-C1A	4.43	126.53	121.24
9	B	101	BCL	C2D-C1D-ND	4.43	114.51	110.13
9	W	101	BCL	C1D-ND-C4D	-4.43	103.20	106.31
9	g	101	BCL	O2D-CGD-O1D	-4.43	115.23	123.85
15	Z	101	CRT	C21-C20-C19	-4.43	114.46	123.52
9	AH	101	BCL	C1D-ND-C4D	-4.43	103.21	106.31
9	X	102	BCL	O2D-CGD-CBD	4.42	118.96	111.23
9	L	301	BCL	C1D-ND-C4D	-4.42	103.21	106.31
15	R	101	CRT	C18-C17-C16	4.42	124.84	118.09
9	AA	101	BCL	O2D-CGD-O1D	-4.42	115.25	123.85
9	AE	102	BCL	C2D-C1D-ND	4.42	114.50	110.13
9	0	101	BCL	CMB-C2B-C1B	-4.41	118.70	125.42
9	c	102	BCL	C2D-C1D-ND	4.41	114.49	110.13
9	AJ	102	BCL	CMB-C2B-C1B	-4.41	118.71	125.42
15	z	101	CRT	C21-C22-C23	-4.41	121.10	127.28
9	G	102	BCL	CMB-C2B-C1B	-4.40	118.72	125.42
9	s	102	BCL	C2D-C1D-ND	4.39	114.47	110.13
9	AD	101	BCL	C4D-CHA-C1A	4.39	126.48	121.24
9	T	102	BCL	C2D-C1D-ND	4.39	114.47	110.13
9	P	101	BCL	C1D-ND-C4D	-4.39	103.23	106.31
7	o	504	HEM	C3B-C4B-NB	-4.38	106.32	109.47
9	M	401	BCL	C1D-ND-C4D	-4.38	103.24	106.31
9	h	101	BCL	CHA-C1A-NA	-4.38	116.48	126.39
15	k	101	CRT	C25-C23-C22	4.37	125.89	119.01
9	m	103	BCL	CMB-C2B-C1B	-4.37	118.76	125.42
11	x	304	UQ8	C25-C24-C26	4.37	122.81	115.23
9	e	102	BCL	C1C-NC-C4C	-4.37	104.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	101	BCL	CMB-C2B-C1B	-4.36	118.78	125.42
9	o	101	BCL	O2D-CGD-O1D	-4.36	115.36	123.85
15	p	103	CRT	C21-C22-C23	-4.36	121.16	127.28
9	y	401	BCL	C1D-ND-C4D	-4.35	103.26	106.31
15	AC	101	CRT	C31-C32-C33	-4.35	121.18	127.28
15	N	101	CRT	C26-C27-C28	-4.35	121.18	127.28
15	9	102	CRT	C15-C14-C12	-4.35	121.18	127.28
9	i	102	BCL	C2D-C1D-ND	4.34	114.42	110.13
9	F	101	BCL	CMB-C2B-C1B	-4.34	118.81	125.42
9	r	101	BCL	C1D-ND-C4D	-4.34	103.27	106.31
15	T	101	CRT	C31-C32-C33	-4.34	121.20	127.28
15	p	103	CRT	C9-C10-C11	-4.33	110.65	123.20
9	x	303	BCL	CMB-C2B-C1B	-4.32	118.84	125.42
9	D	102	BCL	C2D-C1D-ND	4.32	114.40	110.13
15	n	101	CRT	C5-C6-C7	-4.32	119.37	125.89
10	L	302	BPH	O2D-CGD-CBD	4.31	115.69	110.95
9	R	102	BCL	C2D-C1D-ND	4.31	114.39	110.13
9	r	101	BCL	O2D-CGD-O1D	-4.31	115.45	123.85
9	r	101	BCL	C4D-CHA-C1A	4.31	126.38	121.24
9	L	303	BCL	C4D-CHA-C1A	4.31	126.38	121.24
9	d	101	BCL	C1D-ND-C4D	-4.30	103.29	106.31
9	L	301	BCL	C12-C11-C10	-4.30	93.99	113.28
9	O	101	BCL	C4D-CHA-C1A	4.30	126.38	121.24
9	i	102	BCL	C1C-NC-C4C	-4.30	104.72	106.68
9	c	102	BCL	O2D-CGD-O1D	-4.30	115.48	123.85
15	k	101	CRT	C20-C19-C17	-4.30	121.25	127.28
9	m	103	BCL	C4D-CHA-C1A	4.30	126.37	121.24
9	O	101	BCL	O2D-CGD-O1D	-4.30	115.49	123.85
9	T	102	BCL	C4D-CHA-C1A	4.30	126.37	121.24
7	C	501	HEM	CHB-C1B-NB	4.29	129.67	124.37
9	m	102	BCL	C2D-C1D-ND	4.29	114.37	110.13
9	x	305	BCL	C1C-NC-C4C	-4.29	104.72	106.68
9	Q	101	BCL	CHA-C1A-NA	-4.28	116.70	126.39
9	Q	101	BCL	O2D-CGD-CBD	4.28	118.71	111.23
9	k	102	BCL	CGD-CBD-CAD	-4.27	97.04	110.85
9	w	101	BCL	CMB-C2B-C1B	-4.26	118.93	125.42
15	p	103	CRT	C5-C6-C7	-4.26	119.45	125.89
9	r	101	BCL	CMB-C2B-C1B	-4.26	118.94	125.42
9	L	305	BCL	CMA-C3A-C4A	-4.26	100.33	111.77
9	w	101	BCL	C4D-CHA-C1A	4.26	126.32	121.24
15	e	101	CRT	C37-C36-C35	-4.25	118.94	124.91
12	M	406	PEF	O2-C10-O4	-4.25	114.79	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	HEM	CHB-C1B-NB	4.24	129.62	124.37
9	J	102	BCL	C1C-NC-C4C	-4.24	104.74	106.68
15	n	101	CRT	C4-C5-C6	-4.24	118.96	124.91
15	6	101	CRT	C32-C31-C30	-4.24	110.92	123.20
9	P	101	BCL	CHA-C1A-NA	-4.24	116.80	126.39
15	AL	101	CRT	C37-C36-C35	-4.24	118.97	124.91
9	W	101	BCL	C1C-NC-C4C	-4.23	104.75	106.68
9	Y	101	BCL	CBC-CAC-C3C	4.22	122.37	113.41
15	v	101	CRT	C29-C28-C30	4.22	124.53	118.09
9	Y	101	BCL	C4D-CHA-C1A	4.22	126.27	121.24
9	l	102	BCL	C1D-ND-C4D	-4.21	103.36	106.31
9	w	101	BCL	O2D-CGD-CBD	4.21	118.59	111.23
15	v	101	CRT	C21-C20-C19	-4.21	114.90	123.52
9	O	101	BCL	C2D-C1D-ND	4.20	114.29	110.13
9	AK	101	BCL	CHB-C4A-NA	-4.20	118.33	124.40
9	v	102	BCL	CMB-C2B-C1B	-4.20	119.02	125.42
11	L	304	UQ8	C40-C39-C41	4.20	122.52	115.23
9	D	102	BCL	C4D-CHA-C1A	4.20	126.25	121.24
9	AK	101	BCL	C4D-CHA-C1A	4.20	126.25	121.24
9	0	101	BCL	C1D-ND-C4D	-4.20	103.37	106.31
9	R	102	BCL	O2D-CGD-O1D	-4.20	115.68	123.85
9	J	102	BCL	O2D-CGD-O1D	-4.19	115.69	123.85
9	8	102	BCL	CMB-C2B-C1B	-4.19	119.04	125.42
9	L	301	BCL	CBB-CAB-C3B	4.18	129.22	120.40
15	6	101	CRT	C4-C5-C6	-4.18	119.04	124.91
9	AL	102	BCL	CHA-C1A-NA	-4.18	116.92	126.39
12	y	408	PEF	O2-C10-C11	4.18	118.54	111.09
15	c	101	CRT	C4-C5-C6	-4.18	119.05	124.91
15	E	101	CRT	C21-C22-C23	-4.17	121.42	127.28
9	S	102	BCL	C1D-ND-C4D	-4.17	103.39	106.31
12	H	303	PEF	O2-C10-C11	4.17	118.52	111.09
9	r	101	BCL	CHD-C1D-ND	-4.16	118.95	124.80
17	AE	101	PGW	O01-C1-C2	4.15	118.48	111.09
9	M	401	BCL	CBB-CAB-C3B	4.14	129.14	120.40
9	3	101	BCL	CHD-C1D-ND	-4.14	118.97	124.80
9	AK	101	BCL	CMB-C2B-C1B	-4.14	119.11	125.42
9	l	101	BCL	O2D-CGD-O1D	-4.13	115.81	123.85
15	s	101	CRT	C20-C19-C17	-4.13	121.49	127.28
9	W	101	BCL	O2D-CGD-O1D	-4.13	115.81	123.85
9	p	104	BCL	C2D-C1D-ND	4.13	114.21	110.13
9	p	102	BCL	CHA-C1A-NA	-4.12	117.05	126.39
9	AE	104	BCL	C2D-C1D-ND	4.12	114.20	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AC	102	BCL	CMB-C2B-C1B	-4.12	119.15	125.42
9	g	101	BCL	CMB-C2B-C1B	-4.12	119.15	125.42
9	S	102	BCL	CHA-C1A-NA	-4.11	117.08	126.39
9	Z	102	BCL	CBB-CAB-C3B	4.11	129.07	120.40
15	z	101	CRT	C31-C32-C33	-4.11	121.52	127.28
9	M	401	BCL	CHA-C1A-NA	-4.10	117.10	126.39
9	c	102	BCL	C4D-CHA-C1A	4.10	126.14	121.24
9	L	301	BCL	O2A-CGA-O1A	-4.10	113.37	123.63
15	v	101	CRT	C31-C32-C33	-4.10	121.53	127.28
9	AE	102	BCL	CMB-C2B-C1B	-4.10	119.18	125.42
7	o	502	HEM	CHD-C1D-ND	4.09	128.82	124.42
9	W	101	BCL	C4A-NA-C1A	4.09	108.54	106.68
9	AI	101	BCL	C4D-CHA-C1A	4.08	126.11	121.24
9	Y	101	BCL	CMB-C2B-C1B	-4.08	119.21	125.42
9	x	303	BCL	O2A-CGA-O1A	-4.08	113.42	123.63
15	J	101	CRT	C26-C27-C28	-4.08	121.56	127.28
9	4	102	BCL	CHD-C1D-ND	-4.07	119.07	124.80
9	U	101	BCL	CHA-C1A-NA	-4.07	117.17	126.39
9	5	102	BCL	C2A-C1A-CHA	4.07	130.94	123.87
9	k	102	BCL	C2D-C1D-ND	4.07	114.15	110.13
9	k	102	BCL	C2A-C1A-CHA	4.06	130.92	123.87
15	2	101	CRT	C21-C22-C23	-4.06	121.58	127.28
9	k	102	BCL	O2D-CGD-O1D	-4.06	115.94	123.85
9	x	303	BCL	CAC-C3C-C4C	4.06	121.59	112.58
9	L	301	BCL	CMA-C3A-C4A	-4.06	100.87	111.77
9	AE	102	BCL	O2D-CGD-O1D	-4.06	115.95	123.85
9	G	102	BCL	O2D-CGD-O1D	-4.05	115.95	123.85
9	5	102	BCL	C2D-C1D-ND	4.05	114.14	110.13
15	e	101	CRT	C20-C19-C17	-4.05	121.60	127.28
9	AB	101	BCL	C4D-CHA-C1A	4.05	126.08	121.24
9	L	301	BCL	O2D-CGD-CBD	4.05	118.31	111.23
9	AC	102	BCL	C2D-C1D-ND	4.05	114.13	110.13
7	o	501	HEM	C4D-ND-C1D	4.05	110.00	105.21
9	L	303	BCL	CHA-C1A-NA	-4.05	117.23	126.39
12	x	306	PEF	O2-C10-C11	4.04	118.30	111.09
15	6	101	CRT	C34-C33-C35	4.04	124.26	118.09
9	p	102	BCL	CMB-C2B-C1B	-4.04	119.27	125.42
7	o	501	HEM	CHD-C1D-ND	4.04	128.77	124.42
9	5	101	BCL	C4D-CHA-C1A	4.03	126.05	121.24
9	Y	101	BCL	CHD-C1D-ND	-4.02	119.14	124.80
9	x	303	BCL	O2D-CGD-CBD	4.02	118.26	111.23
7	o	501	HEM	CBD-CAD-C3D	-4.02	101.42	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	102	BCL	C2A-C1A-CHA	4.02	130.84	123.87
9	h	101	BCL	CHD-C1D-ND	-4.01	119.15	124.80
15	AC	101	CRT	C21-C22-C23	-4.01	121.65	127.28
9	l	101	BCL	C4D-CHA-C1A	4.01	126.03	121.24
9	c	102	BCL	CMB-C2B-C1B	-4.01	119.31	125.42
9	Y	101	BCL	CAC-C3C-C4C	4.01	121.48	112.58
9	A	102	BCL	CMB-C2B-C1B	-4.01	119.31	125.42
9	K	101	BCL	C4D-CHA-C1A	4.01	126.03	121.24
7	C	503	HEM	CAB-C3B-C2B	-4.01	115.40	128.43
9	P	101	BCL	C1C-NC-C4C	-4.01	104.85	106.68
9	AA	101	BCL	CHA-C1A-NA	-4.00	117.33	126.39
9	F	101	BCL	C4D-CHA-C1A	4.00	126.02	121.24
9	7	101	BCL	C2D-C1D-ND	4.00	114.08	110.13
9	AB	101	BCL	C1D-ND-C4D	-4.00	103.51	106.31
15	U	102	CRT	C26-C27-C28	-3.99	121.68	127.28
15	n	101	CRT	C15-C14-C12	-3.99	121.68	127.28
15	A	103	CRT	C21-C22-C23	-3.99	121.68	127.28
9	L	301	BCL	C2A-C1A-CHA	3.99	130.79	123.87
9	W	101	BCL	C7-C6-C5	-3.99	102.64	113.26
9	G	102	BCL	C1C-NC-C4C	-3.98	104.86	106.68
15	R	101	CRT	C10-C9-C7	-3.98	121.70	127.28
9	x	303	BCL	CMA-C3A-C4A	-3.97	101.09	111.77
15	G	101	CRT	C20-C19-C17	-3.97	121.71	127.28
9	Z	102	BCL	CHB-C4A-NA	-3.97	118.67	124.40
9	L	305	BCL	CMC-C2C-C1C	-3.97	101.11	111.77
9	5	102	BCL	C1D-ND-C4D	-3.96	103.53	106.31
7	C	504	HEM	CHB-C1B-NB	3.96	129.27	124.37
9	A	102	BCL	C4D-CHA-C1A	3.96	125.97	121.24
11	x	304	UQ8	O5-C5-C6	-3.96	114.14	121.79
15	4	101	CRT	C31-C32-C33	-3.95	121.73	127.28
9	l	101	BCL	OBB-CAB-CBB	-3.95	110.92	119.77
9	P	101	BCL	C4D-CHA-C1A	3.95	125.96	121.24
7	C	503	HEM	CHC-C4B-C3B	3.95	132.96	125.07
9	AA	101	BCL	CMB-C2B-C1B	-3.95	119.41	125.42
9	e	102	BCL	CBB-CAB-C3B	3.95	128.72	120.40
9	AE	102	BCL	C4D-CHA-C1A	3.95	125.95	121.24
9	f	101	BCL	C4D-CHA-C1A	3.94	125.95	121.24
7	C	504	HEM	CHD-C4C-C3C	-3.94	118.56	125.21
15	v	101	CRT	C4-C5-C6	3.94	130.45	124.91
9	w	101	BCL	C2D-C1D-ND	3.94	114.03	110.13
15	v	101	CRT	C9-C10-C11	-3.94	111.79	123.20
9	AL	102	BCL	C2D-C1D-ND	3.94	114.02	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	101	BCL	O2D-CGD-CBD	3.94	118.11	111.23
10	L	302	BPH	CMC-C2C-C1C	-3.94	106.13	114.61
9	i	102	BCL	C4D-CHA-C1A	3.94	125.94	121.24
9	y	401	BCL	C1C-NC-C4C	-3.93	104.89	106.68
9	AH	103	BCL	C1C-NC-C4C	-3.93	104.89	106.68
9	K	101	BCL	CED-O2D-CGD	-3.93	107.00	115.92
11	x	304	UQ8	C40-C39-C41	3.93	122.04	115.23
15	R	101	CRT	C5-C6-C7	-3.92	119.96	125.89
15	N	101	CRT	C20-C19-C17	-3.92	121.78	127.28
11	L	304	UQ8	C30-C29-C31	3.92	122.03	115.23
15	f	102	CRT	C37-C36-C35	-3.92	119.41	124.91
9	s	102	BCL	OBb-CAB-CBB	-3.92	111.00	119.77
9	AK	101	BCL	C2D-C1D-ND	3.91	114.00	110.13
7	C	502	HEM	CHD-C4C-NC	3.91	128.71	124.45
9	K	101	BCL	C2D-C1D-ND	3.90	113.99	110.13
9	S	102	BCL	C1C-NC-C4C	-3.90	104.90	106.68
15	p	103	CRT	C26-C27-C28	-3.90	121.81	127.28
7	o	503	HEM	C1B-NB-C4B	3.90	109.83	105.21
9	K	101	BCL	CMB-C2B-C1B	-3.90	119.48	125.42
9	M	401	BCL	CMB-C2B-C1B	-3.90	119.48	125.42
9	z	102	BCL	C2D-C1D-ND	3.90	113.98	110.13
9	AH	103	BCL	OBb-CAB-CBB	-3.90	111.04	119.77
15	f	102	CRT	C32-C31-C30	3.90	134.49	123.20
10	y	402	BPH	O2D-CGD-CBD	3.89	115.22	110.95
9	AH	101	BCL	OBb-CAB-CBB	-3.89	111.06	119.77
9	J	102	BCL	C2D-C1D-ND	3.89	113.98	110.13
9	r	101	BCL	CHA-C1A-NA	-3.88	117.60	126.39
12	L	306	PEF	O3P-C1-C2	3.88	119.83	108.51
10	y	402	BPH	CGD-CBD-CAD	-3.88	98.28	110.85
9	3	101	BCL	CMC-C2C-C3C	-3.88	98.99	113.98
15	AC	101	CRT	C20-C19-C17	-3.87	121.84	127.28
9	7	101	BCL	O2D-CGD-O1D	-3.87	116.31	123.85
9	1	102	BCL	CHA-C1A-NA	-3.87	117.62	126.39
9	f	101	BCL	CHD-C1D-ND	-3.87	119.35	124.80
15	N	101	CRT	C29-C28-C30	3.87	124.00	118.09
9	d	101	BCL	CMB-C2B-C1B	-3.87	119.53	125.42
9	L	301	BCL	CHA-C1A-NA	-3.86	117.66	126.39
15	c	101	CRT	C10-C9-C7	-3.86	121.87	127.28
9	s	102	BCL	CHA-C1A-NA	-3.86	117.66	126.39
9	s	102	BCL	C1C-NC-C4C	-3.86	104.92	106.68
9	AE	104	BCL	CHA-C1A-NA	-3.85	117.66	126.39
9	AL	102	BCL	C1-C2-C3	-3.85	119.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AK	101	BCL	C4A-NA-C1A	3.84	108.43	106.68
9	k	102	BCL	C7-C6-C5	-3.84	103.02	113.26
9	I	101	BCL	CHA-C1A-NA	-3.84	117.69	126.39
14	M	403	MQ8	C14-C13-C15	3.84	121.89	115.23
12	A	101	PEF	C2-O2-C10	-3.84	111.06	117.85
15	2	101	CRT	C37-C36-C35	-3.83	119.53	124.91
7	C	501	HEM	C1B-NB-C4B	3.83	109.75	105.21
9	m	102	BCL	OBb-CAB-CBB	-3.83	111.19	119.77
9	D	101	BCL	CHD-C1D-ND	-3.83	119.41	124.80
9	m	103	BCL	C2D-C1D-ND	3.83	113.91	110.13
9	4	102	BCL	C2D-C1D-ND	3.83	113.91	110.13
9	U	101	BCL	O2A-CGA-O1A	-3.83	114.06	123.63
9	x	303	BCL	C2D-C1D-ND	3.82	113.91	110.13
9	v	102	BCL	C2A-C1A-CHA	3.82	130.49	123.87
15	e	101	CRT	C21-C22-C23	-3.81	121.93	127.28
9	Z	102	BCL	CHA-C1A-NA	-3.81	117.76	126.39
9	f	101	BCL	CHB-C1B-NB	3.81	129.76	124.05
9	7	101	BCL	C4D-CHA-C1A	3.81	125.79	121.24
15	AD	102	CRT	C21-C22-C23	-3.81	121.94	127.28
9	P	101	BCL	C4A-NA-C1A	3.81	108.42	106.68
15	U	102	CRT	C21-C22-C23	-3.80	121.94	127.28
9	g	101	BCL	C2D-C1D-ND	3.80	113.89	110.13
9	L	303	BCL	CMD-C2D-C1D	3.80	131.41	124.73
15	J	101	CRT	C15-C14-C12	-3.79	121.96	127.28
9	AI	101	BCL	C2D-C1D-ND	3.79	113.87	110.13
9	I	101	BCL	C1C-NC-C4C	-3.79	104.95	106.68
9	U	101	BCL	C2D-C1D-ND	3.78	113.87	110.13
15	4	101	CRT	C16-C17-C19	-3.78	113.06	119.01
9	U	101	BCL	CMB-C2B-C1B	-3.78	119.66	125.42
9	AL	102	BCL	CMB-C2B-C1B	-3.78	119.67	125.42
12	M	406	PEF	C3-O3-C30	3.78	126.40	117.08
9	z	102	BCL	OBb-CAB-CBB	-3.78	111.31	119.77
15	9	102	CRT	C21-C20-C19	-3.78	115.79	123.52
9	1	102	BCL	C4D-CHA-C1A	3.78	125.75	121.24
9	0	101	BCL	CHA-C1A-NA	-3.77	117.85	126.39
15	E	101	CRT	C21-C20-C19	-3.77	115.81	123.52
9	9	103	BCL	C4D-CHA-C1A	3.77	125.74	121.24
11	L	304	UQ8	C27-C28-C29	-3.76	119.01	127.62
15	e	101	CRT	C4-C5-C6	-3.76	119.63	124.91
15	J	101	CRT	C9-C10-C11	-3.76	112.30	123.20
9	L	305	BCL	C4D-CHA-C1A	3.76	125.73	121.24
9	3	101	BCL	C1D-ND-C4D	-3.76	103.67	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	101	BCL	C1C-NC-C4C	-3.76	104.96	106.68
9	u	101	BCL	CMC-C2C-C3C	-3.76	99.45	113.98
15	n	101	CRT	C10-C11-C12	-3.76	116.06	126.36
9	L	301	BCL	O2A-CGA-CBA	3.75	123.28	111.83
9	D	101	BCL	C16-C15-C13	-3.75	103.49	115.97
9	4	102	BCL	C4D-CHA-C1A	3.75	125.72	121.24
9	g	101	BCL	CHA-C1A-NA	-3.75	117.90	126.39
9	x	301	BCL	CBB-CAB-C3B	3.75	128.31	120.40
9	z	102	BCL	CMB-C2B-C1B	-3.75	119.71	125.42
9	X	102	BCL	C4D-CHA-C1A	3.75	125.71	121.24
9	J	102	BCL	CMB-C2B-C1B	-3.75	119.72	125.42
9	R	102	BCL	CHD-C1D-ND	-3.74	119.53	124.80
9	s	102	BCL	C4D-CHA-C1A	3.74	125.71	121.24
7	o	503	HEM	CAB-C3B-C2B	-3.74	116.28	128.43
9	e	102	BCL	CHA-C1A-NA	-3.74	117.93	126.39
12	A	101	PEF	C3-O3-C30	3.73	126.29	117.08
9	5	102	BCL	OBB-CAB-CBB	-3.73	111.42	119.77
9	D	101	BCL	CMB-C2B-C1B	-3.72	119.75	125.42
9	8	102	BCL	C2D-C1D-ND	3.72	113.81	110.13
9	R	102	BCL	CBB-CAB-C3B	3.72	128.25	120.40
9	B	101	BCL	CHA-C1A-NA	-3.72	117.96	126.39
15	Z	101	CRT	C18-C17-C16	3.72	123.77	118.09
9	x	305	BCL	O2D-CGD-O1D	-3.72	116.60	123.85
9	Q	101	BCL	C2D-C1D-ND	3.72	113.81	110.13
9	W	101	BCL	CHA-C1A-NA	-3.72	117.97	126.39
7	C	501	HEM	CBA-CAA-C2A	-3.72	102.25	112.53
9	h	101	BCL	C4D-CHA-C1A	3.72	125.68	121.24
9	8	102	BCL	C4D-CHA-C1A	3.72	125.68	121.24
9	u	101	BCL	CMB-C2B-C1B	-3.72	119.76	125.42
15	X	101	CRT	C9-C10-C11	3.72	133.97	123.20
9	I	101	BCL	C2D-C1D-ND	3.71	113.80	110.13
7	C	502	HEM	CHA-C1A-NA	3.71	130.59	123.86
15	E	101	CRT	C10-C9-C7	-3.71	122.07	127.28
15	e	101	CRT	C34-C33-C35	3.71	123.75	118.09
9	AD	101	BCL	C2D-C1D-ND	3.71	113.79	110.13
9	0	101	BCL	C4D-CHA-C1A	3.70	125.66	121.24
9	L	305	BCL	C7-C6-C5	-3.70	103.40	113.26
9	v	102	BCL	C2D-C1D-ND	3.70	113.79	110.13
9	3	101	BCL	C4D-CHA-C1A	3.70	125.66	121.24
9	x	301	BCL	CHD-C1D-ND	-3.70	119.60	124.80
9	x	301	BCL	C12-C11-C10	-3.70	96.72	113.28
9	R	102	BCL	OBB-CAB-CBB	-3.70	111.49	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	102	BCL	C2D-C1D-ND	3.70	113.78	110.13
12	t	303	PEF	O2-C10-O4	-3.69	115.86	122.99
9	AD	101	BCL	CHA-C1A-NA	-3.69	118.03	126.39
9	P	101	BCL	C2A-C1A-CHA	3.69	130.27	123.87
9	x	301	BCL	CHA-C1A-NA	-3.69	118.04	126.39
9	x	305	BCL	C1-O2A-CGA	3.68	125.57	116.65
14	y	403	MQ8	C26-C27-C28	-3.68	119.19	127.62
9	N	102	BCL	C7-C6-C5	-3.68	103.45	113.26
9	l	101	BCL	C2D-C1D-ND	3.68	113.77	110.13
9	Q	101	BCL	C1-O2A-CGA	3.68	125.56	116.65
9	L	303	BCL	O2D-CGD-O1D	-3.68	116.69	123.85
9	x	305	BCL	CBB-CAB-C3B	3.67	128.14	120.40
9	N	102	BCL	C4D-CHA-C1A	3.67	125.62	121.24
9	AK	101	BCL	CMC-C2C-C3C	-3.67	99.80	113.98
9	z	102	BCL	C4D-CHA-C1A	3.67	125.62	121.24
9	p	104	BCL	CHA-C1A-NA	-3.67	118.09	126.39
11	L	304	UQ8	C10-C9-C11	3.67	121.59	115.23
9	5	101	BCL	CHA-C1A-NA	-3.66	118.09	126.39
9	AK	101	BCL	CED-O2D-CGD	-3.66	107.61	115.92
15	i	101	CRT	C10-C9-C7	-3.66	122.14	127.28
9	y	401	BCL	C1-O2A-CGA	3.65	125.50	116.65
9	x	301	BCL	CMD-C2D-C1D	3.65	131.16	124.73
9	J	102	BCL	CMA-C3A-C4A	-3.65	101.96	111.77
15	G	101	CRT	C4-C5-C6	-3.65	119.78	124.91
15	U	102	CRT	C9-C10-C11	-3.65	112.62	123.20
15	Z	101	CRT	C4-C5-C6	-3.65	119.79	124.91
9	e	102	BCL	C2D-C1D-ND	3.64	113.73	110.13
9	l	101	BCL	CHB-C1B-NB	3.64	129.51	124.05
9	d	101	BCL	C4A-NA-C1A	3.64	108.34	106.68
9	l	101	BCL	CBB-CAB-C3B	3.64	128.07	120.40
15	AH	102	CRT	C21-C22-C23	-3.64	122.18	127.28
9	F	101	BCL	CMA-C3A-C4A	-3.64	102.00	111.77
9	AE	102	BCL	C7-C6-C5	-3.63	103.58	113.26
9	AE	102	BCL	OBB-CAB-CBB	-3.63	111.63	119.77
9	N	102	BCL	OBB-CAB-CBB	-3.62	111.65	119.77
15	2	101	CRT	C14-C15-C16	-3.62	112.70	123.20
9	j	101	BCL	C4D-CHA-C1A	3.62	125.56	121.24
7	C	503	HEM	CBD-CAD-C3D	-3.62	102.52	112.53
9	Q	101	BCL	OBB-CAB-CBB	-3.62	111.66	119.77
9	M	401	BCL	C12-C11-C10	-3.62	97.07	113.28
9	5	102	BCL	CMB-C2B-C1B	-3.62	119.91	125.42
9	u	101	BCL	C4D-CHA-C1A	3.61	125.56	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	CRT	C21-C22-C23	-3.61	122.21	127.28
9	j	101	BCL	CHB-C1B-NB	3.61	129.47	124.05
9	G	102	BCL	C2D-C1D-ND	3.61	113.70	110.13
9	AI	101	BCL	O2A-CGA-O1A	-3.61	114.59	123.63
9	h	101	BCL	C2D-C1D-ND	3.61	113.69	110.13
9	p	104	BCL	CGD-CBD-CAD	-3.60	99.19	110.85
9	m	103	BCL	CHD-C1D-ND	-3.60	119.74	124.80
9	4	102	BCL	CHA-C1A-NA	-3.60	118.25	126.39
9	9	103	BCL	C1-O2A-CGA	3.60	125.36	116.65
9	l	101	BCL	C11-C10-C8	-3.60	104.01	115.97
9	k	102	BCL	CHA-C1A-NA	-3.60	118.25	126.39
9	AB	101	BCL	CHA-C1A-NA	-3.59	118.25	126.39
9	AH	101	BCL	CHB-C1B-NB	3.59	129.44	124.05
9	p	102	BCL	CHD-C1D-ND	-3.59	119.75	124.80
9	W	101	BCL	C2D-C1D-ND	3.59	113.68	110.13
15	AD	102	CRT	C10-C9-C7	-3.59	122.24	127.28
9	AD	101	BCL	C16-C15-C13	-3.59	104.03	115.97
9	AB	101	BCL	C1-C2-C3	-3.59	120.32	126.20
9	L	303	BCL	CBB-CAB-C3B	3.59	127.96	120.40
9	u	101	BCL	C2D-C1D-ND	3.58	113.67	110.13
9	O	101	BCL	CHB-C1B-NB	3.58	129.42	124.05
9	V	101	BCL	C16-C15-C13	-3.58	104.07	115.97
9	0	101	BCL	OBB-CAB-CBB	-3.58	111.76	119.77
9	Z	102	BCL	C1C-NC-C4C	-3.57	105.05	106.68
9	L	305	BCL	CMB-C2B-C1B	-3.57	119.99	125.42
9	x	305	BCL	C2B-C1B-NB	-3.57	106.63	110.33
9	X	102	BCL	CMB-C2B-C1B	-3.56	119.99	125.42
9	s	102	BCL	C2A-C1A-CHA	3.56	130.05	123.87
9	k	102	BCL	CMB-C2B-C1B	-3.56	120.00	125.42
15	Z	101	CRT	C24-C23-C25	3.56	123.52	118.09
9	AB	101	BCL	CHB-C1B-NB	3.55	129.38	124.05
9	p	104	BCL	C3B-C4B-NB	-3.55	105.07	109.76
9	4	102	BCL	CMB-C2B-C1B	-3.55	120.01	125.42
9	Z	102	BCL	CMB-C2B-C1B	-3.55	120.01	125.42
9	x	305	BCL	C3D-C2D-C1D	-3.55	100.99	105.83
9	W	101	BCL	CHB-C4A-NA	-3.55	119.28	124.40
9	D	101	BCL	CHA-C1A-NA	-3.54	118.37	126.39
15	AL	101	CRT	C21-C20-C19	-3.54	116.27	123.52
9	j	101	BCL	OBB-CAB-CBB	-3.54	111.83	119.77
9	m	103	BCL	C1-C2-C3	3.54	132.00	126.20
9	x	305	BCL	CHA-C1A-NA	-3.54	118.38	126.39
9	AC	102	BCL	C4D-CHA-C1A	3.54	125.47	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	102	BCL	C1D-ND-C4D	-3.54	103.83	106.31
9	0	101	BCL	C2D-C1D-ND	3.54	113.63	110.13
9	y	401	BCL	O2A-CGA-O1A	-3.54	114.78	123.63
9	u	101	BCL	CHD-C1D-ND	-3.54	119.83	124.80
9	K	101	BCL	C16-C15-C13	-3.54	104.21	115.97
11	x	304	UQ8	C32-C33-C34	-3.54	119.53	127.62
15	y	404	CRT	C20-C19-C17	-3.53	122.32	127.28
9	I	101	BCL	O2D-CGD-O1D	-3.53	116.97	123.85
7	o	502	HEM	CHA-C1A-NA	3.53	130.26	123.86
9	N	102	BCL	C2D-C1D-ND	3.53	113.62	110.13
9	9	103	BCL	CMD-C2D-C1D	3.53	130.94	124.73
9	AK	101	BCL	C3B-C4B-NB	-3.53	105.10	109.76
10	y	402	BPH	OBB-CAB-C3B	3.53	125.89	119.99
9	i	102	BCL	CHA-C1A-NA	-3.53	118.40	126.39
14	M	403	MQ8	C26-C27-C28	-3.53	119.55	127.62
15	T	101	CRT	C13-C12-C11	3.52	123.47	118.09
7	C	503	HEM	C4C-NC-C1C	3.52	111.56	105.82
15	T	101	CRT	C10-C9-C7	-3.52	122.35	127.28
9	Z	102	BCL	OBB-CAB-CBB	-3.52	111.90	119.77
9	L	303	BCL	C6-C5-C3	3.51	122.03	113.47
9	D	101	BCL	CED-O2D-CGD	-3.51	107.94	115.92
9	w	101	BCL	CHA-C1A-NA	-3.51	118.44	126.39
9	M	401	BCL	C4A-NA-C1A	3.51	108.28	106.68
9	K	101	BCL	CMA-C3A-C4A	-3.51	102.34	111.77
9	x	303	BCL	CHA-C1A-NA	-3.51	118.45	126.39
9	5	102	BCL	C16-C15-C13	-3.51	104.31	115.97
9	y	401	BCL	CMC-C2C-C3C	-3.51	100.42	113.98
9	9	103	BCL	C11-C10-C8	-3.51	104.31	115.97
9	AA	101	BCL	C2D-C1D-ND	3.51	113.60	110.13
9	y	401	BCL	CMB-C2B-C1B	-3.50	120.08	125.42
9	AK	101	BCL	CHA-C1A-NA	-3.50	118.46	126.39
9	J	102	BCL	OBB-CAB-CBB	-3.50	111.93	119.77
9	1	101	BCL	CHD-C1D-ND	-3.50	119.88	124.80
9	f	101	BCL	C3B-C4B-NB	-3.50	105.14	109.76
9	w	101	BCL	CHD-C1D-ND	-3.50	119.88	124.80
9	F	101	BCL	OBB-CAB-CBB	-3.50	111.94	119.77
9	9	103	BCL	C2D-C1D-ND	3.50	113.59	110.13
9	Y	101	BCL	OBB-CAB-CBB	-3.50	111.94	119.77
9	O	101	BCL	C11-C10-C8	-3.49	104.35	115.97
9	X	102	BCL	CBB-CAB-C3B	3.49	127.77	120.40
9	v	102	BCL	C11-C10-C8	-3.49	104.36	115.97
9	7	101	BCL	OBB-CAB-CBB	-3.49	111.95	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	BCL	CHA-C1A-NA	-3.49	118.49	126.39
14	y	403	MQ8	O4-C4-C3	-3.49	115.07	120.67
9	Y	101	BCL	CHA-C1A-NA	-3.48	118.50	126.39
15	c	101	CRT	C27-C26-C25	-3.48	113.11	123.20
9	m	103	BCL	CHA-C1A-NA	-3.48	118.50	126.39
9	X	102	BCL	C2D-C1D-ND	3.48	113.57	110.13
15	4	101	CRT	C25-C23-C22	-3.48	113.54	119.01
15	AL	101	CRT	C32-C31-C30	-3.48	113.13	123.20
15	2	101	CRT	C13-C12-C11	3.48	123.40	118.09
9	D	102	BCL	CHB-C1B-NB	3.48	129.26	124.05
9	e	102	BCL	CHB-C1B-NB	3.47	129.26	124.05
9	m	102	BCL	C1C-NC-C4C	-3.47	105.09	106.68
9	O	101	BCL	CHA-C1A-NA	-3.47	118.53	126.39
15	J	101	CRT	C20-C19-C17	-3.47	122.41	127.28
9	l	101	BCL	CBB-CAB-C3B	3.47	127.72	120.40
9	1	101	BCL	C2D-C1D-ND	3.47	113.56	110.13
9	u	101	BCL	CMA-C3A-C4A	-3.47	102.45	111.77
15	6	101	CRT	C21-C20-C19	-3.47	116.42	123.52
9	AH	103	BCL	CBB-CAB-C3B	3.47	127.72	120.40
9	s	102	BCL	CBB-CAB-C3B	3.47	127.71	120.40
15	AD	102	CRT	C10-C11-C12	-3.47	116.86	126.36
9	K	101	BCL	CHA-C1A-NA	-3.46	118.55	126.39
9	W	101	BCL	OBB-CAB-CBB	-3.46	112.02	119.77
12	y	408	PEF	C3-C2-C1	3.46	119.86	111.78
15	6	101	CRT	C21-C22-C23	-3.46	122.42	127.28
9	L	305	BCL	OBB-CAB-CBB	-3.46	112.02	119.77
9	U	101	BCL	OBB-CAB-CBB	-3.46	112.02	119.77
9	V	101	BCL	CHA-C1A-NA	-3.46	118.56	126.39
9	1	102	BCL	CMB-C2B-C1B	-3.46	120.15	125.42
15	c	101	CRT	C14-C15-C16	-3.46	113.19	123.20
9	AI	101	BCL	OBB-CAB-CBB	-3.45	112.03	119.77
9	5	101	BCL	OBB-CAB-CBB	-3.45	112.04	119.77
9	y	401	BCL	CHA-C1A-NA	-3.45	118.58	126.39
9	AL	102	BCL	C16-C15-C13	-3.45	104.51	115.97
7	o	502	HEM	CHC-C1C-NC	3.45	128.21	124.45
9	1	102	BCL	CHB-C1B-NB	3.44	129.21	124.05
9	y	401	BCL	C3C-C4C-CHD	-3.44	116.13	123.39
9	N	102	BCL	C4A-NA-C1A	3.44	108.25	106.68
9	AH	101	BCL	CBB-CAB-C3B	3.44	127.66	120.40
9	9	103	BCL	CMB-C2B-C1B	-3.44	120.18	125.42
11	L	304	UQ8	C15-C14-C16	3.44	121.20	115.23
9	V	101	BCL	C2D-C1D-ND	3.44	113.53	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	101	BCL	O2D-CGD-O1D	-3.43	117.16	123.85
9	AJ	102	BCL	C3C-C4C-CHD	-3.43	116.15	123.39
9	J	102	BCL	CMD-C2D-C1D	3.43	130.77	124.73
9	M	401	BCL	C1-C2-C3	-3.43	120.57	126.20
9	O	101	BCL	CHD-C1D-ND	-3.43	119.98	124.80
17	AE	101	PGW	C02-O01-C1	3.42	123.89	117.85
9	9	103	BCL	CHD-C1D-ND	-3.42	119.98	124.80
9	J	102	BCL	C4A-NA-C1A	3.42	108.24	106.68
9	L	303	BCL	C2D-C1D-ND	3.42	113.51	110.13
15	4	101	CRT	C18-C17-C16	3.42	123.31	118.09
9	d	101	BCL	CHA-C1A-NA	-3.41	118.66	126.39
15	N	101	CRT	C1-C4-C5	3.41	121.84	112.98
15	AJ	101	CRT	C20-C21-C22	-3.41	116.54	123.52
9	L	305	BCL	C2D-C1D-ND	3.41	113.50	110.13
9	AI	101	BCL	O2A-CGA-CBA	3.41	122.23	111.83
15	6	101	CRT	C35-C33-C32	-3.41	113.65	119.01
9	x	303	BCL	CHB-C1B-NB	3.41	129.16	124.05
9	AL	102	BCL	CBB-CAB-C3B	3.41	127.58	120.40
9	7	101	BCL	C1-O2A-CGA	3.40	124.89	116.65
9	G	102	BCL	CHA-C1A-NA	-3.40	118.68	126.39
9	X	102	BCL	CHA-C1A-NA	-3.40	118.69	126.39
9	x	303	BCL	C3B-C4B-NB	-3.40	105.27	109.76
9	W	101	BCL	C1-O2A-CGA	3.40	124.88	116.65
9	v	102	BCL	OBb-CAB-CBB	-3.40	112.16	119.77
9	5	101	BCL	C2D-C1D-ND	3.40	113.49	110.13
15	X	101	CRT	C37-C36-C35	-3.40	120.14	124.91
9	e	102	BCL	OBb-CAB-CBB	-3.40	112.16	119.77
15	8	101	CRT	C25-C23-C22	3.40	124.35	119.01
9	X	102	BCL	CMA-C3A-C4A	-3.40	102.65	111.77
9	L	303	BCL	CGD-CBD-CAD	-3.40	99.85	110.85
9	AB	101	BCL	CMC-C2C-C3C	-3.39	100.86	113.98
9	AB	101	BCL	C2D-C1D-ND	3.39	113.48	110.13
15	k	101	CRT	C26-C25-C23	-3.39	117.07	126.36
9	L	305	BCL	C11-C10-C8	-3.39	104.70	115.97
9	M	401	BCL	OBd-CAD-C3D	3.39	136.33	128.42
9	m	102	BCL	CHA-C1A-NA	-3.39	118.72	126.39
9	x	303	BCL	C2A-C1A-CHA	3.38	129.74	123.87
9	AD	101	BCL	CMB-C2B-C1B	-3.38	120.27	125.42
9	K	101	BCL	C1C-NC-C4C	-3.38	105.14	106.68
9	Q	101	BCL	CMB-C2B-C1B	-3.38	120.27	125.42
9	T	102	BCL	C7-C6-C5	-3.38	104.26	113.26
7	o	501	HEM	CAA-CBA-CGA	-3.38	104.70	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	102	BCL	CMB-C2B-C1B	-3.38	120.28	125.42
9	c	102	BCL	C16-C15-C13	-3.38	104.74	115.97
9	7	101	BCL	C1C-NC-C4C	-3.38	105.14	106.68
9	K	101	BCL	C4A-NA-C1A	3.38	108.22	106.68
9	A	102	BCL	OBB-CAB-CBB	-3.37	112.21	119.77
15	AJ	101	CRT	C21-C20-C19	3.37	130.42	123.52
9	p	104	BCL	C4D-CHA-C1A	3.37	125.27	121.24
9	T	102	BCL	C1-O2A-CGA	3.37	124.81	116.65
9	m	103	BCL	OBB-CAB-CBB	-3.37	112.23	119.77
10	x	302	BPH	O1D-CGD-CBD	-3.37	119.62	124.72
15	2	101	CRT	C20-C19-C17	-3.36	122.56	127.28
9	N	102	BCL	C16-C15-C13	-3.36	104.79	115.97
9	e	102	BCL	C11-C12-C13	-3.36	104.79	115.97
9	c	102	BCL	CHA-C1A-NA	-3.36	118.79	126.39
15	A	103	CRT	C21-C20-C19	-3.36	116.65	123.52
7	C	503	HEM	C3C-C2C-C1C	3.36	110.22	107.05
9	AE	104	BCL	CMC-C2C-C3C	-3.36	101.00	113.98
17	S	101	PGW	O01-C1-C2	3.35	117.07	111.09
7	o	501	HEM	C3B-C4B-NB	-3.35	107.06	109.47
9	U	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
9	AH	103	BCL	C4D-CHA-C1A	3.35	125.24	121.24
9	M	401	BCL	C16-C15-C13	-3.35	104.83	115.97
9	AI	101	BCL	C1C-NC-C4C	-3.35	105.15	106.68
9	j	101	BCL	CHA-C1A-NA	-3.35	118.81	126.39
9	y	401	BCL	CBB-CAB-C3B	3.35	127.46	120.40
9	Z	102	BCL	CHB-C1B-NB	3.35	129.07	124.05
15	z	101	CRT	C21-C20-C19	-3.35	116.67	123.52
7	o	503	HEM	CHB-C1B-NB	3.35	128.50	124.37
9	T	102	BCL	CHD-C1D-ND	-3.34	120.10	124.80
9	U	101	BCL	CBB-CAB-C3B	3.34	127.45	120.40
9	D	102	BCL	C2A-C1A-CHA	3.34	129.66	123.87
9	z	102	BCL	C16-C15-C13	-3.34	104.87	115.97
9	x	305	BCL	C7-C6-C5	-3.34	104.37	113.26
9	9	103	BCL	CHA-C1A-NA	-3.33	118.84	126.39
15	9	102	CRT	C10-C11-C12	-3.33	117.22	126.36
9	v	102	BCL	CHA-C1A-NA	-3.33	118.85	126.39
9	i	102	BCL	CMB-C2B-C1B	-3.33	120.35	125.42
15	E	101	CRT	C4-C5-C6	-3.33	120.24	124.91
9	x	305	BCL	C2A-C1A-CHA	3.33	129.65	123.87
15	P	102	CRT	C32-C31-C30	-3.33	113.55	123.20
15	AJ	101	CRT	C34-C33-C35	3.33	123.17	118.09
15	U	102	CRT	C35-C33-C32	-3.33	113.78	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AC	101	CRT	C18-C17-C16	3.33	123.17	118.09
9	8	102	BCL	OBB-CAB-CBB	-3.33	112.32	119.77
9	k	102	BCL	OBB-CAB-CBB	-3.33	112.32	119.77
15	AJ	101	CRT	C36-C35-C33	3.32	130.92	125.89
15	J	101	CRT	C21-C20-C19	-3.32	116.72	123.52
15	T	101	CRT	C34-C33-C35	3.32	123.16	118.09
7	C	502	HEM	CHC-C1C-NC	3.32	128.07	124.45
9	G	102	BCL	C2C-C3C-C4C	-3.32	96.37	101.34
9	f	101	BCL	C1D-ND-C4D	-3.32	103.98	106.31
9	AE	104	BCL	CHB-C1B-NB	3.32	129.02	124.05
15	n	101	CRT	C20-C19-C17	-3.32	122.63	127.28
9	AE	104	BCL	C1C-NC-C4C	-3.31	105.17	106.68
16	t	302	PO4	O4-P-O2	3.31	118.22	107.91
9	K	101	BCL	OBB-CAB-CBB	-3.31	112.36	119.77
9	A	102	BCL	C1C-NC-C4C	-3.31	105.17	106.68
9	AK	101	BCL	C2A-C1A-CHA	3.31	129.60	123.87
9	p	102	BCL	C2D-C1D-ND	3.30	113.40	110.13
11	x	304	UQ8	C40-C39-C38	-3.30	115.14	123.63
9	T	102	BCL	CHA-C1A-NA	-3.30	118.91	126.39
9	AI	101	BCL	CHA-C1A-NA	-3.30	118.91	126.39
9	AL	102	BCL	OBB-CAB-CBB	-3.30	112.38	119.77
9	x	305	BCL	C12-C11-C10	-3.30	98.49	113.28
9	l	101	BCL	CMC-C2C-C3C	-3.30	101.23	113.98
15	f	102	CRT	C14-C15-C16	-3.30	113.65	123.20
9	T	102	BCL	CMC-C2C-C3C	-3.29	101.24	113.98
9	j	101	BCL	C2D-C1D-ND	3.29	113.39	110.13
9	AE	102	BCL	CHA-C1A-NA	-3.29	118.93	126.39
9	T	102	BCL	C3B-C4B-NB	-3.29	105.41	109.76
9	f	101	BCL	CHA-C1A-NA	-3.29	118.94	126.39
9	9	103	BCL	C7-C6-C5	-3.29	104.49	113.26
9	1	101	BCL	CAA-CBA-CGA	-3.29	103.86	113.21
9	z	102	BCL	CHA-C1A-NA	-3.29	118.94	126.39
9	x	303	BCL	CMD-C2D-C1D	3.29	130.52	124.73
9	AL	102	BCL	CHB-C4A-NA	-3.29	119.65	124.40
9	x	301	BCL	CAA-CBA-CGA	-3.29	103.87	113.21
9	R	102	BCL	C11-C10-C8	-3.29	105.05	115.97
9	D	101	BCL	O2A-CGA-O1A	-3.28	115.41	123.63
9	5	101	BCL	CBB-CAB-C3B	3.28	127.32	120.40
15	s	101	CRT	C21-C22-C23	-3.28	122.67	127.28
9	S	102	BCL	C2D-C1D-ND	3.28	113.37	110.13
9	K	101	BCL	O2A-CGA-O1A	-3.28	115.43	123.63
9	y	401	BCL	C11-C10-C8	-3.28	105.07	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	101	BCL	CHB-C1B-NB	3.28	128.97	124.05
9	A	102	BCL	CMC-C2C-C3C	-3.28	101.31	113.98
9	N	102	BCL	CHA-C1A-NA	-3.27	118.98	126.39
10	L	302	BPH	O1D-CGD-CBD	-3.27	119.76	124.72
9	3	101	BCL	CHA-C1A-NA	-3.27	118.98	126.39
12	M	407	PEF	O2P-P-O1P	3.27	127.66	112.44
9	c	102	BCL	CHD-C1D-ND	-3.27	120.20	124.80
7	o	502	HEM	C3A-C4A-NA	-3.27	104.90	110.14
9	5	101	BCL	O2A-CGA-O1A	-3.27	115.46	123.63
12	t	303	PEF	O3-C30-C31	3.27	126.24	112.38
9	AH	103	BCL	CHA-C1A-NA	-3.26	119.00	126.39
9	O	101	BCL	C3C-C4C-CHD	-3.26	116.51	123.39
9	M	401	BCL	C6-C5-C3	-3.26	105.52	113.47
15	E	101	CRT	C18-C17-C16	3.26	123.07	118.09
9	A	102	BCL	CHA-C1A-NA	-3.26	119.01	126.39
9	y	401	BCL	C4D-CHA-C1A	3.26	125.13	121.24
9	8	102	BCL	C16-C15-C13	-3.26	105.13	115.97
9	D	101	BCL	CHB-C1B-NB	3.26	128.94	124.05
9	AJ	102	BCL	CHA-C1A-NA	-3.26	119.01	126.39
9	p	102	BCL	CMD-C2D-C1D	3.26	130.47	124.73
9	8	102	BCL	CGD-CBD-CAD	-3.26	100.30	110.85
9	G	102	BCL	C3B-C4B-NB	-3.26	105.46	109.76
9	c	102	BCL	C7-C6-C5	-3.26	104.58	113.26
7	o	504	HEM	CHD-C4C-C3C	-3.26	119.72	125.21
14	y	403	MQ8	C14-C13-C15	3.26	120.88	115.23
9	l	102	BCL	C3B-C4B-NB	-3.25	105.47	109.76
9	d	101	BCL	CHD-C1D-ND	-3.25	120.23	124.80
12	t	301	PEF	O4P-C4-C5	-3.25	97.28	109.17
9	9	103	BCL	CMC-C2C-C3C	-3.25	101.43	113.98
9	c	102	BCL	O2A-C1-C2	3.25	120.60	108.11
9	p	104	BCL	CMA-C3A-C4A	-3.25	103.05	111.77
7	C	503	HEM	CHC-C1C-NC	3.24	127.98	124.45
9	Z	102	BCL	C2A-C1A-CHA	3.24	129.49	123.87
9	0	101	BCL	CBB-CAB-C3B	3.24	127.23	120.40
9	y	401	BCL	C3B-C4B-NB	-3.24	105.48	109.76
7	C	502	HEM	C3A-C4A-NA	-3.24	104.95	110.14
9	8	102	BCL	CMA-C3A-C4A	-3.24	103.08	111.77
9	D	102	BCL	CMC-C2C-C3C	-3.23	101.48	113.98
9	AH	101	BCL	CHD-C1D-ND	-3.23	120.26	124.80
9	Q	101	BCL	CED-O2D-CGD	-3.23	108.59	115.92
9	AD	101	BCL	C4A-NA-C1A	3.23	108.15	106.68
9	x	305	BCL	C3C-C2C-C1C	3.23	107.08	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	102	BCL	CBB-CAB-C3B	3.22	127.20	120.40
9	R	102	BCL	CHB-C1B-NB	3.22	128.88	124.05
15	4	101	CRT	C24-C23-C25	3.22	123.01	118.09
9	V	101	BCL	C2C-C3C-C4C	-3.22	96.52	101.34
9	O	101	BCL	C3B-C4B-NB	-3.22	105.51	109.76
11	x	304	UQ8	C37-C38-C39	-3.22	120.26	127.62
15	Z	101	CRT	C16-C17-C19	-3.21	113.95	119.01
9	0	101	BCL	CMC-C2C-C3C	-3.21	101.55	113.98
9	c	102	BCL	OBB-CAB-CBB	-3.21	112.57	119.77
9	r	101	BCL	CHB-C1B-NB	3.21	128.87	124.05
9	m	102	BCL	C2B-C1B-NB	-3.21	106.99	110.33
9	F	101	BCL	C1-O2A-CGA	3.21	124.43	116.65
9	F	101	BCL	CBB-CAB-C3B	3.21	127.17	120.40
9	L	303	BCL	C3B-C4B-NB	-3.21	105.53	109.76
9	AE	102	BCL	C4A-NA-C1A	3.20	108.14	106.68
9	AK	101	BCL	CGD-CBD-CAD	-3.20	100.47	110.85
9	F	101	BCL	CHB-C1B-NB	3.20	128.85	124.05
9	w	101	BCL	CHB-C1B-NB	3.20	128.85	124.05
9	O	101	BCL	C3D-C2D-C1D	-3.20	101.47	105.83
9	Z	102	BCL	C4D-CHA-C1A	3.20	125.06	121.24
9	M	401	BCL	CMD-C2D-C1D	3.20	130.36	124.73
9	y	401	BCL	CHB-C1B-NB	3.20	128.84	124.05
9	j	101	BCL	C3B-C4B-NB	-3.20	105.54	109.76
15	z	101	CRT	C9-C10-C11	-3.19	113.95	123.20
9	f	101	BCL	C2B-C1B-NB	-3.19	107.02	110.33
9	p	102	BCL	O2A-CGA-O1A	-3.19	115.64	123.63
9	AK	101	BCL	C1C-NC-C4C	-3.19	105.22	106.68
9	P	101	BCL	C3B-C4B-NB	-3.19	105.55	109.76
15	AJ	101	CRT	C4-C5-C6	-3.19	120.43	124.91
15	y	404	CRT	C13-C12-C14	-3.19	117.65	122.82
15	s	101	CRT	C34-C33-C35	3.19	122.96	118.09
9	p	104	BCL	CHB-C1B-NB	3.19	128.83	124.05
9	z	102	BCL	C4A-NA-C1A	3.19	108.13	106.68
9	x	303	BCL	C3D-C2D-C1D	-3.19	101.48	105.83
9	AE	104	BCL	C7-C6-C5	-3.19	104.77	113.26
15	A	103	CRT	C10-C9-C7	-3.18	122.81	127.28
15	n	101	CRT	C9-C10-C11	3.18	132.42	123.20
9	d	101	BCL	C2D-C1D-ND	3.18	113.27	110.13
9	S	102	BCL	CHD-C1D-ND	-3.18	120.33	124.80
9	Q	101	BCL	C16-C15-C13	-3.18	105.40	115.97
9	G	102	BCL	OBB-CAB-CBB	-3.18	112.65	119.77
9	3	101	BCL	C3B-C4B-NB	-3.18	105.57	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	p	102	BCL	CHB-C1B-NB	3.18	128.81	124.05
9	S	102	BCL	CMA-C3A-C4A	-3.18	103.24	111.77
9	P	101	BCL	C2C-C3C-C4C	-3.17	96.58	101.34
9	w	101	BCL	CED-O2D-CGD	-3.17	108.71	115.92
9	P	101	BCL	O2A-CGA-O1A	-3.17	115.69	123.63
9	7	101	BCL	CMB-C2B-C1B	-3.17	120.59	125.42
9	p	104	BCL	CBB-CAB-C3B	3.17	127.09	120.40
9	m	102	BCL	CHD-C1D-ND	-3.17	120.34	124.80
9	r	101	BCL	O2A-CGA-O1A	-3.17	115.70	123.63
9	p	104	BCL	O2A-CGA-O1A	-3.17	115.70	123.63
11	L	304	UQ8	C7-C6-C1	-3.17	119.46	124.89
9	N	102	BCL	CMD-C2D-C1D	3.17	130.31	124.73
9	V	101	BCL	OBB-CAB-CBB	-3.17	112.68	119.77
9	K	101	BCL	C11-C10-C8	-3.16	105.45	115.97
9	L	303	BCL	C3C-C4C-CHD	-3.16	116.72	123.39
9	k	102	BCL	C3D-C2D-C1D	-3.16	101.52	105.83
15	2	101	CRT	C26-C27-C28	-3.16	122.84	127.28
9	T	102	BCL	C2C-C3C-C4C	-3.16	96.60	101.34
15	AD	102	CRT	C18-C17-C16	3.16	122.92	118.09
9	V	101	BCL	CHB-C1B-NB	3.16	128.79	124.05
15	k	101	CRT	C15-C14-C12	-3.16	122.85	127.28
15	J	101	CRT	C8-C7-C6	3.16	122.91	118.09
9	AE	102	BCL	CBB-CAB-C3B	3.16	127.06	120.40
9	p	104	BCL	CHD-C1D-ND	-3.16	120.36	124.80
9	8	102	BCL	CBB-CAB-C3B	3.15	127.05	120.40
9	7	101	BCL	CBB-CAB-C3B	3.15	127.05	120.40
9	i	102	BCL	OBB-CAB-CBB	-3.15	112.71	119.77
9	z	102	BCL	CBB-CAB-C3B	3.15	127.05	120.40
9	AH	103	BCL	CED-O2D-CGD	-3.15	108.76	115.92
9	P	101	BCL	CHB-C4A-NA	-3.15	119.85	124.40
9	e	102	BCL	C16-C15-C13	-3.15	105.49	115.97
15	v	101	CRT	C13-C12-C11	3.15	122.90	118.09
9	N	102	BCL	C1C-NC-C4C	-3.15	105.24	106.68
15	P	102	CRT	C14-C15-C16	-3.15	114.08	123.20
9	AC	102	BCL	C1-C2-C3	-3.15	121.04	126.20
7	C	501	HEM	CAA-CBA-CGA	-3.15	105.32	113.67
9	G	102	BCL	C2A-C1A-CHA	3.15	129.33	123.87
9	F	101	BCL	C2D-C1D-ND	3.15	113.24	110.13
9	P	101	BCL	C2D-C1D-ND	3.15	113.24	110.13
9	AH	103	BCL	CMC-C2C-C3C	-3.14	101.82	113.98
9	AH	103	BCL	CMB-C2B-C1B	-3.14	120.63	125.42
15	AD	102	CRT	C21-C20-C19	-3.14	117.09	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	102	BCL	C3B-C4B-NB	-3.14	105.61	109.76
15	AL	101	CRT	C26-C27-C28	-3.14	122.87	127.28
10	M	402	BPH	OBB-CAB-CBB	-3.14	113.49	120.19
9	AI	101	BCL	C2A-C1A-CHA	3.14	129.32	123.87
9	l	101	BCL	CHD-C1D-ND	-3.14	120.38	124.80
15	i	101	CRT	C21-C22-C23	-3.14	122.87	127.28
9	D	101	BCL	C3C-C4C-CHD	-3.14	116.77	123.39
15	6	101	CRT	C14-C15-C16	-3.14	114.10	123.20
9	1	101	BCL	OBB-CAB-CBB	-3.14	112.74	119.77
9	z	102	BCL	CHD-C1D-ND	-3.14	120.39	124.80
9	J	102	BCL	CHA-C1A-NA	-3.14	119.29	126.39
9	p	102	BCL	C7-C6-C5	-3.14	104.90	113.26
9	I	101	BCL	C2B-C1B-NB	-3.14	107.07	110.33
15	A	103	CRT	C4-C5-C6	-3.13	120.51	124.91
9	5	101	BCL	C2B-C1B-NB	-3.13	107.08	110.33
9	D	101	BCL	C7-C6-C5	-3.13	104.91	113.26
9	9	103	BCL	CHB-C1B-NB	3.13	128.75	124.05
9	e	102	BCL	C4D-CHA-C1A	3.13	124.98	121.24
9	I	101	BCL	CMC-C2C-C3C	-3.13	101.88	113.98
9	D	102	BCL	C16-C15-C13	-3.13	105.56	115.97
15	4	101	CRT	C27-C26-C25	-3.13	114.14	123.20
15	A	103	CRT	C31-C32-C33	-3.13	122.89	127.28
15	k	101	CRT	C32-C31-C30	-3.13	114.14	123.20
9	M	401	BCL	C2A-C1A-CHA	3.12	129.28	123.87
9	AC	102	BCL	CHD-C1D-ND	-3.12	120.41	124.80
9	G	102	BCL	C4D-CHA-C1A	3.12	124.97	121.24
9	5	101	BCL	CMC-C2C-C3C	-3.12	101.92	113.98
9	O	101	BCL	CMC-C2C-C3C	-3.12	101.92	113.98
9	1	102	BCL	C11-C12-C13	-3.12	105.60	115.97
9	O	101	BCL	C7-C6-C5	-3.12	104.95	113.26
15	A	103	CRT	C34-C33-C35	3.12	122.85	118.09
9	v	102	BCL	C7-C6-C5	-3.11	104.96	113.26
9	U	101	BCL	CHC-C1C-NC	3.11	128.89	124.40
9	Z	102	BCL	CMC-C2C-C3C	-3.11	101.95	113.98
9	V	101	BCL	C3B-C4B-NB	-3.11	105.65	109.76
14	M	403	MQ8	C35-C33-C32	-3.11	114.19	121.17
9	c	102	BCL	C1-O2A-CGA	3.11	124.18	116.65
9	D	102	BCL	OBB-CAB-CBB	-3.11	112.81	119.77
9	u	101	BCL	C3B-C4B-NB	-3.11	105.66	109.76
15	N	101	CRT	C32-C31-C30	-3.11	114.20	123.20
9	L	305	BCL	C6-C5-C3	-3.10	105.91	113.47
9	P	101	BCL	OBB-CAB-CBB	-3.10	112.82	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	p	103	CRT	C20-C19-C17	-3.10	122.93	127.28
9	D	102	BCL	C3B-C4B-NB	-3.10	105.67	109.76
9	l	101	BCL	O2A-CGA-O1A	-3.10	115.88	123.63
15	c	101	CRT	C18-C17-C16	3.10	122.82	118.09
9	l	101	BCL	CHA-C1A-NA	-3.10	119.38	126.39
9	f	101	BCL	CBB-CAB-C3B	3.10	126.93	120.40
9	l	101	BCL	C16-C15-C13	-3.09	105.68	115.97
9	p	102	BCL	C16-C15-C13	-3.09	105.68	115.97
9	p	104	BCL	C2A-C1A-CHA	3.09	129.23	123.87
9	m	103	BCL	OBD-CAD-C3D	3.09	135.64	128.42
10	L	302	BPH	O2A-CGA-CBA	3.09	121.26	111.83
9	I	101	BCL	CHB-C1B-NB	3.09	128.69	124.05
9	j	101	BCL	CBB-CAB-C3B	3.09	126.92	120.40
15	i	101	CRT	C14-C15-C16	-3.09	114.25	123.20
7	o	504	HEM	C4C-NC-C1C	3.09	110.86	105.82
15	P	102	CRT	C31-C32-C33	-3.09	122.95	127.28
9	4	102	BCL	C16-C15-C13	-3.09	105.70	115.97
9	m	102	BCL	CMC-C2C-C3C	-3.09	102.04	113.98
15	AJ	101	CRT	C26-C27-C28	-3.09	122.95	127.28
7	C	503	HEM	CHD-C4C-C3C	-3.09	120.00	125.21
9	L	305	BCL	CBB-CAB-C3B	3.09	126.91	120.40
9	T	102	BCL	C1-C2-C3	-3.08	121.14	126.20
9	B	101	BCL	C3D-C2D-C1D	-3.08	101.62	105.83
9	h	101	BCL	O2A-CGA-O1A	-3.08	115.92	123.63
9	L	301	BCL	O2D-CGD-O1D	-3.08	117.85	123.85
7	C	503	HEM	CAB-C3B-C4B	3.08	138.00	124.39
9	w	101	BCL	CMC-C2C-C3C	-3.08	102.08	113.98
9	AA	101	BCL	O2A-CGA-O1A	-3.08	115.93	123.63
9	B	101	BCL	C1-O2A-CGA	3.08	124.10	116.65
9	u	101	BCL	CHA-C1A-NA	-3.07	119.43	126.39
10	M	402	BPH	O2A-CGA-CBA	3.07	121.21	111.83
9	AJ	102	BCL	CMC-C2C-C3C	-3.07	102.11	113.98
9	AH	101	BCL	O2A-CGA-O1A	-3.07	115.94	123.63
9	w	101	BCL	C3D-C2D-C1D	-3.07	101.64	105.83
15	Z	101	CRT	C25-C23-C22	-3.07	114.18	119.01
9	y	401	BCL	CMA-C3A-C4A	-3.07	103.52	111.77
9	Y	101	BCL	C1D-ND-C4D	-3.07	104.16	106.31
9	x	303	BCL	CGD-CBD-CAD	-3.07	100.91	110.85
9	AH	103	BCL	C16-C15-C13	-3.07	105.77	115.97
9	W	101	BCL	CGD-CBD-CAD	-3.07	100.92	110.85
9	4	102	BCL	CHB-C1B-NB	3.07	128.65	124.05
9	U	101	BCL	C7-C6-C5	-3.06	105.09	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	404	CRT	C15-C14-C12	-3.06	122.99	127.28
9	S	102	BCL	CHC-C1C-NC	3.06	128.81	124.40
9	4	102	BCL	C7-C6-C5	-3.06	105.11	113.26
9	B	101	BCL	C1C-NC-C4C	-3.05	105.29	106.68
15	4	101	CRT	C21-C20-C19	-3.05	117.27	123.52
9	G	102	BCL	CGD-CBD-CAD	-3.05	100.96	110.85
9	8	102	BCL	CMC-C2C-C3C	-3.05	102.18	113.98
9	AC	102	BCL	CMC-C2C-C3C	-3.05	102.18	113.98
9	g	101	BCL	CGD-CBD-CAD	-3.05	100.97	110.85
9	D	102	BCL	C3D-C2D-C1D	-3.05	101.67	105.83
9	V	101	BCL	CBB-CAB-C3B	3.05	126.83	120.40
9	P	101	BCL	CBB-CAB-C3B	3.05	126.82	120.40
9	5	102	BCL	CBB-CAB-C3B	3.05	126.82	120.40
15	J	101	CRT	C34-C33-C35	3.04	122.74	118.09
9	AC	102	BCL	CHA-C1A-NA	-3.04	119.50	126.39
9	AI	101	BCL	CBB-CAB-C3B	3.04	126.82	120.40
9	W	101	BCL	O2A-CGA-O1A	-3.04	116.02	123.63
9	O	101	BCL	CMA-C3A-C4A	-3.04	103.61	111.77
9	g	101	BCL	C2A-C1A-CHA	3.04	129.14	123.87
9	c	102	BCL	CBB-CAB-C3B	3.04	126.81	120.40
9	AA	101	BCL	C7-C6-C5	-3.04	105.17	113.26
9	X	102	BCL	OBB-CAB-CBB	-3.04	112.97	119.77
9	d	101	BCL	OBB-CAB-CBB	-3.04	112.97	119.77
15	X	101	CRT	C20-C21-C22	-3.03	117.31	123.52
9	O	101	BCL	O2A-CGA-O1A	-3.03	116.04	123.63
9	AI	101	BCL	C2B-C1B-NB	-3.03	107.18	110.33
9	L	305	BCL	O2A-CGA-O1A	-3.03	116.05	123.63
9	B	101	BCL	CHB-C1B-NB	3.03	128.59	124.05
9	X	102	BCL	O2A-CGA-O1A	-3.03	116.05	123.63
9	T	102	BCL	C1C-NC-C4C	-3.03	105.30	106.68
9	A	102	BCL	C2B-C1B-NB	-3.03	107.19	110.33
15	AL	101	CRT	C14-C15-C16	-3.03	114.42	123.20
9	8	102	BCL	C7-C6-C5	-3.03	105.19	113.26
9	k	102	BCL	CMD-C2D-C1D	3.03	130.06	124.73
9	z	102	BCL	C11-C10-C8	-3.03	105.90	115.97
9	AC	102	BCL	C3B-C4B-NB	-3.02	105.77	109.76
15	z	101	CRT	C27-C26-C25	-3.02	114.44	123.20
9	AA	101	BCL	C2B-C1B-NB	-3.02	107.19	110.33
9	v	102	BCL	C3B-C4B-NB	-3.02	105.77	109.76
15	X	101	CRT	C15-C14-C12	-3.02	123.04	127.28
15	y	404	CRT	C36-C35-C33	3.02	130.46	125.89
9	AE	104	BCL	CHD-C1D-ND	-3.02	120.55	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	102	BCL	C3B-C4B-NB	-3.02	105.78	109.76
9	AE	102	BCL	C2A-C1A-CHA	3.02	129.11	123.87
9	V	101	BCL	CMC-C2C-C3C	-3.02	102.31	113.98
9	L	301	BCL	CMD-C2D-C1D	3.02	130.04	124.73
9	x	303	BCL	CBB-CAB-C3B	3.01	126.75	120.40
9	L	301	BCL	C2D-C1D-ND	3.01	113.11	110.13
14	M	403	MQ8	C34-C33-C35	3.01	120.46	115.23
9	L	301	BCL	CBC-CAC-C3C	3.01	119.80	113.41
9	r	101	BCL	OBB-CAB-CBB	-3.01	113.03	119.77
9	AJ	102	BCL	OBB-CAB-CBB	-3.01	113.03	119.77
9	P	101	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
7	o	503	HEM	CBD-CAD-C3D	-3.01	104.22	112.53
9	I	101	BCL	O2A-CGA-O1A	-3.01	116.11	123.63
9	R	102	BCL	C3D-C2D-C1D	-3.00	101.73	105.83
9	P	101	BCL	CHB-C1B-NB	3.00	128.56	124.05
9	d	101	BCL	C2B-C1B-NB	-3.00	107.21	110.33
9	AB	101	BCL	C3B-C4B-NB	-3.00	105.80	109.76
9	u	101	BCL	OBB-CAB-CBB	-3.00	113.05	119.77
9	M	401	BCL	CGD-CBD-CAD	-3.00	101.13	110.85
15	P	102	CRT	C34-C33-C35	3.00	122.67	118.09
9	h	101	BCL	CMC-C2C-C3C	-3.00	102.39	113.98
9	w	101	BCL	CMD-C2D-C1D	3.00	130.01	124.73
9	x	303	BCL	CBC-CAC-C3C	3.00	119.77	113.41
15	J	101	CRT	C29-C28-C30	3.00	122.67	118.09
9	AH	101	BCL	CHC-C1C-NC	3.00	128.72	124.40
9	I	101	BCL	C3B-C4B-NB	-3.00	105.81	109.76
9	B	101	BCL	C3B-C4B-NB	-2.99	105.81	109.76
9	AA	101	BCL	OBB-CAB-CBB	-2.99	113.06	119.77
9	m	103	BCL	C11-C10-C8	-2.99	106.02	115.97
9	k	102	BCL	CHB-C4A-NA	-2.99	120.08	124.40
9	AE	104	BCL	OBB-CAB-CBB	-2.99	113.07	119.77
9	G	102	BCL	CBB-CAB-C3B	2.99	126.70	120.40
12	H	304	PEF	O3-C3-C2	2.99	117.01	108.40
9	5	101	BCL	CHB-C4A-NA	-2.99	120.08	124.40
7	C	501	HEM	C3B-C4B-NB	-2.99	107.32	109.47
9	3	101	BCL	CMD-C2D-C1D	2.99	129.99	124.73
9	AC	102	BCL	CHB-C1B-NB	2.99	128.53	124.05
9	F	101	BCL	CHA-C1A-NA	-2.99	119.63	126.39
9	D	102	BCL	CBB-CAB-C3B	2.99	126.69	120.40
9	1	102	BCL	C16-C15-C13	-2.98	106.04	115.97
15	J	101	CRT	C4-C5-C6	2.98	129.10	124.91
9	y	401	BCL	CHD-C1D-ND	-2.98	120.60	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	101	BCL	C2A-C1A-CHA	2.98	129.04	123.87
9	5	101	BCL	CHB-C1B-NB	2.98	128.52	124.05
15	AC	101	CRT	C27-C26-C25	-2.98	114.56	123.20
9	k	102	BCL	O2A-C1-C2	2.98	119.58	108.11
9	7	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
9	W	101	BCL	CBB-CAB-C3B	2.98	126.68	120.40
15	U	102	CRT	C6-C7-C9	-2.98	114.32	119.01
9	Y	101	BCL	CBB-CAB-C3B	2.98	126.68	120.40
9	m	103	BCL	CHB-C4A-NA	-2.98	120.10	124.40
15	y	404	CRT	C14-C15-C16	-2.97	114.58	123.20
9	O	101	BCL	CBB-CAB-C3B	2.97	126.67	120.40
9	3	101	BCL	CBB-CAB-C3B	2.97	126.67	120.40
9	l	101	BCL	C4A-NA-C1A	2.97	108.03	106.68
15	6	101	CRT	C10-C9-C7	-2.97	123.11	127.28
9	J	102	BCL	C2B-C1B-NB	-2.97	107.25	110.33
15	9	102	CRT	C29-C28-C30	2.97	122.62	118.09
9	9	103	BCL	CBB-CAB-C3B	2.97	126.66	120.40
15	AE	103	CRT	C14-C15-C16	-2.97	114.60	123.20
9	l	101	BCL	C7-C6-C5	-2.97	105.35	113.26
15	AE	103	CRT	C20-C19-C17	-2.97	123.11	127.28
9	w	101	BCL	OBB-CAB-CBB	-2.97	113.12	119.77
9	j	101	BCL	C7-C6-C5	-2.97	105.35	113.26
9	x	305	BCL	C16-C15-C13	-2.97	106.11	115.97
9	9	103	BCL	C3D-C2D-C1D	-2.96	101.79	105.83
9	AC	102	BCL	C16-C15-C13	-2.96	106.12	115.97
15	N	101	CRT	C15-C14-C12	-2.96	123.12	127.28
9	AD	101	BCL	OBB-CAB-CBB	-2.96	113.14	119.77
9	4	102	BCL	C1-O2A-CGA	2.96	123.82	116.65
9	AI	101	BCL	CHB-C1B-NB	2.96	128.49	124.05
9	8	102	BCL	CHD-C1D-ND	-2.96	120.64	124.80
15	E	101	CRT	C34-C33-C35	2.96	122.61	118.09
10	M	402	BPH	CED-O2D-CGD	2.96	122.62	115.92
9	I	101	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
9	AH	101	BCL	CED-O2D-CGD	-2.95	109.21	115.92
14	M	403	MQ8	C20-C18-C17	-2.95	114.54	121.17
9	e	102	BCL	CMC-C2C-C3C	-2.95	102.57	113.98
15	f	102	CRT	C13-C12-C11	2.95	122.60	118.09
7	C	503	HEM	C2C-C1C-NC	-2.95	104.18	109.64
9	M	401	BCL	CHB-C1B-NB	2.95	128.47	124.05
15	Z	101	CRT	C32-C31-C30	-2.95	114.65	123.20
9	AE	102	BCL	C3C-C2C-C1C	2.95	106.63	101.87
9	h	101	BCL	CBB-CAB-C3B	2.95	126.62	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	CRT	C21-C20-C19	-2.95	117.49	123.52
9	Z	102	BCL	C4A-NA-C1A	2.95	108.02	106.68
9	v	102	BCL	CBB-CAB-C3B	2.94	126.61	120.40
15	n	101	CRT	C13-C12-C14	-2.94	118.05	122.82
12	H	301	PEF	C3-C2-C1	-2.94	104.92	111.78
16	t	302	PO4	O4-P-O1	-2.94	100.55	110.95
9	J	102	BCL	C11-C10-C8	-2.94	106.19	115.97
9	J	102	BCL	C2A-C1A-CHA	2.94	128.97	123.87
7	C	502	HEM	C4D-ND-C1D	2.94	108.69	105.21
9	x	305	BCL	CMC-C2C-C1C	-2.94	103.88	111.77
9	0	101	BCL	C7-C6-C5	-2.94	105.44	113.26
9	AE	104	BCL	C3D-C2D-C1D	-2.94	101.82	105.83
15	6	101	CRT	C8-C7-C6	2.93	122.57	118.09
9	AH	103	BCL	C2B-C1B-NB	-2.93	107.28	110.33
9	k	102	BCL	C16-C15-C13	-2.93	106.21	115.97
15	Z	101	CRT	C13-C12-C11	2.93	122.57	118.09
15	Z	101	CRT	C34-C33-C35	2.93	122.57	118.09
15	9	102	CRT	C20-C19-C17	-2.93	123.17	127.28
9	z	102	BCL	C3D-C2D-C1D	-2.93	101.83	105.83
9	U	101	BCL	C16-C15-C13	-2.93	106.23	115.97
9	z	102	BCL	CMC-C2C-C3C	-2.93	102.66	113.98
15	y	404	CRT	C15-C14-C12	-2.93	123.17	127.28
9	I	101	BCL	C11-C10-C8	-2.93	106.24	115.97
9	5	101	BCL	C6-C5-C3	-2.93	106.34	113.47
15	v	101	CRT	C27-C26-C25	-2.92	114.73	123.20
9	m	102	BCL	CHB-C1B-NB	2.92	128.44	124.05
15	T	101	CRT	C27-C26-C25	-2.92	114.73	123.20
9	k	102	BCL	CBB-CAB-C3B	2.92	126.56	120.40
9	5	102	BCL	C1C-NC-C4C	-2.92	105.35	106.68
9	X	102	BCL	C16-C15-C13	-2.92	106.25	115.97
15	i	101	CRT	C34-C33-C35	2.92	122.55	118.09
9	AE	104	BCL	CBB-CAB-C3B	2.92	126.56	120.40
15	y	404	CRT	C21-C22-C23	-2.92	123.19	127.28
9	5	101	BCL	C11-C12-C13	-2.92	106.27	115.97
9	k	102	BCL	CHD-C1D-ND	-2.92	120.70	124.80
15	e	101	CRT	C8-C7-C6	2.92	122.54	118.09
9	K	101	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
9	AD	101	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
9	m	102	BCL	O2A-CGA-O1A	-2.92	116.33	123.63
9	AH	101	BCL	C2D-C1D-ND	2.91	113.01	110.13
9	AB	101	BCL	CBB-CAB-C3B	2.91	126.55	120.40
15	U	102	CRT	C32-C31-C30	-2.91	114.76	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	502	HEM	CAA-CBA-CGA	-2.91	105.94	113.67
9	AB	101	BCL	C1-O2A-CGA	2.91	123.70	116.65
15	AH	102	CRT	C24-C23-C25	2.91	122.53	118.09
9	R	102	BCL	CHA-C1A-NA	-2.91	119.80	126.39
9	B	101	BCL	CMC-C2C-C3C	-2.91	102.73	113.98
9	R	102	BCL	CMC-C2C-C3C	-2.91	102.74	113.98
9	d	101	BCL	CBB-CAB-C3B	2.91	126.53	120.40
9	L	301	BCL	CGD-CBD-CAD	-2.91	101.44	110.85
9	0	101	BCL	C1C-NC-C4C	-2.91	105.35	106.68
9	p	102	BCL	C2B-C1B-NB	-2.91	107.31	110.33
9	g	101	BCL	C3C-C4C-CHD	-2.91	117.27	123.39
9	v	102	BCL	C4D-CHA-C1A	2.91	124.71	121.24
9	4	102	BCL	OBB-CAB-CBB	-2.90	113.26	119.77
9	0	101	BCL	C1-C2-C3	-2.90	121.44	126.20
9	AE	104	BCL	C3C-C4C-CHD	-2.90	117.27	123.39
9	AE	104	BCL	C3B-C4B-NB	-2.90	105.93	109.76
7	C	501	HEM	O2D-CGD-CBD	2.90	123.17	114.00
15	c	101	CRT	C21-C20-C19	-2.90	117.58	123.52
9	S	102	BCL	OBB-CAB-CBB	-2.90	113.27	119.77
9	y	401	BCL	OBD-CAD-C3D	2.90	135.20	128.42
9	AK	101	BCL	O2A-CGA-O1A	-2.90	116.37	123.63
9	Q	101	BCL	CBB-CAB-C3B	2.90	126.52	120.40
9	F	101	BCL	CMC-C2C-C3C	-2.90	102.77	113.98
15	A	103	CRT	C1-C4-C5	2.90	120.51	112.98
9	w	101	BCL	C3B-C4B-NB	-2.90	105.93	109.76
9	y	401	BCL	C2D-C1D-ND	2.90	113.00	110.13
15	s	101	CRT	C31-C32-C33	-2.90	123.21	127.28
9	j	101	BCL	CMC-C2C-C3C	-2.90	102.78	113.98
7	o	503	HEM	CAB-C3B-C4B	2.90	137.19	124.39
9	AK	101	BCL	OBB-CAB-CBB	-2.90	113.28	119.77
7	o	501	HEM	CHB-C1B-NB	2.90	127.95	124.37
9	AB	101	BCL	OBB-CAB-CBB	-2.89	113.29	119.77
9	A	102	BCL	C3D-C2D-C1D	-2.89	101.88	105.83
9	u	101	BCL	CHB-C1B-NB	2.89	128.39	124.05
7	o	502	HEM	C4D-ND-C1D	2.89	108.63	105.21
15	y	404	CRT	C13-C12-C11	2.89	122.51	118.09
15	v	101	CRT	C20-C19-C17	-2.89	123.22	127.28
9	l	101	BCL	CMA-C3A-C4A	-2.89	104.00	111.77
9	AL	102	BCL	CBC-CAC-C3C	2.89	119.54	113.41
9	5	102	BCL	CMC-C2C-C3C	-2.89	102.82	113.98
9	g	101	BCL	C2B-C1B-NB	-2.89	107.33	110.33
11	x	304	UQ8	C12-C13-C14	-2.89	121.02	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	304	UQ8	C6-C1-C2	2.89	121.45	119.17
11	x	304	UQ8	O4-C4-C5	2.88	126.37	116.64
7	o	502	HEM	C4A-NA-C1A	2.88	110.52	105.82
9	4	102	BCL	O2A-CGA-O1A	-2.88	116.42	123.63
9	z	102	BCL	C7-C6-C5	-2.88	105.58	113.26
9	x	301	BCL	CMC-C2C-C3C	-2.88	102.84	113.98
15	T	101	CRT	C9-C10-C11	-2.88	114.85	123.20
9	0	101	BCL	CHB-C1B-NB	2.88	128.37	124.05
9	K	101	BCL	C2B-C1B-NB	-2.88	107.34	110.33
15	AC	101	CRT	C21-C20-C19	-2.88	117.63	123.52
9	Z	102	BCL	C16-C15-C13	-2.88	106.40	115.97
15	4	101	CRT	C35-C33-C32	2.88	123.54	119.01
9	z	102	BCL	C3C-C4C-CHD	-2.88	117.33	123.39
9	x	305	BCL	C6-C5-C3	-2.88	106.46	113.47
14	y	403	MQ8	C15-C13-C12	-2.88	114.71	121.17
9	G	102	BCL	C7-C6-C5	-2.88	105.60	113.26
9	P	101	BCL	CBC-CAC-C3C	2.88	119.51	113.41
9	AE	102	BCL	C2B-C1B-NB	-2.87	107.34	110.33
9	5	101	BCL	C3C-C4C-CHD	-2.87	117.33	123.39
12	y	406	PEF	C2-O2-C10	-2.87	112.78	117.85
9	D	101	BCL	C3B-C4B-NB	-2.87	105.97	109.76
9	m	103	BCL	CBB-CAB-C3B	2.87	126.45	120.40
9	x	301	BCL	C2D-C1D-ND	2.87	112.97	110.13
7	C	504	HEM	C3B-C2B-C1B	2.86	108.56	106.41
9	5	101	BCL	C3B-C4B-NB	-2.86	105.98	109.76
9	N	102	BCL	CMC-C2C-C3C	-2.86	102.91	113.98
15	v	101	CRT	C15-C14-C12	-2.86	123.26	127.28
9	N	102	BCL	CHB-C1B-NB	2.86	128.34	124.05
15	R	101	CRT	C21-C20-C19	-2.86	117.67	123.52
9	u	101	BCL	CGD-CBD-CAD	-2.86	101.59	110.85
9	k	102	BCL	CMC-C2C-C3C	-2.86	102.94	113.98
15	2	101	CRT	C10-C9-C7	-2.86	123.27	127.28
15	P	102	CRT	C26-C25-C23	-2.85	118.53	126.36
12	t	303	PEF	C3-O3-C30	2.85	124.12	117.08
9	AL	102	BCL	C3B-C4B-NB	-2.85	105.99	109.76
15	9	102	CRT	C27-C26-C25	-2.85	114.94	123.20
9	v	102	BCL	CHB-C4A-NA	-2.85	120.28	124.40
9	h	101	BCL	C2B-C1B-NB	-2.85	107.37	110.33
9	B	101	BCL	CBB-CAB-C3B	2.85	126.41	120.40
15	f	102	CRT	C4-C5-C6	-2.85	120.91	124.91
9	M	401	BCL	CAA-CBA-CGA	-2.85	105.12	113.21
9	0	101	BCL	CMA-C3A-C4A	-2.85	104.12	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	101	BCL	C4A-NA-C1A	2.85	107.98	106.68
9	Y	101	BCL	O2A-CGA-O1A	-2.85	116.51	123.63
9	P	101	BCL	CHD-C1D-ND	-2.84	120.80	124.80
9	D	102	BCL	C11-C12-C13	-2.84	106.52	115.97
9	c	102	BCL	C3D-C2D-C1D	-2.84	101.95	105.83
9	4	102	BCL	CBB-CAB-C3B	2.84	126.39	120.40
9	A	102	BCL	CHD-C1D-ND	-2.84	120.80	124.80
9	8	102	BCL	CHB-C1B-NB	2.84	128.31	124.05
9	AH	103	BCL	C7-C6-C5	-2.84	105.69	113.26
9	5	102	BCL	C3D-C2D-C1D	-2.84	101.95	105.83
9	F	101	BCL	CBC-CAC-C3C	2.84	119.44	113.41
15	9	102	CRT	C10-C9-C7	2.84	131.25	127.28
9	9	103	BCL	OBB-CAB-CBB	-2.83	113.42	119.77
9	3	101	BCL	C1-C2-C3	2.83	130.84	126.20
15	N	101	CRT	C13-C12-C11	2.83	122.41	118.09
9	S	102	BCL	O2A-CGA-O1A	-2.83	116.55	123.63
15	A	103	CRT	C26-C27-C28	-2.83	123.31	127.28
15	AL	101	CRT	C34-C33-C35	2.83	122.41	118.09
9	B	101	BCL	OBB-CAB-CBB	-2.83	113.43	119.77
9	F	101	BCL	C4A-NA-C1A	2.83	107.97	106.68
9	c	102	BCL	CHB-C1B-NB	2.83	128.29	124.05
11	L	304	UQ8	C35-C34-C36	2.83	120.14	115.23
9	J	102	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
9	AC	102	BCL	C1C-NC-C4C	-2.83	105.39	106.68
9	w	101	BCL	C1-O2A-CGA	2.83	123.50	116.65
14	y	403	MQ8	C7-C8-C9	-2.83	116.75	120.24
15	AE	103	CRT	C13-C12-C11	2.83	122.41	118.09
9	r	101	BCL	C7-C6-C5	-2.82	105.73	113.26
9	L	303	BCL	CAA-CBA-CGA	2.82	121.22	113.21
9	G	102	BCL	C16-C15-C13	-2.82	106.59	115.97
15	AJ	101	CRT	C13-C12-C11	2.82	122.39	118.09
15	M	404	CRT	C20-C19-C17	-2.82	123.33	127.28
9	S	102	BCL	C2B-C1B-NB	-2.82	107.40	110.33
9	0	101	BCL	C2C-C3C-C4C	-2.82	97.12	101.34
9	7	101	BCL	CMC-C2C-C3C	-2.82	103.09	113.98
9	i	102	BCL	C16-C15-C13	-2.82	106.60	115.97
9	T	102	BCL	CHB-C1B-NB	2.82	128.28	124.05
9	U	101	BCL	CHB-C1B-NB	2.82	128.28	124.05
7	o	503	HEM	CHC-C4B-C3B	2.82	130.69	125.07
7	C	504	HEM	CAC-C3C-C4C	-2.82	118.10	124.82
9	k	102	BCL	C2B-C1B-NB	-2.81	107.41	110.33
9	AA	101	BCL	C16-C15-C13	-2.81	106.61	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	y	403	MQ8	C21-C22-C23	-2.81	121.18	127.62
15	M	404	CRT	C36-C35-C33	-2.81	121.64	125.89
9	I	101	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
9	L	305	BCL	CHA-C1A-NA	-2.81	120.02	126.39
9	O	101	BCL	OBB-CAB-CBB	-2.81	113.47	119.77
15	AH	102	CRT	C9-C10-C11	-2.81	115.05	123.20
9	O	101	BCL	C2A-C1A-CHA	2.81	128.75	123.87
9	s	102	BCL	CHB-C1B-NB	2.81	128.27	124.05
9	f	101	BCL	C1-O2A-CGA	2.81	123.46	116.65
11	x	304	UQ8	C30-C29-C28	-2.81	116.41	123.63
15	T	101	CRT	C29-C28-C30	2.81	122.38	118.09
15	z	101	CRT	C24-C23-C25	2.81	122.38	118.09
15	AH	102	CRT	C4-C5-C6	-2.81	120.97	124.91
9	h	101	BCL	OBB-CAB-CBB	-2.81	113.48	119.77
9	i	102	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
9	p	102	BCL	OBB-CAB-CBB	-2.81	113.48	119.77
11	x	304	UQ8	C26-C24-C23	-2.81	114.87	121.17
9	y	401	BCL	C7-C6-C5	-2.81	105.78	113.26
9	x	305	BCL	OBB-CAB-CBB	-2.81	113.49	119.77
9	s	102	BCL	C16-C15-C13	-2.80	106.64	115.97
9	D	102	BCL	C4A-NA-C1A	2.80	107.96	106.68
9	Z	102	BCL	C3B-C4B-NB	-2.80	106.06	109.76
9	Y	101	BCL	CHB-C4A-NA	-2.80	120.36	124.40
9	l	101	BCL	CGD-CBD-CAD	-2.80	101.79	110.85
9	3	101	BCL	CAA-CBA-CGA	-2.80	105.26	113.21
15	G	101	CRT	C9-C10-C11	-2.80	115.09	123.20
9	x	301	BCL	C11-C10-C8	-2.80	106.67	115.97
15	c	101	CRT	C21-C22-C23	-2.79	123.36	127.28
9	R	102	BCL	C3B-C4B-NB	-2.79	106.07	109.76
9	AI	101	BCL	CMC-C2C-C3C	-2.79	103.19	113.98
9	AL	102	BCL	CMC-C2C-C3C	-2.79	103.20	113.98
9	N	102	BCL	CMA-C3A-C4A	-2.79	104.28	111.77
9	4	102	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
9	O	101	BCL	CMB-C2B-C3B	2.79	134.47	125.67
7	C	503	HEM	CHB-C4A-NA	2.79	128.91	123.86
9	s	102	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
15	s	101	CRT	C26-C25-C23	-2.78	118.73	126.36
9	1	102	BCL	CMC-C2C-C3C	-2.78	103.22	113.98
9	3	101	BCL	C7-C6-C5	-2.78	105.84	113.26
9	U	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	z	102	BCL	CMD-C2D-C1D	2.78	129.63	124.73
9	T	102	BCL	C16-C15-C13	-2.78	106.71	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	503	HEM	CAD-C3D-C4D	2.78	129.55	124.70
9	N	102	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	W	101	BCL	CMB-C2B-C1B	-2.78	121.18	125.42
9	AE	102	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
9	s	102	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
15	2	101	CRT	C4-C5-C6	-2.78	121.01	124.91
15	2	101	CRT	C31-C32-C33	-2.78	123.38	127.28
9	p	102	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
7	C	502	HEM	CMC-C2C-C1C	-2.78	119.84	124.73
9	l	101	BCL	C1C-NC-C4C	-2.78	105.41	106.68
9	D	101	BCL	CMC-C2C-C3C	-2.78	103.25	113.98
7	C	504	HEM	CAA-CBA-CGA	-2.77	106.31	113.67
12	t	303	PEF	O5-C30-C31	-2.77	114.95	124.77
9	AA	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
9	AC	102	BCL	C4A-NA-C1A	2.77	107.94	106.68
9	K	101	BCL	CHB-C1B-NB	2.77	128.21	124.05
15	J	101	CRT	C32-C31-C30	-2.77	115.17	123.20
9	N	102	BCL	CHD-C1D-ND	-2.77	120.90	124.80
9	AL	102	BCL	CAA-CBA-CGA	-2.77	105.34	113.21
9	AH	103	BCL	CHD-C1D-ND	-2.77	120.91	124.80
9	8	102	BCL	CHA-C1A-NA	-2.77	120.12	126.39
9	T	102	BCL	C11-C10-C8	-2.77	106.76	115.97
15	e	101	CRT	C15-C14-C12	-2.77	123.40	127.28
9	5	102	BCL	CAA-CBA-CGA	-2.77	105.35	113.21
9	S	102	BCL	CHB-C1B-NB	2.77	128.20	124.05
15	8	101	CRT	C5-C6-C7	-2.76	121.72	125.89
9	F	101	BCL	C16-C15-C13	-2.76	106.78	115.97
9	AB	101	BCL	C11-C10-C8	-2.76	106.78	115.97
9	d	101	BCL	C2A-C3A-C4A	-2.76	97.40	101.87
15	AC	101	CRT	C14-C15-C16	-2.76	115.19	123.20
9	AK	101	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
9	L	301	BCL	CMB-C2B-C1B	-2.76	121.22	125.42
9	l	101	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
9	p	104	BCL	C16-C15-C13	-2.76	106.80	115.97
9	e	102	BCL	O2A-CGA-O1A	-2.76	116.73	123.63
12	y	408	PEF	C2-O2-C10	-2.76	112.98	117.85
9	h	101	BCL	CHB-C4A-NA	-2.76	120.42	124.40
9	AH	103	BCL	C4A-NA-C1A	2.76	107.94	106.68
9	p	104	BCL	C11-C12-C13	-2.75	106.81	115.97
9	3	101	BCL	CHB-C4A-NA	-2.75	120.42	124.40
9	M	401	BCL	OBB-CAB-CBB	-2.75	113.61	119.77
9	v	102	BCL	C3D-C2D-C1D	-2.75	102.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
9	0	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
7	o	503	HEM	O2D-CGD-CBD	2.75	122.69	114.00
15	i	101	CRT	C4-C5-C6	-2.75	121.05	124.91
9	J	102	BCL	C3C-C4C-CHD	-2.75	117.60	123.39
9	AJ	102	BCL	CHD-C1D-ND	-2.75	120.94	124.80
15	AC	101	CRT	C26-C27-C28	-2.75	123.42	127.28
9	l	101	BCL	C2A-C1A-CHA	2.74	128.63	123.87
9	AH	101	BCL	C7-C6-C5	-2.74	105.95	113.26
10	x	302	BPH	CMA-C3A-C4A	-2.74	108.70	114.61
9	I	101	BCL	OBB-CAB-CBB	-2.74	113.63	119.77
9	j	101	BCL	CED-O2D-CGD	-2.74	109.69	115.92
9	0	101	BCL	C3B-C4B-NB	-2.74	106.14	109.76
9	Z	102	BCL	C2B-C1B-NB	-2.74	107.48	110.33
7	C	504	HEM	CHA-C1A-NA	2.74	128.83	123.86
9	w	101	BCL	C2A-C1A-CHA	2.74	128.62	123.87
9	AK	101	BCL	CHB-C1B-NB	2.74	128.16	124.05
9	g	101	BCL	CHB-C1B-NB	2.74	128.16	124.05
15	AE	103	CRT	C9-C10-C11	-2.74	115.26	123.20
9	S	102	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
9	j	101	BCL	O2A-CGA-O1A	-2.74	116.78	123.63
9	x	305	BCL	O2A-CGA-CBA	2.74	120.19	111.83
15	E	101	CRT	C35-C33-C32	-2.74	114.70	119.01
15	U	102	CRT	C15-C14-C12	-2.74	123.44	127.28
9	O	101	BCL	C16-C15-C13	-2.74	106.87	115.97
9	AD	101	BCL	CHB-C1B-NB	2.74	128.16	124.05
9	AC	102	BCL	C3D-C2D-C1D	-2.74	102.10	105.83
9	G	102	BCL	C12-C11-C10	-2.74	101.02	113.28
7	C	502	HEM	C4A-C3A-C2A	2.73	109.95	106.82
9	A	102	BCL	C7-C6-C5	-2.73	105.98	113.26
12	H	304	PEF	O2-C10-O4	-2.73	117.72	122.99
9	m	102	BCL	CBB-CAB-C3B	2.73	126.16	120.40
9	Q	101	BCL	CBC-CAC-C3C	2.73	119.21	113.41
9	m	103	BCL	O2A-CGA-O1A	-2.73	116.80	123.63
7	C	504	HEM	C4C-NC-C1C	2.73	110.27	105.82
9	r	101	BCL	C2D-C1D-ND	2.73	112.83	110.13
9	I	101	BCL	C4A-NA-C1A	2.73	107.92	106.68
15	s	101	CRT	C35-C33-C32	-2.73	114.72	119.01
15	G	101	CRT	C21-C20-C19	-2.73	117.94	123.52
15	4	101	CRT	C10-C9-C7	-2.73	123.46	127.28
