Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 10:19 AM UTC

PDB ID	:	5B5N / pdb_00005b5n
Title	:	Crystal structure of the Ba-substituted LH1-RC complex from Tch. tepidum
Authors	:	Wang-Otomo, Z.-Y.; Yu, L.-J.
Deposited on	:	2016-05-12
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

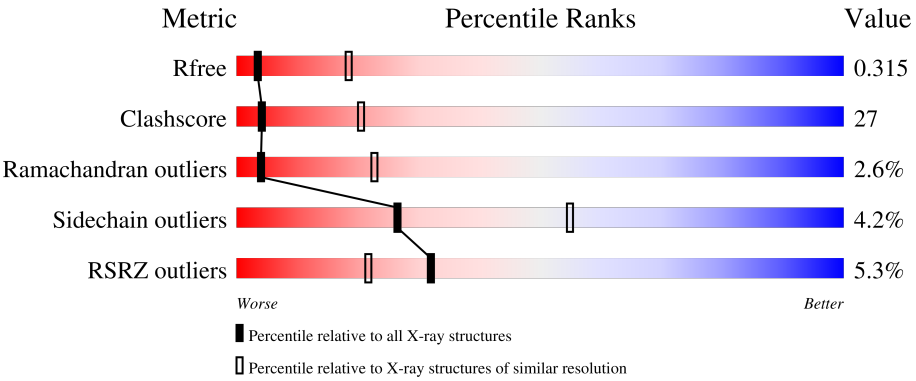
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 <=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	6% 48% 37% 10% • 5%
1	o	333	5% 46% 39% 9% • 5%
2	L	281	5% 51% 38% 11%
2	x	281	4% 45% 44% 10%
3	M	319	5% 40% 48% 12%

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Mol	Chain	Length	Quality of chain
3	y	319	5% 42% 49% 8%
4	H	259	2% 44% 45% 10%
4	t	259	3% 46% 42% 9%
5	1	61	5% 39% 49% 8%
5	3	61	11% 57% 33% 8%
5	5	61	11% 61% 31% 7%
5	7	61	3% 48% 46% 5%
5	9	61	3% 44% 44% 10%
5	A	61	5% 44% 46% 8%
5	AA	61	7% 61% 28% 10%
5	AC	61	10% 52% 44%
5	AE	61	7% 38% 57%
5	AG	61	5% 48% 46% 5%
5	AI	61	10% 54% 36% 8%
5	AK	61	11% 49% 43% 7%
5	D	61	3% 54% 41%
5	F	61	5% 48% 46% 5%
5	I	61	3% 43% 49% 7%
5	K	61	10% 67% 26% 5%
5	O	61	7% 59% 33%
5	Q	61	11% 39% 56%
5	S	61	2% 46% 48% 5%
5	U	61	11% 43% 49% 7%
5	W	61	5% 41% 54%
5	Y	61	8% 52% 41% 5%

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Mol	Chain	Length	Quality of chain
5	d	61	5% 56% 34% 8%
5	f	61	8% 48% 43% 8%
5	h	61	8% 52% 41% 5%
5	j	61	2% 41% 54%
5	l	61	11% 41% 54%
5	m	61	8% 56% 39%
5	p	61	10% 48% 46% 5%
5	r	61	8% 31% 62% 5%
5	u	61	11% 43% 44% 10%
5	w	61	2% 61% 36%
6	0	47	2% 45% 38% 15%
6	2	47	49% 34% 15%
6	4	47	2% 60% 26% 15%
6	6	47	57% 26% 15%
6	8	47	4% 49% 36% 15%
6	AB	47	6% 47% 38% 15%
6	AD	47	2% 45% 40% 15%
6	AF	47	2% 49% 34% 15%
6	AH	47	9% 53% 32% 15%
6	AJ	47	2% 45% 34% 15%
6	AL	47	4% 55% 30% 15%
6	B	47	4% 38% 45% 15%
6	E	47	6% 51% 30% 15%
6	G	47	4% 45% 40% 15%
6	J	47	4% 32% 53% 15%

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Mol	Chain	Length	Quality of chain
6	N	47	4% 68% 15% 15%
6	P	47	6% 55% 28% 15%
6	R	47	6% 55% 30% 15%
6	T	47	4% 51% 34% 15%
6	V	47	51% 34% 15%
6	X	47	51% 28% 6% 15%
6	Z	47	68% 17% 15%
6	c	47	6% 57% 28% 15%
6	e	47	2% 51% 32% 15%
6	g	47	2% 51% 32% 15%
6	i	47	2% 60% 21% 15%
6	k	47	2% 51% 34% 15%
6	n	47	2% 47% 38% 15%
6	q	47	4% 60% 26% 15%
6	s	47	2% 51% 34% 15%
6	v	47	2% 51% 34% 15%
6	z	47	45% 40% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CRT	X	101	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 51893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

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

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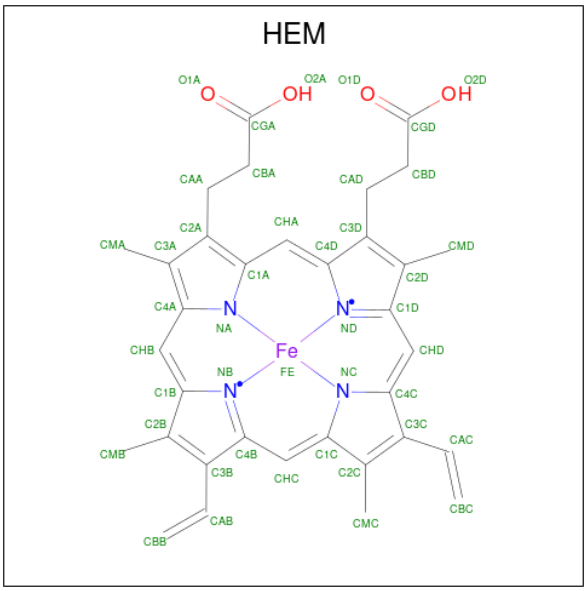
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	4	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	6	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	8	40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

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



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

- Molecule 8 is BARIUM ION (CCD ID: BA) (formula: Ba).

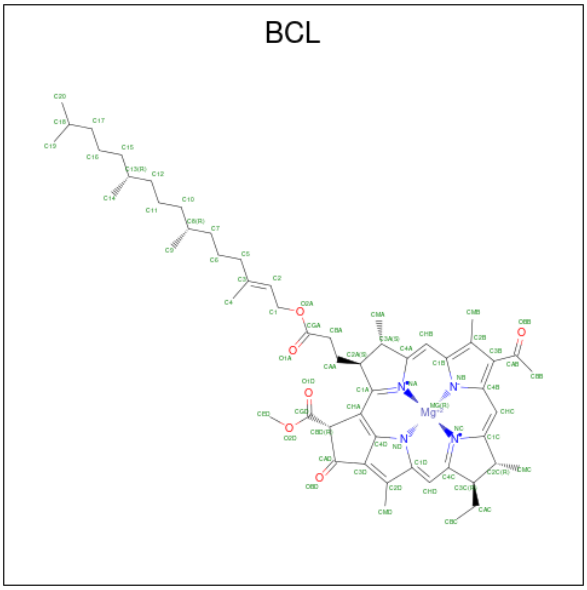
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ba 1 1	0	0
8	L	2	Total Ba 2 2	0	0
8	A	2	Total Ba 2 2	0	0
8	D	1	Total Ba 1 1	0	0
8	F	1	Total Ba 1 1	0	0
8	I	1	Total Ba 1 1	0	0
8	K	1	Total Ba 1 1	0	0
8	O	1	Total Ba 1 1	0	0
8	Q	1	Total Ba 1 1	0	0
8	S	1	Total Ba 1 1	0	0
8	U	1	Total Ba 1 1	0	0
8	W	1	Total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

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

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



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

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

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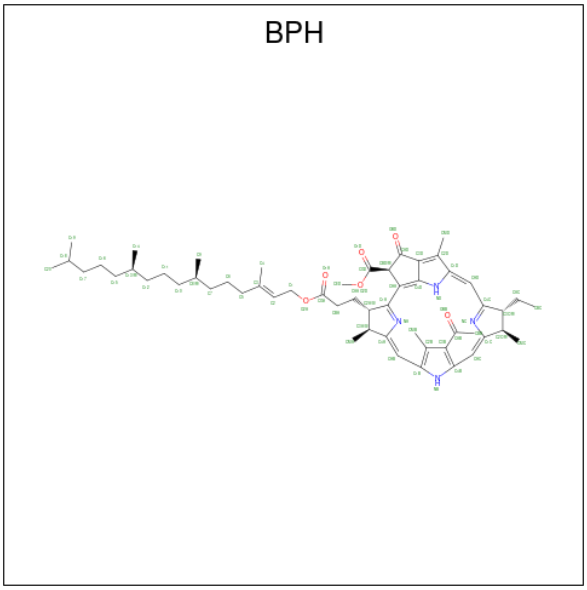
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	q	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	r	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	s	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	u	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	u	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	w	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	z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

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

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



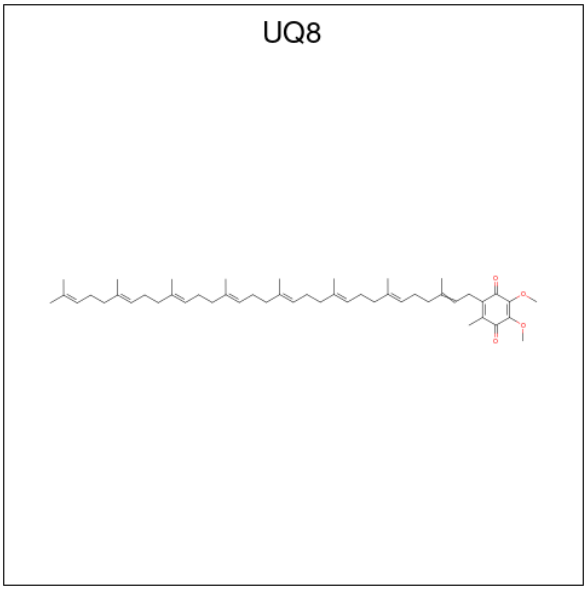
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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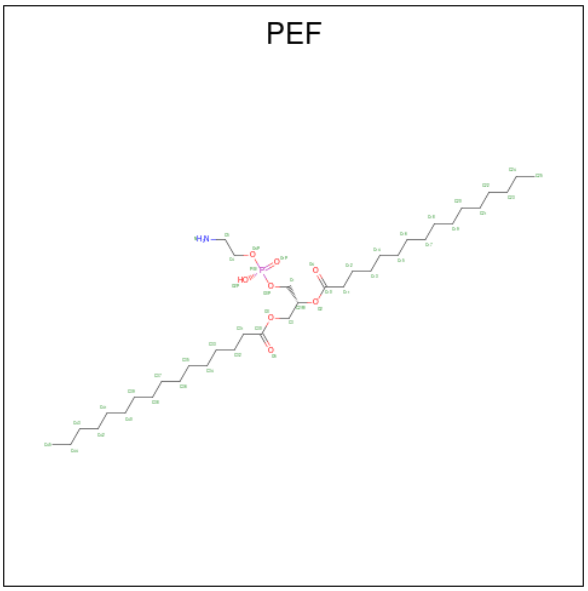
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

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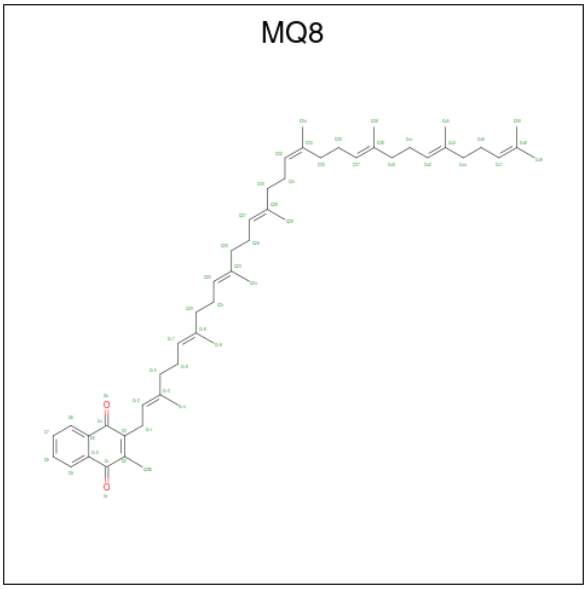
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	m	1	Total C N O P 19 9 1 8 1	0	0
12	p	1	Total C N O P 16 7 1 7 1	0	0

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

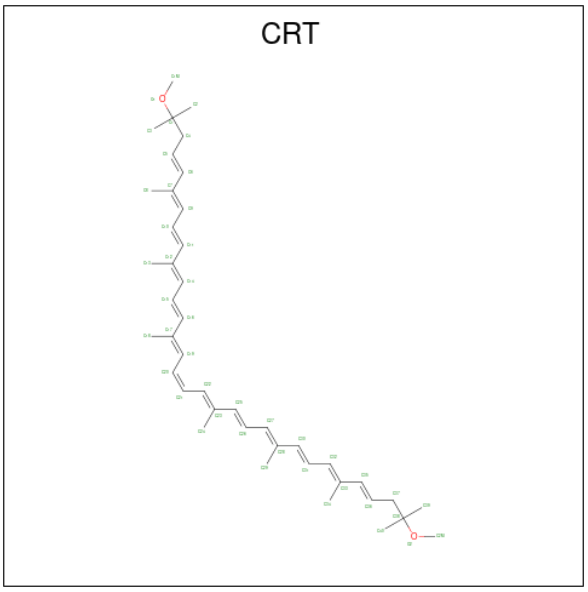
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	1	Total Fe 1 1	0	0
13	x	1	Total Fe 1 1	0	0

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



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

- Molecule 15 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



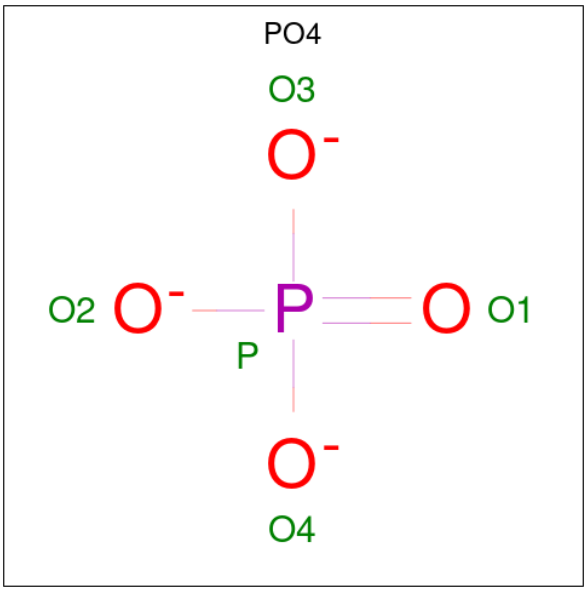
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total C O 44 42 2	0	0
15	E	1	Total C O 44 42 2	0	0
15	G	1	Total C O 44 42 2	0	0
15	I	1	Total C O 44 42 2	0	0
15	O	1	Total C O 44 42 2	0	0
15	P	1	Total C O 44 42 2	0	0
15	R	1	Total C O 44 42 2	0	0
15	T	1	Total C O 44 42 2	0	0
15	V	1	Total C O 44 42 2	0	0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

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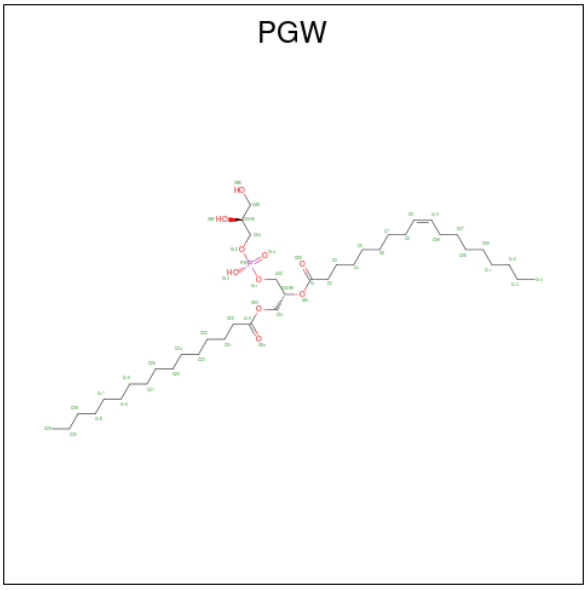
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	7	1	Total C O 44 42 2	0	0
15	9	1	Total C O 44 42 2	0	0
15	0	1	Total C O 44 42 2	0	0
15	y	1	Total C O 44 42 2	0	0
15	m	1	Total C O 44 42 2	0	0
15	n	1	Total C O 44 42 2	0	0
15	q	1	Total C O 44 42 2	0	0
15	s	1	Total C O 44 42 2	0	0
15	v	1	Total C O 44 42 2	0	0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

- Molecule 16 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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



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.

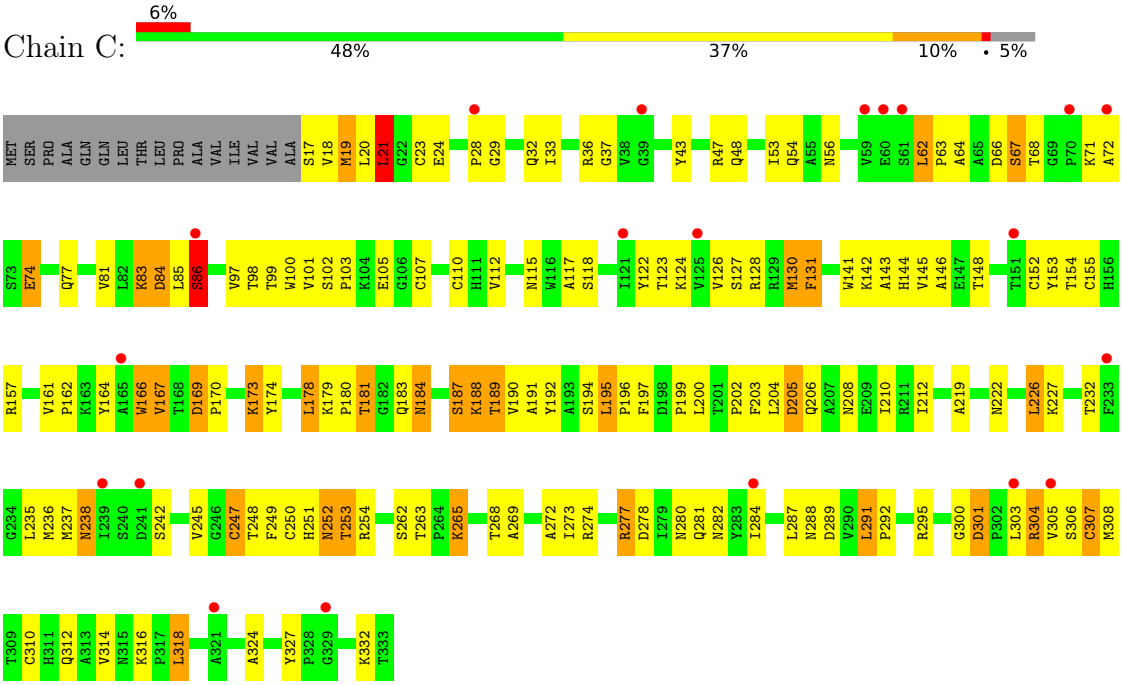
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	2	Total	O	0	0
			2	2		
18	W	1	Total	O	0	0
			1	1		
18	x	2	Total	O	0	0
			2	2		
18	AI	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

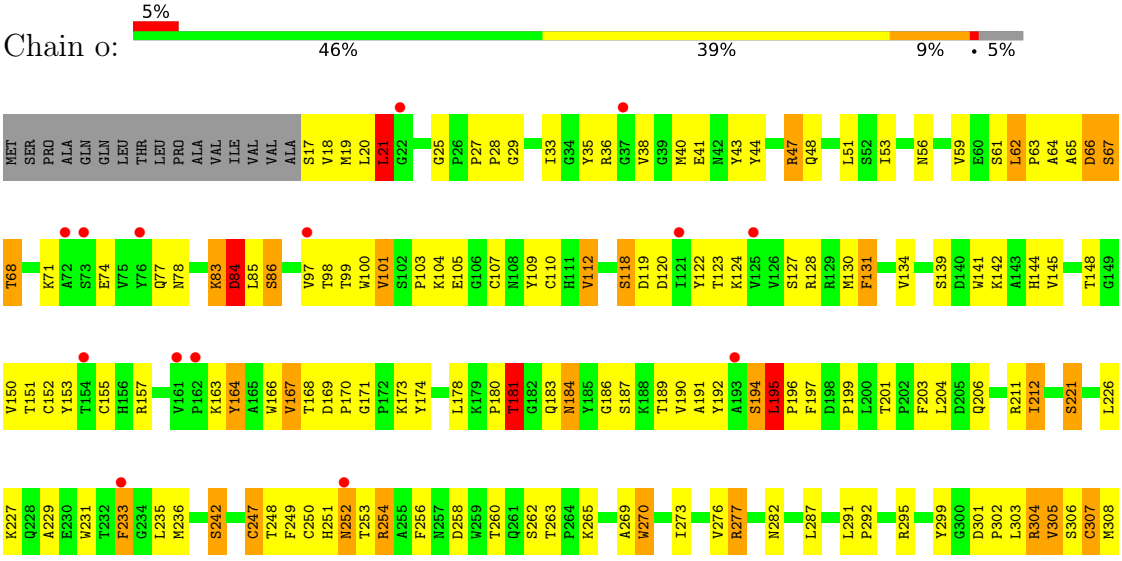
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

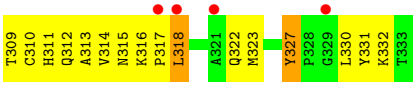
Chain C:



• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain o:

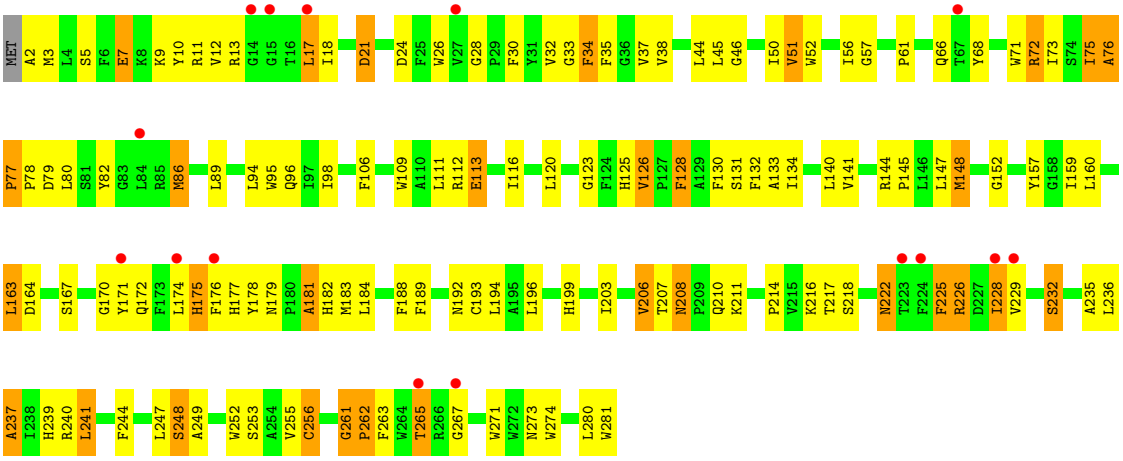




• Molecule 2: Photosynthetic reaction center L subunit

Chain L:

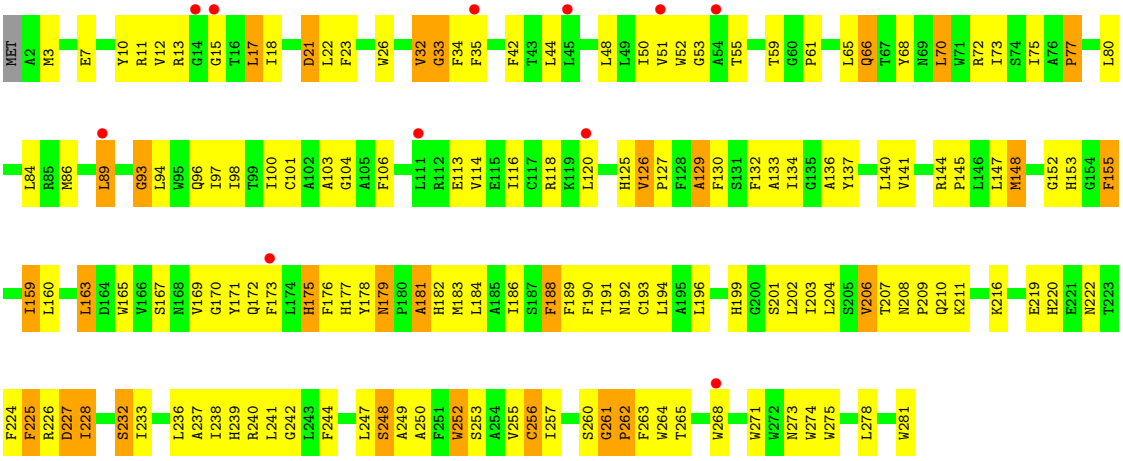




• Molecule 2: Photosynthetic reaction center L subunit

Chain x:

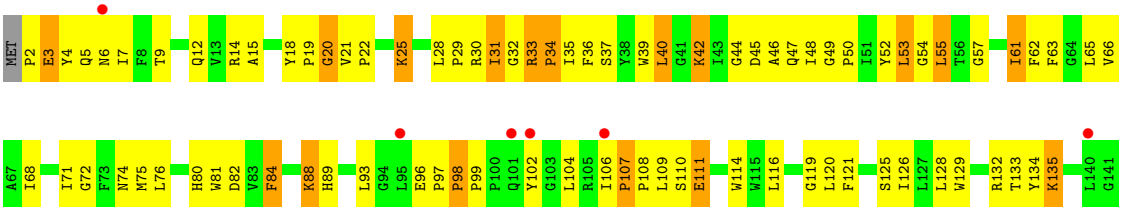


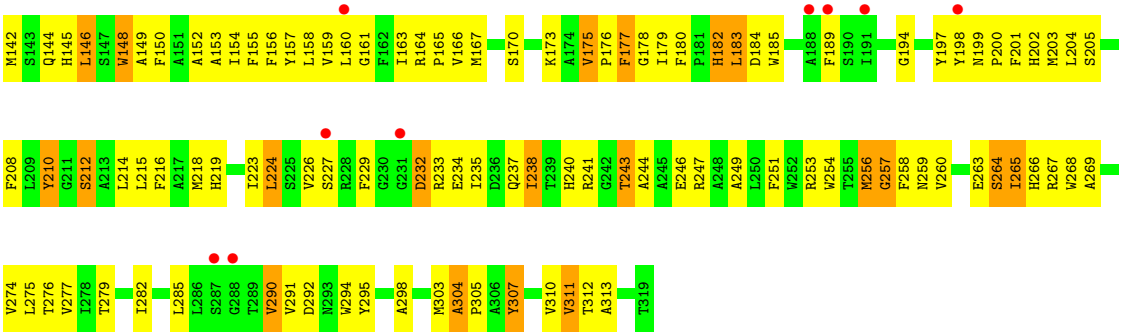


• Molecule 3: Photosynthetic reaction center M subunit

Chain M:



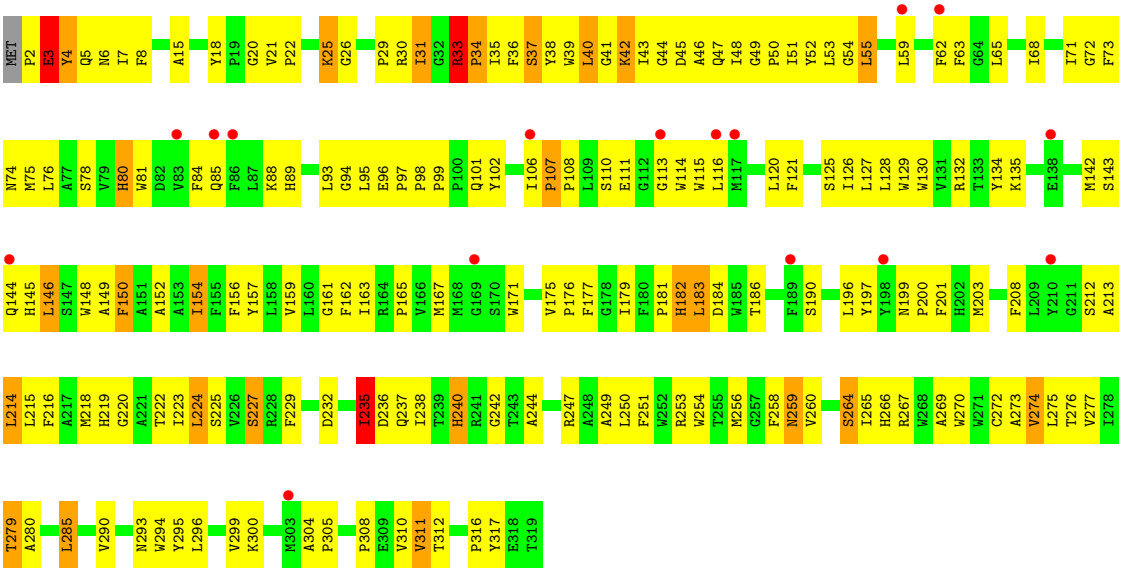




• Molecule 3: Photosynthetic reaction center M subunit

Chain y:

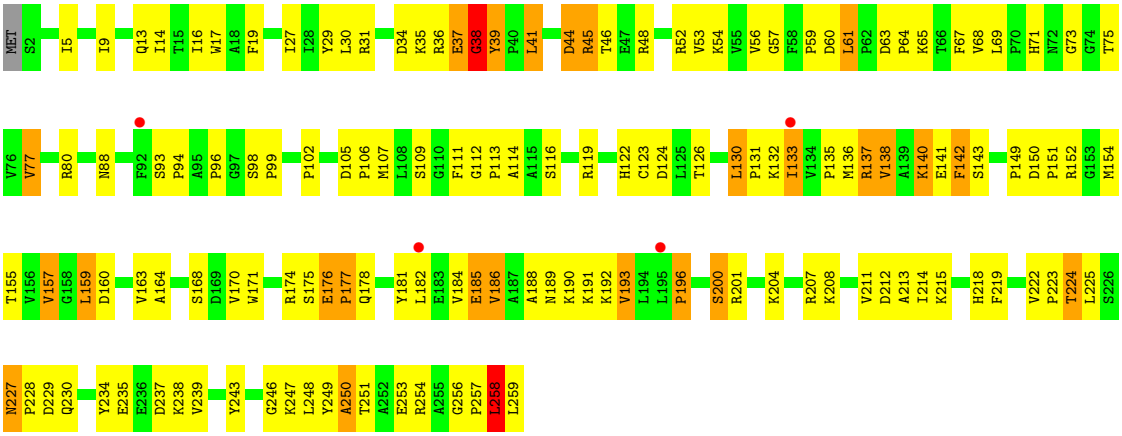




• Molecule 4: Photosynthetic reaction center H subunit

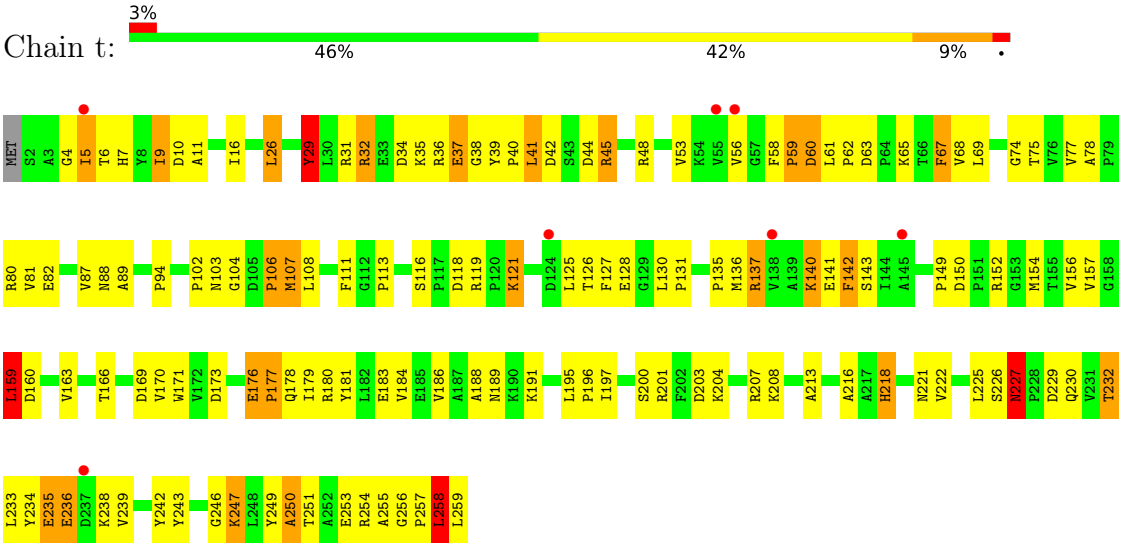
Chain H:





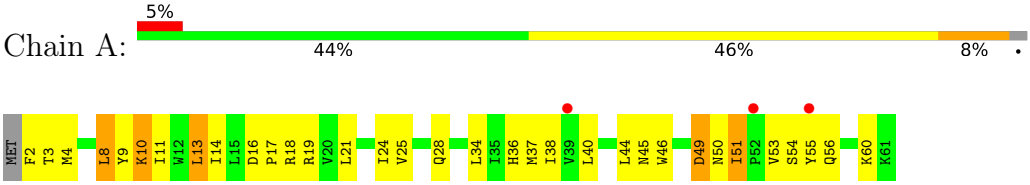
• Molecule 4: Photosynthetic reaction center H subunit

Chain t:



• Molecule 5: LH1 alpha polypeptide

Chain A:



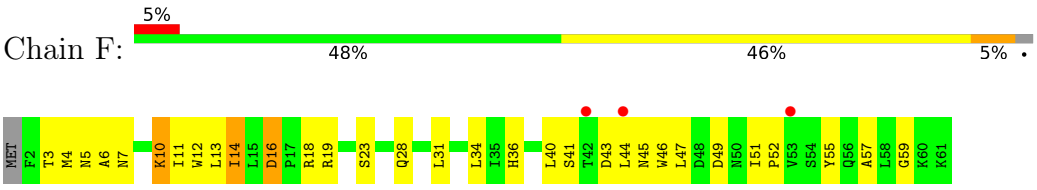
• Molecule 5: LH1 alpha polypeptide

Chain D:



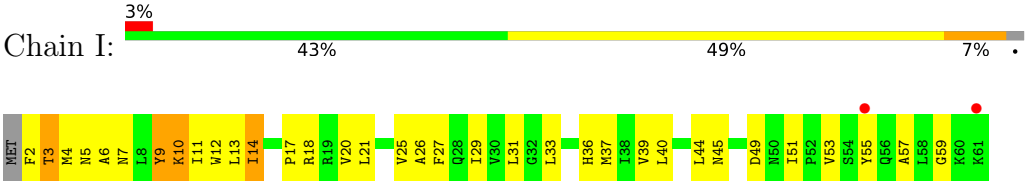
• Molecule 5: LH1 alpha polypeptide

Chain F:



• Molecule 5: LH1 alpha polypeptide

Chain I:



• Molecule 5: LH1 alpha polypeptide

Chain K:

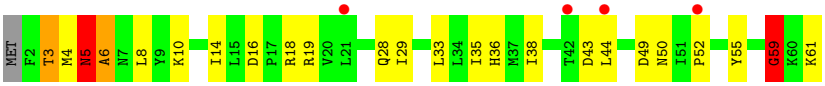




• Molecule 5: LH1 alpha polypeptide

Chain O:

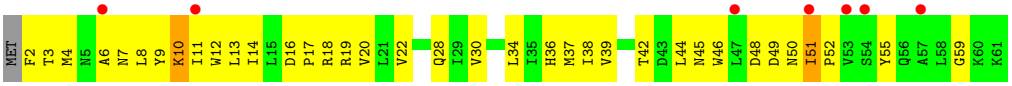




• Molecule 5: LH1 alpha polypeptide

Chain Q:

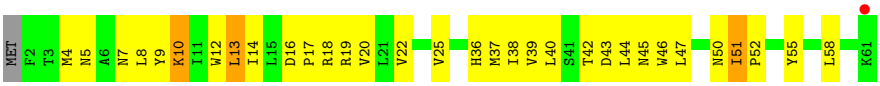




• Molecule 5: LH1 alpha polypeptide

Chain S:

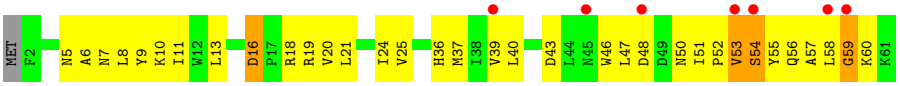




• Molecule 5: LH1 alpha polypeptide

Chain U:

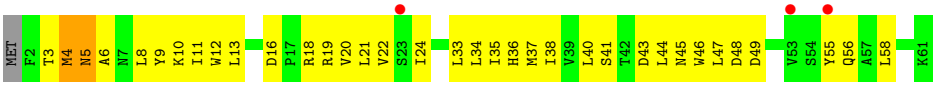




• Molecule 5: LH1 alpha polypeptide

Chain W:

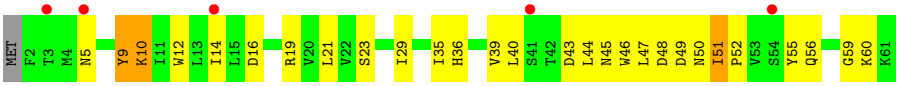




• Molecule 5: LH1 alpha polypeptide

Chain Y:

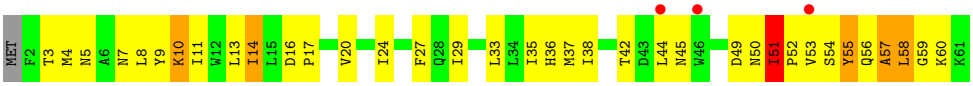




• Molecule 5: LH1 alpha polypeptide

Chain 1:

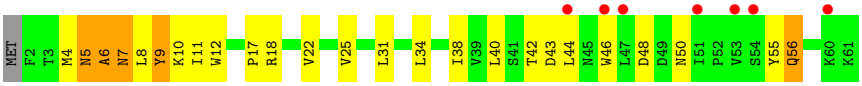




• Molecule 5: LH1 alpha polypeptide

Chain 3:

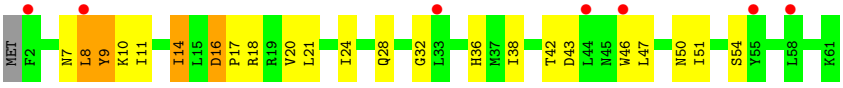




• Molecule 5: LH1 alpha polypeptide

Chain 5:

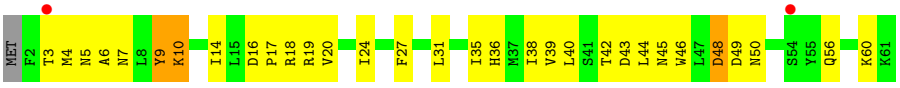




• Molecule 5: LH1 alpha polypeptide

Chain 7:





• Molecule 5: LH1 alpha polypeptide

Chain 9:

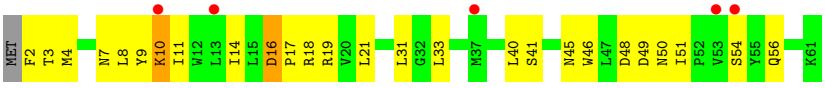




• Molecule 5: LH1 alpha polypeptide

Chain m:

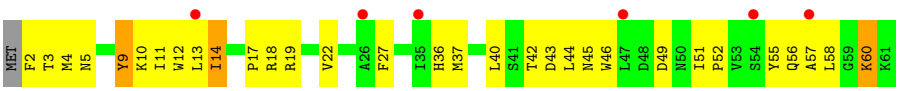




• Molecule 5: LH1 alpha polypeptide

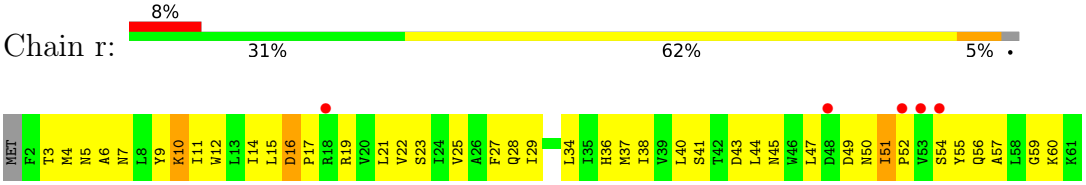
Chain p:





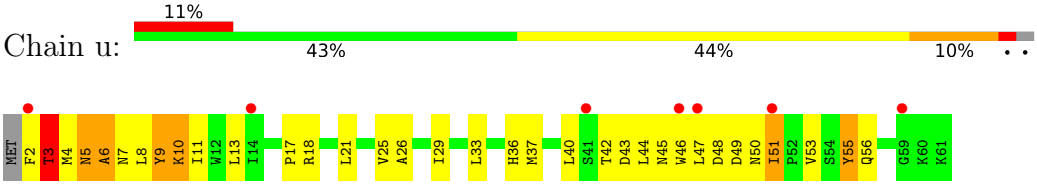
• Molecule 5: LH1 alpha polypeptide

Chain r:



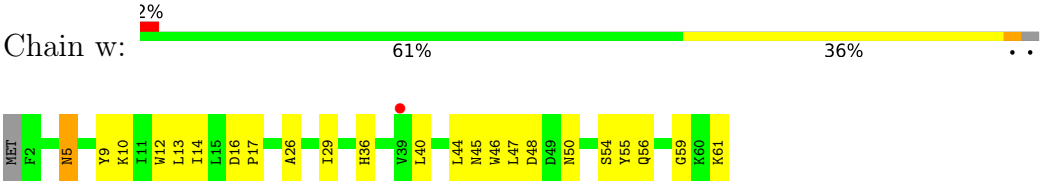
• Molecule 5: LH1 alpha polypeptide

Chain u:



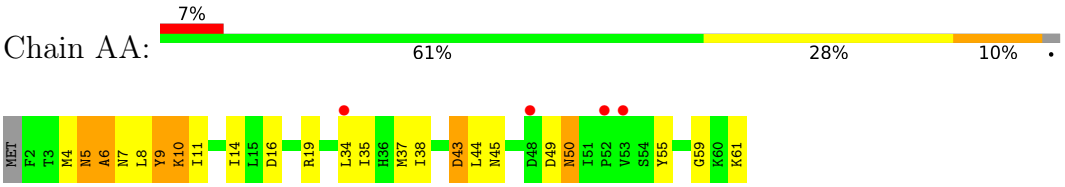
• Molecule 5: LH1 alpha polypeptide

Chain w:



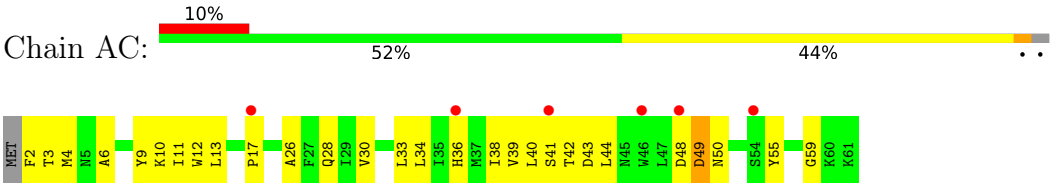
• Molecule 5: LH1 alpha polypeptide

Chain AA:



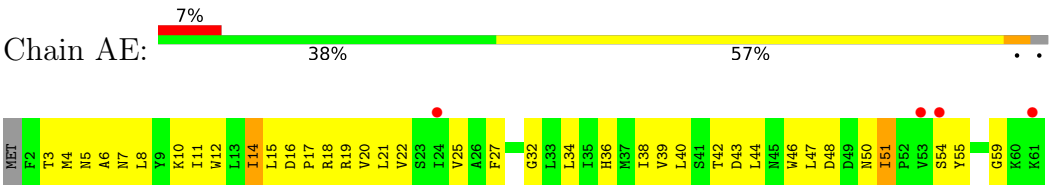
• Molecule 5: LH1 alpha polypeptide

Chain AC:



• Molecule 5: LH1 alpha polypeptide

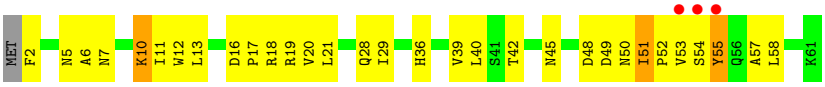
Chain AE:



• Molecule 5: LH1 alpha polypeptide

Chain AG:

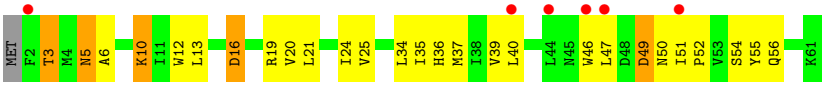




• Molecule 5: LH1 alpha polypeptide

Chain AI:

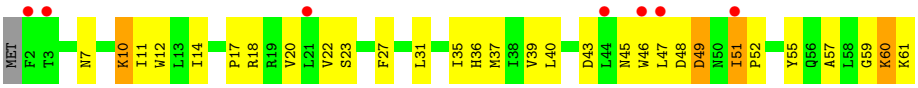




• Molecule 5: LH1 alpha polypeptide

Chain AK:

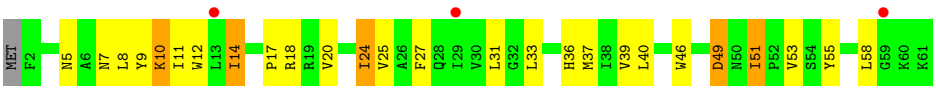




• Molecule 5: LH1 alpha polypeptide

Chain d:

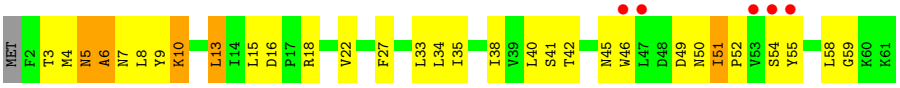




• Molecule 5: LH1 alpha polypeptide

Chain f:

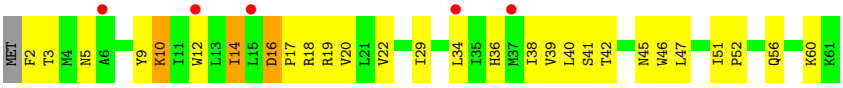




• Molecule 5: LH1 alpha polypeptide

Chain h:

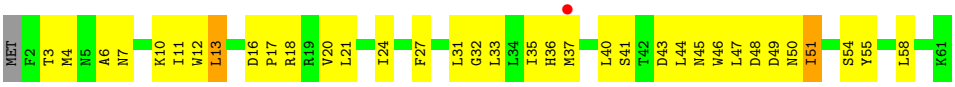




• Molecule 5: LH1 alpha polypeptide

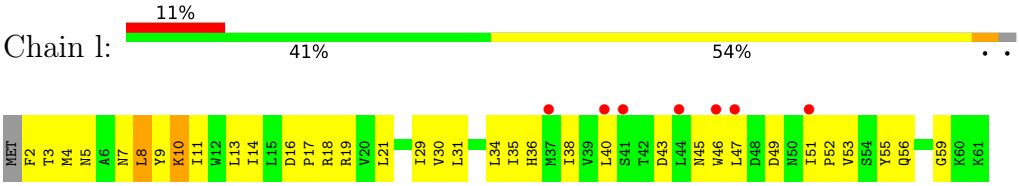
Chain j:





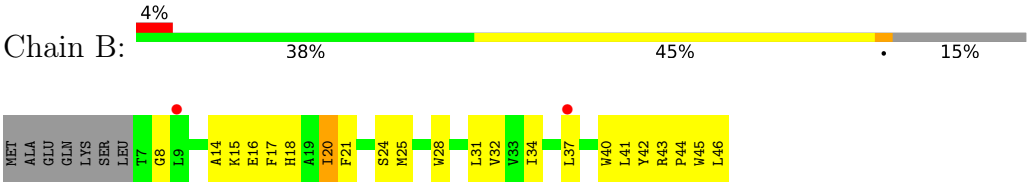
• Molecule 5: LH1 alpha polypeptide

Chain l:



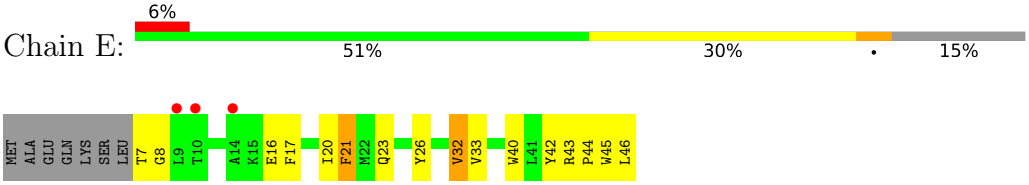
• Molecule 6: LH1 beta polypeptide

Chain B:



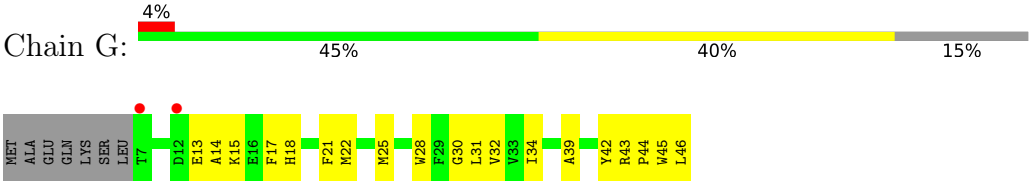
• Molecule 6: LH1 beta polypeptide

Chain E:



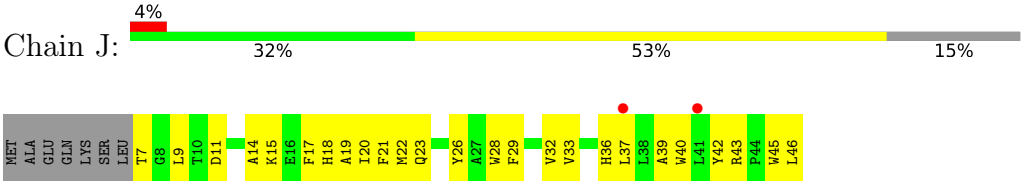
• Molecule 6: LH1 beta polypeptide

Chain G:



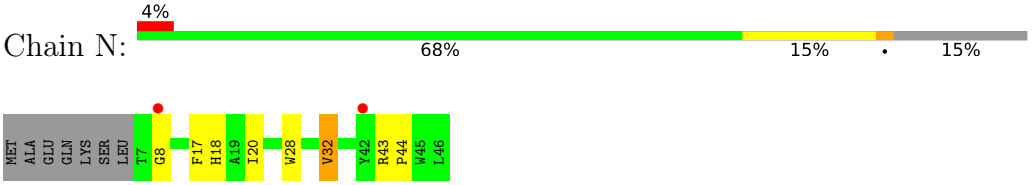
• Molecule 6: LH1 beta polypeptide

Chain J:



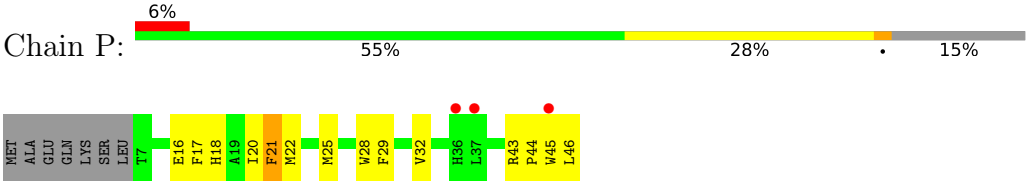
• Molecule 6: LH1 beta polypeptide

Chain N:



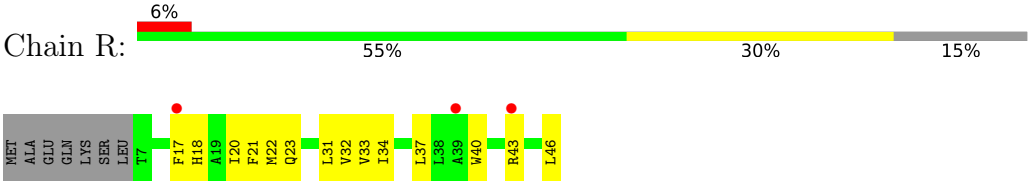
• Molecule 6: LH1 beta polypeptide

Chain P:



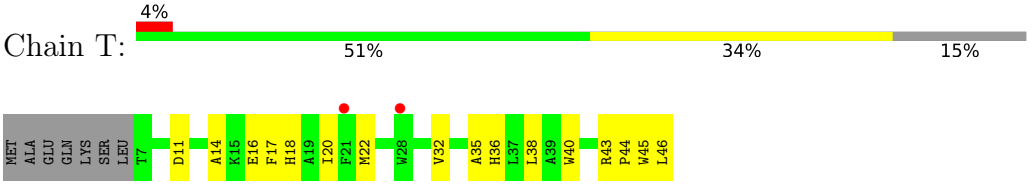
• Molecule 6: LH1 beta polypeptide

Chain R:



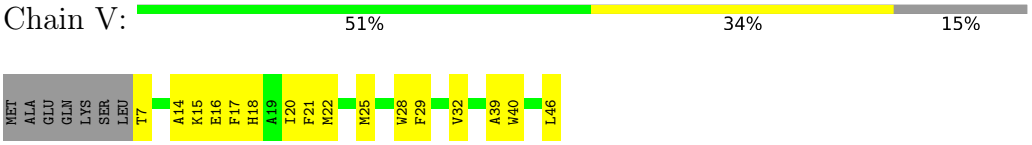
• Molecule 6: LH1 beta polypeptide

Chain T:



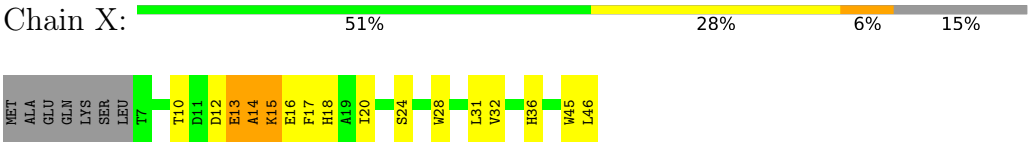
• Molecule 6: LH1 beta polypeptide

Chain V:



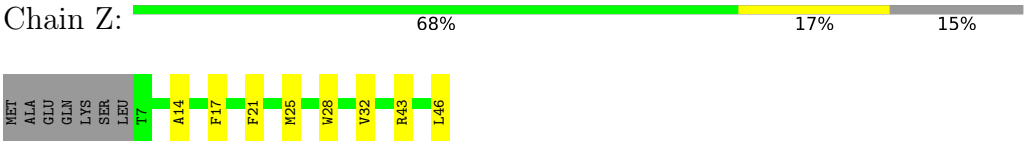
• Molecule 6: LH1 beta polypeptide

Chain X:



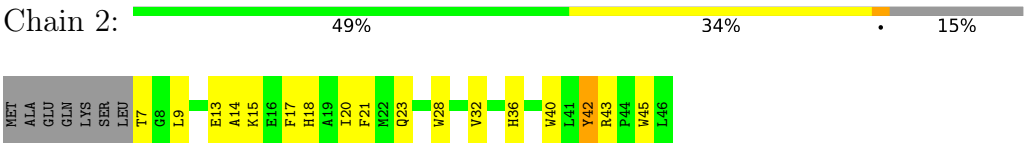
• Molecule 6: LH1 beta polypeptide

Chain Z:



• Molecule 6: LH1 beta polypeptide

Chain 2:



• Molecule 6: LH1 beta polypeptide

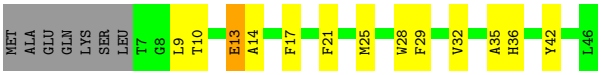
Chain 4:



• Molecule 6: LH1 beta polypeptide

Chain 6:

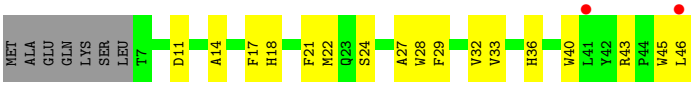




• Molecule 6: LH1 beta polypeptide

Chain 8:





• Molecule 6: LH1 beta polypeptide

Chain 0:

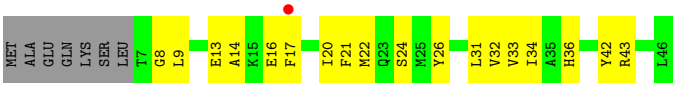




• Molecule 6: LH1 beta polypeptide

Chain n:

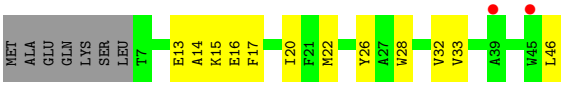




• Molecule 6: LH1 beta polypeptide

Chain q:

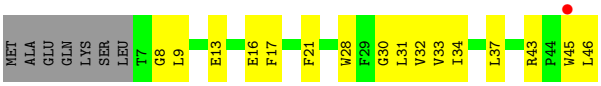




• Molecule 6: LH1 beta polypeptide

Chain s:

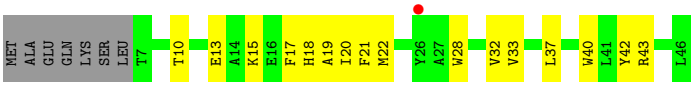




• Molecule 6: LH1 beta polypeptide

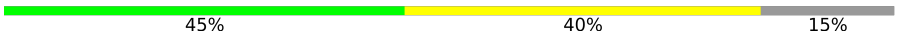
Chain v:

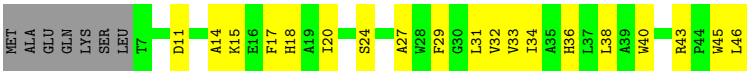




• Molecule 6: LH1 beta polypeptide

Chain z:

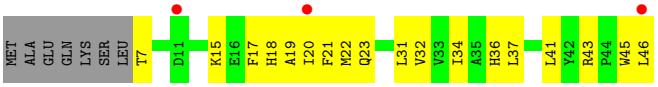




• Molecule 6: LH1 beta polypeptide

Chain AB:

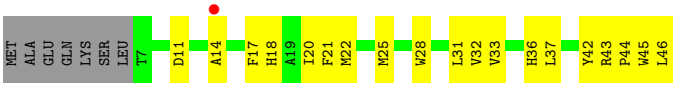




• Molecule 6: LH1 beta polypeptide

Chain AD:





• Molecule 6: LH1 beta polypeptide

Chain AF:

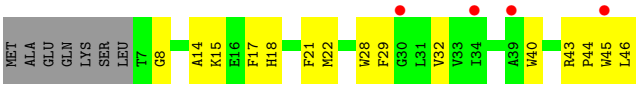




• Molecule 6: LH1 beta polypeptide

Chain AH:





• Molecule 6: LH1 beta polypeptide

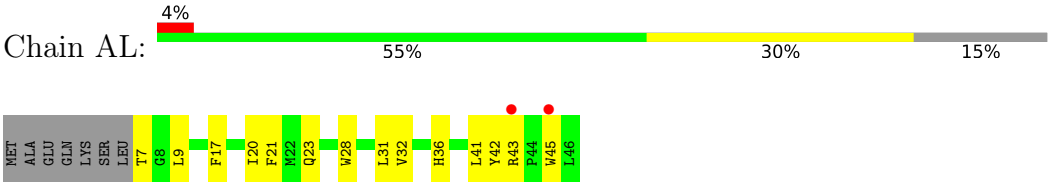
Chain AJ:





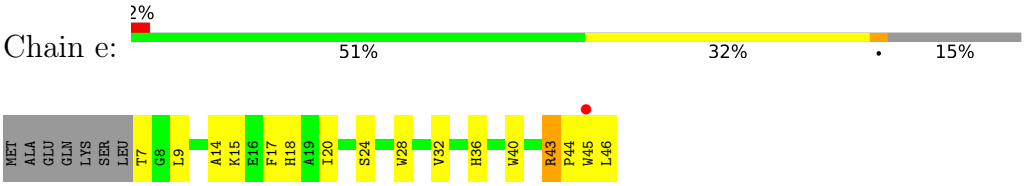
• Molecule 6: LH1 beta polypeptide

Chain AL:



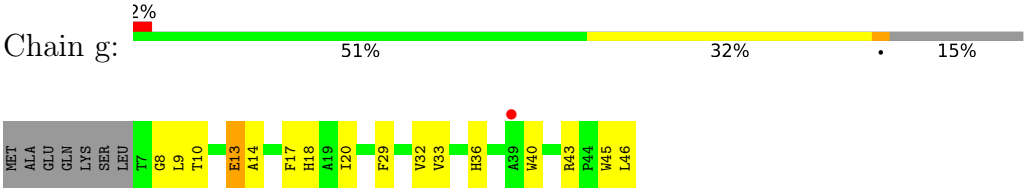
• Molecule 6: LH1 beta polypeptide

Chain e:



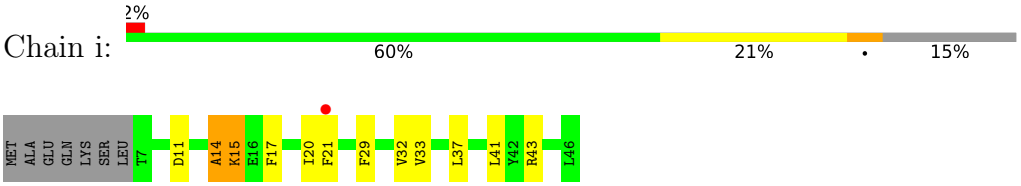
• Molecule 6: LH1 beta polypeptide

Chain g:



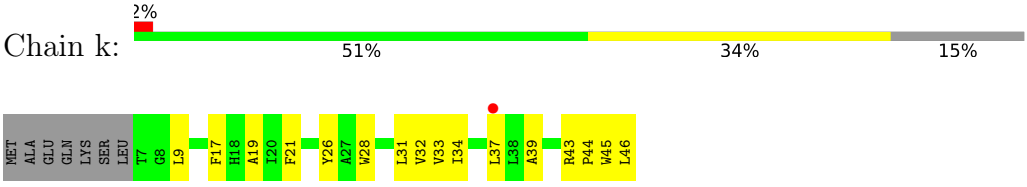
• Molecule 6: LH1 beta polypeptide

Chain i:



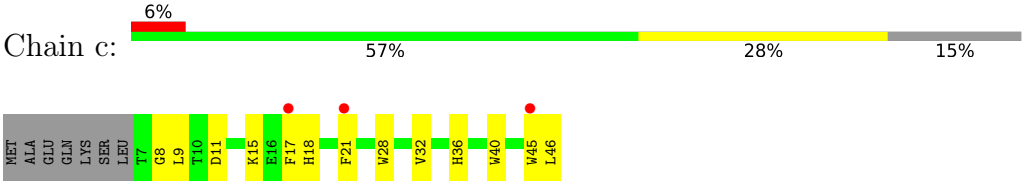
• Molecule 6: LH1 beta polypeptide

Chain k:



• Molecule 6: LH1 beta polypeptide

Chain c:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	163.83Å 148.56Å 210.00Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	49.90 – 3.30 49.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.90-3.30) 92.5 (49.90-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.279 , 0.313 0.281 , 0.315	Depositor DCC
R_{free} test set	6658 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 96.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.95	0/2528	1.55	47/3451 (1.4%)
1	o	0.90	0/2528	1.49	40/3451 (1.2%)
2	L	0.98	3/2318 (0.1%)	1.44	37/3167 (1.2%)
2	x	1.02	2/2318 (0.1%)	1.48	35/3167 (1.1%)
3	M	0.93	1/2646 (0.0%)	1.49	53/3621 (1.5%)
3	y	0.92	1/2646 (0.0%)	1.42	28/3621 (0.8%)
4	H	0.95	2/2037 (0.1%)	1.50	29/2776 (1.0%)
4	t	0.99	1/2037 (0.0%)	1.51	29/2776 (1.0%)
5	1	0.72	1/485 (0.2%)	1.34	7/664 (1.1%)
5	3	0.65	0/485	1.19	3/664 (0.5%)
5	5	0.66	0/485	1.12	3/664 (0.5%)
5	7	0.64	0/485	1.23	4/664 (0.6%)
5	9	0.60	0/485	1.09	1/664 (0.2%)
5	A	0.66	0/485	1.22	6/664 (0.9%)
5	AA	0.61	0/485	1.20	4/664 (0.6%)
5	AC	0.63	0/485	1.07	0/664
5	AE	0.58	0/491	1.10	2/672 (0.3%)
5	AG	0.62	0/485	1.14	2/664 (0.3%)
5	AI	0.67	0/485	1.18	5/664 (0.8%)
5	AK	0.72	0/485	1.16	2/664 (0.3%)
5	D	0.60	0/485	1.20	4/664 (0.6%)
5	F	0.59	0/485	1.17	3/664 (0.5%)
5	I	0.64	0/485	1.20	3/664 (0.5%)
5	K	0.61	0/485	1.16	4/664 (0.6%)
5	O	0.62	0/485	1.15	2/664 (0.3%)
5	Q	0.65	0/485	1.27	6/664 (0.9%)
5	S	0.69	0/491	1.03	2/672 (0.3%)
5	U	0.74	0/485	1.17	3/664 (0.5%)
5	W	0.75	0/485	1.20	2/664 (0.3%)
5	Y	0.72	0/485	1.14	2/664 (0.3%)
5	d	0.66	0/485	1.19	3/664 (0.5%)
5	f	0.75	0/485	1.28	7/664 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	h	0.71	0/485	1.21	3/664 (0.5%)
5	j	0.61	0/485	1.19	5/664 (0.8%)
5	l	0.59	0/485	1.11	2/664 (0.3%)
5	m	0.60	0/485	1.15	3/664 (0.5%)
5	p	0.67	0/485	1.20	3/664 (0.5%)
5	r	0.65	0/485	1.16	3/664 (0.5%)
5	u	0.66	0/485	1.13	4/664 (0.6%)
5	w	0.59	0/485	1.18	4/664 (0.6%)
6	0	0.51	0/350	1.07	1/476 (0.2%)
6	2	0.58	0/350	1.10	4/476 (0.8%)
6	4	0.56	0/350	1.01	1/476 (0.2%)
6	6	0.55	0/350	0.97	1/476 (0.2%)
6	8	0.53	0/350	0.92	0/476
6	AB	0.54	0/350	1.04	0/476
6	AD	0.53	0/350	0.95	0/476
6	AF	0.51	0/350	0.92	2/476 (0.4%)
6	AH	0.49	0/350	1.02	2/476 (0.4%)
6	AJ	0.60	0/350	0.94	1/476 (0.2%)
6	AL	0.59	0/350	1.02	1/476 (0.2%)
6	B	0.54	0/350	1.10	3/476 (0.6%)
6	E	0.59	0/350	1.14	1/476 (0.2%)
6	G	0.55	0/350	0.98	1/476 (0.2%)
6	J	0.56	0/350	1.10	1/476 (0.2%)
6	N	0.52	0/350	0.96	1/476 (0.2%)
6	P	0.49	0/350	0.98	0/476
6	R	0.51	0/350	0.97	0/476
6	T	0.56	0/350	1.03	1/476 (0.2%)
6	V	0.55	0/350	0.98	1/476 (0.2%)
6	X	0.58	0/350	1.15	3/476 (0.6%)
6	Z	0.56	0/350	0.89	0/476
6	c	0.54	0/350	0.95	0/476
6	e	0.63	0/350	0.92	2/476 (0.4%)
6	g	0.53	0/350	0.99	2/476 (0.4%)
6	i	0.55	0/350	0.98	2/476 (0.4%)
6	k	0.46	0/350	0.84	0/476
6	n	0.64	0/350	1.04	0/476
6	q	0.59	0/350	1.05	2/476 (0.4%)
6	s	0.59	0/350	0.98	0/476
6	v	0.55	0/350	1.01	1/476 (0.2%)
6	z	0.53	0/350	1.12	1/476 (0.2%)
All	All	0.77	11/45790 (0.0%)	1.28	440/62526 (0.7%)

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

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	241	LEU	CA-C	-5.75	1.45	1.52
4	H	39	TYR	CA-C	5.74	1.60	1.52
3	y	106	ILE	CA-C	-5.56	1.49	1.53
2	x	252	TRP	C-O	-5.45	1.17	1.24
2	L	237	ALA	C-O	-5.25	1.18	1.24
2	L	265	THR	CA-CB	-5.22	1.46	1.54
3	M	53	LEU	CA-C	-5.21	1.47	1.53
5	1	51	ILE	CA-C	5.15	1.58	1.52
4	H	38	GLY	C-O	-5.12	1.17	1.23
4	t	67	PHE	CA-C	-5.11	1.46	1.52
2	x	179	ASN	CA-C	-5.05	1.46	1.52

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	x	228	ILE	N-CA-C	12.90	122.66	110.53
1	o	195	LEU	CA-C-N	-12.79	105.67	120.13
1	o	195	LEU	C-N-CA	-12.79	105.67	120.13
3	M	33	ARG	CA-C-N	11.09	133.70	119.84
3	M	33	ARG	C-N-CA	11.09	133.70	119.84
4	H	71	HIS	N-CA-C	10.69	126.25	111.17
5	7	16	ASP	CA-C-N	10.64	130.30	119.24
5	7	16	ASP	C-N-CA	10.64	130.30	119.24
3	y	33	ARG	CA-C-N	10.57	133.05	119.84
3	y	33	ARG	C-N-CA	10.57	133.05	119.84
2	L	17	LEU	N-CA-C	-10.47	100.24	113.43
1	C	29	GLY	N-CA-C	-10.04	98.31	112.37
3	y	146	LEU	N-CA-C	-10.02	99.91	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	258	LEU	N-CA-C	-9.91	103.33	114.62
5	p	9	TYR	N-CA-C	-9.71	95.30	110.36
1	C	195	LEU	CA-C-N	-9.34	109.58	120.13
1	C	195	LEU	C-N-CA	-9.34	109.58	120.13
3	M	15	ALA	N-CA-C	-9.24	97.53	108.25
3	y	183	LEU	N-CA-C	-9.11	100.49	111.69
1	o	332	LYS	N-CA-C	8.89	123.04	110.50
2	L	280	LEU	N-CA-C	-8.79	102.97	114.31
3	M	55	LEU	N-CA-C	-8.78	101.28	111.03
1	o	194	SER	N-CA-C	8.78	124.05	113.16
2	x	33	GLY	N-CA-C	-8.76	101.64	112.68
5	Q	51	ILE	N-CA-C	8.71	117.39	107.89
3	M	304	ALA	CA-C-N	8.69	128.72	119.78
3	M	304	ALA	C-N-CA	8.69	128.72	119.78
4	H	185	GLU	N-CA-C	-8.55	95.42	108.67
3	y	15	ALA	N-CA-C	-8.46	98.44	108.25
3	M	146	LEU	N-CA-C	-8.40	101.71	111.03
4	t	176	GLU	CA-C-N	8.39	130.32	119.84
4	t	176	GLU	C-N-CA	8.39	130.32	119.84
5	j	58	LEU	N-CA-C	-8.35	102.81	113.16
5	K	9	TYR	N-CA-C	-8.34	100.86	112.45
1	o	62	LEU	CA-C-N	-8.28	111.45	119.90
1	o	62	LEU	C-N-CA	-8.28	111.45	119.90
2	L	77	PRO	CA-C-N	-8.26	112.34	120.52
2	L	77	PRO	C-N-CA	-8.26	112.34	120.52
5	j	16	ASP	CA-C-N	8.26	128.74	119.32
5	j	16	ASP	C-N-CA	8.26	128.74	119.32
2	x	77	PRO	CA-C-N	-8.26	112.34	120.52
2	x	77	PRO	C-N-CA	-8.26	112.34	120.52
3	M	154	ILE	N-CA-C	-8.26	102.49	110.42
4	H	61	LEU	CA-C-N	8.22	128.86	120.14
4	H	61	LEU	C-N-CA	8.22	128.86	120.14
1	C	64	ALA	CA-C-N	-8.21	111.02	122.93
1	C	64	ALA	C-N-CA	-8.21	111.02	122.93
5	Q	7	ASN	N-CA-C	-8.19	101.30	112.03
3	y	264	SER	N-CA-C	8.16	121.09	111.71
1	C	112	VAL	N-CA-C	-8.13	99.55	107.76
5	7	9	TYR	N-CA-C	-8.11	101.17	112.45
5	3	7	ASN	N-CA-C	-8.08	99.97	112.99
3	y	80	HIS	N-CA-C	8.03	123.03	113.23
2	L	128	PHE	N-CA-C	-8.03	102.47	111.14
1	C	62	LEU	N-CA-C	-7.99	99.27	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	281	GLN	N-CA-C	7.96	121.47	111.69
2	x	17	LEU	N-CA-C	-7.95	103.41	113.43
6	J	15	LYS	N-CA-C	-7.94	101.92	111.69
3	y	30	ARG	N-CA-C	-7.91	97.38	109.95
5	r	16	ASP	CA-C-N	7.88	127.80	119.05
5	r	16	ASP	C-N-CA	7.88	127.80	119.05
1	o	65	ALA	N-CA-C	-7.88	96.91	109.59
1	o	118	SER	N-CA-C	7.79	121.49	110.50
5	U	16	ASP	CA-C-N	7.78	127.69	119.05
5	U	16	ASP	C-N-CA	7.78	127.69	119.05
3	M	210	TYR	N-CA-C	-7.76	102.90	111.36
5	d	51	ILE	N-CA-C	7.70	117.14	108.05
1	C	305	VAL	N-CA-C	7.69	120.89	108.97
5	AK	49	ASP	N-CA-C	-7.67	104.15	113.97
3	y	213	ALA	N-CA-C	-7.67	102.86	111.14
4	t	74	GLY	N-CA-C	7.62	120.14	110.38
6	4	15	LYS	N-CA-C	-7.59	102.35	111.69
5	Q	16	ASP	CA-C-N	7.59	127.47	119.05
5	Q	16	ASP	C-N-CA	7.59	127.47	119.05
1	C	102	SER	CA-C-N	7.57	127.22	119.19
1	C	102	SER	C-N-CA	7.57	127.22	119.19
1	C	301	ASP	CA-C-N	7.55	128.90	120.66
1	C	301	ASP	C-N-CA	7.55	128.90	120.66
5	AA	16	ASP	CA-C-N	7.55	127.93	119.32
5	AA	16	ASP	C-N-CA	7.55	127.93	119.32
3	M	257	GLY	N-CA-C	7.54	125.39	115.36
5	F	16	ASP	CA-C-N	7.53	127.41	119.05
5	F	16	ASP	C-N-CA	7.53	127.41	119.05
1	C	101	VAL	CA-C-N	-7.51	115.38	122.37
1	C	101	VAL	C-N-CA	-7.51	115.38	122.37
3	M	20	GLY	N-CA-C	7.50	123.90	112.81
4	t	125	LEU	N-CA-C	7.47	121.67	109.72
2	x	159	ILE	N-CA-C	7.46	118.19	110.36
5	w	13	LEU	N-CA-C	-7.46	104.18	113.28
3	y	85	GLN	N-CA-C	-7.44	103.17	111.28
3	y	214	LEU	N-CA-C	7.44	119.08	110.97
2	x	34	PHE	N-CA-C	7.37	120.19	111.71
3	M	135	LYS	N-CA-C	-7.34	102.97	110.97
3	M	128	LEU	N-CA-C	-7.33	103.30	112.90
2	x	155	PHE	CA-C-N	7.32	127.48	120.31
2	x	155	PHE	C-N-CA	7.32	127.48	120.31
3	M	226	VAL	N-CA-C	-7.32	104.12	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	y	40	LEU	N-CA-C	-7.30	103.32	111.28
5	AI	49	ASP	N-CA-C	-7.28	104.65	113.97
6	X	15	LYS	N-CA-C	-7.18	102.48	112.45
1	o	247	CYS	CA-CB-SG	-7.17	97.92	114.40
5	S	9	TYR	N-CA-C	-7.15	102.51	112.45
2	L	181	ALA	N-CA-C	-7.14	103.57	111.36
5	f	58	LEU	N-CA-C	7.13	122.31	112.04
3	M	40	LEU	N-CA-C	-7.13	103.51	111.28
1	o	112	VAL	N-CA-C	-7.10	100.59	107.76
6	0	8	GLY	N-CA-C	7.09	129.99	113.18
1	o	199	PRO	N-CA-C	-6.99	106.60	114.92
2	L	228	ILE	CB-CA-C	-6.98	102.87	112.02
4	t	116	SER	CA-C-N	-6.98	111.11	119.84
4	t	116	SER	C-N-CA	-6.98	111.11	119.84
1	C	131	PHE	N-CA-C	-6.97	103.45	112.23
4	H	73	GLY	N-CA-C	6.97	122.71	113.37
6	B	14	ALA	N-CA-C	-6.97	104.39	113.17
6	G	15	LYS	N-CA-C	-6.96	103.13	111.69
3	M	307	TYR	CA-C-N	-6.94	112.33	119.83
3	M	307	TYR	C-N-CA	-6.94	112.33	119.83
5	5	16	ASP	CA-C-N	6.92	126.16	118.97
5	5	16	ASP	C-N-CA	6.92	126.16	118.97
6	g	8	GLY	N-CA-C	6.88	123.52	113.48
5	f	7	ASN	N-CA-C	-6.85	103.06	112.03
5	3	9	TYR	N-CA-C	-6.84	102.94	112.45
5	p	14	ILE	N-CA-C	-6.84	106.36	111.90
4	H	138	VAL	N-CA-C	-6.83	102.72	112.35
2	x	114	VAL	N-CA-C	-6.83	104.11	110.53
5	Q	13	LEU	N-CA-C	-6.83	104.95	113.28
6	X	15	LYS	CA-C-N	6.83	129.31	120.44
6	X	15	LYS	C-N-CA	6.83	129.31	120.44
4	H	41	LEU	N-CA-C	6.82	119.13	110.33
3	y	150	PHE	N-CA-C	-6.82	103.78	111.07
4	t	67	PHE	N-CA-C	-6.75	98.23	109.24
2	x	261	GLY	N-CA-C	-6.74	98.59	112.34
5	j	51	ILE	N-CA-C	6.74	115.23	107.89
1	o	101	VAL	CA-C-N	-6.73	116.11	122.37
1	o	101	VAL	C-N-CA	-6.73	116.11	122.37
5	9	7	ASN	N-CA-C	-6.70	105.86	112.97
6	i	15	LYS	N-CA-C	-6.70	103.22	111.40
1	C	166	TRP	N-CA-C	6.70	118.69	109.18
5	AG	58	LEU	N-CA-C	-6.70	105.11	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	7	ILE	N-CA-C	-6.68	105.32	111.67
2	L	72	ARG	N-CA-C	6.68	121.43	113.28
1	C	122	TYR	N-CA-C	6.68	120.30	111.75
5	h	5	ASN	N-CA-C	6.68	119.91	109.96
1	C	291	LEU	CA-C-N	6.67	126.64	120.03
1	C	291	LEU	C-N-CA	6.67	126.64	120.03
1	C	118	SER	N-CA-C	6.65	119.87	110.50
5	1	14	ILE	CB-CA-C	-6.61	104.96	111.30
3	M	183	LEU	N-CA-C	-6.60	103.57	111.69
4	t	29	TYR	CA-CB-CG	6.60	125.79	113.90
6	2	15	LYS	N-CA-C	-6.60	103.35	111.40
3	y	154	ILE	N-CA-C	-6.56	104.12	110.42
5	w	5	ASN	N-CA-C	6.54	119.25	111.33
2	x	129	ALA	N-CA-C	-6.53	104.16	111.28
5	f	8	LEU	N-CA-C	-6.53	105.62	112.93
2	L	228	ILE	N-CA-C	6.52	116.66	110.53
5	I	9	TYR	N-CA-C	-6.52	103.38	112.45
2	x	227	ASP	N-CA-C	-6.52	104.09	111.07
5	W	4	MET	N-CA-C	-6.50	103.69	111.69
5	AE	14	ILE	CB-CA-C	-6.50	105.06	111.30
6	AH	15	LYS	N-CA-C	-6.48	103.49	111.40
5	I	51	ILE	N-CA-C	6.48	115.11	107.73
1	o	168	THR	N-CA-C	-6.47	100.25	109.96
1	C	222	ASN	CA-C-N	6.45	128.70	120.89
1	C	222	ASN	C-N-CA	6.45	128.70	120.89
4	H	256	GLY	N-CA-C	-6.44	99.20	112.34
1	o	233	PHE	N-CA-C	-6.44	104.34	111.36
3	y	4	TYR	N-CA-C	-6.44	101.17	110.24
5	h	16	ASP	CA-C-N	6.40	126.61	119.32
5	h	16	ASP	C-N-CA	6.40	126.61	119.32
3	M	150	PHE	N-CA-C	-6.39	103.44	111.11
1	o	252	ASN	N-CA-C	-6.39	92.84	107.48
2	L	214	PRO	CA-C-O	-6.38	114.28	122.13
1	o	29	GLY	N-CA-C	-6.38	103.44	112.37
5	Y	50	ASN	N-CA-C	-6.38	103.37	111.92
5	D	9	TYR	N-CA-C	-6.36	100.00	109.86
1	o	25	GLY	CA-C-N	6.35	126.92	120.38
1	o	25	GLY	C-N-CA	6.35	126.92	120.38
4	H	44	ASP	N-CA-C	-6.35	105.40	113.02
5	m	3	THR	N-CA-C	-6.34	105.42	113.02
3	M	264	SER	N-CA-C	6.32	118.97	111.71
6	q	15	LYS	N-CA-C	-6.30	103.94	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	120	LEU	N-CA-C	6.30	120.43	112.87
4	H	176	GLU	CA-C-N	6.29	127.71	119.84
4	H	176	GLU	C-N-CA	6.29	127.71	119.84
1	o	331	TYR	N-CA-C	-6.26	99.61	109.50
1	C	247	CYS	CA-CB-SG	-6.24	100.06	114.40
5	K	16	ASP	CA-C-N	6.23	125.96	119.05
5	K	16	ASP	C-N-CA	6.23	125.96	119.05
3	M	9	THR	N-CA-C	-6.22	100.96	110.30
1	o	327	TYR	CA-C-N	6.22	125.90	119.56
1	o	327	TYR	C-N-CA	6.22	125.90	119.56
5	u	51	ILE	N-CA-C	6.21	114.72	107.77
3	y	129	TRP	N-CA-C	-6.20	104.63	111.82
1	C	300	GLY	N-CA-C	-6.20	106.77	115.32
3	M	237	GLN	N-CA-C	-6.18	105.22	112.89
3	y	224	LEU	N-CA-C	-6.16	105.62	113.01
2	x	70	LEU	N-CA-C	6.15	118.78	111.71
2	L	232	SER	N-CA-C	-6.15	97.56	108.13
3	y	135	LYS	N-CA-C	-6.10	104.32	110.97
4	t	159	LEU	CA-C-N	-6.10	112.91	122.73
4	t	159	LEU	C-N-CA	-6.10	112.91	122.73
1	C	169	ASP	CA-C-N	6.10	127.00	120.47
1	C	169	ASP	C-N-CA	6.10	127.00	120.47
1	o	78	ASN	N-CA-C	6.09	117.88	109.54
1	o	186	GLY	N-CA-C	-6.08	98.77	113.18
5	f	51	ILE	N-CA-C	6.08	113.86	108.63
1	C	265	LYS	N-CA-C	-6.07	105.36	112.89
3	M	107	PRO	N-CA-C	6.07	118.10	110.70
6	E	32	VAL	N-CA-C	6.06	116.11	110.42
5	F	7	ASN	N-CA-C	-6.05	104.10	112.03
5	D	16	ASP	CA-C-N	6.05	125.76	119.05
5	D	16	ASP	C-N-CA	6.05	125.76	119.05
5	d	14	ILE	CB-CA-C	-6.05	105.49	111.30
2	x	126	VAL	CA-C-N	-6.03	113.47	119.56
2	x	126	VAL	C-N-CA	-6.03	113.47	119.56
3	y	227	SER	N-CA-C	-6.03	105.89	113.18
6	AH	14	ALA	N-CA-C	-6.03	105.89	113.72
3	M	290	VAL	N-CA-C	6.02	117.18	112.12
5	f	16	ASP	CA-C-N	6.02	125.73	119.05
5	f	16	ASP	C-N-CA	6.02	125.73	119.05
1	C	199	PRO	N-CA-C	-6.01	107.76	114.92
5	S	13	LEU	N-CA-C	-6.01	105.94	113.28
2	L	76	ALA	CA-C-N	6.01	126.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	76	ALA	C-N-CA	6.01	126.57	120.38
5	AI	3	THR	N-CA-C	-6.00	100.40	108.86
2	x	72	ARG	N-CA-C	5.98	120.58	113.28
2	L	37	VAL	N-CA-C	-5.98	104.48	111.00
4	t	258	LEU	N-CA-C	-5.98	107.81	114.62
2	L	7	GLU	N-CA-C	5.98	120.73	112.90
2	L	211	LYS	N-CA-C	-5.98	101.56	110.23
4	H	164	ALA	N-CA-C	-5.97	105.07	112.72
2	x	120	LEU	N-CA-C	5.97	120.04	112.87
2	L	226	ARG	N-CA-C	-5.96	104.71	112.23
1	o	181	THR	N-CA-C	5.96	119.66	112.38
3	y	55	LEU	N-CA-C	-5.95	104.43	111.03
1	o	62	LEU	N-CA-C	-5.93	102.11	110.29
5	A	51	ILE	N-CA-C	5.93	114.35	107.89
1	C	324	ALA	N-CA-C	5.92	118.49	111.33
1	C	62	LEU	CA-C-N	-5.92	113.86	119.90
1	C	62	LEU	C-N-CA	-5.92	113.86	119.90
4	H	130	LEU	N-CA-C	-5.91	102.70	110.39
4	t	37	GLU	N-CA-C	-5.90	100.60	108.74
5	u	9	TYR	N-CA-C	-5.90	104.25	112.45
5	AA	50	ASN	N-CA-C	-5.89	104.02	111.92
1	o	305	VAL	N-CA-C	5.89	118.09	108.97
5	W	58	LEU	N-CA-C	-5.88	105.76	113.17
5	K	13	LEU	N-CA-C	-5.88	106.11	113.28
4	H	228	PRO	N-CA-C	5.87	121.69	114.35
1	o	330	LEU	N-CA-C	5.86	119.74	112.59
3	M	106	ILE	CB-CA-C	-5.85	104.16	110.95
3	y	107	PRO	N-CA-C	5.85	117.83	110.70
1	C	115	ASN	N-CA-C	5.84	118.12	108.49
4	H	192	LYS	N-CA-C	5.83	118.73	109.24
1	C	327	TYR	CA-C-N	5.82	125.44	119.56
1	C	327	TYR	C-N-CA	5.82	125.44	119.56
4	t	9	ILE	N-CA-C	5.82	116.24	107.80
5	AI	51	ILE	N-CA-C	5.82	114.91	108.05
5	AI	16	ASP	CA-C-N	5.81	125.50	119.05
5	AI	16	ASP	C-N-CA	5.81	125.50	119.05
5	A	25	VAL	N-CA-C	5.81	116.00	110.42
3	M	170	SER	N-CA-C	5.80	117.06	107.20
4	H	38	GLY	N-CA-C	5.80	126.92	113.18
2	x	169	VAL	N-CA-C	-5.75	103.73	111.44
5	Y	48	ASP	N-CA-C	5.75	119.61	110.70
4	H	137	ARG	N-CA-C	-5.74	105.39	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	146	ALA	CB-CA-C	-5.73	108.97	115.79
2	L	206	VAL	N-CA-C	5.73	116.74	111.81
4	t	232	THR	N-CA-C	5.73	119.30	110.42
5	l	9	TYR	N-CA-C	-5.72	104.50	112.45
1	C	251	HIS	N-CA-C	5.72	118.19	109.95
1	C	86	SER	N-CA-C	-5.72	102.98	110.53
2	L	123	GLY	CA-C-N	-5.71	114.03	122.83
2	L	123	GLY	C-N-CA	-5.71	114.03	122.83
4	H	224	THR	N-CA-C	5.71	118.99	110.14
4	t	127	PHE	N-CA-C	-5.70	105.15	111.36
4	t	247	LYS	N-CA-C	-5.70	105.43	112.38
1	o	109	TYR	N-CA-C	5.69	117.29	111.14
2	L	261	GLY	CA-C-N	5.69	126.95	119.84
2	L	261	GLY	C-N-CA	5.69	126.95	119.84
5	O	59	GLY	N-CA-C	5.69	126.67	113.18
4	t	41	LEU	N-CA-C	5.69	117.67	110.33
2	x	188	PHE	N-CA-C	-5.68	105.01	111.14
4	H	155	THR	CA-C-N	-5.67	115.06	122.37
4	H	155	THR	C-N-CA	-5.67	115.06	122.37
2	L	217	THR	N-CA-C	5.67	118.48	109.81
4	t	121	LYS	N-CA-C	-5.66	103.79	111.55
3	M	61	ILE	N-CA-C	-5.66	104.85	110.62
2	L	261	GLY	N-CA-C	-5.66	100.80	112.34
2	x	66	GLN	N-CA-C	-5.65	102.66	110.35
5	r	51	ILE	N-CA-C	5.65	114.05	107.89
2	L	86	MET	N-CA-C	-5.65	100.77	109.76
5	1	16	ASP	CA-C-N	5.64	124.84	118.97
5	1	16	ASP	C-N-CA	5.64	124.84	118.97
3	M	224	LEU	N-CA-C	-5.64	104.75	111.69
2	L	113	GLU	N-CA-C	-5.64	105.13	112.23
2	L	34	PHE	N-CA-C	5.64	118.19	111.71
1	o	122	TYR	N-CA-C	5.63	118.96	111.75
5	AE	51	ILE	N-CA-C	5.62	114.69	108.05
4	t	227	ASN	CA-C-N	-5.61	114.22	120.45
4	t	227	ASN	C-N-CA	-5.61	114.22	120.45
3	M	119	GLY	N-CA-C	-5.60	105.71	112.49
3	M	148	TRP	N-CA-C	-5.60	106.28	113.23
2	x	126	VAL	CB-CA-C	-5.60	106.67	114.00
1	o	64	ALA	CA-C-N	-5.59	114.83	122.93
1	o	64	ALA	C-N-CA	-5.59	114.83	122.93
1	o	131	PHE	N-CA-C	-5.58	105.19	112.23
2	x	228	ILE	CB-CA-C	-5.58	104.71	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AF	43	ARG	CA-C-N	5.58	125.50	119.76
6	AF	43	ARG	C-N-CA	5.58	125.50	119.76
2	x	93	GLY	N-CA-C	-5.58	105.74	112.49
3	M	175	VAL	CA-C-N	5.57	126.04	120.14
3	M	175	VAL	C-N-CA	5.57	126.04	120.14
6	e	43	ARG	CA-C-N	5.56	125.84	119.83
6	e	43	ARG	C-N-CA	5.56	125.84	119.83
2	L	159	ILE	N-CA-C	5.56	116.19	110.36
2	L	267	GLY	N-CA-C	-5.54	105.45	112.54
3	y	175	VAL	CA-C-N	5.53	126.00	120.14
3	y	175	VAL	C-N-CA	5.53	126.00	120.14
1	C	189	THR	N-CA-C	-5.51	104.79	112.45
3	M	106	ILE	N-CA-C	-5.50	102.55	107.56
1	C	288	ASN	N-CA-C	5.49	118.02	111.71
2	L	222	ASN	N-CA-C	5.49	117.27	111.28
2	x	126	VAL	N-CA-C	5.49	118.93	112.35
2	x	53	GLY	N-CA-C	-5.49	105.75	112.77
5	w	16	ASP	CA-C-N	5.48	125.13	119.05
5	w	16	ASP	C-N-CA	5.48	125.13	119.05
4	t	222	VAL	N-CA-C	-5.47	103.00	108.96
1	C	169	ASP	N-CA-CB	-5.46	101.03	110.10
5	O	3	THR	N-CA-C	5.46	118.06	108.56
6	2	43	ARG	CA-C-N	5.46	125.38	119.76
6	2	43	ARG	C-N-CA	5.46	125.38	119.76
5	AA	9	TYR	N-CA-C	-5.45	104.88	112.45
5	I	14	ILE	CB-CA-C	-5.44	106.08	111.30
2	x	232	SER	N-CA-C	-5.44	98.69	108.48
6	6	13	GLU	N-CA-C	-5.44	106.50	113.02
1	C	187	SER	N-CA-C	5.43	117.25	108.34
6	g	13	GLU	N-CA-C	-5.42	106.51	113.02
5	f	13	LEU	N-CA-C	-5.42	106.67	113.28
3	M	111	GLU	CA-C-N	-5.40	115.79	123.08
3	M	111	GLU	C-N-CA	-5.40	115.79	123.08
6	z	14	ALA	N-CA-C	-5.39	106.71	113.72
5	l	53	VAL	N-CA-C	5.39	116.44	108.45
1	C	252	ASN	N-CA-C	-5.38	96.45	107.70
2	x	113	GLU	N-CA-C	-5.38	105.45	112.23
2	L	51	VAL	N-CA-C	-5.38	105.47	110.53
3	M	177	PHE	N-CA-C	5.37	117.47	108.23
2	L	126	VAL	CA-C-N	-5.36	114.14	119.56
2	L	126	VAL	C-N-CA	-5.36	114.14	119.56
3	M	84	PHE	N-CA-C	-5.36	104.87	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	x	103	ALA	N-CA-C	-5.36	105.36	111.14
5	1	3	THR	N-CA-C	5.35	118.44	110.52
5	1	57	ALA	CA-C-N	5.35	131.33	121.70
5	1	57	ALA	C-N-CA	5.35	131.33	121.70
6	q	14	ALA	N-CA-C	-5.35	106.80	113.38
5	A	3	THR	N-CA-C	-5.35	106.94	112.93
3	y	237	GLN	N-CA-C	-5.34	106.26	112.89
5	d	49	ASP	N-CA-C	-5.34	107.42	114.31
2	L	206	VAL	CB-CA-C	-5.34	105.41	111.55
1	o	164	TYR	N-CA-C	5.33	119.50	112.25
3	y	235	ILE	CB-CA-C	-5.33	105.03	112.02
3	M	98	PRO	CA-C-N	-5.33	114.89	120.38
3	M	98	PRO	C-N-CA	-5.33	114.89	120.38
4	H	37	GLU	N-CA-C	-5.33	101.39	108.74
1	C	226	LEU	N-CA-C	-5.32	105.56	111.36
1	C	205	ASP	N-CA-C	-5.32	99.47	110.80
4	H	133	ILE	N-CA-C	5.30	115.23	108.12
1	o	254	ARG	N-CA-C	-5.30	106.31	112.89
5	3	8	LEU	N-CA-C	-5.30	106.40	112.92
1	o	171	GLY	N-CA-C	-5.29	101.55	112.34
3	M	19	PRO	N-CA-C	-5.29	107.53	114.03
4	t	137	ARG	N-CA-C	-5.29	105.57	112.23
2	x	181	ALA	N-CA-C	-5.28	105.61	111.36
5	7	3	THR	CB-CA-C	-5.28	109.51	115.79
2	x	206	VAL	N-CA-C	5.28	116.35	111.81
5	u	55	TYR	N-CA-C	-5.28	105.99	112.90
1	o	270	TRP	N-CA-C	-5.27	105.45	111.14
4	H	123	CYS	N-CA-C	5.27	118.65	110.17
6	B	40	TRP	N-CA-C	-5.26	105.72	111.82
5	A	13	LEU	N-CA-C	-5.24	106.88	113.28
2	x	127	PRO	CA-C-N	5.24	127.57	120.44
2	x	127	PRO	C-N-CA	5.24	127.57	120.44
5	AG	55	TYR	N-CA-C	5.24	118.13	111.69
3	M	88	LYS	N-CA-C	5.23	116.98	111.28
1	C	197	PHE	N-CA-C	5.22	121.93	110.80
5	j	13	LEU	N-CA-C	-5.22	106.91	113.28
4	H	196	PRO	CA-C-O	-5.22	115.31	121.67
3	M	212	SER	N-CA-C	-5.21	106.18	112.54
2	x	51	VAL	N-CA-C	-5.20	105.64	110.53
2	L	229	VAL	N-CA-C	5.19	117.38	111.88
4	t	26	LEU	N-CA-C	-5.19	105.27	111.03
6	AJ	15	LYS	N-CA-C	-5.19	105.31	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	13	LEU	N-CA-C	-5.19	106.95	113.28
4	t	32	ARG	N-CA-C	-5.18	105.70	112.23
3	M	194	GLY	N-CA-C	5.17	124.50	114.16
3	M	25	LYS	N-CA-C	-5.17	103.22	110.50
3	M	30	ARG	N-CA-C	-5.16	101.46	109.72
5	AK	57	ALA	N-CA-C	-5.15	106.96	114.12
3	M	49	GLY	C-N-CD	-5.15	109.28	120.60
6	v	15	LYS	N-CA-C	-5.15	105.12	111.40
4	H	200	SER	N-CA-C	5.14	117.35	109.07
6	2	42	TYR	N-CA-C	5.14	117.78	111.82
5	5	9	TYR	N-CA-C	-5.14	105.37	111.69
1	o	51	LEU	N-CA-C	-5.14	105.76	111.36
6	V	15	LYS	N-CA-C	-5.13	105.38	111.69
5	u	3	THR	N-CA-C	5.13	119.58	112.45
3	M	205	SER	N-CA-C	-5.12	105.70	111.28
4	t	235	GLU	N-CA-C	5.11	117.75	111.82
4	t	236	GLU	N-CA-C	-5.11	105.62	111.14
3	M	66	VAL	N-CA-C	-5.11	105.52	110.42
6	N	32	VAL	N-CA-C	5.11	115.33	110.53
4	t	128	GLU	N-CA-C	5.10	116.92	111.36
2	L	33	GLY	N-CA-C	-5.09	106.26	112.68
6	i	14	ALA	N-CA-C	-5.09	106.75	113.17
4	H	68	VAL	N-CA-CB	-5.09	106.60	111.89
3	y	240	HIS	N-CA-C	5.09	117.38	107.71
6	B	15	LYS	N-CA-C	-5.08	104.72	112.04
3	M	47	GLN	CA-C-N	-5.08	116.21	123.11
3	M	47	GLN	C-N-CA	-5.08	116.21	123.11
5	A	49	ASP	N-CA-C	-5.08	107.76	114.31
5	Q	14	ILE	CB-CA-C	-5.07	106.43	111.30
3	y	259	ASN	N-CA-C	5.06	115.21	108.38
4	t	203	ASP	N-CA-C	-5.06	100.25	109.56
4	H	105	ASP	CA-C-N	5.06	126.16	119.84
4	H	105	ASP	C-N-CA	5.06	126.16	119.84
3	y	49	GLY	C-N-CD	-5.05	109.48	120.60
5	D	14	ILE	CB-CA-C	-5.05	106.45	111.30
1	C	143	ALA	N-CA-C	-5.05	106.81	112.87
6	T	14	ALA	N-CA-C	-5.05	107.16	113.72
5	m	16	ASP	CA-C-N	5.04	125.07	119.32
5	m	16	ASP	C-N-CA	5.04	125.07	119.32
3	M	82	ASP	N-CA-C	-5.04	99.13	107.99
5	U	48	ASP	N-CA-C	5.04	117.28	108.52
5	A	14	ILE	N-CA-C	5.03	115.97	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	243	THR	N-CA-C	-5.02	106.98	113.01
4	t	225	LEU	N-CA-C	5.02	117.75	109.76
1	o	197	PHE	N-CA-C	5.02	121.49	110.80
2	x	165	TRP	N-CA-C	-5.02	105.72	111.14
5	p	42	THR	N-CA-C	5.02	117.48	109.65
1	o	242	SER	N-CA-C	5.01	116.75	111.28
6	AL	41	LEU	N-CA-C	5.00	116.54	111.14

There are no chirality outliers.

All (8) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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	147	0
1	o	2458	0	2385	152	1
2	L	2231	0	2192	154	0
2	x	2231	0	2192	164	0
3	M	2546	0	2521	197	0
3	y	2546	0	2521	189	0
4	H	1982	0	1981	121	0
4	t	1982	0	1981	113	0
5	1	475	0	486	46	1
5	3	475	0	486	21	0
5	5	475	0	486	26	0
5	7	475	0	486	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9	475	0	486	42	0
5	A	475	0	486	38	0
5	AA	475	0	486	21	0
5	AC	475	0	486	36	0
5	AE	481	0	490	35	0
5	AG	475	0	486	30	0
5	AI	475	0	486	28	0
5	AK	475	0	486	30	0
5	D	475	0	486	30	0
5	F	475	0	486	28	0
5	I	475	0	486	52	0
5	K	475	0	486	18	0
5	O	475	0	486	30	0
5	Q	475	0	486	37	0
5	S	481	0	490	39	0
5	U	475	0	486	42	0
5	W	475	0	486	36	0
5	Y	475	0	486	42	0
5	d	475	0	486	32	0
5	f	475	0	486	23	0
5	h	475	0	486	28	0
5	j	475	0	486	37	0
5	l	475	0	486	50	0
5	m	475	0	486	34	0
5	p	475	0	486	39	0
5	r	475	0	486	43	0
5	u	475	0	486	48	0
5	w	475	0	486	26	0
6	0	337	0	323	22	0
6	2	337	0	323	17	0
6	4	337	0	323	16	0
6	6	337	0	323	14	0
6	8	337	0	323	17	0
6	AB	337	0	323	18	0
6	AD	337	0	323	23	0
6	AF	337	0	323	20	0
6	AH	337	0	323	17	0
6	AJ	337	0	323	26	0
6	AL	337	0	323	19	0
6	B	337	0	323	37	0
6	E	337	0	323	27	0
6	G	337	0	323	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	337	0	323	31	0
6	N	337	0	323	11	0
6	P	337	0	323	19	0
6	R	337	0	323	19	0
6	T	337	0	323	20	0
6	V	337	0	323	23	0
6	X	337	0	323	23	0
6	Z	337	0	323	13	0
6	c	337	0	323	19	0
6	e	337	0	323	20	0
6	g	337	0	323	15	0
6	i	337	0	323	15	0
6	k	337	0	323	22	0
6	n	337	0	323	31	0
6	q	337	0	323	16	0
6	s	337	0	323	21	0
6	v	337	0	323	20	0
6	z	337	0	323	17	0
7	C	172	0	120	28	0
7	o	172	0	120	30	0
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	5	1	0	0	0	0
8	7	1	0	0	0	0
8	A	2	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	AG	1	0	0	0	0
8	AI	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	m	2	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	u	1	0	0	0	0
8	w	1	0	0	0	0
8	x	2	0	0	0	0
9	0	66	0	74	5	0
9	1	66	0	74	10	0
9	2	66	0	74	9	0
9	3	66	0	74	10	0
9	4	66	0	74	10	0
9	5	66	0	74	12	0
9	6	66	0	74	10	0
9	7	66	0	74	7	0
9	8	66	0	74	12	0
9	9	66	0	74	8	0
9	A	132	0	148	16	0
9	AB	132	0	148	18	0
9	AC	132	0	148	16	0
9	AE	66	0	74	9	0
9	AF	66	0	74	8	0
9	AG	66	0	74	6	0
9	AH	66	0	74	8	0
9	AI	132	0	148	22	0
9	AK	66	0	74	9	0
9	AL	66	0	74	11	0
9	D	132	0	148	16	0
9	F	66	0	74	4	0
9	G	66	0	74	12	0
9	I	132	0	148	22	0
9	K	66	0	74	6	0
9	L	132	0	148	28	0
9	M	132	0	148	21	0
9	N	66	0	74	4	0
9	O	66	0	74	6	0
9	P	66	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Q	66	0	74	3	0
9	R	66	0	74	5	0
9	S	66	0	74	11	0
9	T	66	0	74	12	0
9	U	66	0	74	9	0
9	V	66	0	74	8	0
9	W	66	0	74	8	0
9	X	66	0	74	8	0
9	Y	66	0	74	9	0
9	Z	66	0	74	16	0
9	c	66	0	74	14	0
9	d	66	0	74	12	0
9	e	66	0	74	12	0
9	f	66	0	74	7	0
9	g	66	0	74	6	0
9	h	66	0	74	8	0
9	i	66	0	74	8	0
9	j	66	0	74	8	0
9	k	66	0	74	12	0
9	l	66	0	74	8	0
9	m	132	0	148	16	0
9	p	66	0	74	12	0
9	q	66	0	74	11	0
9	r	66	0	74	11	0
9	s	66	0	74	11	0
9	u	132	0	148	19	0
9	w	66	0	74	8	0
9	x	198	0	222	26	0
9	y	66	0	74	16	0
9	z	66	0	74	6	0
10	L	65	0	76	5	0
10	M	65	0	76	14	0
10	x	65	0	76	4	0
10	y	65	0	76	10	0
11	L	53	0	74	12	0
11	x	53	0	74	18	0
12	A	19	0	11	2	0
12	H	76	0	44	26	0
12	L	12	0	9	0	0
12	M	35	0	22	2	0
12	m	19	0	11	3	0
12	p	16	0	11	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	t	38	0	22	7	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	4	0
14	y	53	0	72	8	0
15	0	44	0	60	12	0
15	2	44	0	60	7	0
15	4	44	0	60	14	0
15	7	88	0	120	20	0
15	9	44	0	60	16	0
15	AC	44	0	60	11	0
15	AD	44	0	60	8	0
15	AF	44	0	60	14	0
15	AH	44	0	60	9	0
15	AJ	44	0	60	12	0
15	AL	44	0	60	10	0
15	E	44	0	60	14	0
15	G	44	0	60	9	0
15	I	44	0	60	10	0
15	M	44	0	60	13	0
15	O	44	0	60	9	0
15	P	44	0	60	9	0
15	R	44	0	60	11	0
15	T	44	0	60	11	0
15	V	44	0	60	10	0
15	X	44	0	60	21	0
15	Z	44	0	60	8	0
15	e	44	0	60	10	0
15	g	44	0	60	12	0
15	i	44	0	60	4	0
15	k	44	0	60	15	0
15	m	44	0	60	8	0
15	n	44	0	60	17	0
15	q	44	0	60	9	0
15	s	44	0	60	10	0
15	v	44	0	60	7	0
15	y	44	0	60	11	0
15	z	44	0	60	6	0
16	H	5	0	0	0	0
16	M	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	t	5	0	0	0	0
16	y	5	0	0	1	0
17	AE	21	0	12	2	0
17	S	21	0	12	3	0
18	AI	1	0	0	0	0
18	L	2	0	0	0	0
18	W	1	0	0	1	0
18	x	2	0	0	0	0
All	All	51893	0	52456	2857	1

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 27.