12	m	101	PEF	O3-C3-C2	2.73	116.25	108.40
9	O	101	BCL	C2B-C1B-NB	-2.73	107.50	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	y	403	MQ8	C24-C23-C25	2.72	119.96	115.23
9	l	101	BCL	CMC-C2C-C3C	-2.72	103.45	113.98
15	i	101	CRT	C21-C20-C19	-2.72	117.95	123.52
9	l	101	BCL	C3B-C4B-NB	-2.72	106.17	109.76
9	x	305	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
9	y	401	BCL	CAA-CBA-CGA	-2.72	105.48	113.21
9	p	102	BCL	C1-O2A-CGA	2.72	123.24	116.65
9	5	102	BCL	CBC-CAC-C3C	2.72	119.19	113.41
9	0	101	BCL	C5-C3-C2	2.72	127.27	121.17
9	AK	101	BCL	C11-C10-C8	-2.72	106.92	115.97
9	Z	102	BCL	CHD-C1D-ND	-2.72	120.97	124.80
9	g	101	BCL	C12-C11-C10	-2.72	101.09	113.28
9	AC	102	BCL	OBB-CAB-CBB	-2.72	113.68	119.77
15	AD	102	CRT	C14-C15-C16	2.72	131.07	123.20
15	AL	101	CRT	C24-C23-C25	2.72	122.24	118.09
11	x	304	UQ8	O4-C4-C3	-2.72	113.37	123.64
9	x	305	BCL	C11-C10-C8	-2.71	106.94	115.97
9	F	101	BCL	C11-C12-C13	-2.71	106.95	115.97
7	C	504	HEM	CHD-C1D-ND	2.71	127.34	124.42
9	A	102	BCL	CHB-C1B-NB	2.71	128.12	124.05
15	c	101	CRT	C24-C23-C25	2.71	122.23	118.09
9	f	101	BCL	C16-C15-C13	-2.71	106.96	115.97
15	2	101	CRT	C18-C17-C16	2.71	122.23	118.09
15	z	101	CRT	C18-C17-C16	2.71	122.22	118.09
7	C	502	HEM	C4A-NA-C1A	2.71	110.23	105.82
15	Z	101	CRT	C26-C27-C28	-2.71	123.48	127.28
15	N	101	CRT	C21-C20-C19	-2.71	117.98	123.52
9	Z	102	BCL	C3D-C2D-C1D	-2.71	102.14	105.83
10	y	402	BPH	O2A-CGA-CBA	2.71	120.08	111.83
15	U	102	CRT	C13-C12-C11	2.71	122.22	118.09
9	V	101	BCL	CHD-C1D-ND	-2.71	121.00	124.80
9	J	102	BCL	C7-C6-C5	-2.70	106.05	113.26
9	j	101	BCL	C2B-C1B-NB	-2.70	107.52	110.33
9	G	102	BCL	CMC-C2C-C3C	-2.70	103.53	113.98
9	S	102	BCL	C7-C6-C5	-2.70	106.06	113.26
15	n	101	CRT	C26-C27-C28	-2.70	123.49	127.28
9	R	102	BCL	CMD-C2D-C1D	2.70	129.49	124.73
9	AA	101	BCL	C2C-C3C-C4C	-2.70	97.29	101.34
9	F	101	BCL	CHD-C1D-ND	-2.70	121.00	124.80
9	W	101	BCL	CMC-C2C-C3C	-2.70	103.54	113.98
9	I	101	BCL	CGD-CBD-CAD	-2.70	102.10	110.85
15	E	101	CRT	C8-C7-C6	2.70	122.21	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AE	104	BCL	C1-O2A-CGA	2.70	123.19	116.65
9	j	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
15	G	101	CRT	C31-C30-C28	-2.70	118.97	126.36
15	R	101	CRT	C32-C31-C30	-2.70	115.39	123.20
10	x	302	BPH	C1-C2-C3	-2.70	121.78	126.20
11	x	304	UQ8	C7-C6-C5	-2.70	115.38	118.52
9	AI	101	BCL	C4A-NA-C1A	2.69	107.91	106.68
9	D	102	BCL	CMA-C3A-C4A	-2.69	104.53	111.77
15	4	101	CRT	C29-C28-C30	2.69	122.20	118.09
9	AI	101	BCL	CMD-C2D-C3D	2.69	133.86	127.69
9	X	102	BCL	C7-C6-C5	-2.69	106.09	113.26
9	G	102	BCL	C11-C10-C8	-2.69	107.02	115.97
9	9	103	BCL	C2B-C1B-NB	-2.69	107.54	110.33
9	Z	102	BCL	C7-C6-C5	-2.69	106.09	113.26
9	AL	102	BCL	CHD-C1D-ND	-2.69	121.02	124.80
9	s	102	BCL	C11-C12-C13	-2.69	107.03	115.97
9	L	303	BCL	C1C-NC-C4C	2.69	107.91	106.68
15	i	101	CRT	C32-C31-C30	-2.69	115.41	123.20
9	A	102	BCL	CBB-CAB-C3B	2.69	126.07	120.40
9	P	101	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
9	h	101	BCL	C3B-C4B-NB	-2.69	106.21	109.76
9	r	101	BCL	CMC-C2C-C3C	-2.69	103.60	113.98
15	f	102	CRT	C31-C30-C28	2.69	133.73	126.36
15	2	101	CRT	C11-C12-C14	-2.69	114.78	119.01
9	g	101	BCL	CBB-CAB-C3B	2.68	126.06	120.40
9	AL	102	BCL	CMD-C2D-C1D	2.68	129.46	124.73
9	AA	101	BCL	CHB-C1B-NB	2.68	128.07	124.05
9	i	102	BCL	C1-O2A-CGA	2.68	123.15	116.65
9	7	101	BCL	CMA-C3A-C4A	-2.68	104.56	111.77
9	O	101	BCL	C3C-C2C-C1C	2.68	106.20	101.87
9	z	102	BCL	C3C-C2C-C1C	2.68	106.20	101.87
9	3	101	BCL	OBB-CAB-CBB	-2.68	113.76	119.77
14	M	403	MQ8	C21-C22-C23	-2.68	121.49	127.62
15	AJ	101	CRT	C20-C19-C17	2.68	131.04	127.28
9	p	104	BCL	OBB-CAB-CBB	-2.68	113.77	119.77
15	AH	102	CRT	C5-C6-C7	-2.68	121.84	125.89
9	AC	102	BCL	C11-C10-C8	-2.68	107.06	115.97
15	p	103	CRT	C24-C23-C25	2.68	122.18	118.09
15	AJ	101	CRT	C9-C10-C11	2.68	130.95	123.20
7	o	503	HEM	C4D-ND-C1D	2.68	108.38	105.21
9	K	101	BCL	C11-C12-C13	-2.67	107.08	115.97
9	T	102	BCL	C3D-C2D-C1D	-2.67	102.18	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	4	102	BCL	C12-C11-C10	-2.67	101.30	113.28
9	R	102	BCL	C2B-C1B-NB	-2.67	107.56	110.33
9	R	102	BCL	C16-C15-C13	-2.67	107.09	115.97
9	p	102	BCL	C3B-C4B-NB	-2.67	106.24	109.76
9	R	102	BCL	C2C-C3C-C4C	-2.67	97.35	101.34
15	k	101	CRT	C10-C9-C7	-2.67	123.54	127.28
9	8	102	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
9	J	102	BCL	C16-C15-C13	-2.66	107.11	115.97
15	AE	103	CRT	C29-C28-C30	2.66	122.16	118.09
17	S	101	PGW	O03-C01-C02	2.66	116.07	108.40
15	P	102	CRT	C13-C12-C11	2.66	122.15	118.09
9	p	104	BCL	C7-C6-C5	-2.66	106.17	113.26
9	u	101	BCL	C3C-C4C-CHD	-2.66	117.78	123.39
9	d	101	BCL	CHC-C1C-NC	2.66	128.24	124.40
10	y	402	BPH	CMC-C2C-C1C	-2.66	108.88	114.61
9	g	101	BCL	CMC-C2C-C3C	-2.66	103.71	113.98
9	AA	101	BCL	CBB-CAB-C3B	2.66	126.00	120.40
15	U	102	CRT	C20-C19-C17	-2.66	123.55	127.28
9	8	102	BCL	C3B-C4B-NB	-2.66	106.25	109.76
9	M	401	BCL	CHD-C1D-ND	-2.66	121.06	124.80
15	p	103	CRT	C14-C15-C16	-2.66	115.50	123.20
9	l	101	BCL	CMD-C2D-C1D	2.66	129.41	124.73
9	1	101	BCL	CHA-C1A-NA	-2.66	120.38	126.39
9	c	102	BCL	C11-C12-C13	-2.65	107.14	115.97
9	AJ	102	BCL	C2D-C1D-ND	2.65	112.75	110.13
7	C	503	HEM	CAA-CBA-CGA	-2.65	106.63	113.67
9	g	101	BCL	C16-C15-C13	-2.65	107.15	115.97
9	L	303	BCL	CMB-C2B-C1B	-2.65	121.38	125.42
9	1	101	BCL	CMB-C2B-C3B	2.65	134.04	125.67
9	s	102	BCL	CMC-C2C-C3C	-2.65	103.73	113.98
9	k	102	BCL	C3B-C4B-NB	-2.65	106.26	109.76
9	5	102	BCL	C4D-CHA-C1A	2.65	124.40	121.24
9	X	102	BCL	CHD-C1D-ND	-2.65	121.08	124.80
9	F	101	BCL	C3B-C4B-NB	-2.65	106.27	109.76
15	AD	102	CRT	C15-C16-C17	2.65	133.62	126.36
9	L	305	BCL	C1D-CHD-C4C	-2.65	120.24	126.62
9	w	101	BCL	C16-C15-C13	-2.65	107.17	115.97
9	k	102	BCL	CAA-CBA-CGA	-2.64	105.70	113.21
7	o	504	HEM	CHB-C1B-NB	2.64	127.64	124.37
15	AC	101	CRT	C9-C10-C11	-2.64	115.54	123.20
9	AK	101	BCL	C3C-C4C-CHD	-2.64	117.82	123.39
9	D	101	BCL	C11-C12-C13	-2.64	107.18	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	102	CRT	C18-C17-C16	2.64	122.12	118.09
9	W	101	BCL	C4D-CHA-C1A	2.64	124.39	121.24
9	Q	101	BCL	C2C-C3C-C4C	-2.64	97.38	101.34
9	g	101	BCL	OBb-CAB-CBB	-2.64	113.86	119.77
15	U	102	CRT	C20-C21-C22	-2.64	118.12	123.52
9	Q	101	BCL	C3B-C4B-NB	-2.64	106.28	109.76
15	P	102	CRT	C9-C10-C11	-2.64	115.56	123.20
9	K	101	BCL	C2A-C1A-CHA	2.64	128.44	123.87
9	5	101	BCL	CHD-C1D-ND	-2.64	121.09	124.80
9	AE	102	BCL	CHD-C1D-ND	-2.64	121.09	124.80
7	o	503	HEM	CMD-C2D-C1D	2.64	129.15	125.03
9	Z	102	BCL	C11-C10-C8	-2.64	107.20	115.97
9	g	101	BCL	C3B-C4B-NB	-2.64	106.28	109.76
9	R	102	BCL	C1-O2A-CGA	2.63	123.03	116.65
9	X	102	BCL	C1C-NC-C4C	-2.63	105.48	106.68
9	p	104	BCL	CHB-C4A-NA	-2.63	120.60	124.40
9	3	101	BCL	C3D-C2D-C1D	-2.63	102.24	105.83
9	1	101	BCL	C4D-CHA-C1A	2.63	124.39	121.24
9	AE	102	BCL	CMC-C2C-C3C	-2.63	103.80	113.98
9	P	101	BCL	CMB-C2B-C3B	2.63	133.97	125.67
9	w	101	BCL	C3C-C4C-CHD	-2.63	117.84	123.39
9	AC	102	BCL	CBB-CAB-C3B	2.63	125.95	120.40
9	R	102	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
9	p	104	BCL	C3C-C2C-C1C	2.63	106.12	101.87
9	AK	101	BCL	CBB-CAB-C3B	2.63	125.95	120.40
9	x	301	BCL	C3B-C4B-NB	-2.63	106.29	109.76
12	t	301	PEF	C3-O3-C30	2.63	123.57	117.08
9	p	104	BCL	CHC-C1C-NC	2.63	128.19	124.40
9	m	103	BCL	C2A-C1A-CHA	2.63	128.43	123.87
15	A	103	CRT	C18-C17-C16	2.63	122.10	118.09
9	AJ	102	BCL	C4D-CHA-C1A	2.63	124.38	121.24
9	D	101	BCL	C2B-C1B-NB	-2.62	107.61	110.33
9	O	101	BCL	C11-C12-C13	-2.62	107.24	115.97
9	X	102	BCL	CMC-C2C-C3C	-2.62	103.84	113.98
15	y	404	CRT	C26-C27-C28	-2.62	123.60	127.28
9	5	102	BCL	C6-C5-C3	-2.62	107.08	113.47
7	o	502	HEM	CHD-C4C-C3C	-2.62	120.79	125.21
9	A	102	BCL	C3C-C4C-CHD	-2.62	117.87	123.39
10	M	402	BPH	OBb-CAB-C3B	2.62	124.37	119.99
9	1	101	BCL	C11-C10-C8	-2.62	107.25	115.97
9	L	303	BCL	C3D-C2D-C1D	-2.62	102.25	105.83
15	v	101	CRT	C26-C25-C23	-2.62	119.18	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AH	101	BCL	C3B-C4B-NB	-2.62	106.30	109.76
9	3	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
9	z	102	BCL	C2B-C1B-NB	-2.62	107.61	110.33
9	8	102	BCL	OBD-CAD-C3D	2.62	134.54	128.42
9	B	101	BCL	C1D-CHD-C4C	-2.62	120.31	126.62
9	i	102	BCL	CBB-CAB-C3B	2.61	125.91	120.40
7	C	504	HEM	C4C-C3C-C2C	2.61	109.08	106.81
9	AD	101	BCL	C2B-C1B-NB	-2.61	107.61	110.33
9	M	401	BCL	CMB-C2B-C3B	2.61	133.91	125.67
9	y	401	BCL	C2A-C1A-CHA	2.61	128.40	123.87
9	h	101	BCL	C11-C10-C8	-2.61	107.28	115.97
15	6	101	CRT	C20-C19-C17	-2.61	123.61	127.28
9	g	101	BCL	C1C-NC-C4C	-2.61	105.49	106.68
9	AD	101	BCL	CMC-C2C-C3C	-2.61	103.89	113.98
9	AJ	102	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
11	L	304	UQ8	C45-C44-C43	-2.61	114.83	122.66
9	Y	101	BCL	C7-C6-C5	-2.61	106.31	113.26
9	Y	101	BCL	C2B-C1B-NB	-2.61	107.62	110.33
15	s	101	CRT	C36-C35-C33	2.61	129.83	125.89
9	x	305	BCL	CHB-C1B-NB	2.61	127.96	124.05
7	C	502	HEM	CHB-C4A-NA	2.61	128.59	123.86
9	D	102	BCL	CMB-C2B-C3B	2.61	133.89	125.67
9	p	104	BCL	CMC-C2C-C3C	-2.61	103.91	113.98
9	c	102	BCL	C2A-C1A-CHA	2.60	128.39	123.87
7	o	503	HEM	C4C-NC-C1C	2.60	110.07	105.82
7	o	504	HEM	CHD-C1D-ND	2.60	127.22	124.42
9	g	101	BCL	O2A-CGA-O1A	-2.60	117.12	123.63
9	r	101	BCL	CHB-C4A-NA	-2.60	120.64	124.40
9	j	101	BCL	CHD-C1D-ND	-2.60	121.14	124.80
15	4	101	CRT	C14-C15-C16	-2.60	115.67	123.20
9	3	101	BCL	C2B-C1B-NB	-2.60	107.63	110.33
9	D	102	BCL	CHC-C1C-NC	2.60	128.15	124.40
15	4	101	CRT	C20-C21-C22	-2.60	118.20	123.52
9	R	102	BCL	C7-C6-C5	-2.60	106.34	113.26
9	k	102	BCL	C1C-NC-C4C	-2.60	105.49	106.68
15	6	101	CRT	C9-C10-C11	-2.60	115.67	123.20
14	M	403	MQ8	C24-C23-C25	2.60	119.73	115.23
9	l	101	BCL	CHB-C1B-NB	2.60	127.94	124.05
15	U	102	CRT	C24-C23-C22	-2.59	118.61	122.82
15	f	102	CRT	C1-C4-C5	2.59	119.72	112.98
9	f	101	BCL	CMC-C2C-C3C	-2.59	103.96	113.98
11	L	304	UQ8	C40-C39-C38	-2.59	116.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AD	101	BCL	C3C-C4C-CHD	-2.59	117.94	123.39
9	L	301	BCL	C11-C10-C8	-2.59	107.36	115.97
9	9	103	BCL	C3B-C4B-NB	-2.59	106.34	109.76
14	y	403	MQ8	C2M-C2-C3	-2.59	120.20	124.45
9	K	101	BCL	C3C-C2C-C1C	2.59	106.05	101.87
9	AB	101	BCL	CMB-C2B-C3B	2.59	133.83	125.67
9	7	101	BCL	CHD-C1D-ND	-2.59	121.16	124.80
15	T	101	CRT	C18-C17-C16	2.59	122.04	118.09
11	x	304	UQ8	O3-C3-C2	2.59	125.36	116.64
15	f	102	CRT	C6-C7-C9	2.58	123.07	119.01
15	z	101	CRT	C14-C15-C16	-2.58	115.72	123.20
9	P	101	BCL	C16-C15-C13	-2.58	107.38	115.97
9	i	102	BCL	CHC-C1C-NC	2.58	128.13	124.40
9	f	101	BCL	OBB-CAB-CBB	-2.58	113.99	119.77
9	m	102	BCL	C3D-C2D-C1D	-2.58	102.31	105.83
9	K	101	BCL	CHD-C1D-ND	-2.58	121.17	124.80
9	L	305	BCL	CHD-C1D-ND	-2.58	121.18	124.80
15	f	102	CRT	C5-C6-C7	-2.57	122.00	125.89
9	J	102	BCL	C11-C12-C13	-2.57	107.41	115.97
9	j	101	BCL	CMB-C2B-C3B	2.57	133.79	125.67
15	y	404	CRT	C34-C33-C35	2.57	122.02	118.09
9	AI	101	BCL	C3B-C4B-NB	-2.57	106.37	109.76
9	I	101	BCL	CHC-C1C-NC	2.57	128.11	124.40
7	C	501	HEM	C2A-C1A-NA	-2.57	107.30	110.15
9	g	101	BCL	CHD-C1D-ND	-2.57	121.19	124.80
15	e	101	CRT	C26-C25-C23	-2.57	119.32	126.36
15	Z	101	CRT	C21-C22-C23	-2.57	123.68	127.28
9	y	401	BCL	OBB-CAB-CBB	-2.57	114.02	119.77
9	m	103	BCL	C3C-C4C-CHD	-2.57	117.98	123.39
7	C	502	HEM	C4C-CHD-C1D	-2.57	120.57	126.02
10	L	302	BPH	C1-O2A-CGA	2.57	122.86	116.65
9	0	101	BCL	O2A-CGA-O1A	-2.56	117.21	123.63
9	Q	101	BCL	C3D-C2D-C1D	-2.56	102.33	105.83
12	y	407	PEF	O3-C3-C2	2.56	115.79	108.40
7	o	503	HEM	CHC-C1C-NC	2.56	127.25	124.45
15	6	101	CRT	C18-C17-C16	2.56	122.00	118.09
15	s	101	CRT	C26-C27-C28	-2.56	123.68	127.28
9	U	101	BCL	CMC-C2C-C3C	-2.56	104.07	113.98
10	M	402	BPH	CBA-CAA-C2A	-2.56	106.23	113.78
15	G	101	CRT	C26-C25-C23	-2.56	119.34	126.36
9	Q	101	BCL	C2B-C1B-NB	-2.56	107.67	110.33
9	d	101	BCL	CMC-C2C-C3C	-2.56	104.08	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	x	302	BPH	CBA-CAA-C2A	-2.56	106.23	113.78
9	z	102	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
9	x	305	BCL	O2A-CGA-O1A	-2.56	117.22	123.63
9	c	102	BCL	C4A-NA-C1A	2.56	107.85	106.68
9	K	101	BCL	C3C-C4C-CHD	-2.56	118.00	123.39
9	AH	101	BCL	C2B-C1B-NB	-2.56	107.67	110.33
9	4	102	BCL	CED-O2D-CGD	-2.56	110.11	115.92
9	AL	102	BCL	C3C-C2C-C1C	2.56	106.00	101.87
9	L	303	BCL	C1D-CHD-C4C	-2.55	120.46	126.62
9	w	101	BCL	CBB-CAB-C3B	2.55	125.79	120.40
9	AB	101	BCL	CGD-CBD-CAD	-2.55	102.58	110.85
15	f	102	CRT	C10-C9-C7	-2.55	123.70	127.28
15	J	101	CRT	C6-C7-C9	-2.55	114.99	119.01
9	A	102	BCL	C16-C15-C13	-2.55	107.48	115.97
15	AE	103	CRT	C32-C31-C30	-2.55	115.81	123.20
9	AA	101	BCL	C3B-C4B-NB	-2.55	106.39	109.76
9	v	102	BCL	CED-O2D-CGD	-2.55	110.13	115.92
9	X	102	BCL	C1-O2A-CGA	2.55	122.83	116.65
15	v	101	CRT	C30-C28-C27	-2.55	115.00	119.01
9	X	102	BCL	C3B-C4B-NB	-2.55	106.39	109.76
15	AE	103	CRT	C5-C6-C7	-2.55	122.04	125.89
7	o	502	HEM	CAD-CBD-CGD	-2.55	106.90	113.67
15	k	101	CRT	C21-C22-C23	-2.55	123.70	127.28
9	P	101	BCL	CED-O2D-CGD	-2.55	110.13	115.92
9	3	101	BCL	C1-O2A-CGA	2.55	122.82	116.65
9	X	102	BCL	C2A-C1A-CHA	2.55	128.29	123.87
9	r	101	BCL	C3B-C4B-NB	-2.55	106.40	109.76
9	F	101	BCL	C11-C10-C8	-2.55	107.50	115.97
9	AD	101	BCL	CBB-CAB-C3B	2.55	125.77	120.40
9	h	101	BCL	C7-C6-C5	-2.55	106.47	113.26
9	j	101	BCL	CMD-C2D-C1D	2.55	129.22	124.73
9	v	102	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
9	S	102	BCL	CMA-C3A-C2A	-2.55	104.13	113.98
9	x	305	BCL	O2A-C1-C2	2.55	117.91	108.11
7	C	502	HEM	C2B-C1B-NB	-2.55	106.91	109.84
9	AH	103	BCL	C2A-C1A-CHA	2.54	128.28	123.87
9	7	101	BCL	C3D-C2D-C1D	-2.54	102.36	105.83
9	W	101	BCL	CHD-C1D-ND	-2.54	121.23	124.80
15	2	101	CRT	C34-C33-C35	2.54	121.97	118.09
9	J	102	BCL	C3B-C4B-NB	-2.54	106.41	109.76
9	l	101	BCL	C6-C5-C3	-2.54	107.28	113.47
15	P	102	CRT	C8-C7-C6	2.54	121.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AJ	101	CRT	C35-C33-C32	-2.54	115.02	119.01
15	2	101	CRT	C21-C20-C19	-2.54	118.33	123.52
9	7	101	BCL	C11-C12-C13	-2.54	107.53	115.97
9	AI	101	BCL	C3D-C2D-C1D	-2.54	102.37	105.83
15	AC	101	CRT	C29-C28-C30	2.54	121.96	118.09
15	v	101	CRT	C15-C16-C17	-2.53	119.42	126.36
9	A	102	BCL	C3B-C4B-NB	-2.53	106.42	109.76
9	x	301	BCL	O2A-C1-C2	2.53	117.86	108.11
9	Y	101	BCL	CMD-C2D-C1D	2.53	129.19	124.73
9	g	101	BCL	CAA-CBA-CGA	-2.53	106.02	113.21
7	o	502	HEM	C2A-C1A-NA	-2.53	107.34	110.15
9	AJ	102	BCL	C2B-C1B-NB	-2.53	107.70	110.33
15	8	101	CRT	C4-C5-C6	-2.53	121.36	124.91
7	o	504	HEM	C4D-ND-C1D	2.53	108.20	105.21
9	I	101	BCL	C7-C6-C5	-2.53	106.52	113.26
15	AL	101	CRT	C10-C9-C7	-2.53	123.73	127.28
9	p	102	BCL	CHC-C1C-NC	2.53	128.05	124.40
9	x	303	BCL	C1C-NC-C4C	-2.53	105.53	106.68
9	f	101	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
9	k	102	BCL	C1-O2A-CGA	2.53	122.77	116.65
15	z	101	CRT	C29-C28-C30	2.53	121.95	118.09
9	m	103	BCL	C2B-C1B-NB	-2.53	107.71	110.33
9	7	101	BCL	C11-C10-C8	-2.53	107.57	115.97
9	7	101	BCL	CHB-C1B-NB	2.52	127.84	124.05
7	C	503	HEM	O2A-CGA-CBA	2.52	121.97	114.00
9	x	303	BCL	C16-C15-C13	-2.52	107.58	115.97
9	AD	101	BCL	C11-C12-C13	-2.52	107.58	115.97
9	N	102	BCL	C3B-C4B-NB	-2.52	106.43	109.76
9	y	401	BCL	O2A-CGA-CBA	2.52	119.52	111.83
9	AB	101	BCL	C2B-C1B-NB	-2.52	107.71	110.33
9	L	305	BCL	CED-O2D-CGD	-2.52	110.20	115.92
10	x	302	BPH	C1-O2A-CGA	2.52	122.74	116.65
7	C	503	HEM	CHB-C1B-C2B	-2.51	119.80	126.95
9	m	103	BCL	CHB-C1B-NB	2.51	127.82	124.05
15	U	102	CRT	C14-C15-C16	-2.51	115.92	123.20
7	o	502	HEM	C2B-C1B-NB	-2.51	106.95	109.84
9	B	101	BCL	O2A-CGA-O1A	-2.51	117.34	123.63
9	AD	101	BCL	CHD-C1D-ND	-2.51	121.27	124.80
9	l	102	BCL	C2B-C1B-NB	-2.51	107.72	110.33
15	p	103	CRT	C35-C33-C32	-2.51	115.06	119.01
9	r	101	BCL	C1C-NC-C4C	-2.51	105.53	106.68
15	AE	103	CRT	C36-C35-C33	-2.51	122.10	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	504	HEM	C4C-CHD-C1D	-2.51	120.69	126.02
9	W	101	BCL	C3B-C4B-NB	-2.51	106.45	109.76
9	AJ	102	BCL	C11-C10-C8	-2.51	107.63	115.97
9	AH	101	BCL	CMC-C2C-C3C	-2.51	104.28	113.98
9	x	303	BCL	CED-O2D-CGD	-2.51	110.22	115.92
9	e	102	BCL	CMA-C3A-C4A	-2.51	105.03	111.77
15	A	103	CRT	C14-C15-C16	-2.51	115.94	123.20
9	AB	101	BCL	CHD-C1D-ND	-2.51	121.28	124.80
9	7	101	BCL	C16-C15-C13	-2.51	107.63	115.97
7	o	501	HEM	CAD-C3D-C4D	2.51	129.06	124.70
9	AJ	102	BCL	C1D-CHD-C4C	-2.51	120.58	126.62
9	U	101	BCL	C11-C12-C13	-2.50	107.64	115.97
9	L	305	BCL	C3D-C2D-C1D	-2.50	102.41	105.83
9	i	102	BCL	C1D-CHD-C4C	-2.50	120.58	126.62
7	o	502	HEM	C4C-CHD-C1D	-2.50	120.70	126.02
15	z	101	CRT	C30-C28-C27	-2.50	115.07	119.01
9	Q	101	BCL	CHB-C1B-NB	2.50	127.80	124.05
9	4	102	BCL	C2B-C1B-NB	-2.50	107.73	110.33
15	AJ	101	CRT	C15-C14-C12	-2.50	123.77	127.28
9	AD	101	BCL	C12-C11-C10	-2.50	102.08	113.28
7	C	502	HEM	CAA-CBA-CGA	-2.50	107.04	113.67
9	y	401	BCL	O2A-C1-C2	2.50	117.73	108.11
9	AC	102	BCL	C3C-C4C-CHD	-2.50	118.12	123.39
9	c	102	BCL	CGD-CBD-CAD	-2.50	102.76	110.85
9	T	102	BCL	C11-C12-C13	-2.50	107.66	115.97
7	o	504	HEM	C4B-C3B-C2B	-2.49	104.99	107.28
9	e	102	BCL	C3D-C2D-C1D	-2.49	102.43	105.83
9	m	103	BCL	CMC-C2C-C3C	-2.49	104.34	113.98
15	2	101	CRT	C32-C31-C30	-2.49	115.98	123.20
9	AK	101	BCL	C6-C5-C3	-2.49	107.40	113.47
15	E	101	CRT	C32-C31-C30	-2.49	115.98	123.20
9	T	102	BCL	CED-O2D-CGD	-2.49	110.26	115.92
9	c	102	BCL	C3C-C4C-CHD	-2.49	118.14	123.39
7	o	502	HEM	CHB-C4A-NA	2.49	128.38	123.86
9	AH	101	BCL	C1C-NC-C4C	-2.49	105.54	106.68
15	y	404	CRT	C1-C4-C5	2.49	119.45	112.98
15	8	101	CRT	C24-C23-C22	-2.49	118.78	122.82
9	AJ	102	BCL	CBB-CAB-C3B	2.49	125.65	120.40
9	7	101	BCL	C3B-C4B-NB	-2.49	106.47	109.76
7	o	503	HEM	CHD-C4C-C3C	-2.49	121.02	125.21
9	AE	104	BCL	CHC-C1C-NC	2.49	127.99	124.40
9	J	102	BCL	CBA-CAA-C2A	2.49	121.19	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	101	BCL	OBB-CAB-CBB	-2.49	114.20	119.77
9	x	301	BCL	CMA-C3A-C4A	-2.49	105.09	111.77
9	5	102	BCL	C7-C6-C5	-2.49	106.64	113.26
12	t	301	PEF	O2P-P-O1P	2.48	124.00	112.44
9	s	102	BCL	C3B-C4B-NB	-2.48	106.48	109.76
15	U	102	CRT	C8-C7-C6	2.48	121.88	118.09
9	l	101	BCL	C11-C12-C13	-2.48	107.71	115.97
9	AI	101	BCL	C3C-C4C-CHD	-2.48	118.16	123.39
9	5	102	BCL	C12-C11-C10	-2.48	102.15	113.28
9	AE	102	BCL	CHB-C1B-NB	2.48	127.77	124.05
15	f	102	CRT	C30-C28-C27	-2.48	115.11	119.01
9	m	103	BCL	CBC-CAC-C3C	2.48	118.67	113.41
9	AH	103	BCL	C12-C11-C10	-2.48	102.17	113.28
9	AA	101	BCL	CHD-C1D-ND	-2.48	121.31	124.80
15	AH	102	CRT	C35-C33-C32	-2.48	115.11	119.01
9	J	102	BCL	CMC-C2C-C3C	-2.48	104.41	113.98
9	L	301	BCL	CHD-C1D-ND	-2.48	121.32	124.80
9	k	102	BCL	CHC-C1C-NC	2.48	127.97	124.40
9	c	102	BCL	C3B-C4B-NB	-2.48	106.49	109.76
9	J	102	BCL	CHD-C1D-ND	-2.47	121.32	124.80
15	p	103	CRT	C6-C7-C9	-2.47	115.12	119.01
9	K	101	BCL	CMC-C2C-C3C	-2.47	104.42	113.98
9	g	101	BCL	C7-C6-C5	-2.47	106.67	113.26
9	8	102	BCL	O2A-C1-C2	2.47	117.63	108.11
9	3	101	BCL	C4A-NA-C1A	2.47	107.81	106.68
9	w	101	BCL	C7-C6-C5	-2.47	106.67	113.26
9	f	101	BCL	CMB-C2B-C3B	2.47	133.47	125.67
9	AH	103	BCL	C11-C10-C8	-2.47	107.75	115.97
9	p	104	BCL	CMB-C2B-C3B	2.47	133.46	125.67
9	m	103	BCL	CHC-C1C-NC	2.47	127.97	124.40
9	AH	103	BCL	C1-C2-C3	2.47	130.24	126.20
9	G	102	BCL	O2A-CGA-O1A	-2.47	117.45	123.63
15	4	101	CRT	C37-C36-C35	-2.47	121.45	124.91
9	h	101	BCL	CMA-C3A-C2A	-2.47	104.44	113.98
9	x	303	BCL	CMB-C2B-C3B	2.47	133.45	125.67
9	y	401	BCL	C3D-C2D-C1D	-2.47	102.46	105.83
7	C	501	HEM	CHB-C1B-C2B	-2.47	119.94	126.95
9	AC	102	BCL	C7-C6-C5	-2.47	106.69	113.26
9	Y	101	BCL	C2A-C1A-CHA	2.46	128.14	123.87
15	e	101	CRT	C35-C33-C32	-2.46	115.13	119.01
9	g	101	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
9	j	101	BCL	C3D-C2D-C1D	-2.46	102.47	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	101	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
7	C	504	HEM	C4D-ND-C1D	2.46	108.12	105.21
15	G	101	CRT	C27-C26-C25	-2.46	116.07	123.20
9	AH	101	BCL	CMD-C2D-C1D	2.46	129.06	124.73
15	U	102	CRT	C24-C23-C25	2.46	121.84	118.09
9	7	101	BCL	C2C-C3C-C4C	-2.46	97.66	101.34
9	z	102	BCL	C1D-CHD-C4C	-2.45	120.70	126.62
9	3	101	BCL	CMB-C2B-C3B	2.45	133.41	125.67
9	AE	104	BCL	C11-C12-C13	-2.45	107.81	115.97
9	Z	102	BCL	O2A-CGA-O1A	-2.45	117.49	123.63
9	i	102	BCL	O2A-CGA-O1A	-2.45	117.50	123.63
9	F	101	BCL	C1C-NC-C4C	-2.45	105.56	106.68
9	F	101	BCL	CAA-CBA-CGA	-2.45	106.25	113.21
9	A	102	BCL	O2A-C1-C2	2.45	117.54	108.11
15	P	102	CRT	C10-C9-C7	-2.45	123.84	127.28
11	L	304	UQ8	C7-C6-C5	2.45	121.36	118.52
9	B	101	BCL	C4A-NA-C1A	2.45	107.80	106.68
9	G	102	BCL	C2B-C1B-NB	-2.45	107.79	110.33
9	p	102	BCL	CMC-C2C-C3C	-2.45	104.52	113.98
9	9	103	BCL	C2A-C1A-CHA	2.45	128.11	123.87
12	t	303	PEF	O2P-P-O1P	2.45	123.82	112.44
9	Z	102	BCL	C2C-C3C-C4C	-2.44	97.68	101.34
9	u	101	BCL	C2A-C1A-CHA	2.44	128.11	123.87
15	s	101	CRT	C9-C10-C11	-2.44	116.12	123.20
9	B	101	BCL	C3C-C2C-C1C	2.44	105.81	101.87
9	h	101	BCL	C3D-C2D-C1D	-2.44	102.50	105.83
9	c	102	BCL	C1-C2-C3	-2.44	122.20	126.20
9	x	305	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
15	R	101	CRT	C16-C17-C19	-2.44	115.17	119.01
15	AD	102	CRT	C11-C12-C14	2.44	122.85	119.01
15	AD	102	CRT	C26-C25-C23	-2.44	119.67	126.36
9	D	101	BCL	C3C-C2C-C1C	2.44	105.81	101.87
9	M	401	BCL	C10-C8-C7	-2.44	99.72	112.07
9	L	301	BCL	C2A-C3A-C4A	-2.44	97.93	101.87
9	p	102	BCL	CBB-CAB-C3B	2.44	125.54	120.40
7	o	503	HEM	CBA-CAA-C2A	2.44	119.27	112.53
11	x	304	UQ8	O5-C5-C4	2.44	126.19	121.03
9	I	101	BCL	C1D-CHD-C4C	-2.44	120.75	126.62
9	AB	101	BCL	C6-C5-C3	-2.43	107.54	113.47
9	S	102	BCL	C3B-C4B-NB	-2.43	106.55	109.76
9	T	102	BCL	C3C-C4C-CHD	-2.43	118.26	123.39
15	f	102	CRT	C8-C7-C9	-2.43	118.87	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	102	BCL	C3D-C2D-C1D	-2.43	102.51	105.83
9	D	102	BCL	C12-C11-C10	-2.43	102.38	113.28
9	AI	101	BCL	C7-C6-C5	-2.43	106.78	113.26
9	5	102	BCL	C2B-C1B-NB	-2.43	107.80	110.33
9	s	102	BCL	C2B-C1B-NB	-2.43	107.81	110.33
9	c	102	BCL	C12-C11-C10	-2.43	102.39	113.28
9	x	303	BCL	OBB-CAB-CBB	-2.43	114.33	119.77
9	R	102	BCL	C4A-NA-C1A	2.43	107.79	106.68
9	u	101	BCL	C1C-NC-C4C	-2.43	105.57	106.68
9	B	101	BCL	C2A-C1A-CHA	2.43	128.08	123.87
9	AL	102	BCL	CHC-C1C-NC	2.43	127.90	124.40
9	A	102	BCL	O2A-CGA-O1A	-2.43	117.56	123.63
9	c	102	BCL	C2B-C1B-NB	-2.43	107.81	110.33
15	e	101	CRT	C26-C27-C28	-2.43	123.88	127.28
9	AK	101	BCL	C7-C6-C5	-2.43	106.80	113.26
7	C	501	HEM	CAD-CBD-CGD	2.42	120.10	113.67
9	r	101	BCL	C2B-C1B-NB	-2.42	107.81	110.33
15	n	101	CRT	C18-C17-C16	2.42	121.79	118.09
9	M	401	BCL	C3B-C4B-NB	-2.42	106.56	109.76
9	x	303	BCL	C2B-C1B-NB	-2.42	107.81	110.33
9	F	101	BCL	C3D-C2D-C1D	-2.42	102.53	105.83
9	f	101	BCL	C2D-C1D-ND	2.42	112.52	110.13
15	n	101	CRT	C24-C23-C25	2.42	121.78	118.09
9	B	101	BCL	CMB-C2B-C3B	2.42	133.30	125.67
9	e	102	BCL	C2B-C1B-NB	-2.42	107.82	110.33
15	U	102	CRT	C34-C33-C35	2.42	121.78	118.09
9	M	401	BCL	C2D-C1D-ND	2.42	112.52	110.13
9	r	101	BCL	C11-C12-C13	-2.42	107.93	115.97
9	D	102	BCL	C11-C10-C8	-2.42	107.93	115.97
10	x	302	BPH	O2A-CGA-CBA	2.42	119.20	111.83
9	AH	101	BCL	C16-C15-C13	-2.42	107.94	115.97
9	p	104	BCL	C11-C10-C8	-2.41	107.94	115.97
9	I	101	BCL	C2A-C1A-CHA	2.41	128.05	123.87
9	3	101	BCL	C11-C12-C13	-2.41	107.95	115.97
9	AH	101	BCL	C3D-C2D-C1D	-2.41	102.54	105.83
9	X	102	BCL	CHB-C1B-NB	2.41	127.66	124.05
9	Y	101	BCL	CMC-C2C-C1C	-2.41	105.31	111.77
9	d	101	BCL	CMC-C2C-C1C	-2.41	105.31	111.77
9	M	401	BCL	C3D-C2D-C1D	-2.40	102.55	105.83
9	5	102	BCL	CMD-C2D-C3D	2.40	133.20	127.69
9	AL	102	BCL	C11-C12-C13	-2.40	107.97	115.97
11	L	304	UQ8	C20-C19-C21	2.40	119.40	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	4	102	BCL	C6-C5-C3	-2.40	107.61	113.47
9	AD	101	BCL	C11-C10-C8	-2.40	107.98	115.97
9	N	102	BCL	C3C-C4C-CHD	-2.40	118.33	123.39
15	T	101	CRT	C16-C17-C19	-2.40	115.23	119.01
9	i	102	BCL	CHB-C1B-NB	2.40	127.65	124.05
15	R	101	CRT	C34-C33-C35	2.40	121.76	118.09
15	i	101	CRT	C9-C10-C11	-2.40	116.24	123.20
9	G	102	BCL	CMA-C3A-C4A	-2.40	105.32	111.77
9	3	101	BCL	C2D-C1D-ND	2.40	112.50	110.13
15	k	101	CRT	C4-C5-C6	-2.40	121.54	124.91
9	AH	101	BCL	CMB-C2B-C3B	2.40	133.24	125.67
9	AI	101	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
9	AD	101	BCL	C1-O2A-CGA	2.40	122.46	116.65
9	y	401	BCL	CMD-C2D-C1D	2.40	128.95	124.73
9	0	101	BCL	C4A-NA-C1A	2.40	107.77	106.68
9	AE	104	BCL	C11-C10-C8	-2.40	108.00	115.97
7	C	502	HEM	C2A-C1A-NA	-2.40	107.49	110.15
9	x	303	BCL	C1D-CHD-C4C	-2.40	120.84	126.62
9	AH	101	BCL	C11-C10-C8	-2.40	108.00	115.97
9	8	102	BCL	C1D-CHD-C4C	-2.40	120.84	126.62
9	AB	101	BCL	C16-C15-C13	-2.40	108.00	115.97
9	L	303	BCL	C4D-C3D-CAD	2.40	110.71	108.11
9	R	102	BCL	CMA-C3A-C2A	-2.40	104.72	113.98
9	B	101	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
9	g	101	BCL	C1-C2-C3	-2.39	122.28	126.20
15	AE	103	CRT	C4-C5-C6	-2.39	121.55	124.91
9	AD	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
9	v	102	BCL	CMC-C2C-C3C	-2.39	104.73	113.98
9	m	102	BCL	C2A-C1A-CHA	2.39	128.02	123.87
9	h	101	BCL	C3C-C4C-CHD	-2.39	118.35	123.39
9	O	101	BCL	C1-O2A-CGA	2.39	122.44	116.65
9	N	102	BCL	CHC-C1C-NC	2.39	127.85	124.40
9	AL	102	BCL	C3D-C2D-C1D	-2.39	102.57	105.83
9	K	101	BCL	C7-C6-C5	-2.39	106.89	113.26
9	4	102	BCL	CMC-C2C-C3C	-2.39	104.75	113.98
9	c	102	BCL	CMC-C2C-C3C	-2.39	104.75	113.98
9	i	102	BCL	C2A-C1A-CHA	2.39	128.01	123.87
9	T	102	BCL	CBB-CAB-C3B	2.39	125.43	120.40
9	AE	104	BCL	CMB-C2B-C3B	2.39	133.20	125.67
9	J	102	BCL	C1-O2A-CGA	2.39	122.42	116.65
9	d	101	BCL	C3B-C4B-NB	-2.39	106.61	109.76
9	N	102	BCL	C2B-C1B-NB	-2.38	107.85	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	101	BCL	C2B-C1B-NB	-2.38	107.86	110.33
14	M	403	MQ8	C11-C3-C2	-2.38	120.81	124.89
11	x	304	UQ8	C32-C31-C29	2.38	121.08	113.19
9	p	104	BCL	OBD-CAD-C3D	2.38	133.98	128.42
9	s	102	BCL	C4A-NA-C1A	2.38	107.77	106.68
7	o	504	HEM	C4A-C3A-C2A	2.38	109.54	106.82
10	M	402	BPH	C6-C7-C8	-2.38	108.06	115.97
9	4	102	BCL	C1C-NC-C4C	-2.38	105.59	106.68
9	AE	102	BCL	C1-O2A-CGA	2.38	122.41	116.65
11	x	304	UQ8	O3-C3-C4	-2.38	114.64	123.64
15	e	101	CRT	C9-C10-C11	-2.38	116.31	123.20
9	T	102	BCL	O2A-CGA-O1A	-2.38	117.69	123.63
15	AL	101	CRT	C9-C10-C11	-2.37	116.32	123.20
15	T	101	CRT	C14-C15-C16	-2.37	116.32	123.20
9	F	101	BCL	CHC-C1C-NC	2.37	127.83	124.40
15	s	101	CRT	C6-C7-C9	-2.37	115.28	119.01
9	9	103	BCL	C3C-C4C-CHD	-2.37	118.39	123.39
7	o	502	HEM	C4A-C3A-C2A	2.37	109.53	106.82
7	C	504	HEM	O2D-CGD-CBD	2.37	121.50	114.00
9	D	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
9	AD	101	BCL	C1C-NC-C4C	-2.37	105.60	106.68
15	A	103	CRT	C16-C17-C19	-2.37	115.28	119.01
9	u	101	BCL	CBB-CAB-C3B	2.37	125.40	120.40
9	N	102	BCL	C12-C11-C10	-2.37	102.66	113.28
9	R	102	BCL	O2A-C1-C2	2.37	117.23	108.11
14	y	403	MQ8	C41-C42-C43	-2.37	122.20	127.62
9	9	103	BCL	C16-C15-C13	-2.37	108.09	115.97
9	0	101	BCL	O2A-C1-C2	2.37	117.22	108.11
9	J	102	BCL	C4D-C3D-CAD	2.37	110.68	108.11
9	V	101	BCL	CAA-CBA-CGA	-2.37	106.49	113.21
9	W	101	BCL	C3D-C2D-C1D	-2.37	102.60	105.83
15	y	404	CRT	C40-C38-C39	2.37	114.75	110.43
9	AK	101	BCL	CHD-C1D-ND	-2.37	121.47	124.80
9	5	102	BCL	C3B-C4B-NB	-2.37	106.64	109.76
9	1	101	BCL	C2B-C1B-NB	-2.37	107.87	110.33
15	i	101	CRT	C26-C27-C28	-2.37	123.96	127.28
9	m	103	BCL	O2A-C1-C2	2.37	117.21	108.11
9	i	102	BCL	C2B-C1B-NB	-2.36	107.87	110.33
7	o	504	HEM	C3B-C2B-C1B	2.36	108.19	106.41
15	y	404	CRT	C29-C28-C27	-2.36	118.99	122.82
9	AA	101	BCL	CMC-C2C-C3C	-2.36	104.84	113.98
15	f	102	CRT	C11-C12-C14	-2.36	115.29	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AA	101	BCL	CGD-CBD-CAD	-2.36	103.20	110.85
9	L	303	BCL	OBD-CAD-C3D	2.36	133.93	128.42
9	L	305	BCL	C16-C15-C13	-2.36	108.12	115.97
15	c	101	CRT	C34-C33-C35	2.36	121.69	118.09
9	A	102	BCL	C2A-C1A-CHA	2.36	127.96	123.87
9	d	101	BCL	CAA-CBA-CGA	-2.36	106.51	113.21
9	K	101	BCL	C3B-C4B-NB	-2.36	106.65	109.76
7	o	502	HEM	C3B-C2B-C1B	2.36	108.18	106.41
9	L	301	BCL	C5-C3-C2	2.36	126.45	121.17
9	x	301	BCL	C16-C15-C13	-2.36	108.14	115.97
9	Q	101	BCL	CMC-C2C-C3C	-2.35	104.88	113.98
9	r	101	BCL	CMD-C2D-C1D	2.35	128.87	124.73
9	U	101	BCL	CED-O2D-CGD	-2.35	110.58	115.92
9	D	102	BCL	C1-O2A-CGA	2.35	122.35	116.65
9	AJ	102	BCL	C16-C15-C13	-2.35	108.15	115.97
9	5	101	BCL	O2A-CGA-CBA	2.35	119.00	111.83
9	1	102	BCL	C3D-C2D-C1D	-2.35	102.62	105.83
15	J	101	CRT	C14-C15-C16	-2.35	116.39	123.20
9	d	101	BCL	CHB-C1B-NB	2.35	127.57	124.05
9	w	101	BCL	C11-C10-C8	-2.35	108.16	115.97
9	5	101	BCL	CMA-C3A-C2A	-2.35	104.90	113.98
10	L	302	BPH	CBA-CAA-C2A	-2.35	106.86	113.78
9	AE	104	BCL	CMA-C3A-C4A	-2.35	105.46	111.77
9	h	101	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
15	AL	101	CRT	C8-C7-C6	2.35	121.67	118.09
9	D	102	BCL	C1D-CHD-C4C	-2.34	120.97	126.62
9	L	305	BCL	C2B-C1B-NB	-2.34	107.90	110.33
9	R	102	BCL	C3C-C4C-CHD	-2.34	118.45	123.39
9	1	101	BCL	C3D-C2D-C1D	-2.34	102.64	105.83
9	w	101	BCL	C2A-C3A-C4A	-2.34	98.09	101.87
12	H	301	PEF	O3-C3-C2	-2.34	101.65	108.40
9	j	101	BCL	C1-O2A-CGA	2.34	122.31	116.65
9	x	301	BCL	CAC-C3C-C4C	2.34	117.77	112.58
15	c	101	CRT	C13-C12-C11	2.34	121.66	118.09
15	R	101	CRT	C26-C27-C28	-2.34	124.00	127.28
9	A	102	BCL	CHB-C4A-NA	-2.34	121.03	124.40
10	L	302	BPH	C11-C10-C8	-2.34	108.20	115.97
9	U	101	BCL	C3B-C4B-NB	-2.34	106.68	109.76
15	AL	101	CRT	C18-C17-C16	2.34	121.66	118.09
9	I	101	BCL	CHD-C1D-ND	-2.34	121.52	124.80
7	o	501	HEM	CHA-C4D-ND	2.33	127.25	124.37
9	h	101	BCL	C16-C15-C13	-2.33	108.20	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	102	BCL	CMD-C2D-C1D	2.33	128.84	124.73
15	X	101	CRT	C32-C31-C30	-2.33	116.44	123.20
9	z	102	BCL	C11-C12-C13	-2.33	108.21	115.97
15	e	101	CRT	C10-C11-C12	-2.33	119.97	126.36
12	t	303	PEF	O3P-P-O1P	-2.33	99.69	108.94
9	p	102	BCL	C11-C12-C13	-2.33	108.22	115.97
9	D	102	BCL	C7-C6-C5	-2.33	107.05	113.26
9	y	401	BCL	CMB-C2B-C3B	2.33	133.02	125.67
10	y	402	BPH	O2A-CGA-O1A	-2.33	117.80	123.63
9	p	104	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
9	r	101	BCL	O2A-CGA-CBA	2.33	118.93	111.83
7	C	501	HEM	CHC-C1C-NC	2.33	126.99	124.45
9	AC	102	BCL	CMA-C3A-C4A	-2.33	105.52	111.77
9	AE	102	BCL	C12-C11-C10	-2.33	102.85	113.28
9	0	101	BCL	C16-C15-C13	-2.33	108.23	115.97
15	G	101	CRT	C34-C33-C35	2.33	121.64	118.09
9	d	101	BCL	C3D-C2D-C1D	-2.33	102.66	105.83
15	P	102	CRT	C27-C26-C25	-2.32	116.47	123.20
15	AJ	101	CRT	C32-C31-C30	-2.32	116.47	123.20
9	W	101	BCL	C2B-C1B-NB	-2.32	107.92	110.33
9	z	102	BCL	O2A-CGA-O1A	-2.32	117.82	123.63
9	O	101	BCL	C12-C11-C10	-2.32	102.88	113.28
9	J	102	BCL	CBB-CAB-C3B	2.32	125.29	120.40
9	AH	103	BCL	C3D-C2D-C1D	-2.32	102.67	105.83
15	AH	102	CRT	C27-C26-C25	-2.32	116.48	123.20
15	E	101	CRT	C26-C27-C28	-2.32	124.03	127.28
11	x	304	UQ8	C35-C34-C36	2.32	119.25	115.23
9	AA	101	BCL	CMA-C3A-C4A	-2.32	105.55	111.77
9	AK	101	BCL	CMA-C3A-C4A	-2.32	105.55	111.77
15	R	101	CRT	C15-C16-C17	2.32	132.71	126.36
9	AH	101	BCL	CMA-C3A-C4A	-2.31	105.55	111.77
9	N	102	BCL	CMB-C2B-C3B	2.31	132.97	125.67
9	f	101	BCL	C3D-C2D-C1D	-2.31	102.67	105.83
7	C	504	HEM	C4B-C3B-C2B	-2.31	105.15	107.28
12	H	304	PEF	C2-O2-C10	-2.31	113.76	117.85
9	T	102	BCL	C12-C11-C10	-2.31	102.91	113.28
9	5	101	BCL	C3C-C2C-C1C	2.31	105.61	101.87
9	7	101	BCL	C6-C5-C3	-2.31	107.84	113.47
9	AC	102	BCL	C12-C11-C10	-2.31	102.92	113.28
9	s	102	BCL	CHD-C1D-ND	-2.31	121.55	124.80
9	e	102	BCL	C7-C6-C5	-2.31	107.10	113.26
15	X	101	CRT	C10-C11-C12	2.31	132.70	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	101	BCL	CMC-C2C-C1C	-2.31	105.56	111.77
9	AC	102	BCL	C2B-C1B-NB	-2.31	107.93	110.33
11	L	304	UQ8	C37-C38-C39	-2.31	122.34	127.62
15	Z	101	CRT	C35-C33-C32	-2.31	115.38	119.01
9	AD	101	BCL	O2A-CGA-O1A	-2.31	117.86	123.63
15	2	101	CRT	C5-C6-C7	-2.31	122.41	125.89
9	1	101	BCL	C2A-C1A-CHA	2.31	127.87	123.87
9	D	102	BCL	C3C-C4C-CHD	-2.31	118.53	123.39
9	i	102	BCL	CMC-C2C-C3C	-2.31	105.07	113.98
9	7	101	BCL	CAA-CBA-CGA	-2.31	106.66	113.21
9	c	102	BCL	C11-C10-C8	-2.31	108.30	115.97
9	K	101	BCL	C1-O2A-CGA	2.30	122.23	116.65
15	AJ	101	CRT	C24-C23-C25	2.30	121.61	118.09
9	1	101	BCL	C1-O2A-CGA	2.30	122.22	116.65
9	Z	102	BCL	CMA-C3A-C4A	-2.30	105.58	111.77
9	0	101	BCL	CMB-C2B-C3B	2.30	132.93	125.67
12	y	406	PEF	O2-C10-O4	-2.30	118.55	122.99
15	N	101	CRT	C14-C15-C16	-2.30	116.53	123.20
9	K	101	BCL	CBB-CAB-C3B	2.30	125.25	120.40
9	3	101	BCL	C11-C10-C8	-2.30	108.32	115.97
9	D	102	BCL	C1C-NC-C4C	-2.30	105.63	106.68
15	AH	102	CRT	C14-C15-C16	-2.30	116.54	123.20
15	E	101	CRT	C24-C23-C25	2.30	121.60	118.09
9	i	102	BCL	C3B-C4B-NB	-2.30	106.73	109.76
15	G	101	CRT	C18-C17-C16	2.30	121.59	118.09
9	k	102	BCL	C11-C10-C8	-2.30	108.33	115.97
7	o	503	HEM	CHA-C4D-ND	2.30	127.21	124.37
15	A	103	CRT	C32-C31-C30	-2.29	116.55	123.20
15	P	102	CRT	C18-C17-C16	2.29	121.59	118.09
9	AH	103	BCL	O2A-CGA-O1A	-2.29	117.89	123.63
9	s	102	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
9	u	101	BCL	C11-C12-C13	-2.29	108.35	115.97
9	x	305	BCL	CGD-CBD-CAD	-2.29	103.43	110.85
9	O	101	BCL	C6-C5-C3	-2.29	107.89	113.47
9	Y	101	BCL	C11-C10-C8	-2.29	108.36	115.97
9	e	102	BCL	C11-C10-C8	-2.29	108.36	115.97
7	o	503	HEM	CAA-C2A-C1A	2.29	129.41	124.94
9	X	102	BCL	CAA-C2A-C3A	2.29	119.17	113.00
15	J	101	CRT	C35-C33-C32	-2.28	115.42	119.01
9	AI	101	BCL	O2A-C1-C2	2.28	116.90	108.11
9	5	102	BCL	C11-C12-C13	-2.28	108.38	115.97
9	4	102	BCL	CMD-C2D-C1D	2.28	128.75	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AE	102	BCL	CMC-C2C-C1C	-2.28	105.64	111.77
15	6	101	CRT	C8-C7-C9	-2.28	119.12	122.82
9	AE	102	BCL	O2A-CGA-O1A	-2.28	117.92	123.63
9	9	103	BCL	C4A-NA-C1A	2.28	107.72	106.68
9	D	102	BCL	CMD-C2D-C3D	2.28	132.92	127.69
15	T	101	CRT	C32-C31-C30	-2.28	116.59	123.20
9	AL	102	BCL	C3C-C4C-CHD	-2.28	118.58	123.39
9	Z	102	BCL	CAB-C3B-C2B	-2.28	123.00	127.74
12	m	101	PEF	C3-C2-C1	-2.28	106.47	111.78
9	I	101	BCL	CBB-CAB-C3B	2.28	125.21	120.40
9	5	102	BCL	CAC-C3C-C4C	2.28	117.64	112.58
9	9	103	BCL	C1C-NC-C4C	-2.28	105.64	106.68
9	AB	101	BCL	C1C-NC-C4C	-2.28	105.64	106.68
15	M	404	CRT	C9-C10-C11	-2.28	116.59	123.20
9	T	102	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
9	A	102	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
15	J	101	CRT	C13-C12-C11	2.28	121.57	118.09
9	V	101	BCL	C3D-C2D-C1D	-2.28	102.72	105.83
9	l	101	BCL	C2B-C1B-NB	-2.28	107.97	110.33
9	w	101	BCL	O2A-CGA-O1A	-2.28	117.94	123.63
9	V	101	BCL	C3C-C4C-CHD	-2.28	118.59	123.39
9	L	303	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
9	D	102	BCL	C2C-C3C-C4C	-2.28	97.93	101.34
15	k	101	CRT	C24-C23-C22	-2.28	119.13	122.82
9	Q	101	BCL	CHD-C1D-ND	-2.27	121.60	124.80
9	X	102	BCL	CHC-C1C-NC	2.27	127.68	124.40
9	AB	101	BCL	C11-C12-C13	-2.27	108.41	115.97
15	T	101	CRT	C34-C33-C32	-2.27	119.13	122.82
9	9	103	BCL	C3C-C2C-C1C	2.27	105.54	101.87
7	C	504	HEM	C4C-CHD-C1D	-2.27	121.19	126.02
15	R	101	CRT	C13-C12-C14	-2.27	119.14	122.82
9	Q	101	BCL	C12-C11-C10	-2.27	103.10	113.28
15	f	102	CRT	C24-C23-C25	2.27	121.56	118.09
9	5	101	BCL	CMB-C2B-C3B	2.27	132.83	125.67
9	i	102	BCL	CMA-C3A-C4A	-2.27	105.67	111.77
9	I	101	BCL	CED-O2D-CGD	-2.27	110.77	115.92
15	9	102	CRT	C4-C5-C6	-2.27	121.73	124.91
10	L	302	BPH	C11-C12-C13	-2.27	108.42	115.97
9	e	102	BCL	CMB-C2B-C3B	2.27	132.82	125.67
9	G	102	BCL	CMB-C2B-C3B	2.27	132.82	125.67
15	f	102	CRT	C29-C28-C30	2.27	121.55	118.09
9	y	401	BCL	C16-C15-C13	-2.27	108.44	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	101	CRT	C27-C26-C25	-2.27	116.64	123.20
15	4	101	CRT	C31-C30-C28	2.26	132.57	126.36
15	2	101	CRT	C20-C21-C22	-2.26	118.89	123.52
7	o	501	HEM	O2D-CGD-CBD	2.26	121.15	114.00
14	M	403	MQ8	C2M-C2-C3	-2.26	120.73	124.45
9	u	101	BCL	C14-C13-C12	-2.26	103.21	111.27
9	r	101	BCL	CBB-CAB-C3B	2.26	125.17	120.40
15	z	101	CRT	C36-C35-C33	-2.26	122.47	125.89
9	D	101	BCL	CBB-CAB-C3B	2.26	125.17	120.40
9	S	102	BCL	C6-C5-C3	-2.26	107.96	113.47
9	m	102	BCL	C11-C10-C8	-2.26	108.45	115.97
9	f	101	BCL	O2A-CGA-O1A	-2.26	117.97	123.63
9	p	104	BCL	CBC-CAC-C3C	2.26	118.21	113.41
15	E	101	CRT	C14-C15-C16	-2.26	116.65	123.20
7	o	504	HEM	C3C-C2C-C1C	2.26	109.18	107.05
9	AK	101	BCL	C1D-CHD-C4C	-2.26	121.18	126.62
9	S	102	BCL	CMC-C2C-C3C	-2.26	105.26	113.98
10	L	302	BPH	C1-C2-C3	-2.26	122.50	126.20
9	l	101	BCL	C3B-C4B-NB	-2.26	106.78	109.76
9	B	101	BCL	C3C-C4C-CHD	-2.26	118.64	123.39
9	m	102	BCL	C12-C11-C10	-2.25	103.17	113.28
9	4	102	BCL	CHC-C1C-NC	2.25	127.65	124.40
15	T	101	CRT	C40-C38-C39	-2.25	106.31	110.43
9	AJ	102	BCL	CMB-C2B-C3B	2.25	132.78	125.67
15	k	101	CRT	C13-C12-C11	2.25	121.53	118.09
9	v	102	BCL	C2C-C3C-C4C	-2.25	97.97	101.34
7	o	503	HEM	CHB-C1B-C2B	-2.25	120.55	126.95
15	A	103	CRT	C10-C11-C12	-2.25	120.19	126.36
9	AB	101	BCL	C3D-C2D-C1D	-2.25	102.76	105.83
9	G	102	BCL	C11-C12-C13	-2.25	108.49	115.97
7	C	501	HEM	CHD-C1D-C2D	-2.25	121.48	125.03
9	L	305	BCL	C2A-C1A-CHA	2.25	127.77	123.87
9	x	303	BCL	O2A-CGA-CBA	2.25	118.69	111.83
9	AH	101	BCL	C11-C12-C13	-2.25	108.50	115.97
9	U	101	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
9	l	101	BCL	CGD-CBD-CAD	-2.24	103.58	110.85
9	p	102	BCL	C1C-NC-C4C	-2.24	105.66	106.68
9	u	101	BCL	C3D-C2D-C1D	-2.24	102.77	105.83
10	y	402	BPH	C6-C5-C3	-2.24	108.00	113.47
9	AH	101	BCL	OBD-CAD-C3D	2.24	133.66	128.42
9	y	401	BCL	CBA-CAA-C2A	2.24	120.47	113.79
15	8	101	CRT	C20-C19-C17	-2.24	124.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AL	102	BCL	C11-C10-C8	-2.24	108.52	115.97
15	4	101	CRT	C30-C28-C27	-2.24	115.48	119.01
9	X	102	BCL	C1D-CHD-C4C	-2.24	121.22	126.62
9	G	102	BCL	CHB-C1B-NB	2.24	127.41	124.05
9	M	401	BCL	CMC-C2C-C3C	-2.24	105.32	113.98
11	L	304	UQ8	C12-C13-C14	-2.24	122.50	127.62
9	x	303	BCL	C4D-CHA-C1A	2.24	123.92	121.24
12	M	408	PEF	O2P-P-O1P	2.24	122.86	112.44
9	v	102	BCL	C2B-C1B-NB	-2.24	108.00	110.33
9	G	102	BCL	C3C-C4C-CHD	-2.24	118.68	123.39
9	D	102	BCL	C2B-C1B-NB	-2.24	108.01	110.33
9	S	102	BCL	CBB-CAB-C3B	2.24	125.12	120.40
12	x	306	PEF	O3-C30-C31	2.24	121.87	112.38
9	e	102	BCL	C3C-C2C-C1C	2.24	105.48	101.87
9	i	102	BCL	C12-C11-C10	-2.24	103.26	113.28
9	p	102	BCL	C3C-C2C-C1C	2.23	105.48	101.87
9	u	101	BCL	O2A-CGA-O1A	-2.23	118.04	123.63
9	x	305	BCL	C3B-C4B-NB	-2.23	106.81	109.76
7	o	503	HEM	O2A-CGA-CBA	2.23	121.06	114.00
9	F	101	BCL	C7-C6-C5	-2.23	107.31	113.26
9	R	102	BCL	C11-C12-C13	-2.23	108.54	115.97
7	o	504	HEM	C2C-C1C-NC	-2.23	105.50	109.64
9	U	101	BCL	C2B-C1B-NB	-2.23	108.01	110.33
15	T	101	CRT	C36-C35-C33	2.23	129.27	125.89
9	h	101	BCL	C3C-C2C-C1C	2.23	105.47	101.87
9	X	102	BCL	O2A-C1-C2	2.23	116.70	108.11
9	y	401	BCL	C6-C5-C3	-2.23	108.03	113.47
9	u	101	BCL	C11-C10-C8	-2.23	108.55	115.97
9	V	101	BCL	O2A-CGA-O1A	-2.23	118.05	123.63
9	S	102	BCL	O2A-CGA-CBA	2.23	118.63	111.83
15	E	101	CRT	C9-C10-C11	-2.23	116.75	123.20
9	F	101	BCL	C2A-C1A-CHA	2.23	127.73	123.87
15	G	101	CRT	C13-C12-C11	2.23	121.49	118.09
9	U	101	BCL	C3C-C4C-CHD	-2.23	118.70	123.39
15	N	101	CRT	C27-C26-C25	-2.23	116.75	123.20
15	AL	101	CRT	C21-C22-C23	-2.23	124.16	127.28
9	AD	101	BCL	CAA-CBA-CGA	-2.23	106.89	113.21
15	p	103	CRT	C20-C21-C22	-2.23	118.97	123.52
9	h	101	BCL	CHB-C1B-NB	2.22	127.39	124.05
9	k	102	BCL	CHB-C1B-NB	2.22	127.39	124.05
7	o	502	HEM	CMB-C2B-C1B	2.22	128.51	125.03
17	S	101	PGW	O01-C02-C03	2.22	116.32	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	101	BCL	O2A-CGA-O1A	-2.22	118.07	123.63
9	k	102	BCL	CED-O2D-CGD	-2.22	110.87	115.92
9	AI	101	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
12	y	408	PEF	O5-C30-C31	-2.22	116.90	124.77
9	l	102	BCL	CHD-C1D-ND	-2.22	121.68	124.80
9	J	102	BCL	CAA-C2A-C3A	2.22	119.00	113.00
9	l	101	BCL	C3C-C2C-C1C	2.22	105.46	101.87
7	o	502	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
9	M	401	BCL	C7-C6-C5	-2.22	107.34	113.26
15	p	103	CRT	C21-C20-C19	-2.22	118.98	123.52
9	AH	103	BCL	CHB-C1B-NB	2.22	127.38	124.05
15	n	101	CRT	C21-C20-C19	-2.22	118.98	123.52
9	f	101	BCL	O2A-C1-C2	2.22	116.64	108.11
9	AE	102	BCL	CMA-C3A-C4A	-2.22	105.81	111.77
9	e	102	BCL	CGD-CBD-CAD	-2.22	103.67	110.85
9	AC	102	BCL	CGD-CBD-CAD	-2.21	103.68	110.85
9	AE	102	BCL	OBD-CAD-C3D	2.21	133.59	128.42
9	5	101	BCL	O2A-C1-C2	2.21	116.63	108.11
9	8	102	BCL	C1-C2-C3	2.21	129.82	126.20
14	M	403	MQ8	C11-C3-C4	2.21	120.91	118.58
9	P	101	BCL	C11-C10-C8	-2.21	108.61	115.97
15	9	102	CRT	C18-C17-C16	2.21	121.47	118.09
15	N	101	CRT	C18-C17-C16	2.21	121.47	118.09
9	z	102	BCL	C3B-C4B-NB	-2.21	106.84	109.76
9	p	102	BCL	CHB-C4A-NA	-2.21	121.21	124.40
9	Q	101	BCL	CHC-C1C-NC	2.21	127.59	124.40
9	j	101	BCL	C6-C5-C3	-2.21	108.08	113.47
9	P	101	BCL	C2B-C1B-NB	-2.21	108.04	110.33
9	AE	102	BCL	C1C-NC-C4C	-2.21	105.67	106.68
15	6	101	CRT	C20-C21-C22	-2.21	119.00	123.52
9	V	101	BCL	C2B-C1B-NB	-2.21	108.04	110.33
9	AA	101	BCL	CED-O2D-CGD	-2.21	110.91	115.92
9	g	101	BCL	C3C-C2C-C1C	2.21	105.43	101.87
9	AD	101	BCL	C3B-C4B-NB	-2.21	106.85	109.76
9	B	101	BCL	C11-C10-C8	-2.20	108.64	115.97
9	G	102	BCL	CHD-C1D-ND	-2.20	121.70	124.80
9	h	101	BCL	C12-C11-C10	-2.20	103.40	113.28
11	L	304	UQ8	C17-C18-C19	-2.20	122.58	127.62
9	v	102	BCL	CGD-CBD-CAD	-2.20	103.72	110.85
9	AK	101	BCL	C1-C2-C3	-2.20	122.59	126.20
7	C	503	HEM	CHB-C4A-C3A	-2.20	121.03	127.43
15	T	101	CRT	C11-C12-C14	-2.20	115.55	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	y	403	MQ8	C45-C43-C44	2.20	119.04	115.23
9	P	101	BCL	C12-C11-C10	-2.20	103.43	113.28
9	AC	102	BCL	C1-O2A-CGA	2.20	121.97	116.65
9	AJ	102	BCL	CHB-C1B-NB	2.20	127.34	124.05
9	AH	101	BCL	CHB-C4A-NA	-2.19	121.23	124.40
9	W	101	BCL	C11-C10-C8	-2.19	108.67	115.97
9	V	101	BCL	C2A-C1A-CHA	2.19	127.67	123.87
9	1	102	BCL	CMA-C3A-C4A	-2.19	105.88	111.77
9	P	101	BCL	CHC-C1C-NC	2.19	127.56	124.40
9	AA	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
12	x	306	PEF	O2P-P-O3P	-2.19	97.63	107.57
9	AD	101	BCL	CED-O2D-CGD	-2.19	110.94	115.92
15	s	101	CRT	C5-C6-C7	-2.19	122.58	125.89
15	N	101	CRT	C24-C23-C22	-2.19	119.27	122.82
9	A	102	BCL	C4A-NA-C1A	2.19	107.68	106.68
15	8	101	CRT	C1-C4-C5	2.18	118.66	112.98
9	e	102	BCL	C1D-CHD-C4C	-2.18	121.35	126.62
9	L	301	BCL	C1-C2-C3	-2.18	122.62	126.20
9	T	102	BCL	C2B-C1B-NB	-2.18	108.06	110.33
15	s	101	CRT	C29-C28-C30	2.18	121.42	118.09
7	o	504	HEM	CAA-CBA-CGA	-2.18	107.88	113.67
9	3	101	BCL	O2A-C1-C2	2.18	116.50	108.11
9	w	101	BCL	C11-C12-C13	-2.18	108.72	115.97
9	0	101	BCL	C11-C12-C13	-2.18	108.72	115.97
9	e	102	BCL	C12-C11-C10	-2.18	103.52	113.28
9	J	102	BCL	CHB-C1B-NB	2.18	127.32	124.05
9	AD	101	BCL	C1D-CHD-C4C	-2.18	121.37	126.62
9	F	101	BCL	CMB-C2B-C3B	2.18	132.54	125.67
15	AH	102	CRT	C13-C12-C11	2.18	121.41	118.09
9	F	101	BCL	O2A-CGA-O1A	-2.18	118.19	123.63
15	9	102	CRT	C9-C10-C11	2.17	129.50	123.20
9	j	101	BCL	C16-C15-C13	-2.17	108.74	115.97
9	3	101	BCL	C12-C11-C10	-2.17	103.53	113.28
12	H	304	PEF	O2-C2-C3	2.17	116.14	108.34
7	C	503	HEM	CHA-C1A-NA	2.17	127.80	123.86
15	AC	101	CRT	C32-C31-C30	-2.17	116.91	123.20
9	x	305	BCL	CMD-C2D-C3D	2.17	132.67	127.69
9	B	101	BCL	CGD-CBD-CAD	-2.17	103.81	110.85
12	H	303	PEF	C2-O2-C10	-2.17	114.01	117.85
15	c	101	CRT	C16-C17-C19	-2.17	115.60	119.01
7	o	502	HEM	CHB-C1B-NB	2.17	127.05	124.37
15	6	101	CRT	C24-C23-C25	2.17	121.40	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	CRT	C29-C28-C30	2.17	121.40	118.09
9	X	102	BCL	C12-C11-C10	-2.17	103.57	113.28
9	A	102	BCL	CED-O2D-CGD	-2.17	111.00	115.92
9	m	102	BCL	C3B-C4B-NB	-2.17	106.90	109.76
14	M	403	MQ8	C34-C33-C32	-2.16	118.07	123.63
9	z	102	BCL	C1-O2A-CGA	2.16	121.89	116.65
9	AE	102	BCL	C3B-C4B-NB	-2.16	106.90	109.76
9	AK	101	BCL	C2B-C1B-NB	-2.16	108.08	110.33
9	AJ	102	BCL	C1-O2A-CGA	2.16	121.88	116.65
9	m	103	BCL	C3C-C2C-C1C	2.16	105.36	101.87
9	m	103	BCL	C3B-C4B-NB	-2.16	106.91	109.76
9	S	102	BCL	C16-C15-C13	-2.16	108.78	115.97
9	V	101	BCL	CMB-C2B-C3B	2.16	132.48	125.67
15	2	101	CRT	C27-C26-C25	-2.16	116.94	123.20
9	s	102	BCL	CMB-C2B-C3B	2.16	132.48	125.67
14	y	403	MQ8	C29-C28-C27	-2.16	118.09	123.63
9	k	102	BCL	C4D-CHA-C1A	2.16	123.82	121.24
9	Q	101	BCL	CAA-CBA-CGA	-2.16	107.08	113.21
9	AE	104	BCL	C2C-C3C-C4C	-2.16	98.11	101.34
15	e	101	CRT	C6-C7-C9	-2.16	115.62	119.01
15	2	101	CRT	C24-C23-C25	2.16	121.38	118.09
9	L	305	BCL	CAA-C2A-C3A	2.16	118.82	113.00
9	B	101	BCL	CHC-C1C-NC	2.16	127.51	124.40
15	y	404	CRT	C6-C7-C9	2.15	122.40	119.01
14	M	403	MQ8	C9-C10-C1	2.15	123.24	120.10
9	z	102	BCL	C2A-C1A-CHA	2.15	127.60	123.87
9	AB	101	BCL	C12-C11-C10	-2.15	103.63	113.28
9	Z	102	BCL	C1-C2-C3	-2.15	122.67	126.20
12	t	301	PEF	O2-C10-C11	2.15	114.93	111.09
15	k	101	CRT	C8-C7-C9	-2.15	119.33	122.82
9	P	101	BCL	C11-C12-C13	-2.15	108.81	115.97
9	M	401	BCL	CAC-C3C-C4C	2.15	117.36	112.58
9	W	101	BCL	OBD-CAD-C3D	2.15	133.44	128.42
9	j	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
9	V	101	BCL	C7-C6-C5	-2.15	107.53	113.26
9	5	102	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
9	w	101	BCL	CMB-C2B-C3B	2.15	132.45	125.67
15	p	103	CRT	C32-C31-C30	-2.15	116.97	123.20
9	1	102	BCL	CHB-C4A-NA	-2.15	121.30	124.40
15	AE	103	CRT	C8-C7-C6	2.15	121.37	118.09
9	AH	103	BCL	O2A-C1-C2	2.15	116.37	108.11
7	C	503	HEM	CMC-C2C-C3C	-2.15	123.23	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	y	401	BCL	C11-C12-C13	-2.15	108.83	115.97
9	P	101	BCL	O2A-C1-C2	2.15	116.37	108.11
9	v	102	BCL	CMB-C2B-C3B	2.15	132.44	125.67
9	j	101	BCL	C2A-C1A-CHA	2.14	127.59	123.87
9	K	101	BCL	O2A-CGA-CBA	2.14	118.37	111.83
12	p	101	PEF	O3-C30-C31	2.14	121.47	112.38
9	Q	101	BCL	CMA-C3A-C4A	-2.14	106.02	111.77
15	i	101	CRT	C18-C17-C16	2.14	121.36	118.09
9	Z	102	BCL	CHC-C1C-NC	2.14	127.49	124.40
15	y	404	CRT	C31-C30-C28	-2.14	120.50	126.36
9	J	102	BCL	C4D-CHA-C1A	2.14	123.80	121.24
15	U	102	CRT	O1-C1-C2	2.14	123.67	108.97
14	M	403	MQ8	O4-C4-C5	-2.14	118.16	121.57
15	AH	102	CRT	C29-C28-C27	-2.14	119.36	122.82
9	u	101	BCL	CED-O2D-CGD	-2.13	111.07	115.92
7	o	502	HEM	CMC-C2C-C1C	-2.13	120.97	124.73
9	0	101	BCL	C12-C11-C10	-2.13	103.72	113.28
9	AK	101	BCL	CMB-C2B-C3B	2.13	132.40	125.67
9	4	102	BCL	CGD-CBD-CAD	-2.13	103.94	110.85
9	z	102	BCL	C12-C11-C10	-2.13	103.72	113.28
15	v	101	CRT	C14-C15-C16	-2.13	117.03	123.20
15	k	101	CRT	C1-C4-C5	2.13	118.51	112.98
9	7	101	BCL	CGD-CBD-CAD	-2.13	103.95	110.85
9	L	301	BCL	C4D-CHA-C1A	2.13	123.78	121.24
9	r	101	BCL	C3D-C2D-C1D	-2.13	102.92	105.83
9	J	102	BCL	O2A-CGA-O1A	-2.13	118.30	123.63
9	AB	101	BCL	C2A-C1A-CHA	2.13	127.56	123.87
9	m	102	BCL	C3C-C4C-CHD	-2.13	118.91	123.39
15	AH	102	CRT	C32-C31-C30	-2.13	117.03	123.20
15	M	404	CRT	C21-C20-C19	-2.13	119.17	123.52
9	Z	102	BCL	C11-C12-C13	-2.13	108.90	115.97
7	C	503	HEM	C4D-ND-C1D	2.13	107.72	105.21
9	r	101	BCL	C5-C3-C2	2.13	125.94	121.17
9	g	101	BCL	O2A-CGA-CBA	2.13	118.31	111.83
7	C	502	HEM	CAD-C3D-C4D	2.12	128.40	124.70
7	C	503	HEM	O2D-CGD-CBD	2.12	120.71	114.00
9	R	102	BCL	CMB-C2B-C3B	2.12	132.37	125.67
9	h	101	BCL	C1C-NC-C4C	-2.12	105.71	106.68
9	r	101	BCL	C16-C15-C13	-2.12	108.91	115.97
9	5	101	BCL	CGD-CBD-CAD	-2.12	103.97	110.85
9	I	101	BCL	CMB-C2B-C3B	2.12	132.37	125.67
9	F	101	BCL	O2A-CGA-CBA	2.12	118.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	g	101	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
9	F	101	BCL	C1D-CHD-C4C	-2.12	121.51	126.62
10	L	302	BPH	C6-C7-C8	-2.12	108.92	115.97
11	L	304	UQ8	C46-C44-C45	2.12	119.46	114.59
7	o	502	HEM	CMB-C2B-C3B	-2.12	123.30	128.43
7	C	501	HEM	CHA-C4D-ND	2.12	126.98	124.37
9	S	102	BCL	CBC-CAC-C3C	2.12	117.90	113.41
14	y	403	MQ8	C26-C25-C23	-2.11	106.18	113.19
9	x	301	BCL	C2A-C1A-CHA	2.11	127.54	123.87
9	v	102	BCL	C11-C12-C13	-2.11	108.94	115.97
11	x	304	UQ8	C42-C41-C39	2.11	120.19	113.19
14	M	403	MQ8	O1-C1-C2	-2.11	117.67	120.45
9	F	101	BCL	C3C-C4C-CHD	-2.11	118.94	123.39
9	O	101	BCL	CMD-C2D-C1D	2.11	128.45	124.73
9	7	101	BCL	CBC-CAC-C3C	2.11	117.89	113.41
7	C	501	HEM	C1C-CHC-C4B	-2.11	121.53	126.02
9	L	301	BCL	O2A-C1-C2	2.11	116.24	108.11
15	N	101	CRT	C24-C23-C25	2.11	121.31	118.09
9	0	101	BCL	CHD-C1D-ND	-2.11	121.83	124.80
9	u	101	BCL	C2B-C1B-NB	-2.11	108.14	110.33
15	AL	101	CRT	C31-C32-C33	-2.11	124.32	127.28
15	c	101	CRT	C34-C33-C32	-2.11	119.40	122.82
15	4	101	CRT	C1-C4-C5	2.11	118.46	112.98
9	5	102	BCL	C1-O2A-CGA	2.11	121.75	116.65
9	s	102	BCL	O2A-CGA-O1A	-2.11	118.36	123.63
9	Y	101	BCL	CHB-C1B-NB	2.11	127.21	124.05
15	AE	103	CRT	C31-C32-C33	-2.11	124.32	127.28
9	p	104	BCL	O2A-CGA-CBA	2.10	118.25	111.83
9	r	101	BCL	CMA-C3A-C4A	-2.10	106.12	111.77
9	AB	101	BCL	C7-C6-C5	-2.10	107.66	113.26
7	C	502	HEM	CBB-CAB-C3B	-2.10	117.02	127.53
15	k	101	CRT	C13-C12-C14	-2.10	119.41	122.82
9	x	301	BCL	C10-C8-C7	-2.10	101.42	112.07
9	l	101	BCL	C12-C11-C10	-2.10	103.86	113.28
7	o	504	HEM	CAD-C3D-C4D	2.10	128.36	124.70
7	C	501	HEM	O2D-CGD-O1D	-2.10	117.94	123.33
15	Z	101	CRT	C29-C28-C27	-2.10	119.42	122.82
9	L	305	BCL	CHB-C1B-NB	2.10	127.20	124.05
9	S	102	BCL	CHB-C4A-NA	-2.10	121.37	124.40
15	N	101	CRT	C29-C28-C27	-2.10	119.42	122.82
9	G	102	BCL	OBD-CAD-C3D	2.10	133.32	128.42
12	M	407	PEF	C3-O3-C30	2.10	122.25	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	101	BCL	C3C-C2C-C1C	2.10	105.25	101.87
15	AE	103	CRT	C26-C25-C23	-2.10	120.62	126.36
9	D	101	BCL	C1-O2A-CGA	2.10	121.72	116.65
9	p	102	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
9	AH	103	BCL	C3B-C4B-NB	-2.09	107.00	109.76
9	8	102	BCL	C4A-NA-C1A	2.09	107.63	106.68
9	T	102	BCL	CMA-C3A-C4A	-2.09	106.15	111.77
14	y	403	MQ8	C8-C9-C10	2.09	123.58	119.80
7	o	503	HEM	CHB-C4A-NA	2.09	127.65	123.86
11	L	304	UQ8	C3M-O3-C3	2.09	123.82	116.47
9	x	303	BCL	C6-C5-C3	-2.09	108.38	113.47
9	1	101	BCL	CMA-C3A-C4A	-2.09	106.16	111.77
9	F	101	BCL	C2B-C1B-NB	-2.09	108.16	110.33
9	Y	101	BCL	C2D-C1D-ND	2.09	112.19	110.13
15	AH	102	CRT	C8-C7-C6	2.09	121.28	118.09
15	G	101	CRT	C26-C27-C28	-2.09	124.35	127.28
9	S	102	BCL	CED-O2D-CGD	-2.09	111.18	115.92
9	4	102	BCL	C11-C10-C8	-2.09	109.03	115.97
11	x	304	UQ8	C15-C14-C13	-2.09	118.27	123.63
9	m	103	BCL	C11-C12-C13	-2.08	109.04	115.97
9	5	102	BCL	C2C-C3C-C4C	-2.08	98.22	101.34
9	AH	103	BCL	C1-O2A-CGA	2.08	121.69	116.65
9	A	102	BCL	CMA-C3A-C4A	-2.08	106.17	111.77
9	AA	101	BCL	O2A-CGA-CBA	2.08	118.18	111.83
9	d	101	BCL	C14-C13-C12	-2.08	103.86	111.27
9	9	103	BCL	O2A-C1-C2	2.08	116.11	108.11
9	h	101	BCL	CHC-C1C-NC	2.08	127.40	124.40
9	l	101	BCL	C3C-C2C-C1C	2.08	105.23	101.87
9	9	103	BCL	CED-O2D-CGD	-2.08	111.20	115.92
9	5	102	BCL	O2A-CGA-O1A	-2.08	118.43	123.63
9	D	102	BCL	CHD-C1D-ND	-2.08	121.88	124.80
9	P	101	BCL	CMC-C2C-C3C	-2.08	105.95	113.98
9	Y	101	BCL	C3D-C2D-C1D	-2.08	103.00	105.83
15	M	404	CRT	C13-C12-C11	2.08	121.26	118.09
15	A	103	CRT	C29-C28-C30	2.08	121.26	118.09
9	I	101	BCL	O2A-CGA-CBA	2.07	118.16	111.83
9	c	102	BCL	C3C-C2C-C1C	2.07	105.22	101.87
9	g	101	BCL	C2A-C3A-C4A	-2.07	98.52	101.87
9	4	102	BCL	C4A-NA-C1A	2.07	107.62	106.68
9	m	102	BCL	CHB-C4A-NA	-2.07	121.41	124.40
9	Y	101	BCL	CMC-C2C-C3C	-2.07	105.98	113.98
9	x	301	BCL	C1-C2-C3	-2.07	122.81	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	102	BCL	O2A-CGA-CBA	2.07	118.15	111.83
9	0	101	BCL	C1D-CHD-C4C	-2.07	121.63	126.62
15	A	103	CRT	C27-C26-C25	-2.07	117.20	123.20
7	C	504	HEM	CHC-C1C-NC	2.07	126.71	124.45
7	C	504	HEM	CBC-CAC-C3C	-2.07	117.19	127.53
15	X	101	CRT	C34-C33-C35	2.07	121.25	118.09
15	4	101	CRT	C32-C31-C30	2.07	129.19	123.20
9	i	102	BCL	C11-C12-C13	-2.07	109.10	115.97
9	S	102	BCL	CMB-C2B-C3B	2.07	132.18	125.67
9	AB	101	BCL	C3C-C4C-CHD	-2.07	119.04	123.39
9	P	101	BCL	C7-C6-C5	-2.07	107.76	113.26
15	R	101	CRT	C4-C5-C6	-2.06	122.02	124.91
9	y	401	BCL	CAA-C2A-C3A	2.06	118.57	113.00
9	L	301	BCL	CAC-C3C-C4C	2.06	117.16	112.58
9	N	102	BCL	O2A-CGA-O1A	-2.06	118.47	123.63
9	V	101	BCL	C11-C10-C8	-2.06	109.11	115.97
9	8	102	BCL	CMB-C2B-C3B	2.06	132.17	125.67
9	X	102	BCL	C2B-C1B-NB	-2.06	108.19	110.33
9	k	102	BCL	C1D-CHD-C4C	-2.06	121.65	126.62
9	9	103	BCL	C6-C5-C3	-2.06	108.45	113.47
9	f	101	BCL	CED-O2D-CGD	-2.06	111.24	115.92
9	9	103	BCL	O2A-CGA-O1A	-2.06	118.47	123.63
15	AE	103	CRT	C27-C26-C25	-2.06	117.23	123.20
15	8	101	CRT	C9-C10-C11	-2.06	117.24	123.20
15	s	101	CRT	O1-C1-C2	2.06	123.12	108.97
9	K	101	BCL	CHC-C1C-NC	2.06	127.37	124.40
15	Z	101	CRT	C27-C26-C25	-2.06	117.24	123.20
15	p	103	CRT	C24-C23-C22	-2.06	119.48	122.82
15	i	101	CRT	C29-C28-C30	2.06	121.23	118.09
7	C	504	HEM	CMC-C2C-C1C	2.06	128.35	124.73
12	y	407	PEF	C3-O3-C30	2.06	122.16	117.08
9	u	101	BCL	CMD-C2D-C1D	2.06	128.35	124.73
9	h	101	BCL	C1-O2A-CGA	2.06	121.62	116.65
9	v	102	BCL	CHD-C1D-ND	-2.05	121.91	124.80
9	AE	102	BCL	C11-C10-C8	-2.05	109.14	115.97
9	8	102	BCL	CHC-C1C-NC	2.05	127.36	124.40
15	k	101	CRT	C8-C7-C6	2.05	121.22	118.09
7	o	501	HEM	CHD-C4C-NC	2.05	126.69	124.45
14	M	403	MQ8	C15-C13-C12	-2.05	116.56	121.17
9	O	101	BCL	CBA-CAA-C2A	2.05	119.90	113.79
9	l	101	BCL	C3C-C4C-CHD	-2.05	119.07	123.39
9	A	102	BCL	C11-C12-C13	-2.05	109.15	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	101	BCL	C1-O2A-CGA	2.05	121.61	116.65
9	AJ	102	BCL	C3D-C2D-C1D	-2.05	103.04	105.83
10	L	302	BPH	C7-C6-C5	-2.05	107.80	113.26
9	z	102	BCL	CHB-C1B-NB	2.05	127.12	124.05
9	m	103	BCL	CMB-C2B-C3B	2.05	132.12	125.67
9	L	305	BCL	C3C-C2C-C1C	2.05	105.17	101.87
9	w	101	BCL	O2A-C1-C2	2.04	115.97	108.11
9	Z	102	BCL	O2A-CGA-CBA	2.04	118.07	111.83
9	P	101	BCL	CMD-C2D-C1D	2.04	128.33	124.73
9	AE	104	BCL	C3C-C2C-C1C	2.04	105.17	101.87
9	u	101	BCL	C12-C11-C10	-2.04	104.12	113.28
9	AH	103	BCL	C3C-C2C-C1C	2.04	105.17	101.87
9	e	102	BCL	CAC-C3C-C4C	-2.04	108.05	112.58
15	c	101	CRT	C36-C35-C33	-2.04	122.81	125.89
9	S	102	BCL	CMC-C2C-C1C	-2.04	106.28	111.77
9	L	303	BCL	C6-C7-C8	2.04	122.75	115.97
15	AH	102	CRT	C21-C20-C19	-2.04	119.34	123.52
9	l	101	BCL	CMB-C2B-C3B	2.04	132.11	125.67
9	AH	103	BCL	C1D-CHD-C4C	-2.04	121.70	126.62
15	f	102	CRT	C21-C20-C19	-2.04	119.34	123.52
9	g	101	BCL	C2C-C3C-C4C	-2.04	98.29	101.34
9	AC	102	BCL	C11-C12-C13	-2.04	109.19	115.97
9	J	102	BCL	C12-C11-C10	-2.04	104.14	113.28
15	9	102	CRT	C30-C28-C27	-2.04	115.80	119.01
15	AD	102	CRT	C32-C31-C30	-2.04	117.30	123.20
7	o	504	HEM	CHB-C4A-NA	2.04	127.56	123.86
9	W	101	BCL	O2A-CGA-CBA	2.04	118.05	111.83
9	v	102	BCL	C3C-C4C-CHD	-2.04	119.10	123.39
7	o	504	HEM	O2D-CGD-CBD	2.04	120.44	114.00
9	AE	104	BCL	C16-C15-C13	-2.04	109.20	115.97
15	M	404	CRT	C21-C22-C23	-2.04	124.42	127.28
9	Q	101	BCL	C3C-C4C-CHD	-2.04	119.10	123.39
15	c	101	CRT	C31-C30-C28	-2.04	120.78	126.36
9	s	102	BCL	O2A-C1-C2	2.04	115.94	108.11
9	8	102	BCL	C11-C10-C8	-2.03	109.20	115.97
7	o	503	HEM	CAA-CBA-CGA	-2.03	108.27	113.67
15	k	101	CRT	C24-C23-C25	-2.03	114.98	118.09
9	AD	101	BCL	CMD-C2D-C1D	2.03	128.31	124.73
12	M	408	PEF	O2-C10-O4	-2.03	119.07	122.99
9	AK	101	BCL	CHC-C1C-NC	2.03	127.33	124.40
15	n	101	CRT	C18-C17-C19	-2.03	119.53	122.82
9	x	301	BCL	CBC-CAC-C3C	2.03	117.72	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	304	UQ8	O5-C5-C6	2.03	125.72	121.79
15	6	101	CRT	C13-C12-C11	2.03	121.19	118.09
9	AI	101	BCL	CHB-C4A-NA	-2.03	121.47	124.40
9	8	102	BCL	C3C-C2C-C1C	2.03	105.14	101.87
9	4	102	BCL	C3B-C4B-NB	-2.03	107.08	109.76
7	o	504	HEM	CAA-C2A-C1A	2.03	128.90	124.94
9	L	305	BCL	CHC-C1C-NC	2.02	127.32	124.40
9	v	102	BCL	O2A-CGA-O1A	-2.02	118.56	123.63
15	AD	102	CRT	C16-C17-C19	-2.02	115.83	119.01
15	s	101	CRT	C27-C26-C25	-2.02	117.33	123.20
9	x	305	BCL	C4-C3-C5	-2.02	111.72	115.23
15	E	101	CRT	C16-C17-C19	-2.02	115.83	119.01
9	G	102	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
10	M	402	BPH	O2A-CGA-O1A	-2.02	118.58	123.63
9	M	401	BCL	C11-C10-C8	-2.02	109.25	115.97
9	AE	104	BCL	O2A-CGA-O1A	-2.02	118.58	123.63
15	f	102	CRT	C27-C26-C25	-2.02	117.35	123.20
10	y	402	BPH	O1D-CGD-CBD	-2.02	121.66	124.72
9	j	101	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
9	W	101	BCL	CBA-CAA-C2A	2.02	119.79	113.79
9	5	102	BCL	CHB-C4A-NA	-2.02	121.49	124.40
12	t	303	PEF	O3-C3-C2	2.01	114.20	108.40
11	x	304	UQ8	C35-C34-C33	-2.01	118.45	123.63
9	f	101	BCL	C1D-CHD-C4C	-2.01	121.76	126.62
7	C	502	HEM	C1D-C2D-C3D	2.01	109.10	106.98
9	5	102	BCL	CGD-CBD-CAD	-2.01	104.33	110.85
9	AL	102	BCL	CGD-CBD-CAD	-2.01	104.33	110.85
9	AE	104	BCL	C12-C11-C10	-2.01	104.26	113.28
9	V	101	BCL	C12-C11-C10	-2.01	104.26	113.28
9	p	102	BCL	C12-C11-C10	-2.01	104.26	113.28
9	X	102	BCL	CED-O2D-CGD	-2.01	111.35	115.92
9	g	101	BCL	CBC-CAC-C3C	2.01	117.68	113.41
9	m	103	BCL	C12-C11-C10	-2.01	104.27	113.28
15	N	101	CRT	C9-C10-C11	-2.01	117.38	123.20
15	T	101	CRT	C29-C28-C27	-2.01	119.56	122.82
9	7	101	BCL	O2A-CGA-O1A	-2.01	118.60	123.63
9	f	101	BCL	CHB-C4A-NA	-2.01	121.50	124.40
9	g	101	BCL	C11-C10-C8	-2.01	109.29	115.97
9	l	102	BCL	CMD-C2D-C3D	2.01	132.30	127.69
9	d	101	BCL	CMA-C3A-C4A	-2.01	106.37	111.77
9	r	101	BCL	C1-O2A-CGA	2.01	121.51	116.65
15	e	101	CRT	C29-C28-C30	2.01	121.15	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AC	102	BCL	CMB-C2B-C3B	2.01	132.00	125.67
10	M	402	BPH	C5-C3-C2	-2.01	116.67	121.17
9	X	102	BCL	C2C-C3C-C4C	-2.01	98.34	101.34
15	P	102	CRT	C30-C28-C27	-2.01	115.86	119.01
9	S	102	BCL	C1D-CHD-C4C	-2.00	121.79	126.62
9	L	303	BCL	O2A-CGA-O1A	-2.00	118.62	123.63
9	N	102	BCL	C11-C10-C8	-2.00	109.31	115.97
9	p	102	BCL	C3C-C4C-CHD	-2.00	119.17	123.39
15	f	102	CRT	C16-C17-C19	-2.00	115.86	119.01
9	p	102	BCL	CMB-C2B-C3B	2.00	131.98	125.67
9	m	102	BCL	CMB-C2B-C3B	2.00	131.98	125.67
9	AE	104	BCL	C2B-C1B-NB	-2.00	108.25	110.33
9	d	101	BCL	CMD-C2D-C1D	2.00	128.25	124.73
9	h	101	BCL	CMD-C2D-C1D	2.00	128.25	124.73
9	m	102	BCL	CGD-CBD-CAD	-2.00	104.37	110.85

There are no chirality outliers.

All (1749) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	503	HEM	C2B-C3B-CAB-CBB
7	o	501	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C4B-C3B-CAB-CBB
7	o	503	HEM	C2B-C3B-CAB-CBB
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	303	BCL	C1A-C2A-CAA-CBA
9	L	303	BCL	C3A-C2A-CAA-CBA
9	L	303	BCL	C2C-C3C-CAC-CBC
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	L	303	BCL	CBD-CGD-O2D-CED
9	L	305	BCL	C4C-C3C-CAC-CBC
9	L	305	BCL	CHA-CBD-CGD-O2D
9	M	401	BCL	C2C-C3C-CAC-CBC
9	M	401	BCL	C4C-C3C-CAC-CBC
9	A	102	BCL	C1A-C2A-CAA-CBA
9	A	102	BCL	C3A-C2A-CAA-CBA
9	A	102	BCL	CBA-CGA-O2A-C1
9	A	102	BCL	O1A-CGA-O2A-C1
9	A	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	B	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C3A-C2A-CAA-CBA
9	B	101	BCL	C2C-C3C-CAC-CBC
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	C4C-C3C-CAC-CBC
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	I	101	BCL	C2C-C3C-CAC-CBC
9	I	101	BCL	C4C-C3C-CAC-CBC
9	I	101	BCL	CBD-CGD-O2D-CED
9	J	102	BCL	C1A-C2A-CAA-CBA
9	J	102	BCL	C3A-C2A-CAA-CBA
9	J	102	BCL	C4C-C3C-CAC-CBC
9	J	102	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	CBD-CGD-O2D-CED
9	N	102	BCL	C3A-C2A-CAA-CBA
9	N	102	BCL	C2C-C3C-CAC-CBC
9	N	102	BCL	C4C-C3C-CAC-CBC
9	N	102	BCL	CBD-CGD-O2D-CED
9	N	102	BCL	O1D-CGD-O2D-CED
9	O	101	BCL	C3A-C2A-CAA-CBA
9	O	101	BCL	C2C-C3C-CAC-CBC
9	O	101	BCL	C4C-C3C-CAC-CBC
9	O	101	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	C2C-C3C-CAC-CBC
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	C4-C3-C5-C6
9	R	102	BCL	C4C-C3C-CAC-CBC
9	R	102	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	CHA-CBD-CGD-O1D
9	S	102	BCL	CHA-CBD-CGD-O2D
9	T	102	BCL	C1A-C2A-CAA-CBA
9	T	102	BCL	C3A-C2A-CAA-CBA
9	T	102	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	U	101	BCL	CBD-CGD-O2D-CED
9	V	101	BCL	C1A-C2A-CAA-CBA
9	V	101	BCL	C3A-C2A-CAA-CBA
9	V	101	BCL	CBD-CGD-O2D-CED
9	W	101	BCL	CHA-CBD-CGD-O1D
9	W	101	BCL	CHA-CBD-CGD-O2D
9	X	102	BCL	C3A-C2A-CAA-CBA
9	X	102	BCL	C2-C1-O2A-CGA
9	X	102	BCL	C2C-C3C-CAC-CBC
9	X	102	BCL	C4C-C3C-CAC-CBC
9	X	102	BCL	CBD-CGD-O2D-CED
9	Y	101	BCL	C3A-C2A-CAA-CBA
9	Y	101	BCL	C2C-C3C-CAC-CBC
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	1	101	BCL	C2C-C3C-CAC-CBC
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D
9	1	102	BCL	C3A-C2A-CAA-CBA
9	1	102	BCL	CBD-CGD-O2D-CED
9	3	101	BCL	CBD-CGD-O2D-CED
9	4	102	BCL	C3A-C2A-CAA-CBA
9	4	102	BCL	C2C-C3C-CAC-CBC
9	4	102	BCL	CBD-CGD-O2D-CED
9	5	101	BCL	C2C-C3C-CAC-CBC
9	5	101	BCL	C4C-C3C-CAC-CBC
9	5	102	BCL	C3A-C2A-CAA-CBA
9	5	102	BCL	C2C-C3C-CAC-CBC
9	5	102	BCL	C4C-C3C-CAC-CBC
9	5	102	BCL	CBD-CGD-O2D-CED
9	7	101	BCL	C2C-C3C-CAC-CBC
9	8	102	BCL	C1A-C2A-CAA-CBA
9	8	102	BCL	C3A-C2A-CAA-CBA
9	8	102	BCL	CBA-CGA-O2A-C1
9	8	102	BCL	O1A-CGA-O2A-C1
9	8	102	BCL	C2C-C3C-CAC-CBC
9	8	102	BCL	C4C-C3C-CAC-CBC
9	8	102	BCL	CHA-CBD-CGD-O1D
9	8	102	BCL	CHA-CBD-CGD-O2D
9	8	102	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	9	103	BCL	C4C-C3C-CAC-CBC
9	0	101	BCL	C3A-C2A-CAA-CBA
9	x	301	BCL	C2C-C3C-CAC-CBC
9	x	301	BCL	C4C-C3C-CAC-CBC
9	x	303	BCL	C3A-C2A-CAA-CBA
9	x	303	BCL	C2C-C3C-CAC-CBC
9	x	303	BCL	C4C-C3C-CAC-CBC
9	x	305	BCL	C4C-C3C-CAC-CBC
9	x	305	BCL	CHA-CBD-CGD-O1D
9	x	305	BCL	CHA-CBD-CGD-O2D
9	y	401	BCL	C3A-C2A-CAA-CBA
9	y	401	BCL	C4C-C3C-CAC-CBC
9	m	102	BCL	C4C-C3C-CAC-CBC
9	m	102	BCL	C14-C13-C15-C16
9	m	103	BCL	C3A-C2A-CAA-CBA
9	m	103	BCL	CBA-CGA-O2A-C1
9	m	103	BCL	O1A-CGA-O2A-C1
9	m	103	BCL	C2C-C3C-CAC-CBC
9	m	103	BCL	C4C-C3C-CAC-CBC
9	m	103	BCL	O2A-C1-C2-C3
9	p	102	BCL	C3A-C2A-CAA-CBA
9	p	102	BCL	CBD-CGD-O2D-CED
9	p	104	BCL	C1A-C2A-CAA-CBA
9	p	104	BCL	C2C-C3C-CAC-CBC
9	r	101	BCL	C1A-C2A-CAA-CBA
9	r	101	BCL	C3A-C2A-CAA-CBA
9	s	102	BCL	C1A-C2A-CAA-CBA
9	s	102	BCL	C3A-C2A-CAA-CBA
9	s	102	BCL	C2C-C3C-CAC-CBC
9	s	102	BCL	C4C-C3C-CAC-CBC
9	s	102	BCL	CBD-CGD-O2D-CED
9	u	101	BCL	C1A-C2A-CAA-CBA
9	u	101	BCL	CBD-CGD-O2D-CED
9	v	102	BCL	C3A-C2A-CAA-CBA
9	v	102	BCL	C2C-C3C-CAC-CBC
9	v	102	BCL	CBD-CGD-O2D-CED
9	w	101	BCL	C1A-C2A-CAA-CBA
9	w	101	BCL	C4C-C3C-CAC-CBC
9	w	101	BCL	CBD-CGD-O2D-CED
9	z	102	BCL	C3A-C2A-CAA-CBA
9	z	102	BCL	C2C-C3C-CAC-CBC
9	z	102	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	AA	101	BCL	C2C-C3C-CAC-CBC
9	AB	101	BCL	C1A-C2A-CAA-CBA
9	AB	101	BCL	C3A-C2A-CAA-CBA
9	AB	101	BCL	C4C-C3C-CAC-CBC
9	AB	101	BCL	CBD-CGD-O2D-CED
9	AC	102	BCL	C3A-C2A-CAA-CBA
9	AC	102	BCL	C4C-C3C-CAC-CBC
9	AC	102	BCL	CBD-CGD-O2D-CED
9	AD	101	BCL	C1A-C2A-CAA-CBA
9	AD	101	BCL	C3A-C2A-CAA-CBA
9	AD	101	BCL	C4C-C3C-CAC-CBC
9	AD	101	BCL	CBD-CGD-O2D-CED
9	AE	104	BCL	C3A-C2A-CAA-CBA
9	AE	104	BCL	C4C-C3C-CAC-CBC
9	AE	104	BCL	CBD-CGD-O2D-CED
9	AH	101	BCL	C1A-C2A-CAA-CBA
9	AI	101	BCL	C1A-C2A-CAA-CBA
9	AJ	102	BCL	C1A-C2A-CAA-CBA
9	AJ	102	BCL	C3A-C2A-CAA-CBA
9	AJ	102	BCL	C4C-C3C-CAC-CBC
9	AJ	102	BCL	CBD-CGD-O2D-CED
9	AK	101	BCL	C2C-C3C-CAC-CBC
9	AK	101	BCL	C4C-C3C-CAC-CBC
9	AK	101	BCL	CBD-CGD-O2D-CED
9	AL	102	BCL	C1A-C2A-CAA-CBA
9	AL	102	BCL	C3A-C2A-CAA-CBA
9	AL	102	BCL	C2C-C3C-CAC-CBC
9	AL	102	BCL	C4C-C3C-CAC-CBC
9	AL	102	BCL	CBD-CGD-O2D-CED
9	d	101	BCL	C1A-C2A-CAA-CBA
9	d	101	BCL	C2C-C3C-CAC-CBC
9	d	101	BCL	CBD-CGD-O2D-CED
9	e	102	BCL	C3A-C2A-CAA-CBA
9	e	102	BCL	CBA-CGA-O2A-C1
9	e	102	BCL	C2C-C3C-CAC-CBC
9	e	102	BCL	C4C-C3C-CAC-CBC
9	e	102	BCL	CBD-CGD-O2D-CED
9	f	101	BCL	CBD-CGD-O2D-CED
9	g	101	BCL	C3A-C2A-CAA-CBA
9	g	101	BCL	CBA-CGA-O2A-C1
9	g	101	BCL	O1A-CGA-O2A-C1
9	g	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	h	101	BCL	C2C-C3C-CAC-CBC
9	h	101	BCL	C4C-C3C-CAC-CBC
9	i	102	BCL	C3A-C2A-CAA-CBA
9	i	102	BCL	CBD-CGD-O2D-CED
9	i	102	BCL	C4-C3-C5-C6
9	j	101	BCL	C2C-C3C-CAC-CBC
9	j	101	BCL	C4C-C3C-CAC-CBC
9	k	102	BCL	C1A-C2A-CAA-CBA
9	k	102	BCL	C3A-C2A-CAA-CBA
9	k	102	BCL	C2C-C3C-CAC-CBC
9	k	102	BCL	C4C-C3C-CAC-CBC
9	k	102	BCL	CHA-CBD-CGD-O1D
9	k	102	BCL	CHA-CBD-CGD-O2D
9	k	102	BCL	O2A-C1-C2-C3
9	l	101	BCL	CBD-CGD-O2D-CED
9	c	102	BCL	C1A-C2A-CAA-CBA
9	c	102	BCL	C3A-C2A-CAA-CBA
9	c	102	BCL	C4C-C3C-CAC-CBC
10	M	402	BPH	C4C-C3C-CAC-CBC
10	M	402	BPH	C2C-C3C-CAC-CBC
10	M	402	BPH	O2A-C1-C2-C3
10	x	302	BPH	CBD-CGD-O2D-CED
10	x	302	BPH	C4C-C3C-CAC-CBC
10	x	302	BPH	C2C-C3C-CAC-CBC
10	y	402	BPH	C4C-C3C-CAC-CBC
12	L	306	PEF	O3P-C1-C2-C3
12	L	306	PEF	O3P-C1-C2-O2
12	L	306	PEF	C4-O4P-P-O1P
12	L	306	PEF	C4-O4P-P-O2P
12	L	306	PEF	C4-O4P-P-O3P
12	M	406	PEF	C1-O3P-P-O1P
12	M	406	PEF	C1-O3P-P-O4P
12	M	406	PEF	C4-O4P-P-O1P
12	M	406	PEF	C4-O4P-P-O2P
12	M	407	PEF	O4P-C4-C5-N
12	M	407	PEF	C1-O3P-P-O2P
12	M	407	PEF	C1-O3P-P-O4P
12	M	408	PEF	O4P-C4-C5-N
12	M	408	PEF	C1-O3P-P-O1P
12	M	408	PEF	C1-O3P-P-O2P
12	M	408	PEF	C1-O3P-P-O4P
12	H	301	PEF	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
12	H	301	PEF	C1-O3P-P-O1P
12	H	303	PEF	C1-O3P-P-O1P
12	H	303	PEF	C4-O4P-P-O1P
12	H	303	PEF	C4-O4P-P-O3P
12	H	304	PEF	O4P-C4-C5-N
12	H	304	PEF	C1-O3P-P-O1P
12	H	304	PEF	C1-O3P-P-O2P
12	H	304	PEF	C1-O3P-P-O4P
12	A	101	PEF	O4P-C4-C5-N
12	A	101	PEF	C1-O3P-P-O1P
12	A	101	PEF	C1-O3P-P-O4P
12	x	306	PEF	O4P-C4-C5-N
12	x	306	PEF	C1-O3P-P-O2P
12	x	306	PEF	C1-O3P-P-O4P
12	y	408	PEF	O4P-C4-C5-N
12	y	408	PEF	C1-O3P-P-O2P
12	y	408	PEF	C1-O3P-P-O4P
12	t	301	PEF	O4P-C4-C5-N
12	t	301	PEF	C1-O3P-P-O2P
12	t	303	PEF	C1-O3P-P-O2P
12	t	303	PEF	C1-O3P-P-O4P
12	t	303	PEF	C4-O4P-P-O1P
12	m	101	PEF	C5-C4-O4P-P
12	m	101	PEF	C4-O4P-P-O1P
12	p	101	PEF	C1-C2-C3-O3
12	p	101	PEF	C1-O3P-P-O2P
12	p	101	PEF	C1-O3P-P-O4P
14	M	403	MQ8	C15-C16-C17-C18
14	M	403	MQ8	C26-C27-C28-C30
14	M	403	MQ8	C31-C32-C33-C34
14	M	403	MQ8	C31-C32-C33-C35
14	M	403	MQ8	C46-C47-C48-C49
14	y	403	MQ8	C11-C12-C13-C15
14	y	403	MQ8	C16-C17-C18-C19
14	y	403	MQ8	C16-C17-C18-C20
14	y	403	MQ8	C34-C33-C35-C36
14	y	403	MQ8	C36-C37-C38-C40
15	M	404	CRT	C1-C4-C5-C6
15	M	404	CRT	C32-C33-C35-C36
15	M	404	CRT	C34-C33-C35-C36
15	M	404	CRT	C35-C36-C37-C38
15	A	103	CRT	C2-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
15	E	101	CRT	C22-C23-C25-C26
15	E	101	CRT	C36-C37-C38-C39
15	E	101	CRT	C36-C37-C38-C40
15	E	101	CRT	C36-C37-C38-O2
15	G	101	CRT	O1-C1-C4-C5
15	G	101	CRT	C2-C1-C4-C5
15	G	101	CRT	C3-C1-C4-C5
15	G	101	CRT	C27-C28-C30-C31
15	G	101	CRT	C29-C28-C30-C31
15	J	101	CRT	C5-C6-C7-C8
15	J	101	CRT	C5-C6-C7-C9
15	J	101	CRT	C36-C37-C38-C39
15	J	101	CRT	C36-C37-C38-C40
15	J	101	CRT	C36-C37-C38-O2
15	J	101	CRT	C40-C38-O2-C2M
15	N	101	CRT	O1-C1-C4-C5
15	N	101	CRT	C2-C1-C4-C5
15	N	101	CRT	C3-C1-C4-C5
15	P	102	CRT	O1-C1-C4-C5
15	P	102	CRT	C22-C23-C25-C26
15	P	102	CRT	C24-C23-C25-C26
15	P	102	CRT	C27-C28-C30-C31
15	P	102	CRT	C29-C28-C30-C31
15	R	101	CRT	C3-C1-O1-C1M
15	R	101	CRT	C5-C6-C7-C9
15	T	101	CRT	C2-C1-O1-C1M
15	T	101	CRT	C5-C6-C7-C9
15	T	101	CRT	C15-C16-C17-C19
15	U	102	CRT	O1-C1-C4-C5
15	U	102	CRT	C2-C1-C4-C5
15	U	102	CRT	C3-C1-C4-C5
15	U	102	CRT	C10-C11-C12-C14
15	U	102	CRT	C15-C16-C17-C19
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	C17-C19-C20-C21
15	Z	101	CRT	C5-C6-C7-C8
15	Z	101	CRT	C5-C6-C7-C9
15	Z	101	CRT	C10-C11-C12-C14
15	Z	101	CRT	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	Z	101	CRT	C15-C16-C17-C19
15	Z	101	CRT	C36-C37-C38-C39
15	Z	101	CRT	C36-C37-C38-C40
15	Z	101	CRT	C36-C37-C38-O2
15	2	101	CRT	C15-C16-C17-C19
15	2	101	CRT	C36-C37-C38-C39
15	2	101	CRT	C36-C37-C38-C40
15	2	101	CRT	C36-C37-C38-O2
15	4	101	CRT	C15-C16-C17-C19
15	4	101	CRT	C27-C28-C30-C31
15	6	101	CRT	C5-C6-C7-C8
15	6	101	CRT	C5-C6-C7-C9
15	8	101	CRT	O1-C1-C4-C5
15	8	101	CRT	C2-C1-C4-C5
15	8	101	CRT	C3-C1-C4-C5
15	9	102	CRT	C3-C1-O1-C1M
15	9	102	CRT	C1-C4-C5-C6
15	9	102	CRT	C15-C16-C17-C19
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-C4-C5
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	n	101	CRT	C40-C38-O2-C2M
15	p	103	CRT	C36-C37-C38-C39
15	s	101	CRT	C2-C1-O1-C1M
15	s	101	CRT	C5-C6-C7-C8
15	s	101	CRT	C5-C6-C7-C9
15	s	101	CRT	C15-C16-C17-C19
15	v	101	CRT	C1-C4-C5-C6
15	v	101	CRT	C22-C23-C25-C26
15	v	101	CRT	C24-C23-C25-C26
15	v	101	CRT	C27-C28-C30-C31
15	AC	101	CRT	C3-C1-O1-C1M
15	AC	101	CRT	O1-C1-C4-C5
15	AC	101	CRT	C2-C1-C4-C5
15	AC	101	CRT	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
15	AD	102	CRT	C3-C1-O1-C1M
15	AD	102	CRT	C36-C37-C38-C40
15	AD	102	CRT	C36-C37-C38-O2
15	AE	103	CRT	C5-C6-C7-C8
15	AE	103	CRT	C5-C6-C7-C9
15	AH	102	CRT	C3-C1-O1-C1M
15	AH	102	CRT	O1-C1-C4-C5
15	AH	102	CRT	C15-C16-C17-C18
15	AH	102	CRT	C15-C16-C17-C19
15	AH	102	CRT	C22-C23-C25-C26
15	AH	102	CRT	C36-C37-C38-C39
15	AH	102	CRT	C36-C37-C38-C40
15	AH	102	CRT	C36-C37-C38-O2
15	AJ	101	CRT	C17-C19-C20-C21
15	AJ	101	CRT	C27-C28-C30-C31
15	AJ	101	CRT	C29-C28-C30-C31
15	AL	101	CRT	C15-C16-C17-C19
15	AL	101	CRT	C22-C23-C25-C26
15	AL	101	CRT	C24-C23-C25-C26
15	AL	101	CRT	C35-C36-C37-C38
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	e	101	CRT	C10-C11-C12-C13
15	e	101	CRT	C10-C11-C12-C14
15	e	101	CRT	C22-C23-C25-C26
15	f	102	CRT	C2-C1-O1-C1M
15	i	101	CRT	C3-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	O1-C1-C4-C5
15	k	101	CRT	C2-C1-C4-C5
15	k	101	CRT	C3-C1-C4-C5
17	S	101	PGW	C04-C05-CAD-OAE
17	S	101	PGW	C04-O12-P-O11
17	S	101	PGW	C04-O12-P-O13
17	S	101	PGW	C2-C1-O01-C02
17	AE	101	PGW	OAF-C05-CAD-OAE
17	AE	101	PGW	C04-C05-CAD-OAE
17	AE	101	PGW	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
9	D	101	BCL	O1D-CGD-O2D-CED
9	G	102	BCL	O1D-CGD-O2D-CED
9	Q	101	BCL	O1D-CGD-O2D-CED
9	R	102	BCL	O1D-CGD-O2D-CED
9	U	101	BCL	O1D-CGD-O2D-CED
9	V	101	BCL	O1D-CGD-O2D-CED
9	Z	102	BCL	O1D-CGD-O2D-CED
9	4	102	BCL	O1D-CGD-O2D-CED
9	5	102	BCL	O1D-CGD-O2D-CED
9	m	102	BCL	O1D-CGD-O2D-CED
9	s	102	BCL	O1D-CGD-O2D-CED
9	u	101	BCL	O1D-CGD-O2D-CED
9	AB	101	BCL	O1D-CGD-O2D-CED
9	AC	102	BCL	O1D-CGD-O2D-CED
9	AE	102	BCL	O1D-CGD-O2D-CED
9	k	102	BCL	O1D-CGD-O2D-CED
9	l	101	BCL	O1D-CGD-O2D-CED
12	H	303	PEF	C11-C10-O2-C2
12	H	304	PEF	C11-C10-O2-C2
12	x	306	PEF	C11-C10-O2-C2
12	t	303	PEF	C11-C10-O2-C2
17	S	101	PGW	O02-C1-O01-C02
9	J	102	BCL	O1D-CGD-O2D-CED
9	K	101	BCL	O1D-CGD-O2D-CED
9	P	101	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	O1D-CGD-O2D-CED
9	T	102	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	O1D-CGD-O2D-CED
9	x	303	BCL	O1D-CGD-O2D-CED
9	p	102	BCL	O1D-CGD-O2D-CED
9	v	102	BCL	O1D-CGD-O2D-CED
9	z	102	BCL	O1D-CGD-O2D-CED
9	AH	101	BCL	O1D-CGD-O2D-CED
9	AH	103	BCL	O1D-CGD-O2D-CED
9	AI	101	BCL	O1D-CGD-O2D-CED
9	AL	102	BCL	O1D-CGD-O2D-CED
9	e	102	BCL	O1D-CGD-O2D-CED
9	i	102	BCL	O1D-CGD-O2D-CED
17	AE	101	PGW	O02-C1-O01-C02
9	L	301	BCL	CBD-CGD-O2D-CED
9	A	102	BCL	CBD-CGD-O2D-CED
9	D	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	F	101	BCL	CBD-CGD-O2D-CED
9	Q	101	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	CBD-CGD-O2D-CED
9	7	101	BCL	CBD-CGD-O2D-CED
9	x	303	BCL	CBD-CGD-O2D-CED
9	x	305	BCL	CBD-CGD-O2D-CED
9	m	102	BCL	CBD-CGD-O2D-CED
9	m	103	BCL	CBD-CGD-O2D-CED
9	p	104	BCL	CBD-CGD-O2D-CED
9	r	101	BCL	CBD-CGD-O2D-CED
9	AE	102	BCL	CBD-CGD-O2D-CED
9	AH	101	BCL	CBD-CGD-O2D-CED
9	AH	103	BCL	CBD-CGD-O2D-CED
9	AI	101	BCL	CBD-CGD-O2D-CED
9	h	101	BCL	CBD-CGD-O2D-CED
9	j	101	BCL	CBD-CGD-O2D-CED
9	k	102	BCL	CBD-CGD-O2D-CED
10	L	302	BPH	CBD-CGD-O2D-CED
9	G	102	BCL	O1A-CGA-O2A-C1
9	J	102	BCL	O1A-CGA-O2A-C1
9	W	101	BCL	O1A-CGA-O2A-C1
9	l	102	BCL	O1A-CGA-O2A-C1
9	s	102	BCL	O1A-CGA-O2A-C1
9	e	102	BCL	O1A-CGA-O2A-C1
9	k	102	BCL	O1A-CGA-O2A-C1
9	L	303	BCL	O1D-CGD-O2D-CED
9	O	101	BCL	O1D-CGD-O2D-CED
9	X	102	BCL	O1D-CGD-O2D-CED
9	AE	104	BCL	O1D-CGD-O2D-CED
9	AJ	102	BCL	O1D-CGD-O2D-CED
12	y	407	PEF	C11-C10-O2-C2
9	L	301	BCL	O1D-CGD-O2D-CED
9	D	102	BCL	O1D-CGD-O2D-CED
9	7	101	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	O1D-CGD-O2D-CED
9	g	101	BCL	O1D-CGD-O2D-CED
9	j	101	BCL	O1D-CGD-O2D-CED
10	L	302	BPH	O1D-CGD-O2D-CED
9	G	102	BCL	CBA-CGA-O2A-C1
9	l	102	BCL	CBA-CGA-O2A-C1
9	s	102	BCL	CBA-CGA-O2A-C1
9	k	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	x	306	PEF	O4-C10-O2-C2
9	L	305	BCL	CBD-CGD-O2D-CED
9	O	101	BCL	O1A-CGA-O2A-C1
9	R	102	BCL	O1A-CGA-O2A-C1
9	X	102	BCL	O1A-CGA-O2A-C1
9	4	102	BCL	O1A-CGA-O2A-C1
9	v	102	BCL	O1A-CGA-O2A-C1
9	z	102	BCL	O1A-CGA-O2A-C1
9	AE	104	BCL	O1A-CGA-O2A-C1
9	I	101	BCL	O1D-CGD-O2D-CED
9	l	102	BCL	O1D-CGD-O2D-CED
9	m	103	BCL	O1D-CGD-O2D-CED
9	p	104	BCL	O1D-CGD-O2D-CED
9	w	101	BCL	O1D-CGD-O2D-CED
9	AK	101	BCL	O1D-CGD-O2D-CED
9	f	101	BCL	O1D-CGD-O2D-CED
9	AD	101	BCL	O1D-CGD-O2D-CED
9	d	101	BCL	O1D-CGD-O2D-CED
10	x	302	BPH	O1D-CGD-O2D-CED
12	M	408	PEF	C11-C10-O2-C2
12	H	303	PEF	O4-C10-O2-C2
12	H	304	PEF	O4-C10-O2-C2
9	d	101	BCL	O1A-CGA-O2A-C1
9	J	102	BCL	C3-C5-C6-C7
9	K	101	BCL	C3-C5-C6-C7
9	N	102	BCL	C3-C5-C6-C7
9	W	101	BCL	C3-C5-C6-C7
9	X	102	BCL	C3-C5-C6-C7
9	8	102	BCL	C3-C5-C6-C7
9	9	103	BCL	C3-C5-C6-C7
9	w	101	BCL	C3-C5-C6-C7
9	z	102	BCL	C3-C5-C6-C7
9	AH	103	BCL	C3-C5-C6-C7
9	k	102	BCL	C3-C5-C6-C7
9	J	102	BCL	CBA-CGA-O2A-C1
9	O	101	BCL	CBA-CGA-O2A-C1
9	T	102	BCL	CBA-CGA-O2A-C1
9	W	101	BCL	CBA-CGA-O2A-C1
9	Z	102	BCL	CBA-CGA-O2A-C1
9	4	102	BCL	CBA-CGA-O2A-C1
9	v	102	BCL	CBA-CGA-O2A-C1
9	AH	103	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	i	102	BCL	CBA-CGA-O2A-C1
9	B	101	BCL	CBD-CGD-O2D-CED
9	5	101	BCL	CBD-CGD-O2D-CED
9	8	102	BCL	CBD-CGD-O2D-CED
9	AA	101	BCL	CBD-CGD-O2D-CED
9	c	102	BCL	CBD-CGD-O2D-CED
12	y	408	PEF	C11-C10-O2-C2
12	t	303	PEF	O4-C10-O2-C2
9	P	101	BCL	C4-C3-C5-C6
9	T	102	BCL	C4-C3-C5-C6
9	W	101	BCL	C4-C3-C5-C6
9	Z	102	BCL	C4-C3-C5-C6
9	l	102	BCL	C4-C3-C5-C6
9	s	102	BCL	C4-C3-C5-C6
9	w	101	BCL	C4-C3-C5-C6
9	AE	102	BCL	C4-C3-C5-C6
9	d	101	BCL	C4-C3-C5-C6
9	e	102	BCL	C4-C3-C5-C6
10	y	402	BPH	C4-C3-C5-C6
14	M	403	MQ8	C14-C13-C15-C16
14	y	403	MQ8	C14-C13-C15-C16
9	P	101	BCL	C2-C3-C5-C6
9	Q	101	BCL	C2-C3-C5-C6
9	T	102	BCL	C2-C3-C5-C6
9	W	101	BCL	C2-C3-C5-C6
9	l	102	BCL	C2-C3-C5-C6
9	s	102	BCL	C2-C3-C5-C6
9	AE	102	BCL	C2-C3-C5-C6
9	e	102	BCL	C2-C3-C5-C6
9	i	102	BCL	C2-C3-C5-C6
10	y	402	BPH	C2-C3-C5-C6
14	M	403	MQ8	C32-C33-C35-C36
14	M	403	MQ8	C46-C47-C48-C50
9	0	101	BCL	O1A-CGA-O2A-C1
9	D	102	BCL	C3-C5-C6-C7
9	U	101	BCL	C3-C5-C6-C7
9	x	303	BCL	C3-C5-C6-C7
9	p	104	BCL	C3-C5-C6-C7
9	AJ	102	BCL	C3-C5-C6-C7
9	g	101	BCL	C3-C5-C6-C7
9	i	102	BCL	C3-C5-C6-C7
10	M	402	BPH	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	K	101	BCL	CBA-CGA-O2A-C1
9	R	102	BCL	CBA-CGA-O2A-C1
9	X	102	BCL	CBA-CGA-O2A-C1
9	5	102	BCL	CBA-CGA-O2A-C1
9	z	102	BCL	CBA-CGA-O2A-C1
9	AB	101	BCL	CBA-CGA-O2A-C1
9	AC	102	BCL	CBA-CGA-O2A-C1
9	AE	104	BCL	CBA-CGA-O2A-C1
9	c	102	BCL	CBA-CGA-O2A-C1
14	M	403	MQ8	C16-C17-C18-C19
14	y	403	MQ8	C11-C12-C13-C14
14	y	403	MQ8	C36-C37-C38-C39
14	y	403	MQ8	C41-C42-C43-C45
14	y	403	MQ8	C41-C42-C43-C44
15	9	102	CRT	C11-C10-C9-C7
15	AH	102	CRT	C25-C26-C27-C28
9	K	101	BCL	O1A-CGA-O2A-C1
9	T	102	BCL	O1A-CGA-O2A-C1
9	V	101	BCL	O1A-CGA-O2A-C1
9	Z	102	BCL	O1A-CGA-O2A-C1
9	AB	101	BCL	O1A-CGA-O2A-C1
9	AC	102	BCL	O1A-CGA-O2A-C1
9	AH	103	BCL	O1A-CGA-O2A-C1
9	i	102	BCL	O1A-CGA-O2A-C1
9	c	102	BCL	O1A-CGA-O2A-C1
9	F	101	BCL	O1D-CGD-O2D-CED
9	h	101	BCL	O1D-CGD-O2D-CED
9	L	303	BCL	C13-C15-C16-C17
12	M	408	PEF	O5-C30-O3-C3
12	H	304	PEF	C31-C30-O3-C3
9	AD	101	BCL	C3-C5-C6-C7
10	x	302	BPH	C3-C5-C6-C7
9	9	103	BCL	CBD-CGD-O2D-CED
9	x	305	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	CBA-CGA-O2A-C1
9	1	101	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	CBA-CGA-O2A-C1
12	y	407	PEF	O5-C30-O3-C3
12	p	101	PEF	O2-C2-C3-O3
12	t	301	PEF	C11-C10-O2-C2
9	F	101	BCL	O1A-CGA-O2A-C1
12	M	408	PEF	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
9	A	102	BCL	O1D-CGD-O2D-CED
9	V	101	BCL	CBA-CGA-O2A-C1
9	0	101	BCL	CBA-CGA-O2A-C1
9	d	101	BCL	CBA-CGA-O2A-C1
9	X	102	BCL	C4-C3-C5-C6
9	AD	101	BCL	C4-C3-C5-C6
9	Z	102	BCL	C2-C3-C5-C6
9	w	101	BCL	C2-C3-C5-C6
9	AD	101	BCL	C2-C3-C5-C6
14	y	403	MQ8	C42-C43-C44-C46
12	y	408	PEF	O5-C30-O3-C3
12	H	303	PEF	C31-C30-O3-C3
9	1	101	BCL	O1A-CGA-O2A-C1
9	5	102	BCL	O1A-CGA-O2A-C1
11	L	304	UQ8	C29-C31-C32-C33
11	x	304	UQ8	C29-C31-C32-C33
11	x	304	UQ8	C19-C21-C22-C23
14	M	403	MQ8	C18-C20-C21-C22
14	M	403	MQ8	C33-C35-C36-C37
14	M	403	MQ8	C43-C44-C46-C47
14	y	403	MQ8	C28-C30-C31-C32
14	y	403	MQ8	C33-C35-C36-C37
14	y	403	MQ8	C38-C40-C41-C42
14	y	403	MQ8	C43-C44-C46-C47
9	x	305	BCL	C15-C16-C17-C18
7	o	502	HEM	C3D-CAD-CBD-CGD
9	AD	101	BCL	C2A-CAA-CBA-CGA
9	L	305	BCL	O1D-CGD-O2D-CED
9	j	101	BCL	O1A-CGA-O2A-C1
9	N	102	BCL	CBA-CGA-O2A-C1
9	AA	101	BCL	CBA-CGA-O2A-C1
9	AJ	102	BCL	CBA-CGA-O2A-C1
14	M	403	MQ8	C36-C37-C38-C39
9	R	102	BCL	C15-C16-C17-C18
9	Y	101	BCL	CBD-CGD-O2D-CED
12	y	407	PEF	C31-C30-O3-C3
9	x	305	BCL	C3-C5-C6-C7
12	A	101	PEF	C11-C10-O2-C2
15	n	101	CRT	C11-C10-C9-C7
9	N	102	BCL	O1A-CGA-O2A-C1
17	S	101	PGW	O12-C04-C05-CAD
9	D	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	U	101	BCL	CBA-CGA-O2A-C1
9	7	101	BCL	CBA-CGA-O2A-C1
9	x	303	BCL	CBA-CGA-O2A-C1
9	m	102	BCL	CBA-CGA-O2A-C1
9	AL	102	BCL	CBA-CGA-O2A-C1
9	h	101	BCL	CBA-CGA-O2A-C1
10	M	402	BPH	CBD-CGD-O2D-CED
12	y	408	PEF	C31-C30-O3-C3
9	8	102	BCL	O1D-CGD-O2D-CED
9	AA	101	BCL	O1D-CGD-O2D-CED
9	AJ	102	BCL	O1A-CGA-O2A-C1
9	G	102	BCL	C4-C3-C5-C6
9	AA	101	BCL	C4-C3-C5-C6
14	y	403	MQ8	C45-C43-C44-C46
9	G	102	BCL	C2-C3-C5-C6
9	AA	101	BCL	C2-C3-C5-C6
9	d	101	BCL	C2-C3-C5-C6
14	M	403	MQ8	C12-C13-C15-C16
14	y	403	MQ8	C12-C13-C15-C16
14	y	403	MQ8	C32-C33-C35-C36
9	u	101	BCL	C3-C5-C6-C7
9	B	101	BCL	C11-C12-C13-C14
9	N	102	BCL	C6-C7-C8-C9
9	Q	101	BCL	C11-C12-C13-C14
9	S	102	BCL	C6-C7-C8-C9
9	T	102	BCL	C6-C7-C8-C9
9	W	101	BCL	C11-C10-C8-C9
9	Y	101	BCL	C14-C13-C15-C16
9	1	101	BCL	C11-C12-C13-C14
9	5	101	BCL	C14-C13-C15-C16
9	5	102	BCL	C6-C7-C8-C9
9	0	101	BCL	C14-C13-C15-C16
9	m	103	BCL	C6-C7-C8-C9
9	m	103	BCL	C14-C13-C15-C16
9	p	102	BCL	C11-C10-C8-C9
9	w	101	BCL	C6-C7-C8-C9
9	AI	101	BCL	C11-C12-C13-C14
9	AJ	102	BCL	C6-C7-C8-C9
9	g	101	BCL	C14-C13-C15-C16
9	c	102	BCL	O1D-CGD-O2D-CED
12	y	407	PEF	O4-C10-O2-C2
12	M	407	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
17	S	101	PGW	O12-C04-C05-OAF
9	B	101	BCL	O1D-CGD-O2D-CED
15	A	103	CRT	C5-C6-C7-C8
15	E	101	CRT	C24-C23-C25-C26
15	N	101	CRT	C5-C6-C7-C8
15	R	101	CRT	C5-C6-C7-C8
15	R	101	CRT	C15-C16-C17-C18
15	T	101	CRT	C5-C6-C7-C8
15	T	101	CRT	C15-C16-C17-C18
15	U	102	CRT	C10-C11-C12-C13
15	U	102	CRT	C15-C16-C17-C18
15	Z	101	CRT	C10-C11-C12-C13
15	2	101	CRT	C15-C16-C17-C18
15	4	101	CRT	C5-C6-C7-C8
15	4	101	CRT	C15-C16-C17-C18
15	4	101	CRT	C29-C28-C30-C31
15	6	101	CRT	C24-C23-C25-C26
15	9	102	CRT	C15-C16-C17-C18
15	n	101	CRT	C5-C6-C7-C8
15	s	101	CRT	C15-C16-C17-C18
15	v	101	CRT	C29-C28-C30-C31
15	AH	102	CRT	C24-C23-C25-C26
15	AL	101	CRT	C15-C16-C17-C18
15	e	101	CRT	C24-C23-C25-C26
15	c	101	CRT	C5-C6-C7-C8
15	A	103	CRT	C5-C6-C7-C9
15	9	102	CRT	C5-C6-C7-C9
15	n	101	CRT	C5-C6-C7-C9
9	3	101	BCL	C2A-CAA-CBA-CGA
9	p	104	BCL	C2A-CAA-CBA-CGA
9	w	101	BCL	C2A-CAA-CBA-CGA
9	D	102	BCL	O1A-CGA-O2A-C1
9	x	303	BCL	O1A-CGA-O2A-C1
9	y	401	BCL	CBA-CGA-O2A-C1
9	p	104	BCL	CBA-CGA-O2A-C1
9	AD	101	BCL	CBA-CGA-O2A-C1
9	x	305	BCL	C2-C1-O2A-CGA
9	5	101	BCL	O1D-CGD-O2D-CED
9	A	102	BCL	C8-C10-C11-C12
9	G	102	BCL	C15-C16-C17-C18
9	P	101	BCL	C5-C6-C7-C8
9	X	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	AC	102	BCL	C13-C15-C16-C17
9	AK	101	BCL	C13-C15-C16-C17
9	h	101	BCL	C15-C16-C17-C18
9	i	102	BCL	C8-C10-C11-C12
17	S	101	PGW	OAF-C05-CAD-OAE
9	N	102	BCL	C11-C12-C13-C15
9	Y	101	BCL	C11-C12-C13-C15
9	8	102	BCL	C11-C12-C13-C15
9	r	101	BCL	C11-C10-C8-C7
9	AI	101	BCL	C12-C13-C15-C16
9	p	104	BCL	C4-C3-C5-C6
9	F	101	BCL	C5-C6-C7-C8
9	AE	104	BCL	C5-C6-C7-C8
11	L	304	UQ8	C39-C41-C42-C43
11	L	304	UQ8	C14-C16-C17-C18
11	x	304	UQ8	C24-C26-C27-C28
9	F	101	BCL	C3-C5-C6-C7
9	z	102	BCL	C5-C6-C7-C8
9	AD	101	BCL	C8-C10-C11-C12
12	H	303	PEF	O5-C30-O3-C3
12	H	304	PEF	O5-C30-O3-C3
9	U	101	BCL	O1A-CGA-O2A-C1
9	y	401	BCL	O1A-CGA-O2A-C1
9	m	102	BCL	O1A-CGA-O2A-C1
9	AD	101	BCL	O1A-CGA-O2A-C1
9	h	101	BCL	O1A-CGA-O2A-C1
9	M	401	BCL	C5-C6-C7-C8
9	T	102	BCL	C13-C15-C16-C17
9	3	101	BCL	C5-C6-C7-C8
9	5	101	BCL	C8-C10-C11-C12
9	8	102	BCL	C15-C16-C17-C18
9	m	102	BCL	C15-C16-C17-C18
7	C	502	HEM	C3D-CAD-CBD-CGD
9	L	303	BCL	C2A-CAA-CBA-CGA
9	x	301	BCL	C2A-CAA-CBA-CGA
9	x	303	BCL	C2A-CAA-CBA-CGA
9	r	101	BCL	C2A-CAA-CBA-CGA
9	AI	101	BCL	C2A-CAA-CBA-CGA
9	T	102	BCL	C5-C6-C7-C8
9	W	101	BCL	C13-C15-C16-C17
9	Z	102	BCL	C8-C10-C11-C12
9	Z	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	4	102	BCL	C5-C6-C7-C8
9	AA	101	BCL	C8-C10-C11-C12
9	L	301	BCL	C13-C15-C16-C17
9	F	101	BCL	C10-C11-C12-C13
9	F	101	BCL	C13-C15-C16-C17
9	G	102	BCL	C8-C10-C11-C12
9	N	102	BCL	C13-C15-C16-C17
9	N	102	BCL	C15-C16-C17-C18
9	R	102	BCL	C13-C15-C16-C17
9	U	101	BCL	C15-C16-C17-C18
9	X	102	BCL	C10-C11-C12-C13
9	X	102	BCL	C13-C15-C16-C17
9	8	102	BCL	C10-C11-C12-C13
9	x	301	BCL	C13-C15-C16-C17
9	r	101	BCL	C8-C10-C11-C12
9	AD	101	BCL	C5-C6-C7-C8
9	AH	103	BCL	C8-C10-C11-C12
9	AJ	102	BCL	C8-C10-C11-C12
9	e	102	BCL	C5-C6-C7-C8
9	k	102	BCL	C10-C11-C12-C13
9	k	102	BCL	C15-C16-C17-C18
12	M	408	PEF	O4-C10-O2-C2
9	7	101	BCL	O1A-CGA-O2A-C1
9	AA	101	BCL	O1A-CGA-O2A-C1
9	AL	102	BCL	O1A-CGA-O2A-C1
9	Q	101	BCL	C8-C10-C11-C12
9	m	103	BCL	C5-C6-C7-C8
9	AE	104	BCL	C8-C10-C11-C12
9	i	102	BCL	C13-C15-C16-C17
9	j	101	BCL	C10-C11-C12-C13
9	l	101	BCL	C8-C10-C11-C12
14	y	403	MQ8	C46-C47-C48-C50
9	L	303	BCL	C5-C6-C7-C8
9	1	102	BCL	C8-C10-C11-C12
9	4	102	BCL	C8-C10-C11-C12
9	x	305	BCL	C13-C15-C16-C17
9	v	102	BCL	C5-C6-C7-C8
9	z	102	BCL	C10-C11-C12-C13
10	L	302	BPH	C5-C6-C7-C8
9	X	102	BCL	C2-C3-C5-C6
9	AI	101	BCL	C13-C15-C16-C17
9	p	104	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	W	101	BCL	C10-C11-C12-C13
9	AA	101	BCL	C5-C6-C7-C8
9	AH	101	BCL	C5-C6-C7-C8
15	AL	101	CRT	C30-C31-C32-C33
9	0	101	BCL	C8-C10-C11-C12
9	AH	103	BCL	C13-C15-C16-C17
9	L	301	BCL	C2A-CAA-CBA-CGA
9	Q	101	BCL	C2A-CAA-CBA-CGA
9	s	102	BCL	C2A-CAA-CBA-CGA
9	AH	101	BCL	C2A-CAA-CBA-CGA
9	g	101	BCL	C2A-CAA-CBA-CGA
9	9	103	BCL	O1D-CGD-O2D-CED
9	P	101	BCL	CBA-CGA-O2A-C1
9	AK	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	CBA-CGA-O2A-C1
9	l	101	BCL	CBA-CGA-O2A-C1
9	B	101	BCL	C13-C15-C16-C17
9	R	102	BCL	C10-C11-C12-C13
9	S	102	BCL	C8-C10-C11-C12
9	x	301	BCL	C5-C6-C7-C8
9	p	102	BCL	C15-C16-C17-C18
9	r	101	BCL	C13-C15-C16-C17
9	s	102	BCL	C5-C6-C7-C8
9	AK	101	BCL	C8-C10-C11-C12
9	f	101	BCL	C5-C6-C7-C8
9	c	102	BCL	C13-C15-C16-C17
14	y	403	MQ8	C46-C47-C48-C49
9	D	102	BCL	C15-C16-C17-C18
9	AE	104	BCL	C13-C15-C16-C17
9	g	101	BCL	C15-C16-C17-C18
9	k	102	BCL	C8-C10-C11-C12
9	Q	101	BCL	C5-C6-C7-C8
9	x	301	BCL	C15-C16-C17-C18
12	y	408	PEF	O4-C10-O2-C2
9	AI	101	BCL	C4-C3-C5-C6
9	3	101	BCL	C15-C16-C17-C18
9	AB	101	BCL	C15-C16-C17-C18
14	M	403	MQ8	C41-C42-C43-C45
9	p	102	BCL	CBA-CGA-O2A-C1
9	u	101	BCL	CBA-CGA-O2A-C1
9	L	303	BCL	C16-C17-C18-C20
9	M	401	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	AC	102	BCL	C16-C17-C18-C19
9	AI	101	BCL	C16-C17-C18-C19
9	Y	101	BCL	C8-C10-C11-C12
15	X	101	CRT	C10-C11-C12-C13
15	X	101	CRT	C24-C23-C25-C26
15	9	102	CRT	C5-C6-C7-C8
15	n	101	CRT	C24-C23-C25-C26
15	p	103	CRT	C5-C6-C7-C8
15	v	101	CRT	C15-C16-C17-C18
15	AD	102	CRT	C29-C28-C30-C31
15	AL	101	CRT	C5-C6-C7-C8
15	6	101	CRT	C22-C23-C25-C26
9	k	102	BCL	C2A-CAA-CBA-CGA
9	c	102	BCL	C2A-CAA-CBA-CGA
9	7	101	BCL	C8-C10-C11-C12
9	z	102	BCL	C13-C15-C16-C17
9	y	401	BCL	O2A-C1-C2-C3
9	AH	103	BCL	O2A-C1-C2-C3
12	x	306	PEF	C1-C2-O2-C10
9	5	102	BCL	C16-C17-C18-C20
9	z	102	BCL	C16-C17-C18-C19
9	d	101	BCL	C16-C17-C18-C19
9	e	102	BCL	C15-C16-C17-C18
9	p	104	BCL	C2-C3-C5-C6
9	I	101	BCL	CBA-CGA-O2A-C1
9	y	401	BCL	C2-C1-O2A-CGA
9	L	301	BCL	C16-C17-C18-C19
9	L	305	BCL	C16-C17-C18-C19
9	Q	101	BCL	C16-C17-C18-C19
9	Z	102	BCL	C16-C17-C18-C19
9	Z	102	BCL	C16-C17-C18-C20
9	u	101	BCL	C16-C17-C18-C19
9	AK	101	BCL	C16-C17-C18-C19
9	d	101	BCL	C16-C17-C18-C20
12	t	301	PEF	O4-C10-O2-C2
9	f	101	BCL	O1A-CGA-O2A-C1
9	7	101	BCL	C10-C11-C12-C13
9	D	102	BCL	C13-C15-C16-C17
9	g	101	BCL	C8-C10-C11-C12
9	Q	101	BCL	CBA-CGA-O2A-C1
9	AI	101	BCL	C5-C6-C7-C8
9	L	303	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	M	401	BCL	C16-C17-C18-C20
9	Q	101	BCL	C16-C17-C18-C20
9	m	103	BCL	C16-C17-C18-C19
9	m	103	BCL	C16-C17-C18-C20
9	AC	102	BCL	C16-C17-C18-C20
9	AI	101	BCL	C16-C17-C18-C20
9	AK	101	BCL	C16-C17-C18-C20
9	g	101	BCL	C16-C17-C18-C19
9	j	101	BCL	C16-C17-C18-C20
9	l	101	BCL	C16-C17-C18-C19
9	AB	101	BCL	C8-C10-C11-C12
9	j	101	BCL	C15-C16-C17-C18
9	5	101	BCL	C11-C10-C8-C7
9	9	103	BCL	C11-C12-C13-C15
9	L	301	BCL	C15-C16-C17-C18
9	M	401	BCL	C15-C16-C17-C18
9	P	101	BCL	O1A-CGA-O2A-C1
9	AK	101	BCL	O1A-CGA-O2A-C1
9	l	101	BCL	C4-C3-C5-C6
9	p	104	BCL	C3A-C2A-CAA-CBA
9	u	101	BCL	C3A-C2A-CAA-CBA
9	AH	101	BCL	C3A-C2A-CAA-CBA
9	AH	103	BCL	C3A-C2A-CAA-CBA
9	d	101	BCL	C3A-C2A-CAA-CBA
10	M	402	BPH	C15-C16-C17-C18
9	L	301	BCL	C16-C17-C18-C20
9	L	305	BCL	C16-C17-C18-C20
9	5	102	BCL	C16-C17-C18-C19
9	u	101	BCL	C16-C17-C18-C20
9	z	102	BCL	C16-C17-C18-C20
9	f	101	BCL	C16-C17-C18-C20
9	l	101	BCL	O1A-CGA-O2A-C1
9	AE	102	BCL	CBA-CGA-O2A-C1
9	I	101	BCL	O1A-CGA-O2A-C1
9	Q	101	BCL	O1A-CGA-O2A-C1
12	M	407	PEF	C31-C30-O3-C3
9	Y	101	BCL	C16-C17-C18-C19
9	p	102	BCL	O1A-CGA-O2A-C1
9	u	101	BCL	O1A-CGA-O2A-C1
9	S	102	BCL	C13-C15-C16-C17
9	u	101	BCL	C13-C15-C16-C17
9	f	101	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	L	305	BCL	C3-C5-C6-C7
12	x	306	PEF	C31-C30-O3-C3
7	o	501	HEM	C2A-CAA-CBA-CGA
9	w	101	BCL	C5-C6-C7-C8
9	l	101	BCL	C2-C3-C5-C6
9	AI	101	BCL	C2-C3-C5-C6
10	M	402	BPH	O1D-CGD-O2D-CED
9	D	101	BCL	CBA-CGA-O2A-C1
9	5	101	BCL	CBA-CGA-O2A-C1
9	D	101	BCL	C11-C10-C8-C9
12	M	407	PEF	C2-C3-O3-C30
9	V	101	BCL	C8-C10-C11-C12
9	5	102	BCL	C10-C11-C12-C13
9	AI	101	BCL	C15-C16-C17-C18
9	l	101	BCL	C10-C11-C12-C13
9	AE	102	BCL	O1A-CGA-O2A-C1
15	J	101	CRT	C11-C10-C9-C7
15	c	101	CRT	C25-C26-C27-C28
9	AH	103	BCL	C16-C17-C18-C19
9	g	101	BCL	C16-C17-C18-C20
9	l	101	BCL	C16-C17-C18-C20
9	J	102	BCL	C5-C6-C7-C8
9	c	102	BCL	C10-C11-C12-C13
9	G	102	BCL	C5-C6-C7-C8
9	u	101	BCL	C8-C10-C11-C12
15	i	101	CRT	C34-C33-C35-C36
9	I	101	BCL	C3-C5-C6-C7
15	4	101	CRT	C5-C6-C7-C9
9	P	101	BCL	C16-C17-C18-C19
9	j	101	BCL	C16-C17-C18-C19
11	x	304	UQ8	C20-C19-C21-C22
11	x	304	UQ8	C18-C19-C21-C22
9	Y	101	BCL	O1D-CGD-O2D-CED
9	O	101	BCL	C8-C10-C11-C12
9	8	102	BCL	C8-C10-C11-C12
9	x	305	BCL	C5-C6-C7-C8
9	AJ	102	BCL	C15-C16-C17-C18
9	h	101	BCL	C10-C11-C12-C13
7	C	502	HEM	C4B-C3B-CAB-CBB
7	o	501	HEM	C4B-C3B-CAB-CBB
17	AE	101	PGW	C20-C19-O03-C01
9	L	301	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	y	401	BCL	C13-C15-C16-C17
9	AI	101	BCL	C10-C11-C12-C13
10	M	402	BPH	C8-C10-C11-C12
12	H	304	PEF	O2-C2-C3-O3
10	y	402	BPH	CBA-CGA-O2A-C1
9	r	101	BCL	C15-C16-C17-C18
12	A	101	PEF	O4-C10-O2-C2
9	9	103	BCL	C2-C1-O2A-CGA
10	y	402	BPH	C2C-C3C-CAC-CBC
9	AH	103	BCL	C16-C17-C18-C20
9	e	102	BCL	C10-C11-C12-C13
9	i	102	BCL	C2A-CAA-CBA-CGA
9	S	102	BCL	C5-C6-C7-C8
9	AB	101	BCL	C10-C11-C12-C13
9	D	101	BCL	O1A-CGA-O2A-C1
9	5	101	BCL	O1A-CGA-O2A-C1
9	AL	102	BCL	C3-C5-C6-C7
9	D	102	BCL	C1A-C2A-CAA-CBA
9	G	102	BCL	C1A-C2A-CAA-CBA
9	N	102	BCL	C1A-C2A-CAA-CBA
9	O	101	BCL	C1A-C2A-CAA-CBA
9	X	102	BCL	C1A-C2A-CAA-CBA
9	Y	101	BCL	C1A-C2A-CAA-CBA
9	1	102	BCL	C1A-C2A-CAA-CBA
9	4	102	BCL	C1A-C2A-CAA-CBA
9	5	102	BCL	C1A-C2A-CAA-CBA
9	0	101	BCL	C1A-C2A-CAA-CBA
9	x	303	BCL	C1A-C2A-CAA-CBA
9	y	401	BCL	C1A-C2A-CAA-CBA
9	m	103	BCL	C1A-C2A-CAA-CBA
9	p	102	BCL	C1A-C2A-CAA-CBA
9	v	102	BCL	C1A-C2A-CAA-CBA
9	z	102	BCL	C1A-C2A-CAA-CBA
9	AC	102	BCL	C1A-C2A-CAA-CBA
9	AE	104	BCL	C1A-C2A-CAA-CBA
9	e	102	BCL	C1A-C2A-CAA-CBA
9	g	101	BCL	C1A-C2A-CAA-CBA
9	i	102	BCL	C1A-C2A-CAA-CBA
17	S	101	PGW	C01-C02-C03-O11
9	L	303	BCL	C11-C12-C13-C15
9	B	101	BCL	C11-C12-C13-C15
9	D	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	G	102	BCL	C11-C12-C13-C15
9	Y	101	BCL	C12-C13-C15-C16
9	5	102	BCL	C6-C7-C8-C10
9	8	102	BCL	C6-C7-C8-C10
9	m	103	BCL	C12-C13-C15-C16
9	v	102	BCL	C11-C12-C13-C15
9	w	101	BCL	C11-C10-C8-C7
9	AC	102	BCL	C11-C12-C13-C15
9	AD	101	BCL	C11-C10-C8-C7
9	AH	101	BCL	C11-C12-C13-C15
9	AH	103	BCL	C11-C12-C13-C15
9	AL	102	BCL	C6-C7-C8-C10
9	f	101	BCL	C11-C12-C13-C15
10	L	302	BPH	C11-C10-C8-C7
9	Y	101	BCL	C16-C17-C18-C20
9	AD	101	BCL	C16-C17-C18-C20
9	L	301	BCL	C2C-C3C-CAC-CBC
9	y	401	BCL	C2C-C3C-CAC-CBC
9	m	102	BCL	C2C-C3C-CAC-CBC
9	AJ	102	BCL	C2C-C3C-CAC-CBC
15	M	404	CRT	C2-C1-C4-C5
15	M	404	CRT	C3-C1-C4-C5
15	A	103	CRT	C2-C1-C4-C5
15	A	103	CRT	C3-C1-C4-C5
15	N	101	CRT	C36-C37-C38-C39
15	P	102	CRT	C2-C1-C4-C5
15	U	102	CRT	C36-C37-C38-C39
15	X	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	C3-C1-C4-C5
15	n	101	CRT	C3-C1-C4-C5
15	p	103	CRT	C36-C37-C38-C40
15	AD	102	CRT	C36-C37-C38-C39
15	f	102	CRT	C3-C1-C4-C5
15	i	101	CRT	C36-C37-C38-C40
9	R	102	BCL	C5-C6-C7-C8
9	AH	101	BCL	C10-C11-C12-C13
9	g	101	BCL	C4-C3-C5-C6
14	M	403	MQ8	C29-C28-C30-C31
9	z	102	BCL	C15-C16-C17-C18
9	l	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	z	102	BCL	C2A-CAA-CBA-CGA
9	e	102	BCL	C2A-CAA-CBA-CGA
9	D	101	BCL	C6-C7-C8-C9
9	D	102	BCL	C14-C13-C15-C16
9	Y	101	BCL	C11-C12-C13-C14
9	8	102	BCL	C6-C7-C8-C9
9	9	103	BCL	C14-C13-C15-C16
9	p	102	BCL	C6-C7-C8-C9
9	p	104	BCL	C14-C13-C15-C16
9	r	101	BCL	C6-C7-C8-C9
9	v	102	BCL	C11-C12-C13-C14
9	AB	101	BCL	C11-C10-C8-C9
9	AE	102	BCL	C14-C13-C15-C16
9	AH	101	BCL	C11-C12-C13-C14
9	AH	103	BCL	C11-C12-C13-C14
9	j	101	BCL	C11-C10-C8-C9
10	y	402	BPH	C11-C10-C8-C9
7	o	504	HEM	C4D-C3D-CAD-CBD
9	1	101	BCL	C13-C15-C16-C17
9	3	101	BCL	C10-C11-C12-C13
11	x	304	UQ8	C39-C41-C42-C43
12	M	408	PEF	C1-C2-C3-O3
12	H	304	PEF	C1-C2-C3-O3
9	D	101	BCL	C8-C10-C11-C12
9	W	101	BCL	C8-C10-C11-C12
9	p	102	BCL	C8-C10-C11-C12
9	j	101	BCL	C5-C6-C7-C8
9	F	101	BCL	C16-C17-C18-C20
9	I	101	BCL	C10-C11-C12-C13
10	y	402	BPH	O1A-CGA-O2A-C1
14	M	403	MQ8	C22-C23-C25-C26
9	AL	102	BCL	C8-C10-C11-C12
15	s	101	CRT	C10-C11-C12-C13
15	v	101	CRT	C15-C16-C17-C19
9	B	101	BCL	C8-C10-C11-C12
9	AC	102	BCL	C15-C16-C17-C18
9	AH	101	BCL	C13-C15-C16-C17
9	AL	102	BCL	C15-C16-C17-C18
9	7	101	BCL	C5-C6-C7-C8
9	A	102	BCL	O2A-C1-C2-C3
9	i	102	BCL	O2A-C1-C2-C3
10	y	402	BPH	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
17	AE	101	PGW	C03-C02-O01-C1
9	D	101	BCL	C15-C16-C17-C18
9	5	101	BCL	C15-C16-C17-C18
15	p	103	CRT	C11-C10-C9-C7
9	S	102	BCL	C16-C17-C18-C19
12	M	407	PEF	O3P-C1-C2-C3
9	U	101	BCL	C10-C11-C12-C13
9	W	101	BCL	C15-C16-C17-C18
9	S	102	BCL	CBA-CGA-O2A-C1
9	p	102	BCL	C5-C6-C7-C8
9	R	102	BCL	C2-C3-C5-C6
9	U	101	BCL	C2-C3-C5-C6
9	g	101	BCL	C2-C3-C5-C6
12	M	407	PEF	O5-C30-O3-C3
10	x	302	BPH	C10-C11-C12-C13
15	M	404	CRT	C2-C1-O1-C1M
15	A	103	CRT	C3-C1-O1-C1M
15	E	101	CRT	C2-C1-O1-C1M
15	G	101	CRT	C2-C1-O1-C1M
15	J	101	CRT	C3-C1-O1-C1M
15	J	101	CRT	C39-C38-O2-C2M
15	N	101	CRT	C2-C1-O1-C1M
15	R	101	CRT	C2-C1-O1-C1M
15	T	101	CRT	C3-C1-O1-C1M
15	U	102	CRT	C2-C1-O1-C1M
15	4	101	CRT	C2-C1-O1-C1M
15	6	101	CRT	C2-C1-O1-C1M
15	8	101	CRT	C2-C1-O1-C1M
15	9	102	CRT	C2-C1-O1-C1M
15	y	404	CRT	C3-C1-O1-C1M
15	y	404	CRT	C39-C38-O2-C2M
15	y	404	CRT	C40-C38-O2-C2M
15	n	101	CRT	C3-C1-O1-C1M
15	n	101	CRT	C39-C38-O2-C2M
15	p	103	CRT	C3-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	AE	103	CRT	C2-C1-O1-C1M
15	AH	102	CRT	C2-C1-O1-C1M
15	i	101	CRT	C2-C1-O1-C1M
15	k	101	CRT	C2-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
15	c	101	CRT	C2-C1-O1-C1M
9	O	101	BCL	C15-C16-C17-C18
9	A	102	BCL	C15-C16-C17-C18
9	d	101	BCL	C15-C16-C17-C18
9	R	102	BCL	C4-C3-C5-C6
10	L	302	BPH	C4-C3-C5-C6
10	M	402	BPH	CBA-CGA-O2A-C1
9	1	102	BCL	C5-C6-C7-C8
9	L	303	BCL	C11-C12-C13-C14
9	L	305	BCL	C11-C10-C8-C9
9	G	102	BCL	C11-C12-C13-C14
9	V	101	BCL	C6-C7-C8-C9
9	x	305	BCL	C11-C10-C8-C9
9	m	102	BCL	C11-C10-C8-C9
9	w	101	BCL	C11-C10-C8-C9
9	AC	102	BCL	C11-C12-C13-C14
9	AD	101	BCL	C11-C10-C8-C9
9	AL	102	BCL	C6-C7-C8-C9
9	f	101	BCL	C11-C12-C13-C14
10	L	302	BPH	C6-C7-C8-C9
10	L	302	BPH	C11-C10-C8-C9
9	W	101	BCL	C5-C6-C7-C8
9	1	101	BCL	C5-C6-C7-C8
14	M	403	MQ8	C41-C42-C43-C44
12	M	408	PEF	O3P-C1-C2-C3
12	H	303	PEF	O3P-C1-C2-C3
12	y	408	PEF	O3P-C1-C2-C3
17	AE	101	PGW	C01-C02-C03-O11
12	x	306	PEF	O5-C30-O3-C3
9	L	305	BCL	C11-C10-C8-C7
9	D	102	BCL	C12-C13-C15-C16
9	K	101	BCL	C11-C10-C8-C7
9	Q	101	BCL	C11-C12-C13-C15
9	S	102	BCL	C12-C13-C15-C16
9	X	102	BCL	C11-C10-C8-C7
9	5	101	BCL	C12-C13-C15-C16
9	9	103	BCL	C12-C13-C15-C16
9	x	305	BCL	C11-C10-C8-C7
9	m	102	BCL	C11-C10-C8-C7
9	p	102	BCL	C6-C7-C8-C10
9	p	104	BCL	C12-C13-C15-C16
9	r	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	AB	101	BCL	C11-C10-C8-C7
9	AE	102	BCL	C12-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C7
9	j	101	BCL	C11-C10-C8-C7
10	M	402	BPH	C11-C10-C8-C7
10	y	402	BPH	C11-C10-C8-C7
12	H	301	PEF	C31-C30-O3-C3
9	9	103	BCL	C16-C17-C18-C20
9	R	102	BCL	C3A-C2A-CAA-CBA
9	U	101	BCL	C4-C3-C5-C6
9	l	101	BCL	C3A-C2A-CAA-CBA
9	w	101	BCL	C3A-C2A-CAA-CBA
9	AH	101	BCL	C4-C3-C5-C6
9	AI	101	BCL	C3A-C2A-CAA-CBA
10	y	402	BPH	C3A-C2A-CAA-CBA
9	B	101	BCL	C5-C6-C7-C8
15	c	101	CRT	C11-C10-C9-C7
10	L	302	BPH	C3-C5-C6-C7
9	L	305	BCL	CBA-CGA-O2A-C1
12	x	306	PEF	C1-C2-C3-O3
9	c	102	BCL	C8-C10-C11-C12
10	L	302	BPH	C2-C3-C5-C6
12	H	303	PEF	O3P-C1-C2-O2
9	Y	101	BCL	C10-C11-C12-C13
9	P	101	BCL	C16-C17-C18-C20
9	f	101	BCL	C16-C17-C18-C19
9	l	101	BCL	C2A-CAA-CBA-CGA
12	M	408	PEF	O2-C2-C3-O3
12	t	303	PEF	O2-C2-C3-O3
10	M	402	BPH	C13-C15-C16-C17
9	AH	101	BCL	C2-C3-C5-C6
14	y	403	MQ8	C22-C23-C25-C26
9	l	101	BCL	C15-C16-C17-C18
9	x	305	BCL	C4B-C3B-CAB-OB
9	j	101	BCL	C3-C5-C6-C7
9	S	102	BCL	C14-C13-C15-C16
9	5	102	BCL	C11-C12-C13-C14
9	f	101	BCL	C11-C10-C8-C9
9	k	102	BCL	C6-C7-C8-C9
10	M	402	BPH	C11-C12-C13-C14
12	M	406	PEF	C31-C30-O3-C3
9	AH	103	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	o	504	HEM	C2D-C3D-CAD-CBD
9	P	101	BCL	C4C-C3C-CAC-CBC
9	Q	101	BCL	C4C-C3C-CAC-CBC
9	3	101	BCL	C4C-C3C-CAC-CBC
9	4	102	BCL	C4C-C3C-CAC-CBC
9	7	101	BCL	C4C-C3C-CAC-CBC
9	d	101	BCL	C4C-C3C-CAC-CBC
9	F	101	BCL	C15-C16-C17-C18
9	0	101	BCL	C15-C16-C17-C18
9	x	305	BCL	CBA-CGA-O2A-C1
9	I	101	BCL	C4-C3-C5-C6
9	9	103	BCL	C5-C6-C7-C8
9	AH	101	BCL	C3-C5-C6-C7
9	y	401	BCL	C15-C16-C17-C18
12	x	306	PEF	O3P-C1-C2-C3
9	x	305	BCL	O1A-CGA-O2A-C1
9	AA	101	BCL	C13-C15-C16-C17
15	6	101	CRT	C34-C33-C35-C36
9	1	101	BCL	C11-C10-C8-C7
9	5	102	BCL	C11-C12-C13-C15
9	x	301	BCL	C12-C13-C15-C16
9	AJ	102	BCL	C6-C7-C8-C10
9	AJ	102	BCL	C11-C10-C8-C7
9	k	102	BCL	C6-C7-C8-C10
9	k	102	BCL	C11-C12-C13-C15
10	L	302	BPH	C6-C7-C8-C10
10	M	402	BPH	C6-C7-C8-C10
10	M	402	BPH	C11-C12-C13-C15
15	N	101	CRT	C1-C4-C5-C6
15	R	101	CRT	C1-C4-C5-C6
15	AJ	101	CRT	C35-C36-C37-C38
15	f	102	CRT	C1-C4-C5-C6
15	f	102	CRT	C35-C36-C37-C38
9	f	101	BCL	C10-C11-C12-C13
15	R	101	CRT	C15-C16-C17-C19
15	n	101	CRT	C22-C23-C25-C26
15	p	103	CRT	C5-C6-C7-C9
15	c	101	CRT	C5-C6-C7-C9
9	F	101	BCL	C16-C17-C18-C19
9	S	102	BCL	C16-C17-C18-C20
9	AK	101	BCL	C4-C3-C5-C6
9	S	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	M	402	BPH	O1A-CGA-O2A-C1
7	C	502	HEM	C2B-C3B-CAB-CBB
9	5	102	BCL	C3-C5-C6-C7
9	O	101	BCL	C5-C6-C7-C8
17	S	101	PGW	C03-C02-O01-C1
9	AK	101	BCL	C15-C16-C17-C18
9	L	305	BCL	O1A-CGA-O2A-C1
9	9	103	BCL	C10-C11-C12-C13
9	p	104	BCL	C13-C15-C16-C17
9	f	101	BCL	C8-C10-C11-C12
12	x	306	PEF	O3P-C1-C2-O2
17	S	101	PGW	O01-C02-C03-O11
17	AE	101	PGW	O01-C02-C03-O11
12	H	303	PEF	C1-C2-C3-O3
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	503	HEM	C4B-C3B-CAB-CBB
14	y	403	MQ8	C24-C23-C25-C26
9	I	101	BCL	C2-C3-C5-C6
14	M	403	MQ8	C27-C28-C30-C31
9	m	102	BCL	C5-C6-C7-C8
12	H	303	PEF	O2-C2-C3-O3
12	x	306	PEF	O2-C2-C3-O3
9	AB	101	BCL	C6-C7-C8-C9
9	f	101	BCL	C14-C13-C15-C16
10	M	402	BPH	C6-C7-C8-C9
9	L	305	BCL	C5-C6-C7-C8
9	X	102	BCL	C5-C6-C7-C8
9	l	102	BCL	C13-C15-C16-C17
15	M	404	CRT	O1-C1-C4-C5
15	M	404	CRT	C36-C37-C38-O2
15	y	404	CRT	C36-C37-C38-O2
15	n	101	CRT	O1-C1-C4-C5
15	p	103	CRT	C36-C37-C38-O2
15	i	101	CRT	C36-C37-C38-O2
17	AE	101	PGW	O04-C19-O03-C01
9	K	101	BCL	C16-C17-C18-C19
9	AD	101	BCL	C16-C17-C18-C19
9	AH	101	BCL	C16-C17-C18-C19
9	AH	101	BCL	C16-C17-C18-C20
9	R	102	BCL	C3-C5-C6-C7
9	5	101	BCL	C3-C5-C6-C7
9	AA	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	R	102	BCL	C1A-C2A-CAA-CBA
9	1	101	BCL	C1A-C2A-CAA-CBA
9	7	101	BCL	C1A-C2A-CAA-CBA
9	AA	101	BCL	C1A-C2A-CAA-CBA
9	AH	103	BCL	C1A-C2A-CAA-CBA
9	Y	101	BCL	CBA-CGA-O2A-C1
15	N	101	CRT	C5-C6-C7-C9
9	K	101	BCL	C16-C17-C18-C20
9	B	101	BCL	C11-C10-C8-C7
9	N	102	BCL	C11-C10-C8-C7
9	T	102	BCL	C11-C10-C8-C7
9	U	101	BCL	C11-C12-C13-C15
9	Z	102	BCL	C6-C7-C8-C10
9	1	101	BCL	C11-C12-C13-C15
9	7	101	BCL	C11-C12-C13-C15
9	0	101	BCL	C11-C12-C13-C15
9	0	101	BCL	C12-C13-C15-C16
9	s	102	BCL	C11-C12-C13-C15
9	z	102	BCL	C12-C13-C15-C16
9	AA	101	BCL	C11-C12-C13-C15
9	AH	103	BCL	C12-C13-C15-C16
9	g	101	BCL	C12-C13-C15-C16
9	i	102	BCL	C11-C12-C13-C15
9	k	102	BCL	C5-C6-C7-C8
9	V	101	BCL	C2C-C3C-CAC-CBC
9	c	102	BCL	C2C-C3C-CAC-CBC
15	M	404	CRT	C36-C37-C38-C39
15	M	404	CRT	C36-C37-C38-C40
15	P	102	CRT	C3-C1-C4-C5
15	z	101	CRT	C36-C37-C38-C39
15	i	101	CRT	C36-C37-C38-C39
15	c	101	CRT	C36-C37-C38-C40
9	F	101	BCL	C4-C3-C5-C6
14	M	403	MQ8	C24-C23-C25-C26
14	y	403	MQ8	C39-C38-C40-C41
9	r	101	BCL	C16-C17-C18-C19
12	y	407	PEF	O3P-C1-C2-O2
12	y	408	PEF	O3P-C1-C2-O2
9	x	305	BCL	C4B-C3B-CAB-CBB
9	1	101	BCL	C11-C10-C8-C9
9	x	301	BCL	C14-C13-C15-C16
9	AH	103	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	M	402	BPH	C11-C10-C8-C9
9	y	401	BCL	C5-C6-C7-C8
15	Z	101	CRT	C11-C10-C9-C7
15	Z	101	CRT	C12-C14-C15-C16
9	7	101	BCL	C13-C15-C16-C17
7	C	504	HEM	C4D-C3D-CAD-CBD
10	x	302	BPH	O1A-CGA-O2A-C1
10	L	302	BPH	C13-C15-C16-C17
10	M	402	BPH	C16-C17-C18-C19
9	L	305	BCL	C13-C15-C16-C17
14	y	403	MQ8	C37-C38-C40-C41
9	y	401	BCL	CAD-CBD-CGD-O2D
9	8	102	BCL	C2A-CAA-CBA-CGA
9	L	305	BCL	CHA-CBD-CGD-O1D
9	y	401	BCL	CAD-CBD-CGD-O1D
9	d	101	BCL	CHA-CBD-CGD-O1D
9	d	101	BCL	CHA-CBD-CGD-O2D
12	L	306	PEF	O4P-C4-C5-N
12	L	306	PEF	C1-O3P-P-O1P
12	M	406	PEF	O4P-C4-C5-N
12	M	406	PEF	C1-O3P-P-O2P
12	M	406	PEF	C4-O4P-P-O3P
12	A	101	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	C4-O4P-P-O1P
12	t	301	PEF	C1-O3P-P-O4P
17	S	101	PGW	C03-O11-P-O13
9	8	102	BCL	C16-C17-C18-C20
12	m	101	PEF	C11-C10-O2-C2
9	AC	102	BCL	C4-C3-C5-C6
9	8	102	BCL	C5-C6-C7-C8
12	H	304	PEF	C2-C1-O3P-P
15	R	101	CRT	C29-C28-C30-C31
9	W	101	BCL	C16-C17-C18-C20
9	Y	101	BCL	O1A-CGA-O2A-C1
9	U	101	BCL	C13-C15-C16-C17
9	9	103	BCL	C16-C17-C18-C19
9	4	102	BCL	C3-C5-C6-C7
15	R	101	CRT	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	X	101	CRT	C9-C10-C11-C12
15	4	101	CRT	C28-C30-C31-C32
15	AD	102	CRT	C14-C15-C16-C17
15	AJ	101	CRT	C9-C10-C11-C12
15	f	102	CRT	C28-C30-C31-C32
9	x	303	BCL	C13-C15-C16-C17
9	AH	101	BCL	C15-C16-C17-C18
10	M	402	BPH	C16-C17-C18-C20
9	Q	101	BCL	C10-C11-C12-C13
9	M	401	BCL	C11-C10-C8-C9
9	K	101	BCL	C11-C10-C8-C9
9	N	102	BCL	C11-C12-C13-C14
9	O	101	BCL	C6-C7-C8-C9
9	X	102	BCL	C11-C10-C8-C9
9	0	101	BCL	C11-C12-C13-C14
9	r	101	BCL	C11-C10-C8-C9
9	AA	101	BCL	C11-C12-C13-C14
9	AI	101	BCL	C14-C13-C15-C16
9	e	102	BCL	C6-C7-C8-C9
9	i	102	BCL	C11-C12-C13-C14
10	M	402	BPH	C14-C13-C15-C16
9	Q	101	BCL	C12-C13-C15-C16
9	3	101	BCL	C12-C13-C15-C16
9	4	102	BCL	C6-C7-C8-C10
9	m	102	BCL	C6-C7-C8-C10
9	m	103	BCL	C6-C7-C8-C10
9	p	102	BCL	C11-C10-C8-C7
9	AH	103	BCL	C11-C10-C8-C7
10	x	302	BPH	C8-C10-C11-C12
12	M	408	PEF	O3P-C1-C2-O2
9	p	102	BCL	C10-C11-C12-C13
9	O	101	BCL	C16-C17-C18-C20
9	AB	101	BCL	C2A-CAA-CBA-CGA
9	J	102	BCL	C15-C16-C17-C18
12	m	101	PEF	O4-C10-O2-C2
15	N	101	CRT	C15-C16-C17-C18
15	J	101	CRT	C1-C4-C5-C6
15	U	102	CRT	C35-C36-C37-C38
15	6	101	CRT	C35-C36-C37-C38
15	9	102	CRT	C35-C36-C37-C38
15	c	101	CRT	C3-C1-O1-C1M
9	d	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	AD	102	CRT	C27-C28-C30-C31
15	X	101	CRT	C25-C26-C27-C28
9	AC	102	BCL	C2-C3-C5-C6
9	N	102	BCL	C11-C10-C8-C9
9	4	102	BCL	C6-C7-C8-C9
9	5	101	BCL	C11-C10-C8-C9
9	8	102	BCL	C11-C12-C13-C14
9	AH	101	BCL	CBA-CGA-O2A-C1
10	x	302	BPH	CBA-CGA-O2A-C1
9	w	101	BCL	C10-C11-C12-C13
9	p	104	BCL	CAA-CBA-CGA-O2A
15	T	101	CRT	C25-C26-C27-C28
7	C	504	HEM	C4C-C3C-CAC-CBC
9	F	101	BCL	C11-C12-C13-C15
9	O	101	BCL	C11-C10-C8-C7
9	W	101	BCL	C12-C13-C15-C16
9	V	101	BCL	C13-C15-C16-C17
9	x	303	BCL	C16-C17-C18-C20
9	AJ	102	BCL	C16-C17-C18-C20
9	AL	102	BCL	C5-C6-C7-C8
12	H	301	PEF	C11-C10-O2-C2
9	7	101	BCL	C3A-C2A-CAA-CBA
9	9	103	BCL	C3A-C2A-CAA-CBA
9	AB	101	BCL	C4-C3-C5-C6
12	M	406	PEF	O5-C30-O3-C3
15	R	101	CRT	C13-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C34
15	8	101	CRT	C21-C22-C23-C24
15	AD	102	CRT	C13-C12-C14-C15
15	f	102	CRT	C31-C32-C33-C34
15	k	101	CRT	C21-C22-C23-C24
9	L	303	BCL	C15-C16-C17-C18
12	M	406	PEF	C11-C10-O2-C2
9	g	101	BCL	C2-C1-O2A-CGA
15	y	404	CRT	C20-C21-C22-C23
15	AL	101	CRT	C25-C26-C27-C28
9	1	101	BCL	C15-C16-C17-C18
15	AD	102	CRT	C34-C33-C35-C36
7	C	501	HEM	CAA-CBA-CGA-O2A
9	r	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C25-C24-C26-C27
12	H	301	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
9	F	101	BCL	C2-C3-C5-C6
9	x	303	BCL	C16-C17-C18-C19
7	o	502	HEM	CAA-CBA-CGA-O1A
9	M	401	BCL	C6-C7-C8-C9
9	B	101	BCL	C11-C10-C8-C9
9	F	101	BCL	C11-C12-C13-C14
9	O	101	BCL	C11-C10-C8-C9
9	V	101	BCL	C11-C12-C13-C14
9	7	101	BCL	C11-C12-C13-C14
9	m	103	BCL	C11-C12-C13-C14
9	u	101	BCL	C11-C10-C8-C9
9	z	102	BCL	C14-C13-C15-C16
9	AA	101	BCL	C6-C7-C8-C9
9	AH	103	BCL	C11-C10-C8-C9
9	AL	102	BCL	C11-C10-C8-C9
9	h	101	BCL	C14-C13-C15-C16
9	c	102	BCL	C6-C7-C8-C9
10	x	302	BPH	C6-C7-C8-C9
10	y	402	BPH	C14-C13-C15-C16
9	AH	103	BCL	C4-C3-C5-C6
11	L	304	UQ8	C23-C24-C26-C27
7	C	504	HEM	C2D-C3D-CAD-CBD
7	C	502	HEM	CAA-CBA-CGA-O2A
12	H	301	PEF	O5-C30-O3-C3
9	W	101	BCL	C1A-C2A-CAA-CBA
15	R	101	CRT	C11-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C35
15	8	101	CRT	C21-C22-C23-C25
15	AD	102	CRT	C11-C12-C14-C15
15	f	102	CRT	C31-C32-C33-C35
15	k	101	CRT	C21-C22-C23-C25
9	r	101	BCL	C16-C17-C18-C20
7	C	501	HEM	CAA-CBA-CGA-O1A
17	S	101	PGW	C20-C19-O03-C01
11	L	304	UQ8	C30-C29-C31-C32
9	L	303	BCL	C12-C13-C15-C16
9	M	401	BCL	C6-C7-C8-C10
9	P	101	BCL	C11-C10-C8-C7
9	P	101	BCL	C11-C12-C13-C15
9	X	102	BCL	C12-C13-C15-C16
9	m	102	BCL	C11-C12-C13-C15
9	AE	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	AH	101	BCL	C6-C7-C8-C10
10	x	302	BPH	C6-C7-C8-C10
9	1	102	BCL	C2A-CAA-CBA-CGA
9	F	101	BCL	C8-C10-C11-C12
9	p	102	BCL	C2C-C3C-CAC-CBC
15	X	101	CRT	C36-C37-C38-C40
15	4	101	CRT	C2-C1-C4-C5
15	p	103	CRT	C2-C1-C4-C5
15	AH	102	CRT	C3-C1-C4-C5
15	f	102	CRT	C2-C1-C4-C5
9	p	102	BCL	C3-C5-C6-C7
11	L	304	UQ8	C2-C3-O3-C3M
9	7	101	BCL	C16-C17-C18-C20
9	AB	101	BCL	C5-C6-C7-C8
15	y	404	CRT	C5-C6-C7-C8
15	n	101	CRT	C10-C11-C12-C13
9	K	101	BCL	C4-C3-C5-C6
9	8	102	BCL	C4-C3-C5-C6
9	j	101	BCL	C4-C3-C5-C6
9	k	102	BCL	C4-C3-C5-C6
10	M	402	BPH	C4-C3-C5-C6
14	y	403	MQ8	C29-C28-C30-C31
9	r	101	BCL	C2-C3-C5-C6
9	AH	101	BCL	O1A-CGA-O2A-C1
9	1	102	BCL	C4B-C3B-CAB-OB
7	C	502	HEM	CAA-CBA-CGA-O1A
9	L	303	BCL	C14-C13-C15-C16
9	AE	102	BCL	C6-C7-C8-C9
9	g	101	BCL	C11-C12-C13-C14
15	i	101	CRT	C11-C10-C9-C7
9	L	305	BCL	C8-C10-C11-C12
9	m	102	BCL	C8-C10-C11-C12
9	l	101	BCL	C4-C3-C5-C6
9	K	101	BCL	C2-C3-C5-C6
9	AK	101	BCL	C2-C3-C5-C6
11	L	304	UQ8	C28-C29-C31-C32
7	C	504	HEM	CAA-CBA-CGA-O1A
12	t	303	PEF	C1-C2-C3-O3
9	j	101	BCL	C8-C10-C11-C12
9	v	102	BCL	C4C-C3C-CAC-CBC
9	X	102	BCL	C2A-CAA-CBA-CGA
9	5	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	y	401	BCL	C4-C3-C5-C6
14	M	403	MQ8	C39-C38-C40-C41
9	W	101	BCL	C16-C17-C18-C19
9	J	102	BCL	C10-C11-C12-C13
10	L	302	BPH	C8-C10-C11-C12
9	c	102	BCL	C3-C5-C6-C7
9	AI	101	BCL	CAA-CBA-CGA-O2A
9	AB	101	BCL	C16-C17-C18-C20
12	y	407	PEF	O3P-C1-C2-C3
9	c	102	BCL	C4-C3-C5-C6
11	x	304	UQ8	C12-C11-C9-C10
9	j	101	BCL	C2-C3-C5-C6
9	l	101	BCL	C2-C3-C5-C6
9	G	102	BCL	C10-C11-C12-C13
9	g	101	BCL	C11-C12-C13-C15
9	c	102	BCL	C11-C12-C13-C15
7	C	501	HEM	CAD-CBD-CGD-O2D
15	E	101	CRT	C11-C10-C9-C7
9	m	102	BCL	C3-C5-C6-C7
7	C	503	HEM	CAA-CBA-CGA-O2A
7	o	503	HEM	CAA-CBA-CGA-O2A
9	Q	101	BCL	C11-C10-C8-C9
9	T	102	BCL	C11-C10-C8-C9
9	X	102	BCL	C11-C12-C13-C14
9	Z	102	BCL	C6-C7-C8-C9
9	7	101	BCL	C11-C10-C8-C9
9	r	101	BCL	C11-C12-C13-C14
9	c	102	BCL	C11-C12-C13-C14
9	3	101	BCL	C8-C10-C11-C12
9	F	101	BCL	C2A-CAA-CBA-CGA
9	U	101	BCL	C2A-CAA-CBA-CGA
9	Y	101	BCL	C2-C1-O2A-CGA
9	Z	102	BCL	C2-C1-O2A-CGA
9	s	102	BCL	C2-C1-O2A-CGA
9	AE	102	BCL	C2-C1-O2A-CGA
9	AH	101	BCL	C2-C1-O2A-CGA
9	e	102	BCL	C2-C1-O2A-CGA
9	V	101	BCL	C4-C3-C5-C6
9	x	305	BCL	C4-C3-C5-C6
7	C	501	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	CAA-CBA-CGA-O2A
9	x	305	BCL	C2B-C3B-CAB-OB

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Mol	Chain	Res	Type	Atoms
10	L	302	BPH	O2A-C1-C2-C3
9	AH	103	BCL	C2A-CAA-CBA-CGA
9	U	101	BCL	C8-C10-C11-C12
9	0	101	BCL	C10-C11-C12-C13
10	y	402	BPH	C16-C17-C18-C19
7	C	501	HEM	CAD-CBD-CGD-O1D
7	C	503	HEM	CAA-CBA-CGA-O1A
7	o	503	HEM	CAA-CBA-CGA-O1A
14	y	403	MQ8	C15-C16-C17-C18
7	C	501	HEM	C4B-C3B-CAB-CBB
12	x	306	PEF	C5-C4-O4P-P
9	B	101	BCL	C14-C13-C15-C16
9	T	102	BCL	C11-C12-C13-C14
9	U	101	BCL	C11-C12-C13-C14
9	x	305	BCL	C6-C7-C8-C9
9	s	102	BCL	C11-C12-C13-C14
9	u	101	BCL	C14-C13-C15-C16
9	AH	101	BCL	C6-C7-C8-C9
9	AJ	102	BCL	C11-C10-C8-C9
9	8	102	BCL	C16-C17-C18-C19
9	0	101	BCL	C16-C17-C18-C20
15	N	101	CRT	C15-C16-C17-C19
15	i	101	CRT	C32-C33-C35-C36
15	A	103	CRT	O1-C1-C4-C5
15	2	101	CRT	O1-C1-C4-C5
15	c	101	CRT	C36-C37-C38-O2
9	AD	101	BCL	CAA-CBA-CGA-O2A
9	8	102	BCL	C2-C3-C5-C6
9	AK	101	BCL	C2A-CAA-CBA-CGA
9	N	102	BCL	C6-C7-C8-C10
9	Q	101	BCL	C11-C10-C8-C7
9	T	102	BCL	C11-C12-C13-C15
9	X	102	BCL	C11-C12-C13-C15
9	3	101	BCL	C11-C10-C8-C7
9	5	101	BCL	C11-C12-C13-C15
9	7	101	BCL	C11-C10-C8-C7
9	m	102	BCL	C12-C13-C15-C16
9	u	101	BCL	C11-C10-C8-C7
9	v	102	BCL	C12-C13-C15-C16
9	w	101	BCL	C6-C7-C8-C10
9	AI	101	BCL	C11-C12-C13-C15
9	R	102	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	1	102	BCL	C2-C1-O2A-CGA
9	x	303	BCL	C2-C1-O2A-CGA
9	d	101	BCL	C2-C1-O2A-CGA
9	D	101	BCL	C5-C6-C7-C8
9	Y	101	BCL	C13-C15-C16-C17
15	2	101	CRT	C3-C1-O1-C1M
15	v	101	CRT	C2-C1-O1-C1M
15	AE	103	CRT	C39-C38-O2-C2M
15	AH	102	CRT	C39-C38-O2-C2M
15	AJ	101	CRT	C39-C38-O2-C2M
15	AJ	101	CRT	C40-C38-O2-C2M
9	P	101	BCL	CAA-CBA-CGA-O2A
9	1	101	BCL	CAA-CBA-CGA-O2A
9	Y	101	BCL	CAA-CBA-CGA-O2A
7	C	504	HEM	CAA-CBA-CGA-O2A
9	P	101	BCL	C11-C10-C8-C9
9	3	101	BCL	C11-C10-C8-C9
9	5	102	BCL	C11-C10-C8-C9
9	i	102	BCL	CAA-CBA-CGA-O2A
9	AE	104	BCL	C16-C17-C18-C20
9	AD	101	BCL	C15-C16-C17-C18
9	9	103	BCL	C1A-C2A-CAA-CBA
15	R	101	CRT	C27-C28-C30-C31
15	X	101	CRT	C22-C23-C25-C26
15	6	101	CRT	C32-C33-C35-C36
15	n	101	CRT	C10-C11-C12-C14
15	p	103	CRT	C27-C28-C30-C31
15	s	101	CRT	C10-C11-C12-C14
15	AL	101	CRT	C5-C6-C7-C9
9	f	101	BCL	CAA-CBA-CGA-O2A
9	s	102	BCL	C13-C15-C16-C17
11	L	304	UQ8	C41-C42-C43-C44
17	AE	101	PGW	O12-C04-C05-CAD
9	D	101	BCL	C11-C10-C8-C7
9	O	101	BCL	C11-C12-C13-C15
9	r	101	BCL	C11-C12-C13-C15
9	u	101	BCL	C12-C13-C15-C16
9	AB	101	BCL	C11-C12-C13-C15
9	l	101	BCL	C11-C10-C8-C7
9	p	102	BCL	C13-C15-C16-C17
10	x	302	BPH	C13-C15-C16-C17
9	X	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	x	302	BPH	O2A-C1-C2-C3
9	8	102	BCL	C13-C15-C16-C17
12	m	101	PEF	C31-C30-O3-C3
9	L	303	BCL	C3-C5-C6-C7
9	W	101	BCL	C2C-C3C-CAC-CBC
15	s	101	CRT	C36-C37-C38-C39
15	c	101	CRT	C36-C37-C38-C39
9	e	102	BCL	C13-C15-C16-C17
7	o	501	HEM	CAA-CBA-CGA-O1A
9	W	101	BCL	C3A-C2A-CAA-CBA
9	Q	101	BCL	C15-C16-C17-C18
9	AE	102	BCL	C16-C17-C18-C19
12	M	406	PEF	O4-C10-O2-C2
9	AB	101	BCL	C2-C3-C5-C6
10	M	402	BPH	C2-C3-C5-C6
9	P	101	BCL	CAA-CBA-CGA-O1A
9	P	101	BCL	C11-C12-C13-C14
9	Q	101	BCL	C14-C13-C15-C16
9	x	301	BCL	C11-C12-C13-C14
9	AB	101	BCL	C11-C12-C13-C14
9	l	101	BCL	C11-C10-C8-C9
9	Z	102	BCL	C5-C6-C7-C8
14	M	403	MQ8	C16-C17-C18-C20
11	L	304	UQ8	C12-C11-C9-C10
9	AH	103	BCL	C2-C3-C5-C6
15	J	101	CRT	C35-C36-C37-C38
15	X	101	CRT	C35-C36-C37-C38
15	X	101	CRT	C10-C11-C12-C14
15	AD	102	CRT	C32-C33-C35-C36
15	f	102	CRT	C15-C16-C17-C19
9	l	101	BCL	CAA-CBA-CGA-O1A
9	AD	101	BCL	CAA-CBA-CGA-O1A
9	f	101	BCL	CAA-CBA-CGA-O1A
9	x	301	BCL	C4-C3-C5-C6
9	V	101	BCL	C15-C16-C17-C18
9	i	102	BCL	CAA-CBA-CGA-O1A
9	e	102	BCL	CAD-CBD-CGD-O2D
10	L	302	BPH	C4C-C3C-CAC-CBC
9	Y	101	BCL	CAA-CBA-CGA-O1A
17	AE	101	PGW	O12-C04-C05-OAF
9	G	102	BCL	C2-C1-O2A-CGA
9	l	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
7	C	504	HEM	CAD-CBD-CGD-O2D
7	o	501	HEM	CAD-CBD-CGD-O2D
9	j	101	BCL	CAA-CBA-CGA-O2A
9	I	101	BCL	C8-C10-C11-C12
9	5	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

141 monomers are involved in 1156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	403	MQ8	9	0
9	k	102	BCL	12	0
9	3	101	BCL	11	0
7	o	504	HEM	12	0
9	p	104	BCL	6	0
12	L	306	PEF	1	0
9	5	101	BCL	9	0
15	G	101	CRT	10	0
9	j	101	BCL	11	0
15	A	103	CRT	8	0
15	AC	101	CRT	7	0
12	M	406	PEF	2	0
7	C	504	HEM	11	0
12	t	303	PEF	8	0
9	A	102	BCL	9	0
15	M	404	CRT	11	0
12	y	406	PEF	4	0
12	y	408	PEF	3	0
9	m	102	BCL	4	0
9	u	101	BCL	9	0
9	x	305	BCL	17	0
9	AE	104	BCL	7	0
9	AJ	102	BCL	5	0
9	c	102	BCL	7	0
15	9	102	CRT	14	0
12	x	306	PEF	11	0
9	v	102	BCL	9	0
15	AJ	101	CRT	10	0
15	4	101	CRT	10	0
10	x	302	BPH	12	0
9	G	102	BCL	7	0
10	y	402	BPH	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	z	101	CRT	3	0
7	o	503	HEM	5	0
9	f	101	BCL	10	0
9	P	101	BCL	6	0
9	l	101	BCL	13	0
9	R	102	BCL	6	0
15	p	103	CRT	9	0
9	AK	101	BCL	7	0
9	AB	101	BCL	10	0
7	C	503	HEM	7	0
9	8	102	BCL	14	0
7	C	501	HEM	10	0
9	0	101	BCL	8	0
9	F	101	BCL	10	0
9	y	401	BCL	11	0
9	g	101	BCL	12	0
15	Z	101	CRT	9	0
9	B	101	BCL	9	0
9	s	102	BCL	4	0
9	Z	102	BCL	9	0
9	AC	102	BCL	8	0
12	H	301	PEF	4	0
15	6	101	CRT	5	0
17	AE	101	PGW	1	0
9	AH	103	BCL	9	0
12	M	407	PEF	5	0
12	y	407	PEF	2	0
15	AE	103	CRT	13	0
15	e	101	CRT	11	0
9	D	101	BCL	11	0
9	AD	101	BCL	12	0
9	e	102	BCL	11	0
15	AL	101	CRT	11	0
9	m	103	BCL	9	0
12	M	408	PEF	3	0
9	r	101	BCL	12	0
9	O	101	BCL	8	0
9	i	102	BCL	8	0
9	AL	102	BCL	10	0
9	J	102	BCL	12	0
12	H	304	PEF	6	0
9	z	102	BCL	6	0

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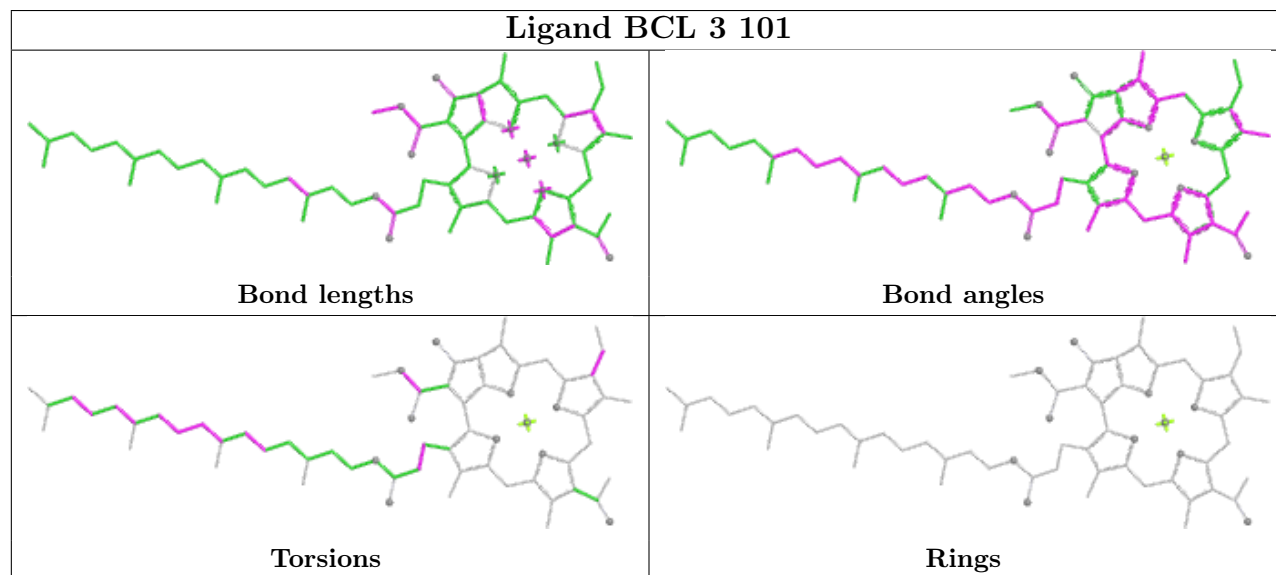
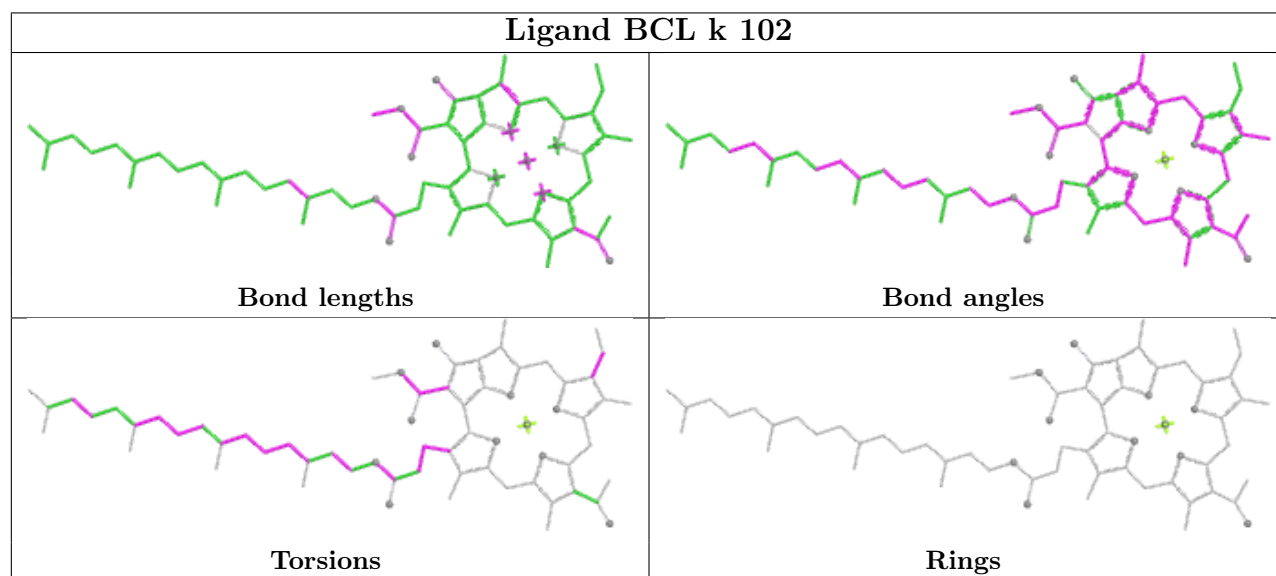
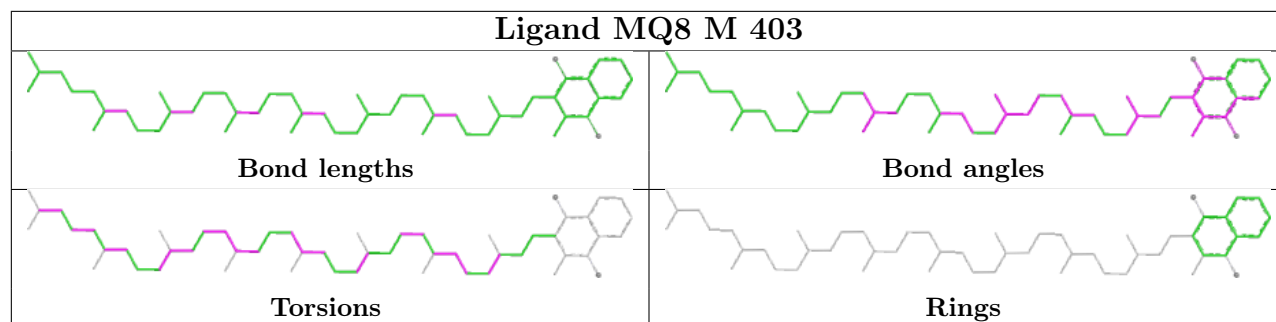
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	101	CRT	15	0
7	o	501	HEM	9	0
15	8	101	CRT	14	0
14	y	403	MQ8	10	0
9	S	102	BCL	8	0
9	7	101	BCL	8	0
9	x	301	BCL	12	0
9	L	305	BCL	10	0
15	c	101	CRT	6	0
9	X	102	BCL	12	0
15	v	101	CRT	7	0
9	AE	102	BCL	6	0
17	S	101	PGW	3	0
9	Y	101	BCL	13	0
15	k	101	CRT	11	0
9	l	101	BCL	5	0
7	o	502	HEM	10	0
12	A	101	PEF	3	0
9	h	101	BCL	10	0
9	T	102	BCL	12	0
9	p	102	BCL	12	0
15	U	102	CRT	5	0
9	5	102	BCL	5	0
12	m	101	PEF	4	0
9	Q	101	BCL	5	0
15	n	101	CRT	15	0
15	X	101	CRT	12	0
9	D	102	BCL	7	0
15	y	404	CRT	10	0
9	d	101	BCL	9	0
9	I	101	BCL	9	0
15	AD	102	CRT	10	0
15	i	101	CRT	6	0
15	T	101	CRT	13	0
9	AI	101	BCL	11	0
10	M	402	BPH	13	0
7	C	502	HEM	5	0
9	AA	101	BCL	8	0
12	p	101	PEF	5	0
15	E	101	CRT	9	0
15	f	102	CRT	12	0
9	W	101	BCL	12	0

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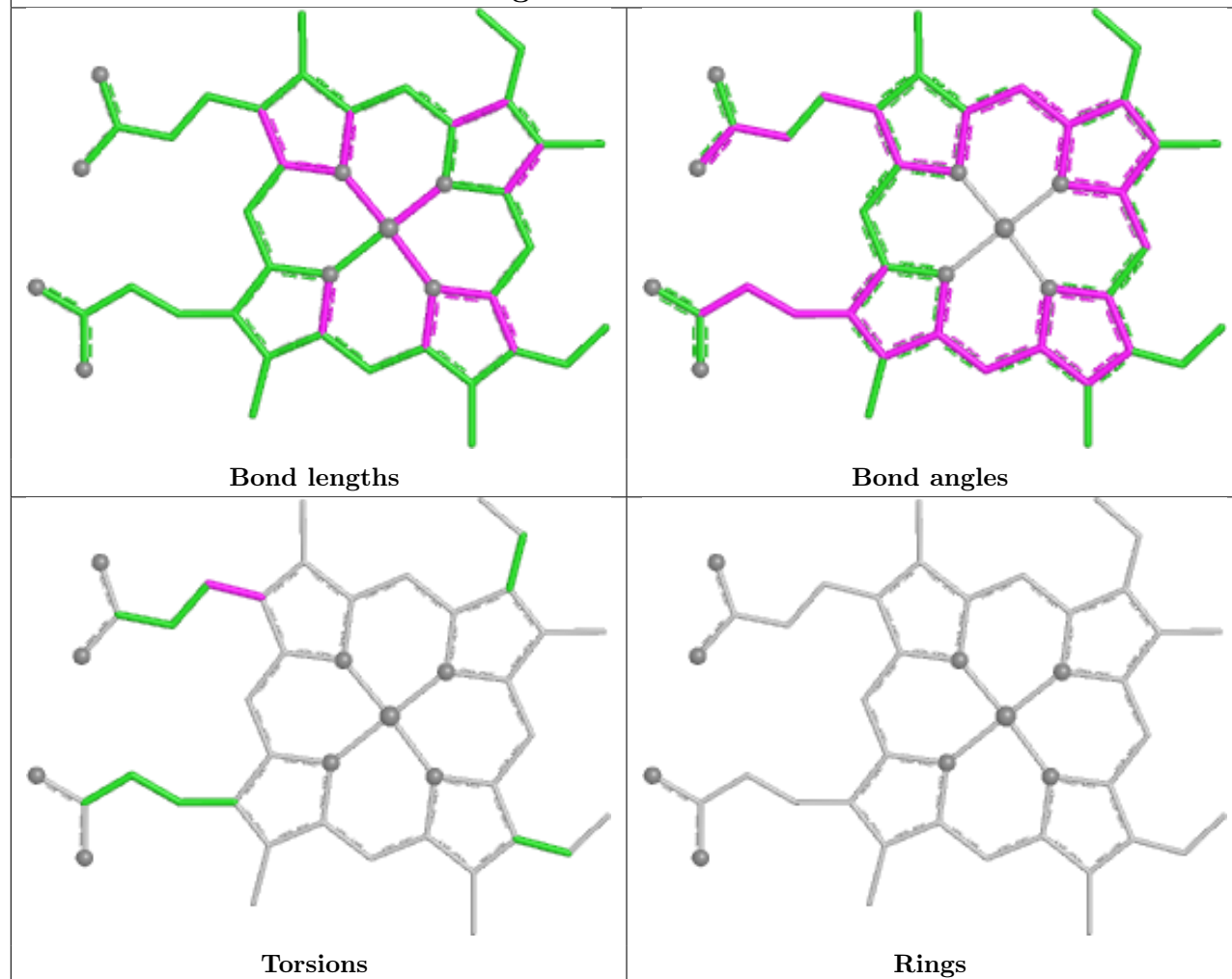
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	4	102	BCL	13	0
9	w	101	BCL	12	0
9	1	102	BCL	9	0
9	AH	101	BCL	13	0
12	H	303	PEF	3	0
9	U	101	BCL	10	0
16	y	405	PO4	1	0
15	s	101	CRT	13	0
15	2	101	CRT	14	0
9	9	103	BCL	10	0
15	J	101	CRT	12	0
9	M	401	BCL	12	0
12	t	301	PEF	5	0
15	R	101	CRT	8	0
9	L	303	BCL	11	0
15	P	102	CRT	9	0
9	x	303	BCL	9	0
11	L	304	UQ8	18	0
9	L	301	BCL	11	0
11	x	304	UQ8	20	0
9	N	102	BCL	5	0
9	K	101	BCL	5	0
9	V	101	BCL	9	0
10	L	302	BPH	14	0
15	AH	102	CRT	8	0

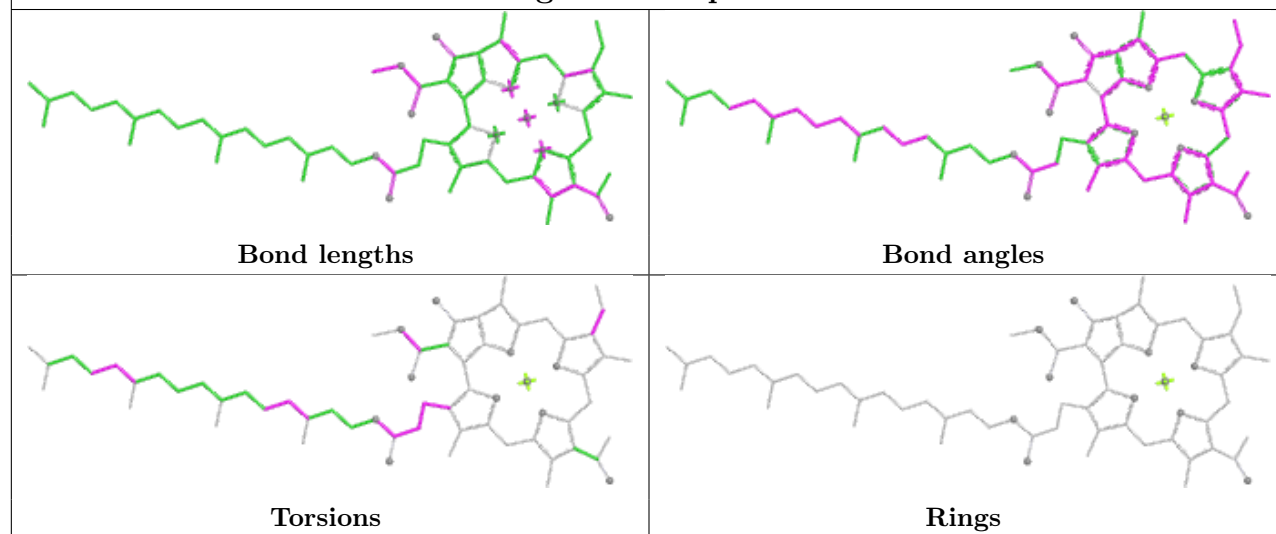
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



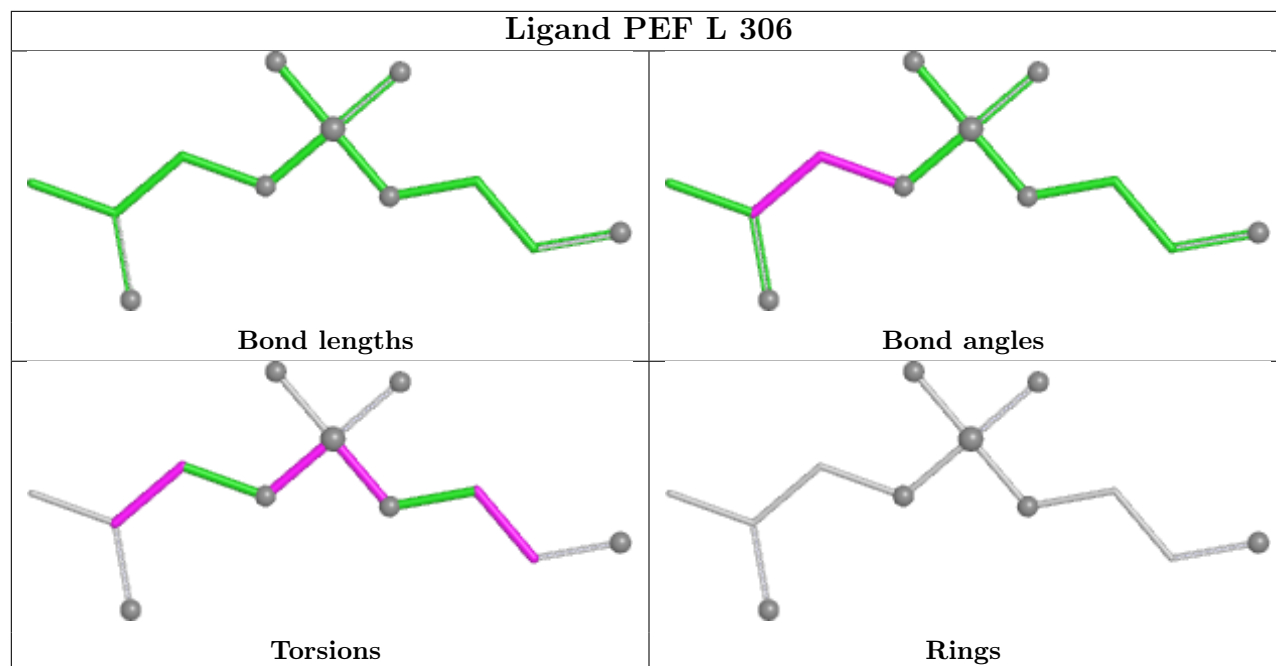
Ligand HEM o 504



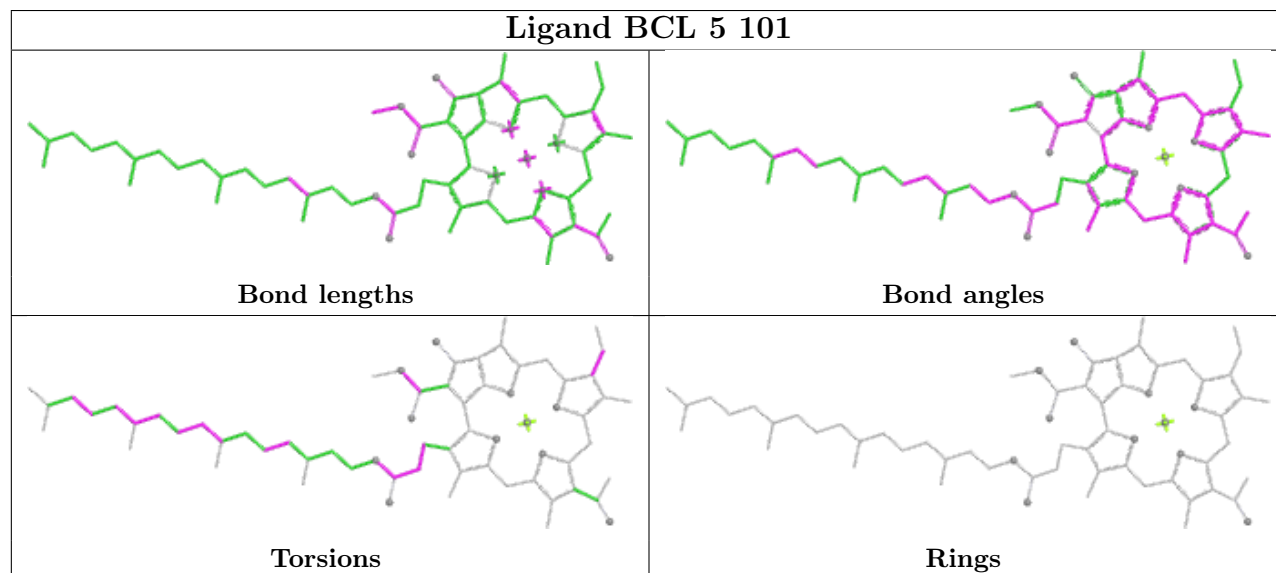
Ligand BCL p 104

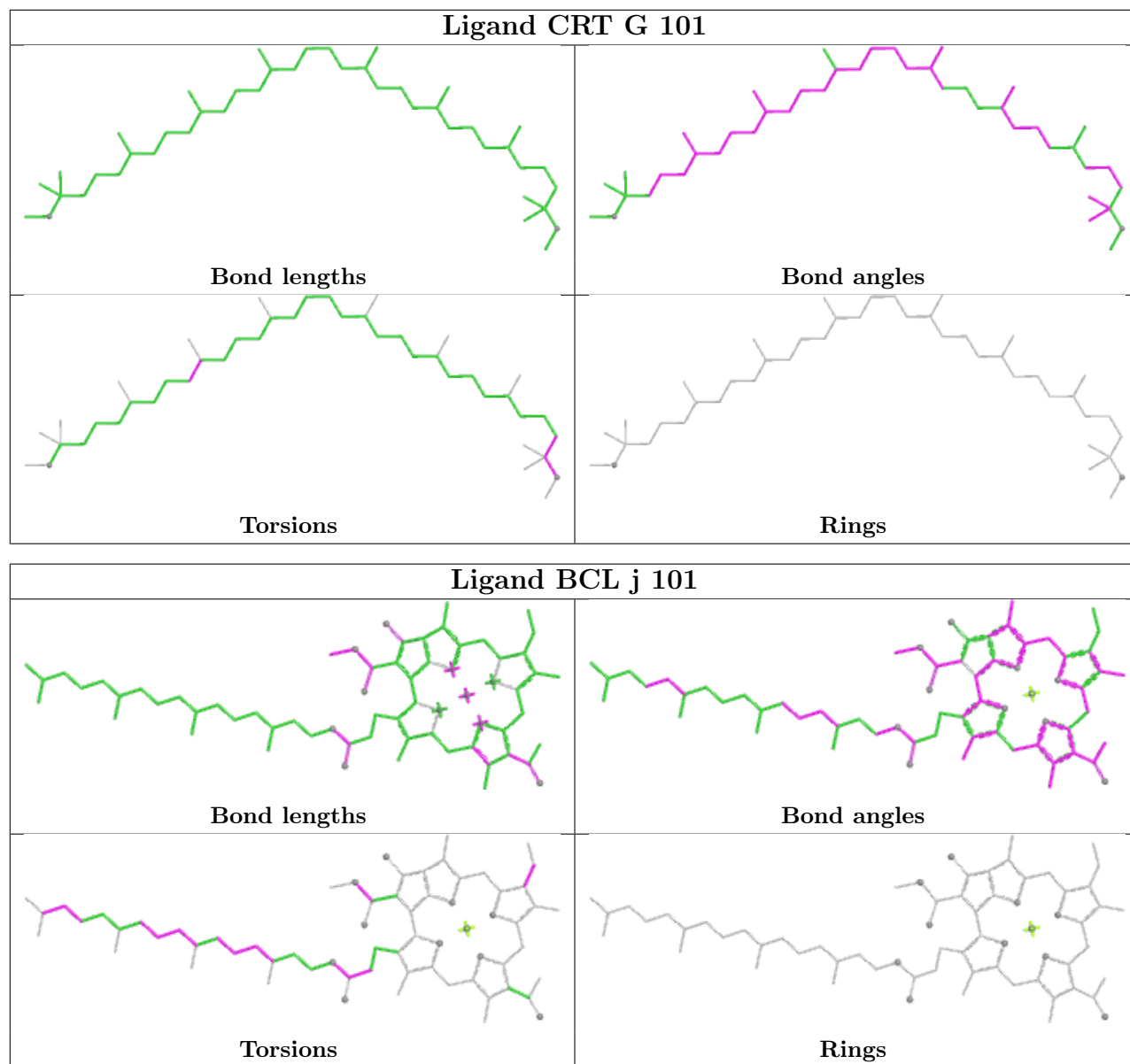


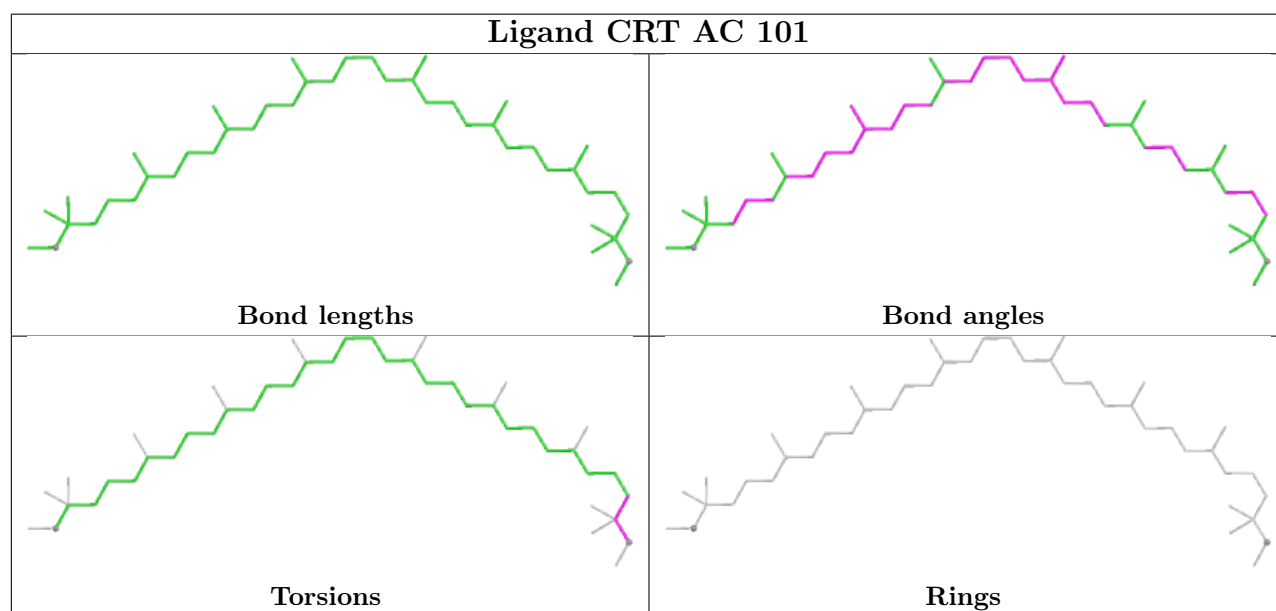
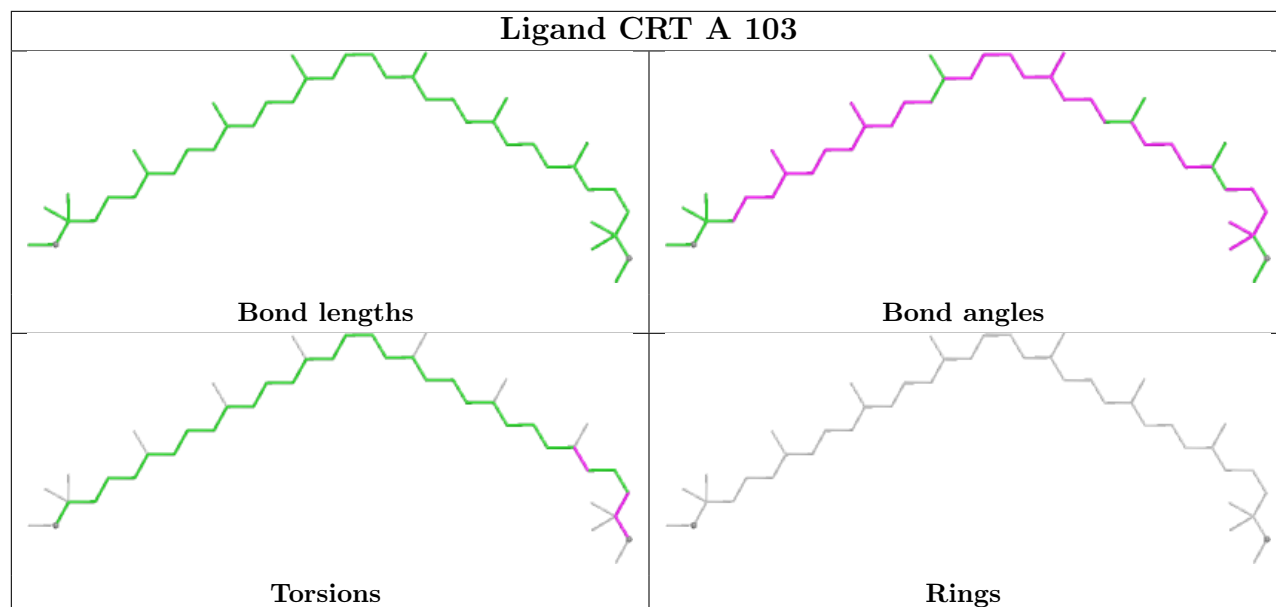
Ligand PEF L 306