All (2857) 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:AA:45:ASN:O	5:AA:49:ASP:OD2	1.57	1.23
5:7:45:ASN:O	5:7:49:ASP:OD2	1.71	1.06
3:M:277:VAL:HG11	10:M:403:BPH:HAC2	1.42	0.98
3:y:25:LYS:HD3	3:y:26:GLY:H	1.27	0.98
5:p:56:GLN:O	5:p:58:LEU:N	1.98	0.96
5:j:35:ILE:HB	9:k:102:BCL:HED1	1.46	0.96
5:1:57:ALA:H	5:1:58:LEU:C	1.72	0.95
6:AJ:25:MET:HG3	15:AJ:101:CRT:H21	1.50	0.93
12:x:306:PEF:H51	4:t:68:VAL:H	1.33	0.93
1:o:107:CYS:SG	7:o:501:HEM:HAB	2.09	0.92
9:G:102:BCL:H12	9:G:102:BCL:H3A	1.49	0.92
3:y:277:VAL:HG11	10:y:402:BPH:HAC2	1.52	0.92
2:L:46:GLY:HA3	10:L:302:BPH:H9C3	1.52	0.91
1:C:307:CYS:SG	7:C:504:HEM:HAB	2.09	0.91
6:T:17:PHE:HA	15:T:101:CRT:H6	1.54	0.90
2:x:188:PHE:CD2	2:x:248:SER:HB3	2.06	0.90
9:f:101:BCL:H121	9:f:101:BCL:H62	1.52	0.89
6:R:17:PHE:HA	15:R:101:CRT:H6	1.55	0.88
9:y:401:BCL:H2	10:y:402:BPH:HHC	1.55	0.88
1:o:20:LEU:HA	1:o:21:LEU:HB2	1.52	0.87
5:9:3:THR:HB	5:9:8:LEU:HB2	1.54	0.87
5:m:45:ASN:HB3	5:p:56:GLN:HE22	1.39	0.87
1:C:152:CYS:SG	7:C:502:HEM:HAB	2.15	0.87
3:y:34:PRO:HG3	3:y:50:PRO:HD3	1.55	0.87
4:H:159:LEU:HD22	4:H:254:ARG:NH2	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:176:PHE:HE1	2:x:179:ASN:HD22	1.20	0.86
6:R:21:PHE:HA	15:R:101:CRT:H15	1.57	0.86
12:m:101:PEF:H51	5:l:19:ARG:HH22	1.41	0.86
5:m:14:ILE:HG23	5:p:18:ARG:HG2	1.58	0.85
2:L:188:PHE:CD2	2:L:248:SER:HB3	2.12	0.85
5:I:45:ASN:O	5:I:49:ASP:OD2	1.95	0.85
5:w:50:ASN:HB2	5:w:54:SER:HA	1.57	0.85
5:j:45:ASN:O	5:j:49:ASP:OD2	1.93	0.85
4:H:122:HIS:HB3	4:t:121:LYS:HZ2	1.41	0.85
5:r:45:ASN:O	5:r:49:ASP:OD2	1.93	0.85
1:C:32:GLN:NE2	2:L:79:ASP:OD1	2.09	0.85
5:AE:43:ASP:HB2	5:AG:48:ASP:HA	1.59	0.85
2:L:188:PHE:HD2	2:L:248:SER:HB3	1.42	0.85
2:x:189:PHE:CD1	2:x:249:ALA:HB1	2.12	0.84
4:H:39:TYR:OH	12:H:301:PEF:N	2.10	0.84
1:o:178:LEU:HA	3:y:110:SER:HB2	1.60	0.84
5:7:14:ILE:HD11	15:0:101:CRT:H5	1.58	0.84
2:x:188:PHE:HD2	2:x:248:SER:HB3	1.42	0.84
5:U:5:ASN:OD1	5:U:7:ASN:N	2.10	0.84
1:C:189:THR:O	1:C:238:ASN:ND2	2.10	0.84
3:y:265:ILE:HD13	14:y:403:MQ8:H121	1.59	0.83
4:H:150:ASP:O	4:H:207:ARG:NH2	2.11	0.83
5:j:32:GLY:HA2	9:k:102:BCL:HED2	1.59	0.83
5:A:40:LEU:O	5:A:45:ASN:ND2	2.10	0.83
2:L:21:ASP:O	5:9:18:ARG:NH2	2.12	0.83
5:j:35:ILE:HG12	15:k:101:CRT:H403	1.61	0.82
3:M:214:LEU:O	3:M:218:MET:HG3	1.80	0.81
5:j:10:LYS:HA	5:j:13:LEU:HD13	1.60	0.81
5:p:12:TRP:HB3	5:p:17:PRO:HG3	1.62	0.81
9:u:102:BCL:HBA2	6:v:32:VAL:HG21	1.61	0.81
2:L:44:LEU:HD23	5:9:30:VAL:HG11	1.61	0.81
4:H:56:VAL:H	12:H:302:PEF:HN2	1.28	0.81
9:8:101:BCL:H8	9:8:101:BCL:H2	1.61	0.81
6:V:21:PHE:HA	15:V:101:CRT:H14	1.62	0.81
1:o:67:SER:OG	1:o:86:SER:OG	1.97	0.81
6:G:32:VAL:HG21	9:G:102:BCL:HBA2	1.63	0.81
5:O:43:ASP:OD2	5:Q:50:ASN:ND2	2.13	0.81
5:U:5:ASN:HB3	5:U:8:LEU:HB2	1.63	0.81
6:n:21:PHE:HA	15:n:101:CRT:H14	1.63	0.81
6:AH:17:PHE:HA	15:AH:102:CRT:H6	1.62	0.81
5:I:40:LEU:O	5:I:45:ASN:ND2	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:44:LEU:HD23	5:l:30:VAL:HG11	1.63	0.80
6:n:17:PHE:HD1	15:n:101:CRT:H5	1.46	0.80
4:H:63:ASP:OD1	5:F:19:ARG:NH2	2.15	0.80
3:y:3:GLU:OE2	4:t:247:LYS:NZ	2.13	0.80
5:I:45:ASN:O	6:J:43:ARG:NH1	2.13	0.80
2:x:281:TRP:HB2	3:y:88:LYS:HD2	1.62	0.80
9:AC:103:BCL:HBA2	6:AD:32:VAL:HG21	1.64	0.80
3:M:267:ARG:NH1	12:H:305:PEF:O3	2.15	0.80
6:X:45:TRP:HD1	6:X:46:LEU:HG	1.47	0.80
6:2:17:PHE:HA	15:2:101:CRT:H6	1.64	0.79
2:x:86:MET:HG3	5:j:41:SER:HB3	1.64	0.79
2:x:202:LEU:HD23	11:x:304:UQ8:H3MA	1.64	0.79
4:H:186:VAL:HG23	4:H:191:LYS:O	1.82	0.79
6:q:13:GLU:HB3	15:q:101:CRT:H21A	1.63	0.79
5:Y:44:LEU:HA	5:1:55:TYR:CE2	2.18	0.79
5:A:13:LEU:O	5:D:18:ARG:NH2	2.16	0.79
6:E:17:PHE:HA	15:E:101:CRT:H6	1.64	0.78
6:B:17:PHE:HD1	15:9:101:CRT:H5	1.48	0.78
6:AF:44:PRO:O	5:AG:55:TYR:OH	1.99	0.78
4:H:96:PRO:HD3	6:0:7:THR:HA	1.66	0.78
2:L:189:PHE:CD1	2:L:249:ALA:HB1	2.18	0.78
1:C:107:CYS:SG	7:C:501:HEM:HAB	2.24	0.78
4:H:113:PRO:HG3	4:H:248:LEU:HB3	1.66	0.78
5:A:45:ASN:O	5:A:49:ASP:OD2	2.02	0.78
5:1:51:ILE:HG22	5:1:52:PRO:HA	1.66	0.78
1:C:227:LYS:NZ	3:M:96:GLU:OE2	2.15	0.78
4:H:31:ARG:NH1	4:H:34:ASP:OD2	2.16	0.78
1:o:19:MET:HB2	1:o:21:LEU:HD13	1.66	0.78
1:C:247:CYS:HG	7:C:503:HEM:CAB	1.97	0.78
3:M:267:ARG:NH1	12:H:305:PEF:O1P	2.16	0.78
6:AL:21:PHE:HD1	15:AL:101:CRT:H14	1.48	0.78
5:S:43:ASP:CG	5:U:50:ASN:HA	2.09	0.78
5:5:50:ASN:HB2	5:5:54:SER:HA	1.65	0.77
4:t:65:LYS:HE2	4:t:67:PHE:CE1	2.19	0.77
4:t:150:ASP:O	4:t:207:ARG:NH2	2.16	0.77
3:M:62:PHE:HB3	5:Q:30:VAL:HG21	1.66	0.77
4:t:31:ARG:NH1	4:t:34:ASP:OD2	2.17	0.77
1:o:67:SER:HA	1:o:68:THR:HG22	1.67	0.77
1:C:247:CYS:SG	7:C:503:HEM:CAB	2.72	0.77
5:u:49:ASP:OD2	6:v:43:ARG:NH1	2.18	0.77
6:B:44:PRO:HG2	5:D:52:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:247:CYS:SG	7:o:503:HEM:CAB	2.73	0.77
6:q:28:TRP:NE1	9:q:102:BCL:O1A	2.17	0.77
3:M:126:ILE:HD13	9:M:402:BCL:H91	1.67	0.77
6:B:20:ILE:O	6:B:24:SER:OG	2.01	0.76
5:d:5:ASN:HB3	5:d:8:LEU:HB2	1.67	0.76
1:C:24:GLU:OE2	2:L:265:THR:OG1	2.02	0.76
5:u:50:ASN:HB2	5:w:59:GLY:HA3	1.66	0.76
5:AA:43:ASP:HB2	5:AC:48:ASP:HA	1.66	0.76
6:AF:17:PHE:HA	15:AF:102:CRT:H6	1.68	0.76
5:W:10:LYS:HA	5:W:13:LEU:HD13	1.66	0.76
5:AI:10:LYS:HA	5:AI:13:LEU:HD13	1.67	0.76
5:AK:49:ASP:OD2	6:AL:43:ARG:NH1	2.19	0.76
5:f:42:THR:HG21	5:h:47:LEU:HB3	1.67	0.76
9:i:102:BCL:HMA1	9:j:101:BCL:HMA1	1.67	0.76
5:I:25:VAL:HG13	9:I:101:BCL:H62	1.68	0.76
15:4:101:CRT:H292	9:5:101:BCL:H71	1.67	0.76
5:AI:49:ASP:O	5:AK:60:LYS:N	2.17	0.76
15:I:102:CRT:H14	6:J:21:PHE:HA	1.65	0.76
6:Z:17:PHE:HA	15:Z:101:CRT:H6	1.67	0.76
15:9:101:CRT:H11	15:9:101:CRT:H81	1.67	0.76
3:M:65:LEU:HD21	10:M:403:BPH:H102	1.66	0.75
15:AH:102:CRT:H292	9:AI:101:BCL:H43	1.67	0.75
3:y:25:LYS:HD3	3:y:26:GLY:N	1.99	0.75
5:AK:14:ILE:HD12	15:e:101:CRT:H82	1.68	0.75
5:A:49:ASP:OD2	6:B:43:ARG:NH1	2.20	0.75
6:s:32:VAL:HG21	9:s:102:BCL:HBA2	1.67	0.75
2:L:175:HIS:NE2	3:M:184:ASP:OD1	2.20	0.75
2:L:252:TRP:HE1	11:L:304:UQ8:H35A	1.52	0.75
5:Y:14:ILE:HD11	15:2:101:CRT:H32A	1.67	0.74
4:H:14:ILE:HA	4:H:17:TRP:HD1	1.52	0.74
1:o:247:CYS:SG	7:o:503:HEM:HAB	2.27	0.74
1:C:247:CYS:SG	7:C:503:HEM:HAB	2.28	0.74
4:H:45:ARG:HH11	4:H:53:VAL:HG11	1.50	0.74
5:l:45:ASN:O	5:l:49:ASP:OD2	2.06	0.74
9:AG:101:BCL:HAA2	9:AG:101:BCL:HED3	1.70	0.74
9:AI:102:BCL:HBA2	6:AJ:32:VAL:HG21	1.69	0.74
6:k:21:PHE:HA	15:k:101:CRT:H11	1.70	0.74
3:M:240:HIS:CE1	4:H:69:LEU:HD11	2.23	0.74
5:Y:5:ASN:HA	6:2:23:GLN:HE22	1.53	0.74
4:t:108:LEU:HD21	4:t:221:ASN:HD22	1.52	0.74
6:E:43:ARG:HG3	5:F:55:TYR:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:306:PEF:H32	12:x:306:PEF:H52	1.69	0.73
15:n:101:CRT:H241	9:p:102:BCL:H71	1.69	0.73
5:r:51:ILE:HD13	6:s:43:ARG:HH22	1.53	0.73
6:G:17:PHE:HA	15:G:101:CRT:H6	1.70	0.73
2:L:232:SER:OG	11:L:304:UQ8:O5	2.06	0.73
6:N:32:VAL:HG21	9:N:101:BCL:HBA2	1.71	0.73
9:AI:101:BCL:HED2	9:AI:101:BCL:H2A	1.71	0.73
3:M:277:VAL:CG1	10:M:403:BPH:HAC2	2.19	0.73
6:B:21:PHE:HA	15:9:101:CRT:H14	1.70	0.73
15:k:101:CRT:H27	9:k:102:BCL:H41	1.71	0.72
1:C:20:LEU:HA	1:C:21:LEU:HB2	1.70	0.72
3:y:4:TYR:CE1	3:y:6:ASN:HA	2.24	0.72
5:l:31:LEU:HD23	9:c:101:BCL:HED2	1.71	0.72
3:M:84:PHE:CD1	5:W:37:MET:HG3	2.23	0.72
4:H:94:PRO:HG2	6:0:8:GLY:HA2	1.71	0.72
1:o:295:ARG:NH2	7:o:502:HEM:O1A	2.22	0.72
5:l:3:THR:HB	5:l:8:LEU:HB2	1.69	0.72
5:f:15:LEU:HD23	5:h:18:ARG:HG3	1.72	0.72
5:u:43:ASP:CG	5:w:50:ASN:HD21	1.97	0.72
5:Y:39:VAL:HG11	9:Y:101:BCL:HBC1	1.70	0.72
4:t:45:ARG:HD2	4:t:53:VAL:HG11	1.71	0.72
1:C:292:PRO:HG2	1:C:295:ARG:HG2	1.70	0.72
3:y:62:PHE:HB3	5:AC:30:VAL:HG21	1.72	0.72
9:Y:101:BCL:H2	6:Z:28:TRP:CH2	2.24	0.72
9:m:103:BCL:HBA2	6:n:32:VAL:HG21	1.71	0.72
6:s:21:PHE:HA	15:s:101:CRT:H14	1.72	0.72
6:g:32:VAL:HG21	9:g:102:BCL:O1A	1.89	0.72
2:x:21:ASP:O	5:l:18:ARG:NH2	2.23	0.71
5:u:11:ILE:HG12	9:w:101:BCL:H161	1.71	0.71
3:M:18:TYR:CE2	3:M:20:GLY:HA2	2.26	0.71
6:R:43:ARG:HG3	5:S:55:TYR:CZ	2.25	0.71
2:x:144:ARG:HB3	2:x:145:PRO:HD3	1.72	0.71
3:y:179:ILE:O	3:y:182:HIS:ND1	2.22	0.71
6:X:36:HIS:CD2	9:X:102:BCL:H8	2.25	0.71
3:M:177:PHE:HD1	15:M:405:CRT:H16	1.54	0.71
1:o:263:THR:HG22	3:y:311:VAL:HG11	1.73	0.71
9:O:102:BCL:H2	9:O:102:BCL:HBA1	1.71	0.71
1:o:169:ASP:OD1	1:o:170:PRO:HD2	1.90	0.71
3:M:260:VAL:HB	3:M:264:SER:OG	1.90	0.71
6:T:44:PRO:HG2	5:U:52:PRO:HG3	1.71	0.71
2:x:140:LEU:HD11	9:x:301:BCL:HED2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:PHE:O	1:C:277:ARG:NH1	2.24	0.71
6:k:32:VAL:HG11	9:k:102:BCL:HBA2	1.72	0.71
6:X:24:SER:HB2	15:X:101:CRT:H14	1.72	0.71
3:y:201:PHE:HD1	3:y:279:THR:HG22	1.54	0.71
9:A:102:BCL:H122	5:9:2:PHE:HA	1.72	0.70
6:n:31:LEU:HD23	6:n:34:ILE:HD12	1.73	0.70
6:P:43:ARG:HG3	5:Q:55:TYR:CZ	2.26	0.70
5:S:51:ILE:HG22	5:S:52:PRO:HA	1.72	0.70
3:y:37:SER:HB2	12:y:406:PEF:H31	1.73	0.70
4:t:137:ARG:NH2	4:t:229:ASP:OD1	2.24	0.70
5:W:21:LEU:HD11	15:X:101:CRT:H133	1.73	0.70
5:9:5:ASN:O	5:9:7:ASN:N	2.17	0.70
6:c:40:TRP:HH2	6:c:46:LEU:HB2	1.54	0.70
5:W:11:ILE:HD13	15:Z:101:CRT:H10	1.72	0.70
1:o:19:MET:O	1:o:21:LEU:HD22	1.91	0.70
1:C:107:CYS:SG	7:C:501:HEM:CAB	2.80	0.70
3:M:265:ILE:HD13	14:M:404:MQ8:H121	1.72	0.70
2:x:179:ASN:O	2:x:183:MET:HG3	1.91	0.70
1:C:97:VAL:HG21	1:C:131:PHE:CZ	2.26	0.70
1:C:153:TYR:CE1	1:C:157:ARG:HA	2.26	0.70
6:G:43:ARG:HG3	5:I:55:TYR:CZ	2.26	0.70
5:Y:44:LEU:HD23	5:1:55:TYR:HE2	1.57	0.70
5:m:8:LEU:HG	6:q:20:ILE:HD13	1.73	0.70
1:C:152:CYS:SG	7:C:502:HEM:CAB	2.80	0.70
2:L:179:ASN:O	2:L:183:MET:HG3	1.92	0.70
3:M:197:TYR:CZ	9:M:402:BCL:HMC2	2.26	0.70
6:g:17:PHE:HA	15:g:101:CRT:H6	1.74	0.70
3:y:161:GLY:HA3	15:y:404:CRT:H26	1.73	0.69
6:B:20:ILE:HB	15:9:101:CRT:H82	1.73	0.69
5:r:5:ASN:O	5:r:7:ASN:N	2.23	0.69
2:L:176:PHE:HE1	2:L:179:ASN:HD22	1.37	0.69
6:V:29:PHE:CD1	9:V:102:BCL:H2	2.27	0.69
5:r:40:LEU:O	5:r:45:ASN:ND2	2.24	0.69
6:s:17:PHE:HA	15:s:101:CRT:H6	1.75	0.69
3:y:159:VAL:HG13	3:y:285:LEU:HD13	1.74	0.69
9:w:101:BCL:H193	9:w:101:BCL:H71	1.75	0.69
6:z:32:VAL:HG21	9:z:102:BCL:HBA2	1.75	0.69
5:r:23:SER:HB3	9:u:101:BCL:H141	1.73	0.69
5:Q:10:LYS:HB3	15:T:101:CRT:H22A	1.73	0.69
5:AE:11:ILE:HD12	5:AE:14:ILE:HD12	1.74	0.69
2:L:2:ALA:N	12:A:101:PEF:O2P	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:86:MET:HA	2:x:96:GLN:HE22	1.57	0.69
9:x:303:BCL:HMA1	9:x:303:BCL:H121	1.74	0.69
9:g:102:BCL:HMA1	9:h:101:BCL:HMA1	1.75	0.69
5:j:44:LEU:HD13	9:k:102:BCL:HBC2	1.74	0.69
5:W:41:SER:O	18:W:201:HOH:O	2.10	0.69
6:n:43:ARG:HG3	5:p:55:TYR:CZ	2.27	0.69
5:U:16:ASP:OD2	5:U:18:ARG:NH2	2.21	0.69
1:o:164:TYR:CD2	1:o:312:GLN:HG2	2.28	0.69
5:AI:21:LEU:HD11	15:AJ:101:CRT:H133	1.75	0.69
9:AI:101:BCL:HBD	9:AI:101:BCL:HAA1	1.74	0.69
9:e:102:BCL:H12	9:e:102:BCL:H3A	1.75	0.69
5:Q:20:VAL:HG22	9:S:102:BCL:H162	1.73	0.68
5:S:16:ASP:OD2	5:S:19:ARG:HG3	1.93	0.68
2:x:68:TYR:HA	2:x:73:ILE:HD11	1.75	0.68
5:u:42:THR:HG21	5:w:47:LEU:HD13	1.74	0.68
9:AI:101:BCL:HBC2	9:AI:102:BCL:HMD1	1.74	0.68
6:AJ:17:PHE:HA	15:AJ:101:CRT:H6	1.74	0.68
5:l:10:LYS:HA	5:l:13:LEU:HD13	1.75	0.68
1:o:107:CYS:SG	7:o:501:HEM:CAB	2.81	0.68
2:x:209:PRO:HD2	12:x:306:PEF:H12	1.75	0.68
5:AA:10:LYS:HB3	15:AD:101:CRT:H33	1.75	0.68
1:o:152:CYS:SG	7:o:502:HEM:HAB	2.33	0.68
15:AF:102:CRT:H372	5:AG:36:HIS:CD2	2.29	0.68
4:H:60:ASP:OD1	4:H:61:LEU:N	2.26	0.68
6:V:17:PHE:HB2	15:V:101:CRT:H22A	1.75	0.68
5:Y:12:TRP:HB2	6:Z:14:ALA:HB1	1.76	0.68
5:Y:44:LEU:HD23	5:1:55:TYR:CE2	2.28	0.68
4:H:65:LYS:HE2	4:H:67:PHE:CE1	2.28	0.68
2:x:3:MET:HB3	2:x:7:GLU:HB3	1.75	0.68
3:y:63:PHE:HZ	5:AC:33:LEU:HD12	1.58	0.68
6:AB:46:LEU:HD22	6:AD:42:TYR:CE2	2.28	0.68
2:x:167:SER:HA	9:x:301:BCL:HBC1	1.74	0.68
3:y:41:GLY:HA2	3:y:44:GLY:O	1.92	0.68
2:L:225:PHE:CD2	11:L:304:UQ8:H7A	2.29	0.68
3:y:260:VAL:HB	3:y:264:SER:OG	1.93	0.68
9:AH:101:BCL:HBD	9:AH:101:BCL:HAA1	1.75	0.68
1:o:167:VAL:HG13	1:o:303:LEU:HD23	1.75	0.68
6:AD:42:TYR:OH	6:AD:43:ARG:NH2	2.25	0.68
6:e:45:TRP:CD1	6:e:46:LEU:HG	2.28	0.68
2:x:211:LYS:HA	12:x:306:PEF:O2	1.94	0.68
3:M:32:GLY:H	17:S:101:PGW:HADA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:101:CRT:H291	9:5:101:BCL:HBA1	1.77	0.67
9:L:303:BCL:H142	9:L:303:BCL:HMA2	1.76	0.67
1:o:148:THR:HA	1:o:322:GLN:HG2	1.75	0.67
2:L:26:TRP:CZ3	4:H:99:PRO:HB3	2.28	0.67
6:T:32:VAL:HG11	9:T:102:BCL:H2	1.74	0.67
5:Y:51:ILE:HG23	5:Y:52:PRO:HA	1.75	0.67
1:o:43:TYR:CE1	2:x:148:MET:HE1	2.29	0.67
1:C:307:CYS:SG	7:C:504:HEM:CAB	2.83	0.67
6:G:45:TRP:CD1	6:G:46:LEU:HG	2.29	0.67
6:0:17:PHE:HB2	15:0:101:CRT:H31A	1.75	0.67
5:p:18:ARG:HD3	12:p:101:PEF:C30	2.25	0.67
5:f:51:ILE:HD13	6:g:43:ARG:HH22	1.59	0.67
2:x:193:CYS:SG	10:y:402:BPH:HMC3	2.34	0.67
9:m:103:BCL:H142	6:n:33:VAL:HG22	1.75	0.67
6:AB:45:TRP:CD1	6:AB:46:LEU:HG	2.29	0.67
15:m:104:CRT:H6	6:c:17:PHE:HA	1.76	0.67
15:z:101:CRT:H241	9:AB:101:BCL:H91	1.75	0.67
2:x:55:THR:HG1	2:x:68:TYR:HH	1.40	0.67
6:e:32:VAL:HG21	9:e:102:BCL:HBA2	1.75	0.67
2:L:203:ILE:HG13	3:M:266:HIS:CD2	2.30	0.67
3:M:265:ILE:HG23	3:M:266:HIS:ND1	2.10	0.66
15:m:104:CRT:H10	5:j:11:ILE:HD13	1.76	0.66
3:y:18:TYR:CE2	3:y:20:GLY:HA2	2.30	0.66
5:AI:34:LEU:HA	5:AI:37:MET:HE3	1.76	0.66
4:H:190:LYS:HD2	6:s:8:GLY:HA2	1.78	0.66
9:1:101:BCL:HBA1	6:2:28:TRP:HH2	1.59	0.66
2:L:17:LEU:O	4:H:258:LEU:HB2	1.96	0.66
4:t:159:LEU:HD22	4:t:254:ARG:NH2	2.10	0.66
3:M:258:PHE:HB3	12:H:301:PEF:H31	1.78	0.66
5:O:14:ILE:HD11	15:R:101:CRT:H31A	1.77	0.66
4:t:249:TYR:O	4:t:251:THR:N	2.29	0.66
3:M:109:LEU:HD11	5:Q:42:THR:HG22	1.77	0.66
5:9:11:ILE:HD13	15:9:101:CRT:H10	1.77	0.66
6:i:32:VAL:HG21	9:i:102:BCL:HBA2	1.76	0.66
5:A:11:ILE:HD13	15:E:101:CRT:H10	1.77	0.66
6:4:29:PHE:CE1	9:4:102:BCL:H11	2.30	0.66
5:O:4:MET:O	5:O:6:ALA:N	2.30	0.65
9:j:101:BCL:H2	6:k:28:TRP:CH2	2.30	0.65
2:L:240:ARG:NE	3:M:6:ASN:O	2.29	0.65
6:B:20:ILE:HG23	5:9:5:ASN:HB3	1.77	0.65
5:W:43:ASP:O	5:Y:56:GLN:NE2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:5:ASN:OD1	5:AG:7:ASN:HB2	1.96	0.65
2:L:177:HIS:HB3	3:M:183:LEU:HD13	1.76	0.65
5:K:17:PRO:HB3	6:N:17:PHE:CZ	2.32	0.65
6:s:43:ARG:HG3	5:u:55:TYR:CZ	2.32	0.65
5:D:36:HIS:CD2	15:9:101:CRT:H372	2.31	0.65
1:C:67:SER:HA	1:C:68:THR:OG1	1.96	0.65
9:L:303:BCL:H121	9:L:303:BCL:HMA1	1.78	0.65
1:o:110:CYS:HA	1:o:123:THR:OG1	1.96	0.65
3:y:277:VAL:CG1	10:y:402:BPH:HAC2	2.24	0.65
6:q:33:VAL:HG22	9:q:102:BCL:H92	1.77	0.65
5:u:3:THR:HB	5:u:8:LEU:HB3	1.78	0.65
5:S:44:LEU:HD22	6:T:43:ARG:HD3	1.79	0.65
3:y:214:LEU:O	3:y:218:MET:HG3	1.96	0.65
15:s:101:CRT:H372	5:u:36:HIS:CD2	2.31	0.65
6:c:40:TRP:CH2	6:c:46:LEU:HB2	2.31	0.65
4:H:150:ASP:OD1	4:H:152:ARG:HB2	1.96	0.65
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.79	0.65
6:R:18:HIS:O	6:R:22:MET:HG2	1.96	0.65
2:L:240:ARG:HG2	3:M:224:LEU:HD21	1.77	0.65
2:x:203:ILE:HG13	3:y:266:HIS:CD2	2.32	0.65
3:y:84:PHE:CD1	5:AI:37:MET:HG3	2.32	0.65
5:m:56:GLN:NE2	5:l:43:ASP:O	2.29	0.65
6:AF:21:PHE:HA	15:AF:102:CRT:C14	2.26	0.65
5:7:44:LEU:HD12	5:9:47:LEU:HD22	1.79	0.65
1:o:59:VAL:HG21	1:o:100:TRP:HE1	1.61	0.65
1:C:242:SER:HA	1:C:308:MET:HE2	1.79	0.64
2:L:72:ARG:HD2	3:M:305:PRO:HA	1.79	0.64
2:L:206:VAL:HG13	3:M:142:MET:HE3	1.79	0.64
3:y:65:LEU:HD21	10:y:402:BPH:H102	1.79	0.64
6:AB:17:PHE:HA	15:AC:101:CRT:H6	1.79	0.64
2:x:261:GLY:O	2:x:264:TRP:N	2.29	0.64
5:m:48:ASP:OD1	5:l:43:ASP:N	2.31	0.64
15:n:101:CRT:H342	9:p:102:BCL:HBA2	1.78	0.64
6:e:44:PRO:O	5:f:55:TYR:OH	2.13	0.64
15:k:101:CRT:H27	9:k:102:BCL:C4	2.28	0.64
1:C:67:SER:OG	1:C:86:SER:OG	2.08	0.64
5:I:33:LEU:O	5:I:37:MET:HG2	1.98	0.64
5:p:43:ASP:HA	5:r:56:GLN:HE21	1.62	0.64
5:F:34:LEU:HD21	15:G:101:CRT:H2M2	1.79	0.64
6:X:17:PHE:HA	15:X:101:CRT:H6	1.80	0.64
5:u:45:ASN:HB3	5:w:56:GLN:HE22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:w:101:BCL:HAA1	9:w:101:BCL:HBD	1.78	0.64
6:z:29:PHE:O	6:z:33:VAL:HG23	1.97	0.64
5:d:49:ASP:HB2	5:d:51:ILE:HG13	1.78	0.64
9:d:101:BCL:HBC2	9:e:102:BCL:HMD1	1.80	0.64
6:i:33:VAL:HG22	9:i:102:BCL:H92	1.78	0.64
1:C:179:LYS:HD2	3:M:111:GLU:HG3	1.78	0.64
1:C:206:GLN:O	1:C:277:ARG:HD2	1.98	0.64
12:x:306:PEF:H51	4:t:68:VAL:N	2.10	0.64
5:1:45:ASN:HB3	5:3:56:GLN:OE1	1.98	0.64
4:t:246:GLY:HA2	4:t:250:ALA:H	1.63	0.64
3:M:145:HIS:HA	3:M:148:TRP:CE3	2.33	0.64
15:Z:101:CRT:H372	5:1:36:HIS:CD2	2.33	0.64
9:Z:102:BCL:HED2	9:Z:102:BCL:HAA2	1.79	0.64
6:AB:45:TRP:HD1	6:AB:46:LEU:HG	1.63	0.64
9:AG:101:BCL:H2	6:AH:29:PHE:CD1	2.32	0.64
9:AK:101:BCL:H2	6:AL:28:TRP:CZ2	2.31	0.64
4:t:45:ARG:HH11	4:t:53:VAL:HG11	1.62	0.64
5:p:40:LEU:O	5:p:45:ASN:ND2	2.31	0.64
5:j:24:ILE:HG12	9:l:101:BCL:H171	1.79	0.64
1:C:263:THR:HG22	3:M:311:VAL:HG11	1.78	0.64
2:L:222:ASN:O	2:L:226:ARG:HG3	1.98	0.64
5:K:43:ASP:OD2	5:O:50:ASN:HA	1.98	0.64
6:n:17:PHE:HA	15:n:101:CRT:H83	1.79	0.64
5:O:5:ASN:OD1	5:O:5:ASN:N	2.30	0.63
9:x:305:BCL:O1D	3:y:203:MET:HB3	1.98	0.63
9:M:402:BCL:C2	10:M:403:BPH:HBB2	2.28	0.63
5:A:17:PRO:HB3	6:B:17:PHE:CZ	2.33	0.63
1:o:301:ASP:HB2	1:o:304:ARG:HH12	1.62	0.63
5:AE:50:ASN:HB3	5:AE:54:SER:HA	1.79	0.63
1:C:301:ASP:HB2	1:C:304:ARG:HH12	1.62	0.63
9:A:103:BCL:HAA2	9:A:103:BCL:HED3	1.79	0.63
9:8:101:BCL:H43	9:8:101:BCL:HMA2	1.81	0.63
1:o:203:PHE:O	1:o:277:ARG:NH1	2.29	0.63
3:M:161:GLY:HA3	15:M:405:CRT:H292	1.80	0.63
5:I:9:TYR:OH	6:J:11:ASP:OD1	2.12	0.63
5:U:25:VAL:HG13	9:U:101:BCL:H41	1.80	0.63
9:u:102:BCL:HED3	9:u:102:BCL:HAA2	1.81	0.63
1:C:200:LEU:HD22	1:C:204:LEU:HD12	1.79	0.63
5:O:43:ASP:HB2	5:Q:48:ASP:OD1	1.98	0.63
6:2:32:VAL:HG21	9:2:102:BCL:HBA2	1.80	0.63
5:AG:45:ASN:HB3	5:AI:56:GLN:HE22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HG13	1:C:287:LEU:HD13	1.81	0.63
5:A:13:LEU:HB2	15:E:101:CRT:H1M1	1.81	0.63
5:Y:5:ASN:OD1	6:2:23:GLN:NE2	2.32	0.63
6:Z:21:PHE:HA	15:Z:101:CRT:H11	1.81	0.63
1:o:110:CYS:O	1:o:124:LYS:HB2	1.99	0.63
2:L:239:HIS:CD2	3:M:223:ILE:HG13	2.34	0.63
9:F:101:BCL:HBC2	9:G:102:BCL:HMD1	1.80	0.63
6:n:31:LEU:HD12	5:l:2:PHE:CE2	2.34	0.63
5:AE:44:LEU:HD13	9:AE:102:BCL:HBC3	1.78	0.63
5:3:5:ASN:ND2	5:3:5:ASN:O	2.32	0.62
2:L:206:VAL:CG1	3:M:142:MET:HE3	2.29	0.62
9:6:101:BCL:HMA1	9:7:102:BCL:HMA1	1.80	0.62
5:u:43:ASP:OD1	5:w:50:ASN:ND2	2.32	0.62
6:k:31:LEU:HD23	6:k:34:ILE:HD12	1.81	0.62
4:H:257:PRO:HG3	5:7:19:ARG:CZ	2.29	0.62
5:K:40:LEU:HG	5:K:46:TRP:CH2	2.35	0.62
5:7:4:MET:HG3	5:7:5:ASN:H	1.64	0.62
1:o:67:SER:HA	1:o:68:THR:CG2	2.29	0.62
2:x:48:LEU:HD13	5:l:34:LEU:HD22	1.81	0.62
12:x:306:PEF:C5	4:t:68:VAL:H	2.10	0.62
3:y:33:ARG:HG2	3:y:34:PRO:HD2	1.80	0.62
3:y:265:ILE:CD1	14:y:403:MQ8:H121	2.28	0.62
1:C:21:LEU:HG	2:L:274:TRP:CD1	2.35	0.62
5:F:45:ASN:O	5:F:49:ASP:OD2	2.17	0.62
5:U:39:VAL:HG11	9:U:101:BCL:HBC1	1.80	0.62
1:o:100:TRP:HE3	1:o:152:CYS:HG	1.46	0.62
3:M:34:PRO:HG3	3:M:50:PRO:HD3	1.81	0.62
5:I:11:ILE:HG12	9:K:101:BCL:H161	1.81	0.62
5:U:43:ASP:CG	5:W:55:TYR:HB2	2.24	0.62
6:Z:32:VAL:HG21	9:Z:102:BCL:HBA2	1.82	0.62
3:M:179:ILE:O	3:M:182:HIS:ND1	2.25	0.62
6:Z:46:LEU:HD22	6:2:42:TYR:CE2	2.35	0.62
9:m:103:BCL:H152	6:n:36:HIS:CD2	2.35	0.62
5:AC:36:HIS:CD2	15:AC:101:CRT:H372	2.34	0.62
1:C:250:CYS:SG	7:C:503:HEM:CAC	2.87	0.62
2:L:157:TYR:CG	10:L:302:BPH:H151	2.34	0.62
4:H:247:LYS:HA	4:H:254:ARG:HH11	1.63	0.62
2:x:206:VAL:HG13	3:y:142:MET:HE3	1.80	0.62
6:n:20:ILE:O	6:n:24:SER:OG	2.11	0.62
5:l:5:ASN:C	5:l:7:ASN:H	2.08	0.62
1:o:119:ASP:OD2	1:o:128:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:211:LYS:HG2	12:x:306:PEF:C10	2.30	0.62
5:p:19:ARG:HH22	12:p:101:PEF:HN2	1.45	0.62
15:v:101:CRT:H372	5:w:36:HIS:CD2	2.35	0.62
4:H:56:VAL:N	12:H:302:PEF:HN2	1.97	0.62
6:4:32:VAL:HG21	9:4:102:BCL:HBA2	1.81	0.62
1:o:47:ARG:HH11	1:o:47:ARG:CG	2.13	0.62
5:m:45:ASN:HB3	5:p:56:GLN:NE2	2.12	0.62
5:m:33:LEU:HD23	15:m:104:CRT:H36	1.82	0.62
9:j:101:BCL:H61	6:k:28:TRP:CZ3	2.35	0.62
1:C:20:LEU:HD23	1:C:21:LEU:HD22	1.80	0.61
1:C:97:VAL:HG21	1:C:131:PHE:HZ	1.66	0.61
3:M:229:PHE:HE2	3:M:247:ARG:HD3	1.65	0.61
9:A:103:BCL:HBA2	6:B:32:VAL:HG21	1.81	0.61
6:E:44:PRO:O	5:F:52:PRO:HD2	2.00	0.61
1:o:100:TRP:HB3	1:o:152:CYS:HB2	1.80	0.61
2:x:42:PHE:CD2	2:x:104:GLY:HA3	2.34	0.61
5:r:12:TRP:CE3	5:r:17:PRO:HG3	2.35	0.61
6:B:44:PRO:O	5:D:55:TYR:OH	2.18	0.61
3:y:229:PHE:HB2	3:y:244:ALA:HB2	1.80	0.61
6:AB:32:VAL:HG21	9:AB:102:BCL:HBA2	1.82	0.61
9:AB:102:BCL:H42	9:AC:102:BCL:H172	1.81	0.61
5:AG:45:ASN:HB3	5:AI:56:GLN:NE2	2.14	0.61
5:h:17:PRO:HB3	6:i:17:PHE:CE1	2.35	0.61
6:c:36:HIS:ND1	9:c:101:BCL:H111	2.16	0.61
5:A:55:TYR:OH	6:0:44:PRO:O	2.14	0.61
5:Q:38:ILE:O	5:Q:42:THR:HG23	2.00	0.61
4:t:48:ARG:HG2	6:n:8:GLY:HA3	1.80	0.61
1:C:178:LEU:HA	3:M:110:SER:HB2	1.80	0.61
2:L:281:TRP:HB2	3:M:88:LYS:HD2	1.82	0.61
5:AC:17:PRO:HB3	6:AD:17:PHE:CZ	2.36	0.61
5:j:43:ASP:O	5:l:56:GLN:NE2	2.33	0.61
3:M:76:LEU:HG	3:M:81:TRP:HA	1.83	0.61
6:B:17:PHE:CD1	15:9:101:CRT:H5	2.34	0.61
3:M:229:PHE:CE2	3:M:247:ARG:HD3	2.36	0.61
5:D:17:PRO:HB3	6:E:17:PHE:CZ	2.35	0.61
6:G:46:LEU:HD22	6:J:42:TYR:CE2	2.36	0.61
5:I:2:PHE:HB3	6:J:26:TYR:HE2	1.64	0.61
1:o:206:GLN:O	1:o:277:ARG:HD2	2.01	0.61
1:o:301:ASP:HB2	1:o:304:ARG:NH1	2.16	0.61
3:y:89:HIS:O	3:y:93:LEU:HG	1.99	0.61
15:y:404:CRT:H2M3	5:AA:38:ILE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:56:GLN:HG2	5:9:43:ASP:CG	2.25	0.61
2:x:15:GLY:O	2:x:118:ARG:NE	2.32	0.61
3:y:63:PHE:CE1	5:AC:30:VAL:HG22	2.35	0.61
5:m:18:ARG:HG3	5:l:14:ILE:HG22	1.83	0.61
5:u:42:THR:HG21	5:w:47:LEU:HB3	1.81	0.61
1:C:164:TYR:HD2	1:C:312:GLN:HG2	1.65	0.61
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.83	0.61
4:H:45:ARG:HH12	12:H:302:PEF:H21	1.66	0.61
5:D:12:TRP:HB3	5:D:17:PRO:HG3	1.83	0.61
1:o:41:GLU:OE1	2:x:153:HIS:ND1	2.33	0.61
2:x:189:PHE:CE1	2:x:249:ALA:HB1	2.35	0.61
12:y:407:PEF:N	12:y:408:PEF:O1P	2.34	0.61
5:AK:7:ASN:OD1	5:AK:10:LYS:HD2	2.00	0.61
6:T:43:ARG:HG3	5:U:55:TYR:OH	2.01	0.61
9:4:102:BCL:HMA1	9:5:101:BCL:HMA1	1.82	0.61
6:0:33:VAL:HG22	9:0:102:BCL:H93	1.83	0.61
5:p:18:ARG:HB3	12:p:101:PEF:O3	2.00	0.61
5:l:5:ASN:O	5:l:7:ASN:N	2.28	0.61
2:L:239:HIS:CG	3:M:223:ILE:HG21	2.36	0.61
6:0:45:TRP:HD1	6:0:46:LEU:HG	1.65	0.61
1:o:105:GLU:N	1:o:105:GLU:OE2	2.34	0.61
3:M:35:ILE:HG13	3:M:48:ILE:HB	1.83	0.60
5:O:36:HIS:HB3	15:O:101:CRT:H393	1.82	0.60
6:P:28:TRP:HH2	9:P:101:BCL:HBA1	1.66	0.60
2:x:188:PHE:HZ	11:x:304:UQ8:H27A	1.66	0.60
9:x:303:BCL:HED3	3:y:179:ILE:HG23	1.83	0.60
3:y:159:VAL:HA	3:y:163:ILE:HB	1.84	0.60
9:c:101:BCL:HAA2	9:c:101:BCL:HED3	1.83	0.60
2:L:244:PHE:HD1	11:L:304:UQ8:H43	1.66	0.60
9:R:102:BCL:H3A	9:R:102:BCL:H2	1.81	0.60
5:U:9:TYR:HB2	6:V:14:ALA:O	2.00	0.60
5:Y:52:PRO:HD2	5:Y:55:TYR:CE2	2.36	0.60
1:o:21:LEU:HD21	2:x:274:TRP:CZ2	2.36	0.60
5:AC:39:VAL:HG11	9:AC:102:BCL:HBC1	1.81	0.60
5:d:7:ASN:HB3	5:d:10:LYS:HD2	1.82	0.60
1:C:287:LEU:O	1:C:291:LEU:HD12	2.00	0.60
6:G:39:ALA:HB1	9:G:102:BCL:HBC1	1.83	0.60
5:S:25:VAL:HG22	9:S:102:BCL:H8	1.83	0.60
9:W:101:BCL:H152	9:W:101:BCL:H93	1.83	0.60
5:Y:23:SER:HB3	9:1:101:BCL:H151	1.82	0.60
9:Z:102:BCL:HMA1	9:1:101:BCL:HMA1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:7:THR:HG23	6:2:9:LEU:H	1.65	0.60
1:o:227:LYS:HZ1	3:y:97:PRO:HD2	1.66	0.60
2:x:132:PHE:CZ	11:x:304:UQ8:H40B	2.35	0.60
5:U:54:SER:O	5:U:58:LEU:N	2.34	0.60
3:M:99:PRO:HD2	3:M:102:TYR:CD2	2.36	0.60
5:W:35:ILE:HG12	15:X:101:CRT:H403	1.83	0.60
5:1:29:ILE:HD11	9:1:101:BCL:H72	1.82	0.60
2:x:199:HIS:CE1	2:x:239:HIS:CE1	2.89	0.60
6:AJ:43:ARG:HG3	5:AK:55:TYR:CE1	2.37	0.60
5:A:16:ASP:OD2	5:A:19:ARG:HG3	2.02	0.60
5:3:5:ASN:O	5:3:7:ASN:N	2.33	0.60
3:y:71:ILE:O	3:y:75:MET:HG3	2.02	0.60
5:AK:59:GLY:O	5:AK:61:LYS:N	2.31	0.60
6:k:45:TRP:CD1	6:k:46:LEU:HG	2.37	0.60
6:T:35:ALA:HA	6:T:38:LEU:HD12	1.83	0.60
5:Y:23:SER:HB3	9:1:101:BCL:H121	1.84	0.60
1:o:103:PRO:HG2	1:o:104:LYS:HD2	1.83	0.60
3:y:35:ILE:HG13	3:y:48:ILE:HB	1.84	0.60
4:t:234:TYR:O	4:t:238:LYS:HG2	2.01	0.60
5:r:55:TYR:C	5:r:57:ALA:H	2.10	0.60
6:AL:32:VAL:HG21	9:AL:102:BCL:HBA2	1.83	0.60
2:L:144:ARG:HB3	2:L:145:PRO:HD3	1.84	0.60
9:G:102:BCL:HMA1	9:I:101:BCL:HMA1	1.83	0.60
9:I:103:BCL:HAA2	9:I:103:BCL:CED	2.31	0.60
6:AJ:20:ILE:HD12	15:AJ:101:CRT:C5	2.31	0.60
6:P:45:TRP:CD1	6:P:46:LEU:HG	2.37	0.60
12:m:101:PEF:H51	5:l:19:ARG:NH2	2.16	0.60
4:H:246:GLY:O	4:H:254:ARG:NH1	2.35	0.60
1:o:47:ARG:HH11	1:o:47:ARG:HG2	1.66	0.60
2:x:201:SER:HG	3:y:270:TRP:CD1	2.20	0.60
2:x:126:VAL:HG11	3:y:251:PHE:CE2	2.37	0.59
1:C:310:CYS:SG	7:C:504:HEM:CAC	2.90	0.59
2:L:170:GLY:HA2	2:L:176:PHE:HD2	1.66	0.59
9:U:101:BCL:HAA2	9:U:101:BCL:HBD	1.84	0.59
9:3:101:BCL:HBC2	9:4:102:BCL:HMD1	1.84	0.59
6:n:20:ILE:HB	15:n:101:CRT:H82	1.83	0.59
2:L:237:ALA:HA	2:L:240:ARG:HD2	1.84	0.59
1:o:152:CYS:SG	7:o:502:HEM:CAB	2.89	0.59
3:y:4:TYR:HE1	3:y:6:ASN:HA	1.67	0.59
6:AB:43:ARG:HG3	5:AC:55:TYR:OH	2.02	0.59
6:AF:21:PHE:HA	15:AF:102:CRT:H14	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:45:TRP:HD1	6:AH:46:LEU:HG	1.67	0.59
5:AK:39:VAL:HG11	9:AK:101:BCL:HBC1	1.85	0.59
1:C:21:LEU:HD11	2:L:274:TRP:CD2	2.37	0.59
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.37	0.59
5:1:57:ALA:N	5:1:58:LEU:C	2.54	0.59
6:AB:18:HIS:O	6:AB:22:MET:HG2	2.02	0.59
9:AG:101:BCL:H2	6:AH:29:PHE:CE1	2.37	0.59
1:C:19:MET:O	1:C:21:LEU:HD22	2.02	0.59
6:B:46:LEU:C	5:D:51:ILE:HG21	2.27	0.59
5:Q:28:GLN:HB3	9:Q:101:BCL:H42	1.84	0.59
3:y:247:ARG:NH2	4:t:113:PRO:O	2.32	0.59
5:r:14:ILE:HG13	5:r:15:LEU:HG	1.83	0.59
2:L:206:VAL:HB	2:L:216:LYS:HB2	1.85	0.59
1:o:127:SER:OG	7:o:501:HEM:HAC	2.03	0.59
9:A:102:BCL:H2	6:B:28:TRP:CH2	2.37	0.59
6:2:13:GLU:HB3	15:2:101:CRT:H23	1.84	0.59
1:o:84:ASP:OD1	1:o:84:ASP:N	2.36	0.59
5:AC:42:THR:HG21	5:AE:47:LEU:HD13	1.85	0.59
5:AG:11:ILE:HD13	15:AJ:101:CRT:C10	2.33	0.59
5:d:5:ASN:ND2	6:g:20:ILE:HA	2.17	0.59
2:L:112:ARG:O	2:L:116:ILE:HG13	2.02	0.59
4:H:159:LEU:HD22	4:H:254:ARG:HH21	1.65	0.59
2:x:175:HIS:CD2	2:x:178:TYR:CE1	2.91	0.59
3:y:52:TYR:O	3:y:132:ARG:NH2	2.33	0.59
4:t:179:ILE:HG22	4:t:197:ILE:HD13	1.85	0.59
6:v:20:ILE:HD12	15:v:101:CRT:C6	2.33	0.59
5:h:19:ARG:HA	5:h:22:VAL:HG22	1.85	0.59
6:i:11:ASP:O	6:i:15:LYS:HG3	2.03	0.59
5:A:28:GLN:OE1	6:B:28:TRP:NE1	2.36	0.59
5:O:36:HIS:CD2	15:O:101:CRT:H372	2.38	0.59
6:P:45:TRP:HD1	6:P:46:LEU:HG	1.67	0.59
6:R:32:VAL:HG21	9:R:102:BCL:HBA2	1.85	0.59
1:C:21:LEU:HD23	2:L:271:TRP:CZ2	2.37	0.58
5:d:25:VAL:HG13	9:d:101:BCL:H72	1.85	0.58
5:j:44:LEU:HD22	6:k:43:ARG:HD3	1.84	0.58
4:H:63:ASP:CG	5:F:19:ARG:HH22	2.10	0.58
6:X:45:TRP:CD1	6:X:46:LEU:HG	2.33	0.58
6:8:43:ARG:HG3	5:9:55:TYR:CZ	2.38	0.58
1:o:181:THR:HB	1:o:183:GLN:O	2.02	0.58
2:x:222:ASN:O	2:x:226:ARG:HG3	2.03	0.58
3:y:290:VAL:HG11	4:t:11:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:18:HIS:O	6:J:22:MET:HG2	2.02	0.58
6:X:32:VAL:HG21	9:X:102:BCL:HBA2	1.85	0.58
5:1:5:ASN:HB3	5:1:8:LEU:HB2	1.86	0.58
3:y:99:PRO:HB2	3:y:101:GLN:HG2	1.84	0.58
5:r:34:LEU:HD21	15:s:101:CRT:H2M2	1.84	0.58
6:P:43:ARG:HG3	5:Q:55:TYR:CE1	2.39	0.58
5:5:9:TYR:HB2	6:6:14:ALA:O	2.03	0.58
5:AE:18:ARG:NH1	17:AE:101:PGW:OAE	2.37	0.58
5:f:27:PHE:CE1	5:h:29:ILE:HD13	2.38	0.58
5:S:25:VAL:HG21	9:S:102:BCL:H152	1.84	0.58
5:3:43:ASP:OD2	5:5:54:SER:OG	2.19	0.58
1:o:292:PRO:HD2	1:o:295:ARG:HG2	1.85	0.58
5:w:40:LEU:O	5:w:45:ASN:ND2	2.35	0.58
5:AC:43:ASP:HB2	5:AE:48:ASP:HA	1.86	0.58
9:j:101:BCL:H2	6:k:28:TRP:CZ2	2.36	0.58
3:M:175:VAL:HG22	3:M:185:TRP:CE2	2.38	0.58
6:R:43:ARG:HG3	5:S:55:TYR:CE1	2.38	0.58
2:x:132:PHE:HZ	11:x:304:UQ8:H40B	1.68	0.58
3:y:177:PHE:CD1	15:y:404:CRT:H19	2.38	0.58
4:t:32:ARG:NH2	4:t:62:PRO:HA	2.18	0.58
4:t:60:ASP:OD1	4:t:60:ASP:N	2.36	0.58
4:t:136:MET:HG3	4:t:170:VAL:O	2.03	0.58
9:AB:101:BCL:HBC2	9:AB:102:BCL:HMD1	1.84	0.58
6:AH:17:PHE:HB2	15:AH:102:CRT:H22A	1.83	0.58
9:g:102:BCL:H3A	9:g:102:BCL:H12	1.84	0.58
4:H:54:LYS:NZ	12:H:304:PEF:O2P	2.36	0.58
9:r:101:BCL:H2	6:s:28:TRP:CZ2	2.38	0.58
9:h:101:BCL:H52	9:h:101:BCL:H142	1.85	0.58
1:C:56:ASN:HB3	1:C:318:LEU:HA	1.85	0.58
6:B:24:SER:HB3	5:9:2:PHE:C	2.29	0.58
6:J:46:LEU:HD21	5:K:46:TRP:HB2	1.85	0.58
1:o:250:CYS:O	1:o:262:SER:HB3	2.04	0.58
15:v:101:CRT:H342	9:w:101:BCL:O1A	2.03	0.58
5:7:9:TYR:OH	6:8:11:ASP:OD2	2.12	0.58
6:AJ:14:ALA:CB	6:AJ:17:PHE:HB3	2.34	0.58
2:L:35:PHE:CD2	2:L:111:LEU:HB3	2.39	0.58
9:S:102:BCL:HBD	9:S:102:BCL:HAA1	1.86	0.58
4:t:44:ASP:HB3	4:t:48:ARG:HH21	1.69	0.58
6:q:17:PHE:HA	15:q:101:CRT:H6	1.86	0.58
5:AK:51:ILE:HG21	6:AL:43:ARG:HH22	1.68	0.58
5:U:11:ILE:HG12	9:W:101:BCL:H142	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:17:PRO:HB3	6:6:17:PHE:CZ	2.39	0.57
9:7:102:BCL:HAA2	9:7:102:BCL:HBD	1.86	0.57
2:x:196:LEU:HD11	3:y:269:ALA:HB1	1.86	0.57
12:x:306:PEF:H51	4:t:67:PHE:HA	1.84	0.57
3:y:201:PHE:CD1	3:y:279:THR:HG22	2.38	0.57
5:u:3:THR:HG23	5:u:5:ASN:H	1.69	0.57
5:d:33:LEU:HB3	5:d:37:MET:HE3	1.86	0.57
9:d:101:BCL:HAC2	9:e:102:BCL:HAC1	1.86	0.57
5:h:40:LEU:O	5:h:45:ASN:ND2	2.36	0.57
2:L:26:TRP:HZ3	4:H:99:PRO:HB3	1.69	0.57
4:H:251:THR:OG1	4:H:254:ARG:HG3	2.03	0.57
5:1:36:HIS:CE1	9:2:102:BCL:HMD3	2.39	0.57
2:x:176:PHE:HE1	2:x:179:ASN:ND2	1.99	0.57
3:y:102:TYR:HE2	3:y:111:GLU:HB3	1.69	0.57
3:y:197:TYR:CZ	9:y:401:BCL:HMC2	2.39	0.57
5:AK:11:ILE:HA	15:e:101:CRT:H83	1.85	0.57
5:AK:27:PHE:CZ	5:AK:31:LEU:HD22	2.39	0.57
2:L:44:LEU:HD23	5:9:30:VAL:CG1	2.33	0.57
15:m:104:CRT:H403	5:l:35:ILE:HG12	1.86	0.57
6:AH:28:TRP:CZ2	9:AH:101:BCL:H2	2.39	0.57
3:M:208:PHE:CD2	3:M:275:LEU:HB3	2.39	0.57
6:E:16:GLU:O	6:E:20:ILE:HG13	2.04	0.57
6:q:20:ILE:HD12	15:q:101:CRT:C6	2.34	0.57
5:AG:12:TRP:HZ3	5:AG:20:VAL:HG21	1.68	0.57
9:AI:102:BCL:HBA2	6:AJ:32:VAL:CG2	2.35	0.57
1:C:110:CYS:HA	1:C:123:THR:OG1	2.03	0.57
5:F:12:TRP:HB2	6:G:14:ALA:HB1	1.85	0.57
5:Y:40:LEU:HG	5:Y:46:TRP:CH2	2.39	0.57
4:t:35:LYS:NZ	4:t:56:VAL:O	2.33	0.57
4:t:36:ARG:NE	4:t:65:LYS:HD2	2.20	0.57
4:t:171:TRP:HB2	4:t:181:TYR:HB2	1.85	0.57
6:AF:45:TRP:HD1	6:AF:46:LEU:HG	1.69	0.57
5:f:4:MET:O	5:f:6:ALA:N	2.38	0.57
3:M:3:GLU:OE2	4:H:212:ASP:HB3	2.05	0.57
4:H:246:GLY:HA2	4:H:250:ALA:H	1.69	0.57
2:x:236:LEU:O	2:x:239:HIS:HB2	2.04	0.57
3:y:177:PHE:HD1	15:y:404:CRT:H19	1.70	0.57
6:s:46:LEU:HD22	6:v:42:TYR:CE2	2.39	0.57
2:L:179:ASN:HB3	2:L:182:HIS:CB	2.35	0.57
6:X:17:PHE:H	15:X:101:CRT:H23	1.69	0.57
2:x:13:ARG:NH2	2:x:21:ASP:OD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AC:102:BCL:H191	6:AD:31:LEU:HD22	1.86	0.57
1:C:191:ALA:HB3	1:C:237:MET:HE3	1.87	0.57
3:M:53:LEU:HD12	3:M:132:ARG:HH12	1.70	0.57
5:F:4:MET:N	6:J:23:GLN:OE1	2.31	0.57
6:X:17:PHE:N	15:X:101:CRT:H23	2.19	0.57
5:7:7:ASN:HB3	5:7:10:LYS:HD2	1.87	0.57
5:r:11:ILE:HD12	5:r:14:ILE:HD11	1.85	0.57
5:u:33:LEU:O	5:u:37:MET:HG2	2.05	0.57
9:i:102:BCL:H52	9:i:102:BCL:H3A	1.86	0.57
4:H:57:GLY:H	12:H:302:PEF:C5	2.18	0.57
2:x:188:PHE:CZ	11:x:304:UQ8:H27A	2.39	0.57
5:AE:5:ASN:C	5:AE:7:ASN:H	2.13	0.57
6:AF:28:TRP:CZ2	9:AF:101:BCL:H43	2.40	0.57
5:d:24:ILE:HD11	9:f:101:BCL:H141	1.87	0.57
1:C:188:LYS:HB2	1:C:192:TYR:CZ	2.39	0.57
2:L:179:ASN:HB3	2:L:182:HIS:HB2	1.86	0.57
2:L:241:LEU:HD21	11:L:304:UQ8:H13	1.86	0.57
1:o:314:VAL:HG12	1:o:316:LYS:H	1.70	0.57
4:t:171:TRP:HE1	4:t:183:GLU:HG3	1.70	0.57
6:s:9:LEU:HD23	6:s:13:GLU:HB3	1.86	0.57
5:w:17:PRO:HB3	6:z:17:PHE:CZ	2.40	0.57
9:AC:103:BCL:HBA2	6:AD:32:VAL:CG2	2.35	0.57
9:AL:102:BCL:H3A	9:AL:102:BCL:CGA	2.35	0.57
6:E:21:PHE:HA	15:E:101:CRT:H11	1.86	0.56
15:7:101:CRT:H392	9:7:102:BCL:HMB2	1.86	0.56
5:m:50:ASN:HB3	5:m:54:SER:HA	1.86	0.56
1:C:21:LEU:HD21	2:L:274:TRP:CZ2	2.40	0.56
3:M:263:GLU:OE1	3:M:267:ARG:NH2	2.35	0.56
5:Q:19:ARG:HD2	5:S:18:ARG:HH22	1.70	0.56
6:e:20:ILE:O	6:e:24:SER:OG	2.22	0.56
2:L:61:PRO:HA	2:L:66:GLN:HG3	1.88	0.56
3:M:72:GLY:HA3	15:M:405:CRT:C6	2.36	0.56
6:E:17:PHE:HB2	15:E:101:CRT:H31A	1.88	0.56
6:G:18:HIS:O	6:G:22:MET:HG2	2.05	0.56
15:R:101:CRT:H372	5:S:36:HIS:CG	2.40	0.56
5:S:14:ILE:HD11	15:V:101:CRT:H31A	1.87	0.56
1:o:97:VAL:HG21	1:o:131:PHE:CZ	2.40	0.56
1:o:310:CYS:SG	7:o:504:HEM:HMC2	2.45	0.56
6:n:31:LEU:HD12	5:l:2:PHE:HE2	1.70	0.56
5:u:2:PHE:O	6:v:22:MET:HE2	2.05	0.56
15:G:101:CRT:H372	5:I:36:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:7:ASN:HB3	5:u:10:LYS:HD2	1.86	0.56
5:I:44:LEU:HD23	6:J:43:ARG:HG2	1.87	0.56
6:N:43:ARG:HG3	5:O:55:TYR:OH	2.04	0.56
6:Z:43:ARG:HD3	5:1:55:TYR:OH	2.04	0.56
2:x:177:HIS:HB3	3:y:183:LEU:HD13	1.88	0.56
9:p:102:BCL:H2	6:q:28:TRP:CH2	2.41	0.56
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.87	0.56
6:4:21:PHE:CD1	15:4:101:CRT:H14	2.41	0.56
6:6:29:PHE:CD1	9:6:101:BCL:H2	2.41	0.56
2:x:86:MET:HG2	5:j:37:MET:O	2.05	0.56
4:t:29:TYR:CZ	12:t:303:PEF:C30	2.89	0.56
5:AA:35:ILE:HG12	15:AC:101:CRT:H403	1.88	0.56
5:j:12:TRP:HZ3	5:j:20:VAL:HG21	1.70	0.56
5:S:13:LEU:HD21	6:T:11:ASP:HA	1.88	0.56
5:3:9:TYR:HB2	6:4:14:ALA:O	2.05	0.56
1:C:203:PHE:CG	1:C:235:LEU:HD22	2.40	0.56
9:D:101:BCL:HAC1	9:D:102:BCL:HAC2	1.88	0.56
9:N:101:BCL:HED2	9:N:101:BCL:HAA2	1.86	0.56
6:T:44:PRO:HG2	5:U:52:PRO:CG	2.36	0.56
15:4:101:CRT:H291	9:5:101:BCL:CBA	2.35	0.56
9:4:102:BCL:H121	9:4:102:BCL:HBB2	1.86	0.56
5:AG:51:ILE:HG22	5:AG:52:PRO:HA	1.87	0.56
3:M:233:ARG:NH1	4:H:133:ILE:HD11	2.21	0.56
3:M:260:VAL:HG12	4:H:34:ASP:OD2	2.06	0.56
6:R:17:PHE:HB2	15:R:101:CRT:H22A	1.88	0.56
5:m:56:GLN:HG2	5:l:43:ASP:CG	2.31	0.56
1:C:20:LEU:HA	1:C:21:LEU:CB	2.36	0.56
1:C:99:THR:HA	1:C:103:PRO:HB3	1.87	0.56
4:H:126:THR:HG23	4:H:130:LEU:O	2.05	0.56
4:H:168:SER:HB3	4:H:185:GLU:HB2	1.87	0.56
9:w:101:BCL:H102	9:w:101:BCL:H171	1.86	0.56
5:AC:44:LEU:HD12	5:AE:47:LEU:HD22	1.87	0.56
6:AF:43:ARG:HG3	5:AG:55:TYR:CE1	2.41	0.56
5:d:9:TYR:HB2	6:e:14:ALA:O	2.06	0.56
4:H:189:ASN:ND2	4:H:191:LYS:HB2	2.20	0.55
1:o:20:LEU:CA	1:o:21:LEU:HB2	2.29	0.55
1:o:164:TYR:HB2	1:o:309:THR:HA	1.87	0.55
15:AF:102:CRT:H372	5:AG:36:HIS:CG	2.40	0.55
6:AH:44:PRO:O	5:AI:55:TYR:OH	2.20	0.55
5:j:17:PRO:HB3	6:k:17:PHE:CZ	2.41	0.55
11:L:304:UQ8:H38	11:L:304:UQ8:H35B	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:59:VAL:HG21	1:o:100:TRP:NE1	2.21	0.55
5:r:43:ASP:OD1	5:u:56:GLN:HG2	2.05	0.55
5:w:40:LEU:HG	5:w:46:TRP:CH2	2.40	0.55
5:j:46:TRP:NE1	9:j:101:BCL:OBB	2.38	0.55
3:M:99:PRO:HD2	3:M:102:TYR:HD2	1.72	0.55
6:B:16:GLU:O	6:B:20:ILE:HG13	2.06	0.55
9:I:103:BCL:H202	6:J:40:TRP:NE1	2.21	0.55
6:R:40:TRP:CH2	6:R:46:LEU:HB2	2.41	0.55
5:U:16:ASP:OD2	5:U:19:ARG:HG3	2.06	0.55
5:1:54:SER:HB2	5:1:57:ALA:HB1	1.88	0.55
1:o:166:TRP:CD1	1:o:306:SER:HB3	2.42	0.55
2:x:17:LEU:O	4:t:258:LEU:HB2	2.06	0.55
9:AE:102:BCL:HBA1	6:AF:32:VAL:HG11	1.87	0.55
6:AJ:45:TRP:HD1	6:AJ:46:LEU:HG	1.71	0.55
6:e:20:ILE:HD12	15:e:101:CRT:H42	1.87	0.55
2:L:207:THR:OG1	2:L:208:ASN:ND2	2.39	0.55
4:H:249:TYR:O	4:H:251:THR:N	2.40	0.55
5:S:19:ARG:NH2	17:S:101:PGW:H04A	2.21	0.55
9:Z:102:BCL:HMB1	9:Z:102:BCL:H93	1.89	0.55
3:y:267:ARG:NH1	12:t:303:PEF:H31	2.21	0.55
4:t:159:LEU:HD21	4:t:251:THR:HG23	1.88	0.55
5:AG:5:ASN:ND2	6:AJ:23:GLN:OE1	2.39	0.55
5:AI:20:VAL:O	5:AI:24:ILE:HG12	2.06	0.55
9:F:101:BCL:HAA2	9:F:101:BCL:HBD	1.89	0.55
5:I:26:ALA:O	5:I:29:ILE:HG22	2.06	0.55
6:0:32:VAL:HG11	9:0:102:BCL:HBA1	1.86	0.55
1:o:270:TRP:CG	3:y:316:PRO:HG2	2.42	0.55
5:d:12:TRP:HZ3	5:d:20:VAL:HG21	1.71	0.55
1:C:173:LYS:HB2	3:M:80:HIS:CG	2.42	0.55
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.89	0.55
9:S:102:BCL:HBC2	9:T:102:BCL:HMD1	1.89	0.55
5:1:33:LEU:HB3	5:1:37:MET:HE3	1.88	0.55
1:o:33:ILE:HG21	1:o:248:THR:O	2.05	0.55
2:x:206:VAL:CG1	3:y:142:MET:HE3	2.36	0.55
5:m:8:LEU:HG	6:q:20:ILE:CD1	2.37	0.55
6:n:24:SER:HB3	5:l:2:PHE:C	2.30	0.55
6:AJ:12:ASP:C	6:AJ:15:LYS:H	2.14	0.55
3:M:63:PHE:CD1	5:Q:30:VAL:HG22	2.42	0.55
5:W:3:THR:HG22	6:X:18:HIS:NE2	2.22	0.55
5:5:24:ILE:HD11	9:7:102:BCL:H151	1.88	0.55
5:9:10:LYS:HB3	15:9:101:CRT:H41	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:101:BCL:H2	6:AL:28:TRP:CH2	2.41	0.55
5:j:51:ILE:HD11	5:l:55:TYR:O	2.07	0.55
9:1:101:BCL:HAC1	9:2:102:BCL:HAC1	1.89	0.55
15:n:101:CRT:H81	15:n:101:CRT:H11	1.87	0.55
5:p:9:TYR:OH	5:p:10:LYS:HE2	2.06	0.55
5:AK:23:SER:OG	9:d:101:BCL:H152	2.06	0.55
6:B:24:SER:OG	5:9:3:THR:HA	2.07	0.55
5:D:9:TYR:C	5:D:11:ILE:H	2.14	0.55
6:G:13:GLU:HB3	15:G:101:CRT:H21A	1.89	0.55
5:U:53:VAL:HG13	5:U:55:TYR:CZ	2.41	0.55
4:t:173:ASP:OD2	4:t:180:ARG:NH2	2.35	0.55
4:t:251:THR:OG1	4:t:254:ARG:HG3	2.07	0.55
9:m:102:BCL:HMB2	15:m:104:CRT:H371	1.89	0.55
5:u:43:ASP:HB2	5:w:48:ASP:OD1	2.07	0.55
6:AJ:18:HIS:O	6:AJ:22:MET:HG2	2.06	0.55
1:C:278:ASP:OD1	1:C:282:ASN:ND2	2.39	0.55
4:H:57:GLY:H	12:H:302:PEF:H52	1.72	0.55
5:I:12:TRP:CZ3	5:I:20:VAL:HG11	2.42	0.55
4:t:141:GLU:HG2	4:t:142:PHE:H	1.72	0.55
2:L:71:TRP:CD2	3:M:303:MET:HE3	2.42	0.54
2:L:183:MET:HE3	9:L:303:BCL:HED2	1.88	0.54
6:B:17:PHE:HA	15:9:101:CRT:H83	1.88	0.54
9:I:101:BCL:HAA2	9:I:101:BCL:HBD	1.88	0.54
6:n:20:ILE:HB	15:n:101:CRT:C8	2.37	0.54
6:AF:45:TRP:CD1	6:AF:46:LEU:HG	2.42	0.54
1:C:167:VAL:HG22	1:C:303:LEU:HD23	1.89	0.54
1:C:187:SER:C	1:C:189:THR:H	2.15	0.54
5:I:44:LEU:HD11	6:J:45:TRP:HB3	1.89	0.54
5:O:36:HIS:CG	15:O:101:CRT:H372	2.42	0.54
5:1:4:MET:HE1	5:1:8:LEU:HD23	1.88	0.54
6:AL:36:HIS:HB3	9:AL:102:BCL:H142	1.89	0.54
5:j:33:LEU:O	5:j:37:MET:HG2	2.07	0.54
12:M:407:PEF:H52	12:M:408:PEF:O2P	2.08	0.54
5:U:53:VAL:O	5:U:55:TYR:N	2.41	0.54
5:9:5:ASN:C	5:9:7:ASN:H	2.12	0.54
1:o:17:SER:HA	1:o:18:VAL:HB	1.89	0.54
3:y:63:PHE:HE1	5:AC:30:VAL:HA	1.72	0.54
3:y:277:VAL:O	3:y:280:ALA:HB3	2.08	0.54
9:AL:102:BCL:HBD	9:AL:102:BCL:HAA1	1.90	0.54
9:h:101:BCL:HAA2	9:h:101:BCL:HBD	1.89	0.54
6:i:29:PHE:CE1	9:i:102:BCL:H2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:49:ASP:HB2	5:A:51:ILE:HG13	1.90	0.54
6:P:28:TRP:CH2	9:P:101:BCL:HBA1	2.42	0.54
5:W:44:LEU:HD12	5:Y:47:LEU:HD22	1.89	0.54
5:5:43:ASP:OD2	5:7:50:ASN:HA	2.07	0.54
1:o:41:GLU:OE2	2:x:80:LEU:HD11	2.07	0.54
1:o:100:TRP:HE3	1:o:152:CYS:SG	2.31	0.54
1:o:128:ARG:HH21	7:o:501:HEM:CAD	2.21	0.54
3:y:73:PHE:N	15:y:404:CRT:H32A	2.23	0.54
15:AL:101:CRT:H371	9:d:101:BCL:HMB2	1.87	0.54
9:AL:102:BCL:HAA1	9:AL:102:BCL:CBD	2.38	0.54
5:j:40:LEU:O	5:j:45:ASN:ND2	2.37	0.54
6:k:33:VAL:O	6:k:37:LEU:HG	2.07	0.54
1:C:43:TYR:CE1	2:L:148:MET:HE1	2.42	0.54
2:L:160:LEU:O	2:L:163:LEU:HB2	2.08	0.54
2:L:175:HIS:CD2	2:L:178:TYR:CE1	2.96	0.54
5:K:40:LEU:O	5:K:45:ASN:ND2	2.36	0.54
9:3:101:BCL:H2	6:4:28:TRP:CH2	2.42	0.54
4:t:44:ASP:O	4:t:48:ARG:HB2	2.07	0.54
5:m:31:LEU:HD23	9:m:103:BCL:HED2	1.89	0.54
5:AG:16:ASP:OD1	5:AG:18:ARG:N	2.38	0.54
15:e:101:CRT:H371	9:f:101:BCL:HMB2	1.88	0.54
5:h:2:PHE:CE1	6:k:26:TYR:HB3	2.42	0.54
5:j:17:PRO:HB3	6:k:17:PHE:CE2	2.43	0.54
9:L:303:BCL:H203	9:L:303:BCL:H141	1.89	0.54
3:M:96:GLU:HG3	3:M:97:PRO:HD2	1.89	0.54
4:H:193:VAL:HB	4:H:222:VAL:HG11	1.88	0.54
6:B:43:ARG:HG3	5:D:55:TYR:CE1	2.42	0.54
15:7:103:CRT:C35	9:9:102:BCL:H3A	2.38	0.54
3:y:208:PHE:CD2	3:y:275:LEU:HB3	2.43	0.54
9:y:401:BCL:H61	10:y:402:BPH:HBB2	1.89	0.54
4:t:218:HIS:HB3	4:t:242:TYR:OH	2.07	0.54
6:AH:45:TRP:CD1	6:AH:46:LEU:HG	2.43	0.54
3:M:12:GLN:OE1	3:M:14:ARG:NH2	2.29	0.54
9:M:402:BCL:H61	10:M:403:BPH:C4B	2.37	0.54
5:S:38:ILE:HD11	5:U:37:MET:HE1	1.89	0.54
6:2:36:HIS:CD2	9:2:102:BCL:H102	2.43	0.54
3:y:75:MET:HE2	3:y:94:GLY:HA2	1.88	0.54
5:r:27:PHE:HB2	9:u:101:BCL:H151	1.88	0.54
6:g:45:TRP:HD1	6:g:46:LEU:HG	1.72	0.54
6:c:32:VAL:CG2	9:c:101:BCL:HBA2	2.37	0.54
1:C:127:SER:OG	7:C:501:HEM:HAC	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:253:ARG:HH22	12:H:301:PEF:H52	1.72	0.54
4:H:64:PRO:HB3	4:H:77:VAL:HG13	1.90	0.54
4:H:184:VAL:HB	4:H:193:VAL:HG22	1.90	0.54
6:N:17:PHE:CD1	15:O:101:CRT:H6	2.43	0.54
9:U:101:BCL:HED2	6:V:32:VAL:HA	1.89	0.54
5:p:2:PHE:O	5:p:3:THR:OG1	2.25	0.54
9:q:102:BCL:HED2	9:q:102:BCL:HBA1	1.90	0.54
5:d:12:TRP:O	6:e:7:THR:HG21	2.07	0.54
5:h:34:LEU:O	5:h:38:ILE:HG13	2.08	0.54
3:M:267:ARG:HD3	12:H:305:PEF:C30	2.38	0.54
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.88	0.54
4:H:44:ASP:O	4:H:48:ARG:HB2	2.07	0.54
4:H:176:GLU:O	4:H:178:GLN:HG2	2.07	0.54
2:x:3:MET:HB2	4:t:42:ASP:HB3	1.88	0.54
2:x:175:HIS:NE2	3:y:184:ASP:OD1	2.37	0.54
5:AC:34:LEU:O	5:AC:38:ILE:HG13	2.07	0.54
5:AE:17:PRO:HG2	6:AF:9:LEU:HD11	1.90	0.54
9:A:102:BCL:C12	5:9:2:PHE:HA	2.36	0.54
5:U:20:VAL:O	5:U:24:ILE:HG12	2.07	0.54
1:o:250:CYS:SG	7:o:503:HEM:CAC	2.95	0.54
3:y:186:THR:HG22	9:y:401:BCL:HBC2	1.90	0.54
6:s:31:LEU:O	6:s:34:ILE:HB	2.08	0.54
5:AG:16:ASP:OD2	5:AG:19:ARG:HG3	2.07	0.54
9:L:301:BCL:NA	9:M:402:BCL:HBB2	2.22	0.53
4:H:44:ASP:HB3	4:H:48:ARG:HH21	1.73	0.53
5:S:39:VAL:HG11	9:S:102:BCL:HBC1	1.90	0.53
5:W:9:TYR:CD2	6:X:15:LYS:HG2	2.43	0.53
5:Y:52:PRO:HD2	5:Y:55:TYR:HE2	1.73	0.53
5:1:5:ASN:OD1	5:1:7:ASN:N	2.41	0.53
1:C:71:LYS:O	1:C:74:GLU:HG2	2.09	0.53
3:M:146:LEU:O	3:M:149:ALA:N	2.38	0.53
5:Y:5:ASN:HA	6:2:23:GLN:NE2	2.23	0.53
5:Y:44:LEU:HA	5:1:55:TYR:HE2	1.69	0.53
5:Y:51:ILE:CG2	5:Y:52:PRO:HA	2.39	0.53
6:6:28:TRP:O	6:6:32:VAL:HG23	2.08	0.53
2:x:248:SER:OG	11:x:304:UQ8:H35A	2.09	0.53
15:q:101:CRT:H393	5:r:36:HIS:HB3	1.90	0.53
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.91	0.53
3:M:120:LEU:HD13	15:M:405:CRT:H371	1.89	0.53
15:4:101:CRT:C32	9:5:101:BCL:HBA2	2.39	0.53
5:5:18:ARG:O	5:5:21:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:293:ASN:CG	3:y:296:LEU:HG	2.34	0.53
5:l:34:LEU:O	5:l:38:ILE:HG13	2.09	0.53
1:C:141:TRP:O	1:C:145:VAL:HG22	2.09	0.53
1:C:316:LYS:HG2	7:C:504:HEM:HAD2	1.89	0.53
2:L:240:ARG:HA	3:M:224:LEU:HD11	1.91	0.53
9:X:102:BCL:HMA1	9:Y:101:BCL:HMA1	1.89	0.53
6:2:20:ILE:HD12	15:2:101:CRT:C6	2.38	0.53
6:n:17:PHE:CD1	15:n:101:CRT:H5	2.36	0.53
5:p:45:ASN:O	5:p:49:ASP:OD2	2.25	0.53
6:AJ:43:ARG:HG3	5:AK:55:TYR:CZ	2.44	0.53
5:I:3:THR:N	5:I:4:MET:HA	2.24	0.53
5:1:56:GLN:HB2	5:1:57:ALA:HA	1.90	0.53
9:9:102:BCL:HBC2	9:0:102:BCL:HMD1	1.90	0.53
1:o:174:TYR:OH	3:y:78:SER:HB2	2.08	0.53
1:o:263:THR:HA	3:y:311:VAL:HG13	1.91	0.53
6:AL:21:PHE:CD1	15:AL:101:CRT:H14	2.37	0.53
1:C:19:MET:C	1:C:21:LEU:HD13	2.34	0.53
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.08	0.53
2:L:164:ASP:OD1	3:M:198:TYR:OH	2.26	0.53
2:L:170:GLY:HA2	2:L:176:PHE:CD2	2.43	0.53
2:L:253:SER:HB3	9:L:301:BCL:O2D	2.08	0.53
5:F:28:GLN:HB3	9:F:101:BCL:H12	1.91	0.53
5:m:17:PRO:HB3	6:n:17:PHE:CZ	2.44	0.53
5:u:3:THR:HB	5:u:8:LEU:CB	2.38	0.53
5:AC:12:TRP:CD1	6:AD:18:HIS:HB2	2.44	0.53
2:L:261:GLY:O	2:L:263:PHE:N	2.42	0.53
3:M:247:ARG:HH22	4:H:113:PRO:C	2.16	0.53
6:B:16:GLU:OE2	5:9:10:LYS:HE3	2.09	0.53
4:t:36:ARG:C	4:t:37:GLU:HG2	2.33	0.53
2:L:9:LYS:HE2	2:L:10:TYR:CZ	2.44	0.53
2:L:109:TRP:CZ2	14:M:404:MQ8:H291	2.44	0.53
6:E:17:PHE:HA	15:E:101:CRT:H42	1.91	0.53
6:J:33:VAL:O	6:J:37:LEU:HG	2.08	0.53
5:K:51:ILE:HG12	5:O:59:GLY:HA2	1.89	0.53
9:K:101:BCL:HED1	6:N:28:TRP:CZ2	2.44	0.53
5:Q:44:LEU:HD12	5:S:47:LEU:HD22	1.91	0.53
5:Y:44:LEU:HA	5:1:55:TYR:CD2	2.44	0.53
5:1:57:ALA:N	5:1:58:LEU:O	2.40	0.53
4:t:232:THR:O	4:t:236:GLU:HG3	2.08	0.53
5:p:19:ARG:NH2	12:p:101:PEF:HN2	2.06	0.53
5:j:35:ILE:HG12	15:k:101:CRT:C40	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:MET:HE1	1:C:284:ILE:HD13	1.91	0.53
5:O:59:GLY:O	5:O:61:LYS:HA	2.09	0.53
1:o:56:ASN:HB3	1:o:318:LEU:HA	1.91	0.53
1:o:236:MET:HB3	7:o:503:HEM:C4B	2.44	0.53
5:f:40:LEU:HG	5:f:46:TRP:CH2	2.43	0.53
2:L:35:PHE:CZ	2:L:111:LEU:HD13	2.44	0.53
2:L:167:SER:HA	9:L:301:BCL:HBC1	1.90	0.53
2:L:183:MET:HE1	3:M:180:PHE:HE1	1.73	0.53
5:F:16:ASP:OD2	5:F:19:ARG:HG3	2.09	0.53
9:G:102:BCL:H3A	9:G:102:BCL:C1	2.33	0.53
6:R:46:LEU:HD11	9:R:102:BCL:H151	1.91	0.53
5:7:36:HIS:CD2	15:7:101:CRT:H393	2.44	0.53
6:0:11:ASP:O	6:0:15:LYS:HG3	2.09	0.53
5:r:29:ILE:HG13	9:r:101:BCL:H43	1.91	0.53
5:d:31:LEU:HD21	15:e:101:CRT:H32	1.91	0.53
1:C:169:ASP:OD1	1:C:170:PRO:HD2	2.09	0.52
1:C:232:THR:O	1:C:236:MET:HG2	2.09	0.52
2:L:183:MET:HB3	9:L:303:BCL:O1D	2.09	0.52
3:M:98:PRO:HG3	3:M:107:PRO:HG3	1.91	0.52
3:M:177:PHE:CD1	15:M:405:CRT:H16	2.41	0.52
5:3:42:THR:OG1	5:5:47:LEU:HD22	2.08	0.52
5:m:8:LEU:HD23	6:q:20:ILE:HG23	1.91	0.52
9:m:103:BCL:HAA2	9:m:103:BCL:HED3	1.90	0.52
6:AH:21:PHE:CD2	15:AH:102:CRT:H14	2.43	0.52
6:k:32:VAL:CG1	9:k:102:BCL:HBA2	2.38	0.52
2:L:71:TRP:CD1	3:M:303:MET:HG2	2.43	0.52
15:X:101:CRT:H181	15:X:101:CRT:H21	1.92	0.52
9:x:301:BCL:H161	9:x:305:BCL:H102	1.89	0.52
6:z:45:TRP:CD1	6:z:46:LEU:HG	2.44	0.52
5:AI:16:ASP:OD2	5:AI:19:ARG:HG3	2.10	0.52
1:C:181:THR:C	1:C:183:GLN:H	2.16	0.52
3:M:4:TYR:CE1	3:M:6:ASN:HA	2.44	0.52
4:H:106:PRO:O	4:H:109:SER:OG	2.24	0.52
9:4:102:BCL:HAA1	9:4:102:BCL:HBD	1.92	0.52
2:x:96:GLN:O	2:x:100:ILE:HG13	2.09	0.52
5:D:10:LYS:O	5:D:14:ILE:HG13	2.10	0.52
5:9:49:ASP:HB2	5:9:51:ILE:HG13	1.92	0.52
3:y:63:PHE:HB2	3:y:125:SER:HB2	1.91	0.52
4:t:135:PRO:HD3	4:t:171:TRP:CZ3	2.43	0.52
6:s:8:GLY:O	6:s:9:LEU:HD12	2.09	0.52
6:s:30:GLY:O	6:s:34:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:36:HIS:CE1	9:AE:102:BCL:HMD3	2.44	0.52
5:h:42:THR:HG21	5:j:47:LEU:HD13	1.91	0.52
1:C:130:MET:HB3	7:C:502:HEM:C4B	2.44	0.52
16:M:406:PO4:O3	5:O:19:ARG:NE	2.42	0.52
5:O:59:GLY:C	5:O:61:LYS:HA	2.34	0.52
5:Y:9:TYR:CE1	5:Y:10:LYS:HG3	2.44	0.52
4:t:88:ASN:OD1	4:t:103:ASN:HB2	2.09	0.52
6:n:20:ILE:HD12	15:n:101:CRT:H82	1.91	0.52
6:n:24:SER:HB3	5:l:2:PHE:O	2.10	0.52
5:AA:4:MET:O	5:AA:6:ALA:N	2.39	0.52
9:AG:101:BCL:HMD1	9:AH:101:BCL:HBC2	1.92	0.52
1:C:155:CYS:SG	7:C:502:HEM:CAC	2.97	0.52
1:C:269:ALA:O	1:C:273:ILE:HG13	2.09	0.52
2:L:248:SER:OG	11:L:304:UQ8:H35B	2.10	0.52
9:I:103:BCL:HBA1	9:I:103:BCL:H2	1.91	0.52
5:AC:9:TYR:HB2	6:AD:14:ALA:O	2.10	0.52
3:M:163:ILE:O	3:M:167:MET:HG3	2.10	0.52
9:W:101:BCL:HAA2	9:W:101:BCL:HBD	1.91	0.52
1:o:118:SER:O	1:o:124:LYS:HD3	2.08	0.52
5:w:9:TYR:HA	6:z:18:HIS:CG	2.44	0.52
5:AI:36:HIS:CE1	9:AI:102:BCL:HMD3	2.44	0.52
1:C:105:GLU:N	1:C:105:GLU:OE2	2.43	0.52
2:L:34:PHE:O	2:L:38:VAL:HG23	2.10	0.52
6:X:10:THR:OG1	6:X:13:GLU:HG3	2.10	0.52
5:Y:35:ILE:HG12	15:Z:101:CRT:H392	1.91	0.52
5:7:9:TYR:HB2	6:8:14:ALA:O	2.09	0.52
5:9:36:HIS:CE1	9:0:102:BCL:HMD3	2.44	0.52
9:y:401:BCL:HAA1	9:y:401:BCL:HBD	1.92	0.52
15:n:101:CRT:H10	5:l:11:ILE:HD13	1.92	0.52
5:AE:34:LEU:O	5:AE:38:ILE:HG13	2.09	0.52
6:g:45:TRP:CD1	6:g:46:LEU:HG	2.45	0.52
6:k:32:VAL:HG21	9:k:102:BCL:H11	1.92	0.52
1:C:250:CYS:O	1:C:262:SER:HB3	2.10	0.52
2:L:235:ALA:N	11:L:304:UQ8:O4	2.42	0.52
3:M:175:VAL:HG13	3:M:185:TRP:CG	2.45	0.52
4:H:149:PRO:HG3	4:H:204:LYS:HD3	1.91	0.52
5:I:11:ILE:HD12	5:I:14:ILE:HD12	1.92	0.52
2:x:211:LYS:HA	12:x:306:PEF:C10	2.40	0.52
4:t:135:PRO:HB3	4:t:171:TRP:NE1	2.25	0.52
6:q:16:GLU:O	6:q:20:ILE:HG13	2.10	0.52
6:k:21:PHE:HA	15:k:101:CRT:H14	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:80:HIS:O	3:M:81:TRP:HB2	2.10	0.52
3:M:178:GLY:O	3:M:182:HIS:HB3	2.10	0.52
3:M:265:ILE:CD1	14:M:404:MQ8:H121	2.38	0.52
5:O:5:ASN:HB3	5:O:8:LEU:HD13	1.92	0.52
5:3:17:PRO:HG2	6:4:9:LEU:HD11	1.91	0.52
1:o:227:LYS:NZ	3:y:96:GLU:OE2	2.43	0.52
3:y:150:PHE:O	3:y:154:ILE:HG13	2.10	0.52
5:AA:7:ASN:OD1	5:AA:9:TYR:HE1	1.93	0.52
6:AD:44:PRO:O	5:AE:55:TYR:OH	2.25	0.52
1:C:236:MET:HB3	7:C:503:HEM:C4B	2.45	0.51
1:C:245:VAL:HG21	1:C:249:PHE:CD2	2.46	0.51
2:L:207:THR:HG21	3:M:238:ILE:HD13	1.91	0.51
9:L:303:BCL:H2	10:M:403:BPH:CMB	2.40	0.51
4:H:138:VAL:HG21	4:H:229:ASP:HB3	1.91	0.51
6:E:21:PHE:C	6:E:21:PHE:CD1	2.87	0.51
5:I:44:LEU:HD21	6:J:45:TRP:HB3	1.92	0.51
5:5:14:ILE:HG21	15:7:103:CRT:H1M1	1.92	0.51
1:o:98:THR:HA	7:o:501:HEM:HMC3	1.92	0.51
9:x:305:BCL:HMD2	9:y:401:BCL:HBB3	1.93	0.51
4:t:7:HIS:CE1	5:u:48:ASP:HB3	2.44	0.51
5:AG:10:LYS:HA	5:AG:13:LEU:HD13	1.92	0.51
5:d:17:PRO:HG2	6:e:9:LEU:HD21	1.92	0.51
3:M:256:MET:HE2	3:M:258:PHE:CE1	2.44	0.51
5:1:54:SER:OG	5:1:60:LYS:O	2.29	0.51
5:3:31:LEU:HD12	5:3:34:LEU:HD23	1.92	0.51
1:o:195:LEU:HB3	1:o:196:PRO:CD	2.39	0.51
3:y:59:LEU:HB3	3:y:128:LEU:HD13	1.91	0.51
5:AA:50:ASN:HB2	5:AC:59:GLY:HA3	1.91	0.51
6:AD:45:TRP:CD1	6:AD:46:LEU:HG	2.46	0.51
9:K:101:BCL:HBD	9:K:101:BCL:HAA2	1.92	0.51
5:W:43:ASP:OD2	5:Y:55:TYR:HB2	2.11	0.51
5:5:8:LEU:HD11	15:7:103:CRT:H133	1.92	0.51
1:o:221:SER:O	1:o:221:SER:OG	2.24	0.51
3:y:2:PRO:HB2	4:t:201:ARG:CZ	2.41	0.51
3:y:260:VAL:HG12	4:t:34:ASP:CG	2.36	0.51
4:t:107:MET:SD	4:t:249:TYR:HB2	2.51	0.51
5:p:11:ILE:HD12	5:p:14:ILE:HD12	1.90	0.51
5:AG:11:ILE:HG12	9:AI:101:BCL:H142	1.92	0.51
5:f:50:ASN:ND2	5:f:54:SER:HB2	2.25	0.51
9:h:101:BCL:HED2	6:i:32:VAL:HA	1.93	0.51
2:L:281:TRP:CB	3:M:88:LYS:HD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:153:ALA:HB2	10:M:403:BPH:HAC1	1.92	0.51
4:H:135:PRO:HA	4:H:171:TRP:HA	1.93	0.51
6:Z:46:LEU:HD22	6:2:42:TYR:CZ	2.45	0.51
3:y:34:PRO:CG	3:y:50:PRO:HD3	2.36	0.51
3:y:253:ARG:HH12	12:t:301:PEF:HN2	1.59	0.51
4:t:61:LEU:HD12	4:t:61:LEU:N	2.25	0.51
9:u:102:BCL:HAA2	9:u:102:BCL:CED	2.39	0.51
5:AK:10:LYS:HD3	15:e:101:CRT:H41	1.90	0.51
1:C:166:TRP:O	1:C:303:LEU:HA	2.10	0.51
2:L:208:ASN:N	2:L:208:ASN:HD22	2.08	0.51
6:J:32:VAL:HG13	6:J:36:HIS:CE1	2.45	0.51
5:U:25:VAL:HG11	9:U:101:BCL:H18	1.92	0.51
5:W:12:TRP:HZ3	5:W:20:VAL:HG21	1.76	0.51
15:s:101:CRT:H372	5:u:36:HIS:CG	2.46	0.51
9:AB:101:BCL:HAA1	9:AB:101:BCL:HBD	1.92	0.51
5:I:3:THR:OG1	5:I:5:ASN:N	2.44	0.51
6:4:46:LEU:HA	5:5:51:ILE:HD13	1.93	0.51
1:o:83:LYS:O	1:o:85:LEU:N	2.41	0.51
3:y:99:PRO:HD2	3:y:102:TYR:CD2	2.45	0.51
3:y:115:TRP:HZ3	3:y:116:LEU:HD12	1.76	0.51
3:y:134:TYR:CE2	3:y:144:GLN:HG3	2.46	0.51
9:p:102:BCL:H2	6:q:28:TRP:CZ2	2.46	0.51
3:M:149:ALA:O	3:M:152:ALA:N	2.39	0.51
4:H:57:GLY:HA3	12:H:301:PEF:O1P	2.11	0.51
9:O:102:BCL:HMD1	9:P:101:BCL:HBC2	1.93	0.51
6:P:21:PHE:C	6:P:21:PHE:CD1	2.88	0.51
5:U:40:LEU:HD13	5:U:46:TRP:CH2	2.44	0.51
9:3:101:BCL:HBA2	9:4:102:BCL:OBD	2.11	0.51
1:o:36:ARG:HD2	2:x:77:PRO:O	2.11	0.51
1:o:164:TYR:CB	1:o:309:THR:HA	2.41	0.51
1:o:258:ASP:OD1	1:o:260:THR:OG1	2.23	0.51
2:x:55:THR:OG1	2:x:68:TYR:OH	2.18	0.51
2:x:140:LEU:HD21	2:x:257:ILE:HG12	1.93	0.51
2:x:241:LEU:HD21	11:x:304:UQ8:H13	1.92	0.51
4:t:36:ARG:O	4:t:37:GLU:HG2	2.09	0.51
1:C:273:ILE:HB	1:C:274:ARG:HH11	1.76	0.51
2:L:75:ILE:N	2:L:75:ILE:HD12	2.25	0.51
4:H:14:ILE:HA	4:H:17:TRP:CD1	2.39	0.51
5:A:9:TYR:HD1	6:B:18:HIS:CE1	2.29	0.51
5:S:5:ASN:OD1	5:S:7:ASN:N	2.43	0.51
9:Z:102:BCL:H52	9:Z:102:BCL:HBA1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:302:PRO:O	1:o:304:ARG:HG2	2.10	0.51
3:y:42:LYS:HE3	12:y:408:PEF:O2P	2.10	0.51
15:AF:102:CRT:H342	9:AH:101:BCL:O1A	2.11	0.51
2:L:86:MET:HA	2:L:96:GLN:HE22	1.75	0.51
10:L:302:BPH:H141	9:M:401:BCL:HBB3	1.93	0.51
3:M:219:HIS:CE1	3:M:266:HIS:HE1	2.27	0.51
6:B:45:TRP:HD1	6:B:46:LEU:HG	1.75	0.51
5:F:10:LYS:HB3	15:I:102:CRT:H42	1.93	0.51
5:r:44:LEU:HD12	5:u:47:LEU:HD22	1.93	0.51
15:g:101:CRT:H292	9:h:101:BCL:H71	1.92	0.51
5:Q:28:GLN:CD	15:R:101:CRT:H25	2.36	0.51
5:9:20:VAL:O	5:9:24:ILE:HG13	2.11	0.51
1:o:181:THR:C	1:o:183:GLN:H	2.19	0.51
1:o:258:ASP:OD1	1:o:260:THR:N	2.44	0.51
5:m:17:PRO:HB3	6:n:17:PHE:CE2	2.46	0.51
6:AB:21:PHE:HA	15:AC:101:CRT:H14	1.92	0.51
5:AG:54:SER:HB3	5:AG:57:ALA:HB3	1.93	0.51
2:L:176:PHE:HB3	9:L:301:BCL:H3C	1.94	0.50
3:M:34:PRO:CG	3:M:50:PRO:HD3	2.41	0.50
3:M:152:ALA:O	3:M:155:PHE:HB3	2.11	0.50
3:M:267:ARG:HH11	12:H:305:PEF:C30	2.23	0.50
5:D:22:VAL:HG22	9:D:101:BCL:H191	1.93	0.50
15:P:102:CRT:H372	5:Q:36:HIS:CD2	2.46	0.50
6:R:33:VAL:O	6:R:37:LEU:HG	2.11	0.50
5:1:54:SER:HB2	5:1:57:ALA:CB	2.41	0.50
5:5:46:TRP:CZ3	9:5:101:BCL:HAC2	2.47	0.50
6:E:21:PHE:C	6:E:21:PHE:HD1	2.20	0.50
6:P:21:PHE:C	6:P:21:PHE:HD1	2.19	0.50
3:y:54:GLY:HA3	16:y:405:PO4:O1	2.10	0.50
9:p:102:BCL:HAC1	9:q:102:BCL:HBC2	1.92	0.50
5:r:4:MET:HG3	6:v:19:ALA:HB1	1.94	0.50
5:AC:13:LEU:HD21	6:AD:11:ASP:HA	1.94	0.50
6:AJ:14:ALA:HB1	6:AJ:17:PHE:HB3	1.93	0.50
5:AK:40:LEU:HD21	5:AK:47:LEU:HD12	1.92	0.50
1:C:124:LYS:HG3	7:C:501:HEM:HMD3	1.93	0.50
6:B:31:LEU:HD23	6:B:34:ILE:HD12	1.94	0.50
6:2:40:TRP:HE3	6:2:45:TRP:CZ3	2.29	0.50
5:7:27:PHE:CZ	5:7:31:LEU:HD22	2.46	0.50
1:o:128:ARG:HH21	7:o:501:HEM:HAD2	1.76	0.50
3:y:114:TRP:HA	3:y:114:TRP:CE3	2.46	0.50
5:AE:36:HIS:O	5:AE:40:LEU:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:PRO:HB2	2:L:152:GLY:HA2	1.94	0.50
4:H:88:ASN:ND2	4:H:109:SER:O	2.41	0.50
5:Y:43:ASP:C	5:Y:45:ASN:H	2.19	0.50
2:x:207:THR:HG21	3:y:238:ILE:HG21	1.92	0.50
6:AD:45:TRP:HD1	6:AD:46:LEU:HG	1.76	0.50
5:AE:14:ILE:HD11	15:AH:102:CRT:C5	2.41	0.50
1:C:128:ARG:HH21	7:C:501:HEM:CAD	2.25	0.50
2:L:228:ILE:HD13	3:M:133:THR:HG22	1.93	0.50
6:6:21:PHE:CE1	9:7:102:BCL:H172	2.46	0.50
1:o:43:TYR:CZ	2:x:148:MET:HE1	2.46	0.50
4:t:126:THR:HG23	4:t:130:LEU:O	2.12	0.50
5:u:11:ILE:HD13	15:z:101:CRT:H10	1.94	0.50
6:c:11:ASP:O	6:c:15:LYS:HG3	2.11	0.50
4:H:157:VAL:HG12	4:H:163:VAL:HA	1.93	0.50
6:T:45:TRP:CZ2	9:T:102:BCL:H151	2.46	0.50
9:3:101:BCL:HBD	9:3:101:BCL:HAA1	1.94	0.50
3:y:37:SER:HB2	12:y:406:PEF:C3	2.42	0.50
5:AE:34:LEU:HD21	15:AF:102:CRT:H2M2	1.93	0.50
3:M:57:GLY:O	3:M:61:ILE:HG13	2.12	0.50
5:I:2:PHE:HA	5:I:4:MET:SD	2.52	0.50
5:S:19:ARG:HH22	17:S:101:PGW:H04A	1.77	0.50
15:X:101:CRT:H181	15:X:101:CRT:C21	2.42	0.50
1:o:194:SER:O	1:o:195:LEU:O	2.30	0.50
3:y:80:HIS:O	3:y:81:TRP:HB2	2.11	0.50
3:y:222:THR:O	3:y:225:SER:OG	2.23	0.50
6:q:22:MET:HE3	6:q:26:TYR:CE2	2.47	0.50
5:d:40:LEU:HG	5:d:46:TRP:CH2	2.47	0.50
15:g:101:CRT:H30	9:g:102:BCL:HMA2	1.93	0.50
6:i:21:PHE:CE1	9:j:101:BCL:H172	2.47	0.50
9:l:101:BCL:H101	9:l:101:BCL:H203	1.92	0.50
9:A:102:BCL:HMB2	15:0:101:CRT:H371	1.94	0.50
5:F:11:ILE:HD12	5:F:14:ILE:HD11	1.92	0.50
5:I:11:ILE:HD13	15:O:101:CRT:H10	1.93	0.50
15:7:101:CRT:H342	9:7:102:BCL:O1A	2.12	0.50
6:0:45:TRP:CD1	6:0:46:LEU:HG	2.46	0.50
2:x:18:ILE:HD12	2:x:35:PHE:HZ	1.76	0.50
4:t:5:ILE:HD12	5:w:56:GLN:O	2.12	0.50
4:t:36:ARG:CZ	4:t:65:LYS:HD2	2.42	0.50
1:C:253:THR:HG21	2:L:171:TYR:HB2	1.92	0.50
5:Q:51:ILE:CD1	6:R:43:ARG:HH22	2.25	0.50
1:o:269:ALA:O	1:o:273:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:MET:SD	2:L:174:LEU:HB3	2.52	0.49
2:L:57:GLY:HA3	2:L:66:GLN:HA	1.94	0.49
3:M:2:PRO:HB2	4:H:201:ARG:CZ	2.41	0.49
5:I:9:TYR:OH	5:I:10:LYS:HE3	2.12	0.49
5:K:9:TYR:CE1	5:K:10:LYS:HG3	2.46	0.49
6:T:36:HIS:CD2	9:T:102:BCL:H71	2.47	0.49
6:8:45:TRP:CD1	6:8:46:LEU:HG	2.47	0.49
6:0:32:VAL:HG21	9:0:102:BCL:HBA2	1.94	0.49
1:o:174:TYR:OH	1:o:181:THR:OG1	2.07	0.49
2:x:61:PRO:O	5:m:41:SER:O	2.29	0.49
2:x:179:ASN:HB3	2:x:182:HIS:CB	2.42	0.49
3:y:26:GLY:HA3	5:AA:19:ARG:HD2	1.93	0.49
3:y:260:VAL:HG12	4:t:34:ASP:OD2	2.12	0.49
6:s:17:PHE:HB2	15:s:101:CRT:H31A	1.94	0.49
5:f:9:TYR:HB2	6:g:14:ALA:O	2.11	0.49
5:l:46:TRP:NE1	9:l:101:BCL:OBB	2.44	0.49
1:C:272:ALA:HB1	7:C:504:HEM:C4B	2.48	0.49
3:M:89:HIS:O	3:M:93:LEU:HG	2.13	0.49
4:H:41:LEU:HD11	12:H:301:PEF:H42	1.93	0.49
5:I:9:TYR:HB2	6:J:14:ALA:O	2.11	0.49
5:O:35:ILE:HG12	15:P:102:CRT:H403	1.94	0.49
5:5:32:GLY:HA2	9:6:101:BCL:O1D	2.13	0.49
3:y:265:ILE:HG23	3:y:266:HIS:ND1	2.27	0.49
4:t:135:PRO:HA	4:t:171:TRP:HA	1.93	0.49
4:t:196:PRO:HD3	4:t:243:TYR:CE2	2.47	0.49
5:m:11:ILE:HD13	15:q:101:CRT:H10	1.93	0.49
5:u:26:ALA:HA	5:u:29:ILE:HG22	1.94	0.49
5:h:3:THR:OG1	6:k:19:ALA:O	2.25	0.49
6:E:7:THR:OG1	6:E:8:GLY:N	2.44	0.49
9:1:101:BCL:H2	6:2:28:TRP:CH2	2.47	0.49
3:y:224:LEU:HA	3:y:227:SER:HB3	1.93	0.49
9:m:103:BCL:HBA1	6:n:32:VAL:HG11	1.94	0.49
6:s:16:GLU:HB3	15:s:101:CRT:H22A	1.93	0.49
5:AC:36:HIS:CE1	9:AC:103:BCL:HMD3	2.47	0.49
1:C:98:THR:HA	7:C:501:HEM:HMC3	1.94	0.49
1:C:100:TRP:HE3	1:C:152:CYS:HG	1.60	0.49
1:C:254:ARG:HH12	3:M:305:PRO:HG2	1.77	0.49
2:L:106:PHE:CE1	9:L:301:BCL:H121	2.48	0.49
2:L:140:LEU:HD11	9:L:301:BCL:HED2	1.94	0.49
5:S:16:ASP:OD1	5:S:18:ARG:N	2.44	0.49
6:X:12:ASP:HA	6:X:15:LYS:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:133:ALA:HB1	9:x:301:BCL:H62	1.94	0.49
2:x:250:ALA:HB2	10:x:302:BPH:HAC2	1.93	0.49
3:y:39:TRP:O	3:y:40:LEU:C	2.53	0.49
3:y:196:LEU:HD12	3:y:294:TRP:CD1	2.47	0.49
5:r:28:GLN:HG3	9:r:101:BCL:H52	1.94	0.49
6:AF:18:HIS:O	6:AF:22:MET:HG2	2.12	0.49
1:C:183:GLN:HA	1:C:196:PRO:HA	1.95	0.49
5:F:31:LEU:HD12	5:F:34:LEU:HD23	1.95	0.49
5:F:40:LEU:HG	5:F:46:TRP:CH2	2.48	0.49
5:Q:10:LYS:HD3	15:T:101:CRT:H21A	1.94	0.49
9:2:102:BCL:H12	9:2:102:BCL:H3A	1.95	0.49
4:t:94:PRO:CG	6:c:8:GLY:HA3	2.42	0.49
9:m:102:BCL:H101	5:l:2:PHE:HA	1.94	0.49
5:AE:15:LEU:C	6:AF:7:THR:HG21	2.37	0.49
5:AE:25:VAL:HG21	9:AF:101:BCL:C15	2.43	0.49
5:AK:40:LEU:HG	5:AK:46:TRP:CH2	2.47	0.49
15:AL:101:CRT:H35	9:d:101:BCL:HMB2	1.93	0.49
6:B:44:PRO:HG2	5:D:52:PRO:CD	2.40	0.49
5:D:40:LEU:HG	5:D:46:TRP:CH2	2.47	0.49
9:D:102:BCL:HAA2	9:D:102:BCL:CED	2.43	0.49
6:P:29:PHE:O	6:P:32:VAL:HB	2.12	0.49
6:X:10:THR:HG1	6:X:13:GLU:HG3	1.77	0.49
5:1:27:PHE:CD2	9:3:101:BCL:H191	2.47	0.49
1:o:107:CYS:CB	7:o:501:HEM:HAB	2.43	0.49
2:x:89:LEU:HA	2:x:93:GLY:HA3	1.93	0.49
9:m:102:BCL:HAA1	9:m:103:BCL:OBD	2.12	0.49
15:m:104:CRT:H14	6:c:21:PHE:HA	1.94	0.49
9:r:101:BCL:HAA1	9:r:101:BCL:HBD	1.95	0.49
15:AH:102:CRT:H342	9:AI:101:BCL:O1A	2.11	0.49
5:d:36:HIS:CE1	9:e:102:BCL:HMD3	2.47	0.49
5:j:43:ASP:HA	5:l:56:GLN:HE21	1.77	0.49
3:M:74:ASN:HD21	3:M:114:TRP:CD1	2.31	0.49
15:M:405:CRT:H2M3	5:O:38:ILE:HG12	1.95	0.49
4:H:211:VAL:HG21	4:H:219:PHE:HZ	1.77	0.49
2:x:50:ILE:HD11	2:x:98:ILE:HG21	1.95	0.49
3:y:115:TRP:CZ3	3:y:116:LEU:HD12	2.46	0.49
4:t:4:GLY:O	4:t:6:THR:N	2.46	0.49
1:C:110:CYS:O	1:C:124:LYS:HB2	2.12	0.49
2:L:28:GLY:HA2	12:A:101:PEF:O2P	2.12	0.49
9:Q:101:BCL:H51	9:Q:101:BCL:H102	1.94	0.49
6:T:40:TRP:CD2	9:T:102:BCL:H162	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:84:LEU:HB2	5:h:41:SER:HB2	1.94	0.49
4:t:58:PHE:CD1	4:t:59:PRO:HA	2.48	0.49
5:m:16:ASP:OD2	5:m:19:ARG:HG3	2.13	0.49
5:r:5:ASN:C	5:r:7:ASN:H	2.19	0.49
5:AA:7:ASN:HB3	5:AA:10:LYS:HD2	1.93	0.49
1:C:17:SER:HA	1:C:18:VAL:HB	1.94	0.49
1:C:110:CYS:SG	7:C:501:HEM:CAC	3.01	0.49
1:C:130:MET:HE1	1:C:284:ILE:CD1	2.43	0.49
9:L:303:BCL:H142	9:L:303:BCL:CMA	2.43	0.49
3:M:155:PHE:O	3:M:159:VAL:HG23	2.12	0.49
4:H:247:LYS:HA	4:H:254:ARG:NH1	2.27	0.49
5:A:51:ILE:HD13	6:B:42:TYR:OH	2.13	0.49
5:S:43:ASP:OD2	5:U:50:ASN:HA	2.13	0.49
5:Y:16:ASP:OD2	5:Y:19:ARG:HB2	2.13	0.49
5:7:43:ASP:C	5:7:45:ASN:H	2.21	0.49
2:x:170:GLY:HA2	2:x:176:PHE:HD2	1.78	0.49
5:AE:38:ILE:O	5:AE:42:THR:HG23	2.12	0.49
6:g:10:THR:OG1	6:g:13:GLU:HG3	2.13	0.49
1:C:194:SER:OG	3:M:184:ASP:OD2	2.23	0.49
3:M:114:TRP:HA	3:M:114:TRP:CE3	2.48	0.49
9:F:101:BCL:H52	6:G:28:TRP:CE2	2.48	0.49
5:S:43:ASP:OD1	5:U:55:TYR:HB2	2.13	0.49
6:V:29:PHE:CE1	9:V:102:BCL:H2	2.48	0.49
5:W:38:ILE:CD1	15:X:101:CRT:H401	2.43	0.49
15:4:101:CRT:H371	9:5:101:BCL:HMB2	1.95	0.49
1:o:252:ASN:OD1	1:o:254:ARG:HG2	2.12	0.49
2:x:199:HIS:HE1	2:x:239:HIS:CE1	2.30	0.49
5:p:27:PHE:CE1	5:r:29:ILE:HD13	2.48	0.49
5:l:17:PRO:HB3	6:c:17:PHE:CZ	2.48	0.49
5:l:29:ILE:HG12	9:l:101:BCL:H11	1.95	0.49
5:Y:43:ASP:CG	5:1:50:ASN:HA	2.38	0.48
5:7:20:VAL:O	5:7:24:ILE:HG13	2.13	0.48
1:o:212:ILE:N	7:o:503:HEM:O1A	2.33	0.48
4:t:135:PRO:HB2	4:t:169:ASP:OD2	2.13	0.48
5:AC:48:ASP:O	5:AC:50:ASN:N	2.45	0.48
5:AE:51:ILE:O	5:AE:55:TYR:HE2	1.96	0.48
6:AF:21:PHE:CZ	15:AF:102:CRT:H19	2.48	0.48
9:d:101:BCL:H2	6:e:28:TRP:CZ3	2.48	0.48
1:C:166:TRP:CD1	1:C:306:SER:HB3	2.49	0.48
1:C:250:CYS:HA	1:C:263:THR:OG1	2.13	0.48
3:M:121:PHE:HZ	5:Q:34:LEU:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:36:ARG:NE	4:H:65:LYS:HD2	2.27	0.48
5:A:9:TYR:HB3	6:B:18:HIS:ND1	2.28	0.48
5:F:4:MET:HE2	6:J:19:ALA:HB1	1.94	0.48
5:7:40:LEU:HG	5:7:46:TRP:CH2	2.48	0.48
1:o:152:CYS:HA	7:o:502:HEM:HAB	1.95	0.48
3:y:146:LEU:O	3:y:149:ALA:N	2.45	0.48
9:r:101:BCL:HBC2	9:s:102:BCL:HHD	1.94	0.48
6:s:45:TRP:CD1	6:s:46:LEU:HG	2.48	0.48
5:u:36:HIS:CE1	9:u:102:BCL:HMD3	2.48	0.48
9:AI:101:BCL:H2A	9:AI:101:BCL:CED	2.42	0.48
6:e:20:ILE:HD12	15:e:101:CRT:H6	1.94	0.48
1:C:242:SER:HA	1:C:308:MET:CE	2.43	0.48
2:L:3:MET:HB3	2:L:7:GLU:CD	2.38	0.48
4:H:35:LYS:NZ	4:H:56:VAL:O	2.34	0.48
6:B:21:PHE:CD1	6:B:21:PHE:C	2.91	0.48
5:D:34:LEU:O	5:D:38:ILE:HG13	2.12	0.48
5:I:29:ILE:HD13	9:I:101:BCL:H61	1.94	0.48
5:O:16:ASP:OD2	5:O:19:ARG:HG3	2.13	0.48
9:8:101:BCL:H8	9:8:101:BCL:C2	2.39	0.48
2:x:42:PHE:O	2:x:101:CYS:HB3	2.14	0.48
9:x:303:BCL:H161	9:x:303:BCL:H141	1.56	0.48
5:p:9:TYR:CZ	5:p:10:LYS:HE2	2.48	0.48
5:1:38:ILE:O	5:1:42:THR:HG23	2.13	0.48
1:o:97:VAL:HG21	1:o:131:PHE:HZ	1.77	0.48
2:x:188:PHE:CE2	2:x:248:SER:HB3	2.45	0.48
4:t:37:GLU:O	4:t:39:TYR:N	2.47	0.48
5:AA:14:ILE:HD11	15:AD:101:CRT:H31A	1.95	0.48
5:AE:22:VAL:HG22	9:AF:101:BCL:H172	1.95	0.48
5:AG:5:ASN:C	5:AG:7:ASN:H	2.21	0.48
1:C:191:ALA:O	1:C:192:TYR:HB2	2.13	0.48
5:D:12:TRP:HZ3	5:D:20:VAL:HG11	1.78	0.48
6:N:17:PHE:HD1	15:O:101:CRT:H6	1.79	0.48
1:o:155:CYS:SG	7:o:502:HEM:CAC	3.01	0.48
5:AE:32:GLY:HA2	9:AE:102:BCL:O1D	2.13	0.48
2:L:225:PHE:CE2	11:L:304:UQ8:H1M	2.49	0.48
5:F:44:LEU:HD23	5:I:55:TYR:CE2	2.48	0.48
5:7:7:ASN:HA	5:7:9:TYR:CE1	2.47	0.48
15:7:103:CRT:C33	9:9:102:BCL:HBA2	2.43	0.48
3:y:7:ILE:HB	12:y:407:PEF:O2P	2.14	0.48
3:y:63:PHE:CZ	5:AC:33:LEU:HD12	2.44	0.48
6:s:45:TRP:HZ2	9:s:102:BCL:H121	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:21:LEU:O	5:AE:25:VAL:HG23	2.14	0.48
5:f:35:ILE:HG12	15:g:101:CRT:H403	1.95	0.48
5:l:7:ASN:HB3	5:l:10:LYS:HD2	1.95	0.48
1:C:164:TYR:CD2	1:C:312:GLN:HG2	2.47	0.48
2:L:222:ASN:HB3	2:L:226:ARG:NH1	2.29	0.48
4:H:102:PRO:HB3	4:H:111:PHE:HD2	1.78	0.48
5:I:2:PHE:HB3	6:J:26:TYR:CE2	2.48	0.48
6:8:40:TRP:HE3	6:8:45:TRP:CZ3	2.32	0.48
2:x:148:MET:HG2	2:x:262:PRO:HG3	1.95	0.48
3:y:63:PHE:CD1	5:AC:30:VAL:HG22	2.48	0.48
9:p:102:BCL:HAA1	9:q:102:BCL:OBD	2.14	0.48
15:AH:102:CRT:H393	5:AI:36:HIS:HB3	1.95	0.48
5:AK:14:ILE:HG22	5:d:18:ARG:HG3	1.94	0.48
1:C:263:THR:C	3:M:313:ALA:HB2	2.38	0.48
3:M:145:HIS:HA	3:M:148:TRP:HE3	1.79	0.48
4:H:60:ASP:CG	4:H:61:LEU:H	2.19	0.48
4:H:122:HIS:CB	4:t:121:LYS:HZ2	2.21	0.48
6:J:7:THR:OG1	6:J:9:LEU:HD13	2.14	0.48
5:O:4:MET:N	6:R:23:GLN:OE1	2.47	0.48
5:7:35:ILE:CG1	15:7:103:CRT:H403	2.44	0.48
9:8:101:BCL:HED2	9:8:101:BCL:H2A	1.94	0.48
1:o:66:ASP:HB3	1:o:67:SER:H	1.55	0.48
1:o:152:CYS:CA	7:o:502:HEM:HAB	2.44	0.48
3:y:71:ILE:HA	3:y:95:LEU:HD22	1.95	0.48
15:m:104:CRT:H403	5:l:35:ILE:CG1	2.42	0.48
1:C:268:THR:HG21	7:C:504:HEM:C2A	2.49	0.48
3:M:81:TRP:CD1	5:U:40:LEU:HG	2.49	0.48
9:A:102:BCL:H8	9:A:102:BCL:H193	1.95	0.48
6:P:25:MET:HG2	6:P:29:PHE:CE2	2.48	0.48
5:W:45:ASN:HB3	5:Y:56:GLN:HE22	1.79	0.48
6:n:24:SER:OG	5:l:3:THR:HA	2.14	0.48
9:AC:102:BCL:H43	6:AD:28:TRP:CZ2	2.49	0.48
3:M:203:MET:HB3	9:M:401:BCL:O1D	2.14	0.48
5:K:12:TRP:CD1	6:N:18:HIS:HB2	2.49	0.48
5:Q:18:ARG:O	5:Q:22:VAL:HG23	2.14	0.48
5:S:4:MET:HE1	5:S:8:LEU:HD23	1.96	0.48
9:U:101:BCL:HBA1	6:V:28:TRP:HH2	1.79	0.48
5:Y:9:TYR:CD1	5:Y:10:LYS:N	2.82	0.48
1:o:21:LEU:HD11	2:x:274:TRP:CD2	2.49	0.48
1:o:315:ASN:O	7:o:504:HEM:HBA1	2.14	0.48
2:x:75:ILE:HD12	2:x:75:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:163:VAL:O	4:t:216:ALA:HB1	2.14	0.48
9:z:102:BCL:H111	9:z:102:BCL:H143	1.57	0.48
9:AC:103:BCL:HED2	9:AC:103:BCL:HAA2	1.96	0.48
5:AG:49:ASP:HB3	5:AG:51:ILE:HD11	1.94	0.48
5:d:39:VAL:HG11	9:d:101:BCL:HBC1	1.96	0.48
15:g:101:CRT:H35	15:g:101:CRT:H31	1.50	0.48
15:i:101:CRT:H372	5:j:36:HIS:CD2	2.49	0.48
1:C:23:CYS:SG	2:L:263:PHE:HB3	2.53	0.47
3:M:39:TRP:O	3:M:40:LEU:C	2.57	0.47
5:S:50:ASN:HB2	5:U:59:GLY:C	2.39	0.47
9:S:102:BCL:H92	9:S:102:BCL:H61	1.75	0.47
6:X:14:ALA:CB	6:X:17:PHE:HB3	2.44	0.47
1:o:139:SER:HA	1:o:142:LYS:HE3	1.95	0.47
4:t:108:LEU:HD23	4:t:108:LEU:HA	1.61	0.47
4:t:189:ASN:OD1	4:t:191:LYS:HB2	2.13	0.47
12:m:101:PEF:C5	5:l:19:ARG:HH22	2.19	0.47
5:r:16:ASP:OD2	5:r:19:ARG:HG3	2.14	0.47
2:L:253:SER:OG	9:L:301:BCL:HBA1	2.15	0.47
3:M:18:TYR:CZ	3:M:20:GLY:HA2	2.49	0.47
1:o:203:PHE:CG	1:o:235:LEU:HD22	2.49	0.47
5:r:45:ASN:C	5:r:49:ASP:OD2	2.56	0.47
5:w:26:ALA:HA	5:w:29:ILE:HG22	1.95	0.47
5:AI:50:ASN:HB3	5:AI:54:SER:HA	1.96	0.47
1:C:33:ILE:HG21	1:C:248:THR:O	2.15	0.47
3:M:275:LEU:HA	3:M:275:LEU:HD23	1.45	0.47
4:H:223:PRO:HG2	4:H:238:LYS:O	2.13	0.47
5:A:36:HIS:CD2	15:0:101:CRT:H372	2.49	0.47
9:D:102:BCL:HAA2	9:D:102:BCL:HED3	1.97	0.47
9:G:102:BCL:H62	9:G:102:BCL:H41	1.47	0.47
5:Q:20:VAL:HG13	9:S:102:BCL:H141	1.95	0.47
5:S:40:LEU:HD13	5:S:46:TRP:CH2	2.50	0.47
6:X:24:SER:CB	15:X:101:CRT:H14	2.43	0.47
9:X:102:BCL:HBB2	9:X:102:BCL:H151	1.95	0.47
9:Y:101:BCL:HBC2	9:Z:102:BCL:HMD1	1.96	0.47
1:o:71:LYS:HB2	1:o:74:GLU:HG2	1.96	0.47
9:y:401:BCL:H2	10:y:402:BPH:CHC	2.38	0.47
4:t:150:ASP:OD1	4:t:152:ARG:HB2	2.14	0.47
6:z:20:ILE:HD12	15:z:101:CRT:C6	2.44	0.47
6:AB:20:ILE:HD12	15:AC:101:CRT:C5	2.43	0.47
5:j:50:ASN:HB3	5:j:54:SER:HB2	1.96	0.47
1:C:205:ASP:CG	1:C:304:ARG:HE	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:135:LYS:HD3	5:O:19:ARG:HH11	1.78	0.47
3:M:240:HIS:HE1	4:H:69:LEU:HD11	1.76	0.47
4:H:196:PRO:HD3	4:H:243:TYR:CE2	2.49	0.47
9:A:103:BCL:HMB2	9:A:103:BCL:H122	1.96	0.47
5:F:13:LEU:HD13	15:I:102:CRT:H1M1	1.96	0.47
5:F:57:ALA:C	5:F:59:GLY:H	2.22	0.47
5:W:5:ASN:OD1	5:W:6:ALA:N	2.48	0.47
6:4:29:PHE:O	6:4:33:VAL:HG23	2.14	0.47
5:7:17:PRO:HB3	6:8:17:PHE:CE2	2.49	0.47
2:x:261:GLY:O	2:x:263:PHE:N	2.46	0.47
3:y:249:ALA:HB1	3:y:259:ASN:ND2	2.30	0.47
3:y:300:LYS:HE2	4:t:10:ASP:OD2	2.15	0.47
15:n:101:CRT:H393	5:p:36:HIS:HB3	1.96	0.47
5:p:44:LEU:HD12	5:r:47:LEU:HD22	1.96	0.47
6:z:36:HIS:CD2	9:z:102:BCL:H8	2.49	0.47
3:M:6:ASN:HD22	3:M:227:SER:HB2	1.80	0.47
3:M:129:TRP:O	3:M:133:THR:HG23	2.14	0.47
5:I:17:PRO:HB3	6:J:17:PHE:CZ	2.50	0.47
5:I:26:ALA:HA	5:I:29:ILE:HG22	1.97	0.47
5:Q:42:THR:HG21	5:S:47:LEU:HD13	1.96	0.47
5:Q:45:ASN:O	5:Q:49:ASP:OD2	2.31	0.47
1:o:27:PRO:HD3	5:f:41:SER:HB2	1.97	0.47
1:o:66:ASP:O	1:o:67:SER:OG	2.25	0.47
2:x:181:ALA:HB3	2:x:256:CYS:HA	1.97	0.47
2:x:240:ARG:HA	3:y:224:LEU:HD11	1.97	0.47
5:m:9:TYR:HB3	6:n:14:ALA:O	2.14	0.47
5:m:14:ILE:HG23	5:p:18:ARG:CG	2.39	0.47
9:AB:101:BCL:HAA1	9:AB:101:BCL:CBD	2.44	0.47
5:h:9:TYR:HB2	6:i:14:ALA:O	2.13	0.47
5:h:42:THR:O	5:h:45:ASN:HB2	2.14	0.47
5:j:44:LEU:HD12	5:l:47:LEU:HD22	1.95	0.47
2:L:132:PHE:CD2	2:L:247:LEU:HB3	2.49	0.47
3:M:161:GLY:CA	15:M:405:CRT:H292	2.45	0.47
4:H:37:GLU:O	4:H:39:TYR:N	2.47	0.47
6:G:46:LEU:HD22	6:J:42:TYR:CZ	2.49	0.47
6:P:18:HIS:O	6:P:22:MET:HG2	2.14	0.47
15:Z:101:CRT:C27	9:Z:102:BCL:H11	2.44	0.47
6:6:21:PHE:CZ	9:7:102:BCL:H172	2.50	0.47
15:7:103:CRT:H27	9:8:101:BCL:H42	1.95	0.47
5:9:39:VAL:HG11	9:9:102:BCL:HBC1	1.95	0.47
2:x:10:TYR:O	2:x:12:VAL:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AL:17:PHE:HA	15:AL:101:CRT:H6	1.95	0.47
9:c:101:BCL:H2	9:c:101:BCL:H3A	1.95	0.47
1:C:54:GLN:OE1	1:C:54:GLN:HA	2.14	0.47
1:C:274:ARG:N	1:C:274:ARG:HD2	2.29	0.47
3:M:65:LEU:HD21	10:M:403:BPH:C10	2.42	0.47
6:E:45:TRP:HD1	6:E:46:LEU:OXT	1.97	0.47
5:I:12:TRP:HZ3	5:I:20:VAL:HG21	1.80	0.47
6:P:16:GLU:O	6:P:20:ILE:HG13	2.15	0.47
6:V:40:TRP:CH2	6:V:46:LEU:HB2	2.50	0.47
5:3:42:THR:HG21	5:5:47:LEU:HD13	1.97	0.47
5:5:7:ASN:C	5:5:9:TYR:H	2.22	0.47
9:9:102:BCL:H2	6:0:28:TRP:CZ2	2.50	0.47
1:o:256:PHE:HZ	2:x:171:TYR:CE2	2.32	0.47
2:x:7:GLU:HB2	3:y:250:LEU:HD21	1.97	0.47
2:x:70:LEU:O	2:x:159:ILE:HD12	2.15	0.47
2:x:155:PHE:CZ	9:x:305:BCL:HMC2	2.50	0.47
2:x:281:TRP:CB	3:y:88:LYS:HD2	2.38	0.47
14:y:403:MQ8:H451	14:y:403:MQ8:H462	1.61	0.47
4:t:249:TYR:C	4:t:251:THR:H	2.23	0.47
5:m:17:PRO:HG2	6:n:9:LEU:HD21	1.96	0.47
9:r:101:BCL:HBC2	9:s:102:BCL:HMD1	1.96	0.47
5:w:14:ILE:HD11	15:AC:101:CRT:H21A	1.95	0.47
5:w:26:ALA:O	5:w:29:ILE:HG22	2.15	0.47
9:w:101:BCL:HAA1	9:w:101:BCL:CBD	2.43	0.47
15:AD:101:CRT:H372	5:AE:36:HIS:CD2	2.50	0.47
9:AF:101:BCL:H112	9:AF:101:BCL:H72	1.49	0.47
5:AG:42:THR:HG21	5:AI:47:LEU:HD13	1.97	0.47
9:AG:101:BCL:HBA1	6:AH:32:VAL:HG11	1.97	0.47
5:d:27:PHE:CZ	5:d:31:LEU:HD22	2.49	0.47
5:h:17:PRO:HB3	6:i:17:PHE:CZ	2.49	0.47
6:i:17:PHE:HA	15:i:101:CRT:H6	1.96	0.47
15:k:101:CRT:H243	9:l:101:BCL:H172	1.96	0.47
1:C:43:TYR:CZ	2:L:148:MET:HE1	2.50	0.47
2:L:199:HIS:HA	11:L:304:UQ8:O2	2.14	0.47
3:M:260:VAL:HG22	14:M:404:MQ8:C4	2.45	0.47
4:H:116:SER:OG	4:H:237:ASP:HB3	2.15	0.47
12:H:302:PEF:C10	5:D:18:ARG:HB3	2.45	0.47
5:U:24:ILE:HD11	9:W:101:BCL:H202	1.97	0.47
9:V:102:BCL:HBC3	9:V:102:BCL:H2C	1.60	0.47
5:W:40:LEU:HD21	5:W:47:LEU:HD12	1.96	0.47
6:X:31:LEU:HD23	6:X:31:LEU:HA	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:101:BCL:H2	6:Z:28:TRP:CZ2	2.50	0.47
1:o:164:TYR:HD2	1:o:312:GLN:HG2	1.74	0.47
3:y:31:ILE:HD11	3:y:53:LEU:HB2	1.96	0.47
3:y:59:LEU:HB3	3:y:128:LEU:CD1	2.44	0.47
3:y:80:HIS:O	3:y:80:HIS:CG	2.67	0.47
3:y:121:PHE:N	3:y:121:PHE:HD1	2.13	0.47
3:y:253:ARG:NH1	12:t:301:PEF:HN2	2.13	0.47
10:y:402:BPH:HBA2	10:y:402:BPH:H3A	1.70	0.47
5:p:43:ASP:OD1	5:r:56:GLN:HG2	2.15	0.47
5:u:2:PHE:HB3	5:u:4:MET:SD	2.55	0.47
5:AE:12:TRP:CZ3	5:AE:20:VAL:HG11	2.49	0.47
5:AE:16:ASP:OD2	5:AE:19:ARG:HG3	2.14	0.47
15:AJ:101:CRT:H10	15:AJ:101:CRT:H81	1.59	0.47
1:C:314:VAL:HG12	1:C:316:LYS:H	1.80	0.47
2:L:51:VAL:CG1	5:A:37:MET:HG3	2.45	0.47
3:M:104:LEU:HD11	3:M:166:VAL:HA	1.97	0.47
15:E:101:CRT:H372	5:F:36:HIS:CD2	2.49	0.47
15:V:101:CRT:H393	5:W:36:HIS:CD2	2.50	0.47
9:X:102:BCL:H161	9:X:102:BCL:H122	1.69	0.47
5:Y:43:ASP:OD2	5:1:50:ASN:HA	2.14	0.47
5:9:46:TRP:CD2	9:9:102:BCL:H2C	2.50	0.47
6:0:21:PHE:CD1	15:0:101:CRT:H14	2.50	0.47
2:x:191:THR:HG23	9:x:303:BCL:H42	1.96	0.47
4:t:102:PRO:HB3	4:t:111:PHE:HD2	1.80	0.47
6:AF:28:TRP:CE2	9:AF:101:BCL:H43	2.50	0.47
6:i:21:PHE:CZ	9:j:101:BCL:H172	2.50	0.47
2:L:45:LEU:HB2	5:9:30:VAL:HG13	1.96	0.47
5:A:21:LEU:HD23	5:A:21:LEU:HA	1.76	0.47
5:F:4:MET:O	5:F:6:ALA:N	2.45	0.47
6:G:21:PHE:CZ	15:G:101:CRT:H19	2.50	0.47
5:I:39:VAL:HG11	9:I:101:BCL:HAC2	1.97	0.47
9:R:102:BCL:H18	9:R:102:BCL:H152	1.52	0.47
5:1:33:LEU:O	5:1:37:MET:HG3	2.15	0.47
2:x:252:TRP:O	2:x:256:CYS:HB3	2.15	0.47
6:z:32:VAL:HG13	6:z:36:HIS:CE1	2.49	0.47
5:AA:11:ILE:HD12	5:AA:14:ILE:HD12	1.96	0.47
5:AI:40:LEU:HG	5:AI:46:TRP:CZ3	2.49	0.47
1:C:77:GLN:HB2	1:C:117:ALA:CB	2.46	0.46
10:L:302:BPH:H141	9:M:401:BCL:CBB	2.46	0.46
3:M:109:LEU:CD1	5:Q:42:THR:HG22	2.43	0.46
4:H:136:MET:SD	4:H:152:ARG:NH2	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:235:GLU:O	4:H:239:VAL:HG23	2.15	0.46
9:W:101:BCL:H112	9:W:101:BCL:H91	1.55	0.46
2:x:199:HIS:HA	11:x:304:UQ8:O2	2.15	0.46
2:x:253:SER:CB	9:x:301:BCL:HBA1	2.46	0.46
3:y:156:PHE:HZ	9:y:401:BCL:HBD	1.80	0.46
5:u:26:ALA:O	5:u:29:ILE:HG22	2.15	0.46
9:u:101:BCL:HAC1	9:u:102:BCL:HAC2	1.96	0.46
2:L:184:LEU:HD23	2:L:252:TRP:CD2	2.50	0.46
2:L:225:PHE:HD1	2:L:225:PHE:HA	1.53	0.46
4:H:77:VAL:O	4:H:80:ARG:NE	2.46	0.46
6:G:31:LEU:O	6:G:34:ILE:HB	2.16	0.46
5:U:8:LEU:HD23	6:V:18:HIS:HE2	1.80	0.46
5:1:49:ASP:O	5:1:51:ILE:HG13	2.14	0.46
6:4:21:PHE:HA	15:4:101:CRT:H11	1.96	0.46
5:7:43:ASP:N	5:9:48:ASP:OD1	2.48	0.46
5:9:40:LEU:HD21	5:9:47:LEU:HD12	1.97	0.46
6:0:21:PHE:HA	15:0:101:CRT:H14	1.98	0.46
9:x:303:BCL:HBD	9:x:303:BCL:HAA1	1.97	0.46
4:t:141:GLU:HG2	4:t:142:PHE:HD1	1.79	0.46
5:f:34:LEU:O	5:f:38:ILE:HG13	2.14	0.46
6:g:10:THR:HG23	6:g:13:GLU:CD	2.41	0.46
9:c:101:BCL:H3A	9:c:101:BCL:HBA1	1.45	0.46
3:M:241:ARG:NH2	3:M:246:GLU:OE1	2.47	0.46
4:H:141:GLU:HG2	4:H:142:PHE:N	2.30	0.46
5:A:13:LEU:HB2	15:E:101:CRT:C1M	2.45	0.46
5:I:12:TRP:HE1	6:J:18:HIS:HA	1.80	0.46
10:y:402:BPH:H6C2	10:y:402:BPH:H4C1	1.73	0.46
5:AA:8:LEU:HD11	15:AD:101:CRT:H133	1.96	0.46
9:AB:102:BCL:HMA1	9:AC:102:BCL:HMA1	1.98	0.46
5:d:12:TRP:HE1	6:e:18:HIS:CA	2.29	0.46
1:C:142:LYS:C	1:C:144:HIS:N	2.73	0.46
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.96	0.46
9:M:401:BCL:CHD	9:M:401:BCL:HBC2	2.45	0.46
4:H:106:PRO:HB3	4:H:249:TYR:CD1	2.51	0.46
4:H:137:ARG:NH1	4:H:229:ASP:OD1	2.40	0.46
5:A:24:ILE:HG13	9:D:101:BCL:H143	1.97	0.46
15:I:102:CRT:H371	9:K:101:BCL:HMB2	1.98	0.46
6:V:25:MET:HG3	15:V:101:CRT:C21	2.45	0.46
5:7:10:LYS:NZ	6:8:11:ASP:OD1	2.35	0.46
3:y:74:ASN:HD21	3:y:114:TRP:CG	2.33	0.46
3:y:102:TYR:CZ	3:y:108:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:121:PHE:N	3:y:121:PHE:CD1	2.82	0.46
3:y:267:ARG:HH12	12:t:303:PEF:H31	1.79	0.46
9:u:101:BCL:HAA1	9:u:102:BCL:OBD	2.15	0.46
5:AE:3:THR:OG1	5:AE:4:MET:N	2.47	0.46
9:AI:102:BCL:HBD	9:AI:102:BCL:HAA1	1.98	0.46
9:j:101:BCL:H51	9:j:101:BCL:H8	1.68	0.46
2:L:133:ALA:HB1	9:L:301:BCL:H62	1.97	0.46
2:L:236:LEU:HD21	3:M:6:ASN:OD1	2.15	0.46
9:L:303:BCL:HED3	3:M:183:LEU:HD21	1.97	0.46
3:M:219:HIS:CE1	3:M:266:HIS:CE1	3.04	0.46
3:M:304:ALA:HA	3:M:305:PRO:HD2	1.67	0.46
6:G:43:ARG:HG3	5:I:55:TYR:CE1	2.51	0.46
9:V:102:BCL:H192	9:V:102:BCL:H161	1.72	0.46
5:9:10:LYS:HA	5:9:13:LEU:HD22	1.97	0.46
1:o:35:TYR:O	1:o:38:VAL:HG23	2.16	0.46
3:y:33:ARG:HA	3:y:34:PRO:HD3	1.69	0.46
4:t:32:ARG:HG3	4:t:59:PRO:HG2	1.98	0.46
5:w:50:ASN:HB3	5:w:55:TYR:CD2	2.51	0.46
5:AC:36:HIS:CG	15:AC:101:CRT:H372	2.50	0.46
6:AH:44:PRO:O	5:AI:52:PRO:HD2	2.16	0.46
6:AJ:31:LEU:HD23	6:AJ:31:LEU:HA	1.82	0.46
9:e:102:BCL:H3A	9:e:102:BCL:HBA1	1.62	0.46
1:C:263:THR:C	1:C:265:LYS:H	2.23	0.46
3:M:159:VAL:HA	3:M:163:ILE:HB	1.98	0.46
4:H:52:ARG:HA	12:H:304:PEF:O3P	2.15	0.46
9:D:102:BCL:H92	6:E:33:VAL:HG22	1.97	0.46
6:X:14:ALA:HB1	6:X:17:PHE:HB3	1.98	0.46
2:x:177:HIS:CE1	9:y:401:BCL:CBC	2.98	0.46
2:x:219:GLU:HB3	3:y:18:TYR:OH	2.15	0.46
2:x:244:PHE:HE2	11:x:304:UQ8:H21	1.80	0.46
3:y:37:SER:HB2	12:y:406:PEF:H21	1.97	0.46
3:y:267:ARG:NH2	12:t:303:PEF:O1P	2.31	0.46
4:t:94:PRO:HB2	6:c:8:GLY:HA3	1.96	0.46
5:p:19:ARG:HH12	12:p:101:PEF:HN2	1.64	0.46
6:AL:32:VAL:CG2	9:AL:102:BCL:HBA2	2.44	0.46
9:e:102:BCL:HBD	9:e:102:BCL:HAA1	1.98	0.46
1:C:174:TYR:CE2	1:C:180:PRO:HA	2.51	0.46
2:L:35:PHE:CE2	2:L:111:LEU:HB3	2.50	0.46
2:L:106:PHE:CD2	9:L:301:BCL:H91	2.51	0.46
2:L:192:ASN:HD21	3:M:212:SER:C	2.24	0.46
3:M:208:PHE:CZ	3:M:275:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:BCL:HAA2	9:I:103:BCL:HED3	1.96	0.46
5:S:5:ASN:HB3	5:S:8:LEU:N	2.30	0.46
9:S:102:BCL:H3A	9:S:102:BCL:HBA1	1.53	0.46
15:T:101:CRT:H22A	15:T:101:CRT:H5	1.66	0.46
5:U:43:ASP:OD2	5:W:55:TYR:HB2	2.14	0.46
6:X:20:ILE:HD12	15:X:101:CRT:C5	2.46	0.46
6:Z:43:ARG:HB3	5:1:55:TYR:OH	2.16	0.46
2:x:89:LEU:HA	2:x:89:LEU:HD23	1.74	0.46
2:x:204:LEU:HD21	3:y:267:ARG:HG3	1.97	0.46
3:y:219:HIS:ND1	14:y:403:MQ8:O1	2.46	0.46
4:t:136:MET:HE2	4:t:136:MET:HB3	1.69	0.46
9:q:102:BCL:HBD	9:q:102:BCL:HAA2	1.97	0.46
5:u:11:ILE:HG21	9:w:101:BCL:H152	1.98	0.46
9:AK:101:BCL:HED1	6:AL:31:LEU:HB3	1.98	0.46
15:k:101:CRT:H372	5:l:36:HIS:CD2	2.50	0.46
5:l:35:ILE:HD12	9:c:101:BCL:O1D	2.16	0.46
1:C:219:ALA:HB2	3:M:292:ASP:HB2	1.97	0.46
3:M:31:ILE:H	3:M:31:ILE:HG12	1.47	0.46
3:M:198:TYR:HB3	3:M:298:ALA:HB2	1.98	0.46
4:H:35:LYS:HG2	4:H:39:TYR:CZ	2.50	0.46
9:D:101:BCL:H11	15:9:101:CRT:H291	1.97	0.46
5:K:10:LYS:HG2	5:K:13:LEU:HD12	1.98	0.46
6:4:17:PHE:CE1	15:4:101:CRT:H9	2.50	0.46
15:4:101:CRT:H2M1	5:5:36:HIS:HB3	1.98	0.46
1:o:163:LYS:HD2	1:o:164:TYR:CE2	2.51	0.46
2:x:175:HIS:CD2	2:x:178:TYR:HE1	2.33	0.46
12:x:306:PEF:O4	12:x:306:PEF:H11	2.13	0.46
3:y:72:GLY:HA3	15:y:404:CRT:H33	1.98	0.46
4:t:135:PRO:HB3	4:t:171:TRP:CD1	2.50	0.46
5:u:9:TYR:HA	6:v:18:HIS:CG	2.51	0.46
9:AB:101:BCL:H162	9:AB:101:BCL:H101	1.98	0.46
6:AD:25:MET:HG3	15:AD:101:CRT:C21	2.46	0.46
5:AG:11:ILE:HG23	5:AG:12:TRP:CD2	2.51	0.46
15:g:101:CRT:H32	15:g:101:CRT:H291	1.97	0.46
1:C:173:LYS:HB2	3:M:80:HIS:CD2	2.51	0.46
2:L:18:ILE:HD12	2:L:35:PHE:CZ	2.51	0.46
3:M:63:PHE:CE1	5:Q:30:VAL:HG22	2.50	0.46
3:M:202:HIS:HB2	9:M:402:BCL:HED2	1.97	0.46
9:M:402:BCL:HBA2	9:M:402:BCL:H3A	1.65	0.46
5:D:39:VAL:HG21	9:D:102:BCL:H3C	1.98	0.46
9:D:102:BCL:HBA2	6:E:32:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:17:PRO:HB3	6:N:17:PHE:CE2	2.51	0.46
9:O:102:BCL:HHD	9:P:101:BCL:HBC2	1.98	0.46
9:Q:101:BCL:HBC3	9:Q:101:BCL:H2C	1.77	0.46
9:W:101:BCL:H112	9:W:101:BCL:H143	1.70	0.46
5:1:10:LYS:HB3	15:4:101:CRT:H22A	1.98	0.46
5:5:36:HIS:CE1	9:6:101:BCL:HMD3	2.51	0.46
6:8:21:PHE:C	6:8:21:PHE:CD1	2.94	0.46
1:o:311:HIS:NE2	7:o:504:HEM:NB	2.64	0.46
2:x:233:ILE:HG12	2:x:237:ALA:CB	2.46	0.46
14:y:403:MQ8:H242	14:y:403:MQ8:H192	1.98	0.46
4:t:104:GLY:O	4:t:106:PRO:HD3	2.15	0.46
4:t:226:SER:O	4:t:227:ASN:HB2	2.16	0.46
9:p:102:BCL:HAC1	9:q:102:BCL:CBC	2.46	0.46
6:q:46:LEU:HD22	5:r:52:PRO:HB3	1.98	0.46
5:AK:20:VAL:HA	9:d:101:BCL:H143	1.98	0.46
5:f:5:ASN:ND2	6:i:20:ILE:HG12	2.31	0.46
6:g:40:TRP:NE1	9:g:102:BCL:H201	2.30	0.46
2:L:78:PRO:HB2	2:L:82:TYR:CD2	2.51	0.46
4:H:151:PRO:HA	4:H:154:MET:SD	2.56	0.46
9:O:102:BCL:HBA1	9:O:102:BCL:C2	2.44	0.46
5:S:17:PRO:HB3	6:T:17:PHE:CE1	2.51	0.46
9:T:102:BCL:C2	9:T:102:BCL:H3A	2.46	0.46
5:U:40:LEU:HD11	5:U:47:LEU:HD12	1.98	0.46
5:W:38:ILE:HD12	15:X:101:CRT:H401	1.98	0.46
9:5:101:BCL:HAC1	9:6:101:BCL:CBC	2.46	0.46
6:8:29:PHE:O	6:8:33:VAL:HG23	2.16	0.46
1:o:97:VAL:HG22	1:o:152:CYS:SG	2.56	0.46
2:x:65:LEU:CD1	3:y:308:PRO:HG3	2.46	0.46
2:x:106:PHE:CD2	9:x:301:BCL:H91	2.51	0.46
3:y:256:MET:HE2	3:y:258:PHE:CE1	2.51	0.46
5:d:12:TRP:HE1	6:e:18:HIS:HA	1.80	0.46
2:L:177:HIS:HB3	3:M:183:LEU:HD22	1.98	0.45
3:M:33:ARG:HA	3:M:34:PRO:HD3	1.59	0.45
9:A:102:BCL:H112	9:A:102:BCL:H192	1.98	0.45
5:D:35:ILE:HG12	15:E:101:CRT:H403	1.98	0.45
6:P:17:PHE:CD1	15:P:102:CRT:H9	2.52	0.45
15:X:101:CRT:H372	5:Y:36:HIS:CD2	2.51	0.45
5:5:14:ILE:HD13	15:7:103:CRT:H1M1	1.97	0.45
9:5:101:BCL:H112	9:5:101:BCL:H72	1.39	0.45
1:o:44:TYR:HA	2:x:265:THR:HB	1.99	0.45
2:x:225:PHE:HD1	2:x:225:PHE:HA	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:127:LEU:O	3:y:130:TRP:HB3	2.16	0.45
5:m:14:ILE:CG2	5:p:18:ARG:HG2	2.35	0.45
6:AB:19:ALA:O	6:AB:23:GLN:HG2	2.16	0.45
9:AC:102:BCL:H101	6:AD:28:TRP:CE3	2.51	0.45
9:i:102:BCL:H41	9:i:102:BCL:H61	1.66	0.45
6:k:31:LEU:O	6:k:34:ILE:HB	2.16	0.45
1:C:28:PRO:HD3	2:L:262:PRO:HA	1.98	0.45
3:M:39:TRP:O	3:M:42:LYS:HB2	2.17	0.45
5:A:44:LEU:HD23	5:D:55:TYR:CE2	2.50	0.45
6:P:44:PRO:O	5:Q:52:PRO:HD2	2.17	0.45
6:V:29:PHE:O	6:V:32:VAL:HB	2.16	0.45
5:Y:36:HIS:HE1	9:Z:102:BCL:OBD	1.99	0.45
9:Y:101:BCL:HMC2	9:Y:101:BCL:HHC	1.69	0.45
2:x:274:TRP:CZ3	2:x:278:LEU:HD21	2.51	0.45
3:y:97:PRO:HD3	3:y:176:PRO:HB3	1.97	0.45
4:t:80:ARG:HH11	4:t:82:GLU:CD	2.24	0.45
5:m:40:LEU:HG	5:m:46:TRP:CH2	2.51	0.45
6:AJ:13:GLU:HA	6:AJ:14:ALA:HA	1.77	0.45
5:d:9:TYR:HB2	6:e:15:LYS:HA	1.97	0.45
5:f:10:LYS:HG2	5:f:13:LEU:HD12	1.98	0.45
5:h:12:TRP:HZ3	5:h:20:VAL:HG21	1.79	0.45
6:k:39:ALA:O	6:k:43:ARG:N	2.50	0.45
9:T:102:BCL:O2D	9:T:102:BCL:HAA2	2.17	0.45
9:2:102:BCL:HMA1	9:3:101:BCL:HMA1	1.99	0.45
6:4:16:GLU:O	6:4:20:ILE:HG13	2.16	0.45
3:y:190:SER:CB	9:y:401:BCL:HAC2	2.47	0.45
3:y:295:TYR:O	3:y:299:VAL:HG23	2.17	0.45
4:t:156:VAL:HG21	4:t:184:VAL:HG13	1.98	0.45
15:n:101:CRT:H371	9:p:102:BCL:HMB2	1.98	0.45
9:AC:103:BCL:H91	6:AD:36:HIS:CD2	2.52	0.45
5:AG:39:VAL:HG11	9:AH:101:BCL:HBC1	1.97	0.45
5:h:39:VAL:HG11	9:h:101:BCL:HBC1	1.98	0.45
3:M:232:ASP:C	3:M:234:GLU:H	2.25	0.45
9:M:402:BCL:H61	10:M:403:BPH:CHC	2.47	0.45
5:A:10:LYS:HD2	6:E:20:ILE:CD1	2.46	0.45
9:A:103:BCL:H102	9:A:103:BCL:H62	1.49	0.45
9:G:102:BCL:H203	9:G:102:BCL:H161	1.70	0.45
5:S:22:VAL:HG22	9:S:102:BCL:H18	1.99	0.45
5:U:18:ARG:HE	5:U:18:ARG:HB2	1.64	0.45
5:U:54:SER:OG	5:U:57:ALA:HB3	2.17	0.45
6:V:17:PHE:HA	15:V:101:CRT:H6	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:4:MET:O	5:3:6:ALA:N	2.50	0.45
5:3:11:ILE:HD13	15:7:101:CRT:H132	1.98	0.45
1:o:183:GLN:O	1:o:184:ASN:HB2	2.17	0.45
2:x:179:ASN:HB3	2:x:182:HIS:HB3	1.97	0.45
2:x:224:PHE:O	2:x:228:ILE:HG13	2.17	0.45
9:x:301:BCL:HAA2	9:x:301:BCL:CBD	2.47	0.45
15:s:101:CRT:H36	5:u:33:LEU:HD23	1.98	0.45
5:u:44:LEU:HD12	5:w:47:LEU:HD23	1.97	0.45
6:v:17:PHE:CD1	15:v:101:CRT:H6	2.51	0.45
5:AI:12:TRP:HE1	6:AJ:18:HIS:CB	2.29	0.45
9:k:102:BCL:H151	9:k:102:BCL:H111	1.75	0.45
2:L:5:SER:N	4:H:38:GLY:O	2.43	0.45
3:M:121:PHE:CD1	3:M:121:PHE:N	2.85	0.45
9:A:102:BCL:H91	9:A:102:BCL:H121	1.97	0.45
5:1:29:ILE:O	5:1:33:LEU:HG	2.16	0.45
5:7:27:PHE:CE2	5:7:31:LEU:HD22	2.52	0.45
5:p:22:VAL:HG13	9:p:102:BCL:H18	1.99	0.45
9:r:101:BCL:H151	9:r:101:BCL:H18	1.41	0.45
5:u:46:TRP:HA	5:u:49:ASP:OD2	2.16	0.45
9:u:102:BCL:H193	6:v:40:TRP:CD2	2.51	0.45
6:v:10:THR:OG1	6:v:13:GLU:N	2.48	0.45
6:v:21:PHE:CD2	15:v:101:CRT:H14	2.51	0.45
5:AI:5:ASN:HB3	6:AL:23:GLN:OE1	2.16	0.45
9:c:101:BCL:H141	9:c:101:BCL:H161	1.66	0.45
2:L:128:PHE:O	2:L:131:SER:HB2	2.17	0.45
6:T:45:TRP:HE1	9:T:102:BCL:H143	1.80	0.45
15:V:101:CRT:H36	5:W:33:LEU:HD23	1.97	0.45
1:o:21:LEU:HD21	2:x:274:TRP:CE2	2.52	0.45
1:o:178:LEU:HA	3:y:110:SER:CB	2.41	0.45
1:o:250:CYS:HA	1:o:263:THR:OG1	2.17	0.45
3:y:62:PHE:CB	5:AC:30:VAL:HG21	2.45	0.45
3:y:200:PRO:HB2	4:t:16:ILE:CD1	2.47	0.45
5:r:56:GLN:OE1	5:r:56:GLN:HA	2.16	0.45
2:L:3:MET:HB3	2:L:7:GLU:HB3	1.99	0.45
4:H:46:THR:OG1	4:H:53:VAL:O	2.32	0.45
4:H:65:LYS:HB2	4:H:65:LYS:HE3	1.76	0.45
5:Q:19:ARG:HD2	5:S:18:ARG:NH2	2.32	0.45
5:U:5:ASN:OD1	5:U:6:ALA:N	2.50	0.45
5:Y:49:ASP:HB2	5:Y:51:ILE:HB	1.98	0.45
5:7:50:ASN:HD22	5:9:60:LYS:HA	1.82	0.45
1:o:21:LEU:HD23	2:x:271:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:58:PHE:CG	4:t:59:PRO:HA	2.51	0.45
9:p:102:BCL:H142	9:p:102:BCL:H111	1.69	0.45
5:d:49:ASP:HB2	5:d:51:ILE:CG1	2.46	0.45
5:f:35:ILE:CG1	15:g:101:CRT:H403	2.47	0.45
9:l:101:BCL:HBC3	9:l:101:BCL:H2C	1.58	0.45
1:C:21:LEU:HD21	2:L:274:TRP:CE2	2.51	0.45
1:C:100:TRP:HE3	1:C:152:CYS:SG	2.40	0.45
2:L:106:PHE:CE1	10:L:302:BPH:H2	2.51	0.45
3:M:52:TYR:O	3:M:132:ARG:NH2	2.50	0.45
3:M:164:ARG:NH2	3:M:173:LYS:O	2.50	0.45
4:H:35:LYS:NZ	4:H:59:PRO:O	2.50	0.45
6:B:20:ILE:CB	15:9:101:CRT:H82	2.44	0.45
6:B:37:LEU:O	6:B:41:LEU:HG	2.17	0.45
5:K:10:LYS:O	5:K:13:LEU:HB2	2.16	0.45
6:N:20:ILE:HD12	15:O:101:CRT:C6	2.46	0.45
5:U:16:ASP:CG	5:U:18:ARG:HH21	2.17	0.45
5:U:43:ASP:OD1	5:W:56:GLN:HG2	2.17	0.45
9:U:101:BCL:CED	6:V:32:VAL:HA	2.47	0.45
5:W:36:HIS:CE1	9:X:102:BCL:HMD3	2.52	0.45
9:1:101:BCL:O2D	9:1:101:BCL:H2A	2.17	0.45
9:5:101:BCL:HED2	6:6:35:ALA:HB2	1.99	0.45
6:6:32:VAL:HG21	9:6:101:BCL:O1A	2.16	0.45
6:0:21:PHE:HA	15:0:101:CRT:C14	2.47	0.45
1:o:83:LYS:C	1:o:85:LEU:H	2.25	0.45
1:o:307:CYS:SG	7:o:504:HEM:CAB	3.05	0.45
2:x:84:LEU:HB2	5:h:41:SER:CB	2.47	0.45
2:x:86:MET:CG	5:j:41:SER:HB3	2.42	0.45
2:x:126:VAL:HG11	3:y:251:PHE:HE2	1.80	0.45
9:x:301:BCL:H51	10:x:302:BPH:HBB2	1.99	0.45
3:y:38:TYR:CD1	3:y:38:TYR:C	2.94	0.45
3:y:163:ILE:O	3:y:167:MET:HG3	2.16	0.45
5:AC:17:PRO:HB3	6:AD:17:PHE:CE1	2.51	0.45
5:AI:35:ILE:HG12	15:AJ:101:CRT:H403	1.99	0.45
9:AI:102:BCL:HBA1	9:AI:102:BCL:H3A	1.66	0.45
2:L:163:LEU:HD13	3:M:197:TYR:CD1	2.52	0.45
2:L:241:LEU:CD2	11:L:304:UQ8:H13	2.46	0.45
5:I:55:TYR:C	5:I:57:ALA:H	2.24	0.45
5:Q:12:TRP:CH2	6:R:17:PHE:HE2	2.34	0.45
6:8:32:VAL:HG21	9:8:101:BCL:H11	1.98	0.45
1:o:153:TYR:CD1	1:o:157:ARG:HA	2.52	0.45
4:t:80:ARG:HG3	4:t:82:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:36:HIS:CE1	9:q:102:BCL:HMD3	2.52	0.45
9:AE:102:BCL:H121	6:AF:45:TRP:HZ2	1.81	0.45
6:AF:31:LEU:O	6:AF:34:ILE:HB	2.17	0.45
6:AJ:44:PRO:O	5:AK:52:PRO:HD2	2.17	0.45
15:AJ:101:CRT:H393	5:AK:36:HIS:CD2	2.51	0.45
5:AK:45:ASN:OD1	5:AK:47:LEU:N	2.39	0.45
15:AL:101:CRT:H10	15:AL:101:CRT:H81	1.79	0.45
6:e:43:ARG:HA	6:e:44:PRO:HD2	1.87	0.45
4:H:16:ILE:HD12	4:H:16:ILE:HA	1.90	0.45
4:H:224:THR:OG1	4:H:225:LEU:N	2.50	0.45
5:I:31:LEU:HD21	15:I:102:CRT:H32	1.99	0.45
5:I:44:LEU:HD13	9:I:103:BCL:HAC1	1.99	0.45
1:o:67:SER:CA	1:o:68:THR:HG22	2.40	0.45
2:x:129:ALA:HB1	2:x:247:LEU:HD21	1.99	0.45
3:y:161:GLY:HA3	15:y:404:CRT:C26	2.44	0.45
3:y:162:PHE:C	3:y:165:PRO:HD2	2.42	0.45
9:u:101:BCL:H12	6:v:28:TRP:HZ2	1.82	0.45
5:AE:25:VAL:CG2	9:AF:101:BCL:H121	2.46	0.45
5:d:40:LEU:HG	5:d:46:TRP:CZ3	2.52	0.45
1:C:47:ARG:HD2	1:C:47:ARG:HA	1.74	0.44
1:C:254:ARG:HD2	3:M:295:TYR:HE1	1.82	0.44
2:L:50:ILE:HD11	2:L:98:ILE:HG21	1.98	0.44
2:L:164:ASP:OD2	3:M:307:TYR:OH	2.35	0.44
3:M:2:PRO:HB2	4:H:201:ARG:NH1	2.33	0.44
4:H:29:TYR:OH	12:H:305:PEF:C30	2.65	0.44
5:A:18:ARG:HH12	5:9:19:ARG:NH1	2.15	0.44
5:O:29:ILE:O	5:O:33:LEU:HG	2.17	0.44
6:T:18:HIS:O	6:T:22:MET:HG2	2.18	0.44
15:X:101:CRT:H10	15:X:101:CRT:H81	1.73	0.44
5:Y:9:TYR:HD1	5:Y:9:TYR:H	1.66	0.44
2:x:202:LEU:HA	2:x:202:LEU:HD12	1.51	0.44
2:x:237:ALA:HA	2:x:240:ARG:HD2	1.98	0.44
3:y:128:LEU:HD23	3:y:128:LEU:HA	1.75	0.44
15:n:101:CRT:H20	15:n:101:CRT:H181	1.85	0.44
5:r:17:PRO:HB3	6:s:17:PHE:CZ	2.51	0.44
6:s:45:TRP:HD1	6:s:46:LEU:HG	1.83	0.44
6:AD:18:HIS:O	6:AD:22:MET:HG2	2.17	0.44
5:h:51:ILE:HA	5:h:52:PRO:HA	1.82	0.44
15:k:101:CRT:H20	15:k:101:CRT:H181	1.76	0.44
1:C:24:GLU:O	2:L:263:PHE:HA	2.17	0.44
4:H:45:ARG:HH12	12:H:302:PEF:C10	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:BCL:H122	6:J:45:TRP:HZ2	1.82	0.44
6:T:45:TRP:NE1	9:T:102:BCL:H143	2.32	0.44
9:W:101:BCL:HBC2	9:X:102:BCL:HMD1	1.99	0.44
9:1:101:BCL:H2A	9:1:101:BCL:CED	2.47	0.44
5:5:9:TYR:C	5:5:11:ILE:H	2.25	0.44
1:o:61:SER:HA	1:o:327:TYR:OH	2.17	0.44
1:o:62:LEU:O	1:o:63:PRO:C	2.59	0.44
1:o:311:HIS:HE1	7:o:504:HEM:NA	2.15	0.44
2:x:225:PHE:CD2	11:x:304:UQ8:H7A	2.52	0.44
3:y:76:LEU:HD12	3:y:76:LEU:HA	1.78	0.44
3:y:143:SER:HB2	3:y:145:HIS:HD1	1.82	0.44
3:y:149:ALA:O	3:y:152:ALA:N	2.48	0.44
4:t:53:VAL:HG22	12:p:101:PEF:O5	2.17	0.44
4:t:234:TYR:CE1	4:t:238:LYS:HG3	2.52	0.44
6:z:40:TRP:CE2	9:z:102:BCL:H202	2.52	0.44
9:AB:102:BCL:H93	9:AB:102:BCL:H61	1.76	0.44
5:AK:35:ILE:HG12	15:AL:101:CRT:H403	1.97	0.44
9:AK:101:BCL:HBC2	9:AL:102:BCL:HMD1	1.98	0.44
6:AL:21:PHE:CE1	15:AL:101:CRT:H16	2.51	0.44
9:d:101:BCL:H2	6:e:28:TRP:CH2	2.53	0.44
9:d:101:BCL:HAA2	9:d:101:BCL:HBD	2.00	0.44
5:f:5:ASN:ND2	6:i:20:ILE:HA	2.32	0.44
5:h:40:LEU:HG	5:h:46:TRP:CH2	2.52	0.44
6:k:43:ARG:HA	5:l:55:TYR:OH	2.17	0.44
1:C:124:LYS:HE3	7:C:501:HEM:C3D	2.52	0.44
4:H:136:MET:HG3	4:H:170:VAL:O	2.16	0.44
4:H:136:MET:HE3	4:H:142:PHE:HB3	1.99	0.44
5:A:8:LEU:HD23	6:E:20:ILE:HG12	2.00	0.44
5:A:34:LEU:O	5:A:38:ILE:HG13	2.18	0.44
9:D:101:BCL:HAA2	9:D:101:BCL:HBD	2.00	0.44
6:P:17:PHE:HD1	15:P:102:CRT:H6	1.82	0.44
9:4:102:BCL:H3A	9:4:102:BCL:HBA1	1.75	0.44
15:7:103:CRT:H241	15:7:103:CRT:H26	1.66	0.44
1:o:153:TYR:CE1	1:o:157:ARG:HA	2.52	0.44
1:o:316:LYS:HE3	7:o:504:HEM:O1A	2.17	0.44
2:x:61:PRO:HA	2:x:66:GLN:HG3	1.99	0.44
9:x:303:BCL:H3A	9:x:303:BCL:HBA2	1.61	0.44
4:t:65:LYS:HE2	4:t:67:PHE:HE1	1.79	0.44
5:m:2:PHE:HB3	5:m:4:MET:H	1.82	0.44
15:n:101:CRT:H372	5:p:36:HIS:CD2	2.52	0.44
9:z:102:BCL:H3A	9:z:102:BCL:HBA1	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:9:TYR:CE2	6:AB:15:LYS:HG3	2.52	0.44
5:AC:33:LEU:O	15:AC:101:CRT:H2M1	2.17	0.44
5:AC:36:HIS:HB3	15:AC:101:CRT:H393	1.99	0.44
5:AI:12:TRP:HE1	6:AJ:18:HIS:HB2	1.82	0.44
6:AJ:46:LEU:HD22	6:AL:42:TYR:CE2	2.52	0.44
6:g:9:LEU:HD23	6:g:13:GLU:O	2.17	0.44
9:h:101:BCL:H112	9:h:101:BCL:H72	1.84	0.44
6:c:32:VAL:HG22	9:c:101:BCL:HBA2	1.97	0.44
1:C:128:ARG:NE	7:C:501:HEM:O2D	2.49	0.44
4:H:45:ARG:NH1	12:H:302:PEF:H21	2.32	0.44
6:T:45:TRP:CD1	6:T:46:LEU:HG	2.52	0.44
6:Z:43:ARG:HG2	5:1:55:TYR:HE1	1.82	0.44
3:y:25:LYS:HD2	6:AB:7:THR:HG22	1.98	0.44
9:m:102:BCL:H41	9:m:102:BCL:H72	1.99	0.44
5:AE:27:PHE:HZ	15:AF:102:CRT:H31	1.83	0.44
5:AI:39:VAL:HG11	9:AI:101:BCL:HBC1	1.99	0.44
6:e:45:TRP:HD1	6:e:46:LEU:HG	1.79	0.44
6:e:46:LEU:N	5:f:52:PRO:HD3	2.33	0.44
2:L:189:PHE:CE1	2:L:249:ALA:HB1	2.53	0.44
4:H:124:ASP:OD2	4:H:132:LYS:NZ	2.39	0.44
6:B:46:LEU:OXT	5:D:51:ILE:HG21	2.18	0.44
6:N:32:VAL:HG12	9:N:101:BCL:H92	2.00	0.44
5:S:5:ASN:HB3	5:S:8:LEU:HB2	2.00	0.44
5:5:16:ASP:O	5:5:20:VAL:HG23	2.18	0.44
5:AI:12:TRP:HB2	6:AJ:14:ALA:HB3	2.00	0.44
5:j:27:PHE:CE1	5:l:29:ILE:HD13	2.52	0.44
6:k:44:PRO:O	5:l:52:PRO:HD2	2.18	0.44
1:C:36:ARG:HD2	2:L:77:PRO:O	2.17	0.44
1:C:142:LYS:C	1:C:144:HIS:H	2.25	0.44
2:L:75:ILE:O	2:L:95:TRP:HD1	1.99	0.44
2:L:116:ILE:HD13	3:M:254:TRP:HB2	2.00	0.44
12:H:302:PEF:P	12:H:302:PEF:HN1	2.41	0.44
9:O:102:BCL:H2	6:P:32:VAL:HG11	2.00	0.44
9:T:102:BCL:HMA1	9:T:102:BCL:HHB	1.82	0.44
5:Y:29:ILE:HG13	9:Y:101:BCL:H43	1.99	0.44
5:7:42:THR:OG1	5:9:47:LEU:HB3	2.18	0.44
1:o:299:TYR:HB2	1:o:301:ASP:OD1	2.18	0.44
2:x:133:ALA:HB2	10:x:302:BPH:C4C	2.47	0.44
3:y:157:TYR:HB2	9:y:401:BCL:H92	1.98	0.44
4:t:9:ILE:HG12	5:r:41:SER:HB3	1.99	0.44
5:p:9:TYR:C	5:p:11:ILE:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AB:102:BCL:HBD	9:AB:102:BCL:HED2	1.66	0.44
6:AD:33:VAL:O	6:AD:37:LEU:HG	2.18	0.44
15:AJ:101:CRT:H393	5:AK:36:HIS:HD2	1.82	0.44
5:f:45:ASN:HB3	5:h:56:GLN:OE1	2.18	0.44
15:g:101:CRT:H2M1	5:h:36:HIS:HB3	1.98	0.44
5:j:21:LEU:HD23	5:j:21:LEU:HA	1.74	0.44
1:C:21:LEU:HG	2:L:274:TRP:NE1	2.32	0.44
2:L:193:CYS:SG	10:M:403:BPH:HMC2	2.58	0.44
3:M:199:ASN:HA	3:M:294:TRP:CE3	2.52	0.44
9:D:101:BCL:H142	9:D:101:BCL:H111	1.79	0.44
9:S:102:BCL:HAA1	9:S:102:BCL:CBD	2.47	0.44
9:U:101:BCL:H2	6:V:28:TRP:CH2	2.52	0.44
5:Y:23:SER:CB	9:1:101:BCL:H151	2.47	0.44
5:3:40:LEU:HG	5:3:46:TRP:CZ3	2.53	0.44
6:4:46:LEU:HD22	6:6:42:TYR:CE2	2.53	0.44
9:4:102:BCL:H93	9:4:102:BCL:H111	1.81	0.44
1:o:144:HIS:CD2	1:o:144:HIS:C	2.95	0.44
1:o:187:SER:C	1:o:189:THR:H	2.25	0.44
2:x:22:LEU:HG	2:x:23:PHE:CE2	2.53	0.44
3:y:98:PRO:HB2	3:y:171:TRP:HB2	2.00	0.44
5:p:37:MET:HA	5:p:40:LEU:HB2	2.00	0.44
9:AE:102:BCL:HAA2	9:AE:102:BCL:CED	2.48	0.44
6:AF:25:MET:HG3	15:AF:102:CRT:C21	2.47	0.44
9:AG:101:BCL:HBA2	6:AH:32:VAL:HG21	2.00	0.44
6:AJ:14:ALA:HB2	6:AJ:17:PHE:HB3	2.00	0.44
1:C:210:ILE:O	1:C:232:THR:OG1	2.32	0.44
9:L:301:BCL:HHB	9:M:402:BCL:HMB2	2.00	0.44
5:A:17:PRO:HB3	6:B:17:PHE:CE1	2.52	0.44
9:3:101:BCL:H2C	9:3:101:BCL:HBC3	1.75	0.44
9:6:101:BCL:HAA2	9:6:101:BCL:O2D	2.17	0.44
1:o:141:TRP:O	1:o:145:VAL:HG22	2.18	0.44
2:x:97:ILE:HD13	2:x:100:ILE:HD12	1.99	0.44
2:x:160:LEU:HD23	2:x:160:LEU:HA	1.82	0.44
4:t:176:GLU:O	4:t:178:GLN:HG2	2.17	0.44
9:s:102:BCL:HBA1	9:s:102:BCL:H3A	1.77	0.44
5:u:21:LEU:HD21	15:v:101:CRT:C14	2.48	0.44
6:AB:37:LEU:HD23	6:AB:37:LEU:HA	1.71	0.44
9:AC:103:BCL:HMA1	9:AF:101:BCL:HMA1	1.99	0.44
5:AE:27:PHE:CD1	5:AG:29:ILE:HD13	2.53	0.44
9:AE:102:BCL:HBD	9:AE:102:BCL:HED2	1.75	0.44
9:AI:101:BCL:H41	9:AI:101:BCL:H201	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLN:HB2	1:C:117:ALA:HB1	2.00	0.44
3:M:200:PRO:HD2	3:M:294:TRP:CZ3	2.53	0.44
3:M:210:TYR:OH	9:M:402:BCL:HBB3	2.18	0.44
5:D:46:TRP:CD2	9:D:101:BCL:H2C	2.53	0.44
5:Q:10:LYS:HB3	15:T:101:CRT:H5	1.99	0.44
6:T:16:GLU:HB3	15:T:101:CRT:H33	2.00	0.44
5:W:18:ARG:O	5:W:22:VAL:HG23	2.18	0.44
9:Z:102:BCL:H62	9:Z:102:BCL:H41	1.42	0.44
1:o:142:LYS:C	1:o:144:HIS:N	2.75	0.44
1:o:276:VAL:HG21	7:o:504:HEM:HAB	2.00	0.44
5:u:37:MET:CE	5:u:40:LEU:HD12	2.48	0.44
5:AG:28:GLN:HB3	9:AH:101:BCL:H12	2.00	0.44
9:e:102:BCL:HED3	9:e:102:BCL:HAA2	2.00	0.44
2:L:181:ALA:HB3	2:L:256:CYS:HA	2.00	0.43
3:M:6:ASN:HD22	3:M:227:SER:CB	2.31	0.43
6:E:20:ILE:HD12	15:E:101:CRT:C6	2.48	0.43
5:I:9:TYR:C	5:I:11:ILE:N	2.75	0.43
5:1:35:ILE:HG12	15:2:101:CRT:H392	2.00	0.43
5:5:38:ILE:O	5:5:42:THR:HG23	2.17	0.43
9:5:101:BCL:HHC	9:5:101:BCL:OBB	2.18	0.43
5:7:38:ILE:HD13	15:7:103:CRT:H2M3	1.99	0.43
5:9:11:ILE:HG23	5:9:12:TRP:CD2	2.52	0.43
1:o:134:VAL:HG13	1:o:150:VAL:HG23	2.00	0.43
2:x:136:ALA:CB	9:x:301:BCL:H43	2.48	0.43
4:t:121:LYS:HE3	4:t:234:TYR:CD2	2.53	0.43
12:t:301:PEF:H12	12:t:301:PEF:O4	2.18	0.43
9:u:102:BCL:C9	6:v:33:VAL:HG22	2.48	0.43
17:AE:101:PGW:O02	17:AE:101:PGW:H03A	2.17	0.43
6:AJ:40:TRP:HZ3	6:AJ:46:LEU:H	1.66	0.43
2:L:72:ARG:HH11	3:M:305:PRO:HA	1.82	0.43
3:M:84:PHE:HD1	5:W:37:MET:HG3	1.81	0.43
5:F:23:SER:HB3	9:I:101:BCL:H143	2.00	0.43
6:G:21:PHE:HA	15:G:101:CRT:C14	2.48	0.43
5:U:36:HIS:CE1	9:V:102:BCL:HMD3	2.53	0.43
15:V:101:CRT:H5	15:V:101:CRT:H33	1.44	0.43
15:Z:101:CRT:H27	9:Z:102:BCL:H11	2.00	0.43
9:Z:102:BCL:H162	9:Z:102:BCL:H141	1.74	0.43
5:1:57:ALA:H	5:1:59:GLY:N	2.13	0.43
2:x:42:PHE:CE2	2:x:104:GLY:HA3	2.53	0.43
2:x:125:HIS:CE1	3:y:5:GLN:OE1	2.71	0.43
9:x:303:BCL:H13	9:x:303:BCL:H172	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:x:304:UQ8:H30B	11:x:304:UQ8:C35	2.49	0.43
3:y:219:HIS:O	3:y:223:ILE:HG12	2.18	0.43
4:t:26:LEU:HD12	4:t:29:TYR:CD2	2.53	0.43
6:n:43:ARG:HG3	5:p:55:TYR:CE1	2.52	0.43
5:r:7:ASN:HA	5:r:9:TYR:CE1	2.53	0.43
9:s:102:BCL:HHB	9:s:102:BCL:HMB1	1.78	0.43
5:AE:12:TRP:HZ3	5:AE:20:VAL:HG11	1.82	0.43
9:AF:101:BCL:H192	9:AF:101:BCL:H162	1.76	0.43
9:AK:101:BCL:H102	9:AK:101:BCL:H61	1.74	0.43
6:c:45:TRP:HZ2	9:c:101:BCL:H122	1.82	0.43
3:M:253:ARG:HH22	12:H:301:PEF:C5	2.31	0.43
5:A:44:LEU:HD12	5:D:47:LEU:HD22	2.01	0.43
9:D:101:BCL:H13	9:D:101:BCL:H102	1.70	0.43
6:G:30:GLY:O	6:G:34:ILE:HG12	2.18	0.43
5:I:55:TYR:C	5:I:57:ALA:N	2.77	0.43
5:K:40:LEU:HD21	5:K:47:LEU:HD12	2.00	0.43
5:Y:51:ILE:HG12	5:1:59:GLY:HA3	2.00	0.43
3:y:145:HIS:HA	3:y:148:TRP:CE3	2.53	0.43
14:y:403:MQ8:H161	14:y:403:MQ8:H141	1.80	0.43
4:t:135:PRO:HD3	4:t:171:TRP:CH2	2.54	0.43
5:m:9:TYR:O	5:m:11:ILE:N	2.51	0.43
5:m:49:ASP:HB3	5:m:51:ILE:HG13	2.00	0.43
6:n:22:MET:HE3	6:n:26:TYR:CE2	2.54	0.43
5:p:51:ILE:HG23	5:p:52:PRO:HA	2.01	0.43
5:AC:43:ASP:HB2	5:AE:48:ASP:OD1	2.18	0.43
15:AL:101:CRT:H372	5:d:36:HIS:CD2	2.53	0.43
5:h:38:ILE:O	5:h:42:THR:HG23	2.18	0.43
2:L:68:TYR:HA	2:L:73:ILE:HD11	1.99	0.43
9:L:303:BCL:H91	9:L:303:BCL:H112	1.89	0.43
4:H:9:ILE:HD11	5:F:41:SER:HB2	2.01	0.43
6:G:32:VAL:HG11	9:G:102:BCL:HBA1	2.01	0.43
6:N:44:PRO:O	5:O:52:PRO:HD3	2.18	0.43
5:U:13:LEU:C	6:V:7:THR:HG23	2.43	0.43
9:V:102:BCL:H112	9:V:102:BCL:H142	1.69	0.43
5:1:17:PRO:HA	5:1:20:VAL:HG22	2.00	0.43
15:4:101:CRT:H32	9:5:101:BCL:HBA2	2.01	0.43
5:7:50:ASN:HB2	5:9:59:GLY:C	2.43	0.43
2:x:184:LEU:HD12	2:x:184:LEU:HA	1.63	0.43
11:x:304:UQ8:H7	11:x:304:UQ8:H10	1.73	0.43
3:y:220:GLY:O	3:y:224:LEU:HD12	2.19	0.43
14:y:403:MQ8:H362	14:y:403:MQ8:H341	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:65:LYS:HE2	4:t:67:PHE:CZ	2.54	0.43
6:z:40:TRP:CZ3	6:z:46:LEU:HB2	2.53	0.43
5:AA:45:ASN:C	5:AA:49:ASP:OD2	2.51	0.43
6:AD:28:TRP:O	6:AD:32:VAL:HG23	2.18	0.43
5:AK:11:ILE:HD12	15:e:101:CRT:H81	1.99	0.43
5:l:17:PRO:HB3	6:c:17:PHE:CE1	2.53	0.43
9:L:301:BCL:H162	9:L:301:BCL:H141	1.63	0.43
3:M:126:ILE:HD11	9:M:402:BCL:H142	2.00	0.43
4:H:13:GLN:O	4:H:16:ILE:HG22	2.19	0.43
4:H:60:ASP:CG	4:H:61:LEU:N	2.76	0.43
5:D:43:ASP:C	5:D:45:ASN:H	2.26	0.43
15:I:102:CRT:H31	5:K:29:ILE:HD11	2.00	0.43
5:U:54:SER:HG	5:U:57:ALA:HB3	1.83	0.43
5:W:45:ASN:HB3	5:Y:56:GLN:NE2	2.33	0.43
5:1:9:TYR:HA	6:2:18:HIS:CG	2.53	0.43
5:7:39:VAL:HG12	5:7:46:TRP:HZ3	1.84	0.43
2:x:137:TYR:O	2:x:141:VAL:HG22	2.18	0.43
3:y:40:LEU:O	3:y:44:GLY:N	2.50	0.43
3:y:73:PHE:CZ	3:y:81:TRP:HH2	2.36	0.43
4:t:149:PRO:HB2	4:t:154:MET:HE1	2.00	0.43
6:n:31:LEU:HD23	6:n:31:LEU:HA	1.79	0.43
5:u:46:TRP:CD1	9:u:101:BCL:HMC2	2.53	0.43
9:u:101:BCL:H142	9:u:101:BCL:H112	1.61	0.43
9:u:102:BCL:HBC3	9:u:102:BCL:H2C	1.76	0.43
6:z:34:ILE:O	6:z:38:LEU:HG	2.19	0.43
6:AB:17:PHE:HB2	15:AC:101:CRT:H32A	2.01	0.43
6:AH:43:ARG:HG3	5:AI:55:TYR:CE1	2.53	0.43
5:AI:40:LEU:HD23	5:AI:40:LEU:HA	1.86	0.43
6:AL:20:ILE:HD12	15:AL:101:CRT:C6	2.48	0.43
5:h:14:ILE:HD13	15:k:101:CRT:H1M1	2.00	0.43
9:c:101:BCL:HBD	9:c:101:BCL:HAA1	1.99	0.43
1:C:183:GLN:HG3	1:C:184:ASN:OD1	2.19	0.43
3:M:120:LEU:HD22	5:Q:37:MET:HE2	2.01	0.43
5:A:44:LEU:CD1	5:D:47:LEU:HD22	2.49	0.43
6:B:20:ILE:CG2	5:9:5:ASN:HB3	2.45	0.43
5:I:12:TRP:HB2	6:J:14:ALA:HB1	2.01	0.43
5:K:29:ILE:O	5:K:33:LEU:HG	2.19	0.43
15:X:101:CRT:H393	5:Y:36:HIS:CD2	2.54	0.43
5:5:28:GLN:HE22	15:7:101:CRT:H27	1.84	0.43
2:x:202:LEU:HD23	11:x:304:UQ8:C3M	2.40	0.43
3:y:156:PHE:CE2	9:y:401:BCL:H43	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:z:101:CRT:H342	9:AB:101:BCL:HBA1	2.00	0.43
5:AC:40:LEU:HD23	5:AC:40:LEU:HA	1.89	0.43
5:AG:11:ILE:HG12	9:AI:101:BCL:C14	2.49	0.43
15:k:101:CRT:H15	15:k:101:CRT:H131	1.85	0.43
1:C:141:TRP:O	1:C:144:HIS:HB3	2.19	0.43
1:C:153:TYR:O	1:C:154:THR:C	2.61	0.43
1:C:252:ASN:OD1	1:C:254:ARG:HG2	2.18	0.43
3:M:40:LEU:O	3:M:44:GLY:N	2.47	0.43
3:M:121:PHE:N	3:M:121:PHE:HD1	2.16	0.43
3:M:125:SER:OG	10:M:403:BPH:H2	2.18	0.43
15:M:405:CRT:H31	15:M:405:CRT:H291	1.86	0.43
4:H:57:GLY:N	12:H:302:PEF:H52	2.33	0.43
9:P:101:BCL:H62	9:P:101:BCL:H41	1.83	0.43
5:S:8:LEU:O	5:S:8:LEU:HG	2.19	0.43
9:4:102:BCL:HAA1	9:4:102:BCL:CBD	2.48	0.43
1:o:201:THR:O	1:o:206:GLN:HB2	2.18	0.43
2:x:242:GLY:HA3	3:y:216:PHE:CE1	2.53	0.43
9:y:401:BCL:OBB	9:y:401:BCL:HHC	2.19	0.43
15:y:404:CRT:H401	5:AA:37:MET:HG3	1.99	0.43
4:t:39:TYR:CZ	4:t:41:LEU:HD21	2.54	0.43
4:t:63:ASP:CG	5:r:19:ARG:HH12	2.26	0.43
15:n:101:CRT:H31	15:n:101:CRT:H291	1.79	0.43
5:p:9:TYR:O	5:p:10:LYS:HB2	2.18	0.43
5:u:43:ASP:O	5:w:56:GLN:NE2	2.52	0.43
5:AK:43:ASP:O	5:d:55:TYR:HB2	2.18	0.43
1:C:254:ARG:CZ	3:M:307:TYR:HE1	2.31	0.43
3:M:156:PHE:CZ	3:M:160:LEU:HD11	2.54	0.43
3:M:204:LEU:HD13	4:H:19:PHE:CE2	2.53	0.43
4:H:193:VAL:HB	4:H:222:VAL:CG1	2.49	0.43
5:A:8:LEU:HB2	6:E:20:ILE:HD13	2.00	0.43
9:I:101:BCL:HAC1	9:I:103:BCL:HAC2	2.00	0.43
5:Q:8:LEU:HD11	15:T:101:CRT:H133	2.00	0.43
5:U:21:LEU:HA	5:U:21:LEU:HD23	1.80	0.43
5:3:18:ARG:O	5:3:22:VAL:HG22	2.18	0.43
5:9:9:TYR:HB2	6:0:14:ALA:O	2.18	0.43
1:o:47:ARG:CG	1:o:47:ARG:NH1	2.78	0.43
1:o:112:VAL:HG21	1:o:120:ASP:HB3	2.01	0.43
9:x:301:BCL:O1A	9:x:305:BCL:HBC1	2.18	0.43
3:y:256:MET:HE3	3:y:256:MET:HB2	1.85	0.43
4:t:169:ASP:CG	4:t:170:VAL:H	2.26	0.43
5:u:5:ASN:HA	5:u:6:ALA:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:w:12:TRP:CD1	6:z:18:HIS:HB2	2.54	0.43
9:AB:101:BCL:H93	9:AB:101:BCL:H61	1.88	0.43
15:AF:102:CRT:H10	15:AF:102:CRT:H81	1.78	0.43
9:f:101:BCL:H192	9:f:101:BCL:H161	1.73	0.43
9:f:101:BCL:HMD1	6:g:36:HIS:CE1	2.54	0.43
6:g:40:TRP:CD1	9:g:102:BCL:H191	2.54	0.43
5:h:10:LYS:HD3	15:k:101:CRT:H22A	2.01	0.43
9:k:102:BCL:H141	9:k:102:BCL:H162	1.65	0.43
1:C:203:PHE:CB	1:C:235:LEU:HD22	2.48	0.43
3:M:36:PHE:HA	3:M:46:ALA:O	2.18	0.43
3:M:116:LEU:HD12	3:M:116:LEU:HA	1.89	0.43
4:H:215:LYS:HB2	4:H:218:HIS:CD2	2.53	0.43
6:E:46:LEU:HD22	5:F:51:ILE:HG21	2.01	0.43
5:I:21:LEU:HD23	5:I:21:LEU:HA	1.74	0.43
6:J:29:PHE:O	6:J:33:VAL:HG23	2.19	0.43
15:R:101:CRT:H10	15:R:101:CRT:H81	1.94	0.43
5:7:14:ILE:HD11	15:0:101:CRT:C5	2.39	0.43
5:7:36:HIS:CD2	15:7:101:CRT:H372	2.54	0.43
5:9:3:THR:O	5:9:5:ASN:N	2.51	0.43
2:x:116:ILE:HG23	3:y:254:TRP:HE3	1.84	0.43
3:y:235:ILE:HG22	3:y:236:ASP:N	2.32	0.43
5:r:38:ILE:HD13	15:s:101:CRT:H391	2.00	0.43
5:u:25:VAL:HG13	9:u:101:BCL:H71	2.00	0.43
5:w:44:LEU:HD23	5:AA:55:TYR:CD2	2.54	0.43
6:AH:43:ARG:HG3	5:AI:55:TYR:CZ	2.53	0.43
9:AI:101:BCL:HAA1	9:AI:101:BCL:CBD	2.40	0.43
5:d:5:ASN:OD1	5:d:7:ASN:N	2.52	0.43
5:d:27:PHE:HB2	9:f:101:BCL:H201	2.01	0.43
1:C:37:GLY:HA3	2:L:76:ALA:HB1	2.00	0.43
1:C:187:SER:C	1:C:189:THR:N	2.77	0.43
11:L:304:UQ8:H32	11:L:304:UQ8:H35	1.75	0.43
3:M:197:TYR:CE1	9:M:402:BCL:HMC2	2.53	0.43
3:M:267:ARG:NH1	12:H:305:PEF:C30	2.80	0.43
15:I:102:CRT:H26	15:I:102:CRT:H241	1.87	0.43
6:Z:25:MET:O	6:Z:28:TRP:HB3	2.19	0.43
5:1:44:LEU:HD23	5:3:55:TYR:CE2	2.54	0.43
5:3:25:VAL:HG22	9:3:101:BCL:H8	2.01	0.43
1:o:195:LEU:HD11	1:o:233:PHE:CD2	2.54	0.43
1:o:316:LYS:O	1:o:317:PRO:C	2.60	0.43
2:x:125:HIS:HE1	3:y:5:GLN:OE1	2.01	0.43
2:x:278:LEU:HD12	2:x:281:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:r:12:TRP:CH2	6:s:17:PHE:HE2	2.36	0.43
9:r:101:BCL:H143	9:r:101:BCL:H162	1.64	0.43
9:AB:102:BCL:HBD	9:AB:102:BCL:HAA1	2.01	0.43
9:AC:102:BCL:H62	9:AC:102:BCL:H41	1.35	0.43
5:AI:25:VAL:HG22	9:AI:101:BCL:H51	2.00	0.43
5:f:18:ARG:O	5:f:22:VAL:HG22	2.19	0.43
5:h:42:THR:HG21	5:j:47:LEU:HB3	2.01	0.43
5:h:47:LEU:HD23	5:h:47:LEU:HA	1.83	0.43
5:j:20:VAL:O	5:j:24:ILE:HG13	2.19	0.43
5:j:40:LEU:HD23	5:j:40:LEU:HA	1.93	0.43
3:M:96:GLU:HA	3:M:97:PRO:HD3	1.86	0.42
5:A:2:PHE:C	5:A:4:MET:H	2.27	0.42
5:A:2:PHE:HB3	5:A:4:MET:HB2	2.01	0.42
9:D:102:BCL:H192	9:D:102:BCL:H161	1.75	0.42
6:E:17:PHE:CA	15:E:101:CRT:H42	2.49	0.42
5:I:12:TRP:CH2	5:I:20:VAL:HG11	2.53	0.42
5:W:4:MET:HG2	5:W:8:LEU:HD22	2.01	0.42
15:X:101:CRT:H393	5:Y:36:HIS:HD2	1.84	0.42
6:2:21:PHE:CZ	15:2:101:CRT:H19	2.53	0.42
5:7:18:ARG:H	5:7:18:ARG:HG2	1.59	0.42
1:o:99:THR:HA	1:o:103:PRO:HB3	1.99	0.42
2:x:268:TRP:O	2:x:271:TRP:N	2.48	0.42
6:s:8:GLY:C	6:s:9:LEU:HD12	2.43	0.42
5:u:49:ASP:HB2	5:u:51:ILE:HG12	2.00	0.42
5:u:50:ASN:ND2	5:w:61:LYS:O	2.52	0.42
15:AJ:101:CRT:H371	9:AK:101:BCL:HMB2	2.01	0.42
6:c:28:TRP:O	6:c:32:VAL:HG23	2.19	0.42
2:L:9:LYS:HE3	4:H:116:SER:C	2.44	0.42
2:L:125:HIS:CE1	3:M:5:GLN:OE1	2.72	0.42
2:L:179:ASN:HB3	2:L:182:HIS:HB3	2.02	0.42
3:M:114:TRP:CZ2	5:S:37:MET:HE1	2.54	0.42
3:M:243:THR:O	3:M:247:ARG:HD2	2.19	0.42
3:M:285:LEU:HD23	3:M:285:LEU:HA	1.67	0.42
15:M:405:CRT:C2M	5:O:38:ILE:HA	2.50	0.42
4:H:251:THR:C	4:H:253:GLU:H	2.27	0.42
6:T:45:TRP:CZ3	9:T:102:BCL:HBC3	2.54	0.42
5:7:7:ASN:O	5:7:10:LYS:HB2	2.19	0.42
15:9:101:CRT:H81	15:9:101:CRT:C11	2.39	0.42
1:o:249:PHE:O	1:o:263:THR:OG1	2.23	0.42
1:o:263:THR:C	1:o:265:LYS:H	2.27	0.42
11:x:304:UQ8:H15	11:x:304:UQ8:H12	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:107:PRO:HG2	3:y:113:GLY:N	2.34	0.42
5:m:51:ILE:HG12	5:p:60:LYS:CB	2.50	0.42
5:p:46:TRP:CD2	9:p:102:BCL:H2C	2.54	0.42
5:u:50:ASN:CB	5:w:59:GLY:HA3	2.44	0.42
9:u:101:BCL:H12	6:v:28:TRP:CZ2	2.54	0.42
6:v:18:HIS:O	6:v:22:MET:HG2	2.19	0.42
5:AA:59:GLY:C	5:AA:61:LYS:HA	2.45	0.42
6:AJ:20:ILE:HD12	15:AJ:101:CRT:C6	2.49	0.42
15:i:101:CRT:H10	15:i:101:CRT:H81	1.91	0.42
9:k:102:BCL:HMA1	9:k:102:BCL:H62	2.01	0.42
7:C:504:HEM:HHA	7:C:504:HEM:HBD1	2.01	0.42
2:L:3:MET:HG2	2:L:11:ARG:NH2	2.34	0.42
2:L:208:ASN:ND2	2:L:208:ASN:N	2.67	0.42
3:M:65:LEU:HD21	10:M:403:BPH:H7C2	2.00	0.42
3:M:183:LEU:HD23	3:M:183:LEU:HA	1.74	0.42
3:M:229:PHE:CZ	3:M:247:ARG:NH1	2.86	0.42
3:M:249:ALA:HB1	3:M:259:ASN:ND2	2.34	0.42
15:M:405:CRT:H10	15:M:405:CRT:H81	1.86	0.42
5:A:9:TYR:HD1	6:B:18:HIS:NE2	2.17	0.42
9:A:103:BCL:HAA2	9:A:103:BCL:CED	2.49	0.42
9:I:103:BCL:H161	9:I:103:BCL:H192	1.78	0.42
5:W:4:MET:O	5:W:5:ASN:HB2	2.18	0.42
5:W:45:ASN:O	5:W:49:ASP:OD2	2.37	0.42
6:6:36:HIS:CD2	9:6:101:BCL:H102	2.54	0.42
1:o:204:LEU:HD22	7:o:504:HEM:HBB1	2.01	0.42
2:x:163:LEU:HD13	3:y:197:TYR:CD1	2.54	0.42
3:y:120:LEU:HD11	5:AA:34:LEU:HD11	2.01	0.42
5:m:4:MET:CE	5:m:7:ASN:HD22	2.32	0.42
5:u:25:VAL:HG13	9:u:101:BCL:C7	2.49	0.42
6:v:33:VAL:O	6:v:37:LEU:HG	2.18	0.42
5:h:16:ASP:HA	5:h:17:PRO:HD3	1.87	0.42
9:i:102:BCL:H52	9:i:102:BCL:HBA1	2.01	0.42
6:c:32:VAL:HG21	9:c:101:BCL:HBA2	2.00	0.42
2:L:253:SER:CB	9:L:301:BCL:HBA1	2.49	0.42
9:M:401:BCL:H122	9:M:401:BCL:H162	1.65	0.42
4:H:142:PHE:HZ	4:H:174:ARG:HA	1.84	0.42
4:H:225:LEU:C	4:H:227:ASN:H	2.27	0.42
5:A:46:TRP:HA	5:A:49:ASP:OD2	2.19	0.42
9:I:103:BCL:HAA2	9:I:103:BCL:HED2	2.00	0.42
5:Q:39:VAL:HG12	5:Q:46:TRP:HZ3	1.83	0.42
6:X:13:GLU:HA	6:X:14:ALA:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:102:BCL:H93	9:Z:102:BCL:CMB	2.50	0.42
5:3:34:LEU:O	5:3:38:ILE:HG13	2.19	0.42
5:7:36:HIS:NE2	15:7:101:CRT:H372	2.34	0.42
5:7:42:THR:HG21	5:9:47:LEU:HB2	2.01	0.42
1:o:191:ALA:O	1:o:192:TYR:HB2	2.20	0.42
3:y:200:PRO:HB2	4:t:16:ILE:HD13	2.01	0.42
15:y:404:CRT:H33	15:y:404:CRT:C6	2.45	0.42
15:AF:102:CRT:H22A	15:AF:102:CRT:H5	1.49	0.42
6:AH:18:HIS:O	6:AH:22:MET:HG2	2.20	0.42
9:AL:102:BCL:H111	9:AL:102:BCL:H93	1.57	0.42
1:C:263:THR:O	1:C:265:LYS:N	2.53	0.42
9:L:303:BCL:HBA2	9:L:303:BCL:H3A	1.42	0.42
3:M:158:LEU:HD23	3:M:158:LEU:HA	1.88	0.42
4:H:14:ILE:HG21	5:I:37:MET:SD	2.59	0.42
4:H:29:TYR:HH	12:H:305:PEF:C10	2.32	0.42
4:H:119:ARG:O	4:H:234:TYR:HB2	2.20	0.42
6:G:44:PRO:O	5:I:55:TYR:OH	2.29	0.42
6:R:40:TRP:CZ3	6:R:46:LEU:HB2	2.54	0.42
9:R:102:BCL:H142	9:R:102:BCL:H112	1.70	0.42
15:T:101:CRT:H27	9:T:102:BCL:O1A	2.18	0.42
6:Z:43:ARG:HD3	5:1:55:TYR:CZ	2.54	0.42
5:1:7:ASN:HB3	5:1:10:LYS:HD2	2.02	0.42
5:3:31:LEU:O	5:3:34:LEU:HB3	2.19	0.42
6:8:24:SER:O	6:8:27:ALA:HB3	2.20	0.42
5:9:35:ILE:HG12	15:0:101:CRT:H403	2.01	0.42
1:o:292:PRO:HD2	1:o:295:ARG:CG	2.49	0.42
2:x:190:PHE:CZ	9:y:401:BCL:HBA2	2.55	0.42
11:x:304:UQ8:H35	11:x:304:UQ8:H32	1.35	0.42
3:y:126:ILE:HD11	9:y:401:BCL:H142	2.02	0.42
3:y:293:ASN:OD1	3:y:293:ASN:C	2.62	0.42
4:t:118:ASP:OD1	4:t:238:LYS:NZ	2.36	0.42
5:p:56:GLN:C	5:p:58:LEU:H	2.15	0.42
5:u:49:ASP:O	5:u:50:ASN:HB2	2.18	0.42
6:z:11:ASP:O	6:z:15:LYS:HB2	2.19	0.42
6:e:40:TRP:NE1	9:e:102:BCL:H201	2.34	0.42
5:f:9:TYR:HA	6:g:18:HIS:HB2	2.01	0.42
5:j:17:PRO:HG2	6:k:9:LEU:HD21	2.01	0.42
1:C:128:ARG:HH21	7:C:501:HEM:HAD1	1.84	0.42
1:C:141:TRP:C	1:C:145:VAL:HG22	2.45	0.42
1:C:332:LYS:HE2	1:C:332:LYS:HB3	1.86	0.42
2:L:199:HIS:CE1	2:L:239:HIS:CE1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:405:CRT:H26	15:M:405:CRT:H241	1.81	0.42
4:H:214:ILE:HB	4:H:218:HIS:HB2	2.00	0.42
5:D:9:TYR:CZ	5:D:10:LYS:HE2	2.54	0.42
15:I:102:CRT:C6	6:J:20:ILE:HD12	2.50	0.42
5:O:43:ASP:HB2	5:Q:48:ASP:HA	2.01	0.42
5:U:6:ALA:C	5:U:8:LEU:H	2.27	0.42
6:V:39:ALA:HB1	9:V:102:BCL:HBC1	2.02	0.42
9:Z:102:BCL:H52	9:Z:102:BCL:H3A	2.02	0.42
6:8:32:VAL:CG2	9:8:101:BCL:HBA2	2.50	0.42
1:o:40:MET:HE3	1:o:251:HIS:O	2.20	0.42
1:o:312:GLN:O	1:o:313:ALA:HB3	2.20	0.42
3:y:36:PHE:HA	3:y:46:ALA:O	2.19	0.42
4:t:87:VAL:HG12	4:t:89:ALA:N	2.35	0.42
5:m:21:LEU:HD23	5:m:21:LEU:HA	1.69	0.42
9:m:102:BCL:H162	9:m:102:BCL:H192	1.83	0.42
15:AD:101:CRT:H241	15:AD:101:CRT:H26	1.64	0.42
5:AE:39:VAL:HG21	9:AE:102:BCL:H3C	2.00	0.42
6:AH:40:TRP:HZ3	6:AH:46:LEU:H	1.67	0.42
5:d:10:LYS:HB3	15:g:101:CRT:H22A	2.02	0.42
6:i:43:ARG:HG3	5:j:55:TYR:OH	2.19	0.42
5:j:4:MET:HE1	5:j:7:ASN:HB2	2.00	0.42
15:k:101:CRT:H26	15:k:101:CRT:H241	1.64	0.42
9:k:102:BCL:H3A	9:k:102:BCL:HBA1	1.77	0.42
1:C:83:LYS:O	1:C:85:LEU:N	2.51	0.42
1:C:161:VAL:O	1:C:162:PRO:C	2.61	0.42
6:P:17:PHE:CD1	15:P:102:CRT:H6	2.55	0.42
6:V:20:ILE:HD12	15:V:101:CRT:C6	2.50	0.42
5:W:34:LEU:O	5:W:38:ILE:HG13	2.20	0.42
5:1:9:TYR:HB2	6:2:14:ALA:O	2.20	0.42
5:5:9:TYR:C	5:5:11:ILE:N	2.77	0.42
5:7:35:ILE:HG12	15:7:103:CRT:H403	2.01	0.42
15:7:101:CRT:H10	15:7:101:CRT:H81	1.86	0.42
15:9:101:CRT:H20	15:9:101:CRT:H181	1.81	0.42
2:x:192:ASN:HD21	3:y:212:SER:C	2.27	0.42
3:y:256:MET:HE3	14:y:403:MQ8:H262	2.02	0.42
9:p:102:BCL:H141	9:p:102:BCL:H162	1.73	0.42
5:r:9:TYR:OH	5:r:10:LYS:HE2	2.20	0.42
5:r:9:TYR:C	5:r:11:ILE:H	2.27	0.42
9:r:101:BCL:HBA2	9:s:102:BCL:HED3	2.02	0.42
9:AH:101:BCL:HAA1	9:AH:101:BCL:CBD	2.47	0.42
9:AI:101:BCL:HMB3	9:AI:101:BCL:HHB	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:176:PHE:HE1	2:L:179:ASN:ND2	2.13	0.42
2:L:271:TRP:O	2:L:273:ASN:N	2.52	0.42
4:H:149:PRO:HB2	4:H:154:MET:CE	2.49	0.42
5:A:10:LYS:HD2	6:E:20:ILE:HD11	2.01	0.42
6:B:17:PHE:HB2	15:9:101:CRT:H32A	2.02	0.42
9:G:102:BCL:HAA2	9:G:102:BCL:HED2	2.00	0.42
9:I:103:BCL:HBA2	6:J:32:VAL:HG21	2.02	0.42
15:O:101:CRT:H15	15:O:101:CRT:H131	1.89	0.42
6:P:17:PHE:HA	15:P:102:CRT:H6	2.01	0.42
6:V:28:TRP:O	6:V:32:VAL:HG23	2.19	0.42
15:V:101:CRT:H393	5:W:36:HIS:HB3	2.01	0.42
9:W:101:BCL:H52	6:X:28:TRP:CE3	2.55	0.42
5:1:24:ILE:HD13	9:3:101:BCL:H18	2.01	0.42
6:8:28:TRP:O	6:8:32:VAL:HG23	2.19	0.42
1:o:166:TRP:HE1	1:o:305:VAL:C	2.27	0.42
2:x:196:LEU:HD12	2:x:196:LEU:HA	1.70	0.42
3:y:229:PHE:CB	3:y:244:ALA:HB2	2.49	0.42
3:y:229:PHE:CZ	3:y:247:ARG:NH1	2.88	0.42
4:t:48:ARG:CG	6:n:8:GLY:HA3	2.48	0.42
15:q:101:CRT:H372	5:r:36:HIS:CD2	2.55	0.42
9:AB:101:BCL:HBC3	9:AB:101:BCL:H2C	1.86	0.42
5:AC:12:TRP:HD1	6:AD:18:HIS:HB2	1.85	0.42
6:AD:20:ILE:HD12	15:AD:101:CRT:C6	2.50	0.42
9:AI:101:BCL:H121	9:AI:101:BCL:H161	1.84	0.42
9:e:102:BCL:HHB	9:e:102:BCL:HMB3	1.86	0.42
5:j:31:LEU:O	5:j:35:ILE:HG13	2.20	0.42
5:l:46:TRP:CE2	9:l:101:BCL:HHC	2.55	0.42
3:M:134:TYR:CE1	3:M:144:GLN:HG3	2.54	0.42
4:H:112:GLY:C	4:H:114:ALA:N	2.76	0.42
6:E:46:LEU:HD23	6:G:42:TYR:HE1	1.85	0.42
6:G:25:MET:HG3	15:G:101:CRT:C20	2.49	0.42
5:I:3:THR:HB	6:J:18:HIS:NE2	2.35	0.42
9:N:101:BCL:HBA1	9:N:101:BCL:H3A	1.59	0.42
5:O:18:ARG:HE	5:O:18:ARG:HB2	1.68	0.42
6:X:20:ILE:HB	15:X:101:CRT:C9	2.49	0.42
5:Y:36:HIS:CE1	9:Z:102:BCL:HMD3	2.54	0.42
5:1:11:ILE:HD12	5:1:14:ILE:HD12	2.02	0.42
5:3:9:TYR:HB2	6:4:14:ALA:C	2.45	0.42
1:o:101:VAL:CG2	1:o:152:CYS:HB3	2.50	0.42
1:o:254:ARG:HH12	3:y:305:PRO:HG2	1.84	0.42
2:x:130:PHE:O	2:x:134:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:8:PHE:N	12:y:407:PEF:O2P	2.44	0.42
3:y:59:LEU:HD13	5:AC:26:ALA:HA	2.02	0.42
15:y:404:CRT:H2M1	5:AA:38:ILE:HG12	2.02	0.42
6:n:20:ILE:HG23	5:l:5:ASN:HB3	2.02	0.42
6:n:42:TYR:CE2	6:c:46:LEU:HD22	2.54	0.42
5:r:12:TRP:HE3	5:r:17:PRO:HG3	1.83	0.42
9:r:101:BCL:H71	9:r:101:BCL:H112	1.83	0.42
5:u:17:PRO:HB3	6:v:17:PHE:CZ	2.54	0.42
9:u:102:BCL:HBA1	6:v:32:VAL:HG11	2.01	0.42
6:v:17:PHE:HA	15:v:101:CRT:H6	2.02	0.42
9:i:102:BCL:HBB2	9:i:102:BCL:H143	2.02	0.42
1:C:153:TYR:CD1	1:C:157:ARG:HA	2.53	0.42
1:C:301:ASP:HB2	1:C:304:ARG:NH1	2.32	0.42
2:L:30:PHE:CE1	3:M:257:GLY:HA3	2.55	0.42
2:L:126:VAL:HG11	3:M:251:PHE:CE2	2.55	0.42
2:L:140:LEU:HD11	9:L:301:BCL:CED	2.49	0.42
4:H:27:ILE:HA	4:H:27:ILE:HD13	1.71	0.42
4:H:36:ARG:C	4:H:37:GLU:HG2	2.45	0.42
4:H:36:ARG:O	4:H:37:GLU:HG2	2.19	0.42
4:H:93:SER:HB3	4:H:98:SER:OG	2.20	0.42
4:H:122:HIS:HB3	4:t:121:LYS:NZ	2.22	0.42
15:E:101:CRT:H10	15:E:101:CRT:H81	1.88	0.42
15:P:102:CRT:H20	15:P:102:CRT:H181	1.83	0.42
15:R:101:CRT:H393	5:S:36:HIS:HB3	2.01	0.42
5:W:40:LEU:HG	5:W:46:TRP:CH2	2.55	0.42
5:1:51:ILE:HG13	5:1:51:ILE:H	1.43	0.42
9:2:102:BCL:H93	9:2:102:BCL:H111	1.82	0.42
6:4:20:ILE:HD12	15:4:101:CRT:H6	2.02	0.42
5:9:40:LEU:HD12	5:9:40:LEU:HA	1.71	0.42
6:0:40:TRP:HH2	6:0:46:LEU:OXT	2.02	0.42
2:x:18:ILE:HD12	2:x:35:PHE:CZ	2.54	0.42
2:x:194:LEU:HD12	10:y:402:BPH:C4C	2.50	0.42
3:y:81:TRP:CD1	5:AG:40:LEU:HG	2.55	0.42
4:t:235:GLU:O	4:t:239:VAL:HG23	2.19	0.42
4:t:251:THR:HG1	4:t:254:ARG:HG3	1.85	0.42
5:p:4:MET:O	5:p:5:ASN:HB2	2.19	0.42
15:AC:101:CRT:H20	15:AC:101:CRT:H181	1.84	0.42
6:AL:45:TRP:O	5:d:51:ILE:HG22	2.20	0.42
1:C:202:PRO:O	1:C:208:ASN:HB2	2.20	0.41
1:C:254:ARG:NH1	3:M:305:PRO:HG2	2.35	0.41
2:L:177:HIS:NE2	9:L:301:BCL:HMC2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:301:BCL:HAA2	9:L:301:BCL:HBD	2.02	0.41
6:B:25:MET:HG3	15:9:101:CRT:C21	2.50	0.41
5:F:43:ASP:O	5:I:55:TYR:HB2	2.21	0.41
5:O:3:THR:O	5:O:4:MET:HG2	2.20	0.41
5:O:49:ASP:O	5:O:50:ASN:HB2	2.20	0.41
5:U:51:ILE:HG23	5:U:52:PRO:HA	2.02	0.41
6:V:32:VAL:HG11	9:V:102:BCL:HBA1	2.01	0.41
15:X:101:CRT:H342	9:Y:101:BCL:HBA2	2.02	0.41
9:8:101:BCL:H141	9:8:101:BCL:H162	1.77	0.41
9:9:102:BCL:H112	9:9:102:BCL:H91	1.78	0.41
2:x:140:LEU:CD2	2:x:257:ILE:HG12	2.50	0.41
2:x:226:ARG:HH21	3:y:47:GLN:HB3	1.85	0.41
2:x:233:ILE:HG12	2:x:237:ALA:HB1	2.02	0.41
2:x:238:ILE:HG12	11:x:304:UQ8:C1	2.50	0.41
3:y:242:GLY:HA2	4:t:119:ARG:HD2	2.02	0.41
9:m:103:BCL:H11	9:m:103:BCL:H3A	2.02	0.41
9:r:101:BCL:HBA1	9:r:101:BCL:H3A	1.57	0.41
5:u:10:LYS:O	5:u:13:LEU:HB2	2.20	0.41
6:AB:37:LEU:O	6:AB:41:LEU:HG	2.20	0.41
9:AC:102:BCL:HBD	9:AC:102:BCL:HAA1	2.01	0.41
5:AG:12:TRP:HB3	5:AG:17:PRO:HG3	2.01	0.41
9:d:101:BCL:HMD1	6:e:36:HIS:ND1	2.35	0.41
1:C:167:VAL:HG12	1:C:301:ASP:OD2	2.20	0.41
3:M:89:HIS:C	3:M:93:LEU:HG	2.44	0.41
5:A:50:ASN:HB3	5:A:54:SER:HA	2.02	0.41
9:G:102:BCL:H3A	9:G:102:BCL:HBA1	1.76	0.41
5:I:10:LYS:HA	5:I:13:LEU:HG	2.02	0.41
5:I:18:ARG:HE	5:I:18:ARG:HB2	1.69	0.41
5:S:10:LYS:O	5:S:14:ILE:HG13	2.19	0.41
5:W:10:LYS:HD3	15:Z:101:CRT:H31A	2.02	0.41
6:8:46:LEU:HD22	6:0:42:TYR:CZ	2.55	0.41
5:9:10:LYS:HB3	15:9:101:CRT:C4	2.50	0.41
2:x:77:PRO:HB2	2:x:152:GLY:HA2	2.01	0.41
2:x:173:PHE:CZ	2:x:260:SER:HB3	2.55	0.41
3:y:181:PRO:O	3:y:184:ASP:HB2	2.20	0.41
4:t:195:LEU:HA	4:t:196:PRO:HD3	1.77	0.41
5:m:2:PHE:C	5:m:4:MET:H	2.29	0.41
5:AG:16:ASP:OD1	5:AG:16:ASP:C	2.62	0.41
5:AG:21:LEU:HD23	5:AG:21:LEU:HA	1.66	0.41
5:AI:34:LEU:O	5:AI:37:MET:HB3	2.20	0.41
9:AI:102:BCL:HAA1	9:AI:102:BCL:CBD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AJ:11:ASP:O	6:AJ:15:LYS:HG3	2.19	0.41
6:g:29:PHE:O	6:g:33:VAL:HG23	2.20	0.41
5:l:8:LEU:HG	6:c:18:HIS:NE2	2.35	0.41
1:C:253:THR:HG21	2:L:171:TYR:CB	2.50	0.41
3:M:185:TRP:CH2	3:M:189:PHE:CD2	3.09	0.41
5:D:12:TRP:CZ3	5:D:20:VAL:HG11	2.56	0.41
6:E:23:GLN:HA	6:E:26:TYR:HB2	2.02	0.41
6:E:43:ARG:HG3	5:F:55:TYR:OH	2.19	0.41
5:I:7:ASN:OD1	5:I:9:TYR:HE2	2.03	0.41
9:Y:101:BCL:H111	9:Y:101:BCL:H151	1.64	0.41
15:0:101:CRT:H15	15:0:101:CRT:H131	1.89	0.41
1:o:242:SER:HA	1:o:308:MET:HE2	2.02	0.41
2:x:52:TRP:CH2	5:l:38:ILE:HG23	2.55	0.41
2:x:199:HIS:NE2	3:y:266:HIS:NE2	2.69	0.41
4:t:256:GLY:HA2	4:t:257:PRO:O	2.20	0.41
5:m:4:MET:HE2	5:m:7:ASN:HD22	1.86	0.41
5:m:50:ASN:CB	5:m:54:SER:HA	2.50	0.41
9:s:102:BCL:H52	9:s:102:BCL:H12	1.85	0.41
5:AC:9:TYR:C	5:AC:11:ILE:N	2.78	0.41
5:AC:28:GLN:HB3	9:AC:102:BCL:H42	2.02	0.41
9:AH:101:BCL:H3A	9:AH:101:BCL:HBA1	1.66	0.41
9:AL:102:BCL:CGA	9:AL:102:BCL:C3A	2.98	0.41
5:d:14:ILE:HG12	15:g:101:CRT:H1M1	2.03	0.41
5:f:33:LEU:HA	5:f:33:LEU:HD23	1.79	0.41
6:k:21:PHE:CA	15:k:101:CRT:H11	2.46	0.41
15:k:101:CRT:H10	15:k:101:CRT:H81	1.92	0.41
9:l:101:BCL:H121	9:l:101:BCL:H161	1.97	0.41
6:c:36:HIS:HE1	9:c:101:BCL:NB	2.18	0.41
2:L:17:LEU:HD23	2:L:17:LEU:HA	1.71	0.41
2:L:218:SER:HB3	4:H:175:SER:HB3	2.03	0.41
9:L:301:BCL:C4A	9:M:402:BCL:HBB2	2.50	0.41
3:M:260:VAL:HG12	4:H:34:ASP:CG	2.46	0.41
6:E:17:PHE:HD1	15:E:101:CRT:H33	1.86	0.41
15:G:101:CRT:H20	15:G:101:CRT:H181	1.76	0.41
5:I:27:PHE:HE2	15:I:102:CRT:C28	2.33	0.41
5:I:44:LEU:CD1	9:I:103:BCL:HMC1	2.49	0.41
15:I:102:CRT:H21A	15:I:102:CRT:H5	1.65	0.41
9:K:101:BCL:H122	9:K:101:BCL:H162	1.74	0.41
5:O:28:GLN:HE21	6:P:28:TRP:HE1	1.67	0.41
9:P:101:BCL:H102	9:P:101:BCL:H13	1.95	0.41
6:T:20:ILE:HD12	15:T:101:CRT:C6	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:16:GLU:O	6:V:20:ILE:HG13	2.20	0.41
6:X:16:GLU:HB3	15:X:101:CRT:H21A	2.02	0.41
9:2:102:BCL:H3A	9:2:102:BCL:HBA1	1.78	0.41
6:6:10:THR:OG1	6:6:13:GLU:HG3	2.20	0.41
5:9:17:PRO:HG2	6:0:9:LEU:HD11	2.02	0.41
6:0:20:ILE:HD13	6:0:20:ILE:HG21	1.88	0.41
1:o:151:THR:HG21	1:o:323:MET:HE2	2.02	0.41
2:x:17:LEU:HD23	2:x:17:LEU:HA	1.82	0.41
3:y:159:VAL:HG21	3:y:285:LEU:HD22	2.03	0.41
4:t:135:PRO:HB3	4:t:171:TRP:CE2	2.56	0.41
9:m:103:BCL:HBA1	9:m:103:BCL:H12	1.76	0.41
15:z:101:CRT:H20	15:z:101:CRT:H181	1.94	0.41
6:AB:31:LEU:O	6:AB:34:ILE:HB	2.20	0.41
6:AJ:9:LEU:HB3	6:AJ:13:GLU:O	2.20	0.41
5:AK:39:VAL:HG11	9:AK:101:BCL:CBC	2.48	0.41
5:d:11:ILE:HD12	5:d:14:ILE:HD12	2.01	0.41
9:c:101:BCL:HBB2	9:c:101:BCL:H121	2.02	0.41
1:C:263:THR:HG22	3:M:311:VAL:CG1	2.46	0.41
2:L:113:GLU:OE2	2:L:126:VAL:HG12	2.21	0.41
2:L:281:TRP:CE3	3:M:88:LYS:HB2	2.55	0.41
3:M:65:LEU:HD11	10:M:403:BPH:H122	2.01	0.41
15:E:101:CRT:H393	5:F:36:HIS:HB3	2.02	0.41
9:I:103:BCL:H193	6:J:40:TRP:CZ2	2.55	0.41
5:K:35:ILE:HD11	15:O:101:CRT:H403	2.03	0.41
15:P:102:CRT:H2M1	5:Q:37:MET:HG2	2.03	0.41
9:Z:102:BCL:HBA1	9:Z:102:BCL:H3A	1.86	0.41
5:5:43:ASP:OD1	5:7:56:GLN:HG2	2.20	0.41
6:6:25:MET:HG3	15:7:101:CRT:C21	2.50	0.41
9:8:101:BCL:HBD	9:8:101:BCL:HAA1	2.03	0.41
1:o:17:SER:OG	1:o:19:MET:HG2	2.19	0.41
1:o:256:PHE:CZ	2:x:171:TYR:CE2	3.07	0.41
10:x:302:BPH:H3A	10:x:302:BPH:HBA2	1.69	0.41
4:t:36:ARG:NH1	4:t:62:PRO:HG2	2.34	0.41
4:t:39:TYR:HA	4:t:40:PRO:C	2.46	0.41
4:t:253:GLU:C	4:t:255:ALA:H	2.27	0.41
9:m:103:BCL:H111	9:m:103:BCL:H71	1.86	0.41
6:AD:21:PHE:CD1	6:AD:21:PHE:C	2.98	0.41
5:AE:11:ILE:HD13	15:AH:102:CRT:H10	2.02	0.41
6:i:37:LEU:O	6:i:41:LEU:HG	2.20	0.41
2:L:52:TRP:O	2:L:56:ILE:HG23	2.20	0.41
2:L:196:LEU:HD13	3:M:216:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:63:PHE:HB2	3:M:125:SER:HB2	2.02	0.41
3:M:201:PHE:CE1	3:M:282:ILE:HG21	2.56	0.41
4:H:133:ILE:HG22	4:H:171:TRP:HE3	1.86	0.41
4:H:182:LEU:HD23	4:H:182:LEU:HA	1.72	0.41
15:X:101:CRT:H15	15:X:101:CRT:H131	1.94	0.41
6:8:36:HIS:CD2	9:8:101:BCL:H161	2.56	0.41
2:x:11:ARG:HG2	2:x:26:TRP:CZ2	2.55	0.41
2:x:177:HIS:CE1	9:y:401:BCL:HBC1	2.56	0.41
2:x:182:HIS:CE1	2:x:186:ILE:HD11	2.55	0.41
3:y:99:PRO:HD2	3:y:102:TYR:HD2	1.85	0.41
6:q:32:VAL:HG21	9:q:102:BCL:CGA	2.51	0.41
5:r:9:TYR:C	5:r:11:ILE:N	2.78	0.41
9:s:102:BCL:H62	9:s:102:BCL:H41	1.90	0.41
5:u:37:MET:HE1	5:u:40:LEU:HD12	2.02	0.41
15:AF:102:CRT:H36	15:AF:102:CRT:H341	1.95	0.41
5:AK:17:PRO:HG2	6:AL:9:LEU:HD11	2.01	0.41
5:AK:18:ARG:O	5:AK:22:VAL:HG23	2.20	0.41
1:C:187:SER:OG	1:C:189:THR:HB	2.20	0.41
3:M:234:GLU:OE2	3:M:266:HIS:CE1	2.74	0.41
6:B:31:LEU:HD23	6:B:31:LEU:HA	1.70	0.41
5:D:31:LEU:HD12	5:D:34:LEU:HD23	2.03	0.41
6:G:17:PHE:CD1	15:G:101:CRT:H9	2.56	0.41
9:G:102:BCL:H141	9:G:102:BCL:H162	1.69	0.41
5:K:5:ASN:HB2	5:K:8:LEU:HB2	2.02	0.41
5:O:44:LEU:HD23	5:Q:55:TYR:CD2	2.56	0.41
6:R:20:ILE:HD12	15:R:101:CRT:C6	2.51	0.41
15:2:101:CRT:H10	15:2:101:CRT:H81	1.82	0.41
5:3:12:TRP:CD1	6:4:17:PHE:HD2	2.39	0.41
9:6:101:BCL:H3A	9:6:101:BCL:C1	2.50	0.41
5:9:51:ILE:HD11	6:0:43:ARG:HH22	1.85	0.41
6:0:9:LEU:HD23	6:0:14:ALA:HA	2.03	0.41
1:o:242:SER:HA	1:o:308:MET:CE	2.51	0.41
2:x:227:ASP:O	3:y:51:ILE:HG13	2.21	0.41
2:x:240:ARG:NH1	3:y:43:ILE:HA	2.35	0.41
2:x:273:ASN:C	2:x:275:TRP:N	2.79	0.41
3:y:143:SER:HB2	3:y:145:HIS:ND1	2.35	0.41
4:t:233:LEU:HD23	4:t:233:LEU:HA	1.92	0.41
9:q:102:BCL:HBA1	9:q:102:BCL:CED	2.50	0.41
6:z:24:SER:O	6:z:27:ALA:HB3	2.21	0.41
9:z:102:BCL:HMA1	9:AB:101:BCL:HMA1	2.02	0.41
6:AB:36:HIS:CD2	9:AB:102:BCL:H102	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AB:101:BCL:HBA1	9:AB:101:BCL:H3A	1.87	0.41
5:AC:28:GLN:HB3	9:AC:102:BCL:H12	2.03	0.41
5:AE:46:TRP:HA	6:AF:43:ARG:HH12	1.84	0.41
9:AE:102:BCL:H192	6:AF:40:TRP:NE1	2.35	0.41
6:AF:20:ILE:HD12	15:AF:102:CRT:C6	2.50	0.41
9:AL:102:BCL:H3A	9:AL:102:BCL:H12	2.03	0.41
9:e:102:BCL:H92	9:e:102:BCL:H61	1.89	0.41
1:C:72:ALA:N	1:C:85:LEU:O	2.42	0.41
2:L:196:LEU:HD12	2:L:196:LEU:HA	1.64	0.41
3:M:42:LYS:HE3	12:M:408:PEF:O2P	2.21	0.41
9:A:103:BCL:HBA1	9:A:103:BCL:H3A	1.74	0.41
9:D:101:BCL:H11	9:D:101:BCL:H51	1.93	0.41
5:I:4:MET:O	5:I:5:ASN:HB2	2.20	0.41
15:R:101:CRT:H20	15:R:101:CRT:H181	1.94	0.41
15:0:101:CRT:H10	15:0:101:CRT:H81	1.90	0.41
1:o:287:LEU:O	1:o:291:LEU:HD12	2.20	0.41
2:x:167:SER:HA	9:x:301:BCL:CBC	2.48	0.41
2:x:186:ILE:HD13	9:x:303:BCL:HMD2	2.01	0.41
2:x:216:LYS:HD3	2:x:220:HIS:CE1	2.56	0.41
2:x:225:PHE:CD2	11:x:304:UQ8:C7	3.04	0.41
3:y:108:PRO:HA	5:AC:41:SER:O	2.21	0.41
3:y:162:PHE:HB2	15:y:404:CRT:H291	2.01	0.41
3:y:219:HIS:CE1	3:y:223:ILE:HD11	2.56	0.41
3:y:304:ALA:HA	3:y:305:PRO:HD2	1.96	0.41
4:t:149:PRO:HG3	4:t:204:LYS:HD3	2.03	0.41
5:p:49:ASP:O	5:p:51:ILE:HD12	2.20	0.41
6:q:17:PHE:HD1	15:q:101:CRT:H6	1.86	0.41
6:AH:40:TRP:CE3	6:AH:44:PRO:HA	2.55	0.41
5:AI:3:THR:HG22	6:AJ:18:HIS:HE2	1.86	0.41
15:i:101:CRT:H2M1	5:j:36:HIS:HB3	2.03	0.41
5:l:17:PRO:HG2	6:c:9:LEU:HD11	2.02	0.41
1:C:47:ARG:NE	5:3:48:ASP:OD1	2.53	0.41
1:C:81:VAL:HB	7:C:501:HEM:O1D	2.21	0.41
2:L:175:HIS:CD2	2:L:178:TYR:HE1	2.36	0.41
2:L:196:LEU:HD11	3:M:269:ALA:HB1	2.02	0.41
3:M:268:TRP:CD2	4:H:30:LEU:HD13	2.56	0.41
15:M:405:CRT:H15	15:M:405:CRT:H131	1.95	0.41
4:H:136:MET:HE2	4:H:136:MET:HB3	1.83	0.41
5:A:11:ILE:HD11	5:D:21:LEU:HD11	2.02	0.41
6:B:28:TRP:O	6:B:32:VAL:HG23	2.21	0.41
5:D:44:LEU:HD12	5:F:47:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:39:VAL:CG2	9:I:103:BCL:H3C	2.51	0.41
5:Q:9:TYR:C	5:Q:11:ILE:H	2.29	0.41
6:R:17:PHE:HA	15:R:101:CRT:C6	2.37	0.41
5:S:5:ASN:HD22	6:V:20:ILE:HG23	1.86	0.41
6:V:18:HIS:O	6:V:22:MET:HG2	2.20	0.41
9:X:102:BCL:HBA1	9:X:102:BCL:H3A	1.87	0.41
6:4:17:PHE:CD1	15:4:101:CRT:H9	2.56	0.41
15:4:101:CRT:H15	15:4:101:CRT:H131	1.81	0.41
15:7:103:CRT:H342	9:9:102:BCL:HBA2	2.02	0.41
1:o:174:TYR:CE1	1:o:180:PRO:HA	2.56	0.41
1:o:196:PRO:HG2	1:o:231:TRP:CD2	2.56	0.41
1:o:226:LEU:O	1:o:229:ALA:HB3	2.21	0.41
2:x:116:ILE:HD13	3:y:254:TRP:CB	2.51	0.41
2:x:211:LYS:HG2	12:x:306:PEF:C11	2.51	0.41
2:x:240:ARG:NE	3:y:6:ASN:O	2.51	0.41
3:y:218:MET:HG3	3:y:218:MET:H	1.52	0.41
15:m:104:CRT:H20	15:m:104:CRT:H181	1.95	0.41
9:q:102:BCL:H111	9:q:102:BCL:H93	1.87	0.41
5:r:50:ASN:HB3	5:r:54:SER:HB3	2.03	0.41
6:z:31:LEU:HA	6:z:31:LEU:HD23	1.74	0.41
6:z:43:ARG:HG3	5:AA:55:TYR:OH	2.20	0.41
5:AC:49:ASP:O	5:AC:50:ASN:HB2	2.21	0.41
6:AL:43:ARG:HG2	5:d:55:TYR:CZ	2.56	0.41
5:h:12:TRP:CH2	5:h:20:VAL:HG11	2.56	0.41
5:j:18:ARG:H	5:j:18:ARG:HG2	1.58	0.41
2:L:12:VAL:HG22	2:L:13:ARG:N	2.36	0.41
2:L:18:ILE:HD12	2:L:35:PHE:HZ	1.86	0.41
2:L:116:ILE:HD13	3:M:254:TRP:CB	2.51	0.41
2:L:130:PHE:CE2	2:L:134:ILE:HD11	2.56	0.41
2:L:140:LEU:HA	2:L:140:LEU:HD23	1.85	0.41
3:M:71:ILE:O	3:M:75:MET:HG3	2.22	0.41
3:M:126:ILE:HD12	3:M:157:TYR:CZ	2.56	0.41
3:M:156:PHE:CD2	9:M:402:BCL:H43	2.56	0.41
12:H:302:PEF:C31	5:A:19:ARG:HB2	2.51	0.41
5:D:14:ILE:HG22	5:F:18:ARG:HG2	2.03	0.41
9:K:101:BCL:HHB	9:K:101:BCL:HMB3	1.86	0.41
9:O:102:BCL:H172	9:O:102:BCL:H13	1.78	0.41
5:S:42:THR:HG21	5:U:47:LEU:HD13	2.02	0.41
5:Y:21:LEU:HD23	5:Y:21:LEU:HA	1.92	0.41
5:5:17:PRO:HG2	6:6:9:LEU:HD11	2.03	0.41
6:0:12:ASP:O	6:0:15:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:28:PRO:HD3	2:x:262:PRO:HA	2.02	0.41
1:o:142:LYS:C	1:o:144:HIS:H	2.28	0.41
1:o:311:HIS:NE2	7:o:504:HEM:NC	2.69	0.41
1:o:311:HIS:CE1	7:o:504:HEM:NA	2.89	0.41
2:x:32:VAL:HG12	2:x:33:GLY:O	2.20	0.41
2:x:155:PHE:CE2	9:x:305:BCL:HMC2	2.56	0.41
5:u:46:TRP:HA	6:v:43:ARG:HH12	1.86	0.41
5:AC:9:TYR:C	5:AC:11:ILE:H	2.29	0.41
9:AI:101:BCL:H41	9:AI:101:BCL:H62	1.90	0.41
9:AI:102:BCL:HMB3	9:AI:102:BCL:HHB	1.84	0.41
15:AJ:101:CRT:H2M1	5:AK:37:MET:HG3	2.03	0.41
5:l:51:ILE:HA	5:l:52:PRO:HA	1.77	0.41
1:C:144:HIS:CD2	1:C:144:HIS:C	2.99	0.40
9:M:401:BCL:H92	9:M:401:BCL:H62	1.80	0.40
9:A:102:BCL:HBA2	15:0:101:CRT:H342	2.02	0.40
6:E:40:TRP:HZ3	6:E:46:LEU:H	1.69	0.40
5:S:12:TRP:CZ3	5:S:20:VAL:HG11	2.55	0.40
6:T:40:TRP:HZ3	6:T:45:TRP:H	1.67	0.40
5:Y:36:HIS:CE1	9:Z:102:BCL:OBD	2.74	0.40
5:1:24:ILE:HD11	9:3:101:BCL:H152	2.03	0.40
5:5:43:ASP:HB2	5:7:48:ASP:HA	2.04	0.40
1:o:59:VAL:H	1:o:59:VAL:HG22	1.59	0.40
2:x:106:PHE:CE1	9:x:301:BCL:H121	2.56	0.40
9:x:301:BCL:HAA2	9:x:301:BCL:HBD	2.03	0.40
15:s:101:CRT:H181	15:s:101:CRT:H20	1.84	0.40
9:u:102:BCL:H112	9:u:102:BCL:H91	1.74	0.40
6:AB:32:VAL:CG2	9:AB:102:BCL:HBA2	2.48	0.40
5:AG:50:ASN:ND2	5:AG:54:SER:OG	2.53	0.40
9:AK:101:BCL:H61	9:AK:101:BCL:H41	1.67	0.40
9:AL:102:BCL:H141	9:AL:102:BCL:H162	1.70	0.40
5:f:51:ILE:HA	5:f:52:PRO:HA	1.95	0.40
5:l:16:ASP:HB3	5:l:19:ARG:HE	1.85	0.40
1:C:62:LEU:O	1:C:63:PRO:C	2.64	0.40
1:C:144:HIS:NE2	7:C:504:HEM:NC	2.69	0.40
3:M:199:ASN:ND2	3:M:294:TRP:CE2	2.89	0.40
5:K:14:ILE:HD11	15:P:102:CRT:H21A	2.03	0.40
6:R:31:LEU:O	6:R:34:ILE:HB	2.22	0.40
5:S:50:ASN:ND2	5:U:60:LYS:HA	2.36	0.40
5:W:16:ASP:OD2	5:W:19:ARG:HG3	2.21	0.40
1:o:211:ARG:HD3	3:y:317:TYR:CE2	2.56	0.40
2:x:232:SER:OG	11:x:304:UQ8:O5	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:199:ASN:O	3:y:203:MET:HG3	2.21	0.40
4:t:65:LYS:HG2	4:t:78:ALA:O	2.21	0.40
9:m:103:BCL:HAA1	9:m:103:BCL:HBD	2.02	0.40
5:r:21:LEU:HD23	5:r:21:LEU:HA	1.87	0.40
5:r:22:VAL:O	5:r:25:VAL:HB	2.21	0.40
6:s:33:VAL:O	6:s:37:LEU:HG	2.22	0.40
9:s:102:BCL:HBA1	9:s:102:BCL:H12	1.72	0.40
5:w:44:LEU:HD22	6:z:43:ARG:HD3	2.03	0.40
5:f:49:ASP:O	5:f:50:ASN:HB2	2.20	0.40
5:l:3:THR:CB	5:l:8:LEU:HB2	2.46	0.40
2:L:21:ASP:HA	2:L:24:ASP:HB3	2.02	0.40
2:L:194:LEU:HD11	10:M:403:BPH:ND	2.36	0.40
9:L:301:BCL:HAA2	9:M:401:BCL:HBC1	2.02	0.40
3:M:63:PHE:CB	3:M:125:SER:HB2	2.51	0.40
3:M:215:LEU:HD23	3:M:215:LEU:HA	1.81	0.40
15:M:405:CRT:H2M3	5:O:38:ILE:HA	2.02	0.40
4:H:238:LYS:HA	4:H:238:LYS:HD3	1.94	0.40
6:E:42:TYR:HE2	6:E:43:ARG:HE	1.66	0.40
9:I:101:BCL:H12	6:J:28:TRP:CZ2	2.56	0.40
9:I:103:BCL:HBC1	6:J:39:ALA:HB1	2.04	0.40
5:Q:51:ILE:HD13	6:R:43:ARG:HH22	1.84	0.40
5:9:49:ASP:O	5:9:50:ASN:HB2	2.21	0.40
2:x:176:PHE:HB3	9:x:301:BCL:H3C	2.03	0.40
3:y:253:ARG:HG3	3:y:253:ARG:HH11	1.87	0.40
4:t:135:PRO:HD3	4:t:171:TRP:CE3	2.56	0.40
5:m:10:LYS:HB3	15:q:101:CRT:H1M1	2.03	0.40
5:p:19:ARG:NH1	12:p:101:PEF:HN2	2.20	0.40
6:q:17:PHE:CD1	15:q:101:CRT:H9	2.56	0.40
9:w:101:BCL:H203	15:z:101:CRT:H131	2.04	0.40
5:AK:49:ASP:HB3	5:AK:51:ILE:HG22	2.03	0.40
6:e:17:PHE:N	15:e:101:CRT:H23	2.35	0.40
15:g:101:CRT:H392	9:h:101:BCL:HMB2	2.02	0.40
5:l:21:LEU:HD23	5:l:21:LEU:HA	1.90	0.40
2:L:179:ASN:OD1	2:L:179:ASN:C	2.65	0.40
3:M:21:VAL:HA	3:M:22:PRO:HD3	1.84	0.40
3:M:256:MET:HE3	3:M:256:MET:HB2	1.88	0.40
5:A:18:ARG:HG3	5:9:15:LEU:HD23	2.03	0.40
9:A:102:BCL:H72	9:A:102:BCL:H41	2.04	0.40
9:A:103:BCL:H142	9:A:103:BCL:H112	1.83	0.40
5:I:10:LYS:O	5:I:13:LEU:HB2	2.21	0.40
5:K:35:ILE:HG12	5:K:38:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:101:CRT:H26	15:T:101:CRT:H241	1.91	0.40
9:U:101:BCL:H2	6:V:28:TRP:CZ2	2.57	0.40
5:W:21:LEU:HA	5:W:21:LEU:HD23	1.76	0.40
5:W:35:ILE:O	5:W:38:ILE:N	2.54	0.40
5:1:36:HIS:CE1	9:2:102:BCL:CMD	3.04	0.40
6:6:32:VAL:HG11	9:6:101:BCL:H12	2.03	0.40
7:o:504:HEM:HBB2	7:o:504:HEM:HMB2	2.03	0.40
2:x:61:PRO:HB3	5:m:41:SER:HA	2.02	0.40
3:y:21:VAL:HA	3:y:22:PRO:HD3	1.87	0.40
3:y:37:SER:HB2	12:y:406:PEF:C2	2.51	0.40
3:y:229:PHE:CE2	3:y:247:ARG:HD3	2.55	0.40
3:y:273:ALA:O	3:y:274:VAL:C	2.63	0.40
6:n:13:GLU:HG2	6:n:16:GLU:OE1	2.22	0.40
15:n:101:CRT:C11	5:l:3:THR:HG23	2.52	0.40
5:r:15:LEU:O	5:r:17:PRO:HD3	2.20	0.40
5:r:55:TYR:C	5:r:57:ALA:N	2.74	0.40
9:s:102:BCL:H3A	9:s:102:BCL:H12	2.03	0.40
15:AD:101:CRT:H81	15:AD:101:CRT:H10	1.84	0.40
15:AH:102:CRT:H20	15:AH:102:CRT:H181	1.97	0.40
15:e:101:CRT:C37	9:f:101:BCL:HMB2	2.52	0.40
9:e:102:BCL:H192	9:e:102:BCL:H161	1.76	0.40
1:C:32:GLN:HB2	2:L:80:LEU:HG	2.03	0.40
1:C:178:LEU:HA	3:M:110:SER:CB	2.49	0.40
9:L:301:BCL:HAA2	9:L:301:BCL:CBD	2.52	0.40
9:D:101:BCL:H111	9:D:101:BCL:H93	1.72	0.40
5:I:12:TRP:CD1	6:J:17:PHE:HD2	2.39	0.40
9:I:103:BCL:HMC2	9:I:103:BCL:HHC	1.86	0.40
5:S:45:ASN:HB3	5:U:56:GLN:OE1	2.20	0.40
15:T:101:CRT:H10	15:T:101:CRT:H81	1.95	0.40
6:X:24:SER:HB2	15:X:101:CRT:C14	2.46	0.40
5:3:40:LEU:HD23	5:3:40:LEU:HA	1.87	0.40
6:8:18:HIS:O	6:8:22:MET:HG2	2.21	0.40
6:8:36:HIS:CG	9:8:101:BCL:H13	2.56	0.40
9:8:101:BCL:HHB	9:8:101:BCL:HMB1	1.90	0.40
1:o:310:CYS:SG	7:o:504:HEM:CAC	3.10	0.40
3:y:240:HIS:NE2	4:t:69:LEU:HD11	2.37	0.40
3:y:253:ARG:NH1	3:y:253:ARG:HG3	2.36	0.40
4:t:16:ILE:HD12	4:t:16:ILE:HA	1.89	0.40
9:m:103:BCL:HBA1	9:m:103:BCL:H3A	1.76	0.40
5:p:13:LEU:HD23	5:p:13:LEU:HA	1.84	0.40
5:r:27:PHE:CZ	5:u:29:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:44:LEU:HD12	5:w:47:LEU:HA	2.03	0.40
5:AK:12:TRP:O	6:AL:7:THR:OG1	2.27	0.40
5:d:14:ILE:HD11	15:g:101:CRT:C7	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:52:PRO:O	1:o:77:GLN:NE2[1_554]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	315/333 (95%)	274 (87%)	33 (10%)	8 (2%)	4 23
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	4 23
2	L	278/281 (99%)	248 (89%)	26 (9%)	4 (1%)	9 33
2	x	278/281 (99%)	247 (89%)	28 (10%)	3 (1%)	11 39
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	9 35
3	y	316/319 (99%)	286 (90%)	26 (8%)	4 (1%)	9 35
4	H	256/259 (99%)	216 (84%)	31 (12%)	9 (4%)	3 18
4	t	256/259 (99%)	214 (84%)	32 (12%)	10 (4%)	2 16
5	1	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3 18
5	3	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1 7
5	5	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3 18
5	7	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1 11
5	9	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3 18
5	AA	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1 11
5	AC	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1 7
5	AE	59/61 (97%)	49 (83%)	7 (12%)	3 (5%)	1 11
5	AG	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3 18
5	AI	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3 18
5	AK	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3 18
5	D	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7 30
5	F	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1 11
5	I	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1 11
5	K	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7 30
5	O	58/61 (95%)	46 (79%)	8 (14%)	4 (7%)	1 7
5	Q	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1 7
5	S	59/61 (97%)	49 (83%)	8 (14%)	2 (3%)	3 18
5	U	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1 11
5	W	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7 30
5	Y	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1 11
5	d	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3 18
5	f	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1 7
5	h	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3 18
5	j	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3 18
5	l	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1 11
5	m	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7 30
5	p	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3 18
5	r	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	0 4
5	u	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1 11
5	w	58/61 (95%)	49 (84%)	8 (14%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	8	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AB	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	AJ	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AL	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	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%)	38 (100%)	0	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	P	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	Z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	38 (100%)	0	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100
6	s	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	v	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4783 (88%)	483 (9%)	138 (3%)	4	23