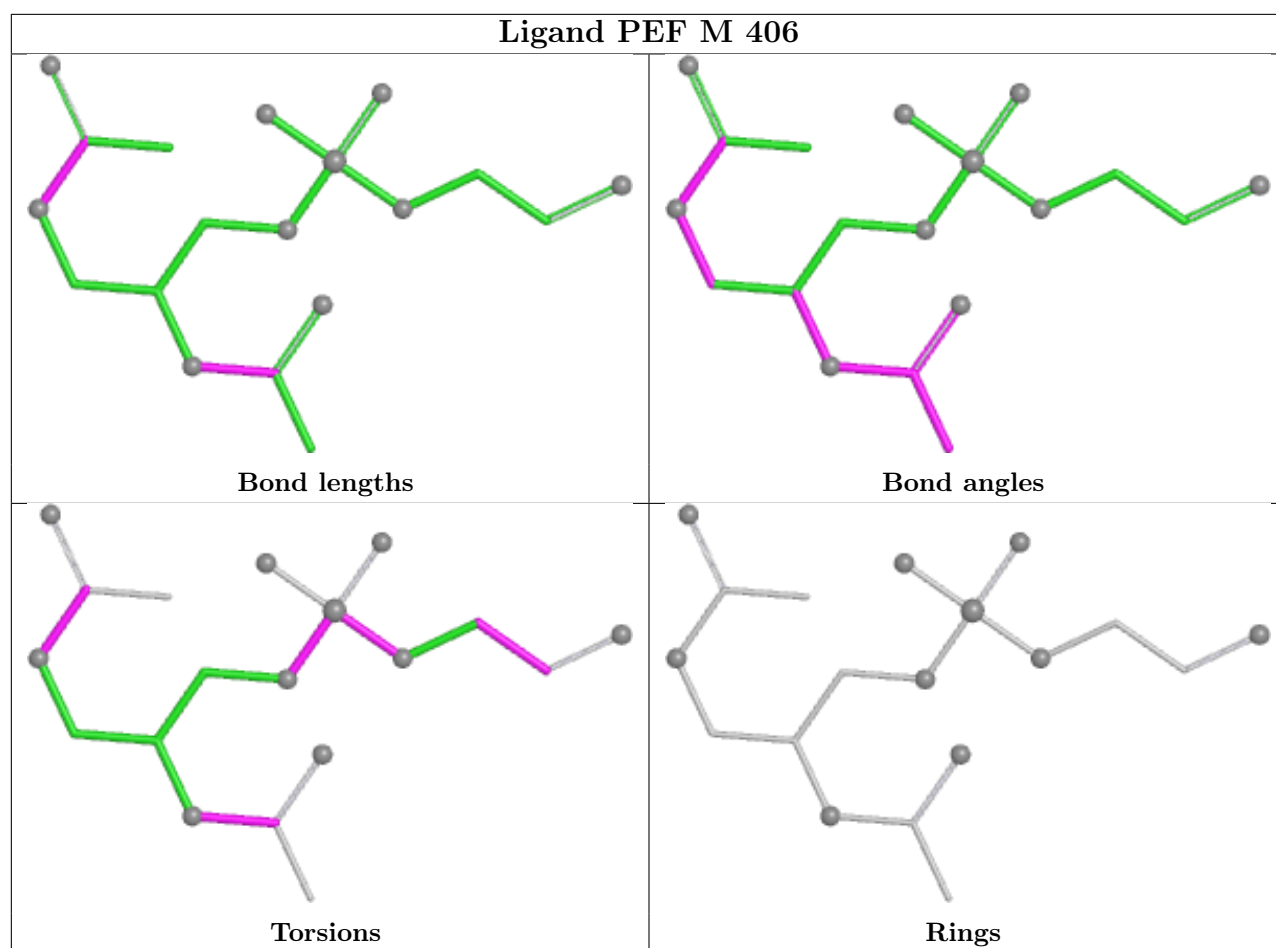


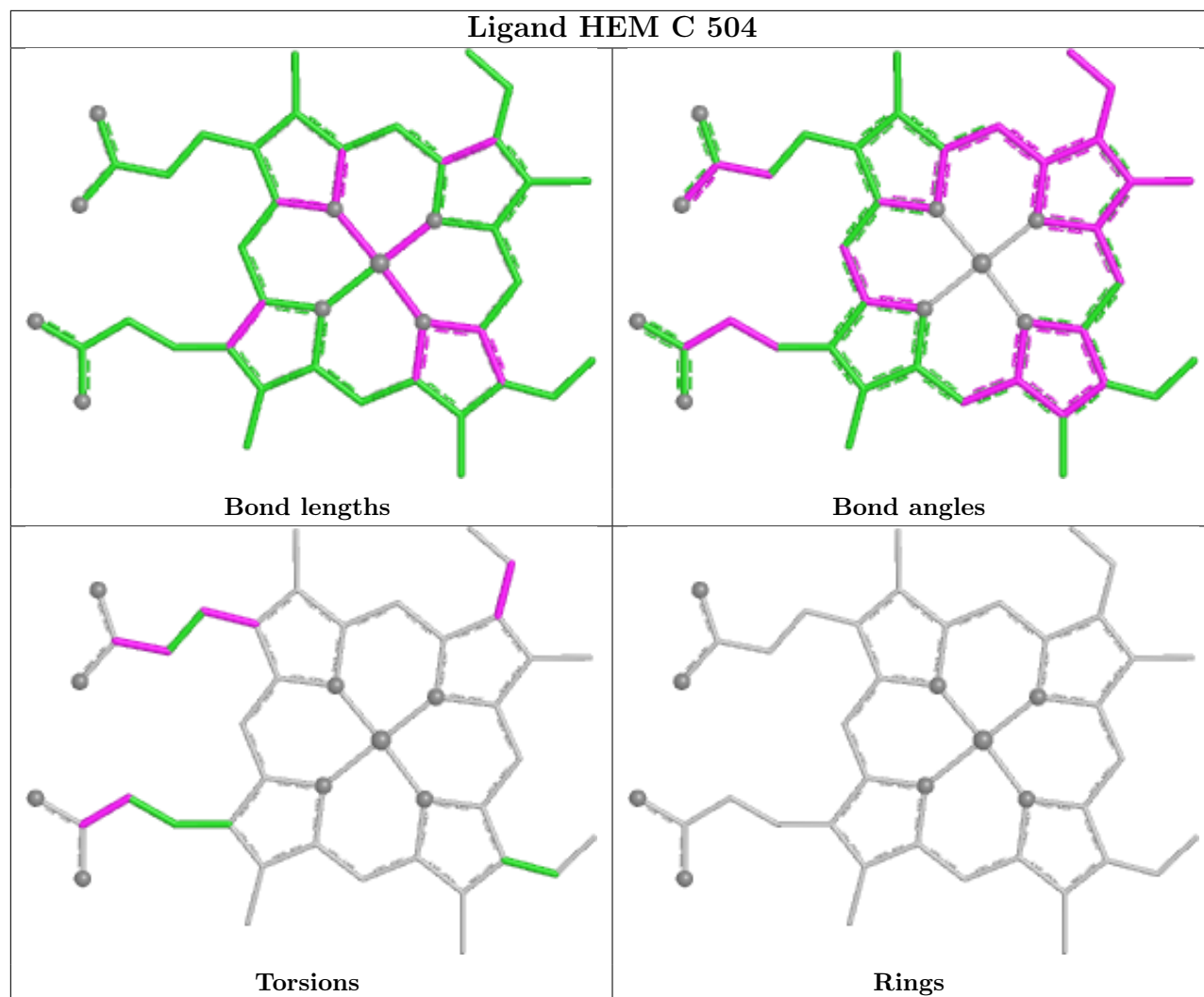
Ligand BCL 5 101



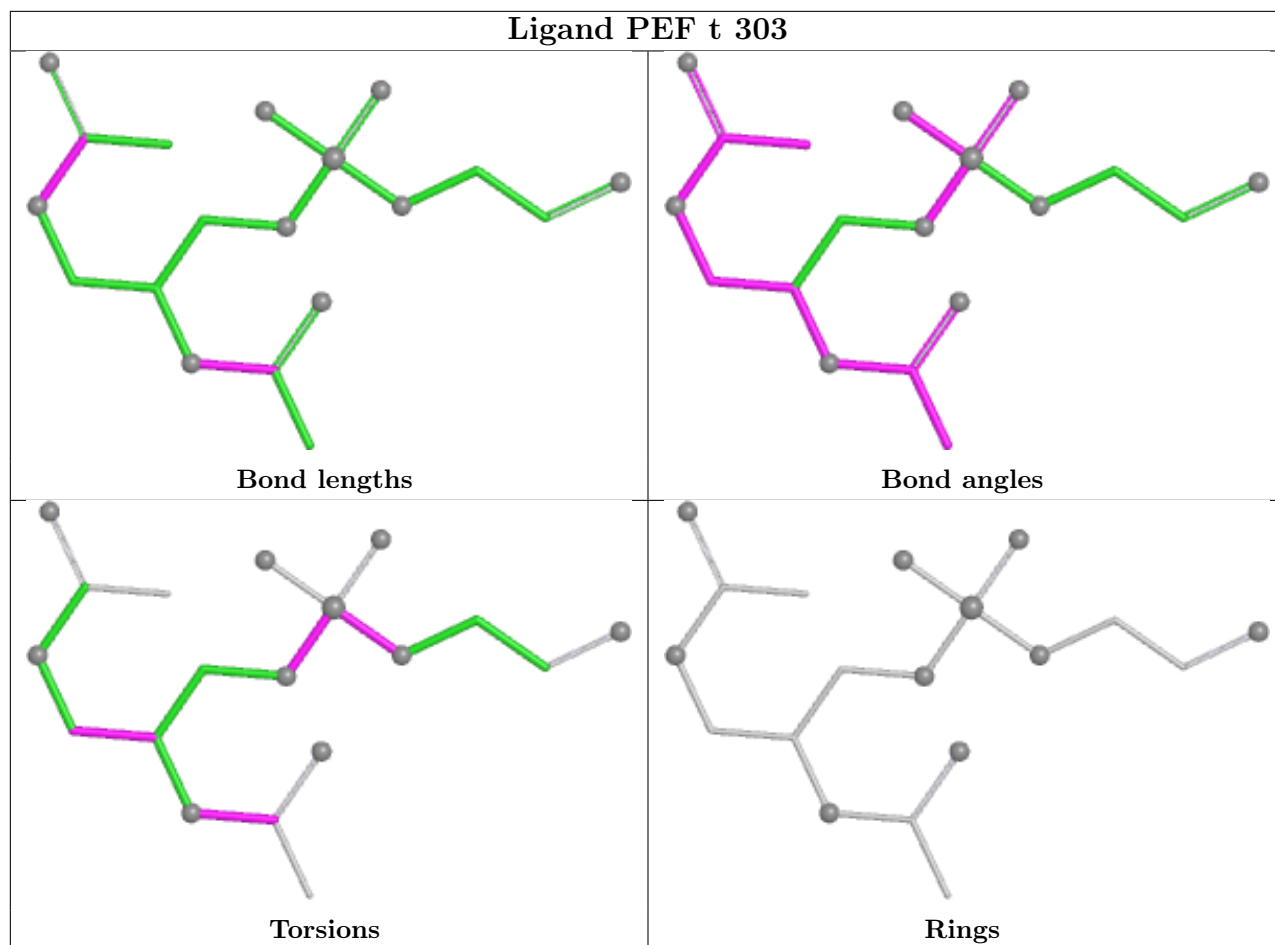




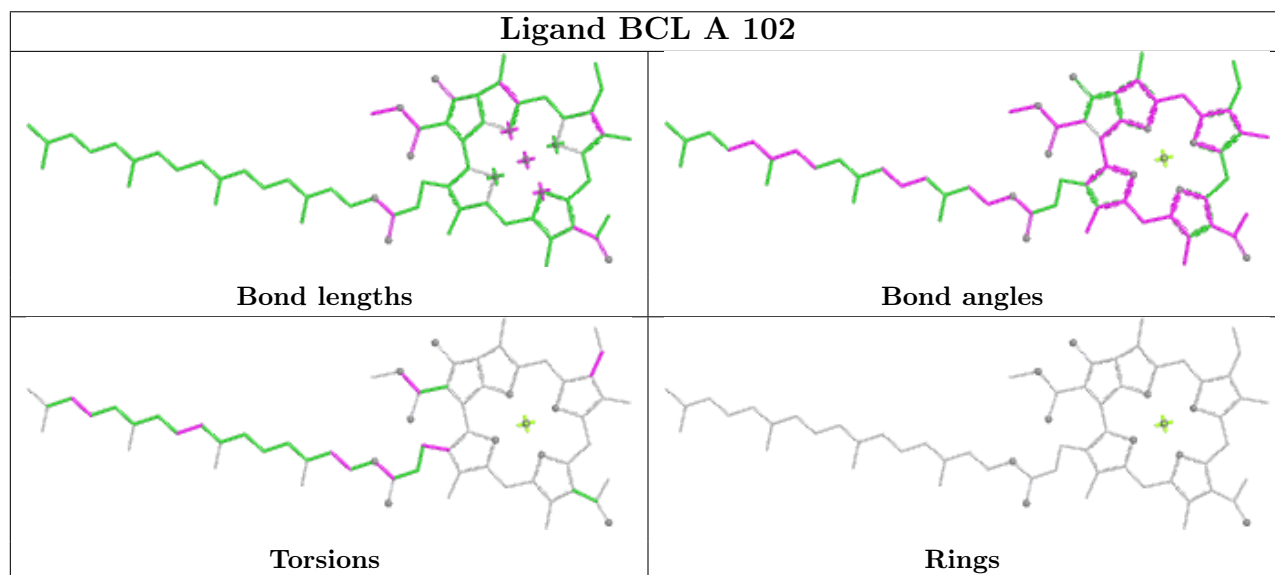


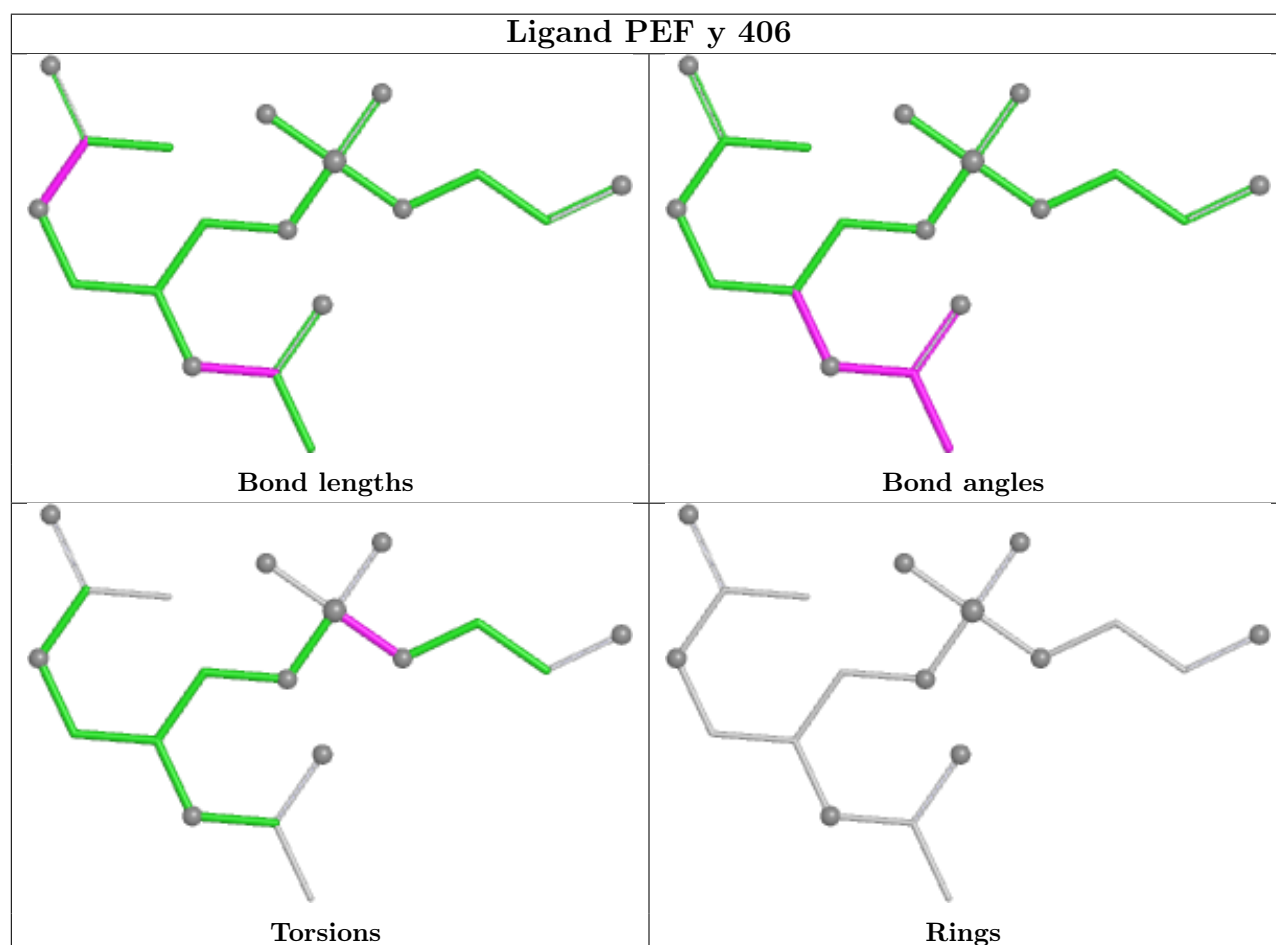
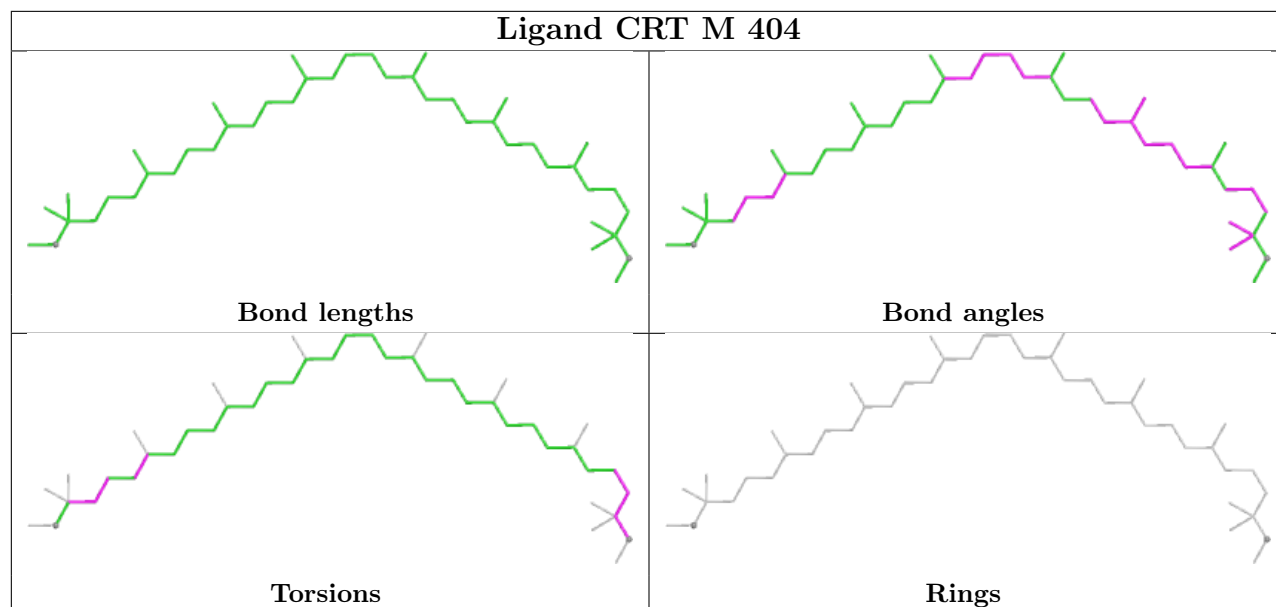


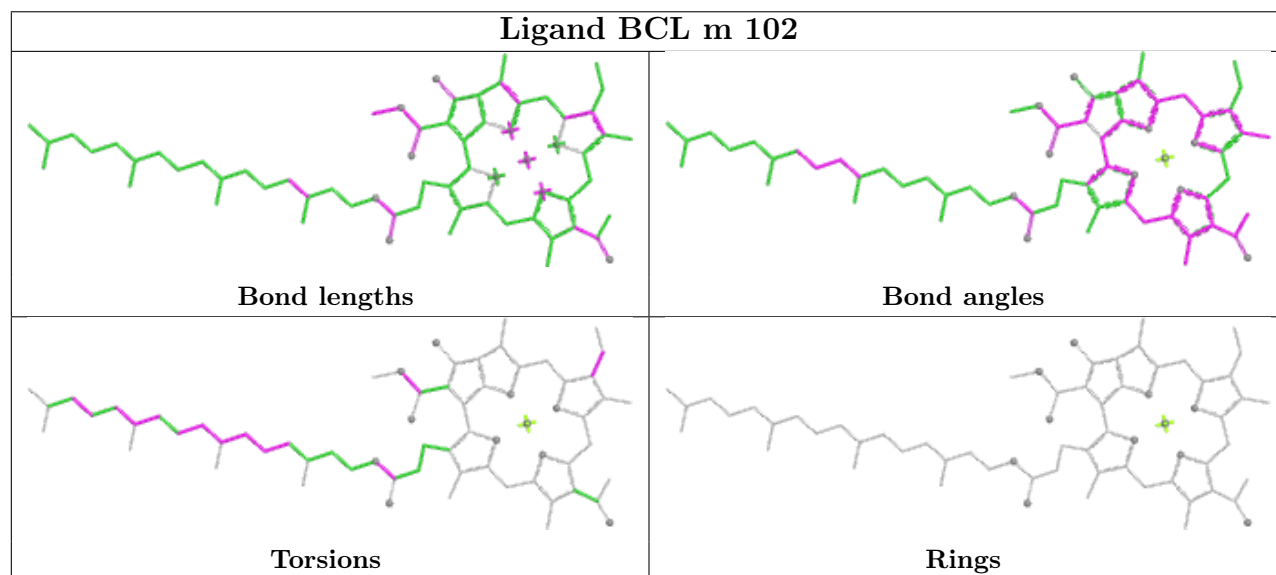
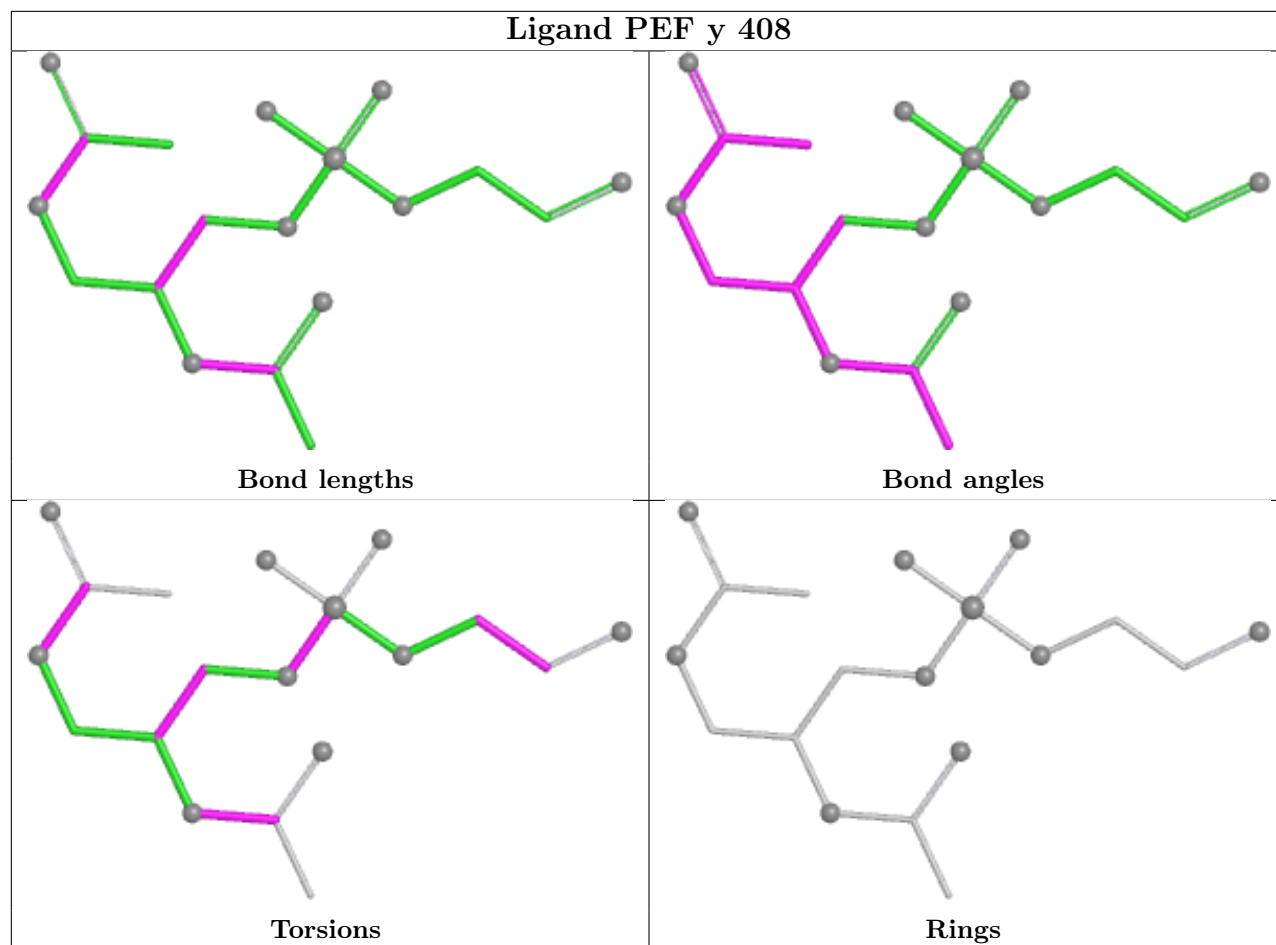
Ligand PEF t 303

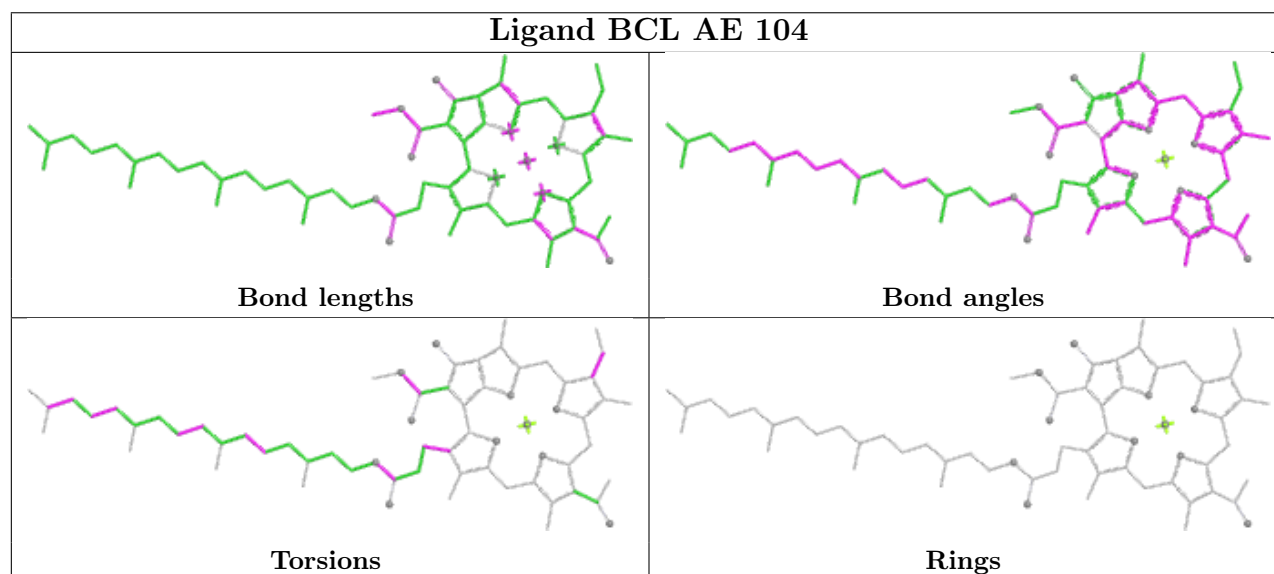
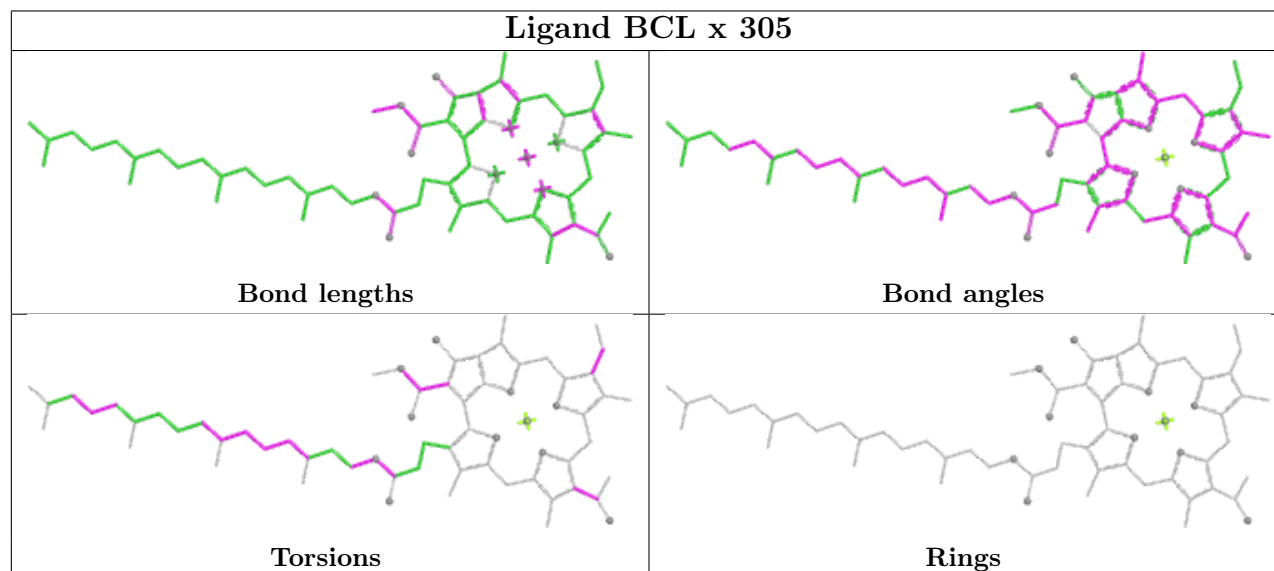
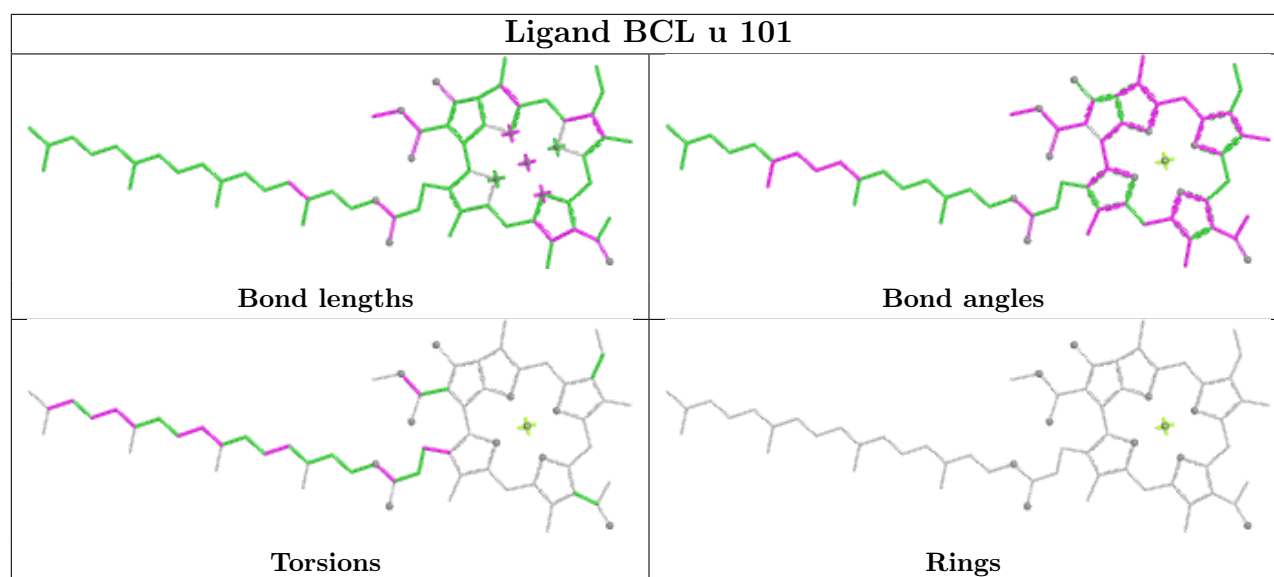


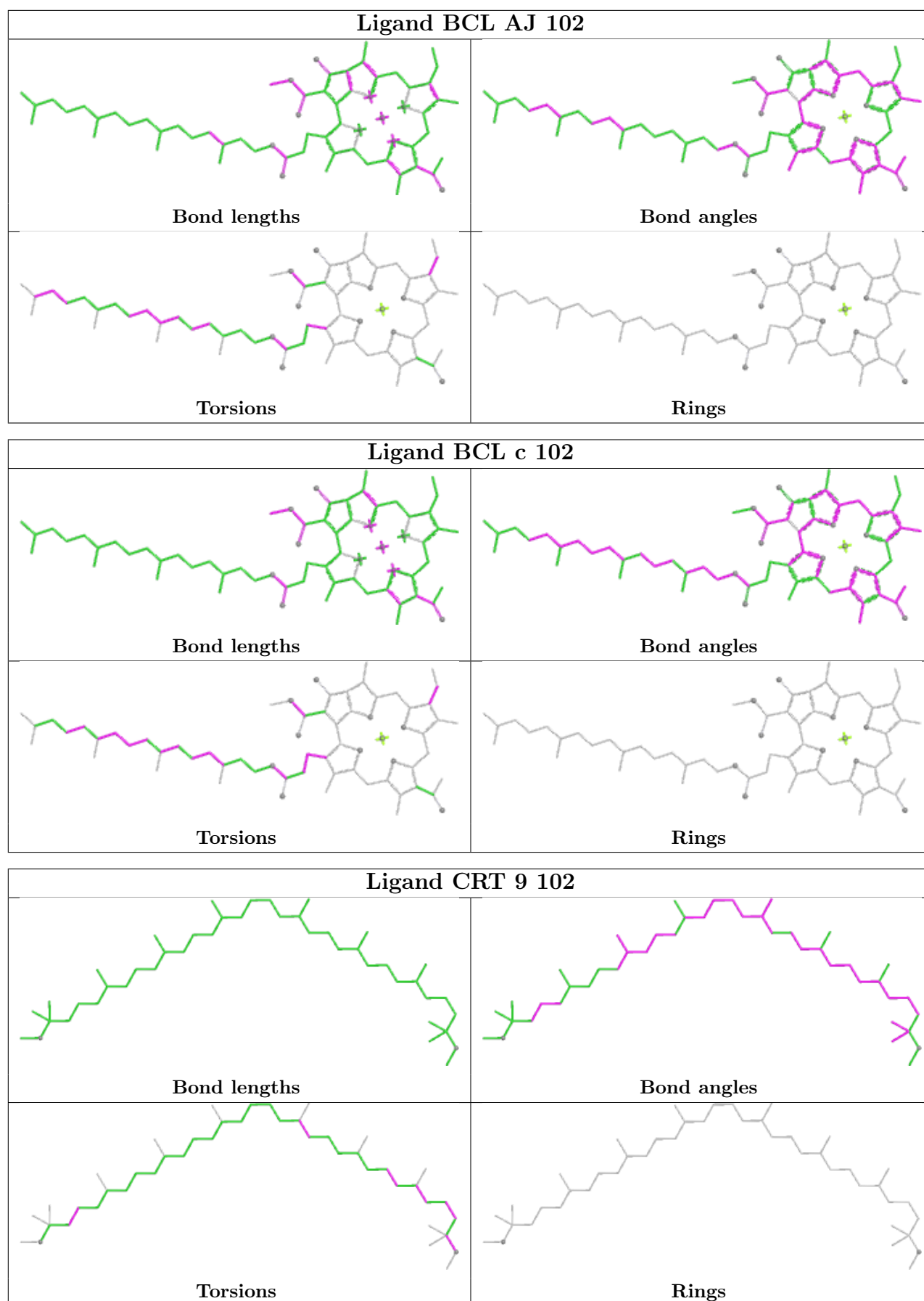
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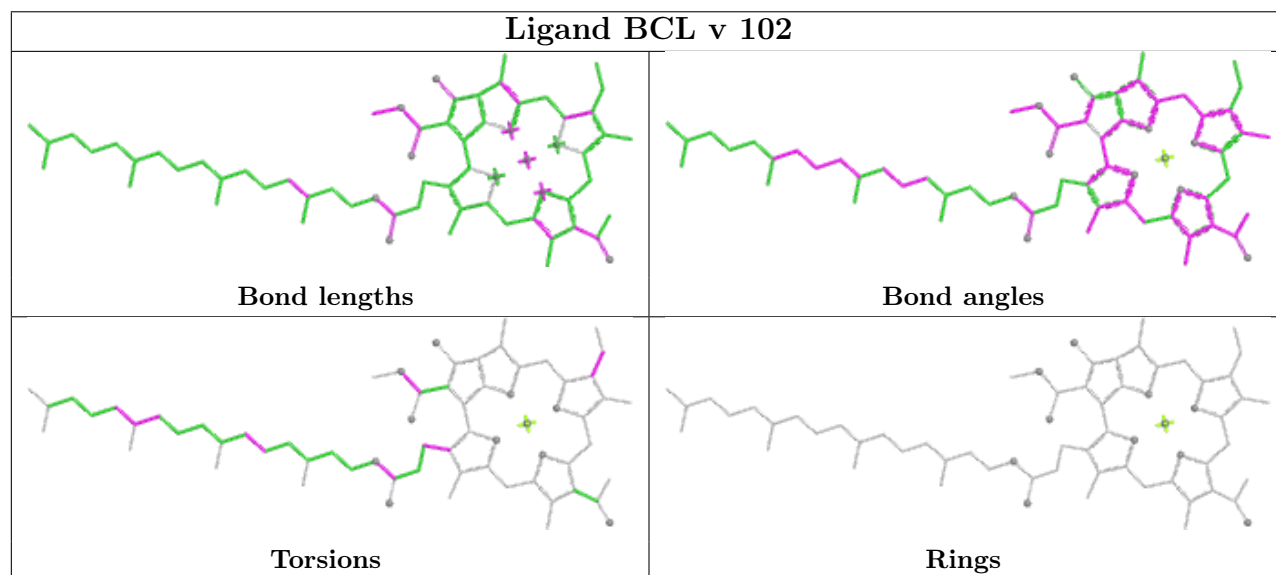
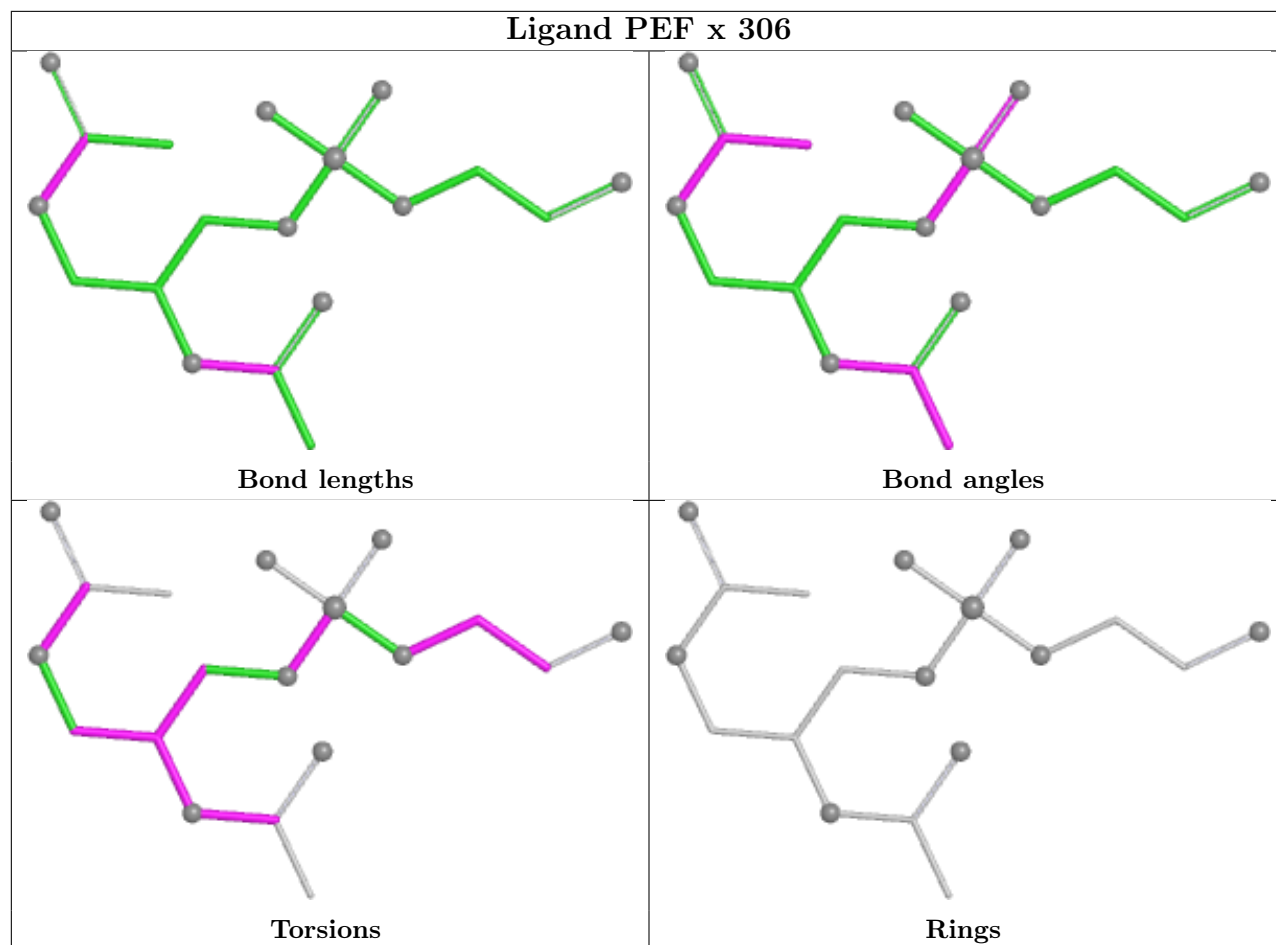


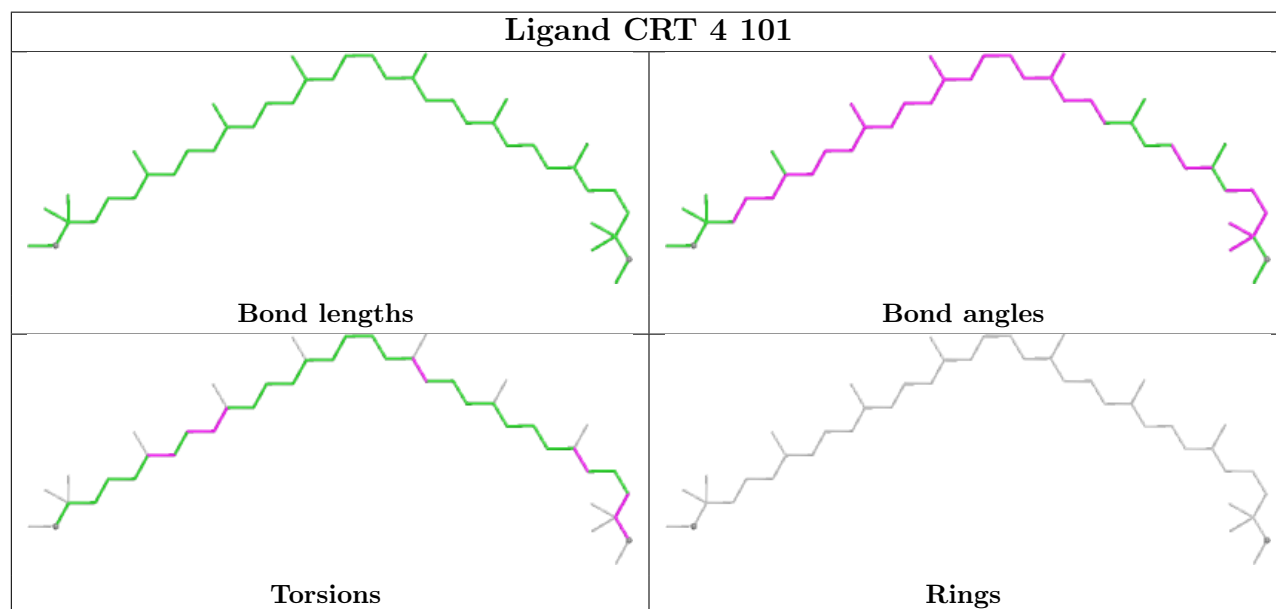
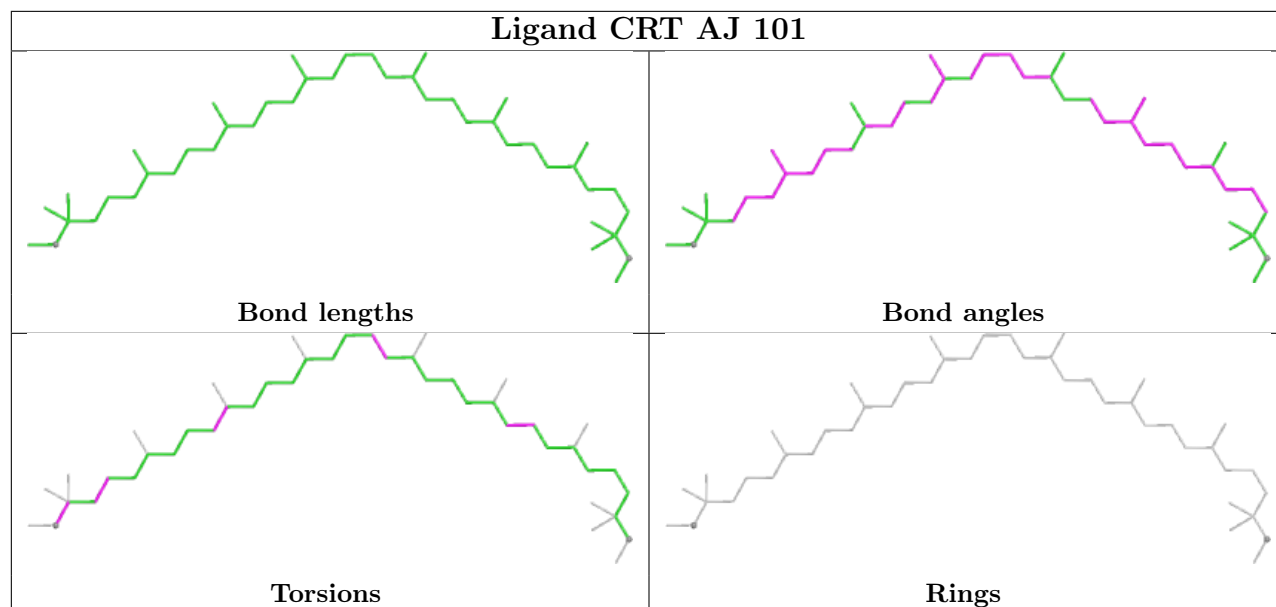




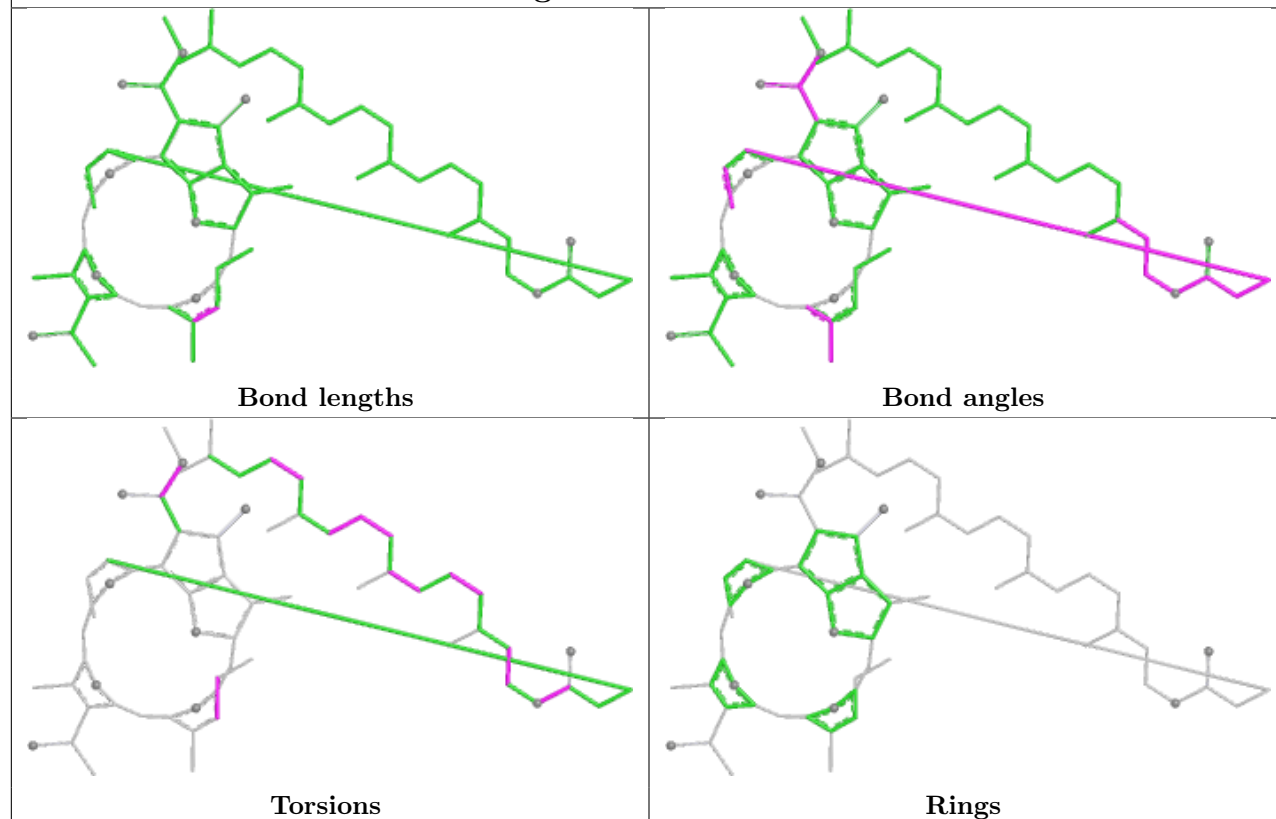




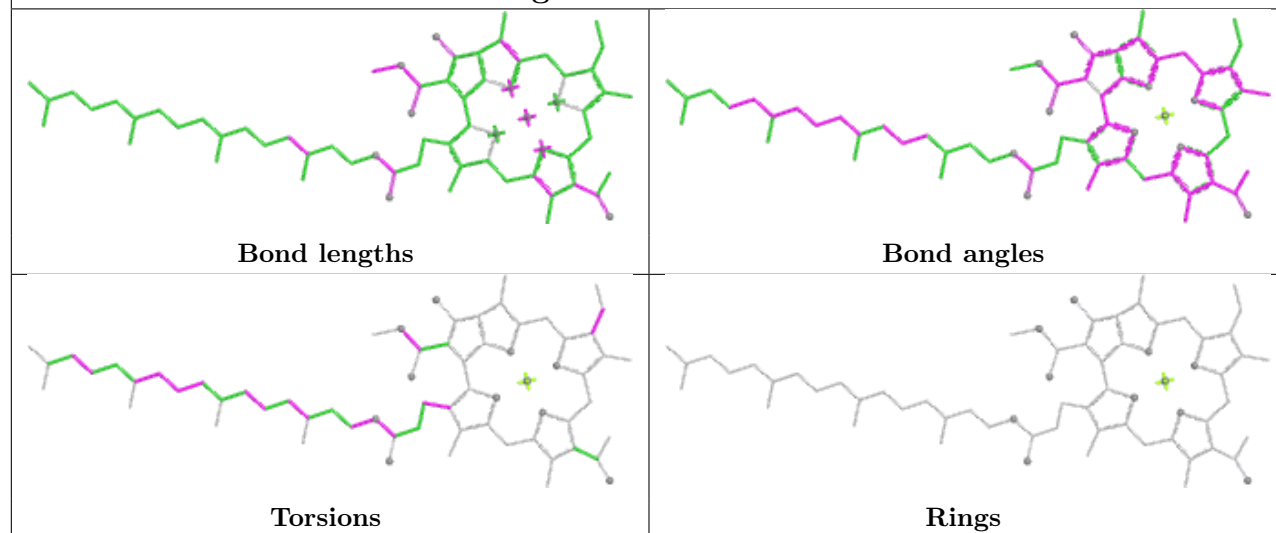




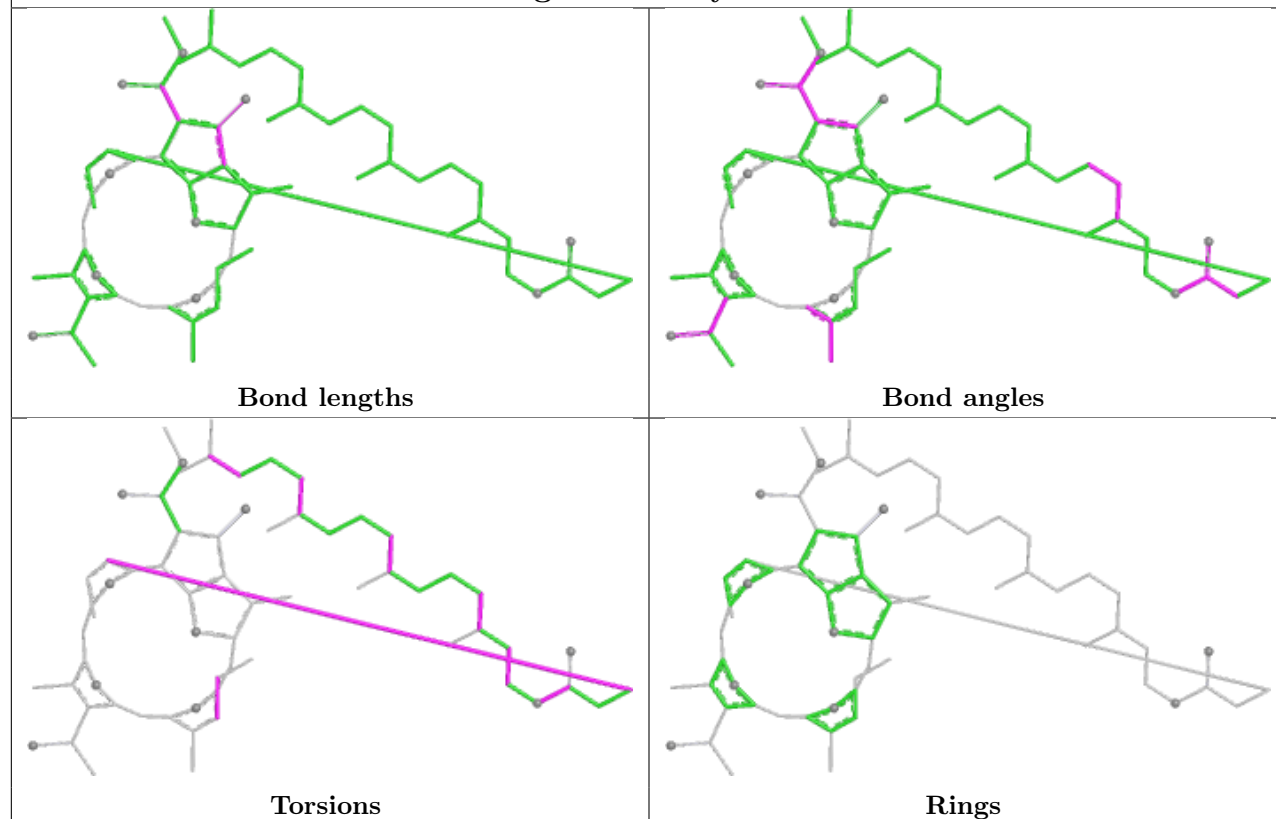
Ligand BPH x 302



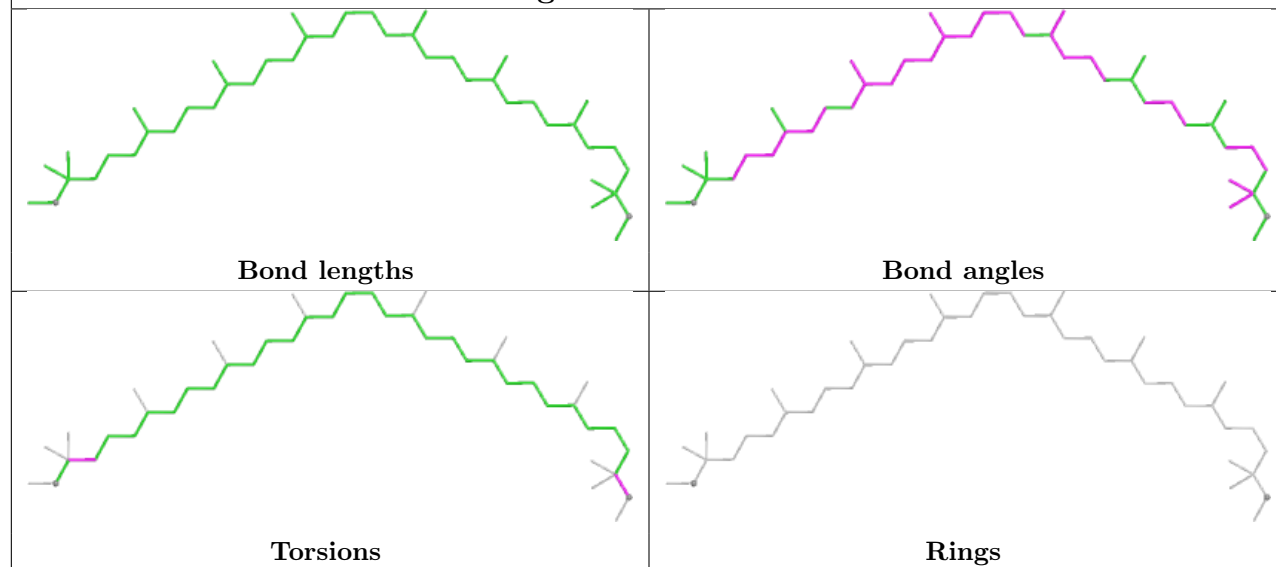
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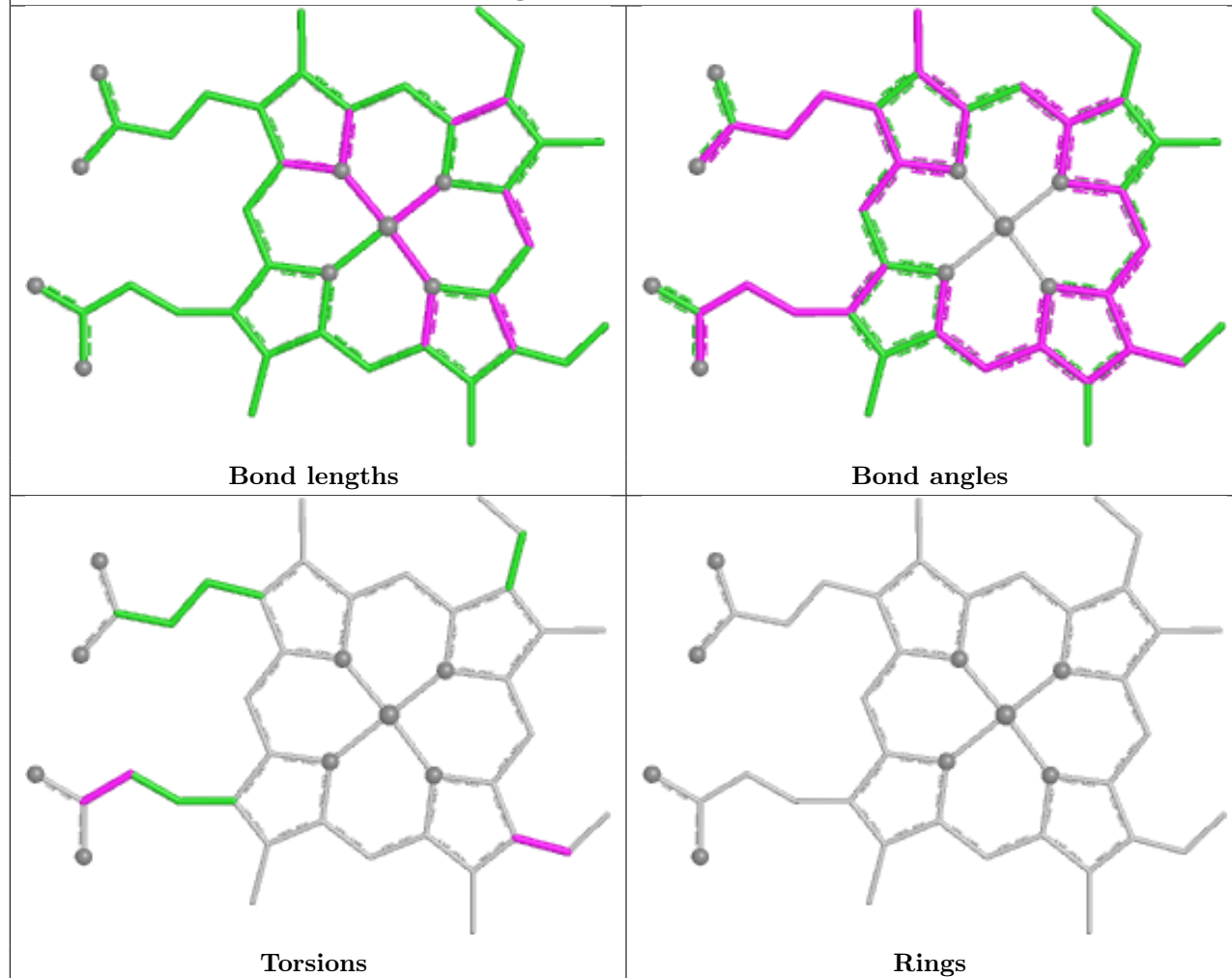
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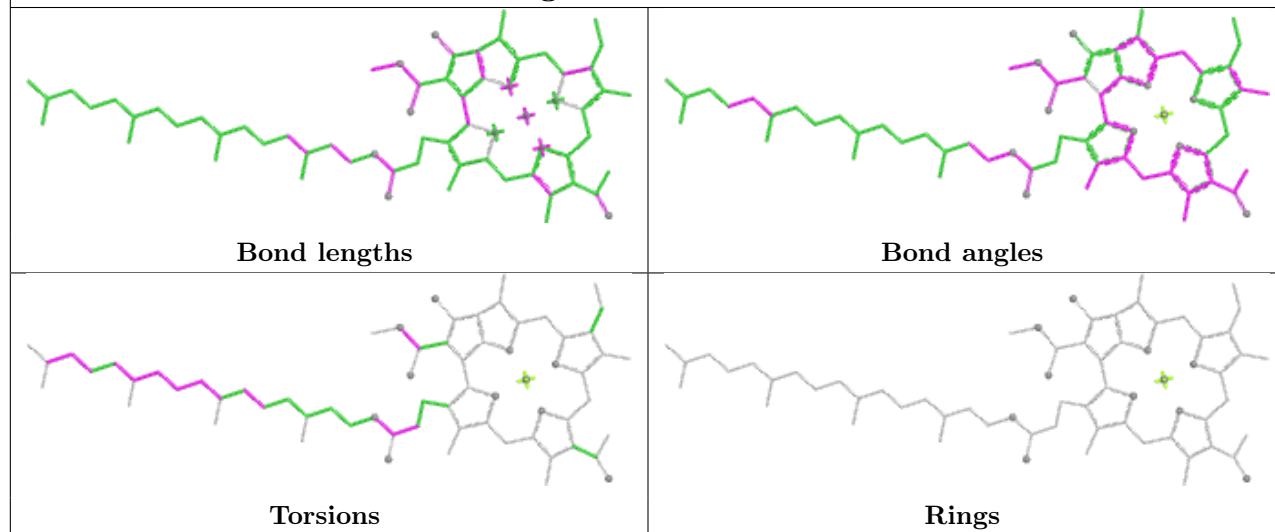
Ligand CRT z 101

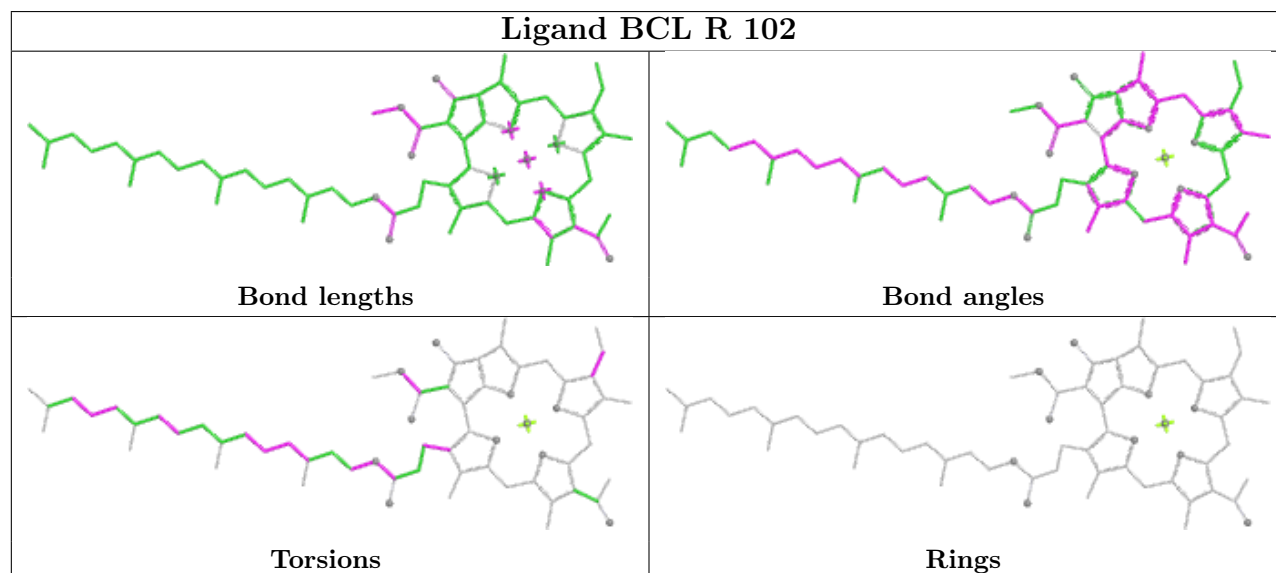
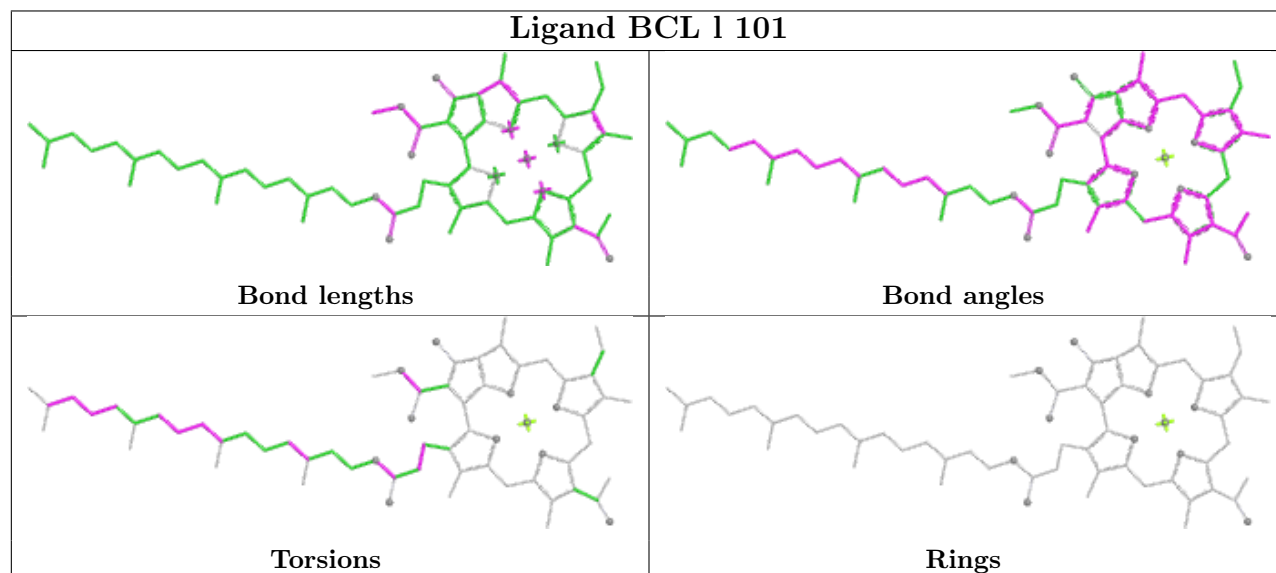
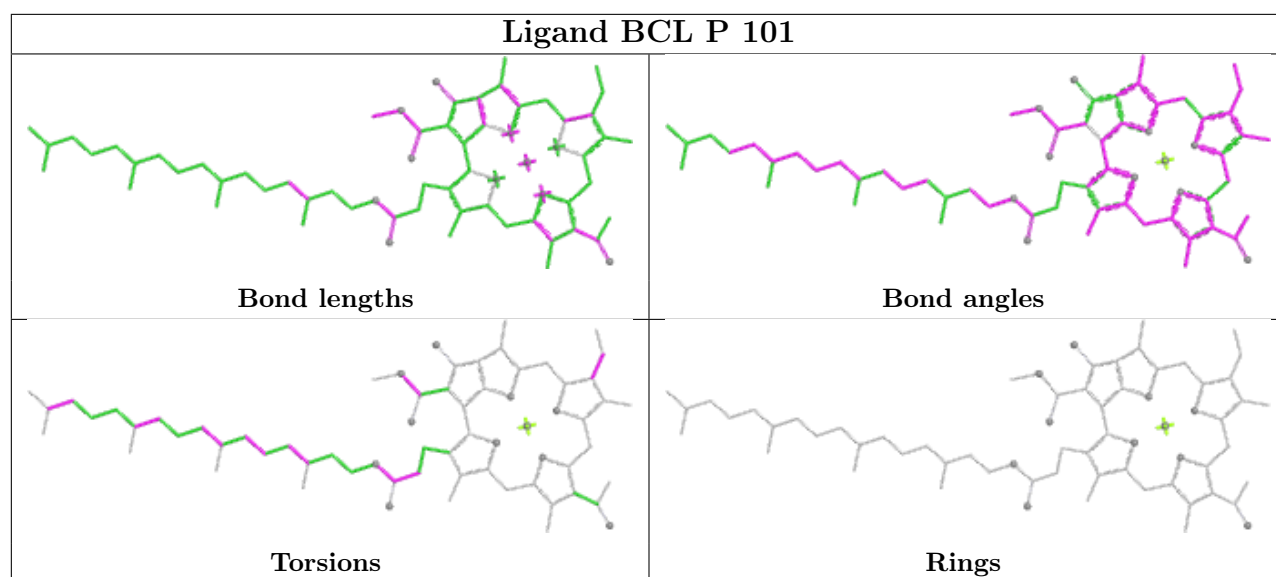


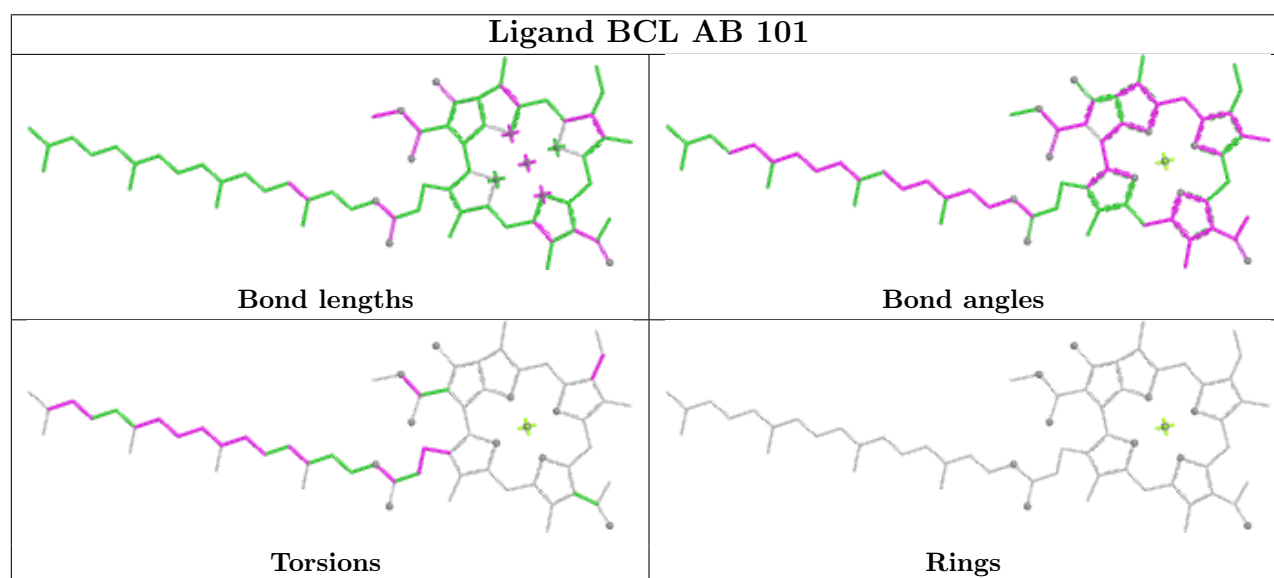
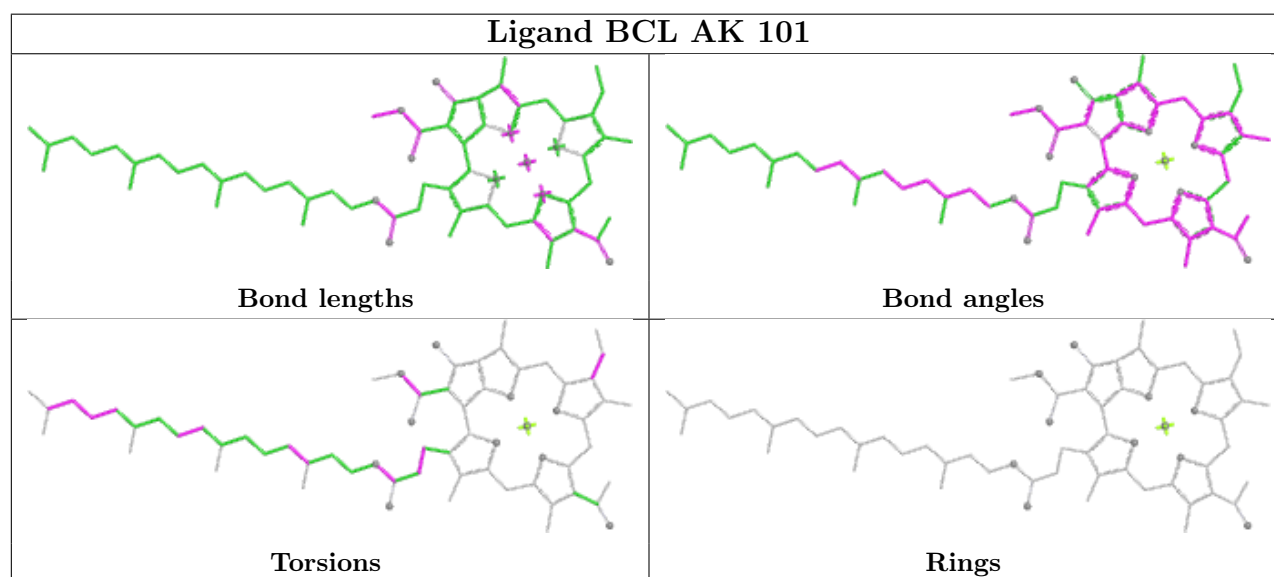
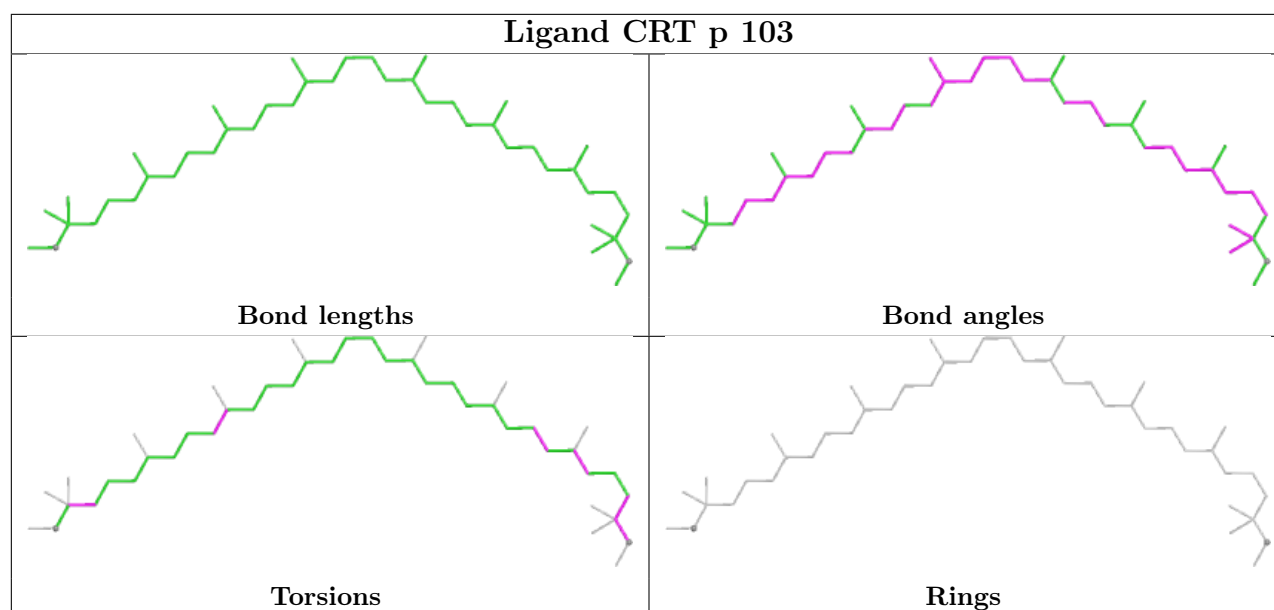
Ligand HEM o 503

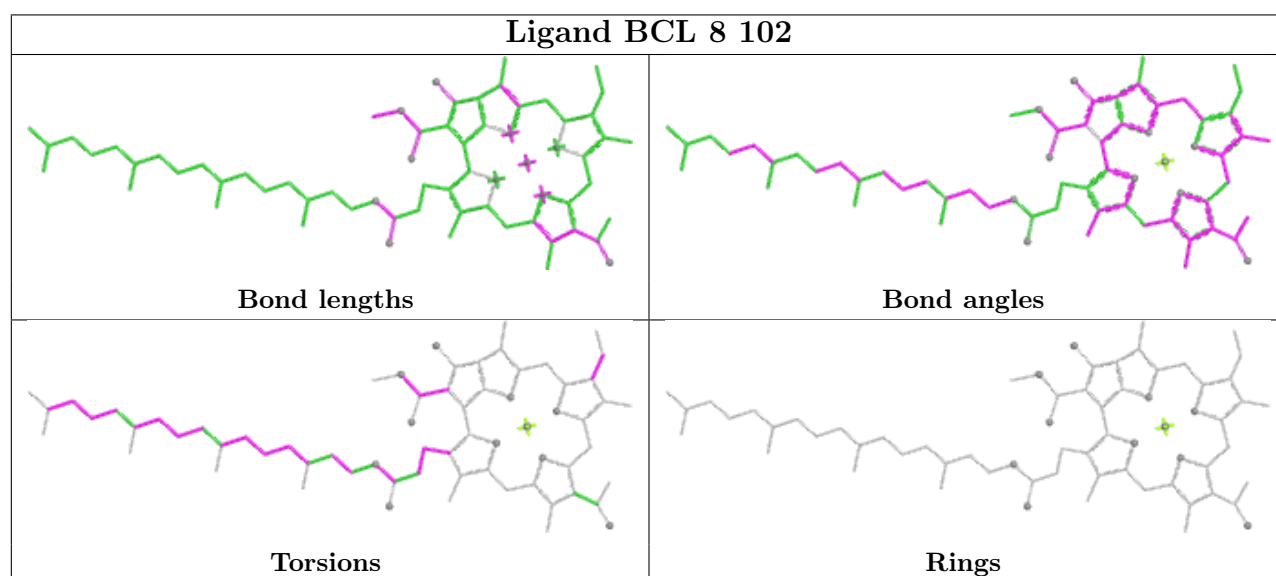
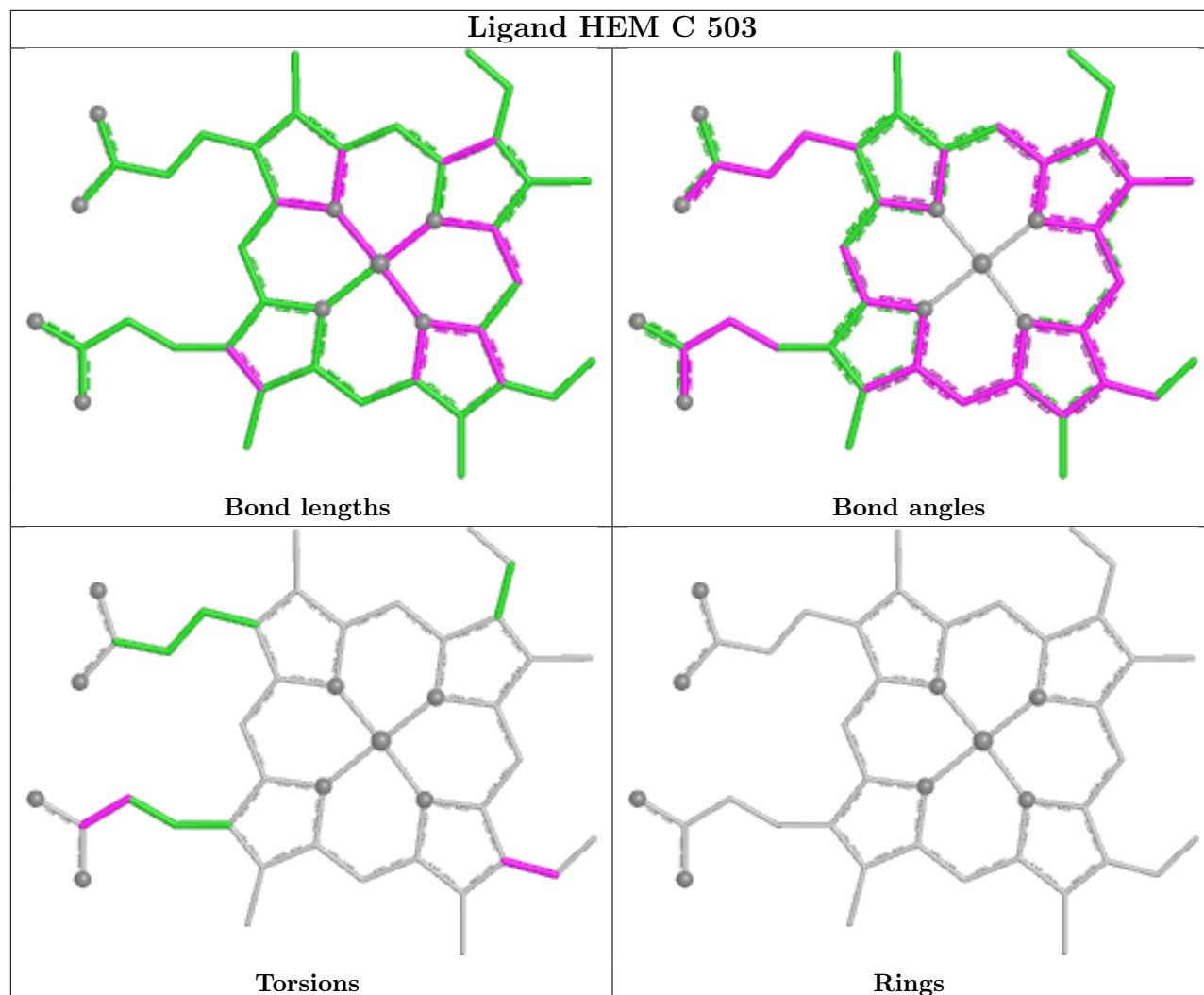


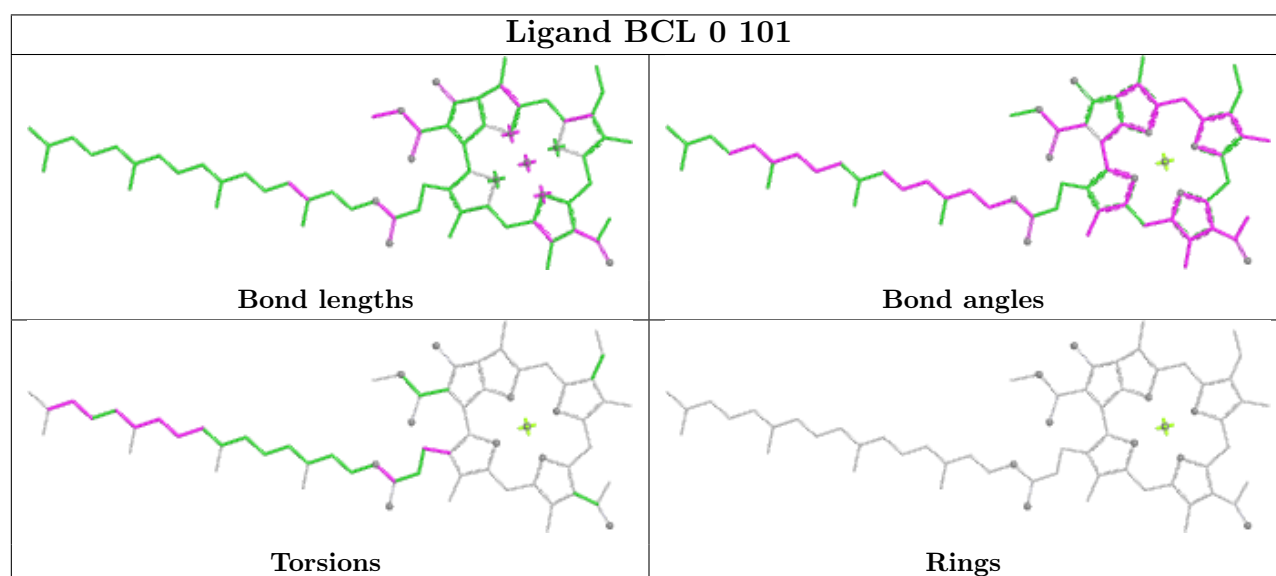
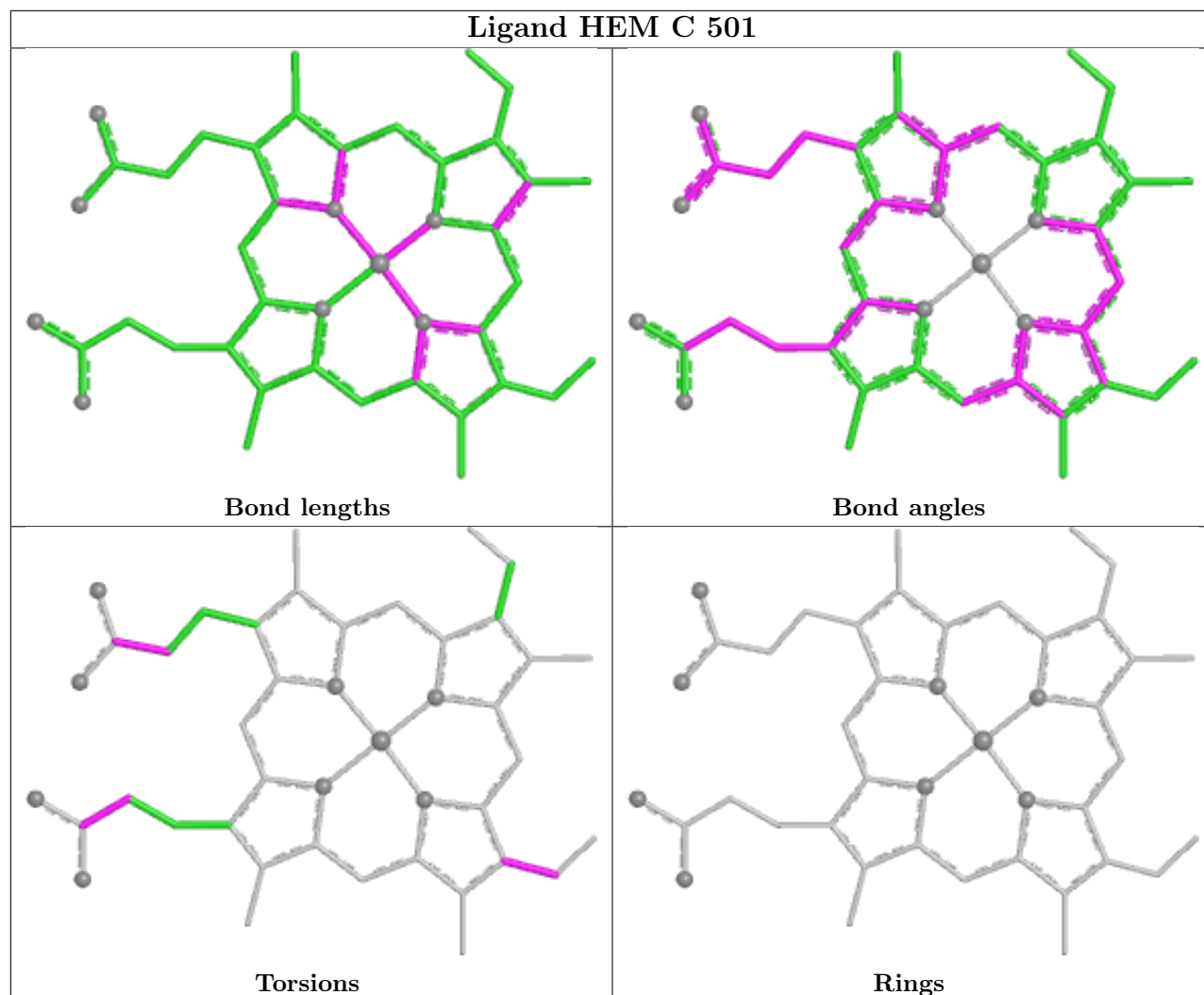
Ligand BCL f 101

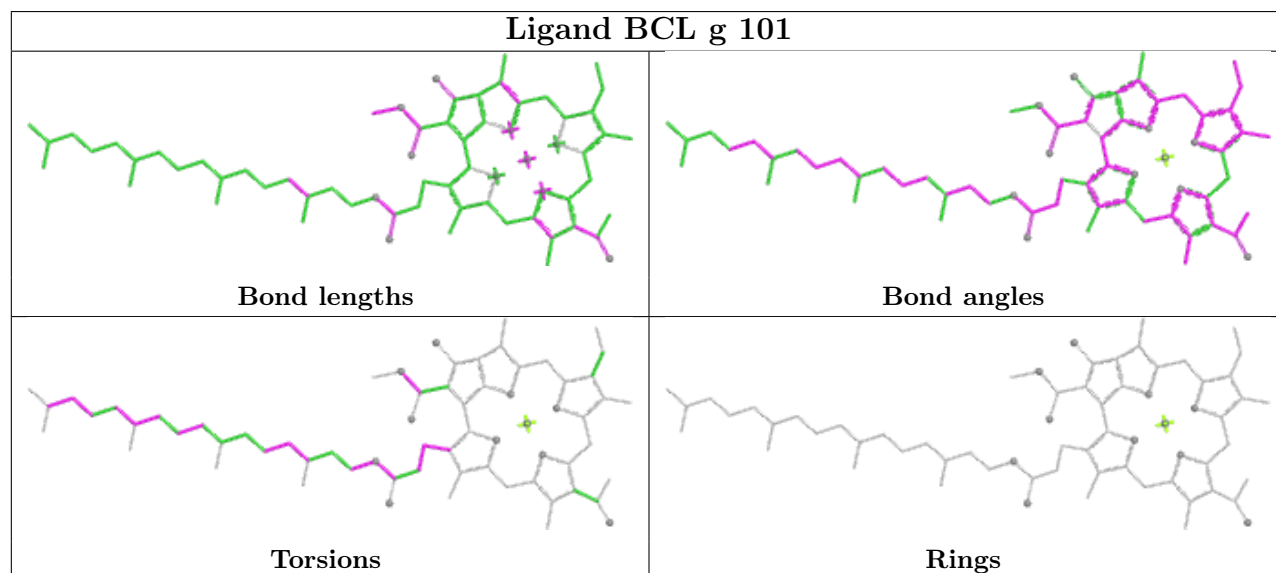
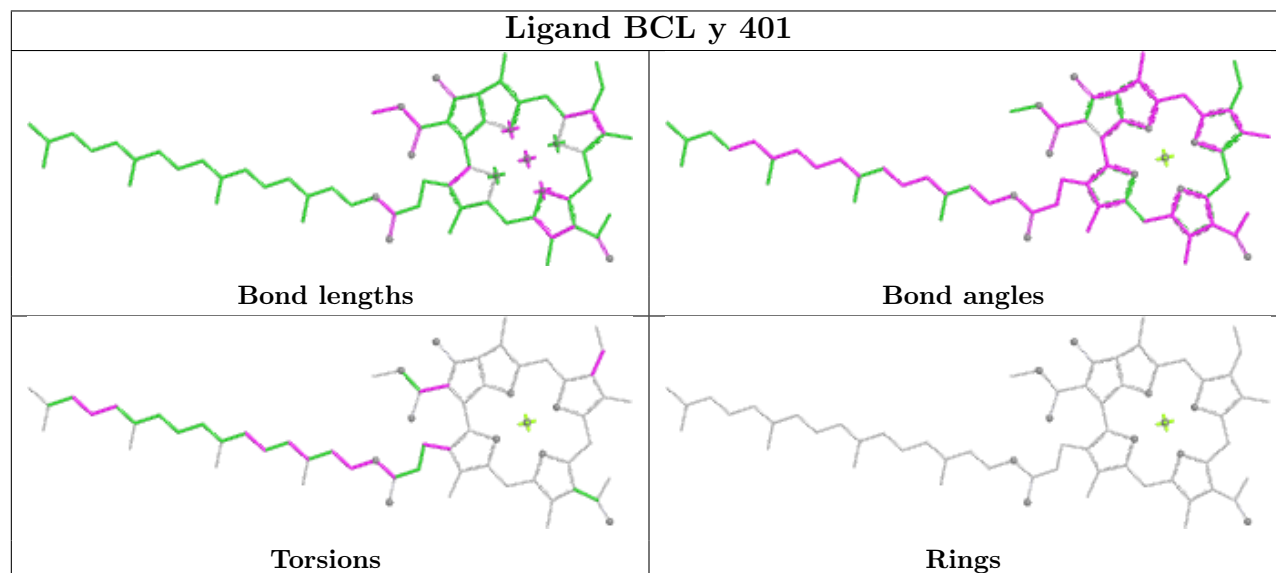
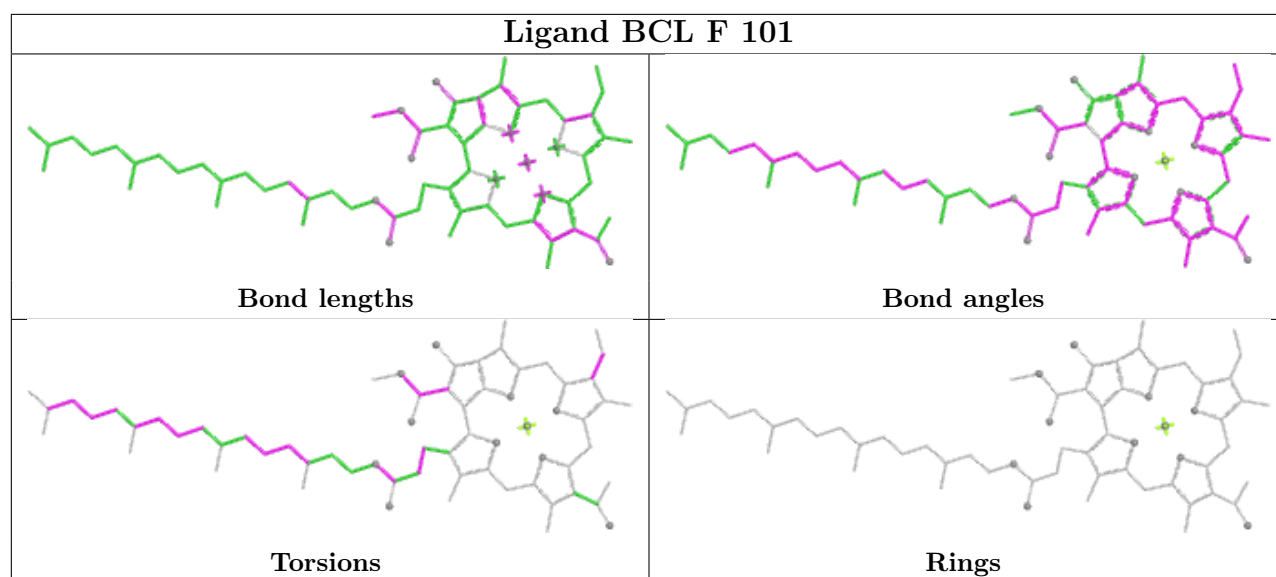


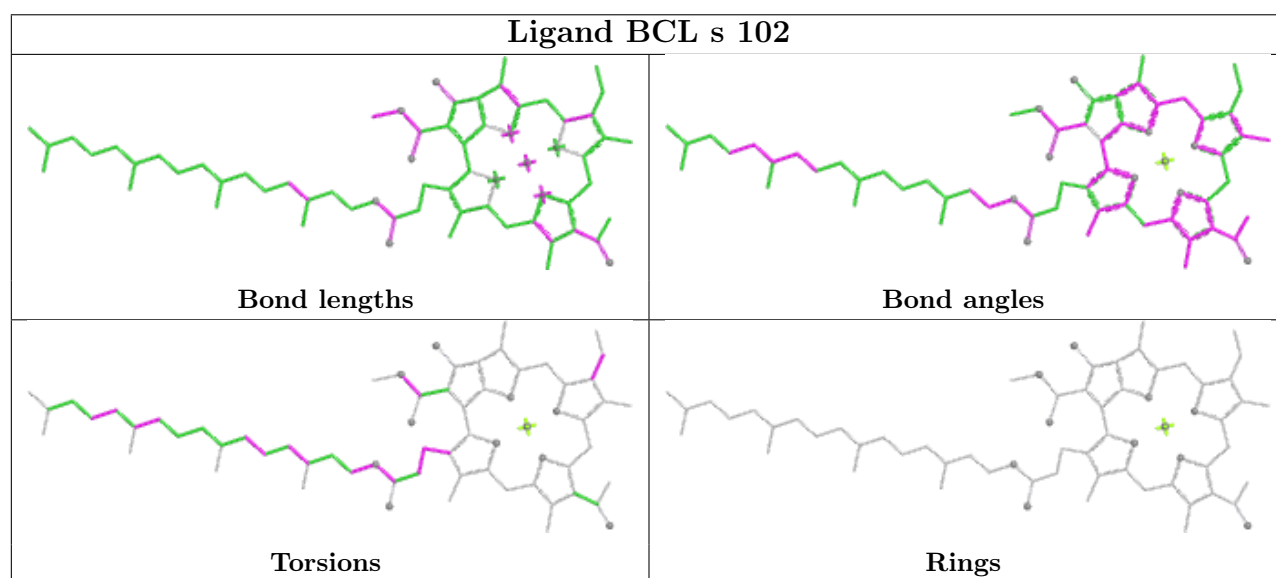
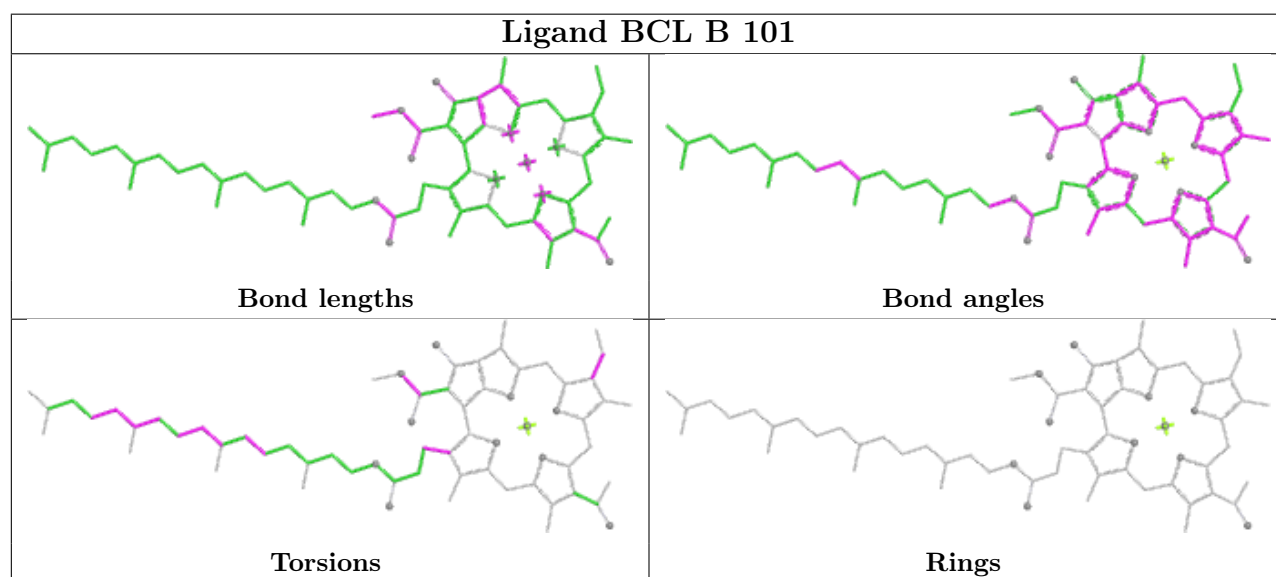
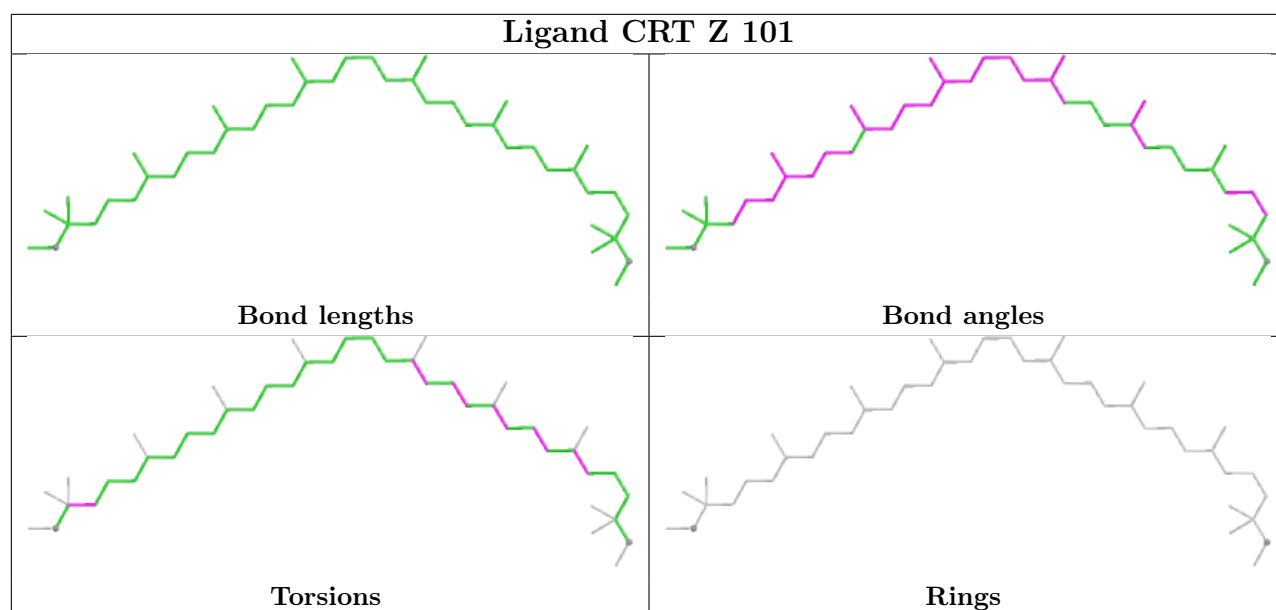


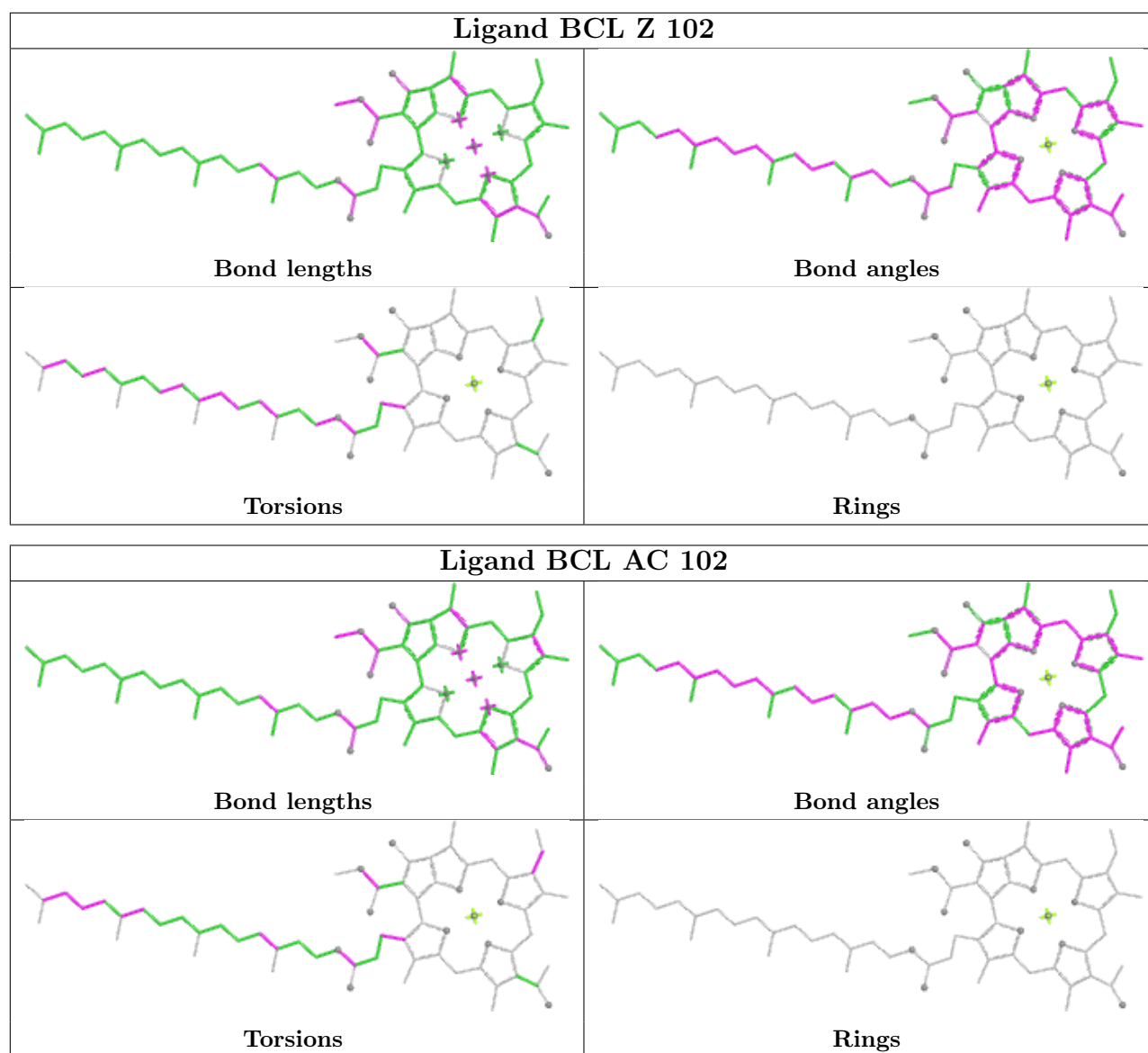


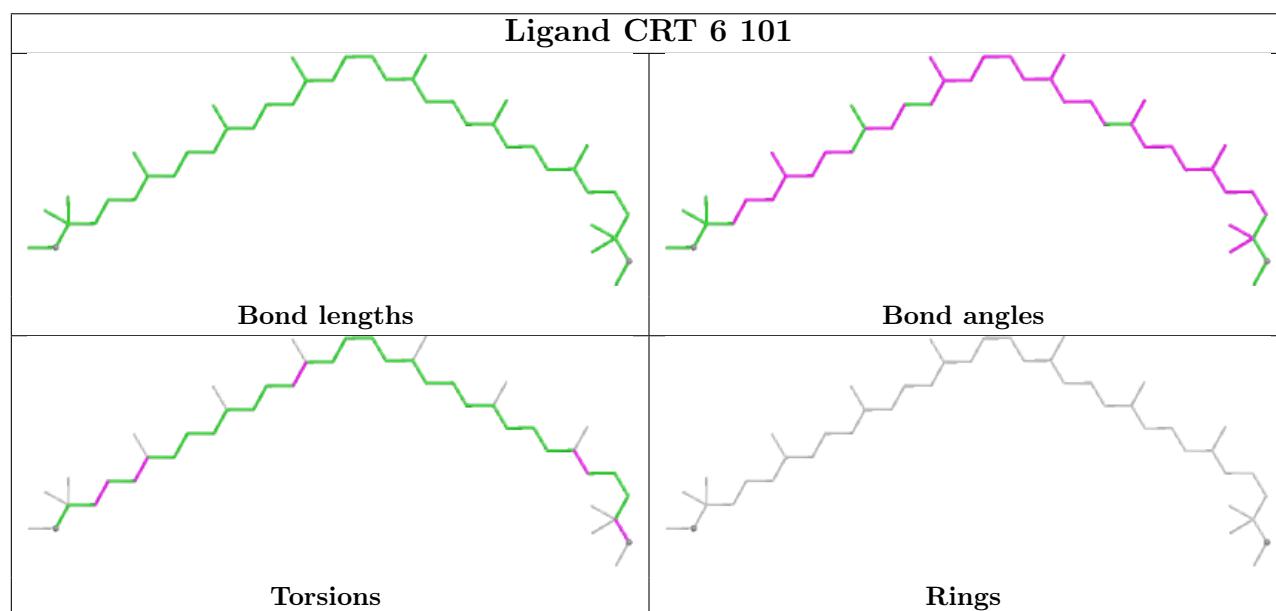
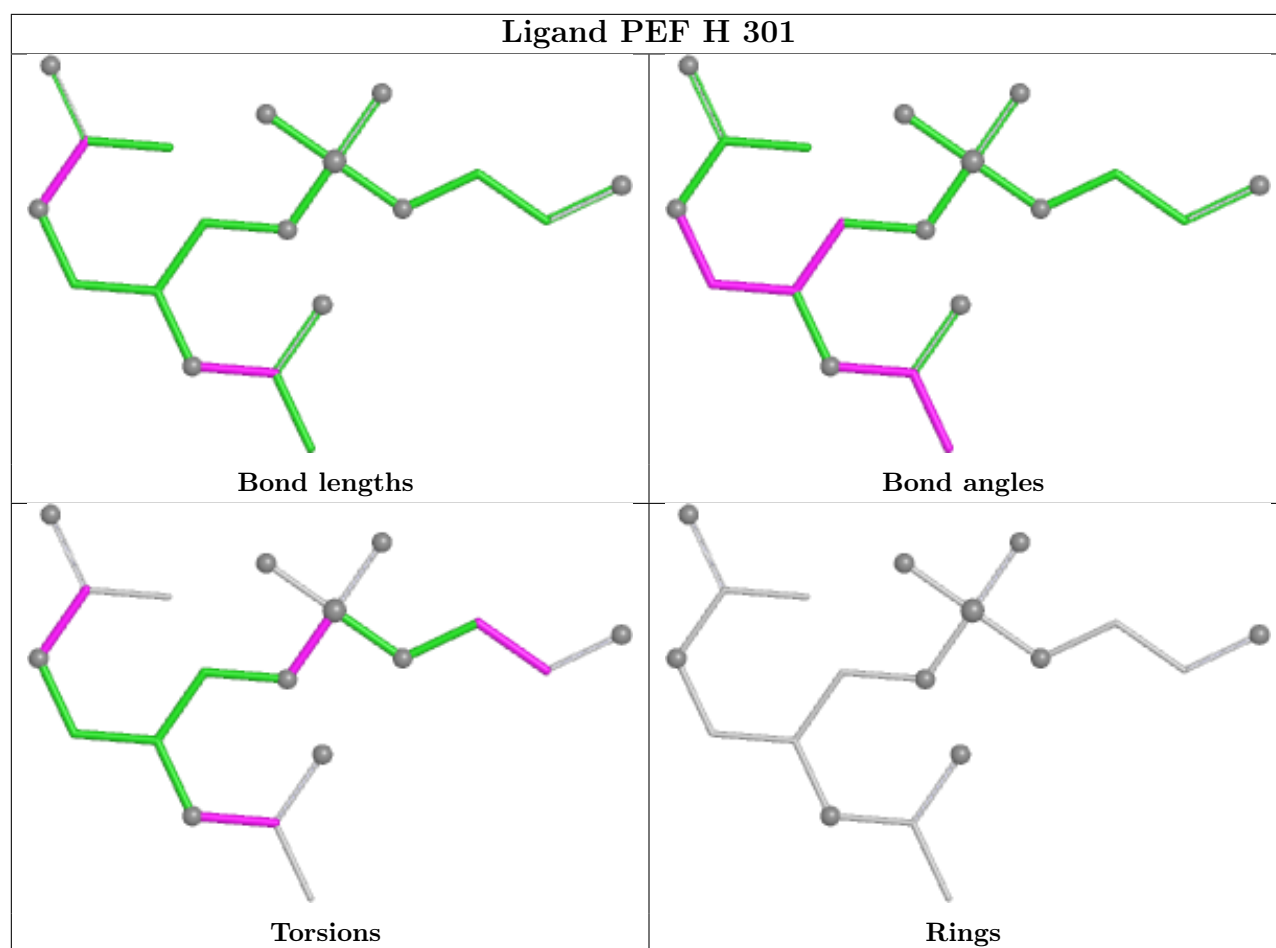