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASP
1	C	195	LEU
2	L	262	PRO
4	H	142	PHE
4	H	250	ALA
5	A	10	LYS
5	A	60	LYS
5	F	3	THR
5	F	5	ASN
5	O	5	ASN
5	O	59	GLY
5	Y	60	LYS
5	3	5	ASN
6	0	8	GLY
1	o	21	LEU
1	o	66	ASP
1	o	195	LEU
2	x	262	PRO
4	t	5	ILE
4	t	142	PHE
4	t	250	ALA
5	m	10	LYS
5	p	57	ALA
5	p	60	LYS
5	r	3	THR
5	r	6	ALA
5	r	60	LYS
5	AA	5	ASN
5	AA	6	ALA
5	AC	4	MET
5	AC	49	ASP
5	AK	60	LYS
5	d	58	LEU
5	f	5	ASN
1	C	21	LEU
1	C	83	LYS
1	C	84	ASP
2	L	21	ASP
4	H	5	ILE
4	H	38	GLY
4	H	188	ALA
5	F	10	LYS
5	I	10	LYS

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Mol	Chain	Res	Type
5	K	10	LYS
5	O	6	ALA
5	O	10	LYS
5	Q	6	ALA
5	Q	10	LYS
5	S	10	LYS
5	S	58	LEU
5	U	10	LYS
5	U	54	SER
5	W	5	ASN
5	1	10	LYS
5	1	58	LEU
5	3	6	ALA
5	5	10	LYS
5	7	10	LYS
5	7	60	LYS
5	9	10	LYS
5	9	59	GLY
1	o	83	LYS
1	o	84	ASP
2	x	21	ASP
4	t	38	GLY
4	t	140	LYS
4	t	188	ALA
5	r	10	LYS
5	r	59	GLY
5	u	10	LYS
5	w	10	LYS
5	AA	10	LYS
5	AC	6	ALA
5	AC	10	LYS
5	AE	6	ALA
5	AE	59	GLY
5	AG	6	ALA
5	AG	10	LYS
5	AI	10	LYS
5	AK	10	LYS
5	d	10	LYS
5	f	59	GLY
5	h	10	LYS
5	l	10	LYS
3	M	3	GLU

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Mol	Chain	Res	Type
3	M	29	PRO
4	H	140	LYS
4	H	177	PRO
5	D	5	ASN
5	I	6	ALA
5	Y	59	GLY
5	5	8	LEU
5	9	4	MET
5	9	6	ALA
3	y	3	GLU
3	y	29	PRO
3	y	34	PRO
4	t	177	PRO
5	u	5	ASN
5	AE	10	LYS
5	f	10	LYS
5	j	6	ALA
5	l	4	MET
1	C	67	SER
1	C	253	THR
3	M	34	PRO
3	M	276	THR
5	U	59	GLY
5	3	10	LYS
5	7	6	ALA
5	j	3	THR
1	C	184	ASN
5	I	59	GLY
5	Y	10	LYS
5	3	56	GLN
1	o	67	SER
1	o	184	ASN
1	o	253	THR
3	y	276	THR
5	f	6	ALA
5	h	60	LYS
5	l	59	GLY
4	H	213	ALA
6	B	8	GLY
5	Q	4	MET
5	9	5	ASN
4	t	213	ALA

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Mol	Chain	Res	Type
5	u	6	ALA
5	AI	6	ALA
2	L	32	VAL
2	x	32	VAL
5	Q	59	GLY
4	t	227	ASN
6	AH	8	GLY
2	L	141	VAL
6	N	8	GLY
4	H	227	ASN
4	t	59	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/278 (95%)	243 (92%)	22 (8%)	10	34
1	o	265/278 (95%)	246 (93%)	19 (7%)	13	40
2	L	228/229 (100%)	214 (94%)	14 (6%)	17	45
2	x	228/229 (100%)	214 (94%)	14 (6%)	17	45
3	M	256/257 (100%)	239 (93%)	17 (7%)	15	43
3	y	256/257 (100%)	238 (93%)	18 (7%)	14	41
4	H	210/211 (100%)	192 (91%)	18 (9%)	10	33
4	t	210/211 (100%)	188 (90%)	22 (10%)	6	25
5	1	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	3	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	5	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	7	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	9	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	A	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	AA	52/56 (93%)	49 (94%)	3 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	49 (94%)	3 (6%)	18	47
5	AI	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	AK	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	D	52/56 (93%)	52 (100%)	0	100	100
5	F	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	I	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	Q	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	S	53/56 (95%)	52 (98%)	1 (2%)	50	68
5	U	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	W	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	Y	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	d	52/56 (93%)	50 (96%)	2 (4%)	29	57
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%)	51 (98%)	1 (2%)	50	68
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%)	49 (94%)	3 (6%)	18	47
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	32 (97%)	1 (3%)	36	61
6	E	33/39 (85%)	32 (97%)	1 (3%)	36	61
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
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%)	33 (100%)	0	100	100
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	33 (100%)	0	100	100
6	g	33/39 (85%)	33 (100%)	0	100	100
6	i	33/39 (85%)	33 (100%)	0	100	100
6	k	33/39 (85%)	33 (100%)	0	100	100
6	n	33/39 (85%)	33 (100%)	0	100	100
6	q	33/39 (85%)	33 (100%)	0	100	100
6	s	33/39 (85%)	33 (100%)	0	100	100
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%)	4444 (96%)	196 (4%)	26	55

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	MET
1	C	21	LEU

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Mol	Chain	Res	Type
1	C	48	GLN
1	C	53	ILE
1	C	74	GLU
1	C	84	ASP
1	C	86	SER
1	C	130	MET
1	C	148	THR
1	C	167	VAL
1	C	173	LYS
1	C	178	LEU
1	C	181	THR
1	C	190	VAL
1	C	212	ILE
1	C	226	LEU
1	C	238	ASN
1	C	277	ARG
1	C	289	ASP
1	C	304	ARG
1	C	307	CYS
1	C	318	LEU
2	L	75	ILE
2	L	89	LEU
2	L	94	LEU
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
3	M	25	LYS
3	M	31	ILE
3	M	37	SER
3	M	42	LYS
3	M	45	ASP
3	M	55	LEU
3	M	68	ILE
3	M	182	HIS

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Mol	Chain	Res	Type
3	M	232	ASP
3	M	235	ILE
3	M	238	ILE
3	M	256	MET
3	M	274	VAL
3	M	279	THR
3	M	310	VAL
3	M	311	VAL
3	M	312	THR
4	H	45	ARG
4	H	75	THR
4	H	77	VAL
4	H	107	MET
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
5	A	53	VAL
6	B	20	ILE
6	E	21	PHE
5	F	14	ILE
5	I	3	THR
5	I	53	VAL
5	O	5	ASN
6	P	21	PHE
5	Q	2	PHE
5	Q	3	THR
5	S	51	ILE
5	U	53	VAL
5	W	24	ILE
5	W	48	ASP

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Mol	Chain	Res	Type
6	X	13	GLU
5	Y	9	TYR
5	Y	51	ILE
5	1	51	ILE
5	1	53	VAL
5	1	55	TYR
5	3	44	LEU
5	3	50	ASN
5	5	14	ILE
5	7	48	ASP
5	9	8	LEU
5	9	13	LEU
1	o	21	LEU
1	o	47	ARG
1	o	48	GLN
1	o	53	ILE
1	o	68	THR
1	o	84	ASP
1	o	86	SER
1	o	130	MET
1	o	167	VAL
1	o	173	LYS
1	o	181	THR
1	o	190	VAL
1	o	212	ILE
1	o	221	SER
1	o	277	ARG
1	o	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	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

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Mol	Chain	Res	Type
2	x	248	SER
2	x	255	VAL
2	x	256	CYS
3	y	3	GLU
3	y	25	LYS
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	232	ASP
3	y	235	ILE
3	y	274	VAL
3	y	279	THR
3	y	285	LEU
3	y	310	VAL
3	y	311	VAL
3	y	312	THR
4	t	45	ARG
4	t	60	ASP
4	t	75	THR
4	t	77	VAL
4	t	81	VAL
4	t	106	PRO
4	t	107	MET
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
4	t	230	GLN
4	t	258	LEU

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Mol	Chain	Res	Type
4	t	259	LEU
5	r	37	MET
5	u	3	THR
5	u	18	ARG
5	u	53	VAL
5	w	5	ASN
5	AA	5	ASN
5	AA	43	ASP
5	AA	44	LEU
5	AC	2	PHE
5	AC	3	THR
5	AE	8	LEU
5	AG	2	PHE
5	AG	51	ILE
5	AG	53	VAL
5	AI	5	ASN
6	AJ	13	GLU
5	AK	48	ASP
5	AK	51	ILE
5	d	24	ILE
5	d	53	VAL
5	f	3	THR
5	h	14	ILE
5	j	48	ASP
5	l	8	LEU
5	l	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	80	GLN
1	C	183	GLN
1	C	208	ASN
1	C	312	GLN
2	L	96	GLN
2	L	125	HIS
2	L	208	ASN
3	M	85	GLN
3	M	240	HIS
3	M	259	ASN
4	H	7	HIS
4	H	122	HIS

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Mol	Chain	Res	Type
4	H	189	ASN
4	H	218	HIS
4	H	230	GLN
5	F	5	ASN
5	I	56	GLN
5	O	28	GLN
6	T	23	GLN
5	U	36	HIS
5	Y	36	HIS
5	1	56	GLN
6	2	23	GLN
6	4	18	HIS
6	6	36	HIS
1	o	208	ASN
1	o	238	ASN
2	x	125	HIS
2	x	182	HIS
3	y	74	ASN
3	y	259	ASN
4	t	221	ASN
5	m	7	ASN
5	m	50	ASN
5	p	50	ASN
5	r	56	GLN
5	w	5	ASN
5	w	50	ASN
5	AA	36	HIS
5	AA	56	GLN
5	AI	5	ASN
5	AK	36	HIS
6	e	18	HIS
5	f	5	ASN
5	h	36	HIS
5	j	28	GLN
5	j	56	GLN
5	l	56	GLN
6	c	36	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
15	CRT	AC	101	-	43,43,43	0.70	0	48,54,54	2.35	18 (37%)
7	HEM	o	502	1	50,50,50	2.48	9 (18%)	67,82,82	2.17	24 (35%)
9	BCL	m	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.08	25 (31%)
9	BCL	j	101	-	69,74,74	1.71	13 (18%)	79,115,115	2.12	26 (32%)
9	BCL	AG	101	-	69,74,74	1.71	12 (17%)	79,115,115	2.20	30 (37%)
9	BCL	y	401	-	69,74,74	1.80	14 (20%)	79,115,115	2.09	29 (36%)
12	PEF	p	101	-	15,15,46	0.95	1 (6%)	17,19,51	0.98	1 (5%)
15	CRT	4	101	-	43,43,43	0.83	0	48,54,54	2.41	24 (50%)
12	PEF	M	408	-	18,18,46	1.79	2 (11%)	21,23,51	1.63	2 (9%)
9	BCL	AK	101	-	69,74,74	1.72	13 (18%)	79,115,115	2.11	29 (36%)
12	PEF	x	306	-	18,18,46	1.75	2 (11%)	21,23,51	1.34	3 (14%)
10	BPH	L	302	-	59,70,70	0.55	1 (1%)	59,101,101	1.97	13 (22%)
15	CRT	7	103	-	43,43,43	0.99	2 (4%)	48,54,54	1.87	10 (20%)
9	BCL	W	101	-	69,74,74	1.74	14 (20%)	79,115,115	1.98	25 (31%)
9	BCL	u	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.09	27 (34%)
9	BCL	A	103	-	69,74,74	1.78	16 (23%)	79,115,115	2.11	28 (35%)
9	BCL	P	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.07	27 (34%)
9	BCL	AB	102	-	69,74,74	1.69	15 (21%)	79,115,115	2.07	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	p	102	-	69,74,74	1.72	14 (20%)	79,115,115	2.11	26 (32%)
9	BCL	z	102	-	69,74,74	1.69	12 (17%)	79,115,115	2.03	28 (35%)
9	BCL	0	102	-	69,74,74	1.78	14 (20%)	79,115,115	2.06	26 (32%)
9	BCL	x	301	-	69,74,74	1.78	14 (20%)	79,115,115	2.27	25 (31%)
12	PEF	H	305	-	18,18,46	1.47	2 (11%)	21,23,51	1.55	3 (14%)
7	HEM	C	502	1	50,50,50	2.49	10 (20%)	67,82,82	2.07	20 (29%)
9	BCL	U	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.04	28 (35%)
9	BCL	r	101	-	69,74,74	1.78	15 (21%)	79,115,115	1.98	27 (34%)
9	BCL	w	101	-	69,74,74	1.76	13 (18%)	79,115,115	2.10	29 (36%)
9	BCL	AL	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.04	28 (35%)
9	BCL	9	102	-	69,74,74	1.70	13 (18%)	79,115,115	2.00	22 (27%)
9	BCL	I	103	-	69,74,74	1.74	14 (20%)	79,115,115	2.08	26 (32%)
11	UQ8	x	304	-	53,53,53	1.57	4 (7%)	66,67,67	1.94	19 (28%)
12	PEF	t	301	-	18,18,46	1.60	2 (11%)	21,23,51	1.30	3 (14%)
10	BPH	M	403	-	59,70,70	0.74	1 (1%)	59,101,101	1.79	7 (11%)
9	BCL	AC	103	-	69,74,74	1.65	13 (18%)	79,115,115	2.11	26 (32%)
9	BCL	O	102	-	69,74,74	1.72	12 (17%)	79,115,115	2.18	33 (41%)
15	CRT	M	405	-	43,43,43	0.78	0	48,54,54	2.17	13 (27%)
15	CRT	O	101	-	43,43,43	0.65	0	48,54,54	2.48	18 (37%)
12	PEF	m	101	-	18,18,46	1.55	2 (11%)	21,23,51	1.64	3 (14%)
15	CRT	Z	101	-	43,43,43	0.79	0	48,54,54	2.18	18 (37%)
7	HEM	o	503	1	50,50,50	2.55	10 (20%)	67,82,82	2.00	19 (28%)
9	BCL	m	103	-	69,74,74	1.73	15 (21%)	79,115,115	2.03	28 (35%)
15	CRT	AD	101	-	43,43,43	0.85	0	48,54,54	2.35	17 (35%)
9	BCL	2	102	-	69,74,74	1.78	14 (20%)	79,115,115	2.13	27 (34%)
17	PGW	S	101	-	20,20,50	1.04	1 (5%)	23,26,56	1.32	1 (4%)
15	CRT	T	101	-	43,43,43	0.71	0	48,54,54	2.27	14 (29%)
9	BCL	7	102	-	69,74,74	1.66	12 (17%)	79,115,115	2.07	27 (34%)
12	PEF	y	407	-	18,18,46	1.68	2 (11%)	21,23,51	1.27	3 (14%)
15	CRT	V	101	-	43,43,43	0.71	0	48,54,54	2.44	16 (33%)
12	PEF	A	101	-	18,18,46	1.46	2 (11%)	21,23,51	1.97	4 (19%)
9	BCL	q	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.07	26 (32%)
12	PEF	H	302	-	18,18,46	1.57	2 (11%)	21,23,51	1.82	2 (9%)
12	PEF	H	304	-	18,18,46	1.65	2 (11%)	21,23,51	1.61	2 (9%)
9	BCL	6	101	-	69,74,74	1.78	14 (20%)	79,115,115	2.10	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	h	101	-	69,74,74	1.71	13 (18%)	79,115,115	2.06	27 (34%)
9	BCL	G	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.00	25 (31%)
15	CRT	AL	101	-	43,43,43	0.79	0	48,54,54	2.04	15 (31%)
17	PGW	AE	101	-	20,20,50	1.00	1 (5%)	23,26,56	1.38	3 (13%)
15	CRT	AH	102	-	43,43,43	0.74	0	48,54,54	2.11	13 (27%)
9	BCL	R	102	-	69,74,74	1.71	15 (21%)	79,115,115	2.22	30 (37%)
15	CRT	g	101	-	43,43,43	0.83	0	48,54,54	2.33	14 (29%)
9	BCL	d	101	-	69,74,74	1.81	15 (21%)	79,115,115	2.06	28 (35%)
12	PEF	L	305	-	11,11,46	0.79	0	13,14,51	1.15	1 (7%)
15	CRT	n	101	-	43,43,43	0.77	0	48,54,54	2.42	21 (43%)
15	CRT	R	101	-	43,43,43	0.85	0	48,54,54	2.17	14 (29%)
9	BCL	L	303	-	69,74,74	1.80	15 (21%)	79,115,115	2.15	26 (32%)
9	BCL	s	102	-	69,74,74	1.80	14 (20%)	79,115,115	2.18	27 (34%)
15	CRT	I	102	-	43,43,43	0.76	0	48,54,54	2.38	14 (29%)
15	CRT	v	101	-	43,43,43	0.70	0	48,54,54	2.55	18 (37%)
9	BCL	e	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.08	28 (35%)
9	BCL	f	101	-	69,74,74	1.83	16 (23%)	79,115,115	2.08	26 (32%)
15	CRT	0	101	-	43,43,43	0.76	0	48,54,54	2.34	20 (41%)
9	BCL	g	102	-	69,74,74	1.73	15 (21%)	79,115,115	2.15	31 (39%)
12	PEF	t	303	-	18,18,46	1.46	2 (11%)	21,23,51	2.28	8 (38%)
7	HEM	C	501	1	50,50,50	2.57	8 (16%)	67,82,82	2.18	22 (32%)
9	BCL	1	101	-	69,74,74	1.74	14 (20%)	79,115,115	2.05	24 (30%)
15	CRT	AJ	101	-	43,43,43	0.79	0	48,54,54	2.38	14 (29%)
9	BCL	AI	101	-	69,74,74	1.75	14 (20%)	79,115,115	2.12	30 (37%)
9	BCL	Q	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.12	28 (35%)
9	BCL	M	401	-	69,74,74	1.72	14 (20%)	79,115,115	2.20	25 (31%)
9	BCL	AB	101	-	69,74,74	1.72	12 (17%)	79,115,115	2.05	26 (32%)
9	BCL	x	305	-	69,74,74	1.81	13 (18%)	79,115,115	2.26	28 (35%)
9	BCL	k	102	-	69,74,74	1.75	14 (20%)	79,115,115	2.16	30 (37%)
9	BCL	u	102	-	69,74,74	1.77	14 (20%)	79,115,115	2.20	25 (31%)
9	BCL	AI	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.08	23 (29%)
9	BCL	A	102	-	69,74,74	1.74	11 (15%)	79,115,115	2.03	26 (32%)
9	BCL	l	101	-	69,74,74	1.69	13 (18%)	79,115,115	2.18	30 (37%)
12	PEF	y	408	-	18,18,46	1.73	2 (11%)	21,23,51	2.44	6 (28%)
16	PO4	M	406	-	4,4,4	0.53	0	6,6,6	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BPH	y	402	-	59,70,70	0.88	3 (5%)	59,101,101	1.59	9 (15%)
15	CRT	i	101	-	43,43,43	0.75	0	48,54,54	2.19	15 (31%)
9	BCL	AE	102	-	69,74,74	1.69	12 (17%)	79,115,115	2.14	29 (36%)
7	HEM	o	504	1	50,50,50	2.55	11 (22%)	67,82,82	1.81	16 (23%)
9	BCL	I	101	-	69,74,74	1.76	14 (20%)	79,115,115	2.08	28 (35%)
9	BCL	Y	101	-	69,74,74	1.76	11 (15%)	79,115,115	2.03	25 (31%)
9	BCL	T	102	-	69,74,74	1.72	14 (20%)	79,115,115	2.23	31 (39%)
9	BCL	AF	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.04	28 (35%)
7	HEM	C	504	1	50,50,50	2.54	10 (20%)	67,82,82	1.93	16 (23%)
15	CRT	AF	102	-	43,43,43	0.70	0	48,54,54	2.33	14 (29%)
14	MQ8	M	404	-	54,54,54	1.03	6 (11%)	67,69,69	1.46	11 (16%)
15	CRT	X	101	-	43,43,43	0.90	0	48,54,54	1.94	10 (20%)
15	CRT	q	101	-	43,43,43	0.73	0	48,54,54	2.13	14 (29%)
12	PEF	M	407	-	15,15,46	1.10	1 (6%)	17,19,51	1.15	1 (5%)
15	CRT	P	102	-	43,43,43	0.66	0	48,54,54	2.15	15 (31%)
15	CRT	9	101	-	43,43,43	0.72	0	48,54,54	2.43	19 (39%)
9	BCL	3	101	-	69,74,74	1.71	14 (20%)	79,115,115	2.06	26 (32%)
15	CRT	m	104	-	43,43,43	0.67	0	48,54,54	2.34	20 (41%)
9	BCL	i	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.15	34 (43%)
15	CRT	k	101	-	43,43,43	0.76	0	48,54,54	2.15	14 (29%)
9	BCL	L	301	-	69,74,74	1.79	15 (21%)	79,115,115	2.19	32 (40%)
14	MQ8	y	403	-	54,54,54	1.10	5 (9%)	67,69,69	1.59	17 (25%)
9	BCL	X	102	-	69,74,74	1.76	12 (17%)	79,115,115	2.21	29 (36%)
12	PEF	H	301	-	18,18,46	1.46	2 (11%)	21,23,51	1.67	3 (14%)
15	CRT	s	101	-	43,43,43	0.77	1 (2%)	48,54,54	2.22	15 (31%)
15	CRT	7	101	-	43,43,43	0.79	0	48,54,54	2.50	17 (35%)
9	BCL	4	102	-	69,74,74	1.76	15 (21%)	79,115,115	2.21	28 (35%)
9	BCL	AH	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.10	27 (34%)
11	UQ8	L	304	-	53,53,53	1.53	4 (7%)	66,67,67	1.71	17 (25%)
16	PO4	H	303	-	4,4,4	0.67	0	6,6,6	0.76	0
16	PO4	y	405	-	4,4,4	0.79	0	6,6,6	1.15	0
15	CRT	G	101	-	43,43,43	0.68	0	48,54,54	2.16	15 (31%)
9	BCL	K	101	-	69,74,74	1.71	12 (17%)	79,115,115	2.09	28 (35%)
9	BCL	x	303	-	69,74,74	1.89	15 (21%)	79,115,115	2.14	28 (35%)
16	PO4	t	302	-	4,4,4	0.92	0	6,6,6	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	Z	102	-	69,74,74	1.73	12 (17%)	79,115,115	2.28	29 (36%)
9	BCL	AC	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.11	28 (35%)
9	BCL	S	102	-	69,74,74	1.74	13 (18%)	79,115,115	2.05	24 (30%)
9	BCL	M	402	-	69,74,74	1.75	13 (18%)	79,115,115	2.33	30 (37%)
15	CRT	E	101	-	43,43,43	0.81	0	48,54,54	2.00	14 (29%)
9	BCL	F	101	-	69,74,74	1.72	14 (20%)	79,115,115	2.12	29 (36%)
9	BCL	D	101	-	69,74,74	1.70	12 (17%)	79,115,115	2.13	24 (30%)
9	BCL	D	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.16	33 (41%)
9	BCL	c	101	-	69,74,74	1.70	13 (18%)	79,115,115	2.06	27 (34%)
9	BCL	5	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.08	25 (31%)
9	BCL	V	102	-	69,74,74	1.73	14 (20%)	79,115,115	2.11	31 (39%)
15	CRT	y	404	-	43,43,43	0.83	0	48,54,54	2.06	12 (25%)
15	CRT	e	101	-	43,43,43	0.68	0	48,54,54	2.15	16 (33%)
10	BPH	x	302	-	59,70,70	0.71	1 (1%)	59,101,101	1.80	13 (22%)
7	HEM	o	501	1	50,50,50	2.58	9 (18%)	67,82,82	1.93	16 (23%)
12	PEF	y	406	-	18,18,46	1.55	2 (11%)	21,23,51	2.10	4 (19%)
9	BCL	N	101	-	69,74,74	1.69	13 (18%)	79,115,115	2.11	27 (34%)
7	HEM	C	503	1	50,50,50	2.55	10 (20%)	67,82,82	2.29	23 (34%)
9	BCL	8	101	-	69,74,74	1.74	14 (20%)	79,115,115	2.12	24 (30%)
15	CRT	2	101	-	43,43,43	0.79	0	48,54,54	1.87	15 (31%)
15	CRT	z	101	-	43,43,43	0.73	0	48,54,54	2.31	19 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AC	101	-	-	10/51/51/51	-
7	HEM	o	502	1	-	3/14/54/54	-
9	BCL	m	102	-	-	13/41/137/137	-
9	BCL	j	101	-	-	17/41/137/137	-
9	BCL	AG	101	-	-	17/41/137/137	-
9	BCL	y	401	-	-	12/41/137/137	-
12	PEF	p	101	-	-	3/16/16/50	-
15	CRT	4	101	-	-	17/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	M	408	-	-	11/20/20/50	-
9	BCL	AK	101	-	-	14/41/137/137	-
12	PEF	x	306	-	-	10/20/20/50	-
10	BPH	L	302	-	-	16/37/105/105	0/5/6/6
15	CRT	7	103	-	-	7/51/51/51	-
9	BCL	W	101	-	-	18/41/137/137	-
9	BCL	u	101	-	-	20/41/137/137	-
9	BCL	A	103	-	-	10/41/137/137	-
9	BCL	P	101	-	-	12/41/137/137	-
9	BCL	AB	102	-	-	16/41/137/137	-
9	BCL	p	102	-	-	12/41/137/137	-
9	BCL	z	102	-	-	17/41/137/137	-
9	BCL	0	102	-	-	16/41/137/137	-
9	BCL	x	301	-	-	12/41/137/137	-
12	PEF	H	305	-	-	10/20/20/50	-
7	HEM	C	502	1	-	5/14/54/54	-
9	BCL	U	101	-	-	16/41/137/137	-
9	BCL	r	101	-	-	17/41/137/137	-
9	BCL	w	101	-	-	15/41/137/137	-
9	BCL	AL	102	-	-	16/41/137/137	-
9	BCL	9	102	-	-	10/41/137/137	-
9	BCL	I	103	-	-	13/41/137/137	-
11	UQ8	x	304	-	-	16/51/75/75	0/1/1/1
12	PEF	t	301	-	-	6/20/20/50	-
10	BPH	M	403	-	-	15/37/105/105	0/5/6/6
9	BCL	AC	103	-	-	16/41/137/137	-
9	BCL	O	102	-	-	14/41/137/137	-
15	CRT	M	405	-	-	13/51/51/51	-
15	CRT	O	101	-	-	7/51/51/51	-
12	PEF	m	101	-	-	8/20/20/50	-
15	CRT	Z	101	-	-	10/51/51/51	-
7	HEM	o	503	1	-	5/14/54/54	-
9	BCL	m	103	-	-	16/41/137/137	-
15	CRT	AD	101	-	-	9/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	2	102	-	-	12/41/137/137	-
17	PGW	S	101	-	-	11/23/23/55	-
15	CRT	T	101	-	-	6/51/51/51	-
9	BCL	7	102	-	-	18/41/137/137	-
12	PEF	y	407	-	-	5/20/20/50	-
15	CRT	V	101	-	-	16/51/51/51	-
12	PEF	A	101	-	-	8/20/20/50	-
9	BCL	q	102	-	-	17/41/137/137	-
12	PEF	H	302	-	-	6/20/20/50	-
12	PEF	H	304	-	-	11/20/20/50	-
9	BCL	6	101	-	-	13/41/137/137	-
9	BCL	h	101	-	-	9/41/137/137	-
9	BCL	G	102	-	-	16/41/137/137	-
15	CRT	AL	101	-	-	8/51/51/51	-
17	PGW	AE	101	-	-	10/23/23/55	-
15	CRT	AH	102	-	-	12/51/51/51	-
9	BCL	R	102	-	-	15/41/137/137	-
15	CRT	g	101	-	-	5/51/51/51	-
9	BCL	d	101	-	-	11/41/137/137	-
12	PEF	L	305	-	-	4/11/11/50	-
15	CRT	n	101	-	-	14/51/51/51	-
15	CRT	R	101	-	-	14/51/51/51	-
9	BCL	L	303	-	-	18/41/137/137	-
9	BCL	s	102	-	-	15/41/137/137	-
15	CRT	I	102	-	-	7/51/51/51	-
15	CRT	v	101	-	-	8/51/51/51	-
9	BCL	e	102	-	-	14/41/137/137	-
9	BCL	f	101	-	-	17/41/137/137	-
15	CRT	0	101	-	-	10/51/51/51	-
9	BCL	g	102	-	-	17/41/137/137	-
12	PEF	t	303	-	-	8/20/20/50	-
7	HEM	C	501	1	-	7/14/54/54	-
9	BCL	1	101	-	-	16/41/137/137	-
15	CRT	AJ	101	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AI	101	-	-	14/41/137/137	-
9	BCL	Q	101	-	-	14/41/137/137	-
9	BCL	M	401	-	-	16/41/137/137	-
9	BCL	AB	101	-	-	13/41/137/137	-
9	BCL	x	305	-	-	16/41/137/137	-
9	BCL	k	102	-	-	22/41/137/137	-
9	BCL	u	102	-	-	10/41/137/137	-
9	BCL	AI	102	-	-	17/41/137/137	-
9	BCL	A	102	-	-	13/41/137/137	-
9	BCL	l	101	-	-	16/41/137/137	-
12	PEF	y	408	-	-	8/20/20/50	-
10	BPH	y	402	-	-	13/37/105/105	0/5/6/6
15	CRT	i	101	-	-	8/51/51/51	-
9	BCL	AE	102	-	-	13/41/137/137	-
7	HEM	o	504	1	-	3/14/54/54	-
9	BCL	I	101	-	-	9/41/137/137	-
9	BCL	Y	101	-	-	12/41/137/137	-
9	BCL	T	102	-	-	13/41/137/137	-
9	BCL	AF	101	-	-	13/41/137/137	-
7	HEM	C	504	1	-	5/14/54/54	-
15	CRT	AF	102	-	-	5/51/51/51	-
14	MQ8	M	404	-	-	20/47/67/67	0/2/2/2
15	CRT	X	101	-	-	15/51/51/51	-
15	CRT	q	101	-	-	7/51/51/51	-
12	PEF	M	407	-	-	3/16/16/50	-
15	CRT	P	102	-	-	7/51/51/51	-
15	CRT	9	101	-	-	12/51/51/51	-
9	BCL	3	101	-	-	12/41/137/137	-
15	CRT	m	104	-	-	3/51/51/51	-
9	BCL	i	102	-	-	17/41/137/137	-
15	CRT	k	101	-	-	9/51/51/51	-
9	BCL	L	301	-	-	9/41/137/137	-
14	MQ8	y	403	-	-	24/47/67/67	0/2/2/2
9	BCL	X	102	-	-	18/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	H	301	-	-	8/20/20/50	-
15	CRT	s	101	-	-	10/51/51/51	-
15	CRT	7	101	-	-	8/51/51/51	-
9	BCL	4	102	-	-	14/41/137/137	-
9	BCL	AH	101	-	-	20/41/137/137	-
11	UQ8	L	304	-	-	10/51/75/75	0/1/1/1
15	CRT	G	101	-	-	12/51/51/51	-
9	BCL	K	101	-	-	11/41/137/137	-
9	BCL	x	303	-	-	16/41/137/137	-
9	BCL	Z	102	-	-	14/41/137/137	-
9	BCL	AC	102	-	-	23/41/137/137	-
9	BCL	S	102	-	-	16/41/137/137	-
9	BCL	M	402	-	-	14/41/137/137	-
15	CRT	E	101	-	-	8/51/51/51	-
9	BCL	F	101	-	-	18/41/137/137	-
9	BCL	D	101	-	-	8/41/137/137	-
9	BCL	D	102	-	-	13/41/137/137	-
9	BCL	c	101	-	-	19/41/137/137	-
9	BCL	5	101	-	-	8/41/137/137	-
9	BCL	V	102	-	-	11/41/137/137	-
15	CRT	y	404	-	-	14/51/51/51	-
15	CRT	e	101	-	-	13/51/51/51	-
10	BPH	x	302	-	-	11/37/105/105	0/5/6/6
7	HEM	o	501	1	-	7/14/54/54	-
12	PEF	y	406	-	-	6/20/20/50	-
9	BCL	N	101	-	-	15/41/137/137	-
7	HEM	C	503	1	-	3/14/54/54	-
9	BCL	8	101	-	-	23/41/137/137	-
15	CRT	2	101	-	-	6/51/51/51	-
15	CRT	z	101	-	-	2/51/51/51	-

All (1118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	FE-NB	14.40	2.39	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	501	HEM	FE-NB	14.11	2.38	1.94
7	C	503	HEM	FE-NB	14.05	2.38	1.94
7	o	503	HEM	FE-NB	13.96	2.37	1.94
7	C	501	HEM	FE-NB	13.85	2.37	1.94
7	o	502	HEM	FE-NB	13.78	2.37	1.94
7	C	504	HEM	FE-NB	13.62	2.36	1.94
7	C	502	HEM	FE-NB	13.51	2.36	1.94
11	L	304	UQ8	C6-C1	8.34	1.50	1.35
11	x	304	UQ8	C6-C1	8.27	1.50	1.35
9	x	303	BCL	MG-ND	-7.44	1.91	2.05
9	f	101	BCL	MG-ND	-6.33	1.93	2.05
9	L	301	BCL	MG-ND	-6.20	1.93	2.05
9	S	102	BCL	MG-ND	-6.19	1.93	2.05
9	0	102	BCL	MG-ND	-6.13	1.93	2.05
9	I	101	BCL	MG-ND	-6.13	1.93	2.05
9	L	303	BCL	MG-ND	-6.11	1.93	2.05
9	M	401	BCL	MG-ND	-6.04	1.93	2.05
9	6	101	BCL	MG-ND	-6.04	1.93	2.05
9	X	102	BCL	MG-ND	-6.03	1.93	2.05
9	w	101	BCL	MG-ND	-6.02	1.93	2.05
9	2	102	BCL	MG-ND	-6.02	1.93	2.05
9	U	101	BCL	MG-ND	-6.00	1.93	2.05
9	e	102	BCL	MG-ND	-6.00	1.93	2.05
9	I	103	BCL	MG-ND	-5.99	1.93	2.05
9	s	102	BCL	MG-ND	-5.99	1.93	2.05
9	A	102	BCL	MG-ND	-5.98	1.93	2.05
9	AI	101	BCL	MG-ND	-5.95	1.94	2.05
9	A	103	BCL	MG-ND	-5.94	1.94	2.05
12	M	408	PEF	O2-C10	5.93	1.48	1.35
9	4	102	BCL	MG-ND	-5.93	1.94	2.05
9	x	305	BCL	MG-ND	-5.92	1.94	2.05
9	P	101	BCL	MG-ND	-5.91	1.94	2.05
9	y	401	BCL	MG-ND	-5.89	1.94	2.05
9	K	101	BCL	MG-ND	-5.86	1.94	2.05
9	d	101	BCL	MG-ND	-5.85	1.94	2.05
9	Z	102	BCL	MG-ND	-5.84	1.94	2.05
9	i	102	BCL	MG-ND	-5.80	1.94	2.05
9	Y	101	BCL	MG-ND	-5.80	1.94	2.05
9	g	102	BCL	MG-ND	-5.80	1.94	2.05
9	Q	101	BCL	MG-ND	-5.79	1.94	2.05
9	r	101	BCL	MG-ND	-5.78	1.94	2.05
9	AL	102	BCL	MG-ND	-5.78	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AF	101	BCL	MG-ND	-5.77	1.94	2.05
9	AC	102	BCL	MG-ND	-5.76	1.94	2.05
9	u	102	BCL	MG-ND	-5.74	1.94	2.05
12	H	302	PEF	O2-C10	5.70	1.47	1.35
9	AK	101	BCL	MG-ND	-5.69	1.94	2.05
9	F	101	BCL	MG-ND	-5.68	1.94	2.05
9	5	101	BCL	MG-ND	-5.67	1.94	2.05
9	AB	101	BCL	MG-ND	-5.67	1.94	2.05
9	k	102	BCL	MG-ND	-5.65	1.94	2.05
12	x	306	PEF	O2-C10	5.65	1.47	1.35
9	O	102	BCL	MG-ND	-5.65	1.94	2.05
9	D	101	BCL	MG-ND	-5.64	1.94	2.05
9	N	101	BCL	MG-ND	-5.64	1.94	2.05
9	q	102	BCL	MG-ND	-5.64	1.94	2.05
9	p	102	BCL	MG-ND	-5.64	1.94	2.05
9	R	102	BCL	MG-ND	-5.64	1.94	2.05
9	e	102	BCL	MG-NB	-5.62	1.94	2.05
9	m	102	BCL	MG-ND	-5.61	1.94	2.05
9	T	102	BCL	MG-ND	-5.60	1.94	2.05
9	9	102	BCL	MG-ND	-5.60	1.94	2.05
9	G	102	BCL	MG-ND	-5.60	1.94	2.05
9	V	102	BCL	MG-ND	-5.60	1.94	2.05
9	h	101	BCL	MG-ND	-5.58	1.94	2.05
9	M	402	BCL	MG-ND	-5.57	1.94	2.05
9	y	401	BCL	MG-NB	-5.57	1.94	2.05
9	AE	102	BCL	MG-ND	-5.57	1.94	2.05
9	x	301	BCL	MG-ND	-5.54	1.94	2.05
9	AI	102	BCL	MG-ND	-5.54	1.94	2.05
12	H	304	PEF	O2-C10	5.53	1.47	1.35
9	4	102	BCL	MG-NB	-5.48	1.94	2.05
9	z	102	BCL	MG-ND	-5.46	1.95	2.05
9	s	102	BCL	MG-NB	-5.45	1.95	2.05
12	y	408	PEF	O2-C10	5.45	1.47	1.35
9	c	101	BCL	MG-ND	-5.43	1.95	2.05
9	AB	102	BCL	MG-ND	-5.41	1.95	2.05
12	y	407	PEF	O2-C10	5.41	1.47	1.35
9	1	101	BCL	MG-ND	-5.41	1.95	2.05
9	AG	101	BCL	MG-ND	-5.40	1.95	2.05
9	AH	101	BCL	MG-ND	-5.38	1.95	2.05
12	t	301	PEF	O2-C10	5.38	1.47	1.35
9	u	102	BCL	MG-NB	-5.37	1.95	2.05
9	f	101	BCL	MG-NB	-5.36	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AL	102	BCL	MG-NB	-5.36	1.95	2.05
9	8	101	BCL	MG-ND	-5.35	1.95	2.05
9	l	101	BCL	MG-ND	-5.35	1.95	2.05
9	O	102	BCL	MG-NB	-5.35	1.95	2.05
9	3	101	BCL	MG-ND	-5.34	1.95	2.05
7	C	501	HEM	FE-NC	5.34	2.12	1.95
9	W	101	BCL	MG-ND	-5.32	1.95	2.05
9	D	102	BCL	MG-ND	-5.31	1.95	2.05
9	x	303	BCL	MG-NB	-5.31	1.95	2.05
9	p	102	BCL	MG-NB	-5.31	1.95	2.05
9	r	101	BCL	MG-NB	-5.31	1.95	2.05
9	m	103	BCL	MG-ND	-5.29	1.95	2.05
9	L	303	BCL	MG-NB	-5.29	1.95	2.05
9	u	101	BCL	MG-ND	-5.28	1.95	2.05
9	j	101	BCL	MG-ND	-5.26	1.95	2.05
9	AC	103	BCL	MG-ND	-5.26	1.95	2.05
9	L	301	BCL	MG-NB	-5.24	1.95	2.05
9	AF	101	BCL	OBD-CAD	5.23	1.31	1.22
9	j	101	BCL	MG-NB	-5.22	1.95	2.05
9	Y	101	BCL	MG-NB	-5.22	1.95	2.05
9	Y	101	BCL	OBD-CAD	5.22	1.31	1.22
9	q	102	BCL	MG-NB	-5.21	1.95	2.05
9	5	101	BCL	MG-NB	-5.20	1.95	2.05
9	AF	101	BCL	MG-NB	-5.17	1.95	2.05
9	A	102	BCL	MG-NB	-5.16	1.95	2.05
9	A	103	BCL	MG-NB	-5.15	1.95	2.05
9	W	101	BCL	OBD-CAD	5.15	1.31	1.22
9	w	101	BCL	MG-NB	-5.14	1.95	2.05
9	m	102	BCL	MG-NB	-5.13	1.95	2.05
9	I	101	BCL	MG-NB	-5.13	1.95	2.05
9	u	101	BCL	MG-NB	-5.13	1.95	2.05
9	AB	101	BCL	OBD-CAD	5.12	1.31	1.22
9	5	101	BCL	OBD-CAD	5.11	1.31	1.22
9	k	102	BCL	MG-NB	-5.11	1.95	2.05
9	2	102	BCL	MG-NB	-5.10	1.95	2.05
9	AI	101	BCL	MG-NB	-5.10	1.95	2.05
9	Z	102	BCL	MG-NB	-5.09	1.95	2.05
9	m	103	BCL	MG-NB	-5.09	1.95	2.05
9	0	102	BCL	MG-NB	-5.09	1.95	2.05
9	Q	101	BCL	MG-NB	-5.09	1.95	2.05
9	d	101	BCL	MG-NB	-5.08	1.95	2.05
9	7	102	BCL	MG-ND	-5.08	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCL	OBD-CAD	5.07	1.31	1.22
9	M	401	BCL	MG-NB	-5.07	1.95	2.05
12	m	101	PEF	O2-C10	5.07	1.46	1.35
9	x	305	BCL	OBD-CAD	5.06	1.31	1.22
9	d	101	BCL	OBD-CAD	5.06	1.31	1.22
9	x	301	BCL	MG-NB	-5.05	1.95	2.05
9	8	101	BCL	MG-NB	-5.04	1.95	2.05
9	AB	101	BCL	MG-NB	-5.04	1.95	2.05
9	AH	101	BCL	OBD-CAD	5.03	1.31	1.22
9	i	102	BCL	MG-NB	-5.02	1.95	2.05
9	AC	102	BCL	MG-NB	-5.02	1.95	2.05
9	W	101	BCL	MG-NB	-5.02	1.95	2.05
9	F	101	BCL	MG-NB	-5.01	1.95	2.05
9	AE	102	BCL	MG-NB	-5.01	1.95	2.05
9	AK	101	BCL	MG-NB	-5.00	1.95	2.05
9	D	102	BCL	MG-NB	-5.00	1.95	2.05
9	U	101	BCL	MG-NB	-5.00	1.95	2.05
9	AB	102	BCL	OBD-CAD	5.00	1.31	1.22
9	L	301	BCL	OBD-CAD	4.99	1.31	1.22
9	1	101	BCL	OBD-CAD	4.99	1.31	1.22
9	z	102	BCL	OBD-CAD	4.98	1.31	1.22
9	6	101	BCL	MG-NB	-4.98	1.95	2.05
9	7	102	BCL	OBD-CAD	4.98	1.31	1.22
9	G	102	BCL	MG-NB	-4.97	1.95	2.05
9	0	102	BCL	OBD-CAD	4.97	1.31	1.22
9	T	102	BCL	OBD-CAD	4.96	1.31	1.22
9	N	101	BCL	OBD-CAD	4.96	1.31	1.22
9	O	102	BCL	OBD-CAD	4.96	1.31	1.22
9	M	402	BCL	MG-NB	-4.96	1.96	2.05
9	D	101	BCL	MG-NB	-4.95	1.96	2.05
9	3	101	BCL	MG-NB	-4.95	1.96	2.05
9	1	101	BCL	MG-NB	-4.95	1.96	2.05
9	I	103	BCL	OBD-CAD	4.95	1.31	1.22
9	AI	102	BCL	MG-NB	-4.95	1.96	2.05
9	K	101	BCL	MG-NB	-4.94	1.96	2.05
9	P	101	BCL	MG-NB	-4.94	1.96	2.05
9	AK	101	BCL	OBD-CAD	4.94	1.31	1.22
9	I	101	BCL	OBD-CAD	4.93	1.31	1.22
9	w	101	BCL	OBD-CAD	4.92	1.31	1.22
9	I	103	BCL	MG-NB	-4.92	1.96	2.05
9	G	102	BCL	OBD-CAD	4.92	1.30	1.22
9	g	102	BCL	MG-NB	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	HEM	C3B-C4B	4.91	1.54	1.44
9	V	102	BCL	MG-NB	-4.91	1.96	2.05
9	R	102	BCL	MG-NB	-4.89	1.96	2.05
9	9	102	BCL	OBD-CAD	4.88	1.30	1.22
9	g	102	BCL	OBD-CAD	4.88	1.30	1.22
9	D	102	BCL	OBD-CAD	4.88	1.30	1.22
9	AG	101	BCL	OBD-CAD	4.87	1.30	1.22
9	u	102	BCL	OBD-CAD	4.86	1.30	1.22
9	AC	102	BCL	OBD-CAD	4.86	1.30	1.22
9	l	101	BCL	MG-NB	-4.86	1.96	2.05
9	AI	102	BCL	OBD-CAD	4.86	1.30	1.22
9	V	102	BCL	OBD-CAD	4.85	1.30	1.22
9	K	101	BCL	OBD-CAD	4.85	1.30	1.22
9	Q	101	BCL	OBD-CAD	4.85	1.30	1.22
9	A	103	BCL	OBD-CAD	4.84	1.30	1.22
9	X	102	BCL	MG-NB	-4.84	1.96	2.05
9	3	101	BCL	OBD-CAD	4.84	1.30	1.22
9	y	401	BCL	OBD-CAD	4.83	1.30	1.22
9	7	102	BCL	MG-NB	-4.83	1.96	2.05
9	AI	101	BCL	OBD-CAD	4.82	1.30	1.22
9	l	101	BCL	OBD-CAD	4.82	1.30	1.22
9	T	102	BCL	MG-NB	-4.81	1.96	2.05
9	c	101	BCL	OBD-CAD	4.81	1.30	1.22
9	M	401	BCL	OBD-CAD	4.81	1.30	1.22
9	2	102	BCL	OBD-CAD	4.80	1.30	1.22
9	P	101	BCL	OBD-CAD	4.80	1.30	1.22
9	h	101	BCL	OBD-CAD	4.78	1.30	1.22
9	c	101	BCL	MG-NB	-4.77	1.96	2.05
9	u	101	BCL	OBD-CAD	4.77	1.30	1.22
9	x	301	BCL	OBD-CAD	4.76	1.30	1.22
9	m	102	BCL	OBD-CAD	4.75	1.30	1.22
9	9	102	BCL	MG-NB	-4.75	1.96	2.05
9	6	101	BCL	OBD-CAD	4.75	1.30	1.22
9	N	101	BCL	MG-NB	-4.74	1.96	2.05
9	j	101	BCL	OBD-CAD	4.74	1.30	1.22
9	U	101	BCL	OBD-CAD	4.74	1.30	1.22
9	f	101	BCL	OBD-CAD	4.73	1.30	1.22
7	o	504	HEM	C1B-NB	-4.73	1.32	1.40
9	R	102	BCL	OBD-CAD	4.72	1.30	1.22
9	M	402	BCL	OBD-CAD	4.72	1.30	1.22
9	A	102	BCL	OBD-CAD	4.72	1.30	1.22
7	C	501	HEM	C4D-ND	-4.72	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	y	406	PEF	O2-C10	4.71	1.45	1.35
9	S	102	BCL	OBD-CAD	4.70	1.30	1.22
9	S	102	BCL	MG-NB	-4.70	1.96	2.05
9	k	102	BCL	OBD-CAD	4.69	1.30	1.22
9	x	305	BCL	MG-NB	-4.69	1.96	2.05
9	AH	101	BCL	MG-NB	-4.68	1.96	2.05
9	s	102	BCL	OBD-CAD	4.67	1.30	1.22
9	q	102	BCL	OBD-CAD	4.66	1.30	1.22
7	o	501	HEM	FE-NC	4.65	2.10	1.95
9	e	102	BCL	OBD-CAD	4.63	1.30	1.22
9	x	303	BCL	OBD-CAD	4.63	1.30	1.22
12	H	301	PEF	O2-C10	4.63	1.45	1.35
9	m	103	BCL	OBD-CAD	4.63	1.30	1.22
7	o	502	HEM	FE-NC	4.62	2.10	1.95
12	t	303	PEF	O2-C10	4.59	1.45	1.35
9	i	102	BCL	OBD-CAD	4.55	1.30	1.22
7	C	502	HEM	FE-NC	4.55	2.10	1.95
9	D	101	BCL	OBD-CAD	4.53	1.30	1.22
9	4	102	BCL	OBD-CAD	4.51	1.30	1.22
9	AC	103	BCL	MG-NB	-4.51	1.96	2.05
9	F	101	BCL	OBD-CAD	4.50	1.30	1.22
9	AC	103	BCL	OBD-CAD	4.49	1.30	1.22
7	o	504	HEM	FE-NC	4.48	2.09	1.95
9	z	102	BCL	MG-NB	-4.47	1.96	2.05
9	8	101	BCL	OBD-CAD	4.47	1.30	1.22
9	X	102	BCL	OBD-CAD	4.46	1.30	1.22
9	AE	102	BCL	OBD-CAD	4.45	1.30	1.22
9	x	305	BCL	O1D-CGD	-4.44	1.10	1.21
12	H	305	PEF	O2-C10	4.44	1.45	1.35
9	AG	101	BCL	MG-NB	-4.42	1.97	2.05
7	C	502	HEM	C1B-NB	-4.38	1.32	1.40
9	x	301	BCL	O1D-CGD	-4.34	1.10	1.21
9	s	102	BCL	O1D-CGD	-4.32	1.10	1.21
9	AB	102	BCL	MG-NB	-4.32	1.97	2.05
12	A	101	PEF	O2-C10	4.30	1.44	1.35
7	o	503	HEM	FE-NC	4.30	2.09	1.95
9	L	303	BCL	OBD-CAD	4.29	1.29	1.22
9	p	102	BCL	OBD-CAD	4.28	1.29	1.22
7	C	504	HEM	C1B-NB	-4.27	1.32	1.40
7	o	501	HEM	C4D-ND	-4.25	1.32	1.40
9	2	102	BCL	O1D-CGD	-4.24	1.10	1.21
9	T	102	BCL	O1D-CGD	-4.22	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	102	BCL	OBD-CAD	4.20	1.29	1.22
9	h	101	BCL	MG-NB	-4.19	1.97	2.05
9	4	102	BCL	O1D-CGD	-4.18	1.10	1.21
7	o	501	HEM	C1B-NB	-4.17	1.33	1.40
9	V	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	AC	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	y	401	BCL	O2D-CED	4.13	1.54	1.45
9	k	102	BCL	O1D-CGD	-4.11	1.10	1.21
9	h	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	AL	102	BCL	OBD-CAD	4.10	1.29	1.22
7	C	504	HEM	C3C-C4C	-4.09	1.38	1.46
9	AG	101	BCL	O1D-CGD	-4.07	1.11	1.21
9	c	101	BCL	O1D-CGD	-4.06	1.11	1.21
9	X	102	BCL	O1D-CGD	-4.04	1.11	1.21
7	C	501	HEM	C1B-NB	-4.02	1.33	1.40
9	D	102	BCL	O1D-CGD	-4.02	1.11	1.21
9	f	101	BCL	O1D-CGD	-4.01	1.11	1.21
9	0	102	BCL	O1D-CGD	-4.01	1.11	1.21
9	AE	102	BCL	O1D-CGD	-4.00	1.11	1.21
9	AF	101	BCL	O1D-CGD	-4.00	1.11	1.21
9	u	101	BCL	O1D-CGD	-3.99	1.11	1.21
9	x	305	BCL	O1A-CGA	-3.98	1.10	1.22
9	5	101	BCL	O1D-CGD	-3.98	1.11	1.21
9	m	103	BCL	O2D-CED	3.97	1.54	1.45
9	L	303	BCL	O1D-CGD	-3.97	1.11	1.21
9	W	101	BCL	O1D-CGD	-3.97	1.11	1.21
9	d	101	BCL	O2D-CED	3.97	1.54	1.45
9	G	102	BCL	O1D-CGD	-3.96	1.11	1.21
9	m	102	BCL	O1D-CGD	-3.96	1.11	1.21
9	x	301	BCL	O2D-CED	3.95	1.54	1.45
9	p	102	BCL	O1D-CGD	-3.95	1.11	1.21
9	q	102	BCL	O1D-CGD	-3.94	1.11	1.21
9	AI	101	BCL	O1D-CGD	-3.94	1.11	1.21
9	AB	101	BCL	O1D-CGD	-3.94	1.11	1.21
9	AL	102	BCL	O1D-CGD	-3.93	1.11	1.21
9	M	402	BCL	O2D-CED	3.93	1.54	1.45
9	A	102	BCL	O1D-CGD	-3.93	1.11	1.21
9	P	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	Q	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	U	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	g	102	BCL	O1D-CGD	-3.91	1.11	1.21
9	x	305	BCL	O2D-CED	3.91	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	101	BCL	O1D-CGD	-3.90	1.11	1.21
9	9	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	w	101	BCL	O1D-CGD	-3.90	1.11	1.21
9	e	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	AI	102	BCL	O1D-CGD	-3.90	1.11	1.21
9	A	103	BCL	O1D-CGD	-3.89	1.11	1.21
9	Y	101	BCL	O2D-CED	3.89	1.53	1.45
9	m	103	BCL	O1D-CGD	-3.88	1.11	1.21
9	D	101	BCL	O1D-CGD	-3.88	1.11	1.21
9	8	101	BCL	O2D-CED	3.88	1.53	1.45
9	6	101	BCL	O1D-CGD	-3.87	1.11	1.21
9	Z	102	BCL	O1D-CGD	-3.87	1.11	1.21
9	i	102	BCL	O1D-CGD	-3.87	1.11	1.21
9	AH	101	BCL	O1D-CGD	-3.86	1.11	1.21
9	u	101	BCL	O2D-CED	3.85	1.53	1.45
9	I	101	BCL	O1D-CGD	-3.85	1.11	1.21
7	o	503	HEM	C4D-ND	-3.85	1.33	1.40
9	AK	101	BCL	O1D-CGD	-3.85	1.11	1.21
9	AL	102	BCL	O2D-CED	3.84	1.53	1.45
9	1	101	BCL	O2D-CED	3.84	1.53	1.45
9	AI	102	BCL	O2D-CED	3.83	1.53	1.45
7	C	504	HEM	FE-NC	3.83	2.07	1.95
9	AC	103	BCL	O1D-CGD	-3.83	1.11	1.21
7	C	502	HEM	C4D-ND	-3.82	1.33	1.40
9	M	401	BCL	O1D-CGD	-3.82	1.11	1.21
9	x	303	BCL	O2D-CED	3.82	1.53	1.45
9	z	102	BCL	O1D-CGD	-3.81	1.11	1.21
9	M	401	BCL	O2D-CED	3.81	1.53	1.45
9	M	402	BCL	O2A-CGA	-3.81	1.22	1.33
7	C	503	HEM	C3C-C4C	-3.81	1.39	1.46
9	S	102	BCL	O1D-CGD	-3.81	1.11	1.21
9	x	303	BCL	O1D-CGD	-3.80	1.11	1.21
9	m	102	BCL	O2D-CED	3.80	1.53	1.45
9	F	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	l	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	j	101	BCL	O1D-CGD	-3.78	1.11	1.21
7	o	502	HEM	C1B-NB	-3.78	1.33	1.40
9	R	102	BCL	O1D-CGD	-3.78	1.11	1.21
7	C	504	HEM	C4D-ND	-3.76	1.33	1.40
9	f	101	BCL	O2D-CED	3.74	1.53	1.45
9	1	101	BCL	O1D-CGD	-3.74	1.11	1.21
9	j	101	BCL	O2D-CED	3.74	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AK	101	BCL	O2D-CED	3.74	1.53	1.45
9	u	102	BCL	O1D-CGD	-3.73	1.11	1.21
9	F	101	BCL	O2D-CED	3.73	1.53	1.45
9	N	101	BCL	O1D-CGD	-3.73	1.11	1.21
9	L	301	BCL	O1D-CGD	-3.73	1.11	1.21
9	G	102	BCL	O2D-CED	3.73	1.53	1.45
7	o	501	HEM	C4B-NB	-3.72	1.31	1.38
9	6	101	BCL	O2D-CED	3.72	1.53	1.45
7	o	503	HEM	C1B-NB	-3.72	1.33	1.40
9	K	101	BCL	O1D-CGD	-3.72	1.11	1.21
9	x	305	BCL	O2A-CGA	-3.72	1.22	1.33
9	3	101	BCL	O2D-CED	3.70	1.53	1.45
9	l	101	BCL	O2D-CED	3.70	1.53	1.45
9	z	102	BCL	O2D-CED	3.69	1.53	1.45
9	c	101	BCL	O2D-CED	3.69	1.53	1.45
9	r	101	BCL	O2D-CED	3.68	1.53	1.45
9	A	102	BCL	O2D-CED	3.68	1.53	1.45
9	p	102	BCL	O2D-CED	3.67	1.53	1.45
9	I	103	BCL	O1D-CGD	-3.67	1.12	1.21
9	Y	101	BCL	O1D-CGD	-3.66	1.12	1.21
9	AB	102	BCL	O1D-CGD	-3.66	1.12	1.21
9	7	102	BCL	O2D-CED	3.66	1.53	1.45
9	S	102	BCL	O2D-CED	3.66	1.53	1.45
9	D	102	BCL	O2D-CED	3.65	1.53	1.45
7	o	502	HEM	C4D-ND	-3.64	1.33	1.40
9	9	102	BCL	O2D-CED	3.64	1.53	1.45
9	O	102	BCL	O2D-CED	3.63	1.53	1.45
9	r	101	BCL	O1D-CGD	-3.62	1.12	1.21
9	M	402	BCL	O1D-CGD	-3.60	1.12	1.21
9	AE	102	BCL	O2D-CED	3.60	1.53	1.45
7	C	503	HEM	C1B-NB	-3.58	1.34	1.40
9	V	102	BCL	O2D-CED	3.58	1.53	1.45
9	g	102	BCL	O2D-CED	3.58	1.53	1.45
7	C	501	HEM	C4B-NB	-3.58	1.31	1.38
9	0	102	BCL	O2D-CED	3.57	1.53	1.45
9	W	101	BCL	O2D-CED	3.57	1.53	1.45
9	y	401	BCL	O1D-CGD	-3.57	1.12	1.21
7	C	501	HEM	FE-ND	-3.57	1.83	1.94
9	I	101	BCL	O2D-CED	3.56	1.53	1.45
9	d	101	BCL	O1D-CGD	-3.56	1.12	1.21
9	AH	101	BCL	O2D-CED	3.54	1.53	1.45
9	O	102	BCL	O1D-CGD	-3.54	1.12	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	504	HEM	FE-ND	-3.53	1.84	1.94
9	e	102	BCL	O2D-CED	3.53	1.53	1.45
9	AC	103	BCL	O2D-CED	3.52	1.53	1.45
9	u	102	BCL	O2D-CED	3.51	1.53	1.45
9	AB	102	BCL	O2D-CED	3.51	1.53	1.45
9	h	101	BCL	O2D-CED	3.50	1.53	1.45
9	N	101	BCL	O2D-CED	3.50	1.53	1.45
9	A	103	BCL	O2D-CED	3.50	1.53	1.45
9	q	102	BCL	O2D-CED	3.50	1.53	1.45
9	X	102	BCL	O2D-CED	3.47	1.53	1.45
9	3	101	BCL	O1D-CGD	-3.47	1.12	1.21
9	4	102	BCL	O2D-CED	3.46	1.53	1.45
9	7	102	BCL	O1D-CGD	-3.46	1.12	1.21
9	K	101	BCL	O2D-CED	3.46	1.53	1.45
7	C	502	HEM	C4B-NB	-3.46	1.32	1.38
9	P	101	BCL	O2D-CED	3.45	1.53	1.45
9	I	103	BCL	O2D-CED	3.44	1.52	1.45
7	o	501	HEM	FE-ND	-3.44	1.84	1.94
9	5	101	BCL	O2D-CED	3.43	1.52	1.45
9	i	102	BCL	O2D-CED	3.42	1.52	1.45
9	y	401	BCL	O2A-CGA	-3.42	1.23	1.33
9	AB	101	BCL	O2D-CED	3.41	1.52	1.45
9	L	303	BCL	O2D-CED	3.41	1.52	1.45
9	AG	101	BCL	O2D-CED	3.40	1.52	1.45
9	D	101	BCL	O2D-CED	3.40	1.52	1.45
9	Q	101	BCL	O2D-CED	3.40	1.52	1.45
9	Z	102	BCL	O2D-CED	3.40	1.52	1.45
9	w	101	BCL	O2D-CED	3.39	1.52	1.45
9	AI	101	BCL	O2D-CED	3.38	1.52	1.45
9	x	301	BCL	C3C-C4C	3.35	1.55	1.51
9	3	101	BCL	O2A-CGA	-3.34	1.23	1.33
9	V	102	BCL	O2D-CGD	-3.33	1.25	1.33
9	U	101	BCL	O2D-CGD	-3.33	1.25	1.33
7	o	503	HEM	FE-ND	-3.33	1.84	1.94
9	y	401	BCL	O1A-CGA	-3.32	1.12	1.22
9	k	102	BCL	O2D-CGD	-3.32	1.25	1.33
9	A	102	BCL	O2A-CGA	-3.31	1.23	1.33
9	R	102	BCL	O2D-CGD	-3.30	1.25	1.33
7	C	503	HEM	C4D-ND	-3.30	1.34	1.40
9	AF	101	BCL	O2D-CED	3.30	1.52	1.45
9	AC	102	BCL	O2D-CED	3.30	1.52	1.45
9	R	102	BCL	O2D-CED	3.30	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	k	102	BCL	O2D-CED	3.28	1.52	1.45
9	Q	101	BCL	O2D-CGD	-3.27	1.25	1.33
9	q	102	BCL	O2A-CGA	-3.27	1.23	1.33
9	0	102	BCL	C3C-C4C	3.26	1.55	1.51
9	8	101	BCL	O2A-CGA	-3.25	1.23	1.33
7	C	504	HEM	C3B-C4B	3.25	1.51	1.44
9	D	101	BCL	O2D-CGD	-3.24	1.25	1.33
9	G	102	BCL	O2D-CGD	-3.23	1.25	1.33
9	q	102	BCL	O1A-CGA	-3.21	1.12	1.22
7	C	503	HEM	FE-NC	3.21	2.05	1.95
12	H	305	PEF	O3-C30	3.21	1.48	1.33
12	M	408	PEF	O3-C30	3.21	1.48	1.33
9	2	102	BCL	O2D-CGD	-3.20	1.25	1.33
9	6	101	BCL	O1A-CGA	-3.20	1.12	1.22
9	w	101	BCL	O2D-CGD	-3.20	1.25	1.33
9	i	102	BCL	O2D-CGD	-3.19	1.25	1.33
9	T	102	BCL	O2D-CED	3.19	1.52	1.45
9	AC	102	BCL	O2D-CGD	-3.18	1.25	1.33
7	o	504	HEM	C4D-ND	-3.18	1.34	1.40
9	L	303	BCL	O2D-CGD	-3.17	1.25	1.33
9	2	102	BCL	O2D-CED	3.16	1.52	1.45
9	D	101	BCL	O2A-CGA	-3.16	1.24	1.33
9	s	102	BCL	O2D-CGD	-3.15	1.25	1.33
9	AB	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	r	101	BCL	C3C-C4C	3.15	1.55	1.51
9	I	103	BCL	O2A-CGA	-3.14	1.24	1.33
9	d	101	BCL	C3C-C4C	3.13	1.55	1.51
9	g	102	BCL	O2D-CGD	-3.13	1.25	1.33
9	AG	101	BCL	O2D-CGD	-3.13	1.25	1.33
9	T	102	BCL	O2D-CGD	-3.12	1.25	1.33
9	AL	102	BCL	C3C-C4C	3.11	1.55	1.51
9	m	102	BCL	O2D-CGD	-3.11	1.25	1.33
9	A	103	BCL	O2A-CGA	-3.10	1.24	1.33
9	3	101	BCL	O1A-CGA	-3.10	1.13	1.22
9	L	303	BCL	C1B-C2B	-3.09	1.35	1.43
9	AF	101	BCL	O2D-CGD	-3.09	1.25	1.33
9	I	101	BCL	O2D-CGD	-3.09	1.25	1.33
9	AL	102	BCL	O2A-CGA	-3.08	1.24	1.33
9	AH	101	BCL	O2D-CGD	-3.08	1.25	1.33
9	P	101	BCL	O2D-CGD	-3.08	1.25	1.33
9	h	101	BCL	O2D-CGD	-3.08	1.25	1.33
7	C	504	HEM	C1D-ND	-3.07	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	x	305	BCL	O2D-CGD	-3.07	1.25	1.33
9	L	301	BCL	O2D-CED	3.07	1.52	1.45
9	x	301	BCL	C3B-CAB	3.07	1.56	1.46
12	y	407	PEF	O3-C30	3.07	1.48	1.33
9	X	102	BCL	C1D-C2D	-3.06	1.39	1.45
9	I	101	BCL	O2A-CGA	-3.06	1.24	1.33
9	M	402	BCL	O1A-CGA	-3.06	1.13	1.22
9	w	101	BCL	O1A-CGA	-3.06	1.13	1.22
7	o	503	HEM	C3B-C4B	3.05	1.50	1.44
9	L	301	BCL	O1A-CGA	-3.04	1.13	1.22
9	AI	102	BCL	O2A-CGA	-3.04	1.24	1.33
12	A	101	PEF	O3-C30	3.04	1.47	1.33
7	o	502	HEM	C4B-NB	-3.03	1.32	1.38
9	e	102	BCL	OBB-CAB	-3.03	1.16	1.23
9	m	103	BCL	O2A-CGA	-3.03	1.24	1.33
9	x	303	BCL	C1D-C2D	-3.02	1.39	1.45
9	s	102	BCL	O2D-CED	3.02	1.52	1.45
9	x	301	BCL	O2D-CGD	-3.02	1.25	1.33
9	Y	101	BCL	O2D-CGD	-3.02	1.25	1.33
9	AC	102	BCL	O1A-CGA	-3.01	1.13	1.22
9	m	102	BCL	O2A-CGA	-3.01	1.24	1.33
9	U	101	BCL	O2A-CGA	-3.00	1.24	1.33
9	j	101	BCL	O2A-CGA	-3.00	1.24	1.33
12	x	306	PEF	O3-C30	3.00	1.47	1.33
9	W	101	BCL	O2D-CGD	-2.99	1.25	1.33
9	m	102	BCL	C1D-C2D	-2.99	1.39	1.45
9	AC	102	BCL	O2A-CGA	-2.98	1.24	1.33
9	0	102	BCL	O2A-CGA	-2.98	1.24	1.33
9	AI	101	BCL	O2D-CGD	-2.98	1.25	1.33
17	S	101	PGW	O01-C1	2.97	1.41	1.35
9	AG	101	BCL	O1A-CGA	-2.97	1.13	1.22
9	u	102	BCL	O2A-CGA	-2.97	1.24	1.33
9	AH	101	BCL	O1A-CGA	-2.97	1.13	1.22
9	x	303	BCL	C1B-C2B	-2.96	1.36	1.43
10	x	302	BPH	C2C-C3C	-2.96	1.52	1.54
9	G	102	BCL	O2A-CGA	-2.96	1.24	1.33
9	AH	101	BCL	O2A-CGA	-2.96	1.24	1.33
9	x	305	BCL	C1D-C2D	-2.96	1.39	1.45
9	s	102	BCL	O2A-CGA	-2.95	1.24	1.33
17	AE	101	PGW	O01-C1	2.95	1.41	1.35
9	D	102	BCL	O2A-CGA	-2.95	1.24	1.33
12	t	303	PEF	O3-C30	2.95	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	C4B-NB	-2.95	1.33	1.38
9	u	102	BCL	C1D-C2D	-2.95	1.39	1.45
9	S	102	BCL	O2D-CGD	-2.94	1.26	1.33
9	D	102	BCL	O2D-CGD	-2.94	1.26	1.33
9	u	102	BCL	O2D-CGD	-2.94	1.26	1.33
9	W	101	BCL	O2A-CGA	-2.94	1.24	1.33
9	d	101	BCL	C5-C3	2.93	1.57	1.51
9	L	301	BCL	O2D-CGD	-2.93	1.26	1.33
9	R	102	BCL	O2A-CGA	-2.93	1.24	1.33
9	AG	101	BCL	O2A-CGA	-2.92	1.24	1.33
9	AB	102	BCL	O2D-CGD	-2.92	1.26	1.33
9	j	101	BCL	O2D-CGD	-2.91	1.26	1.33
9	U	101	BCL	O2D-CED	2.91	1.51	1.45
9	I	101	BCL	O1A-CGA	-2.91	1.13	1.22
9	AE	102	BCL	O2D-CGD	-2.91	1.26	1.33
9	g	102	BCL	O1A-CGA	-2.91	1.13	1.22
9	I	103	BCL	O1A-CGA	-2.91	1.13	1.22
9	Y	101	BCL	C3B-CAB	2.91	1.55	1.46
9	l	101	BCL	O2A-CGA	-2.90	1.24	1.33
7	o	503	HEM	C3C-C4C	-2.90	1.41	1.46
9	AG	101	BCL	C3B-CAB	2.90	1.55	1.46
9	z	102	BCL	O2A-CGA	-2.90	1.24	1.33
9	1	101	BCL	O2A-CGA	-2.90	1.24	1.33
9	f	101	BCL	C5-C3	2.90	1.57	1.51
9	4	102	BCL	O2A-CGA	-2.89	1.24	1.33
9	X	102	BCL	O1A-CGA	-2.89	1.13	1.22
9	6	101	BCL	O2D-CGD	-2.89	1.26	1.33
10	y	402	BPH	C3B-C4B	2.88	1.46	1.41
9	c	101	BCL	O2A-CGA	-2.88	1.25	1.33
9	AB	101	BCL	O2A-CGA	-2.88	1.25	1.33
9	AF	101	BCL	O2A-CGA	-2.88	1.25	1.33
9	5	101	BCL	O1A-CGA	-2.87	1.13	1.22
12	t	301	PEF	O3-C30	2.87	1.47	1.33
12	H	304	PEF	O3-C30	2.87	1.47	1.33
9	0	102	BCL	O2D-CGD	-2.87	1.26	1.33
9	X	102	BCL	O2A-CGA	-2.87	1.25	1.33
9	9	102	BCL	O2A-CGA	-2.87	1.25	1.33
9	AK	101	BCL	O2D-CGD	-2.87	1.26	1.33
12	m	101	PEF	O3-C30	2.87	1.47	1.33
9	5	101	BCL	O2A-CGA	-2.87	1.25	1.33
9	k	102	BCL	O2A-CGA	-2.87	1.25	1.33
9	Z	102	BCL	C1D-C2D	-2.86	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	102	BCL	O2A-CGA	-2.86	1.25	1.33
9	8	101	BCL	O2D-CGD	-2.86	1.26	1.33
9	Q	101	BCL	C3B-CAB	2.85	1.55	1.46
9	F	101	BCL	O1A-CGA	-2.85	1.14	1.22
9	P	101	BCL	O2A-CGA	-2.85	1.25	1.33
9	F	101	BCL	O2A-CGA	-2.84	1.25	1.33
9	f	101	BCL	O2A-CGA	-2.84	1.25	1.33
12	M	407	PEF	O3-C30	2.83	1.47	1.33
9	i	102	BCL	O2A-CGA	-2.83	1.25	1.33
9	x	303	BCL	O2D-CGD	-2.83	1.26	1.33
9	m	103	BCL	O1A-CGA	-2.82	1.14	1.22
9	X	102	BCL	O2D-CGD	-2.82	1.26	1.33
9	N	101	BCL	O2A-CGA	-2.82	1.25	1.33
9	T	102	BCL	O2A-CGA	-2.82	1.25	1.33
9	8	101	BCL	O1A-CGA	-2.82	1.14	1.22
9	AB	102	BCL	O2A-CGA	-2.82	1.25	1.33
9	V	102	BCL	O2A-CGA	-2.82	1.25	1.33
9	F	101	BCL	O2D-CGD	-2.81	1.26	1.33
9	M	401	BCL	O2D-CGD	-2.81	1.26	1.33
9	5	101	BCL	O2D-CGD	-2.80	1.26	1.33
12	y	408	PEF	O3-C30	2.80	1.46	1.33
9	D	101	BCL	O1A-CGA	-2.80	1.14	1.22
12	y	406	PEF	O3-C30	2.80	1.46	1.33
9	K	101	BCL	C3B-CAB	2.80	1.55	1.46
9	l	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	s	102	BCL	O1A-CGA	-2.79	1.14	1.22
7	C	502	HEM	FE-ND	-2.79	1.86	1.94
10	M	403	BPH	C3B-C4B	2.79	1.46	1.41
9	m	103	BCL	C3C-C4C	2.79	1.55	1.51
9	r	101	BCL	O2A-CGA	-2.78	1.25	1.33
9	j	101	BCL	O1A-CGA	-2.78	1.14	1.22
12	H	301	PEF	O3-C30	2.78	1.46	1.33
9	AB	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	1	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	AE	102	BCL	O2A-CGA	-2.78	1.25	1.33
9	f	101	BCL	C3C-C4C	2.78	1.55	1.51
9	P	101	BCL	C3C-C4C	2.77	1.55	1.51
9	AI	101	BCL	O1A-CGA	-2.77	1.14	1.22
7	o	501	HEM	C1D-ND	-2.77	1.33	1.38
9	z	102	BCL	O2D-CGD	-2.77	1.26	1.33
9	d	101	BCL	O2D-CGD	-2.77	1.26	1.33
9	u	101	BCL	O2D-CGD	-2.77	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	102	BCL	O2A-CGA	-2.77	1.25	1.33
9	4	102	BCL	O1A-CGA	-2.77	1.14	1.22
9	x	303	BCL	O2A-CGA	-2.76	1.25	1.33
9	O	102	BCL	O1A-CGA	-2.76	1.14	1.22
9	R	102	BCL	O1A-CGA	-2.76	1.14	1.22
9	Z	102	BCL	O1A-CGA	-2.76	1.14	1.22
9	1	101	BCL	O2D-CGD	-2.75	1.26	1.33
9	AL	102	BCL	O2D-CGD	-2.75	1.26	1.33
9	P	101	BCL	O1A-CGA	-2.75	1.14	1.22
9	L	303	BCL	O2A-CGA	-2.75	1.25	1.33
9	AB	102	BCL	C3C-C4C	2.75	1.55	1.51
9	7	102	BCL	C3B-CAB	2.75	1.55	1.46
9	AL	102	BCL	OBB-CAB	-2.74	1.17	1.23
9	G	102	BCL	O1A-CGA	-2.74	1.14	1.22
9	p	102	BCL	C3B-CAB	2.74	1.55	1.46
9	A	102	BCL	O1A-CGA	-2.74	1.14	1.22
9	Z	102	BCL	O2D-CGD	-2.73	1.26	1.33
9	O	102	BCL	O2A-CGA	-2.73	1.25	1.33
9	x	301	BCL	C5-C3	2.73	1.56	1.51
7	o	502	HEM	FE-ND	-2.73	1.86	1.94
9	c	101	BCL	O2D-CGD	-2.73	1.26	1.33
9	D	102	BCL	OBB-CAB	-2.73	1.17	1.23
9	AE	102	BCL	O1A-CGA	-2.72	1.14	1.22
9	h	101	BCL	O1A-CGA	-2.72	1.14	1.22
9	g	102	BCL	O2A-CGA	-2.72	1.25	1.33
9	6	101	BCL	C3B-CAB	2.72	1.55	1.46
9	2	102	BCL	C1D-C2D	-2.72	1.40	1.45
9	AK	101	BCL	O2A-CGA	-2.71	1.25	1.33
9	AC	103	BCL	C3B-CAB	2.71	1.55	1.46
9	A	102	BCL	O2D-CGD	-2.71	1.26	1.33
9	s	102	BCL	C5-C3	2.71	1.56	1.51
9	AF	101	BCL	O1A-CGA	-2.71	1.14	1.22
7	o	503	HEM	C4B-NB	-2.71	1.33	1.38
9	u	101	BCL	O2A-CGA	-2.71	1.25	1.33
9	L	303	BCL	C5-C3	2.71	1.56	1.51
9	m	102	BCL	O1A-CGA	-2.71	1.14	1.22
14	y	403	MQ8	C42-C43	2.71	1.39	1.33
9	q	102	BCL	O2D-CGD	-2.71	1.26	1.33
7	o	504	HEM	FE-ND	-2.70	1.86	1.94
9	W	101	BCL	O1A-CGA	-2.70	1.14	1.22
9	x	303	BCL	O1A-CGA	-2.70	1.14	1.22
9	A	103	BCL	O2D-CGD	-2.70	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	101	BCL	C1D-C2D	-2.70	1.40	1.45
9	AH	101	BCL	C3B-CAB	2.69	1.55	1.46
9	f	101	BCL	O2D-CGD	-2.69	1.26	1.33
9	U	101	BCL	O1A-CGA	-2.69	1.14	1.22
9	M	401	BCL	O2A-CGA	-2.69	1.25	1.33
9	W	101	BCL	C3C-C4C	2.69	1.55	1.51
9	9	102	BCL	O2D-CGD	-2.69	1.26	1.33
9	p	102	BCL	O1A-CGA	-2.69	1.14	1.22
9	d	101	BCL	O1A-CGA	-2.68	1.14	1.22
11	x	304	UQ8	C4-C3	2.68	1.46	1.36
9	4	102	BCL	C3C-C4C	2.68	1.55	1.51
9	u	101	BCL	O1A-CGA	-2.68	1.14	1.22
9	w	101	BCL	O2A-CGA	-2.68	1.25	1.33
12	p	101	PEF	O3-C30	2.68	1.46	1.33
9	f	101	BCL	O1A-CGA	-2.68	1.14	1.22
9	AC	103	BCL	O2A-CGA	-2.68	1.25	1.33
9	N	101	BCL	O2D-CGD	-2.67	1.26	1.33
9	A	103	BCL	O1A-CGA	-2.67	1.14	1.22
7	C	504	HEM	C4B-NB	-2.67	1.33	1.38
9	8	101	BCL	C3B-CAB	2.67	1.55	1.46
14	y	403	MQ8	C37-C38	2.67	1.39	1.33
9	K	101	BCL	O2D-CGD	-2.66	1.26	1.33
9	M	402	BCL	OBB-CAB	-2.66	1.17	1.23
9	f	101	BCL	OBB-CAB	-2.66	1.17	1.23
9	S	102	BCL	C3B-CAB	2.66	1.55	1.46
9	5	101	BCL	OBB-CAB	-2.66	1.17	1.23
9	z	102	BCL	O1A-CGA	-2.66	1.14	1.22
9	0	102	BCL	O1A-CGA	-2.66	1.14	1.22
9	u	102	BCL	OBB-CAB	-2.66	1.17	1.23
9	O	102	BCL	O2D-CGD	-2.66	1.26	1.33
9	I	103	BCL	O2D-CGD	-2.65	1.26	1.33
9	q	102	BCL	C3C-C4C	2.65	1.54	1.51
9	A	102	BCL	C1D-C2D	-2.65	1.40	1.45
7	o	504	HEM	C1C-C2C	-2.64	1.40	1.45
9	k	102	BCL	O1A-CGA	-2.64	1.14	1.22
9	O	102	BCL	OBB-CAB	-2.64	1.17	1.23
9	K	101	BCL	O1A-CGA	-2.64	1.14	1.22
9	f	101	BCL	C1D-C2D	-2.64	1.40	1.45
9	AC	103	BCL	O2D-CGD	-2.64	1.26	1.33
9	V	102	BCL	O1A-CGA	-2.64	1.14	1.22
9	1	101	BCL	OBB-CAB	-2.63	1.17	1.23
9	Y	101	BCL	O2A-CGA	-2.63	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	m	102	BCL	C3B-CAB	2.63	1.54	1.46
9	2	102	BCL	O2A-CGA	-2.63	1.25	1.33
9	AF	101	BCL	C3B-CAB	2.63	1.54	1.46
9	AG	101	BCL	C1D-C2D	-2.63	1.40	1.45
9	h	101	BCL	C5-C3	2.62	1.56	1.51
9	S	102	BCL	O2A-CGA	-2.62	1.25	1.33
9	y	401	BCL	O2D-CGD	-2.62	1.26	1.33
9	S	102	BCL	O1A-CGA	-2.62	1.14	1.22
9	T	102	BCL	O1A-CGA	-2.62	1.14	1.22
9	AH	101	BCL	C1B-C2B	-2.61	1.37	1.43
9	L	301	BCL	C1B-C2B	-2.61	1.37	1.43
9	Z	102	BCL	C3B-CAB	2.61	1.54	1.46
9	L	303	BCL	OBB-CAB	-2.61	1.17	1.23
9	AK	101	BCL	C1D-C2D	-2.61	1.40	1.45
9	Q	101	BCL	O1A-CGA	-2.60	1.14	1.22
9	i	102	BCL	OBB-CAB	-2.60	1.17	1.23
7	o	503	HEM	C1D-ND	-2.60	1.33	1.38
9	w	101	BCL	C3B-CAB	2.60	1.54	1.46
9	9	102	BCL	O1A-CGA	-2.60	1.14	1.22
9	A	103	BCL	C3C-C4C	2.60	1.54	1.51
9	s	102	BCL	C3C-C4C	2.60	1.54	1.51
9	Q	101	BCL	O2A-CGA	-2.60	1.25	1.33
9	D	102	BCL	O1A-CGA	-2.59	1.14	1.22
9	u	102	BCL	O1A-CGA	-2.59	1.14	1.22
9	s	102	BCL	C3B-CAB	2.59	1.54	1.46
9	s	102	BCL	C1B-C2B	-2.59	1.37	1.43
9	0	102	BCL	C1D-C2D	-2.59	1.40	1.45
9	x	305	BCL	C2C-C3C	-2.59	1.47	1.54
9	e	102	BCL	O1A-CGA	-2.59	1.14	1.22
9	Y	101	BCL	O1A-CGA	-2.58	1.14	1.22
9	m	102	BCL	C5-C3	2.58	1.56	1.51
9	Y	101	BCL	C3C-C4C	2.58	1.54	1.51
9	G	102	BCL	C3B-CAB	2.58	1.54	1.46
9	4	102	BCL	O2D-CGD	-2.58	1.26	1.33
9	z	102	BCL	C3B-CAB	2.58	1.54	1.46
9	K	101	BCL	O2A-CGA	-2.58	1.25	1.33
9	3	101	BCL	C1B-C2B	-2.57	1.37	1.43
9	L	303	BCL	O1A-CGA	-2.57	1.14	1.22
9	L	301	BCL	C3B-CAB	2.57	1.54	1.46
9	AK	101	BCL	O1A-CGA	-2.57	1.14	1.22
9	h	101	BCL	O2A-CGA	-2.57	1.25	1.33
9	AI	101	BCL	O2A-CGA	-2.56	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	401	BCL	O1A-CGA	-2.56	1.14	1.22
9	AI	102	BCL	C1B-C2B	-2.56	1.37	1.43
9	h	101	BCL	C3B-CAB	2.56	1.54	1.46
9	AI	101	BCL	C1B-C2B	-2.56	1.37	1.43
9	l	101	BCL	O2D-CGD	-2.55	1.27	1.33
9	q	102	BCL	C1B-C2B	-2.55	1.37	1.43
9	u	102	BCL	C1B-C2B	-2.55	1.37	1.43
9	AB	102	BCL	O1A-CGA	-2.55	1.14	1.22
9	AE	102	BCL	OBB-CAB	-2.54	1.17	1.23
7	o	502	HEM	C3C-C4C	-2.54	1.41	1.46
9	l	101	BCL	C3B-CAB	2.54	1.54	1.46
9	r	101	BCL	O2D-CGD	-2.54	1.27	1.33
9	I	103	BCL	C1D-C2D	-2.54	1.40	1.45
9	r	101	BCL	O1A-CGA	-2.54	1.14	1.22
9	u	101	BCL	C5-C3	2.53	1.56	1.51
9	q	102	BCL	C1D-C2D	-2.53	1.40	1.45
9	AL	102	BCL	O1A-CGA	-2.53	1.15	1.22
9	S	102	BCL	C3C-C4C	2.52	1.54	1.51
9	R	102	BCL	OBB-CAB	-2.52	1.17	1.23
9	e	102	BCL	O2A-CGA	-2.52	1.26	1.33
9	x	305	BCL	OBB-CAB	-2.52	1.17	1.23
14	M	404	MQ8	C42-C43	2.52	1.38	1.33
9	R	102	BCL	C3B-CAB	2.51	1.54	1.46
7	C	503	HEM	CHC-C1C	2.51	1.43	1.38
9	N	101	BCL	C3B-CAB	2.51	1.54	1.46
9	u	101	BCL	C3C-C4C	2.50	1.54	1.51
9	I	101	BCL	C1D-C2D	-2.49	1.40	1.45
9	AH	101	BCL	C3C-C4C	2.49	1.54	1.51
9	d	101	BCL	C3B-CAB	2.49	1.54	1.46
9	T	102	BCL	OBB-CAB	-2.49	1.17	1.23
9	4	102	BCL	C3B-CAB	2.49	1.54	1.46
9	AI	101	BCL	C3B-CAB	2.49	1.54	1.46
9	g	102	BCL	C3B-CAB	2.49	1.54	1.46
9	P	101	BCL	C1B-C2B	-2.49	1.37	1.43
9	c	101	BCL	OBB-CAB	-2.48	1.17	1.23
9	P	101	BCL	OBB-CAB	-2.48	1.17	1.23
9	AC	102	BCL	OBB-CAB	-2.48	1.17	1.23
9	q	102	BCL	OBB-CAB	-2.47	1.17	1.23
9	4	102	BCL	C1D-C2D	-2.47	1.40	1.45
9	i	102	BCL	O1A-CGA	-2.47	1.15	1.22
7	C	502	HEM	C3C-C2C	2.47	1.42	1.37
9	X	102	BCL	OBB-CAB	-2.46	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	u	101	BCL	C1B-C2B	-2.46	1.37	1.43
9	0	102	BCL	C3B-CAB	2.46	1.54	1.46
15	7	103	CRT	C4-C5	2.46	1.53	1.50
9	V	102	BCL	C3B-CAB	2.46	1.54	1.46
9	s	102	BCL	OBB-CAB	-2.46	1.17	1.23
9	k	102	BCL	OBB-CAB	-2.46	1.17	1.23
9	e	102	BCL	O2D-CGD	-2.46	1.27	1.33
9	N	101	BCL	O1A-CGA	-2.45	1.15	1.22
9	6	101	BCL	C3C-C4C	2.45	1.54	1.51
9	I	101	BCL	OBB-CAB	-2.45	1.17	1.23
9	I	101	BCL	C3B-CAB	2.45	1.54	1.46
9	AI	102	BCL	O1A-CGA	-2.45	1.15	1.22
9	c	101	BCL	C1B-C2B	-2.44	1.37	1.43
7	C	503	HEM	FE-ND	-2.44	1.87	1.94
9	AC	103	BCL	O1A-CGA	-2.44	1.15	1.22
9	I	103	BCL	C3B-CAB	2.44	1.54	1.46
9	9	102	BCL	OBB-CAB	-2.44	1.17	1.23
9	A	103	BCL	C1D-C2D	-2.43	1.40	1.45
10	y	402	BPH	CBD-CGD	-2.43	1.49	1.52
9	AH	101	BCL	OBB-CAB	-2.43	1.17	1.23
9	6	101	BCL	O2A-CGA	-2.43	1.26	1.33
9	F	101	BCL	C1D-C2D	-2.43	1.40	1.45
9	W	101	BCL	C3B-CAB	2.43	1.54	1.46
9	F	101	BCL	C1B-C2B	-2.43	1.37	1.43
9	F	101	BCL	OBB-CAB	-2.43	1.17	1.23
9	L	301	BCL	O2A-CGA	-2.43	1.26	1.33
9	m	103	BCL	OBB-CAB	-2.42	1.17	1.23
9	AI	102	BCL	C3B-CAB	2.42	1.54	1.46
9	f	101	BCL	C1B-C2B	-2.42	1.37	1.43
9	7	102	BCL	O2A-CGA	-2.42	1.26	1.33
11	L	304	UQ8	C7-C8	2.41	1.54	1.50
9	l	101	BCL	OBB-CAB	-2.41	1.17	1.23
9	T	102	BCL	C5-C3	2.41	1.56	1.51
9	AL	102	BCL	C1B-C2B	-2.41	1.37	1.43
14	M	404	MQ8	C22-C23	2.41	1.38	1.33
9	G	102	BCL	C1B-C2B	-2.41	1.37	1.43
9	r	101	BCL	C1B-C2B	-2.41	1.37	1.43
7	o	502	HEM	C3C-C2C	2.40	1.42	1.37
9	U	101	BCL	C3B-CAB	2.40	1.54	1.46
9	2	102	BCL	C5-C3	2.40	1.56	1.51
9	T	102	BCL	C1D-C2D	-2.40	1.40	1.45
9	K	101	BCL	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	102	BCL	C3C-C4C	2.39	1.54	1.51
9	A	102	BCL	OBB-CAB	-2.39	1.17	1.23
9	2	102	BCL	O1A-CGA	-2.39	1.15	1.22
9	W	101	BCL	OBB-CAB	-2.39	1.17	1.23
9	U	101	BCL	C3C-C4C	2.39	1.54	1.51
9	k	102	BCL	C3D-C2D	-2.39	1.32	1.39
9	i	102	BCL	C1B-C2B	-2.38	1.37	1.43
9	U	101	BCL	C5-C3	2.38	1.56	1.51
9	d	101	BCL	C1B-C2B	-2.38	1.37	1.43
9	AC	102	BCL	C3B-CAB	2.38	1.54	1.46
9	AK	101	BCL	C1B-C2B	-2.38	1.37	1.43
9	x	303	BCL	OBB-CAB	-2.38	1.17	1.23
9	D	101	BCL	C1D-C2D	-2.38	1.40	1.45
9	AB	101	BCL	C3B-CAB	2.38	1.54	1.46
9	R	102	BCL	C1D-C2D	-2.38	1.40	1.45
9	j	101	BCL	OBB-CAB	-2.38	1.17	1.23
9	M	401	BCL	C3B-CAB	2.38	1.54	1.46
9	e	102	BCL	C1B-C2B	-2.38	1.37	1.43
9	s	102	BCL	C1D-C2D	-2.38	1.40	1.45
7	o	504	HEM	C3B-C4B	2.38	1.49	1.44
9	1	101	BCL	C3B-CAB	2.37	1.54	1.46
9	AE	102	BCL	C1B-C2B	-2.37	1.37	1.43
9	x	303	BCL	C3D-C2D	-2.37	1.32	1.39
9	L	301	BCL	C1D-C2D	-2.37	1.40	1.45
9	x	303	BCL	C3D-C4D	-2.37	1.38	1.44
9	x	301	BCL	C1B-C2B	-2.37	1.37	1.43
9	j	101	BCL	C3B-CAB	2.37	1.54	1.46
9	F	101	BCL	C3B-CAB	2.36	1.54	1.46
9	d	101	BCL	O2A-CGA	-2.36	1.26	1.33
9	D	102	BCL	C1B-C2B	-2.36	1.37	1.43
9	D	102	BCL	C1D-C2D	-2.36	1.40	1.45
9	y	401	BCL	C2C-C3C	-2.36	1.48	1.54
9	3	101	BCL	OBB-CAB	-2.36	1.17	1.23
9	y	401	BCL	OBB-CAB	-2.36	1.17	1.23
9	AB	102	BCL	OBB-CAB	-2.36	1.17	1.23
9	M	401	BCL	C1B-C2B	-2.35	1.37	1.43
9	2	102	BCL	C3C-C4C	2.35	1.54	1.51
9	7	102	BCL	O1A-CGA	-2.35	1.15	1.22
14	y	403	MQ8	C17-C18	2.35	1.38	1.33
10	L	302	BPH	C3B-C4B	2.35	1.45	1.41
9	AI	102	BCL	OBB-CAB	-2.35	1.17	1.23
9	m	103	BCL	O2D-CGD	-2.35	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	101	BCL	C3B-CAB	2.35	1.54	1.46
9	p	102	BCL	O2D-CGD	-2.35	1.27	1.33
9	AC	103	BCL	C1D-C2D	-2.35	1.40	1.45
14	M	404	MQ8	C17-C18	2.35	1.38	1.33
9	5	101	BCL	C1D-C2D	-2.35	1.40	1.45
9	G	102	BCL	C1D-C2D	-2.35	1.40	1.45
7	o	503	HEM	C1C-C2C	-2.34	1.40	1.45
9	3	101	BCL	C5-C3	2.34	1.56	1.51
9	x	303	BCL	C1A-CHA	-2.34	1.33	1.43
9	L	303	BCL	C3D-C4D	-2.34	1.38	1.44
9	k	102	BCL	C3B-CAB	2.34	1.54	1.46
9	Z	102	BCL	OBB-CAB	-2.34	1.17	1.23
9	D	102	BCL	C3B-CAB	2.34	1.54	1.46
9	I	103	BCL	C1B-C2B	-2.34	1.37	1.43
9	A	103	BCL	C3B-CAB	2.34	1.54	1.46
9	AF	101	BCL	C5-C3	2.34	1.56	1.51
9	u	102	BCL	C3B-CAB	2.33	1.54	1.46
9	m	103	BCL	C3B-CAB	2.33	1.54	1.46
9	k	102	BCL	C1B-C2B	-2.33	1.37	1.43
9	8	101	BCL	C1B-C2B	-2.33	1.37	1.43
9	X	102	BCL	C3B-CAB	2.33	1.54	1.46
9	AC	102	BCL	C5-C3	2.33	1.56	1.51
9	A	102	BCL	C1B-C2B	-2.33	1.37	1.43
9	L	301	BCL	OBB-CAB	-2.32	1.18	1.23
9	d	101	BCL	C1D-C2D	-2.32	1.40	1.45
9	AC	102	BCL	C3C-C4C	2.32	1.54	1.51
9	c	101	BCL	C3C-C4C	2.32	1.54	1.51
9	2	102	BCL	C3B-CAB	2.32	1.54	1.46
9	AI	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	N	101	BCL	OBB-CAB	-2.31	1.18	1.23
11	L	304	UQ8	C4-C3	2.31	1.44	1.36
9	Q	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	r	101	BCL	C1D-C2D	-2.31	1.40	1.45
9	L	301	BCL	C3C-C4C	2.31	1.54	1.51
9	AK	101	BCL	C3B-CAB	2.31	1.54	1.46
9	L	303	BCL	C3D-C2D	-2.31	1.32	1.39
9	AL	102	BCL	C3D-C4D	-2.31	1.39	1.44
9	8	101	BCL	OBB-CAB	-2.30	1.18	1.23
10	y	402	BPH	CHA-CBD	-2.30	1.49	1.51
9	I	101	BCL	C5-C3	2.30	1.56	1.51
9	l	101	BCL	C1D-C2D	-2.30	1.40	1.45
7	C	502	HEM	C1C-C2C	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	x	301	BCL	O2A-CGA	-2.29	1.26	1.33
9	N	101	BCL	C1B-C2B	-2.29	1.37	1.43
9	K	101	BCL	C1B-C2B	-2.29	1.37	1.43
9	c	101	BCL	O1A-CGA	-2.29	1.15	1.22
9	q	102	BCL	C3B-CAB	2.28	1.53	1.46
9	0	102	BCL	OBB-CAB	-2.28	1.18	1.23
9	AL	102	BCL	C3B-CAB	2.28	1.53	1.46
9	L	303	BCL	C3B-C2B	-2.28	1.34	1.42
9	P	101	BCL	C3B-CAB	2.28	1.53	1.46
9	U	101	BCL	C1B-C2B	-2.28	1.37	1.43
9	W	101	BCL	C3D-CAD	2.28	1.53	1.45
9	AB	102	BCL	C3B-CAB	2.27	1.53	1.46
9	M	402	BCL	C1D-ND	2.27	1.40	1.37
9	AI	102	BCL	O2D-CGD	-2.27	1.27	1.33
9	m	103	BCL	C5-C3	2.27	1.56	1.51
7	o	501	HEM	C1C-C2C	-2.27	1.40	1.45
9	P	101	BCL	C1D-C2D	-2.27	1.40	1.45
9	V	102	BCL	C1B-C2B	-2.27	1.37	1.43
9	U	101	BCL	OBB-CAB	-2.27	1.18	1.23
9	AF	101	BCL	C1D-C2D	-2.26	1.40	1.45
9	M	401	BCL	C3D-C4D	-2.26	1.39	1.44
9	e	102	BCL	C1D-C2D	-2.26	1.40	1.45
12	H	302	PEF	O3-C30	2.26	1.44	1.33
9	r	101	BCL	C5-C3	2.25	1.55	1.51
9	x	301	BCL	C3D-C4D	-2.25	1.39	1.44
9	L	303	BCL	C2C-C3C	-2.25	1.48	1.54
9	3	101	BCL	O2D-CGD	-2.25	1.27	1.33
9	R	102	BCL	C1B-C2B	-2.25	1.37	1.43
7	o	502	HEM	C1A-C2A	-2.25	1.40	1.44
9	9	102	BCL	C1B-C2B	-2.25	1.37	1.43
7	C	502	HEM	C1A-C2A	-2.25	1.40	1.44
9	k	102	BCL	C5-C3	2.25	1.55	1.51
9	W	101	BCL	C1B-C2B	-2.25	1.37	1.43
9	M	402	BCL	C2C-C3C	-2.24	1.48	1.54
9	M	401	BCL	C3B-C2B	-2.24	1.34	1.42
9	w	101	BCL	C3C-C4C	2.24	1.54	1.51
9	O	102	BCL	C1B-C2B	-2.24	1.37	1.43
9	4	102	BCL	OBB-CAB	-2.24	1.18	1.23
9	x	303	BCL	C2C-C3C	-2.24	1.48	1.54
9	u	101	BCL	OBB-CAB	-2.24	1.18	1.23
14	M	404	MQ8	C27-C28	2.24	1.38	1.33
9	A	103	BCL	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	101	BCL	C2C-C3C	-2.23	1.48	1.54
9	AC	102	BCL	C1D-C2D	-2.23	1.40	1.45
9	i	102	BCL	C1D-C2D	-2.23	1.40	1.45
9	9	102	BCL	C3C-C4C	2.23	1.54	1.51
9	r	101	BCL	OBB-CAB	-2.22	1.18	1.23
11	x	304	UQ8	C43-C44	2.22	1.39	1.32
11	L	304	UQ8	C28-C29	2.22	1.38	1.33
9	AI	102	BCL	C5-C3	2.22	1.55	1.51
9	m	102	BCL	OBB-CAB	-2.21	1.18	1.23
9	AE	102	BCL	C3B-CAB	2.21	1.53	1.46
9	I	103	BCL	OBB-CAB	-2.21	1.18	1.23
9	2	102	BCL	C1B-C2B	-2.21	1.37	1.43
9	6	101	BCL	OBB-CAB	-2.21	1.18	1.23
7	C	502	HEM	C1D-ND	-2.21	1.34	1.38
14	y	403	MQ8	C32-C33	2.21	1.38	1.33
9	j	101	BCL	C3D-C4D	-2.21	1.39	1.44
9	r	101	BCL	C3B-CAB	2.20	1.53	1.46
9	O	102	BCL	C1D-C2D	-2.20	1.41	1.45
9	q	102	BCL	C3B-C2B	-2.20	1.35	1.42
9	x	305	BCL	C3D-C4D	-2.20	1.39	1.44
7	C	503	HEM	C4A-NA	-2.20	1.35	1.39
9	AL	102	BCL	C1D-C2D	-2.20	1.41	1.45
9	p	102	BCL	C3C-C4C	2.19	1.54	1.51
9	p	102	BCL	C3D-C4D	-2.19	1.39	1.44
9	g	102	BCL	OBB-CAB	-2.19	1.18	1.23
9	w	101	BCL	C1B-C2B	-2.19	1.38	1.43
9	AI	101	BCL	OBB-CAB	-2.19	1.18	1.23
9	V	102	BCL	C5-C3	2.19	1.55	1.51
9	K	101	BCL	C5-C3	2.19	1.55	1.51
9	e	102	BCL	C3C-C4C	2.18	1.54	1.51
9	p	102	BCL	C2C-C3C	-2.18	1.48	1.54
9	M	402	BCL	C1B-C2B	-2.18	1.38	1.43
9	1	101	BCL	C3C-C4C	2.18	1.54	1.51
9	3	101	BCL	C3D-C2D	-2.18	1.33	1.39
9	N	101	BCL	C1D-C2D	-2.18	1.41	1.45
9	m	103	BCL	C1D-C2D	-2.18	1.41	1.45
9	m	103	BCL	C1B-C2B	-2.18	1.38	1.43
9	A	103	BCL	C1B-C2B	-2.18	1.38	1.43
9	T	102	BCL	C1B-C2B	-2.17	1.38	1.43
9	Q	101	BCL	C2C-C3C	-2.17	1.48	1.54
7	C	501	HEM	C1D-ND	-2.17	1.34	1.38
9	I	103	BCL	C3C-C4C	2.17	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	102	BCL	OBB-CAB	-2.17	1.18	1.23
9	1	101	BCL	C1B-C2B	-2.17	1.38	1.43
9	M	402	BCL	O2D-CGD	-2.17	1.27	1.33
9	9	102	BCL	C1D-C2D	-2.17	1.41	1.45
9	x	305	BCL	C3B-C2B	-2.16	1.35	1.42
9	3	101	BCL	C3D-C4D	-2.16	1.39	1.44
9	z	102	BCL	OBB-CAB	-2.16	1.18	1.23
9	X	102	BCL	C3C-C4C	2.16	1.54	1.51
9	AB	102	BCL	C3D-C4D	-2.16	1.39	1.44
9	5	101	BCL	C3B-CAB	2.16	1.53	1.46
9	h	101	BCL	C3B-C2B	-2.16	1.35	1.42
9	d	101	BCL	C2C-C3C	-2.15	1.48	1.54
9	Z	102	BCL	C1B-C2B	-2.15	1.38	1.43
9	Q	101	BCL	C3C-C4C	2.15	1.54	1.51
9	6	101	BCL	C1B-C2B	-2.15	1.38	1.43
9	1	101	BCL	C5-C3	2.15	1.55	1.51
9	w	101	BCL	C1D-C2D	-2.15	1.41	1.45
9	0	102	BCL	C1B-C2B	-2.15	1.38	1.43
9	AK	101	BCL	C2C-C3C	-2.14	1.48	1.54
9	d	101	BCL	OBB-CAB	-2.14	1.18	1.23
7	C	501	HEM	C1B-C2B	-2.14	1.40	1.44
9	r	101	BCL	C3B-C2B	-2.14	1.35	1.42
9	S	102	BCL	C1D-C2D	-2.14	1.41	1.45
9	6	101	BCL	C3B-C2B	-2.14	1.35	1.42
15	s	101	CRT	C4-C5	2.14	1.53	1.50
9	AB	101	BCL	C1B-C2B	-2.13	1.38	1.43
9	z	102	BCL	C1D-C2D	-2.13	1.41	1.45
9	F	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	AH	101	BCL	CHC-C1C	2.13	1.43	1.37
9	7	102	BCL	C3C-C4C	2.13	1.54	1.51
9	7	102	BCL	O2D-CGD	-2.13	1.28	1.33
14	y	403	MQ8	C12-C13	2.13	1.38	1.33
9	y	401	BCL	C3B-CAB	2.13	1.53	1.46
9	y	401	BCL	C1D-C2D	-2.12	1.41	1.45
9	x	301	BCL	O1A-CGA	-2.12	1.16	1.22
9	1	101	BCL	C1D-C2D	-2.12	1.41	1.45
9	AB	102	BCL	C1D-C2D	-2.12	1.41	1.45
9	c	101	BCL	C1D-C2D	-2.12	1.41	1.45
9	7	102	BCL	OBB-CAB	-2.12	1.18	1.23
14	M	404	MQ8	C37-C38	2.12	1.37	1.33
9	m	103	BCL	C3D-CAD	2.12	1.52	1.45
9	AB	102	BCL	C3D-C2D	-2.11	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	102	BCL	OBB-CAB	-2.11	1.18	1.23
9	T	102	BCL	C2C-C3C	-2.11	1.48	1.54
9	P	101	BCL	C5-C3	2.11	1.55	1.51
9	g	102	BCL	C1D-C2D	-2.11	1.41	1.45
9	U	101	BCL	C1D-C2D	-2.11	1.41	1.45
9	i	102	BCL	C3B-CAB	2.11	1.53	1.46
9	m	102	BCL	C1B-C2B	-2.10	1.38	1.43
9	5	101	BCL	C5-C3	2.10	1.55	1.51
9	AB	101	BCL	C5-C3	2.10	1.55	1.51
9	Q	101	BCL	C1B-C2B	-2.10	1.38	1.43
9	AC	103	BCL	OBB-CAB	-2.10	1.18	1.23
9	u	102	BCL	C3C-C4C	2.10	1.54	1.51
9	Y	101	BCL	C2C-C3C	-2.10	1.48	1.54
9	A	103	BCL	C2C-C3C	-2.10	1.48	1.54
9	D	101	BCL	C3B-CAB	2.10	1.53	1.46
9	k	102	BCL	C3D-C4D	-2.09	1.39	1.44
9	AF	101	BCL	C1B-C2B	-2.09	1.38	1.43
9	g	102	BCL	C1B-C2B	-2.09	1.38	1.43
9	0	102	BCL	C5-C3	2.09	1.55	1.51
9	y	401	BCL	C1B-C2B	-2.09	1.38	1.43
9	R	102	BCL	C5-C3	2.08	1.55	1.51
7	C	503	HEM	C2A-C3A	-2.08	1.33	1.38
9	N	101	BCL	C3D-C4D	-2.08	1.39	1.44
9	5	101	BCL	C1B-C2B	-2.08	1.38	1.43
9	AF	101	BCL	OBB-CAB	-2.08	1.18	1.23
9	S	102	BCL	OBB-CAB	-2.08	1.18	1.23
9	M	402	BCL	CHC-C1C	2.08	1.42	1.37
9	4	102	BCL	C3D-C4D	-2.08	1.39	1.44
9	8	101	BCL	C5-C3	2.08	1.55	1.51
9	y	401	BCL	C3D-C4D	-2.08	1.39	1.44
9	A	103	BCL	OBB-CAB	-2.07	1.18	1.23
9	u	101	BCL	C3B-CAB	2.07	1.53	1.46
9	AG	101	BCL	OBB-CAB	-2.07	1.18	1.23
7	o	504	HEM	C4A-NA	-2.07	1.35	1.39
9	l	101	BCL	C1B-C2B	-2.07	1.38	1.43
9	D	102	BCL	C2C-C3C	-2.07	1.48	1.54
9	AI	102	BCL	C2C-C3C	-2.07	1.48	1.54
9	V	102	BCL	C1D-C2D	-2.07	1.41	1.45
9	m	102	BCL	C2C-C3C	-2.07	1.48	1.54
9	g	102	BCL	C3D-C4D	-2.07	1.39	1.44
9	AB	102	BCL	C1B-C2B	-2.06	1.38	1.43
9	u	101	BCL	C3B-C2B	-2.06	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	l	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	AE	102	BCL	C1D-C2D	-2.06	1.41	1.45
9	AK	101	BCL	OBB-CAB	-2.06	1.18	1.23
9	T	102	BCL	C3B-CAB	2.06	1.53	1.46
9	q	102	BCL	C2C-C3C	-2.06	1.48	1.54
9	R	102	BCL	C3D-C4D	-2.06	1.39	1.44
15	7	103	CRT	C37-C36	2.06	1.53	1.50
9	AC	103	BCL	C5-C3	2.05	1.55	1.51
9	S	102	BCL	C2C-C3C	-2.05	1.48	1.54
9	A	103	BCL	C3D-C2D	-2.05	1.33	1.39
9	AC	103	BCL	C3D-C4D	-2.05	1.39	1.44
9	x	301	BCL	C2C-C3C	-2.05	1.48	1.54
9	W	101	BCL	C1A-CHA	-2.05	1.34	1.43
9	3	101	BCL	C3B-CAB	2.05	1.53	1.46
9	m	102	BCL	C3C-C4C	2.05	1.54	1.51
9	7	102	BCL	C3D-C4D	-2.05	1.39	1.44
9	V	102	BCL	C2C-C3C	-2.04	1.48	1.54
9	u	101	BCL	C2C-C3C	-2.04	1.48	1.54
9	i	102	BCL	C3B-C2B	-2.04	1.35	1.42
9	D	101	BCL	C3C-C4C	2.04	1.54	1.51
9	4	102	BCL	C1B-C2B	-2.04	1.38	1.43
9	R	102	BCL	C3D-C2D	-2.04	1.33	1.39
7	o	504	HEM	C3C-C2C	2.04	1.41	1.37
9	P	101	BCL	C3D-C4D	-2.03	1.39	1.44
9	L	301	BCL	C3D-C4D	-2.03	1.39	1.44
9	AH	101	BCL	C1A-CHA	-2.03	1.34	1.43
9	e	102	BCL	C3B-CAB	2.03	1.53	1.46
9	F	101	BCL	C2C-C3C	-2.03	1.49	1.54
9	V	102	BCL	OBB-CAB	-2.03	1.18	1.23
9	G	102	BCL	OBB-CAB	-2.03	1.18	1.23
7	C	504	HEM	C4D-C3D	2.03	1.48	1.45
9	h	101	BCL	C1B-C2B	-2.03	1.38	1.43
9	u	102	BCL	C5-C3	2.03	1.55	1.51
9	AG	101	BCL	C2C-C3C	-2.03	1.49	1.54
9	w	101	BCL	C3D-C4D	-2.03	1.39	1.44
9	I	103	BCL	C3D-C4D	-2.02	1.39	1.44
9	f	101	BCL	C3D-C4D	-2.02	1.39	1.44
9	f	101	BCL	C2C-C3C	-2.02	1.49	1.54
9	j	101	BCL	C1D-C2D	-2.02	1.41	1.45
9	g	102	BCL	C3D-C2D	-2.02	1.33	1.39
11	x	304	UQ8	C26-C24	2.02	1.55	1.51
9	M	401	BCL	C3D-C2D	-2.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	101	BCL	C3B-C2B	-2.02	1.35	1.42
9	L	301	BCL	C3D-C2D	-2.02	1.33	1.39
7	o	501	HEM	C1A-C2A	-2.02	1.40	1.44
9	4	102	BCL	C2C-C3C	-2.02	1.49	1.54
9	AI	101	BCL	C5-C3	2.02	1.55	1.51
9	O	102	BCL	C3D-C2D	-2.02	1.33	1.39
9	AH	101	BCL	C3D-CAD	2.02	1.52	1.45
9	q	102	BCL	C3D-C4D	-2.02	1.39	1.44
9	g	102	BCL	C5-C3	2.01	1.55	1.51
9	8	101	BCL	C1A-CHA	-2.01	1.34	1.43
9	z	102	BCL	C1B-C2B	-2.01	1.38	1.43
7	o	504	HEM	C1D-ND	-2.01	1.34	1.38
9	AL	102	BCL	C5-C3	2.01	1.55	1.51
9	f	101	BCL	C3A-C2A	2.01	1.59	1.54
9	h	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	M	401	BCL	C1B-NB	-2.01	1.35	1.37
9	D	101	BCL	OBB-CAB	-2.01	1.18	1.23
9	AI	101	BCL	C2C-C3C	-2.01	1.49	1.54
9	I	101	BCL	C3C-C4C	2.00	1.54	1.51
9	p	102	BCL	C1B-C2B	-2.00	1.38	1.43
9	j	101	BCL	C1A-CHA	-2.00	1.34	1.43
9	9	102	BCL	C3B-CAB	2.00	1.53	1.46
9	AB	101	BCL	OBB-CAB	-2.00	1.18	1.23
14	M	404	MQ8	C32-C33	2.00	1.37	1.33
9	I	101	BCL	C2C-C3C	-2.00	1.49	1.54