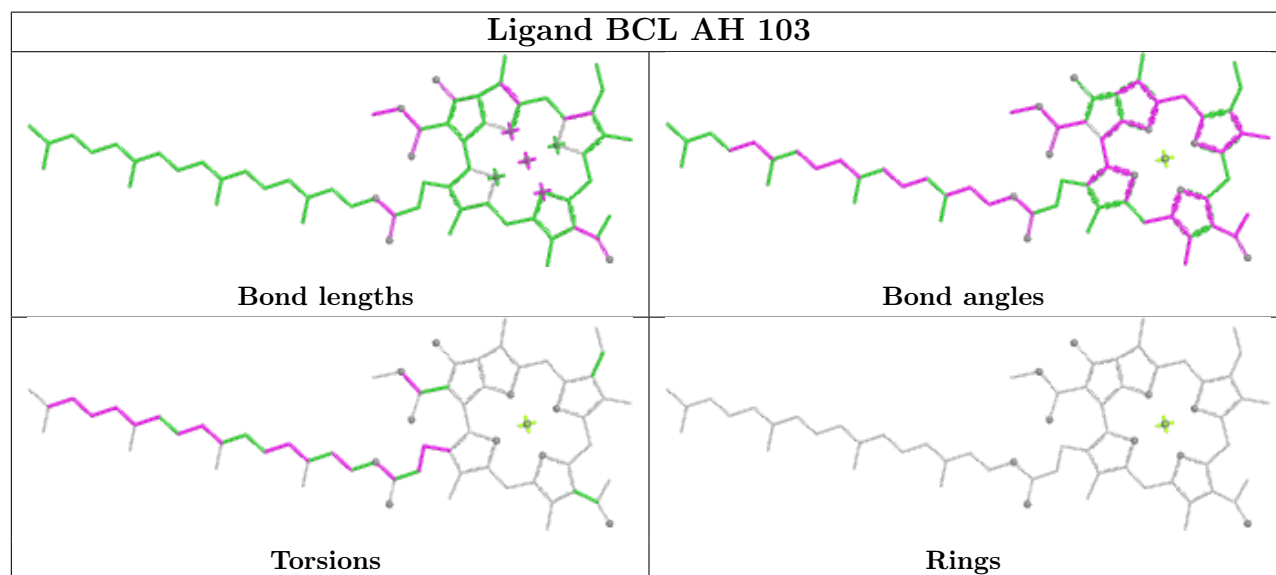
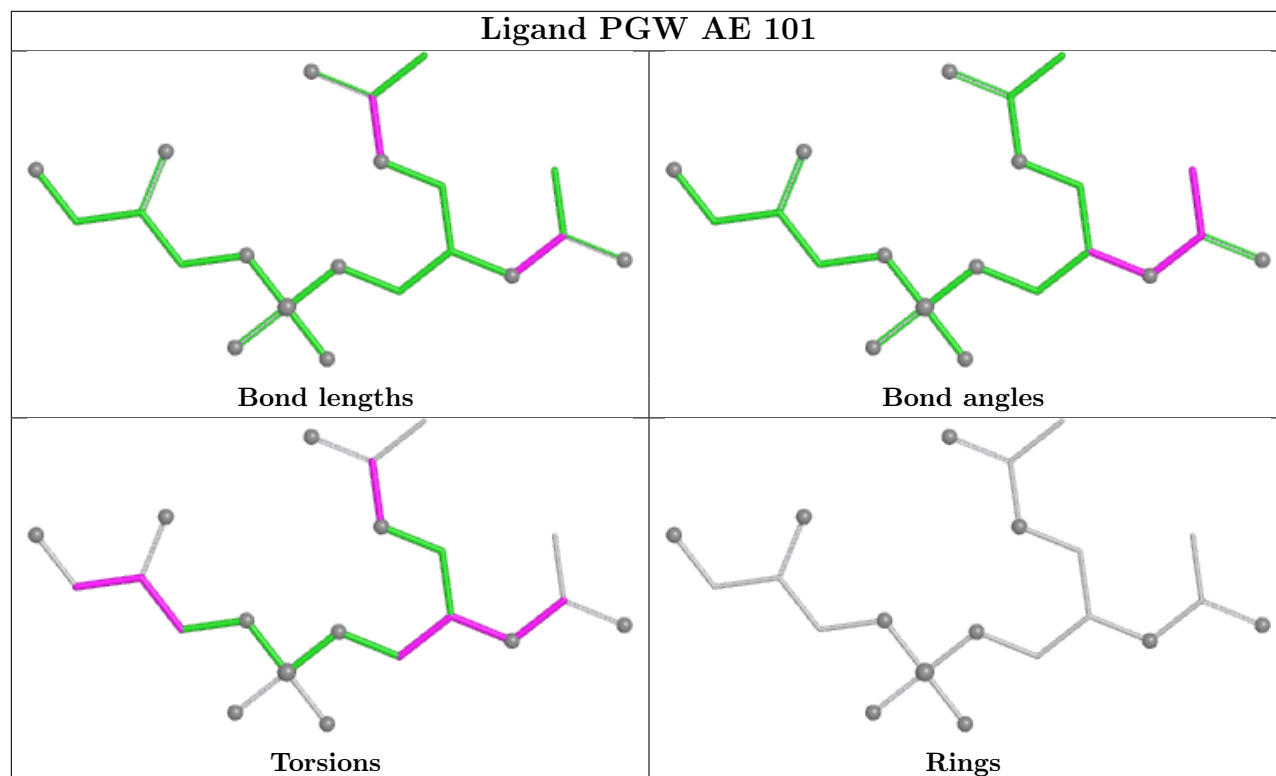


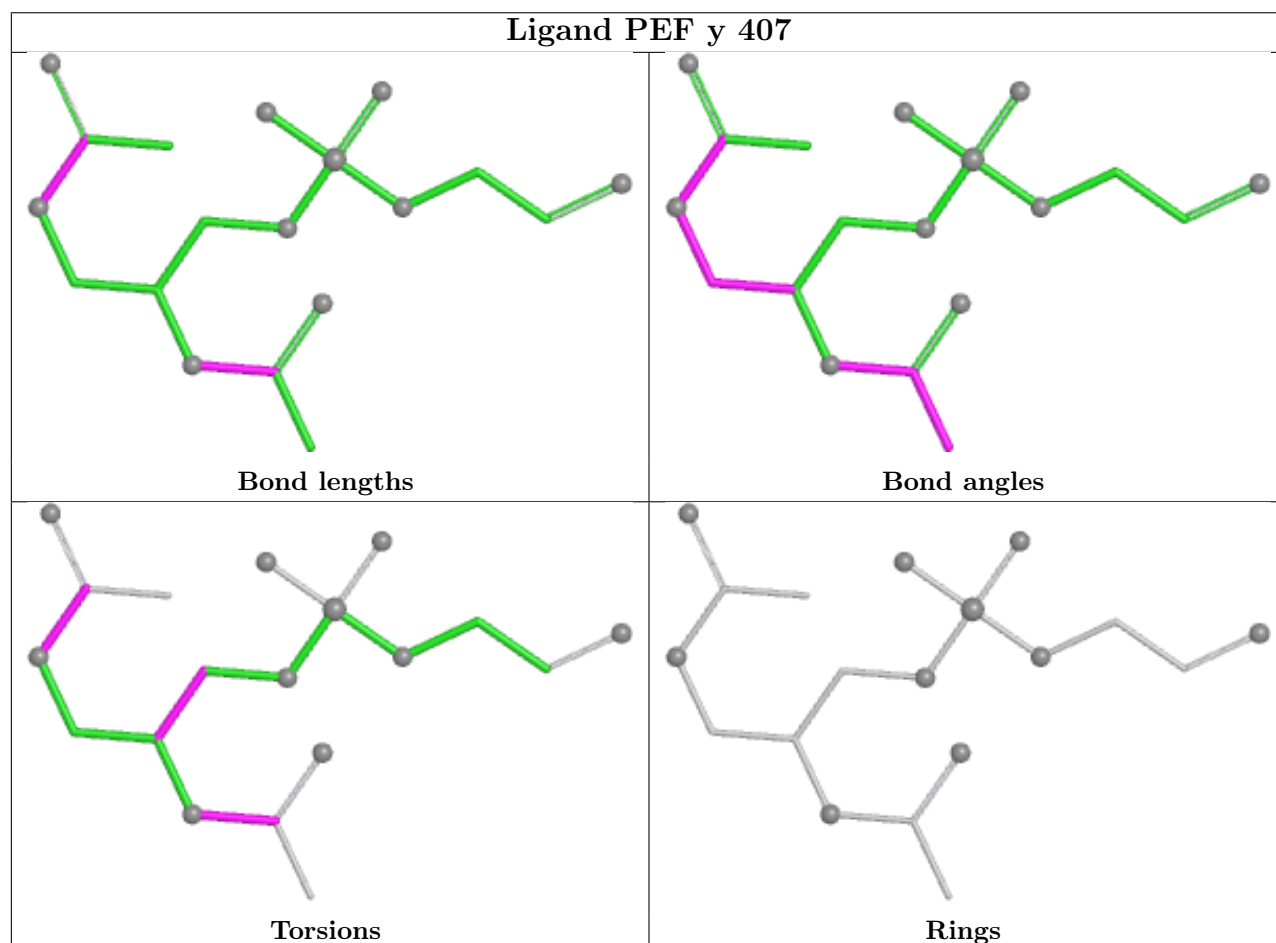
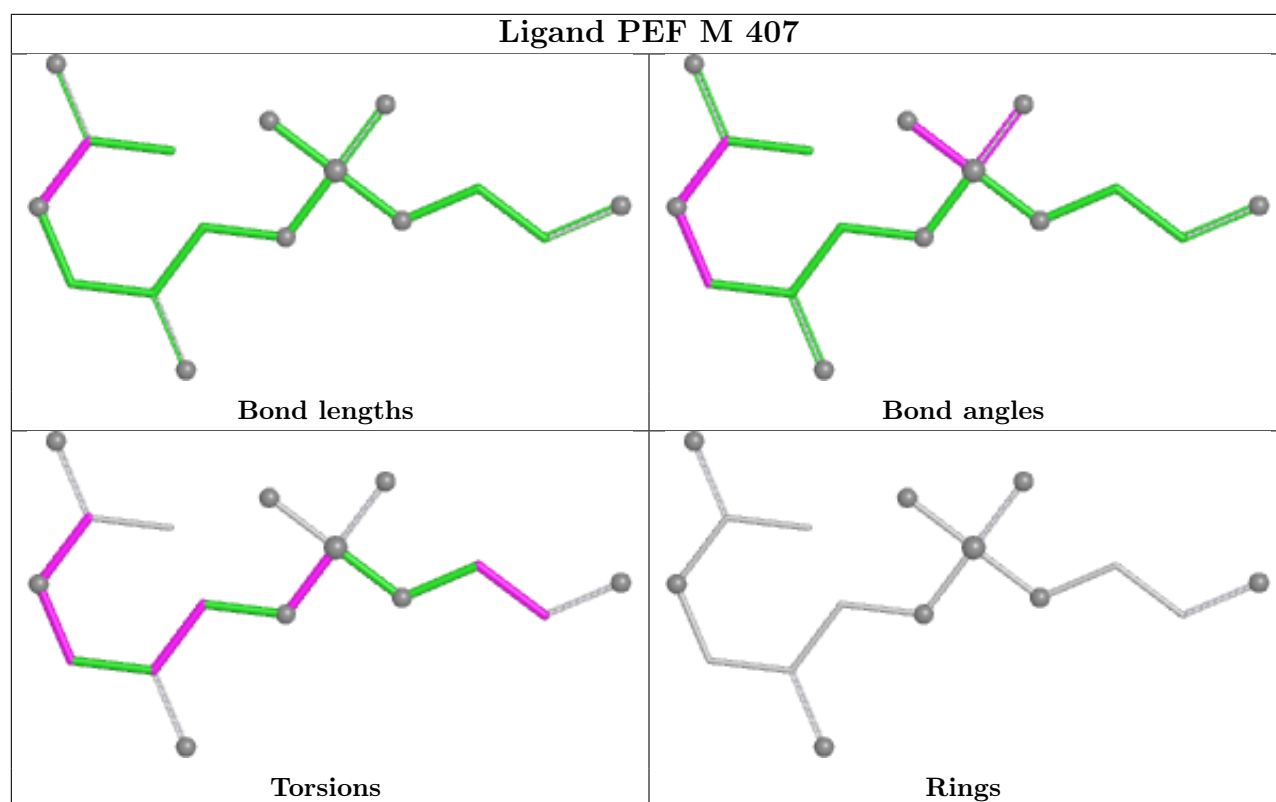


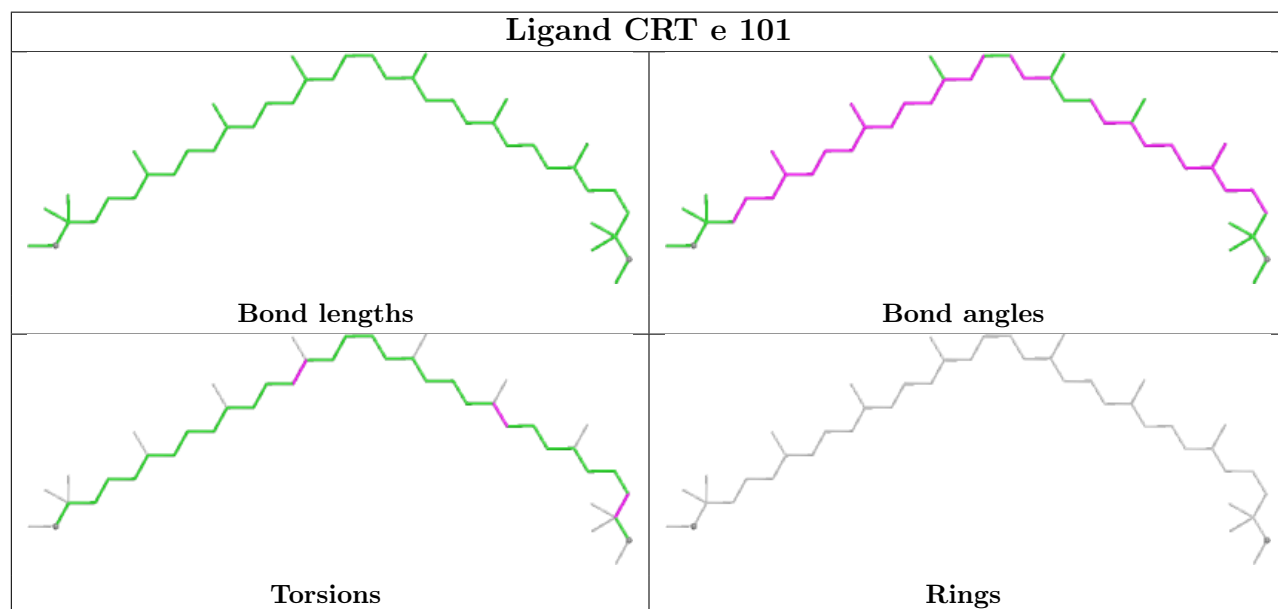
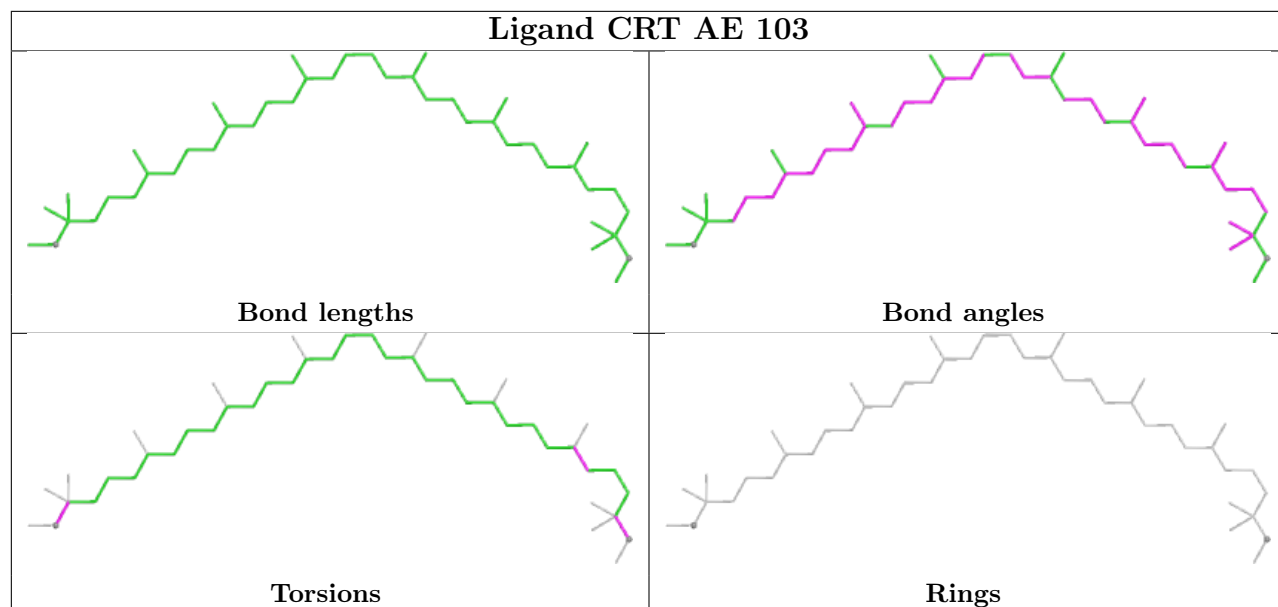


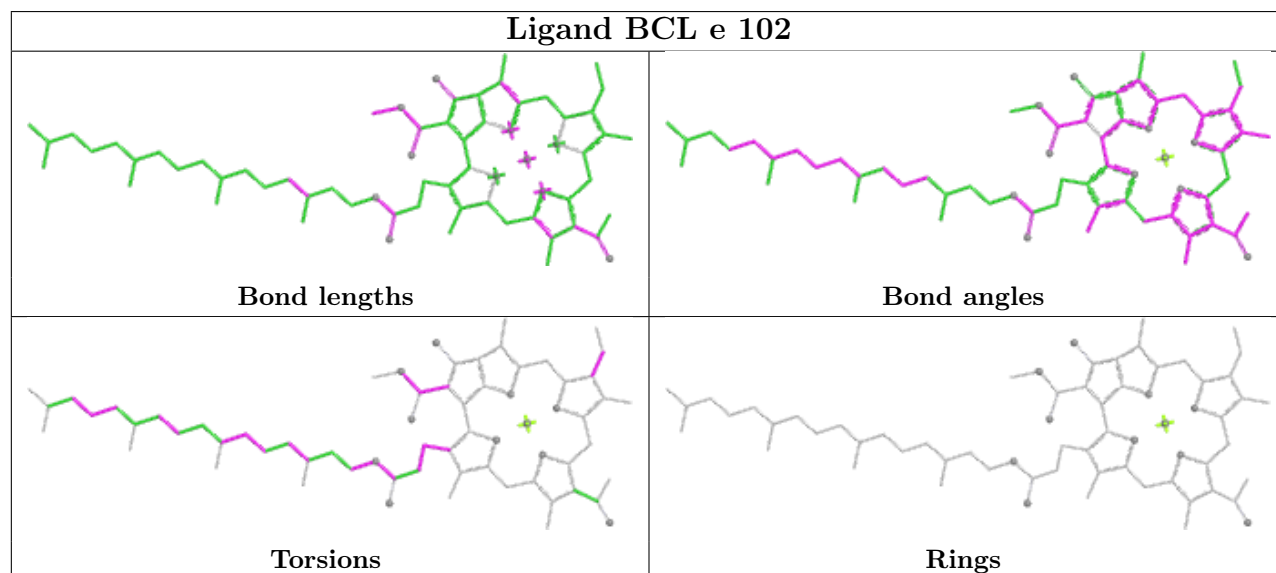
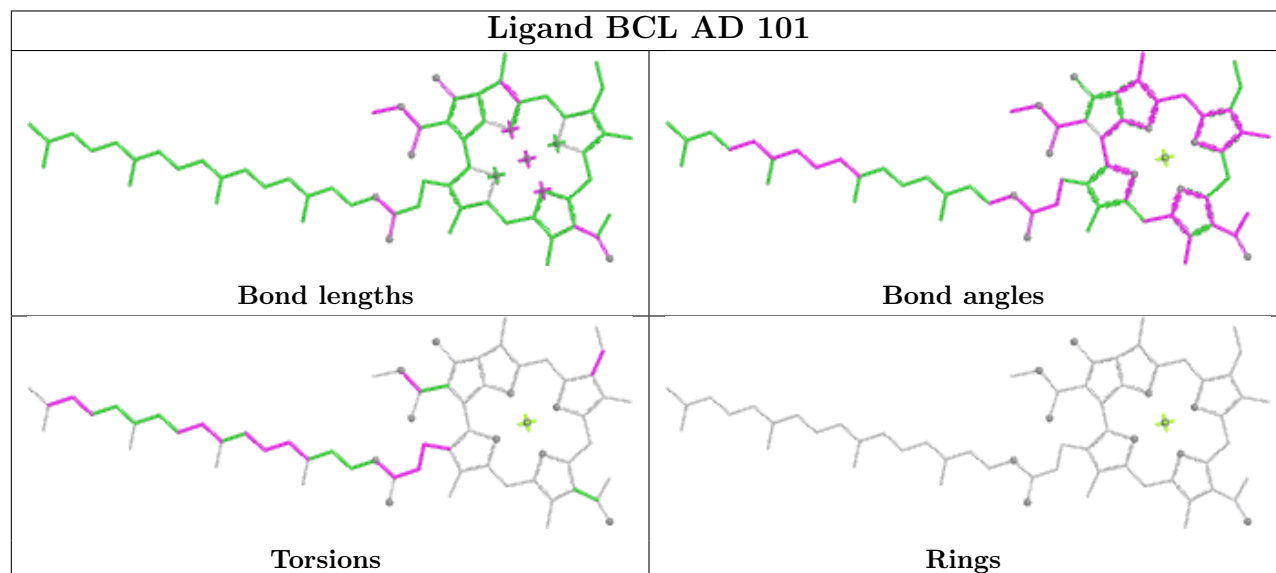
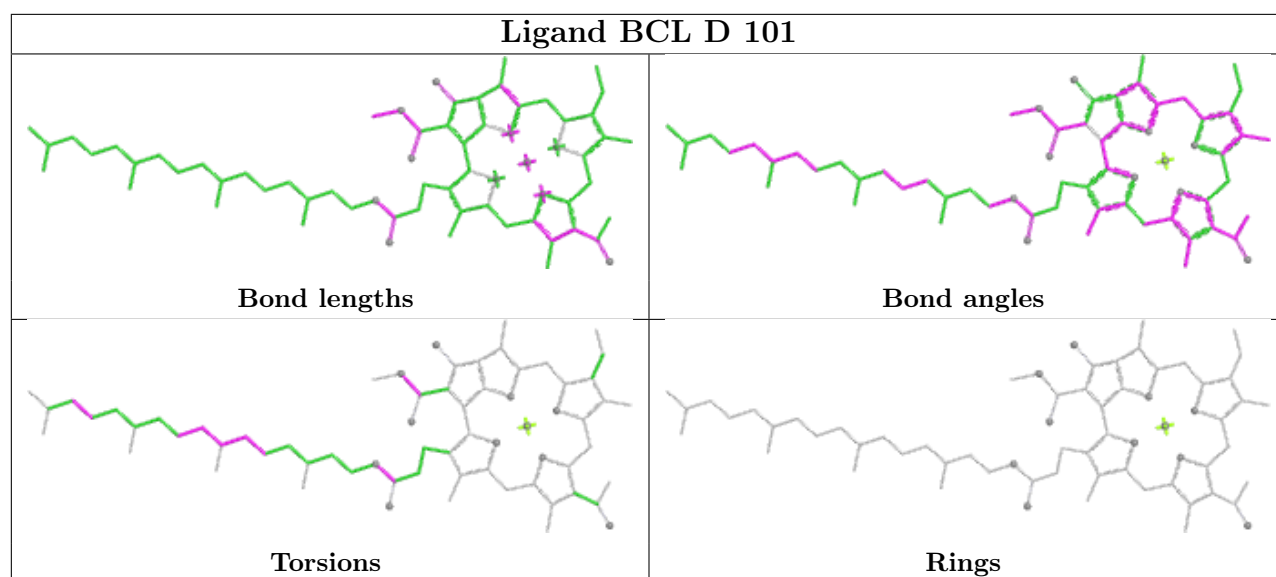


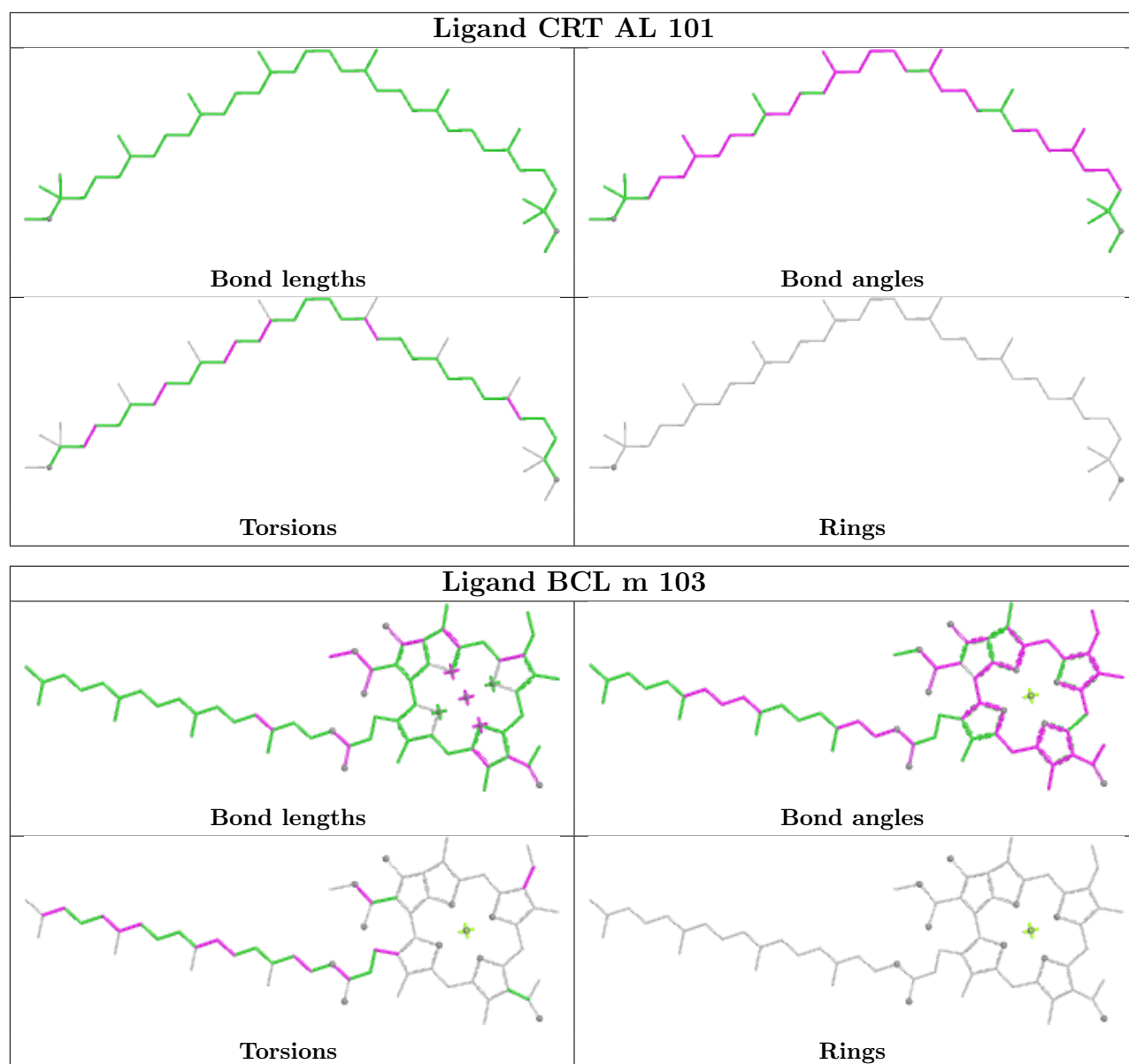


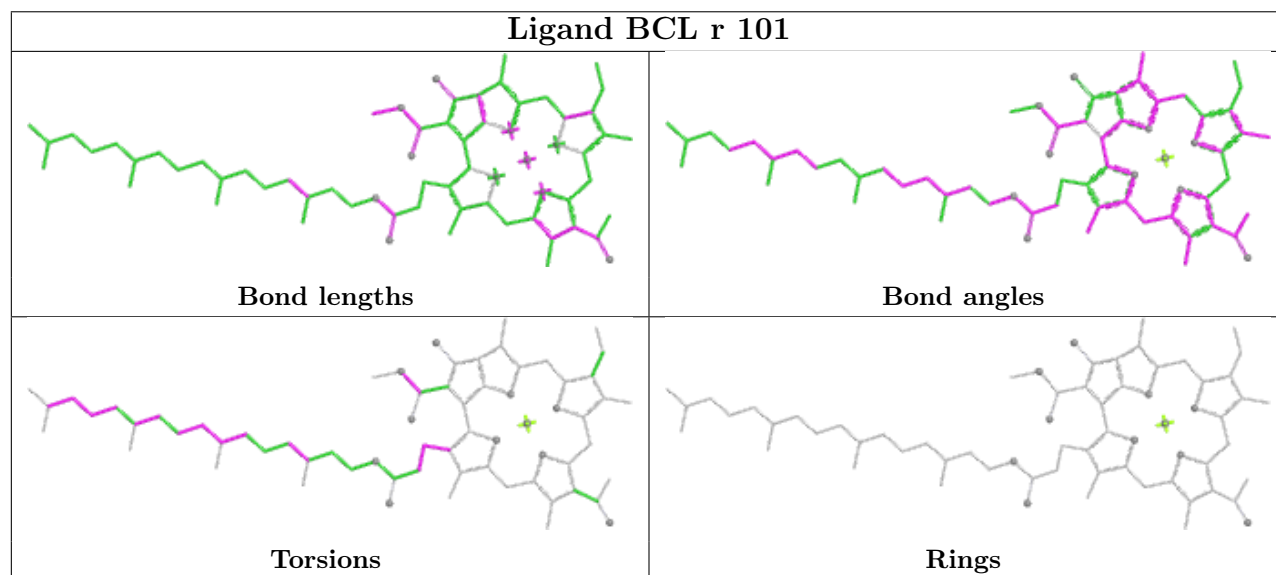
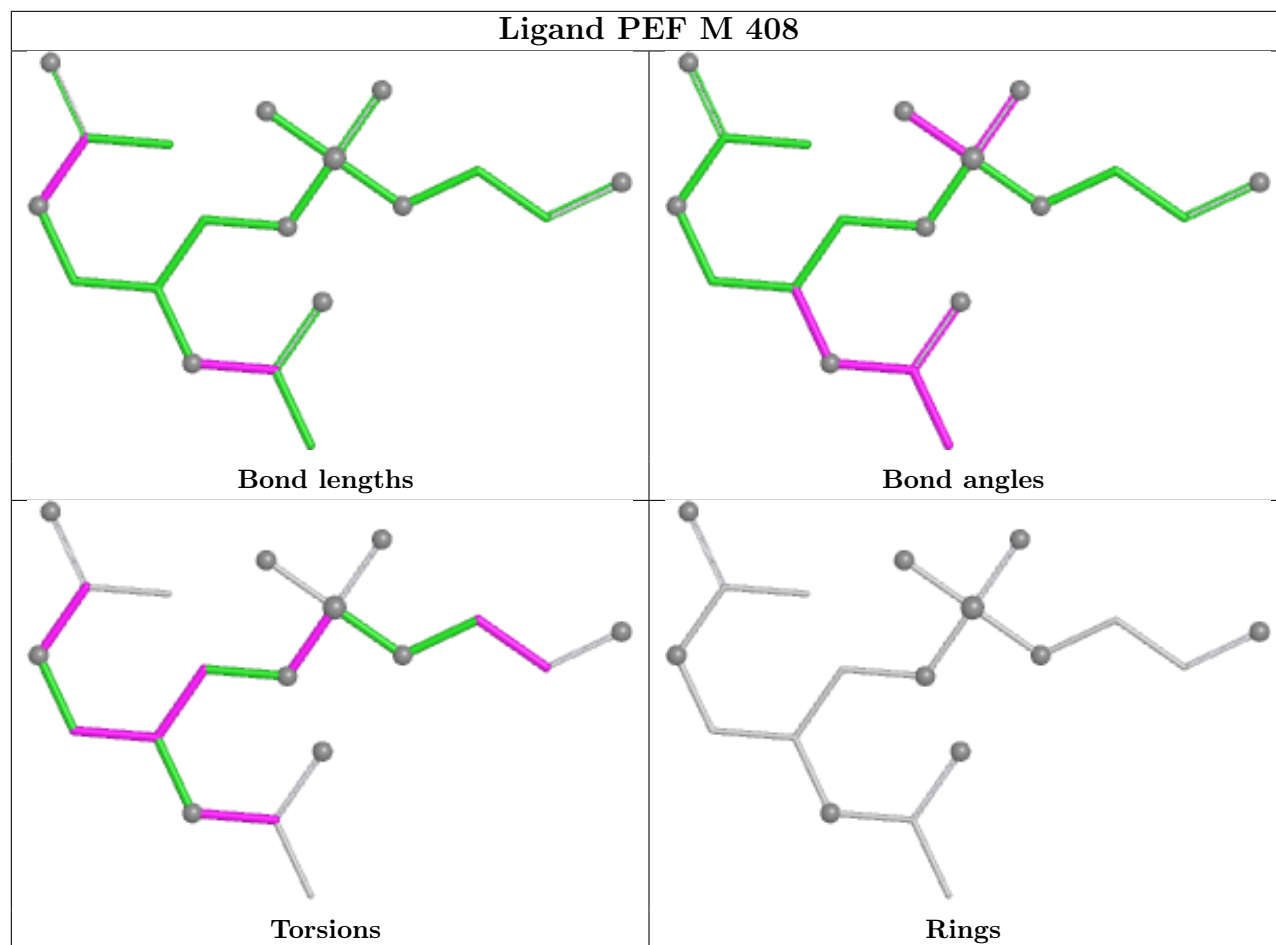


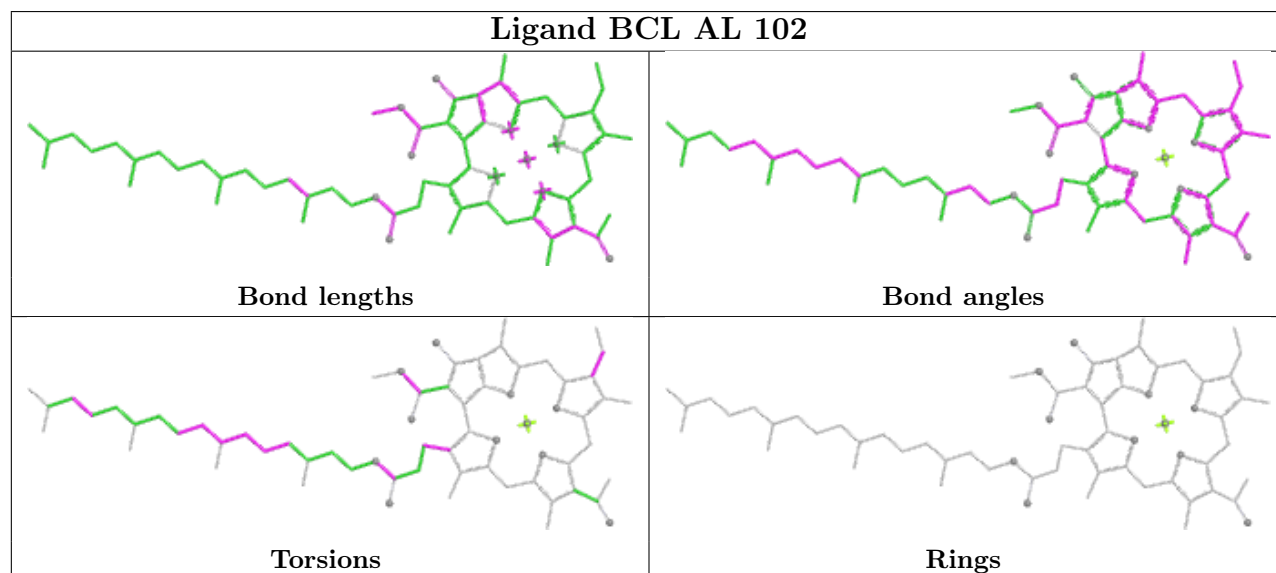
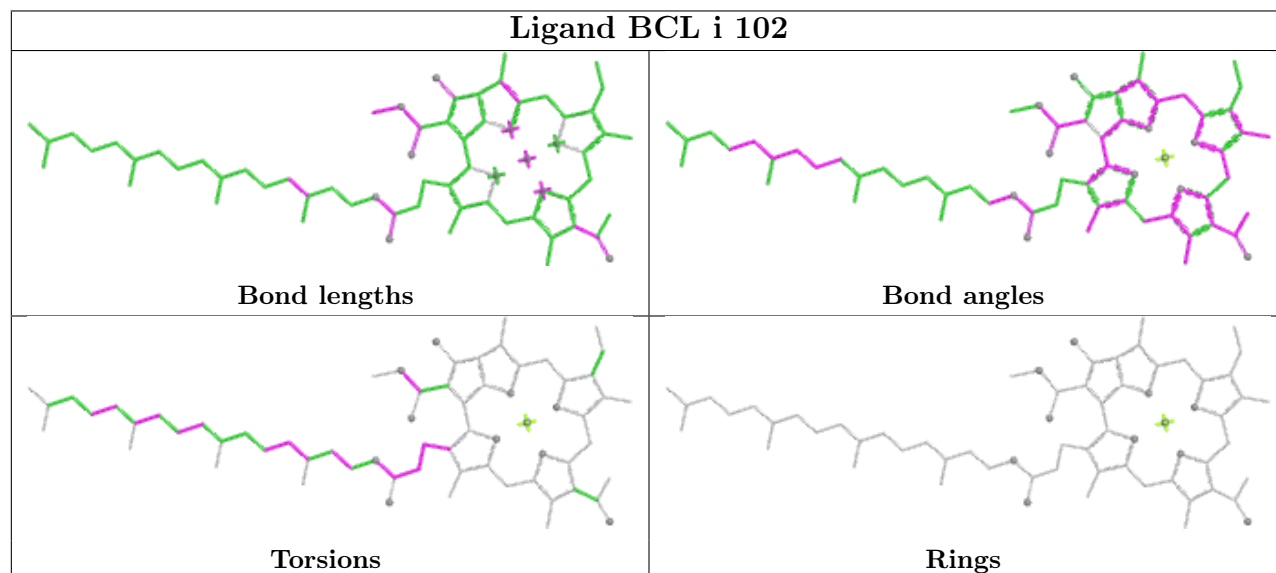
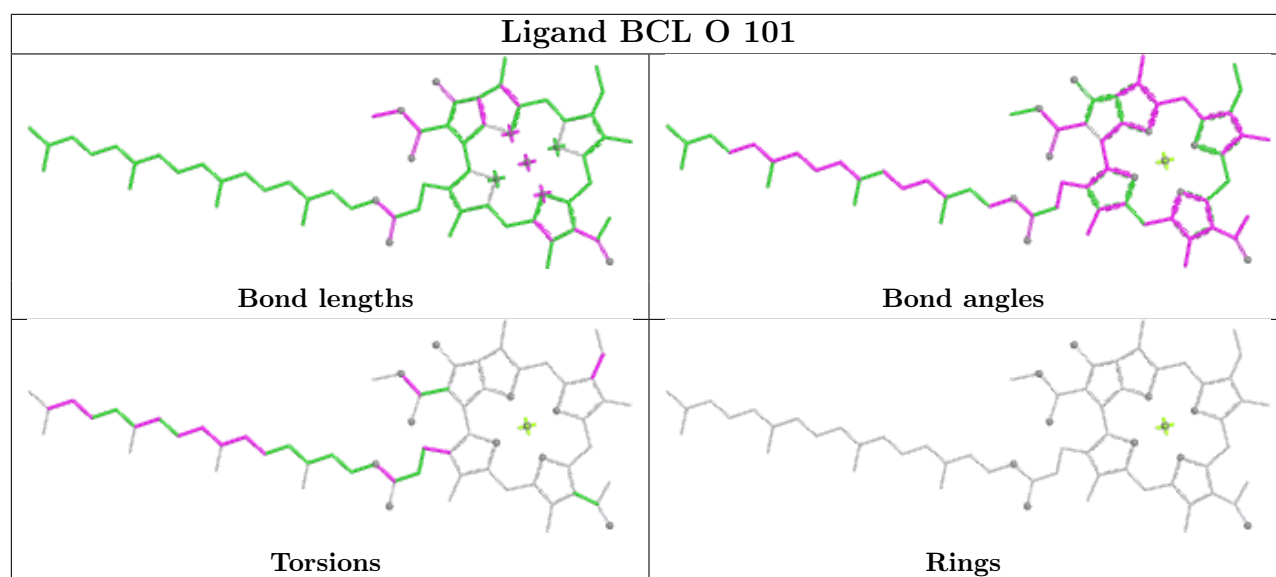




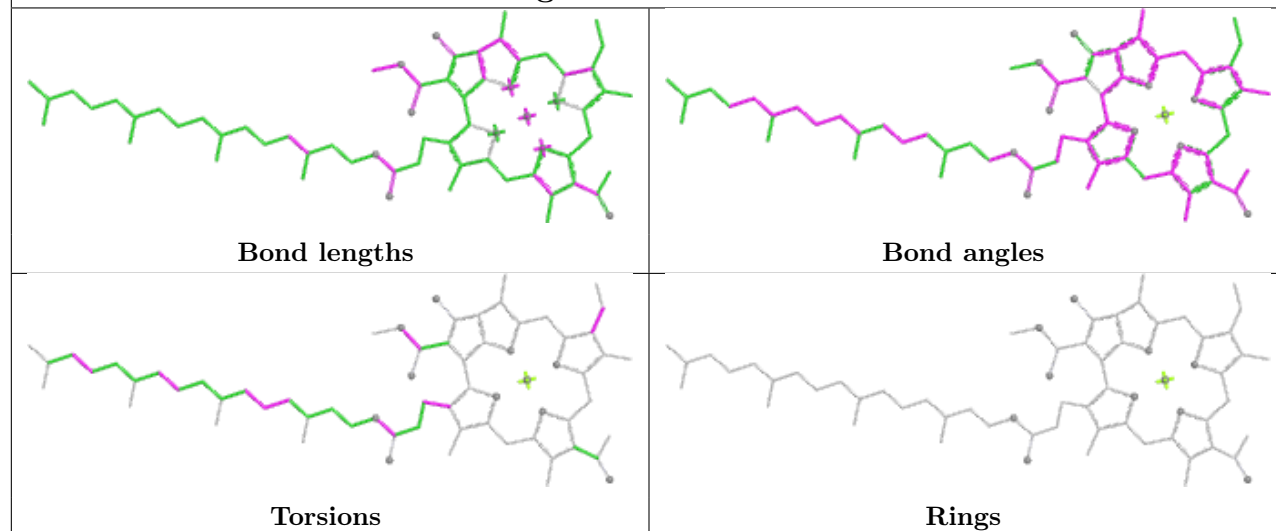




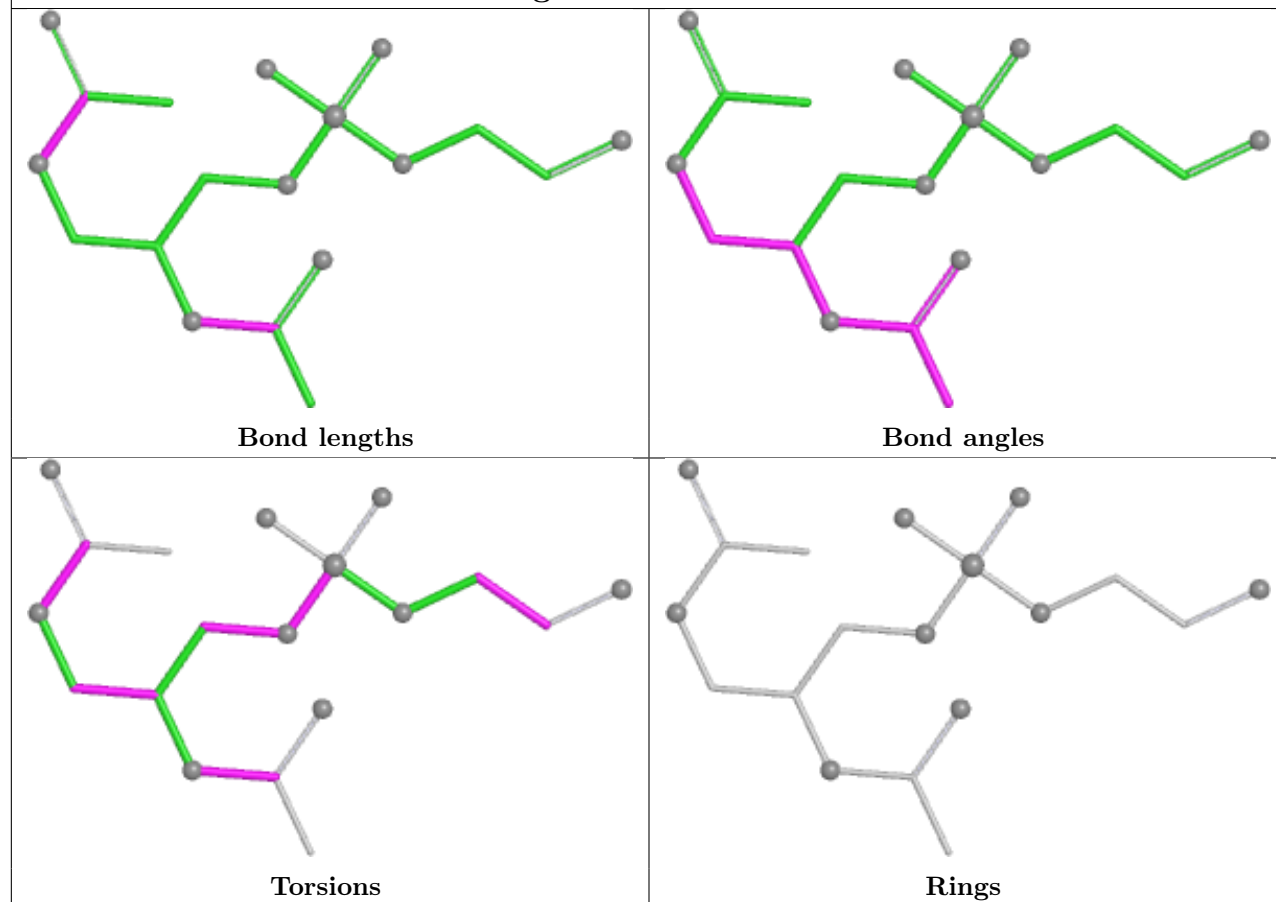


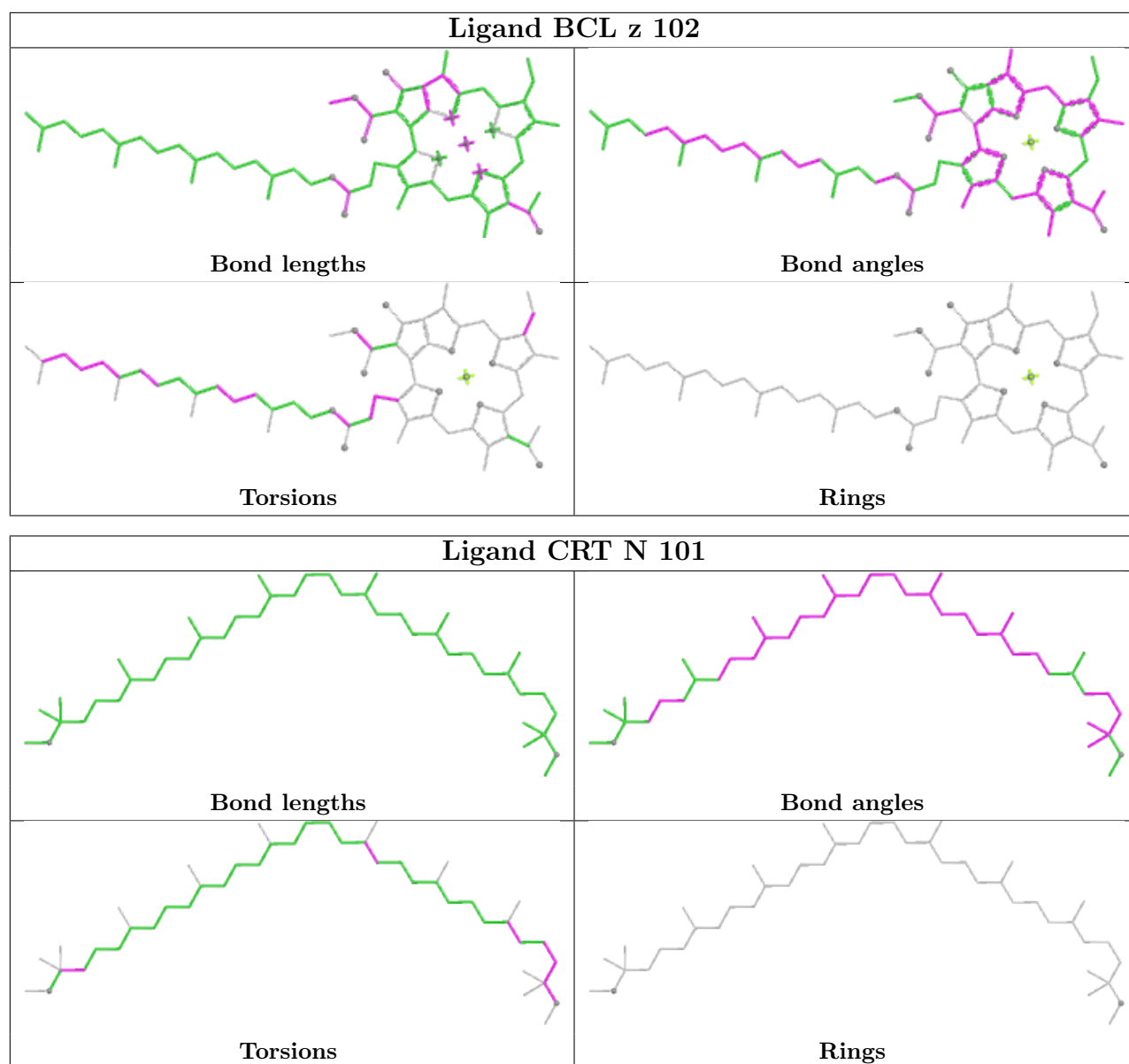


Ligand BCL J 102

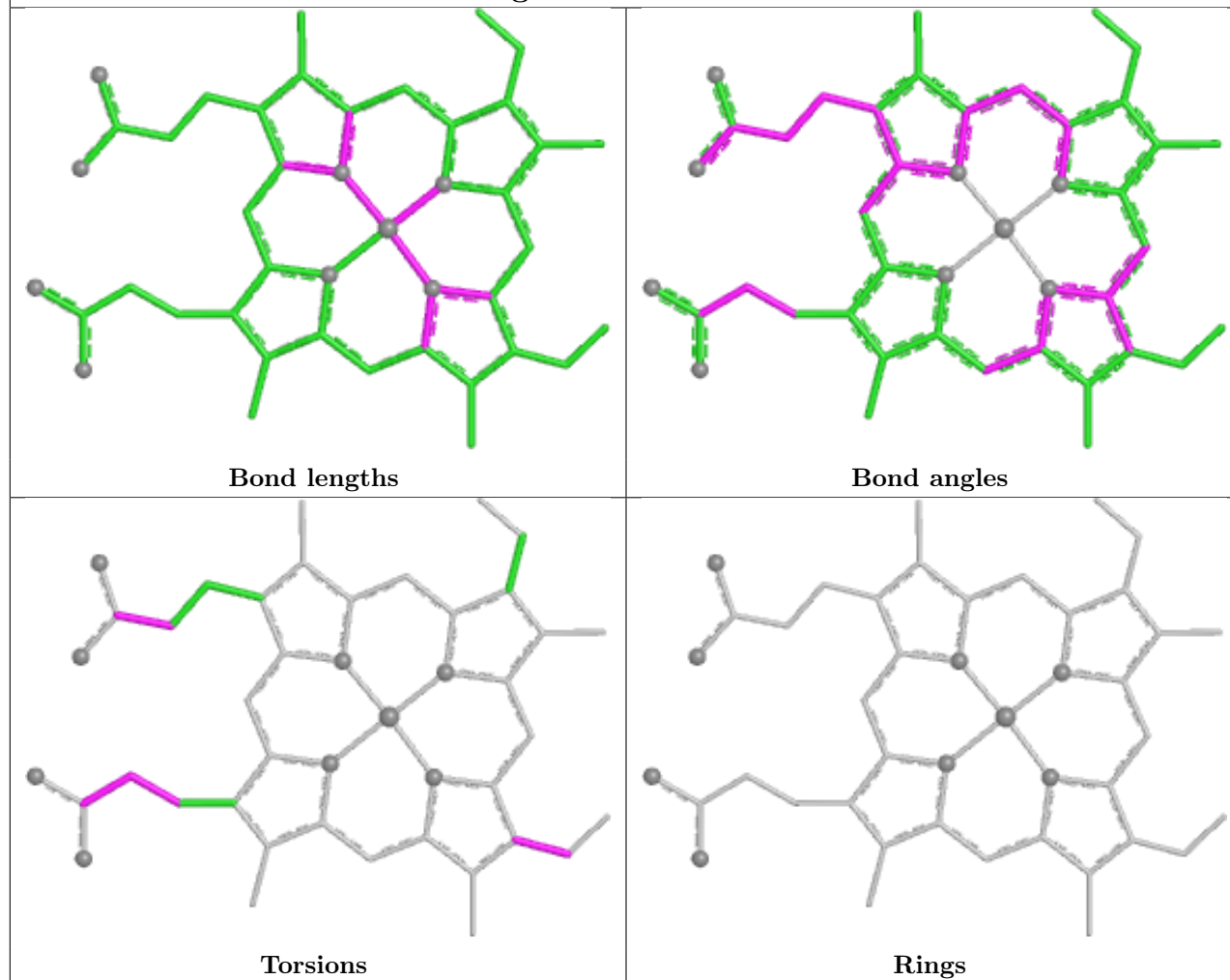


Ligand PEF H 304

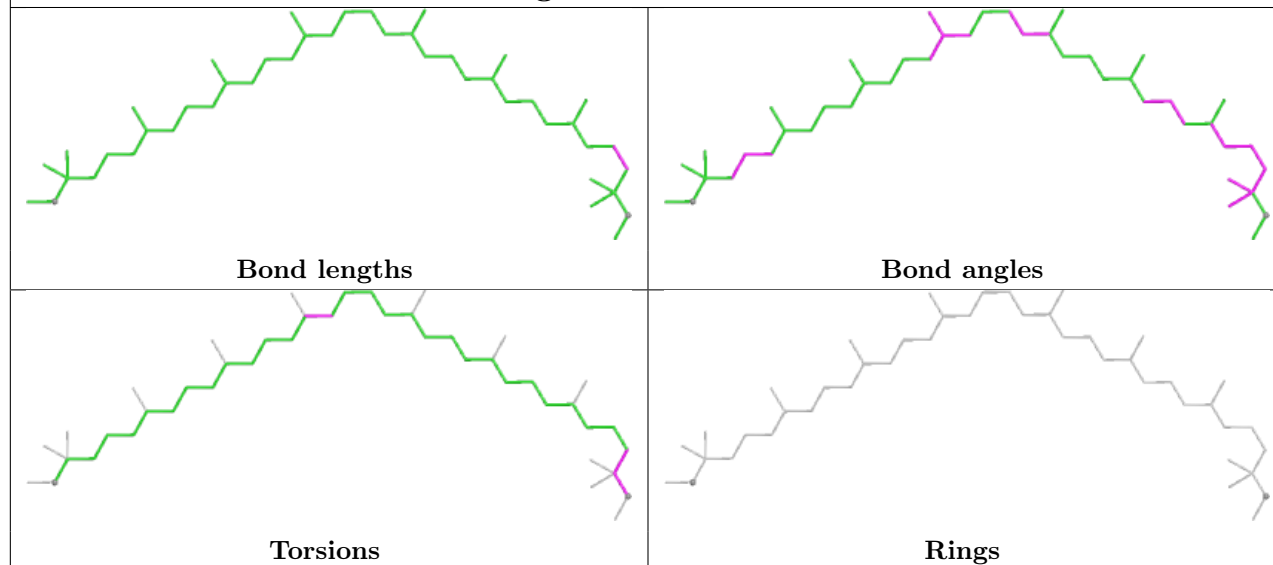


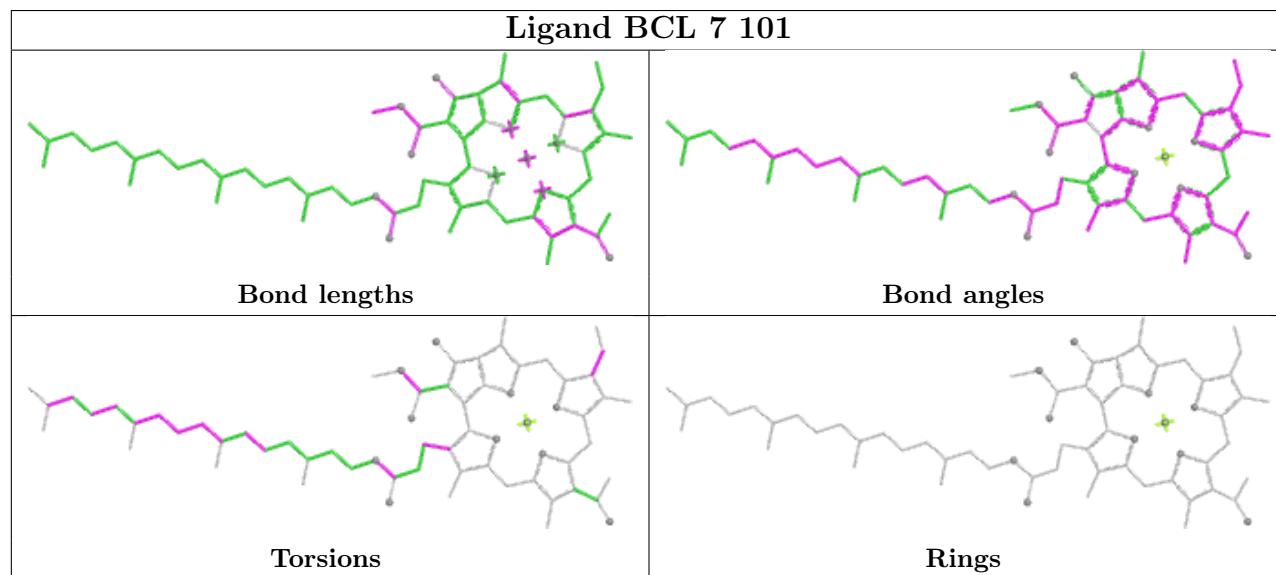
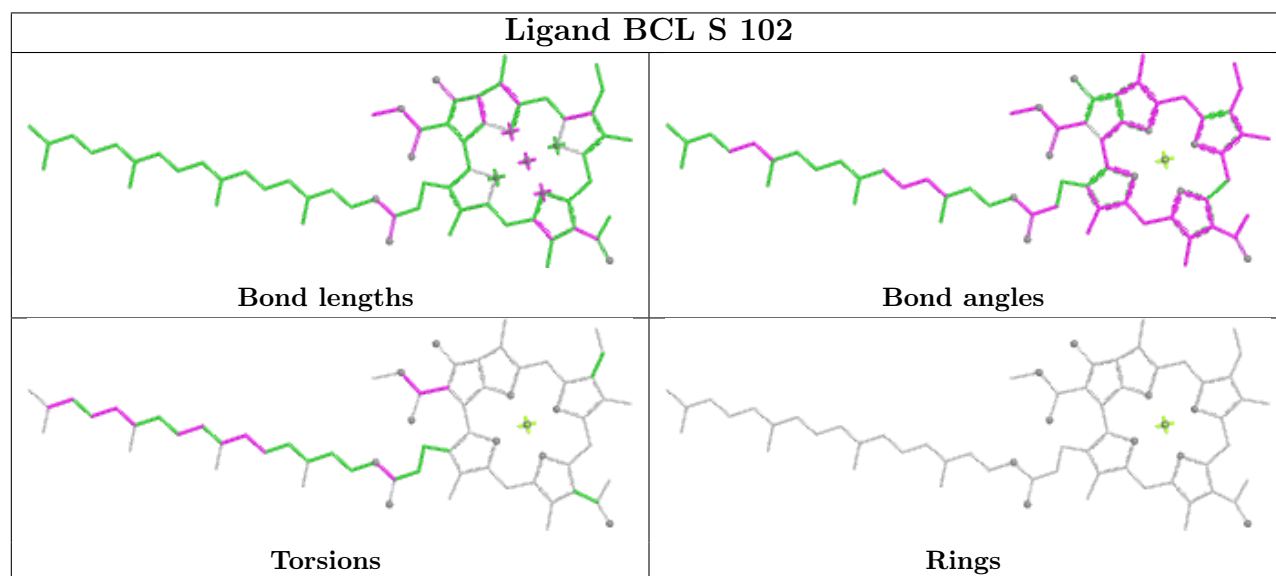
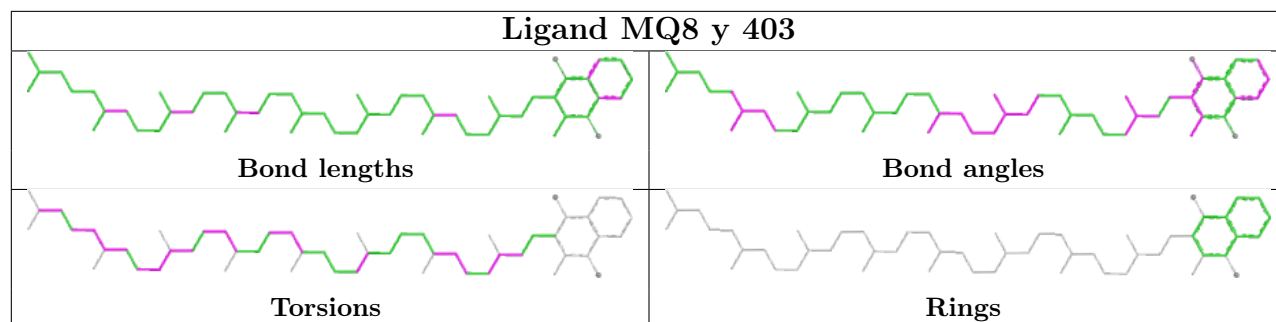


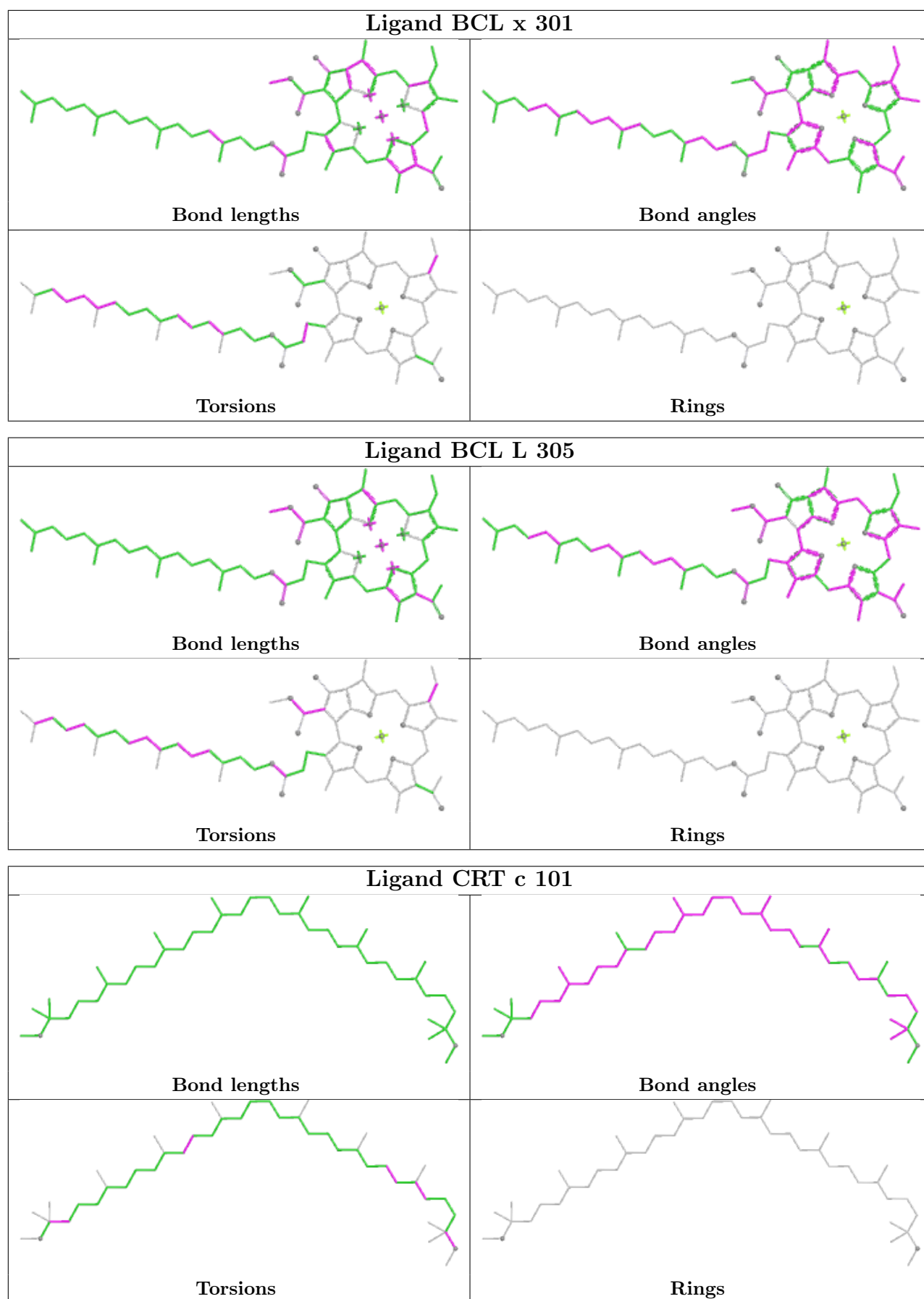
Ligand HEM o 501

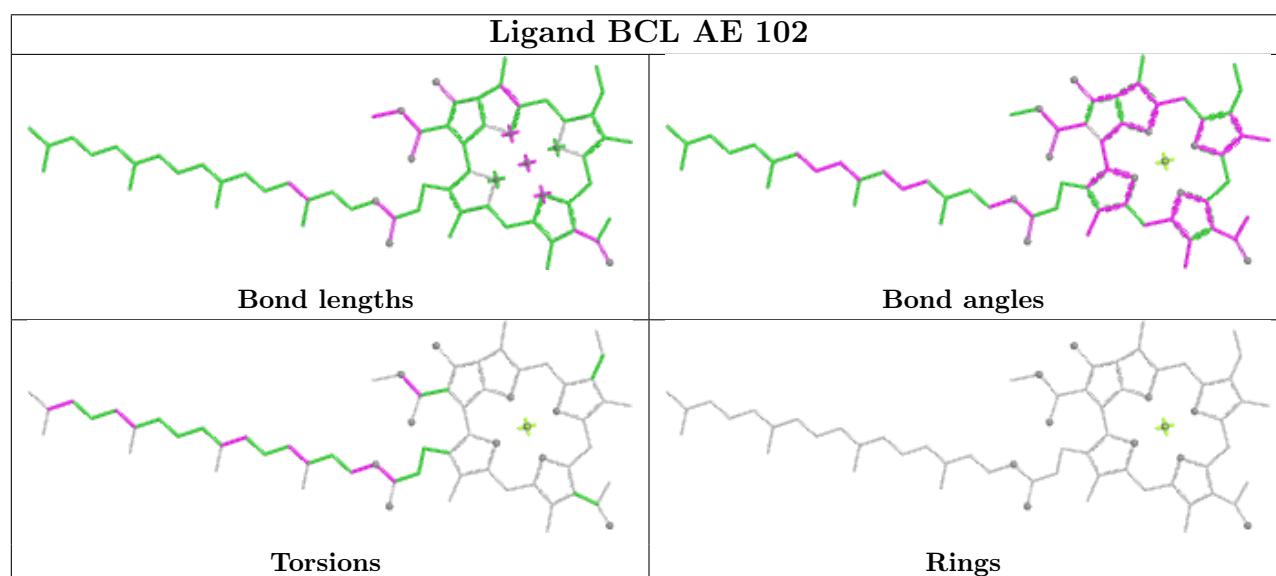
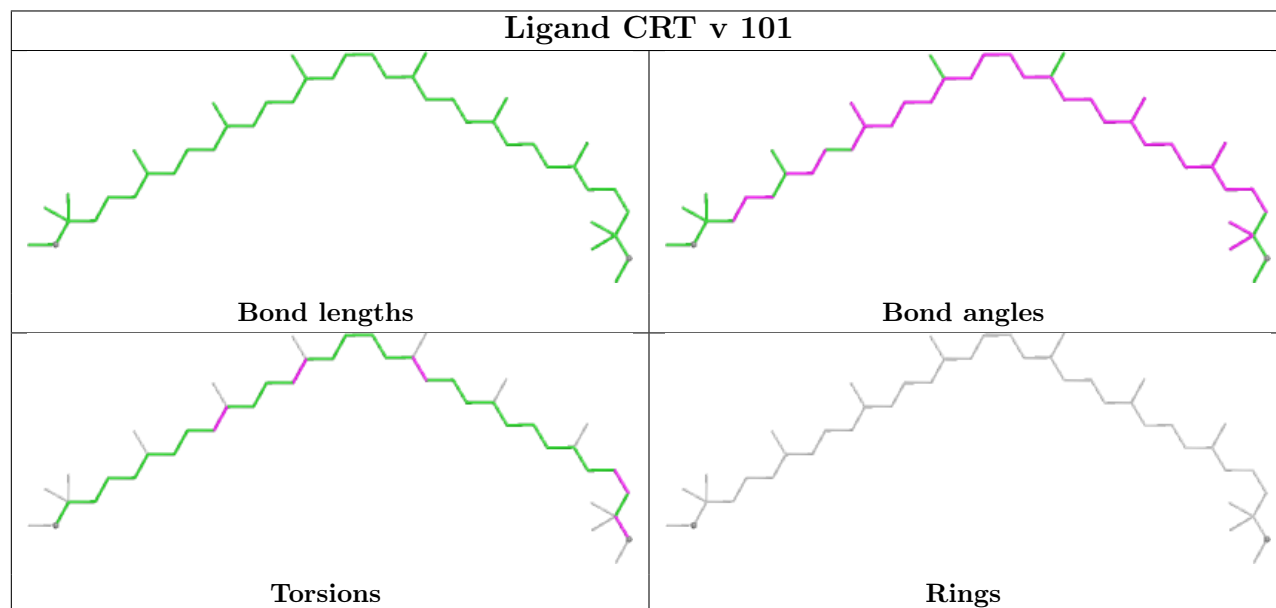
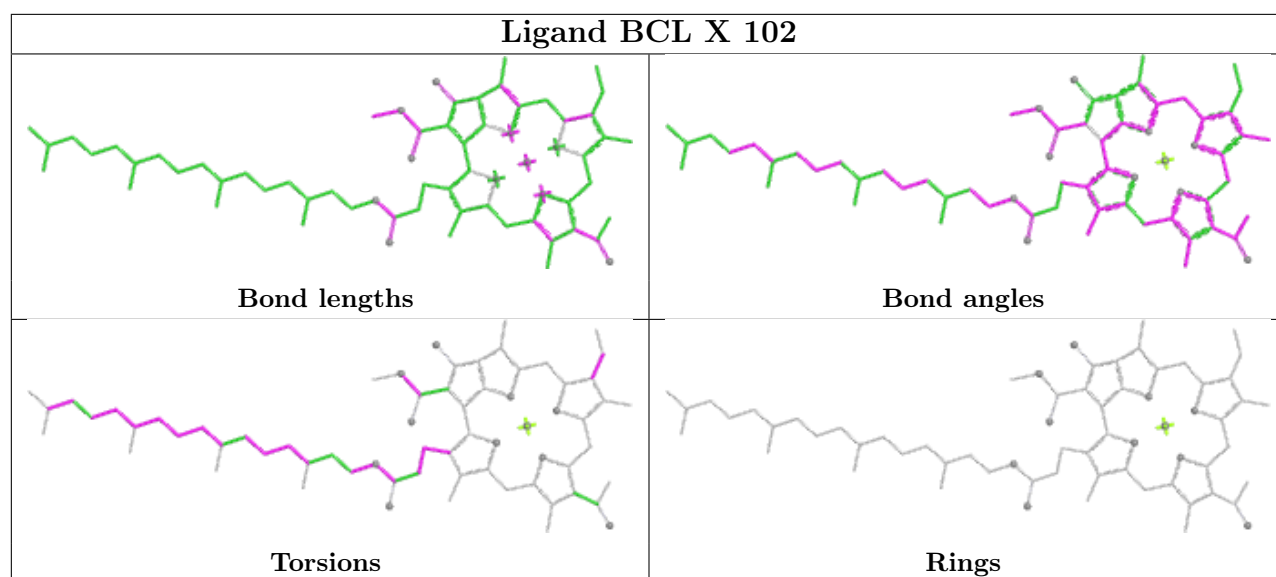


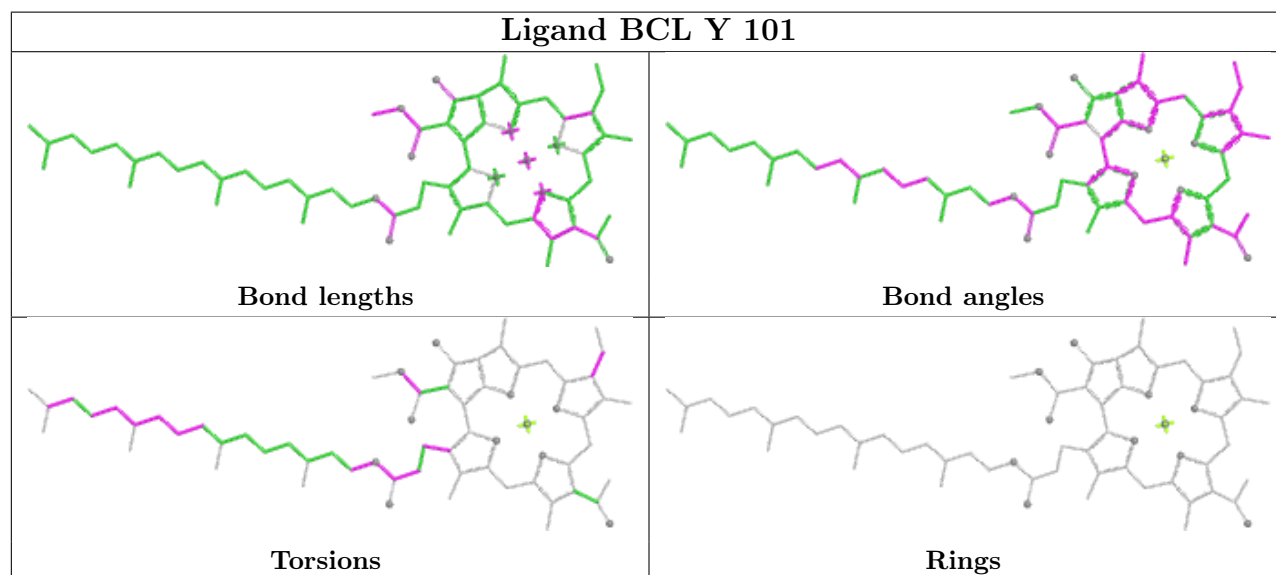
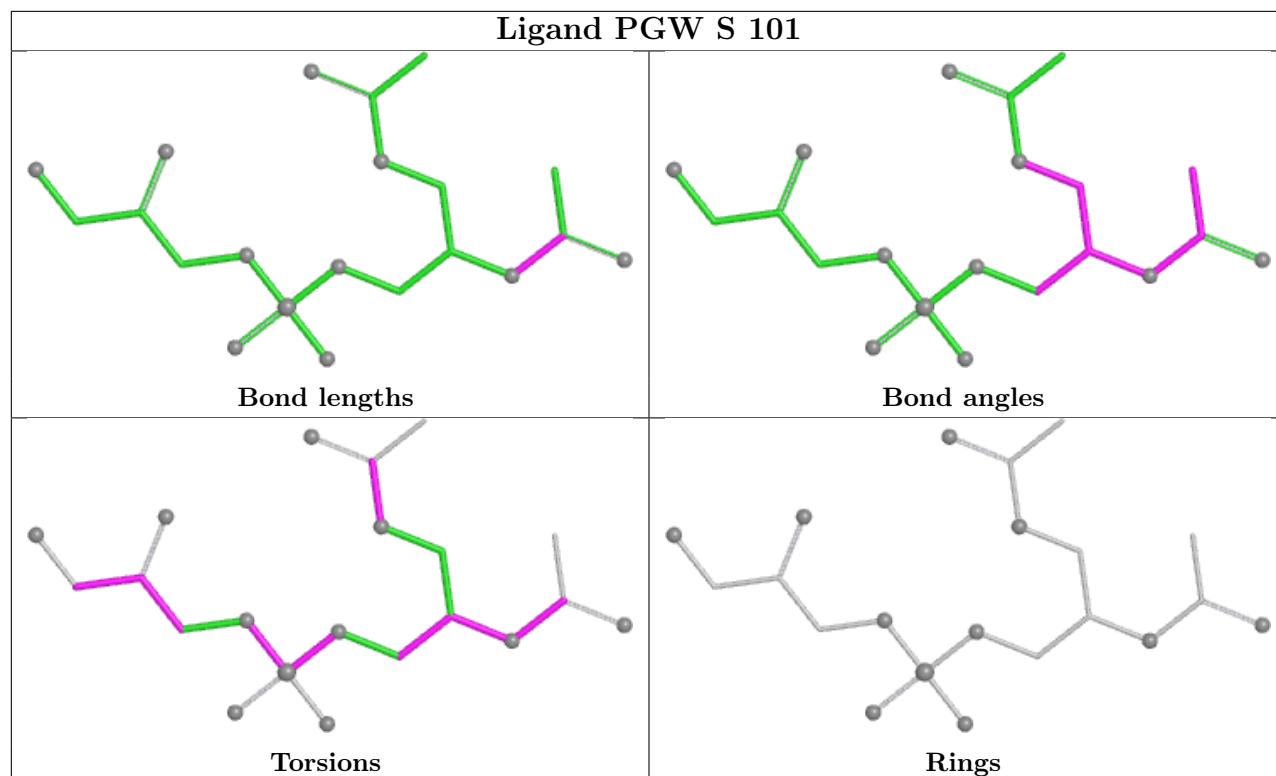
Ligand CRT 8 101

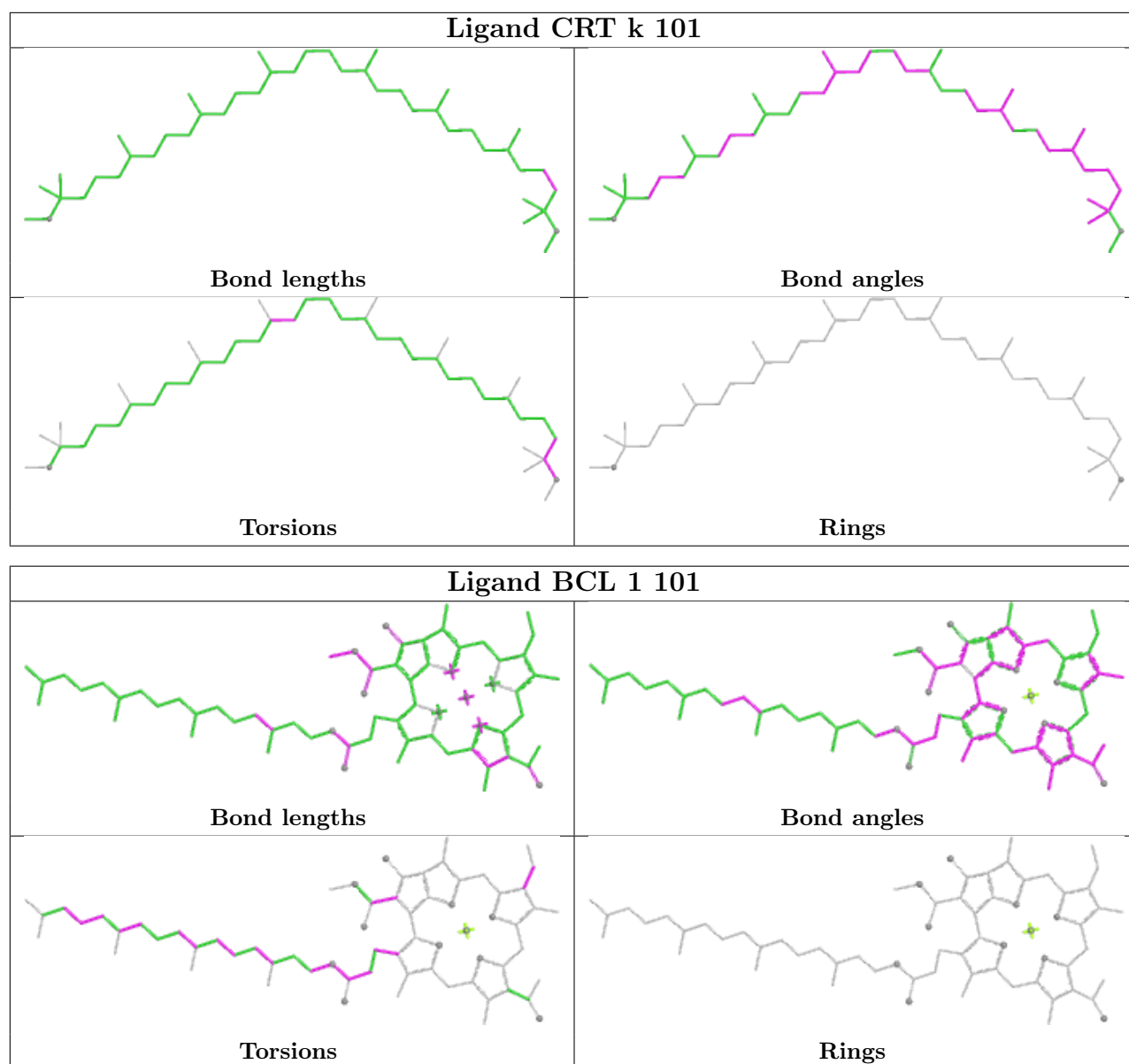




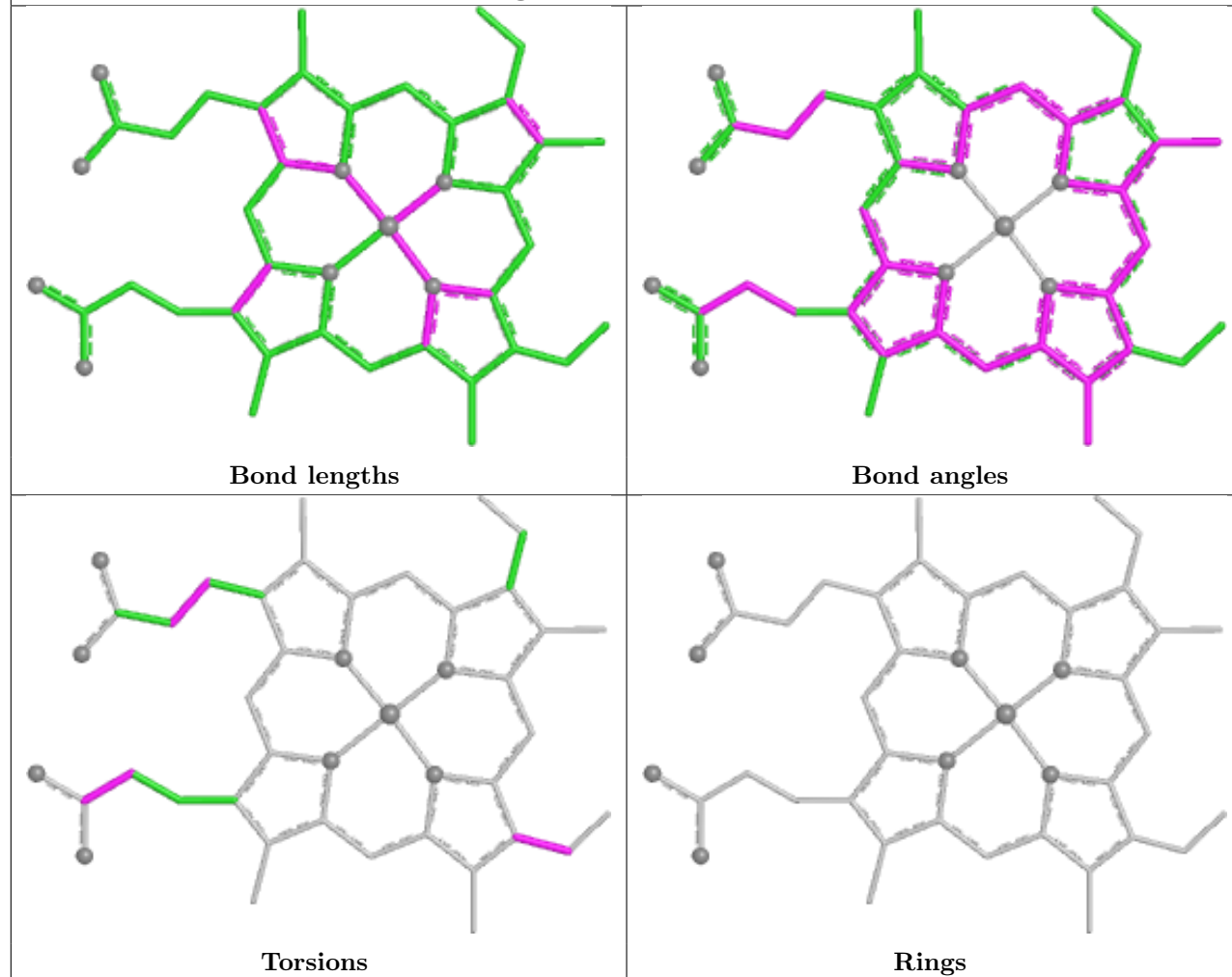




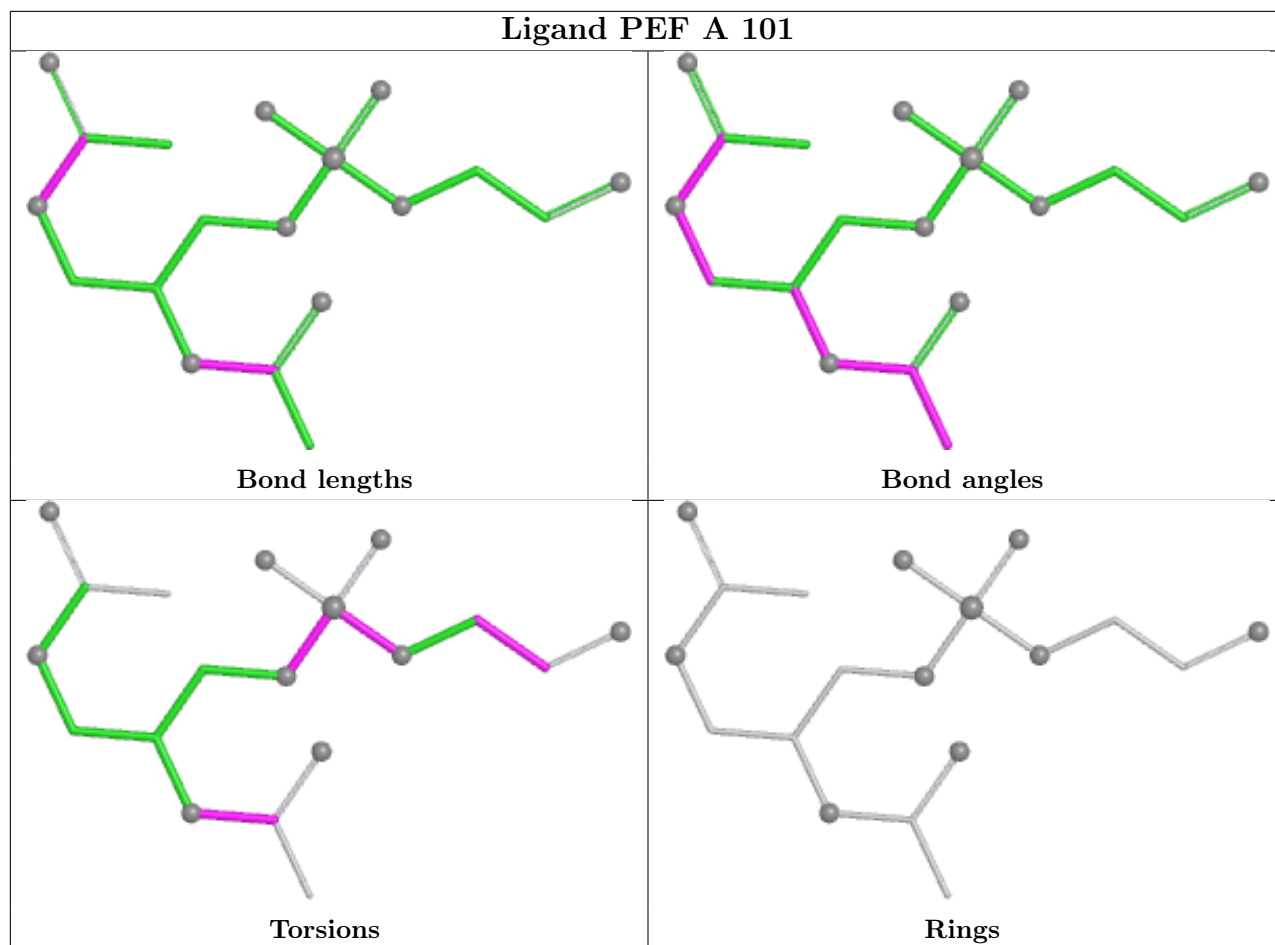




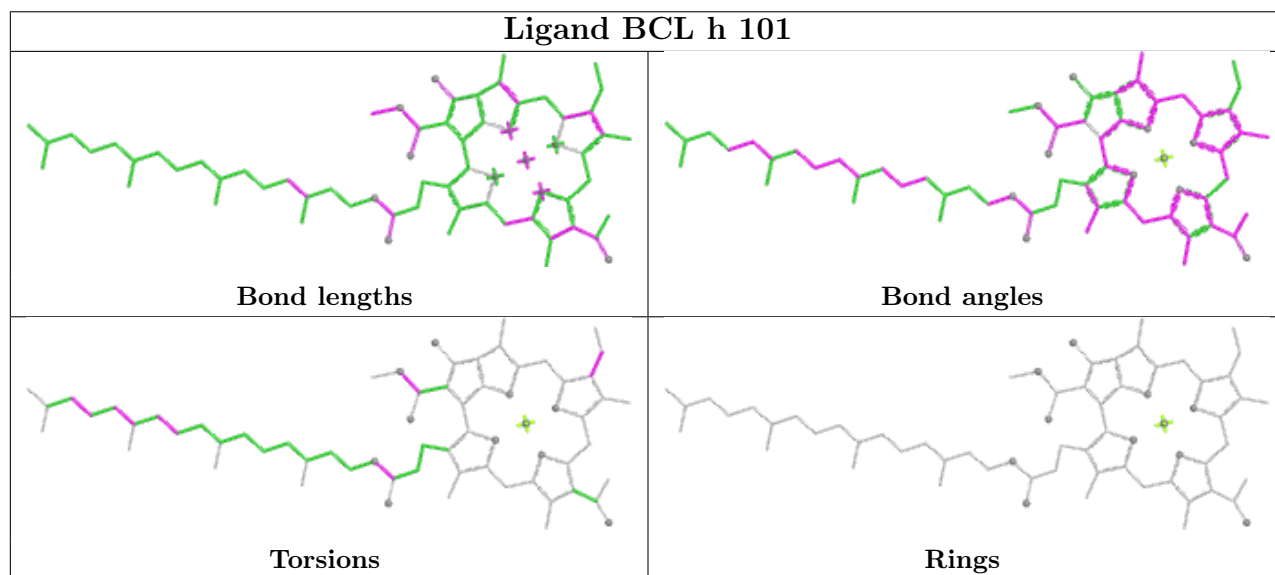
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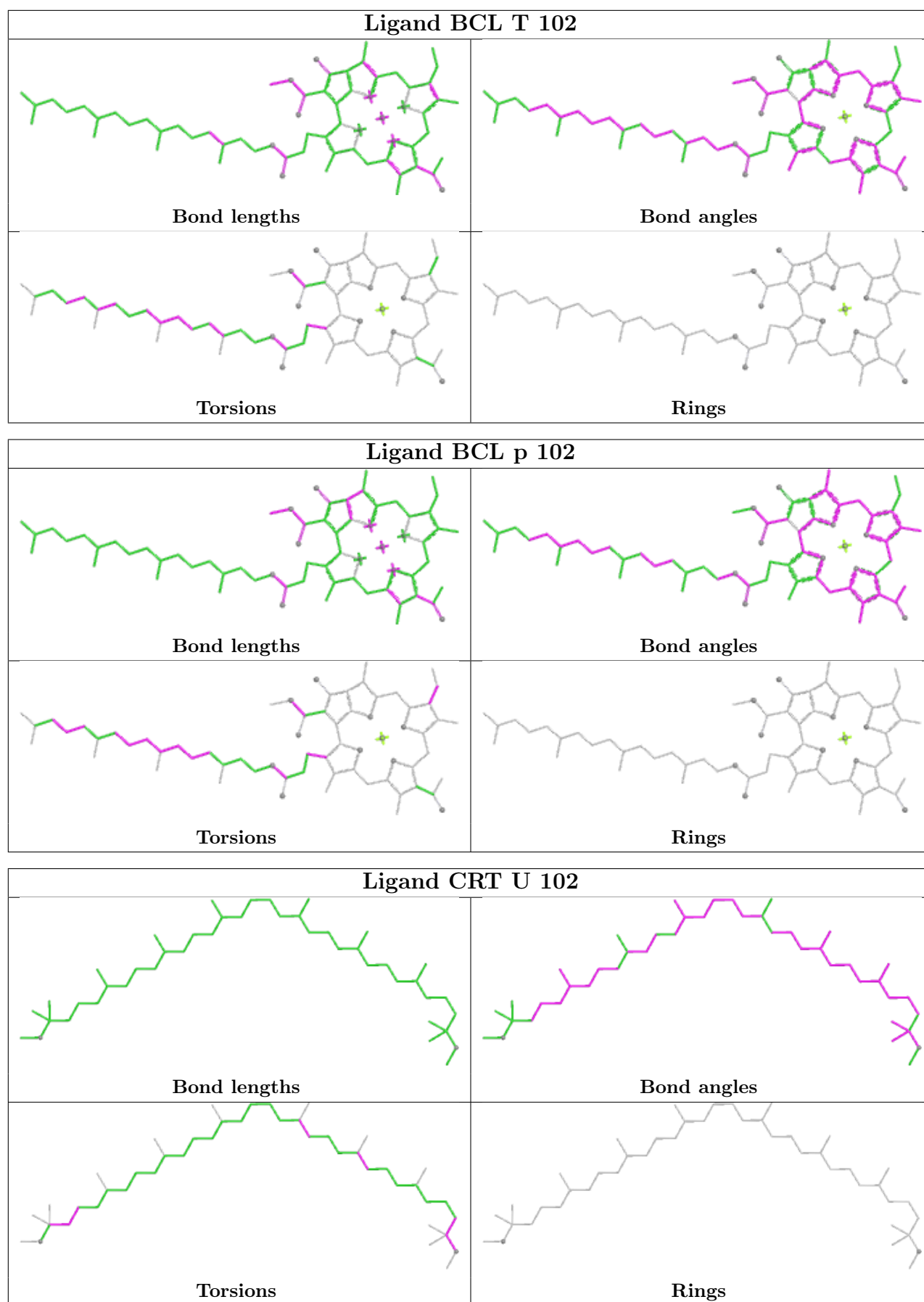


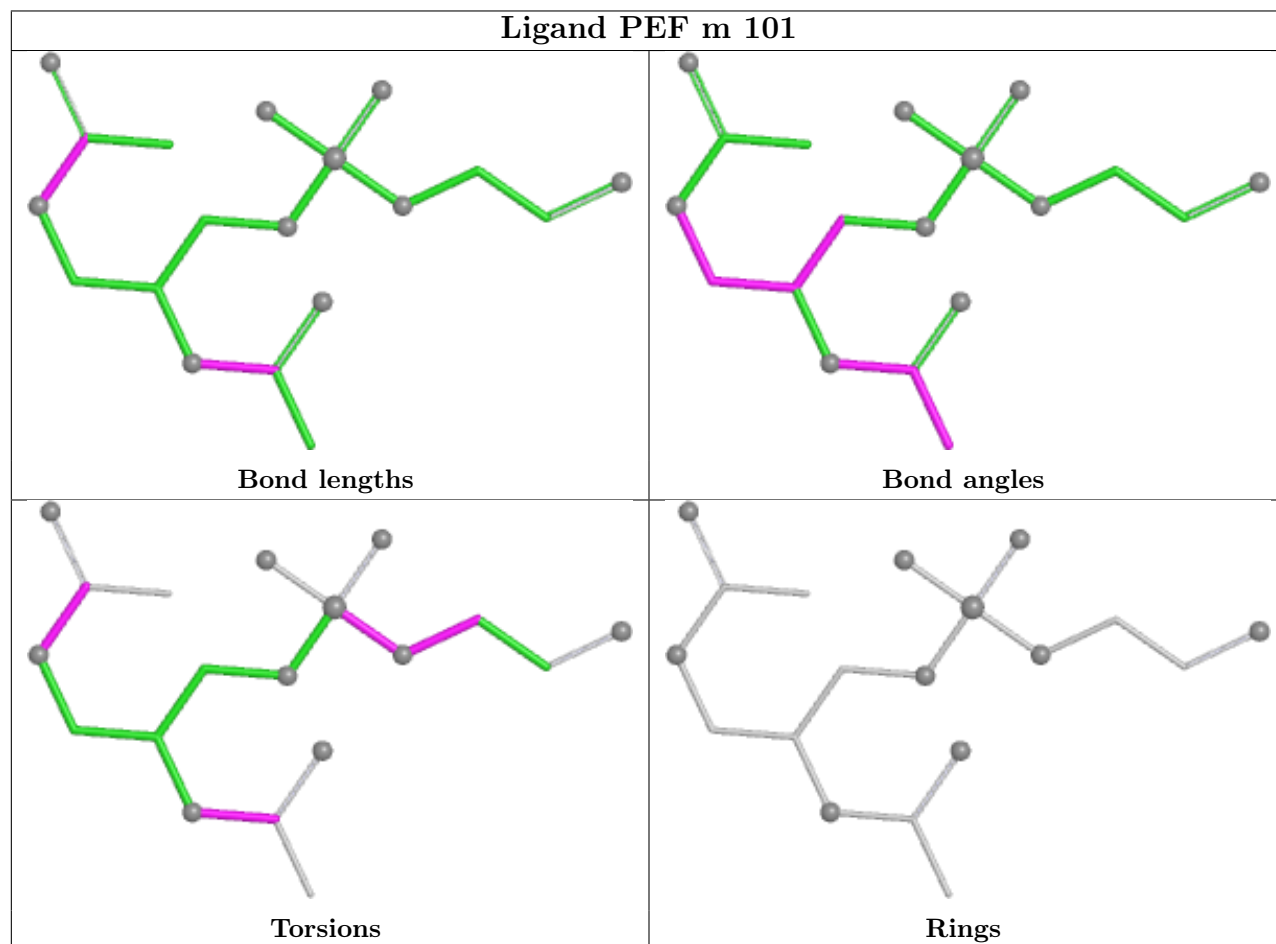
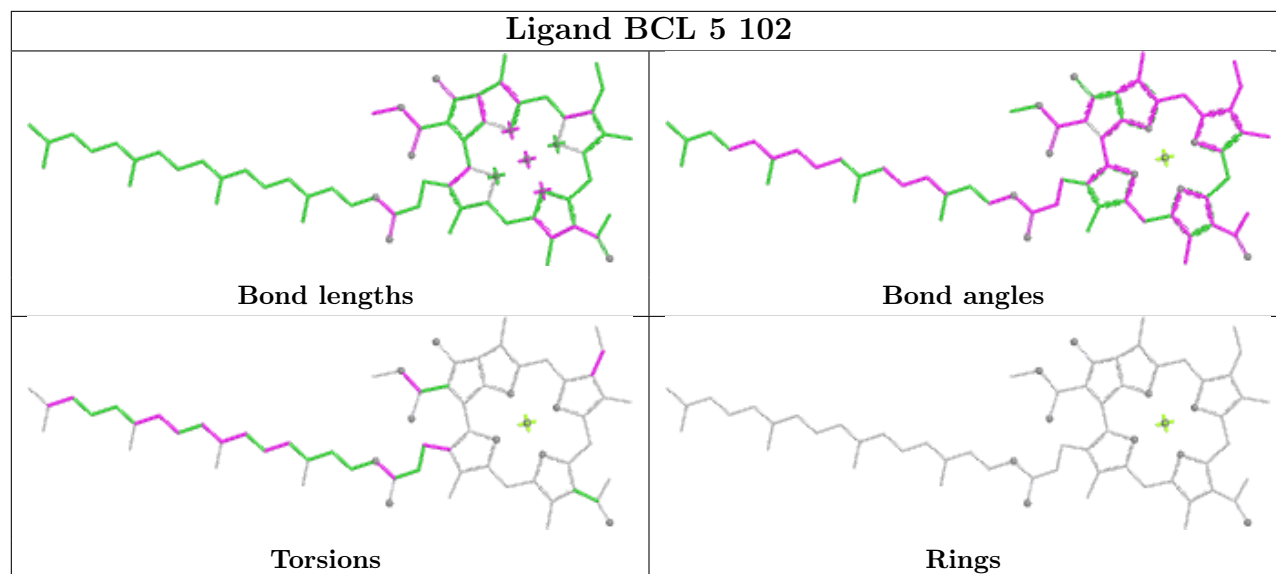
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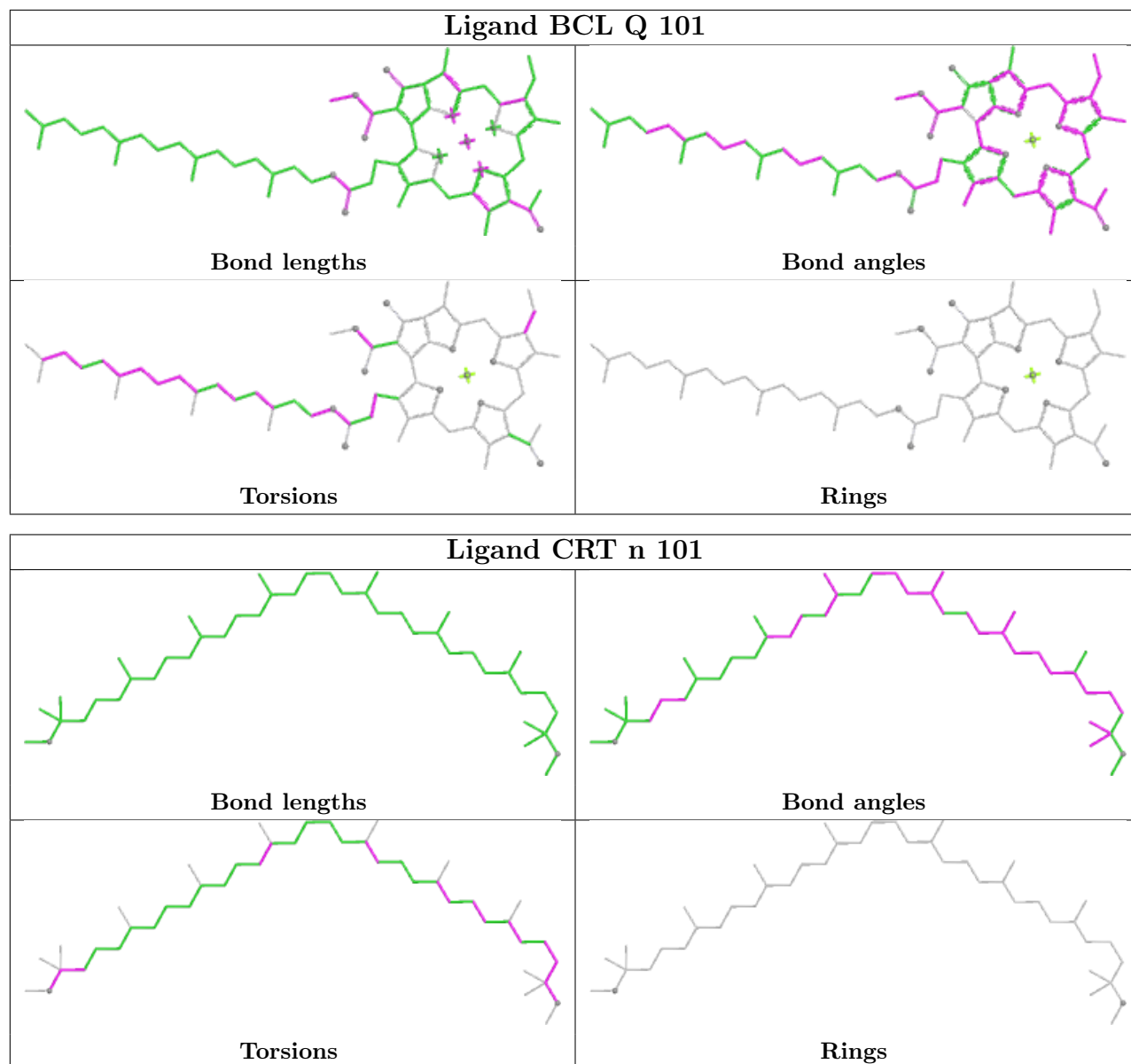