All (2834) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302	BPH	O2D-CGD-CBD	10.00	121.93	110.95
10	M	403	BPH	O2D-CGD-CBD	9.51	121.39	110.95
15	g	101	CRT	C31-C32-C33	-9.13	114.47	127.28
15	AJ	101	CRT	C37-C36-C35	-8.66	112.75	124.91
15	s	101	CRT	C37-C36-C35	-8.23	113.36	124.91
7	C	503	HEM	CHD-C4C-NC	8.06	133.23	124.45
12	y	408	PEF	C2-O2-C10	-7.90	103.90	117.85
15	y	404	CRT	C37-C36-C35	-7.89	113.83	124.91
9	x	301	BCL	C4A-NA-C1A	7.83	110.25	106.68
9	x	301	BCL	O2D-CGD-CBD	7.74	124.76	111.23
15	9	101	CRT	C37-C36-C35	-7.62	114.21	124.91
15	AF	102	CRT	C21-C22-C23	-7.61	116.61	127.28
10	x	302	BPH	O2D-CGD-CBD	7.56	119.26	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	0	101	CRT	C37-C36-C35	-7.45	114.46	124.91
15	AF	102	CRT	C37-C36-C35	-7.39	114.54	124.91
15	7	101	CRT	C37-C36-C35	-7.35	114.59	124.91
10	y	402	BPH	O2D-CGD-CBD	7.34	119.01	110.95
15	M	405	CRT	C3-C1-C2	7.34	123.84	110.43
15	T	101	CRT	C3-C1-C2	7.27	123.72	110.43
15	i	101	CRT	C37-C36-C35	-7.20	114.81	124.91
12	y	406	PEF	O2-C10-C11	7.19	123.90	111.09
9	M	401	BCL	C4A-NA-C1A	7.02	109.88	106.68
9	4	102	BCL	O2D-CGD-CBD	6.99	123.46	111.23
9	AI	102	BCL	O2D-CGD-CBD	6.97	123.41	111.23
15	n	101	CRT	C3-C1-C2	6.92	123.07	110.43
9	Z	102	BCL	O2D-CGD-CBD	6.90	123.29	111.23
15	I	102	CRT	C3-C1-C2	6.90	123.03	110.43
15	m	104	CRT	C37-C36-C35	-6.88	115.25	124.91
9	7	102	BCL	C1D-ND-C4D	-6.83	101.52	106.31
15	V	101	CRT	C37-C36-C35	-6.82	115.33	124.91
15	AD	101	CRT	C3-C1-C2	6.82	122.88	110.43
15	7	101	CRT	C26-C27-C28	-6.81	117.72	127.28
15	AL	101	CRT	C37-C36-C35	-6.75	115.43	124.91
15	O	101	CRT	C21-C22-C23	-6.70	117.88	127.28
15	T	101	CRT	C37-C36-C35	-6.66	115.56	124.91
15	M	405	CRT	C37-C36-C35	-6.60	115.65	124.91
15	q	101	CRT	C37-C36-C35	-6.55	115.72	124.91
7	C	503	HEM	C3B-C4B-NB	-6.53	104.78	109.47
15	O	101	CRT	C4-C5-C6	-6.53	115.74	124.91
15	AH	102	CRT	C3-C1-C2	6.53	122.36	110.43
9	X	102	BCL	O2D-CGD-CBD	6.53	122.64	111.23
7	C	504	HEM	CHD-C4C-NC	6.52	131.55	124.45
15	O	101	CRT	C37-C36-C35	-6.45	115.86	124.91
9	AG	101	BCL	C1D-ND-C4D	-6.42	101.81	106.31
9	L	303	BCL	CMA-C3A-C4A	-6.42	94.52	111.77
15	k	101	CRT	C3-C1-C2	6.41	122.14	110.43
9	q	102	BCL	O2D-CGD-CBD	6.41	122.43	111.23
15	9	101	CRT	C21-C22-C23	-6.40	118.30	127.28
15	V	101	CRT	C21-C22-C23	-6.40	118.30	127.28
15	AJ	101	CRT	C10-C9-C7	-6.38	118.33	127.28
9	j	101	BCL	C1D-ND-C4D	-6.37	101.84	106.31
15	q	101	CRT	C3-C1-C2	6.36	122.05	110.43
15	z	101	CRT	C4-C5-C6	-6.34	116.00	124.91
7	C	502	HEM	CHC-C4B-NB	6.32	131.23	124.42
15	G	101	CRT	C37-C36-C35	-6.29	116.08	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	102	BCL	O2D-CGD-O1D	-6.29	111.61	123.85
9	2	102	BCL	O2D-CGD-CBD	6.28	122.21	111.23
9	A	103	BCL	O2D-CGD-CBD	6.28	122.21	111.23
9	8	101	BCL	O2D-CGD-CBD	6.26	122.17	111.23
12	t	303	PEF	C2-O2-C10	-6.25	106.81	117.85
9	R	102	BCL	C1D-ND-C4D	-6.24	101.93	106.31
9	x	305	BCL	C4A-NA-C1A	6.21	109.51	106.68
15	Z	101	CRT	C37-C36-C35	-6.18	116.24	124.91
9	I	103	BCL	O2D-CGD-CBD	6.14	121.96	111.23
15	R	101	CRT	C3-C1-C2	6.13	121.63	110.43
9	8	101	BCL	C1D-ND-C4D	-6.12	102.02	106.31
15	e	101	CRT	C37-C36-C35	-6.11	116.34	124.91
9	e	102	BCL	O2D-CGD-CBD	6.07	121.84	111.23
9	s	102	BCL	O2D-CGD-CBD	6.06	121.82	111.23
9	M	402	BCL	O2D-CGD-CBD	6.05	121.80	111.23
9	y	401	BCL	C1D-ND-C4D	-6.04	102.07	106.31
9	M	402	BCL	C1D-ND-C4D	-6.04	102.07	106.31
9	N	101	BCL	O2D-CGD-CBD	6.03	121.78	111.23
9	M	401	BCL	C1D-ND-C4D	-6.03	102.08	106.31
9	h	101	BCL	C1D-ND-C4D	-6.02	102.09	106.31
7	o	502	HEM	CHC-C4B-NB	6.01	130.90	124.42
15	I	102	CRT	C37-C36-C35	-6.01	116.47	124.91
9	AC	103	BCL	C1D-ND-C4D	-5.97	102.12	106.31
15	O	101	CRT	C3-C1-C2	5.97	121.34	110.43
9	m	102	BCL	C1D-ND-C4D	-5.94	102.14	106.31
9	f	101	BCL	O2D-CGD-CBD	5.93	121.60	111.23
15	v	101	CRT	C5-C6-C7	5.92	134.84	125.89
9	k	102	BCL	C1D-ND-C4D	-5.92	102.16	106.31
9	i	102	BCL	C1D-ND-C4D	-5.91	102.16	106.31
7	C	502	HEM	C1B-NB-C4B	5.88	112.17	105.21
12	H	302	PEF	O2-C10-C11	5.87	121.56	111.09
9	u	102	BCL	C1D-ND-C4D	-5.87	102.20	106.31
9	m	103	BCL	O2D-CGD-CBD	5.83	121.42	111.23
15	P	102	CRT	C4-C5-C6	-5.83	116.73	124.91
15	v	101	CRT	C3-C1-C2	5.82	121.07	110.43
9	D	101	BCL	C1D-ND-C4D	-5.80	102.24	106.31
15	X	101	CRT	C37-C36-C35	-5.80	116.77	124.91
15	AC	101	CRT	C26-C27-C28	-5.78	119.17	127.28
15	AH	102	CRT	C37-C36-C35	-5.78	116.80	124.91
7	o	502	HEM	C1B-NB-C4B	5.78	112.05	105.21
9	AC	103	BCL	O2D-CGD-CBD	5.77	121.31	111.23
9	l	101	BCL	O2D-CGD-CBD	5.75	121.28	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	7	101	CRT	C3-C1-C2	5.75	120.93	110.43
15	I	102	CRT	C21-C22-C23	-5.74	119.23	127.28
9	l	101	BCL	C1D-ND-C4D	-5.73	102.29	106.31
15	z	101	CRT	C21-C22-C23	-5.72	119.25	127.28
9	AL	102	BCL	O2D-CGD-CBD	5.69	121.18	111.23
15	G	101	CRT	C3-C1-C2	5.68	120.82	110.43
9	M	402	BCL	O2D-CGD-O1D	-5.68	112.79	123.85
9	Q	101	BCL	C1D-ND-C4D	-5.68	102.33	106.31
9	4	102	BCL	C1D-ND-C4D	-5.67	102.33	106.31
9	1	101	BCL	O2D-CGD-CBD	5.67	121.14	111.23
9	AI	102	BCL	O2D-CGD-O1D	-5.66	112.82	123.85
9	5	101	BCL	O2D-CGD-CBD	5.66	121.12	111.23
9	AB	101	BCL	O2D-CGD-CBD	5.66	121.12	111.23
15	0	101	CRT	C3-C1-C2	5.65	120.76	110.43
9	AL	102	BCL	C1D-ND-C4D	-5.65	102.35	106.31
9	T	102	BCL	C1D-ND-C4D	-5.62	102.37	106.31
9	X	102	BCL	O2D-CGD-O1D	-5.62	112.91	123.85
9	X	102	BCL	C1D-ND-C4D	-5.61	102.37	106.31
15	4	101	CRT	C3-C1-C2	5.60	120.67	110.43
9	x	303	BCL	C1D-ND-C4D	-5.60	102.38	106.31
9	3	101	BCL	C1D-ND-C4D	-5.59	102.39	106.31
9	s	102	BCL	C1D-ND-C4D	-5.59	102.39	106.31
9	9	102	BCL	O2D-CGD-CBD	5.59	121.01	111.23
9	A	103	BCL	O2D-CGD-O1D	-5.59	112.96	123.85
9	d	101	BCL	O2D-CGD-O1D	-5.59	112.97	123.85
9	F	101	BCL	O2D-CGD-CBD	5.59	121.00	111.23
10	M	403	BPH	O1D-CGD-CBD	-5.58	116.27	124.72
7	o	501	HEM	CBD-CAD-C3D	-5.57	97.14	112.53
7	o	502	HEM	CHD-C4C-NC	5.57	130.51	124.45
15	AC	101	CRT	C4-C5-C6	-5.57	117.10	124.91
9	L	301	BCL	C1D-ND-C4D	-5.56	102.41	106.31
9	K	101	BCL	C1D-ND-C4D	-5.56	102.41	106.31
9	O	102	BCL	C1D-ND-C4D	-5.56	102.41	106.31
9	AK	101	BCL	O2D-CGD-CBD	5.55	120.94	111.23
9	x	305	BCL	O2D-CGD-CBD	5.55	120.94	111.23
9	p	102	BCL	O2D-CGD-CBD	5.55	120.93	111.23
15	g	101	CRT	C3-C1-C2	5.52	120.51	110.43
9	c	101	BCL	O2D-CGD-CBD	5.51	120.86	111.23
9	9	102	BCL	C1D-ND-C4D	-5.50	102.45	106.31
15	E	101	CRT	C3-C1-C2	5.50	120.48	110.43
15	n	101	CRT	C37-C36-C35	-5.50	117.19	124.91
9	D	102	BCL	O2D-CGD-CBD	5.50	120.84	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	102	CRT	C37-C36-C35	-5.49	117.20	124.91
9	1	101	BCL	O2D-CGD-O1D	-5.47	113.19	123.85
9	T	102	BCL	O2D-CGD-O1D	-5.47	113.19	123.85
9	1	101	BCL	C1D-ND-C4D	-5.46	102.48	106.31
9	AG	101	BCL	O2D-CGD-CBD	5.46	120.77	111.23
9	AE	102	BCL	C4D-CHA-C1A	5.43	127.72	121.24
15	R	101	CRT	C37-C36-C35	-5.43	117.28	124.91
9	5	101	BCL	C1D-ND-C4D	-5.42	102.51	106.31
9	4	102	BCL	O2D-CGD-O1D	-5.42	113.29	123.85
9	AG	101	BCL	O2D-CGD-O1D	-5.42	113.30	123.85
15	k	101	CRT	C37-C36-C35	-5.42	117.31	124.91
9	R	102	BCL	CMB-C2B-C1B	-5.42	117.17	125.42
7	o	503	HEM	C3B-C4B-NB	-5.41	105.58	109.47
9	U	101	BCL	C4D-CHA-C1A	5.41	127.70	121.24
9	u	101	BCL	C1D-ND-C4D	-5.40	102.52	106.31
7	o	504	HEM	CHC-C1C-NC	5.39	130.33	124.45
9	8	101	BCL	O2D-CGD-O1D	-5.39	113.35	123.85
9	d	101	BCL	O2D-CGD-CBD	5.39	120.66	111.23
9	AB	102	BCL	C1D-ND-C4D	-5.38	102.53	106.31
9	s	102	BCL	CMB-C2B-C1B	-5.38	117.23	125.42
9	AC	103	BCL	O2D-CGD-O1D	-5.37	113.39	123.85
9	z	102	BCL	C1D-ND-C4D	-5.36	102.55	106.31
15	y	404	CRT	C3-C1-C2	5.36	120.22	110.43
9	AC	102	BCL	C1D-ND-C4D	-5.36	102.55	106.31
9	w	101	BCL	O2D-CGD-O1D	-5.35	113.44	123.85
9	W	101	BCL	C1D-ND-C4D	-5.34	102.56	106.31
9	AE	102	BCL	C1D-ND-C4D	-5.34	102.57	106.31
7	C	501	HEM	CBD-CAD-C3D	-5.34	97.78	112.53
9	0	102	BCL	O2D-CGD-CBD	5.34	120.56	111.23
9	AC	102	BCL	O2D-CGD-CBD	5.33	120.56	111.23
9	I	103	BCL	C1D-ND-C4D	-5.33	102.57	106.31
12	M	408	PEF	O2-C10-C11	5.33	120.59	111.09
9	V	102	BCL	C1D-ND-C4D	-5.33	102.57	106.31
15	v	101	CRT	C6-C7-C9	-5.33	110.63	119.01
7	o	502	HEM	C3B-C4B-NB	-5.31	105.65	109.47
15	7	103	CRT	C3-C1-C2	5.30	120.12	110.43
9	L	301	BCL	C4A-NA-C1A	5.30	109.10	106.68
9	D	101	BCL	O2D-CGD-O1D	-5.28	113.58	123.85
9	h	101	BCL	O2D-CGD-CBD	5.27	120.44	111.23
9	u	101	BCL	O2D-CGD-CBD	5.25	120.41	111.23
9	AH	101	BCL	C1D-ND-C4D	-5.25	102.63	106.31
9	D	102	BCL	C1D-ND-C4D	-5.24	102.63	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	C1D-ND-C4D	-5.24	102.63	106.31
9	2	102	BCL	O2D-CGD-O1D	-5.24	113.65	123.85
9	Q	101	BCL	C1C-NC-C4C	-5.24	104.29	106.68
9	q	102	BCL	O2D-CGD-O1D	-5.24	113.65	123.85
9	K	101	BCL	O2D-CGD-CBD	5.20	120.33	111.23
9	u	102	BCL	O2D-CGD-CBD	5.19	120.30	111.23
9	AC	102	BCL	O2D-CGD-O1D	-5.18	113.77	123.85
9	x	301	BCL	O2D-CGD-O1D	-5.18	113.77	123.85
9	5	101	BCL	O2D-CGD-O1D	-5.18	113.77	123.85
15	AF	102	CRT	C3-C1-C2	5.17	119.88	110.43
12	A	101	PEF	O2-C10-C11	5.16	120.29	111.09
9	7	102	BCL	O2D-CGD-CBD	5.15	120.24	111.23
9	N	101	BCL	O2D-CGD-O1D	-5.15	113.82	123.85
9	x	305	BCL	C1D-ND-C4D	-5.15	102.70	106.31
9	f	101	BCL	CMB-C2B-C1B	-5.15	117.58	125.42
15	G	101	CRT	C21-C22-C23	-5.14	120.06	127.28
9	z	102	BCL	O2D-CGD-CBD	5.14	120.22	111.23
9	AI	101	BCL	CMB-C2B-C1B	-5.14	117.60	125.42
9	P	101	BCL	C4D-CHA-C1A	5.13	127.36	121.24
9	AE	102	BCL	O2D-CGD-CBD	5.13	120.19	111.23
9	AH	101	BCL	CMB-C2B-C1B	-5.12	117.62	125.42
9	c	101	BCL	C1D-ND-C4D	-5.12	102.72	106.31
15	4	101	CRT	C31-C32-C33	-5.12	120.10	127.28
9	A	103	BCL	C1D-ND-C4D	-5.11	102.72	106.31
9	j	101	BCL	O2D-CGD-O1D	-5.11	113.90	123.85
9	V	102	BCL	C4D-CHA-C1A	5.11	127.34	121.24
15	X	101	CRT	C21-C20-C19	5.11	133.97	123.52
9	P	101	BCL	CMB-C2B-C1B	-5.08	117.68	125.42
15	V	101	CRT	C3-C1-C2	5.08	119.72	110.43
15	AD	101	CRT	C37-C36-C35	-5.08	117.78	124.91
9	F	101	BCL	O2D-CGD-O1D	-5.08	113.97	123.85
15	v	101	CRT	C8-C7-C6	5.07	125.84	118.09
9	p	102	BCL	C1D-ND-C4D	-5.07	102.75	106.31
9	w	101	BCL	C1D-ND-C4D	-5.07	102.75	106.31
9	L	303	BCL	C1-O2A-CGA	5.06	128.91	116.65
9	T	102	BCL	O2D-CGD-CBD	5.06	120.07	111.23
9	6	101	BCL	C1D-ND-C4D	-5.06	102.76	106.31
9	m	102	BCL	O2D-CGD-CBD	5.05	120.06	111.23
9	A	102	BCL	O2D-CGD-CBD	5.05	120.06	111.23
9	AI	102	BCL	C1D-ND-C4D	-5.04	102.77	106.31
9	g	102	BCL	C1D-ND-C4D	-5.04	102.77	106.31
7	C	504	HEM	C3B-C4B-NB	-5.03	105.85	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	j	101	BCL	O2D-CGD-CBD	5.03	120.03	111.23
15	2	101	CRT	C37-C36-C35	-5.03	117.85	124.91
9	AB	101	BCL	O2D-CGD-O1D	-5.03	114.05	123.85
15	4	101	CRT	C21-C20-C19	-5.03	113.23	123.52
9	U	101	BCL	O2D-CGD-O1D	-5.03	114.07	123.85
9	6	101	BCL	O2D-CGD-CBD	5.02	120.01	111.23
9	i	102	BCL	O2D-CGD-O1D	-5.02	114.08	123.85
15	AD	101	CRT	C21-C22-C23	-5.02	120.24	127.28
9	q	102	BCL	C1D-ND-C4D	-5.02	102.79	106.31
9	L	303	BCL	C1D-ND-C4D	-5.00	102.81	106.31
9	I	101	BCL	O2D-CGD-CBD	4.99	119.95	111.23
9	AI	102	BCL	CMB-C2B-C1B	-4.99	117.82	125.42
9	AC	102	BCL	C4D-CHA-C1A	4.99	127.19	121.24
15	I	102	CRT	C5-C6-C7	4.98	133.42	125.89
9	A	102	BCL	C1D-ND-C4D	-4.98	102.82	106.31
9	F	101	BCL	C1D-ND-C4D	-4.98	102.82	106.31
15	AC	101	CRT	C21-C22-C23	-4.97	120.30	127.28
9	AF	101	BCL	C1D-ND-C4D	-4.97	102.82	106.31
15	AC	101	CRT	C37-C36-C35	-4.96	117.95	124.91
12	H	304	PEF	O2-C10-C11	4.96	119.93	111.09
9	x	305	BCL	C4D-CHA-C1A	4.96	127.16	121.24
9	k	102	BCL	O2D-CGD-CBD	4.95	119.89	111.23
15	7	103	CRT	C20-C19-C17	-4.94	120.35	127.28
15	z	101	CRT	C3-C1-C2	4.93	119.44	110.43
15	g	101	CRT	C37-C36-C35	-4.93	117.99	124.91
9	I	101	BCL	C1D-ND-C4D	-4.93	102.86	106.31
15	s	101	CRT	C3-C1-C2	4.93	119.43	110.43
9	3	101	BCL	CMB-C2B-C1B	-4.92	117.92	125.42
9	Y	101	BCL	O2D-CGD-CBD	4.92	119.83	111.23
15	m	104	CRT	C3-C1-C2	4.92	119.41	110.43
9	D	102	BCL	CMB-C2B-C1B	-4.91	117.94	125.42
9	M	401	BCL	O2D-CGD-CBD	4.91	119.81	111.23
9	AK	101	BCL	C1D-ND-C4D	-4.91	102.87	106.31
9	K	101	BCL	CMB-C2B-C1B	-4.91	117.94	125.42
7	C	504	HEM	C1B-NB-C4B	4.90	111.02	105.21
9	m	103	BCL	C1D-ND-C4D	-4.89	102.88	106.31
9	Y	101	BCL	O2D-CGD-O1D	-4.89	114.33	123.85
9	O	102	BCL	CMB-C2B-C1B	-4.89	117.98	125.42
9	r	101	BCL	C1D-ND-C4D	-4.88	102.89	106.31
9	N	101	BCL	CMB-C2B-C1B	-4.88	117.98	125.42
9	Z	102	BCL	C1D-ND-C4D	-4.88	102.89	106.31
9	k	102	BCL	O2D-CGD-O1D	-4.87	114.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	h	101	BCL	O2D-CGD-O1D	-4.87	114.37	123.85
9	x	303	BCL	O2D-CGD-CBD	4.86	119.73	111.23
9	l	101	BCL	O2D-CGD-O1D	-4.86	114.38	123.85
9	G	102	BCL	C4D-CHA-C1A	4.86	127.04	121.24
9	1	101	BCL	CMB-C2B-C1B	-4.85	118.04	125.42
15	E	101	CRT	C37-C36-C35	-4.84	118.11	124.91
7	C	501	HEM	C3B-C4B-NB	-4.84	105.99	109.47
15	i	101	CRT	C3-C1-C2	4.84	119.28	110.43
7	C	502	HEM	C3B-C4B-NB	-4.84	105.99	109.47
9	AI	101	BCL	O2D-CGD-CBD	4.84	119.69	111.23
12	m	101	PEF	O2-C10-C11	4.84	119.72	111.09
9	AB	101	BCL	C1D-ND-C4D	-4.83	102.92	106.31
9	AH	101	BCL	O2D-CGD-CBD	4.83	119.67	111.23
9	x	303	BCL	O2D-CGD-O1D	-4.82	114.46	123.85
9	V	102	BCL	CMB-C2B-C1B	-4.82	118.08	125.42
9	p	102	BCL	CMB-C2B-C1B	-4.81	118.09	125.42
9	m	102	BCL	C4D-CHA-C1A	4.81	126.98	121.24
9	R	102	BCL	C4D-CHA-C1A	4.80	126.97	121.24
9	g	102	BCL	O2D-CGD-CBD	4.79	119.61	111.23
15	0	101	CRT	C21-C22-C23	-4.79	120.56	127.28
7	C	503	HEM	C1B-NB-C4B	4.79	110.88	105.21
15	I	102	CRT	C9-C10-C11	-4.79	109.33	123.20
15	AD	101	CRT	C5-C6-C7	-4.79	118.66	125.89
9	u	102	BCL	C1C-NC-C4C	-4.77	104.50	106.68
9	AH	101	BCL	O2D-CGD-O1D	-4.77	114.56	123.85
9	AK	101	BCL	O2D-CGD-O1D	-4.77	114.56	123.85
9	L	303	BCL	C4D-CHA-C1A	4.77	126.93	121.24
9	AB	102	BCL	C4D-CHA-C1A	4.77	126.93	121.24
9	P	101	BCL	O2D-CGD-CBD	4.77	119.56	111.23
9	O	102	BCL	O2D-CGD-CBD	4.76	119.56	111.23
15	e	101	CRT	C4-C5-C6	-4.74	118.25	124.91
9	R	102	BCL	O2D-CGD-O1D	-4.74	114.61	123.85
9	L	301	BCL	CMA-C3A-C4A	-4.74	99.03	111.77
9	w	101	BCL	O2D-CGD-CBD	4.73	119.51	111.23
11	x	304	UQ8	C6-C1-C2	4.73	122.90	119.17
9	AE	102	BCL	O2D-CGD-O1D	-4.73	114.64	123.85
9	y	401	BCL	O2D-CGD-CBD	4.73	119.50	111.23
15	k	101	CRT	C20-C19-C17	-4.73	120.65	127.28
12	H	305	PEF	O2-C10-C11	4.73	119.52	111.09
9	I	103	BCL	CMB-C2B-C1B	-4.72	118.22	125.42
9	u	102	BCL	CMB-C2B-C1B	-4.72	118.23	125.42
9	AL	102	BCL	O2D-CGD-O1D	-4.72	114.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	c	101	BCL	CMB-C2B-C1B	-4.72	118.23	125.42
9	D	101	BCL	O2D-CGD-CBD	4.71	119.47	111.23
9	s	102	BCL	C4D-CHA-C1A	4.71	126.86	121.24
9	p	102	BCL	O2D-CGD-O1D	-4.71	114.68	123.85
9	I	101	BCL	C4D-CHA-C1A	4.71	126.86	121.24
7	o	501	HEM	CHC-C4B-NB	4.71	129.49	124.42
15	T	101	CRT	C4-C5-C6	-4.70	118.31	124.91
9	c	101	BCL	O2D-CGD-O1D	-4.70	114.71	123.85
9	G	102	BCL	C1D-ND-C4D	-4.69	103.02	106.31
12	y	408	PEF	O2-C10-C11	4.69	119.46	111.09
9	G	102	BCL	CMB-C2B-C1B	-4.69	118.28	125.42
9	2	102	BCL	C1D-ND-C4D	-4.69	103.02	106.31
15	m	104	CRT	C21-C22-C23	-4.68	120.71	127.28
9	F	101	BCL	CMB-C2B-C1B	-4.68	118.30	125.42
9	AI	101	BCL	O2D-CGD-O1D	-4.68	114.75	123.85
9	V	102	BCL	O2D-CGD-CBD	4.67	119.40	111.23
9	u	102	BCL	C4D-CHA-C1A	4.67	126.82	121.24
7	o	501	HEM	C4D-ND-C1D	4.67	110.74	105.21
9	x	303	BCL	CMB-C2B-C1B	-4.67	118.31	125.42
12	t	303	PEF	O2-C10-C11	4.66	119.41	111.09
9	S	102	BCL	O2D-CGD-CBD	4.66	119.38	111.23
15	AC	101	CRT	C31-C32-C33	-4.66	120.74	127.28
9	u	102	BCL	O2D-CGD-O1D	-4.66	114.78	123.85
7	C	501	HEM	CBA-CAA-C2A	-4.65	99.66	112.53
9	AB	102	BCL	CMB-C2B-C1B	-4.64	118.35	125.42
9	AB	102	BCL	O2D-CGD-O1D	-4.64	114.82	123.85
12	A	101	PEF	C2-O2-C10	-4.64	109.65	117.85
9	Q	101	BCL	C4D-CHA-C1A	4.64	126.78	121.24
9	f	101	BCL	O2D-CGD-O1D	-4.62	114.85	123.85
9	s	102	BCL	O2D-CGD-O1D	-4.62	114.85	123.85
9	m	102	BCL	O2D-CGD-O1D	-4.62	114.86	123.85
9	S	102	BCL	O2D-CGD-O1D	-4.62	114.86	123.85
9	d	101	BCL	C1C-NC-C4C	-4.60	104.58	106.68
15	v	101	CRT	C37-C36-C35	-4.60	118.46	124.91
9	Q	101	BCL	O2D-CGD-CBD	4.59	119.26	111.23
9	D	101	BCL	C4D-CHA-C1A	4.59	126.72	121.24
9	e	102	BCL	CMB-C2B-C1B	-4.59	118.43	125.42
15	z	101	CRT	C31-C32-C33	-4.59	120.84	127.28
15	m	104	CRT	C4-C5-C6	-4.59	118.47	124.91
9	M	402	BCL	O2A-CGA-O1A	-4.59	112.16	123.63
9	j	101	BCL	CMB-C2B-C1B	-4.58	118.44	125.42
9	G	102	BCL	O2D-CGD-CBD	4.58	119.23	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AF	101	BCL	CMB-C2B-C1B	-4.58	118.45	125.42
9	2	102	BCL	C4D-CHA-C1A	4.58	126.70	121.24
9	R	102	BCL	C2D-C1D-ND	4.58	114.65	110.13
9	m	103	BCL	C4D-CHA-C1A	4.56	126.69	121.24
9	W	101	BCL	O2D-CGD-CBD	4.56	119.20	111.23
9	k	102	BCL	CMB-C2B-C1B	-4.56	118.48	125.42
9	y	401	BCL	O2D-CGD-O1D	-4.56	114.98	123.85
9	S	102	BCL	CMB-C2B-C1B	-4.56	118.48	125.42
9	D	102	BCL	O2D-CGD-O1D	-4.55	114.98	123.85
9	z	102	BCL	O2D-CGD-O1D	-4.55	114.98	123.85
9	AG	101	BCL	C2D-C1D-ND	4.55	114.63	110.13
9	A	102	BCL	C4D-CHA-C1A	4.55	126.67	121.24
9	X	102	BCL	C2D-C1D-ND	4.55	114.62	110.13
9	L	301	BCL	O2D-CGD-CBD	4.54	119.17	111.23
9	S	102	BCL	C1D-ND-C4D	-4.53	103.13	106.31
9	0	102	BCL	O2D-CGD-O1D	-4.53	115.03	123.85
9	d	101	BCL	C4A-NA-C1A	4.52	108.74	106.68
15	T	101	CRT	C21-C22-C23	-4.52	120.94	127.28
9	g	102	BCL	CMB-C2B-C1B	-4.52	118.54	125.42
9	i	102	BCL	C4D-CHA-C1A	4.51	126.62	121.24
7	C	501	HEM	CHB-C1B-NB	4.51	129.94	124.37
9	i	102	BCL	CMB-C2B-C1B	-4.50	118.56	125.42
9	Y	101	BCL	C1D-ND-C4D	-4.49	103.16	106.31
9	AH	101	BCL	C4D-CHA-C1A	4.49	126.60	121.24
9	AK	101	BCL	CMB-C2B-C1B	-4.48	118.59	125.42
9	P	101	BCL	C1D-ND-C4D	-4.48	103.17	106.31
9	x	305	BCL	O2D-CGD-O1D	-4.48	115.12	123.85
9	K	101	BCL	O2D-CGD-O1D	-4.48	115.13	123.85
9	D	101	BCL	C2D-C1D-ND	4.47	114.55	110.13
9	m	102	BCL	C2D-C1D-ND	4.47	114.55	110.13
9	I	103	BCL	O2D-CGD-O1D	-4.47	115.14	123.85
9	3	101	BCL	O2D-CGD-CBD	4.47	119.04	111.23
15	q	101	CRT	C4-C5-C6	-4.46	118.64	124.91
9	AI	101	BCL	C1D-ND-C4D	-4.46	103.18	106.31
9	A	103	BCL	CMB-C2B-C1B	-4.46	118.62	125.42
9	I	103	BCL	C4D-CHA-C1A	4.46	126.57	121.24
9	Z	102	BCL	CMB-C2B-C1B	-4.46	118.63	125.42
9	u	102	BCL	C2D-C1D-ND	4.46	114.54	110.13
9	AI	101	BCL	C4D-CHA-C1A	4.46	126.56	121.24
9	X	102	BCL	C1C-NC-C4C	-4.45	104.65	106.68
9	P	101	BCL	O2D-CGD-O1D	-4.45	115.18	123.85
9	d	101	BCL	CMB-C2B-C1B	-4.45	118.64	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	102	BCL	C4D-CHA-C1A	4.45	126.55	121.24
9	T	102	BCL	C2D-C1D-ND	4.45	114.53	110.13
9	u	101	BCL	CMA-C3A-C4A	-4.42	99.88	111.77
15	V	101	CRT	C4-C5-C6	-4.42	118.70	124.91
9	q	102	BCL	CMB-C2B-C1B	-4.41	118.71	125.42
9	T	102	BCL	C4D-CHA-C1A	4.40	126.49	121.24
7	o	503	HEM	CHD-C4C-NC	4.40	129.24	124.45
15	s	101	CRT	C26-C27-C28	-4.40	121.11	127.28
15	9	101	CRT	C15-C14-C12	-4.40	121.11	127.28
9	e	102	BCL	C1D-ND-C4D	-4.39	103.23	106.31
9	A	102	BCL	CMB-C2B-C1B	-4.39	118.73	125.42
9	U	101	BCL	CHA-C1A-NA	-4.39	116.45	126.39
9	l	101	BCL	CMB-C2B-C1B	-4.39	118.74	125.42
7	C	502	HEM	CHD-C4C-NC	4.38	129.22	124.45
9	6	101	BCL	C4D-CHA-C1A	4.38	126.47	121.24
9	r	101	BCL	O2D-CGD-CBD	4.37	118.88	111.23
9	AB	101	BCL	C4D-CHA-C1A	4.37	126.46	121.24
9	2	102	BCL	CHA-C1A-NA	-4.37	116.50	126.39
9	x	305	BCL	C2D-C1D-ND	4.36	114.44	110.13
9	AF	101	BCL	C4A-NA-C1A	4.36	108.67	106.68
9	9	102	BCL	O2D-CGD-O1D	-4.36	115.36	123.85
15	M	405	CRT	C4-C5-C6	-4.36	118.79	124.91
9	L	301	BCL	CMB-C2B-C1B	-4.36	118.78	125.42
7	C	501	HEM	C4D-ND-C1D	4.36	110.37	105.21
15	n	101	CRT	C4-C5-C6	-4.35	118.80	124.91
9	e	102	BCL	O2D-CGD-O1D	-4.35	115.38	123.85
7	C	501	HEM	CHC-C4B-NB	4.35	129.11	124.42
9	w	101	BCL	C4D-CHA-C1A	4.35	126.43	121.24
9	U	101	BCL	CMB-C2B-C1B	-4.35	118.79	125.42
9	r	101	BCL	CMB-C2B-C1B	-4.35	118.80	125.42
9	AE	102	BCL	CMB-C2B-C1B	-4.32	118.83	125.42
9	V	102	BCL	O2D-CGD-O1D	-4.32	115.43	123.85
9	g	102	BCL	O2D-CGD-O1D	-4.32	115.44	123.85
9	x	301	BCL	C1D-ND-C4D	-4.32	103.28	106.31
15	4	101	CRT	C27-C26-C25	-4.31	110.71	123.20
9	s	102	BCL	C2D-C1D-ND	4.31	114.39	110.13
9	Q	101	BCL	O2D-CGD-O1D	-4.30	115.47	123.85
17	S	101	PGW	O01-C1-C2	4.29	118.75	111.09
9	G	102	BCL	O2D-CGD-O1D	-4.29	115.49	123.85
7	o	504	HEM	CHD-C4C-NC	4.29	129.12	124.45
9	8	101	BCL	CMB-C2B-C1B	-4.28	118.90	125.42
10	x	302	BPH	CMC-C2C-C1C	-4.28	105.38	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	102	BCL	O2D-CGD-O1D	-4.28	115.52	123.85
9	W	101	BCL	O2D-CGD-O1D	-4.28	115.52	123.85
7	C	501	HEM	C1B-NB-C4B	4.27	110.27	105.21
15	X	101	CRT	C5-C6-C7	-4.26	119.45	125.89
7	o	504	HEM	C1B-NB-C4B	4.26	110.25	105.21
10	L	302	BPH	O1D-CGD-CBD	-4.26	118.26	124.72
11	x	304	UQ8	C15-C14-C16	4.26	122.62	115.23
9	p	102	BCL	C4D-CHA-C1A	4.26	126.32	121.24
12	H	301	PEF	C2-O2-C10	-4.26	110.33	117.85
9	x	305	BCL	C6-C5-C3	-4.26	103.10	113.47
9	w	101	BCL	CMB-C2B-C1B	-4.25	118.95	125.42
9	m	103	BCL	CMB-C2B-C1B	-4.25	118.95	125.42
9	0	102	BCL	C1C-NC-C4C	-4.24	104.74	106.68
9	Q	101	BCL	CMB-C2B-C1B	-4.24	118.96	125.42
9	0	102	BCL	CMB-C2B-C1B	-4.24	118.96	125.42
9	f	101	BCL	C4D-CHA-C1A	4.24	126.30	121.24
9	M	401	BCL	CAC-C3C-C4C	-4.24	103.18	112.58
9	AC	103	BCL	C2D-C1D-ND	4.24	114.32	110.13
9	6	101	BCL	O2D-CGD-O1D	-4.23	115.61	123.85
9	D	102	BCL	C2D-C1D-ND	4.22	114.31	110.13
15	7	103	CRT	C25-C23-C22	4.22	125.65	119.01
7	C	501	HEM	CHD-C1D-ND	4.22	128.96	124.42
15	G	101	CRT	C20-C19-C17	-4.21	121.37	127.28
9	0	102	BCL	C1D-ND-C4D	-4.21	103.36	106.31
11	x	304	UQ8	C32-C33-C34	-4.21	118.00	127.62
9	K	101	BCL	C2D-C1D-ND	4.20	114.29	110.13
9	AB	101	BCL	CMB-C2B-C1B	-4.20	119.02	125.42
15	7	101	CRT	C32-C31-C30	-4.20	111.03	123.20
9	x	303	BCL	C2D-C1D-ND	4.20	114.28	110.13
9	AB	102	BCL	O2D-CGD-CBD	4.20	118.57	111.23
9	I	101	BCL	O2D-CGD-O1D	-4.19	115.68	123.85
12	H	301	PEF	O2-C10-C11	4.19	118.57	111.09
9	d	101	BCL	C1D-ND-C4D	-4.19	103.37	106.31
9	AK	101	BCL	C4D-CHA-C1A	4.19	126.25	121.24
9	5	101	BCL	C4A-NA-C1A	4.19	108.59	106.68
15	AJ	101	CRT	C5-C6-C7	-4.19	119.56	125.89
9	6	101	BCL	CHA-C1A-NA	-4.19	116.91	126.39
9	AH	101	BCL	CHA-C1A-NA	-4.19	116.91	126.39
9	e	102	BCL	C4D-CHA-C1A	4.18	126.23	121.24
7	C	503	HEM	CAB-C3B-C2B	-4.18	114.86	128.43
9	9	102	BCL	C4D-CHA-C1A	4.17	126.22	121.24
9	5	101	BCL	C1C-NC-C4C	-4.17	104.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	102	BCL	O2D-CGD-CBD	4.17	118.52	111.23
9	Z	102	BCL	C2D-C1D-ND	4.17	114.25	110.13
9	x	303	BCL	C2C-C3C-C4C	-4.17	95.10	101.34
7	C	502	HEM	CAD-CBD-CGD	-4.17	102.61	113.67
9	D	102	BCL	C4D-CHA-C1A	4.16	126.21	121.24
9	2	102	BCL	C1C-NC-C4C	-4.16	104.78	106.68
15	e	101	CRT	C32-C31-C30	-4.15	111.16	123.20
9	8	101	BCL	C16-C15-C13	-4.15	102.18	115.97
7	C	503	HEM	CHB-C1B-NB	4.15	129.50	124.37
9	AL	102	BCL	CMB-C2B-C1B	-4.14	119.11	125.42
15	G	101	CRT	C4-C5-C6	-4.14	119.10	124.91
9	0	102	BCL	C4D-CHA-C1A	4.13	126.18	121.24
9	x	301	BCL	CMA-C3A-C4A	-4.13	100.68	111.77
9	W	101	BCL	C4D-CHA-C1A	4.13	126.17	121.24
9	x	301	BCL	CHA-C1A-NA	-4.13	117.05	126.39
9	S	102	BCL	C4D-CHA-C1A	4.12	126.16	121.24
9	U	101	BCL	C1D-ND-C4D	-4.12	103.42	106.31
9	AH	101	BCL	OBB-CAB-CBB	-4.11	110.57	119.77
9	m	102	BCL	CMB-C2B-C1B	-4.11	119.17	125.42
7	o	501	HEM	C1B-NB-C4B	4.10	110.06	105.21
9	Z	102	BCL	C1C-NC-C4C	-4.09	104.81	106.68
14	y	403	MQ8	C26-C27-C28	-4.09	118.27	127.62
9	3	101	BCL	O2D-CGD-O1D	-4.09	115.89	123.85
9	u	101	BCL	O2D-CGD-O1D	-4.07	115.92	123.85
15	e	101	CRT	C15-C14-C12	-4.07	121.58	127.28
9	r	101	BCL	O2D-CGD-O1D	-4.06	115.94	123.85
9	x	303	BCL	C16-C15-C13	-4.06	102.46	115.97
15	n	101	CRT	C5-C6-C7	-4.06	119.76	125.89
15	v	101	CRT	C26-C27-C28	-4.06	121.59	127.28
9	AE	102	BCL	CHA-C1A-NA	-4.06	117.20	126.39
9	4	102	BCL	C2D-C1D-ND	4.06	114.14	110.13
15	7	101	CRT	C35-C33-C32	-4.05	112.63	119.01
15	s	101	CRT	C20-C19-C17	-4.05	121.60	127.28
9	4	102	BCL	C4D-CHA-C1A	4.04	126.07	121.24
9	N	101	BCL	C4D-CHA-C1A	4.03	126.05	121.24
15	AD	101	CRT	C15-C14-C12	-4.03	121.62	127.28
15	AL	101	CRT	C24-C23-C25	4.03	124.24	118.09
9	m	103	BCL	O2D-CGD-O1D	-4.02	116.03	123.85
9	AK	101	BCL	C2D-C1D-ND	4.01	114.10	110.13
9	x	305	BCL	O2A-CGA-O1A	-4.01	113.60	123.63
9	D	101	BCL	C16-C15-C13	-4.00	102.66	115.97
9	x	305	BCL	CHA-C1A-NA	-4.00	117.33	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	303	BCL	C3B-C4B-NB	-4.00	104.48	109.76
9	6	101	BCL	CMB-C2B-C1B	-3.99	119.34	125.42
11	L	304	UQ8	C15-C14-C16	3.99	122.16	115.23
9	M	402	BCL	CBB-CAB-C3B	3.99	128.81	120.40
15	AC	101	CRT	C29-C28-C30	3.99	124.18	118.09
9	AI	101	BCL	CMA-C3A-C4A	-3.99	101.06	111.77
15	AL	101	CRT	C32-C31-C30	-3.98	111.66	123.20
9	2	102	BCL	C2A-C1A-CHA	3.98	130.78	123.87
15	9	101	CRT	C3-C1-C2	3.98	117.70	110.43
9	M	401	BCL	O2D-CGD-O1D	-3.97	116.11	123.85
14	y	403	MQ8	C34-C33-C35	3.97	122.12	115.23
7	o	504	HEM	C4D-ND-C1D	3.97	109.91	105.21
9	L	303	BCL	CMB-C2B-C1B	-3.97	119.38	125.42
9	q	102	BCL	C4D-CHA-C1A	3.97	125.98	121.24
7	o	501	HEM	C3B-C4B-NB	-3.97	106.62	109.47
9	L	303	BCL	CHA-C1A-NA	-3.97	117.41	126.39
9	T	102	BCL	CMB-C2B-C1B	-3.96	119.38	125.42
9	y	401	BCL	C1C-NC-C4C	-3.96	104.87	106.68
9	k	102	BCL	C2D-C1D-ND	3.96	114.04	110.13
9	AG	101	BCL	OBB-CAB-CBB	-3.95	110.91	119.77
9	f	101	BCL	C1D-ND-C4D	-3.95	103.54	106.31
15	9	101	CRT	C5-C6-C7	-3.95	119.92	125.89
9	i	102	BCL	C2D-C1D-ND	3.95	114.03	110.13
15	v	101	CRT	C9-C10-C11	-3.95	111.77	123.20
9	z	102	BCL	C4D-CHA-C1A	3.95	125.95	121.24
9	Z	102	BCL	CHA-C1A-NA	-3.94	117.46	126.39
9	s	102	BCL	CHA-C1A-NA	-3.94	117.47	126.39
9	Y	101	BCL	CHD-C1D-ND	-3.94	119.26	124.80
15	y	404	CRT	C20-C19-C17	-3.93	121.76	127.28
9	Y	101	BCL	C4A-NA-C1A	3.93	108.47	106.68
7	C	503	HEM	CHD-C4C-C3C	-3.93	118.58	125.21
9	AF	101	BCL	C4D-CHA-C1A	3.93	125.93	121.24
9	4	102	BCL	C1C-NC-C4C	-3.93	104.89	106.68
9	6	101	BCL	C2D-C1D-ND	3.93	114.01	110.13
9	U	101	BCL	O2D-CGD-CBD	3.93	118.09	111.23
15	R	101	CRT	C15-C14-C12	-3.92	121.77	127.28
9	g	102	BCL	CHA-C1A-NA	-3.92	117.51	126.39
7	o	503	HEM	C1B-NB-C4B	3.92	109.85	105.21
15	AJ	101	CRT	C15-C14-C12	-3.92	121.78	127.28
15	2	101	CRT	C26-C27-C28	-3.92	121.78	127.28
9	O	102	BCL	C2D-C1D-ND	3.92	114.00	110.13
11	L	304	UQ8	C35-C34-C36	3.92	122.03	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	0	101	CRT	C21-C20-C19	-3.92	115.50	123.52
9	x	303	BCL	CHA-C1A-NA	-3.92	117.52	126.39
9	c	101	BCL	C4D-CHA-C1A	3.91	125.91	121.24
15	R	101	CRT	C18-C17-C16	3.91	124.06	118.09
9	l	101	BCL	C4D-CHA-C1A	3.91	125.90	121.24
15	E	101	CRT	C4-C5-C6	-3.91	119.43	124.91
15	k	101	CRT	C25-C23-C22	3.90	125.15	119.01
15	Z	101	CRT	C32-C31-C30	-3.90	111.89	123.20
15	n	101	CRT	C15-C14-C12	-3.90	121.81	127.28
9	M	402	BCL	CMC-C2C-C3C	-3.89	98.93	113.98
9	3	101	BCL	C4D-CHA-C1A	3.89	125.89	121.24
9	AF	101	BCL	C2D-C1D-ND	3.88	113.97	110.13
9	7	102	BCL	C4A-NA-C1A	3.88	108.45	106.68
9	2	102	BCL	CMB-C2B-C1B	-3.88	119.52	125.42
9	l	101	BCL	C2D-C1D-ND	3.88	113.96	110.13
9	9	102	BCL	CMB-C2B-C1B	-3.87	119.53	125.42
9	X	102	BCL	C4D-CHA-C1A	3.87	125.86	121.24
9	O	102	BCL	CHA-C1A-NA	-3.86	117.65	126.39
9	I	101	BCL	CHA-C1A-NA	-3.86	117.65	126.39
9	M	402	BCL	CMB-C2B-C1B	-3.86	119.54	125.42
9	6	101	BCL	C1-O2A-CGA	3.86	125.99	116.65
9	u	102	BCL	CHA-C1A-NA	-3.85	117.66	126.39
9	j	101	BCL	C4D-CHA-C1A	3.85	125.83	121.24
9	Q	101	BCL	CHA-C1A-NA	-3.85	117.68	126.39
11	L	304	UQ8	C40-C39-C41	3.84	121.90	115.23
9	I	103	BCL	C2D-C1D-ND	3.84	113.93	110.13
15	AF	102	CRT	C10-C9-C7	-3.84	121.89	127.28
15	AH	102	CRT	C26-C27-C28	-3.84	121.89	127.28
15	n	101	CRT	C10-C9-C7	3.84	132.66	127.28
9	I	101	BCL	CMB-C2B-C1B	-3.84	119.57	125.42
15	AC	101	CRT	C20-C19-C17	-3.84	121.89	127.28
9	S	102	BCL	CMA-C3A-C4A	-3.84	101.46	111.77
7	o	502	HEM	CAD-CBD-CGD	-3.84	103.49	113.67
9	z	102	BCL	CMB-C2B-C1B	-3.84	119.58	125.42
9	AF	101	BCL	O2D-CGD-O1D	-3.83	116.39	123.85
9	I	101	BCL	C2D-C1D-ND	3.83	113.92	110.13
15	v	101	CRT	C29-C28-C30	3.83	123.94	118.09
9	AG	101	BCL	CMB-C2B-C1B	-3.83	119.59	125.42
15	v	101	CRT	C4-C5-C6	3.83	130.29	124.91
9	0	102	BCL	CHA-C1A-NA	-3.83	117.73	126.39
15	i	101	CRT	C14-C15-C16	-3.82	112.12	123.20
7	o	501	HEM	CHD-C1D-ND	3.82	128.53	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AE	102	BCL	C2D-C1D-ND	3.82	113.91	110.13
9	j	101	BCL	C1C-NC-C4C	-3.82	104.94	106.68
9	Y	101	BCL	C1-O2A-CGA	3.81	125.88	116.65
9	7	102	BCL	C4D-CHA-C1A	3.81	125.79	121.24
15	X	101	CRT	C10-C9-C7	-3.81	121.93	127.28
7	o	503	HEM	CHB-C1B-NB	3.81	129.08	124.37
7	o	503	HEM	C4D-ND-C1D	3.81	109.72	105.21
15	AJ	101	CRT	C32-C31-C30	-3.81	112.17	123.20
9	Y	101	BCL	CMB-C2B-C1B	-3.81	119.62	125.42
9	F	101	BCL	C4D-CHA-C1A	3.81	125.78	121.24
9	M	402	BCL	CMA-C3A-C4A	-3.80	101.56	111.77
9	x	301	BCL	CHB-C4A-NA	-3.80	118.92	124.40
15	P	102	CRT	C20-C19-C17	-3.79	121.96	127.28
9	5	101	BCL	C2D-C1D-ND	3.79	113.88	110.13
11	x	304	UQ8	C30-C29-C31	3.79	121.81	115.23
9	4	102	BCL	CHA-C1A-NA	-3.79	117.81	126.39
9	L	303	BCL	C3B-C4B-NB	-3.79	104.76	109.76
15	z	101	CRT	C37-C36-C35	-3.79	119.60	124.91
12	y	406	PEF	O2-C10-O4	-3.78	115.69	122.99
15	P	102	CRT	C32-C31-C30	-3.78	112.24	123.20
9	A	102	BCL	C2D-C1D-ND	3.78	113.87	110.13
9	6	101	BCL	OBB-CAB-CBB	-3.77	111.32	119.77
15	R	101	CRT	C21-C22-C23	-3.77	121.99	127.28
9	D	102	BCL	CHA-C1A-NA	-3.77	117.85	126.39
9	e	102	BCL	CHA-C1A-NA	-3.76	117.88	126.39
15	7	101	CRT	C34-C33-C35	3.76	123.83	118.09
9	R	102	BCL	CED-O2D-CGD	-3.75	107.41	115.92
15	i	101	CRT	C21-C22-C23	-3.75	122.02	127.28
9	G	102	BCL	CHA-C1A-NA	-3.74	117.92	126.39
9	u	101	BCL	C4D-CHA-C1A	3.74	125.70	121.24
9	L	301	BCL	CHA-C1A-NA	-3.74	117.93	126.39
9	x	301	BCL	OBB-CAB-CBB	-3.73	111.41	119.77
17	AE	101	PGW	O01-C1-C2	3.73	117.75	111.09
9	AC	103	BCL	C4D-CHA-C1A	3.73	125.69	121.24
15	v	101	CRT	C21-C20-C19	-3.73	115.89	123.52
9	7	102	BCL	C2D-C1D-ND	3.73	113.81	110.13
15	P	102	CRT	C21-C22-C23	-3.72	122.05	127.28
9	c	101	BCL	C2D-C1D-ND	3.72	113.81	110.13
15	Z	101	CRT	C18-C17-C16	3.72	123.77	118.09
9	AB	102	BCL	CHA-C1A-NA	-3.72	117.97	126.39
9	W	101	BCL	OBB-CAB-CBB	-3.72	111.44	119.77
9	4	102	BCL	CMB-C2B-C1B	-3.71	119.77	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	503	HEM	CAB-C3B-C2B	-3.71	116.36	128.43
9	p	102	BCL	CHA-C1A-NA	-3.71	117.99	126.39
9	M	401	BCL	C11-C10-C8	-3.71	103.64	115.97
9	r	101	BCL	C4D-CHA-C1A	3.71	125.67	121.24
9	u	101	BCL	CHD-C1D-ND	-3.71	119.59	124.80
9	z	102	BCL	OBB-CAB-CBB	-3.71	111.47	119.77
9	x	303	BCL	O2A-CGA-O1A	-3.70	114.37	123.63
7	C	504	HEM	CHB-C1B-NB	3.70	128.94	124.37
9	8	101	BCL	OBB-CAB-CBB	-3.70	111.49	119.77
9	P	101	BCL	CHB-C1B-NB	3.70	129.59	124.05
9	W	101	BCL	CMB-C2B-C1B	-3.70	119.79	125.42
9	L	303	BCL	CGD-CBD-CAD	-3.70	98.88	110.85
9	8	101	BCL	C2D-C1D-ND	3.70	113.78	110.13
9	AC	103	BCL	CMB-C2B-C1B	-3.69	119.79	125.42
9	AL	102	BCL	CHA-C1A-NA	-3.69	118.03	126.39
9	AG	101	BCL	C1C-NC-C4C	-3.69	104.99	106.68
9	S	102	BCL	CHA-C1A-NA	-3.69	118.03	126.39
9	R	102	BCL	CHB-C1B-NB	3.69	129.59	124.05
9	A	103	BCL	C2D-C1D-ND	3.68	113.77	110.13
12	A	101	PEF	C3-O3-C30	3.68	126.17	117.08
9	X	102	BCL	CHA-C1A-NA	-3.68	118.05	126.39
9	AC	102	BCL	CHA-C1A-NA	-3.68	118.06	126.39
9	X	102	BCL	CMB-C2B-C1B	-3.68	119.81	125.42
9	k	102	BCL	CMD-C2D-C1D	3.68	131.21	124.73
9	z	102	BCL	CHA-C1A-NA	-3.68	118.06	126.39
9	L	303	BCL	O2D-CGD-O1D	-3.68	116.69	123.85
9	h	101	BCL	CMB-C2B-C1B	-3.67	119.83	125.42
15	I	102	CRT	C4-C5-C6	3.67	130.07	124.91
15	P	102	CRT	C29-C28-C30	3.67	123.69	118.09
9	AC	102	BCL	C1C-NC-C4C	-3.67	105.01	106.68
9	AF	101	BCL	CHA-C1A-NA	-3.66	118.09	126.39
9	3	101	BCL	CHD-C1D-ND	-3.66	119.65	124.80
9	u	101	BCL	CMB-C2B-C1B	-3.66	119.85	125.42
9	M	401	BCL	C6-C5-C3	-3.66	104.55	113.47
9	AK	101	BCL	CHA-C1A-NA	-3.66	118.11	126.39
11	x	304	UQ8	C8-C7-C6	3.66	121.09	112.08
9	I	101	BCL	C7-C6-C5	-3.66	103.52	113.26
9	9	102	BCL	C2D-C1D-ND	3.66	113.75	110.13
9	h	101	BCL	C4D-CHA-C1A	3.65	125.60	121.24
9	5	101	BCL	CMB-C2B-C1B	-3.65	119.86	125.42
15	g	101	CRT	C5-C6-C7	-3.65	120.37	125.89
9	Z	102	BCL	OBB-CAB-CBB	-3.65	111.59	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AF	101	BCL	O2D-CGD-CBD	3.65	117.61	111.23
9	m	103	BCL	CHA-C1A-NA	-3.65	118.13	126.39
15	AL	101	CRT	C26-C27-C28	-3.65	122.16	127.28
9	AC	102	BCL	C2D-C1D-ND	3.65	113.74	110.13
9	M	402	BCL	C16-C15-C13	-3.64	103.86	115.97
9	Y	101	BCL	C4D-CHA-C1A	3.64	125.59	121.24
9	P	101	BCL	CHA-C1A-NA	-3.64	118.15	126.39
15	AJ	101	CRT	C21-C20-C19	3.64	130.97	123.52
9	R	102	BCL	CHD-C1D-ND	-3.64	119.68	124.80
9	e	102	BCL	CHB-C1B-NB	3.64	129.51	124.05
15	AH	102	CRT	C21-C22-C23	-3.64	122.18	127.28
7	C	502	HEM	CHD-C1D-ND	3.63	128.33	124.42
9	N	101	BCL	CHA-C1A-NA	-3.63	118.16	126.39
9	f	101	BCL	CHB-C1B-NB	3.63	129.50	124.05
7	o	502	HEM	CHD-C1D-ND	3.63	128.33	124.42
9	F	101	BCL	C2D-C1D-ND	3.63	113.72	110.13
9	A	102	BCL	CHA-C1A-NA	-3.63	118.17	126.39
15	7	101	CRT	C14-C15-C16	-3.63	112.69	123.20
9	R	102	BCL	O2D-CGD-CBD	3.63	117.57	111.23
9	f	101	BCL	C2D-C1D-ND	3.62	113.71	110.13
9	z	102	BCL	C2D-C1D-ND	3.62	113.71	110.13
9	Z	102	BCL	C4D-CHA-C1A	3.62	125.56	121.24
9	0	102	BCL	C2D-C1D-ND	3.62	113.71	110.13
15	R	101	CRT	C11-C12-C14	3.62	124.70	119.01
15	Z	101	CRT	C34-C33-C35	3.62	123.61	118.09
9	R	102	BCL	CHA-C1A-NA	-3.61	118.21	126.39
9	f	101	BCL	CHA-C1A-NA	-3.61	118.21	126.39
9	m	103	BCL	C2D-C1D-ND	3.61	113.70	110.13
12	x	306	PEF	O2-C10-C11	3.61	117.53	111.09
9	g	102	BCL	C1-O2A-CGA	3.61	125.38	116.65
7	C	504	HEM	CAA-CBA-CGA	-3.61	104.10	113.67
9	Y	101	BCL	CHA-C1A-NA	-3.60	118.23	126.39
9	S	102	BCL	CHD-C1D-ND	-3.60	119.73	124.80
15	AD	101	CRT	C18-C17-C16	3.60	123.59	118.09
15	4	101	CRT	C25-C23-C22	-3.60	113.35	119.01
9	1	101	BCL	C11-C10-C8	-3.60	104.00	115.97
15	R	101	CRT	C5-C6-C7	-3.60	120.46	125.89
9	u	102	BCL	C11-C10-C8	-3.60	104.01	115.97
15	4	101	CRT	C29-C28-C30	3.59	123.58	118.09
9	AG	101	BCL	C4A-NA-C1A	3.59	108.32	106.68
9	AC	103	BCL	CHA-C1A-NA	-3.59	118.26	126.39
9	T	102	BCL	CHA-C1A-NA	-3.59	118.27	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	102	BCL	C4D-CHA-C1A	3.59	125.52	121.24
9	s	102	BCL	CHD-C1D-ND	-3.59	119.75	124.80
15	9	101	CRT	C10-C11-C12	-3.58	116.54	126.36
15	E	101	CRT	C10-C9-C7	-3.58	122.26	127.28
9	Q	101	BCL	OBB-CAB-CBB	-3.58	111.75	119.77
11	x	304	UQ8	C7-C8-C9	-3.57	120.68	126.83
9	N	101	BCL	C7-C6-C5	-3.57	103.74	113.26
15	M	405	CRT	C10-C9-C7	-3.57	122.27	127.28
9	M	401	BCL	CMB-C2B-C1B	-3.57	119.98	125.42
15	q	101	CRT	C5-C6-C7	-3.57	120.50	125.89
15	m	104	CRT	C21-C20-C19	-3.56	116.23	123.52
15	4	101	CRT	C24-C23-C25	3.56	123.53	118.09
9	0	102	BCL	OBB-CAB-CBB	-3.56	111.79	119.77
9	y	401	BCL	CHA-C1A-NA	-3.56	118.33	126.39
15	T	101	CRT	C34-C33-C35	3.56	123.52	118.09
15	9	101	CRT	C21-C20-C19	-3.56	116.24	123.52
9	L	303	BCL	O2D-CGD-CBD	3.56	117.45	111.23
7	o	501	HEM	CAA-CBA-CGA	-3.55	104.24	113.67
15	9	101	CRT	C20-C19-C17	-3.55	122.29	127.28
9	A	103	BCL	C1C-NC-C4C	-3.55	105.06	106.68
9	T	102	BCL	CMC-C2C-C3C	-3.55	100.26	113.98
9	k	102	BCL	C4A-NA-C1A	3.55	108.30	106.68
9	AI	102	BCL	CHD-C1D-ND	-3.55	119.81	124.80
7	C	501	HEM	C2A-C1A-NA	-3.54	106.22	110.15
7	o	503	HEM	CHC-C1C-NC	3.54	128.31	124.45
9	1	101	BCL	C2D-C1D-ND	3.54	113.63	110.13
9	AC	103	BCL	OBB-CAB-CBB	-3.54	111.85	119.77
9	9	102	BCL	CHA-C1A-NA	-3.53	118.41	126.39
9	AI	101	BCL	CHA-C1A-NA	-3.53	118.41	126.39
9	AK	101	BCL	CMC-C2C-C3C	-3.52	100.35	113.98
9	A	102	BCL	C1C-NC-C4C	-3.52	105.07	106.68
15	Z	101	CRT	C10-C9-C7	-3.52	122.33	127.28
9	y	401	BCL	C4D-CHA-C1A	3.52	125.45	121.24
9	e	102	BCL	CBB-CAB-C3B	3.52	127.83	120.40
9	S	102	BCL	C2D-C1D-ND	3.52	113.61	110.13
9	M	402	BCL	CHA-C1A-NA	-3.52	118.42	126.39
9	w	101	BCL	CHA-C1A-NA	-3.52	118.42	126.39
9	q	102	BCL	C2D-C1D-ND	3.52	113.61	110.13
9	W	101	BCL	CHA-C1A-NA	-3.51	118.43	126.39
15	4	101	CRT	C37-C36-C35	-3.51	119.98	124.91
9	AH	101	BCL	CBB-CAB-C3B	3.51	127.81	120.40
9	T	102	BCL	C1-C2-C3	-3.51	120.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	102	BCL	C1C-NC-C4C	-3.51	105.08	106.68
9	F	101	BCL	C7-C6-C5	-3.51	103.91	113.26
9	i	102	BCL	CHA-C1A-NA	-3.51	118.45	126.39
15	q	101	CRT	C21-C20-C19	-3.50	116.35	123.52
9	z	102	BCL	CHD-C1D-ND	-3.50	119.87	124.80
9	w	101	BCL	CMA-C3A-C4A	-3.50	102.36	111.77
15	e	101	CRT	C34-C33-C35	3.50	123.44	118.09
9	A	103	BCL	CHA-C1A-NA	-3.50	118.47	126.39
9	G	102	BCL	C2D-C1D-ND	3.50	113.59	110.13
15	T	101	CRT	C21-C20-C19	-3.50	116.36	123.52
9	V	102	BCL	CHA-C1A-NA	-3.50	118.47	126.39
9	1	101	BCL	C1C-NC-C4C	-3.50	105.08	106.68
15	i	101	CRT	C32-C31-C30	-3.50	113.07	123.20
9	U	101	BCL	CHB-C1B-NB	3.49	129.29	124.05
9	l	101	BCL	OBB-CAB-CBB	-3.49	111.94	119.77
9	S	102	BCL	OBB-CAB-CBB	-3.49	111.95	119.77
9	A	102	BCL	O2D-CGD-O1D	-3.49	117.05	123.85
9	m	102	BCL	CHA-C1A-NA	-3.49	118.49	126.39
9	u	101	BCL	C11-C12-C13	-3.49	104.38	115.97
9	s	102	BCL	CHB-C1B-NB	3.49	129.28	124.05
9	c	101	BCL	C16-C15-C13	-3.48	104.38	115.97
15	q	101	CRT	C21-C22-C23	-3.48	122.40	127.28
9	j	101	BCL	C2D-C1D-ND	3.48	113.57	110.13
9	Q	101	BCL	C2D-C1D-ND	3.48	113.57	110.13
7	C	504	HEM	CHD-C4C-C3C	-3.47	119.35	125.21
12	y	407	PEF	O2-C10-C11	3.47	117.28	111.09
15	s	101	CRT	C34-C33-C35	3.47	123.39	118.09
15	i	101	CRT	C34-C33-C35	3.47	123.39	118.09
9	g	102	BCL	C1-C2-C3	-3.47	120.51	126.20
9	l	101	BCL	CHA-C1A-NA	-3.47	118.54	126.39
9	r	101	BCL	CHB-C1B-NB	3.47	129.25	124.05
9	j	101	BCL	C2B-C1B-NB	-3.47	106.73	110.33
9	i	102	BCL	CHB-C1B-NB	3.47	129.25	124.05
7	C	501	HEM	CAD-CBD-CGD	3.46	122.86	113.67
9	M	402	BCL	C2D-C1D-ND	3.46	113.55	110.13
9	q	102	BCL	CHA-C1A-NA	-3.45	118.57	126.39
9	h	101	BCL	C2D-C1D-ND	3.45	113.54	110.13
9	AC	102	BCL	C16-C15-C13	-3.45	104.50	115.97
15	Z	101	CRT	C13-C12-C11	3.45	123.36	118.09
9	M	401	BCL	CMA-C3A-C4A	-3.45	102.50	111.77
9	V	102	BCL	C2D-C1D-ND	3.45	113.54	110.13
9	2	102	BCL	C2D-C1D-ND	3.45	113.54	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	101	CRT	C32-C31-C30	-3.45	113.21	123.20
9	x	305	BCL	C2B-C1B-NB	-3.45	106.75	110.33
11	x	304	UQ8	C35-C34-C33	-3.44	114.79	123.63
9	AH	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
9	k	102	BCL	CHD-C1D-ND	-3.44	119.96	124.80
7	o	502	HEM	CHA-C1A-NA	3.44	130.10	123.86
9	e	102	BCL	C2D-C1D-ND	3.44	113.53	110.13
9	L	303	BCL	O2A-CGA-O1A	-3.44	115.03	123.63
15	n	101	CRT	C24-C23-C25	3.43	123.33	118.09
9	W	101	BCL	C2D-C1D-ND	3.43	113.52	110.13
9	w	101	BCL	C2D-C1D-ND	3.43	113.52	110.13
15	Z	101	CRT	C16-C17-C19	-3.42	113.62	119.01
9	AF	101	BCL	OBB-CAB-CBB	-3.42	112.10	119.77
9	AH	101	BCL	CHB-C1B-NB	3.42	129.18	124.05
15	m	104	CRT	C18-C17-C16	3.42	123.31	118.09
15	7	101	CRT	C4-C5-C6	-3.42	120.11	124.91
9	p	102	BCL	OBB-CAB-CBB	-3.42	112.11	119.77
7	C	502	HEM	C4D-ND-C1D	3.42	109.25	105.21
9	L	301	BCL	O2D-CGD-O1D	-3.42	117.20	123.85
9	AL	102	BCL	C2D-C1D-ND	3.42	113.51	110.13
9	AB	101	BCL	CHA-C1A-NA	-3.41	118.66	126.39
9	w	101	BCL	CHD-C1D-ND	-3.41	120.00	124.80
15	n	101	CRT	C10-C11-C12	-3.41	117.01	126.36
9	s	102	BCL	OBB-CAB-CBB	-3.41	112.13	119.77
9	U	101	BCL	O2A-CGA-O1A	-3.41	115.09	123.63
9	8	101	BCL	CHD-C1D-ND	-3.41	120.00	124.80
14	M	404	MQ8	C26-C27-C28	-3.41	119.83	127.62
15	AJ	101	CRT	C20-C21-C22	-3.41	116.55	123.52
9	X	102	BCL	CBB-CAB-C3B	3.40	127.58	120.40
9	T	102	BCL	CMA-C3A-C4A	-3.40	102.63	111.77
9	D	102	BCL	OBB-CAB-CBB	-3.40	112.16	119.77
9	M	401	BCL	C2D-C1D-ND	3.40	113.49	110.13
15	P	102	CRT	C26-C25-C23	-3.40	117.05	126.36
9	u	101	BCL	C2D-C1D-ND	3.39	113.49	110.13
9	r	101	BCL	CHA-C1A-NA	-3.39	118.70	126.39
9	i	102	BCL	CBB-CAB-C3B	3.39	127.56	120.40
9	AI	101	BCL	CHB-C1B-NB	3.39	129.14	124.05
7	C	503	HEM	CAB-C3B-C4B	3.39	139.37	124.39
9	A	103	BCL	CHD-C1D-ND	-3.39	120.03	124.80
15	Z	101	CRT	C24-C23-C25	3.39	123.27	118.09
9	D	101	BCL	CHA-C1A-NA	-3.39	118.72	126.39
9	Y	101	BCL	OBB-CAB-CBB	-3.39	112.18	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	x	304	UQ8	C27-C28-C29	-3.39	119.87	127.62
17	AE	101	PGW	C02-O01-C1	3.38	123.82	117.85
9	i	102	BCL	OBB-CAB-CBB	-3.38	112.20	119.77
15	V	101	CRT	C20-C19-C17	-3.38	122.54	127.28
9	N	101	BCL	OBB-CAB-CBB	-3.38	112.20	119.77
9	x	305	BCL	C3D-C2D-C1D	-3.38	101.22	105.83
9	1	101	BCL	OBB-CAB-CBB	-3.38	112.20	119.77
9	V	102	BCL	C16-C15-C13	-3.38	104.74	115.97
15	7	103	CRT	C24-C23-C22	-3.38	117.35	122.82
9	A	102	BCL	C1-O2A-CGA	3.37	124.82	116.65
9	f	101	BCL	CMA-C3A-C4A	-3.37	102.70	111.77
9	AI	101	BCL	OBB-CAB-CBB	-3.37	112.21	119.77
9	G	102	BCL	C16-C15-C13	-3.37	104.76	115.97
15	Z	101	CRT	C21-C20-C19	-3.37	116.62	123.52
9	y	401	BCL	C2D-C1D-ND	3.37	113.46	110.13
9	Z	102	BCL	C16-C15-C13	-3.37	104.77	115.97
9	I	101	BCL	CMA-C3A-C4A	-3.37	102.72	111.77
9	AI	101	BCL	O2A-CGA-O1A	-3.37	115.21	123.63
9	T	102	BCL	C1C-NC-C4C	-3.37	105.14	106.68
9	A	103	BCL	C4D-CHA-C1A	3.37	125.26	121.24
9	3	101	BCL	C4A-NA-C1A	3.36	108.21	106.68
15	P	102	CRT	C34-C33-C35	3.36	123.22	118.09
9	L	301	BCL	OBB-CAB-CBB	-3.36	112.24	119.77
7	o	504	HEM	CHD-C1D-ND	3.36	128.04	124.42
9	A	102	BCL	C4A-NA-C1A	3.36	108.21	106.68
9	F	101	BCL	CHB-C1B-NB	3.36	129.09	124.05
9	N	101	BCL	C16-C15-C13	-3.36	104.81	115.97
9	D	101	BCL	C2B-C1B-NB	-3.36	106.85	110.33
9	r	101	BCL	C2D-C1D-ND	3.35	113.44	110.13
9	AI	102	BCL	C2D-C1D-ND	3.35	113.44	110.13
15	AD	101	CRT	C26-C27-C28	-3.35	122.58	127.28
9	l	101	BCL	C1C-NC-C4C	-3.35	105.15	106.68
9	y	401	BCL	O2A-CGA-O1A	-3.35	115.25	123.63
15	R	101	CRT	C13-C12-C14	-3.35	117.39	122.82
9	u	102	BCL	CHB-C1B-NB	3.35	129.07	124.05
9	G	102	BCL	C1C-NC-C4C	-3.35	105.15	106.68
15	k	101	CRT	C24-C23-C22	-3.35	117.39	122.82
9	h	101	BCL	CHA-C1A-NA	-3.35	118.81	126.39
9	5	101	BCL	CBB-CAB-C3B	3.35	127.46	120.40
9	A	103	BCL	O2A-CGA-O1A	-3.35	115.26	123.63
15	i	101	CRT	C10-C9-C7	-3.34	122.59	127.28
9	AB	102	BCL	C2D-C1D-ND	3.34	113.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	102	BCL	O2D-CGD-O1D	-3.34	117.34	123.85
9	AB	101	BCL	C2D-C1D-ND	3.34	113.43	110.13
15	2	101	CRT	C14-C15-C16	-3.34	113.53	123.20
9	I	101	BCL	O2A-CGA-O1A	-3.34	115.28	123.63
9	M	402	BCL	C2A-C1A-CHA	3.34	129.66	123.87
15	AD	101	CRT	C10-C9-C7	-3.34	122.60	127.28
9	m	102	BCL	C2B-C1B-NB	-3.34	106.87	110.33
7	C	503	HEM	CHC-C4B-C3B	3.34	131.73	125.07
9	P	101	BCL	C2D-C1D-ND	3.33	113.43	110.13
15	7	103	CRT	C37-C36-C35	-3.33	120.23	124.91
15	V	101	CRT	C32-C31-C30	-3.33	113.55	123.20
9	L	301	BCL	C2D-C1D-ND	3.33	113.42	110.13
9	D	102	BCL	C16-C15-C13	-3.33	104.90	115.97
15	0	101	CRT	C34-C33-C35	3.33	123.17	118.09
9	AI	102	BCL	CHA-C1A-NA	-3.33	118.86	126.39
15	I	102	CRT	C15-C14-C12	-3.33	122.61	127.28
15	s	101	CRT	C4-C5-C6	-3.33	120.24	124.91
9	W	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
9	F	101	BCL	CHA-C1A-NA	-3.32	118.87	126.39
9	Z	102	BCL	CBB-CAB-C3B	3.32	127.40	120.40
9	AG	101	BCL	C16-C15-C13	-3.32	104.93	115.97
9	K	101	BCL	CHA-C1A-NA	-3.32	118.87	126.39
9	D	101	BCL	C7-C6-C5	-3.32	104.41	113.26
9	4	102	BCL	CHD-C1D-ND	-3.32	120.13	124.80
9	AI	102	BCL	C4D-CHA-C1A	3.32	125.20	121.24
9	7	102	BCL	OBB-CAB-CBB	-3.32	112.34	119.77
9	3	101	BCL	CMD-C2D-C1D	3.32	130.57	124.73
9	y	401	BCL	CMB-C2B-C1B	-3.32	120.37	125.42
9	X	102	BCL	OBB-CAB-CBB	-3.31	112.35	119.77
9	q	102	BCL	CHB-C1B-NB	3.31	129.01	124.05
9	AC	103	BCL	C4A-NA-C1A	3.31	108.19	106.68
15	m	104	CRT	C14-C15-C16	-3.30	113.63	123.20
9	O	102	BCL	C1-O2A-CGA	3.30	124.64	116.65
15	e	101	CRT	C21-C22-C23	-3.30	122.65	127.28
9	q	102	BCL	OBB-CAB-CBB	-3.30	112.38	119.77
9	V	102	BCL	CHD-C1D-ND	-3.30	120.16	124.80
9	F	101	BCL	OBB-CAB-CBB	-3.30	112.38	119.77
9	k	102	BCL	CHA-C1A-NA	-3.29	118.93	126.39
15	e	101	CRT	C21-C20-C19	-3.29	116.78	123.52
9	5	101	BCL	OBB-CAB-CBB	-3.29	112.39	119.77
9	g	102	BCL	OBB-CAB-CBB	-3.29	112.40	119.77
9	M	402	BCL	OBD-CAD-C3D	3.29	136.11	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	z	102	BCL	C16-C15-C13	-3.29	105.03	115.97
9	N	101	BCL	C2D-C1D-ND	3.29	113.38	110.13
15	AH	102	CRT	C13-C12-C11	3.29	123.11	118.09
9	m	102	BCL	OBB-CAB-CBB	-3.29	112.41	119.77
9	d	101	BCL	CHB-C4A-NA	-3.28	119.66	124.40
9	P	101	BCL	CHD-C1D-ND	-3.28	120.19	124.80
9	r	101	BCL	OBB-CAB-CBB	-3.28	112.43	119.77
15	4	101	CRT	C16-C17-C19	-3.27	113.86	119.01
9	r	101	BCL	CHD-C1D-ND	-3.27	120.20	124.80
9	3	101	BCL	C2D-C1D-ND	3.27	113.36	110.13
9	k	102	BCL	C3D-C2D-C1D	-3.27	101.37	105.83
9	D	101	BCL	CHD-C1D-ND	-3.27	120.20	124.80
15	AF	102	CRT	C14-C15-C16	-3.27	113.73	123.20
9	u	102	BCL	CBB-CAB-C3B	3.27	127.29	120.40
9	1	101	BCL	CHA-C1A-NA	-3.27	118.99	126.39
9	d	101	BCL	CHA-C1A-NA	-3.27	119.00	126.39
15	O	101	CRT	C21-C20-C19	-3.26	116.84	123.52
9	L	301	BCL	C12-C11-C10	-3.26	98.66	113.28
9	AI	102	BCL	C16-C15-C13	-3.26	105.13	115.97
9	x	303	BCL	CHB-C1B-NB	3.26	128.94	124.05
15	O	101	CRT	C9-C10-C11	-3.26	113.76	123.20
9	N	101	BCL	C11-C10-C8	-3.26	105.13	115.97
9	G	102	BCL	OBB-CAB-CBB	-3.26	112.47	119.77
9	AK	101	BCL	CMA-C3A-C4A	-3.26	103.02	111.77
9	u	101	BCL	CHA-C1A-NA	-3.25	119.02	126.39
9	O	102	BCL	CHB-C1B-NB	3.25	128.93	124.05
15	g	101	CRT	C32-C31-C30	3.25	132.62	123.20
9	3	101	BCL	CMC-C2C-C3C	-3.25	101.41	113.98
9	I	101	BCL	C16-C15-C13	-3.25	105.16	115.97
9	l	101	BCL	CMA-C3A-C4A	-3.25	103.04	111.77
15	z	101	CRT	C27-C26-C25	-3.25	113.78	123.20
9	R	102	BCL	C3D-C2D-C1D	-3.25	101.40	105.83
9	R	102	BCL	OBB-CAB-CBB	-3.25	112.49	119.77
9	AK	101	BCL	C1C-NC-C4C	-3.25	105.20	106.68
15	Z	101	CRT	C4-C5-C6	-3.25	120.35	124.91
12	H	302	PEF	C2-O2-C10	-3.25	112.11	117.85
9	c	101	BCL	CHB-C1B-NB	3.25	128.92	124.05
9	AE	102	BCL	CMA-C3A-C4A	-3.25	103.05	111.77
15	V	101	CRT	C26-C25-C23	-3.25	117.46	126.36
15	k	101	CRT	C4-C5-C6	-3.25	120.36	124.91
9	w	101	BCL	C1-C2-C3	-3.24	120.88	126.20
9	D	101	BCL	CMB-C2B-C1B	-3.24	120.48	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	101	CRT	C36-C35-C33	-3.24	120.99	125.89
15	V	101	CRT	C34-C33-C35	3.24	123.04	118.09
9	F	101	BCL	C6-C5-C3	-3.24	105.58	113.47
9	AL	102	BCL	C16-C15-C13	-3.24	105.20	115.97
9	D	101	BCL	CED-O2D-CGD	-3.24	108.57	115.92
12	A	101	PEF	O2-C10-O4	-3.24	116.74	122.99
15	q	101	CRT	C24-C23-C25	3.24	123.03	118.09
9	L	301	BCL	O2A-CGA-O1A	-3.24	115.53	123.63
9	7	102	BCL	CMB-C2B-C1B	-3.24	120.49	125.42
7	C	503	HEM	C4C-NC-C1C	3.24	111.10	105.82
9	3	101	BCL	CHA-C1A-NA	-3.23	119.07	126.39
9	AG	101	BCL	C2B-C1B-NB	-3.23	106.97	110.33
9	9	102	BCL	CHB-C1B-NB	3.23	128.89	124.05
9	AB	102	BCL	OBB-CAB-CBB	-3.23	112.54	119.77
9	Y	101	BCL	C7-C6-C5	-3.23	104.66	113.26
9	Z	102	BCL	C2A-C1A-CHA	3.23	129.47	123.87
9	z	102	BCL	C11-C10-C8	-3.23	105.24	115.97
10	y	402	BPH	OBB-CAB-C3B	3.23	125.38	119.99
9	u	102	BCL	C3B-C4B-NB	-3.22	105.50	109.76
9	x	305	BCL	CAC-C3C-C4C	-3.22	105.43	112.58
9	A	103	BCL	CHB-C1B-NB	3.22	128.88	124.05
15	O	101	CRT	C15-C14-C12	-3.22	122.76	127.28
15	Z	101	CRT	C26-C27-C28	-3.22	122.76	127.28
9	AK	101	BCL	C2A-C1A-CHA	3.22	129.46	123.87
15	I	102	CRT	C8-C7-C6	3.22	123.01	118.09
9	L	301	BCL	C1-C2-C3	-3.22	120.92	126.20
9	K	101	BCL	CHB-C1B-NB	3.22	128.88	124.05
15	m	104	CRT	C27-C26-C25	-3.22	113.87	123.20
9	p	102	BCL	C7-C6-C5	-3.22	104.68	113.26
9	2	102	BCL	CMA-C3A-C4A	-3.22	103.12	111.77
9	AI	102	BCL	OBB-CAB-CBB	-3.22	112.57	119.77
9	M	401	BCL	OBB-CAB-CBB	-3.21	112.57	119.77
15	k	101	CRT	C15-C14-C12	-3.21	122.77	127.28
10	x	302	BPH	CAA-CBA-CGA	-3.21	104.08	113.21
7	o	502	HEM	CHD-C4C-C3C	-3.21	119.79	125.21
9	AE	102	BCL	CHB-C1B-NB	3.21	128.87	124.05
9	T	102	BCL	CHD-C1D-ND	-3.21	120.28	124.80
9	9	102	BCL	CHD-C1D-ND	-3.21	120.28	124.80
15	AF	102	CRT	C20-C19-C17	-3.21	122.77	127.28
9	M	402	BCL	C3B-C4B-NB	-3.21	105.52	109.76
9	Q	101	BCL	C7-C6-C5	-3.21	104.71	113.26
9	j	101	BCL	OBB-CAB-CBB	-3.21	112.58	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	h	101	BCL	CHD-C1D-ND	-3.21	120.29	124.80
9	L	303	BCL	CMC-C2C-C3C	-3.21	101.58	113.98
15	e	101	CRT	C18-C17-C16	3.21	122.99	118.09
9	D	102	BCL	CBB-CAB-C3B	3.21	127.16	120.40
9	AL	102	BCL	CHB-C1B-NB	3.20	128.85	124.05
9	x	303	BCL	CMA-C3A-C4A	-3.20	103.18	111.77
9	1	101	BCL	C4D-CHA-C1A	3.20	125.06	121.24
14	y	403	MQ8	C14-C13-C15	3.20	120.78	115.23
9	q	102	BCL	CHC-C1C-NC	3.20	129.01	124.40
9	8	101	BCL	CBB-CAB-C3B	3.20	127.14	120.40
9	2	102	BCL	C11-C12-C13	-3.19	105.35	115.97
9	x	305	BCL	CGD-CBD-CAD	-3.19	100.51	110.85
15	i	101	CRT	C35-C33-C32	-3.19	113.99	119.01
9	AC	102	BCL	CMB-C2B-C1B	-3.19	120.56	125.42
9	D	102	BCL	CMA-C3A-C4A	-3.19	103.20	111.77
15	9	101	CRT	C32-C31-C30	-3.19	113.96	123.20
9	AF	101	BCL	C7-C6-C5	-3.19	104.77	113.26
9	AC	103	BCL	C1-C2-C3	-3.19	120.98	126.20
15	z	101	CRT	C21-C20-C19	-3.19	117.00	123.52
15	4	101	CRT	C15-C14-C12	-3.19	122.81	127.28
9	h	101	BCL	OBB-CAB-CBB	-3.18	112.64	119.77
9	1	101	BCL	CBB-CAB-C3B	3.18	127.11	120.40
9	AB	102	BCL	CHD-C1D-ND	-3.18	120.32	124.80
9	x	301	BCL	CGD-CBD-CAD	-3.18	100.55	110.85
9	y	401	BCL	CMC-C2C-C3C	-3.18	101.69	113.98
9	6	101	BCL	CBB-CAB-C3B	3.18	127.10	120.40
9	q	102	BCL	CBB-CAB-C3B	3.18	127.10	120.40
9	c	101	BCL	CHA-C1A-NA	-3.18	119.20	126.39
9	d	101	BCL	OBB-CAB-CBB	-3.18	112.66	119.77
9	AI	102	BCL	C3C-C4C-CHD	-3.17	116.70	123.39
9	L	303	BCL	CHD-C1D-ND	-3.17	120.34	124.80
15	AJ	101	CRT	C4-C5-C6	-3.17	120.46	124.91
9	x	305	BCL	CMA-C3A-C4A	-3.17	103.25	111.77
9	h	101	BCL	C1-O2A-CGA	3.17	124.32	116.65
9	3	101	BCL	CHB-C1B-NB	3.17	128.80	124.05
9	M	401	BCL	CHC-C1C-NC	3.17	128.97	124.40
9	M	401	BCL	C16-C15-C13	-3.16	105.45	115.97
9	l	101	BCL	C2A-C1A-CHA	3.16	129.35	123.87
9	e	102	BCL	C1C-NC-C4C	-3.16	105.24	106.68
15	7	101	CRT	C8-C7-C6	3.16	122.92	118.09
9	x	303	BCL	CMC-C2C-C3C	-3.16	101.76	113.98
9	u	102	BCL	CMA-C3A-C4A	-3.16	103.28	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	301	BCL	CHD-C1D-ND	-3.16	120.36	124.80
9	9	102	BCL	CMC-C2C-C3C	-3.16	101.77	113.98
9	s	102	BCL	C1-C2-C3	-3.16	121.02	126.20
9	AG	101	BCL	CBB-CAB-C3B	3.16	127.06	120.40
9	p	102	BCL	C2B-C1B-NB	-3.16	107.05	110.33
9	f	101	BCL	O2A-CGA-O1A	-3.16	115.73	123.63
11	x	304	UQ8	C22-C23-C24	-3.16	120.40	127.62
9	m	103	BCL	CHD-C1D-ND	-3.16	120.36	124.80
9	K	101	BCL	CHD-C1D-ND	-3.16	120.36	124.80
9	j	101	BCL	CHA-C1A-NA	-3.16	119.25	126.39
9	K	101	BCL	C16-C15-C13	-3.16	105.48	115.97
9	u	102	BCL	OBB-CAB-CBB	-3.15	112.71	119.77
9	O	102	BCL	C2B-C1B-NB	-3.15	107.06	110.33
9	f	101	BCL	C16-C15-C13	-3.15	105.50	115.97
9	AC	103	BCL	C1C-NC-C4C	-3.15	105.24	106.68
15	0	101	CRT	C18-C17-C16	3.15	122.90	118.09
9	h	101	BCL	CAA-CBA-CGA	-3.15	104.27	113.21
15	y	404	CRT	C4-C5-C6	-3.15	120.50	124.91
15	E	101	CRT	C21-C22-C23	-3.15	122.87	127.28
9	M	402	BCL	C4D-CHA-C1A	3.14	124.99	121.24
9	3	101	BCL	O2A-CGA-O1A	-3.14	115.78	123.63
7	C	501	HEM	O2D-CGD-CBD	3.14	123.91	114.00
9	I	101	BCL	CHD-C1D-ND	-3.14	120.39	124.80
7	o	503	HEM	CHD-C1D-ND	3.13	127.79	124.42
9	x	301	BCL	CMD-C2D-C1D	3.13	130.24	124.73
11	x	304	UQ8	O3-C3-C2	3.13	127.20	116.64
9	L	303	BCL	CHB-C1B-NB	3.13	128.75	124.05
9	I	103	BCL	CHA-C1A-NA	-3.13	119.30	126.39
9	I	103	BCL	C11-C10-C8	-3.13	105.56	115.97
9	i	102	BCL	C16-C15-C13	-3.13	105.57	115.97
9	V	102	BCL	CHB-C1B-NB	3.13	128.74	124.05
9	1	101	BCL	CHB-C1B-NB	3.12	128.74	124.05
9	AI	102	BCL	CHB-C1B-NB	3.12	128.74	124.05
9	A	102	BCL	CHB-C1B-NB	3.12	128.73	124.05
9	AG	101	BCL	CHA-C1A-NA	-3.12	119.33	126.39
9	l	101	BCL	C16-C15-C13	-3.12	105.61	115.97
15	AH	102	CRT	C32-C31-C30	-3.12	114.17	123.20
9	K	101	BCL	C4D-CHA-C1A	3.11	124.96	121.24
12	L	305	PEF	O3P-C1-C2	3.11	117.59	108.51
15	E	101	CRT	C21-C20-C19	-3.11	117.15	123.52
9	AI	101	BCL	C2D-C1D-ND	3.11	113.21	110.13
9	k	102	BCL	O2A-C1-C2	3.11	120.08	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	y	404	CRT	C32-C31-C30	-3.11	114.19	123.20
9	T	102	BCL	C3B-C4B-NB	-3.11	105.66	109.76
15	0	101	CRT	C4-C5-C6	-3.11	120.55	124.91
9	M	401	BCL	C2B-C1B-NB	-3.11	107.11	110.33
9	I	103	BCL	OBB-CAB-CBB	-3.10	112.82	119.77
9	Q	101	BCL	C16-C15-C13	-3.10	105.66	115.97
9	I	103	BCL	CHB-C1B-NB	3.10	128.70	124.05
9	Y	101	BCL	C2D-C1D-ND	3.10	113.19	110.13
9	K	101	BCL	OBB-CAB-CBB	-3.10	112.83	119.77
14	y	403	MQ8	C31-C32-C33	-3.10	120.53	127.62
9	k	102	BCL	CHB-C1B-NB	3.10	128.70	124.05
9	p	102	BCL	CHD-C1D-ND	-3.10	120.44	124.80
9	d	101	BCL	CMA-C3A-C4A	-3.10	103.45	111.77
9	w	101	BCL	OBB-CAB-CBB	-3.09	112.84	119.77
9	I	101	BCL	C11-C10-C8	-3.09	105.68	115.97
9	Y	101	BCL	CMA-C3A-C4A	-3.09	103.46	111.77
15	P	102	CRT	C26-C27-C28	-3.09	122.94	127.28
9	O	102	BCL	C3B-C4B-NB	-3.09	105.68	109.76
9	x	301	BCL	CBB-CAB-C3B	3.09	126.92	120.40
9	K	101	BCL	C2A-C1A-CHA	3.09	129.23	123.87
9	T	102	BCL	C1-O2A-CGA	3.09	124.13	116.65
15	n	101	CRT	C9-C10-C11	3.09	132.15	123.20
9	AL	102	BCL	C2A-C1A-CHA	3.09	129.23	123.87
9	AL	102	BCL	CBB-CAB-C3B	3.09	126.91	120.40
9	x	301	BCL	C16-C15-C13	-3.08	105.71	115.97
9	O	102	BCL	C16-C15-C13	-3.08	105.72	115.97
9	x	305	BCL	C16-C15-C13	-3.08	105.72	115.97
9	k	102	BCL	CGD-CBD-CAD	-3.08	100.87	110.85
9	W	101	BCL	CHC-C1C-NC	3.08	128.85	124.40
9	4	102	BCL	OBB-CAB-CBB	-3.08	112.87	119.77
9	z	102	BCL	C4A-NA-C1A	3.08	108.08	106.68
9	D	102	BCL	C11-C12-C13	-3.08	105.73	115.97
9	I	103	BCL	CHD-C1D-ND	-3.08	120.47	124.80
15	m	104	CRT	C26-C27-C28	-3.08	122.96	127.28
9	1	101	BCL	CHC-C1C-NC	3.08	128.84	124.40
9	T	102	BCL	C3D-C2D-C1D	-3.08	101.63	105.83
9	S	102	BCL	C2B-C1B-NB	-3.08	107.13	110.33
9	8	101	BCL	C4D-CHA-C1A	3.08	124.92	121.24
15	AJ	101	CRT	C36-C35-C33	3.08	130.54	125.89
9	AH	101	BCL	C7-C6-C5	-3.08	105.06	113.26
15	X	101	CRT	C9-C10-C11	3.08	132.11	123.20
10	x	302	BPH	CMA-C3A-C4A	-3.08	107.98	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	j	101	BCL	CHB-C1B-NB	3.07	128.66	124.05
9	f	101	BCL	CHD-C1D-ND	-3.07	120.48	124.80
9	j	101	BCL	C3B-C4B-NB	-3.07	105.70	109.76
15	O	101	CRT	C20-C19-C17	-3.07	122.97	127.28
9	M	402	BCL	C3C-C4C-CHD	-3.07	116.92	123.39
9	u	101	BCL	C11-C10-C8	-3.07	105.76	115.97
9	2	102	BCL	CHB-C1B-NB	3.07	128.65	124.05
9	0	102	BCL	C7-C6-C5	-3.07	105.08	113.26
9	N	101	BCL	CHB-C1B-NB	3.07	128.65	124.05
7	C	501	HEM	CAA-CBA-CGA	-3.06	105.54	113.67
9	g	102	BCL	C2D-C1D-ND	3.06	113.16	110.13
9	q	102	BCL	O2A-CGA-O1A	-3.06	115.98	123.63
9	u	102	BCL	C2A-C1A-CHA	3.06	129.17	123.87
9	m	103	BCL	OBB-CAB-CBB	-3.06	112.93	119.77
9	8	101	BCL	C7-C6-C5	-3.06	105.12	113.26
9	e	102	BCL	OBB-CAB-CBB	-3.05	112.93	119.77
9	D	102	BCL	C1C-NC-C4C	-3.05	105.29	106.68
9	U	101	BCL	C16-C15-C13	-3.05	105.82	115.97
7	C	503	HEM	CBD-CAD-C3D	-3.05	104.10	112.53
9	X	102	BCL	C1-O2A-CGA	3.05	124.04	116.65
14	M	404	MQ8	C11-C12-C13	-3.05	121.58	126.83
9	u	101	BCL	CGD-CBD-CAD	-3.05	100.98	110.85
9	P	101	BCL	OBB-CAB-CBB	-3.05	112.94	119.77
9	0	102	BCL	CBB-CAB-C3B	3.05	126.82	120.40
15	AL	101	CRT	C21-C20-C19	-3.05	117.29	123.52
9	4	102	BCL	CHB-C1B-NB	3.04	128.62	124.05
9	AH	101	BCL	C2D-C1D-ND	3.04	113.14	110.13
9	V	102	BCL	C1C-NC-C4C	-3.04	105.29	106.68
15	V	101	CRT	C8-C7-C6	3.04	122.73	118.09
9	c	101	BCL	OBB-CAB-CBB	-3.04	112.96	119.77
9	j	101	BCL	O2A-CGA-O1A	-3.04	116.03	123.63
9	p	102	BCL	CHB-C1B-NB	3.04	128.60	124.05
15	7	103	CRT	C32-C31-C30	-3.04	114.40	123.20
9	c	101	BCL	C7-C6-C5	-3.04	105.17	113.26
14	M	404	MQ8	C35-C33-C32	-3.03	114.36	121.17
9	g	102	BCL	O2A-CGA-O1A	-3.03	116.06	123.63
9	Z	102	BCL	C11-C10-C8	-3.02	105.92	115.97
11	x	304	UQ8	O3-C3-C4	-3.02	112.20	123.64
14	M	404	MQ8	C34-C33-C35	3.02	120.47	115.23
14	M	404	MQ8	C14-C13-C15	3.02	120.47	115.23
9	AE	102	BCL	C1C-NC-C4C	-3.02	105.30	106.68
15	V	101	CRT	C9-C10-C11	-3.02	114.45	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AF	101	BCL	CMA-C3A-C4A	-3.02	103.67	111.77
9	AH	101	BCL	C3B-C4B-NB	-3.02	105.78	109.76
9	O	102	BCL	CHD-C1D-ND	-3.01	120.56	124.80
9	m	102	BCL	C1C-NC-C4C	-3.01	105.30	106.68
9	M	402	BCL	O2A-CGA-CBA	3.01	121.02	111.83
9	I	101	BCL	OBB-CAB-CBB	-3.01	113.03	119.77
9	AK	101	BCL	CHB-C4A-NA	-3.01	120.06	124.40
9	8	101	BCL	O2A-C1-C2	3.01	119.68	108.11
9	u	101	BCL	CHB-C1B-NB	3.01	128.56	124.05
9	S	102	BCL	C4A-NA-C1A	3.01	108.05	106.68
9	3	101	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
9	Y	101	BCL	C2B-C1B-NB	-3.01	107.21	110.33
15	k	101	CRT	C26-C25-C23	-3.00	118.12	126.36
9	D	101	BCL	O2A-CGA-O1A	-3.00	116.11	123.63
15	n	101	CRT	C13-C12-C14	-3.00	117.95	122.82
9	x	305	BCL	C7-C6-C5	-3.00	105.26	113.26
15	n	101	CRT	C18-C17-C16	3.00	122.67	118.09
15	X	101	CRT	C15-C14-C12	-3.00	123.07	127.28
15	V	101	CRT	C14-C15-C16	-3.00	114.50	123.20
9	d	101	BCL	C1-O2A-CGA	3.00	123.91	116.65
9	m	102	BCL	O2A-CGA-O1A	-3.00	116.13	123.63
9	X	102	BCL	C3B-C4B-NB	-3.00	105.80	109.76
9	l	101	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
9	AC	103	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
15	v	101	CRT	C21-C22-C23	-3.00	123.08	127.28
9	A	102	BCL	CMA-C3A-C4A	-2.99	103.73	111.77
9	6	101	BCL	C7-C6-C5	-2.99	105.29	113.26
9	O	102	BCL	C3D-C2D-C1D	-2.99	101.75	105.83
9	y	401	BCL	C2A-C1A-CHA	2.99	129.06	123.87
9	9	102	BCL	C7-C6-C5	-2.99	105.29	113.26
15	g	101	CRT	C27-C26-C25	-2.99	114.54	123.20
9	g	102	BCL	C12-C11-C10	-2.99	99.88	113.28
15	7	101	CRT	C20-C21-C22	-2.99	117.41	123.52
9	g	102	BCL	C7-C6-C5	-2.99	105.30	113.26
9	AC	102	BCL	OBB-CAB-CBB	-2.99	113.08	119.77
9	r	101	BCL	C7-C6-C5	-2.98	105.31	113.26
9	AB	102	BCL	CBB-CAB-C3B	2.98	126.69	120.40
9	R	102	BCL	CBB-CAB-C3B	2.98	126.69	120.40
9	k	102	BCL	C16-C15-C13	-2.98	106.05	115.97
7	o	503	HEM	CAA-CBA-CGA	-2.98	105.75	113.67
9	3	101	BCL	C11-C12-C13	-2.98	106.06	115.97
9	A	103	BCL	OBB-CAB-CBB	-2.98	113.10	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	102	BCL	C4A-NA-C1A	2.98	108.04	106.68
9	D	102	BCL	CHB-C1B-NB	2.98	128.51	124.05
11	x	304	UQ8	O4-C4-C3	-2.98	112.38	123.64
9	K	101	BCL	C3D-C2D-C1D	-2.98	101.77	105.83
11	L	304	UQ8	C20-C19-C21	2.98	120.39	115.23
9	U	101	BCL	OBB-CAB-CBB	-2.97	113.11	119.77
9	AB	102	BCL	C11-C10-C8	-2.97	106.08	115.97
9	7	102	BCL	CHA-C1A-NA	-2.97	119.66	126.39
9	s	102	BCL	CMA-C3A-C4A	-2.97	103.79	111.77
9	z	102	BCL	C7-C6-C5	-2.97	105.34	113.26
9	D	101	BCL	C1C-NC-C4C	-2.97	105.32	106.68
15	AL	101	CRT	C18-C17-C16	2.97	122.62	118.09
9	AG	101	BCL	C7-C6-C5	-2.97	105.35	113.26
11	L	304	UQ8	C45-C44-C43	-2.97	113.75	122.66
9	O	102	BCL	C11-C10-C8	-2.97	106.10	115.97
10	x	302	BPH	O1D-CGD-CBD	-2.97	120.22	124.72
9	P	101	BCL	C4A-NA-C1A	2.97	108.03	106.68
15	AC	101	CRT	C34-C33-C35	2.97	122.62	118.09
9	Z	102	BCL	CHB-C1B-NB	2.97	128.50	124.05
9	AK	101	BCL	CED-O2D-CGD	-2.96	109.19	115.92
9	AK	101	BCL	C3B-C4B-NB	-2.96	105.85	109.76
15	V	101	CRT	C15-C14-C12	-2.96	123.12	127.28
9	l	101	BCL	CMC-C2C-C3C	-2.96	102.53	113.98
9	O	102	BCL	O2A-CGA-O1A	-2.96	116.22	123.63
9	T	102	BCL	CBB-CAB-C3B	2.96	126.64	120.40
12	t	303	PEF	C3-O3-C30	2.96	124.39	117.08
9	W	101	BCL	CHB-C4A-NA	-2.96	120.13	124.40
9	e	102	BCL	CHB-C4A-NA	-2.96	120.13	124.40
9	AB	101	BCL	OBB-CAB-CBB	-2.96	113.15	119.77
9	5	101	BCL	C2B-C1B-NB	-2.95	107.26	110.33
9	M	401	BCL	C11-C12-C13	-2.95	106.15	115.97
9	7	102	BCL	CHD-C1D-ND	-2.95	120.65	124.80
15	y	404	CRT	C1-C4-C5	2.95	120.65	112.98
9	k	102	BCL	C2A-C1A-CHA	2.95	128.99	123.87
9	D	101	BCL	C4A-NA-C1A	2.95	108.03	106.68
9	P	101	BCL	CBB-CAB-C3B	2.95	126.62	120.40
9	l	101	BCL	CMD-C2D-C1D	2.95	129.92	124.73
11	x	304	UQ8	C12-C13-C14	-2.95	120.87	127.62
9	y	401	BCL	OBB-CAB-CBB	-2.95	113.17	119.77
9	h	101	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
15	V	101	CRT	C35-C33-C32	-2.95	114.38	119.01
9	c	101	BCL	CHD-C1D-ND	-2.95	120.66	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	BCL	CMC-C2C-C3C	-2.95	102.59	113.98
9	9	102	BCL	C11-C10-C8	-2.94	106.19	115.97
9	d	101	BCL	CBB-CAB-C3B	2.94	126.60	120.40
10	L	302	BPH	CBA-CAA-C2A	-2.94	105.12	113.78
9	m	103	BCL	CHB-C1B-NB	2.94	128.46	124.05
15	s	101	CRT	C35-C33-C32	-2.94	114.39	119.01
9	3	101	BCL	C16-C15-C13	-2.94	106.20	115.97
9	q	102	BCL	C7-C6-C5	-2.94	105.43	113.26
9	u	101	BCL	C2A-C1A-CHA	2.94	128.96	123.87
7	o	502	HEM	C3A-C4A-NA	-2.94	105.44	110.14
9	7	102	BCL	C1C-NC-C4C	-2.93	105.34	106.68
15	M	405	CRT	C20-C19-C17	-2.93	123.16	127.28
9	U	101	BCL	C11-C12-C13	-2.93	106.21	115.97
9	AL	102	BCL	OBB-CAB-CBB	-2.93	113.20	119.77
9	S	102	BCL	O2A-CGA-O1A	-2.93	116.29	123.63
15	AD	101	CRT	C26-C25-C23	-2.93	118.32	126.36
9	4	102	BCL	C7-C6-C5	-2.93	105.45	113.26
9	AB	102	BCL	CHB-C1B-NB	2.93	128.45	124.05
9	L	301	BCL	C11-C10-C8	-2.93	106.22	115.97
9	AB	101	BCL	C3B-C4B-NB	-2.93	105.89	109.76
9	A	103	BCL	CMA-C3A-C4A	-2.93	103.90	111.77
9	p	102	BCL	C11-C12-C13	-2.93	106.23	115.97
9	AC	102	BCL	C2B-C1B-NB	-2.93	107.29	110.33
15	e	101	CRT	C27-C26-C25	-2.93	114.72	123.20
9	k	102	BCL	C7-C6-C5	-2.93	105.46	113.26
9	l	101	BCL	C11-C10-C8	-2.93	106.24	115.97
9	Q	101	BCL	CMC-C2C-C3C	-2.92	102.67	113.98
15	2	101	CRT	C10-C9-C7	-2.92	123.18	127.28
7	o	503	HEM	CBD-CAD-C3D	-2.92	104.45	112.53
9	m	102	BCL	CHB-C1B-NB	2.92	128.43	124.05
12	t	301	PEF	O2-C10-C11	2.92	116.30	111.09
15	AL	101	CRT	C14-C15-C16	-2.92	114.73	123.20
9	7	102	BCL	CBB-CAB-C3B	2.92	126.56	120.40
9	r	101	BCL	C16-C15-C13	-2.92	106.26	115.97
9	D	102	BCL	C3D-C2D-C1D	-2.92	101.85	105.83
9	AB	101	BCL	CHD-C1D-ND	-2.92	120.69	124.80
9	AC	103	BCL	CHD-C1D-ND	-2.92	120.70	124.80
9	X	102	BCL	CMA-C3A-C4A	-2.92	103.93	111.77
9	AH	101	BCL	CMC-C2C-C3C	-2.92	102.70	113.98
9	M	402	BCL	OBB-CAB-CBB	-2.92	113.24	119.77
9	x	301	BCL	CMB-C2B-C1B	-2.91	120.98	125.42
9	AE	102	BCL	C3B-C4B-NB	-2.91	105.92	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	102	BCL	C3B-C4B-NB	-2.91	105.92	109.76
14	y	403	MQ8	C21-C22-C23	-2.91	120.96	127.62
7	C	503	HEM	CAA-C2A-C1A	2.91	130.62	124.94
9	AL	102	BCL	C1-C2-C3	-2.91	121.43	126.20
7	C	504	HEM	C4D-ND-C1D	2.91	108.65	105.21
15	0	101	CRT	C16-C17-C19	-2.91	114.43	119.01
9	7	102	BCL	C2B-C1B-NB	-2.91	107.31	110.33
9	A	102	BCL	C3B-C4B-NB	-2.91	105.92	109.76
9	O	102	BCL	CHC-C1C-NC	2.91	128.60	124.40
9	U	101	BCL	CHD-C1D-ND	-2.91	120.71	124.80
15	m	104	CRT	C10-C9-C7	-2.91	123.20	127.28
9	6	101	BCL	CHC-C1C-NC	2.91	128.59	124.40
9	AB	101	BCL	C16-C15-C13	-2.90	106.31	115.97
14	y	403	MQ8	C11-C12-C13	-2.90	121.83	126.83
9	c	101	BCL	CGD-CBD-CAD	-2.90	101.45	110.85
15	P	102	CRT	C8-C7-C6	2.90	122.52	118.09
15	n	101	CRT	C20-C19-C17	-2.90	123.21	127.28
9	4	102	BCL	C2B-C1B-NB	-2.90	107.32	110.33
9	9	102	BCL	OBB-CAB-CBB	-2.90	113.28	119.77
9	F	101	BCL	C2B-C1B-NB	-2.90	107.32	110.33
9	Z	102	BCL	CHB-C4A-NA	-2.90	120.22	124.40
9	AF	101	BCL	C1C-NC-C4C	-2.90	105.36	106.68
15	n	101	CRT	C26-C27-C28	-2.90	123.22	127.28
9	AG	101	BCL	C4D-CHA-C1A	2.90	124.70	121.24
9	f	101	BCL	C3B-C4B-NB	-2.90	105.94	109.76
15	v	101	CRT	C31-C32-C33	-2.89	123.22	127.28
9	AB	101	BCL	CED-O2D-CGD	-2.89	109.35	115.92
15	z	101	CRT	C18-C17-C16	2.89	122.51	118.09
15	AH	102	CRT	C5-C6-C7	-2.89	121.52	125.89
11	x	304	UQ8	C35-C34-C36	2.89	120.25	115.23
15	7	103	CRT	C1-C4-C5	2.89	120.49	112.98
9	N	101	BCL	CHD-C1D-ND	-2.89	120.73	124.80
9	O	102	BCL	C1C-NC-C4C	-2.89	105.36	106.68
9	l	101	BCL	CBB-CAB-C3B	2.89	126.49	120.40
9	M	402	BCL	CHB-C1B-NB	2.89	128.38	124.05
9	p	102	BCL	C16-C15-C13	-2.89	106.36	115.97
9	e	102	BCL	C11-C12-C13	-2.89	106.37	115.97
15	g	101	CRT	C29-C28-C30	2.89	122.50	118.09
9	AE	102	BCL	C3D-C2D-C1D	-2.88	101.89	105.83
9	s	102	BCL	C16-C15-C13	-2.88	106.38	115.97
9	U	101	BCL	C2D-C1D-ND	2.88	112.98	110.13
9	AI	101	BCL	O2A-CGA-CBA	2.88	120.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	102	BCL	C1C-NC-C4C	-2.88	105.36	106.68
9	w	101	BCL	CHB-C1B-NB	2.88	128.37	124.05
12	y	406	PEF	C2-O2-C10	-2.88	112.76	117.85
9	N	101	BCL	CBB-CAB-C3B	2.88	126.47	120.40
9	R	102	BCL	C11-C10-C8	-2.88	106.39	115.97
9	X	102	BCL	C2A-C1A-CHA	2.88	128.86	123.87
9	T	102	BCL	C3C-C2C-C1C	2.88	106.52	101.87
9	R	102	BCL	C3B-C4B-NB	-2.88	105.96	109.76
9	AK	101	BCL	C3D-C2D-C1D	-2.88	101.91	105.83
15	Z	101	CRT	C25-C23-C22	-2.88	114.48	119.01
9	u	101	BCL	CMC-C2C-C3C	-2.88	102.87	113.98
11	x	304	UQ8	O4-C4-C5	2.87	126.34	116.64
15	Z	101	CRT	C35-C33-C32	-2.87	114.49	119.01
9	D	102	BCL	CMC-C2C-C3C	-2.87	102.88	113.98
9	p	102	BCL	CMD-C2D-C1D	2.87	129.79	124.73
9	k	102	BCL	OBB-CAB-CBB	-2.87	113.34	119.77
15	V	101	CRT	C6-C7-C9	-2.87	114.49	119.01
9	AB	101	BCL	CHB-C1B-NB	2.87	128.35	124.05
9	P	101	BCL	O2A-CGA-O1A	-2.87	116.46	123.63
15	AL	101	CRT	C10-C9-C7	-2.87	123.26	127.28
9	W	101	BCL	CBB-CAB-C3B	2.87	126.45	120.40
9	AL	102	BCL	C3B-C4B-NB	-2.87	105.98	109.76
9	O	102	BCL	CMD-C2D-C1D	2.86	129.77	124.73
9	AF	101	BCL	C2B-C1B-NB	-2.86	107.36	110.33
9	I	101	BCL	C3D-C2D-C1D	-2.86	101.92	105.83
14	M	404	MQ8	C19-C18-C20	2.86	120.19	115.23
9	X	102	BCL	O2A-CGA-O1A	-2.86	116.47	123.63
9	D	101	BCL	C3D-C2D-C1D	-2.86	101.93	105.83
15	z	101	CRT	C24-C23-C25	2.86	122.45	118.09
9	AL	102	BCL	C1C-NC-C4C	-2.86	105.38	106.68
9	AE	102	BCL	CBB-CAB-C3B	2.86	126.43	120.40
9	2	102	BCL	C16-C15-C13	-2.86	106.47	115.97
9	F	101	BCL	CMC-C2C-C3C	-2.85	102.95	113.98
12	H	304	PEF	C3-O3-C30	2.85	124.12	117.08
15	4	101	CRT	C4-C5-C6	-2.85	120.91	124.91
9	g	102	BCL	CBB-CAB-C3B	2.85	126.41	120.40
9	p	102	BCL	O2A-CGA-O1A	-2.85	116.50	123.63
7	C	504	HEM	CAD-CBD-CGD	-2.85	106.11	113.67
9	AL	102	BCL	CMC-C2C-C3C	-2.85	102.97	113.98
15	q	101	CRT	C14-C15-C16	-2.85	114.95	123.20
9	O	102	BCL	CMC-C2C-C3C	-2.85	102.98	113.98
15	0	101	CRT	C27-C26-C25	-2.84	114.96	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	l	101	BCL	O2A-CGA-O1A	-2.84	116.52	123.63
9	K	101	BCL	O2A-CGA-O1A	-2.84	116.52	123.63
9	I	103	BCL	CMA-C3A-C4A	-2.84	104.14	111.77
9	G	102	BCL	CHB-C1B-NB	2.84	128.31	124.05
9	3	101	BCL	C3B-C4B-NB	-2.84	106.01	109.76
15	M	405	CRT	C9-C10-C11	-2.84	114.97	123.20
9	AB	101	BCL	CMC-C2C-C3C	-2.84	103.00	113.98
9	M	401	BCL	O2A-CGA-O1A	-2.84	116.53	123.63
9	0	102	BCL	C3B-C4B-NB	-2.84	106.02	109.76
12	t	303	PEF	O2-C10-O4	-2.84	117.52	122.99
15	AH	102	CRT	C14-C15-C16	-2.84	114.98	123.20
9	S	102	BCL	C11-C10-C8	-2.84	106.54	115.97
9	AI	102	BCL	CBB-CAB-C3B	2.84	126.38	120.40
9	AB	101	BCL	C7-C6-C5	-2.84	105.71	113.26
9	9	102	BCL	C3B-C4B-NB	-2.83	106.02	109.76
9	I	101	BCL	CHB-C1B-NB	2.83	128.30	124.05
9	AF	101	BCL	CGD-CBD-CAD	-2.83	101.68	110.85
9	1	101	BCL	C2B-C1B-NB	-2.83	107.39	110.33
9	AC	103	BCL	CBB-CAB-C3B	2.83	126.37	120.40
9	p	102	BCL	C2D-C1D-ND	2.83	112.93	110.13
9	AC	103	BCL	C16-C15-C13	-2.83	106.56	115.97
9	D	101	BCL	CMC-C2C-C3C	-2.83	103.05	113.98
9	6	101	BCL	C16-C15-C13	-2.83	106.57	115.97
9	e	102	BCL	C16-C15-C13	-2.83	106.57	115.97
9	p	102	BCL	CHC-C1C-NC	2.83	128.48	124.40
9	I	101	BCL	C2B-C1B-NB	-2.83	107.40	110.33
9	X	102	BCL	C11-C12-C13	-2.83	106.57	115.97
15	AC	101	CRT	C14-C15-C16	-2.83	115.01	123.20
9	j	101	BCL	CHD-C1D-ND	-2.82	120.83	124.80
15	9	101	CRT	C34-C33-C35	2.82	122.40	118.09
9	0	102	BCL	CHB-C1B-NB	2.82	128.28	124.05
10	y	402	BPH	O2A-CGA-CBA	2.82	120.44	111.83
9	D	102	BCL	CGD-CBD-CAD	-2.82	101.72	110.85
15	e	101	CRT	C8-C7-C6	2.82	122.39	118.09
15	4	101	CRT	C18-C17-C16	2.82	122.39	118.09
15	R	101	CRT	C32-C31-C30	-2.82	115.03	123.20
9	K	101	BCL	C3C-C2C-C1C	2.82	106.42	101.87
9	3	101	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
10	L	302	BPH	C11-C10-C8	-2.81	106.61	115.97
9	s	102	BCL	CBB-CAB-C3B	2.81	126.33	120.40
9	M	402	BCL	CHC-C1C-NC	2.81	128.46	124.40
9	4	102	BCL	CAA-CBA-CGA	-2.81	105.23	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	301	BCL	CBB-CAB-C3B	2.81	126.33	120.40
9	AE	102	BCL	CHD-C1D-ND	-2.81	120.85	124.80
9	M	401	BCL	CBB-CAB-C3B	2.81	126.32	120.40
9	q	102	BCL	C6-C5-C3	-2.81	106.63	113.47
9	d	101	BCL	C3B-C4B-NB	-2.81	106.06	109.76
15	I	102	CRT	C21-C20-C19	-2.81	117.78	123.52
9	AB	101	BCL	C1-C2-C3	-2.80	121.60	126.20
9	s	102	BCL	C2A-C1A-CHA	2.80	128.73	123.87
9	AF	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
9	8	101	BCL	CHA-C1A-NA	-2.80	120.05	126.39
9	U	101	BCL	CED-O2D-CGD	-2.80	109.56	115.92
15	z	101	CRT	C9-C10-C11	-2.80	115.08	123.20
9	AF	101	BCL	CBB-CAB-C3B	2.80	126.31	120.40
15	T	101	CRT	C31-C30-C28	-2.80	118.68	126.36
7	o	501	HEM	CHB-C4A-NA	2.80	128.93	123.86
9	I	103	BCL	O2A-CGA-O1A	-2.80	116.63	123.63
9	Q	101	BCL	C2B-C1B-NB	-2.80	107.43	110.33
9	k	102	BCL	C1C-NC-C4C	-2.79	105.40	106.68
15	P	102	CRT	C6-C7-C9	-2.79	114.61	119.01
9	F	101	BCL	C3B-C4B-NB	-2.79	106.07	109.76
9	j	101	BCL	CHC-C1C-NC	2.79	128.43	124.40
9	AK	101	BCL	CHC-C1C-NC	2.79	128.43	124.40
9	I	103	BCL	C7-C6-C5	-2.79	105.82	113.26
11	L	304	UQ8	C46-C44-C45	2.79	121.01	114.59
9	P	101	BCL	C3B-C4B-NB	-2.79	106.08	109.76
9	A	103	BCL	C2B-C1B-NB	-2.79	107.44	110.33
9	W	101	BCL	C16-C15-C13	-2.79	106.70	115.97
9	X	102	BCL	CMC-C2C-C3C	-2.79	103.21	113.98
15	m	104	CRT	C16-C17-C19	-2.79	114.63	119.01
7	o	501	HEM	CHD-C4C-NC	2.79	127.49	124.45
9	F	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
9	5	101	BCL	CHA-C1A-NA	-2.79	120.08	126.39
9	0	102	BCL	CMA-C3A-C4A	-2.78	104.29	111.77
9	6	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	i	102	BCL	C11-C10-C8	-2.78	106.71	115.97
7	o	504	HEM	C4B-C3B-C2B	-2.78	104.72	107.28
9	z	102	BCL	CMC-C2C-C3C	-2.78	103.23	113.98
9	O	102	BCL	CBB-CAB-C3B	2.78	126.27	120.40
9	x	303	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
9	AH	101	BCL	O2A-CGA-O1A	-2.78	116.67	123.63
9	K	101	BCL	CMC-C2C-C3C	-2.78	103.23	113.98
9	X	102	BCL	C7-C6-C5	-2.78	105.85	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	101	CRT	C32-C31-C30	-2.78	115.15	123.20
15	2	101	CRT	C4-C5-C6	-2.78	121.01	124.91
15	y	404	CRT	C34-C33-C35	2.78	122.33	118.09
9	N	101	BCL	CHC-C1C-NC	2.78	128.41	124.40
9	L	303	BCL	CMD-C2D-C1D	2.77	129.61	124.73
9	3	101	BCL	OBB-CAB-CBB	-2.77	113.56	119.77
15	z	101	CRT	C6-C7-C9	-2.77	114.65	119.01
7	o	502	HEM	C4A-NA-C1A	2.77	110.34	105.82
9	AB	102	BCL	C3B-C4B-NB	-2.77	106.10	109.76
9	P	101	BCL	CED-O2D-CGD	-2.77	109.62	115.92
9	D	102	BCL	C7-C6-C5	-2.77	105.87	113.26
7	o	502	HEM	C2A-C1A-NA	-2.77	107.08	110.15
9	u	102	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
15	9	101	CRT	C10-C9-C7	2.77	131.16	127.28
15	G	101	CRT	C8-C7-C6	2.77	122.32	118.09
9	A	102	BCL	C3D-C2D-C1D	-2.77	102.06	105.83
9	i	102	BCL	C1-O2A-CGA	2.77	123.35	116.65
9	M	401	BCL	CHA-C1A-NA	-2.76	120.13	126.39
9	Z	102	BCL	C2B-C1B-NB	-2.76	107.46	110.33
9	u	101	BCL	OBB-CAB-CBB	-2.76	113.58	119.77
9	s	102	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
9	AI	101	BCL	O2A-C1-C2	2.76	118.72	108.11
9	A	103	BCL	C3B-C4B-NB	-2.76	106.12	109.76
9	P	101	BCL	CMA-C3A-C4A	-2.76	104.36	111.77
9	AG	101	BCL	CMC-C2C-C3C	-2.76	103.32	113.98
7	o	501	HEM	C2A-C1A-NA	-2.76	107.09	110.15
10	x	302	BPH	O2A-CGA-CBA	2.76	120.24	111.83
9	4	102	BCL	CED-O2D-CGD	-2.76	109.66	115.92
9	AL	102	BCL	C4D-CHA-C1A	2.76	124.53	121.24
15	q	101	CRT	C9-C10-C11	-2.76	115.21	123.20
9	k	102	BCL	CMC-C2C-C3C	-2.76	103.33	113.98
9	j	101	BCL	CMD-C2D-C1D	2.75	129.58	124.73
9	u	102	BCL	O2A-CGA-O1A	-2.75	116.74	123.63
9	m	102	BCL	CMC-C2C-C3C	-2.75	103.33	113.98
9	s	102	BCL	CMC-C2C-C3C	-2.75	103.33	113.98
9	Z	102	BCL	CHC-C1C-NC	2.75	128.37	124.40
15	M	405	CRT	C5-C6-C7	-2.75	121.73	125.89
7	o	504	HEM	CHB-C1B-NB	2.75	127.77	124.37
15	g	101	CRT	C4-C5-C6	-2.75	121.05	124.91
9	X	102	BCL	C2B-C1B-NB	-2.75	107.47	110.33
9	AK	101	BCL	C4A-NA-C1A	2.75	107.93	106.68
9	k	102	BCL	CED-O2D-CGD	-2.75	109.67	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	f	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
9	Q	101	BCL	CHB-C1B-NB	2.75	128.17	124.05
9	z	102	BCL	CBB-CAB-C3B	2.75	126.20	120.40
9	L	303	BCL	C6-C5-C3	2.75	120.16	113.47
9	f	101	BCL	C2A-C1A-CHA	2.75	128.64	123.87
9	P	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
9	AI	102	BCL	CMC-C2C-C3C	-2.75	103.37	113.98
9	R	102	BCL	C11-C12-C13	-2.75	106.84	115.97
9	u	101	BCL	C3B-C4B-NB	-2.74	106.14	109.76
15	s	101	CRT	C26-C25-C23	-2.74	118.84	126.36
9	8	101	BCL	CMC-C2C-C3C	-2.74	103.38	113.98
9	j	101	BCL	CED-O2D-CGD	-2.74	109.69	115.92
9	Q	101	BCL	CHC-C1C-NC	2.74	128.36	124.40
15	4	101	CRT	C13-C12-C14	-2.74	118.38	122.82
9	5	101	BCL	C4D-CHA-C1A	2.74	124.51	121.24
9	T	102	BCL	OBB-CAB-CBB	-2.74	113.64	119.77
15	AC	101	CRT	C32-C31-C30	-2.74	115.27	123.20
9	y	401	BCL	C11-C12-C13	-2.74	106.86	115.97
9	A	102	BCL	C2A-C1A-CHA	2.74	128.62	123.87
9	5	101	BCL	C16-C15-C13	-2.74	106.87	115.97
9	i	102	BCL	C3D-C2D-C1D	-2.74	102.10	105.83
9	e	102	BCL	C3B-C4B-NB	-2.74	106.15	109.76
15	I	102	CRT	C26-C27-C28	-2.74	123.44	127.28
7	C	502	HEM	CHA-C1A-NA	2.73	128.82	123.86
9	AK	101	BCL	O2A-CGA-O1A	-2.73	116.79	123.63
12	t	301	PEF	C3-O3-C30	2.73	123.82	117.08
9	AC	103	BCL	C7-C6-C5	-2.73	105.98	113.26
9	AL	102	BCL	CHC-C1C-NC	2.73	128.34	124.40
9	AK	101	BCL	CHB-C1B-NB	2.73	128.15	124.05
9	A	102	BCL	C2B-C1B-NB	-2.73	107.50	110.33
15	AC	101	CRT	C27-C26-C25	-2.73	115.29	123.20
15	2	101	CRT	C18-C17-C16	2.73	122.26	118.09
9	AF	101	BCL	CHD-C1D-ND	-2.73	120.96	124.80
15	AC	101	CRT	C18-C17-C16	2.73	122.26	118.09
9	0	102	BCL	CMC-C2C-C3C	-2.73	103.43	113.98
10	L	302	BPH	C11-C12-C13	-2.73	106.90	115.97
9	8	101	BCL	CMA-C3A-C4A	-2.73	104.44	111.77
9	AL	102	BCL	CAA-CBA-CGA	-2.73	105.47	113.21
15	G	101	CRT	C6-C7-C9	-2.72	114.72	119.01
7	o	503	HEM	CHA-C4D-ND	2.72	127.74	124.37
9	T	102	BCL	C7-C6-C5	-2.72	106.00	113.26
9	AI	102	BCL	C11-C10-C8	-2.72	106.92	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	y	401	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
9	8	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
9	R	102	BCL	C2B-C1B-NB	-2.72	107.50	110.33
9	K	101	BCL	C1-O2A-CGA	2.72	123.24	116.65
7	o	503	HEM	CAB-C3B-C4B	2.72	136.42	124.39
9	u	101	BCL	C1-C2-C3	-2.72	121.74	126.20
15	4	101	CRT	C29-C28-C27	-2.72	118.41	122.82
9	7	102	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
11	L	304	UQ8	O4-C4-C3	-2.72	113.35	123.64
9	V	102	BCL	CMC-C2C-C3C	-2.72	103.47	113.98
9	X	102	BCL	C11-C10-C8	-2.72	106.93	115.97
9	r	101	BCL	C2A-C1A-CHA	2.72	128.58	123.87
9	d	101	BCL	CHD-C1D-ND	-2.72	120.98	124.80
9	u	102	BCL	CMC-C2C-C3C	-2.72	103.48	113.98
9	k	102	BCL	C3B-C4B-NB	-2.72	106.17	109.76
9	AE	102	BCL	C1-O2A-CGA	2.72	123.22	116.65
9	m	103	BCL	C11-C10-C8	-2.71	106.94	115.97
10	L	302	BPH	O2A-CGA-CBA	2.71	120.11	111.83
9	S	102	BCL	C7-C6-C5	-2.71	106.03	113.26
9	m	103	BCL	CHC-C1C-NC	2.71	128.32	124.40
15	AD	101	CRT	C21-C20-C19	-2.71	117.97	123.52
15	n	101	CRT	C20-C21-C22	-2.71	117.97	123.52
9	0	102	BCL	O2A-CGA-O1A	-2.71	116.84	123.63
9	y	401	BCL	C11-C10-C8	-2.71	106.95	115.97
9	y	401	BCL	CGD-CBD-CAD	-2.71	102.07	110.85
9	AK	101	BCL	OBB-CAB-CBB	-2.71	113.70	119.77
9	g	102	BCL	C2B-C1B-NB	-2.71	107.52	110.33
9	AC	103	BCL	CMC-C2C-C3C	-2.71	103.51	113.98
9	l	101	BCL	CGD-CBD-CAD	-2.71	102.08	110.85
12	x	306	PEF	O3P-P-O1P	-2.71	98.21	108.94
9	D	101	BCL	CMA-C3A-C4A	-2.70	104.50	111.77
9	0	102	BCL	CHD-C1D-ND	-2.70	121.00	124.80
9	e	102	BCL	C7-C6-C5	-2.70	106.06	113.26
15	R	101	CRT	C15-C16-C17	2.70	133.77	126.36
9	d	101	BCL	C2D-C1D-ND	2.70	112.80	110.13
9	7	102	BCL	C11-C10-C8	-2.70	106.99	115.97
9	S	102	BCL	CMC-C2C-C3C	-2.70	103.54	113.98
9	x	303	BCL	C1C-NC-C4C	-2.70	105.45	106.68
9	1	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
11	L	304	UQ8	O3-C3-C2	2.70	125.75	116.64
9	F	101	BCL	C16-C15-C13	-2.70	106.99	115.97
15	AJ	101	CRT	C13-C12-C11	2.70	122.21	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	304	UQ8	C7-C6-C1	-2.70	120.27	124.89
9	c	101	BCL	CBB-CAB-C3B	2.70	126.09	120.40
9	AL	102	BCL	C11-C10-C8	-2.70	107.00	115.97
9	V	102	BCL	CBA-CAA-C2A	2.69	121.81	113.79
9	AB	101	BCL	CMA-C3A-C4A	-2.69	104.53	111.77
7	C	504	HEM	CHD-C1D-ND	2.69	127.32	124.42
9	r	101	BCL	C12-C11-C10	-2.69	101.23	113.28
9	q	102	BCL	CHD-C1D-ND	-2.69	121.02	124.80
9	y	401	BCL	C2B-C1B-NB	-2.69	107.54	110.33
9	Q	101	BCL	CBC-CAC-C3C	2.69	119.11	113.41
9	k	102	BCL	CHC-C1C-NC	2.69	128.28	124.40
9	A	103	BCL	CMD-C2D-C1D	2.69	129.46	124.73
9	4	102	BCL	C3D-C2D-C1D	-2.69	102.17	105.83
9	x	305	BCL	CMC-C2C-C3C	-2.68	103.60	113.98
9	AB	101	BCL	O2A-CGA-O1A	-2.68	116.91	123.63
9	Z	102	BCL	CMA-C3A-C4A	-2.68	104.56	111.77
9	9	102	BCL	C2B-C1B-NB	-2.68	107.55	110.33
9	h	101	BCL	C16-C15-C13	-2.68	107.05	115.97
9	j	101	BCL	CBB-CAB-C3B	2.68	126.05	120.40
9	I	103	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
9	R	102	BCL	CMA-C3A-C2A	-2.68	103.62	113.98
15	T	101	CRT	C27-C26-C25	-2.68	115.44	123.20
12	m	101	PEF	O3-C3-C2	2.68	116.11	108.40
12	y	408	PEF	C3-C2-C1	2.68	118.02	111.78
9	D	102	BCL	C2B-C1B-NB	-2.67	107.55	110.33
9	g	102	BCL	CMD-C2D-C1D	2.67	129.44	124.73
15	G	101	CRT	C9-C10-C11	-2.67	115.45	123.20
9	Z	102	BCL	CMC-C2C-C3C	-2.67	103.65	113.98
9	r	101	BCL	CMC-C2C-C3C	-2.67	103.65	113.98
7	C	502	HEM	CHC-C1C-NC	2.67	127.36	124.45
9	1	101	BCL	CHD-C1D-ND	-2.67	121.04	124.80
9	R	102	BCL	CMC-C2C-C3C	-2.67	103.66	113.98
7	o	502	HEM	CAA-CBA-CGA	-2.67	106.58	113.67
9	AI	101	BCL	CBB-CAB-C3B	2.67	126.03	120.40
9	P	101	BCL	C16-C15-C13	-2.67	107.10	115.97
9	AE	102	BCL	CMC-C2C-C3C	-2.67	103.67	113.98
7	o	502	HEM	CHC-C1C-NC	2.67	127.36	124.45
9	m	103	BCL	CBB-CAB-C3B	2.67	126.02	120.40
9	F	101	BCL	O2A-CGA-O1A	-2.67	116.96	123.63
9	AC	102	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
15	V	101	CRT	C24-C23-C22	-2.66	118.50	122.82
9	AB	102	BCL	CMC-C2C-C3C	-2.66	103.68	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	102	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
9	N	101	BCL	CMA-C3A-C4A	-2.66	104.61	111.77
15	AL	101	CRT	C21-C22-C23	-2.66	123.54	127.28
9	V	102	BCL	C3B-C4B-NB	-2.66	106.25	109.76
9	D	101	BCL	CHB-C1B-NB	2.66	128.04	124.05
9	4	102	BCL	C1-O2A-CGA	2.66	123.09	116.65
9	m	102	BCL	CHD-C1D-ND	-2.66	121.06	124.80
9	L	303	BCL	CBC-CAC-C3C	2.66	119.05	113.41
15	7	101	CRT	C18-C17-C16	2.66	122.15	118.09
9	7	102	BCL	CMD-C2D-C1D	2.66	129.41	124.73
9	5	101	BCL	CMC-C2C-C3C	-2.66	103.70	113.98
9	7	102	BCL	CMC-C2C-C3C	-2.66	103.70	113.98
9	AI	101	BCL	C2A-C1A-CHA	2.66	128.48	123.87
9	F	101	BCL	CHC-C1C-NC	2.66	128.23	124.40
9	w	101	BCL	C2B-C1B-NB	-2.66	107.57	110.33
15	I	102	CRT	C29-C28-C30	2.65	122.14	118.09
9	V	102	BCL	CED-O2D-CGD	-2.65	109.90	115.92
9	x	301	BCL	C3B-C4B-NB	-2.65	106.26	109.76
9	A	102	BCL	C12-C11-C10	-2.65	101.39	113.28
9	I	103	BCL	CBB-CAB-C3B	2.65	125.99	120.40
15	i	101	CRT	C26-C27-C28	-2.65	123.56	127.28
9	p	102	BCL	C12-C11-C10	-2.65	101.40	113.28
9	L	301	BCL	O2A-CGA-CBA	2.65	119.92	111.83
9	I	101	BCL	CMC-C2C-C3C	-2.65	103.74	113.98
9	AE	102	BCL	C2A-C1A-CHA	2.65	128.47	123.87
9	AE	102	BCL	O2A-CGA-O1A	-2.65	117.00	123.63
9	D	101	BCL	C3B-C4B-NB	-2.65	106.26	109.76
9	c	101	BCL	C1-O2A-CGA	2.65	123.06	116.65
15	AD	101	CRT	C15-C16-C17	2.65	133.62	126.36
9	F	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
9	M	401	BCL	CHD-C1D-ND	-2.65	121.08	124.80
9	m	103	BCL	C3B-C4B-NB	-2.65	106.27	109.76
9	AB	101	BCL	C2A-C1A-CHA	2.65	128.46	123.87
9	s	102	BCL	O2A-CGA-O1A	-2.65	117.01	123.63
9	2	102	BCL	CHC-C1C-NC	2.65	128.22	124.40
9	M	402	BCL	C11-C10-C8	-2.65	107.17	115.97
9	AG	101	BCL	C11-C10-C8	-2.64	107.17	115.97
9	7	102	BCL	C16-C15-C13	-2.64	107.18	115.97
9	2	102	BCL	OBB-CAB-CBB	-2.64	113.85	119.77
9	x	303	BCL	CBB-CAB-C3B	2.64	125.97	120.40
7	C	504	HEM	CHC-C1C-NC	2.64	127.33	124.45
9	l	101	BCL	C6-C5-C3	-2.64	107.03	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	501	HEM	O2A-CGA-CBA	2.64	122.34	114.00
9	AB	102	BCL	O2A-CGA-O1A	-2.64	117.02	123.63
15	AD	101	CRT	C32-C31-C30	-2.64	115.55	123.20
9	7	102	BCL	C1-O2A-CGA	2.64	123.04	116.65
9	g	102	BCL	CHB-C1B-NB	2.64	128.01	124.05
9	AC	103	BCL	C1-O2A-CGA	2.64	123.04	116.65
15	P	102	CRT	C14-C15-C16	-2.64	115.55	123.20
9	S	102	BCL	CHB-C1B-NB	2.64	128.01	124.05
9	l	101	BCL	CHB-C1B-NB	2.64	128.01	124.05
9	AE	102	BCL	C6-C5-C3	-2.64	107.04	113.47
15	m	104	CRT	C24-C23-C25	2.64	122.12	118.09
9	5	101	BCL	O2A-CGA-O1A	-2.64	117.03	123.63
9	G	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
15	0	101	CRT	C15-C14-C12	-2.64	123.58	127.28
9	D	101	BCL	C11-C12-C13	-2.64	107.20	115.97
10	x	302	BPH	C1-C2-C3	-2.63	121.88	126.20
9	V	102	BCL	CMA-C3A-C4A	-2.63	104.69	111.77
9	A	102	BCL	CMC-C2C-C3C	-2.63	103.80	113.98
15	n	101	CRT	C34-C33-C35	2.63	122.11	118.09
9	x	305	BCL	C2A-C1A-CHA	2.63	128.44	123.87
9	6	101	BCL	C2A-C1A-CHA	2.63	128.43	123.87
9	O	102	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
9	S	102	BCL	CBB-CAB-C3B	2.63	125.94	120.40
9	w	101	BCL	C1C-NC-C4C	-2.63	105.48	106.68
11	L	304	UQ8	C37-C36-C34	2.63	121.89	113.19
15	i	101	CRT	C11-C12-C14	-2.63	114.88	119.01
9	W	101	BCL	C3B-C4B-NB	-2.63	106.29	109.76
9	6	101	BCL	C1D-CHD-C4C	-2.63	120.29	126.62
9	K	101	BCL	C7-C6-C5	-2.63	106.27	113.26
7	C	504	HEM	CHC-C4B-NB	2.62	127.25	124.42
9	AB	101	BCL	C2B-C1B-NB	-2.62	107.61	110.33
15	4	101	CRT	C5-C6-C7	-2.62	121.93	125.89
9	F	101	BCL	CHD-C1D-ND	-2.62	121.11	124.80
9	AI	101	BCL	C11-C10-C8	-2.62	107.25	115.97
9	x	301	BCL	C11-C10-C8	-2.62	107.25	115.97
12	H	305	PEF	O2-C10-O4	-2.62	117.93	122.99
7	o	502	HEM	C4D-ND-C1D	2.62	108.31	105.21
9	e	102	BCL	CHC-C1C-NC	2.62	128.18	124.40
9	i	102	BCL	C7-C6-C5	-2.62	106.28	113.26
9	P	101	BCL	CMC-C2C-C3C	-2.62	103.86	113.98
9	h	101	BCL	CBB-CAB-C3B	2.62	125.92	120.40
9	N	101	BCL	C1C-NC-C4C	-2.62	105.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	303	BCL	CMB-C2B-C3B	2.62	133.92	125.67
9	AB	102	BCL	C3D-C2D-C1D	-2.62	102.26	105.83
15	AH	102	CRT	C35-C33-C32	-2.62	114.89	119.01
9	F	101	BCL	C1C-NC-C4C	-2.61	105.49	106.68
10	M	403	BPH	CMC-C2C-C1C	-2.61	108.98	114.61
15	z	101	CRT	C34-C33-C32	-2.61	118.58	122.82
7	o	503	HEM	O2A-CGA-CBA	2.61	122.25	114.00
9	Q	101	BCL	CBB-CAB-C3B	2.61	125.91	120.40
15	R	101	CRT	C10-C11-C12	-2.61	119.20	126.36
9	6	101	BCL	CMC-C2C-C3C	-2.61	103.89	113.98
9	y	401	BCL	C3B-C4B-NB	-2.61	106.31	109.76
9	T	102	BCL	CHB-C1B-NB	2.61	127.96	124.05
9	c	101	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
9	g	102	BCL	CGD-CBD-CAD	-2.61	102.40	110.85
15	G	101	CRT	C27-C26-C25	-2.61	115.64	123.20
9	AC	102	BCL	CHC-C1C-NC	2.61	128.16	124.40
9	Q	101	BCL	C2C-C3C-C4C	-2.61	97.43	101.34
7	o	504	HEM	C3C-C2C-C1C	2.61	109.51	107.05
9	AC	103	BCL	C2B-C1B-NB	-2.61	107.62	110.33
15	7	103	CRT	C26-C25-C23	-2.61	119.21	126.36
9	AF	101	BCL	CHB-C1B-NB	2.61	127.96	124.05
9	Y	101	BCL	CED-O2D-CGD	-2.61	110.00	115.92
9	6	101	BCL	CAA-CBA-CGA	-2.60	105.81	113.21
9	Z	102	BCL	C7-C6-C5	-2.60	106.32	113.26
7	o	503	HEM	CAA-C2A-C1A	2.60	130.02	124.94
7	C	501	HEM	C3D-C4D-ND	-2.60	107.32	110.17
9	w	101	BCL	C3D-C2D-C1D	-2.60	102.28	105.83
9	U	101	BCL	CMC-C2C-C3C	-2.60	103.92	113.98
9	m	102	BCL	C3D-C2D-C1D	-2.60	102.28	105.83
9	AC	102	BCL	CHD-C1D-ND	-2.60	121.14	124.80
15	z	101	CRT	C29-C28-C30	2.60	122.06	118.09
9	K	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
7	o	502	HEM	CAD-C3D-C4D	2.60	129.23	124.70
9	AC	102	BCL	CHB-C1B-NB	2.60	127.95	124.05
9	p	102	BCL	C2A-C1A-CHA	2.60	128.38	123.87
7	C	503	HEM	C2C-C1C-NC	-2.60	104.83	109.64
9	L	301	BCL	CMD-C2D-C1D	2.60	129.30	124.73
9	V	102	BCL	OBB-CAB-CBB	-2.60	113.95	119.77
15	AH	102	CRT	C34-C33-C35	2.60	122.05	118.09
9	4	102	BCL	CMC-C2C-C3C	-2.60	103.95	113.98
9	5	101	BCL	CHB-C1B-NB	2.59	127.94	124.05
9	S	102	BCL	C3D-C2D-C1D	-2.59	102.29	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	BCL	C11-C10-C8	-2.59	107.36	115.97
9	w	101	BCL	CMC-C2C-C3C	-2.59	103.97	113.98
9	A	102	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
9	R	102	BCL	C1-O2A-CGA	2.59	122.92	116.65
9	D	102	BCL	CHC-C1C-NC	2.59	128.14	124.40
15	AJ	101	CRT	C9-C10-C11	2.59	130.70	123.20
12	y	408	PEF	C3-O3-C30	2.59	123.47	117.08
9	f	101	BCL	C2B-C1B-NB	-2.59	107.64	110.33
7	o	504	HEM	CMC-C2C-C1C	-2.59	120.17	124.73
9	0	102	BCL	C2B-C1B-NB	-2.59	107.64	110.33
9	A	102	BCL	C3C-C2C-C1C	2.59	106.05	101.87
9	AH	101	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
9	D	102	BCL	C2A-C1A-CHA	2.58	128.35	123.87
9	AB	102	BCL	C12-C11-C10	-2.58	101.70	113.28
9	L	301	BCL	C2A-C1A-CHA	2.58	128.35	123.87
9	Z	102	BCL	C3C-C4C-CHD	-2.58	117.95	123.39
9	L	301	BCL	C5-C3-C2	2.58	126.96	121.17
9	6	101	BCL	CHD-C1D-ND	-2.58	121.17	124.80
9	A	103	BCL	C3D-C2D-C1D	-2.58	102.31	105.83
9	h	101	BCL	CMC-C2C-C3C	-2.58	104.01	113.98
9	6	101	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
12	p	101	PEF	O3-C30-C31	2.58	123.32	112.38
9	AI	102	BCL	C2A-C1A-CHA	2.58	128.34	123.87
9	3	101	BCL	C11-C10-C8	-2.58	107.40	115.97
9	V	102	BCL	CHC-C1C-NC	2.58	128.12	124.40
9	u	101	BCL	CMD-C2D-C1D	2.58	129.26	124.73
9	i	102	BCL	CMC-C2C-C3C	-2.57	104.03	113.98
9	j	101	BCL	CMC-C2C-C3C	-2.57	104.03	113.98
9	F	101	BCL	C2C-C3C-C4C	-2.57	97.48	101.34
9	A	103	BCL	C16-C15-C13	-2.57	107.41	115.97
9	l	101	BCL	CHC-C1C-NC	2.57	128.11	124.40
9	x	303	BCL	CGD-CBD-CAD	-2.57	102.52	110.85
10	x	302	BPH	CBC-CAC-C3C	-2.57	108.72	113.78
15	O	101	CRT	C13-C12-C11	2.57	122.02	118.09
9	m	102	BCL	C3B-C4B-NB	-2.57	106.37	109.76
9	O	102	BCL	CBA-CAA-C2A	2.57	121.44	113.79
9	AI	101	BCL	CMC-C2C-C3C	-2.57	104.04	113.98
15	0	101	CRT	C35-C33-C32	-2.57	114.97	119.01
9	R	102	BCL	C4A-NA-C1A	2.57	107.85	106.68
15	k	101	CRT	C5-C6-C7	-2.57	122.01	125.89
7	C	501	HEM	CHB-C1B-C2B	-2.57	119.65	126.95
9	AB	101	BCL	C3D-C2D-C1D	-2.57	102.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	102	BCL	CED-O2D-CGD	-2.57	110.09	115.92
9	W	101	BCL	O2A-CGA-O1A	-2.57	117.21	123.63
9	A	102	BCL	CHC-C1C-NC	2.57	128.10	124.40
9	D	101	BCL	OBB-CAB-CBB	-2.57	114.02	119.77
9	y	401	BCL	C16-C15-C13	-2.57	107.44	115.97
9	u	102	BCL	C11-C12-C13	-2.57	107.44	115.97
12	y	408	PEF	O2-C10-O4	-2.57	118.04	122.99
7	C	503	HEM	CHC-C1C-NC	2.56	127.25	124.45
15	X	101	CRT	C20-C21-C22	-2.56	118.28	123.52
9	h	101	BCL	CMD-C2D-C1D	2.56	129.24	124.73
10	L	302	BPH	CMC-C2C-C1C	-2.56	109.10	114.61
9	R	102	BCL	C7-C6-C5	-2.56	106.44	113.26
9	d	101	BCL	C4D-CHA-C1A	2.56	124.30	121.24
7	o	501	HEM	C3D-C4D-ND	-2.56	107.37	110.17
9	Y	101	BCL	CMC-C2C-C1C	-2.56	104.90	111.77
9	m	103	BCL	O2A-CGA-O1A	-2.56	117.23	123.63
15	2	101	CRT	C13-C12-C11	2.56	121.99	118.09
14	M	404	MQ8	O1-C1-C2	-2.56	117.09	120.45
9	AI	102	BCL	C7-C6-C5	-2.55	106.45	113.26
9	h	101	BCL	C3B-C4B-NB	-2.55	106.39	109.76
15	Z	101	CRT	C27-C26-C25	-2.55	115.80	123.20
10	L	302	BPH	C1-C2-C3	-2.55	122.01	126.20
9	U	101	BCL	CBB-CAB-C3B	2.55	125.78	120.40
9	AI	101	BCL	C16-C15-C13	-2.55	107.48	115.97
9	x	305	BCL	C1D-CHD-C4C	-2.55	120.46	126.62
9	Y	101	BCL	CMC-C2C-C3C	-2.55	104.11	113.98
15	9	101	CRT	C18-C17-C16	2.55	121.99	118.09
9	z	102	BCL	C3D-C2D-C1D	-2.55	102.35	105.83
15	s	101	CRT	C9-C10-C11	-2.55	115.81	123.20
9	AG	101	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
9	T	102	BCL	CBA-CAA-C2A	2.55	121.38	113.79
9	d	101	BCL	CAA-CBA-CGA	-2.55	105.97	113.21
9	x	301	BCL	C1C-NC-C4C	-2.55	105.52	106.68
9	9	102	BCL	C3D-C2D-C1D	-2.55	102.35	105.83
7	o	504	HEM	O2D-CGD-CBD	2.55	122.05	114.00
15	O	101	CRT	C8-C7-C6	2.55	121.98	118.09
9	AB	102	BCL	C2B-C1B-NB	-2.55	107.69	110.33
9	4	102	BCL	CBB-CAB-C3B	2.55	125.77	120.40
9	AB	102	BCL	CMD-C2D-C1D	2.55	129.21	124.73
9	p	102	BCL	CBB-CAB-C3B	2.55	125.77	120.40
15	X	101	CRT	C32-C31-C30	-2.54	115.83	123.20
15	AF	102	CRT	C8-C7-C6	2.54	121.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AF	101	BCL	C2A-C1A-CHA	2.54	128.28	123.87
15	AL	101	CRT	C8-C7-C9	-2.54	118.70	122.82
9	A	102	BCL	O2A-CGA-O1A	-2.54	117.28	123.63
10	y	402	BPH	CGD-CBD-CAD	-2.54	102.63	110.85
9	AI	101	BCL	C3B-C4B-NB	-2.54	106.41	109.76
9	5	101	BCL	C11-C12-C13	-2.54	107.53	115.97
9	W	101	BCL	OBD-CAD-C3D	2.54	134.34	128.42
9	i	102	BCL	O2A-C1-C2	2.54	117.87	108.11
9	V	102	BCL	CAA-C2A-C3A	2.54	119.85	113.00
9	X	102	BCL	CHB-C1B-NB	2.54	127.85	124.05
9	Y	101	BCL	CMD-C2D-C1D	2.53	129.19	124.73
9	AC	102	BCL	C11-C12-C13	-2.53	107.54	115.97
15	z	101	CRT	C14-C15-C16	-2.53	115.86	123.20
9	5	101	BCL	CHD-C1D-ND	-2.53	121.24	124.80
9	w	101	BCL	C3B-C4B-NB	-2.53	106.42	109.76
15	v	101	CRT	C24-C23-C25	2.53	121.95	118.09
15	I	102	CRT	C32-C31-C30	-2.53	115.87	123.20
15	AF	102	CRT	C9-C10-C11	-2.53	115.88	123.20
9	2	102	BCL	CBB-CAB-C3B	2.53	125.73	120.40
9	5	101	BCL	C12-C11-C10	-2.53	101.96	113.28
9	e	102	BCL	CMC-C2C-C3C	-2.53	104.22	113.98
15	O	101	CRT	C29-C28-C30	2.53	121.95	118.09
9	AF	101	BCL	CHB-C4A-NA	-2.53	120.75	124.40
9	k	102	BCL	C2B-C1B-NB	-2.53	107.71	110.33
9	L	301	BCL	C6-C5-C3	-2.53	107.32	113.47
9	Q	101	BCL	O2A-CGA-O1A	-2.52	117.31	123.63
9	9	102	BCL	CHC-C1C-NC	2.52	128.04	124.40
9	U	101	BCL	C3D-C2D-C1D	-2.52	102.39	105.83
9	s	102	BCL	C3C-C4C-CHD	-2.52	118.08	123.39
9	h	101	BCL	C3D-C2D-C1D	-2.52	102.39	105.83
9	h	101	BCL	C4A-NA-C1A	2.52	107.83	106.68
15	g	101	CRT	C18-C17-C16	2.52	121.93	118.09
9	x	303	BCL	C2B-C1B-NB	-2.52	107.72	110.33
9	x	303	BCL	C1D-CHD-C4C	-2.52	120.55	126.62
9	h	101	BCL	CHC-C1C-NC	2.52	128.03	124.40
9	m	103	BCL	CBC-CAC-C3C	2.52	118.75	113.41
9	V	102	BCL	CHB-C4A-NA	-2.52	120.77	124.40
9	AB	102	BCL	C1-C2-C3	-2.51	122.08	126.20
9	q	102	BCL	C16-C15-C13	-2.51	107.61	115.97
9	O	102	BCL	C4A-NA-C1A	2.51	107.83	106.68
9	w	101	BCL	CBB-CAB-C3B	2.51	125.70	120.40
9	Q	101	BCL	C3B-C4B-NB	-2.51	106.44	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	101	BCL	C3B-C4B-NB	-2.51	106.44	109.76
9	M	402	BCL	C3D-C2D-C1D	-2.51	102.41	105.83
9	4	102	BCL	O2A-C1-C2	2.51	117.76	108.11
9	M	402	BCL	C3C-C2C-C1C	2.51	105.92	101.87
15	g	101	CRT	C14-C15-C16	-2.51	115.94	123.20
9	AG	101	BCL	C3D-C2D-C1D	-2.51	102.41	105.83
9	M	402	BCL	C7-C6-C5	-2.51	106.58	113.26
12	t	303	PEF	O3-C30-C31	2.50	123.01	112.38
9	x	301	BCL	CHC-C1C-NC	2.50	128.01	124.40
9	r	101	BCL	C2B-C1B-NB	-2.50	107.73	110.33
7	C	502	HEM	CAD-C3D-C4D	2.50	129.06	124.70
12	t	303	PEF	O5-C30-C31	-2.50	115.90	124.77
15	AH	102	CRT	C9-C10-C11	-2.50	115.95	123.20
9	AL	102	BCL	C3D-C2D-C1D	-2.50	102.42	105.83
9	W	101	BCL	CMC-C2C-C3C	-2.50	104.30	113.98
9	x	301	BCL	CMC-C2C-C3C	-2.50	104.31	113.98
10	y	402	BPH	O2A-CGA-O1A	-2.50	117.37	123.63
9	K	101	BCL	C3C-C4C-CHD	-2.50	118.12	123.39
9	g	102	BCL	CHD-C1D-ND	-2.50	121.28	124.80
9	d	101	BCL	O2A-C1-C2	2.50	117.73	108.11
7	o	502	HEM	CHB-C1B-NB	2.50	127.46	124.37
9	s	102	BCL	CMB-C2B-C3B	2.50	133.55	125.67
15	v	101	CRT	C34-C33-C35	2.50	121.91	118.09
15	0	101	CRT	C31-C30-C28	-2.50	119.51	126.36
9	l	101	BCL	CHD-C1D-ND	-2.50	121.29	124.80
15	9	101	CRT	C29-C28-C30	2.50	121.90	118.09
9	AG	101	BCL	CHC-C1C-NC	2.50	128.00	124.40
9	e	102	BCL	C2B-C1B-NB	-2.50	107.74	110.33
9	N	101	BCL	C3B-C4B-NB	-2.50	106.47	109.76
14	y	403	MQ8	C20-C18-C17	-2.49	115.57	121.17
9	AG	101	BCL	CED-O2D-CGD	-2.49	110.26	115.92
9	AI	101	BCL	C1C-NC-C4C	-2.49	105.54	106.68
9	g	102	BCL	C3C-C4C-CHD	-2.49	118.13	123.39
9	m	103	BCL	C12-C11-C10	-2.49	102.10	113.28
9	N	101	BCL	C3D-C2D-C1D	-2.49	102.43	105.83
9	T	102	BCL	C16-C15-C13	-2.49	107.68	115.97
9	AE	102	BCL	OBB-CAB-CBB	-2.49	114.19	119.77
9	c	101	BCL	CHC-C1C-NC	2.49	128.00	124.40
9	AB	102	BCL	C1-O2A-CGA	2.49	122.68	116.65
9	f	101	BCL	CMB-C2B-C3B	2.49	133.53	125.67
7	C	503	HEM	CAA-CBA-CGA	-2.49	107.06	113.67
9	f	101	BCL	CMC-C2C-C3C	-2.49	104.36	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	102	BCL	C11-C12-C13	-2.49	107.69	115.97
9	f	101	BCL	CBB-CAB-C3B	2.49	125.64	120.40
15	AD	101	CRT	C11-C12-C14	2.49	122.92	119.01
9	4	102	BCL	C12-C11-C10	-2.49	102.14	113.28
9	I	101	BCL	CBB-CAB-C3B	2.49	125.64	120.40
9	0	102	BCL	C3D-C2D-C1D	-2.49	102.44	105.83
9	L	301	BCL	CGD-CBD-CAD	-2.48	102.81	110.85
9	AI	102	BCL	C3B-C4B-NB	-2.48	106.48	109.76
9	r	101	BCL	CBB-CAB-C3B	2.48	125.63	120.40
11	L	304	UQ8	O3-C3-C4	-2.48	114.26	123.64
9	A	102	BCL	OBB-CAB-CBB	-2.48	114.22	119.77
15	e	101	CRT	C20-C19-C17	-2.48	123.80	127.28
15	E	101	CRT	C8-C7-C9	-2.48	118.80	122.82
15	k	101	CRT	C21-C22-C23	-2.48	123.81	127.28
9	2	102	BCL	C3B-C4B-NB	-2.48	106.49	109.76
9	AH	101	BCL	C16-C15-C13	-2.48	107.74	115.97
9	M	402	BCL	C2B-C1B-NB	-2.48	107.76	110.33
9	D	102	BCL	C3B-C4B-NB	-2.47	106.49	109.76
9	f	101	BCL	O2A-C1-C2	2.47	117.63	108.11
9	w	101	BCL	C6-C5-C3	-2.47	107.44	113.47
10	M	403	BPH	C11-C12-C13	-2.47	107.75	115.97
9	M	401	BCL	C1D-CHD-C4C	-2.47	120.66	126.62
15	v	101	CRT	C29-C28-C27	-2.47	118.81	122.82
10	x	302	BPH	C4-C3-C5	2.47	119.52	115.23
15	4	101	CRT	C10-C9-C7	-2.47	123.81	127.28
7	o	503	HEM	CAD-C3D-C4D	2.47	129.00	124.70
15	g	101	CRT	C21-C20-C19	-2.47	118.46	123.52
9	AB	102	BCL	CHC-C1C-NC	2.47	127.96	124.40
9	3	101	BCL	C7-C6-C5	-2.47	106.68	113.26
15	P	102	CRT	C9-C10-C11	-2.47	116.05	123.20
7	C	501	HEM	CHD-C4C-NC	2.47	127.14	124.45
9	I	101	BCL	C4A-NA-C1A	2.47	107.81	106.68
9	j	101	BCL	C3D-C2D-C1D	-2.47	102.46	105.83
9	U	101	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
9	O	102	BCL	OBB-CAB-CBB	-2.47	114.25	119.77
9	f	101	BCL	OBB-CAB-CBB	-2.47	114.25	119.77
9	R	102	BCL	O2A-CGA-O1A	-2.47	117.46	123.63
9	I	101	BCL	CGD-CBD-CAD	-2.46	102.87	110.85
9	V	102	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
9	F	101	BCL	C4A-NA-C1A	2.46	107.80	106.68
9	Q	101	BCL	CED-O2D-CGD	-2.46	110.33	115.92
9	y	401	BCL	CBB-CAB-C3B	2.46	125.59	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	C1C-NC-C4C	-2.46	105.56	106.68
9	r	101	BCL	C3B-C4B-NB	-2.46	106.52	109.76
14	y	403	MQ8	C29-C28-C30	2.46	119.49	115.23
9	X	102	BCL	C3D-C2D-C1D	-2.46	102.48	105.83
9	K	101	BCL	C2B-C1B-NB	-2.46	107.78	110.33
9	4	102	BCL	C3B-C4B-NB	-2.45	106.52	109.76
15	M	405	CRT	C32-C31-C30	-2.45	116.09	123.20
9	3	101	BCL	O2A-C1-C2	2.45	117.55	108.11
10	M	403	BPH	C6-C5-C3	-2.45	107.49	113.47
12	x	306	PEF	O3-C30-C31	2.45	122.78	112.38
9	L	303	BCL	CMB-C2B-C3B	2.45	133.40	125.67
9	2	102	BCL	O2A-CGA-O1A	-2.45	117.50	123.63
9	AC	102	BCL	C4A-NA-C1A	2.45	107.80	106.68
15	2	101	CRT	C24-C23-C25	2.45	121.83	118.09
9	m	102	BCL	CHC-C1C-NC	2.45	127.93	124.40
9	l	101	BCL	C12-C11-C10	-2.45	102.31	113.28
15	E	101	CRT	C26-C27-C28	-2.45	123.85	127.28
9	AB	101	BCL	CBB-CAB-C3B	2.45	125.56	120.40
9	w	101	BCL	O2A-C1-C2	2.45	117.52	108.11
15	V	101	CRT	C18-C17-C16	2.44	121.82	118.09
9	AC	103	BCL	C12-C11-C10	-2.44	102.32	113.28
15	AJ	101	CRT	C34-C33-C35	2.44	121.82	118.09
9	AE	102	BCL	C11-C12-C13	-2.44	107.84	115.97
9	r	101	BCL	C1C-NC-C4C	-2.44	105.56	106.68
9	7	102	BCL	C3D-C2D-C1D	-2.44	102.50	105.83
15	2	101	CRT	C8-C7-C9	-2.44	118.86	122.82
9	AG	101	BCL	C2A-C1A-CHA	2.44	128.11	123.87
9	T	102	BCL	C4A-NA-C1A	2.44	107.79	106.68
9	2	102	BCL	C2B-C1B-NB	-2.44	107.79	110.33
9	V	102	BCL	C1-O2A-CGA	2.44	122.56	116.65
15	7	101	CRT	C16-C17-C19	-2.44	115.17	119.01
15	2	101	CRT	C21-C20-C19	-2.44	118.53	123.52
9	x	303	BCL	C4D-CHA-C1A	2.44	124.15	121.24
9	AK	101	BCL	C2B-C1B-NB	-2.44	107.80	110.33
9	9	102	BCL	O2A-CGA-O1A	-2.44	117.53	123.63
15	AD	101	CRT	C10-C11-C12	-2.44	119.68	126.36
9	I	101	BCL	C12-C11-C10	-2.44	102.36	113.28
9	AH	101	BCL	CMD-C2D-C1D	2.44	129.02	124.73
7	o	504	HEM	C3B-C4B-NB	-2.44	107.72	109.47
9	x	301	BCL	C1-O2A-CGA	2.44	122.55	116.65
9	R	102	BCL	CMB-C2B-C3B	2.44	133.35	125.67
9	O	102	BCL	C11-C12-C13	-2.43	107.87	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	q	102	BCL	CMC-C2C-C3C	-2.43	104.57	113.98
9	d	101	BCL	CHB-C1B-NB	2.43	127.70	124.05
9	O	102	BCL	C7-C6-C5	-2.43	106.78	113.26
9	9	102	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
9	m	102	BCL	C11-C10-C8	-2.43	107.88	115.97
9	m	103	BCL	OBD-CAD-C3D	2.43	134.10	128.42
9	O	102	BCL	CHB-C4A-NA	-2.43	120.89	124.40
9	Q	101	BCL	CAA-CBA-CGA	-2.43	106.30	113.21
9	m	102	BCL	C12-C11-C10	-2.43	102.38	113.28
9	5	101	BCL	C3D-C2D-C1D	-2.43	102.52	105.83
9	P	101	BCL	CMB-C2B-C3B	2.43	133.33	125.67
9	x	303	BCL	OBB-CAB-CBB	-2.43	114.33	119.77
9	e	102	BCL	C3D-C2D-C1D	-2.43	102.52	105.83
11	L	304	UQ8	C32-C33-C34	-2.43	122.06	127.62
9	AE	102	BCL	CBA-CAA-C2A	2.43	121.02	113.79
15	AF	102	CRT	C13-C12-C11	2.43	121.80	118.09
9	AC	102	BCL	CMC-C2C-C3C	-2.43	104.59	113.98
9	z	102	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
9	4	102	BCL	C11-C12-C13	-2.43	107.90	115.97
9	c	101	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
9	l	101	BCL	C4A-NA-C1A	2.43	107.79	106.68
7	C	502	HEM	C3A-C4A-NA	-2.43	106.25	110.14
9	i	102	BCL	C11-C12-C13	-2.43	107.90	115.97
9	L	301	BCL	CHD-C1D-ND	-2.42	121.39	124.80
9	g	102	BCL	C16-C15-C13	-2.42	107.91	115.97
15	AL	101	CRT	C4-C5-C6	-2.42	121.51	124.91
9	3	101	BCL	CMB-C2B-C3B	2.42	133.31	125.67
15	k	101	CRT	C10-C9-C7	-2.42	123.88	127.28
9	F	101	BCL	CBB-CAB-C3B	2.42	125.51	120.40
7	C	501	HEM	CAD-C3D-C2D	-2.42	123.33	127.87
15	0	101	CRT	C8-C7-C6	2.42	121.79	118.09
9	8	101	BCL	CHB-C1B-NB	2.42	127.68	124.05
15	i	101	CRT	C20-C19-C17	-2.42	123.88	127.28
9	G	102	BCL	CMC-C2C-C3C	-2.42	104.62	113.98
9	G	102	BCL	CHD-C1D-ND	-2.42	121.40	124.80
9	AH	101	BCL	CED-O2D-CGD	-2.42	110.43	115.92
9	AG	101	BCL	C6-C5-C3	-2.42	107.58	113.47
9	I	103	BCL	C11-C12-C13	-2.42	107.93	115.97
9	q	102	BCL	C11-C10-C8	-2.42	107.93	115.97
9	e	102	BCL	C11-C10-C8	-2.42	107.94	115.97
9	L	301	BCL	C16-C15-C13	-2.42	107.94	115.97
9	A	103	BCL	C3C-C4C-CHD	-2.42	118.30	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	101	BCL	CMC-C2C-C3C	-2.41	104.65	113.98
9	L	303	BCL	C6-C7-C8	2.41	123.99	115.97
9	g	102	BCL	C3B-C4B-NB	-2.41	106.57	109.76
9	z	102	BCL	C12-C11-C10	-2.41	102.46	113.28
15	n	101	CRT	C21-C20-C19	-2.41	118.58	123.52
9	f	101	BCL	C1-C2-C3	-2.41	122.25	126.20
15	9	101	CRT	C35-C33-C32	-2.41	115.22	119.01
15	AL	101	CRT	C16-C17-C19	-2.41	115.22	119.01
9	AI	102	BCL	C3D-C2D-C1D	-2.41	102.54	105.83
9	w	101	BCL	C16-C15-C13	-2.41	107.96	115.97
15	9	101	CRT	C4-C5-C6	-2.41	121.53	124.91
9	g	102	BCL	C3D-C2D-C1D	-2.41	102.54	105.83
9	7	102	BCL	CMA-C3A-C2A	-2.41	104.67	113.98
7	o	503	HEM	CHB-C4A-NA	2.41	128.23	123.86
10	L	302	BPH	C4-C3-C5	2.41	119.41	115.23
15	O	101	CRT	C26-C27-C28	-2.41	123.90	127.28
15	7	101	CRT	C21-C20-C19	-2.41	118.60	123.52
9	AF	101	BCL	O2A-CGA-O1A	-2.41	117.61	123.63
9	w	101	BCL	CED-O2D-CGD	-2.40	110.46	115.92
9	AI	102	BCL	CMB-C2B-C3B	2.40	133.25	125.67
9	F	101	BCL	C11-C12-C13	-2.40	107.97	115.97
9	V	102	BCL	CMB-C2B-C3B	2.40	133.24	125.67
9	G	102	BCL	C7-C6-C5	-2.40	106.86	113.26
15	E	101	CRT	C18-C17-C16	2.40	121.75	118.09
9	G	102	BCL	CBB-CAB-C3B	2.40	125.46	120.40
9	G	102	BCL	C3B-C4B-NB	-2.40	106.59	109.76
9	AC	103	BCL	C11-C10-C8	-2.40	108.00	115.97
9	z	102	BCL	C1-O2A-CGA	2.40	122.45	116.65
9	L	301	BCL	C1C-NC-C4C	-2.40	105.59	106.68
9	AC	102	BCL	C11-C10-C8	-2.40	108.00	115.97
9	U	101	BCL	CHC-C1C-NC	2.40	127.86	124.40
15	v	101	CRT	C27-C26-C25	-2.40	116.26	123.20
9	L	301	BCL	CHB-C1B-NB	2.39	127.64	124.05
15	s	101	CRT	C21-C22-C23	-2.39	123.92	127.28
9	p	102	BCL	C1C-NC-C4C	-2.39	105.59	106.68
9	z	102	BCL	C3C-C4C-CHD	-2.39	118.35	123.39
15	M	405	CRT	C18-C17-C16	2.39	121.74	118.09
7	o	503	HEM	O2D-CGD-CBD	2.39	121.56	114.00
7	o	501	HEM	CHB-C1B-NB	2.39	127.33	124.37
15	4	101	CRT	C32-C31-C30	2.39	130.13	123.20
9	D	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
9	y	401	BCL	CMD-C2D-C1D	2.39	128.94	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	y	402	BPH	C6-C5-C3	-2.39	107.64	113.47
9	AG	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
9	G	102	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
7	C	503	HEM	CMC-C2C-C3C	-2.39	122.64	128.43
7	o	503	HEM	CHB-C1B-C2B	-2.39	120.16	126.95
9	9	102	BCL	CMD-C2D-C1D	2.39	128.93	124.73
7	C	501	HEM	CAD-C3D-C4D	2.39	128.86	124.70
9	AE	102	BCL	C3C-C2C-C1C	2.39	105.72	101.87
9	3	101	BCL	CBB-CAB-C3B	2.39	125.43	120.40
9	S	102	BCL	C16-C15-C13	-2.39	108.04	115.97
15	R	101	CRT	C26-C27-C28	-2.39	123.93	127.28
9	i	102	BCL	C2B-C1B-NB	-2.38	107.85	110.33
15	g	101	CRT	C31-C30-C28	2.38	132.90	126.36
9	A	103	BCL	C12-C11-C10	-2.38	102.60	113.28
9	u	101	BCL	O2A-CGA-O1A	-2.38	117.67	123.63
14	y	403	MQ8	C5-C4-C3	2.38	122.63	118.27
9	j	101	BCL	CHB-C4A-NA	-2.38	120.96	124.40
9	j	101	BCL	C4A-NA-C1A	2.38	107.77	106.68
9	S	102	BCL	CMA-C3A-C2A	-2.38	104.78	113.98
15	O	101	CRT	C18-C17-C16	2.38	121.72	118.09
9	4	102	BCL	C11-C10-C8	-2.38	108.06	115.97
9	G	102	BCL	C4A-NA-C1A	2.38	107.76	106.68
15	i	101	CRT	C8-C7-C6	2.38	121.72	118.09
9	AC	103	BCL	CHB-C1B-NB	2.38	127.61	124.05
7	o	504	HEM	C4C-NC-C1C	2.37	109.69	105.82
9	K	101	BCL	C3B-C4B-NB	-2.37	106.63	109.76
15	m	104	CRT	C36-C35-C33	-2.37	122.31	125.89
9	N	101	BCL	O2A-C1-C2	2.37	117.24	108.11
9	W	101	BCL	C7-C6-C5	-2.37	106.94	113.26
9	W	101	BCL	CHB-C1B-NB	2.37	127.61	124.05
9	X	102	BCL	CMA-C3A-C2A	-2.37	104.82	113.98
9	L	301	BCL	C4D-CHA-C1A	2.37	124.07	121.24
15	G	101	CRT	C36-C35-C33	-2.37	122.31	125.89
15	AF	102	CRT	C5-C6-C7	-2.37	122.31	125.89
9	m	103	BCL	C2B-C1B-NB	-2.37	107.87	110.33
9	e	102	BCL	CHD-C1D-ND	-2.37	121.47	124.80
9	q	102	BCL	C3B-C4B-NB	-2.37	106.64	109.76
9	L	303	BCL	OBD-CAD-C3D	2.37	133.94	128.42
9	i	102	BCL	CHD-C1D-ND	-2.37	121.47	124.80
9	z	102	BCL	C11-C12-C13	-2.36	108.11	115.97
9	T	102	BCL	CHB-C4A-NA	-2.36	120.99	124.40
9	1	101	BCL	CAA-CBA-CGA	-2.36	106.50	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	q	101	CRT	C29-C28-C30	2.36	121.70	118.09
9	8	101	BCL	C3C-C2C-C1C	2.36	105.68	101.87
7	o	502	HEM	C4C-CHD-C1D	-2.36	121.00	126.02
9	0	102	BCL	C16-C15-C13	-2.36	108.12	115.97
9	R	102	BCL	CMA-C3A-C4A	-2.36	105.43	111.77
9	AC	102	BCL	CMA-C3A-C4A	-2.36	105.43	111.77
9	y	401	BCL	C3C-C4C-CHD	-2.36	118.42	123.39
9	AI	101	BCL	CHD-C1D-ND	-2.36	121.48	124.80
15	T	101	CRT	C36-C35-C33	2.36	129.46	125.89
9	p	102	BCL	C3D-C2D-C1D	-2.36	102.61	105.83
10	M	403	BPH	O2A-CGA-CBA	2.36	119.02	111.83
9	5	101	BCL	CHC-C1C-NC	2.36	127.80	124.40
9	u	101	BCL	C12-C11-C10	-2.36	102.72	113.28
15	k	101	CRT	C13-C12-C11	2.36	121.69	118.09
9	AI	101	BCL	C11-C12-C13	-2.35	108.14	115.97
9	R	102	BCL	CMD-C2D-C1D	2.35	128.87	124.73
9	d	101	BCL	CMC-C2C-C3C	-2.35	104.89	113.98
7	C	503	HEM	CHB-C1B-C2B	-2.35	120.27	126.95
9	P	101	BCL	C2A-C1A-CHA	2.35	127.95	123.87
9	c	101	BCL	C11-C12-C13	-2.35	108.15	115.97
9	N	101	BCL	C4A-NA-C1A	2.35	107.75	106.68
12	M	407	PEF	O2P-P-O1P	2.35	123.37	112.44
9	m	103	BCL	C2A-C1A-CHA	2.35	127.94	123.87
15	9	101	CRT	C30-C28-C27	-2.35	115.31	119.01
7	C	503	HEM	C3B-C2B-C1B	2.35	108.17	106.41
9	l	101	BCL	C3B-C4B-NB	-2.35	106.66	109.76
9	AC	102	BCL	C1-O2A-CGA	2.35	122.33	116.65
9	W	101	BCL	C12-C11-C10	-2.35	102.77	113.28
9	c	101	BCL	CMC-C2C-C3C	-2.35	104.92	113.98
9	h	101	BCL	O2A-CGA-O1A	-2.34	117.76	123.63
9	u	101	BCL	C3D-C2D-C1D	-2.34	102.63	105.83
9	w	101	BCL	CMD-C2D-C1D	2.34	128.85	124.73
9	Y	101	BCL	C16-C15-C13	-2.34	108.18	115.97
9	K	101	BCL	C11-C10-C8	-2.34	108.18	115.97
9	T	102	BCL	O2A-CGA-O1A	-2.34	117.77	123.63
9	K	101	BCL	CGD-CBD-CAD	-2.34	103.27	110.85
15	s	101	CRT	C14-C15-C16	-2.34	116.42	123.20
9	6	101	BCL	C1C-NC-C4C	-2.34	105.61	106.68
9	AG	101	BCL	C12-C11-C10	-2.34	102.79	113.28
15	e	101	CRT	C29-C28-C30	2.34	121.66	118.09
15	m	104	CRT	C20-C19-C17	-2.34	124.00	127.28
9	I	103	BCL	C16-C15-C13	-2.34	108.19	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	101	BCL	C2A-C1A-CHA	2.34	127.93	123.87
9	L	301	BCL	CMC-C2C-C3C	-2.34	104.94	113.98
15	m	104	CRT	C32-C31-C30	-2.34	116.43	123.20
15	k	101	CRT	C32-C31-C30	-2.34	116.43	123.20
15	E	101	CRT	C34-C33-C35	2.34	121.66	118.09
9	Y	101	BCL	C6-C5-C3	-2.34	107.78	113.47
9	z	102	BCL	C3B-C4B-NB	-2.34	106.68	109.76
9	AL	102	BCL	CAC-C3C-C4C	2.34	117.77	112.58
15	e	101	CRT	C9-C10-C11	-2.33	116.44	123.20
9	x	305	BCL	CHD-C1D-ND	-2.33	121.52	124.80
9	Z	102	BCL	O2A-CGA-O1A	-2.33	117.79	123.63
15	I	102	CRT	C15-C16-C17	-2.33	119.97	126.36
15	G	101	CRT	C14-C15-C16	-2.33	116.44	123.20
9	3	101	BCL	C3C-C2C-C1C	2.33	105.63	101.87
9	w	101	BCL	CAA-CBA-CGA	-2.33	106.60	113.21
10	L	302	BPH	CBC-CAC-C3C	-2.33	109.20	113.78
9	2	102	BCL	CMC-C2C-C3C	-2.33	104.99	113.98
9	T	102	BCL	C11-C12-C13	-2.32	108.24	115.97
7	o	501	HEM	CAD-C3D-C4D	2.32	128.75	124.70
9	m	102	BCL	CMA-C3A-C4A	-2.32	105.53	111.77
12	y	407	PEF	C3-O3-C30	2.32	122.81	117.08
9	V	102	BCL	CBB-CAB-C3B	2.32	125.30	120.40
15	0	101	CRT	C1-C4-C5	2.32	119.01	112.98
9	z	102	BCL	C2B-C1B-NB	-2.32	107.92	110.33
9	I	103	BCL	CMB-C2B-C3B	2.32	132.99	125.67
9	AF	101	BCL	CMC-C2C-C3C	-2.32	105.01	113.98
9	c	101	BCL	C11-C10-C8	-2.32	108.25	115.97
9	O	102	BCL	CMB-C2B-C3B	2.32	132.99	125.67
15	AF	102	CRT	C24-C23-C22	-2.32	119.06	122.82
9	u	102	BCL	CMB-C2B-C3B	2.32	132.99	125.67
15	4	101	CRT	C31-C30-C28	2.32	132.72	126.36
9	x	303	BCL	C4A-NA-C1A	2.32	107.74	106.68
9	AI	101	BCL	CMB-C2B-C3B	2.32	132.98	125.67
9	y	401	BCL	CHB-C1B-NB	2.32	127.53	124.05
9	AK	101	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
15	T	101	CRT	C9-C10-C11	-2.32	116.48	123.20
9	A	103	BCL	CHB-C4A-NA	-2.32	121.05	124.40
9	u	101	BCL	C16-C15-C13	-2.32	108.26	115.97
9	T	102	BCL	C2A-C1A-CHA	2.32	127.89	123.87
9	x	305	BCL	CHC-C1C-NC	2.32	127.74	124.40
9	AI	101	BCL	C6-C5-C3	-2.32	107.83	113.47
9	I	103	BCL	C3C-C2C-C1C	2.32	105.61	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	w	101	BCL	C2A-C1A-CHA	2.32	127.89	123.87
9	q	102	BCL	C2B-C1B-NB	-2.32	107.92	110.33
9	AL	102	BCL	CHD-C1D-ND	-2.31	121.55	124.80
15	M	405	CRT	C26-C27-C28	-2.31	124.03	127.28
9	8	101	BCL	CAA-CBA-CGA	-2.31	106.64	113.21
9	j	101	BCL	C7-C6-C5	-2.31	107.10	113.26
9	6	101	BCL	C10-C8-C7	-2.31	100.35	112.07
9	N	101	BCL	CMB-C2B-C3B	2.31	132.96	125.67
10	L	302	BPH	OBB-CAB-C3B	2.31	123.86	119.99
9	i	102	BCL	CED-O2D-CGD	-2.31	110.67	115.92
7	C	503	HEM	O2A-CGA-CBA	2.31	121.30	114.00
9	l	101	BCL	C11-C12-C13	-2.31	108.29	115.97
9	k	102	BCL	C12-C11-C10	-2.31	102.94	113.28
9	s	102	BCL	CHB-C4A-NA	-2.31	121.07	124.40
9	0	102	BCL	C1-C2-C3	-2.31	122.42	126.20
15	O	101	CRT	C15-C16-C17	-2.31	120.04	126.36
9	AG	101	BCL	O2A-CGA-O1A	-2.31	117.86	123.63
15	s	101	CRT	C31-C32-C33	-2.31	124.04	127.28
7	o	502	HEM	CAC-C3C-C4C	-2.30	119.32	124.82
15	i	101	CRT	C13-C12-C11	2.30	121.61	118.09
9	U	101	BCL	C3B-C4B-NB	-2.30	106.72	109.76
9	Z	102	BCL	C3C-C2C-C1C	2.30	105.59	101.87
7	C	504	HEM	C4C-NC-C1C	2.30	109.57	105.82
15	m	104	CRT	C8-C7-C6	2.30	121.60	118.09
9	4	102	BCL	O2A-CGA-O1A	-2.30	117.88	123.63
9	AH	101	BCL	C11-C10-C8	-2.30	108.32	115.97
15	y	404	CRT	C14-C15-C16	-2.30	116.54	123.20
9	Y	101	BCL	CBB-CAB-C3B	2.30	125.25	120.40
15	9	101	CRT	C18-C17-C19	-2.30	119.09	122.82
9	9	102	BCL	CBB-CAB-C3B	2.30	125.25	120.40
9	P	101	BCL	C2B-C1B-NB	-2.30	107.94	110.33
11	x	304	UQ8	C25-C24-C26	2.30	119.21	115.23
15	7	101	CRT	C8-C7-C9	-2.30	119.10	122.82
15	AD	101	CRT	C13-C12-C14	-2.29	119.10	122.82
9	r	101	BCL	CMD-C2D-C1D	2.29	128.77	124.73
9	s	102	BCL	C11-C12-C13	-2.29	108.34	115.97
9	2	102	BCL	C3C-C2C-C1C	2.29	105.57	101.87
15	AL	101	CRT	C24-C23-C22	-2.29	119.10	122.82
9	S	102	BCL	O2A-CGA-CBA	2.29	118.82	111.83
9	h	101	BCL	C7-C6-C5	-2.29	107.15	113.26
9	AG	101	BCL	C1-O2A-CGA	2.29	122.20	116.65
15	AJ	101	CRT	C13-C12-C14	-2.29	119.10	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	101	BCL	CMC-C2C-C3C	-2.29	105.12	113.98
15	z	101	CRT	C36-C35-C33	-2.29	122.43	125.89
15	Z	101	CRT	C14-C15-C16	-2.29	116.56	123.20
9	w	101	BCL	O2A-CGA-O1A	-2.29	117.90	123.63
9	AK	101	BCL	CGD-CBD-CAD	-2.29	103.44	110.85
9	AB	102	BCL	C6-C5-C3	-2.29	107.89	113.47
9	i	102	BCL	CHB-C4A-NA	-2.29	121.10	124.40
9	AF	101	BCL	C3C-C2C-C1C	2.29	105.56	101.87
15	7	101	CRT	C24-C23-C25	2.29	121.58	118.09
9	r	101	BCL	C3D-C2D-C1D	-2.29	102.71	105.83
9	A	103	BCL	CBB-CAB-C3B	2.29	125.22	120.40
9	N	101	BCL	C1-O2A-CGA	2.29	122.18	116.65
9	g	102	BCL	CMC-C2C-C3C	-2.29	105.15	113.98
15	O	101	CRT	C27-C26-C25	-2.29	116.58	123.20
15	R	101	CRT	C16-C17-C19	-2.28	115.42	119.01
9	K	101	BCL	C11-C12-C13	-2.28	108.37	115.97
9	M	401	BCL	CHB-C1B-NB	2.28	127.47	124.05
15	E	101	CRT	C14-C15-C16	-2.28	116.59	123.20
15	AF	102	CRT	C27-C26-C25	-2.28	116.59	123.20
9	W	101	BCL	C1-O2A-CGA	2.28	122.17	116.65
9	M	402	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
11	L	304	UQ8	C12-C13-C14	-2.28	122.41	127.62
9	6	101	BCL	CHB-C1B-NB	2.28	127.47	124.05
9	G	102	BCL	CMB-C2B-C3B	2.28	132.86	125.67
9	r	101	BCL	C1-O2A-CGA	2.28	122.17	116.65
9	u	101	BCL	CHC-C1C-NC	2.28	127.69	124.40
9	A	102	BCL	CHD-C1D-ND	-2.28	121.60	124.80
9	R	102	BCL	C3C-C4C-CHD	-2.28	118.59	123.39
14	y	403	MQ8	C26-C25-C23	-2.28	105.64	113.19
15	0	101	CRT	C31-C32-C33	-2.28	124.09	127.28
9	c	101	BCL	O2A-C1-C2	2.28	116.86	108.11
9	u	102	BCL	C7-C6-C5	-2.27	107.20	113.26
9	P	101	BCL	CHC-C1C-NC	2.27	127.68	124.40
9	U	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
15	I	102	CRT	C34-C33-C35	2.27	121.56	118.09
15	AD	101	CRT	C14-C15-C16	2.27	129.78	123.20
10	y	402	BPH	O2D-CGD-O1D	-2.27	119.43	123.85
15	s	101	CRT	C13-C12-C11	2.27	121.56	118.09
9	G	102	BCL	CED-O2D-CGD	-2.27	110.76	115.92
14	M	404	MQ8	C20-C18-C17	-2.27	116.07	121.17
9	X	102	BCL	O2A-C1-C2	2.27	116.85	108.11
14	M	404	MQ8	C39-C38-C37	-2.27	117.80	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AI	101	BCL	C3D-C2D-C1D	-2.27	102.73	105.83
9	k	102	BCL	C11-C10-C8	-2.27	108.42	115.97
9	Y	101	BCL	C3D-C2D-C1D	-2.27	102.73	105.83
9	P	101	BCL	C11-C10-C8	-2.27	108.43	115.97
9	L	303	BCL	C1D-CHD-C4C	-2.27	121.16	126.62
15	AF	102	CRT	C8-C7-C9	-2.26	119.15	122.82
9	x	301	BCL	C2A-C1A-CHA	2.26	127.80	123.87
9	Z	102	BCL	C11-C12-C13	-2.26	108.44	115.97
15	E	101	CRT	C13-C12-C11	2.26	121.55	118.09
15	v	101	CRT	C13-C12-C11	2.26	121.55	118.09
9	AB	102	BCL	CED-O2D-CGD	-2.26	110.78	115.92
15	s	101	CRT	C8-C7-C6	2.26	121.54	118.09
9	L	303	BCL	C2D-C1D-ND	2.26	112.36	110.13
15	k	101	CRT	C9-C10-C11	-2.26	116.65	123.20
9	m	103	BCL	C7-C6-C5	-2.26	107.24	113.26
9	x	301	BCL	O2A-CGA-O1A	-2.26	117.98	123.63
9	AH	101	BCL	CMB-C2B-C3B	2.26	132.79	125.67
9	AC	102	BCL	C2A-C1A-CHA	2.26	127.78	123.87
9	9	102	BCL	C3C-C2C-C1C	2.25	105.51	101.87
15	G	101	CRT	C31-C32-C33	-2.25	124.12	127.28
9	s	102	BCL	C3B-C4B-NB	-2.25	106.78	109.76
9	AI	101	BCL	C4-C3-C5	-2.25	111.32	115.23
15	m	104	CRT	C9-C10-C11	-2.25	116.67	123.20
15	Z	101	CRT	C11-C12-C14	-2.25	115.47	119.01
15	AL	101	CRT	C35-C33-C32	-2.25	115.47	119.01
9	W	101	BCL	C11-C10-C8	-2.25	108.48	115.97
9	0	102	BCL	C11-C10-C8	-2.25	108.48	115.97
9	X	102	BCL	C3C-C4C-CHD	-2.25	118.65	123.39
9	c	101	BCL	C4A-NA-C1A	2.25	107.71	106.68
7	C	502	HEM	C2A-C1A-NA	-2.25	107.66	110.15
9	r	101	BCL	O2A-CGA-O1A	-2.25	118.00	123.63
9	c	101	BCL	C2B-C1B-NB	-2.25	107.99	110.33
9	AI	102	BCL	CMA-C3A-C4A	-2.25	105.73	111.77
9	5	101	BCL	C11-C10-C8	-2.25	108.49	115.97
9	V	102	BCL	C7-C6-C5	-2.25	107.27	113.26
9	8	101	BCL	CMD-C2D-C1D	2.25	128.69	124.73
9	q	102	BCL	C11-C12-C13	-2.25	108.50	115.97
9	3	101	BCL	C2B-C1B-NB	-2.25	108.00	110.33
15	7	101	CRT	C31-C32-C33	2.25	130.43	127.28
9	m	103	BCL	C3D-C2D-C1D	-2.25	102.77	105.83
9	Z	102	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
9	R	102	BCL	C2C-C3C-C4C	-2.25	97.98	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	102	BCL	CMA-C3A-C4A	-2.25	105.74	111.77
15	AC	101	CRT	C8-C7-C6	2.25	121.52	118.09
15	e	101	CRT	C30-C28-C27	-2.24	115.48	119.01
15	0	101	CRT	C24-C23-C25	2.24	121.52	118.09
9	AE	102	BCL	CHC-C1C-NC	2.24	127.64	124.40
9	P	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
15	7	101	CRT	C10-C9-C7	-2.24	124.13	127.28
9	i	102	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
9	m	103	BCL	CMC-C2C-C3C	-2.24	105.31	113.98
9	g	102	BCL	CHC-C1C-NC	2.24	127.64	124.40
9	X	102	BCL	CHD-C1D-ND	-2.24	121.65	124.80
9	R	102	BCL	C16-C15-C13	-2.24	108.51	115.97
9	L	303	BCL	CBB-CAB-C3B	2.24	125.13	120.40
9	x	303	BCL	CHC-C1C-NC	2.24	127.64	124.40
9	e	102	BCL	CMA-C3A-C4A	-2.24	105.75	111.77
9	L	301	BCL	CBC-CAC-C3C	2.24	118.17	113.41
9	D	102	BCL	CHD-C1D-ND	-2.24	121.65	124.80
11	L	304	UQ8	C35-C34-C33	-2.24	117.87	123.63
9	AH	101	BCL	C1C-NC-C4C	-2.24	105.66	106.68
9	2	102	BCL	C7-C6-C5	-2.24	107.29	113.26
9	2	102	BCL	CMD-C2D-C3D	2.24	132.82	127.69
9	1	101	BCL	C7-C6-C5	-2.24	107.30	113.26
9	AC	102	BCL	CED-O2D-CGD	-2.24	110.84	115.92
15	0	101	CRT	C32-C31-C30	-2.24	116.72	123.20
9	z	102	BCL	C3C-C2C-C1C	2.24	105.48	101.87
9	AC	102	BCL	CBB-CAB-C3B	2.24	125.12	120.40
9	z	102	BCL	O2A-CGA-O1A	-2.24	118.04	123.63
7	C	501	HEM	CHB-C4A-NA	2.23	127.91	123.86
9	m	102	BCL	C7-C6-C5	-2.23	107.31	113.26
15	AC	101	CRT	C21-C20-C19	-2.23	118.95	123.52
9	e	102	BCL	CMB-C2B-C3B	2.23	132.71	125.67
9	7	102	BCL	O2A-CGA-O1A	-2.23	118.05	123.63
9	AL	102	BCL	C11-C12-C13	-2.23	108.55	115.97
9	e	102	BCL	O2A-CGA-O1A	-2.23	118.05	123.63
9	6	101	BCL	C12-C11-C10	-2.23	103.28	113.28
11	x	304	UQ8	C30-C29-C28	-2.23	117.90	123.63
15	z	101	CRT	C20-C19-C17	-2.23	124.15	127.28
9	V	102	BCL	C11-C10-C8	-2.23	108.55	115.97
10	x	302	BPH	CBA-CAA-C2A	-2.23	107.21	113.78
11	L	304	UQ8	C10-C9-C11	2.23	119.10	115.23
7	C	502	HEM	CHB-C1B-NB	2.23	127.12	124.37
9	m	102	BCL	CBB-CAB-C3B	2.23	125.10	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AC	103	BCL	C11-C12-C13	-2.23	108.56	115.97
9	7	102	BCL	C3B-C4B-NB	-2.23	106.82	109.76
9	AE	102	BCL	C7-C6-C5	-2.23	107.33	113.26
9	D	102	BCL	CMB-C2B-C3B	2.23	132.69	125.67
10	y	402	BPH	CMC-C2C-C3C	-2.22	105.54	114.13
9	Q	101	BCL	C1-O2A-CGA	2.22	122.03	116.65
9	D	101	BCL	C3C-C4C-CHD	-2.22	118.71	123.39
9	Q	101	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
9	AI	101	BCL	C2B-C1B-NB	-2.22	108.02	110.33
12	H	305	PEF	O3-C3-C2	2.22	114.80	108.40
9	y	401	BCL	C7-C6-C5	-2.22	107.34	113.26
9	AB	101	BCL	C1C-NC-C4C	-2.22	105.67	106.68
9	T	102	BCL	CAA-C2A-C3A	2.22	119.00	113.00
9	AB	102	BCL	CMB-C2B-C3B	2.22	132.67	125.67
15	T	101	CRT	C32-C31-C30	-2.22	116.77	123.20
9	i	102	BCL	C3C-C2C-C1C	2.22	105.45	101.87
9	Q	101	BCL	C3D-C2D-C1D	-2.22	102.81	105.83
9	w	101	BCL	C3C-C4C-CHD	-2.22	118.72	123.39
9	AF	101	BCL	C1-O2A-CGA	2.22	122.02	116.65
9	Z	102	BCL	C3B-C4B-NB	-2.22	106.83	109.76
9	8	101	BCL	C1-C2-C3	2.21	129.83	126.20
9	q	102	BCL	C1C-NC-C4C	-2.21	105.67	106.68
9	AK	101	BCL	C2C-C3C-C4C	-2.21	98.02	101.34
9	z	102	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
9	z	102	BCL	CHB-C1B-NB	2.21	127.37	124.05
9	y	401	BCL	O2A-CGA-CBA	2.21	118.58	111.83
7	C	503	HEM	CHB-C4A-NA	2.21	127.87	123.86
9	K	101	BCL	CMB-C2B-C3B	2.21	132.64	125.67
15	O	101	CRT	C32-C31-C30	-2.21	116.79	123.20
9	x	305	BCL	C11-C12-C13	-2.21	108.62	115.97
9	m	102	BCL	C3C-C4C-CHD	-2.21	118.73	123.39
9	AK	101	BCL	CMB-C2B-C3B	2.21	132.64	125.67
9	c	101	BCL	C3B-C4B-NB	-2.21	106.84	109.76
9	6	101	BCL	C2B-C1B-NB	-2.21	108.03	110.33
7	C	503	HEM	CMD-C2D-C1D	2.21	128.49	125.03
9	m	103	BCL	C16-C15-C13	-2.21	108.63	115.97
12	t	303	PEF	O3-C3-C2	2.21	114.76	108.40
9	k	102	BCL	CBB-CAB-C3B	2.21	125.06	120.40
9	I	103	BCL	C3B-C4B-NB	-2.21	106.85	109.76
9	g	102	BCL	CED-O2D-CGD	-2.21	110.91	115.92
9	y	401	BCL	CHD-C1D-ND	-2.21	121.70	124.80
9	AC	102	BCL	C7-C6-C5	-2.20	107.39	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	x	303	BCL	O2A-CGA-CBA	2.20	118.56	111.83
15	2	101	CRT	C8-C7-C6	2.20	121.45	118.09
9	g	102	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
9	7	102	BCL	C11-C12-C13	-2.20	108.64	115.97
9	AK	101	BCL	CHD-C1D-ND	-2.20	121.70	124.80
9	AI	102	BCL	C12-C11-C10	-2.20	103.41	113.28
15	9	101	CRT	C24-C23-C22	-2.20	119.25	122.82
9	j	101	BCL	CMA-C3A-C2A	-2.20	105.47	113.98
12	y	406	PEF	C3-O3-C30	2.20	122.51	117.08
9	T	102	BCL	CMB-C2B-C3B	2.20	132.61	125.67
9	x	301	BCL	C12-C11-C10	-2.20	103.42	113.28
9	4	102	BCL	C16-C15-C13	-2.20	108.66	115.97
9	L	301	BCL	CHC-C1C-NC	2.20	127.57	124.40
12	y	407	PEF	O2P-P-O1P	2.20	122.66	112.44
9	D	102	BCL	C4A-NA-C1A	2.20	107.68	106.68
12	m	101	PEF	C3-C2-C1	-2.20	106.67	111.78
9	M	401	BCL	C3D-C2D-C1D	-2.20	102.83	105.83
9	w	101	BCL	C1-O2A-CGA	2.20	121.96	116.65
9	1	101	BCL	C3D-C2D-C1D	-2.19	102.84	105.83
9	D	102	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
9	U	101	BCL	CHB-C4A-NA	-2.19	121.23	124.40
9	d	101	BCL	C2A-C1A-CHA	2.19	127.67	123.87
15	E	101	CRT	C29-C28-C30	2.19	121.44	118.09
9	AB	101	BCL	C3C-C4C-CHD	-2.19	118.77	123.39
15	n	101	CRT	C21-C22-C23	-2.19	124.20	127.28
15	g	101	CRT	C13-C12-C11	2.19	121.44	118.09
9	I	101	BCL	C1C-NC-C4C	-2.19	105.68	106.68
15	M	405	CRT	C18-C17-C19	-2.19	119.27	122.82
9	K	101	BCL	CMD-C2D-C1D	2.19	128.59	124.73
9	L	303	BCL	C9-C8-C7	2.19	119.08	111.27
14	y	403	MQ8	C2M-C2-C3	-2.19	120.85	124.45
9	AH	101	BCL	C3D-C2D-C1D	-2.19	102.84	105.83
9	i	102	BCL	CMB-C2B-C3B	2.19	132.57	125.67
9	z	102	BCL	CMD-C2D-C1D	2.19	128.58	124.73
9	8	101	BCL	C3B-C4B-NB	-2.19	106.87	109.76
9	l	101	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
7	C	503	HEM	C4C-CHD-C1D	-2.19	121.37	126.02
15	2	101	CRT	C34-C33-C35	2.19	121.43	118.09
9	s	102	BCL	O2A-C1-C2	2.18	116.52	108.11
15	AL	101	CRT	C20-C21-C22	-2.18	119.05	123.52
9	O	102	BCL	C2A-C1A-CHA	2.18	127.66	123.87
15	2	101	CRT	C20-C21-C22	-2.18	119.05	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	i	101	CRT	C4-C5-C6	-2.18	121.85	124.91
9	X	102	BCL	C2C-C3C-C4C	-2.18	98.07	101.34
7	C	502	HEM	C4C-CHD-C1D	-2.18	121.39	126.02
9	U	101	BCL	C2B-C1B-NB	-2.18	108.06	110.33
9	AH	101	BCL	C12-C11-C10	-2.18	103.51	113.28
9	r	101	BCL	CGD-CBD-CAD	-2.18	103.79	110.85
7	o	504	HEM	O2A-CGA-CBA	2.18	120.88	114.00
9	x	305	BCL	C1C-NC-C4C	-2.18	105.69	106.68
9	I	103	BCL	CMC-C2C-C3C	-2.18	105.56	113.98
7	o	503	HEM	C4C-NC-C1C	2.18	109.37	105.82
9	x	305	BCL	C12-C11-C10	-2.18	103.52	113.28
9	x	305	BCL	CHB-C1B-NB	2.18	127.31	124.05
9	1	101	BCL	C1-O2A-CGA	2.18	121.92	116.65
9	6	101	BCL	C2A-C3A-C4A	-2.18	98.35	101.87
14	M	404	MQ8	C44-C43-C42	-2.18	116.28	121.17
14	y	403	MQ8	C35-C33-C32	-2.18	116.28	121.17
9	F	101	BCL	C3C-C4C-CHD	-2.18	118.81	123.39
12	y	408	PEF	P-O4P-C4	-2.18	110.91	121.26
9	I	103	BCL	C2A-C1A-CHA	2.17	127.64	123.87
7	o	504	HEM	CAA-C2A-C1A	2.17	129.19	124.94
9	m	103	BCL	C3C-C4C-CHD	-2.17	118.81	123.39
15	g	101	CRT	C30-C28-C27	-2.17	115.59	119.01
9	m	103	BCL	C1C-NC-C4C	-2.17	105.69	106.68
9	L	301	BCL	CMB-C2B-C3B	2.17	132.52	125.67
9	AF	101	BCL	CMC-C2C-C1C	-2.17	105.94	111.77
7	o	502	HEM	C2B-C1B-NB	-2.17	107.34	109.84
7	o	502	HEM	CHB-C4A-NA	2.17	127.80	123.86
9	AG	101	BCL	O2A-C1-C2	2.17	116.46	108.11
9	7	102	BCL	CHC-C1C-NC	2.17	127.53	124.40
12	H	301	PEF	O2P-P-O1P	2.17	122.53	112.44
15	v	101	CRT	C14-C15-C16	-2.17	116.92	123.20
9	r	101	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
9	q	102	BCL	C12-C11-C10	-2.17	103.57	113.28
15	n	101	CRT	C25-C23-C22	-2.17	115.60	119.01
9	AB	102	BCL	CMA-C3A-C4A	-2.17	105.95	111.77
9	k	102	BCL	CHB-C4A-NA	-2.17	121.27	124.40
9	1	101	BCL	CMB-C2B-C3B	2.17	132.50	125.67
9	I	101	BCL	C11-C12-C13	-2.17	108.77	115.97
15	G	101	CRT	C26-C27-C28	-2.16	124.24	127.28
15	s	101	CRT	C36-C35-C33	2.16	129.16	125.89
7	C	502	HEM	C4A-NA-C1A	2.16	109.35	105.82
9	W	101	BCL	C2A-C1A-CHA	2.16	127.62	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AI	102	BCL	C10-C8-C7	-2.16	101.11	112.07
9	X	102	BCL	CMD-C2D-C3D	2.16	132.65	127.69
9	F	101	BCL	CMB-C2B-C3B	2.16	132.49	125.67
15	2	101	CRT	C35-C33-C32	-2.16	115.61	119.01
9	W	101	BCL	CMA-C3A-C4A	-2.16	105.97	111.77
9	w	101	BCL	CHC-C1C-NC	2.16	127.52	124.40
9	k	102	BCL	CMB-C2B-C3B	2.16	132.48	125.67
9	y	401	BCL	C3D-C2D-C1D	-2.16	102.89	105.83
9	u	102	BCL	C16-C15-C13	-2.16	108.79	115.97
15	Z	101	CRT	C20-C21-C22	-2.16	119.11	123.52
9	u	102	BCL	CMD-C2D-C3D	2.16	132.63	127.69
9	c	101	BCL	CMD-C2D-C1D	2.16	128.52	124.73
9	AI	101	BCL	C7-C6-C5	-2.15	107.52	113.26
9	u	101	BCL	C2B-C1B-NB	-2.15	108.09	110.33
9	O	102	BCL	C12-C11-C10	-2.15	103.63	113.28
9	AF	101	BCL	C3B-C4B-NB	-2.15	106.92	109.76
9	c	101	BCL	CMB-C2B-C3B	2.15	132.46	125.67
9	A	102	BCL	CMB-C2B-C3B	2.15	132.46	125.67
9	d	101	BCL	CMB-C2B-C3B	2.15	132.45	125.67
9	I	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
15	0	101	CRT	O1-C1-C2	2.15	123.75	108.97
9	j	101	BCL	C16-C15-C13	-2.15	108.83	115.97
15	e	101	CRT	C5-C6-C7	-2.15	122.65	125.89
9	7	102	BCL	O2A-C1-C2	2.15	116.37	108.11
7	o	501	HEM	O2D-CGD-CBD	2.15	120.78	114.00
9	M	402	BCL	C12-C11-C10	-2.15	103.66	113.28
9	M	402	BCL	C5-C3-C2	2.14	125.98	121.17
12	M	408	PEF	C2-O2-C10	-2.14	114.06	117.85
15	y	404	CRT	O1-C1-C3	2.14	123.71	108.97
9	AE	102	BCL	C11-C10-C8	-2.14	108.85	115.97
9	m	102	BCL	C2A-C1A-CHA	2.14	127.58	123.87
15	q	101	CRT	C18-C17-C16	2.14	121.36	118.09
9	l	101	BCL	CMB-C2B-C3B	2.14	132.42	125.67
15	7	103	CRT	C5-C6-C7	-2.14	122.66	125.89
9	i	102	BCL	CHC-C1C-NC	2.14	127.49	124.40
9	q	102	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
9	k	102	BCL	C4D-CHA-C1A	2.14	123.79	121.24
7	C	504	HEM	CAD-C3D-C4D	2.14	128.42	124.70
9	M	401	BCL	C3B-C4B-NB	-2.14	106.94	109.76
15	AC	101	CRT	C6-C7-C9	-2.14	115.65	119.01
9	AI	101	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
9	A	103	BCL	CHC-C1C-NC	2.14	127.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	102	BCL	C2B-C1B-NB	-2.13	108.11	110.33
15	e	101	CRT	C26-C25-C23	-2.13	120.52	126.36
9	R	102	BCL	C1C-NC-C4C	-2.13	105.71	106.68
9	AC	102	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
9	r	101	BCL	CMA-C3A-C4A	-2.13	106.05	111.77
7	C	502	HEM	CHB-C4A-NA	2.13	127.72	123.86
7	C	504	HEM	O2D-CGD-CBD	2.13	120.72	114.00
9	AF	101	BCL	C11-C10-C8	-2.13	108.89	115.97
15	M	405	CRT	C36-C35-C33	-2.13	122.68	125.89
9	V	102	BCL	C3C-C4C-CHD	-2.13	118.91	123.39
9	5	101	BCL	CMA-C3A-C4A	-2.12	106.06	111.77
10	x	302	BPH	C11-C12-C13	-2.12	108.90	115.97
9	O	102	BCL	O2A-C1-C2	2.12	116.28	108.11
9	i	102	BCL	C3C-C4C-CHD	-2.12	118.92	123.39
9	K	101	BCL	CED-O2D-CGD	-2.12	111.10	115.92
14	y	403	MQ8	O4-C4-C3	-2.12	117.26	120.67
9	I	101	BCL	O2A-CGA-CBA	2.12	118.31	111.83
9	s	102	BCL	C3C-C2C-C1C	2.12	105.30	101.87
9	j	101	BCL	CAA-C2A-C3A	2.12	118.73	113.00
9	N	101	BCL	CMD-C2D-C1D	2.12	128.46	124.73
9	i	102	BCL	CMA-C3A-C2A	-2.12	105.78	113.98
9	D	102	BCL	C1-O2A-CGA	2.12	121.78	116.65
9	h	101	BCL	CHB-C1B-NB	2.12	127.23	124.05
15	4	101	CRT	C14-C15-C16	-2.12	117.06	123.20
9	M	402	BCL	C6-C5-C3	-2.12	108.31	113.47
9	AB	102	BCL	C11-C12-C13	-2.12	108.93	115.97
9	2	102	BCL	C11-C10-C8	-2.12	108.93	115.97
11	L	304	UQ8	O4-C4-C5	2.12	123.78	116.64
9	i	102	BCL	CAA-C2A-C3A	2.12	118.72	113.00
9	0	102	BCL	C4A-NA-C1A	2.12	107.64	106.68
15	0	101	CRT	C10-C9-C7	-2.11	124.31	127.28
15	P	102	CRT	C18-C17-C16	2.11	121.32	118.09
9	e	102	BCL	C12-C11-C10	-2.11	103.81	113.28
9	D	102	BCL	O2A-CGA-O1A	-2.11	118.34	123.63
9	AC	102	BCL	C12-C11-C10	-2.11	103.81	113.28
9	M	401	BCL	C1C-NC-C4C	-2.11	105.72	106.68
9	U	101	BCL	CMB-C2B-C3B	2.11	132.33	125.67
9	F	101	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
9	AL	102	BCL	CMD-C2D-C1D	2.11	128.45	124.73
15	AH	102	CRT	C8-C7-C6	2.11	121.31	118.09
9	AC	102	BCL	O2A-CGA-O1A	-2.11	118.35	123.63
9	AE	102	BCL	CMB-C2B-C3B	2.11	132.33	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AB	102	BCL	C7-C6-C5	-2.11	107.64	113.26
9	y	401	BCL	OBD-CAD-C3D	2.11	133.35	128.42
9	g	102	BCL	CMB-C2B-C3B	2.11	132.32	125.67
9	f	101	BCL	C3C-C2C-C1C	2.11	105.28	101.87
15	i	101	CRT	C5-C6-C7	-2.11	122.71	125.89
9	d	101	BCL	C2B-C1B-NB	-2.11	108.14	110.33
9	S	102	BCL	C11-C12-C13	-2.11	108.96	115.97
10	y	402	BPH	O1D-CGD-CBD	-2.11	121.53	124.72
9	I	103	BCL	C12-C11-C10	-2.11	103.83	113.28
9	U	101	BCL	C12-C11-C10	-2.11	103.84	113.28
9	i	102	BCL	O2A-CGA-O1A	-2.11	118.36	123.63
15	AC	101	CRT	C26-C25-C23	-2.11	120.59	126.36
9	AL	102	BCL	CMB-C2B-C3B	2.11	132.31	125.67
9	4	102	BCL	CMD-C2D-C1D	2.11	128.44	124.73
15	4	101	CRT	C13-C12-C11	2.10	121.30	118.09
9	x	305	BCL	OBB-CAB-CBB	-2.10	115.06	119.77
9	AL	102	BCL	C12-C11-C10	-2.10	103.85	113.28
9	u	102	BCL	C2C-C3C-C4C	-2.10	98.19	101.34
15	P	102	CRT	C30-C28-C27	-2.10	115.70	119.01
7	C	503	HEM	CMC-C2C-C1C	2.10	128.43	124.73
10	x	302	BPH	C6-C5-C3	-2.10	108.36	113.47
15	O	101	CRT	C34-C33-C35	2.10	121.29	118.09
9	4	102	BCL	CMA-C3A-C2A	-2.10	105.87	113.98
9	7	102	BCL	CHB-C1B-NB	2.10	127.20	124.05
9	2	102	BCL	C1-C2-C3	-2.10	122.76	126.20
9	AI	101	BCL	C4A-NA-C1A	2.10	107.64	106.68
15	AD	101	CRT	C29-C28-C30	2.10	121.29	118.09
9	AE	102	BCL	CED-O2D-CGD	-2.10	111.16	115.92
10	L	302	BPH	O2D-CGD-O1D	-2.10	119.77	123.85
9	L	301	BCL	O2A-C1-C2	2.10	116.18	108.11
9	N	101	BCL	C2B-C1B-NB	-2.10	108.15	110.33
15	4	101	CRT	C20-C19-C17	2.10	130.22	127.28
9	G	102	BCL	O2A-CGA-O1A	-2.10	118.39	123.63
14	y	403	MQ8	C24-C23-C25	2.10	118.87	115.23
14	y	403	MQ8	C45-C43-C44	2.10	118.86	115.23
9	Y	101	BCL	CHB-C1B-NB	2.10	127.19	124.05
9	x	301	BCL	OBD-CAD-C3D	2.10	133.31	128.42
14	y	403	MQ8	C50-C48-C49	2.10	119.41	114.59
9	AB	101	BCL	CMB-C2B-C3B	2.09	132.27	125.67
7	C	503	HEM	CHA-C1A-NA	2.09	127.66	123.86
15	n	101	CRT	C32-C31-C30	-2.09	117.13	123.20
9	AG	101	BCL	C10-C8-C7	-2.09	101.46	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AH	101	BCL	C2B-C1B-NB	-2.09	108.16	110.33
9	AF	101	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
9	d	101	BCL	C11-C10-C8	-2.09	109.01	115.97
9	0	102	BCL	CMB-C2B-C3B	2.09	132.27	125.67
9	M	402	BCL	CGD-CBD-CAD	-2.09	104.07	110.85
9	V	102	BCL	CMD-C2D-C1D	2.09	128.41	124.73
7	o	501	HEM	CHA-C4D-ND	2.09	126.95	124.37
9	h	101	BCL	C1C-NC-C4C	-2.09	105.72	106.68
9	h	101	BCL	O2A-CGA-CBA	2.09	118.21	111.83
7	C	504	HEM	CHB-C1B-C2B	-2.09	121.01	126.95
9	x	301	BCL	C10-C8-C7	-2.09	101.48	112.07
9	x	303	BCL	CHD-C1D-ND	-2.09	121.86	124.80
9	k	102	BCL	CMA-C3A-C4A	-2.09	106.16	111.77
9	d	101	BCL	O2A-CGA-CBA	2.09	118.21	111.83
9	AB	101	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
9	Z	102	BCL	C6-C5-C3	-2.09	108.38	113.47
9	L	303	BCL	C14-C13-C12	-2.09	103.84	111.27
9	L	301	BCL	C1-O2A-CGA	2.09	121.70	116.65
9	A	103	BCL	CMB-C2B-C3B	2.09	132.25	125.67
9	d	101	BCL	C14-C13-C12	-2.09	103.84	111.27
9	q	102	BCL	C1-O2A-CGA	2.09	121.70	116.65
9	s	102	BCL	C7-C6-C5	-2.08	107.71	113.26
9	u	102	BCL	CHC-C1C-NC	2.08	127.41	124.40
9	m	103	BCL	CMB-C2B-C3B	2.08	132.24	125.67
9	D	102	BCL	C11-C10-C8	-2.08	109.04	115.97
9	AE	102	BCL	C2B-C1B-NB	-2.08	108.17	110.33
7	C	501	HEM	C4A-CHB-C1B	-2.08	121.35	126.25
11	x	304	UQ8	C25-C24-C23	-2.08	118.28	123.63
9	Y	101	BCL	CHC-C1C-NC	2.08	127.40	124.40
7	o	501	HEM	CHC-C1C-NC	2.08	126.72	124.45
9	AK	101	BCL	C7-C6-C5	-2.08	107.72	113.26
9	g	102	BCL	CMA-C3A-C2A	-2.08	105.95	113.98
9	x	305	BCL	O2A-CGA-CBA	2.08	118.17	111.83
15	n	101	CRT	C11-C12-C14	2.08	122.28	119.01
7	C	502	HEM	CHD-C4C-C3C	-2.08	121.71	125.21
9	AB	102	BCL	C16-C15-C13	-2.08	109.06	115.97
9	p	102	BCL	CMB-C2B-C3B	2.08	132.22	125.67
15	m	104	CRT	C34-C33-C35	2.08	121.26	118.09
9	P	101	BCL	C3C-C4C-CHD	-2.07	119.02	123.39
9	AC	103	BCL	C3C-C2C-C1C	2.07	105.22	101.87
15	M	405	CRT	C21-C20-C19	-2.07	119.28	123.52
15	n	101	CRT	C35-C33-C32	-2.07	115.75	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AH	101	BCL	O2A-CGA-CBA	2.07	118.16	111.83
9	2	102	BCL	CED-O2D-CGD	-2.07	111.21	115.92
10	x	302	BPH	C11-C10-C8	-2.07	109.08	115.97
9	m	103	BCL	C2A-C3A-C4A	-2.07	98.52	101.87
9	A	103	BCL	C7-C6-C5	-2.07	107.74	113.26
15	O	101	CRT	C14-C15-C16	-2.07	117.20	123.20
15	AF	102	CRT	C4-C5-C6	-2.07	122.00	124.91
15	AH	102	CRT	C15-C14-C12	-2.07	124.37	127.28
15	7	103	CRT	C4-C5-C6	-2.07	122.01	124.91
9	d	101	BCL	C2C-C3C-C4C	-2.07	98.24	101.34
9	p	102	BCL	C6-C5-C3	-2.07	108.43	113.47
9	x	305	BCL	C11-C10-C8	-2.07	109.09	115.97
15	0	101	CRT	C26-C27-C28	-2.07	124.38	127.28
15	y	404	CRT	C31-C30-C28	-2.07	120.70	126.36
7	o	504	HEM	CHA-C4D-ND	2.06	126.92	124.37
9	U	101	BCL	C11-C10-C8	-2.06	109.10	115.97
9	D	102	BCL	OBD-CAD-C3D	2.06	133.24	128.42
9	6	101	BCL	C3B-C4B-NB	-2.06	107.04	109.76
14	y	403	MQ8	C5-C10-C1	-2.06	118.50	120.71
9	AK	101	BCL	C16-C15-C13	-2.06	109.11	115.97
15	R	101	CRT	C35-C33-C32	-2.06	115.77	119.01
7	o	504	HEM	CHC-C4B-NB	2.06	126.64	124.42
9	O	102	BCL	CAA-C2A-C3A	2.06	118.57	113.00
9	I	103	BCL	C3C-C4C-CHD	-2.06	119.05	123.39
9	L	301	BCL	C3D-C2D-C1D	-2.06	103.02	105.83
9	G	102	BCL	C1D-CHD-C4C	-2.06	121.66	126.62
9	D	102	BCL	C12-C11-C10	-2.06	104.06	113.28
15	9	101	CRT	C9-C10-C11	2.06	129.16	123.20
9	V	102	BCL	C2B-C1B-NB	-2.06	108.19	110.33
9	5	101	BCL	C3B-C4B-NB	-2.06	107.05	109.76
9	s	102	BCL	CED-O2D-CGD	-2.06	111.25	115.92
9	L	303	BCL	C11-C10-C8	-2.05	109.14	115.97
9	6	101	BCL	CED-O2D-CGD	-2.05	111.26	115.92
9	AC	103	BCL	CHC-C1C-NC	2.05	127.36	124.40
12	t	303	PEF	O2P-P-O1P	2.05	121.99	112.44
15	X	101	CRT	C31-C32-C33	2.05	130.16	127.28
7	C	501	HEM	CHC-C1C-NC	2.05	126.69	124.45
9	AB	102	BCL	C1C-NC-C4C	-2.05	105.74	106.68
9	I	101	BCL	C2A-C1A-CHA	2.05	127.43	123.87
9	l	101	BCL	C2B-C1B-NB	-2.05	108.20	110.33
10	M	403	BPH	C6-C7-C8	-2.05	109.15	115.97
9	p	102	BCL	CMA-C3A-C4A	-2.05	106.26	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AB	102	BCL	C3C-C2C-C1C	2.05	105.18	101.87
9	AH	101	BCL	OBD-CAD-C3D	2.05	133.21	128.42
9	AL	102	BCL	CBC-CAC-C3C	2.05	117.76	113.41
17	AE	101	PGW	O03-C19-C20	2.05	121.07	112.38
9	A	103	BCL	CED-O2D-CGD	-2.05	111.27	115.92
9	r	101	BCL	CMB-C2B-C3B	2.05	132.12	125.67
7	C	501	HEM	O2D-CGD-O1D	-2.05	118.07	123.33
9	x	303	BCL	CMD-C2D-C1D	2.05	128.33	124.73
9	AC	103	BCL	C3B-C4B-NB	-2.05	107.06	109.76
9	Y	101	BCL	CMA-C3A-C2A	-2.05	106.08	113.98
9	f	101	BCL	C1C-NC-C4C	-2.05	105.75	106.68
7	o	502	HEM	CAC-C3C-C2C	2.04	135.08	128.43
11	L	304	UQ8	C6-C1-C2	2.04	120.78	119.17
9	D	102	BCL	C3C-C2C-C1C	2.04	105.17	101.87
9	e	102	BCL	C1D-CHD-C4C	-2.04	121.69	126.62
7	C	502	HEM	CAD-C3D-C2D	-2.04	124.04	127.87
9	x	303	BCL	C2A-C1A-CHA	2.04	127.41	123.87
15	AC	101	CRT	C29-C28-C27	-2.04	119.51	122.82
9	T	102	BCL	C11-C10-C8	-2.04	109.19	115.97
9	0	102	BCL	CED-O2D-CGD	-2.04	111.29	115.92
7	C	502	HEM	C2B-C1B-NB	-2.04	107.50	109.84
9	Q	101	BCL	C12-C11-C10	-2.04	104.14	113.28
9	AG	101	BCL	CHD-C1D-ND	-2.04	121.93	124.80
7	o	502	HEM	C3B-C2B-C1B	2.04	107.94	106.41
9	u	101	BCL	C1D-CHD-C4C	-2.04	121.71	126.62
15	m	104	CRT	C20-C21-C22	-2.04	119.35	123.52
9	V	102	BCL	C11-C12-C13	-2.04	109.20	115.97
7	C	504	HEM	CHA-C1A-NA	2.03	127.55	123.86
11	x	304	UQ8	C15-C14-C13	-2.03	118.40	123.63
15	Z	101	CRT	C8-C7-C9	-2.03	119.52	122.82
9	f	101	BCL	C11-C10-C8	-2.03	109.20	115.97
15	G	101	CRT	C31-C30-C28	-2.03	120.79	126.36
9	M	401	BCL	C7-C6-C5	-2.03	107.85	113.26
10	L	302	BPH	CMA-C3A-C4A	-2.03	110.23	114.61
15	AJ	101	CRT	C35-C33-C32	-2.03	115.81	119.01
15	q	101	CRT	C32-C31-C30	-2.03	117.31	123.20
9	p	102	BCL	C11-C10-C8	-2.03	109.21	115.97
9	e	102	BCL	C3C-C2C-C1C	2.03	105.15	101.87
9	AK	101	BCL	CBB-CAB-C3B	2.03	124.68	120.40
9	Q	101	BCL	CHD-C1D-ND	-2.03	121.95	124.80
15	T	101	CRT	C31-C32-C33	-2.03	124.43	127.28
15	AC	101	CRT	C9-C10-C11	-2.03	117.32	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	502	HEM	CAD-C3D-C2D	-2.03	124.07	127.87
15	4	101	CRT	C26-C25-C23	2.03	131.92	126.36
9	U	101	BCL	C1C-NC-C4C	-2.03	105.75	106.68
9	h	101	BCL	C3C-C2C-C1C	2.03	105.14	101.87
9	1	101	BCL	O2A-CGA-O1A	-2.02	118.56	123.63
15	y	404	CRT	C13-C12-C14	-2.02	119.54	122.82
9	W	101	BCL	C3D-C2D-C1D	-2.02	103.07	105.83
9	S	102	BCL	CMB-C2B-C3B	2.02	132.05	125.67
9	I	101	BCL	C3C-C2C-C1C	2.02	105.14	101.87
9	AL	102	BCL	C7-C6-C5	-2.02	107.88	113.26
15	X	101	CRT	C29-C28-C30	2.02	121.17	118.09
9	A	102	BCL	CBB-CAB-C3B	2.02	124.66	120.40
9	V	102	BCL	C2A-C1A-CHA	2.02	127.37	123.87
9	i	102	BCL	C12-C11-C10	-2.02	104.23	113.28
9	y	401	BCL	C12-C11-C10	-2.02	104.23	113.28
9	d	101	BCL	O2A-CGA-O1A	-2.02	118.58	123.63
9	D	102	BCL	O2A-C1-C2	2.02	115.88	108.11
9	8	101	BCL	CHB-C4A-NA	-2.02	121.48	124.40
9	h	101	BCL	CMA-C3A-C2A	-2.02	106.18	113.98
15	q	101	CRT	C24-C23-C22	-2.02	119.55	122.82
15	z	101	CRT	C15-C14-C12	-2.02	124.45	127.28
15	T	101	CRT	C35-C33-C32	-2.02	115.83	119.01
9	5	101	BCL	CHB-C4A-NA	-2.02	121.49	124.40
15	z	101	CRT	C30-C28-C27	-2.02	115.84	119.01
9	I	103	BCL	C4A-NA-C1A	2.02	107.60	106.68
12	t	301	PEF	O2P-P-O1P	2.02	121.83	112.44
14	M	404	MQ8	C45-C43-C44	2.02	118.73	115.23
9	f	101	BCL	CHC-C1C-NC	2.02	127.31	124.40
9	N	101	BCL	C12-C11-C10	-2.02	104.25	113.28
15	z	101	CRT	C24-C23-C22	-2.01	119.55	122.82
9	AG	101	BCL	CHB-C1B-NB	2.01	127.07	124.05
15	y	404	CRT	C13-C12-C11	2.01	121.16	118.09
9	0	102	BCL	CHB-C4A-NA	-2.01	121.50	124.40
15	m	104	CRT	C29-C28-C30	2.01	121.16	118.09
9	2	102	BCL	C3D-C2D-C1D	-2.01	103.09	105.83
9	U	101	BCL	O2A-CGA-CBA	2.01	117.97	111.83
15	q	101	CRT	C16-C17-C19	-2.01	115.85	119.01
7	C	502	HEM	CBA-CAA-C2A	-2.01	106.98	112.53
9	u	101	BCL	C3C-C2C-C1C	2.01	105.11	101.87
15	G	101	CRT	C29-C28-C30	2.01	121.16	118.09
9	F	101	BCL	C1-O2A-CGA	2.01	121.51	116.65
9	8	101	BCL	CGD-CBD-CAD	-2.01	104.35	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	502	HEM	C4A-C3A-C2A	2.01	109.12	106.82
15	T	101	CRT	C10-C9-C7	-2.00	124.47	127.28
9	m	102	BCL	CHB-C4A-NA	-2.00	121.51	124.40
9	q	102	BCL	CMB-C2B-C3B	2.00	131.98	125.67
9	g	102	BCL	O2A-CGA-CBA	2.00	117.94	111.83
9	X	102	BCL	C16-C15-C13	-2.00	109.31	115.97
15	4	101	CRT	C1-C4-C5	2.00	118.18	112.98

There are no chirality outliers.

All (1681) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	502	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C3D-CAD-CBD-CGD
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB
7	o	503	HEM	C2B-C3B-CAB-CBB
7	o	503	HEM	C4B-C3B-CAB-CBB
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	301	BCL	CBD-CGD-O2D-CED
9	L	301	BCL	O1D-CGD-O2D-CED
9	L	303	BCL	C3A-C2A-CAA-CBA
9	L	303	BCL	C4C-C3C-CAC-CBC
9	L	303	BCL	CHA-CBD-CGD-O1D
9	L	303	BCL	CHA-CBD-CGD-O2D
9	M	401	BCL	CHA-CBD-CGD-O2D
9	M	402	BCL	C3A-C2A-CAA-CBA
9	M	402	BCL	C4C-C3C-CAC-CBC
9	A	102	BCL	C1A-C2A-CAA-CBA
9	A	102	BCL	C3A-C2A-CAA-CBA
9	A	103	BCL	C3A-C2A-CAA-CBA
9	A	103	BCL	CBA-CGA-O2A-C1
9	A	103	BCL	O1A-CGA-O2A-C1
9	A	103	BCL	C4C-C3C-CAC-CBC
9	D	101	BCL	CBD-CGD-O2D-CED
9	D	102	BCL	C1A-C2A-CAA-CBA
9	D	102	BCL	C3A-C2A-CAA-CBA
9	D	102	BCL	C4C-C3C-CAC-CBC
9	D	102	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CHA-CBD-CGD-O1D
9	F	101	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	G	102	BCL	C3A-C2A-CAA-CBA
9	G	102	BCL	C4C-C3C-CAC-CBC
9	G	102	BCL	CBD-CGD-O2D-CED
9	G	102	BCL	C4-C3-C5-C6
9	I	103	BCL	C4C-C3C-CAC-CBC
9	I	103	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	C3A-C2A-CAA-CBA
9	N	101	BCL	CBD-CGD-O2D-CED
9	O	102	BCL	C1A-C2A-CAA-CBA
9	O	102	BCL	C3A-C2A-CAA-CBA
9	O	102	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	CBD-CGD-O2D-CED
9	Q	101	BCL	C2-C1-O2A-CGA
9	Q	101	BCL	C2C-C3C-CAC-CBC
9	Q	101	BCL	CBD-CGD-O2D-CED
9	R	102	BCL	C1A-C2A-CAA-CBA
9	R	102	BCL	C3A-C2A-CAA-CBA
9	R	102	BCL	C4C-C3C-CAC-CBC
9	R	102	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	C1A-C2A-CAA-CBA
9	S	102	BCL	C3A-C2A-CAA-CBA
9	S	102	BCL	C4C-C3C-CAC-CBC
9	S	102	BCL	CHA-CBD-CGD-O1D
9	S	102	BCL	CHA-CBD-CGD-O2D
9	S	102	BCL	CBD-CGD-O2D-CED
9	T	102	BCL	C3A-C2A-CAA-CBA
9	T	102	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	C4C-C3C-CAC-CBC
9	V	102	BCL	C1A-C2A-CAA-CBA
9	V	102	BCL	C3A-C2A-CAA-CBA
9	V	102	BCL	CBD-CGD-O2D-CED
9	W	101	BCL	CHA-CBD-CGD-O1D
9	W	101	BCL	CHA-CBD-CGD-O2D
9	X	102	BCL	C1A-C2A-CAA-CBA
9	X	102	BCL	C3A-C2A-CAA-CBA
9	X	102	BCL	C2-C1-O2A-CGA
9	X	102	BCL	CBD-CGD-O2D-CED
9	Y	101	BCL	C4C-C3C-CAC-CBC
9	Z	102	BCL	C1A-C2A-CAA-CBA
9	Z	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	Z	102	BCL	CBD-CGD-O2D-CED
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D
9	2	102	BCL	C3A-C2A-CAA-CBA
9	2	102	BCL	CBD-CGD-O2D-CED
9	3	101	BCL	CBD-CGD-O2D-CED
9	4	102	BCL	C1A-C2A-CAA-CBA
9	4	102	BCL	C3A-C2A-CAA-CBA
9	4	102	BCL	C2C-C3C-CAC-CBC
9	4	102	BCL	C4C-C3C-CAC-CBC
9	4	102	BCL	CBD-CGD-O2D-CED
9	6	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	CBD-CGD-O2D-CED
9	7	102	BCL	C2C-C3C-CAC-CBC
9	7	102	BCL	C4C-C3C-CAC-CBC
9	7	102	BCL	CBD-CGD-O2D-CED
9	8	101	BCL	C1A-C2A-CAA-CBA
9	8	101	BCL	C3A-C2A-CAA-CBA
9	8	101	BCL	CHA-CBD-CGD-O1D
9	8	101	BCL	CHA-CBD-CGD-O2D
9	8	101	BCL	O2A-C1-C2-C3
9	9	102	BCL	C4C-C3C-CAC-CBC
9	0	102	BCL	C1A-C2A-CAA-CBA
9	0	102	BCL	C3A-C2A-CAA-CBA
9	0	102	BCL	C4C-C3C-CAC-CBC
9	x	301	BCL	C4C-C3C-CAC-CBC
9	x	301	BCL	CBD-CGD-O2D-CED
9	x	303	BCL	C3A-C2A-CAA-CBA
9	x	305	BCL	C4C-C3C-CAC-CBC
9	x	305	BCL	CHA-CBD-CGD-O1D
9	x	305	BCL	CHA-CBD-CGD-O2D
9	x	305	BCL	CBD-CGD-O2D-CED
9	y	401	BCL	C1A-C2A-CAA-CBA
9	y	401	BCL	C3A-C2A-CAA-CBA
9	y	401	BCL	C4C-C3C-CAC-CBC
9	y	401	BCL	CAD-CBD-CGD-O1D
9	y	401	BCL	CAD-CBD-CGD-O2D
9	m	102	BCL	C4C-C3C-CAC-CBC
9	m	103	BCL	C3A-C2A-CAA-CBA
9	m	103	BCL	CBA-CGA-O2A-C1
9	p	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	p	102	BCL	C3A-C2A-CAA-CBA
9	q	102	BCL	C1A-C2A-CAA-CBA
9	q	102	BCL	CBD-CGD-O2D-CED
9	r	101	BCL	C1A-C2A-CAA-CBA
9	r	101	BCL	C3A-C2A-CAA-CBA
9	r	101	BCL	C4C-C3C-CAC-CBC
9	s	102	BCL	C3A-C2A-CAA-CBA
9	s	102	BCL	CBD-CGD-O2D-CED
9	u	101	BCL	C3A-C2A-CAA-CBA
9	u	101	BCL	CBD-CGD-O2D-CED
9	u	102	BCL	C3A-C2A-CAA-CBA
9	u	102	BCL	CBD-CGD-O2D-CED
9	w	101	BCL	C1A-C2A-CAA-CBA
9	w	101	BCL	C3A-C2A-CAA-CBA
9	w	101	BCL	C4C-C3C-CAC-CBC
9	z	102	BCL	C3A-C2A-CAA-CBA
9	z	102	BCL	CBD-CGD-O2D-CED
9	AB	102	BCL	C3A-C2A-CAA-CBA
9	AB	102	BCL	CBD-CGD-O2D-CED
9	AC	102	BCL	C1A-C2A-CAA-CBA
9	AC	102	BCL	C3A-C2A-CAA-CBA
9	AC	102	BCL	C4C-C3C-CAC-CBC
9	AC	103	BCL	C3A-C2A-CAA-CBA
9	AC	103	BCL	CBD-CGD-O2D-CED
9	AC	103	BCL	O1D-CGD-O2D-CED
9	AE	102	BCL	C1A-C2A-CAA-CBA
9	AE	102	BCL	C3A-C2A-CAA-CBA
9	AE	102	BCL	CBD-CGD-O2D-CED
9	AH	101	BCL	C1A-C2A-CAA-CBA
9	AH	101	BCL	C3A-C2A-CAA-CBA
9	AI	101	BCL	C1A-C2A-CAA-CBA
9	AI	101	BCL	C3A-C2A-CAA-CBA
9	AI	101	BCL	CHA-CBD-CGD-O1D
9	AI	101	BCL	CHA-CBD-CGD-O2D
9	AI	101	BCL	CBD-CGD-O2D-CED
9	AI	102	BCL	C1A-C2A-CAA-CBA
9	AI	102	BCL	C3A-C2A-CAA-CBA
9	AI	102	BCL	C4C-C3C-CAC-CBC
9	AI	102	BCL	CBD-CGD-O2D-CED
9	AK	101	BCL	C2C-C3C-CAC-CBC
9	AL	102	BCL	C1A-C2A-CAA-CBA
9	AL	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	AL	102	BCL	C4C-C3C-CAC-CBC
9	AL	102	BCL	CBD-CGD-O2D-CED
9	d	101	BCL	O1A-CGA-O2A-C1
9	d	101	BCL	CHA-CBD-CGD-O1D
9	d	101	BCL	CHA-CBD-CGD-O2D
9	e	102	BCL	C1A-C2A-CAA-CBA
9	e	102	BCL	C3A-C2A-CAA-CBA
9	e	102	BCL	CBD-CGD-O2D-CED
9	f	101	BCL	CBD-CGD-O2D-CED
9	g	102	BCL	CBD-CGD-O2D-CED
9	i	102	BCL	C3A-C2A-CAA-CBA
9	i	102	BCL	CBD-CGD-O2D-CED
9	j	101	BCL	C2C-C3C-CAC-CBC
9	j	101	BCL	C4C-C3C-CAC-CBC
9	j	101	BCL	CBD-CGD-O2D-CED
9	k	102	BCL	C1A-C2A-CAA-CBA
9	k	102	BCL	C3A-C2A-CAA-CBA
9	k	102	BCL	C2C-C3C-CAC-CBC
9	k	102	BCL	C4C-C3C-CAC-CBC
9	k	102	BCL	O2A-C1-C2-C3
9	l	101	BCL	C2C-C3C-CAC-CBC
9	l	101	BCL	CBD-CGD-O2D-CED
9	c	101	BCL	C3A-C2A-CAA-CBA
9	c	101	BCL	C4C-C3C-CAC-CBC
10	M	403	BPH	C4C-C3C-CAC-CBC
10	x	302	BPH	C4C-C3C-CAC-CBC
10	x	302	BPH	C2C-C3C-CAC-CBC
10	y	402	BPH	C4C-C3C-CAC-CBC
10	y	402	BPH	C3A-C2A-CAA-CBA
11	L	304	UQ8	C40-C39-C41-C42
11	L	304	UQ8	C38-C39-C41-C42
11	x	304	UQ8	C40-C39-C41-C42
11	x	304	UQ8	C24-C26-C27-C28
12	L	305	PEF	O3P-C1-C2-C3
12	L	305	PEF	O3P-C1-C2-O2
12	L	305	PEF	C4-O4P-P-O3P
12	M	407	PEF	C1-O3P-P-O4P
12	M	408	PEF	C1-O3P-P-O2P
12	M	408	PEF	C1-O3P-P-O4P
12	H	301	PEF	C1-O3P-P-O2P
12	H	301	PEF	C1-O3P-P-O4P
12	H	301	PEF	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
12	H	304	PEF	C1-O3P-P-O1P
12	H	304	PEF	C4-O4P-P-O2P
12	H	304	PEF	C4-O4P-P-O3P
12	H	305	PEF	C11-C10-O2-C2
12	H	305	PEF	C1-O3P-P-O1P
12	H	305	PEF	C1-O3P-P-O2P
12	H	305	PEF	C1-O3P-P-O4P
12	A	101	PEF	C1-O3P-P-O4P
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	C11-C10-O2-C2
12	x	306	PEF	C1-O3P-P-O1P
12	y	406	PEF	O4P-C4-C5-N
12	y	406	PEF	C4-O4P-P-O1P
12	y	407	PEF	O4P-C4-C5-N
12	y	408	PEF	C1-O3P-P-O1P
12	y	408	PEF	C1-O3P-P-O2P
12	y	408	PEF	C1-O3P-P-O4P
12	t	301	PEF	O4P-C4-C5-N
12	t	303	PEF	C1-O3P-P-O1P
12	t	303	PEF	C1-O3P-P-O2P
12	t	303	PEF	C1-O3P-P-O4P
12	t	303	PEF	C4-O4P-P-O2P
12	m	101	PEF	O4P-C4-C5-N
12	m	101	PEF	C5-C4-O4P-P
12	m	101	PEF	C1-O3P-P-O1P
12	m	101	PEF	C1-O3P-P-O2P
12	m	101	PEF	C1-O3P-P-O4P
12	m	101	PEF	C4-O4P-P-O1P
12	p	101	PEF	C1-O3P-P-O1P
12	p	101	PEF	C1-O3P-P-O2P
12	p	101	PEF	C1-O3P-P-O4P
14	M	404	MQ8	C16-C17-C18-C19
14	M	404	MQ8	C31-C32-C33-C34
14	M	404	MQ8	C31-C32-C33-C35
14	M	404	MQ8	C36-C37-C38-C40
14	y	403	MQ8	C16-C17-C18-C20
14	y	403	MQ8	C36-C37-C38-C39
14	y	403	MQ8	C36-C37-C38-C40
14	y	403	MQ8	C38-C40-C41-C42
14	y	403	MQ8	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
15	M	405	CRT	C3-C1-C4-C5
15	M	405	CRT	C32-C33-C35-C36
15	M	405	CRT	C34-C33-C35-C36
15	M	405	CRT	C35-C36-C37-C38
15	E	101	CRT	C2-C1-O1-C1M
15	E	101	CRT	C22-C23-C25-C26
15	E	101	CRT	C24-C23-C25-C26
15	G	101	CRT	C5-C6-C7-C8
15	G	101	CRT	C5-C6-C7-C9
15	G	101	CRT	C29-C28-C30-C31
15	G	101	CRT	C32-C33-C35-C36
15	G	101	CRT	C34-C33-C35-C36
15	I	102	CRT	C5-C6-C7-C8
15	I	102	CRT	C5-C6-C7-C9
15	O	101	CRT	C2-C1-O1-C1M
15	O	101	CRT	O1-C1-C4-C5
15	O	101	CRT	C2-C1-C4-C5
15	O	101	CRT	C3-C1-C4-C5
15	O	101	CRT	C15-C16-C17-C19
15	P	102	CRT	O1-C1-C4-C5
15	P	102	CRT	C2-C1-C4-C5
15	P	102	CRT	C3-C1-C4-C5
15	P	102	CRT	C22-C23-C25-C26
15	R	101	CRT	C5-C6-C7-C8
15	R	101	CRT	C5-C6-C7-C9
15	R	101	CRT	C15-C16-C17-C19
15	R	101	CRT	C22-C23-C25-C26
15	R	101	CRT	C24-C23-C25-C26
15	R	101	CRT	C27-C28-C30-C31
15	R	101	CRT	C29-C28-C30-C31
15	T	101	CRT	C3-C1-O1-C1M
15	V	101	CRT	O1-C1-C4-C5
15	V	101	CRT	C2-C1-C4-C5
15	V	101	CRT	C3-C1-C4-C5
15	V	101	CRT	C10-C11-C12-C13
15	V	101	CRT	C10-C11-C12-C14
15	V	101	CRT	C15-C16-C17-C18
15	V	101	CRT	C15-C16-C17-C19
15	V	101	CRT	C36-C37-C38-C39
15	V	101	CRT	C36-C37-C38-C40
15	V	101	CRT	C36-C37-C38-O2
15	X	101	CRT	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
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	Z	101	CRT	C5-C6-C7-C8
15	Z	101	CRT	C5-C6-C7-C9
15	Z	101	CRT	C15-C16-C17-C18
15	Z	101	CRT	C15-C16-C17-C19
15	Z	101	CRT	C27-C28-C30-C31
15	Z	101	CRT	C36-C37-C38-C40
15	Z	101	CRT	C36-C37-C38-O2
15	2	101	CRT	O1-C1-C4-C5
15	2	101	CRT	C5-C6-C7-C8
15	2	101	CRT	C5-C6-C7-C9
15	4	101	CRT	C3-C1-C4-C5
15	4	101	CRT	C5-C6-C7-C8
15	4	101	CRT	C5-C6-C7-C9
15	4	101	CRT	C10-C11-C12-C13
15	4	101	CRT	C10-C11-C12-C14
15	4	101	CRT	C27-C28-C30-C31
15	7	101	CRT	C5-C6-C7-C9
15	7	101	CRT	C22-C23-C25-C26
15	7	101	CRT	C24-C23-C25-C26
15	7	103	CRT	O1-C1-C4-C5
15	7	103	CRT	C2-C1-C4-C5
15	7	103	CRT	C3-C1-C4-C5
15	9	101	CRT	C3-C1-O1-C1M
15	9	101	CRT	C1-C4-C5-C6
15	9	101	CRT	C15-C16-C17-C19
15	0	101	CRT	C2-C1-O1-C1M
15	0	101	CRT	C5-C6-C7-C8
15	0	101	CRT	C5-C6-C7-C9
15	y	404	CRT	C32-C33-C35-C36
15	y	404	CRT	C34-C33-C35-C36
15	y	404	CRT	C35-C36-C37-C38
15	n	101	CRT	C2-C1-O1-C1M
15	n	101	CRT	C3-C1-O1-C1M
15	n	101	CRT	C1-C4-C5-C6
15	n	101	CRT	C15-C16-C17-C18
15	n	101	CRT	C15-C16-C17-C19
15	n	101	CRT	C36-C37-C38-C39
15	n	101	CRT	C36-C37-C38-C40
15	n	101	CRT	C36-C37-C38-O2

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Mol	Chain	Res	Type	Atoms
15	q	101	CRT	C22-C23-C25-C26
15	q	101	CRT	C24-C23-C25-C26
15	s	101	CRT	C5-C6-C7-C8
15	s	101	CRT	C5-C6-C7-C9
15	s	101	CRT	C10-C11-C12-C14
15	s	101	CRT	C22-C23-C25-C26
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	AC	101	CRT	O1-C1-C4-C5
15	AC	101	CRT	C2-C1-C4-C5
15	AD	101	CRT	C3-C1-O1-C1M
15	AF	102	CRT	C27-C28-C30-C31
15	AF	102	CRT	C29-C28-C30-C31
15	AH	102	CRT	C2-C1-O1-C1M
15	AH	102	CRT	C22-C23-C25-C26
15	AJ	101	CRT	C27-C28-C30-C31
15	AJ	101	CRT	C29-C28-C30-C31
15	e	101	CRT	O1-C1-C4-C5
15	e	101	CRT	C2-C1-C4-C5
15	e	101	CRT	C3-C1-C4-C5
15	g	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C10-C11-C12-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-O12-P-O11
17	S	101	PGW	C2-C1-O01-C02
17	AE	101	PGW	C04-C05-CAD-OAE
17	AE	101	PGW	C2-C1-O01-C02
9	A	103	BCL	O1D-CGD-O2D-CED
9	D	102	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	O1D-CGD-O2D-CED
9	G	102	BCL	O1D-CGD-O2D-CED
9	I	101	BCL	O1D-CGD-O2D-CED
9	I	103	BCL	O1D-CGD-O2D-CED
9	R	102	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	O1D-CGD-O2D-CED
9	T	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	U	101	BCL	O1D-CGD-O2D-CED
9	X	102	BCL	O1D-CGD-O2D-CED
9	Z	102	BCL	O1D-CGD-O2D-CED
9	2	102	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	O1D-CGD-O2D-CED
9	7	102	BCL	O1D-CGD-O2D-CED
9	9	102	BCL	O1D-CGD-O2D-CED
9	0	102	BCL	O1D-CGD-O2D-CED
9	x	303	BCL	O1D-CGD-O2D-CED
9	p	102	BCL	O1D-CGD-O2D-CED
9	s	102	BCL	O1D-CGD-O2D-CED
9	w	101	BCL	O1D-CGD-O2D-CED
9	z	102	BCL	O1D-CGD-O2D-CED
9	AC	102	BCL	O1D-CGD-O2D-CED
9	AG	101	BCL	O1D-CGD-O2D-CED
9	AI	102	BCL	O1D-CGD-O2D-CED
9	AK	101	BCL	O1D-CGD-O2D-CED
9	AL	102	BCL	O1D-CGD-O2D-CED
9	d	101	BCL	O1D-CGD-O2D-CED
9	e	102	BCL	O1D-CGD-O2D-CED
9	i	102	BCL	O1D-CGD-O2D-CED
9	j	101	BCL	O1D-CGD-O2D-CED
9	k	102	BCL	O1D-CGD-O2D-CED
9	c	101	BCL	O1D-CGD-O2D-CED
12	H	304	PEF	C11-C10-O2-C2
12	H	305	PEF	O4-C10-O2-C2
9	L	303	BCL	O1D-CGD-O2D-CED
9	D	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	O1D-CGD-O2D-CED
9	O	102	BCL	O1D-CGD-O2D-CED
9	P	101	BCL	O1D-CGD-O2D-CED
9	Q	101	BCL	O1D-CGD-O2D-CED
9	V	102	BCL	O1D-CGD-O2D-CED
9	4	102	BCL	O1D-CGD-O2D-CED
9	6	101	BCL	O1D-CGD-O2D-CED
9	x	301	BCL	O1D-CGD-O2D-CED
9	m	103	BCL	O1D-CGD-O2D-CED
9	q	102	BCL	O1D-CGD-O2D-CED
9	u	102	BCL	O1D-CGD-O2D-CED
9	AE	102	BCL	O1D-CGD-O2D-CED
9	AH	101	BCL	O1D-CGD-O2D-CED
9	g	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	l	101	BCL	O1D-CGD-O2D-CED
12	A	101	PEF	C11-C10-O2-C2
12	x	306	PEF	O4-C10-O2-C2
12	y	407	PEF	C11-C10-O2-C2
12	y	408	PEF	C11-C10-O2-C2
17	S	101	PGW	O02-C1-O01-C02
17	AE	101	PGW	O02-C1-O01-C02
9	L	303	BCL	CBD-CGD-O2D-CED
9	A	102	BCL	CBD-CGD-O2D-CED
9	A	103	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CBD-CGD-O2D-CED
9	I	101	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	CBD-CGD-O2D-CED
9	W	101	BCL	CBD-CGD-O2D-CED
9	Y	101	BCL	CBD-CGD-O2D-CED
9	1	101	BCL	CBD-CGD-O2D-CED
9	5	101	BCL	CBD-CGD-O2D-CED
9	8	101	BCL	CBD-CGD-O2D-CED
9	9	102	BCL	CBD-CGD-O2D-CED
9	0	102	BCL	CBD-CGD-O2D-CED
9	x	303	BCL	CBD-CGD-O2D-CED
9	m	102	BCL	CBD-CGD-O2D-CED
9	m	103	BCL	CBD-CGD-O2D-CED
9	p	102	BCL	CBD-CGD-O2D-CED
9	r	101	BCL	CBD-CGD-O2D-CED
9	w	101	BCL	CBD-CGD-O2D-CED
9	AB	101	BCL	CBD-CGD-O2D-CED
9	AC	102	BCL	CBD-CGD-O2D-CED
9	AF	101	BCL	CBD-CGD-O2D-CED
9	AG	101	BCL	CBD-CGD-O2D-CED
9	AH	101	BCL	CBD-CGD-O2D-CED
9	AK	101	BCL	CBD-CGD-O2D-CED
9	d	101	BCL	CBD-CGD-O2D-CED
9	h	101	BCL	CBD-CGD-O2D-CED
9	k	102	BCL	CBD-CGD-O2D-CED
9	c	101	BCL	CBD-CGD-O2D-CED
10	L	302	BPH	CBD-CGD-O2D-CED
9	4	102	BCL	O1A-CGA-O2A-C1
9	8	101	BCL	O1A-CGA-O2A-C1
9	m	103	BCL	O1A-CGA-O2A-C1
9	s	102	BCL	O1A-CGA-O2A-C1
9	g	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	k	102	BCL	O1A-CGA-O2A-C1
9	u	101	BCL	O1D-CGD-O2D-CED
12	t	303	PEF	C11-C10-O2-C2
14	M	404	MQ8	C46-C47-C48-C49
9	W	101	BCL	O1D-CGD-O2D-CED
9	Y	101	BCL	O1D-CGD-O2D-CED
9	r	101	BCL	O1D-CGD-O2D-CED
9	AB	101	BCL	O1D-CGD-O2D-CED
9	AB	102	BCL	O1D-CGD-O2D-CED
9	AF	101	BCL	O1D-CGD-O2D-CED
10	L	302	BPH	O1D-CGD-O2D-CED
9	8	101	BCL	CBA-CGA-O2A-C1
9	s	102	BCL	CBA-CGA-O2A-C1
9	g	102	BCL	CBA-CGA-O2A-C1
9	k	102	BCL	CBA-CGA-O2A-C1
9	G	102	BCL	O1A-CGA-O2A-C1
9	O	102	BCL	O1A-CGA-O2A-C1
9	2	102	BCL	O1A-CGA-O2A-C1
9	6	101	BCL	O1A-CGA-O2A-C1
9	u	102	BCL	O1A-CGA-O2A-C1
9	AB	102	BCL	O1A-CGA-O2A-C1
9	e	102	BCL	O1A-CGA-O2A-C1
9	AC	103	BCL	C15-C16-C17-C18
9	m	102	BCL	O1D-CGD-O2D-CED
9	f	101	BCL	O1D-CGD-O2D-CED
9	h	101	BCL	O1D-CGD-O2D-CED
9	AI	101	BCL	O1D-CGD-O2D-CED
12	H	304	PEF	O4-C10-O2-C2
9	R	102	BCL	C15-C16-C17-C18
9	K	101	BCL	O1A-CGA-O2A-C1
9	M	401	BCL	C3-C5-C6-C7
9	I	101	BCL	C3-C5-C6-C7
9	I	103	BCL	C3-C5-C6-C7
9	N	101	BCL	C3-C5-C6-C7
9	W	101	BCL	C3-C5-C6-C7
9	6	101	BCL	C3-C5-C6-C7
9	8	101	BCL	C3-C5-C6-C7
9	9	102	BCL	C3-C5-C6-C7
9	u	101	BCL	C3-C5-C6-C7
9	AC	102	BCL	C3-C5-C6-C7
9	AG	101	BCL	C3-C5-C6-C7
9	g	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	k	102	BCL	C3-C5-C6-C7
10	M	403	BPH	C3-C5-C6-C7
9	G	102	BCL	CBA-CGA-O2A-C1
9	O	102	BCL	CBA-CGA-O2A-C1
9	Z	102	BCL	CBA-CGA-O2A-C1
9	4	102	BCL	CBA-CGA-O2A-C1
9	6	101	BCL	CBA-CGA-O2A-C1
9	u	102	BCL	CBA-CGA-O2A-C1
9	d	101	BCL	CBA-CGA-O2A-C1
9	e	102	BCL	CBA-CGA-O2A-C1
9	h	101	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	CBA-CGA-O2A-C1
9	c	101	BCL	CBA-CGA-O2A-C1
9	M	401	BCL	CBD-CGD-O2D-CED
10	x	302	BPH	CBD-CGD-O2D-CED
9	x	305	BCL	O1D-CGD-O2D-CED
12	y	406	PEF	C11-C10-O2-C2
9	I	103	BCL	O1A-CGA-O2A-C1
9	X	102	BCL	O1A-CGA-O2A-C1
9	q	102	BCL	O1A-CGA-O2A-C1
9	Z	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C4-C3-C5-C6
9	7	102	BCL	C4-C3-C5-C6
9	s	102	BCL	C4-C3-C5-C6
9	AB	101	BCL	C4-C3-C5-C6
9	AC	102	BCL	C4-C3-C5-C6
9	i	102	BCL	C4-C3-C5-C6
14	M	404	MQ8	C14-C13-C15-C16
9	G	102	BCL	C2-C3-C5-C6
9	Z	102	BCL	C2-C3-C5-C6
9	2	102	BCL	C2-C3-C5-C6
9	s	102	BCL	C2-C3-C5-C6
9	AB	101	BCL	C2-C3-C5-C6
9	AC	102	BCL	C2-C3-C5-C6
9	i	102	BCL	C2-C3-C5-C6
11	x	304	UQ8	C38-C39-C41-C42
14	M	404	MQ8	C32-C33-C35-C36
14	y	403	MQ8	C12-C13-C15-C16
9	8	101	BCL	O1D-CGD-O2D-CED
9	V	102	BCL	C2A-CAA-CBA-CGA
9	AH	101	BCL	C2A-CAA-CBA-CGA
9	k	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	7	102	BCL	O1A-CGA-O2A-C1
9	V	102	BCL	C3-C5-C6-C7
9	X	102	BCL	C3-C5-C6-C7
9	z	102	BCL	C3-C5-C6-C7
9	AH	101	BCL	C3-C5-C6-C7
9	i	102	BCL	C3-C5-C6-C7
9	I	103	BCL	CBA-CGA-O2A-C1
9	R	102	BCL	CBA-CGA-O2A-C1
9	2	102	BCL	CBA-CGA-O2A-C1
9	7	102	BCL	CBA-CGA-O2A-C1
9	AB	102	BCL	CBA-CGA-O2A-C1
9	AC	103	BCL	CBA-CGA-O2A-C1
9	AE	102	BCL	CBA-CGA-O2A-C1
9	AG	101	BCL	CBA-CGA-O2A-C1
12	H	304	PEF	C31-C30-O3-C3
14	M	404	MQ8	C36-C37-C38-C39
14	y	403	MQ8	C16-C17-C18-C19
14	y	403	MQ8	C41-C42-C43-C45
15	9	101	CRT	C11-C10-C9-C7
15	n	101	CRT	C11-C10-C9-C7
9	R	102	BCL	O1A-CGA-O2A-C1
9	T	102	BCL	O1A-CGA-O2A-C1
9	Z	102	BCL	O1A-CGA-O2A-C1
9	AC	103	BCL	O1A-CGA-O2A-C1
9	AE	102	BCL	O1A-CGA-O2A-C1
9	AG	101	BCL	O1A-CGA-O2A-C1
9	h	101	BCL	O1A-CGA-O2A-C1
9	i	102	BCL	O1A-CGA-O2A-C1
12	t	303	PEF	O4-C10-O2-C2
9	1	101	BCL	O1D-CGD-O2D-CED
14	M	404	MQ8	C46-C47-C48-C50
9	K	101	BCL	C3-C5-C6-C7
9	L	303	BCL	CBA-CGA-O2A-C1
9	D	102	BCL	CBA-CGA-O2A-C1
9	F	101	BCL	CBA-CGA-O2A-C1
9	K	101	BCL	CBA-CGA-O2A-C1
9	P	101	BCL	CBA-CGA-O2A-C1
9	T	102	BCL	CBA-CGA-O2A-C1
9	X	102	BCL	CBA-CGA-O2A-C1
9	0	102	BCL	CBA-CGA-O2A-C1
9	x	303	BCL	CBA-CGA-O2A-C1
9	q	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	z	102	BCL	CBA-CGA-O2A-C1
9	AB	101	BCL	CBA-CGA-O2A-C1
9	f	101	BCL	CBA-CGA-O2A-C1
9	i	102	BCL	CBA-CGA-O2A-C1
9	j	101	BCL	O1A-CGA-O2A-C1
9	c	101	BCL	O1A-CGA-O2A-C1
9	L	303	BCL	O1A-CGA-O2A-C1
12	H	305	PEF	C31-C30-O3-C3
10	x	302	BPH	O1D-CGD-O2D-CED
9	AI	102	BCL	C3-C5-C6-C7
9	A	102	BCL	O1D-CGD-O2D-CED
14	y	403	MQ8	C32-C33-C35-C36
14	y	403	MQ8	C42-C43-C44-C46
12	y	407	PEF	O5-C30-O3-C3
11	L	304	UQ8	C14-C16-C17-C18
11	x	304	UQ8	C39-C41-C42-C43
14	M	404	MQ8	C38-C40-C41-C42
14	M	404	MQ8	C43-C44-C46-C47
14	y	403	MQ8	C33-C35-C36-C37
12	A	101	PEF	O4-C10-O2-C2
12	M	408	PEF	O5-C30-O3-C3
12	y	408	PEF	O5-C30-O3-C3
9	0	102	BCL	O1A-CGA-O2A-C1
9	x	303	BCL	O1A-CGA-O2A-C1
9	z	102	BCL	O1A-CGA-O2A-C1
9	AB	101	BCL	O1A-CGA-O2A-C1
9	f	101	BCL	O1A-CGA-O2A-C1
12	y	407	PEF	O4-C10-O2-C2
9	r	101	BCL	C15-C16-C17-C18
14	M	404	MQ8	C15-C16-C17-C18
9	5	101	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	CBA-CGA-O2A-C1
9	Q	101	BCL	CBA-CGA-O2A-C1
9	W	101	BCL	CBA-CGA-O2A-C1
12	y	407	PEF	C31-C30-O3-C3
9	D	102	BCL	O1A-CGA-O2A-C1
9	F	101	BCL	O1A-CGA-O2A-C1
12	t	301	PEF	C11-C10-O2-C2
15	I	102	CRT	C11-C10-C9-C7
9	N	101	BCL	O1A-CGA-O2A-C1
9	P	101	BCL	O1A-CGA-O2A-C1
9	W	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	I	101	BCL	CBA-CGA-O2A-C1
9	U	101	BCL	CBA-CGA-O2A-C1
9	V	102	BCL	CBA-CGA-O2A-C1
9	Y	101	BCL	CBA-CGA-O2A-C1
9	1	101	BCL	CBA-CGA-O2A-C1
9	5	101	BCL	CBA-CGA-O2A-C1
9	p	102	BCL	CBA-CGA-O2A-C1
9	AI	102	BCL	CBA-CGA-O2A-C1
9	AL	102	BCL	CBA-CGA-O2A-C1
12	y	408	PEF	C31-C30-O3-C3
12	y	408	PEF	O4-C10-O2-C2
14	y	403	MQ8	C14-C13-C15-C16
14	y	403	MQ8	C34-C33-C35-C36
14	y	403	MQ8	C45-C43-C44-C46
9	7	102	BCL	C2-C3-C5-C6
14	M	404	MQ8	C12-C13-C15-C16
9	D	102	BCL	C3-C5-C6-C7
9	M	401	BCL	C6-C7-C8-C9
9	A	102	BCL	C11-C12-C13-C14
9	O	102	BCL	C6-C7-C8-C9
9	6	101	BCL	C6-C7-C8-C9
9	m	103	BCL	C11-C12-C13-C14
9	i	102	BCL	C6-C7-C8-C9
12	M	408	PEF	C31-C30-O3-C3
9	M	401	BCL	O1D-CGD-O2D-CED
9	p	102	BCL	O1A-CGA-O2A-C1
15	O	101	CRT	C15-C16-C17-C18
15	P	102	CRT	C24-C23-C25-C26
15	P	102	CRT	C29-C28-C30-C31
15	R	101	CRT	C15-C16-C17-C18
15	X	101	CRT	C24-C23-C25-C26
15	Z	101	CRT	C29-C28-C30-C31
15	4	101	CRT	C29-C28-C30-C31
15	7	101	CRT	C5-C6-C7-C8
15	7	101	CRT	C29-C28-C30-C31
15	9	101	CRT	C5-C6-C7-C8
15	9	101	CRT	C15-C16-C17-C18
15	9	101	CRT	C29-C28-C30-C31
15	n	101	CRT	C5-C6-C7-C8
15	s	101	CRT	C10-C11-C12-C13
15	s	101	CRT	C15-C16-C17-C18
15	s	101	CRT	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
15	v	101	CRT	C5-C6-C7-C8
15	AC	101	CRT	C15-C16-C17-C18
15	AH	102	CRT	C24-C23-C25-C26
15	AL	101	CRT	C5-C6-C7-C8
15	AL	101	CRT	C24-C23-C25-C26
15	e	101	CRT	C10-C11-C12-C13
15	i	101	CRT	C10-C11-C12-C13
15	G	101	CRT	C27-C28-C30-C31
15	e	101	CRT	C10-C11-C12-C14
9	q	102	BCL	C2A-CAA-CBA-CGA
9	AC	102	BCL	C2A-CAA-CBA-CGA
9	AI	101	BCL	C2A-CAA-CBA-CGA
12	H	302	PEF	C11-C10-O2-C2
9	U	101	BCL	O1A-CGA-O2A-C1
9	Y	101	BCL	O1A-CGA-O2A-C1
9	AI	102	BCL	O1A-CGA-O2A-C1
9	D	101	BCL	CBA-CGA-O2A-C1
9	N	101	BCL	C13-C15-C16-C17
9	i	102	BCL	C2-C1-O2A-CGA
12	H	304	PEF	O5-C30-O3-C3
9	N	101	BCL	C15-C16-C17-C18
9	T	102	BCL	C5-C6-C7-C8
9	AC	102	BCL	C8-C10-C11-C12
9	AG	101	BCL	C13-C15-C16-C17
17	AE	101	PGW	OAF-C05-CAD-OAE
17	S	101	PGW	C20-C19-O03-C01
9	A	102	BCL	C13-C15-C16-C17
9	AK	101	BCL	CBA-CGA-O2A-C1
9	AF	101	BCL	C4-C3-C5-C6
9	AB	101	BCL	C5-C6-C7-C8
15	AJ	101	CRT	C17-C19-C20-C21
11	L	304	UQ8	C29-C31-C32-C33
11	x	304	UQ8	C19-C21-C22-C23
14	y	403	MQ8	C28-C30-C31-C32
9	F	101	BCL	C13-C15-C16-C17
9	8	101	BCL	C10-C11-C12-C13
9	u	102	BCL	C5-C6-C7-C8
12	M	407	PEF	C2-C3-O3-C30
9	V	102	BCL	O1A-CGA-O2A-C1
9	AL	102	BCL	O1A-CGA-O2A-C1
9	I	103	BCL	C5-C6-C7-C8
9	P	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	C15-C16-C17-C18
9	AC	102	BCL	C5-C6-C7-C8
9	AE	102	BCL	C8-C10-C11-C12
9	AG	101	BCL	C8-C10-C11-C12
9	AH	101	BCL	C10-C11-C12-C13
9	AI	102	BCL	C8-C10-C11-C12
9	f	101	BCL	C15-C16-C17-C18
9	h	101	BCL	C10-C11-C12-C13
9	k	102	BCL	C8-C10-C11-C12
10	L	302	BPH	C5-C6-C7-C8
10	L	302	BPH	C8-C10-C11-C12
9	L	303	BCL	C2A-CAA-CBA-CGA
9	I	103	BCL	C2A-CAA-CBA-CGA
9	T	102	BCL	C2A-CAA-CBA-CGA
9	6	101	BCL	C2A-CAA-CBA-CGA
9	g	102	BCL	C2A-CAA-CBA-CGA
12	H	305	PEF	O5-C30-O3-C3
9	A	103	BCL	C8-C10-C11-C12
9	G	102	BCL	C15-C16-C17-C18
9	X	102	BCL	C8-C10-C11-C12
9	3	101	BCL	C5-C6-C7-C8
9	d	101	BCL	C15-C16-C17-C18
9	k	102	BCL	C10-C11-C12-C13
9	k	102	BCL	C15-C16-C17-C18
9	l	101	BCL	C10-C11-C12-C13
9	I	101	BCL	O1A-CGA-O2A-C1
9	5	101	BCL	O1A-CGA-O2A-C1
9	x	303	BCL	C3-C5-C6-C7
9	M	402	BCL	C5-C6-C7-C8
9	F	101	BCL	C15-C16-C17-C18
9	G	102	BCL	C5-C6-C7-C8
9	U	101	BCL	C15-C16-C17-C18
9	W	101	BCL	C10-C11-C12-C13
9	4	102	BCL	C5-C6-C7-C8
9	4	102	BCL	C8-C10-C11-C12
9	5	101	BCL	C15-C16-C17-C18
9	7	102	BCL	C8-C10-C11-C12
9	r	101	BCL	C13-C15-C16-C17
9	z	102	BCL	C5-C6-C7-C8
9	AB	101	BCL	C8-C10-C11-C12
9	AE	102	BCL	C13-C15-C16-C17
9	AK	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	Q	101	BCL	O1A-CGA-O2A-C1
9	1	101	BCL	O1A-CGA-O2A-C1
9	Z	102	BCL	C8-C10-C11-C12
9	g	102	BCL	C8-C10-C11-C12
9	h	101	BCL	C15-C16-C17-C18
9	M	401	BCL	C5-C6-C7-C8
9	F	101	BCL	C5-C6-C7-C8
9	r	101	BCL	C8-C10-C11-C12
9	u	101	BCL	C5-C6-C7-C8
9	AI	102	BCL	C15-C16-C17-C18
9	R	102	BCL	C13-C15-C16-C17
9	U	101	BCL	C13-C15-C16-C17
9	V	102	BCL	C8-C10-C11-C12
9	X	102	BCL	C10-C11-C12-C13
9	AI	101	BCL	C5-C6-C7-C8
9	x	301	BCL	CBA-CGA-O2A-C1
9	y	401	BCL	CBA-CGA-O2A-C1
9	AC	102	BCL	CBA-CGA-O2A-C1
9	l	101	BCL	CBA-CGA-O2A-C1
15	y	404	CRT	C25-C26-C27-C28
9	AK	101	BCL	O1A-CGA-O2A-C1
9	w	101	BCL	C2A-CAA-CBA-CGA
9	AE	102	BCL	C2A-CAA-CBA-CGA
9	3	101	BCL	CBA-CGA-O2A-C1
9	3	101	BCL	C15-C16-C17-C18
9	0	102	BCL	C13-C15-C16-C17
9	s	102	BCL	C5-C6-C7-C8
9	z	102	BCL	C15-C16-C17-C18
9	e	102	BCL	C15-C16-C17-C18
9	c	101	BCL	C13-C15-C16-C17
9	D	101	BCL	C15-C16-C17-C18
9	S	102	BCL	C8-C10-C11-C12
9	u	101	BCL	C13-C15-C16-C17
9	AE	102	BCL	C5-C6-C7-C8
10	M	403	BPH	C13-C15-C16-C17
10	M	403	BPH	C15-C16-C17-C18
12	y	406	PEF	O4-C10-O2-C2
9	D	102	BCL	C13-C15-C16-C17
9	G	102	BCL	C8-C10-C11-C12
9	Q	101	BCL	C8-C10-C11-C12
9	x	301	BCL	C15-C16-C17-C18
9	p	102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	f	101	BCL	C5-C6-C7-C8
9	f	101	BCL	C10-C11-C12-C13
9	i	102	BCL	C13-C15-C16-C17
9	W	101	BCL	C4-C3-C5-C6
9	e	102	BCL	C4-C3-C5-C6
9	AF	101	BCL	C2-C3-C5-C6
9	AB	101	BCL	C13-C15-C16-C17
9	x	305	BCL	C4B-C3B-CAB-OBB
9	c	101	BCL	C6-C7-C8-C9
9	D	101	BCL	O1A-CGA-O2A-C1
14	M	404	MQ8	C18-C20-C21-C22
9	d	101	BCL	C16-C17-C18-C20
9	m	103	BCL	C5-C6-C7-C8
9	r	101	BCL	C5-C6-C7-C8
9	j	101	BCL	C10-C11-C12-C13
15	T	101	CRT	C29-C28-C30-C31
15	X	101	CRT	C10-C11-C12-C13
15	4	101	CRT	C15-C16-C17-C18
15	y	404	CRT	C5-C6-C7-C8
15	AH	102	CRT	C5-C6-C7-C8
15	e	101	CRT	C24-C23-C25-C26
15	k	101	CRT	C10-C11-C12-C13
15	T	101	CRT	C27-C28-C30-C31
15	9	101	CRT	C5-C6-C7-C9
15	9	101	CRT	C27-C28-C30-C31
15	n	101	CRT	C5-C6-C7-C9
15	s	101	CRT	C15-C16-C17-C19
15	AL	101	CRT	C22-C23-C25-C26
9	AC	102	BCL	O1A-CGA-O2A-C1
9	8	101	BCL	C2A-CAA-CBA-CGA
9	x	303	BCL	C2A-CAA-CBA-CGA
9	AG	101	BCL	C2A-CAA-CBA-CGA
9	0	102	BCL	C8-C10-C11-C12
9	x	305	BCL	C2B-C3B-CAB-OBB
9	y	401	BCL	O2A-C1-C2-C3
12	x	306	PEF	C1-C2-O2-C10
9	m	103	BCL	C16-C17-C18-C20
9	AC	103	BCL	C16-C17-C18-C20
9	AK	101	BCL	C16-C17-C18-C20
9	l	101	BCL	C16-C17-C18-C19
9	AK	101	BCL	C3-C5-C6-C7
9	S	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	x	301	BCL	C5-C6-C7-C8
9	u	101	BCL	CBA-CGA-O2A-C1
9	Y	101	BCL	C8-C10-C11-C12
9	z	102	BCL	C13-C15-C16-C17
9	l	101	BCL	C2-C1-O2A-CGA
9	AC	103	BCL	C16-C17-C18-C19
9	g	102	BCL	C16-C17-C18-C19
9	x	301	BCL	O1A-CGA-O2A-C1
9	y	401	BCL	O1A-CGA-O2A-C1
9	U	101	BCL	C8-C10-C11-C12
9	AB	102	BCL	C15-C16-C17-C18
9	l	101	BCL	O1A-CGA-O2A-C1
9	x	303	BCL	C8-C10-C11-C12
9	M	402	BCL	C16-C17-C18-C20
9	W	101	BCL	C16-C17-C18-C20
9	m	103	BCL	C16-C17-C18-C19
9	z	102	BCL	C16-C17-C18-C19
9	AE	102	BCL	C16-C17-C18-C20
9	d	101	BCL	C16-C17-C18-C19
9	l	101	BCL	C16-C17-C18-C20
9	A	102	BCL	C5-C6-C7-C8
9	D	102	BCL	C15-C16-C17-C18
9	I	103	BCL	C15-C16-C17-C18
9	Z	102	BCL	C5-C6-C7-C8
9	AI	101	BCL	C15-C16-C17-C18
9	AI	102	BCL	C13-C15-C16-C17
9	8	101	BCL	C6-C7-C8-C10
9	j	101	BCL	C11-C10-C8-C7
12	t	301	PEF	O4-C10-O2-C2
9	8	101	BCL	C8-C10-C11-C12
9	I	103	BCL	C3A-C2A-CAA-CBA
9	q	102	BCL	C3A-C2A-CAA-CBA
10	y	402	BPH	C4-C3-C5-C6
9	F	101	BCL	C10-C11-C12-C13
9	AC	103	BCL	C13-C15-C16-C17
9	l	101	BCL	C8-C10-C11-C12
12	x	306	PEF	C31-C30-O3-C3
9	W	101	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C20
9	AK	101	BCL	C16-C17-C18-C19
9	g	102	BCL	C16-C17-C18-C20
9	3	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C13-C15-C16-C17
9	S	102	BCL	CBA-CGA-O2A-C1
11	L	304	UQ8	C34-C36-C37-C38
9	7	102	BCL	C10-C11-C12-C13
14	y	403	MQ8	C21-C22-C23-C24
9	X	102	BCL	C16-C17-C18-C19
9	AB	101	BCL	C10-C11-C12-C13
7	o	501	HEM	C2A-CAA-CBA-CGA
7	o	502	HEM	C3D-CAD-CBD-CGD
9	Q	101	BCL	C2A-CAA-CBA-CGA
9	r	101	BCL	C2A-CAA-CBA-CGA
9	AI	101	BCL	C10-C11-C12-C13
9	u	101	BCL	O1A-CGA-O2A-C1
9	A	103	BCL	C15-C16-C17-C18
9	W	101	BCL	C2-C3-C5-C6
9	e	102	BCL	C2-C3-C5-C6
10	x	302	BPH	CBA-CGA-O2A-C1
9	S	102	BCL	C6-C7-C8-C9
9	m	103	BCL	C6-C7-C8-C9
9	AI	102	BCL	C6-C7-C8-C9
9	R	102	BCL	C10-C11-C12-C13
9	O	102	BCL	C5-C6-C7-C8
9	AE	102	BCL	C16-C17-C18-C19
9	AI	101	BCL	C16-C17-C18-C20
12	H	302	PEF	O4-C10-O2-C2
9	L	301	BCL	C5-C6-C7-C8
9	x	301	BCL	C13-C15-C16-C17
10	y	402	BPH	C13-C15-C16-C17
15	e	101	CRT	C15-C16-C17-C18
15	M	405	CRT	C1-C4-C5-C6
15	R	101	CRT	C1-C4-C5-C6
9	F	101	BCL	C3-C5-C6-C7
15	V	101	CRT	C22-C23-C25-C26
15	AC	101	CRT	C15-C16-C17-C19
9	Q	101	BCL	C5-C6-C7-C8
9	8	101	BCL	C16-C17-C18-C20
9	u	101	BCL	C16-C17-C18-C20
9	z	102	BCL	C16-C17-C18-C20
9	AC	102	BCL	C16-C17-C18-C20
9	AK	101	BCL	C4-C3-C5-C6
10	x	302	BPH	O1A-CGA-O2A-C1
7	o	501	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	S	101	PGW	O04-C19-O03-C01
14	y	403	MQ8	C15-C16-C17-C18
9	I	101	BCL	C5-C6-C7-C8
9	R	102	BCL	C5-C6-C7-C8
9	2	102	BCL	C8-C10-C11-C12
9	AB	102	BCL	C5-C6-C7-C8
9	2	102	BCL	C13-C15-C16-C17
7	C	502	HEM	C4B-C3B-CAB-CBB
7	o	501	HEM	C4B-C3B-CAB-CBB
7	o	502	HEM	C4B-C3B-CAB-CBB
9	W	101	BCL	C5-C6-C7-C8
9	y	401	BCL	C5-C6-C7-C8
9	m	102	BCL	C15-C16-C17-C18
12	H	305	PEF	O2-C2-C3-O3
9	S	102	BCL	O1A-CGA-O2A-C1
9	L	303	BCL	C5-C6-C7-C8
9	q	102	BCL	C8-C10-C11-C12
9	AC	102	BCL	C2-C1-O2A-CGA
10	M	403	BPH	C2C-C3C-CAC-CBC
10	y	402	BPH	C2C-C3C-CAC-CBC
9	M	401	BCL	C16-C17-C18-C19
9	M	402	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C19
9	AI	101	BCL	C16-C17-C18-C19
9	0	102	BCL	C4-C3-C5-C6
9	U	101	BCL	C2-C3-C5-C6
9	AC	102	BCL	C15-C16-C17-C18
9	L	301	BCL	C13-C15-C16-C17
9	m	102	BCL	C5-C6-C7-C8
9	c	101	BCL	C3-C5-C6-C7
9	L	303	BCL	C1A-C2A-CAA-CBA
9	M	402	BCL	C1A-C2A-CAA-CBA
9	A	103	BCL	C1A-C2A-CAA-CBA
9	G	102	BCL	C1A-C2A-CAA-CBA
9	I	103	BCL	C1A-C2A-CAA-CBA
9	N	101	BCL	C1A-C2A-CAA-CBA
9	T	102	BCL	C1A-C2A-CAA-CBA
9	2	102	BCL	C1A-C2A-CAA-CBA
9	x	303	BCL	C1A-C2A-CAA-CBA
9	x	305	BCL	C1A-C2A-CAA-CBA
9	m	103	BCL	C1A-C2A-CAA-CBA
9	s	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	u	101	BCL	C1A-C2A-CAA-CBA
9	u	102	BCL	C1A-C2A-CAA-CBA
9	z	102	BCL	C1A-C2A-CAA-CBA
9	AB	102	BCL	C1A-C2A-CAA-CBA
9	AC	103	BCL	C1A-C2A-CAA-CBA
9	i	102	BCL	C1A-C2A-CAA-CBA
9	c	101	BCL	C1A-C2A-CAA-CBA
9	X	102	BCL	C5-C6-C7-C8
9	AL	102	BCL	C8-C10-C11-C12
17	S	101	PGW	C01-C02-C03-O11
9	L	301	BCL	C11-C12-C13-C15
9	L	303	BCL	C11-C12-C13-C15
9	D	101	BCL	C6-C7-C8-C10
9	D	102	BCL	C12-C13-C15-C16
9	F	101	BCL	C11-C12-C13-C15
9	X	102	BCL	C12-C13-C15-C16
9	q	102	BCL	C12-C13-C15-C16
9	r	101	BCL	C11-C12-C13-C15
9	AH	101	BCL	C11-C12-C13-C15
9	e	102	BCL	C12-C13-C15-C16
9	f	101	BCL	C11-C12-C13-C15
10	L	302	BPH	C11-C12-C13-C15
10	M	403	BPH	C6-C7-C8-C10
9	I	101	BCL	C2C-C3C-CAC-CBC
9	N	101	BCL	C2C-C3C-CAC-CBC
9	m	102	BCL	C2C-C3C-CAC-CBC
9	s	102	BCL	C2C-C3C-CAC-CBC
9	u	101	BCL	C2C-C3C-CAC-CBC
9	z	102	BCL	C2C-C3C-CAC-CBC
9	AG	101	BCL	C2C-C3C-CAC-CBC
9	AI	102	BCL	C2C-C3C-CAC-CBC
15	M	405	CRT	C2-C1-C4-C5
15	E	101	CRT	C36-C37-C38-C39
15	E	101	CRT	C36-C37-C38-C40
15	G	101	CRT	C2-C1-C4-C5
15	G	101	CRT	C3-C1-C4-C5
15	I	102	CRT	C36-C37-C38-C39
15	X	101	CRT	C36-C37-C38-C39
15	X	101	CRT	C36-C37-C38-C40
15	Z	101	CRT	C36-C37-C38-C39
15	2	101	CRT	C2-C1-C4-C5
15	2	101	CRT	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
15	4	101	CRT	C2-C1-C4-C5
15	0	101	CRT	C2-C1-C4-C5
15	0	101	CRT	C3-C1-C4-C5
15	n	101	CRT	C2-C1-C4-C5
15	q	101	CRT	C2-C1-C4-C5
15	q	101	CRT	C36-C37-C38-C39
15	q	101	CRT	C36-C37-C38-C40
15	AC	101	CRT	C3-C1-C4-C5
15	AH	102	CRT	C36-C37-C38-C39
15	AH	102	CRT	C36-C37-C38-C40
15	AJ	101	CRT	C36-C37-C38-C39
15	AJ	101	CRT	C36-C37-C38-C40
15	g	101	CRT	C36-C37-C38-C39
9	M	402	BCL	C15-C16-C17-C18
9	AB	102	BCL	C10-C11-C12-C13
9	0	102	BCL	C2-C3-C5-C6
9	Q	101	BCL	C10-C11-C12-C13
9	1	101	BCL	C5-C6-C7-C8
9	x	305	BCL	C4B-C3B-CAB-CBB
9	L	301	BCL	C11-C12-C13-C14
9	M	401	BCL	C11-C10-C8-C9
9	D	101	BCL	C6-C7-C8-C9
9	D	102	BCL	C14-C13-C15-C16
9	F	101	BCL	C11-C12-C13-C14
9	K	101	BCL	C11-C10-C8-C9
9	1	101	BCL	C11-C10-C8-C9
9	8	101	BCL	C6-C7-C8-C9
9	0	102	BCL	C11-C12-C13-C14
9	q	102	BCL	C14-C13-C15-C16
9	u	101	BCL	C6-C7-C8-C9
9	AB	102	BCL	C11-C10-C8-C9
9	AH	101	BCL	C11-C12-C13-C14
9	f	101	BCL	C11-C12-C13-C14
15	X	101	CRT	C17-C19-C20-C21
12	H	302	PEF	C31-C30-O3-C3
11	L	304	UQ8	C39-C41-C42-C43
12	H	304	PEF	C1-C2-C3-O3
15	y	404	CRT	C37-C38-O2-C2M
9	j	101	BCL	C15-C16-C17-C18
9	M	401	BCL	CBA-CGA-O2A-C1
9	L	303	BCL	C16-C17-C18-C19
9	x	303	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
17	S	101	PGW	C02-C01-O03-C19
9	AF	101	BCL	C5-C6-C7-C8
9	U	101	BCL	C4-C3-C5-C6
9	g	102	BCL	C2-C3-C5-C6
14	y	403	MQ8	C37-C38-C40-C41
15	V	101	CRT	C24-C23-C25-C26
15	AF	102	CRT	C5-C6-C7-C8
9	R	102	BCL	C16-C17-C18-C20
15	P	102	CRT	C27-C28-C30-C31
15	AH	102	CRT	C5-C6-C7-C9
9	L	303	BCL	C13-C15-C16-C17
9	A	102	BCL	C8-C10-C11-C12
9	T	102	BCL	C13-C15-C16-C17
9	f	101	BCL	C8-C10-C11-C12
9	S	102	BCL	C2A-CAA-CBA-CGA
9	M	402	BCL	CBA-CGA-O2A-C1
9	A	103	BCL	O2A-C1-C2-C3
9	m	103	BCL	O2A-C1-C2-C3
9	AG	101	BCL	O2A-C1-C2-C3
10	M	403	BPH	O2A-C1-C2-C3
17	AE	101	PGW	C03-C02-O01-C1
9	U	101	BCL	C10-C11-C12-C13
9	0	102	BCL	C15-C16-C17-C18
7	C	504	HEM	C4D-C3D-CAD-CBD
9	AF	101	BCL	CBA-CGA-O2A-C1
10	y	402	BPH	CBA-CGA-O2A-C1
14	y	403	MQ8	C22-C23-C25-C26
9	L	303	BCL	C16-C17-C18-C20
9	u	101	BCL	C16-C17-C18-C19
9	3	101	BCL	C2A-CAA-CBA-CGA
9	AL	102	BCL	C13-C15-C16-C17
15	M	405	CRT	C2-C1-O1-C1M
15	G	101	CRT	C2-C1-O1-C1M
15	I	102	CRT	C3-C1-O1-C1M
15	R	101	CRT	C2-C1-O1-C1M
15	T	101	CRT	C2-C1-O1-C1M
15	V	101	CRT	C2-C1-O1-C1M
15	4	101	CRT	C2-C1-O1-C1M
15	7	101	CRT	C3-C1-O1-C1M
15	7	103	CRT	C2-C1-O1-C1M
15	9	101	CRT	C2-C1-O1-C1M
15	y	404	CRT	C3-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
15	y	404	CRT	C39-C38-O2-C2M
15	m	104	CRT	C2-C1-O1-C1M
15	q	101	CRT	C3-C1-O1-C1M
15	s	101	CRT	C2-C1-O1-C1M
15	v	101	CRT	C3-C1-O1-C1M
15	z	101	CRT	C2-C1-O1-C1M
15	AC	101	CRT	C2-C1-O1-C1M
15	AF	102	CRT	C2-C1-O1-C1M
15	AH	102	CRT	C39-C38-O2-C2M
15	AH	102	CRT	C40-C38-O2-C2M
15	AJ	101	CRT	C3-C1-O1-C1M
15	e	101	CRT	C2-C1-O1-C1M
15	i	101	CRT	C3-C1-O1-C1M
15	k	101	CRT	C2-C1-O1-C1M
9	V	102	BCL	C15-C16-C17-C18
9	AL	102	BCL	C15-C16-C17-C18
9	AH	101	BCL	C4-C3-C5-C6
9	g	102	BCL	C4-C3-C5-C6
10	x	302	BPH	C4-C3-C5-C6
11	x	304	UQ8	C20-C19-C21-C22
17	AE	101	PGW	C20-C19-O03-C01
9	1	101	BCL	C15-C16-C17-C18
9	O	102	BCL	C11-C12-C13-C14
9	m	102	BCL	C11-C10-C8-C9
9	p	102	BCL	C6-C7-C8-C9
9	u	102	BCL	C11-C12-C13-C14
9	AC	103	BCL	C11-C12-C13-C14
9	g	102	BCL	C11-C12-C13-C14
9	j	101	BCL	C11-C10-C8-C9
10	L	302	BPH	C11-C12-C13-C14
10	M	403	BPH	C6-C7-C8-C9
10	y	402	BPH	C11-C10-C8-C9
12	x	306	PEF	O5-C30-O3-C3
9	3	101	BCL	C8-C10-C11-C12
9	c	101	BCL	C8-C10-C11-C12
10	L	302	BPH	CBA-CGA-O2A-C1
9	AB	102	BCL	C8-C10-C11-C12
9	M	402	BCL	CAA-CBA-CGA-O2A
9	M	401	BCL	C11-C10-C8-C7
9	K	101	BCL	C11-C10-C8-C7
9	O	102	BCL	C11-C12-C13-C15
9	1	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	C11-C12-C13-C15
9	9	102	BCL	C12-C13-C15-C16
9	0	102	BCL	C11-C12-C13-C15
9	m	102	BCL	C11-C10-C8-C7
9	p	102	BCL	C6-C7-C8-C10
9	s	102	BCL	C11-C12-C13-C15
9	u	102	BCL	C11-C12-C13-C15
9	AB	102	BCL	C11-C10-C8-C7
9	AB	102	BCL	C11-C12-C13-C15
9	AC	103	BCL	C11-C12-C13-C15
9	g	102	BCL	C11-C12-C13-C15
10	L	302	BPH	C6-C7-C8-C10
10	y	402	BPH	C11-C10-C8-C7
9	W	101	BCL	C8-C10-C11-C12
9	3	101	BCL	C13-C15-C16-C17
9	u	101	BCL	C8-C10-C11-C12
9	l	101	BCL	C15-C16-C17-C18
9	m	102	BCL	C3-C5-C6-C7
9	Y	101	BCL	C3A-C2A-CAA-CBA
9	m	102	BCL	C3A-C2A-CAA-CBA
9	AG	101	BCL	C3A-C2A-CAA-CBA
9	g	102	BCL	C3A-C2A-CAA-CBA
14	y	403	MQ8	C39-C38-C40-C41
9	AH	101	BCL	C5-C6-C7-C8
14	M	404	MQ8	C22-C23-C25-C26
9	M	401	BCL	O1A-CGA-O2A-C1
9	z	102	BCL	C10-C11-C12-C13
9	AH	101	BCL	CBA-CGA-O2A-C1
15	AH	102	CRT	C25-C26-C27-C28
15	AJ	101	CRT	C20-C21-C22-C23
9	x	305	BCL	C13-C15-C16-C17
12	M	408	PEF	C1-C2-C3-O3
12	H	305	PEF	C1-C2-C3-O3
9	U	101	BCL	C3-C5-C6-C7
9	X	102	BCL	C16-C17-C18-C20
10	y	402	BPH	C1A-C2A-CAA-CBA
9	1	101	BCL	C4-C3-C5-C6
14	M	404	MQ8	C24-C23-C25-C26
11	x	304	UQ8	C18-C19-C21-C22
12	H	301	PEF	C31-C30-O3-C3
9	x	303	BCL	C16-C17-C18-C19
17	S	101	PGW	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
9	X	102	BCL	C13-C15-C16-C17
9	6	101	BCL	C5-C6-C7-C8
9	AK	101	BCL	C8-C10-C11-C12
9	8	101	BCL	C16-C17-C18-C19
9	K	101	BCL	C10-C11-C12-C13
9	c	101	BCL	C10-C11-C12-C13
9	AH	101	BCL	C2-C3-C5-C6
10	x	302	BPH	C2-C3-C5-C6
9	q	102	BCL	C16-C17-C18-C19
9	N	101	BCL	C6-C7-C8-C9
9	X	102	BCL	C11-C10-C8-C9
9	r	101	BCL	C11-C12-C13-C14
9	AF	101	BCL	C14-C13-C15-C16
9	f	101	BCL	C11-C10-C8-C9
9	k	102	BCL	C6-C7-C8-C9
9	9	102	BCL	C5-C6-C7-C8
9	AF	101	BCL	O1A-CGA-O2A-C1
9	M	401	BCL	C4C-C3C-CAC-CBC
9	F	101	BCL	C4C-C3C-CAC-CBC
9	P	101	BCL	C4C-C3C-CAC-CBC
9	T	102	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C4C-C3C-CAC-CBC
9	x	303	BCL	C4C-C3C-CAC-CBC
9	AC	103	BCL	C4C-C3C-CAC-CBC
9	AH	101	BCL	C4C-C3C-CAC-CBC
9	AI	101	BCL	C4C-C3C-CAC-CBC
9	h	101	BCL	C4C-C3C-CAC-CBC
9	i	102	BCL	C4C-C3C-CAC-CBC
9	O	102	BCL	C15-C16-C17-C18
15	4	101	CRT	C11-C10-C9-C7
9	I	101	BCL	C2-C3-C5-C6
9	M	401	BCL	C16-C17-C18-C20
10	y	402	BPH	O1A-CGA-O2A-C1
9	AL	102	BCL	C3-C5-C6-C7
12	M	408	PEF	O3P-C1-C2-C3
17	AE	101	PGW	C01-C02-C03-O11
9	0	102	BCL	C10-C11-C12-C13
15	E	101	CRT	C5-C6-C7-C8
9	I	103	BCL	C11-C10-C8-C7
9	X	102	BCL	C11-C10-C8-C7
9	w	101	BCL	C11-C10-C8-C7
9	AF	101	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
9	f	101	BCL	C11-C10-C8-C7
9	k	102	BCL	C6-C7-C8-C10
10	M	403	BPH	C11-C12-C13-C15
15	V	101	CRT	C35-C36-C37-C38
15	AL	101	CRT	C35-C36-C37-C38
15	X	101	CRT	C22-C23-C25-C26
15	4	101	CRT	C15-C16-C17-C19
15	7	101	CRT	C27-C28-C30-C31
15	v	101	CRT	C5-C6-C7-C9
15	AL	101	CRT	C5-C6-C7-C9
15	e	101	CRT	C15-C16-C17-C19
15	e	101	CRT	C22-C23-C25-C26
15	k	101	CRT	C10-C11-C12-C14
9	r	101	BCL	CBA-CGA-O2A-C1
10	M	403	BPH	CBA-CGA-O2A-C1
7	o	503	HEM	C3D-CAD-CBD-CGD
9	M	402	BCL	O1A-CGA-O2A-C1
10	M	403	BPH	O1A-CGA-O2A-C1
10	y	402	BPH	C2-C3-C5-C6
9	q	102	BCL	O2A-C1-C2-C3
9	P	101	BCL	C16-C17-C18-C20
9	AH	101	BCL	O1A-CGA-O2A-C1
10	L	302	BPH	O1A-CGA-O2A-C1
9	AK	101	BCL	C15-C16-C17-C18
9	I	101	BCL	C4-C3-C5-C6
10	L	302	BPH	C4-C3-C5-C6
14	y	403	MQ8	C24-C23-C25-C26
12	M	408	PEF	O2-C2-C3-O3
12	H	304	PEF	O2-C2-C3-O3
12	t	303	PEF	O2-C2-C3-O3
9	9	102	BCL	C14-C13-C15-C16
10	L	302	BPH	C6-C7-C8-C9
9	e	102	BCL	C5-C6-C7-C8
15	M	405	CRT	O1-C1-C4-C5
15	M	405	CRT	C36-C37-C38-O2
15	E	101	CRT	C36-C37-C38-O2
15	G	101	CRT	O1-C1-C4-C5
15	X	101	CRT	C36-C37-C38-O2
15	4	101	CRT	O1-C1-C4-C5
15	y	404	CRT	C36-C37-C38-O2
15	q	101	CRT	C36-C37-C38-O2
15	AH	102	CRT	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
15	AH	102	CRT	C36-C37-C38-O2
9	m	103	BCL	C10-C11-C12-C13
9	x	303	BCL	C10-C11-C12-C13
7	C	504	HEM	C2D-C3D-CAD-CBD
11	x	304	UQ8	C12-C11-C9-C10
9	AC	102	BCL	C10-C11-C12-C13
9	U	101	BCL	C2A-CAA-CBA-CGA
9	p	102	BCL	C16-C17-C18-C19
9	AC	102	BCL	C16-C17-C18-C19
10	M	403	BPH	CBD-CGD-O2D-CED
15	0	101	CRT	C15-C16-C17-C18
9	AK	101	BCL	C2-C3-C5-C6
10	L	302	BPH	C2-C3-C5-C6
15	0	101	CRT	C15-C16-C17-C19
15	V	101	CRT	C17-C19-C20-C21
10	x	302	BPH	C8-C10-C11-C12
7	o	504	HEM	C4D-C3D-CAD-CBD
12	H	304	PEF	O3P-C1-C2-C3
9	M	401	BCL	C6-C7-C8-C10
9	A	102	BCL	C11-C10-C8-C7
9	N	101	BCL	C11-C10-C8-C7
9	P	101	BCL	C11-C12-C13-C15
9	T	102	BCL	C11-C10-C8-C7
9	6	101	BCL	C6-C7-C8-C10
9	7	102	BCL	C11-C12-C13-C15
9	w	101	BCL	C11-C12-C13-C15
9	AB	101	BCL	C11-C12-C13-C15
9	AG	101	BCL	C11-C12-C13-C15
9	AI	102	BCL	C11-C10-C8-C7
9	AL	102	BCL	C6-C7-C8-C10
9	c	101	BCL	C11-C12-C13-C15
9	5	101	BCL	C2C-C3C-CAC-CBC
9	f	101	BCL	C2C-C3C-CAC-CBC
9	g	102	BCL	C2C-C3C-CAC-CBC
15	M	405	CRT	C36-C37-C38-C40
15	G	101	CRT	C36-C37-C38-C39
15	n	101	CRT	C3-C1-C4-C5
9	r	101	BCL	O1A-CGA-O2A-C1
9	R	102	BCL	C4-C3-C5-C6
11	x	304	UQ8	C15-C14-C16-C17
9	R	102	BCL	C16-C17-C18-C19
12	M	408	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	s	102	BCL	C11-C12-C13-C14
9	AB	102	BCL	C11-C12-C13-C14
9	AG	101	BCL	C11-C12-C13-C14
9	W	101	BCL	C13-C15-C16-C17
15	0	101	CRT	C25-C26-C27-C28
12	t	301	PEF	O2-C2-C3-O3
9	P	101	BCL	C16-C17-C18-C19
9	Q	101	BCL	C16-C17-C18-C20
12	x	306	PEF	C1-C2-C3-O3
12	m	101	PEF	C1-C2-C3-O3
9	M	402	BCL	CAD-CBD-CGD-O2D
9	x	303	BCL	CAD-CBD-CGD-O2D
9	j	101	BCL	C13-C15-C16-C17
9	M	401	BCL	CHA-CBD-CGD-O1D
9	M	402	BCL	CAD-CBD-CGD-O1D
9	x	303	BCL	CAD-CBD-CGD-O1D
9	AF	101	BCL	CHA-CBD-CGD-O1D
9	AF	101	BCL	CHA-CBD-CGD-O2D
9	f	101	BCL	CAD-CBD-CGD-O1D
9	k	102	BCL	CHA-CBD-CGD-O1D
9	k	102	BCL	CHA-CBD-CGD-O2D
12	L	305	PEF	C1-O3P-P-O1P
12	M	407	PEF	C1-O3P-P-O1P
12	M	408	PEF	C4-O4P-P-O1P
12	H	301	PEF	C1-O3P-P-O1P
12	H	301	PEF	C4-O4P-P-O2P
12	H	301	PEF	C4-O4P-P-O3P
12	A	101	PEF	O4P-C4-C5-N
12	A	101	PEF	C1-O3P-P-O1P
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	C4-O4P-P-O1P
12	t	303	PEF	C4-O4P-P-O3P
15	E	101	CRT	C11-C10-C9-C7
15	7	101	CRT	C25-C26-C27-C28
15	AL	101	CRT	C30-C31-C32-C33
17	S	101	PGW	C03-O11-P-O14
17	S	101	PGW	C04-O12-P-O14
9	g	102	BCL	C15-C16-C17-C18
9	x	301	BCL	C4-C3-C5-C6
12	H	305	PEF	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
9	AH	101	BCL	C16-C17-C18-C20
9	7	102	BCL	C13-C15-C16-C17
9	Z	102	BCL	C13-C15-C16-C17
9	N	101	BCL	O2A-C1-C2-C3
15	R	101	CRT	C14-C15-C16-C17
15	X	101	CRT	C9-C10-C11-C12
15	4	101	CRT	C28-C30-C31-C32
15	AD	101	CRT	C14-C15-C16-C17
15	AJ	101	CRT	C9-C10-C11-C12
15	g	101	CRT	C28-C30-C31-C32
9	AL	102	BCL	C5-C6-C7-C8
15	X	101	CRT	C12-C14-C15-C16
15	m	104	CRT	C11-C10-C9-C7
9	L	303	BCL	C11-C12-C13-C14
9	L	303	BCL	C14-C13-C15-C16
9	P	101	BCL	C11-C12-C13-C14
9	W	101	BCL	C11-C10-C8-C9
9	7	102	BCL	C11-C12-C13-C14
9	m	103	BCL	C14-C13-C15-C16
9	w	101	BCL	C11-C12-C13-C14
9	z	102	BCL	C6-C7-C8-C9
9	AE	102	BCL	C6-C7-C8-C9
9	AI	102	BCL	C11-C10-C8-C9
9	c	101	BCL	C11-C12-C13-C14
10	M	403	BPH	C11-C12-C13-C14
12	H	302	PEF	O5-C30-O3-C3
9	Y	101	BCL	C11-C12-C13-C15
9	y	401	BCL	C6-C7-C8-C10
9	z	102	BCL	C12-C13-C15-C16
9	AF	101	BCL	C6-C7-C8-C10
9	i	102	BCL	C11-C12-C13-C15
10	L	302	BPH	C11-C10-C8-C7
12	H	302	PEF	O3P-C1-C2-O2
17	AE	101	PGW	O01-C02-C03-O11
9	AG	101	BCL	C16-C17-C18-C19
9	AH	101	BCL	C16-C17-C18-C19
15	m	104	CRT	C25-C26-C27-C28
12	M	408	PEF	C2-C3-O3-C30
7	o	504	HEM	C2D-C3D-CAD-CBD
9	F	101	BCL	C2A-CAA-CBA-CGA
14	y	403	MQ8	C43-C44-C46-C47
15	G	101	CRT	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
15	O	101	CRT	C1-C4-C5-C6
15	T	101	CRT	C39-C38-O2-C2M
15	V	101	CRT	C39-C38-O2-C2M
15	9	101	CRT	C39-C38-O2-C2M
15	y	404	CRT	C40-C38-O2-C2M
15	z	101	CRT	C1-C4-C5-C6
15	AC	101	CRT	C3-C1-O1-C1M
15	AJ	101	CRT	C2-C1-O1-C1M
15	e	101	CRT	C3-C1-O1-C1M
14	y	403	MQ8	C46-C47-C48-C50
9	AC	103	BCL	C2A-CAA-CBA-CGA
12	y	406	PEF	C31-C30-O3-C3
11	x	304	UQ8	C13-C14-C16-C17
11	x	304	UQ8	C12-C11-C9-C8
9	A	102	BCL	C11-C10-C8-C9
9	O	102	BCL	C11-C10-C8-C9
9	AB	101	BCL	C11-C12-C13-C14
9	AF	101	BCL	C6-C7-C8-C9
9	AL	102	BCL	C6-C7-C8-C9
10	L	302	BPH	C11-C10-C8-C9
9	3	101	BCL	C10-C11-C12-C13
9	F	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C30-C29-C31-C32
9	1	101	BCL	C2-C3-C5-C6
7	C	501	HEM	C4B-C3B-CAB-CBB
9	7	102	BCL	C11-C10-C8-C7
9	x	305	BCL	C11-C12-C13-C15
9	u	101	BCL	C11-C10-C8-C7
9	k	102	BCL	C11-C12-C13-C15
9	x	305	BCL	C8-C10-C11-C12
9	M	401	BCL	C13-C15-C16-C17
9	l	101	BCL	C3-C5-C6-C7
9	r	101	BCL	C4-C3-C5-C6
9	1	101	BCL	C2A-CAA-CBA-CGA
10	L	302	BPH	C13-C15-C16-C17
9	r	101	BCL	C16-C17-C18-C19
15	R	101	CRT	C13-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C34
15	7	103	CRT	C21-C22-C23-C24
15	AD	101	CRT	C13-C12-C14-C15
15	g	101	CRT	C31-C32-C33-C34
15	k	101	CRT	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
9	7	102	BCL	C5-C6-C7-C8
9	D	102	BCL	C2-C1-O2A-CGA
15	M	405	CRT	C25-C26-C27-C28
15	Z	101	CRT	C12-C14-C15-C16
15	AJ	101	CRT	C30-C31-C32-C33
15	k	101	CRT	C25-C26-C27-C28
15	AC	101	CRT	C10-C11-C12-C13
17	AE	101	PGW	O04-C19-O03-C01
9	R	102	BCL	C2-C3-C5-C6
9	x	301	BCL	C2-C3-C5-C6
14	M	404	MQ8	C42-C43-C44-C46
12	H	301	PEF	O5-C30-O3-C3
9	M	402	BCL	CAA-CBA-CGA-O1A
9	X	102	BCL	C6-C7-C8-C9
9	2	102	BCL	C6-C7-C8-C9
9	7	102	BCL	C11-C10-C8-C9
9	y	401	BCL	C6-C7-C8-C9
9	u	101	BCL	C11-C10-C8-C9
9	w	101	BCL	C6-C7-C8-C9
9	AC	102	BCL	C6-C7-C8-C9
9	AC	102	BCL	C11-C10-C8-C9
9	W	101	BCL	C15-C16-C17-C18
9	x	305	BCL	C2B-C3B-CAB-CBB
9	c	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C28-C29-C31-C32
9	q	102	BCL	C3-C5-C6-C7
9	4	102	BCL	C2A-CAA-CBA-CGA
9	c	101	BCL	C2A-CAA-CBA-CGA
9	Y	101	BCL	C1A-C2A-CAA-CBA
9	AG	101	BCL	C1A-C2A-CAA-CBA
9	g	102	BCL	C1A-C2A-CAA-CBA
15	R	101	CRT	C11-C12-C14-C15
15	4	101	CRT	C31-C32-C33-C35
15	7	103	CRT	C21-C22-C23-C25
15	AD	101	CRT	C11-C12-C14-C15
15	g	101	CRT	C31-C32-C33-C35
15	k	101	CRT	C21-C22-C23-C25
7	o	501	HEM	CAA-CBA-CGA-O1A
9	h	101	BCL	C4-C3-C5-C6
9	l	101	BCL	C4-C3-C5-C6
11	L	304	UQ8	C20-C19-C21-C22
9	F	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	r	101	BCL	C2-C3-C5-C6
9	L	303	BCL	C12-C13-C15-C16
9	A	102	BCL	C11-C12-C13-C15
9	N	101	BCL	C11-C12-C13-C15
9	O	102	BCL	C11-C10-C8-C7
9	m	103	BCL	C11-C12-C13-C15
9	AH	101	BCL	C6-C7-C8-C10
9	d	101	BCL	C11-C10-C8-C7
9	l	101	BCL	C11-C10-C8-C7
12	M	408	PEF	C11-C10-O2-C2
9	U	101	BCL	C5-C6-C7-C8
9	p	102	BCL	C2C-C3C-CAC-CBC
15	M	405	CRT	C36-C37-C38-C39
15	I	102	CRT	C36-C37-C38-C40
15	0	101	CRT	C36-C37-C38-C39
9	O	102	BCL	C8-C10-C11-C12
15	T	101	CRT	C5-C6-C7-C8
15	AD	101	CRT	C5-C6-C7-C8
15	AL	101	CRT	C10-C11-C12-C13
9	m	103	BCL	C3-C5-C6-C7
9	2	102	BCL	C15-C16-C17-C18
14	M	404	MQ8	C37-C38-C40-C41
9	8	101	BCL	C2-C1-O2A-CGA
10	x	302	BPH	C3-C5-C6-C7
7	C	502	HEM	CAA-CBA-CGA-O2A
9	e	102	BCL	C14-C13-C15-C16
9	i	102	BCL	C11-C12-C13-C14
15	y	404	CRT	C20-C21-C22-C23
9	8	101	BCL	C4-C3-C5-C6
9	AC	103	BCL	C4-C3-C5-C6
9	j	101	BCL	C4-C3-C5-C6
9	k	102	BCL	C4-C3-C5-C6
11	x	304	UQ8	C25-C24-C26-C27
7	C	501	HEM	C2A-CAA-CBA-CGA
7	o	503	HEM	CAA-CBA-CGA-O2A
9	x	305	BCL	C2A-CAA-CBA-CGA
12	H	304	PEF	O3P-C1-C2-O2
9	K	101	BCL	C4-C3-C5-C6
15	AJ	101	CRT	C12-C14-C15-C16
15	i	101	CRT	C11-C10-C9-C7
7	C	501	HEM	CAA-CBA-CGA-O1A
9	Y	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	AI	102	BCL	C16-C17-C18-C20
9	j	101	BCL	C8-C10-C11-C12
7	C	501	HEM	CAD-CBD-CGD-O2D
7	C	502	HEM	CAA-CBA-CGA-O1A
9	G	102	BCL	C16-C17-C18-C20
14	M	404	MQ8	C26-C27-C28-C30
17	AE	101	PGW	O12-C04-C05-CAD
7	o	501	HEM	CAA-CBA-CGA-O2A
7	o	501	HEM	CAD-CBD-CGD-O2D
12	H	302	PEF	O3P-C1-C2-C3
9	K	101	BCL	C16-C17-C18-C19
11	x	304	UQ8	C30-C29-C31-C32
12	m	101	PEF	O2-C2-C3-O3
9	j	101	BCL	C2-C3-C5-C6
11	x	304	UQ8	C23-C24-C26-C27
9	c	101	BCL	C15-C16-C17-C18
15	AD	101	CRT	C35-C36-C37-C38
15	e	101	CRT	C12-C14-C15-C16
15	y	404	CRT	C22-C23-C25-C26
9	L	301	BCL	C14-C13-C15-C16
9	N	101	BCL	C11-C10-C8-C9
9	T	102	BCL	C11-C10-C8-C9
9	4	102	BCL	C11-C12-C13-C14
9	x	301	BCL	C6-C7-C8-C9
9	z	102	BCL	C14-C13-C15-C16
10	y	402	BPH	C11-C12-C13-C14
9	8	101	BCL	C5-C6-C7-C8
9	AB	101	BCL	C2A-CAA-CBA-CGA
9	AI	102	BCL	C2A-CAA-CBA-CGA
9	AK	101	BCL	C2A-CAA-CBA-CGA
9	V	102	BCL	C2-C1-O2A-CGA
9	m	102	BCL	C2-C1-O2A-CGA
9	s	102	BCL	C2-C1-O2A-CGA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	AI	101	BCL	CAA-CBA-CGA-O2A
7	C	501	HEM	CAD-CBD-CGD-O1D
7	o	503	HEM	CAA-CBA-CGA-O1A
9	P	101	BCL	C13-C15-C16-C17
10	x	302	BPH	C15-C16-C17-C18
11	x	304	UQ8	C29-C31-C32-C33
9	q	102	BCL	C16-C17-C18-C20
9	7	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	o	501	HEM	CAD-CBD-CGD-O1D
9	m	102	BCL	C2A-CAA-CBA-CGA
15	AC	101	CRT	C25-C26-C27-C28
9	I	103	BCL	C11-C10-C8-C9
9	u	101	BCL	C14-C13-C15-C16
9	u	102	BCL	C6-C7-C8-C9
9	w	101	BCL	C11-C10-C8-C9
9	AB	102	BCL	C6-C7-C8-C9
9	AH	101	BCL	C6-C7-C8-C9
15	AF	102	CRT	C5-C6-C7-C9
15	I	102	CRT	O1-C1-C4-C5
15	0	101	CRT	O1-C1-C4-C5
15	n	101	CRT	O1-C1-C4-C5
15	v	101	CRT	O1-C1-C4-C5
15	AD	101	CRT	C36-C37-C38-O2
15	AJ	101	CRT	C36-C37-C38-O2
9	8	101	BCL	C2-C3-C5-C6
9	AC	103	BCL	C2-C3-C5-C6
9	G	102	BCL	C11-C12-C13-C15
9	S	102	BCL	C12-C13-C15-C16
9	U	101	BCL	C12-C13-C15-C16
9	4	102	BCL	C11-C12-C13-C15
9	6	101	BCL	C11-C12-C13-C15
9	q	102	BCL	C6-C7-C8-C10
9	AC	102	BCL	C11-C10-C8-C7
9	AG	101	BCL	C12-C13-C15-C16
10	y	402	BPH	C11-C12-C13-C15
9	F	101	BCL	C2-C1-O2A-CGA
9	T	102	BCL	C2-C1-O2A-CGA
9	U	101	BCL	C2-C1-O2A-CGA
9	Z	102	BCL	C2-C1-O2A-CGA
9	x	303	BCL	C2-C1-O2A-CGA
9	AH	101	BCL	C2-C1-O2A-CGA
9	Q	101	BCL	C16-C17-C18-C19
9	j	101	BCL	C5-C6-C7-C8
9	w	101	BCL	O1A-CGA-O2A-C1
9	j	101	BCL	C16-C17-C18-C20
14	M	404	MQ8	C27-C28-C30-C31
15	M	405	CRT	C3-C1-O1-C1M
15	7	103	CRT	C40-C38-O2-C2M
15	9	101	CRT	C40-C38-O2-C2M
15	AL	101	CRT	C39-C38-O2-C2M