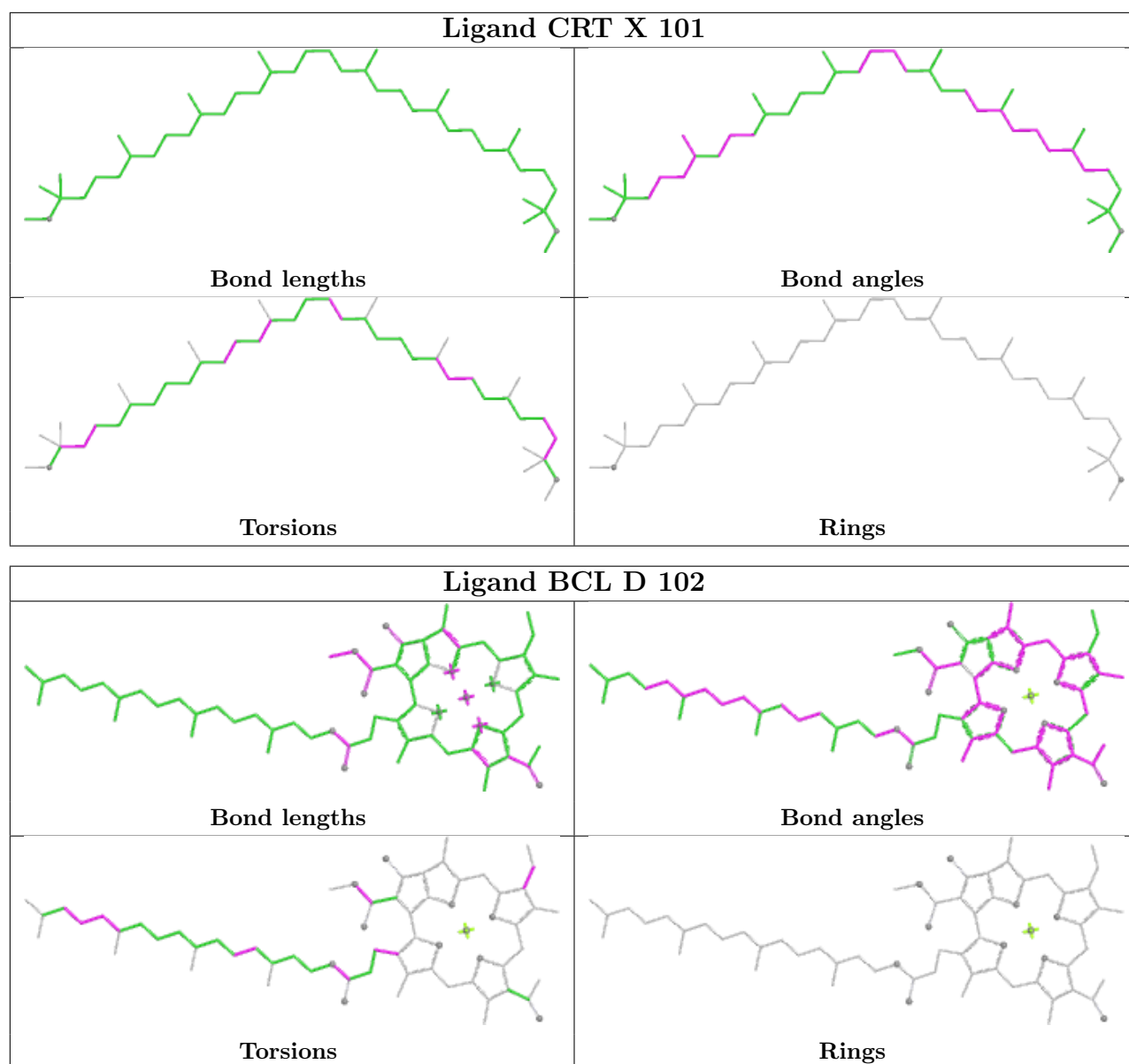
Ligand BCL h 101

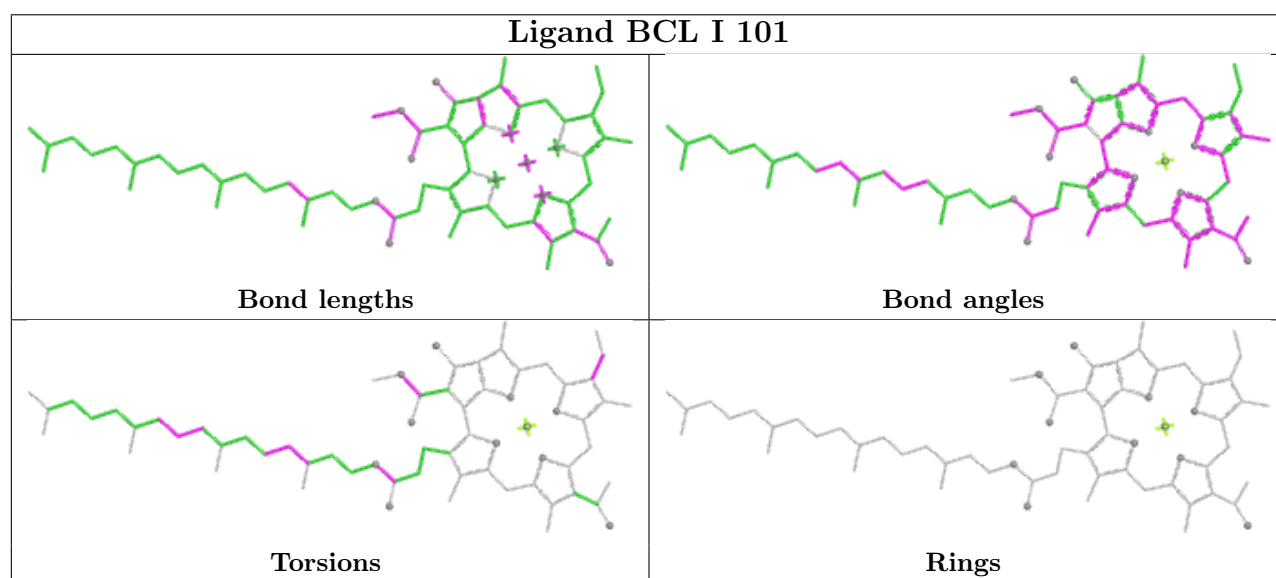
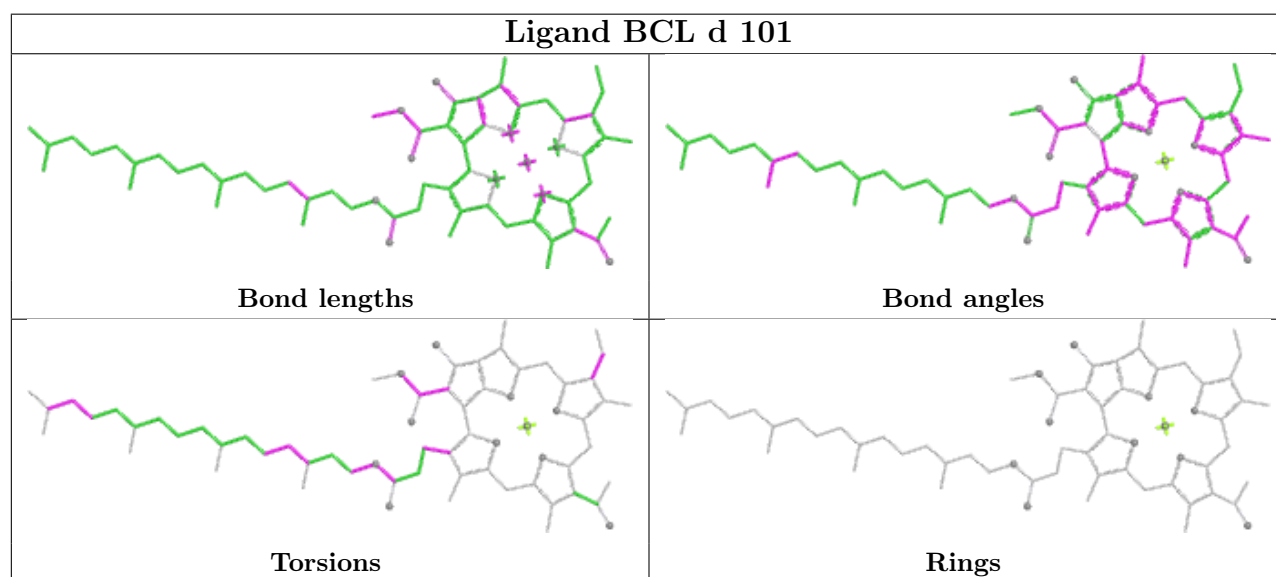
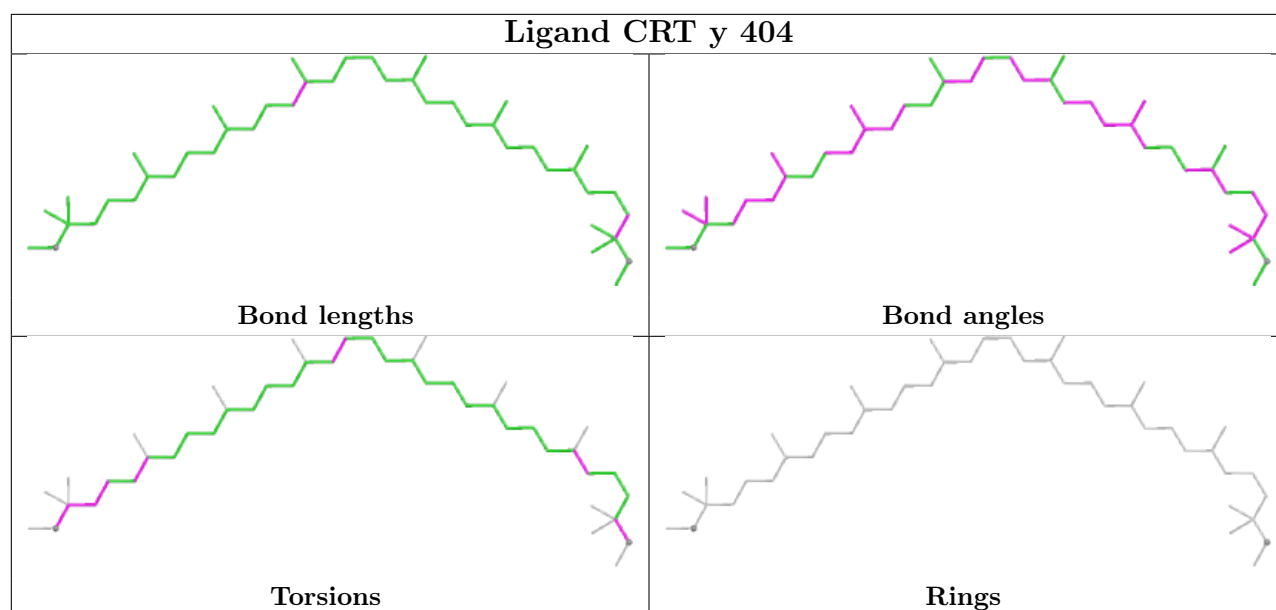


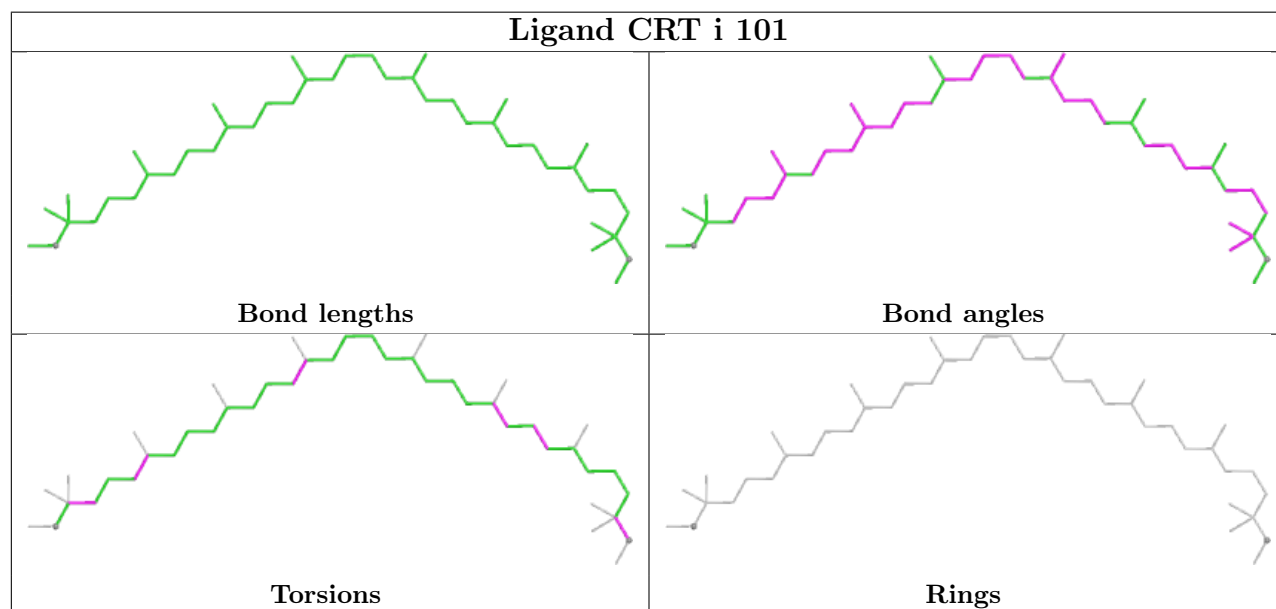
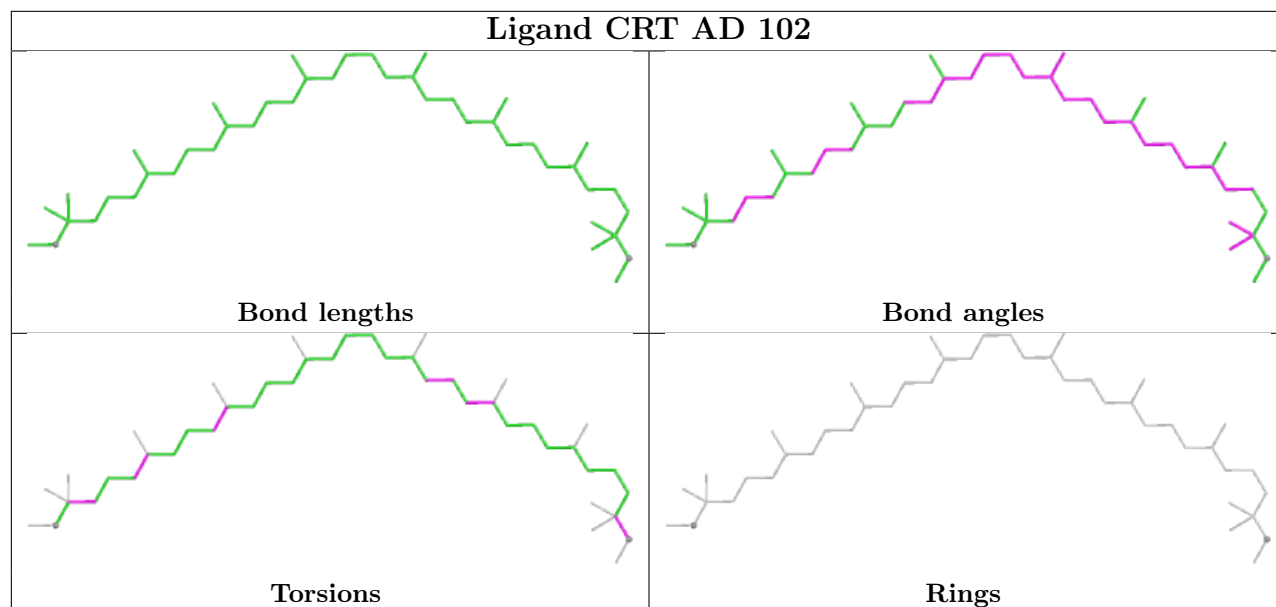


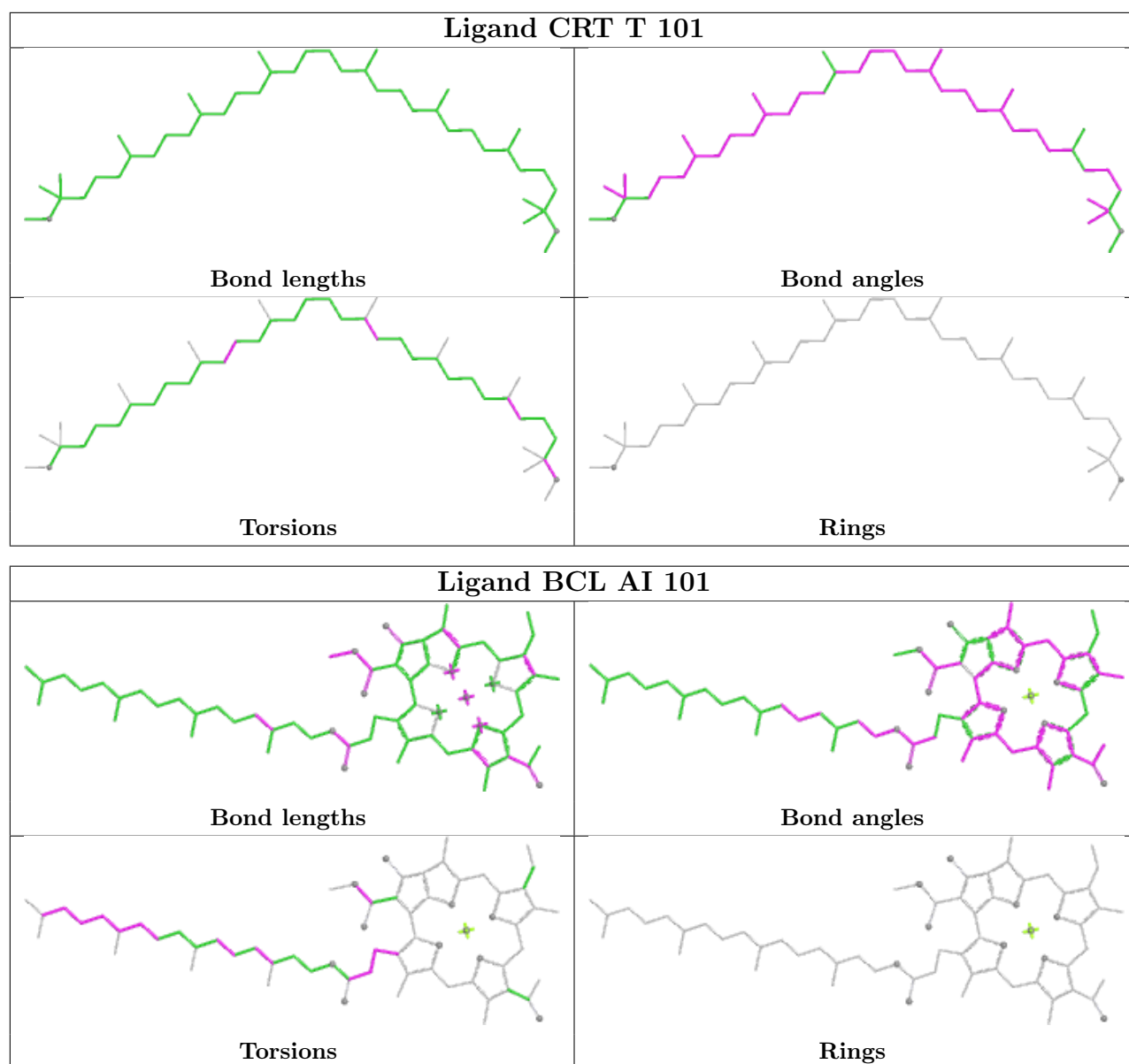


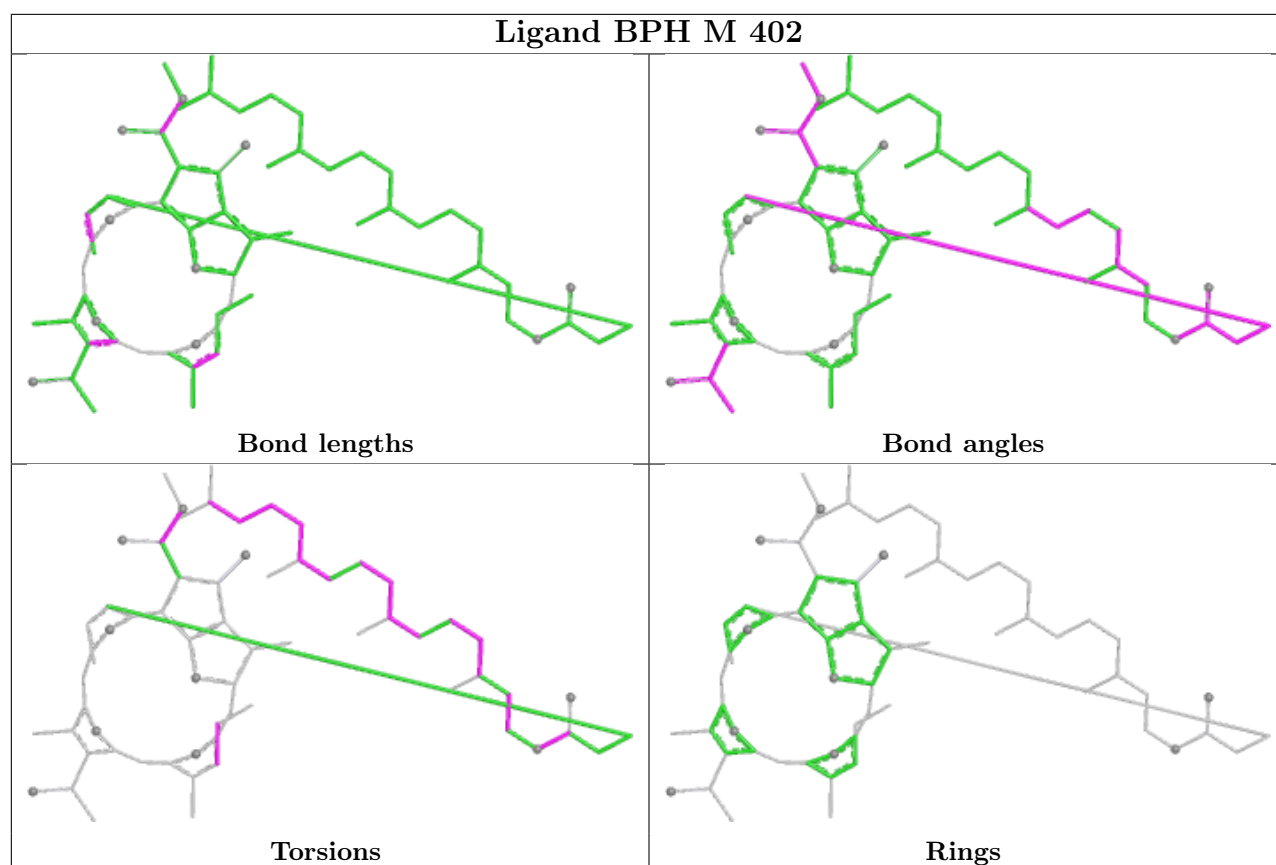


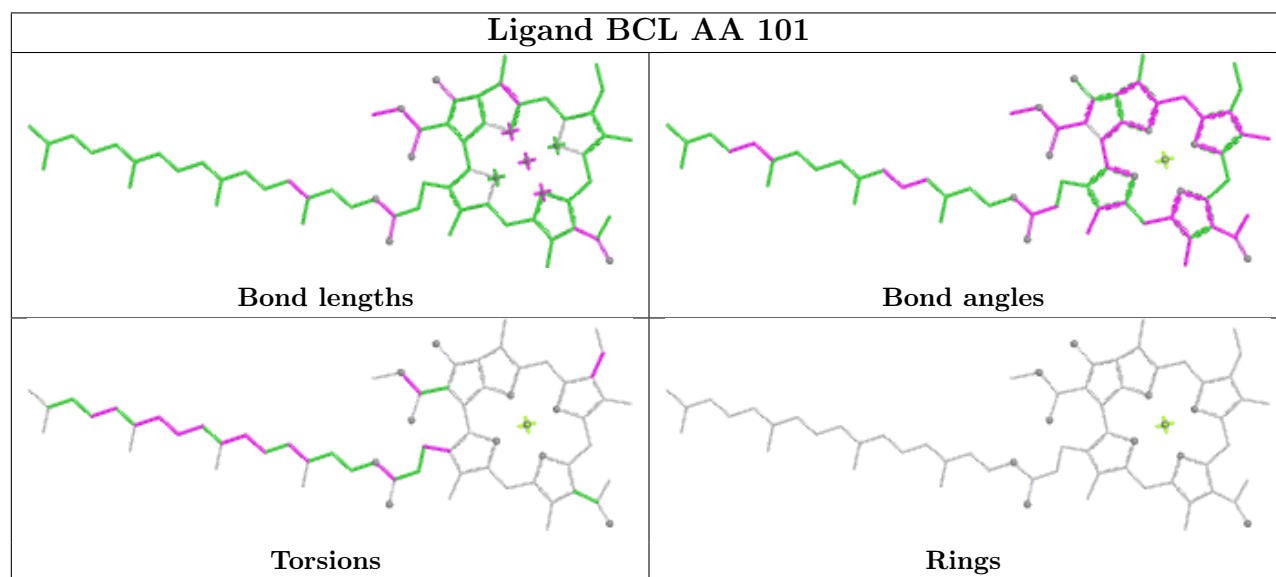
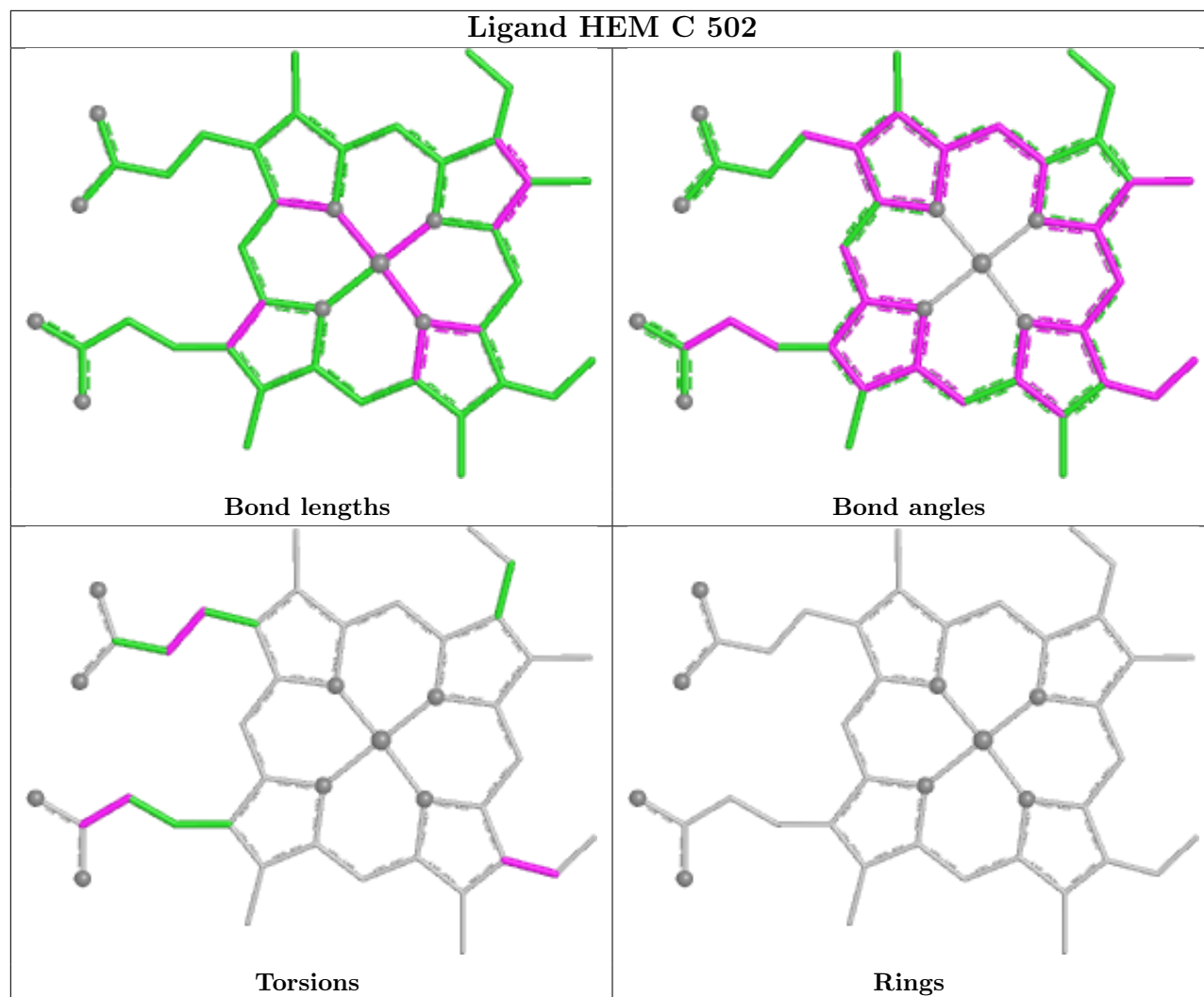


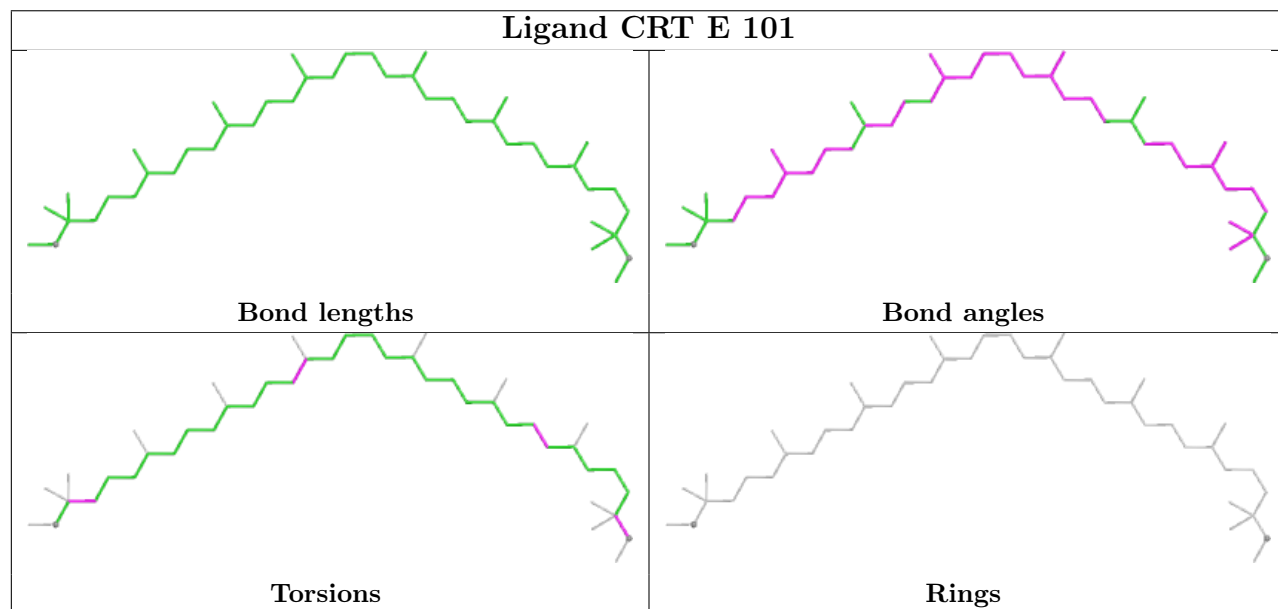
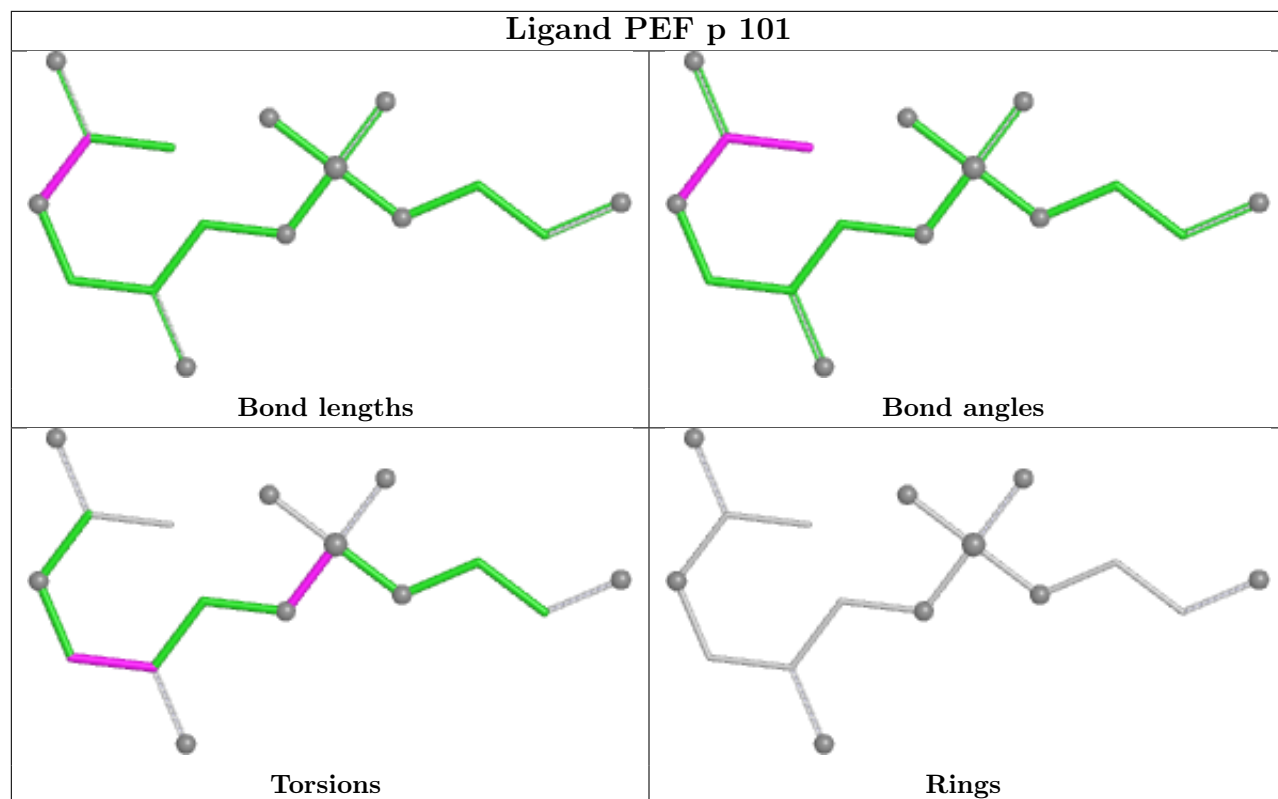


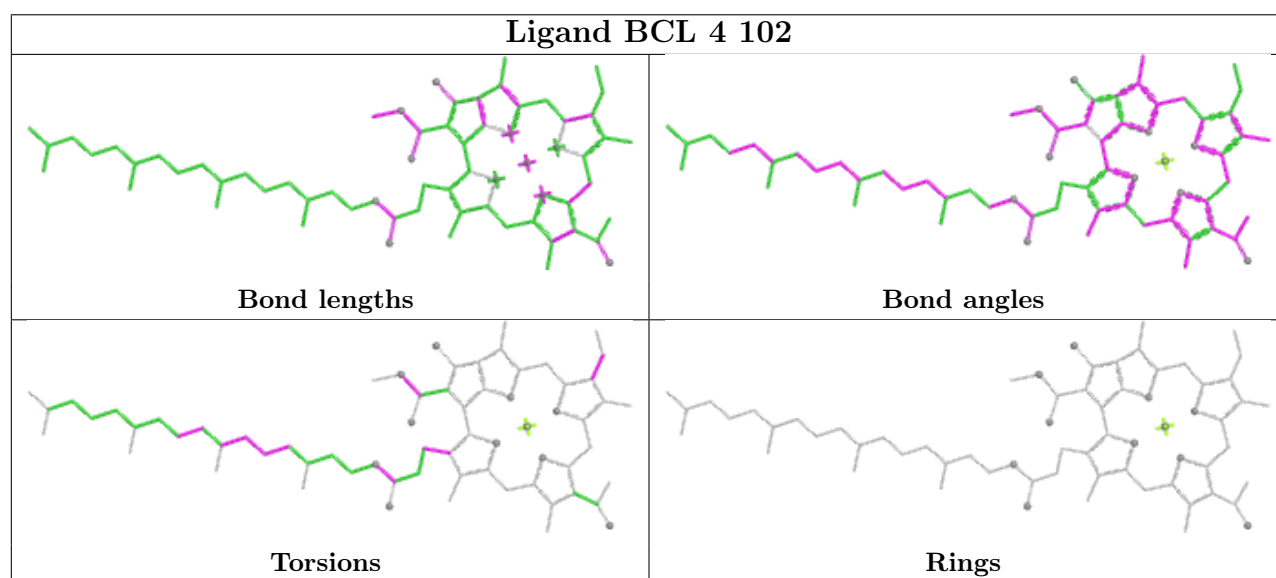
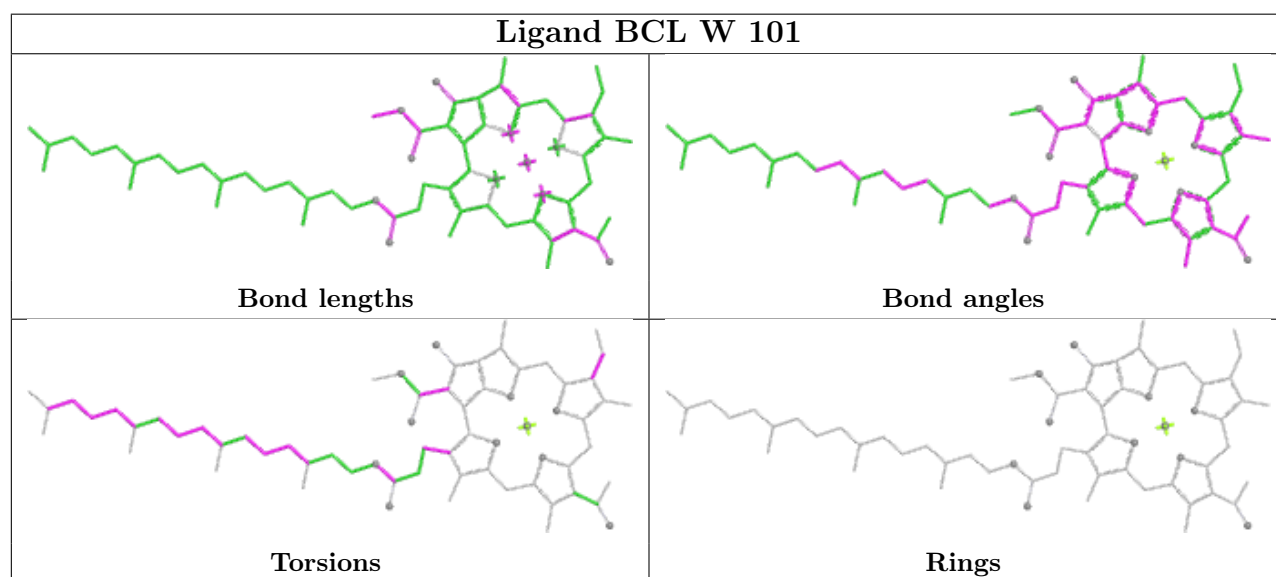
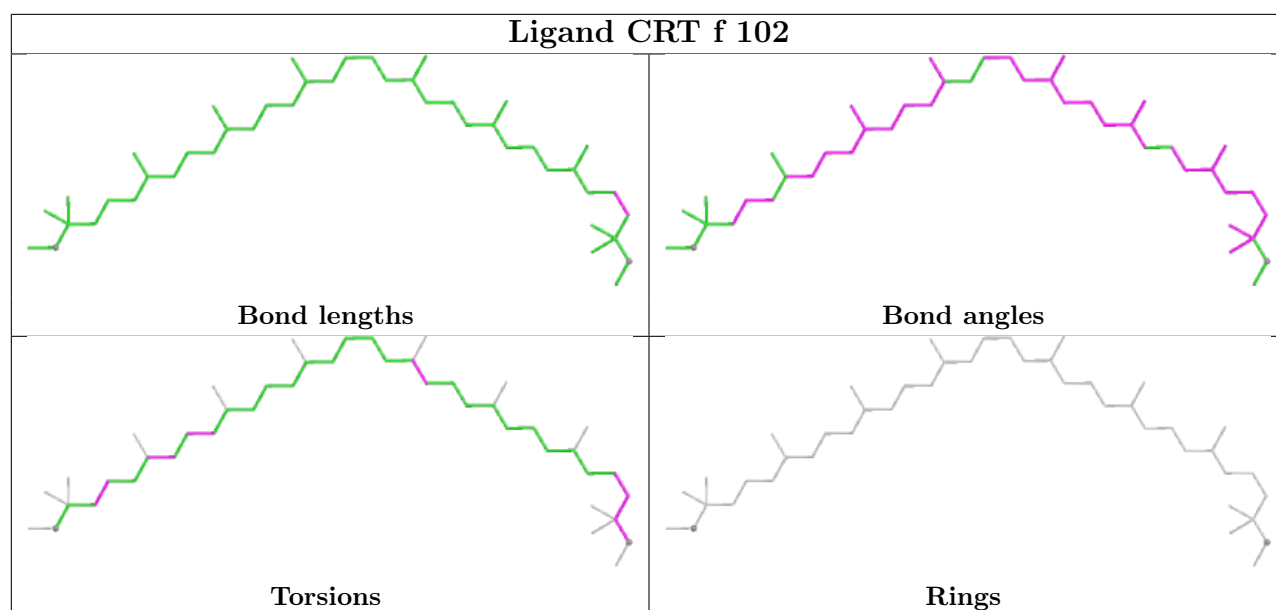


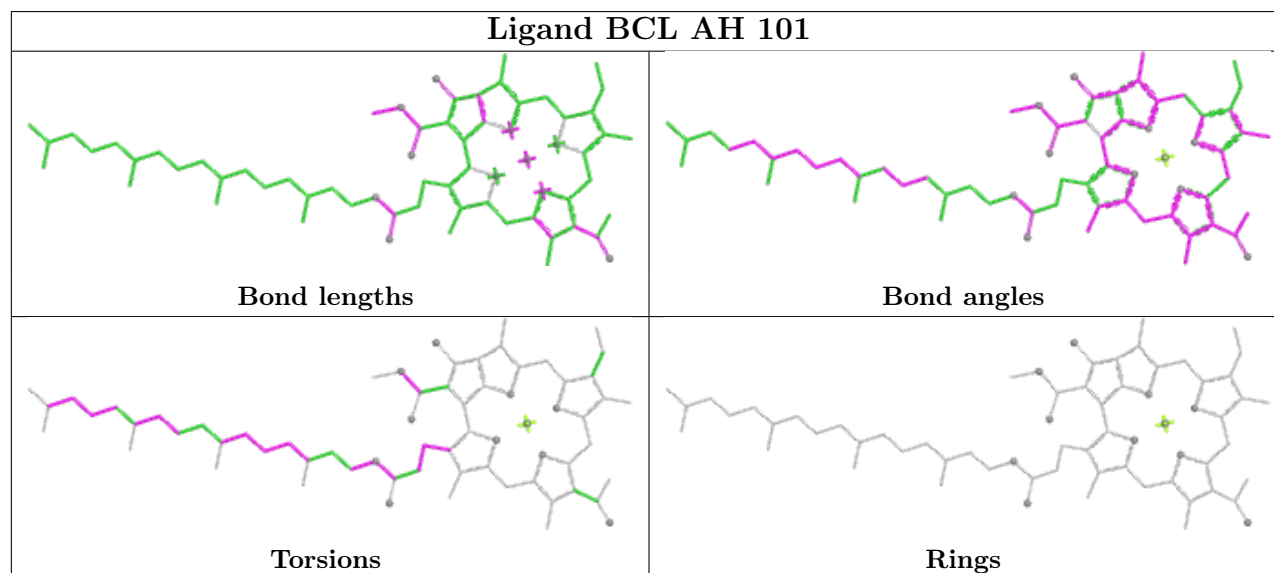
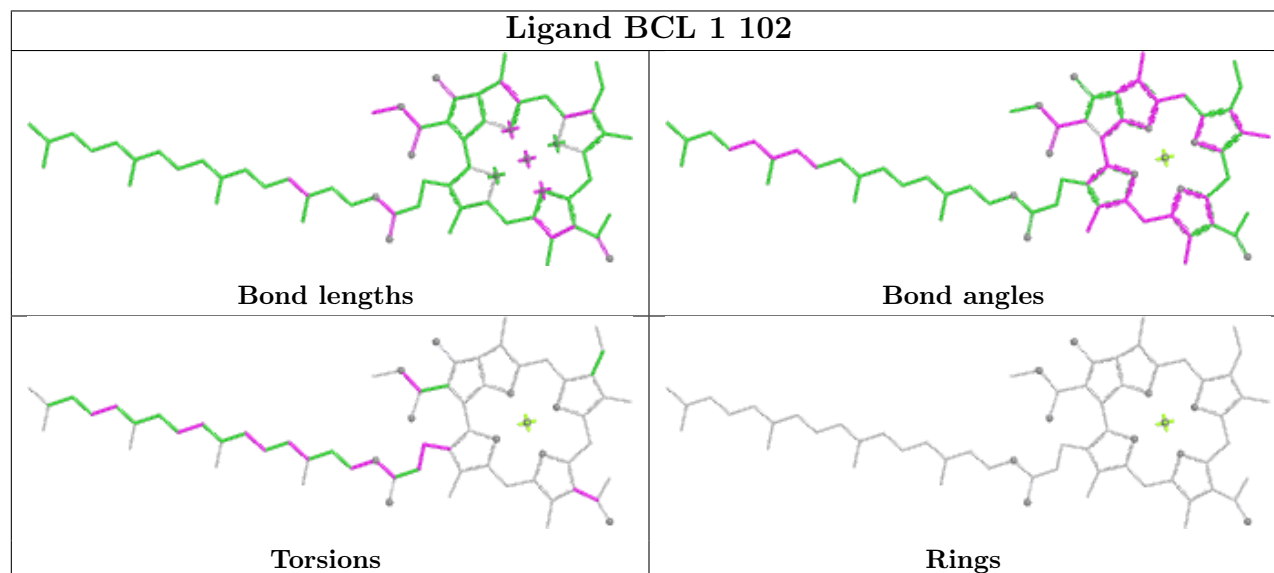
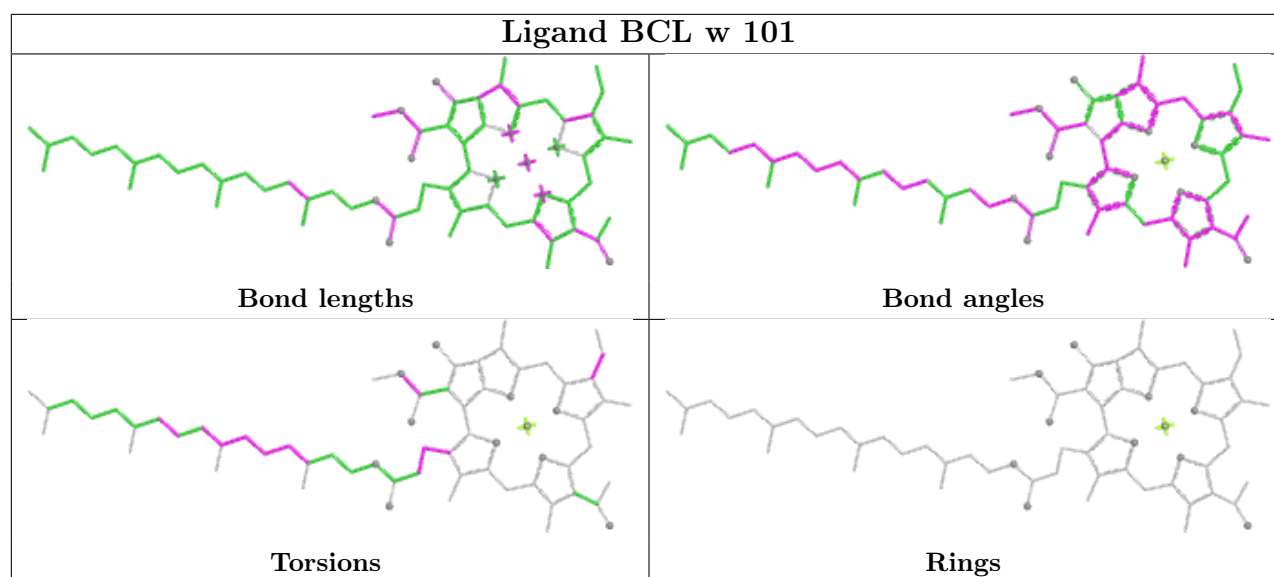




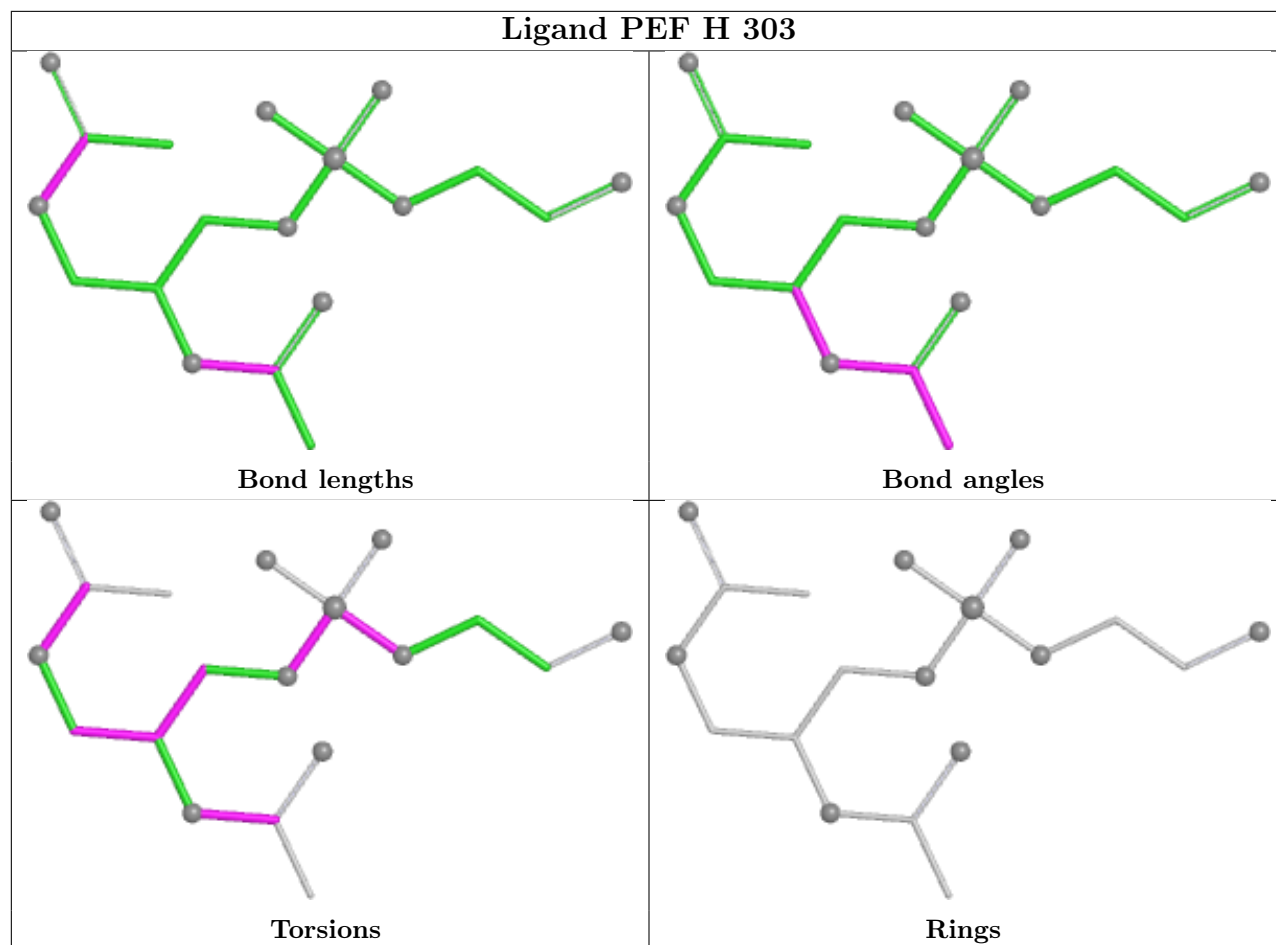




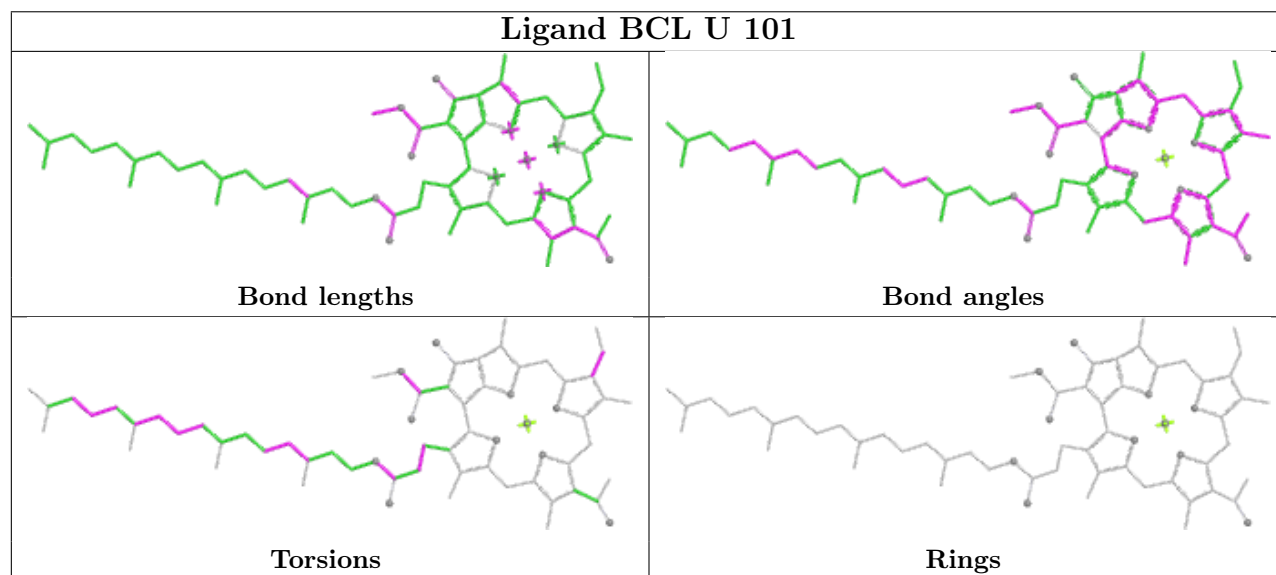


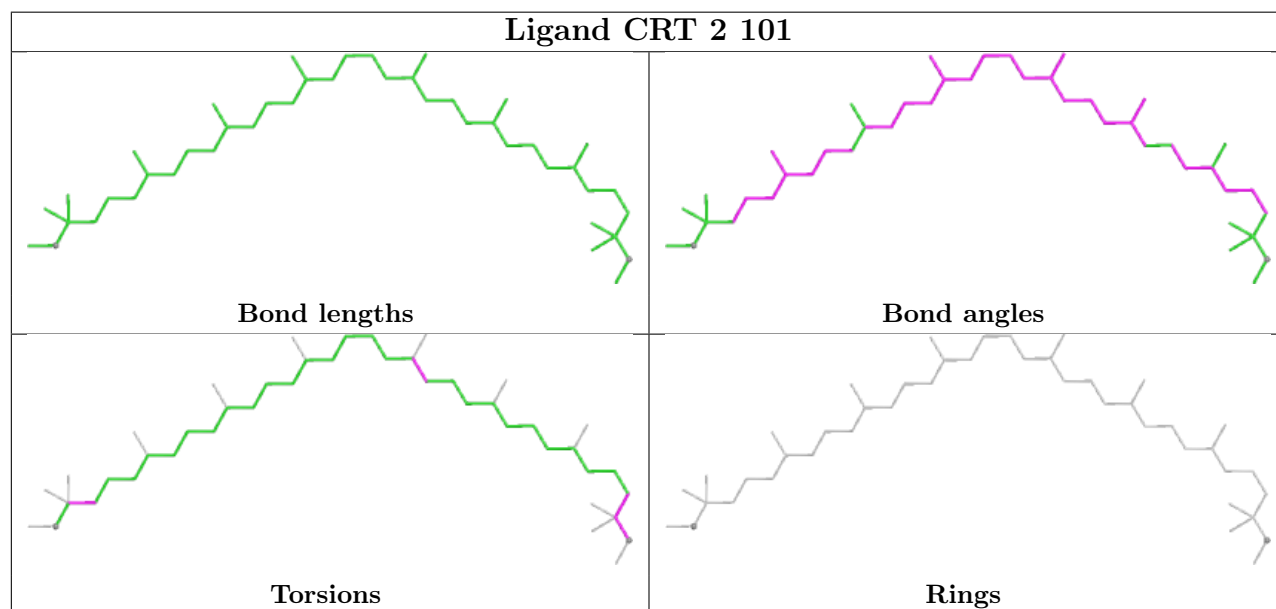
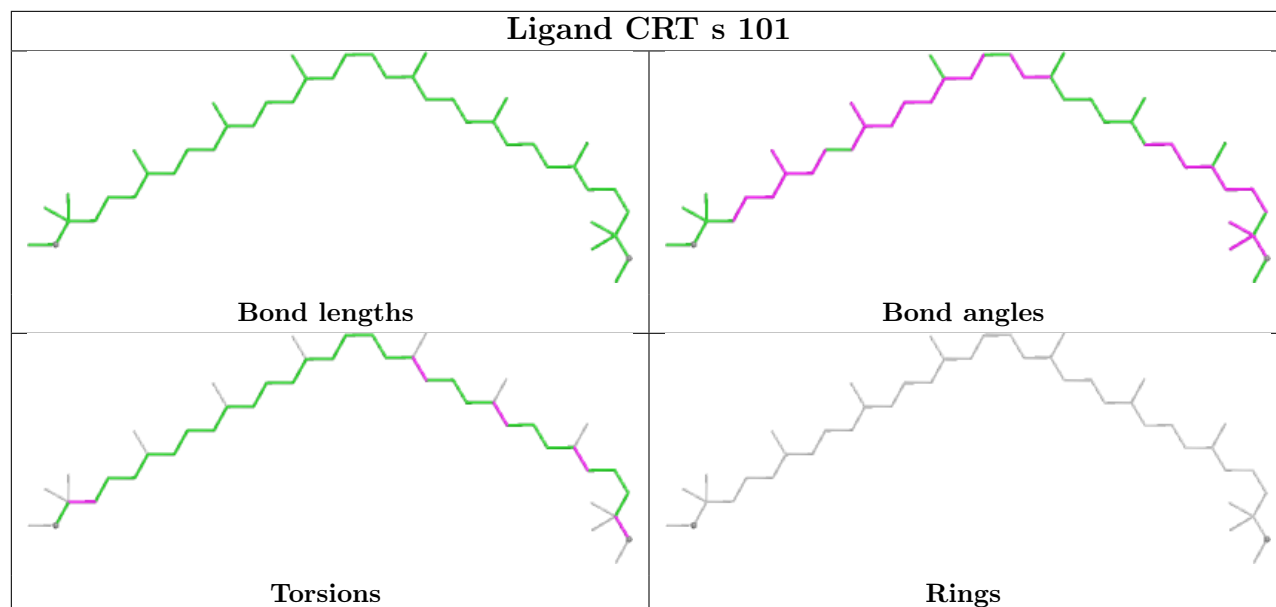


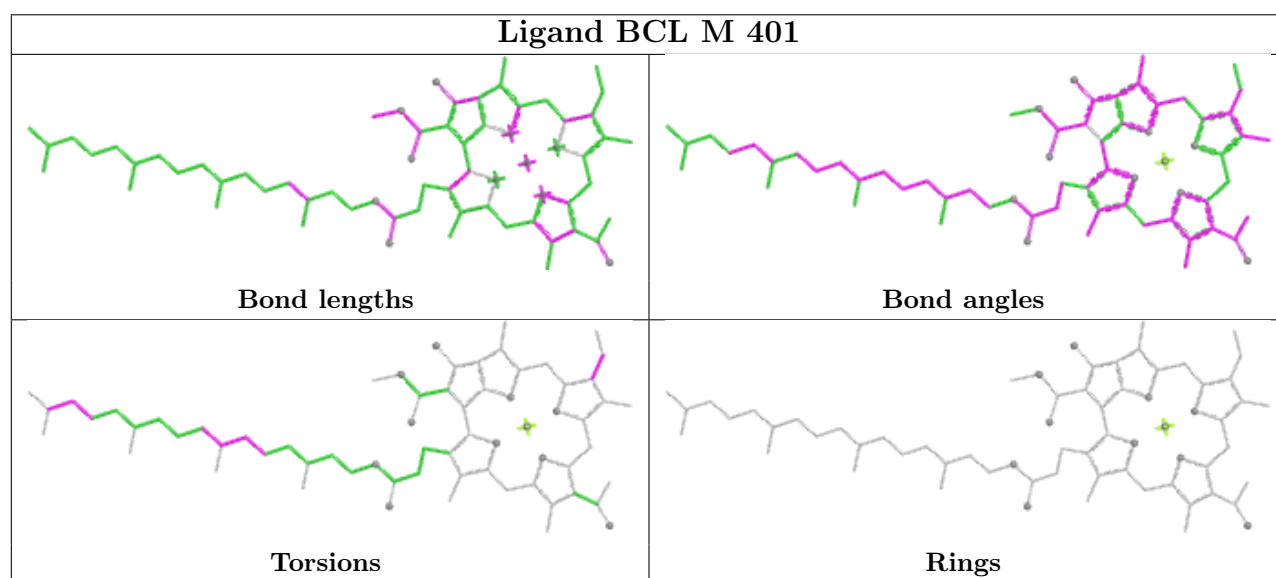
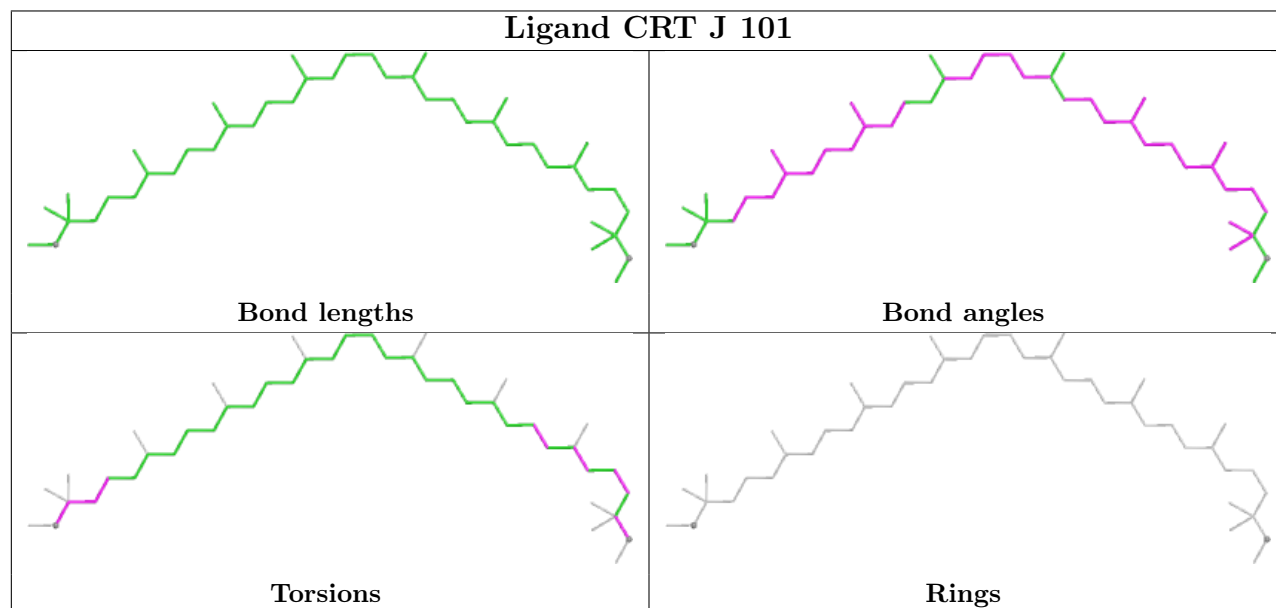
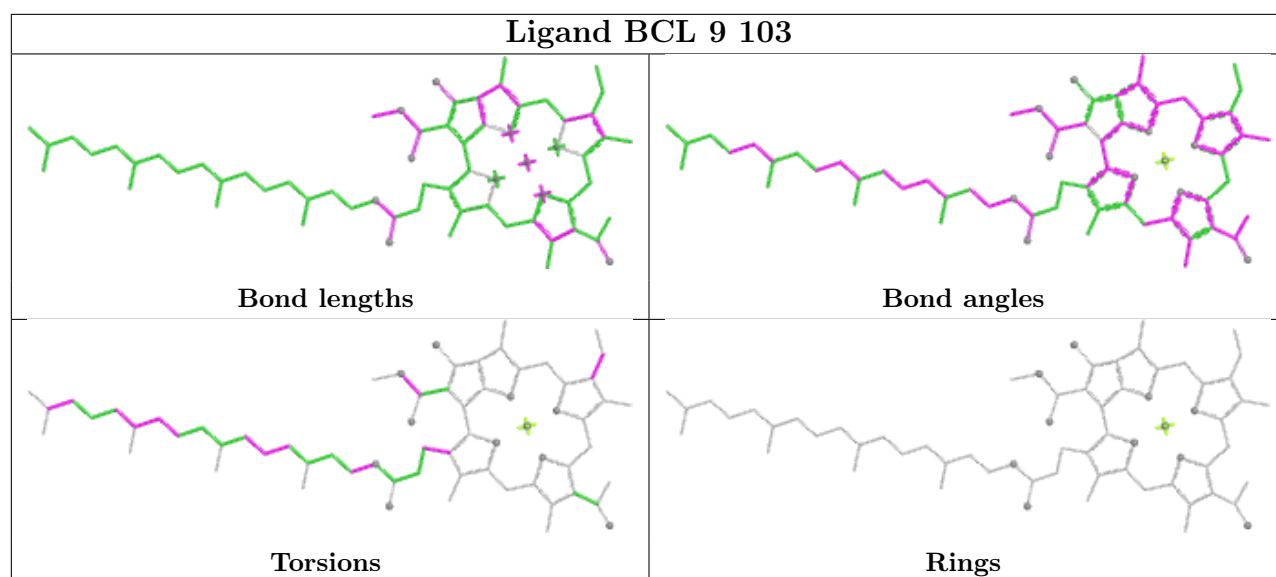
Ligand PEF H 303

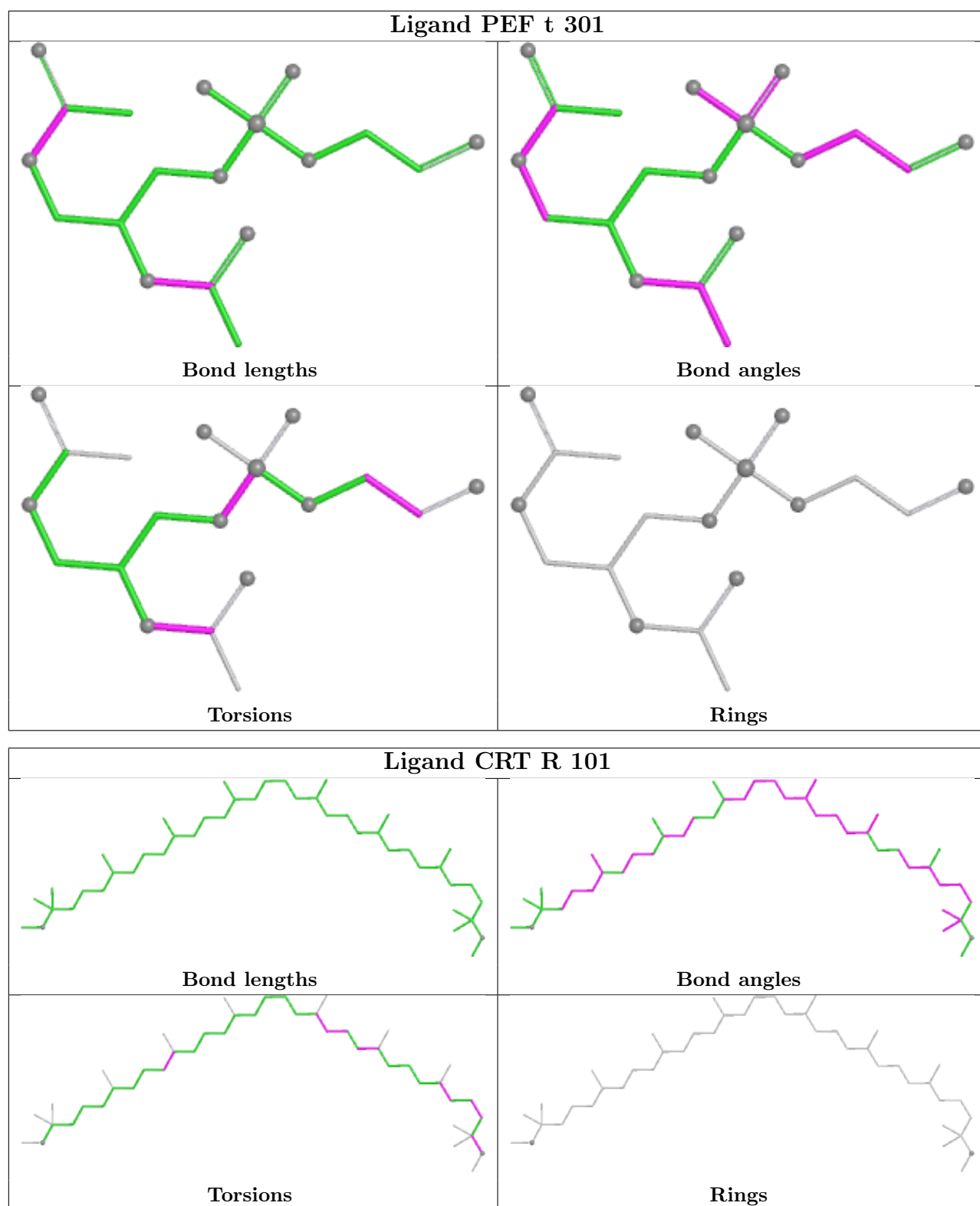


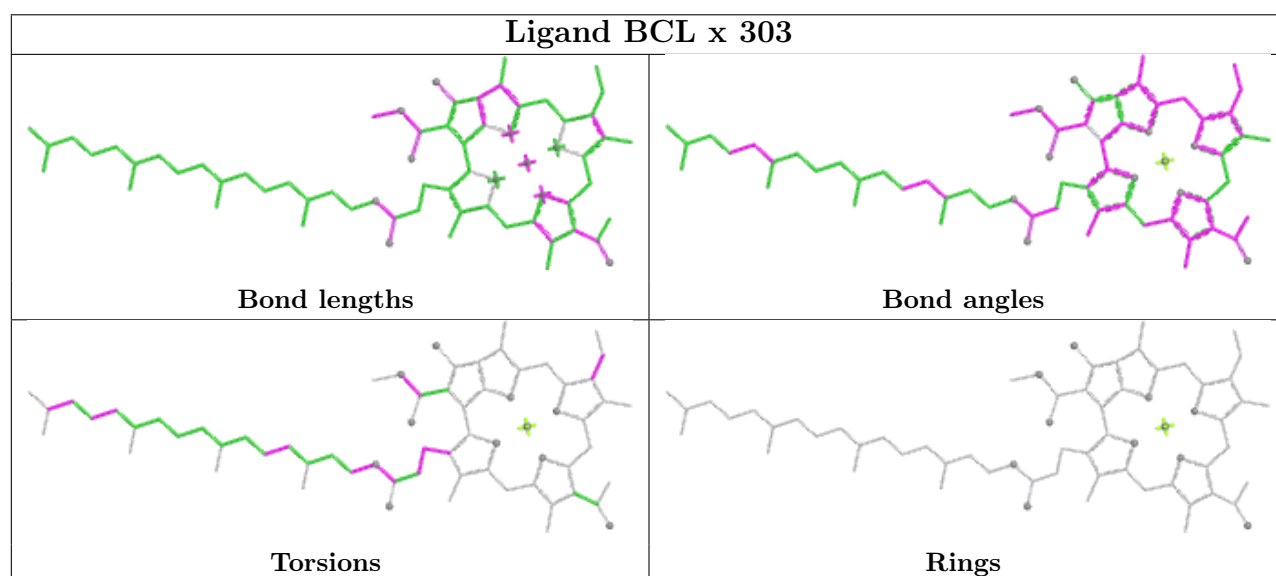
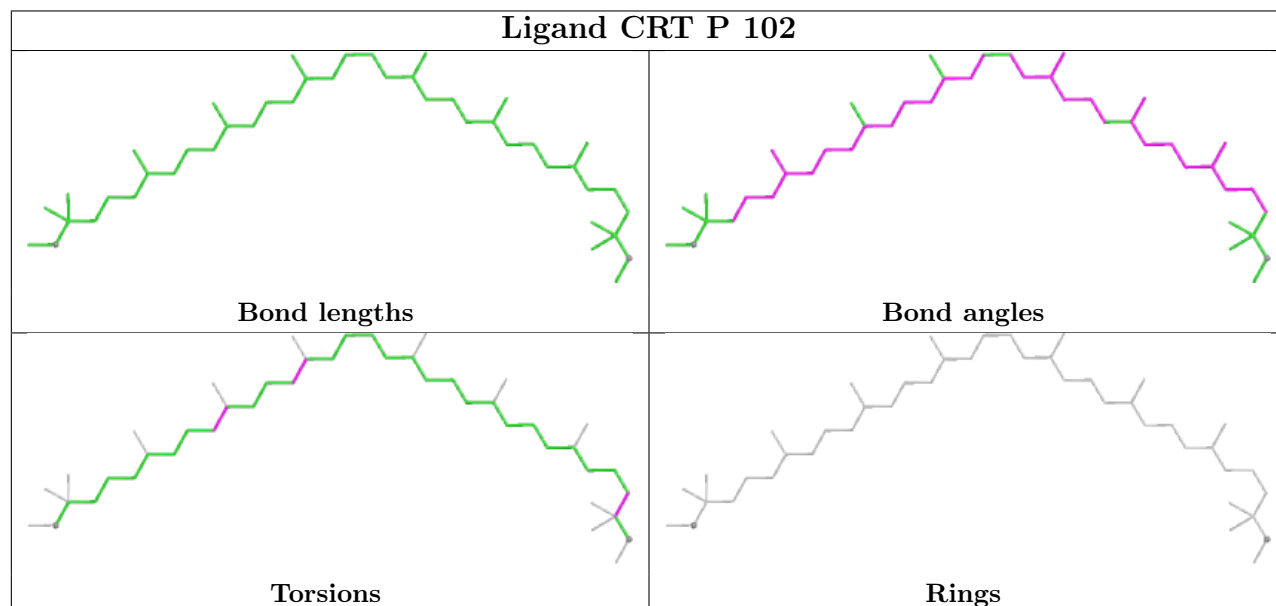
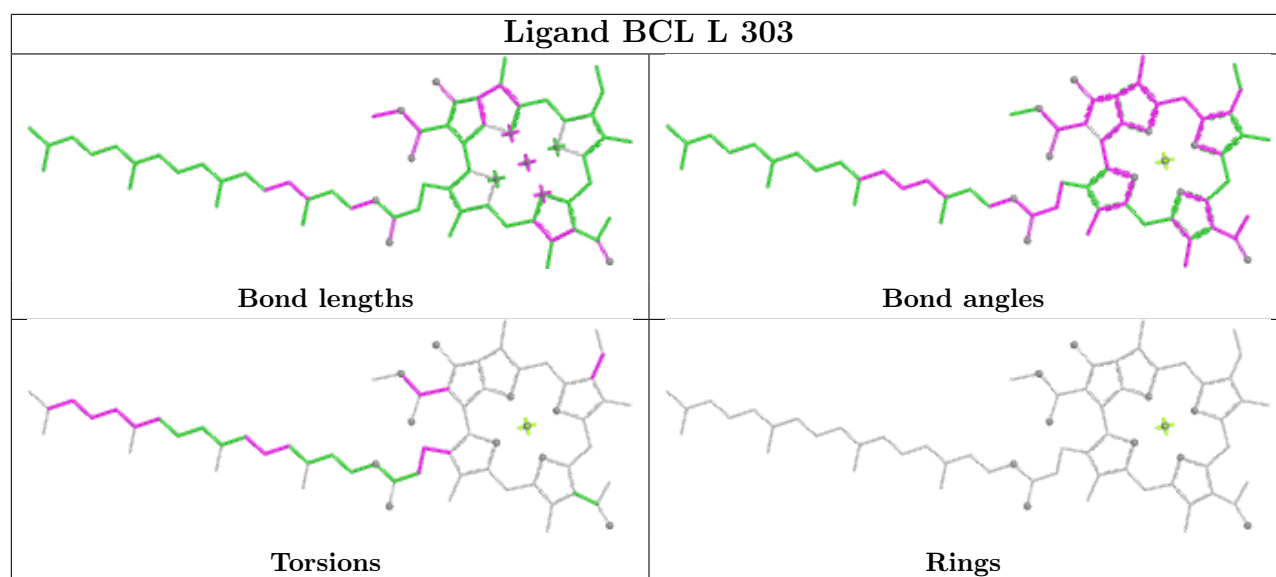
Ligand BCL U 101

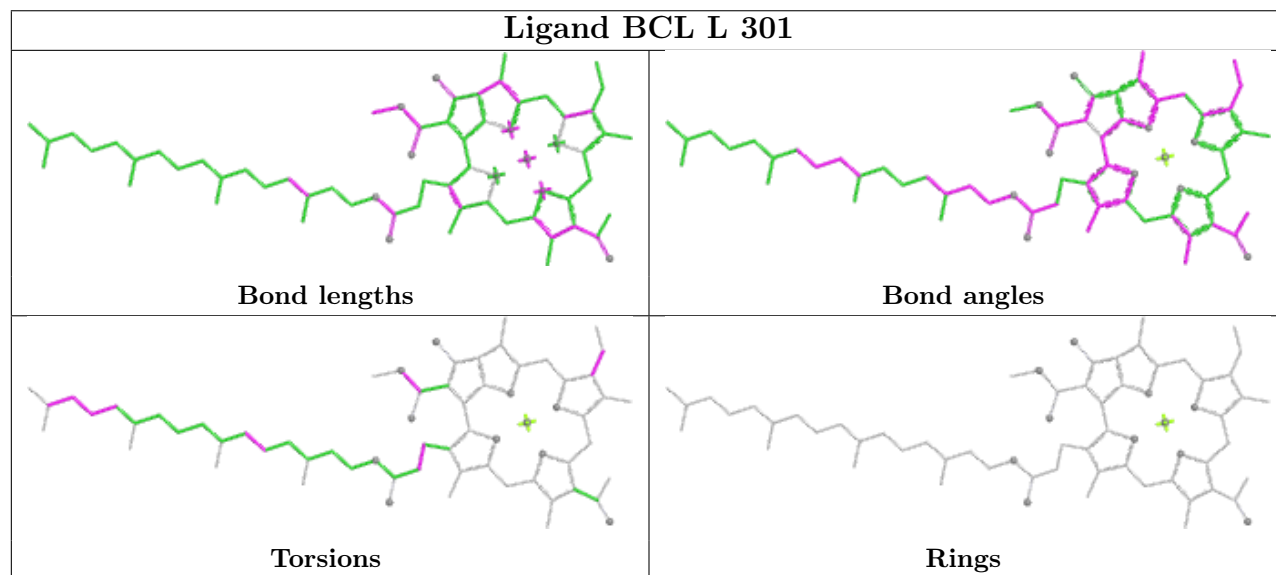
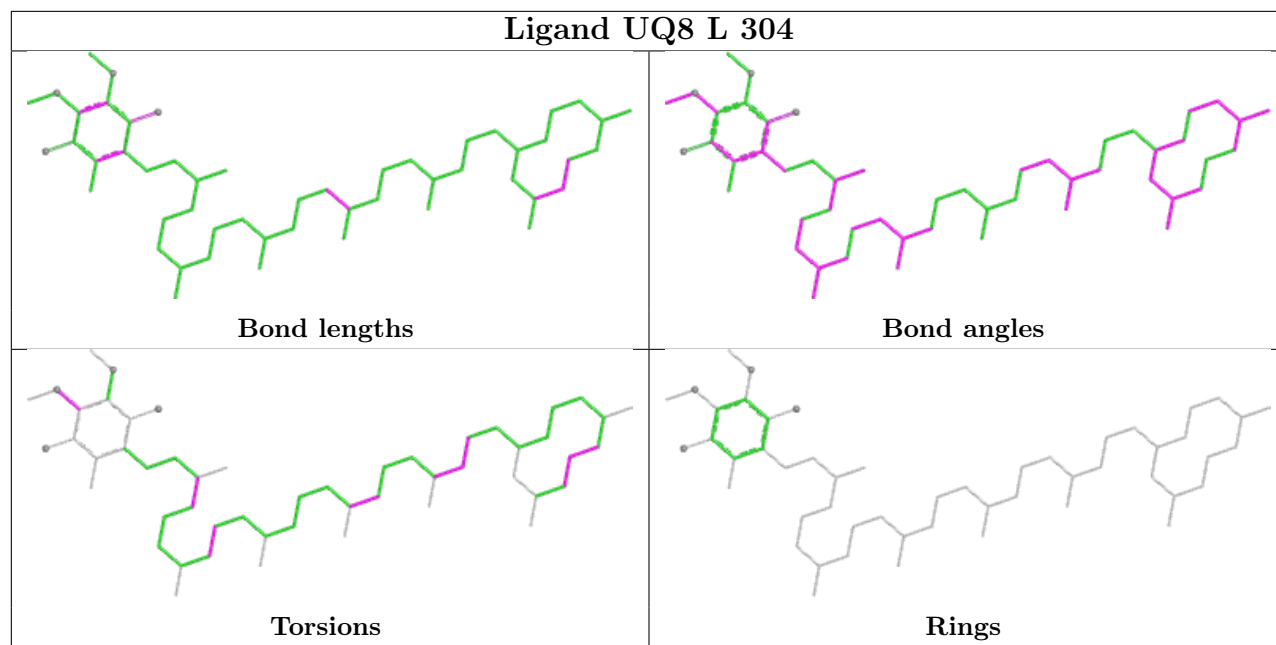


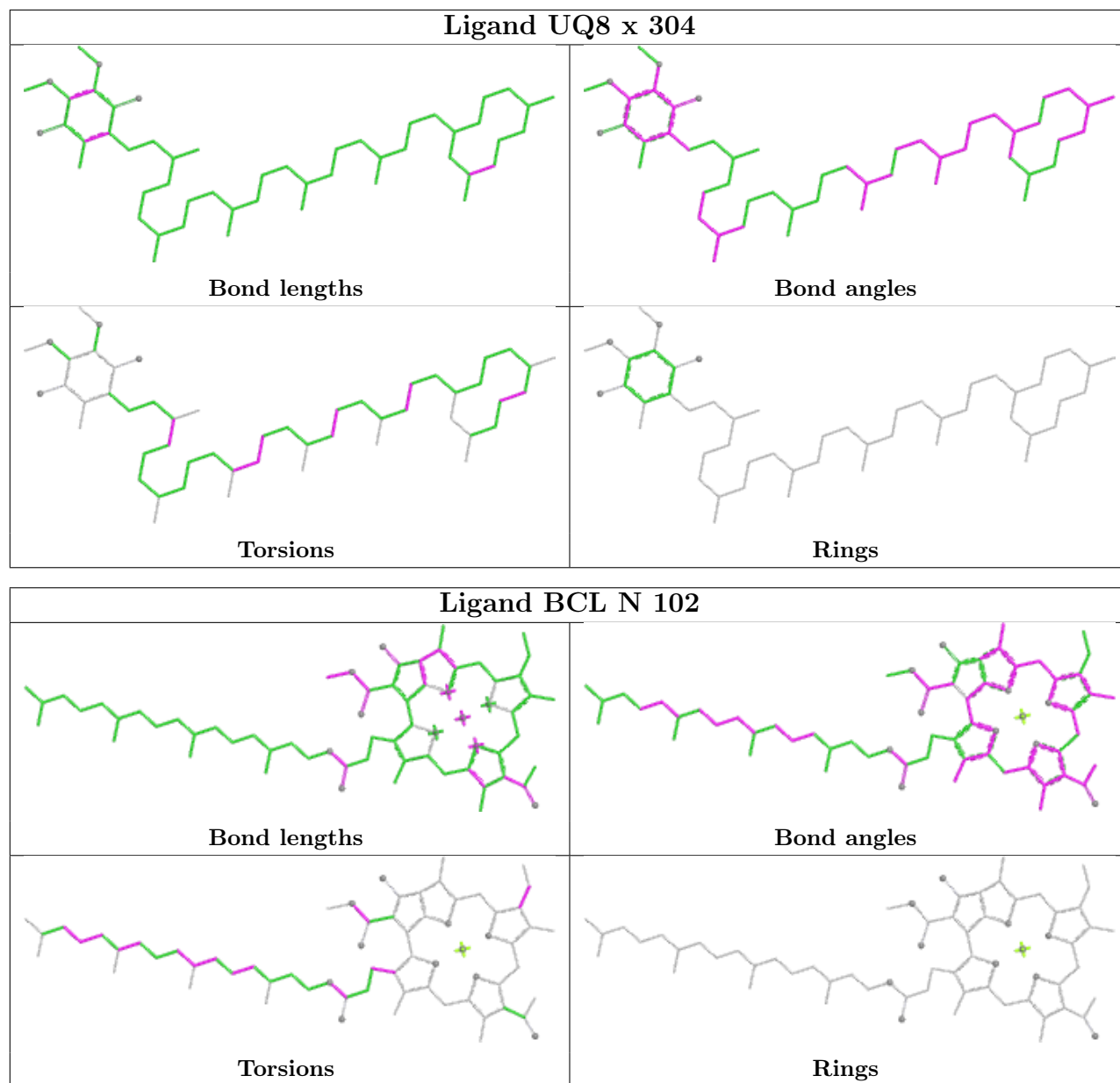


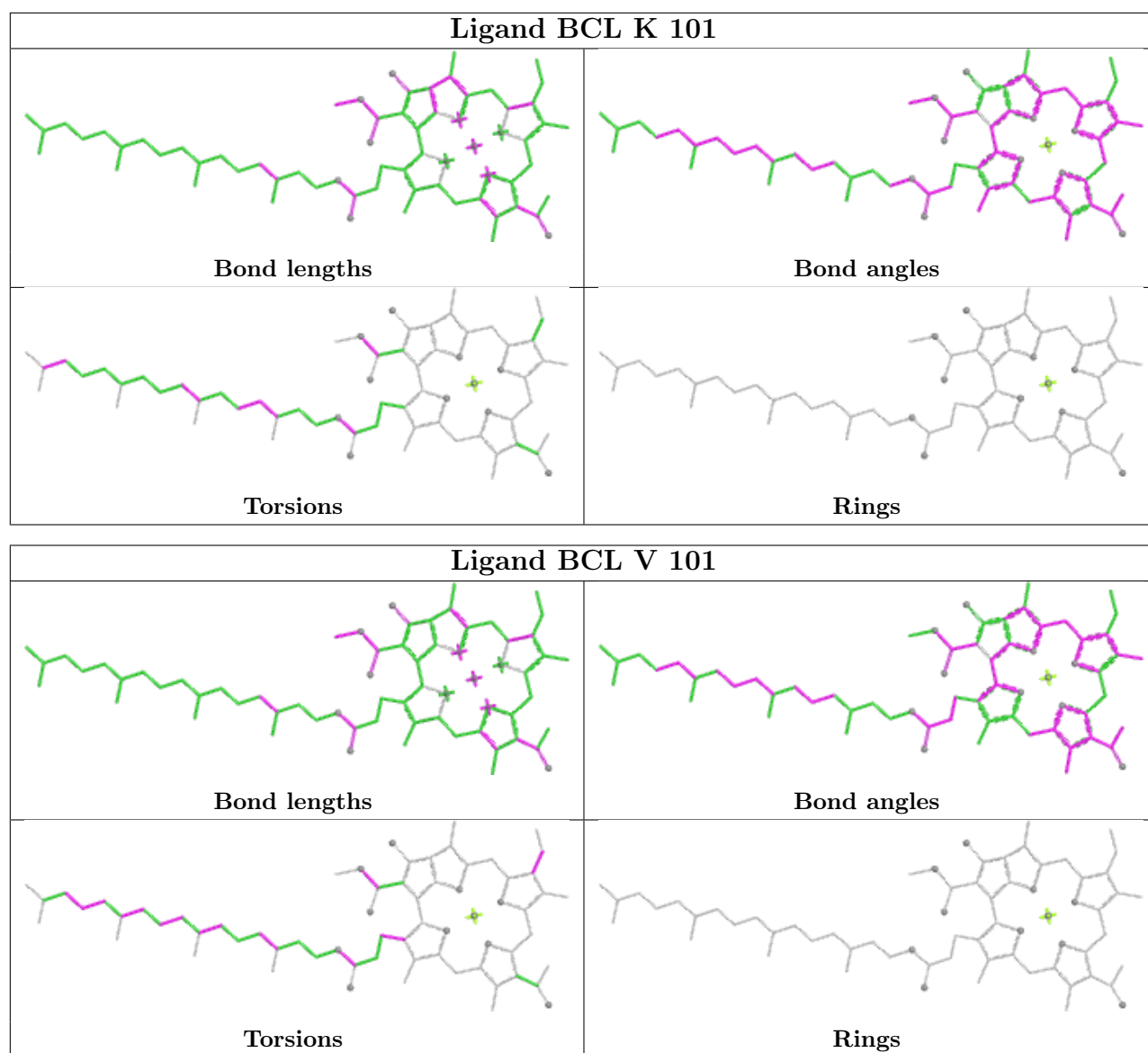


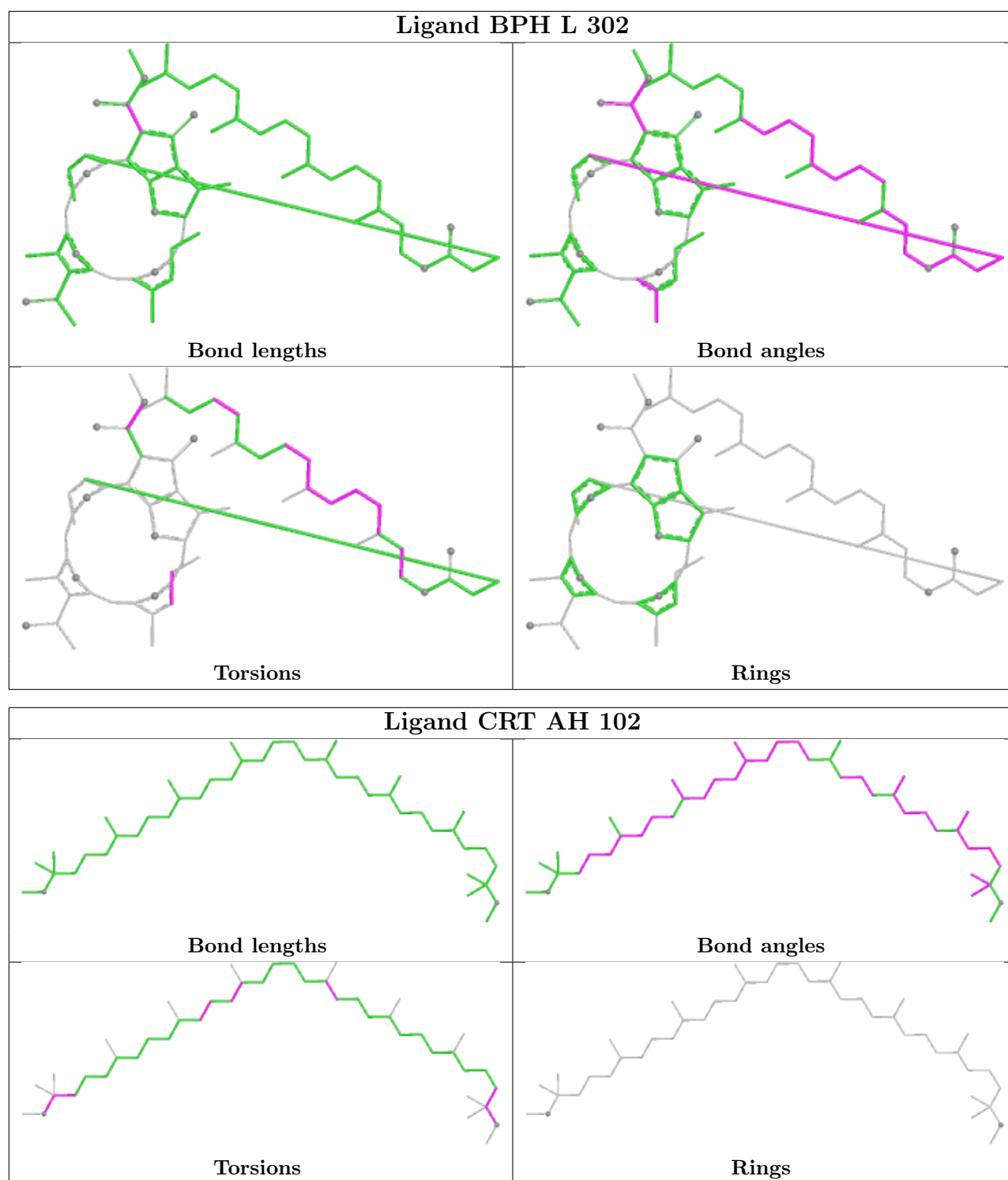












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	317/333 (95%)	0.05	5 (1%) 70 52	79, 112, 143, 161	0
1	o	317/333 (95%)	0.08	10 (3%) 50 34	96, 133, 172, 190	0
2	L	280/281 (99%)	0.20	11 (3%) 43 29	60, 95, 154, 189	0
2	x	280/281 (99%)	0.21	11 (3%) 43 29	63, 97, 147, 181	0
3	M	318/319 (99%)	0.04	9 (2%) 55 36	65, 100, 140, 160	0
3	y	318/319 (99%)	0.10	6 (1%) 66 48	61, 111, 158, 187	0
4	H	258/259 (99%)	-0.09	6 (2%) 61 42	77, 105, 171, 274	0
4	t	258/259 (99%)	-0.08	8 (3%) 51 35	77, 106, 143, 251	0
5	1	60/61 (98%)	-0.00	1 (1%) 69 50	130, 158, 212, 237	0
5	3	60/61 (98%)	0.18	3 (5%) 34 23	129, 157, 225, 232	0
5	5	60/61 (98%)	-0.07	0 100 100	137, 174, 239, 244	0
5	7	60/61 (98%)	0.14	0 100 100	159, 188, 259, 272	0
5	9	60/61 (98%)	0.17	3 (5%) 34 23	163, 204, 239, 243	0
5	A	60/61 (98%)	0.11	4 (6%) 24 16	170, 210, 257, 260	0
5	AA	60/61 (98%)	0.01	2 (3%) 49 33	165, 216, 280, 292	0
5	AC	60/61 (98%)	0.03	1 (1%) 69 50	176, 225, 276, 279	0
5	AE	60/61 (98%)	0.05	3 (5%) 34 23	100, 230, 263, 270	1 (1%)
5	AG	60/61 (98%)	0.01	3 (5%) 34 23	177, 216, 274, 278	0
5	AI	60/61 (98%)	0.15	2 (3%) 49 33	159, 194, 255, 261	0
5	AK	60/61 (98%)	0.20	3 (5%) 34 23	151, 180, 247, 264	0
5	D	60/61 (98%)	-0.07	0 100 100	170, 217, 266, 269	0
5	F	60/61 (98%)	-0.04	0 100 100	174, 215, 261, 264	0
5	I	60/61 (98%)	-0.01	0 100 100	179, 222, 268, 269	0
5	K	60/61 (98%)	-0.15	1 (1%) 69 50	164, 214, 288, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	O	60/61 (98%)	0.01	1 (1%) 69 50	143, 195, 279, 284	0
5	Q	60/61 (98%)	0.15	2 (3%) 49 33	139, 185, 264, 270	0
5	S	60/61 (98%)	0.03	1 (1%) 69 50	81, 193, 256, 260	1 (1%)
5	U	60/61 (98%)	0.12	1 (1%) 69 50	138, 179, 250, 256	0
5	W	60/61 (98%)	-0.15	0 100 100	126, 164, 228, 235	0
5	Y	60/61 (98%)	0.14	1 (1%) 69 50	123, 153, 233, 264	0
5	d	60/61 (98%)	-0.04	2 (3%) 49 33	147, 181, 240, 252	0
5	f	60/61 (98%)	0.07	3 (5%) 34 23	157, 180, 247, 253	0
5	h	60/61 (98%)	-0.07	1 (1%) 69 50	154, 189, 257, 267	0
5	j	60/61 (98%)	-0.17	0 100 100	157, 191, 243, 257	0
5	l	60/61 (98%)	0.11	3 (5%) 34 23	147, 187, 241, 251	0
5	m	60/61 (98%)	0.07	1 (1%) 69 50	146, 186, 255, 259	0
5	p	60/61 (98%)	0.26	3 (5%) 34 23	135, 189, 258, 262	0
5	r	60/61 (98%)	-0.05	2 (3%) 49 33	139, 186, 274, 280	0
5	u	60/61 (98%)	-0.05	4 (6%) 24 16	156, 202, 257, 263	0
5	w	60/61 (98%)	-0.20	1 (1%) 69 50	168, 218, 271, 277	0
6	0	40/47 (85%)	-0.24	0 100 100	178, 236, 246, 250	0
6	2	40/47 (85%)	-0.23	0 100 100	164, 177, 210, 219	0
6	4	40/47 (85%)	-0.29	0 100 100	166, 181, 200, 210	0
6	6	40/47 (85%)	-0.37	0 100 100	178, 203, 222, 224	0
6	8	40/47 (85%)	-0.05	1 (2%) 58 39	194, 230, 240, 241	0
6	AB	40/47 (85%)	0.03	0 100 100	198, 237, 255, 258	0
6	AD	40/47 (85%)	-0.21	0 100 100	210, 245, 256, 257	0
6	AF	40/47 (85%)	-0.04	1 (2%) 58 39	230, 249, 257, 257	0
6	AH	40/47 (85%)	-0.19	1 (2%) 58 39	224, 241, 251, 254	0
6	AJ	40/47 (85%)	-0.30	0 100 100	199, 230, 241, 243	0
6	AL	40/47 (85%)	0.11	0 100 100	190, 211, 236, 238	0
6	B	40/47 (85%)	-0.24	0 100 100	188, 239, 250, 254	0
6	E	40/47 (85%)	-0.19	2 (5%) 34 23	193, 239, 251, 252	0
6	G	40/47 (85%)	-0.04	2 (5%) 34 23	187, 239, 252, 255	0
6	J	40/47 (85%)	-0.06	0 100 100	191, 243, 258, 262	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	N	40/47 (85%)	-0.07	1 (2%) 58 39	175, 225, 247, 254	0
6	P	40/47 (85%)	-0.29	1 (2%) 58 39	170, 220, 241, 245	0
6	R	40/47 (85%)	-0.20	1 (2%) 58 39	170, 223, 236, 236	0
6	T	40/47 (85%)	-0.22	1 (2%) 58 39	184, 218, 236, 237	0
6	V	40/47 (85%)	-0.34	0 100 100	171, 205, 226, 234	0
6	X	40/47 (85%)	-0.15	2 (5%) 34 23	160, 186, 205, 209	0
6	Z	40/47 (85%)	-0.55	0 100 100	159, 173, 197, 202	0
6	c	40/47 (85%)	-0.21	1 (2%) 58 39	160, 217, 245, 247	0
6	e	40/47 (85%)	-0.21	2 (5%) 34 23	189, 204, 236, 240	0
6	g	40/47 (85%)	-0.16	2 (5%) 34 23	195, 213, 235, 239	0
6	i	40/47 (85%)	-0.31	0 100 100	199, 223, 240, 241	0
6	k	40/47 (85%)	-0.30	0 100 100	195, 233, 251, 255	0
6	n	40/47 (85%)	0.01	1 (2%) 58 39	153, 214, 249, 253	0
6	q	40/47 (85%)	-0.41	1 (2%) 58 39	156, 199, 239, 246	0
6	s	40/47 (85%)	0.03	1 (2%) 58 39	151, 198, 236, 238	0
6	v	40/47 (85%)	0.10	2 (5%) 34 23	182, 205, 244, 247	0
6	z	40/47 (85%)	0.02	1 (2%) 58 39	184, 224, 266, 271	0
All	All	5546/5840 (94%)	-0.00	142 (2%) 57 38	60, 169, 252, 303	2 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	3	44	LEU	7.4
6	AF	11	ASP	6.7
5	AK	13	LEU	5.8
6	v	45	TRP	5.8
5	p	47	LEU	5.7
2	x	246	ALA	5.7
6	s	45	TRP	5.6
2	L	176	PHE	5.2
2	x	78	PRO	5.1
5	A	39	VAL	5.0
1	o	97	VAL	4.6
2	x	82	TYR	4.5
2	L	215	VAL	4.3
2	x	120	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	o	204	LEU	3.8
2	x	58	PRO	3.8
4	t	176	GLU	3.6
1	C	241	ASP	3.6
3	M	127	LEU	3.6
1	C	252	ASN	3.6
3	y	198	TYR	3.6
5	AA	8	LEU	3.5
5	r	46	TRP	3.5
6	q	45	TRP	3.5
5	p	46	TRP	3.4
5	9	49	ASP	3.4
2	L	17	LEU	3.4
5	u	47	LEU	3.3
5	u	46	TRP	3.3
4	H	133	ILE	3.3
6	g	39	ALA	3.3
1	o	199	PRO	3.3
2	L	49	LEU	3.2
1	C	59	VAL	3.2
4	t	56	VAL	3.2
5	AA	52	PRO	3.1
1	o	321	ALA	3.0
2	x	80	LEU	3.0
3	y	189	PHE	3.0
4	t	242	TYR	3.0
3	M	110	SER	3.0
5	AG	35	ILE	3.0
1	o	162	PRO	2.9
5	AI	51	ILE	2.9
2	L	15	GLY	2.9
3	M	275	LEU	2.9
5	AG	15	LEU	2.9
5	Q	54	SER	2.8
6	c	17	PHE	2.8
3	y	51	ILE	2.8
1	o	154	THR	2.8
5	S	15	LEU	2.8
4	t	124	ASP	2.7
3	y	195	ASN	2.7
6	G	32	VAL	2.7
5	w	28	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
6	e	45	TRP	2.7
6	E	10	THR	2.6
5	Q	17	PRO	2.6
5	AI	44	LEU	2.6
5	l	47	LEU	2.6
5	l	30	VAL	2.6
5	f	54	SER	2.6
3	M	96	GLU	2.6
5	l	26	ALA	2.6
5	l	44	LEU	2.5
5	u	14	ILE	2.5
6	G	7	THR	2.5
1	C	261	GLN	2.5
6	n	7	THR	2.5
3	M	287	SER	2.5
2	L	174	LEU	2.5
5	AK	44	LEU	2.5
2	x	230	GLY	2.5
3	y	164	ARG	2.4
5	AE	42	THR	2.4
6	T	39	ALA	2.4
6	E	34	ILE	2.4
4	t	75	THR	2.4
5	f	20	VAL	2.4
2	L	265	THR	2.4
6	AH	30	GLY	2.4
2	x	35	PHE	2.4
4	H	124	ASP	2.4
5	U	39	VAL	2.4
6	z	44	PRO	2.4
6	v	26	TYR	2.3
5	O	44	LEU	2.3
4	t	122	HIS	2.3
1	o	315	ASN	2.3
5	AE	54	SER	2.3
3	y	45	ASP	2.3
5	f	22	VAL	2.3
3	M	294	TRP	2.3
5	AC	54	SER	2.3
5	AK	54	SER	2.3
3	M	17	ALA	2.2
5	9	59	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
6	R	39	ALA	2.2
2	L	98	ILE	2.2
5	3	51	ILE	2.2
5	m	55	TYR	2.2
5	r	18	ARG	2.2
2	L	141	VAL	2.2
5	9	30	VAL	2.2
5	AG	44	LEU	2.2
6	X	30	GLY	2.2
6	e	32	VAL	2.2
5	A	52	PRO	2.2
5	d	6	ALA	2.2
6	P	45	TRP	2.2
2	L	14	GLY	2.2
2	x	242	GLY	2.2
5	Y	61	LYS	2.2
5	A	35	ILE	2.1
3	M	95	LEU	2.1
4	H	41	LEU	2.1
5	d	54	SER	2.1
1	C	250	CYS	2.1
2	x	125	HIS	2.1
5	u	51	ILE	2.1
5	p	44	LEU	2.1
5	AE	7	ASN	2.1
5	3	46	TRP	2.1
1	o	233	PHE	2.1
1	o	307	CYS	2.1
4	H	39	TYR	2.1
6	8	27	ALA	2.1
2	x	263	PHE	2.1
6	X	39	ALA	2.1
4	H	202	PHE	2.1
1	o	127	SER	2.0
2	L	232	SER	2.0
3	M	6	ASN	2.0
5	K	21	LEU	2.0
5	h	12	TRP	2.0
6	N	19	ALA	2.0
6	g	26	TYR	2.0
5	A	59	GLY	2.0
4	t	231	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	194	LEU	2.0
4	t	233	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	PEF	y	406	19/47	0.55	0.12	124,132,141,146	0
8	SR	I	102	1/1	0.59	0.17	284,284,284,284	0
16	PO4	y	405	5/5	0.59	0.14	138,141,147,148	0
17	PGW	AE	101	21/51	0.60	0.14	149,167,181,187	0
8	SR	K	102	1/1	0.63	0.19	270,270,270,270	0
12	PEF	A	101	19/47	0.65	0.14	141,149,161,165	0
8	SR	9	101	1/1	0.66	0.19	236,236,236,236	0
12	PEF	m	101	19/47	0.67	0.18	124,130,143,146	0
17	PGW	S	101	21/51	0.68	0.13	118,132,142,148	0
12	PEF	x	306	19/47	0.69	0.10	96,102,108,108	0
15	CRT	J	101	44/44	0.72	0.14	196,214,220,222	0
15	CRT	AL	101	44/44	0.76	0.14	140,190,233,236	0
12	PEF	L	306	12/47	0.76	0.10	113,119,126,127	0
8	SR	7	102	1/1	0.76	0.20	221,221,221,221	0
8	SR	AI	103	1/1	0.76	0.17	228,228,228,228	0
15	CRT	N	101	44/44	0.77	0.14	179,199,209,214	0
16	PO4	t	302	5/5	0.77	0.11	138,140,144,147	0
15	CRT	AH	102	44/44	0.77	0.15	163,220,243,244	0
12	PEF	y	408	19/47	0.77	0.10	93,103,113,116	0
8	SR	5	103	1/1	0.78	0.09	197,197,197,197	0
12	PEF	H	303	19/47	0.78	0.10	164,173,184,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	PEF	t	303	19/47	0.78	0.11	83,87,94,95	0
12	PEF	y	407	19/47	0.79	0.09	91,96,102,105	0
8	SR	p	105	1/1	0.79	0.12	265,265,265,265	0
15	CRT	p	103	44/44	0.79	0.14	158,177,182,187	0
9	BCL	AE	104	66/66	0.80	0.09	208,235,262,264	0
16	PO4	H	302	5/5	0.80	0.07	170,172,178,179	0
8	SR	D	103	1/1	0.81	0.11	269,269,269,269	0
15	CRT	c	101	44/44	0.82	0.14	179,196,203,207	0
15	CRT	8	101	44/44	0.82	0.15	174,203,220,223	0
8	SR	Q	102	1/1	0.82	0.16	256,256,256,256	0
12	PEF	t	301	19/47	0.82	0.10	94,98,103,104	0
12	PEF	H	304	19/47	0.82	0.09	92,98,106,108	0
15	CRT	i	101	44/44	0.82	0.12	163,197,220,226	0
8	SR	U	103	1/1	0.83	0.12	233,233,233,233	0
12	PEF	p	101	16/47	0.83	0.15	132,144,152,156	0
9	BCL	1	101	66/66	0.83	0.12	115,148,161,169	0
12	PEF	M	406	19/47	0.83	0.08	107,115,119,124	0
9	BCL	AC	102	66/66	0.83	0.12	205,236,259,261	0
14	MQ8	M	403	53/53	0.84	0.10	75,98,159,170	0
15	CRT	E	101	44/44	0.84	0.12	182,217,225,226	0
15	CRT	G	101	44/44	0.84	0.12	187,217,225,228	0
12	PEF	M	407	16/47	0.84	0.10	79,83,87,89	0
9	BCL	j	101	66/66	0.84	0.11	177,199,217,223	0
15	CRT	R	101	44/44	0.84	0.14	157,189,197,198	0
9	BCL	m	103	66/66	0.84	0.10	178,209,237,245	0
9	BCL	AH	103	66/66	0.84	0.14	195,211,245,252	0
15	CRT	z	101	44/44	0.84	0.16	179,205,209,210	0
11	UQ8	L	304	53/53	0.85	0.13	75,80,82,83	0
15	CRT	AC	101	44/44	0.85	0.13	195,211,216,218	0
8	SR	j	102	1/1	0.85	0.09	233,233,233,233	0
15	CRT	AJ	101	44/44	0.85	0.11	147,203,240,241	0
9	BCL	G	102	66/66	0.85	0.11	203,233,249,251	0
15	CRT	e	101	44/44	0.85	0.15	149,194,237,241	0
15	CRT	f	102	44/44	0.85	0.12	152,190,223,230	0
9	BCL	N	102	66/66	0.85	0.12	187,219,242,244	0
15	CRT	k	101	44/44	0.85	0.11	172,200,217,220	0
12	PEF	M	408	19/47	0.85	0.07	87,92,97,100	0
9	BCL	T	102	66/66	0.85	0.12	164,188,236,238	0
15	CRT	X	101	44/44	0.85	0.10	118,164,193,198	0
15	CRT	2	101	44/44	0.85	0.09	128,165,195,200	0
9	BCL	f	101	66/66	0.85	0.12	157,181,196,203	0
8	SR	f	103	1/1	0.85	0.06	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	S	102	66/66	0.86	0.12	129,190,203,213	0
15	CRT	n	101	44/44	0.86	0.15	173,188,197,201	0
8	SR	AE	105	1/1	0.86	0.07	257,257,257,257	0
15	CRT	s	101	44/44	0.86	0.11	155,177,181,183	0
15	CRT	v	101	44/44	0.86	0.11	165,192,198,200	0
9	BCL	AD	101	66/66	0.86	0.10	193,224,242,252	0
8	SR	O	102	1/1	0.86	0.11	254,254,254,254	0
12	PEF	H	301	19/47	0.86	0.11	140,163,175,180	0
11	UQ8	x	304	53/53	0.86	0.12	73,85,92,93	0
15	CRT	4	101	44/44	0.86	0.12	136,169,192,198	0
9	BCL	AK	101	66/66	0.87	0.12	168,180,199,220	0
9	BCL	d	101	66/66	0.87	0.11	138,175,187,197	0
9	BCL	K	101	66/66	0.87	0.11	181,215,235,242	0
9	BCL	v	102	66/66	0.87	0.13	182,211,260,262	0
9	BCL	k	102	66/66	0.87	0.11	181,211,246,260	0
8	SR	5	104	1/1	0.87	0.21	206,206,206,206	0
9	BCL	R	102	66/66	0.87	0.10	174,203,233,235	0
9	BCL	AE	102	66/66	0.87	0.10	169,228,244,254	0
9	BCL	1	102	66/66	0.87	0.12	140,153,192,205	0
9	BCL	AH	101	66/66	0.87	0.10	199,218,233,243	0
9	BCL	9	103	66/66	0.87	0.13	169,202,226,235	0
9	BCL	AJ	102	66/66	0.87	0.11	177,189,226,232	0
14	MQ8	y	403	53/53	0.87	0.13	71,88,135,144	0
15	CRT	A	103	44/44	0.87	0.13	186,214,224,225	0
9	BCL	h	101	66/66	0.88	0.10	168,188,207,212	0
9	BCL	z	102	66/66	0.88	0.11	193,228,269,271	0
9	BCL	AB	101	66/66	0.88	0.11	197,232,260,262	0
15	CRT	U	102	44/44	0.88	0.11	132,179,205,208	0
10	BPH	L	302	65/65	0.88	0.14	68,81,108,115	0
15	CRT	M	404	44/44	0.88	0.12	75,96,139,150	0
10	BPH	x	302	65/65	0.88	0.14	71,78,102,105	0
9	BCL	u	101	66/66	0.88	0.12	120,199,218,223	0
9	BCL	p	102	66/66	0.88	0.12	124,199,217,224	0
15	CRT	y	404	44/44	0.89	0.12	96,117,155,166	0
8	SR	AA	102	1/1	0.89	0.06	273,273,273,273	0
9	BCL	J	102	66/66	0.89	0.11	202,233,255,257	0
8	SR	W	102	1/1	0.89	0.10	205,205,205,205	0
15	CRT	T	101	44/44	0.89	0.13	145,187,206,207	0
8	SR	AI	102	1/1	0.89	0.06	245,245,245,245	0
9	BCL	5	102	66/66	0.89	0.11	150,176,224,240	0
9	BCL	c	102	66/66	0.89	0.09	177,211,249,251	0
9	BCL	L	303	66/66	0.89	0.15	62,70,78,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	m	102	66/66	0.89	0.10	160,202,221,229	0
9	BCL	D	102	66/66	0.90	0.11	202,232,246,247	0
9	BCL	F	101	66/66	0.90	0.11	184,220,238,242	0
9	BCL	AL	102	66/66	0.90	0.14	167,178,209,221	0
8	SR	w	103	1/1	0.90	0.18	260,260,260,260	0
15	CRT	AD	102	44/44	0.90	0.13	192,225,232,234	0
9	BCL	w	101	66/66	0.90	0.10	174,206,228,234	0
9	BCL	g	101	66/66	0.90	0.11	169,190,234,245	0
9	BCL	W	101	66/66	0.90	0.10	146,162,172,181	0
9	BCL	AA	101	66/66	0.90	0.09	177,212,237,244	0
9	BCL	Z	102	66/66	0.90	0.10	141,150,181,191	0
9	BCL	I	101	66/66	0.90	0.10	141,226,243,247	0
8	SR	S	103	1/1	0.90	0.12	235,235,235,235	0
8	SR	l	102	1/1	0.90	0.06	245,245,245,245	0
16	PO4	M	405	5/5	0.90	0.11	120,126,128,129	0
15	CRT	6	101	44/44	0.90	0.12	153,180,198,203	0
8	SR	AC	103	1/1	0.90	0.11	265,265,265,265	0
9	BCL	O	101	66/66	0.90	0.10	179,211,234,235	0
9	BCL	P	101	66/66	0.90	0.10	171,205,223,228	0
9	BCL	AI	101	66/66	0.90	0.13	177,195,210,216	0
9	BCL	l	101	66/66	0.91	0.08	161,201,221,228	0
9	BCL	D	101	66/66	0.91	0.11	149,221,243,245	0
8	SR	L	307	1/1	0.91	0.09	205,205,205,205	0
8	SR	w	102	1/1	0.91	0.05	263,263,263,263	0
10	BPH	y	402	65/65	0.91	0.12	80,90,143,155	0
8	SR	A	104	1/1	0.91	0.18	256,256,256,256	0
9	BCL	s	102	66/66	0.91	0.12	171,202,247,248	0
8	SR	m	104	1/1	0.91	0.11	253,253,253,253	0
9	BCL	3	101	66/66	0.91	0.10	134,153,169,173	0
9	BCL	i	102	66/66	0.91	0.10	173,197,242,261	0
9	BCL	L	305	66/66	0.91	0.11	76,88,106,115	0
15	CRT	AE	103	44/44	0.91	0.10	182,236,248,249	0
9	BCL	7	101	66/66	0.91	0.12	162,184,202,209	0
9	BCL	Q	101	66/66	0.92	0.11	165,201,216,224	0
15	CRT	Z	101	44/44	0.92	0.10	114,157,190,195	0
9	BCL	Y	101	66/66	0.92	0.10	139,149,163,175	0
9	BCL	8	102	66/66	0.92	0.07	177,207,239,244	0
8	SR	Y	102	1/1	0.92	0.17	191,191,191,191	0
10	BPH	M	402	65/65	0.92	0.10	72,77,113,123	0
15	CRT	9	102	44/44	0.92	0.14	188,217,226,230	0
9	BCL	x	301	66/66	0.92	0.14	75,81,87,90	0
9	BCL	y	401	66/66	0.92	0.14	78,88,101,108	0