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Mol	Chain	Res	Type	Atoms
9	w	101	BCL	C10-C11-C12-C13
9	A	102	BCL	CAA-CBA-CGA-O2A
9	x	301	BCL	C2A-CAA-CBA-CGA
9	p	102	BCL	C10-C11-C12-C13
9	q	102	BCL	C6-C7-C8-C9
9	d	101	BCL	C6-C7-C8-C9
9	l	101	BCL	C6-C7-C8-C9
9	l	101	BCL	C11-C10-C8-C9
15	R	101	CRT	C10-C11-C12-C13
11	L	304	UQ8	C19-C21-C22-C23
9	m	102	BCL	C1A-C2A-CAA-CBA
12	y	406	PEF	O5-C30-O3-C3
9	u	101	BCL	C4-C3-C5-C6
15	X	101	CRT	C10-C11-C12-C14
15	y	404	CRT	C5-C6-C7-C9
15	v	101	CRT	C15-C16-C17-C19
15	AC	101	CRT	C10-C11-C12-C14
15	AD	101	CRT	C5-C6-C7-C9
9	1	101	BCL	CAA-CBA-CGA-O2A
9	AC	102	BCL	CAA-CBA-CGA-O2A
9	i	102	BCL	CAA-CBA-CGA-O2A
9	j	101	BCL	CAA-CBA-CGA-O2A
9	D	101	BCL	C5-C6-C7-C8
9	Z	102	BCL	C10-C11-C12-C13
9	k	102	BCL	C5-C6-C7-C8
9	P	101	BCL	C4-C3-C5-C6
9	Q	101	BCL	C12-C13-C15-C16
9	3	101	BCL	C11-C10-C8-C7
9	3	101	BCL	C12-C13-C15-C16
9	s	102	BCL	C6-C7-C8-C10
9	u	101	BCL	C12-C13-C15-C16
9	AL	102	BCL	C11-C12-C13-C15
9	e	102	BCL	C11-C12-C13-C15
9	c	101	BCL	C6-C7-C8-C10
10	M	403	BPH	C11-C10-C8-C7
9	h	101	BCL	C2-C3-C5-C6
9	AB	102	BCL	C16-C17-C18-C20
10	L	302	BPH	O2A-C1-C2-C3
12	t	301	PEF	C1-C2-O2-C10
12	t	301	PEF	C3-C2-O2-C10
17	S	101	PGW	C03-C02-O01-C1
9	0	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2C-C3C-CAC-CBC
9	q	102	BCL	C2C-C3C-CAC-CBC
15	4	101	CRT	C36-C37-C38-C39
15	y	404	CRT	C2-C1-C4-C5
15	AD	101	CRT	C36-C37-C38-C40
15	e	101	CRT	C36-C37-C38-C39
15	i	101	CRT	C2-C1-C4-C5
9	e	102	BCL	C2A-CAA-CBA-CGA
9	7	102	BCL	C16-C17-C18-C20
9	y	401	BCL	C16-C17-C18-C20
7	C	501	HEM	CAA-CBA-CGA-O2A
9	Z	102	BCL	C16-C17-C18-C19
7	C	503	HEM	CAA-CBA-CGA-O2A
9	5	101	BCL	C8-C10-C11-C12
14	y	403	MQ8	C25-C26-C27-C28
9	w	101	BCL	CBA-CGA-O2A-C1
9	G	102	BCL	C11-C12-C13-C14
9	Q	101	BCL	C14-C13-C15-C16
9	S	102	BCL	C14-C13-C15-C16
9	x	305	BCL	C11-C12-C13-C14
9	s	102	BCL	C6-C7-C8-C9
9	AG	101	BCL	C14-C13-C15-C16
9	AL	102	BCL	C11-C12-C13-C14
7	o	504	HEM	CAA-CBA-CGA-O2A
9	c	101	BCL	C2-C3-C5-C6
9	K	101	BCL	C13-C15-C16-C17
9	x	305	BCL	C15-C16-C17-C18
15	X	101	CRT	C35-C36-C37-C38
15	2	101	CRT	C1-C4-C5-C6
15	s	101	CRT	C1-C4-C5-C6
15	AJ	101	CRT	C35-C36-C37-C38
9	A	102	BCL	CAA-CBA-CGA-O1A
9	M	402	BCL	C13-C15-C16-C17
9	Y	101	BCL	C15-C16-C17-C18
7	C	504	HEM	CAD-CBD-CGD-O2D
9	AC	102	BCL	CAA-CBA-CGA-O1A
9	f	101	BCL	CAA-CBA-CGA-O2A
7	C	501	HEM	C2B-C3B-CAB-CBB
11	x	304	UQ8	C28-C29-C31-C32
9	G	102	BCL	CAD-CBD-CGD-O2D
9	u	101	BCL	CAD-CBD-CGD-O2D
9	f	101	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	k	102	BCL	CAD-CBD-CGD-O2D
7	C	504	HEM	CAA-CBA-CGA-O1A
10	M	403	BPH	O1D-CGD-O2D-CED
9	i	102	BCL	CAA-CBA-CGA-O1A
9	1	101	BCL	CAA-CBA-CGA-O1A
9	f	101	BCL	CAA-CBA-CGA-O1A
9	5	101	BCL	C10-C11-C12-C13
9	6	101	BCL	C10-C11-C12-C13
9	Y	101	BCL	CAA-CBA-CGA-O2A
9	4	102	BCL	CAA-CBA-CGA-O2A
7	C	504	HEM	CAD-CBD-CGD-O1D
9	S	102	BCL	CAA-CBA-CGA-O2A
9	w	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

141 monomers are involved in 1144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	AC	101	CRT	11	0
7	o	502	HEM	6	0
9	m	102	BCL	5	0
9	j	101	BCL	8	0
9	AG	101	BCL	6	0
9	y	401	BCL	16	0
12	p	101	PEF	7	0
15	4	101	CRT	14	0
12	M	408	PEF	2	0
9	AK	101	BCL	9	0
12	x	306	PEF	11	0
10	L	302	BPH	5	0
15	7	103	CRT	11	0
9	W	101	BCL	8	0
9	u	101	BCL	10	0
9	A	103	BCL	7	0
9	P	101	BCL	6	0
9	AB	102	BCL	9	0
9	p	102	BCL	12	0
9	z	102	BCL	6	0
9	0	102	BCL	5	0
9	x	301	BCL	14	0
12	H	305	PEF	7	0
7	C	502	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	101	BCL	9	0
9	r	101	BCL	11	0
9	w	101	BCL	8	0
9	AL	102	BCL	11	0
9	9	102	BCL	8	0
9	I	103	BCL	15	0
11	x	304	UQ8	18	0
12	t	301	PEF	3	0
10	M	403	BPH	14	0
9	AC	103	BCL	6	0
9	O	102	BCL	6	0
15	M	405	CRT	13	0
15	O	101	CRT	9	0
12	m	101	PEF	3	0
15	Z	101	CRT	8	0
7	o	503	HEM	5	0
9	m	103	BCL	12	0
15	AD	101	CRT	8	0
9	2	102	BCL	9	0
17	S	101	PGW	3	0
15	T	101	CRT	11	0
9	7	102	BCL	7	0
12	y	407	PEF	3	0
15	V	101	CRT	10	0
12	A	101	PEF	2	0
9	q	102	BCL	11	0
12	H	302	PEF	11	0
12	H	304	PEF	2	0
9	6	101	BCL	10	0
9	h	101	BCL	8	0
9	G	102	BCL	12	0
15	AL	101	CRT	10	0
17	AE	101	PGW	2	0
15	AH	102	CRT	9	0
9	R	102	BCL	5	0
15	g	101	CRT	12	0
9	d	101	BCL	12	0
15	n	101	CRT	17	0
15	R	101	CRT	11	0
9	L	303	BCL	10	0
9	s	102	BCL	11	0
15	I	102	CRT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	v	101	CRT	7	0
9	e	102	BCL	12	0
9	f	101	BCL	7	0
15	0	101	CRT	12	0
9	g	102	BCL	6	0
12	t	303	PEF	4	0
7	C	501	HEM	11	0
9	1	101	BCL	10	0
15	AJ	101	CRT	12	0
9	AI	101	BCL	15	0
9	Q	101	BCL	3	0
9	M	401	BCL	7	0
9	AB	101	BCL	10	0
9	x	305	BCL	6	0
9	k	102	BCL	12	0
9	u	102	BCL	11	0
9	AI	102	BCL	8	0
9	A	102	BCL	9	0
9	l	101	BCL	8	0
12	y	408	PEF	2	0
16	M	406	PO4	1	0
10	y	402	BPH	10	0
15	i	101	CRT	4	0
9	AE	102	BCL	9	0
7	o	504	HEM	12	0
9	I	101	BCL	8	0
9	Y	101	BCL	9	0
9	T	102	BCL	12	0
9	AF	101	BCL	8	0
7	C	504	HEM	8	0
15	AF	102	CRT	14	0
14	M	404	MQ8	4	0
15	X	101	CRT	21	0
15	q	101	CRT	9	0
12	M	407	PEF	1	0
15	P	102	CRT	9	0
15	9	101	CRT	16	0
9	3	101	BCL	10	0
15	m	104	CRT	8	0
9	i	102	BCL	8	0
15	k	101	CRT	15	0
9	L	301	BCL	18	0

Continued on next page...

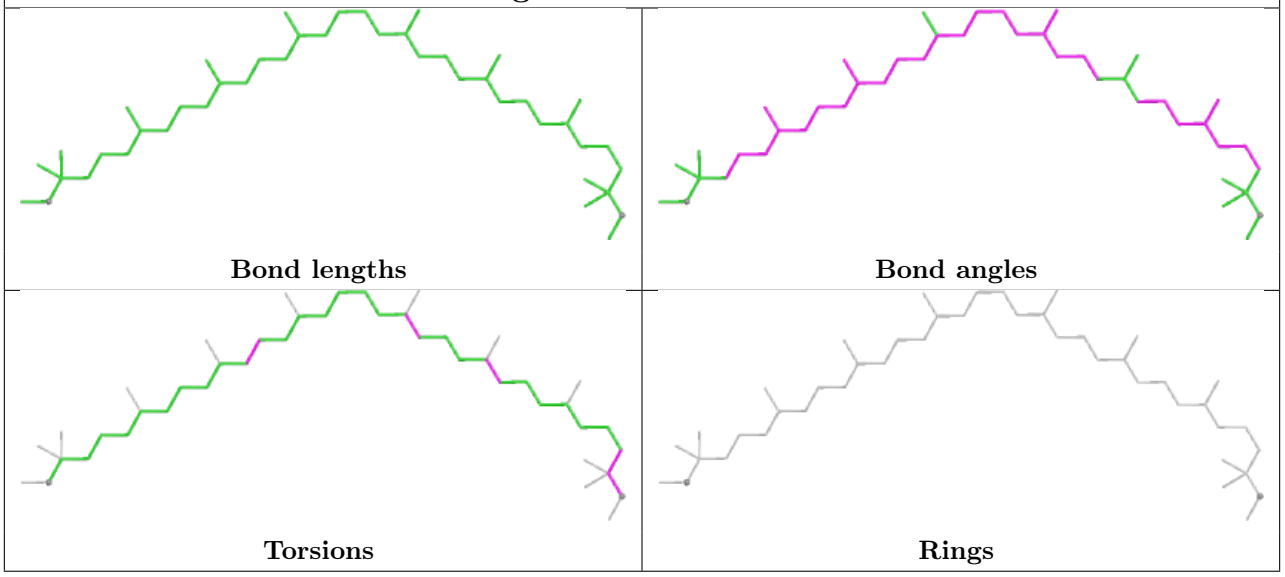
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	y	403	MQ8	8	0
9	X	102	BCL	8	0
12	H	301	PEF	6	0
15	s	101	CRT	10	0
15	7	101	CRT	9	0
9	4	102	BCL	10	0
9	AH	101	BCL	8	0
11	L	304	UQ8	12	0
16	y	405	PO4	1	0
15	G	101	CRT	9	0
9	K	101	BCL	6	0
9	x	303	BCL	8	0
9	Z	102	BCL	16	0
9	AC	102	BCL	10	0
9	S	102	BCL	11	0
9	M	402	BCL	14	0
15	E	101	CRT	14	0
9	F	101	BCL	4	0
9	D	101	BCL	10	0
9	D	102	BCL	7	0
9	c	101	BCL	14	0
9	5	101	BCL	12	0
9	V	102	BCL	8	0
15	y	404	CRT	11	0
15	e	101	CRT	10	0
10	x	302	BPH	4	0
7	o	501	HEM	7	0
12	y	406	PEF	4	0
9	N	101	BCL	4	0
7	C	503	HEM	5	0
9	8	101	BCL	12	0
15	2	101	CRT	7	0
15	z	101	CRT	6	0

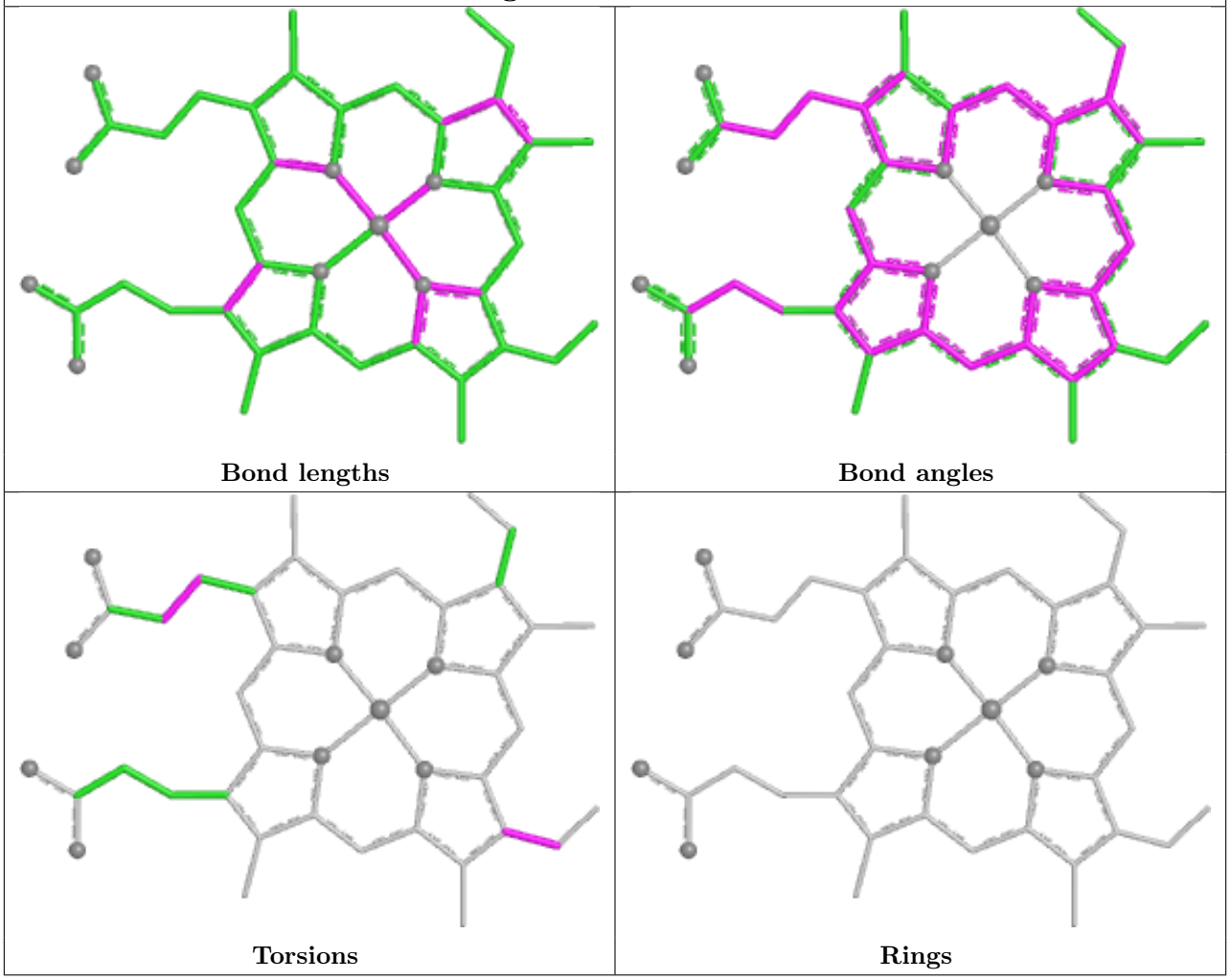
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

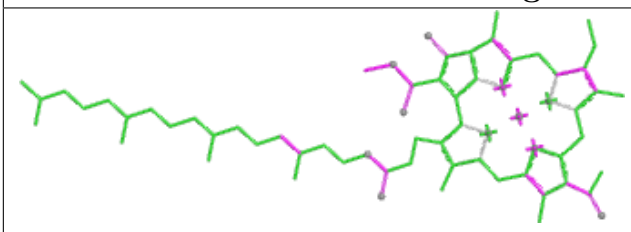
Ligand CRT AC 101



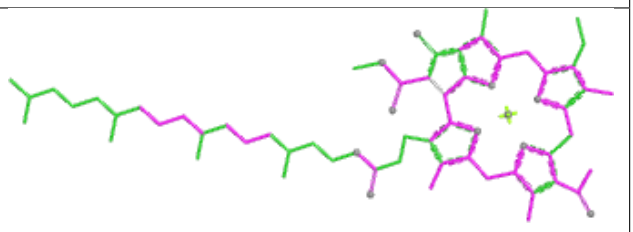
Ligand HEM o 502



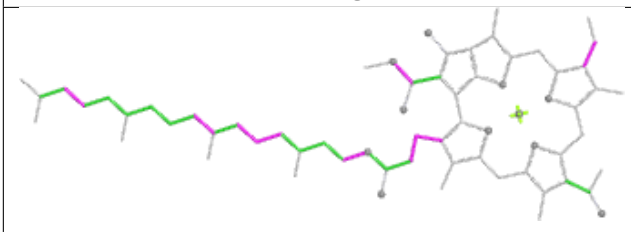
Ligand BCL m 102



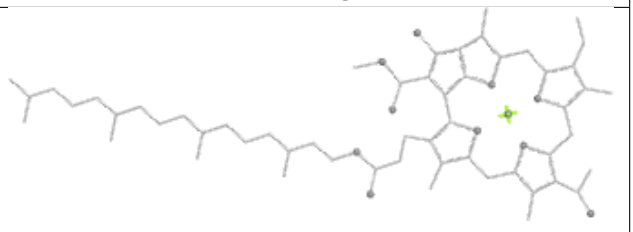
Bond lengths



Bond angles

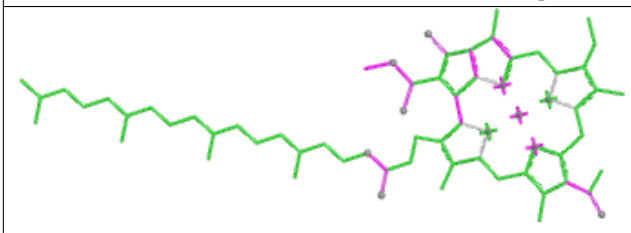


Torsions

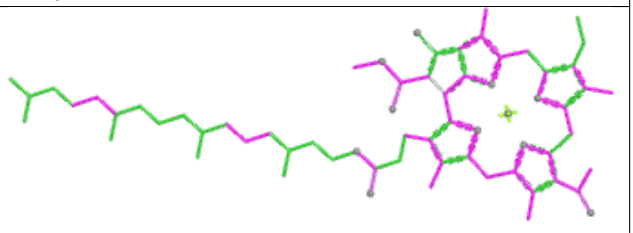


Rings

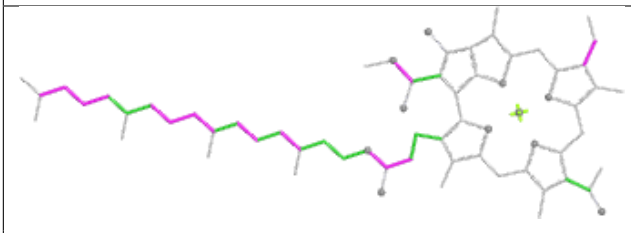
Ligand BCL j 101



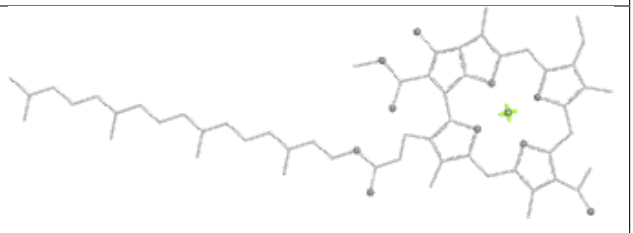
Bond lengths



Bond angles

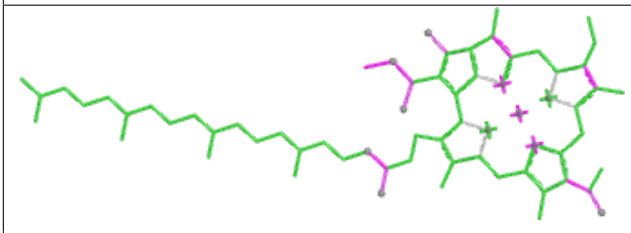


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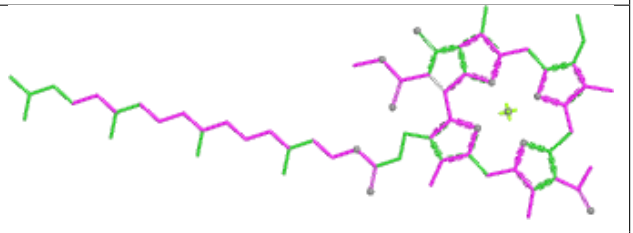


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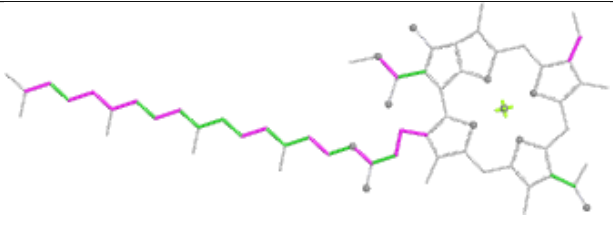
Ligand BCL AG 101



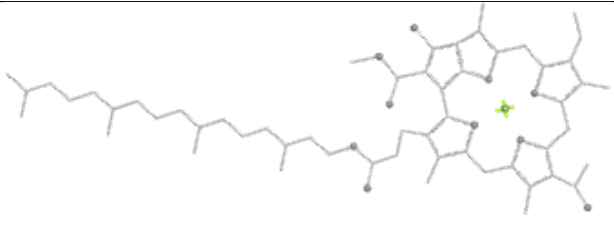
Bond lengths



Bond angles

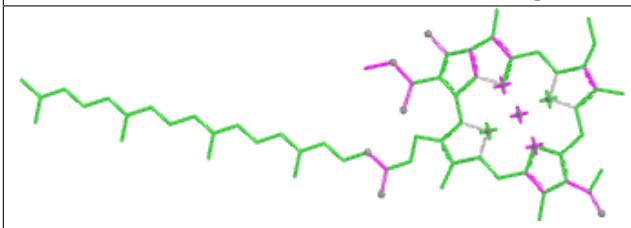


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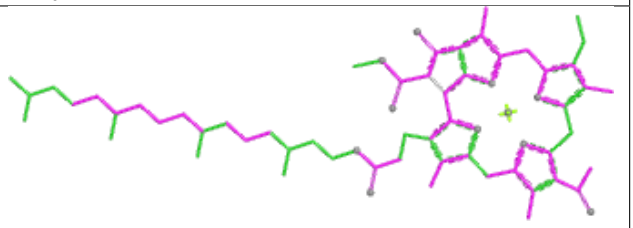


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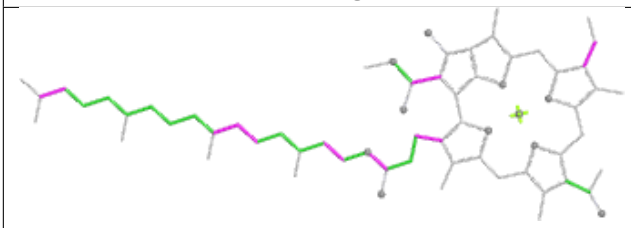
Ligand BCL y 401



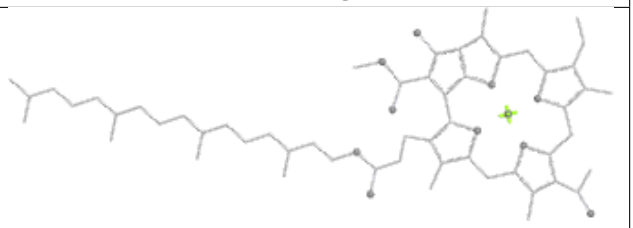
Bond lengths



Bond angles

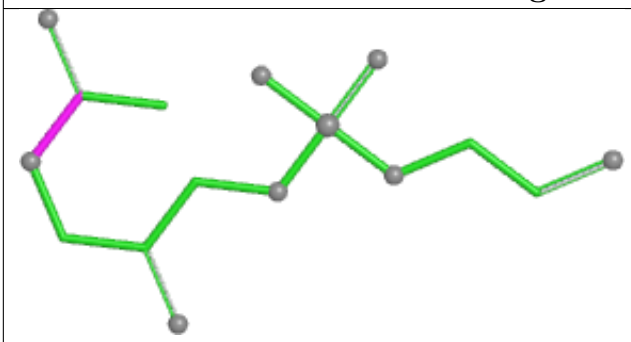


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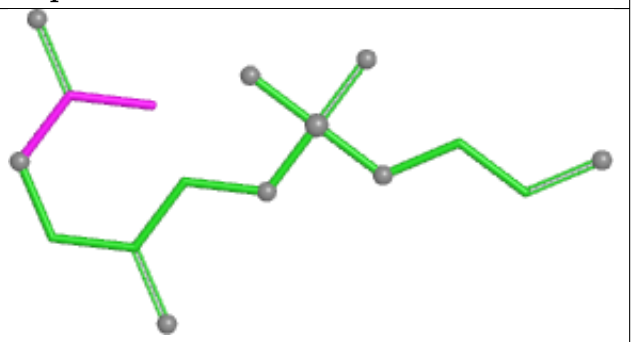


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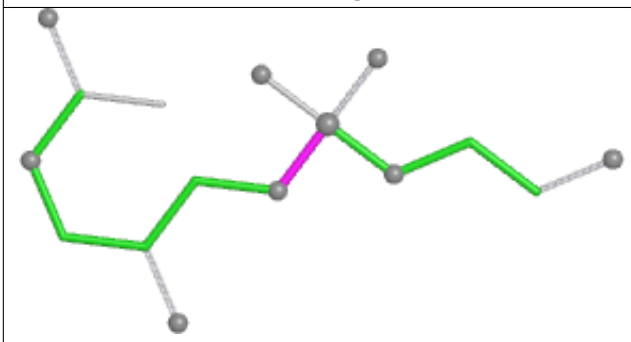
Ligand PEF p 101



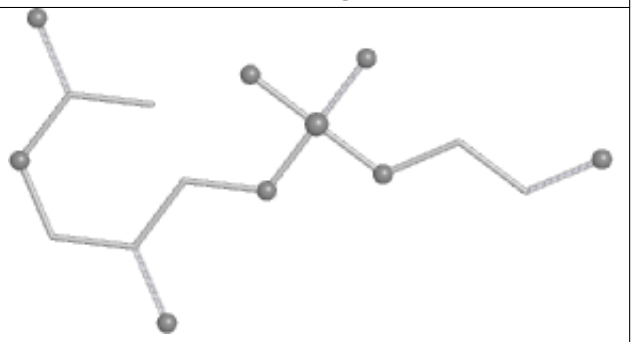
Bond lengths



Bond angles

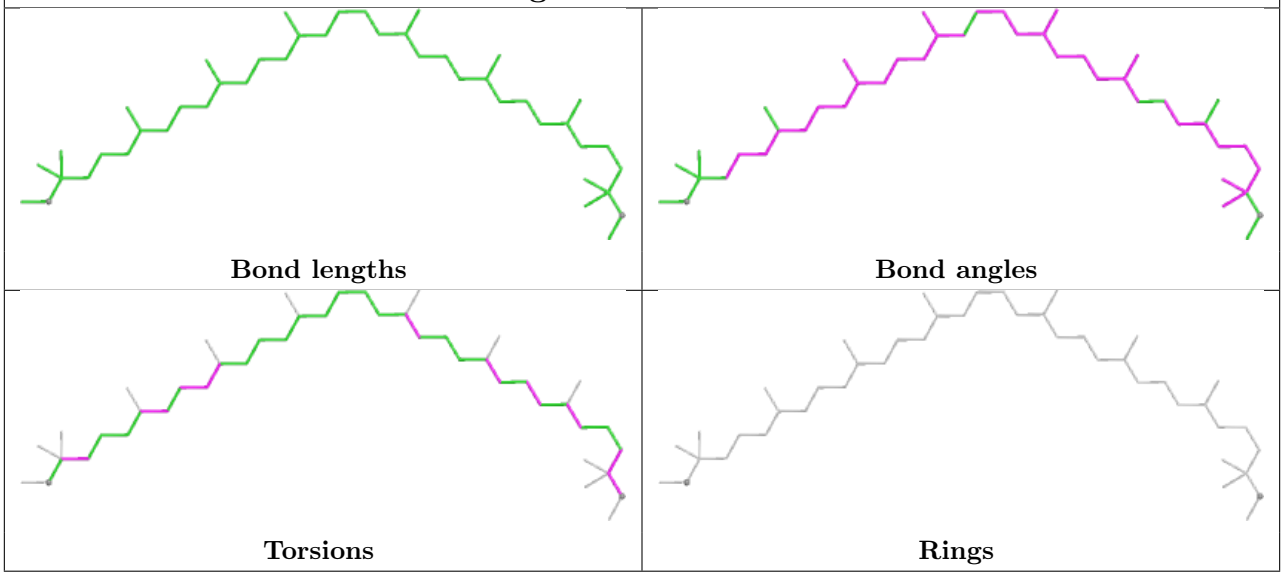


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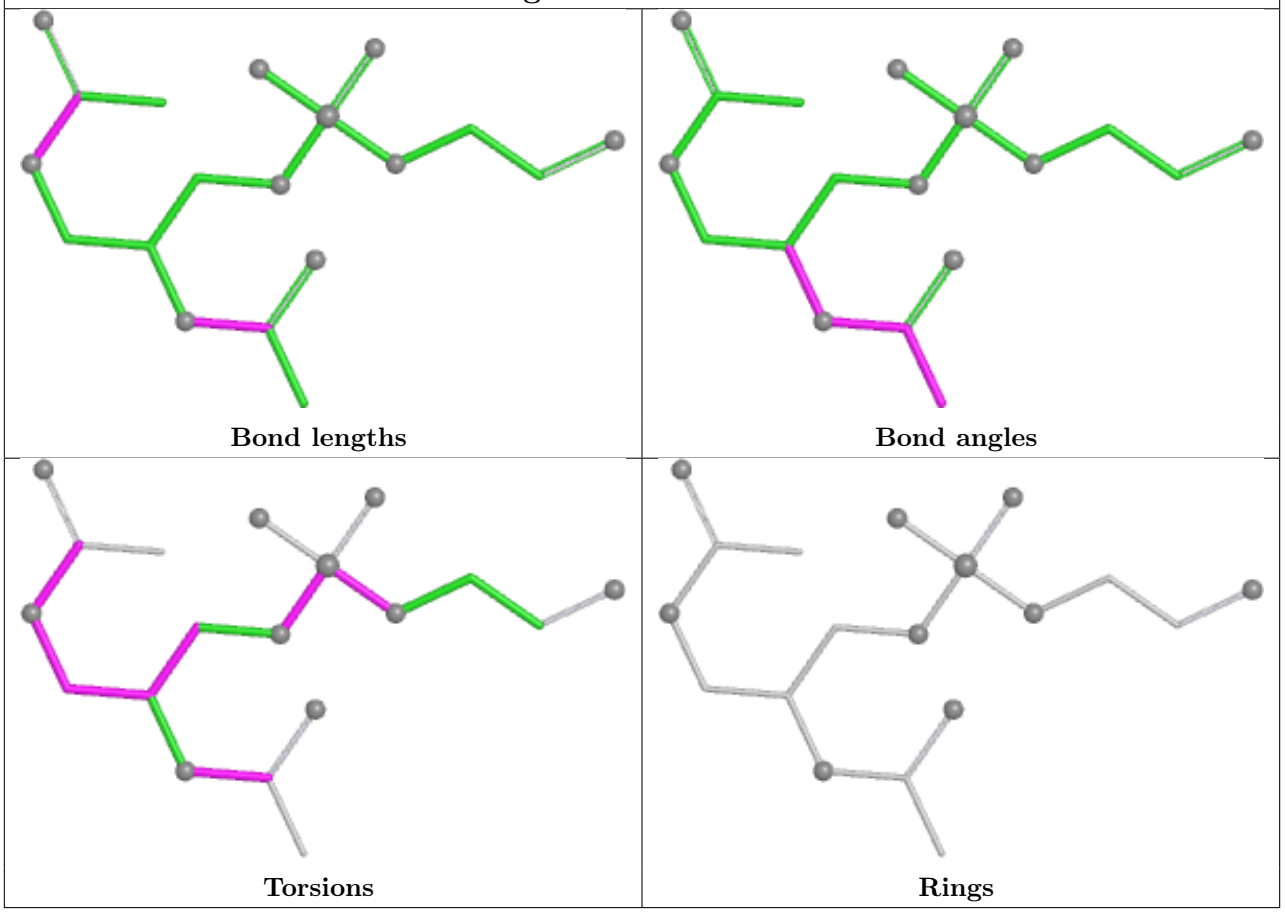


Rings

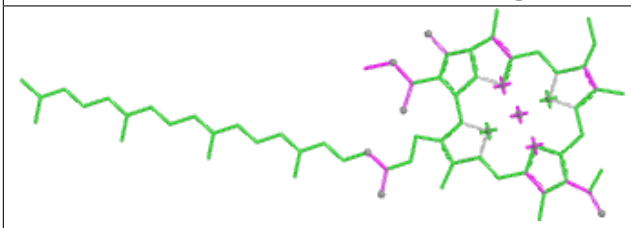
Ligand CRT 4 101



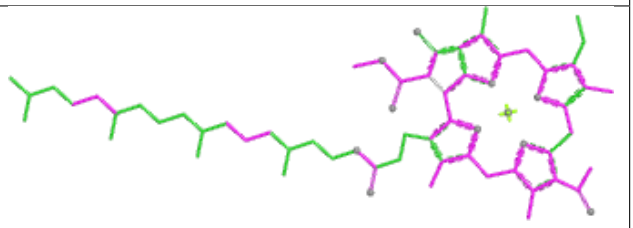
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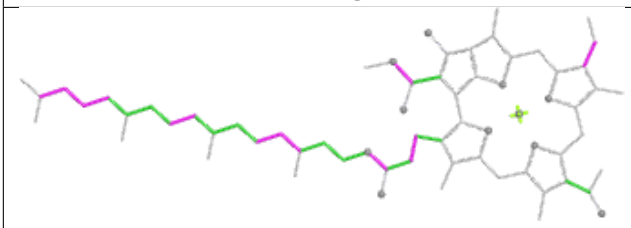
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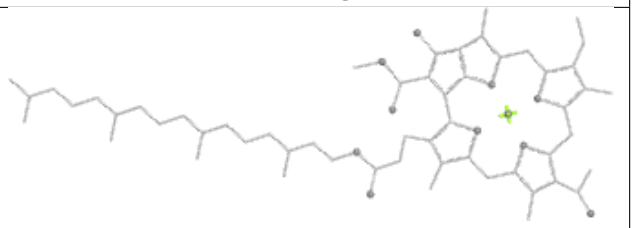
Bond lengths



Bond angles

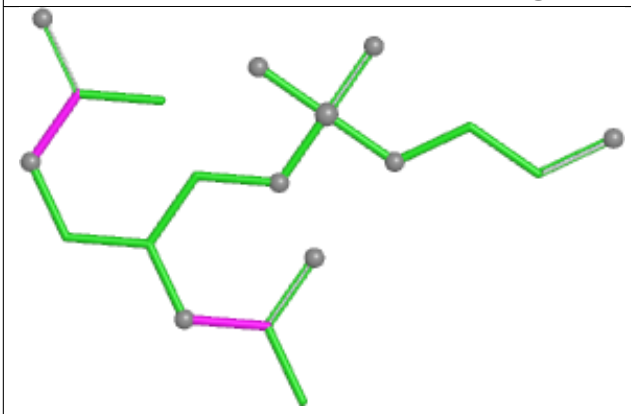


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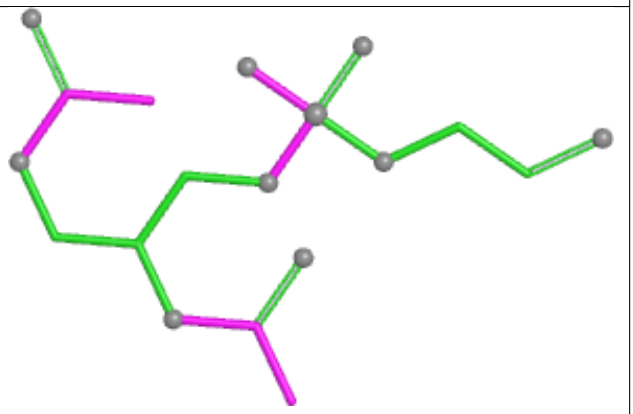


Rings

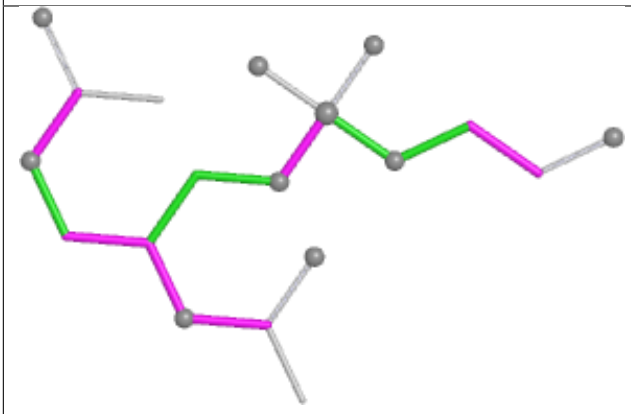
Ligand PEF x 306



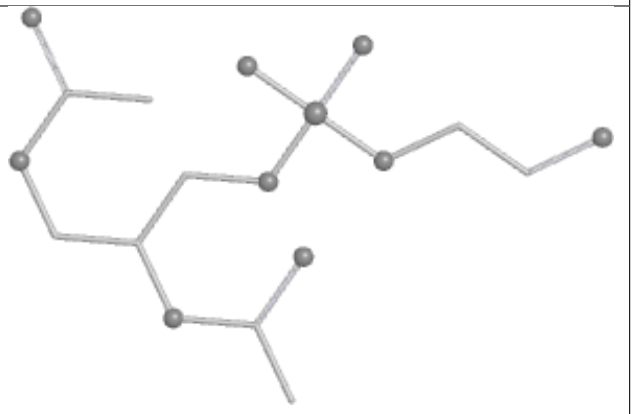
Bond lengths



Bond angles

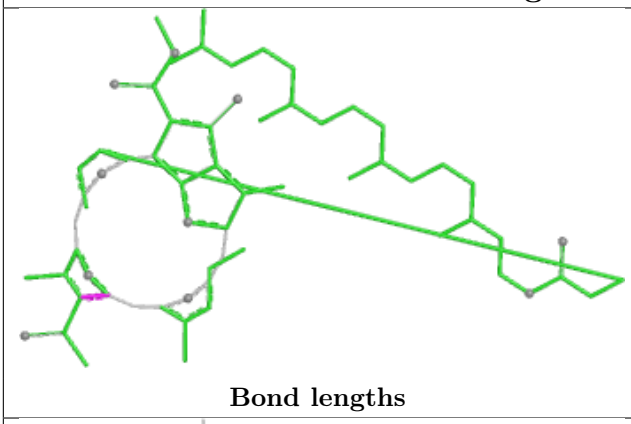


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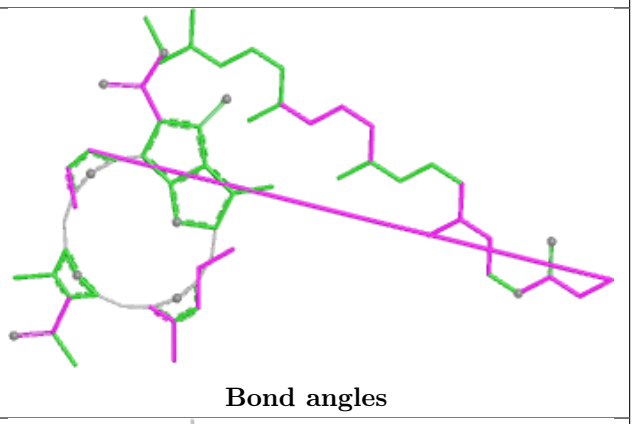


Rings

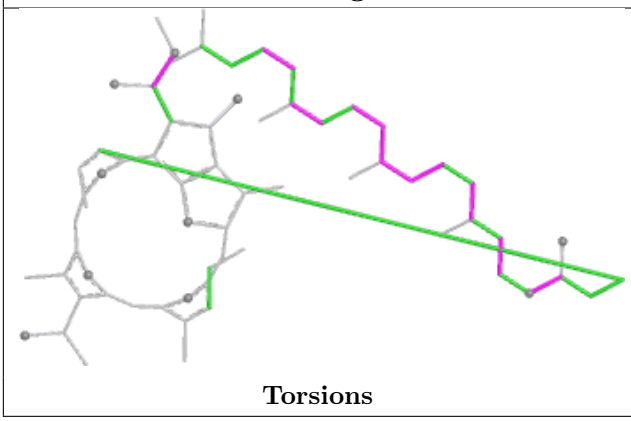
Ligand BPH L 302



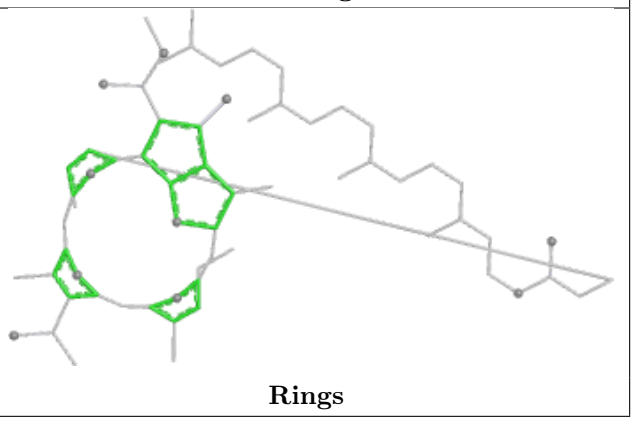
Bond lengths



Bond angles

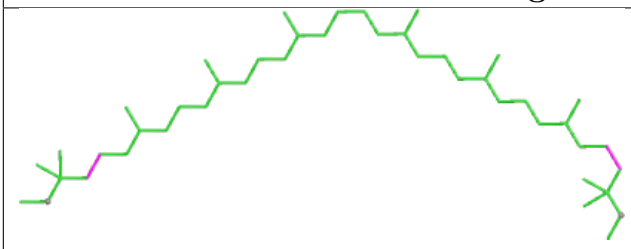


Torsions

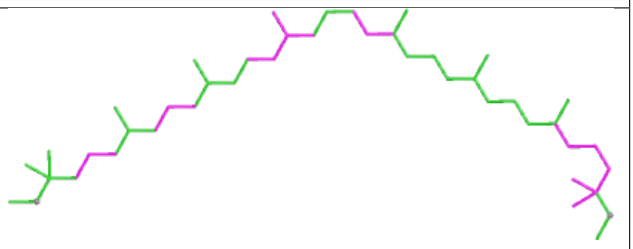


Rings

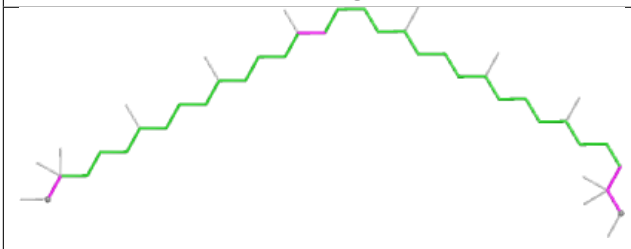
Ligand CRT 7 103



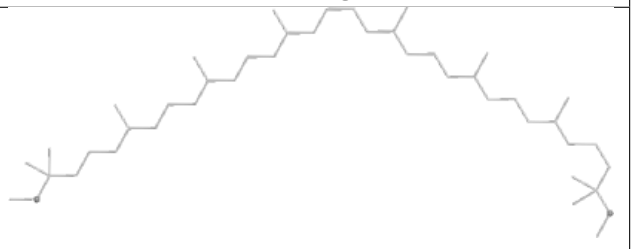
Bond lengths



Bond angles

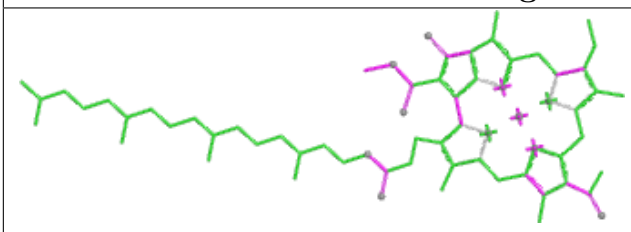


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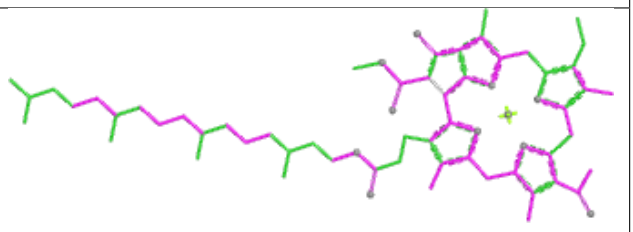


Rings

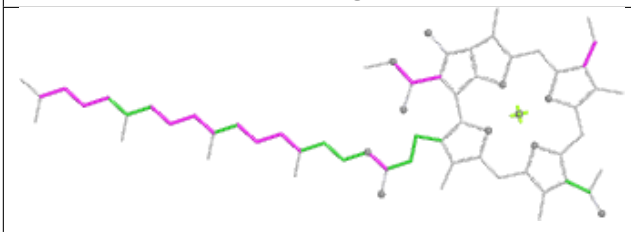
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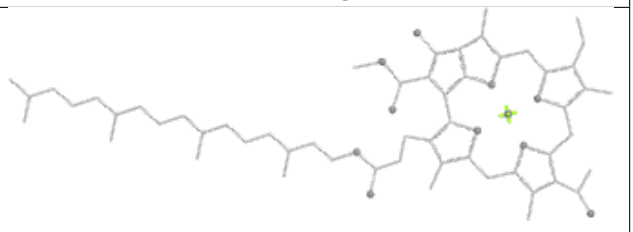
Bond lengths



Bond angles

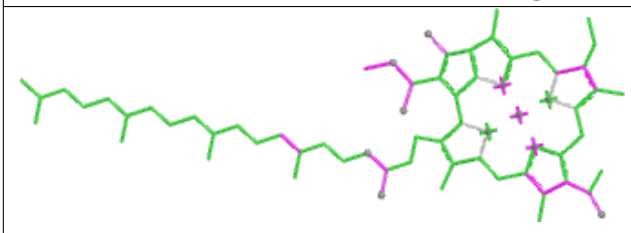


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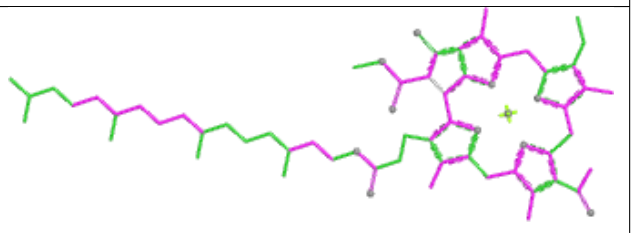


Rings

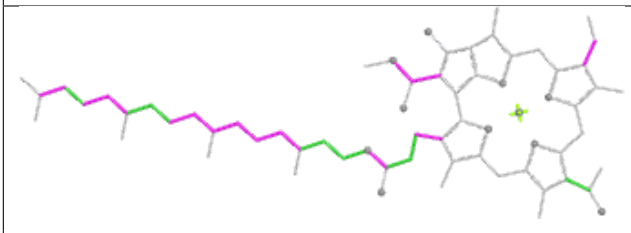
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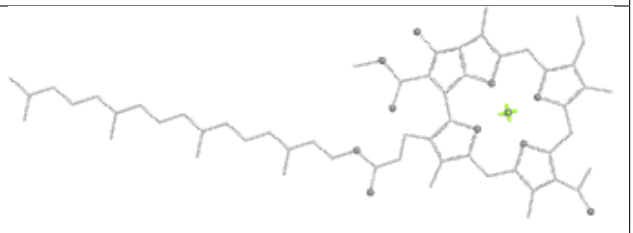
Bond lengths



Bond angles

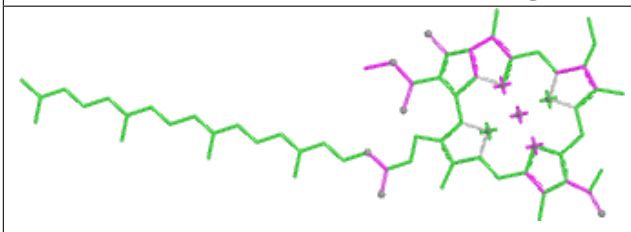


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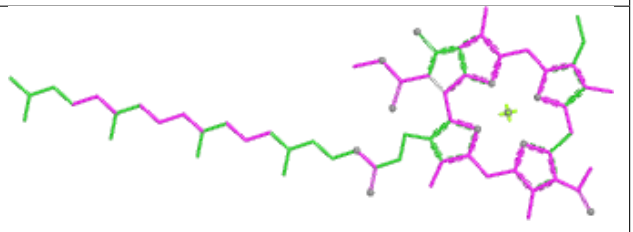


Rings

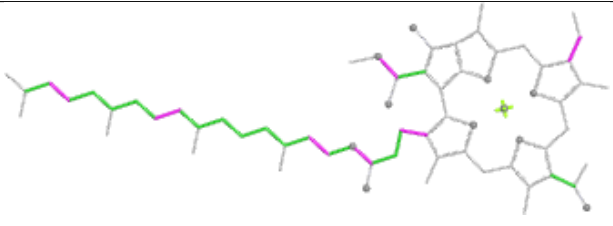
Ligand BCL A 103



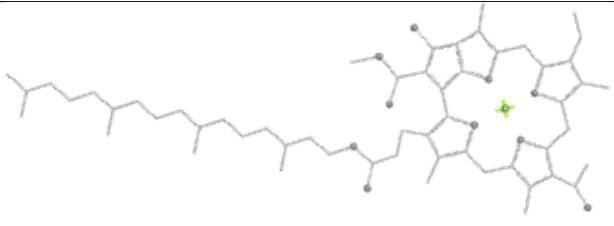
Bond lengths



Bond angles

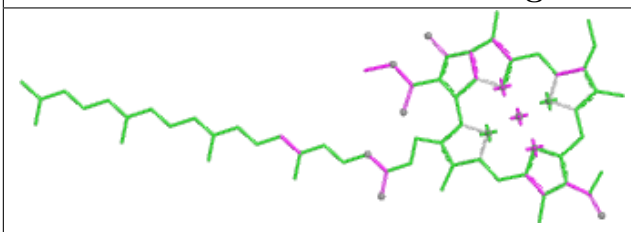


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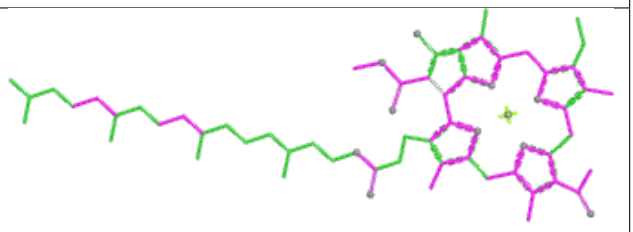


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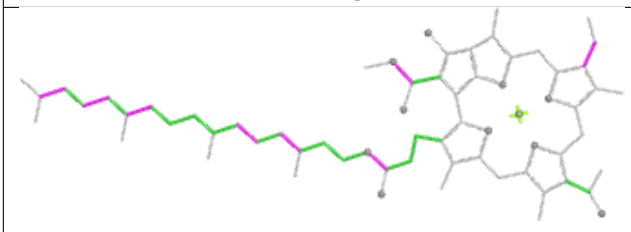
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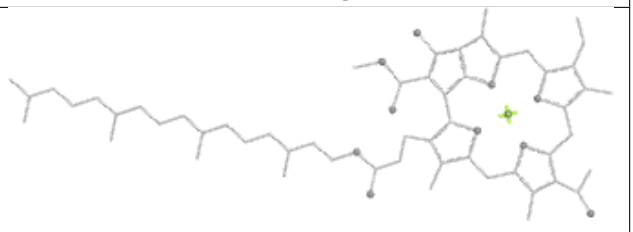
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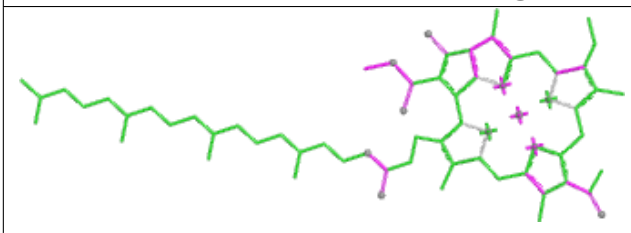


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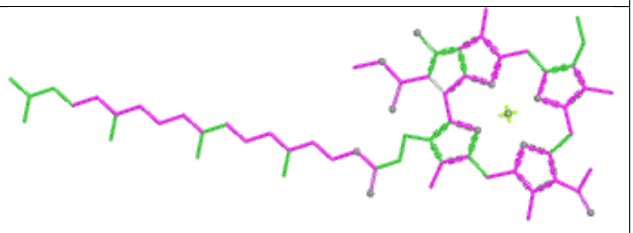


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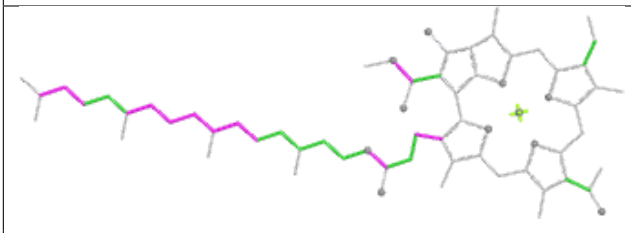
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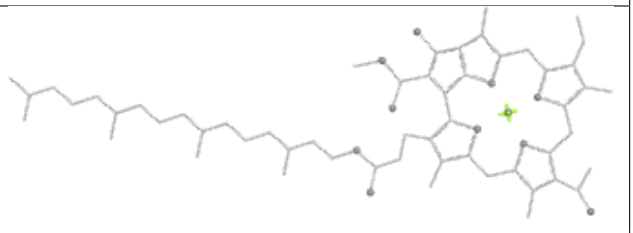
Bond lengths



Bond angles

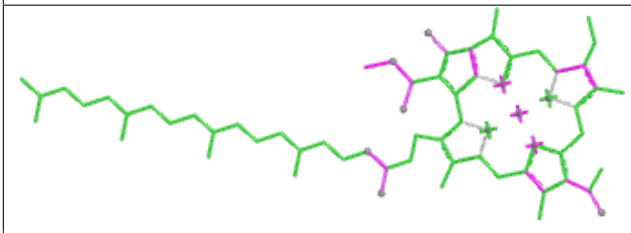


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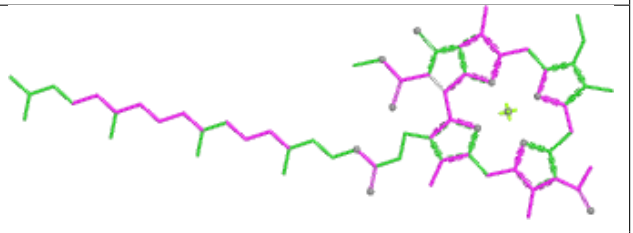


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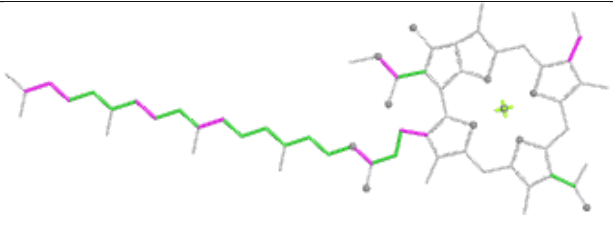
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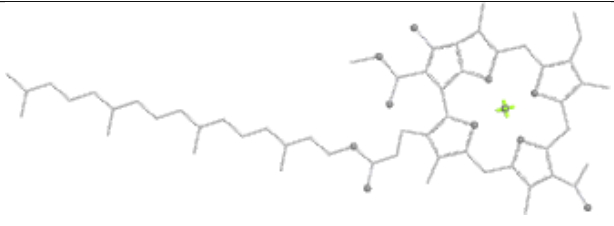
Bond lengths



Bond angles

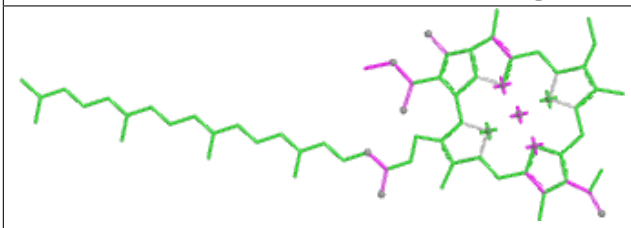


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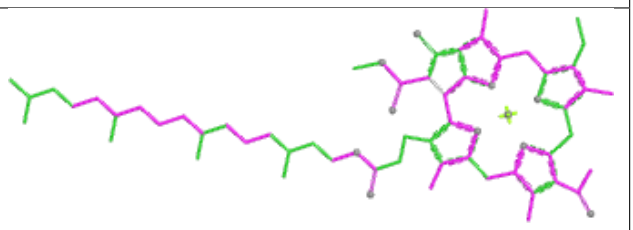


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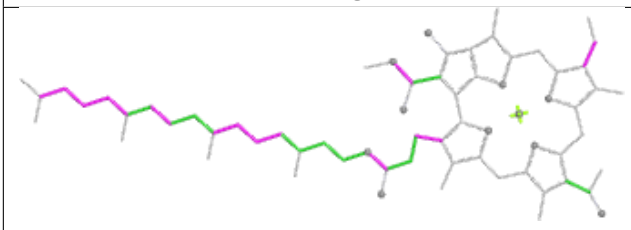
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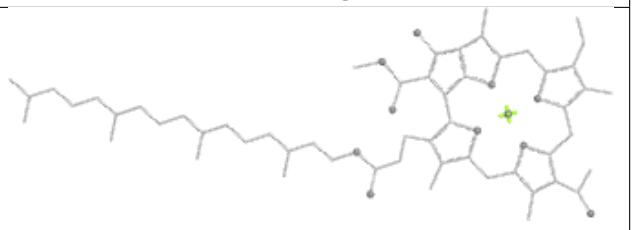
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Bond angles

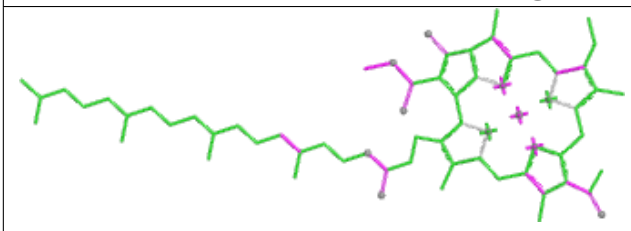


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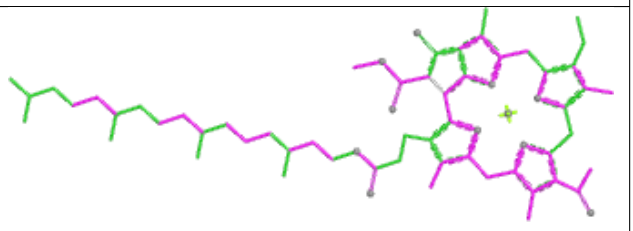


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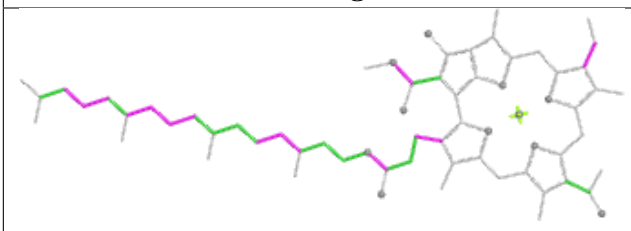
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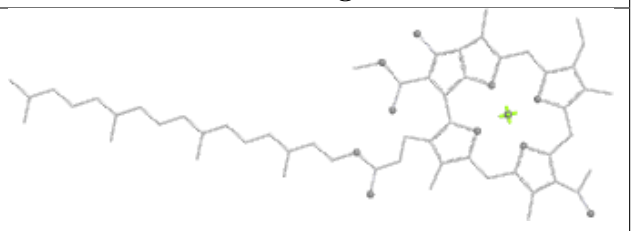
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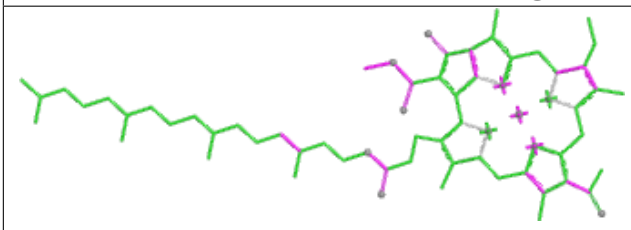


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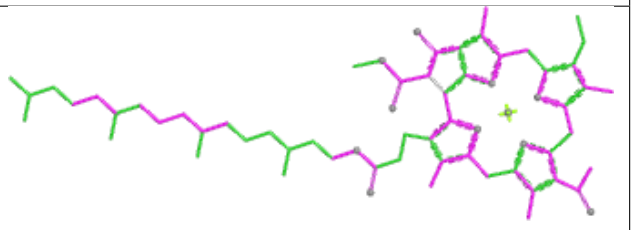


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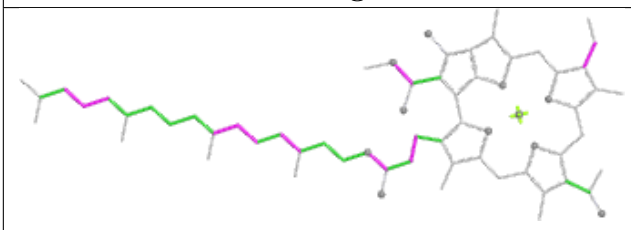
Ligand BCL x 301



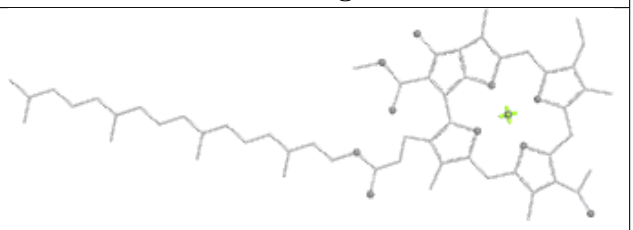
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Bond angles

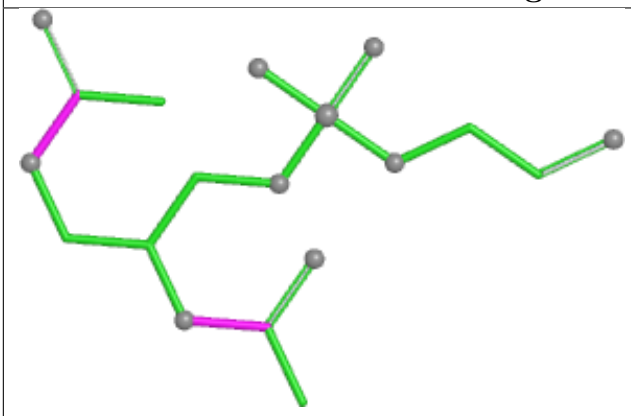


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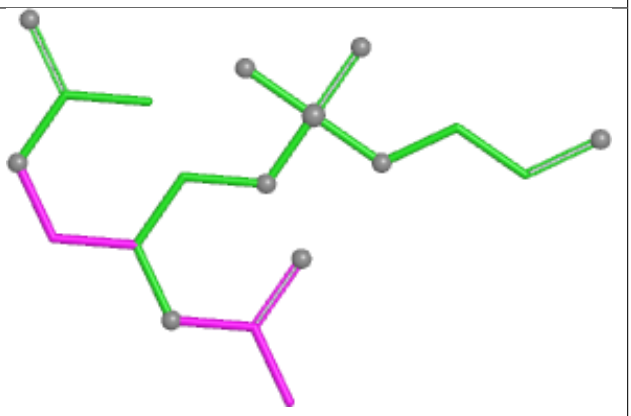


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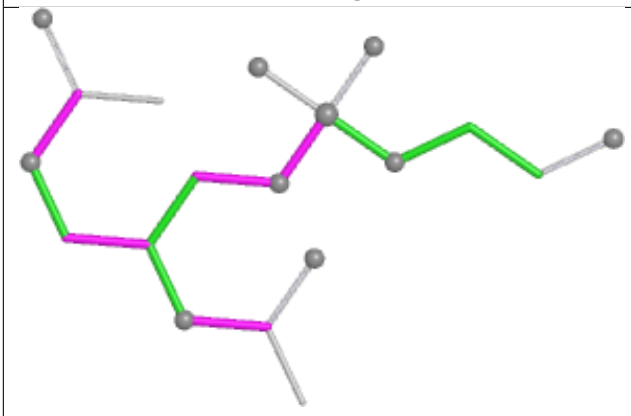
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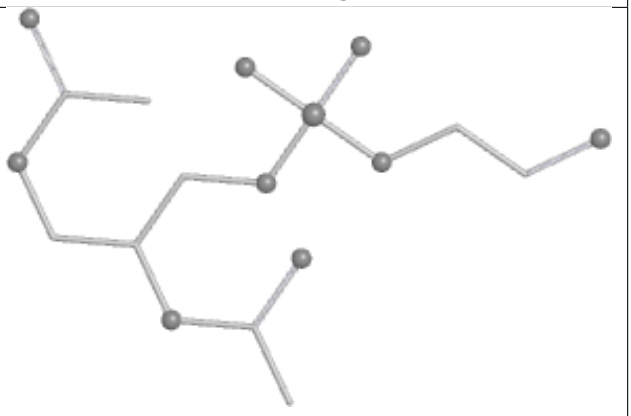
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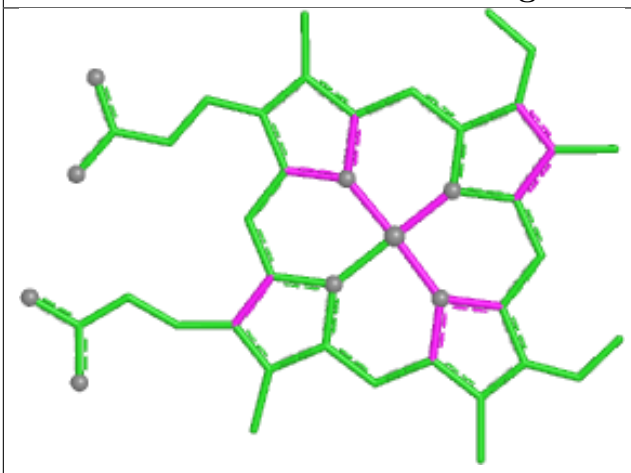


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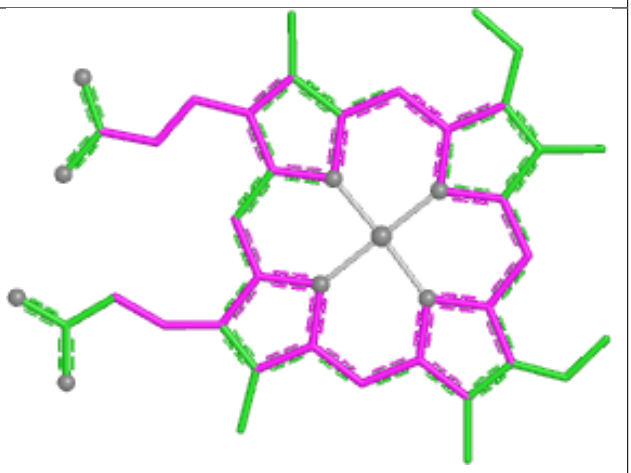


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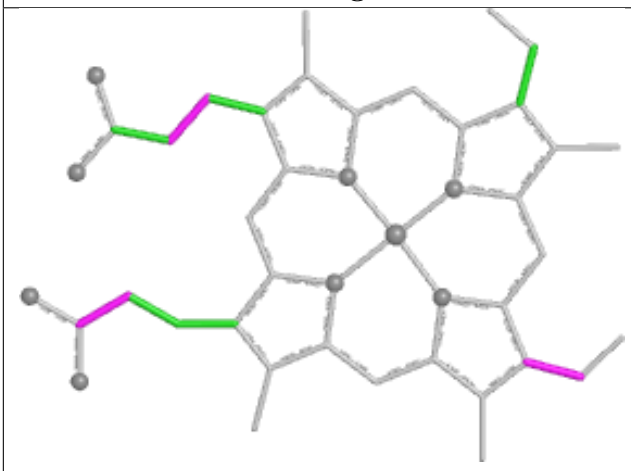
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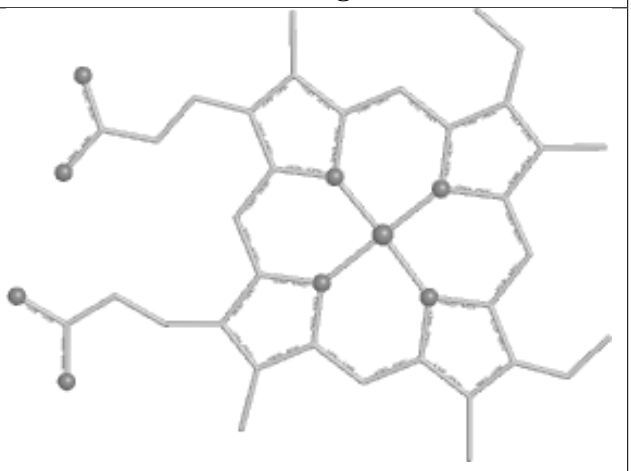
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Bond angles

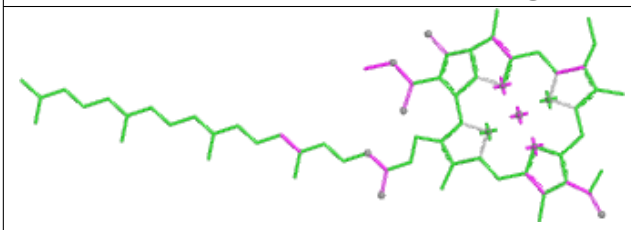


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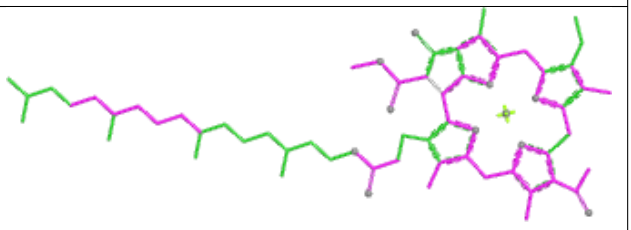


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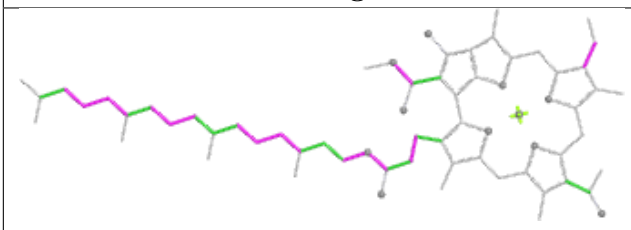
Ligand BCL U 101



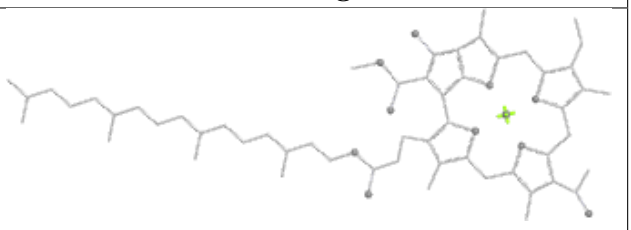
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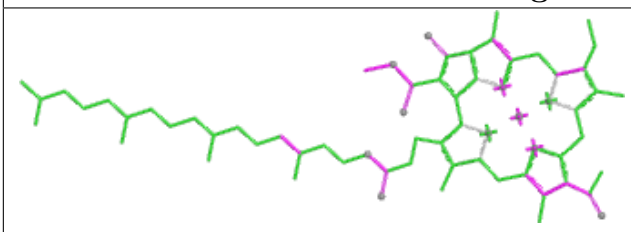


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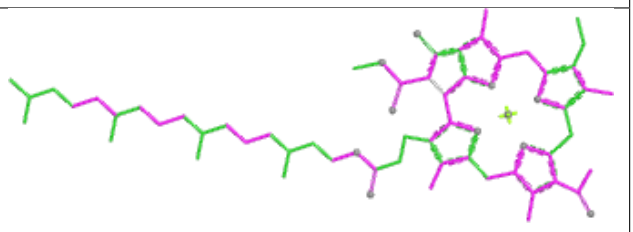


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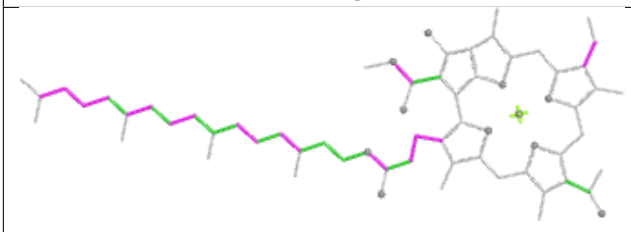
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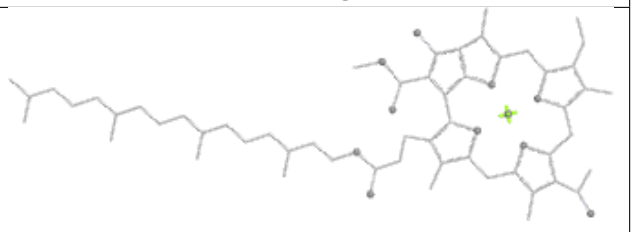
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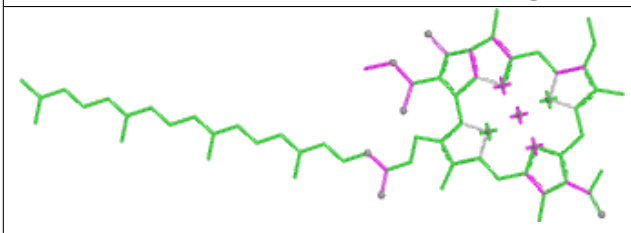


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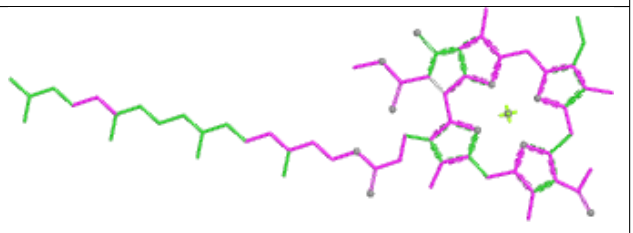


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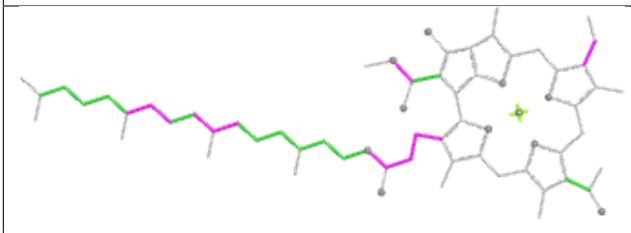
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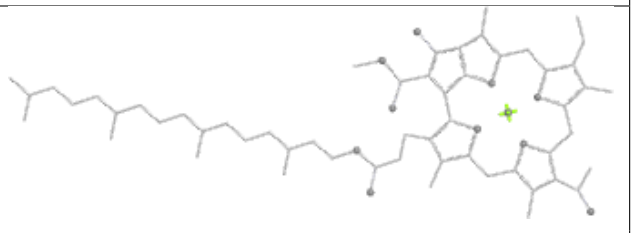
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Bond angles

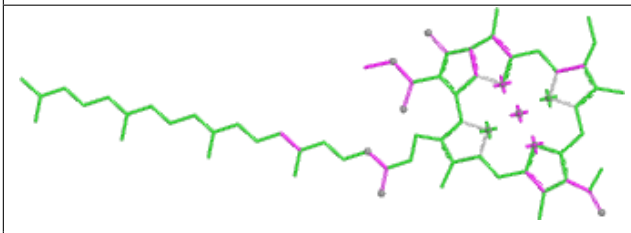


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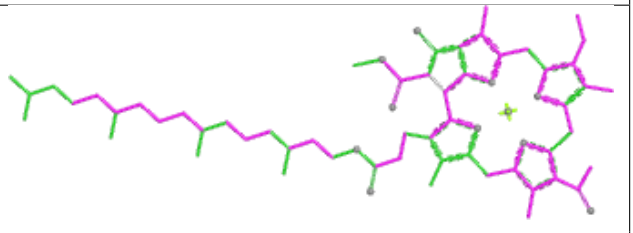


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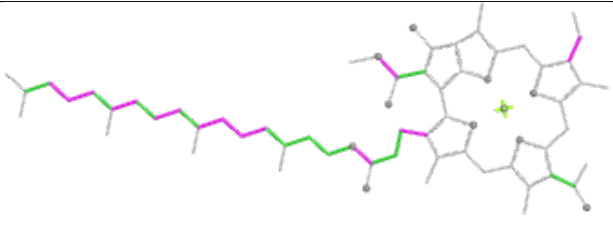
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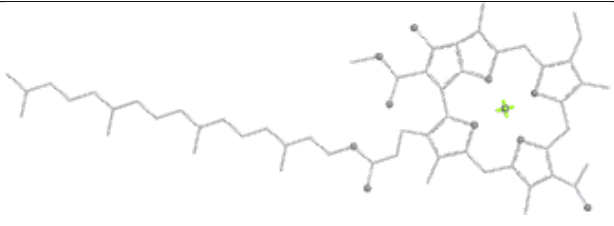
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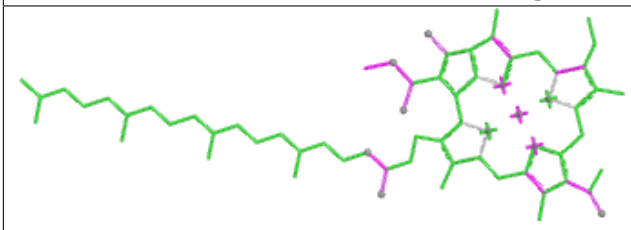
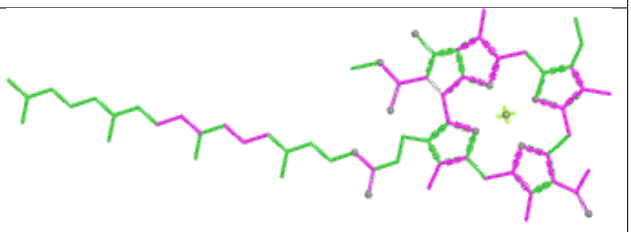
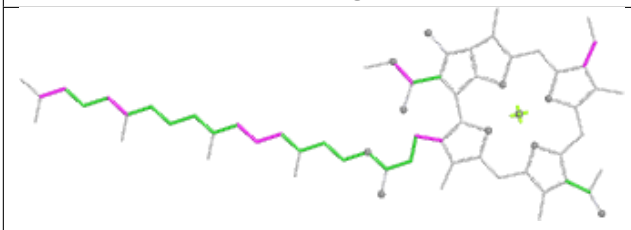
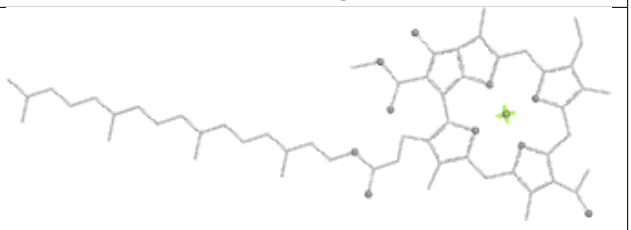
Bond angles

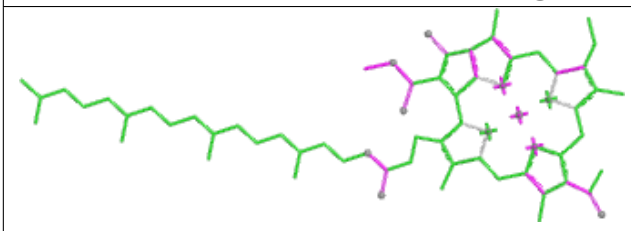
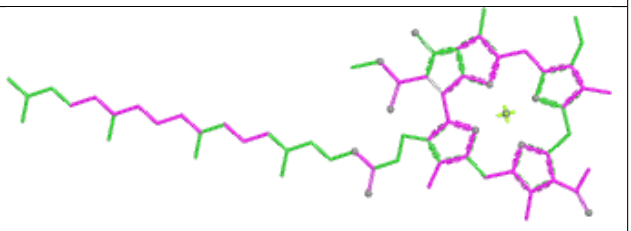
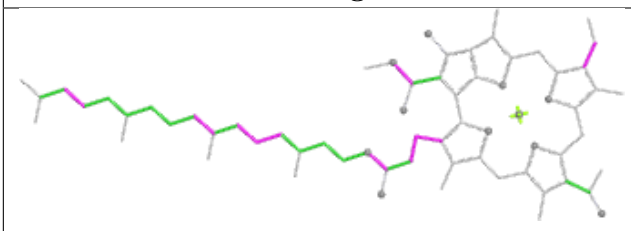
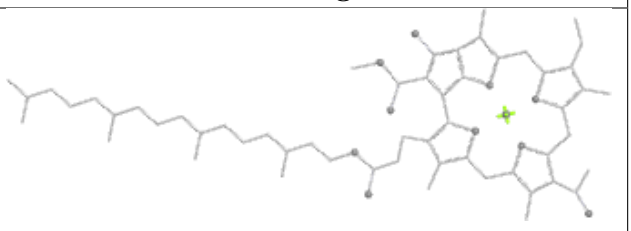


Torsions

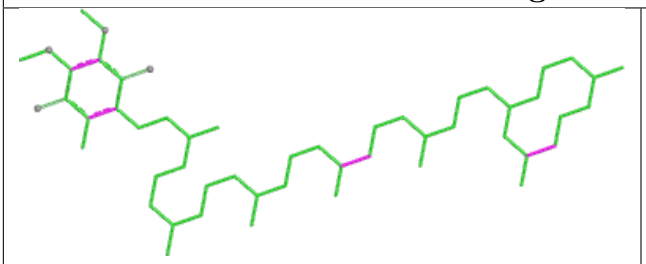


Rings

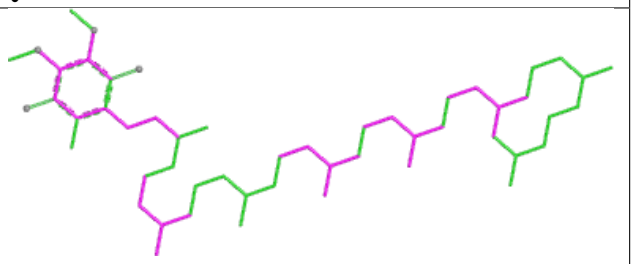
Ligand BCL 9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL I 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

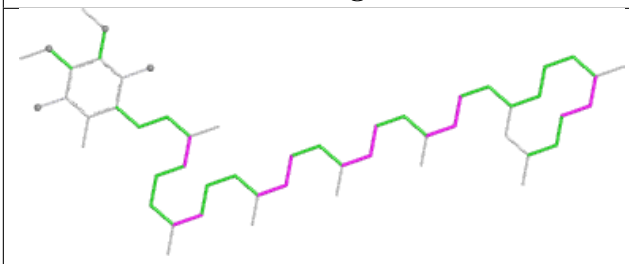
Ligand UQ8 x 304



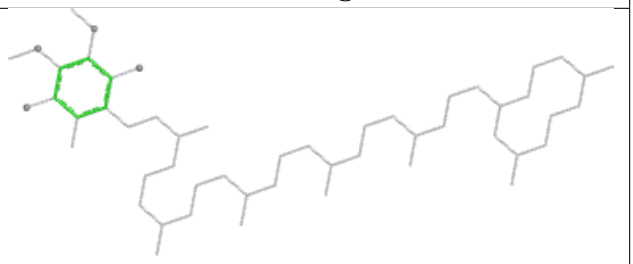
Bond lengths



Bond angles

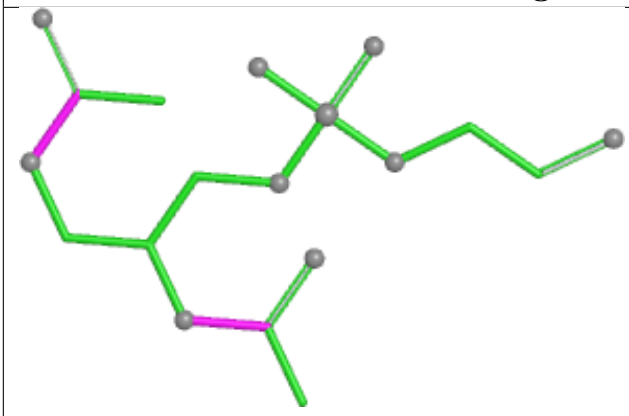


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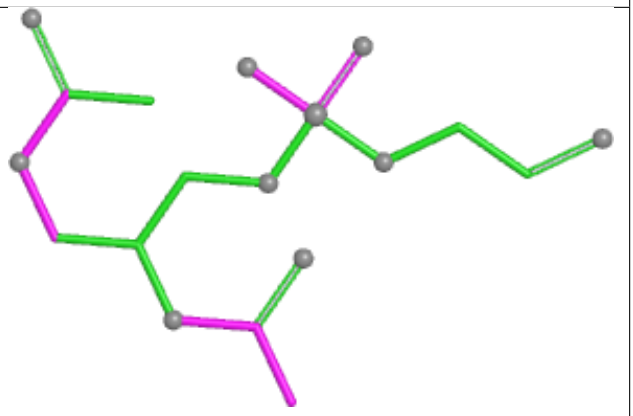


Rings

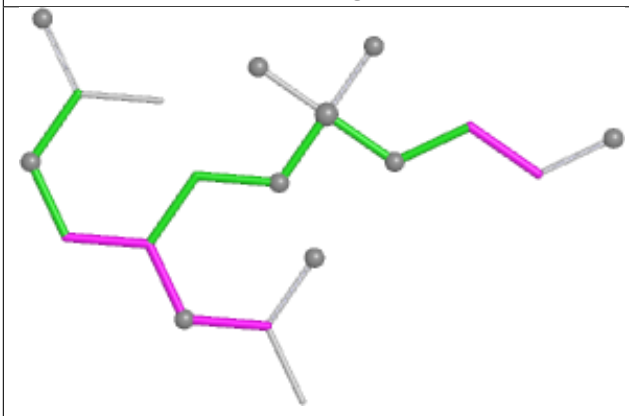
Ligand PEF t 301



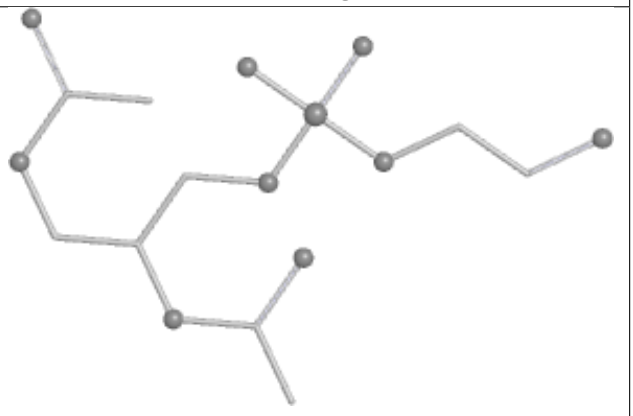
Bond lengths



Bond angles

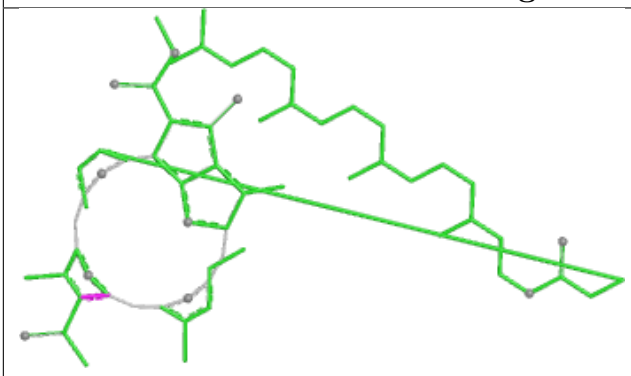


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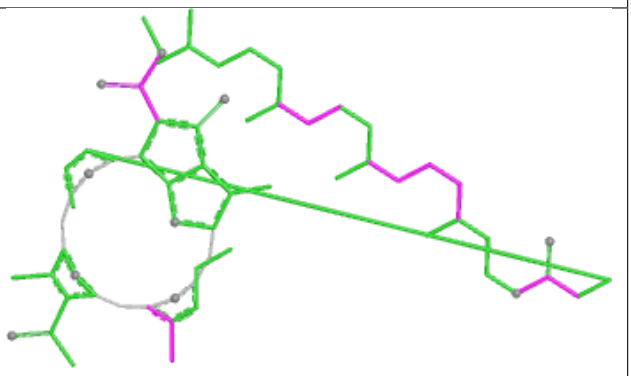


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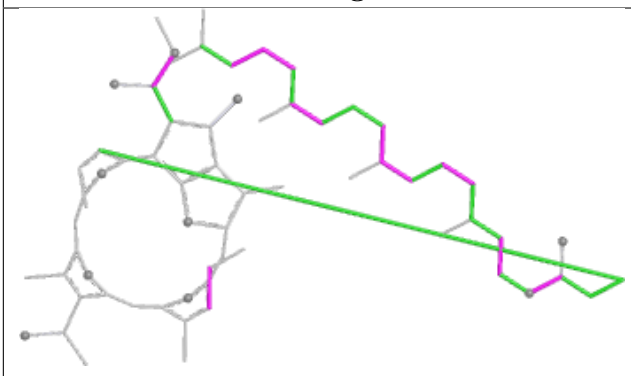
Ligand BPH M 403



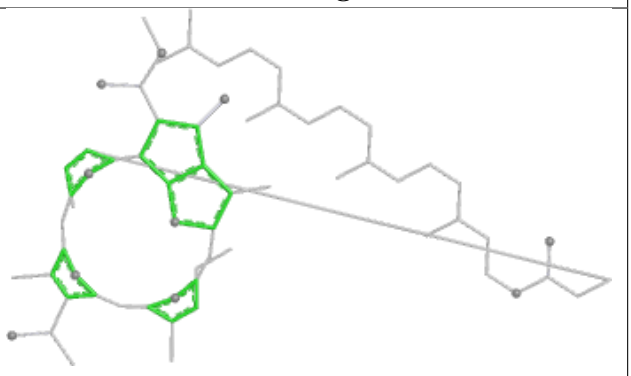
Bond lengths



Bond angles

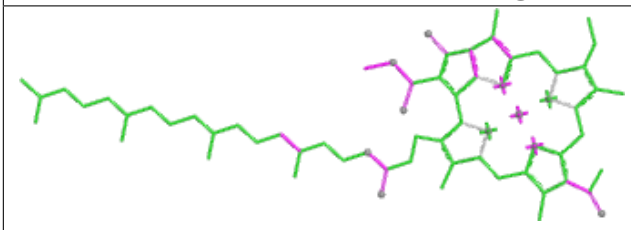


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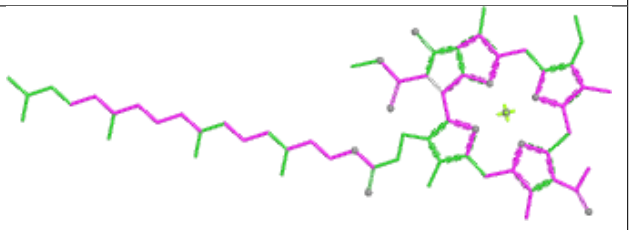


Rings

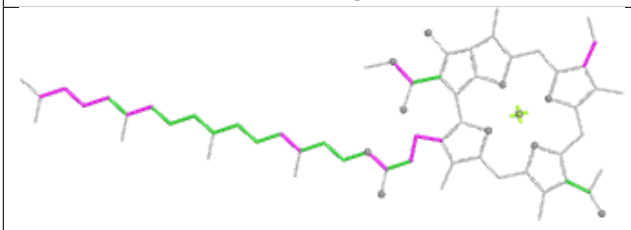
Ligand BCL AC 103



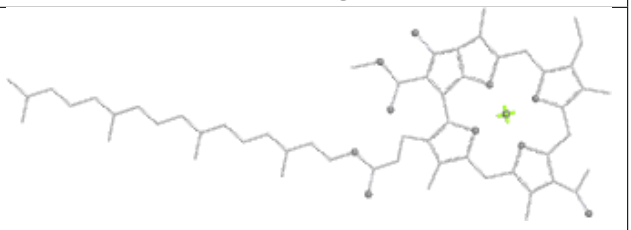
Bond lengths



Bond angles

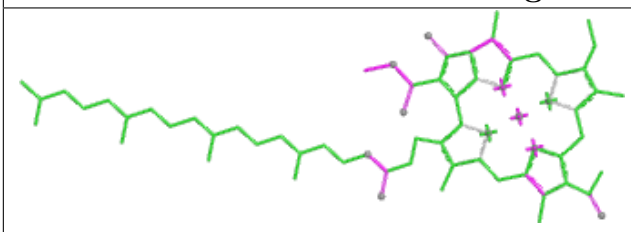


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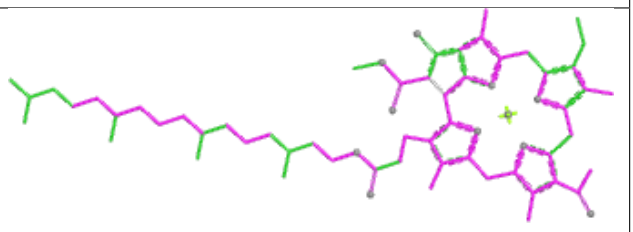


Rings

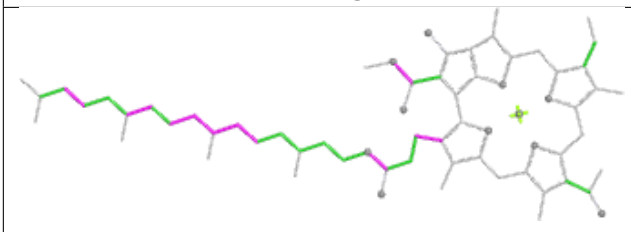
Ligand BCL O 102



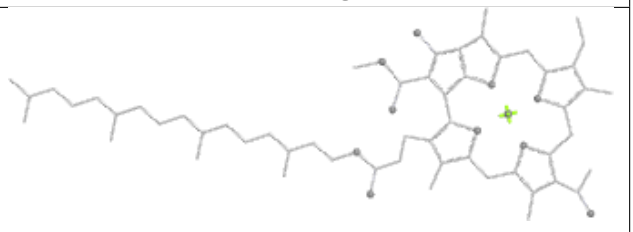
Bond lengths



Bond angles

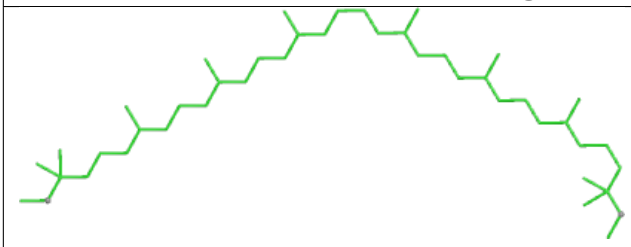


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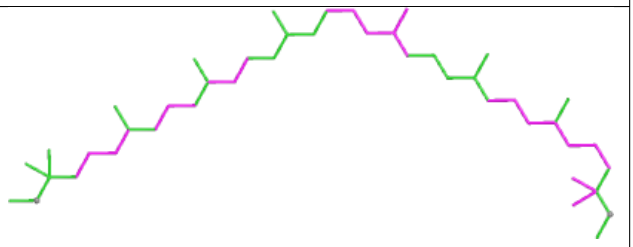