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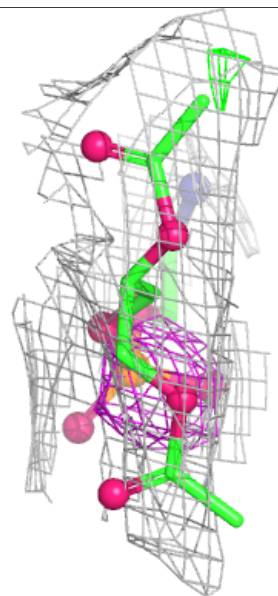
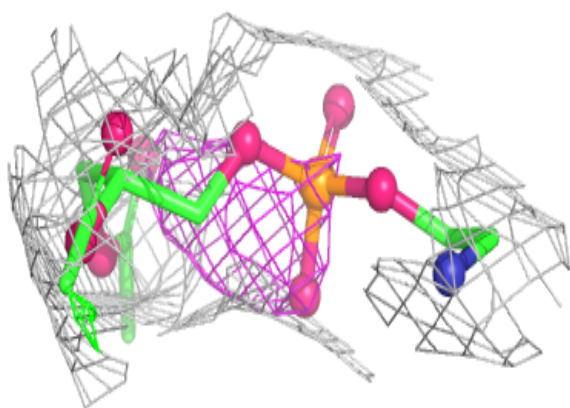
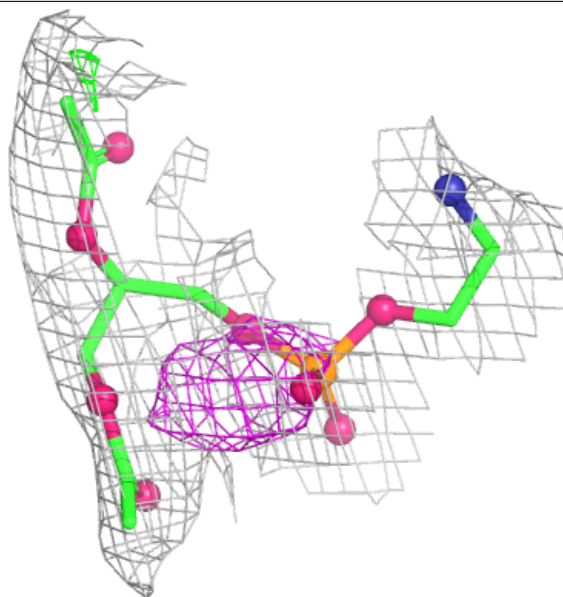
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SR	AK	102	1/1	0.92	0.08	203,203,203,203	0
8	SR	d	102	1/1	0.92	0.09	198,198,198,198	0
15	CRT	P	102	44/44	0.92	0.10	169,193,199,202	0
9	BCL	V	101	66/66	0.92	0.13	159,175,219,232	0
9	BCL	r	101	66/66	0.92	0.09	154,192,211,214	0
9	BCL	5	101	66/66	0.92	0.11	141,165,182,188	0
9	BCL	0	101	66/66	0.93	0.09	190,224,244,245	0
7	HEM	o	501	43/43	0.93	0.15	142,155,165,169	0
9	BCL	U	101	66/66	0.93	0.11	151,179,188,195	0
9	BCL	4	102	66/66	0.93	0.09	138,159,198,209	0
7	HEM	C	501	43/43	0.93	0.13	110,120,129,134	0
8	SR	x	307	1/1	0.93	0.04	168,168,168,168	0
9	BCL	M	401	66/66	0.93	0.10	74,82,88,94	0
9	BCL	e	102	66/66	0.93	0.11	166,180,213,225	0
9	BCL	A	102	66/66	0.93	0.10	202,230,242,244	0
8	SR	L	308	1/1	0.93	0.04	145,145,145,145	0
8	SR	C	505	1/1	0.94	0.06	113,113,113,113	0
9	BCL	x	303	66/66	0.94	0.10	73,82,94,98	0
9	BCL	x	305	66/66	0.94	0.10	72,82,91,99	0
9	BCL	X	102	66/66	0.94	0.10	142,155,182,199	0
8	SR	l	103	1/1	0.94	0.12	176,176,176,176	0
8	SR	F	102	1/1	0.94	0.13	262,262,262,262	0
9	BCL	L	301	66/66	0.94	0.12	67,74,92,98	0
9	BCL	p	104	66/66	0.94	0.10	170,202,241,242	0
8	SR	x	308	1/1	0.94	0.05	196,196,196,196	0
7	HEM	o	503	43/43	0.94	0.17	94,106,122,126	0
7	HEM	o	504	43/43	0.95	0.14	112,116,123,124	0
9	BCL	B	101	66/66	0.95	0.09	187,218,239,241	0
8	SR	r	102	1/1	0.95	0.07	252,252,252,252	0
7	HEM	C	503	43/43	0.96	0.17	85,100,116,119	0
7	HEM	C	504	43/43	0.96	0.16	97,99,104,107	0
8	SR	o	505	1/1	0.96	0.05	111,111,111,111	0
7	HEM	o	502	43/43	0.97	0.13	125,134,142,145	0
7	HEM	C	502	43/43	0.97	0.12	97,104,111,113	0
8	SR	h	102	1/1	0.98	0.11	220,220,220,220	0
13	FE	L	309	1/1	0.98	0.06	65,65,65,65	0
13	FE	x	309	1/1	0.99	0.05	65,65,65,65	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.

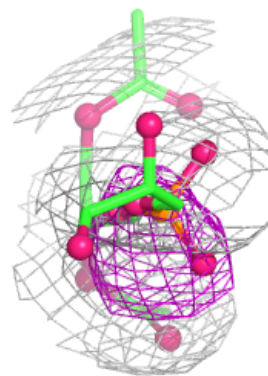
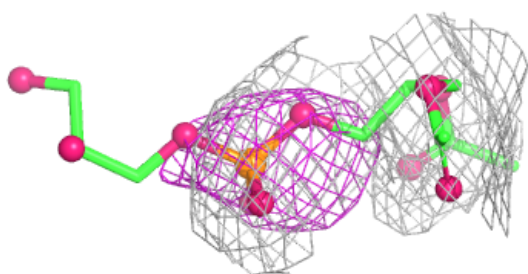
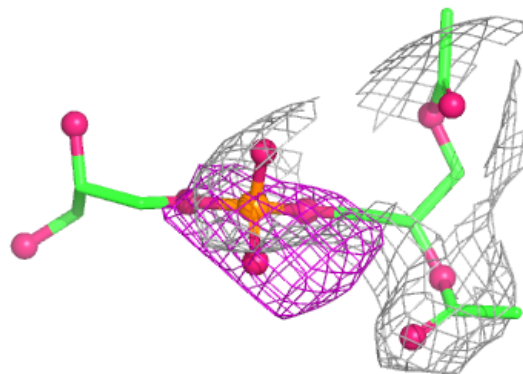
Electron density around PEF y 406:

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



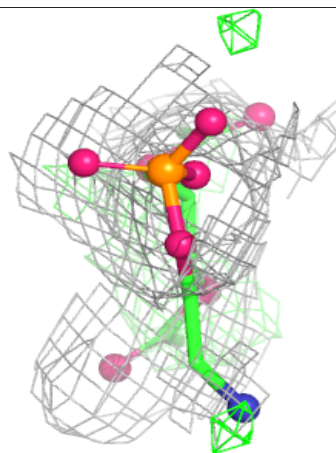
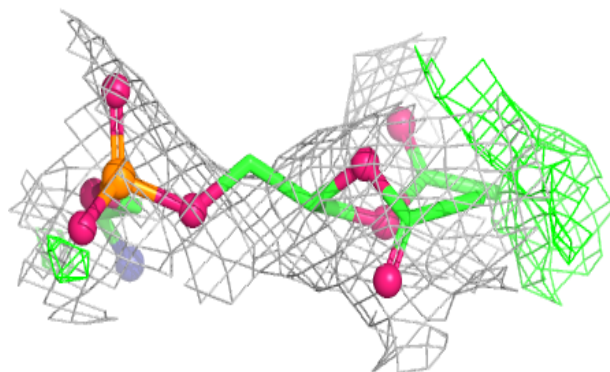
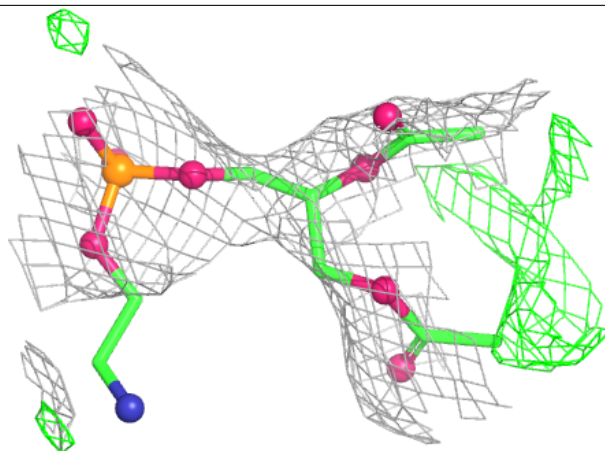
Electron density around PGW AE 101:

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



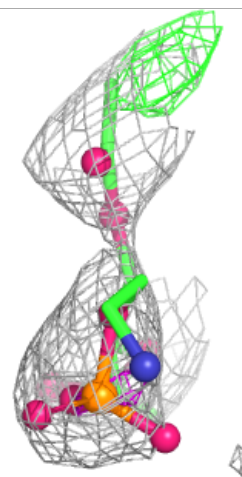
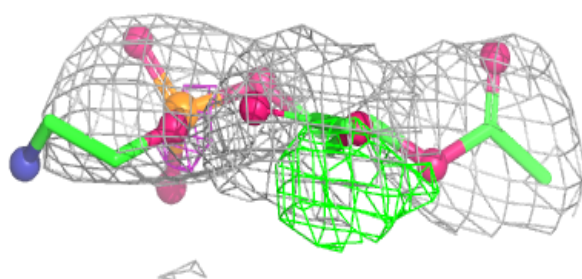
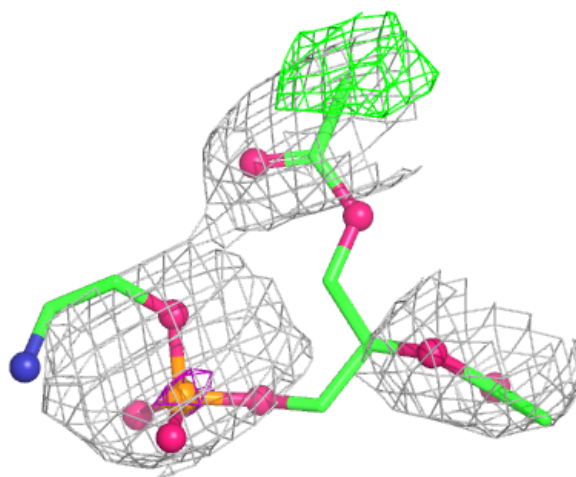
Electron density around PEF A 101:

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



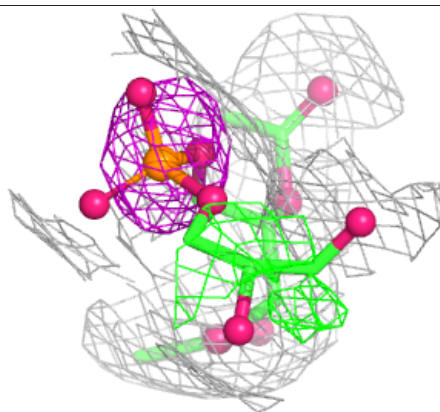
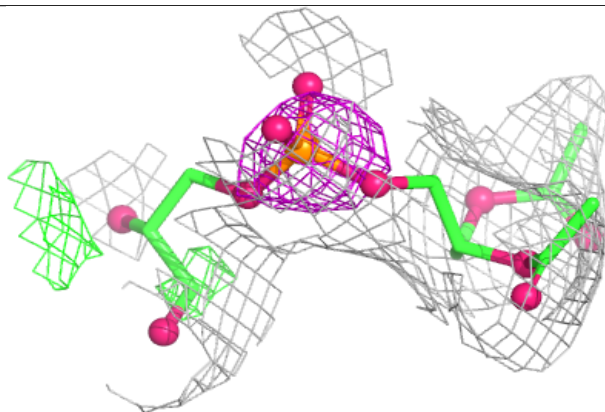
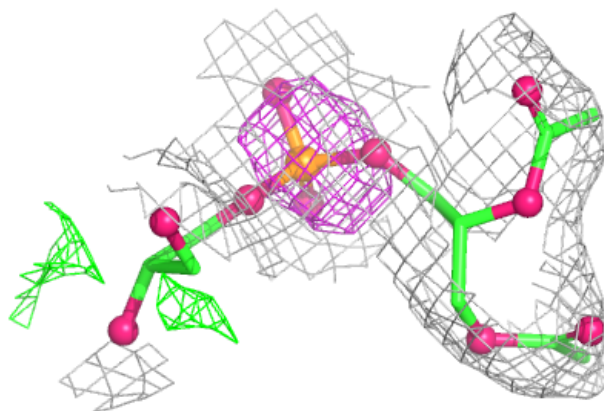
Electron density around PEF m 101:

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



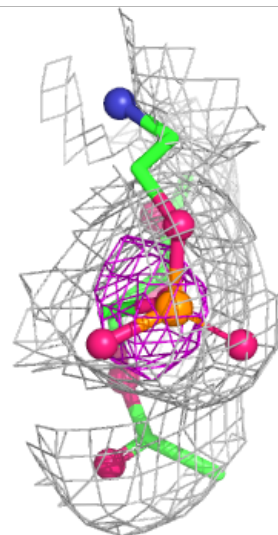
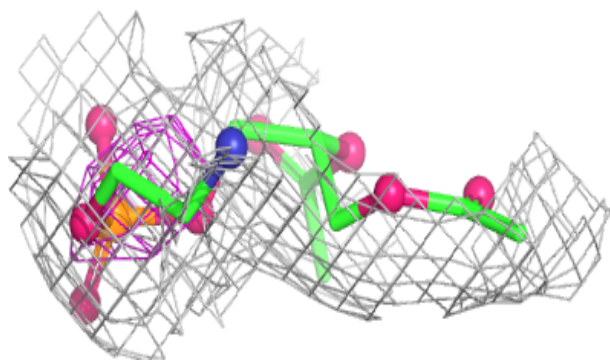
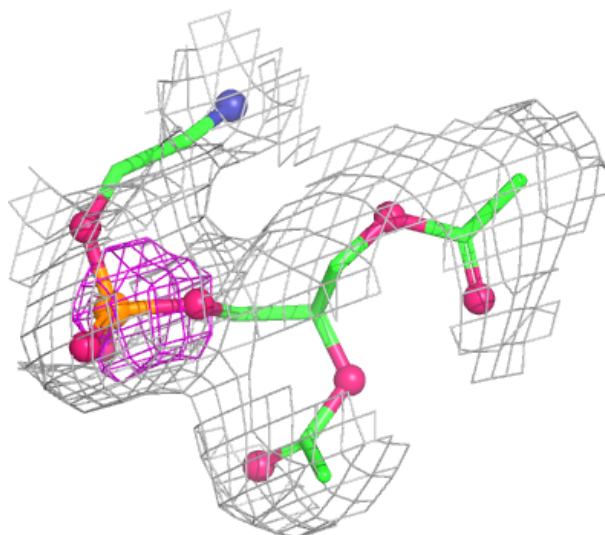
Electron density around PGW S 101:

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



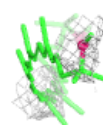
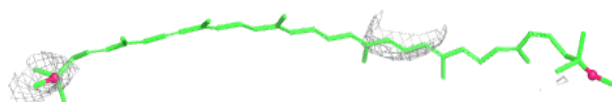
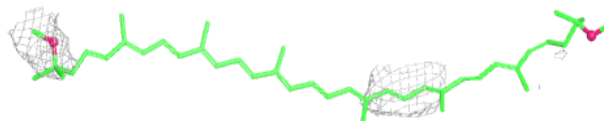
Electron density around PEF x 306:

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

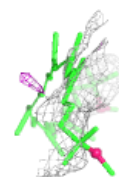
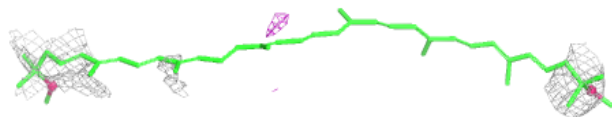
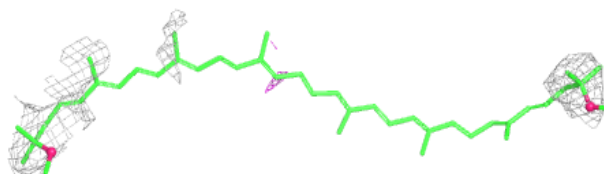


Electron density around CRT J 101:

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

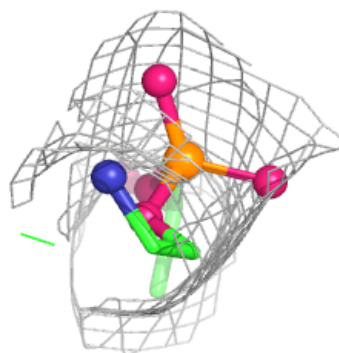
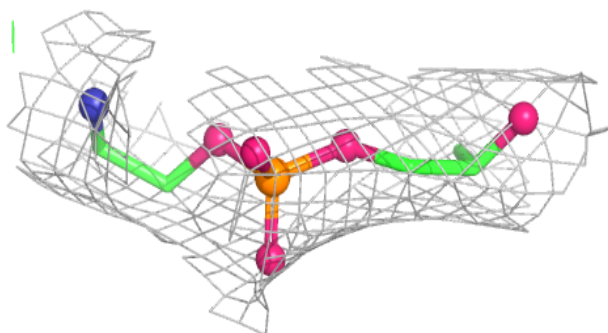
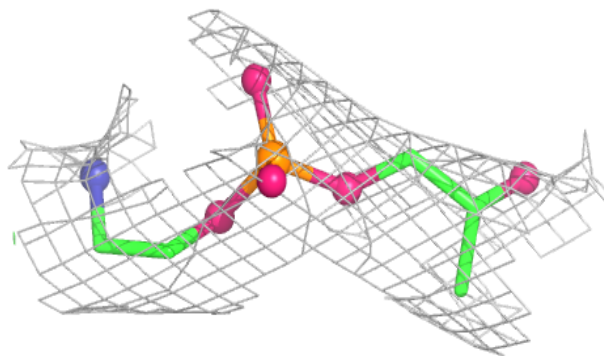
**Electron density around CRT AL 101:**

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

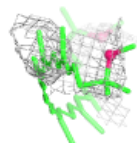
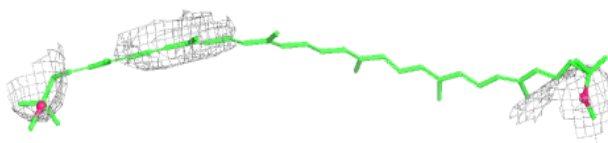
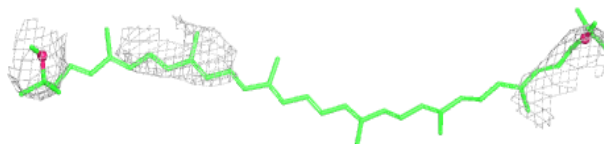


Electron density around PEF L 306:

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

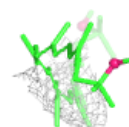
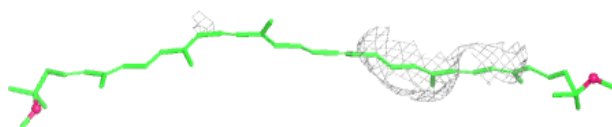
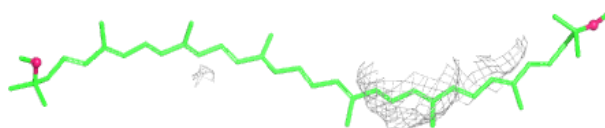
**Electron density around CRT N 101:**

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

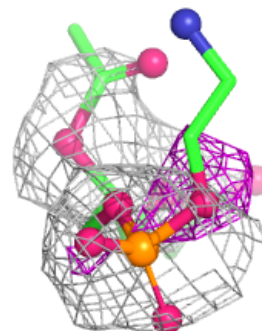
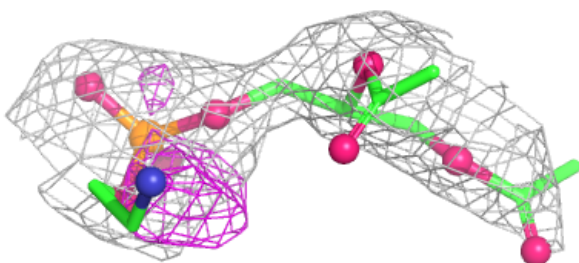
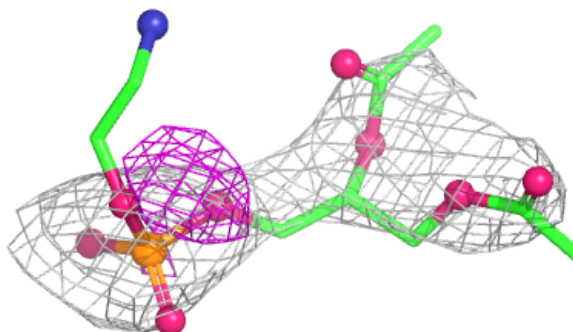


Electron density around CRT AH 102:

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

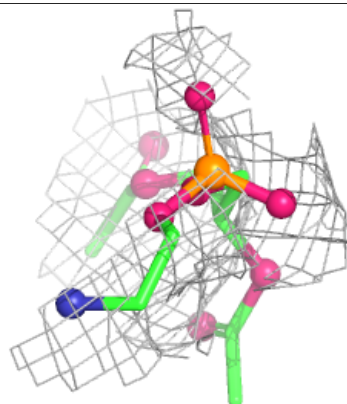
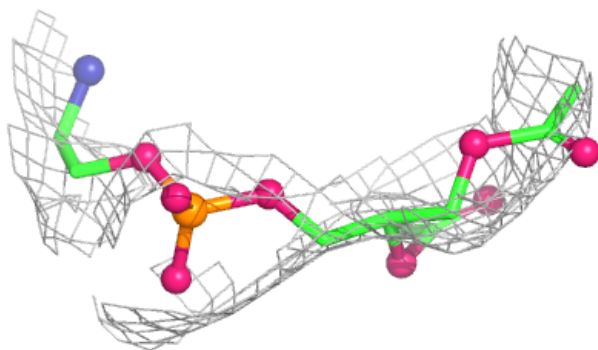
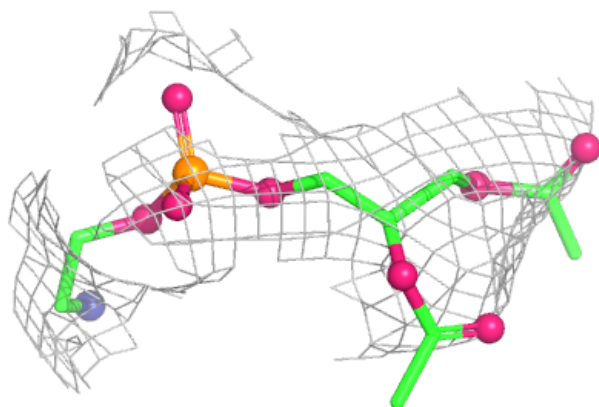
**Electron density around PEF y 408:**

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



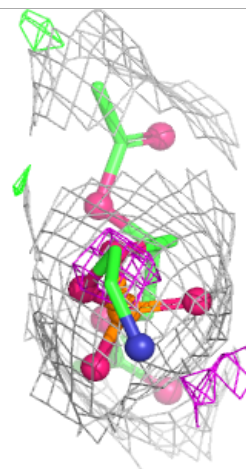
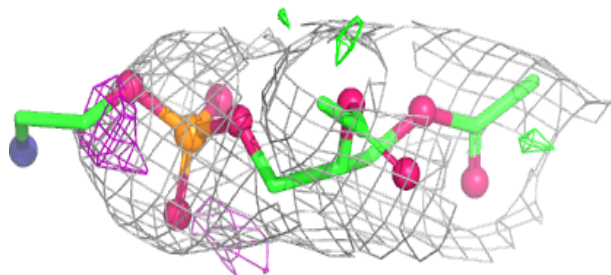
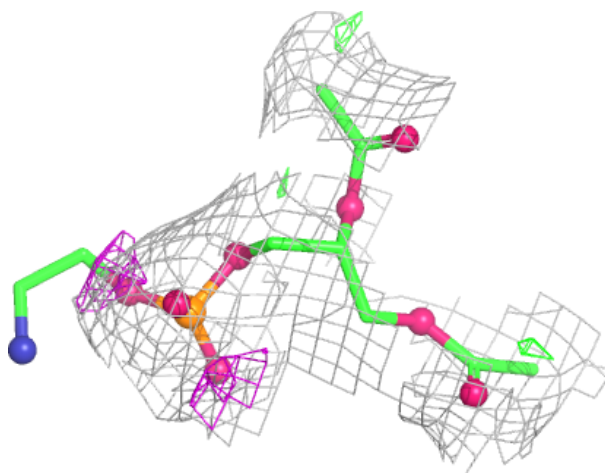
Electron density around PEF H 303:

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



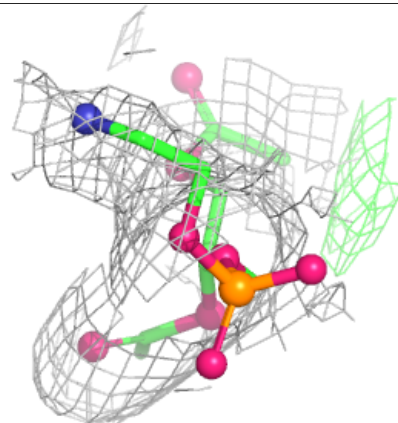
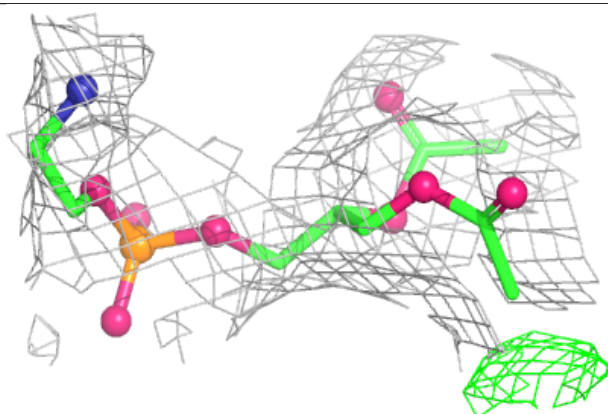
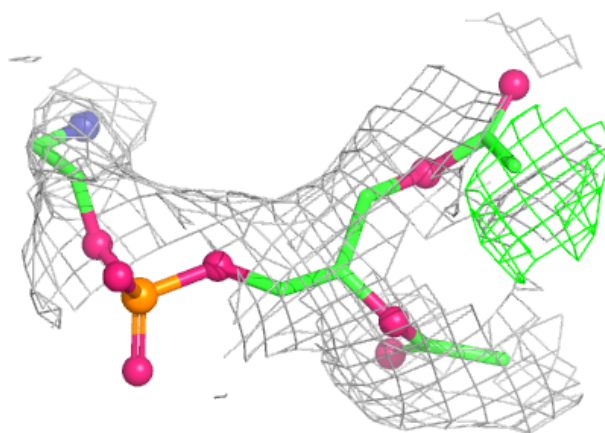
Electron density around PEF t 303:

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

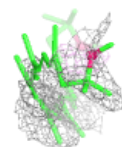
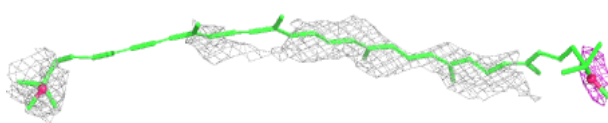
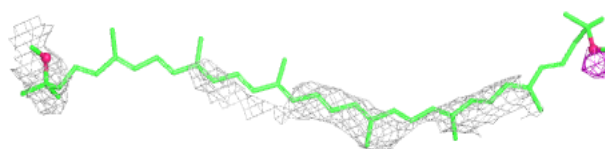


Electron density around PEF y 407:

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

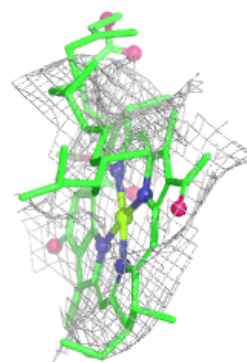
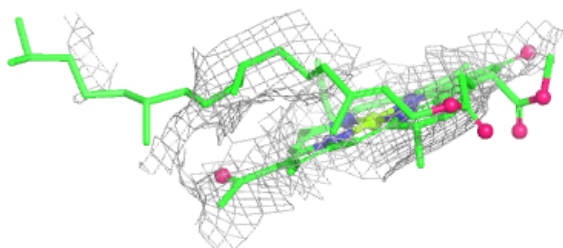
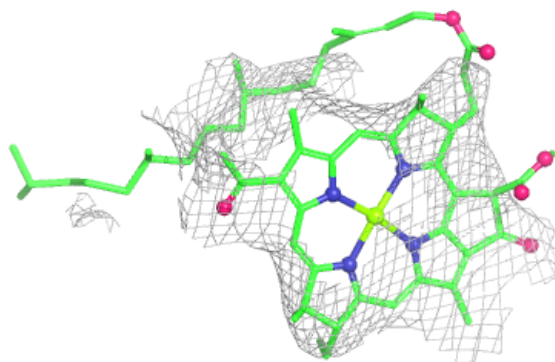
**Electron density around CRT p 103:**

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

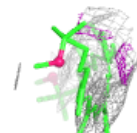
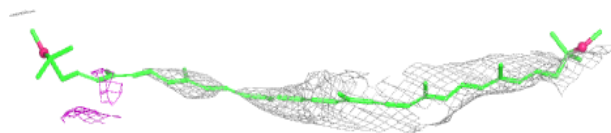
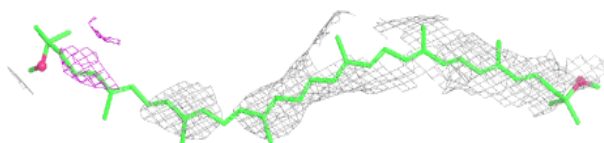


Electron density around BCL AE 104:

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

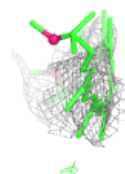
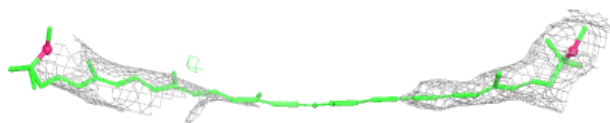
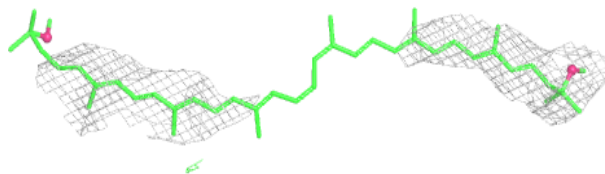
**Electron density around CRT c 101:**

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



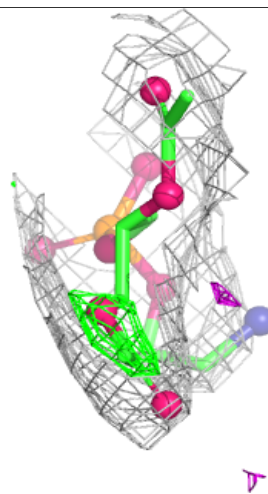
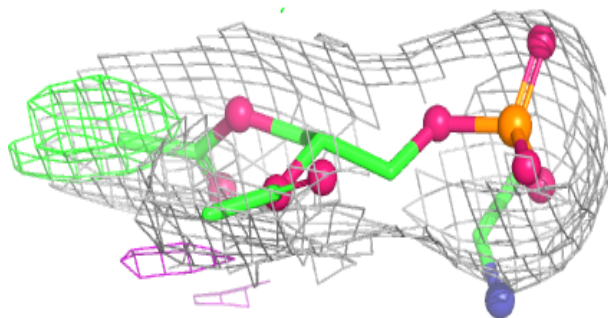
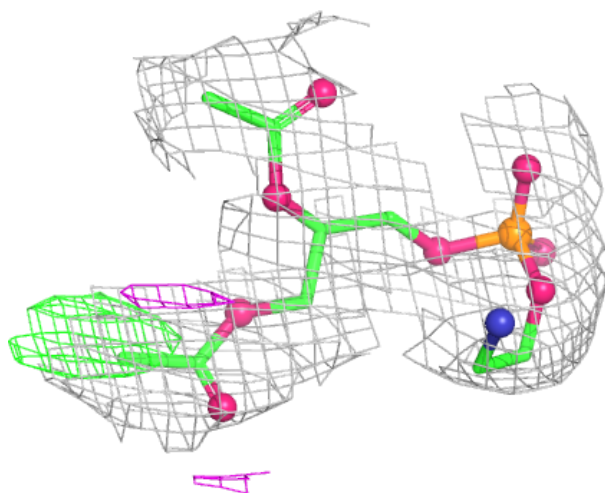
Electron density around CRT 8 101:

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



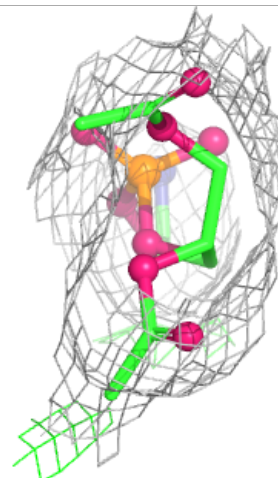
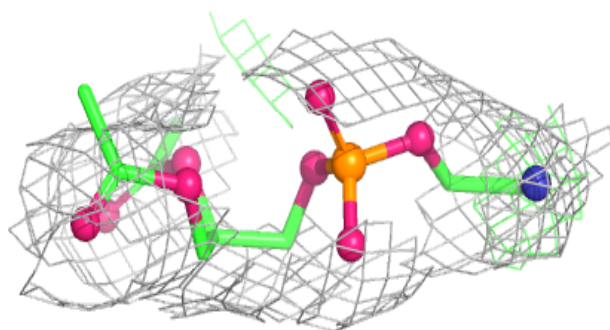
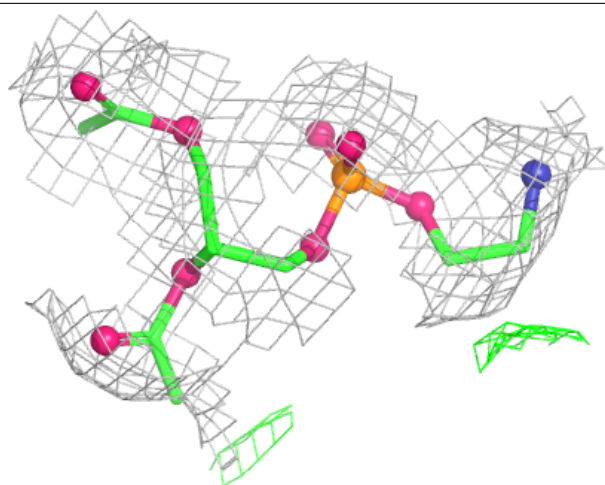
Electron density around PEF t 301:

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



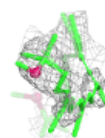
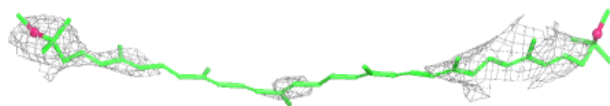
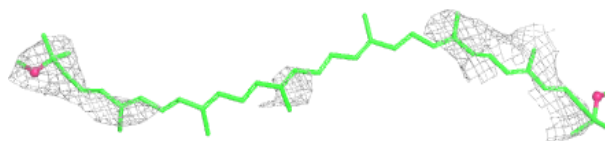
Electron density around PEF H 304:

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



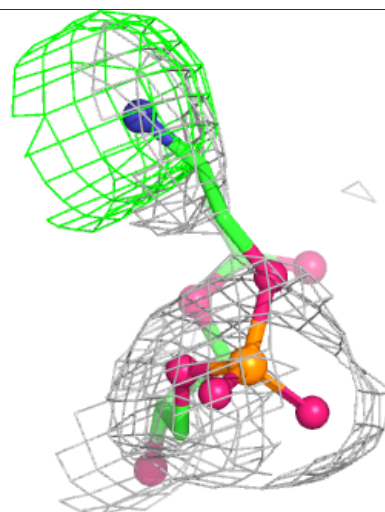
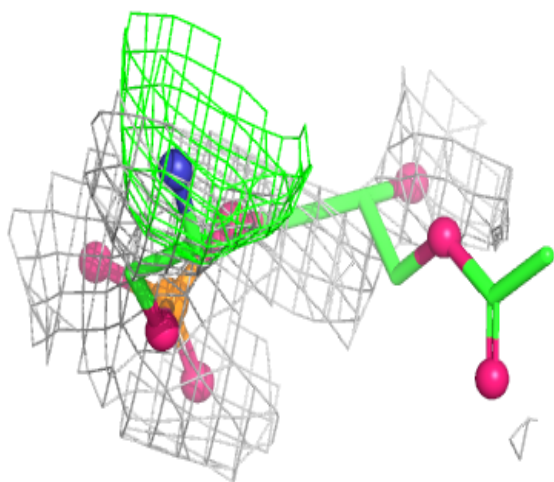
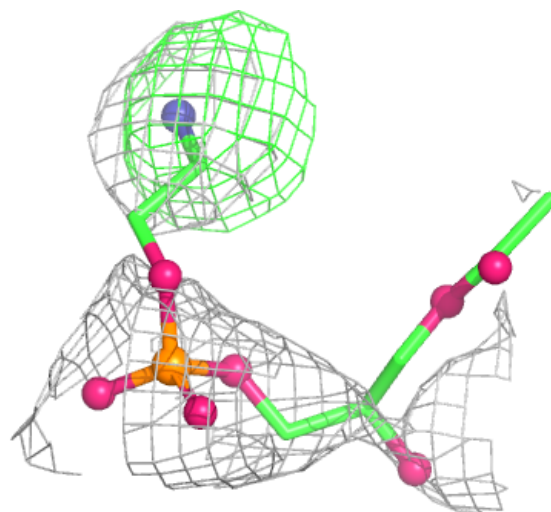
Electron density around CRT i 101:

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



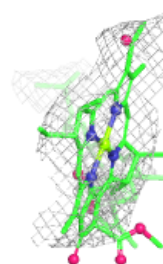
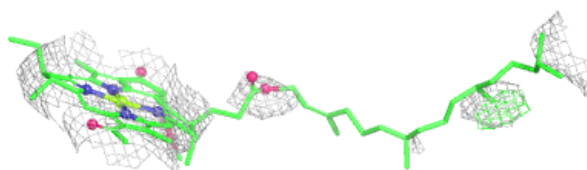
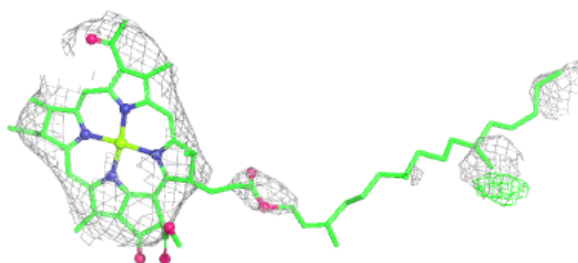
Electron density around PEF p 101:

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



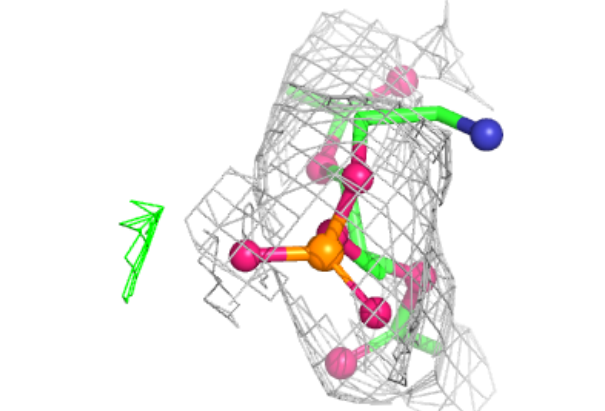
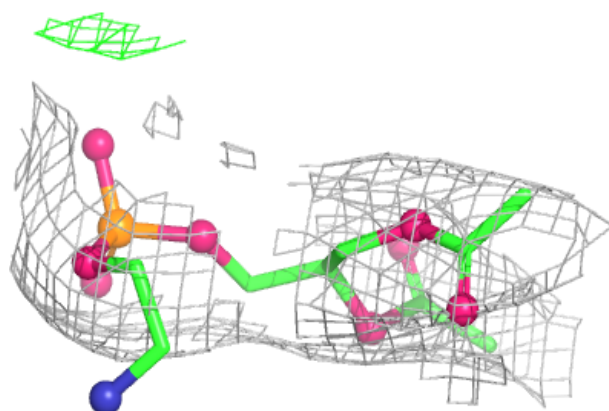
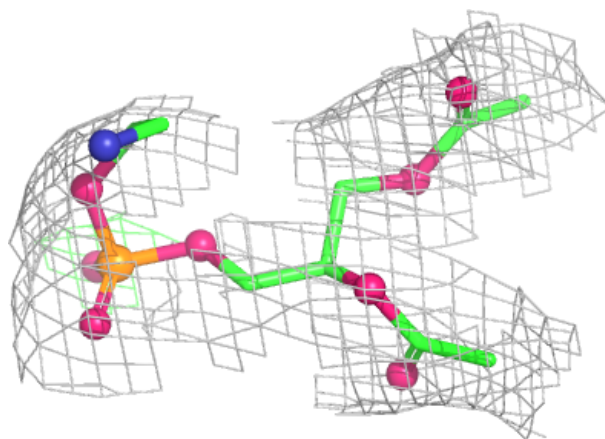
Electron density around BCL 1 101:

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



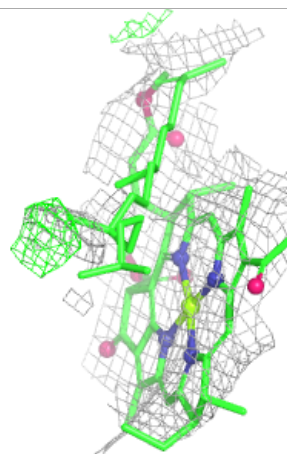
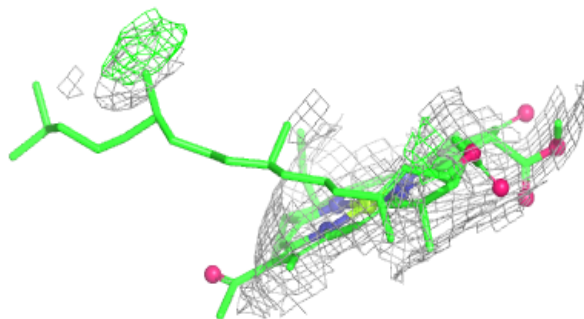
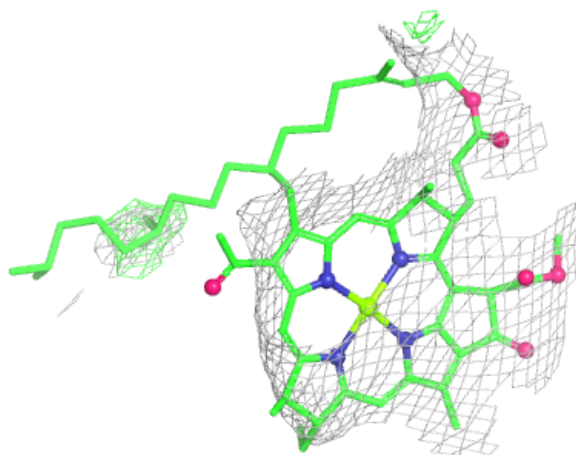
Electron density around PEF M 406:

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



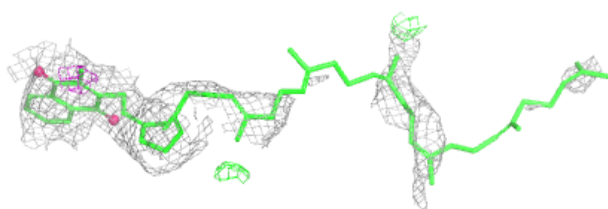
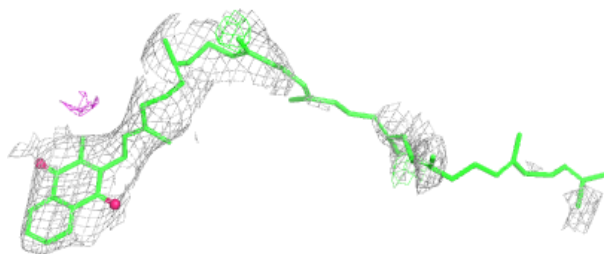
Electron density around BCL AC 102:

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

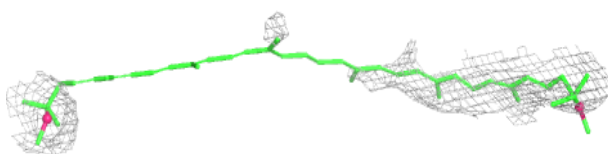
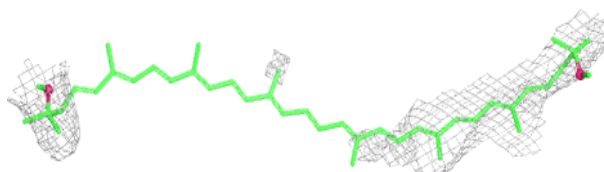


Electron density around MQ8 M 403:

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

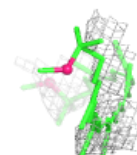
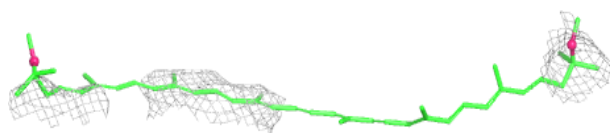
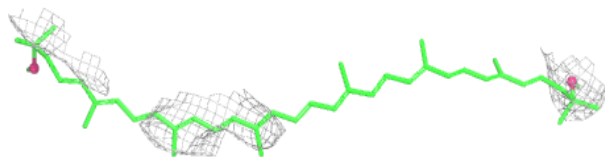
**Electron density around CRT E 101:**

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

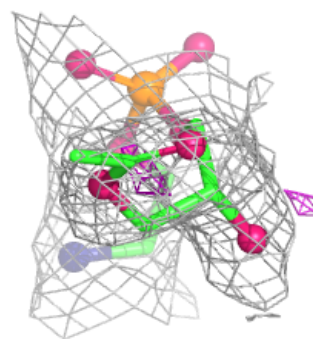
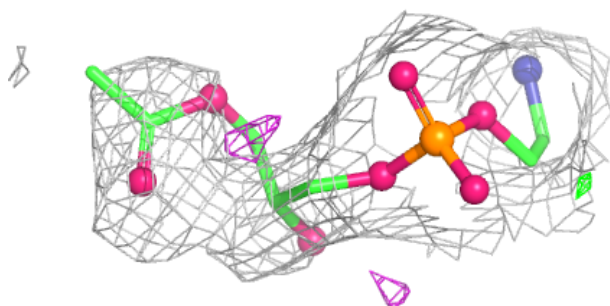
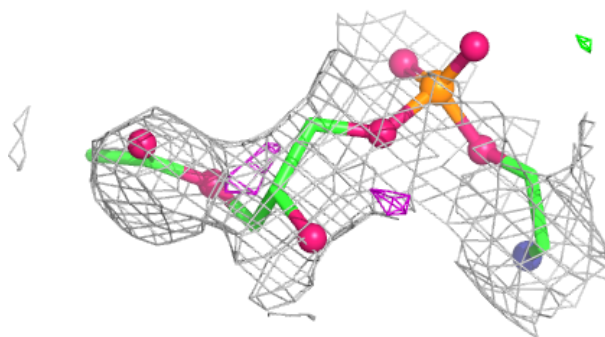


Electron density around CRT G 101:

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

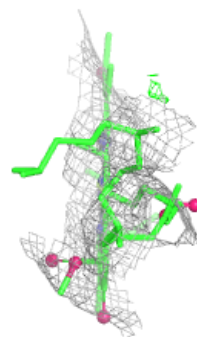
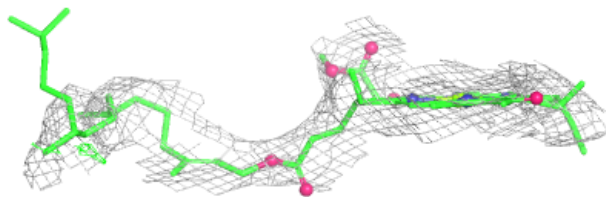
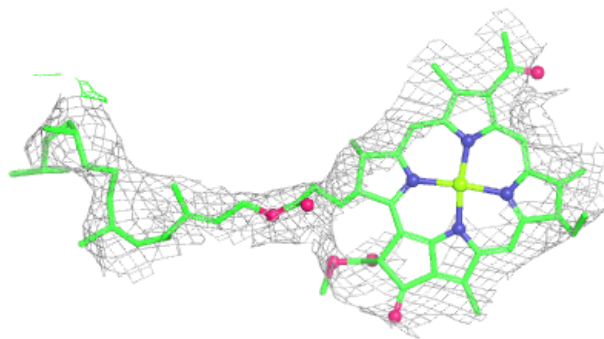
**Electron density around PEF M 407:**

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

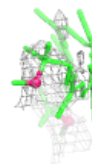
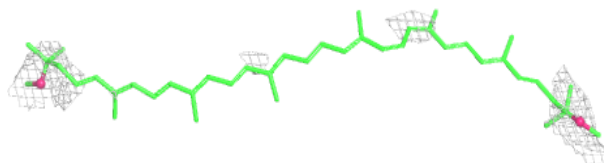


Electron density around BCL j 101:

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

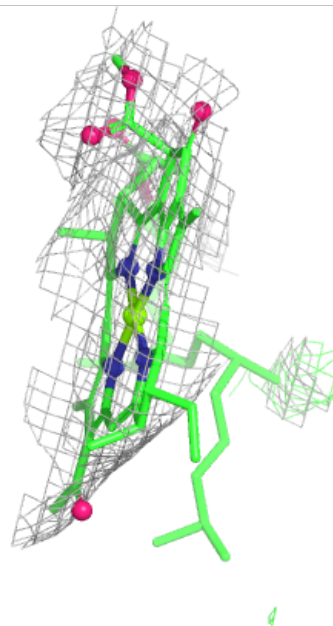
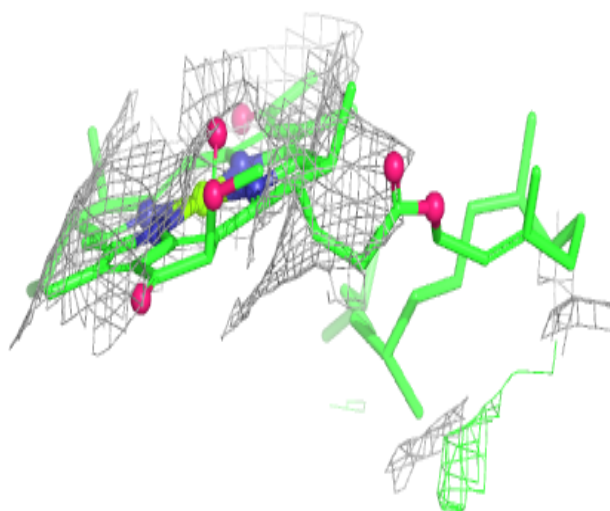
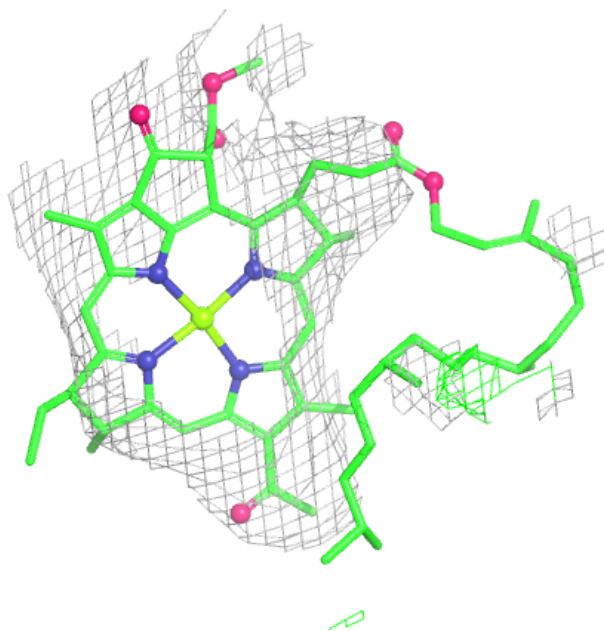
**Electron density around CRT R 101:**

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



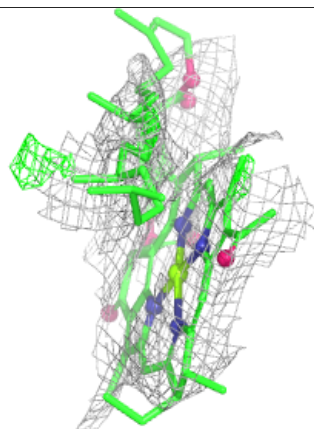
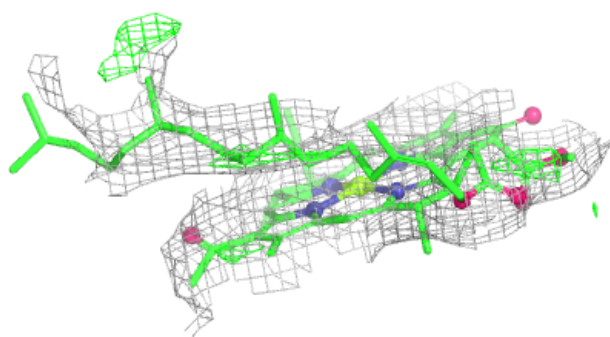
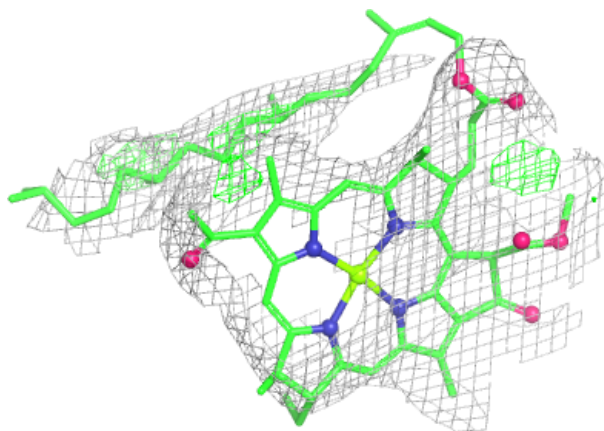
Electron density around BCL m 103:

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

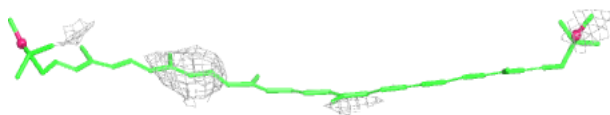
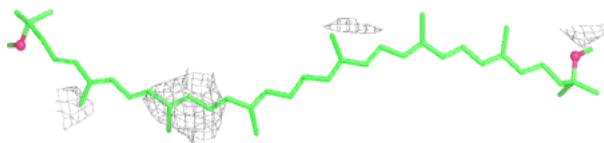


Electron density around BCL AH 103:

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

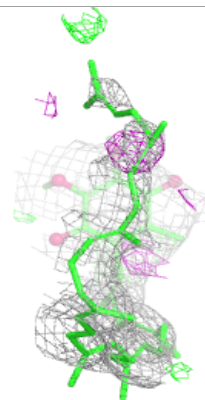
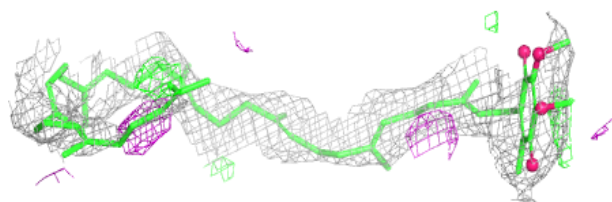
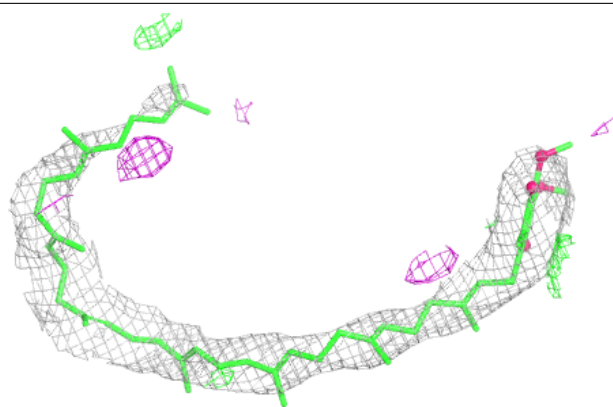
**Electron density around CRT z 101:**

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

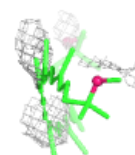
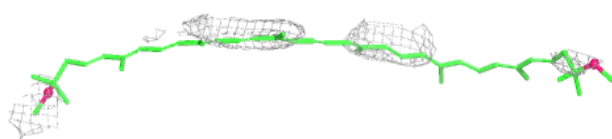


Electron density around UQ8 L 304:

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

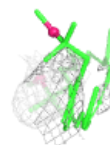
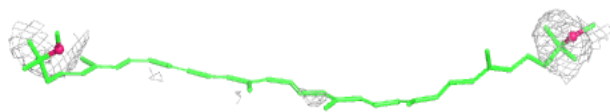
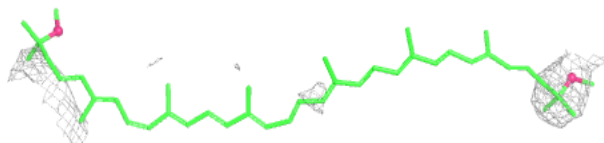
**Electron density around CRT AC 101:**

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

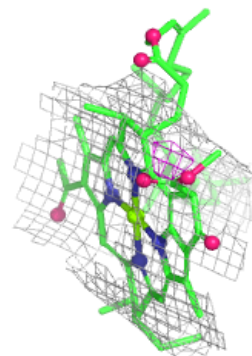
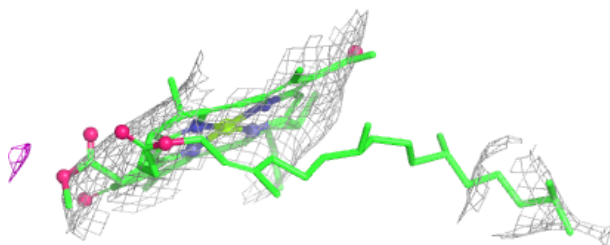
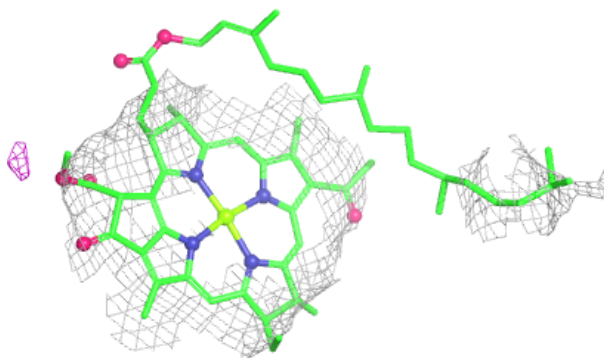


Electron density around CRT AJ 101:

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

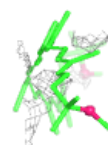
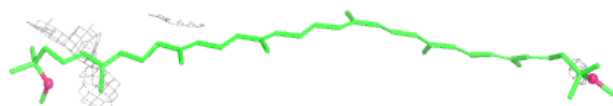
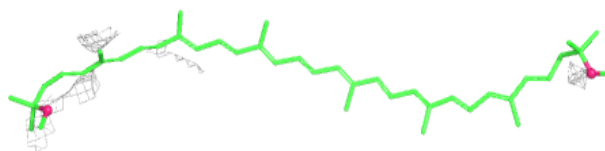
**Electron density around BCL G 102:**

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

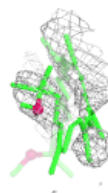
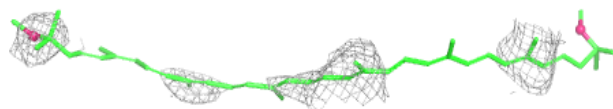
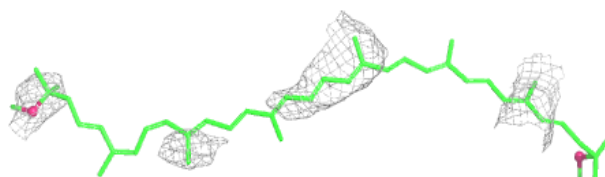


Electron density around CRT e 101:

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

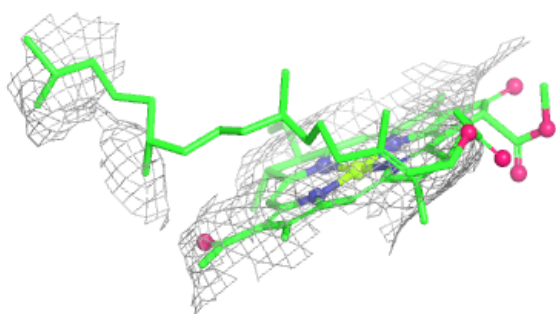
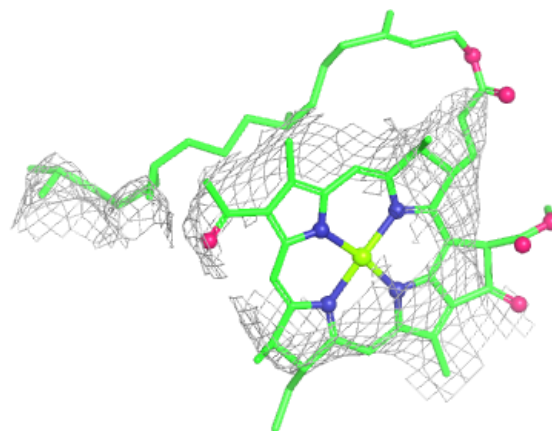
**Electron density around CRT f 102:**

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

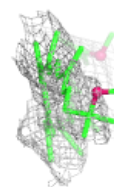
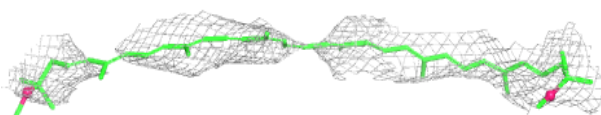
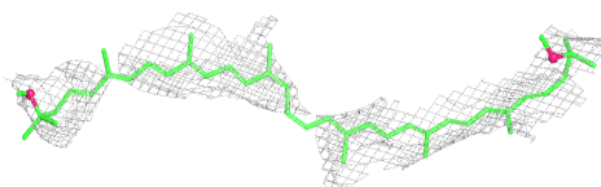


Electron density around BCL N 102:

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

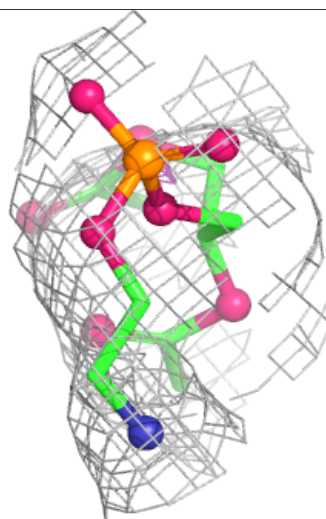
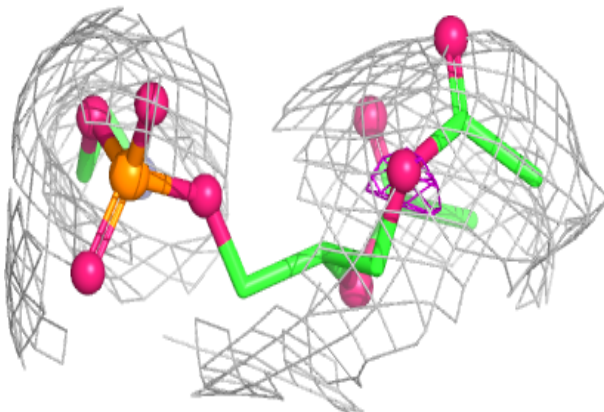
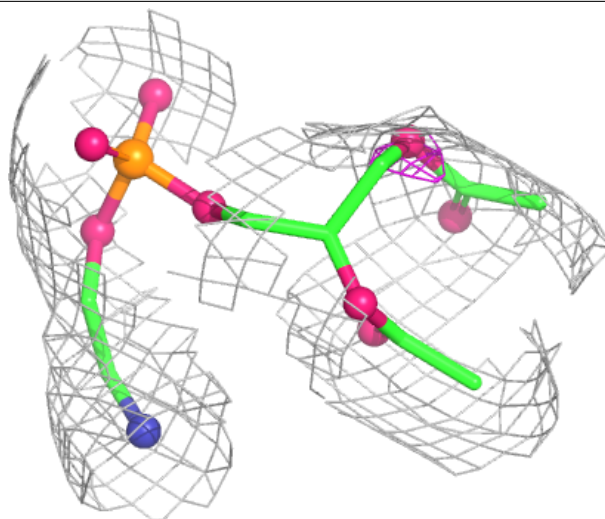
**Electron density around CRT k 101:**

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



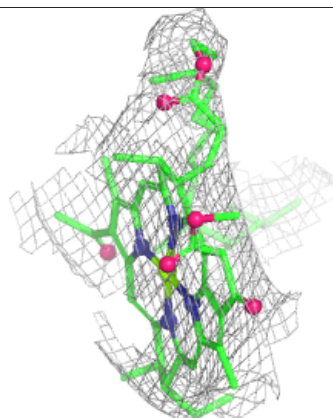
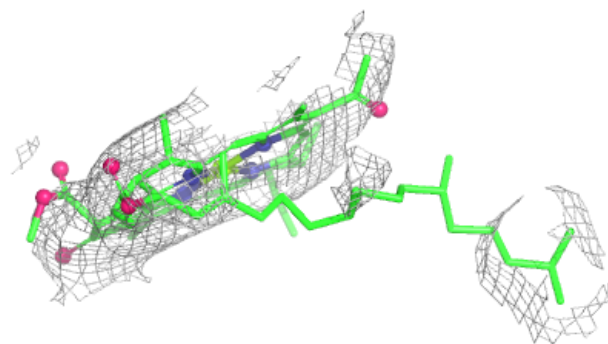
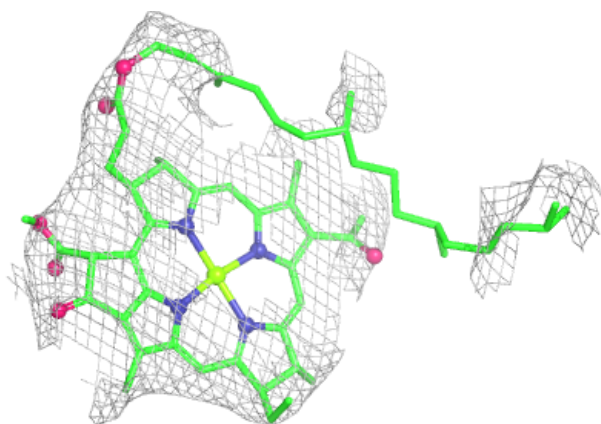
Electron density around PEF M 408:

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

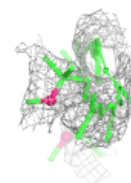
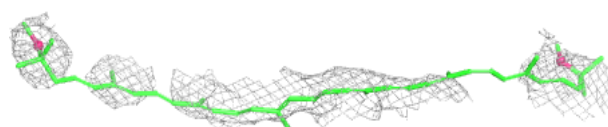
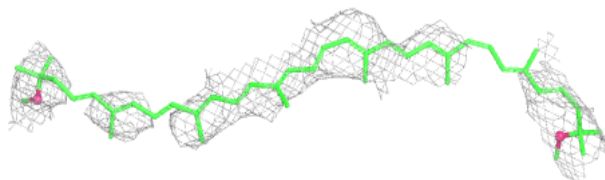


Electron density around BCL T 102:

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

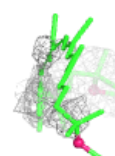
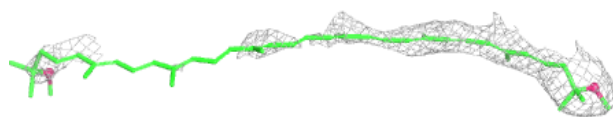
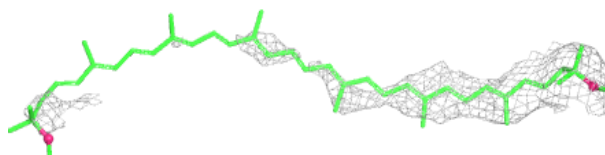
**Electron density around CRT X 101:**

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

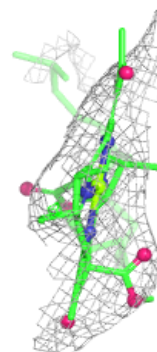
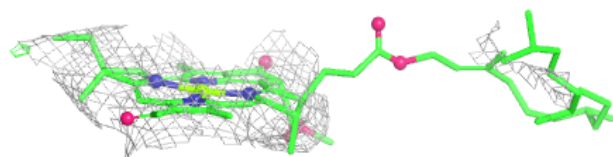
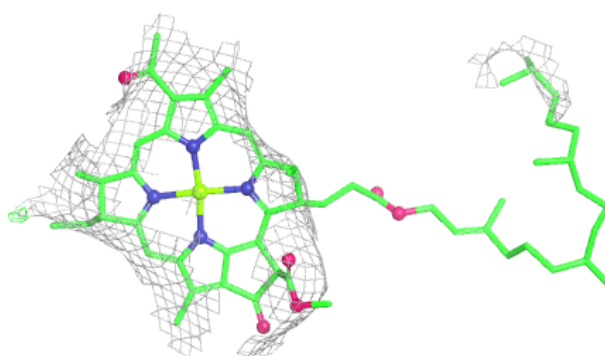


Electron density around CRT 2 101:

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

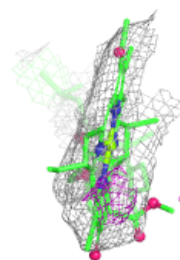
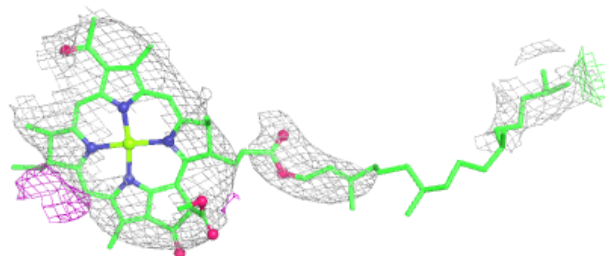
**Electron density around BCL f 101:**

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

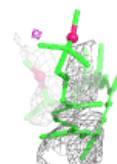
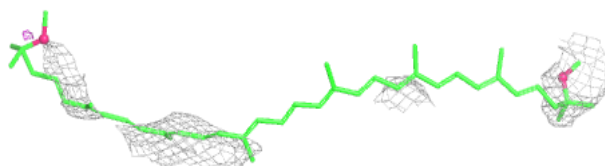


Electron density around BCL S 102:

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

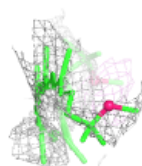
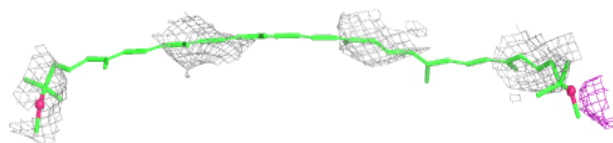
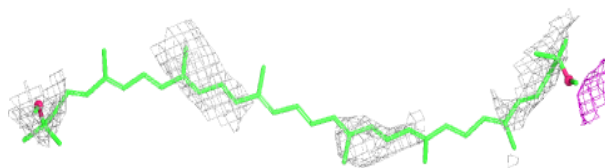
**Electron density around CRT n 101:**

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

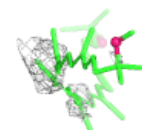
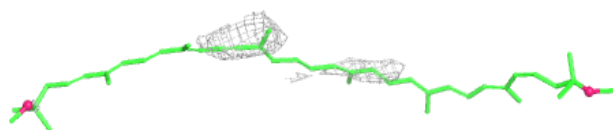


Electron density around CRT s 101:

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

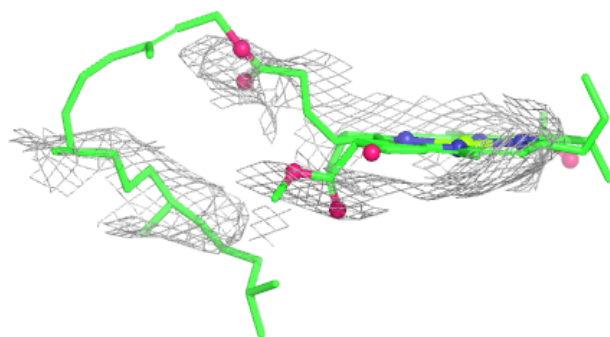
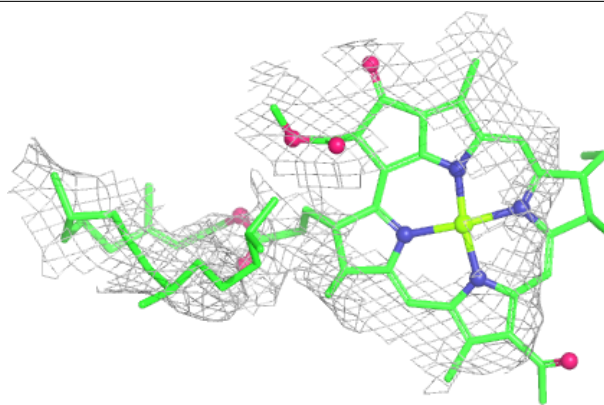
**Electron density around CRT v 101:**

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



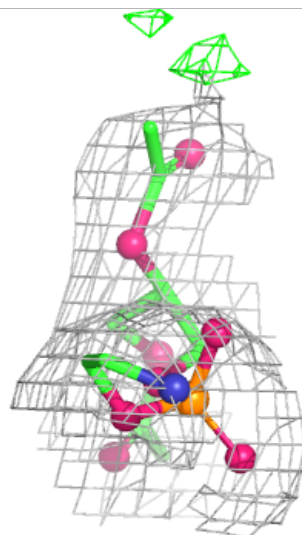
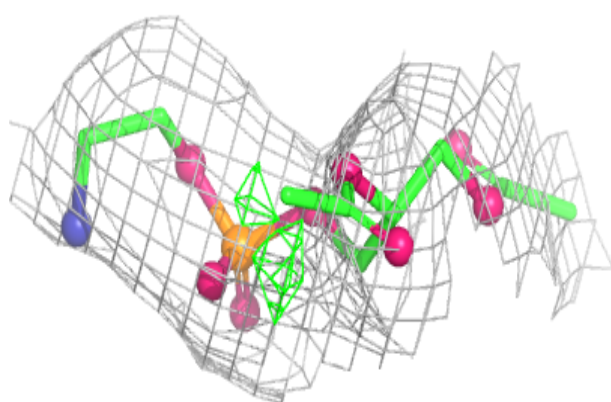
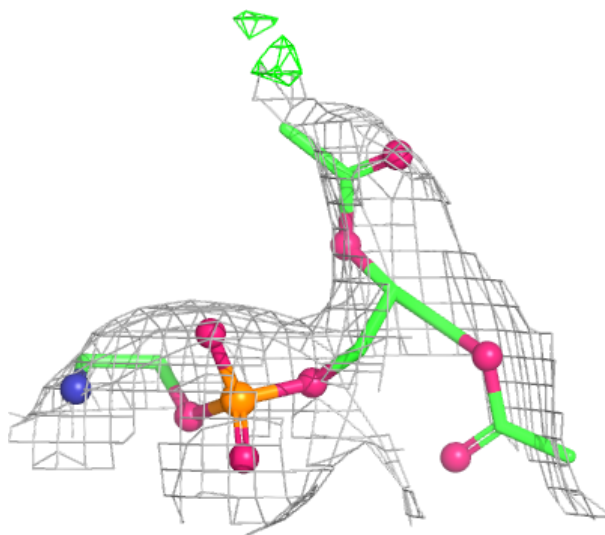
Electron density around BCL AD 101:

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



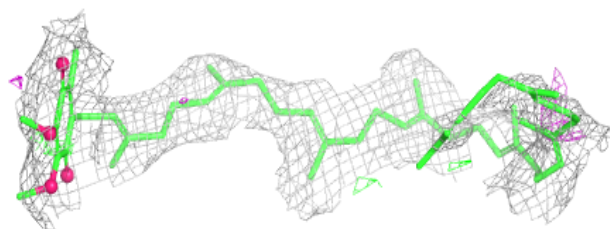
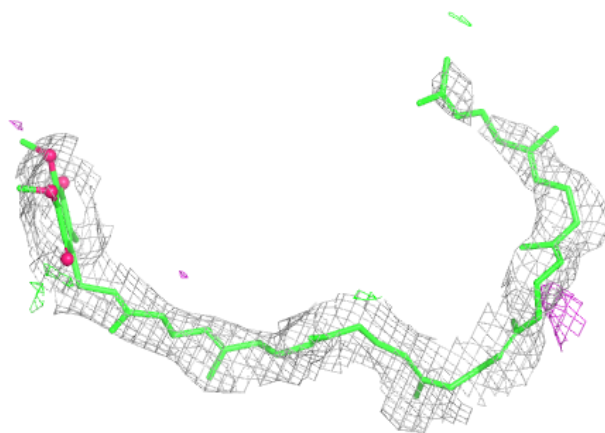
Electron density around PEF H 301:

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

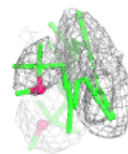
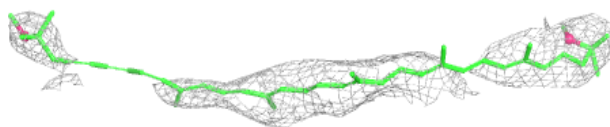
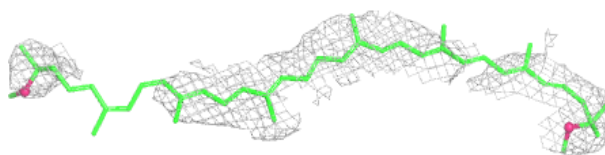


Electron density around UQ8 x 304:

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

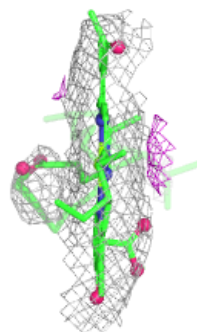
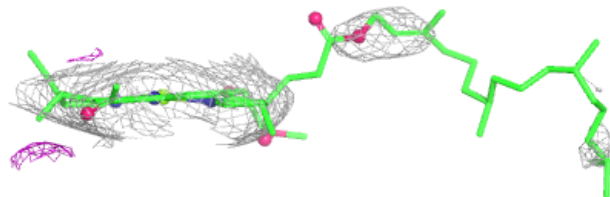
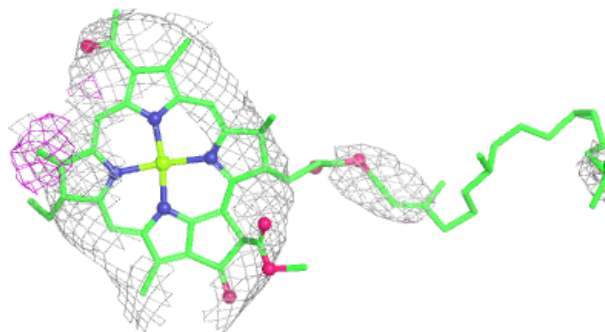
**Electron density around CRT 4 101:**

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

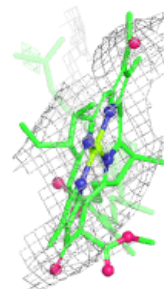
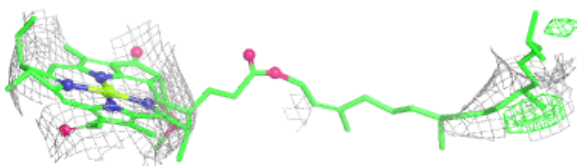
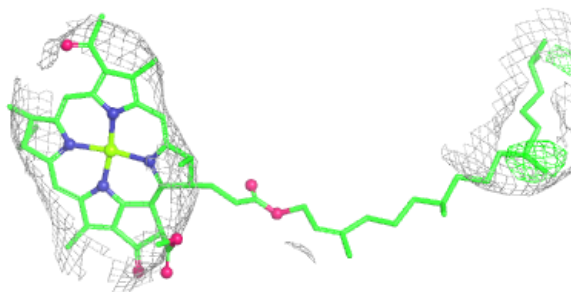


Electron density around BCL AK 101:

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

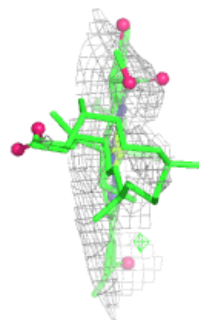
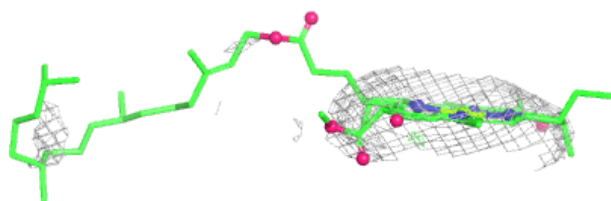
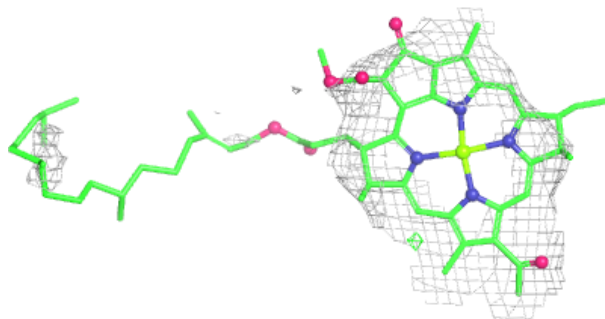
**Electron density around BCL d 101:**

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

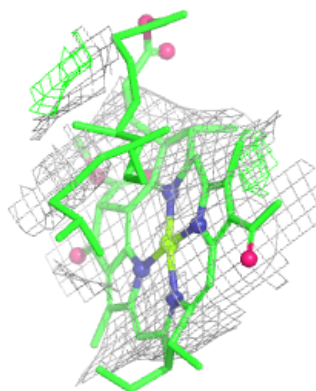
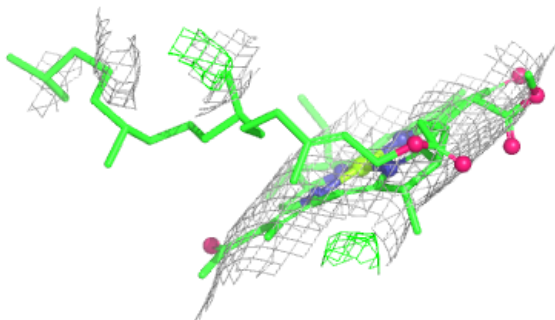
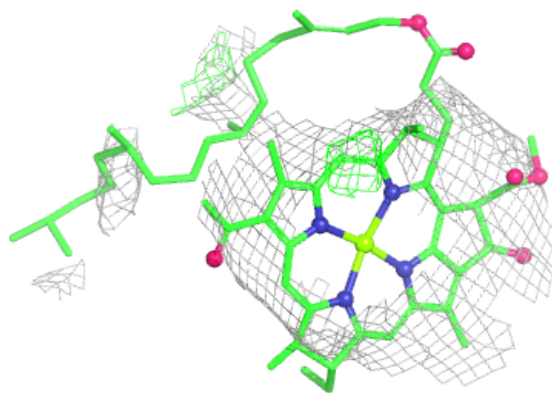


Electron density around BCL K 101:

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

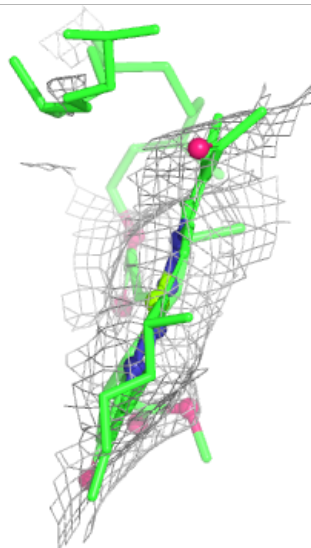
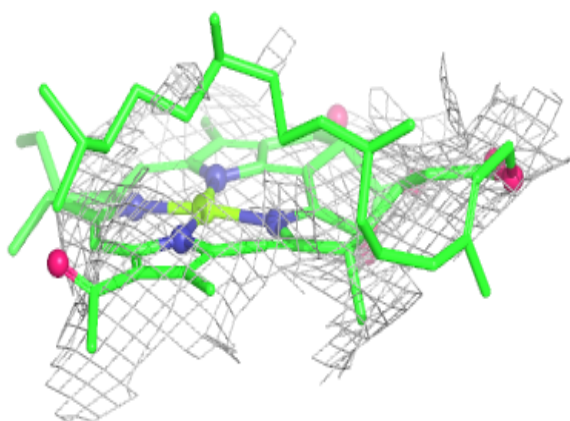
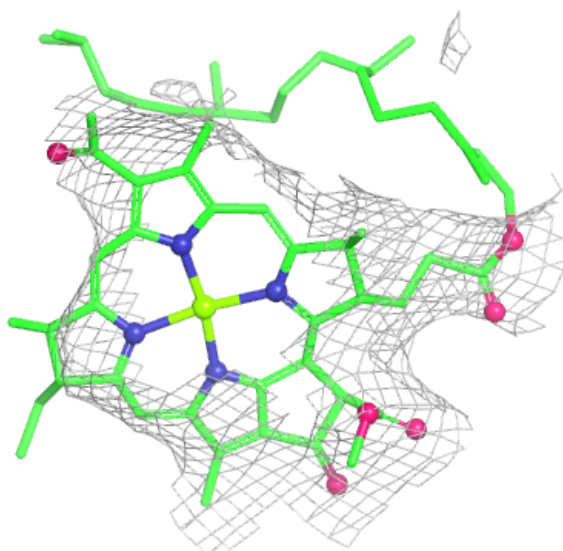
**Electron density around BCL v 102:**

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



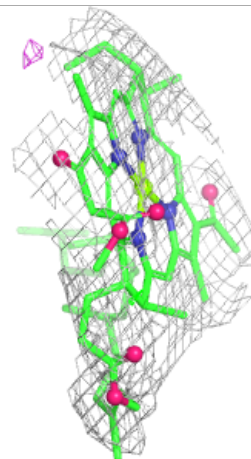
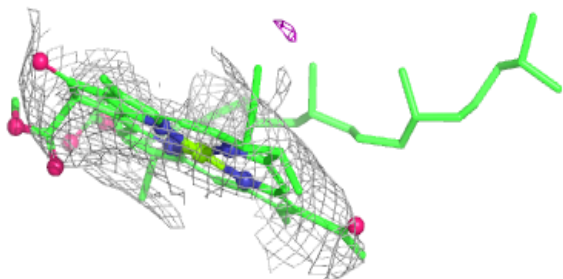
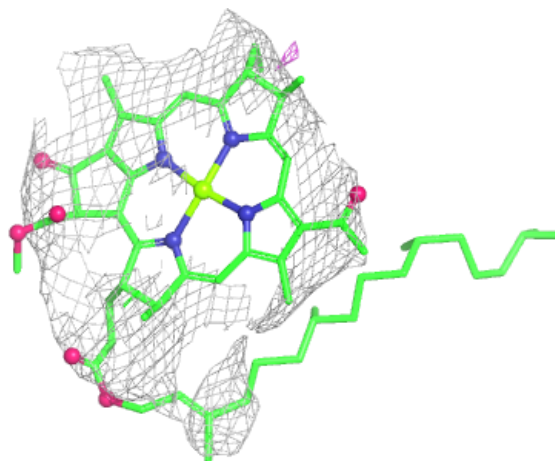
Electron density around BCL k 102:

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



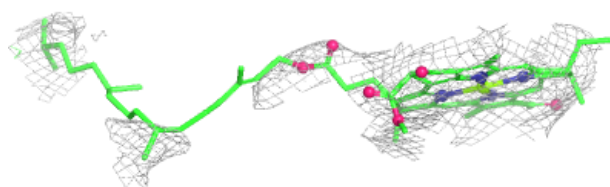
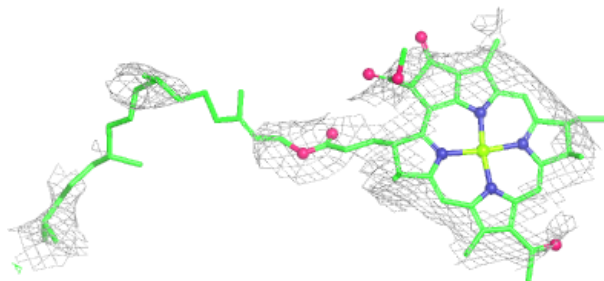
Electron density around BCL R 102:

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

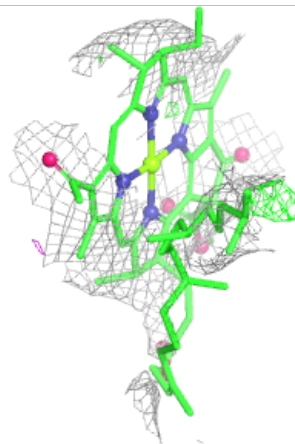
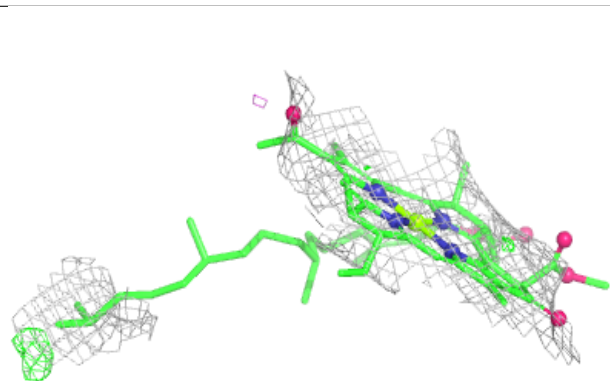
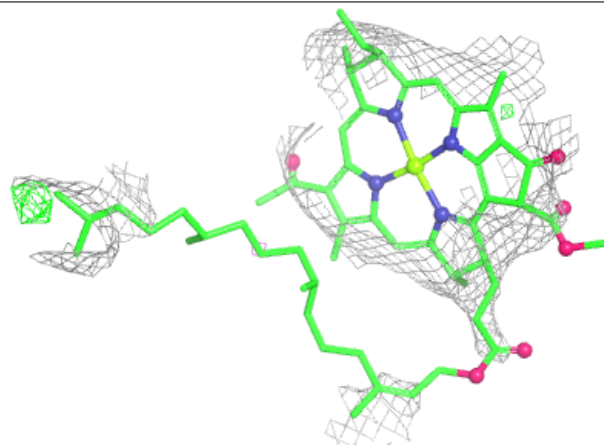


Electron density around BCL AE 102:

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

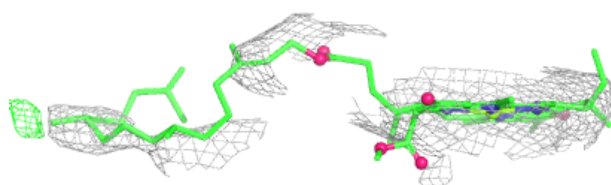
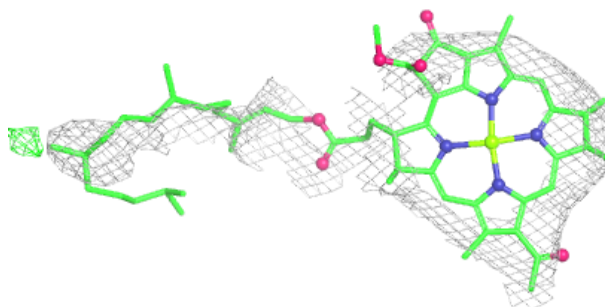
**Electron density around BCL 1 102:**

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

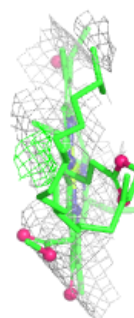
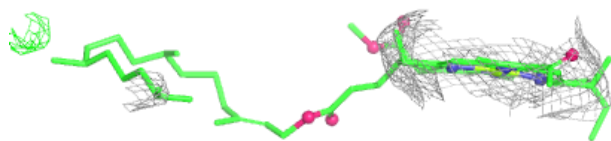
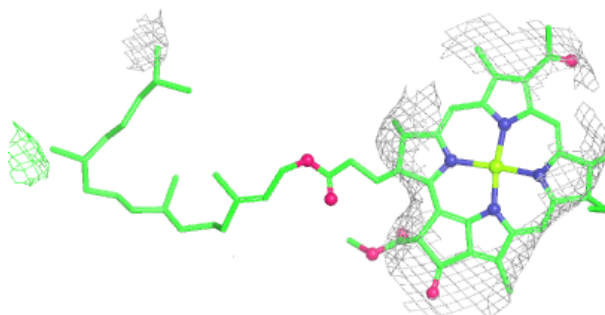


Electron density around BCL AH 101:

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

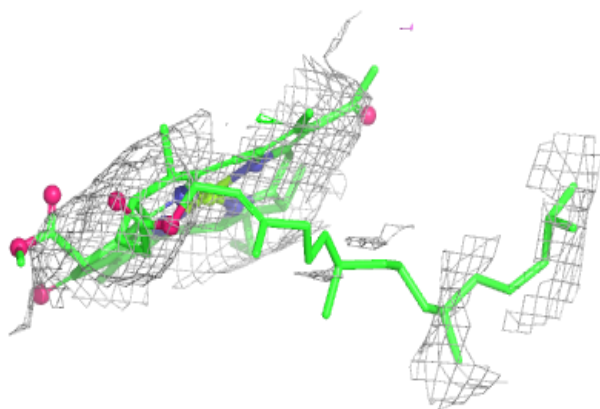
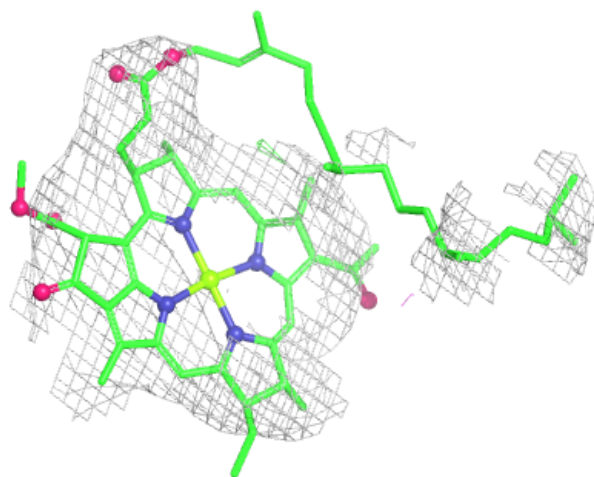
**Electron density around BCL 9 103:**

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



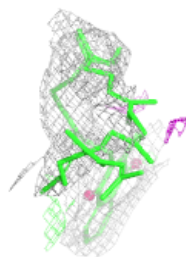
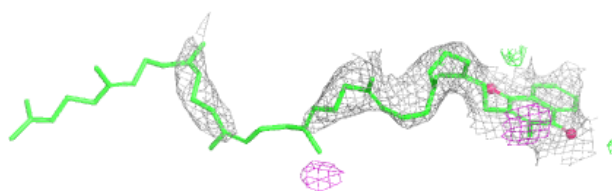
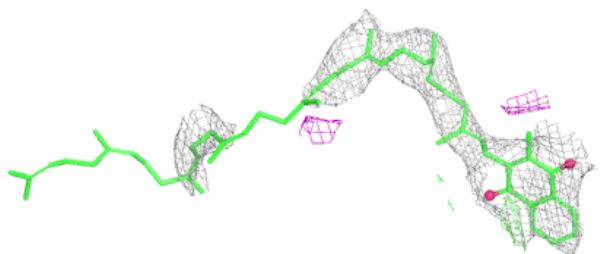
Electron density around BCL AJ 102:

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

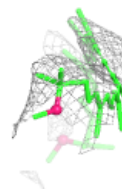
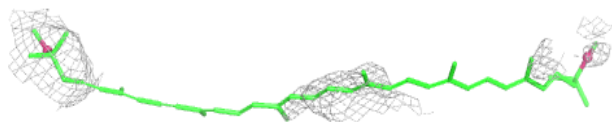
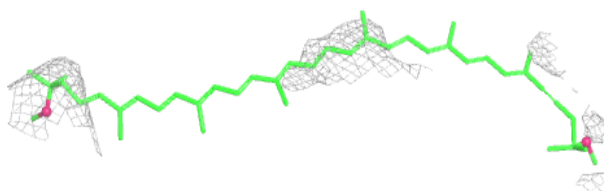


Electron density around MQ8 y 403:

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

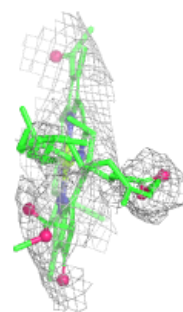
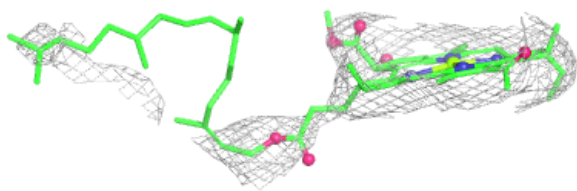
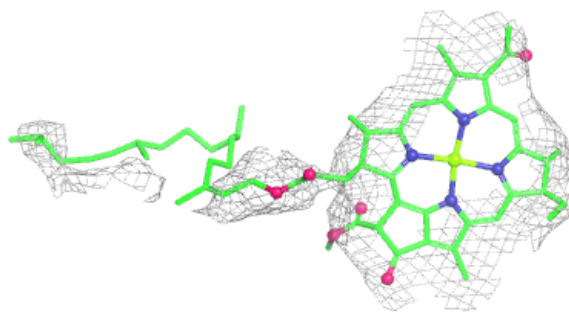
**Electron density around CRT A 103:**

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



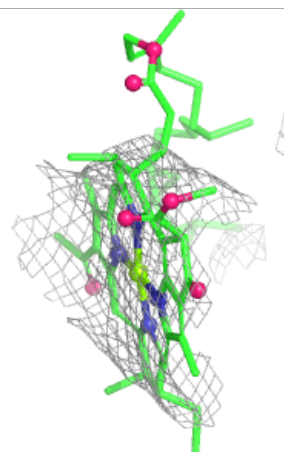
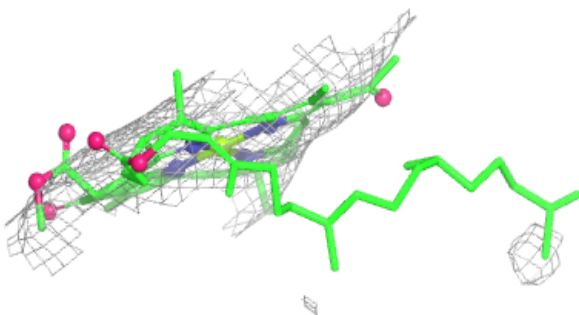
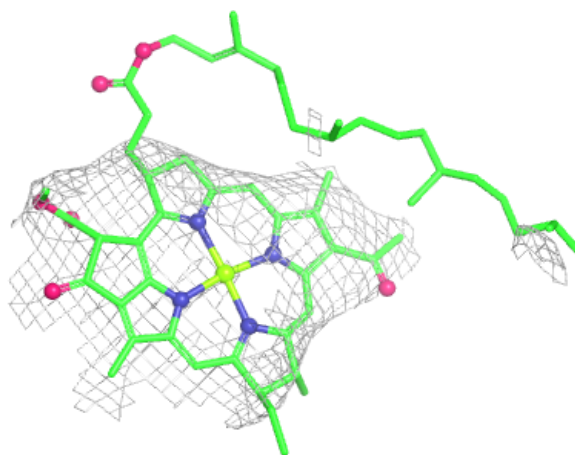
Electron density around BCL h 101:

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



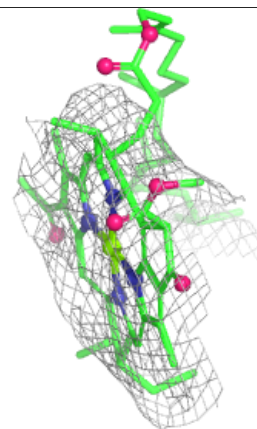
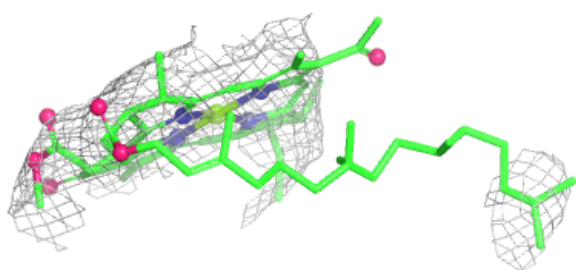
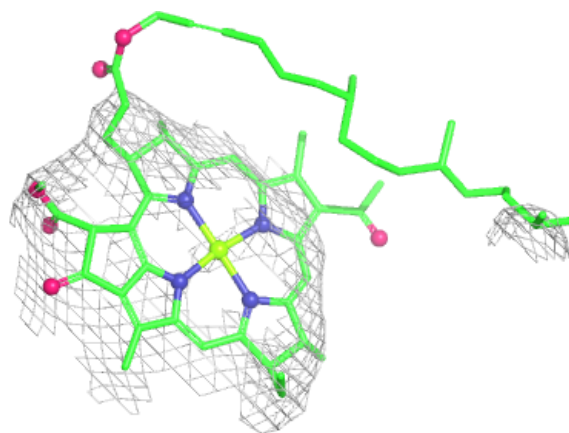
Electron density around BCL z 102:

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



Electron density around 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)

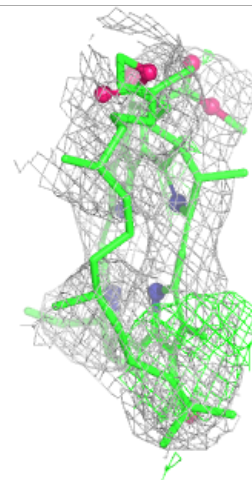
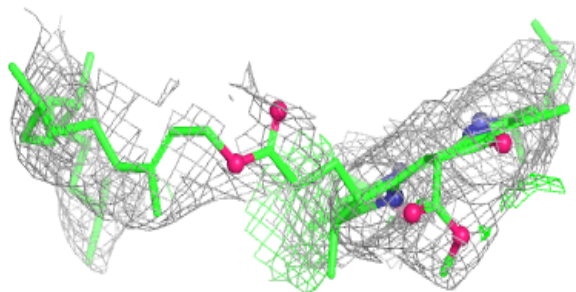
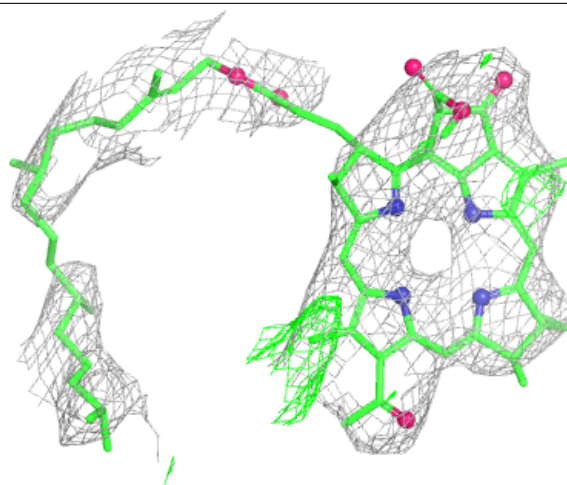
**Electron density around CRT U 102:**

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



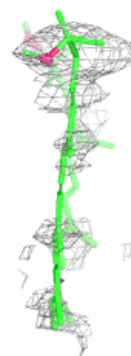
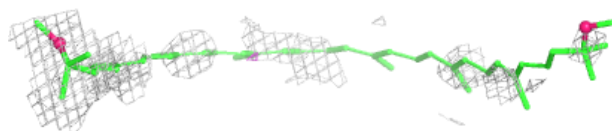
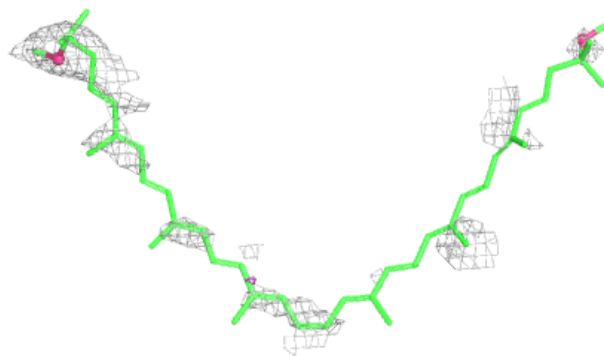
Electron density around BPH L 302:

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

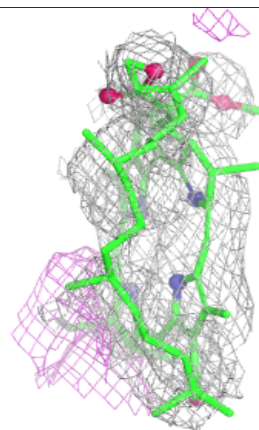
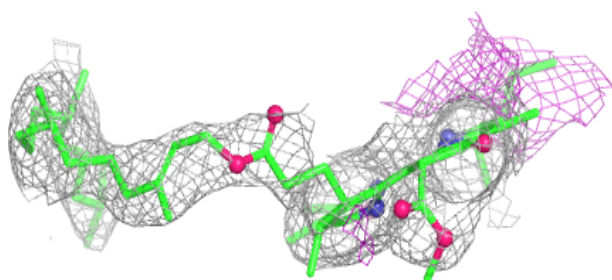
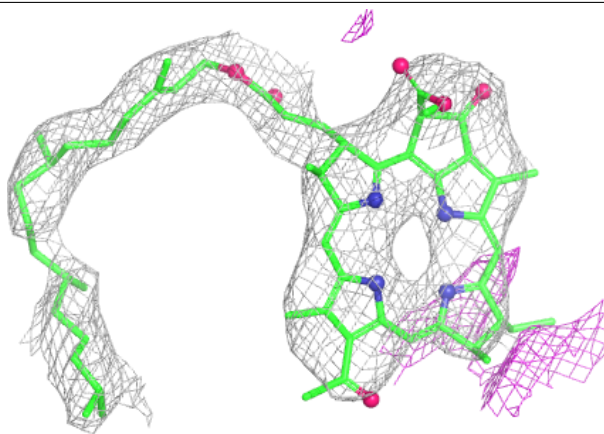


Electron density around CRT M 404:

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

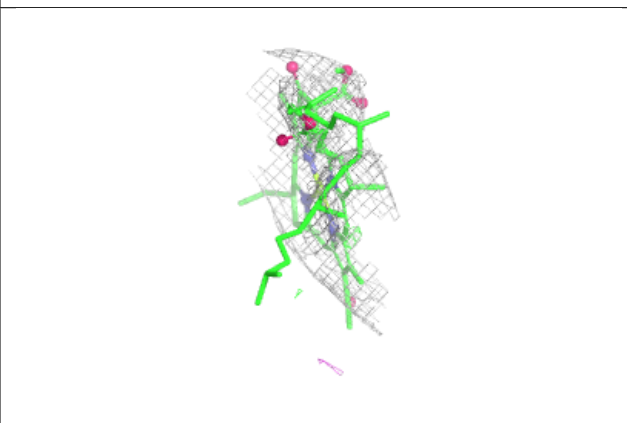
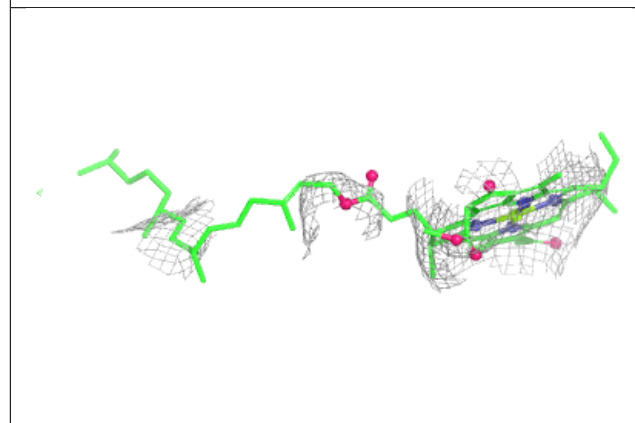
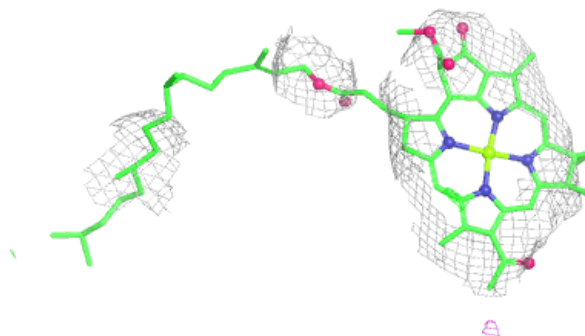
**Electron density around BPH x 302:**

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

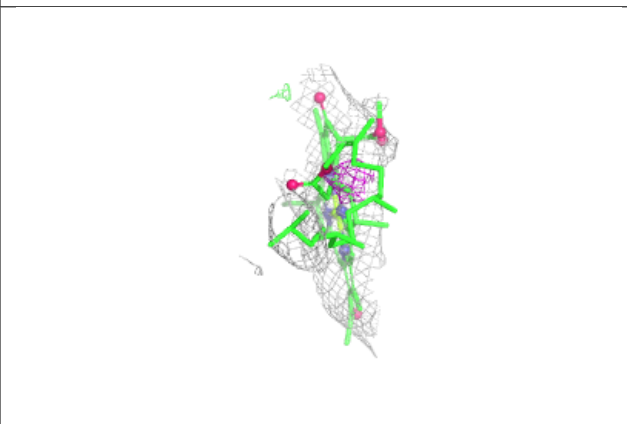
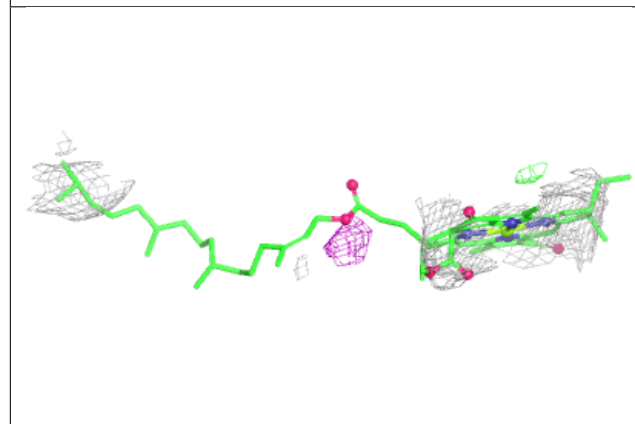
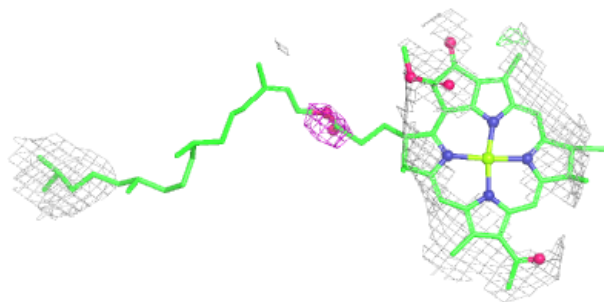


Electron density around BCL u 101:

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

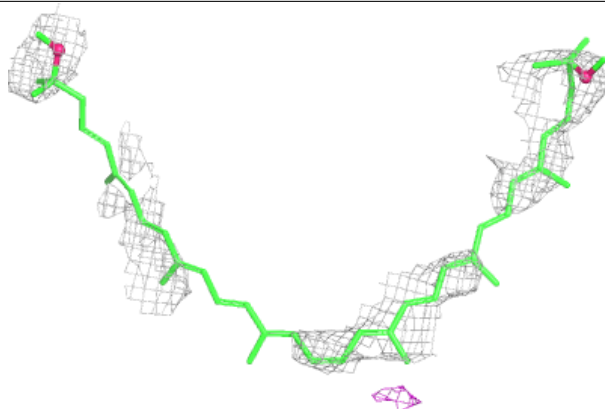
**Electron density around BCL p 102:**

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

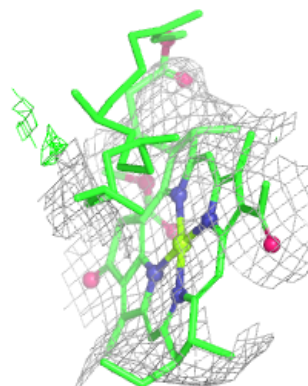
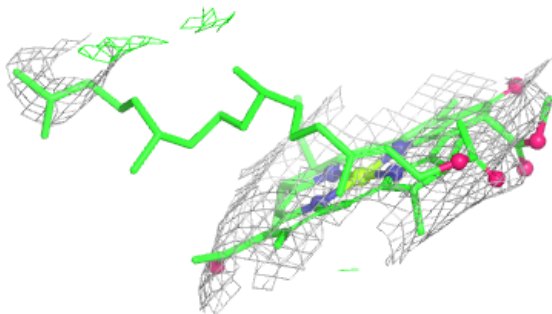
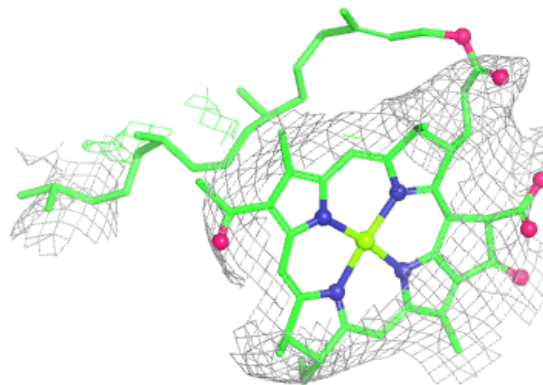


Electron density around CRT y 404:

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

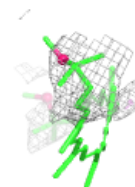
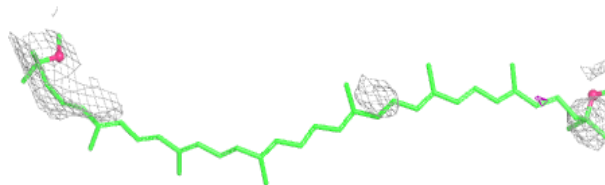
**Electron density around BCL J 102:**

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

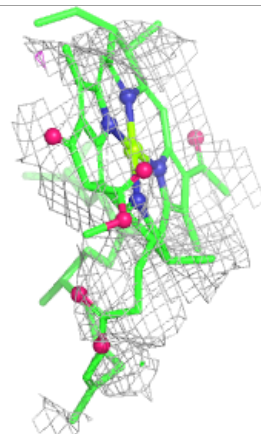
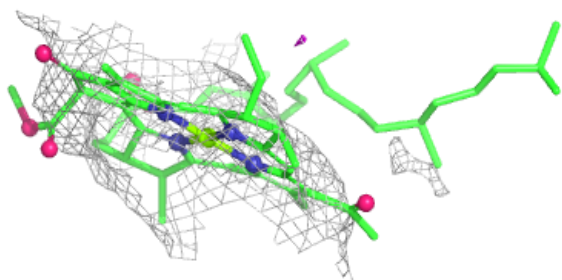
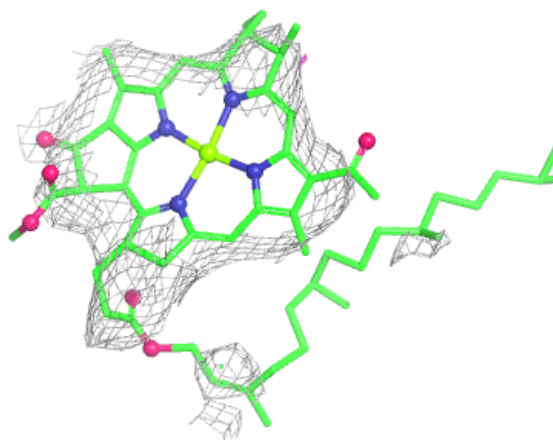


Electron density around CRT T 101:

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

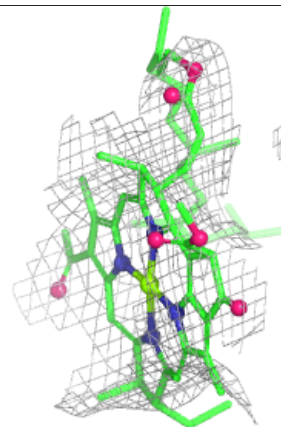
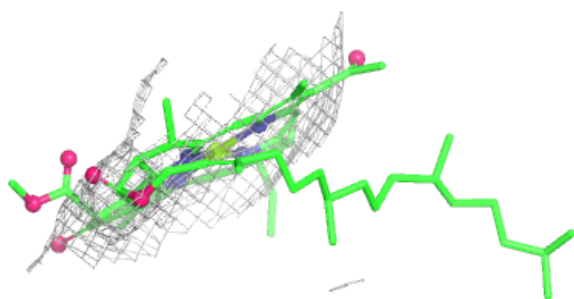
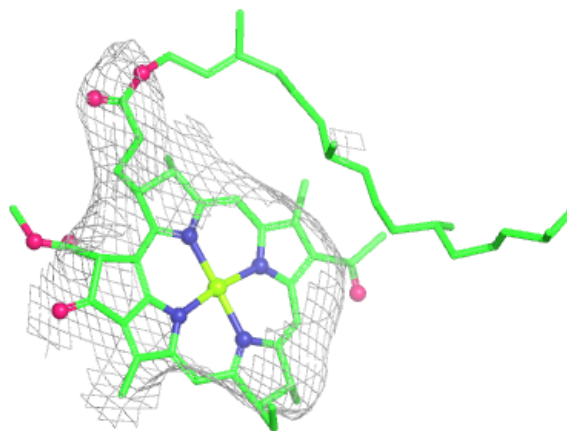
**Electron density around BCL 5 102:**

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



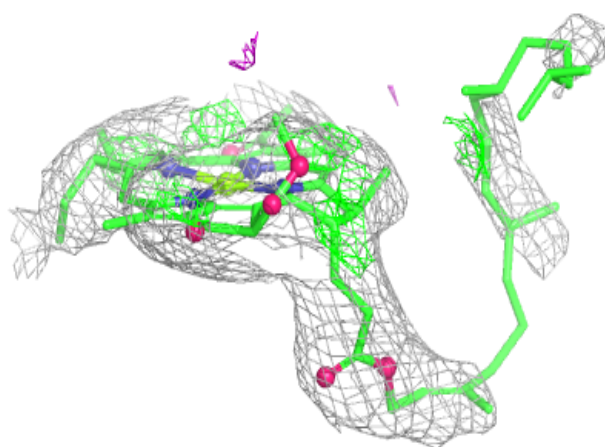
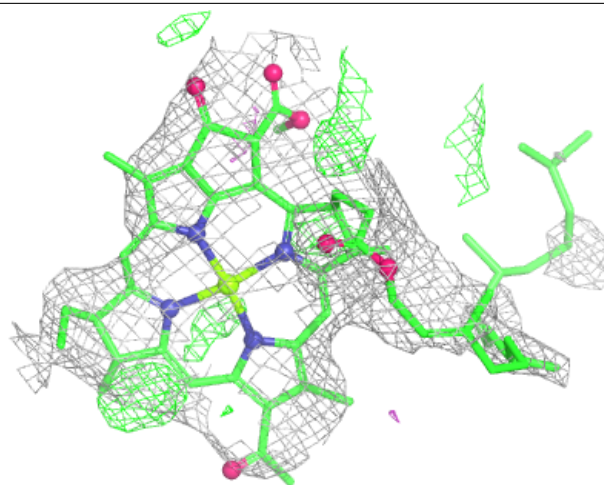
Electron density around BCL c 102:

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



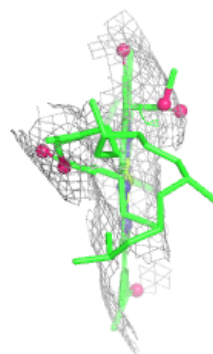
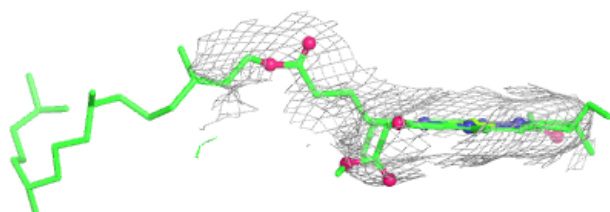
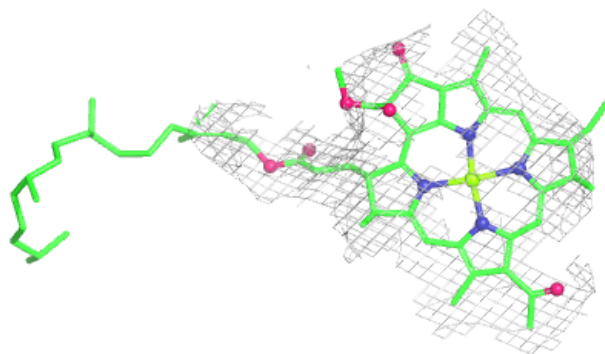
Electron density around BCL L 303:

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

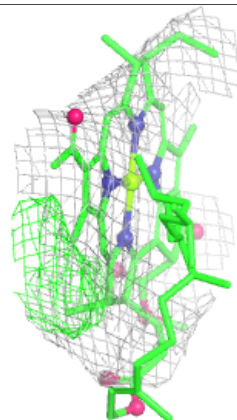
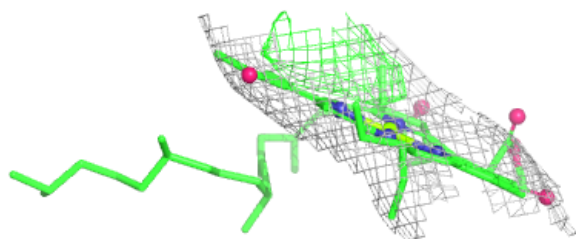
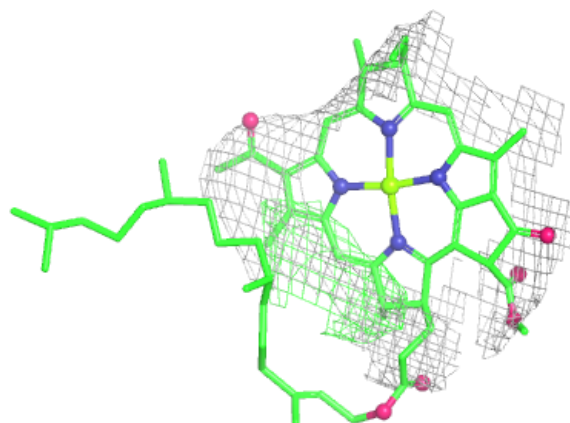


Electron density around BCL m 102:

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

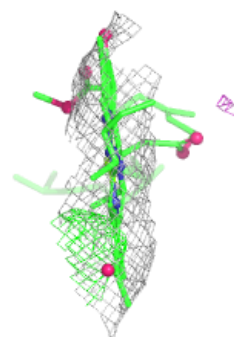
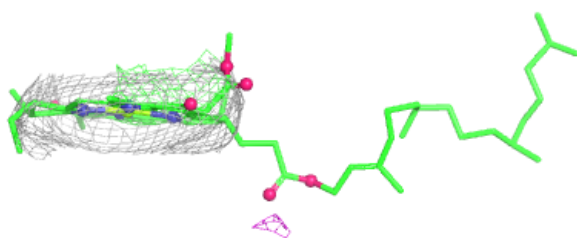
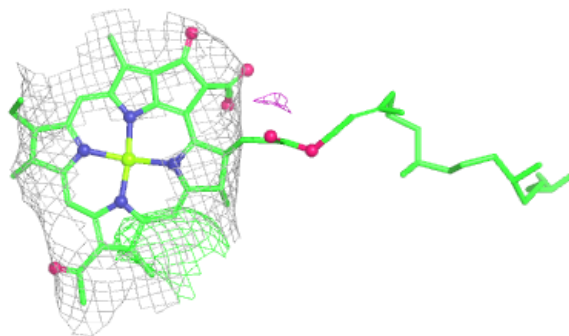
**Electron density around BCL D 102:**

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

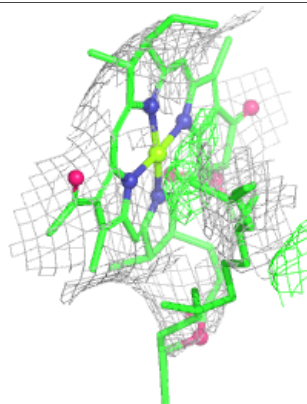
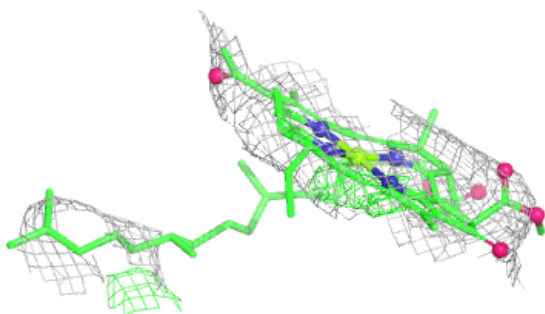
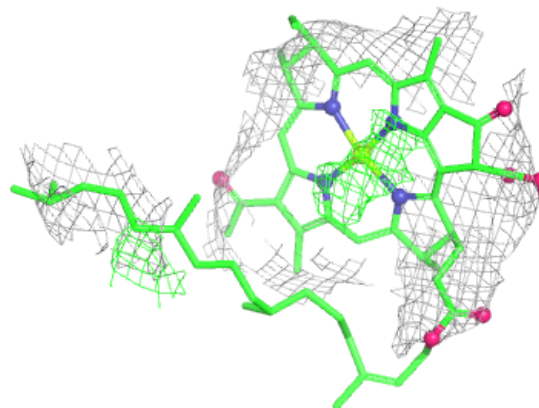


Electron density around BCL F 101:

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

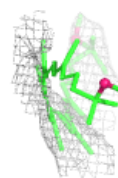
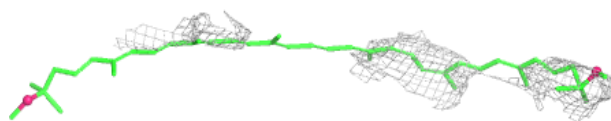
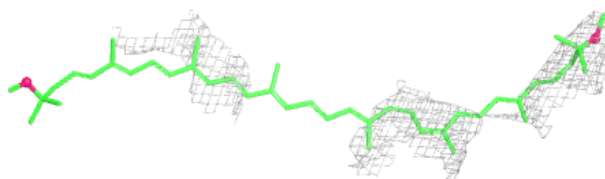
**Electron density around BCL AL 102:**

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

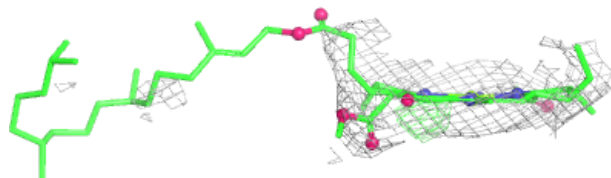
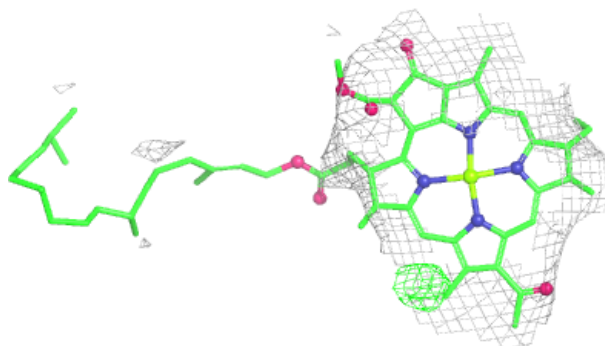


Electron density around CRT AD 102:

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

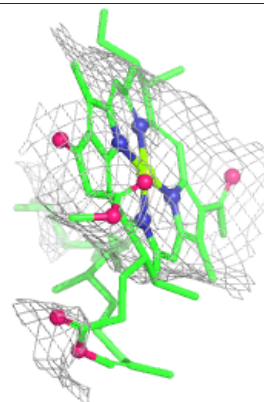
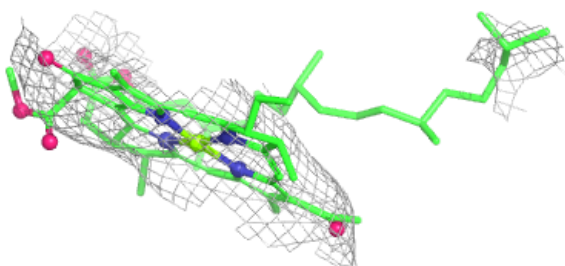
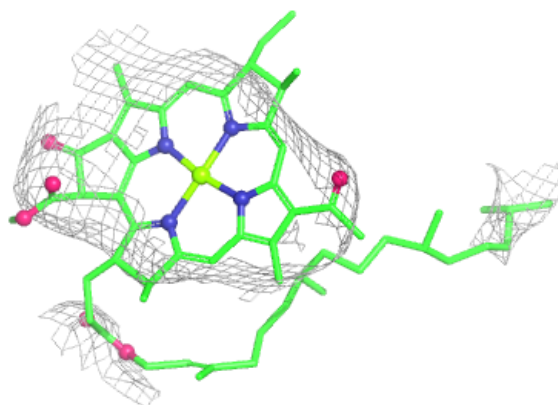
**Electron density around BCL w 101:**

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

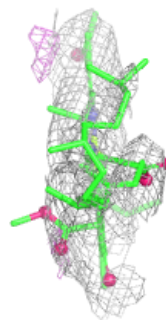
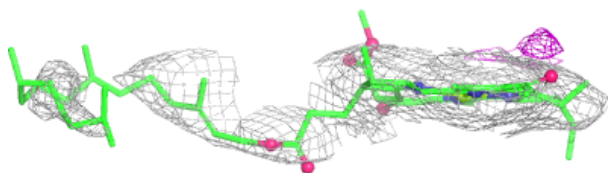
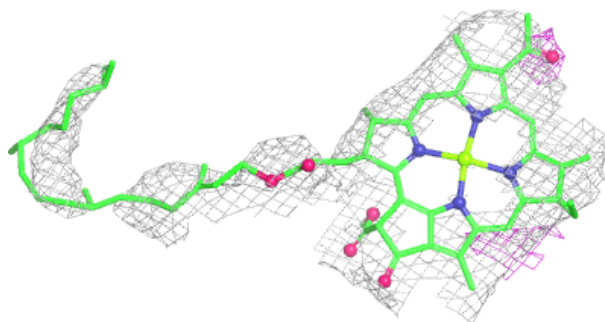


Electron density around BCL g 101:

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

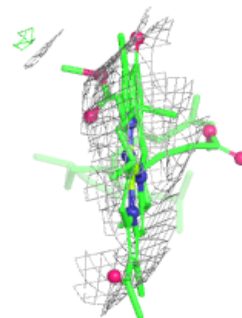
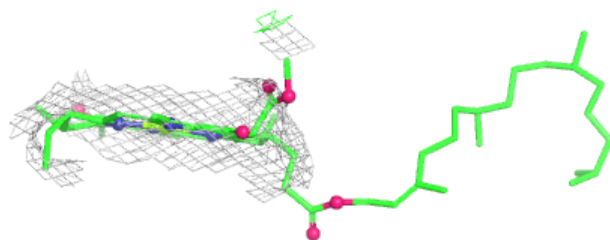
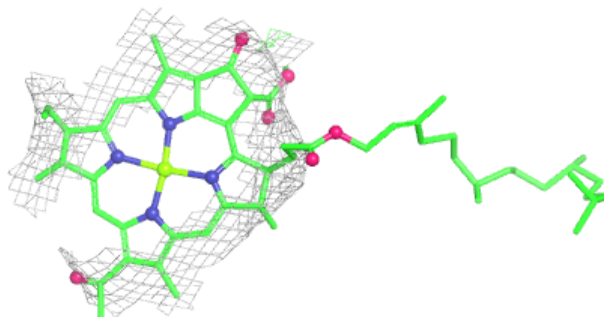
**Electron density around BCL W 101:**

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

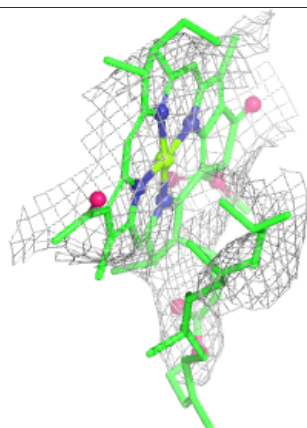
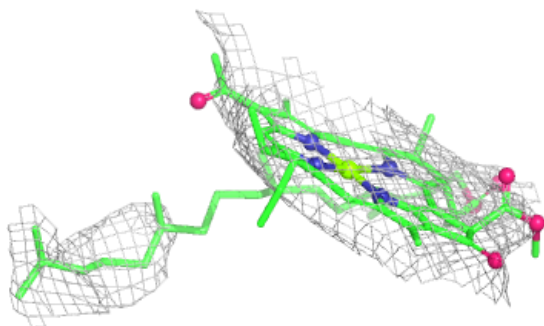
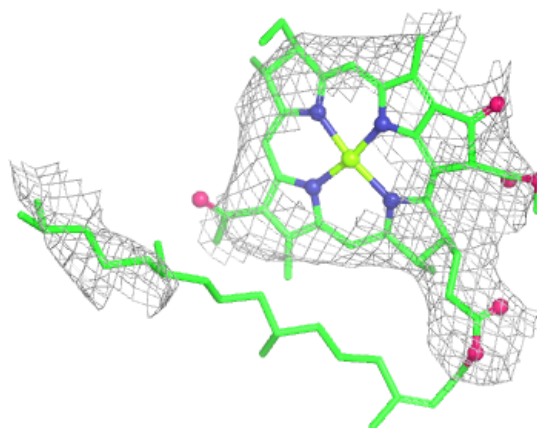


Electron density around BCL AA 101:

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

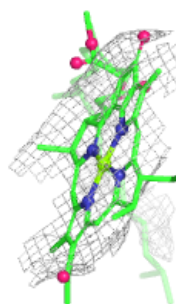
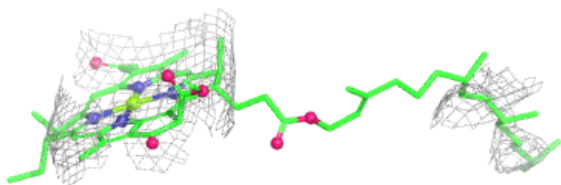
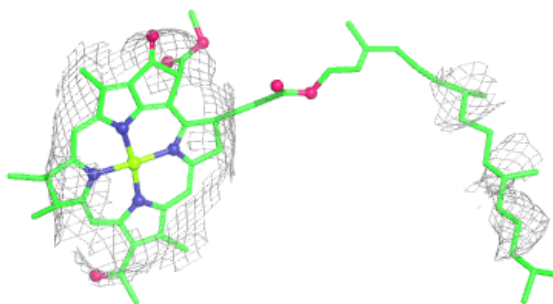
**Electron density around BCL Z 102:**

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

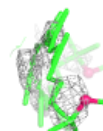
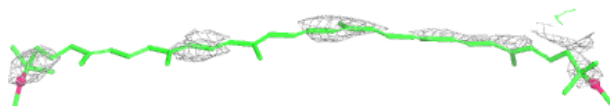
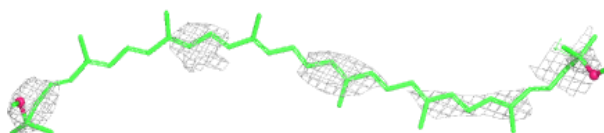


Electron density around BCL I 101:

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

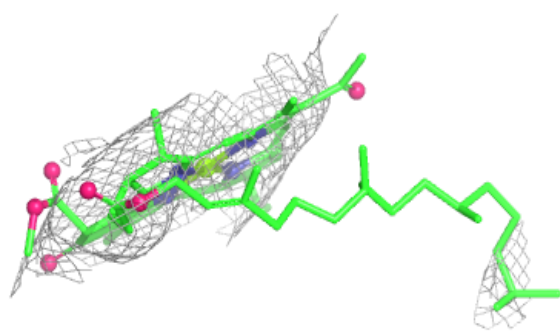
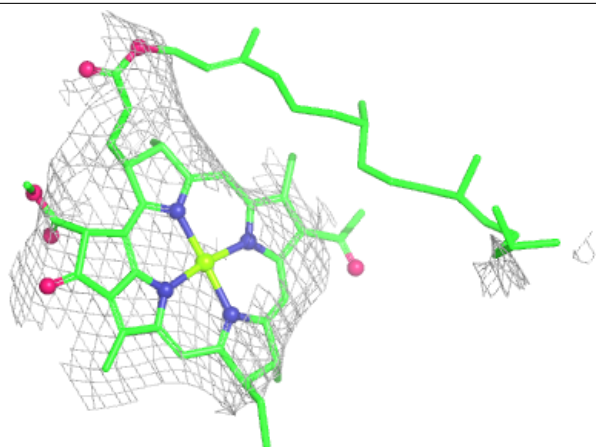
**Electron density around CRT 6 101:**

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

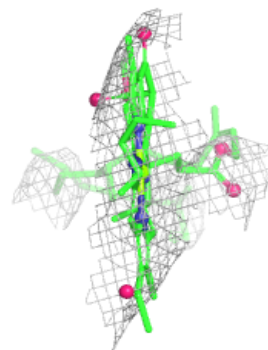
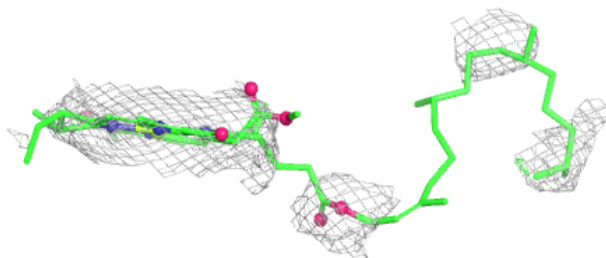
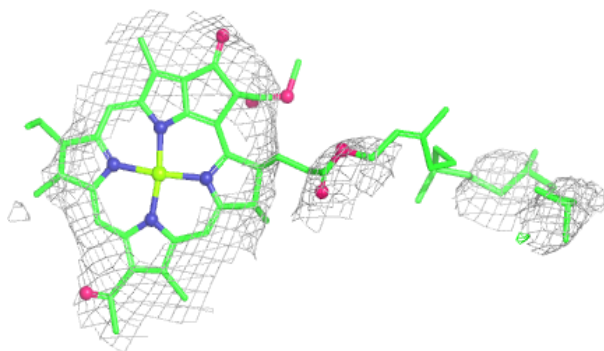


Electron density around BCL O 101:

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

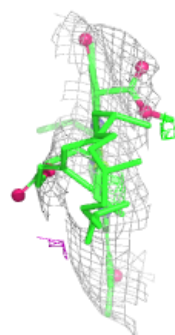
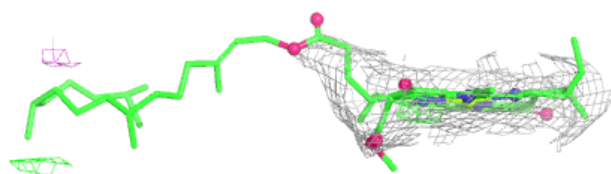
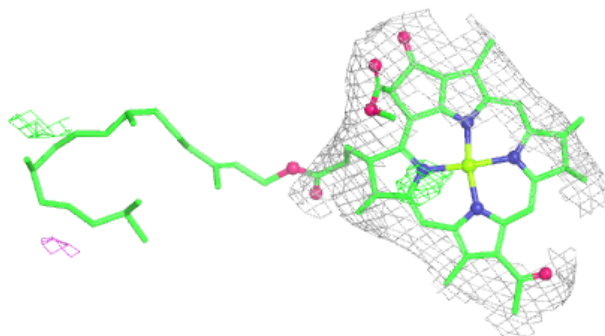
**Electron density around BCL P 101:**

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

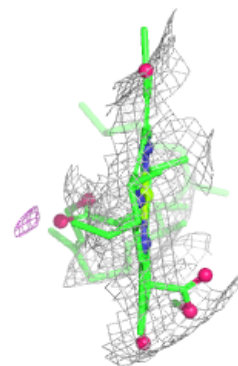
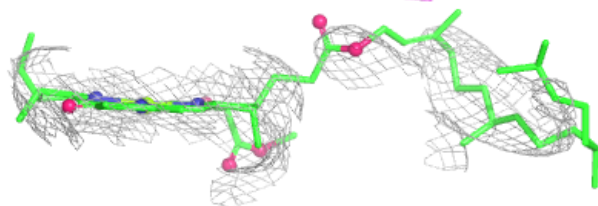
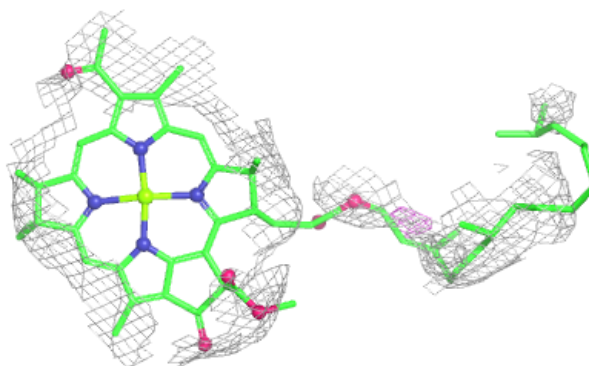


Electron density around BCL AI 101:

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

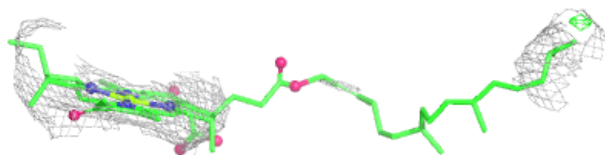
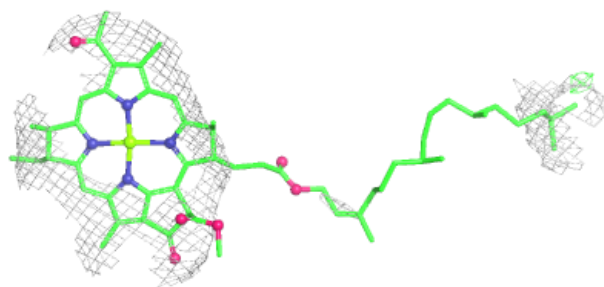
**Electron density around BCL 1 101:**

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

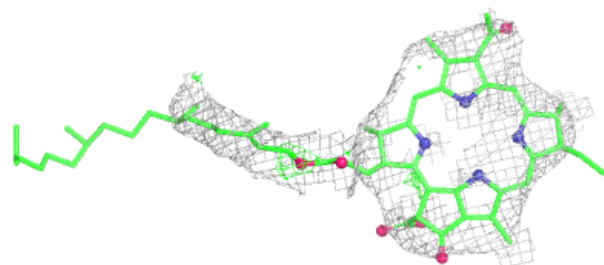


Electron density around BCL D 101:

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

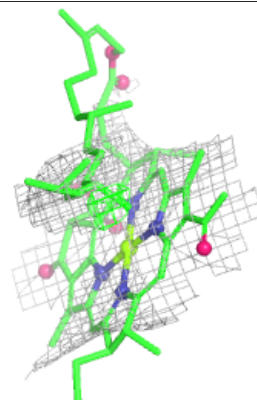
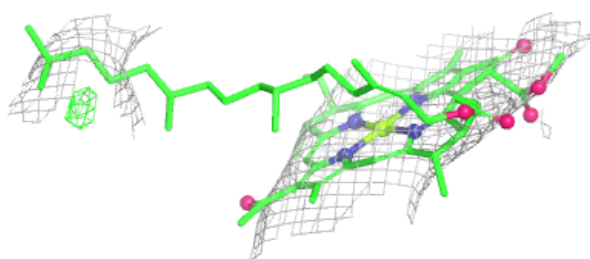
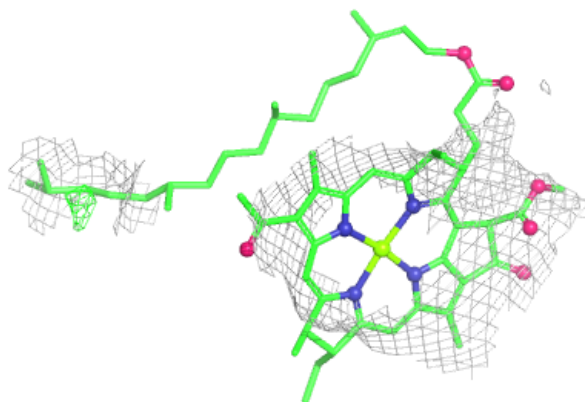
**Electron density around BPH y 402:**

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

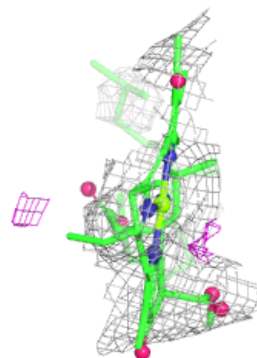
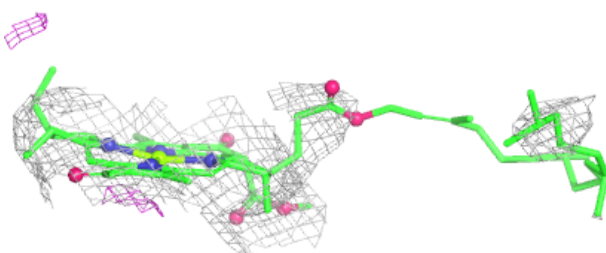
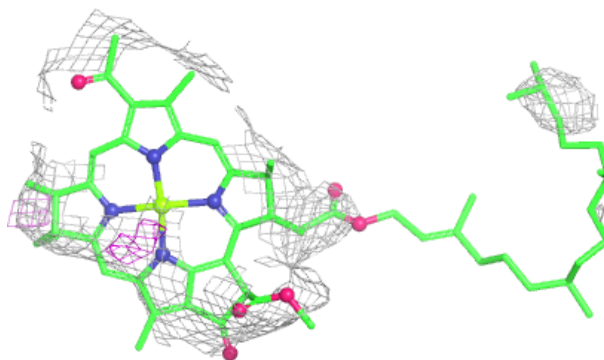


Electron density around BCL s 102:

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

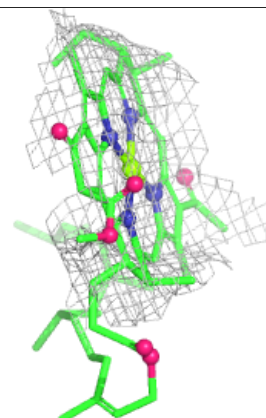
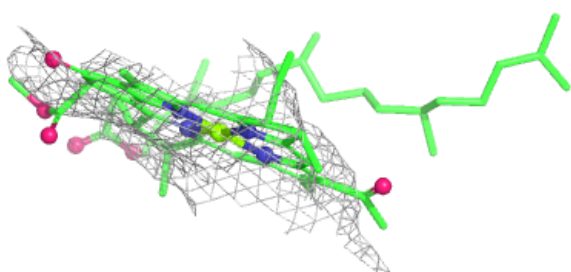
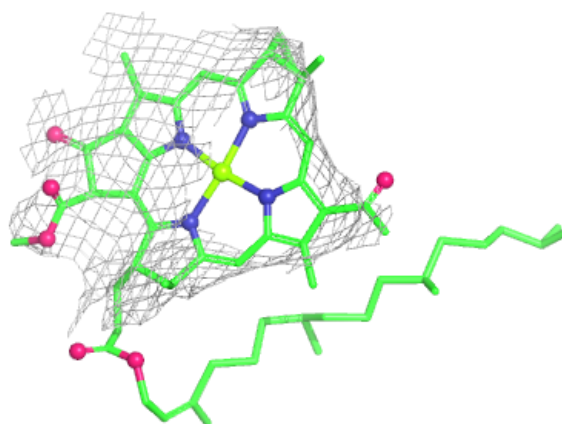
**Electron density around BCL 3 101:**

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

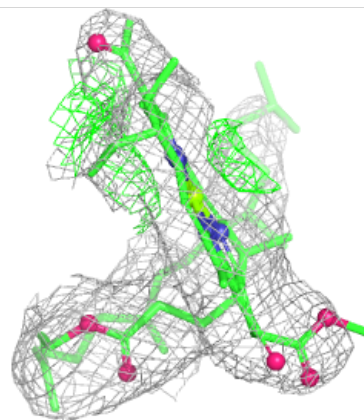
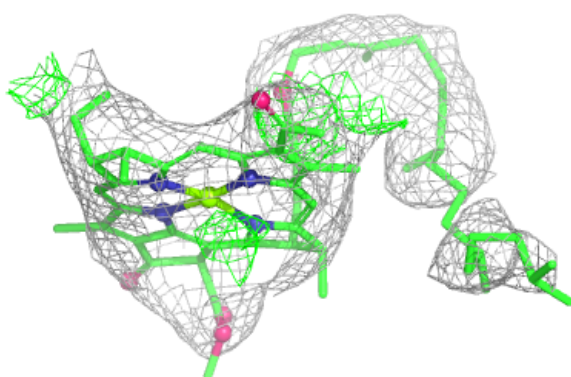
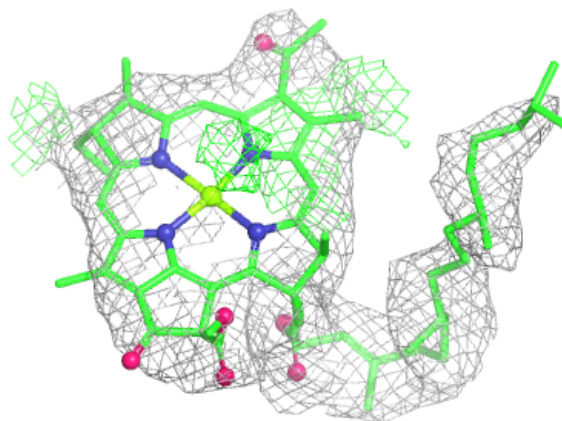


Electron density around BCL i 102:

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

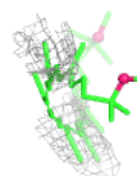
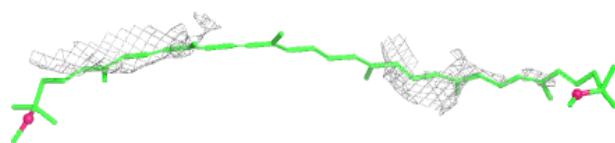
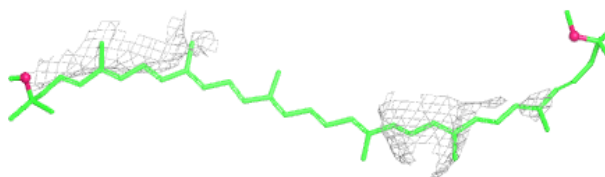
**Electron density around BCL L 305:**

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

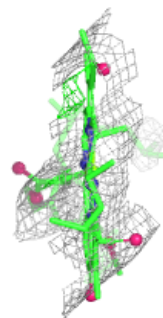
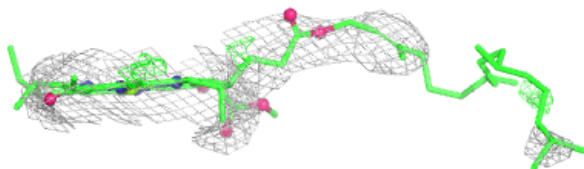
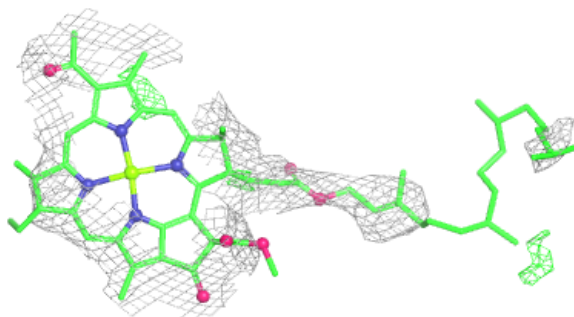


Electron density around CRT AE 103:

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

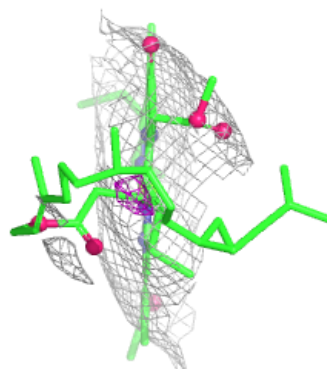
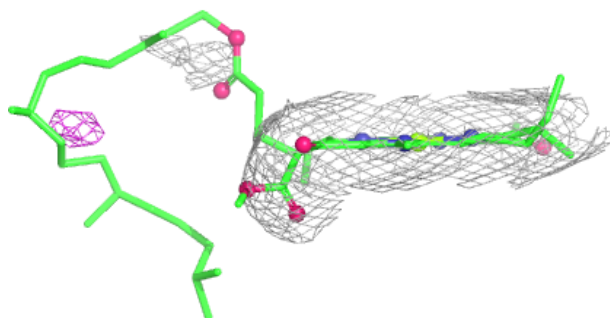
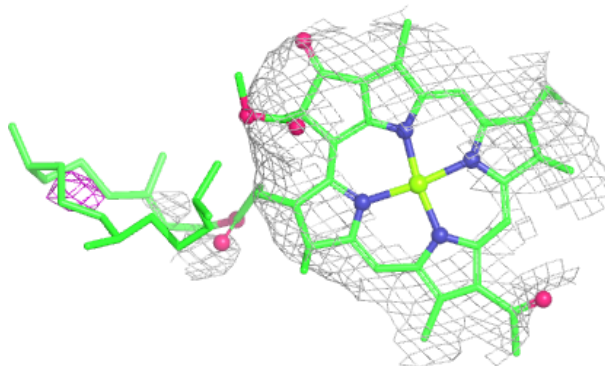
**Electron density around BCL 7 101:**

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

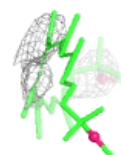
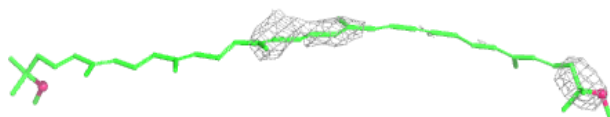
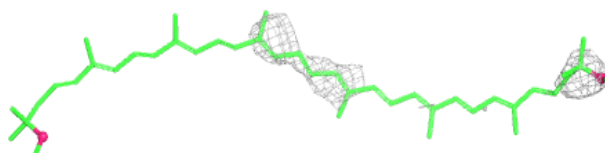


Electron density around BCL Q 101:

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

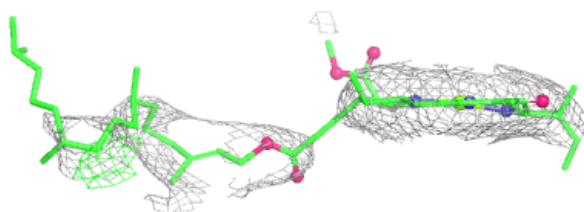
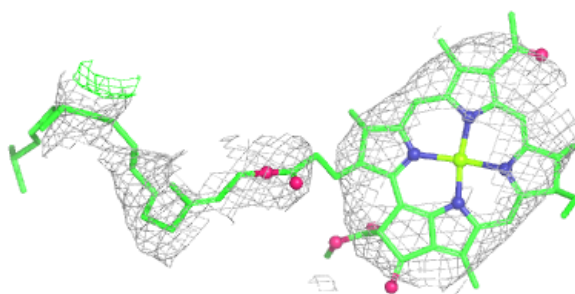
**Electron density around CRT Z 101:**

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



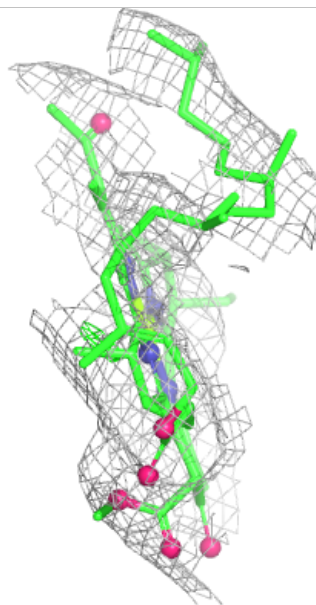
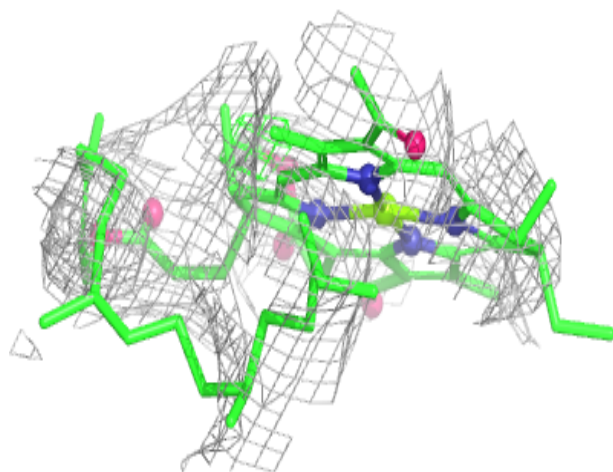
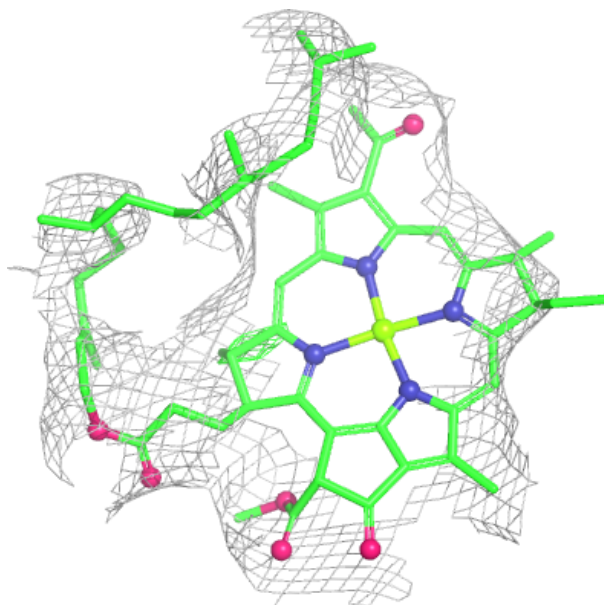
Electron density around BCL Y 101:

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



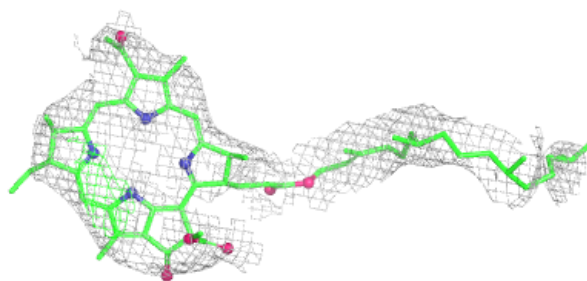
Electron density around BCL 8 102:

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

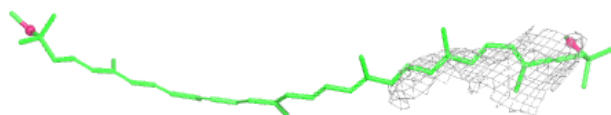
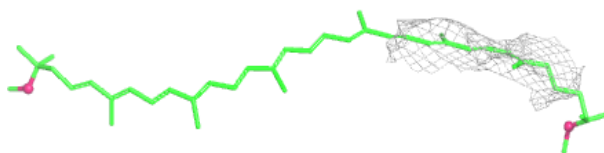


Electron density around BPH M 402:

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

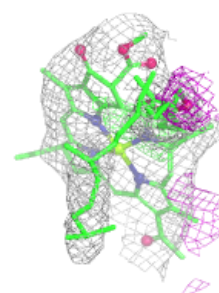
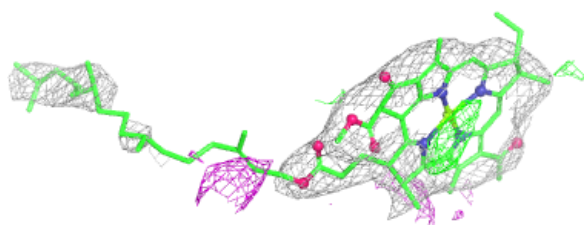
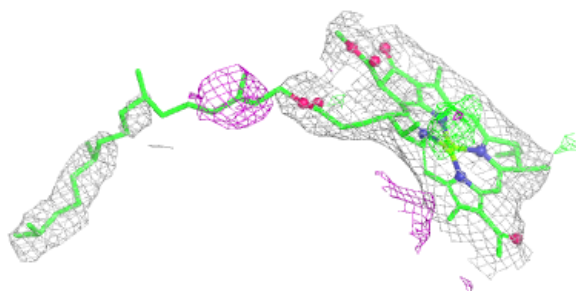
**Electron density around CRT 9 102:**

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

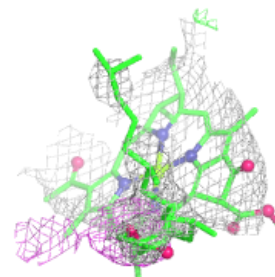
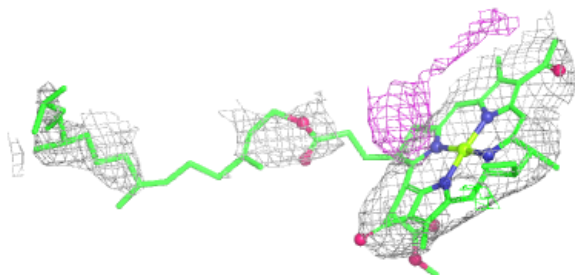
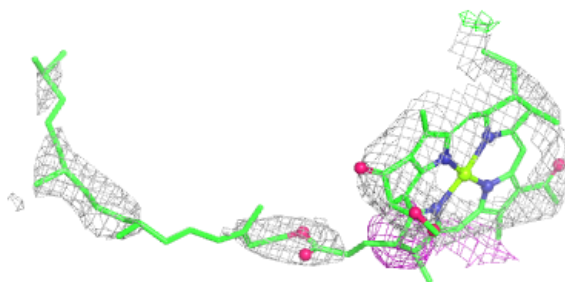


Electron density around BCL x 301:

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

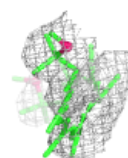
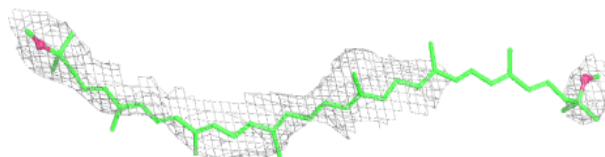
**Electron density around BCL y 401:**

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

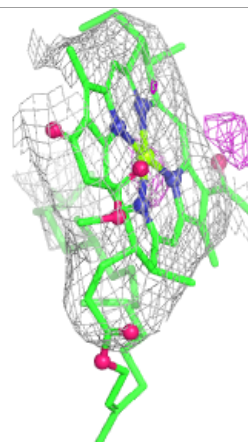
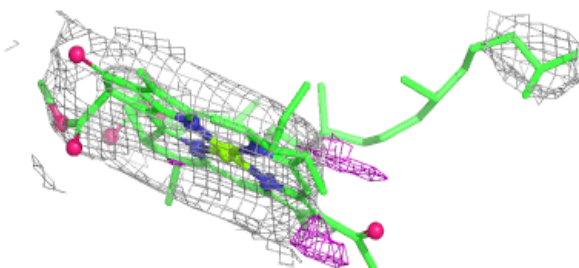
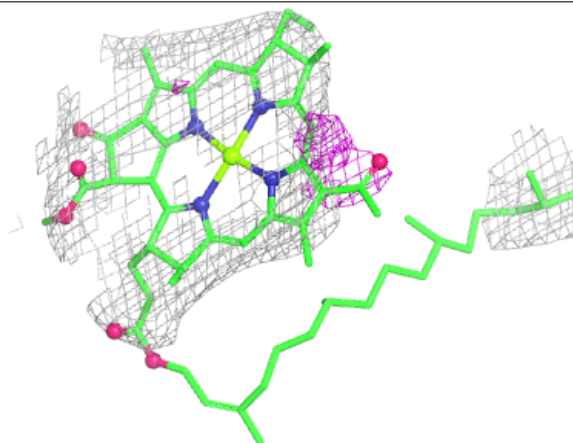


Electron density around CRT P 102:

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

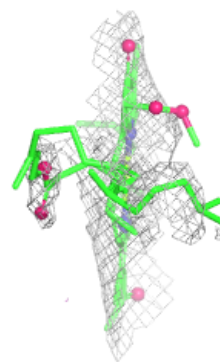
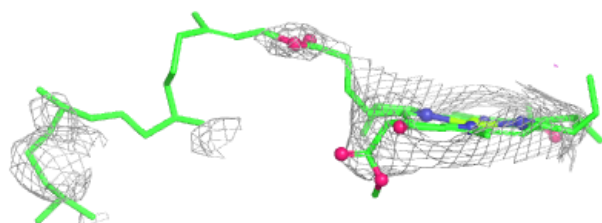
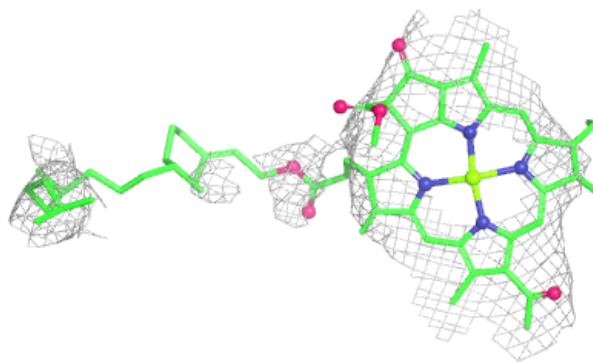
**Electron density around BCL V 101:**

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

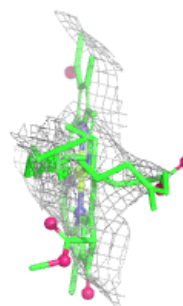
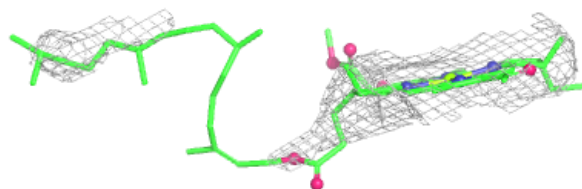
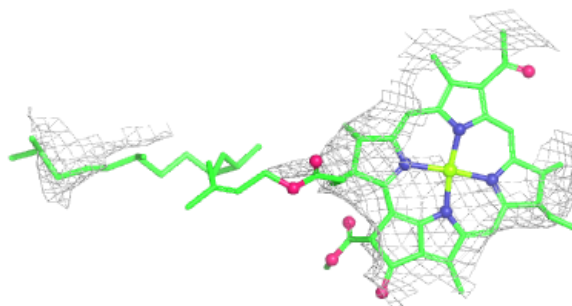


Electron density around BCL r 101:

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

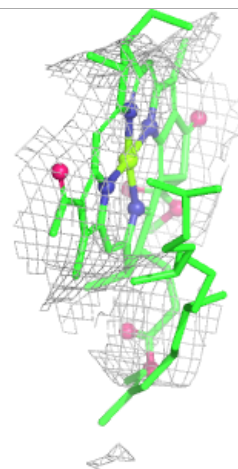
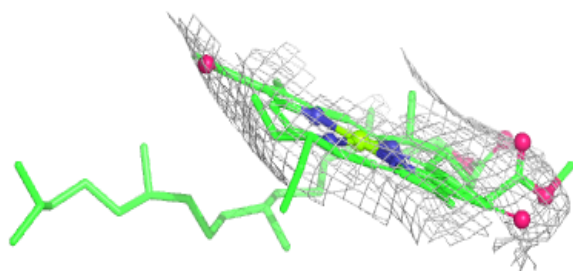
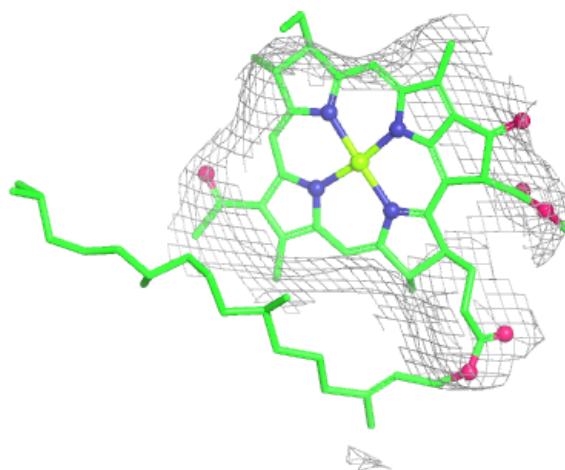
**Electron density around BCL 5 101:**

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



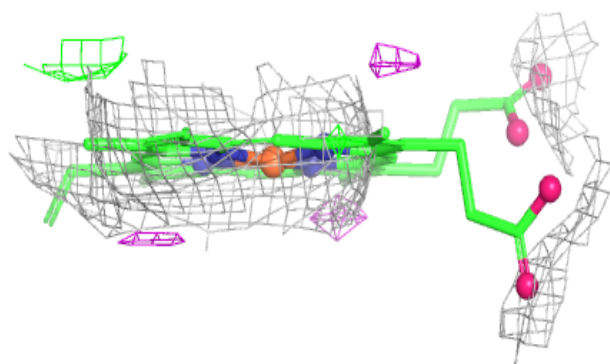
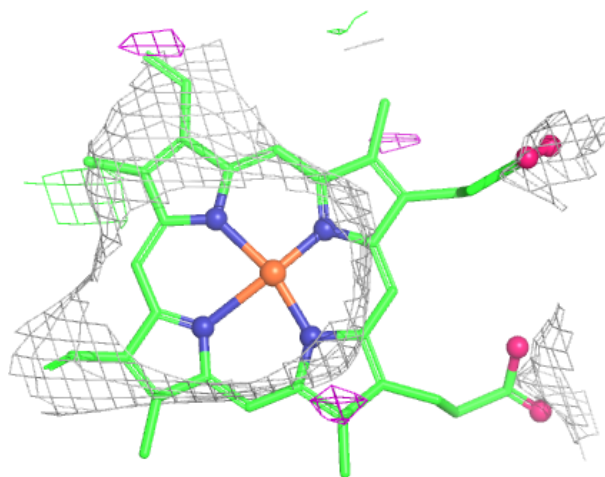
Electron density around BCL 0 101:

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



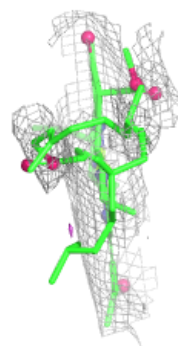
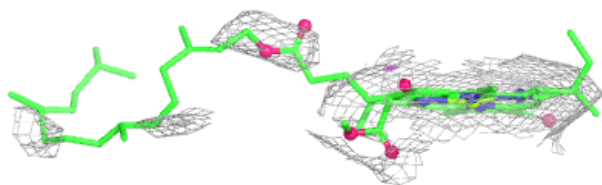
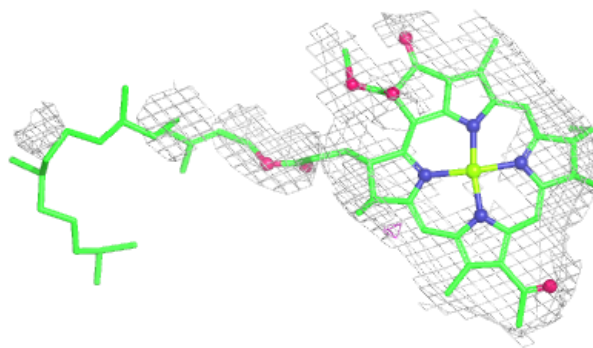
Electron density around HEM o 501:

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



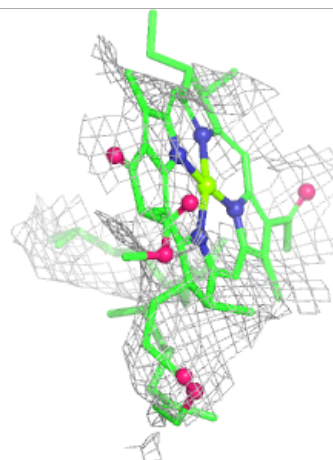
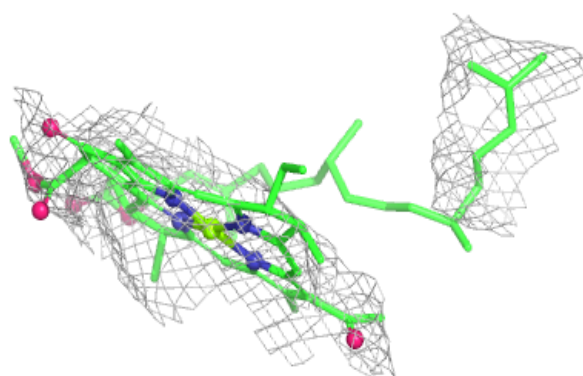
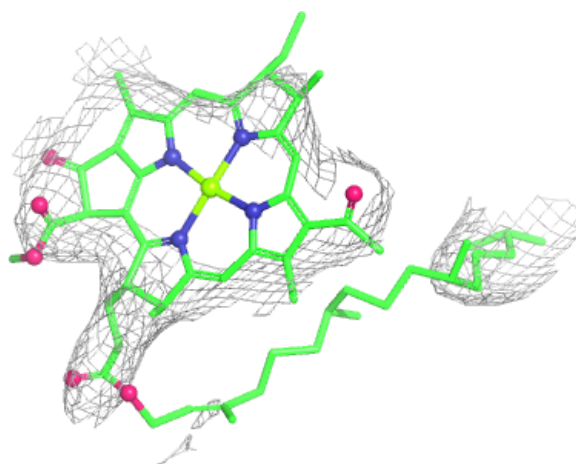
Electron density around BCL U 101:

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



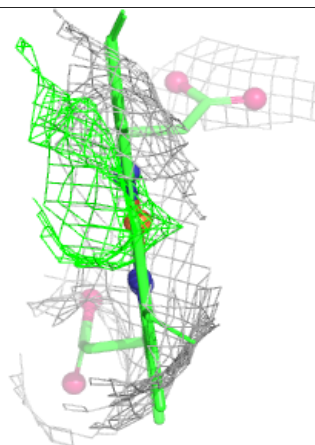
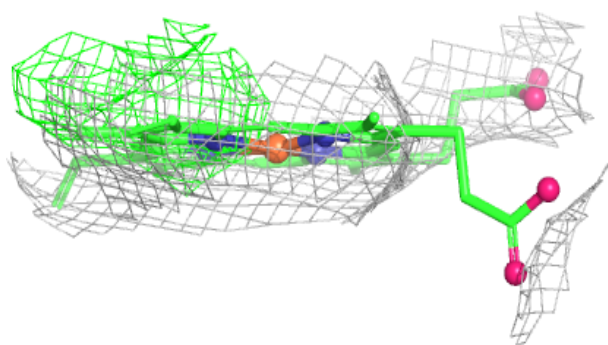
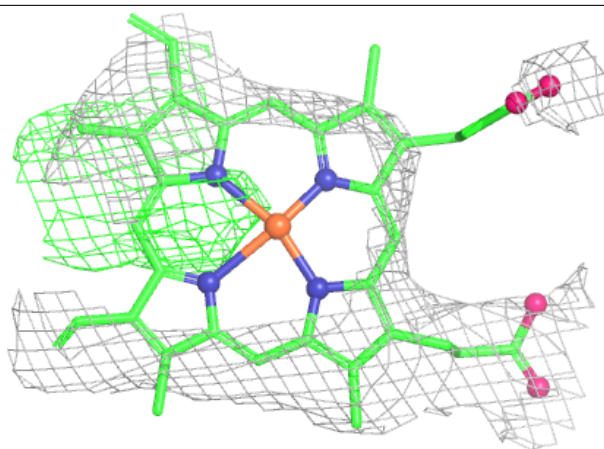
Electron density around BCL 4 102:

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



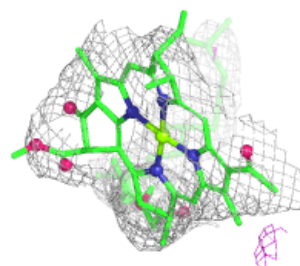
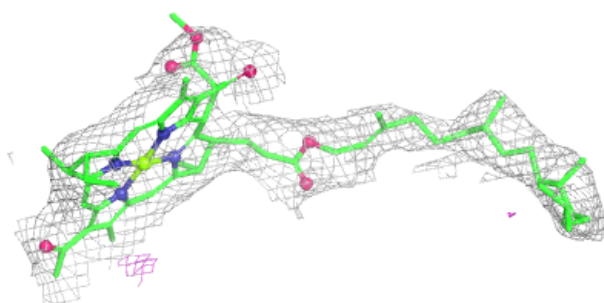
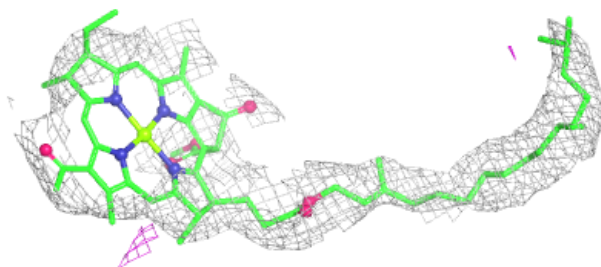
Electron density around HEM C 501:

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

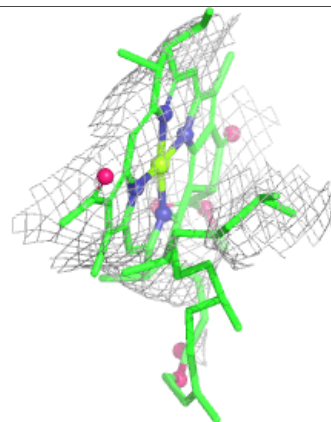
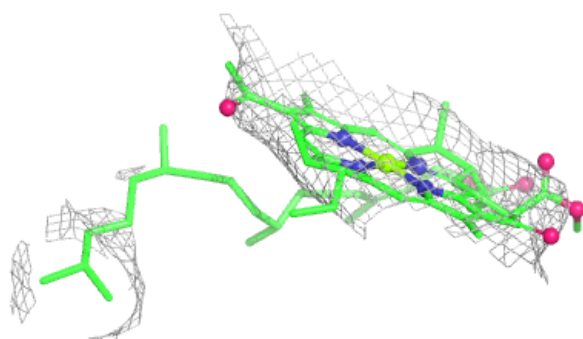
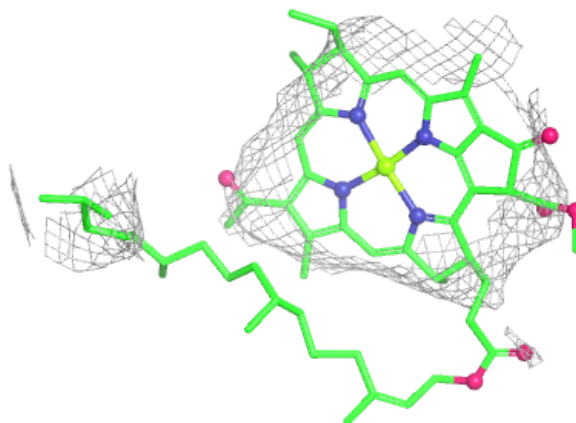


Electron density around BCL M 401:

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

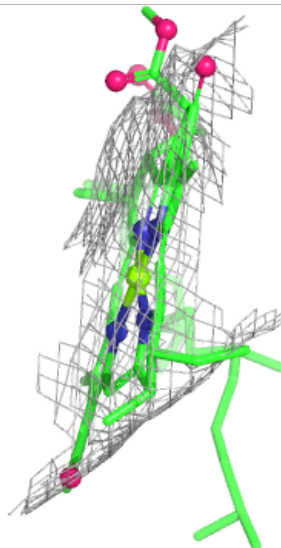
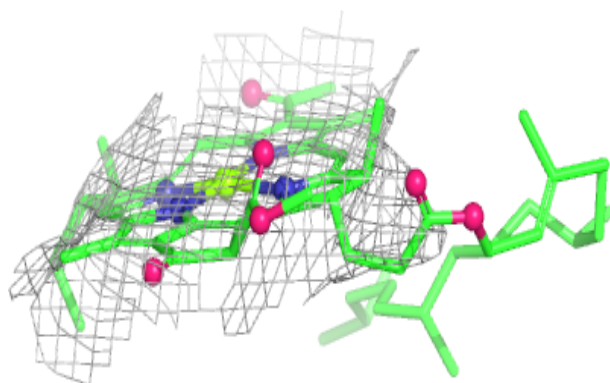
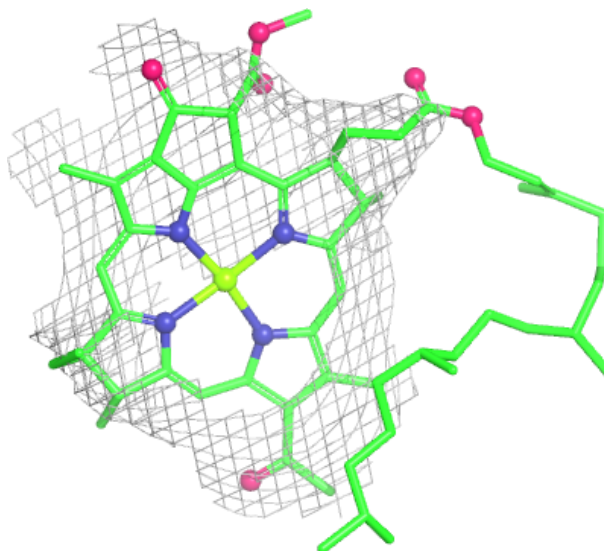
**Electron density around BCL e 102:**

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



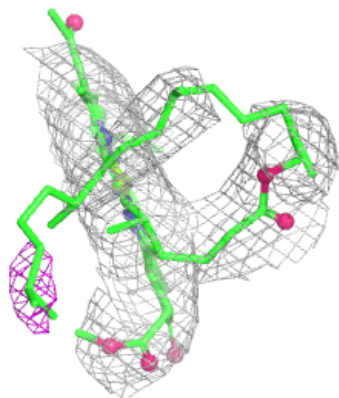
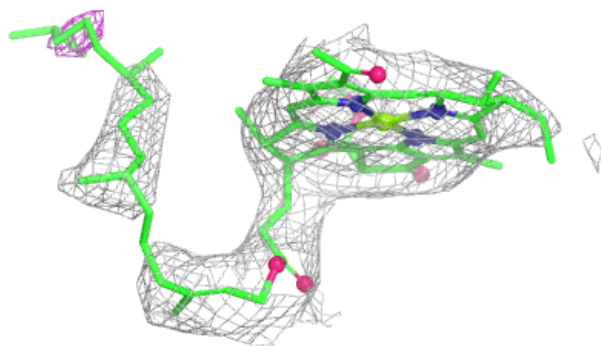
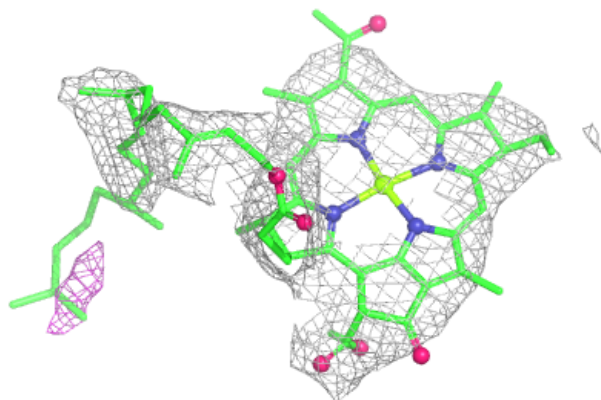
Electron density around BCL A 102:

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

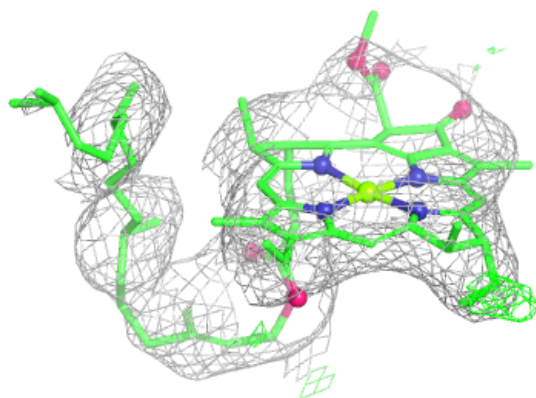
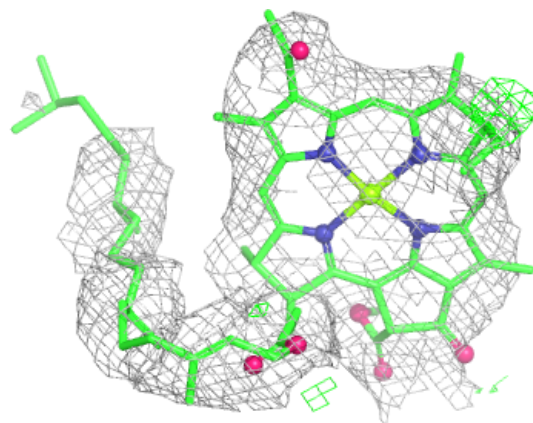


Electron density around BCL x 303:

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

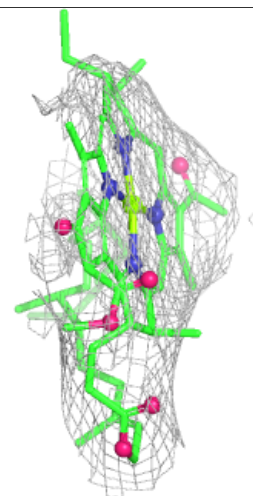
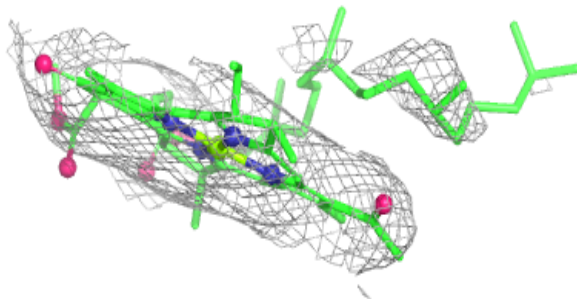
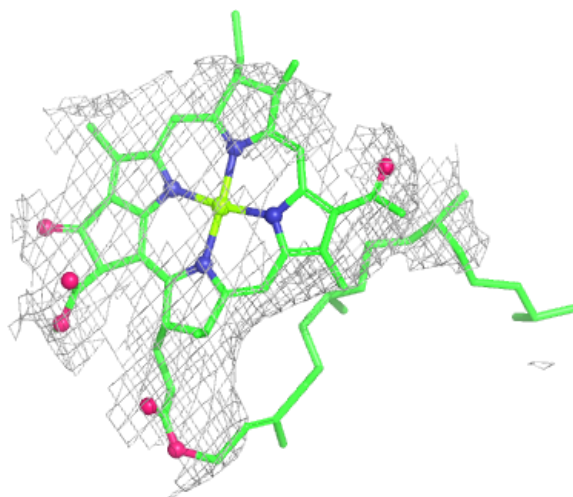
**Electron density around BCL x 305:**

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



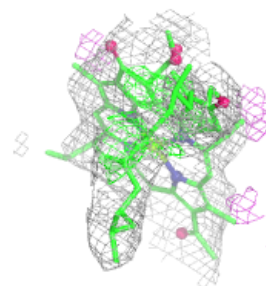
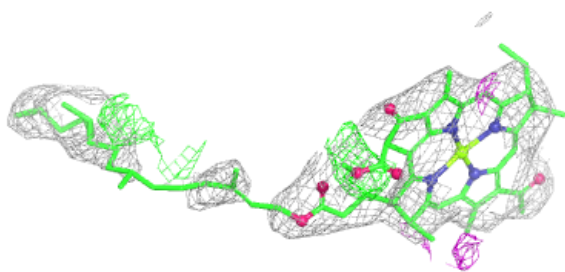
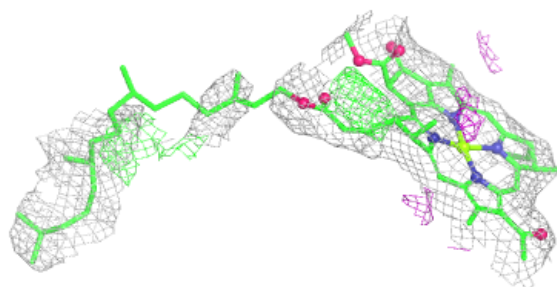
Electron density around BCL X 102:

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



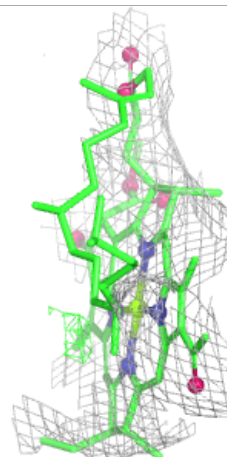
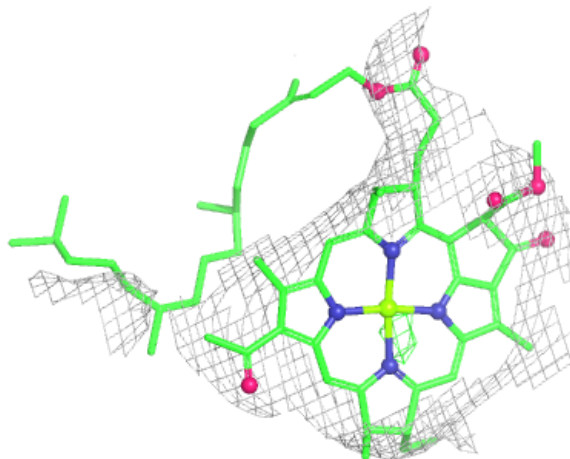
Electron density around BCL L 301:

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



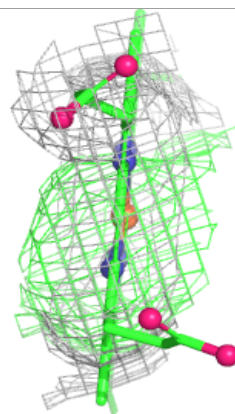
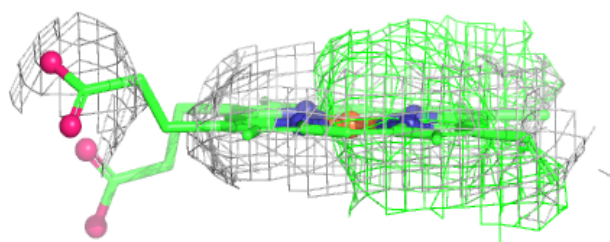
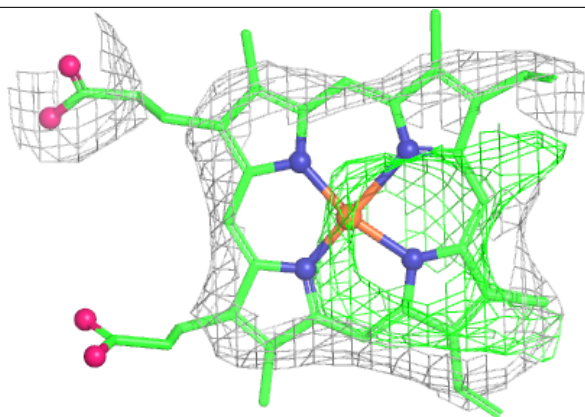
Electron density around BCL p 104:

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



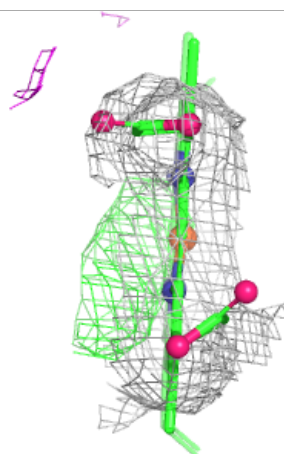
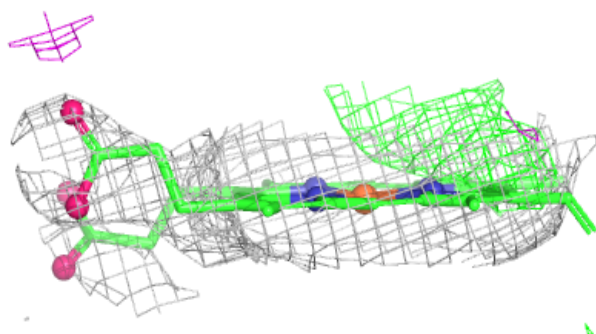
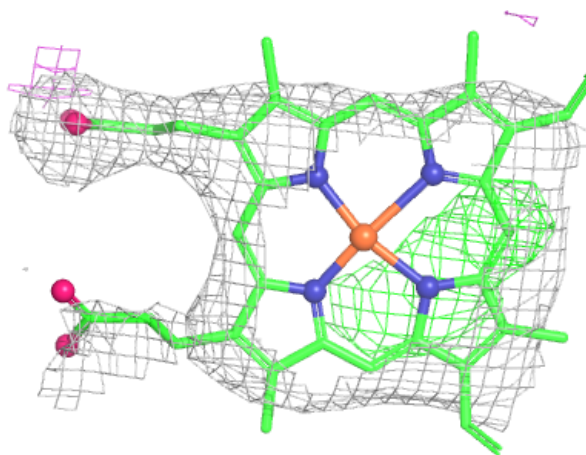
Electron density around HEM o 503:

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



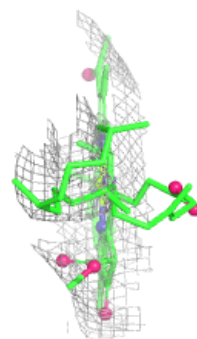
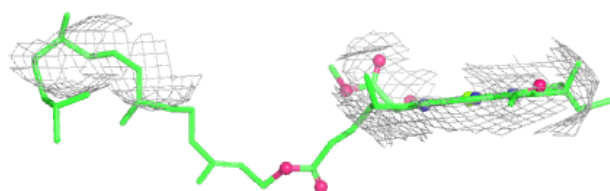
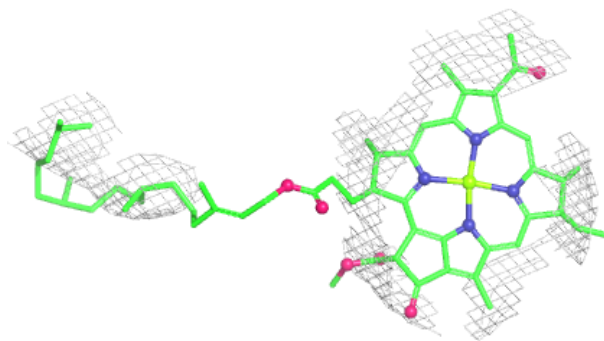
Electron density around HEM o 504:

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



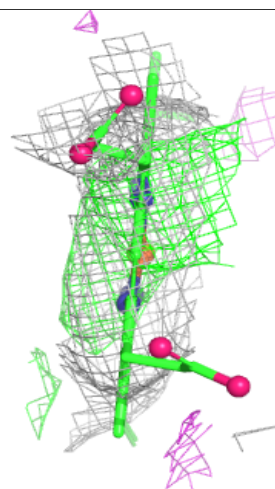
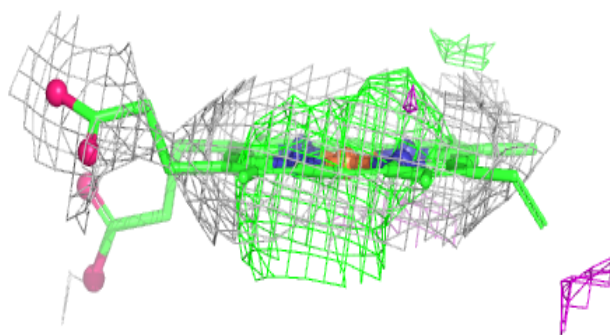
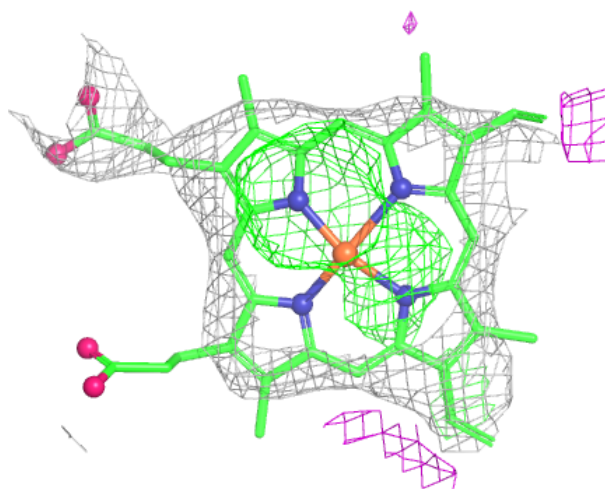
Electron density around BCL B 101:

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



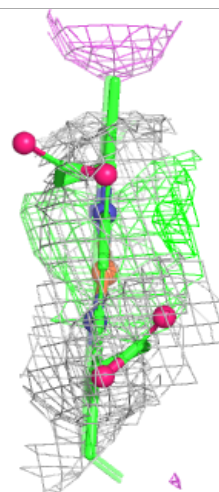
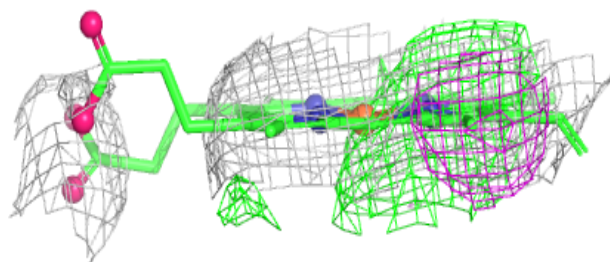
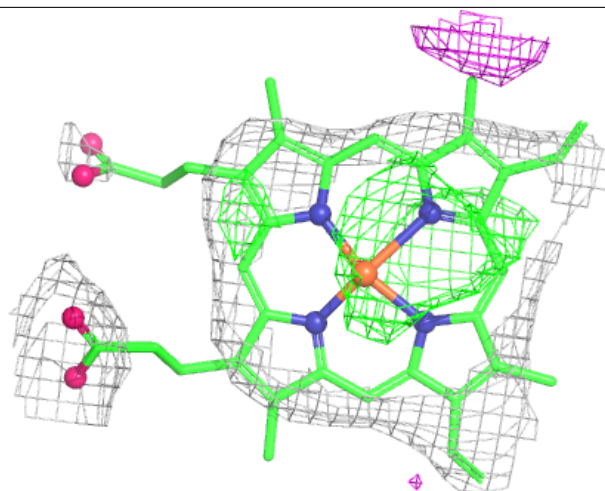
Electron density around HEM C 503:

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



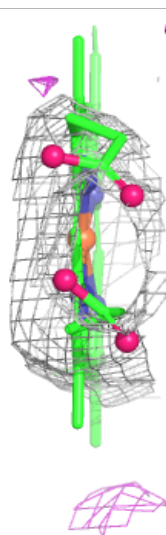
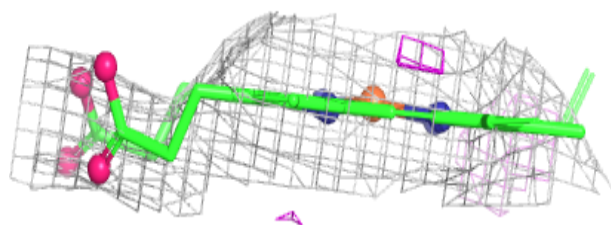
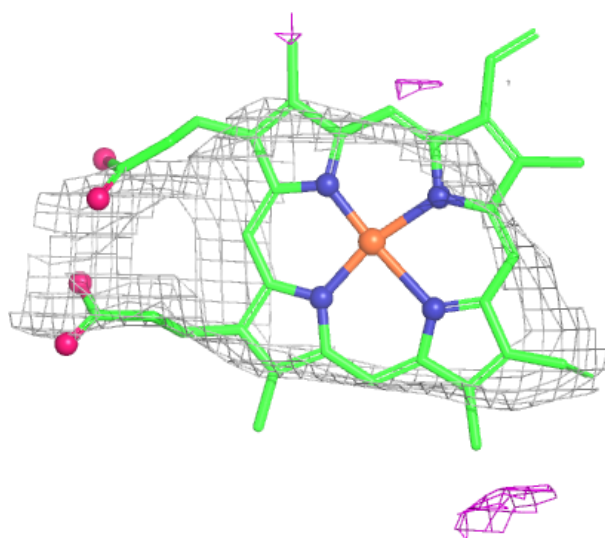
Electron density around HEM C 504:

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



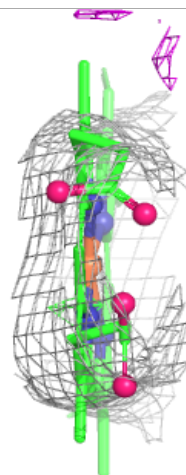
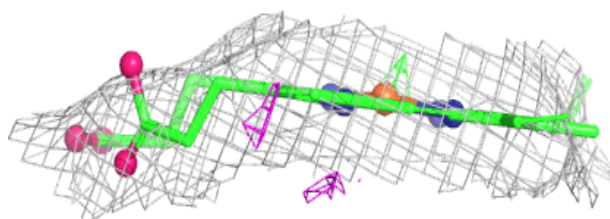
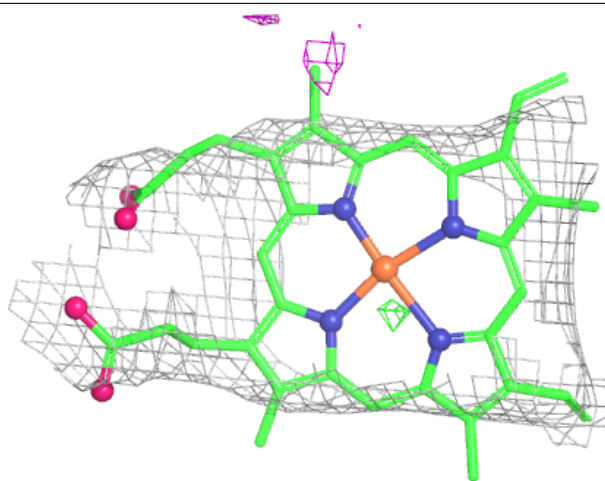
Electron density around HEM o 502:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.