Rings

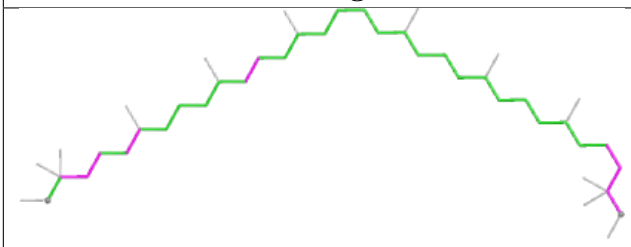
Ligand CRT M 405



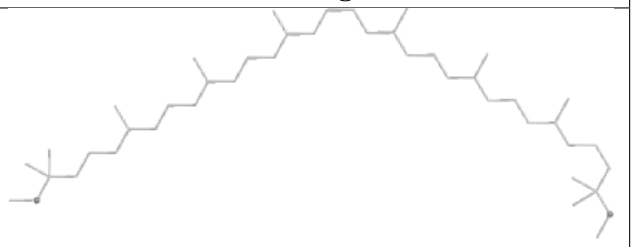
Bond lengths



Bond angles

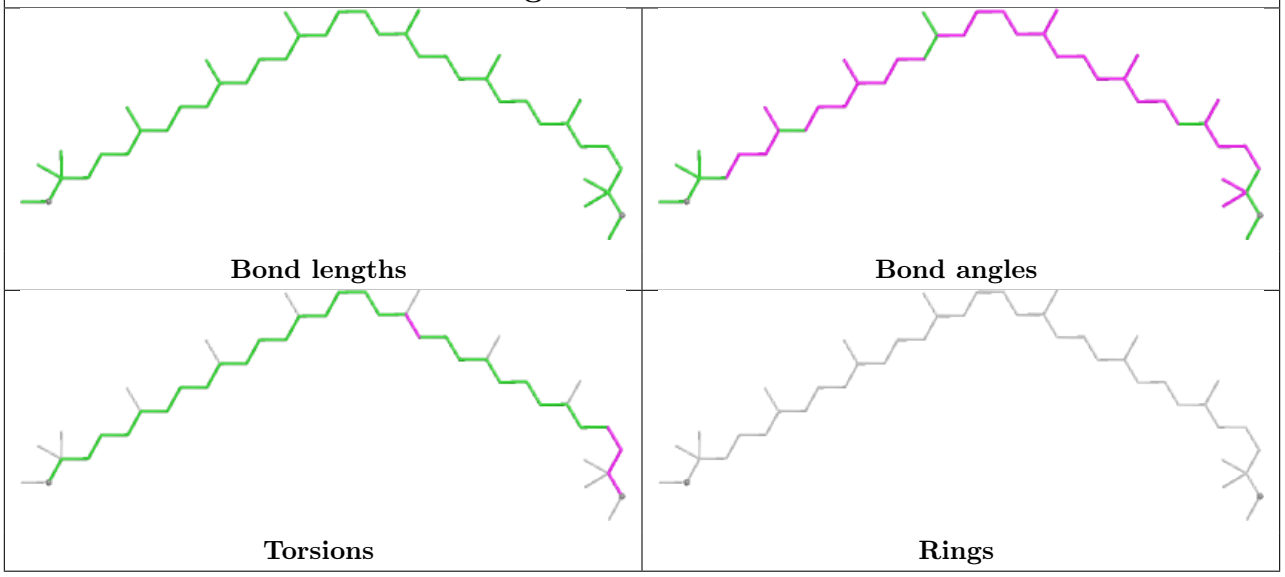


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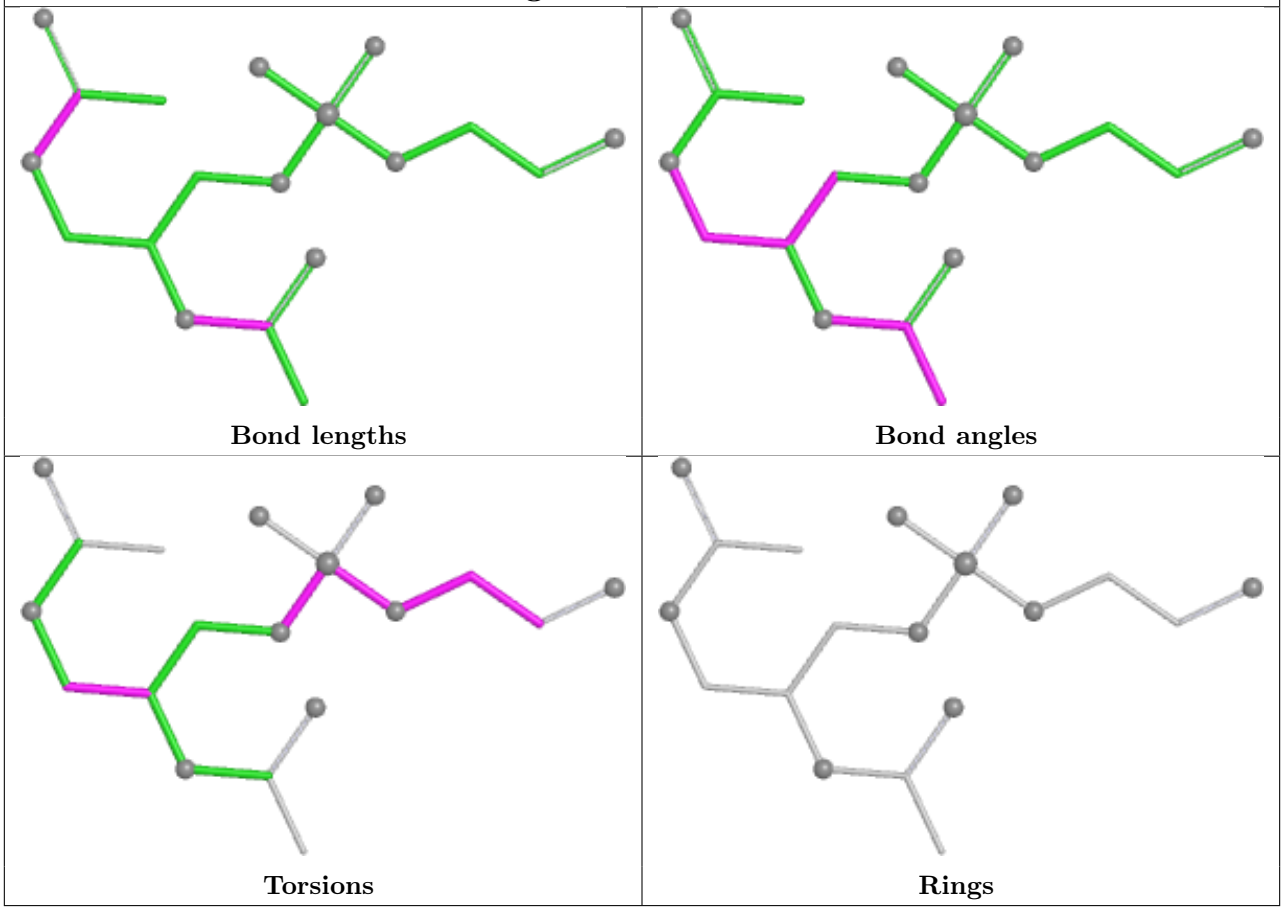


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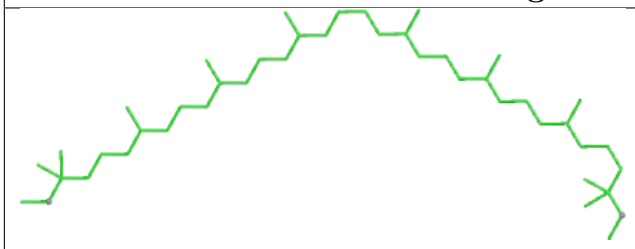
Ligand CRT O 101



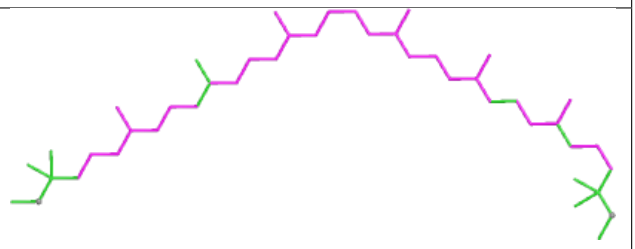
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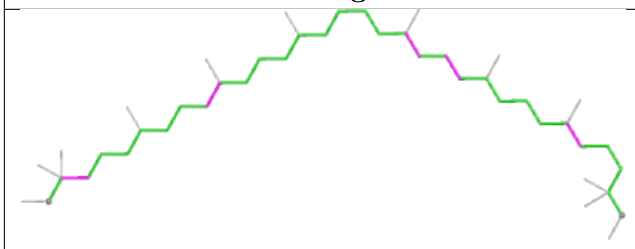
Ligand CRT Z 101



Bond lengths



Bond angles

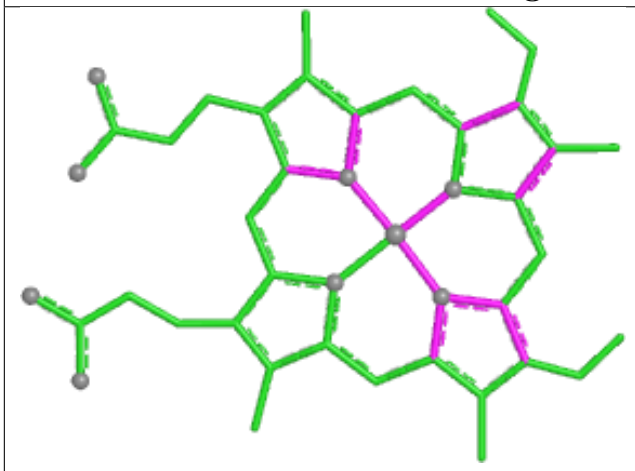


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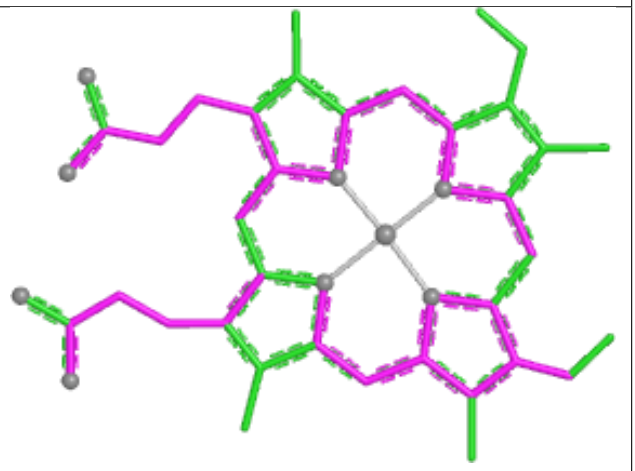


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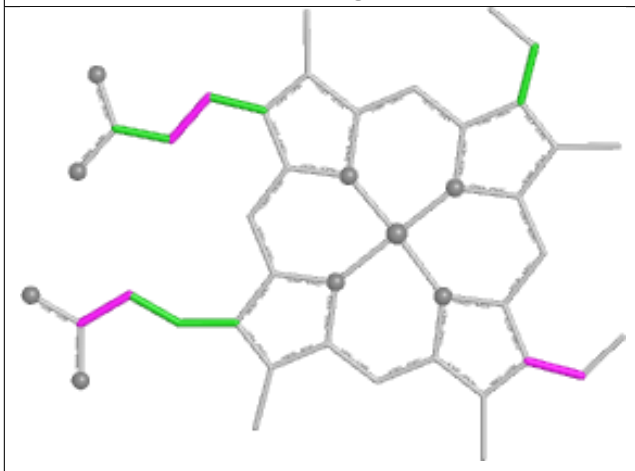
Ligand HEM o 503



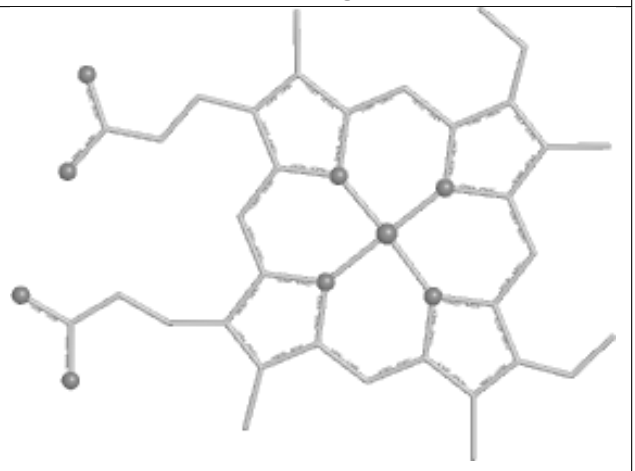
Bond lengths



Bond angles

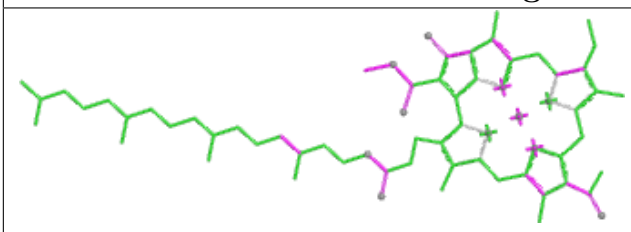


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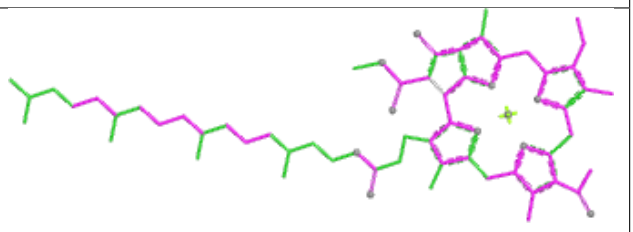


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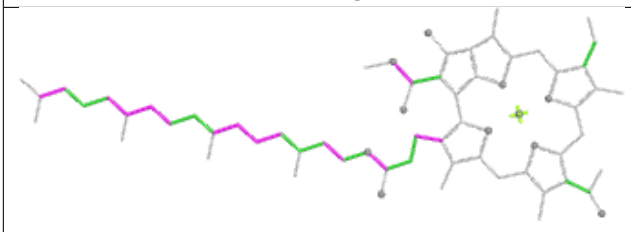
Ligand BCL m 103



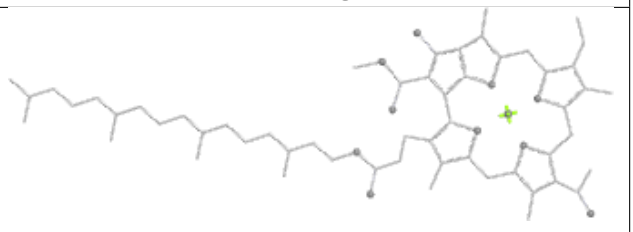
Bond lengths



Bond angles

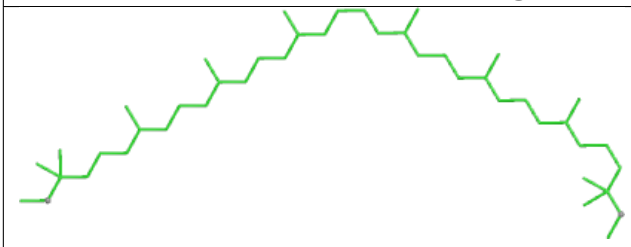


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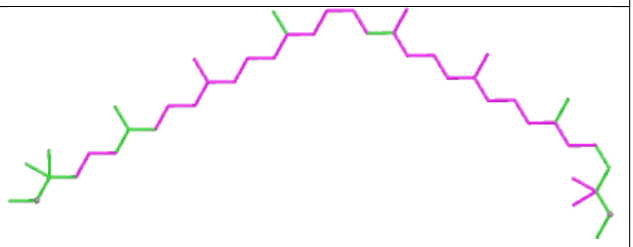


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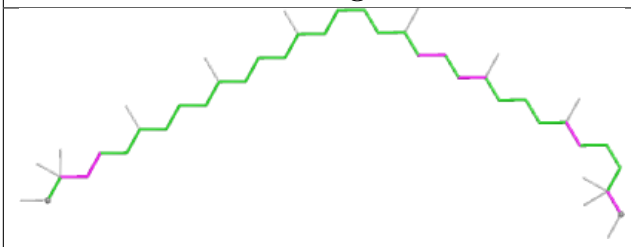
Ligand CRT AD 101



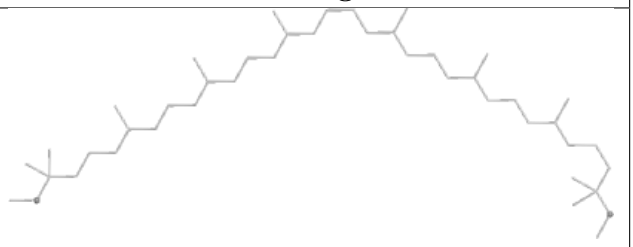
Bond lengths



Bond angles

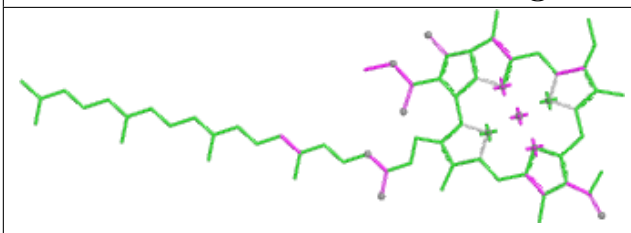


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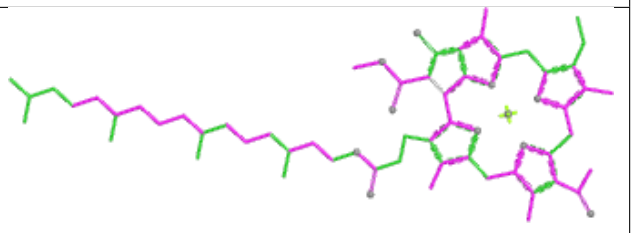


Rings

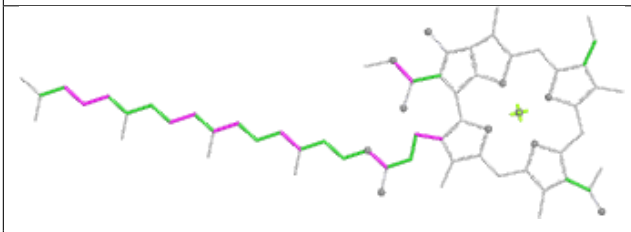
Ligand BCL 2 102



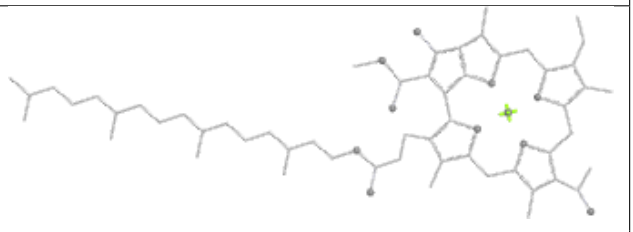
Bond lengths



Bond angles

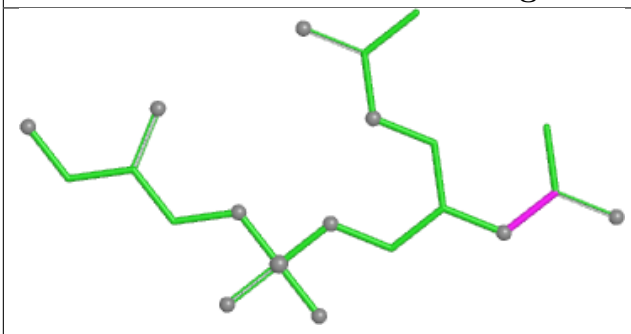


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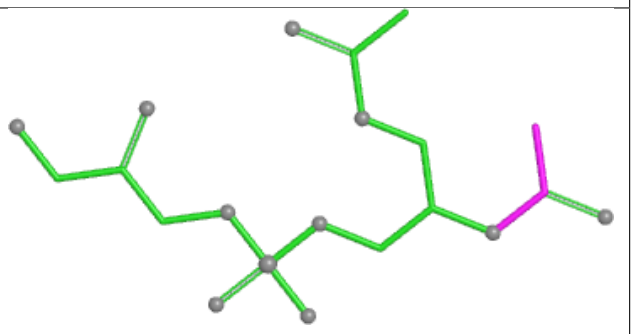


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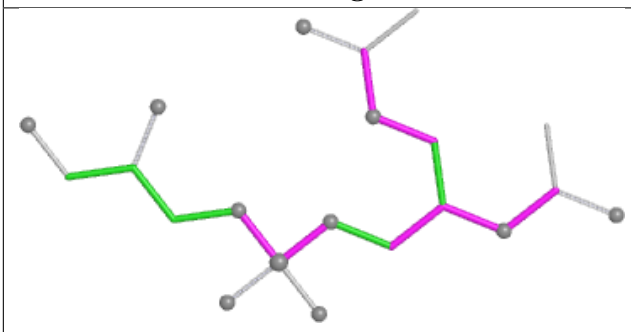
Ligand PGW S 101



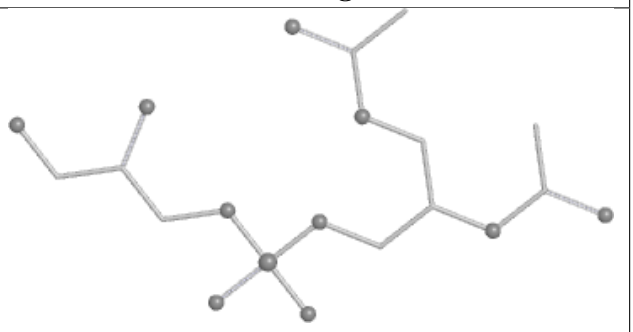
Bond lengths



Bond angles

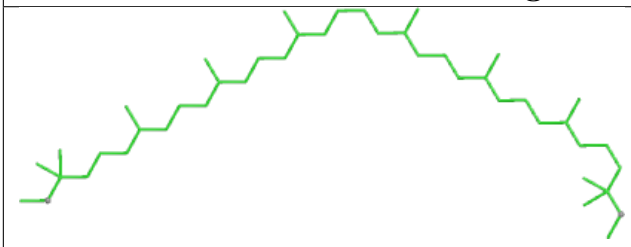


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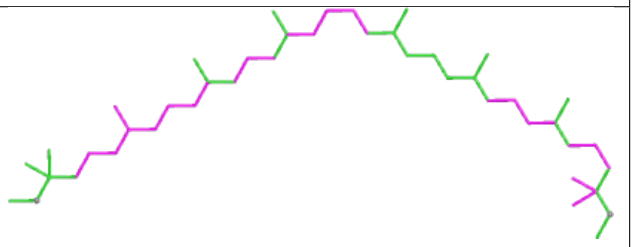


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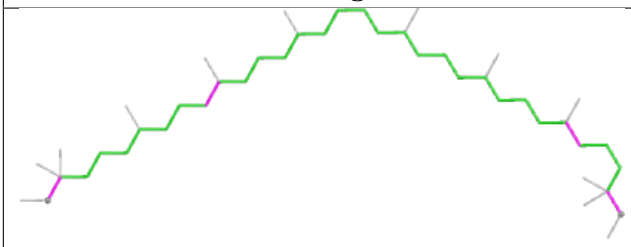
Ligand CRT T 101



Bond lengths



Bond angles

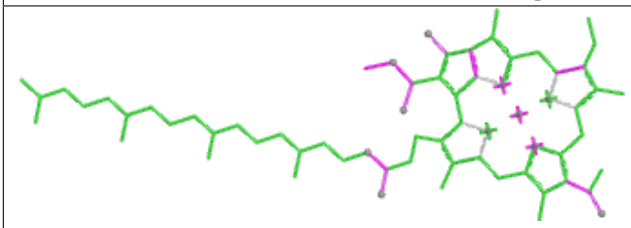


Torsions

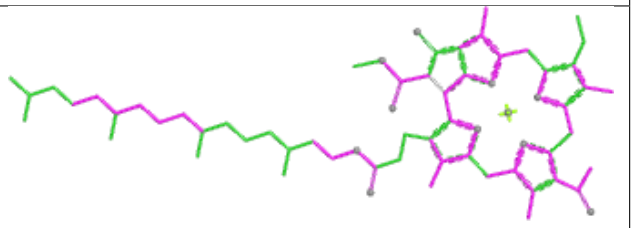


Rings

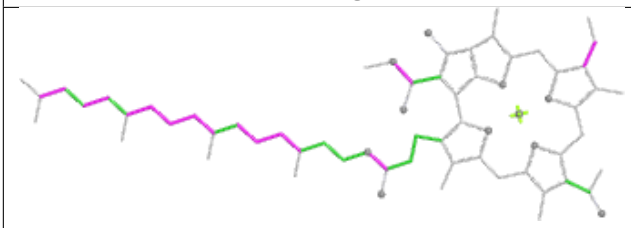
Ligand BCL 7 102



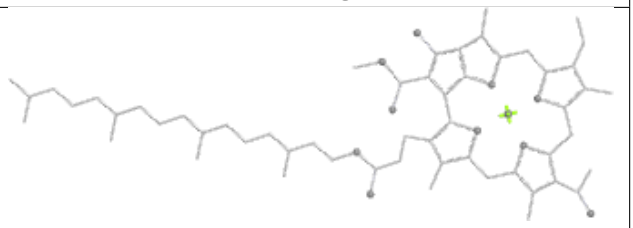
Bond lengths



Bond angles

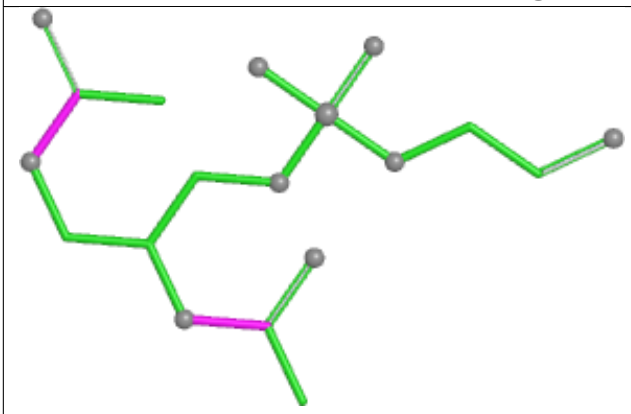


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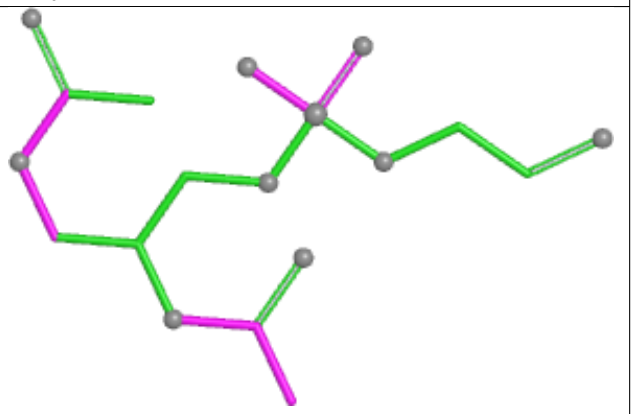


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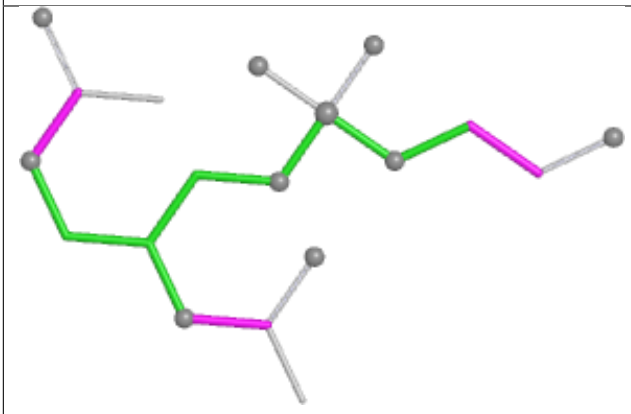
Ligand PEF y 407



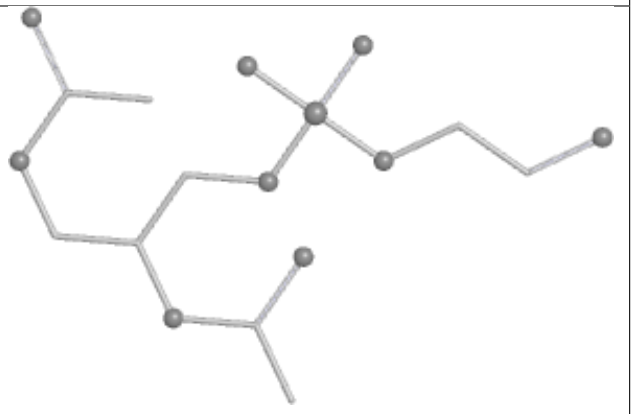
Bond lengths



Bond angles

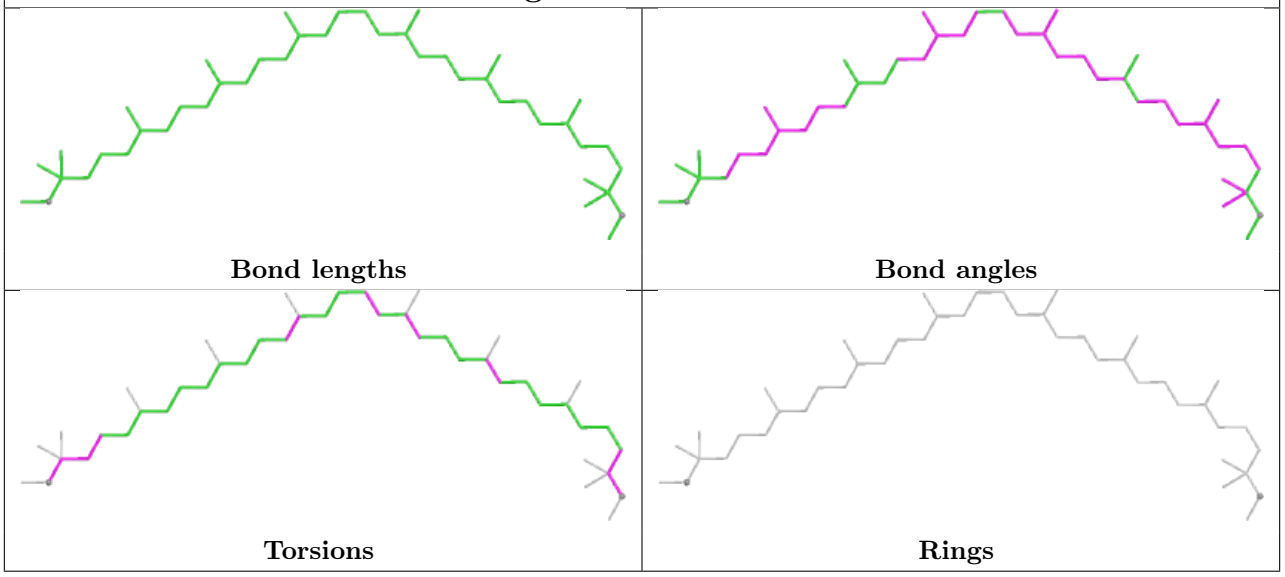


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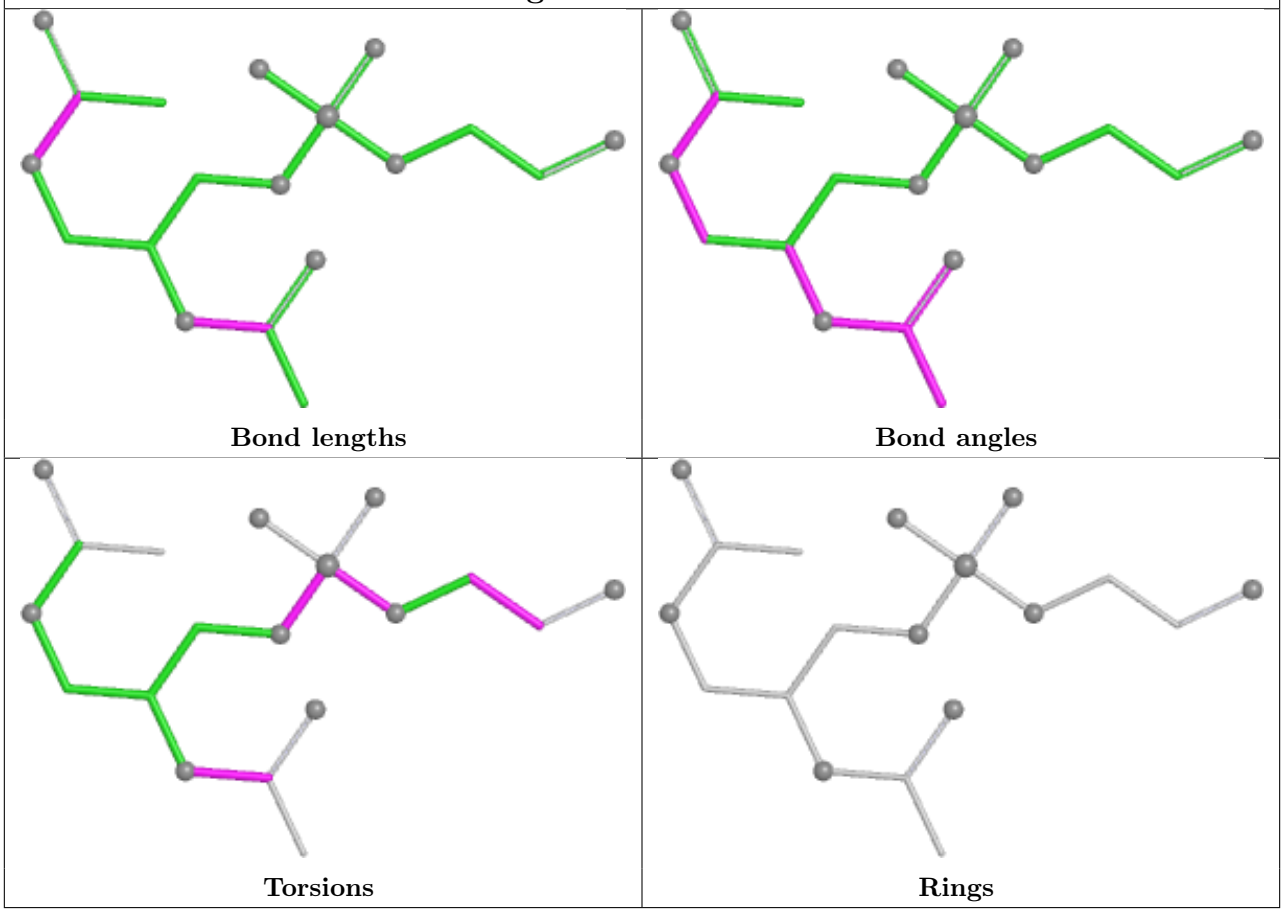


Rings

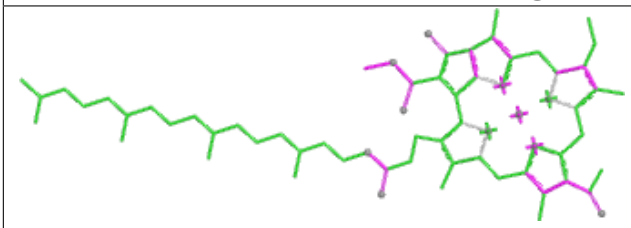
Ligand CRT V 101



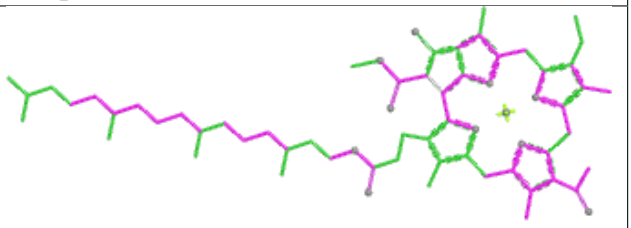
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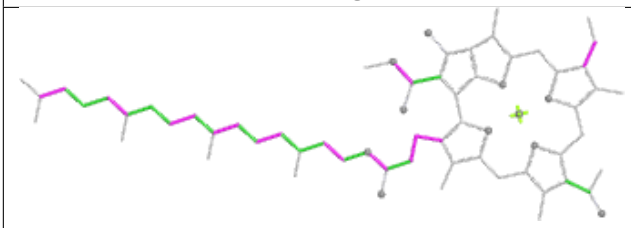
Ligand BCL q 102



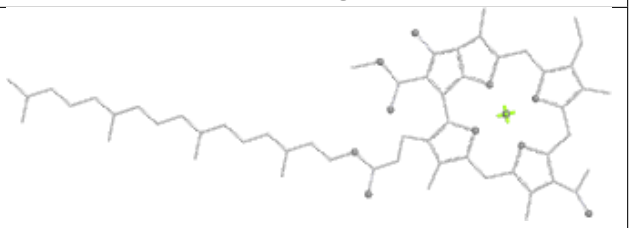
Bond lengths



Bond angles

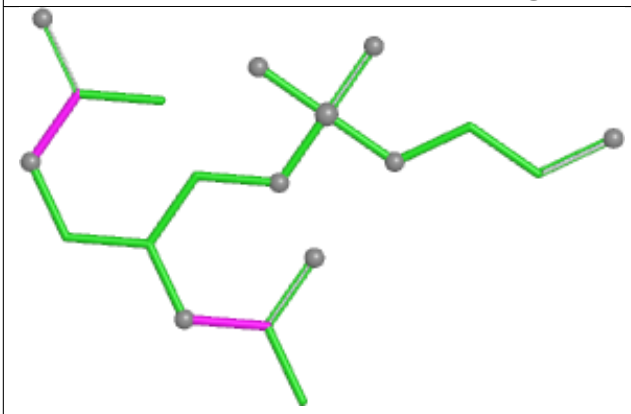


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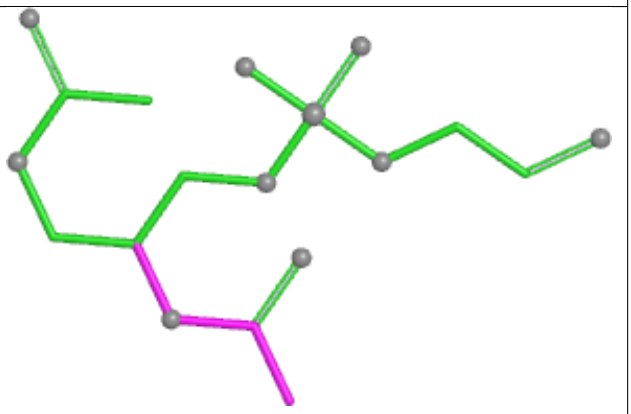


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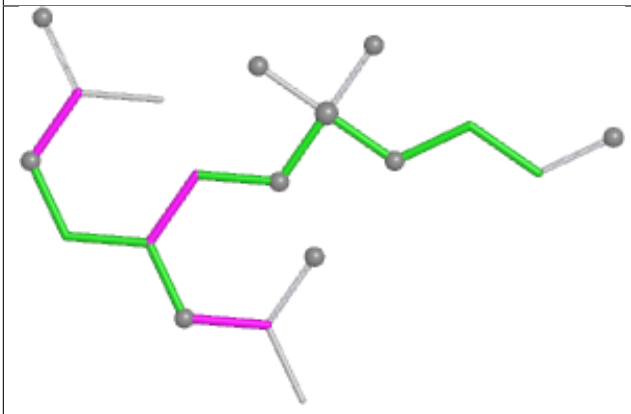
Ligand PEF H 302



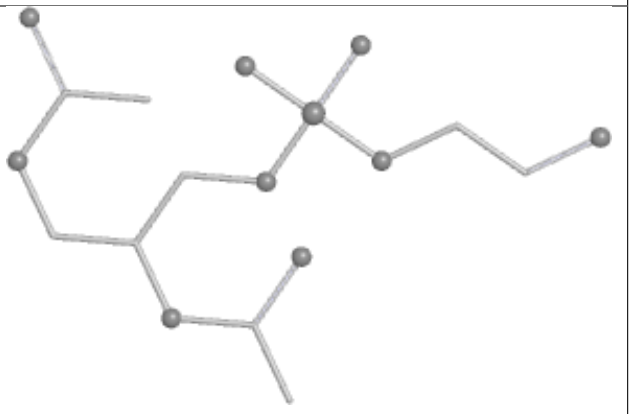
Bond lengths



Bond angles

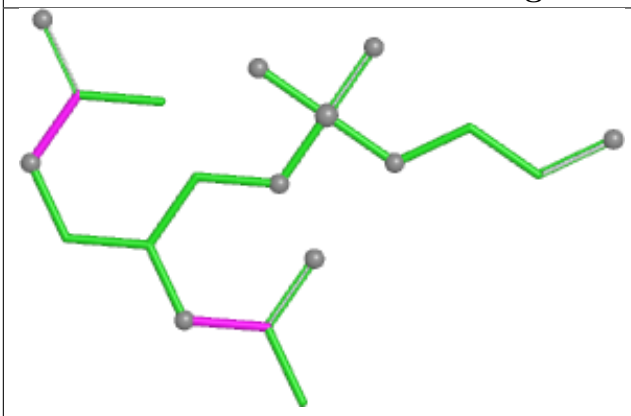


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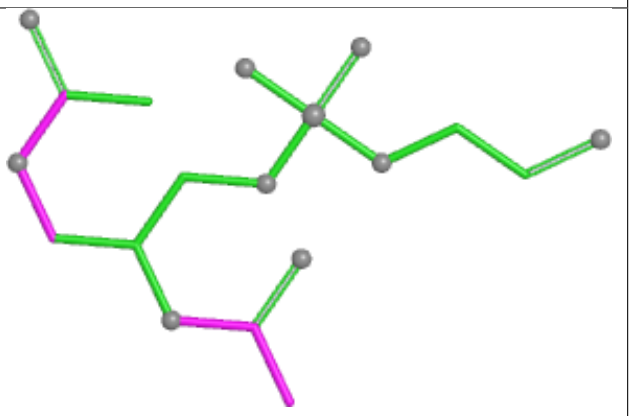


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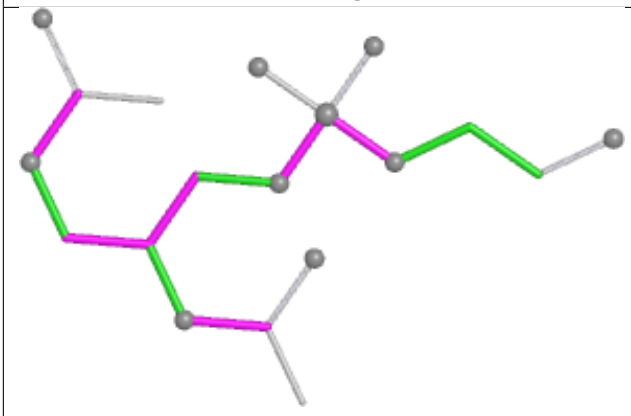
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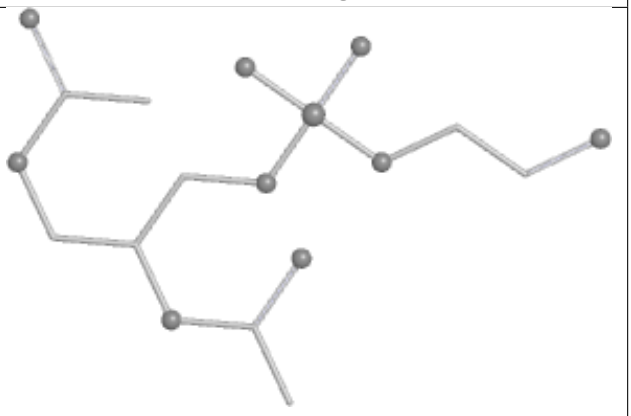
Bond lengths



Bond angles

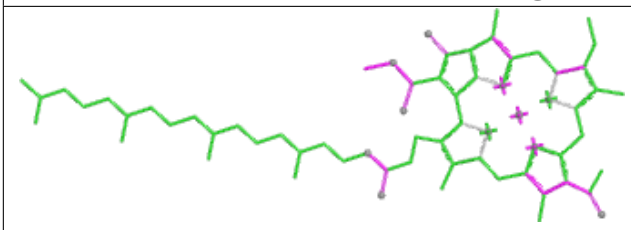


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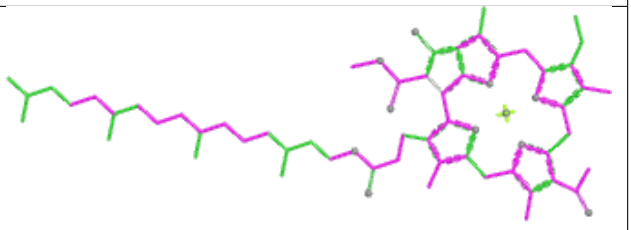


Rings

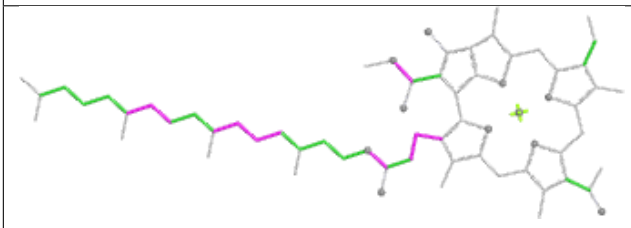
Ligand BCL 6 101



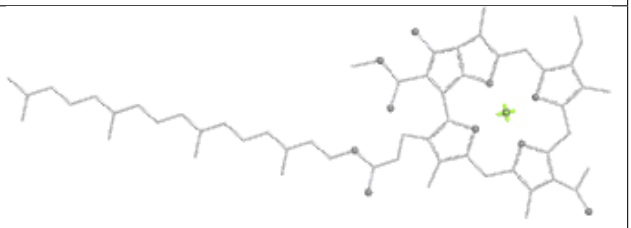
Bond lengths



Bond angles

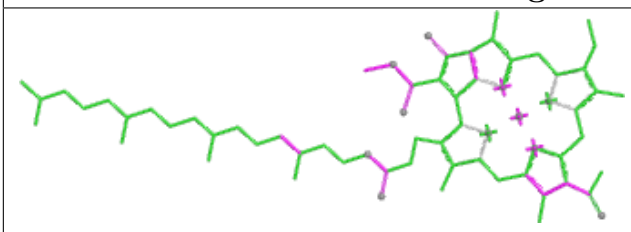


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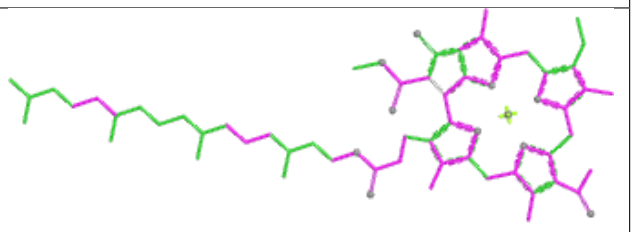


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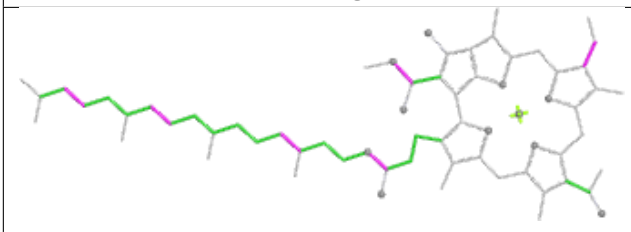
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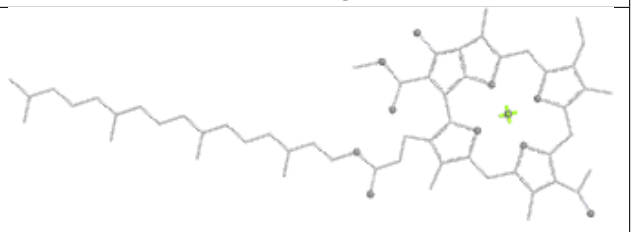
Bond lengths



Bond angles

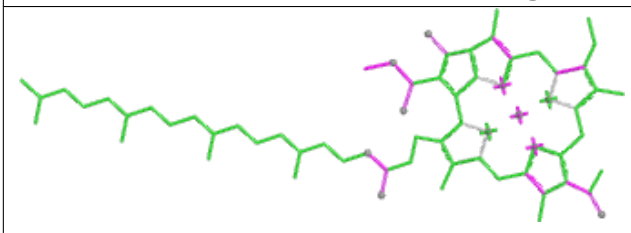


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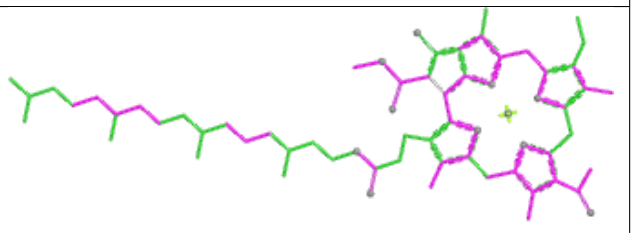


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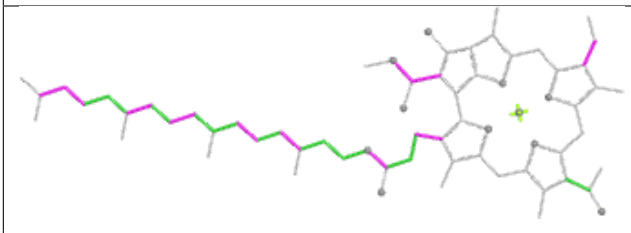
Ligand BCL G 102



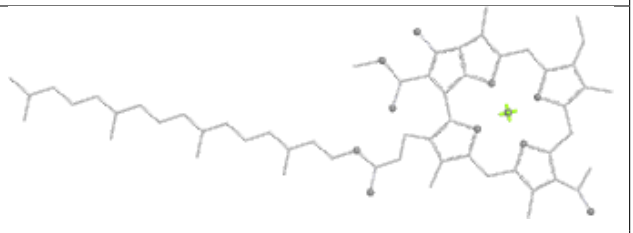
Bond lengths



Bond angles

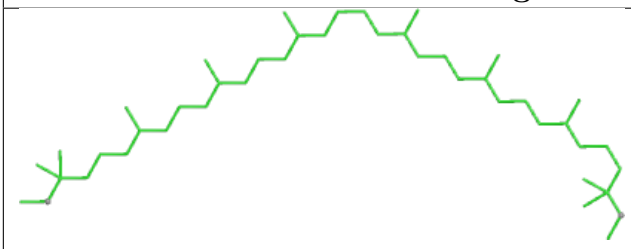


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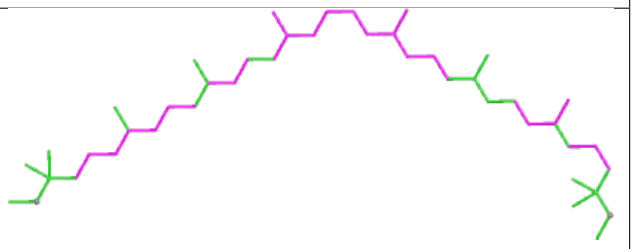


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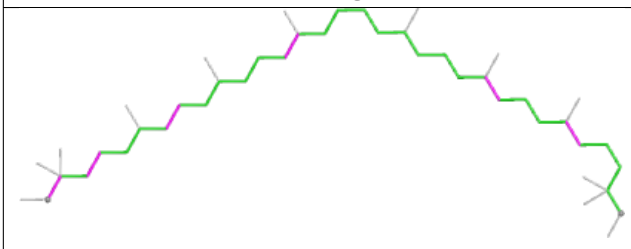
Ligand CRT AL 101



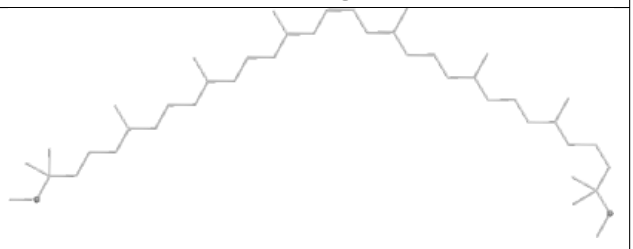
Bond lengths



Bond angles

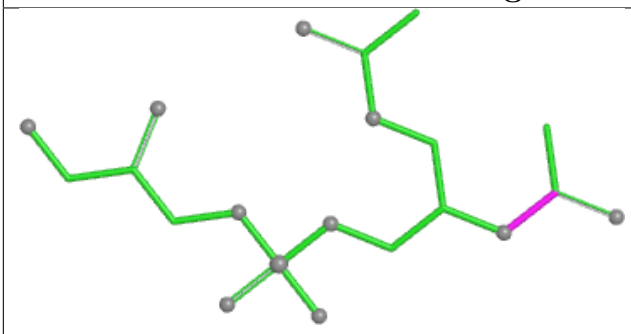


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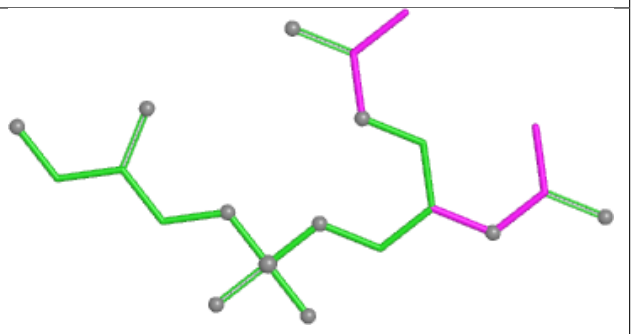


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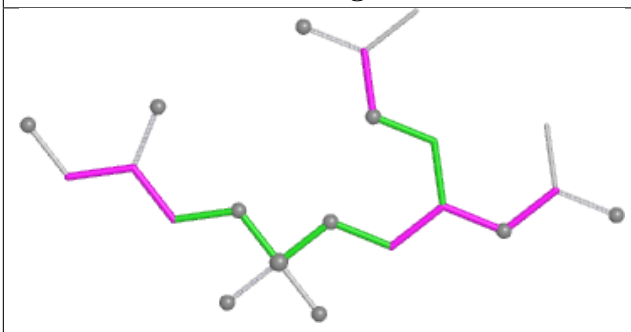
Ligand PGW AE 101



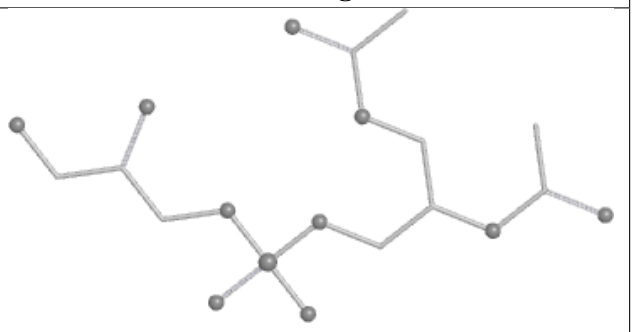
Bond lengths



Bond angles

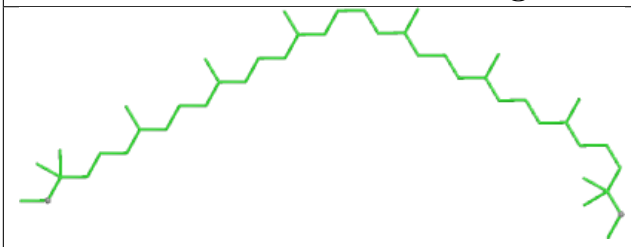


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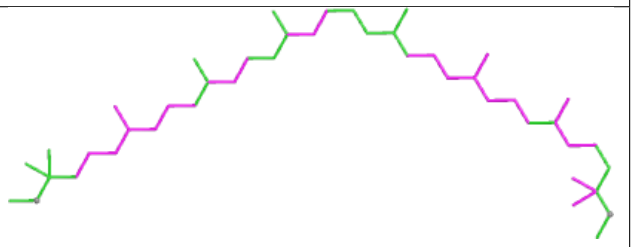


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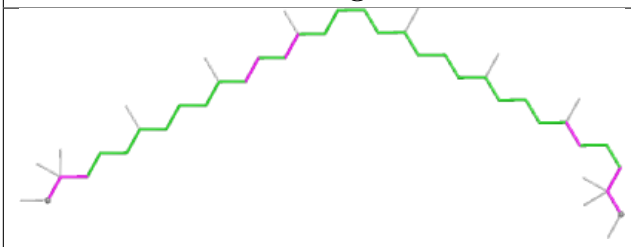
Ligand CRT AH 102



Bond lengths



Bond angles

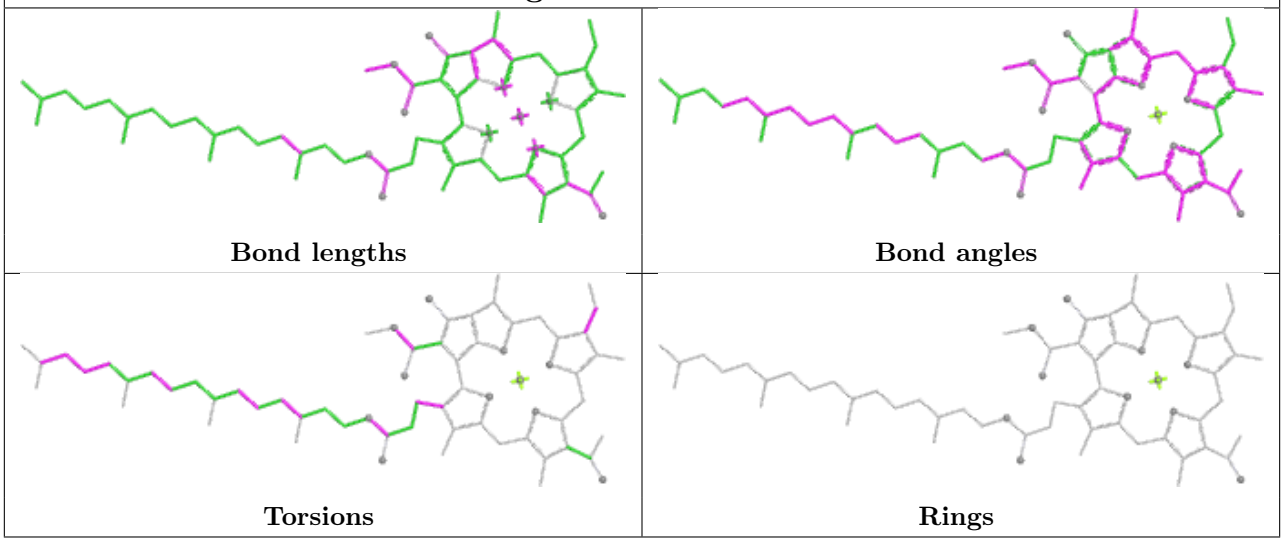


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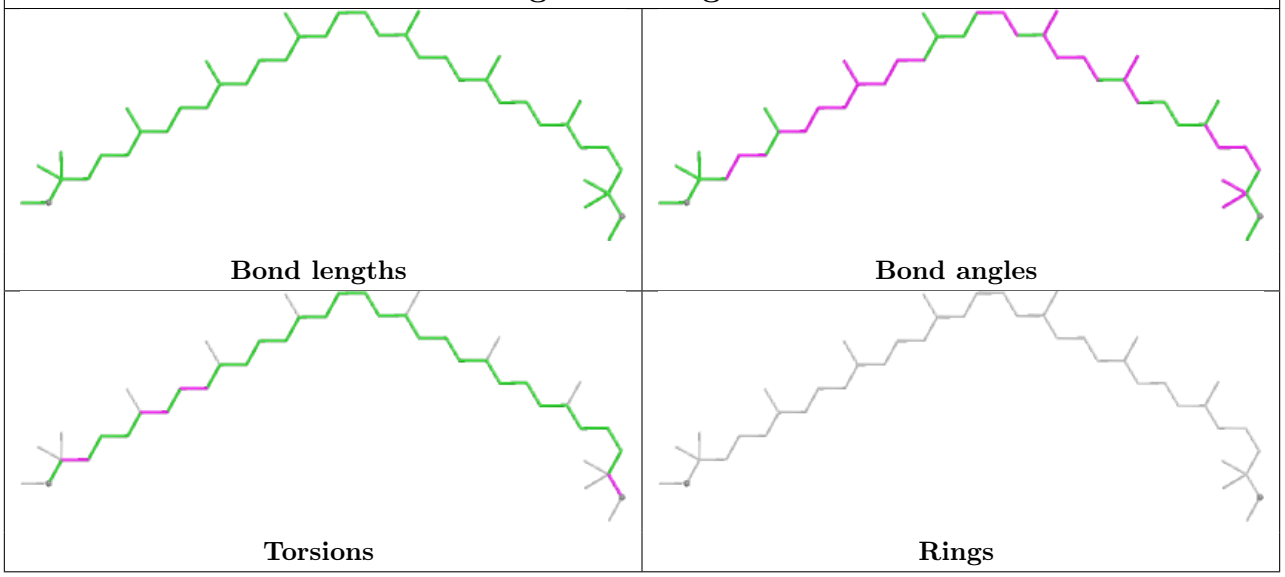


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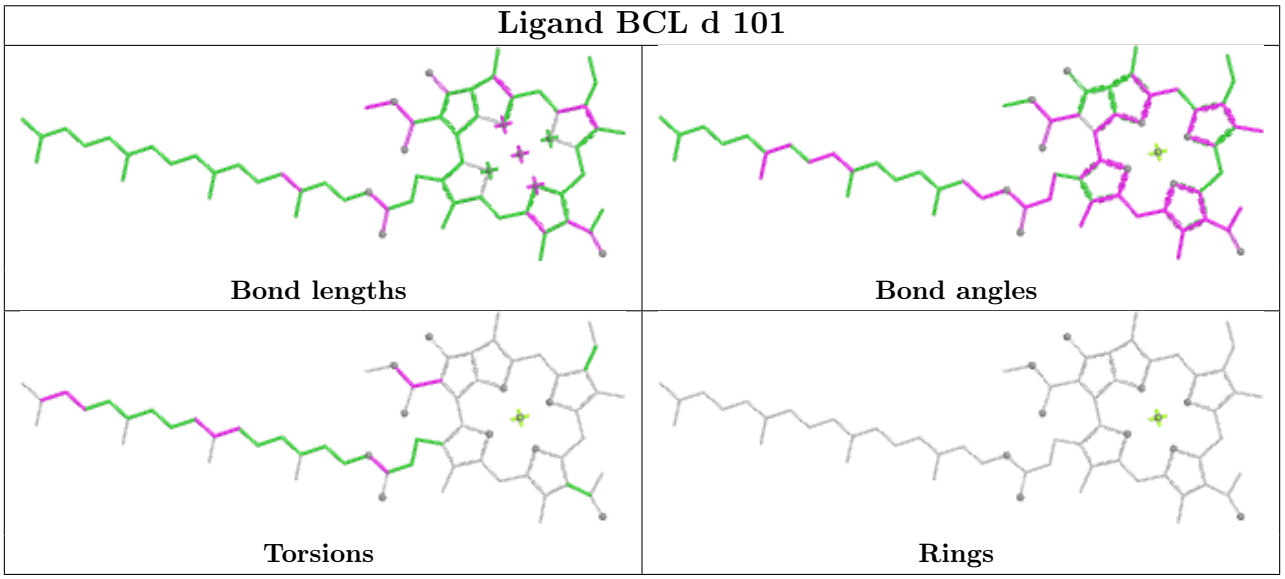
Ligand BCL R 102



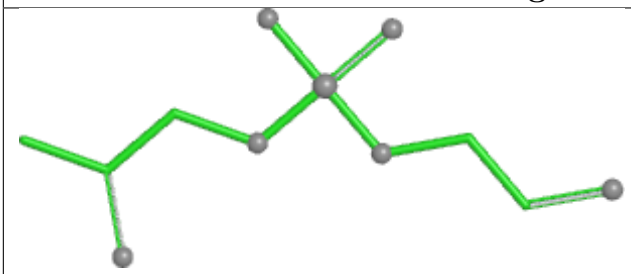
Ligand CRT g 101



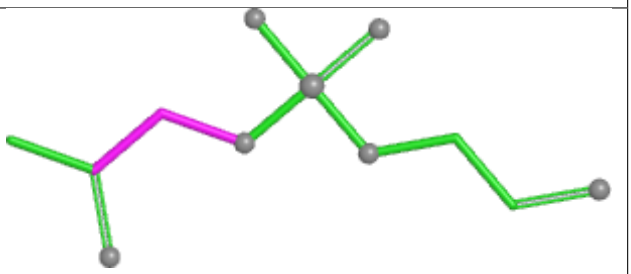
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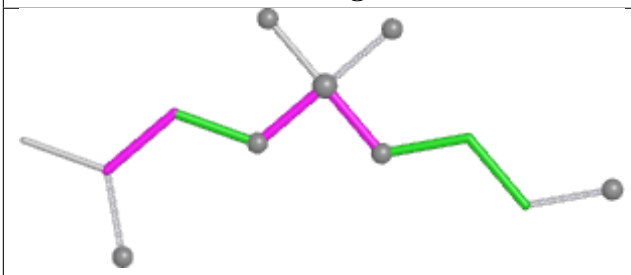
Ligand PEF L 305



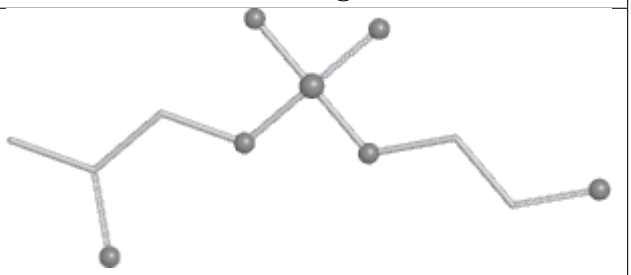
Bond lengths



Bond angles

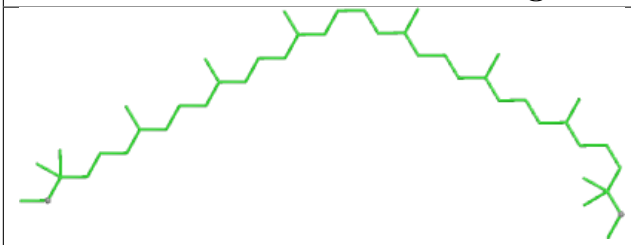


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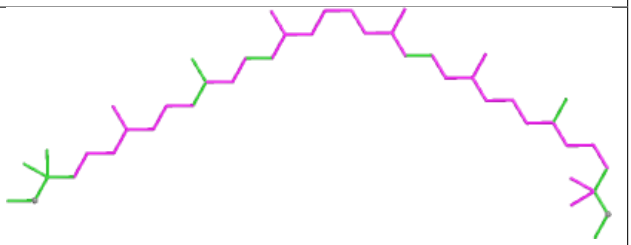


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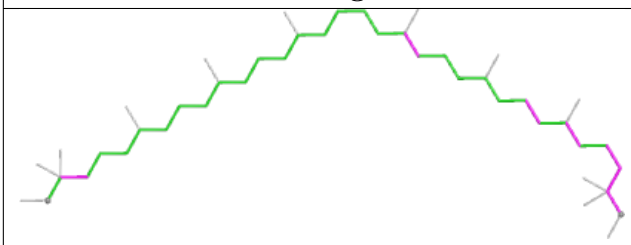
Ligand CRT n 101



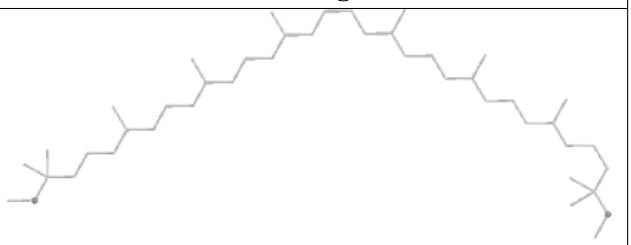
Bond lengths



Bond angles

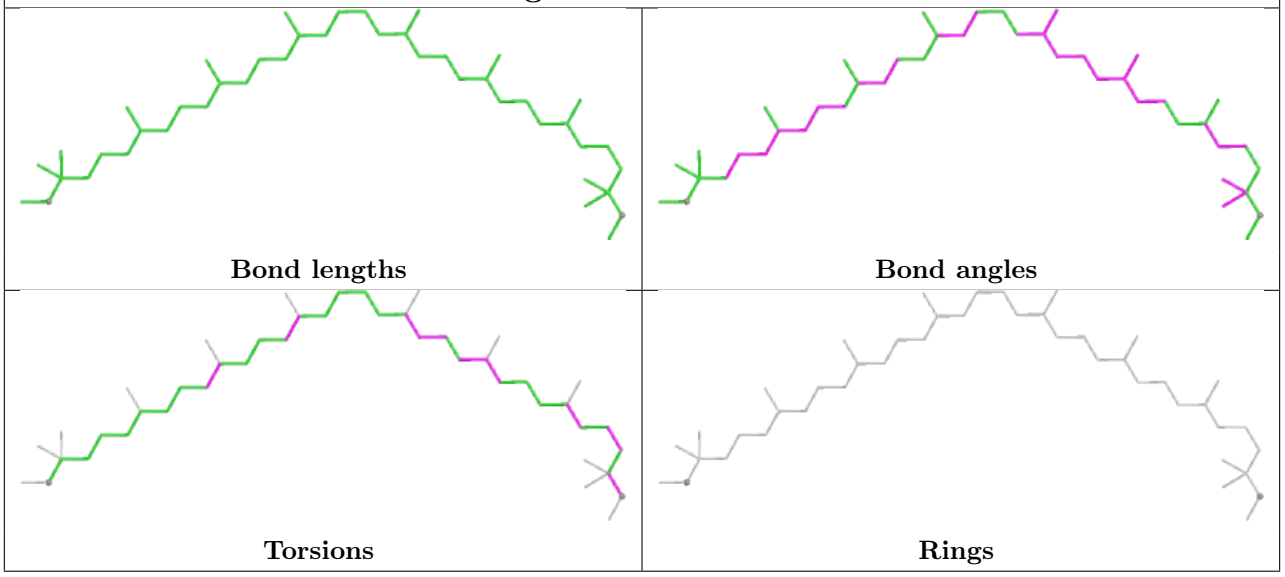


Torsions

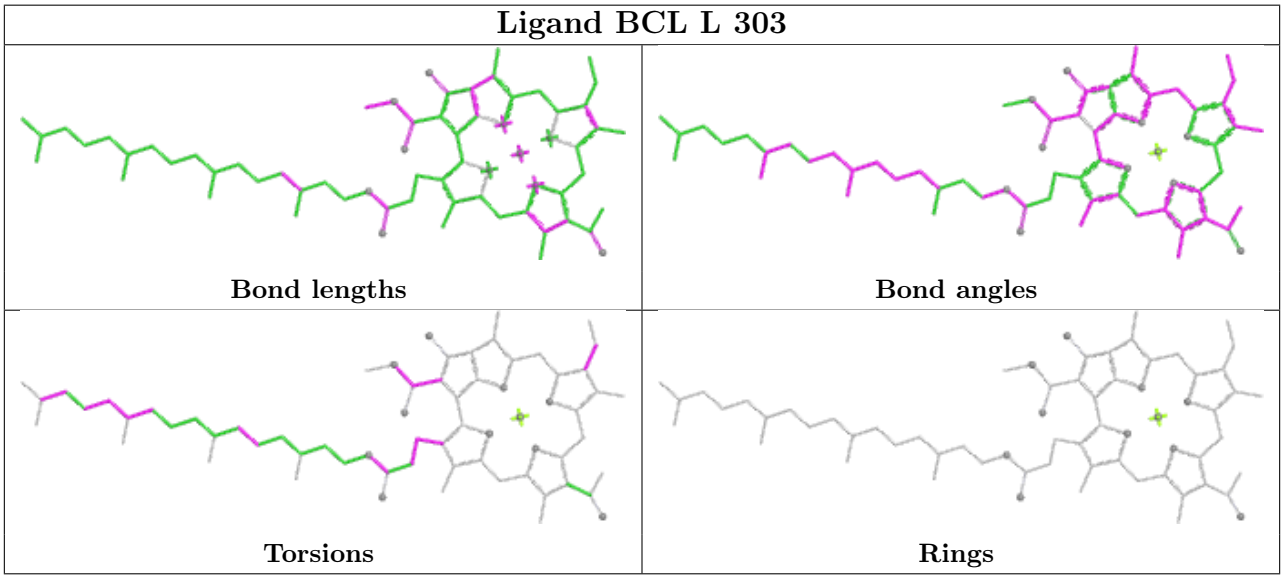


Rings

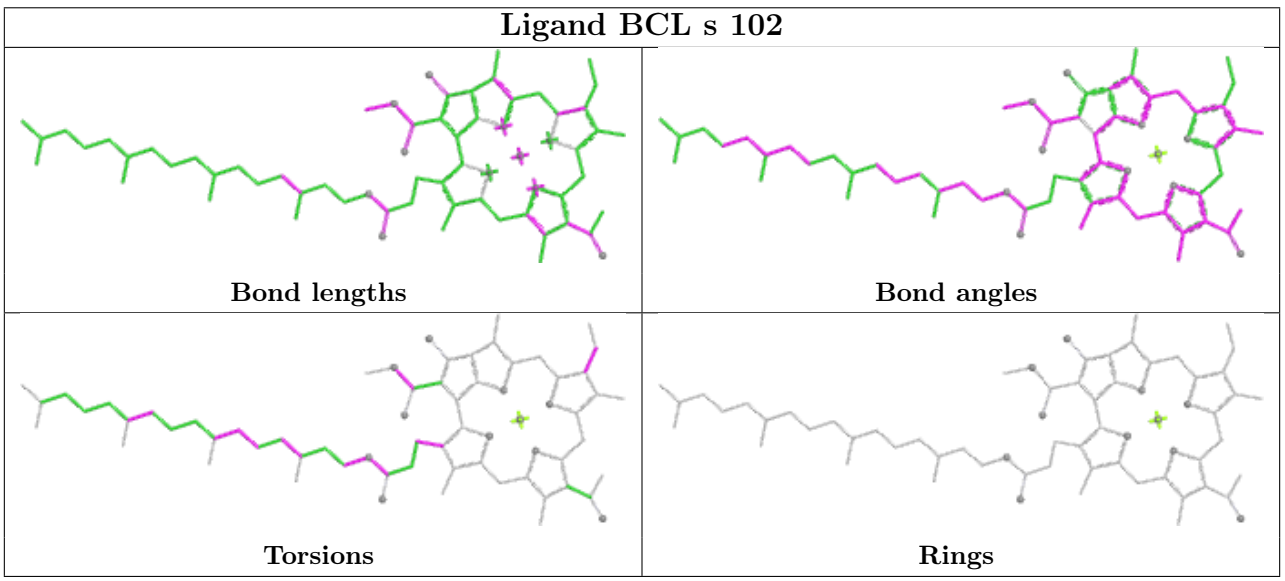
Ligand CRT R 101



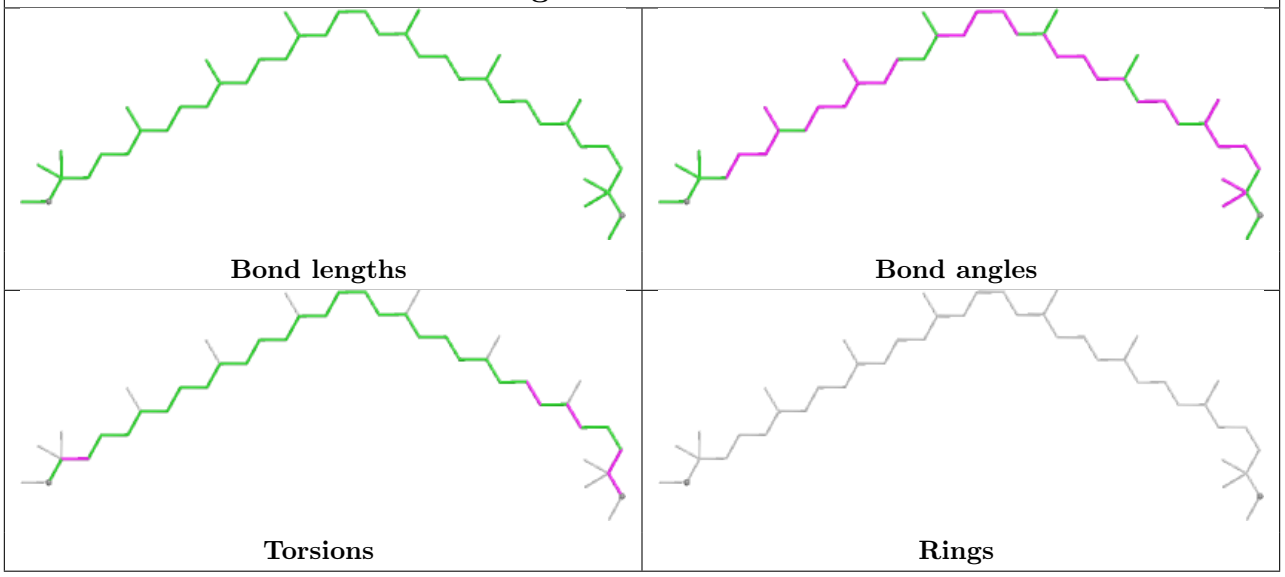
Ligand BCL L 303



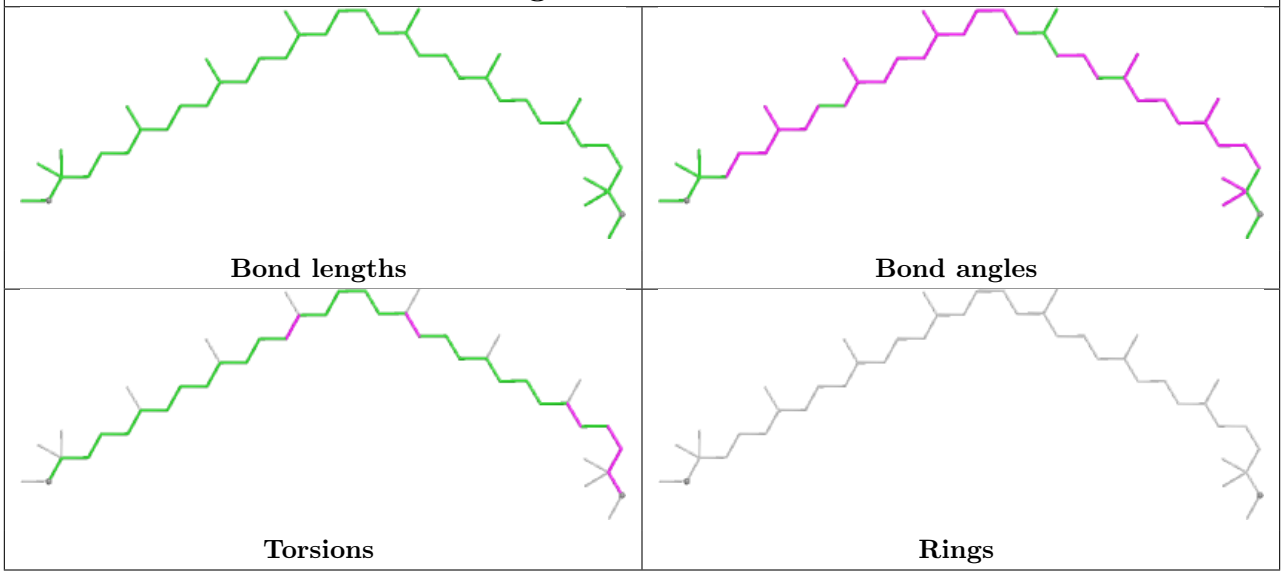
Ligand BCL s 102



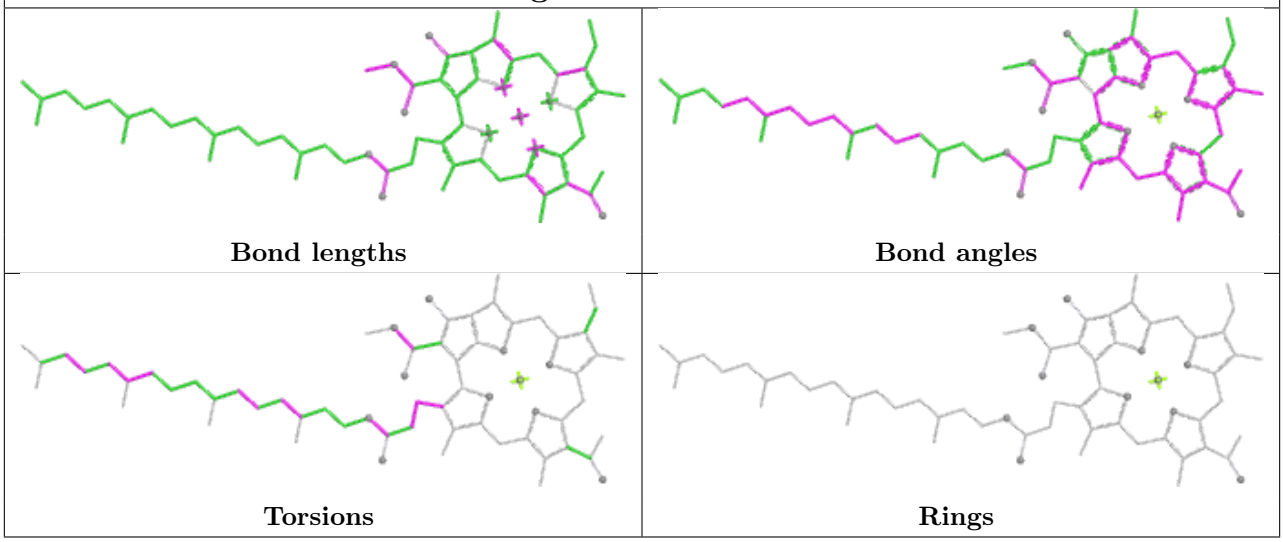
Ligand CRT I 102



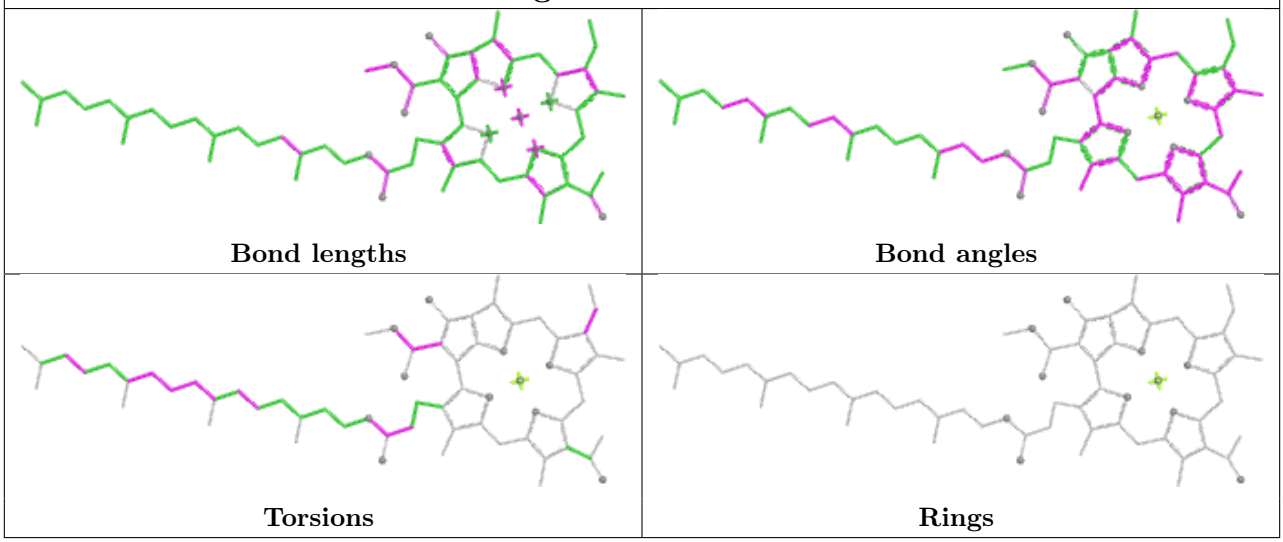
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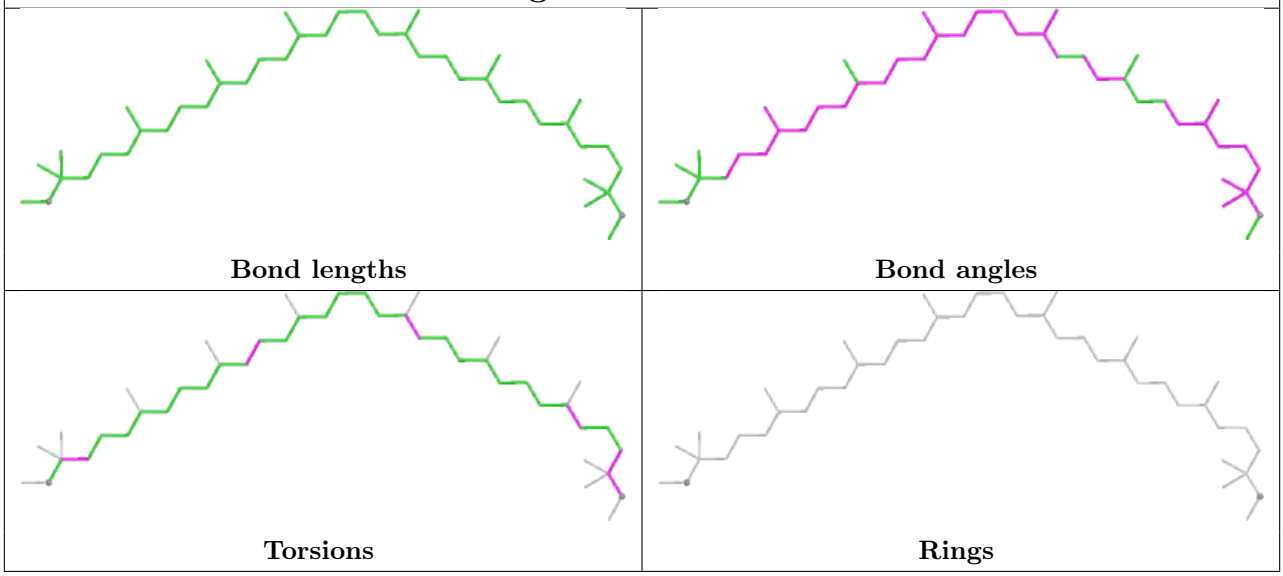
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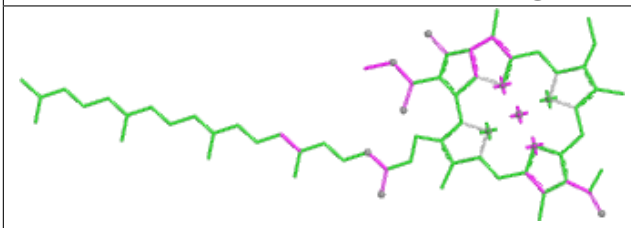
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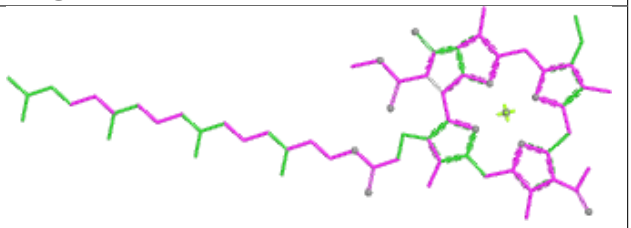
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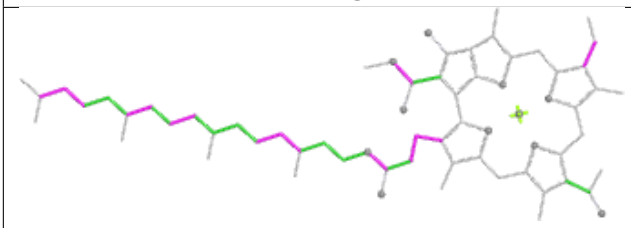
Ligand BCL g 102



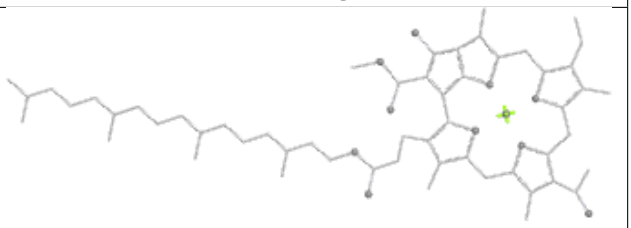
Bond lengths



Bond angles

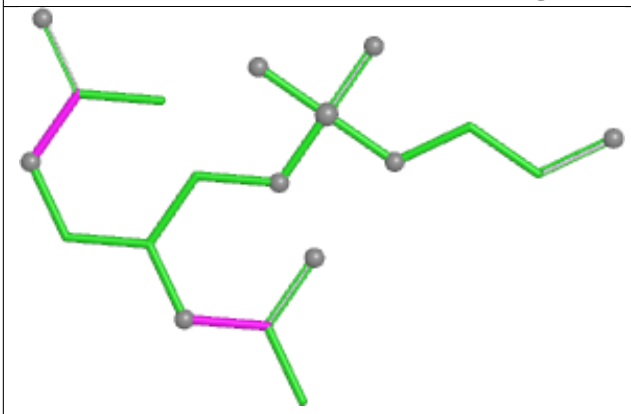


Torsions

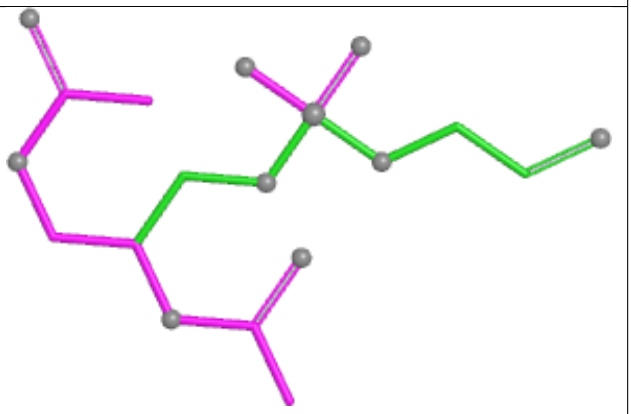


Rings

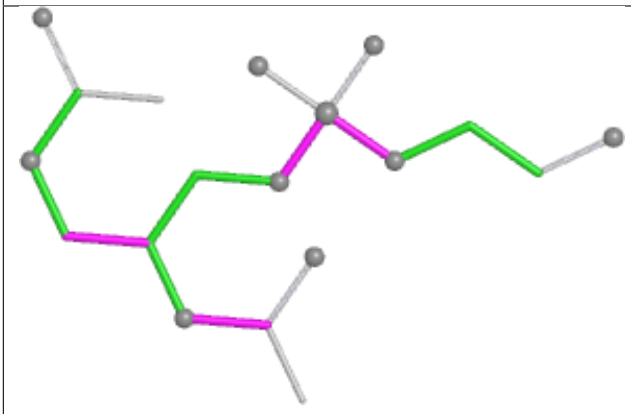
Ligand PEF t 303



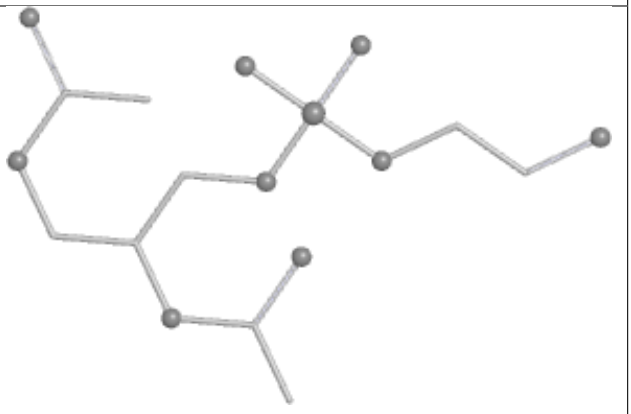
Bond lengths



Bond angles

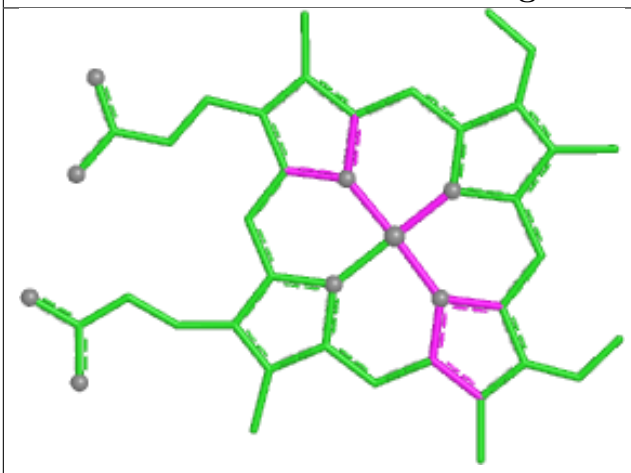


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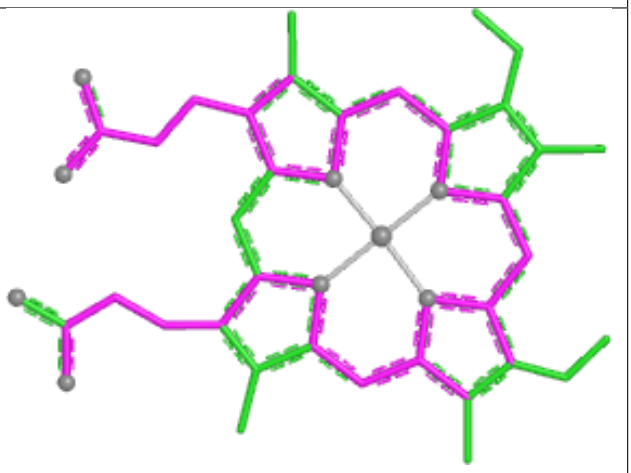


Rings

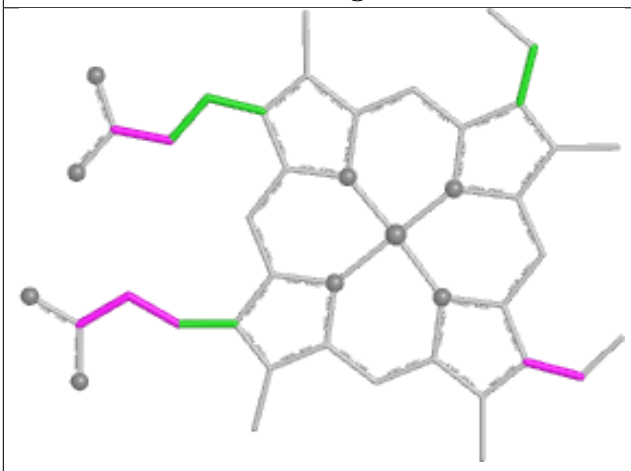
Ligand HEM C 501



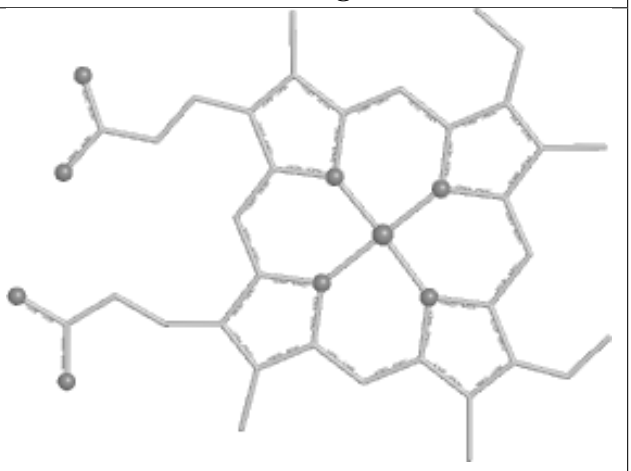
Bond lengths



Bond angles

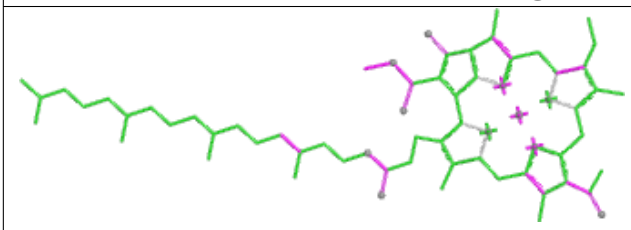


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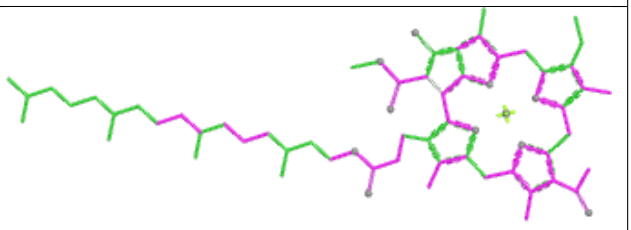


Rings

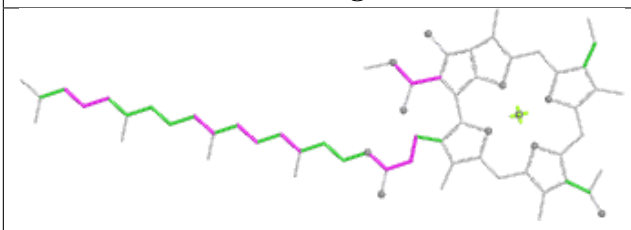
Ligand BCL 1 101



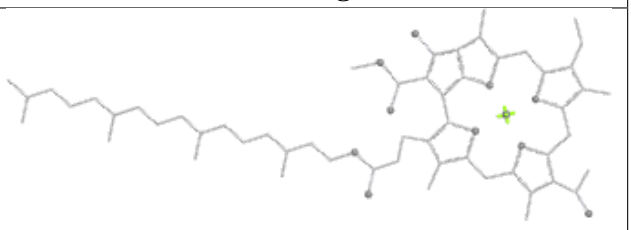
Bond lengths



Bond angles

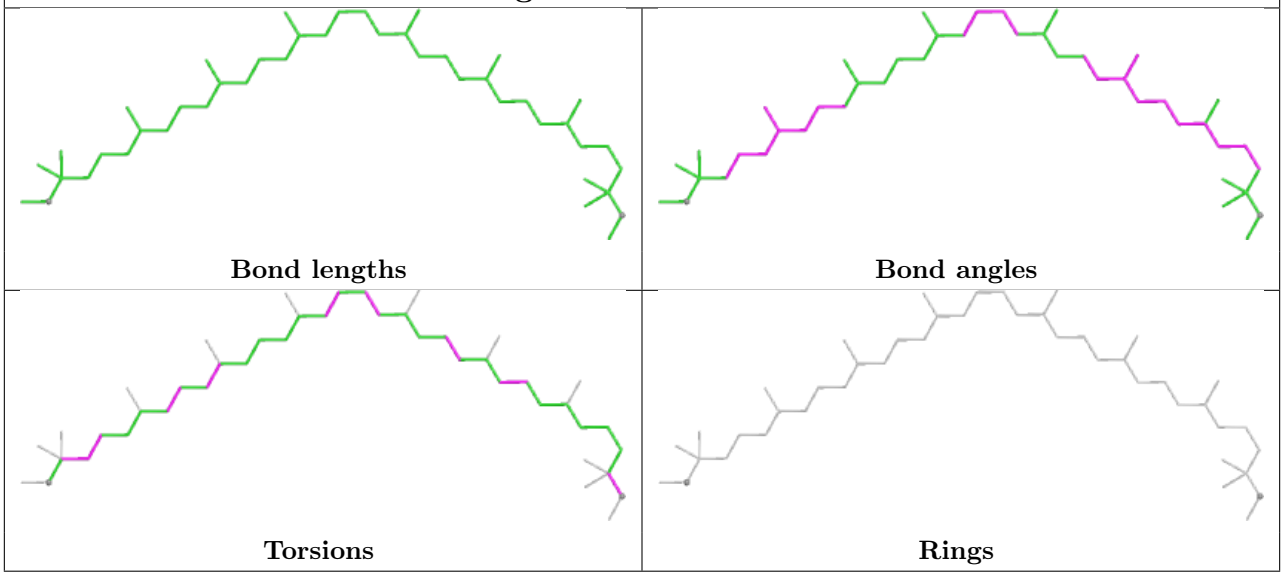


Torsions

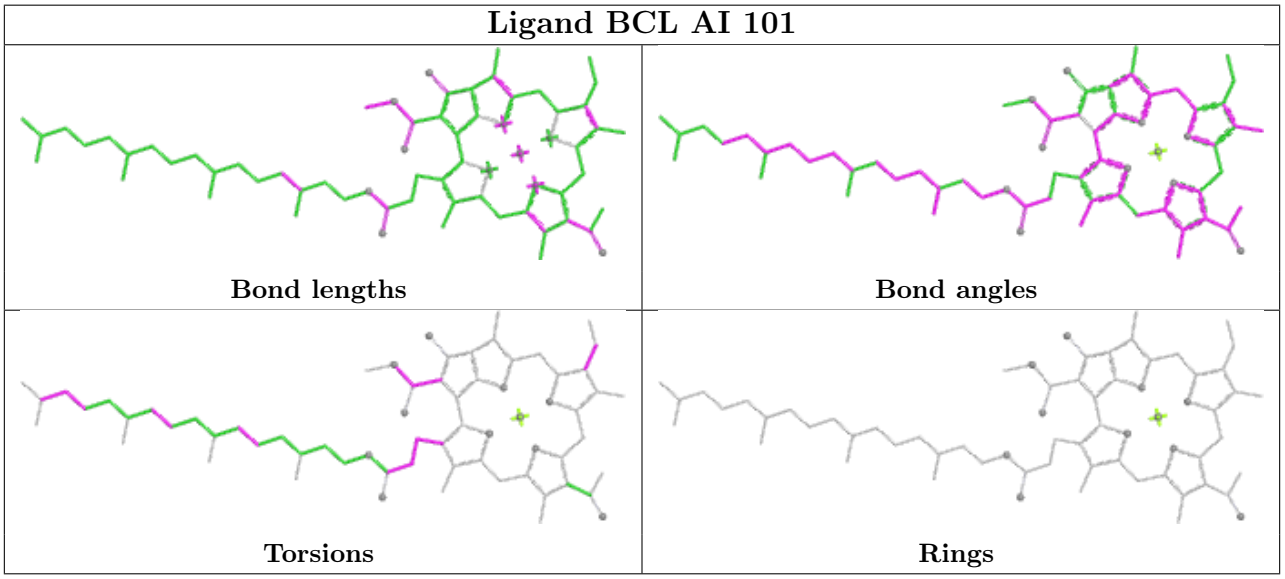


Rings

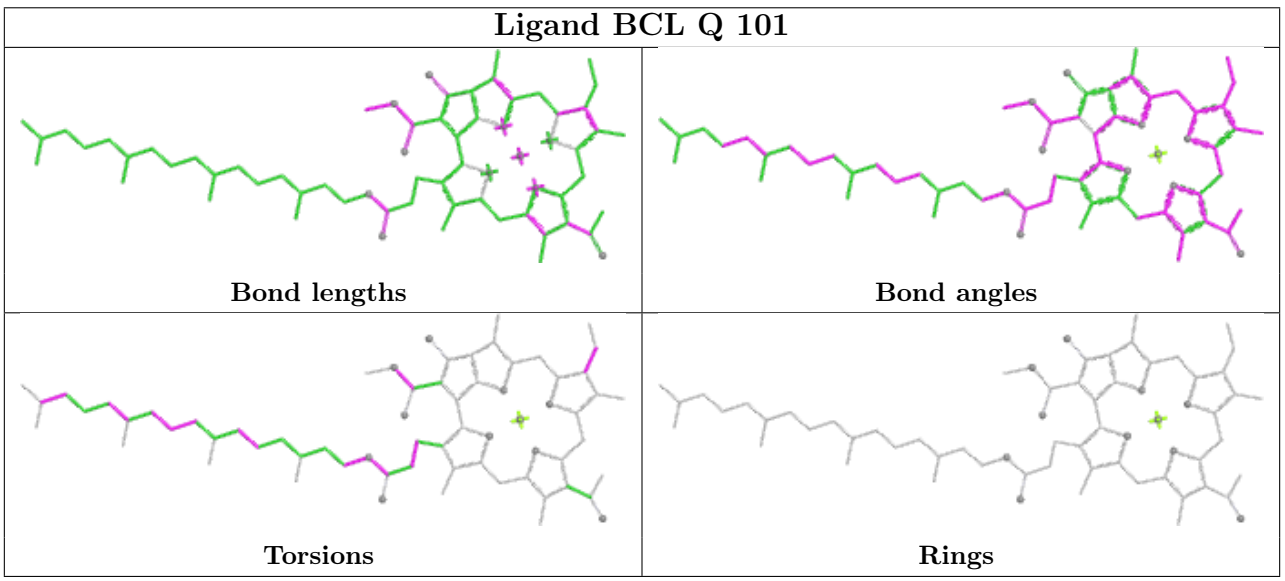
Ligand CRT AJ 101



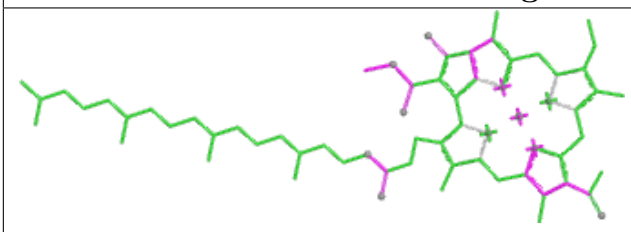
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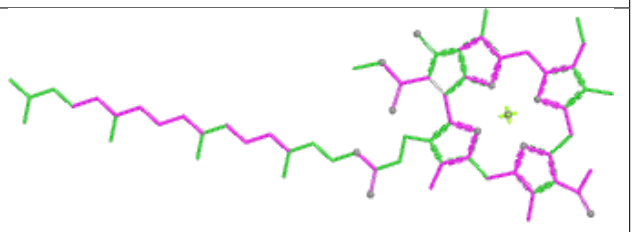
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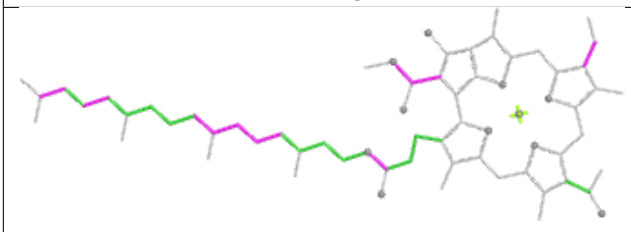
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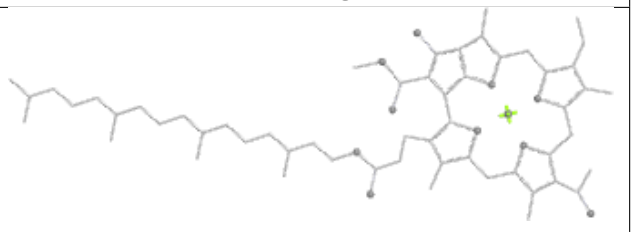
Bond lengths



Bond angles

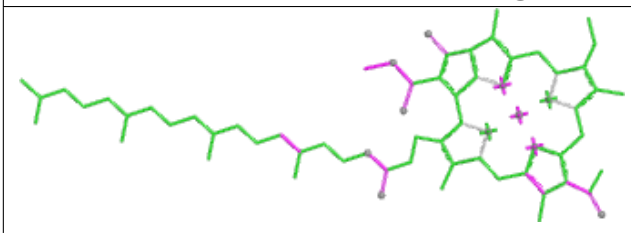


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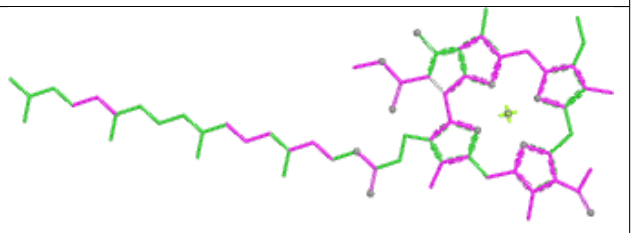


Rings

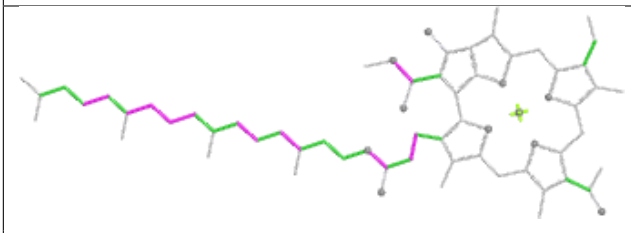
Ligand BCL AB 101



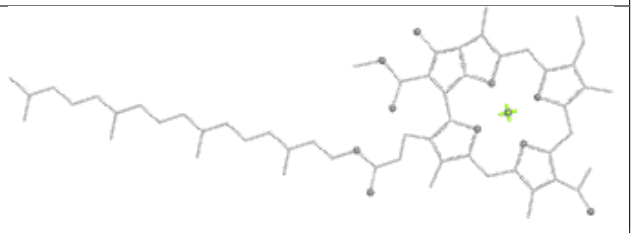
Bond lengths



Bond angles

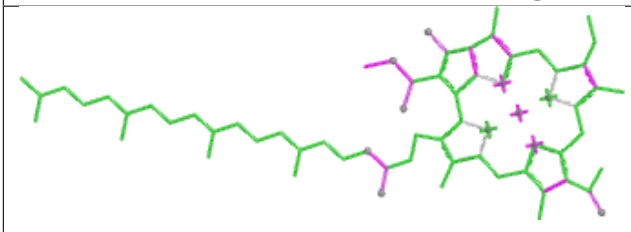


Torsions

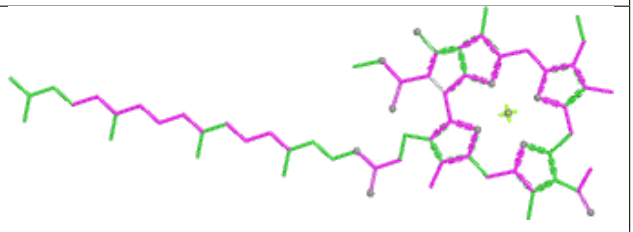


Rings

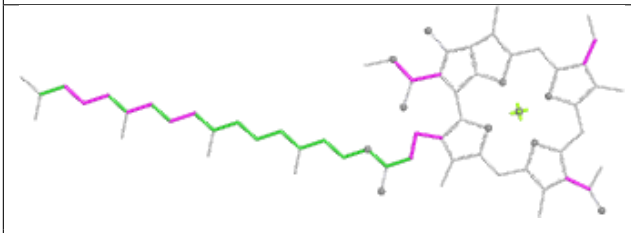
Ligand BCL x 305



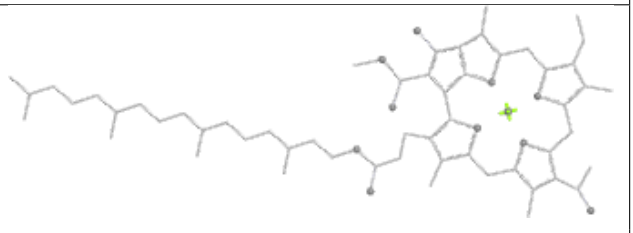
Bond lengths



Bond angles

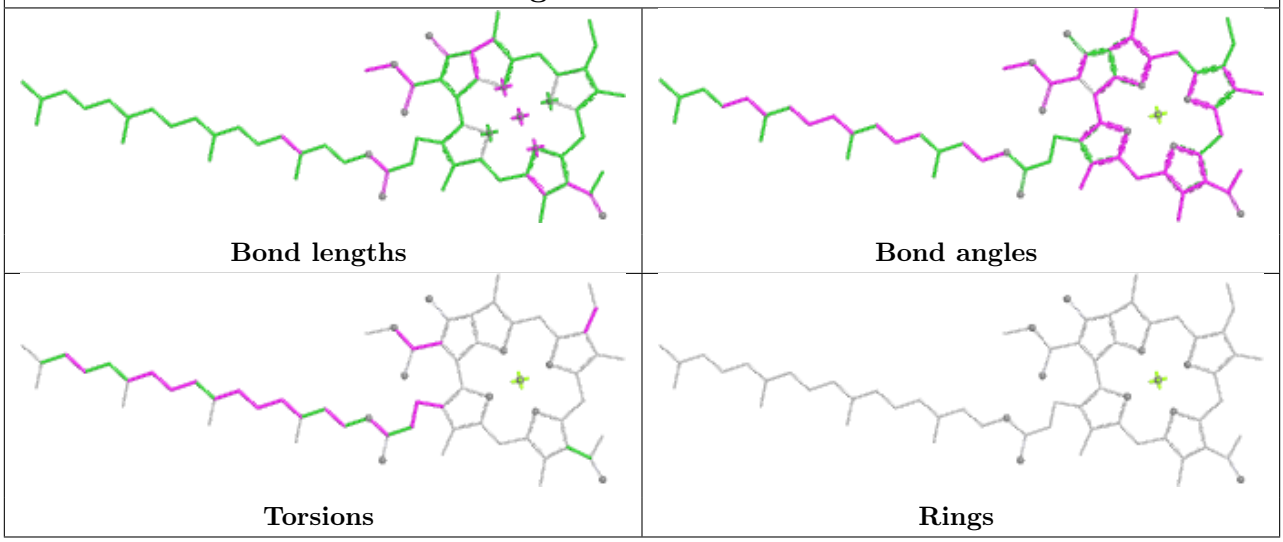


Torsions

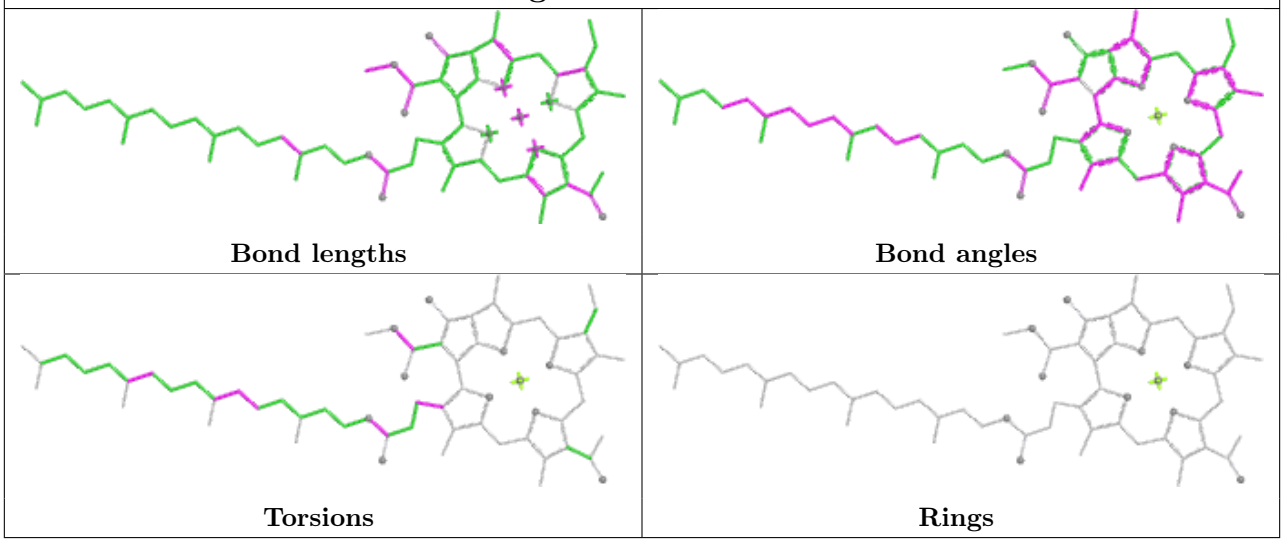


Rings

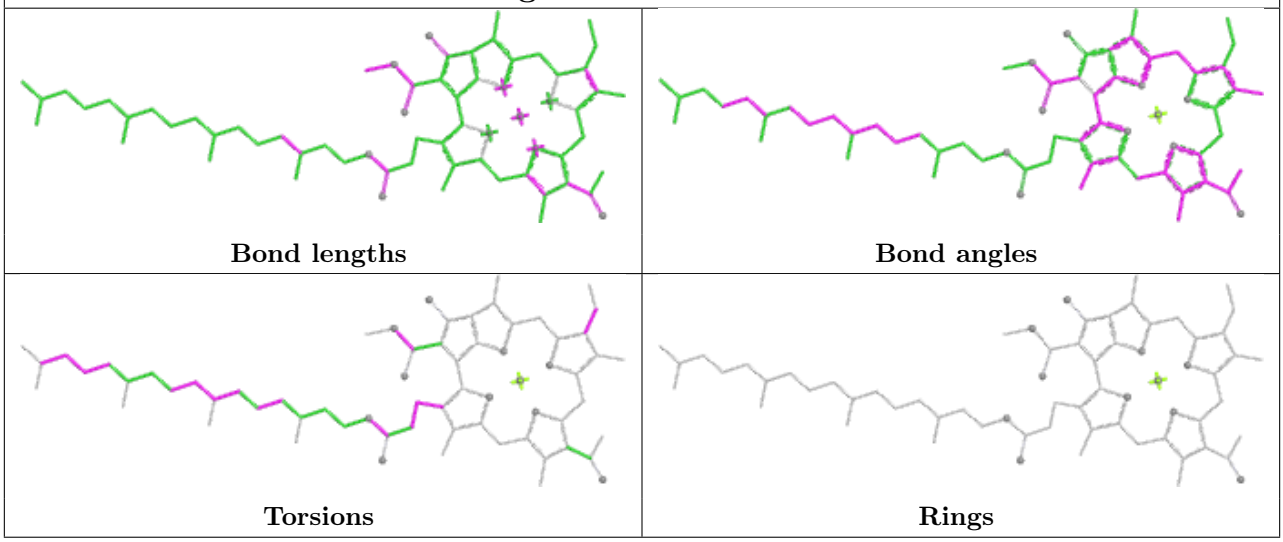
Ligand BCL k 102



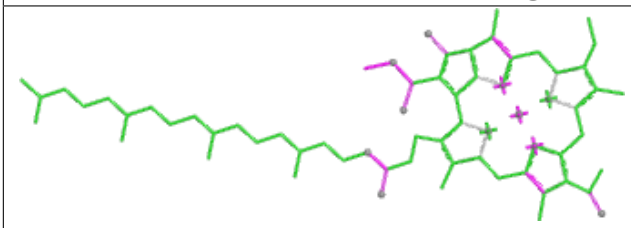
Ligand BCL u 102



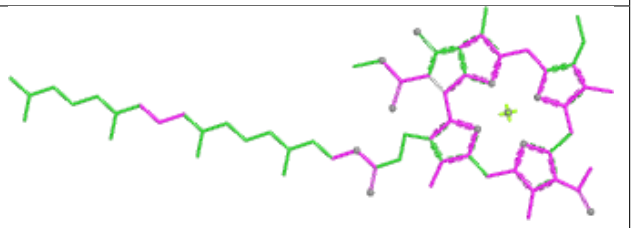
Ligand BCL AI 102



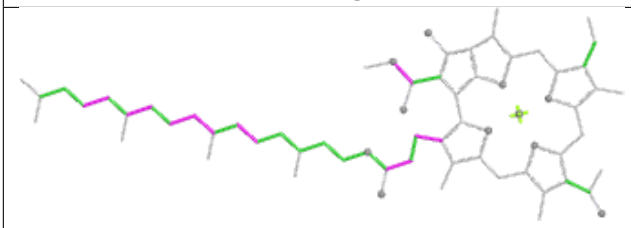
Ligand BCL A 102



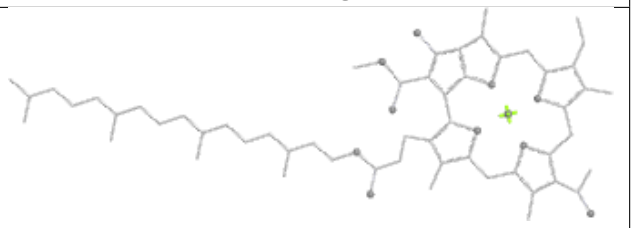
Bond lengths



Bond angles

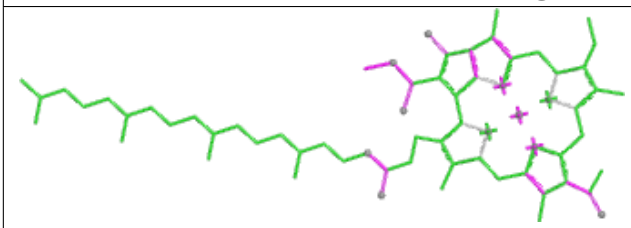


Torsions

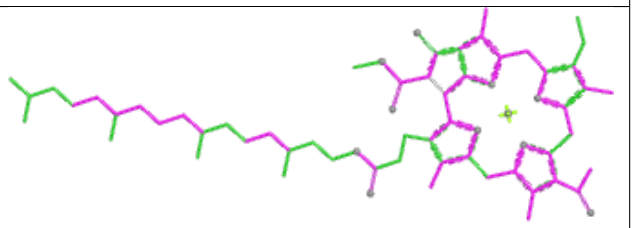


Rings

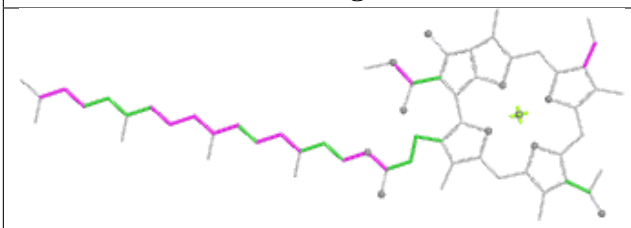
Ligand BCL l 101



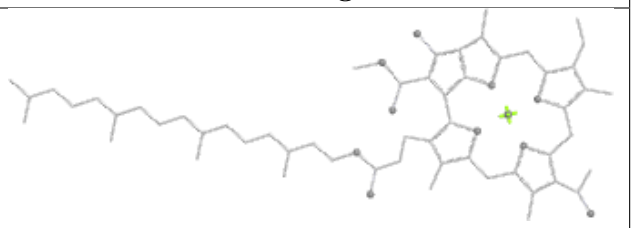
Bond lengths



Bond angles

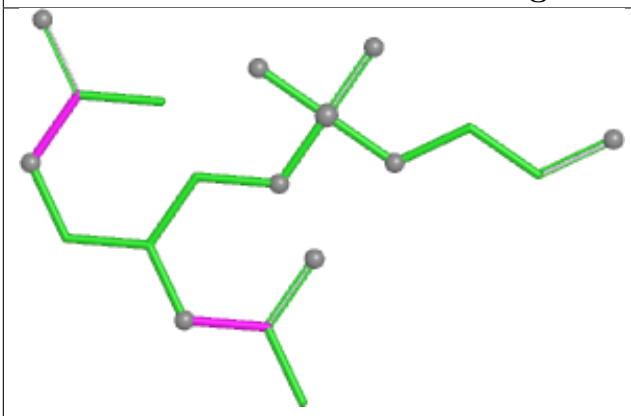


Torsions

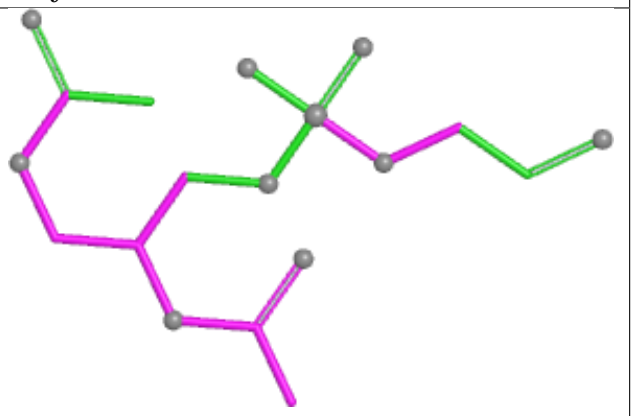


Rings

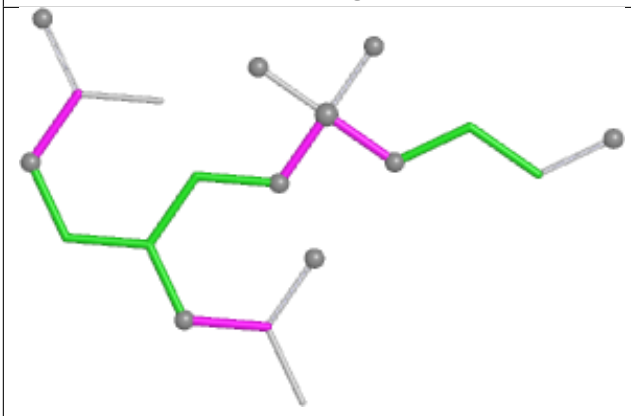
Ligand PEF y 408



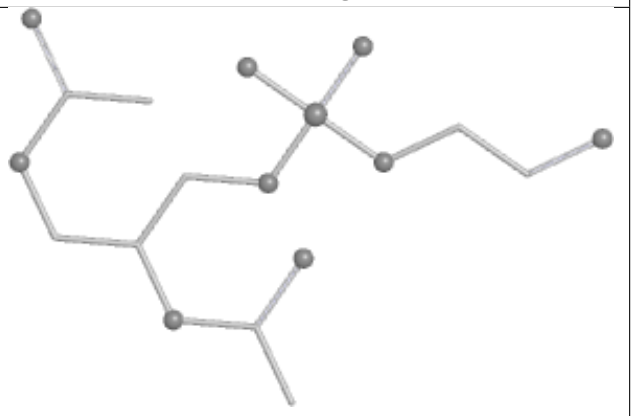
Bond lengths



Bond angles

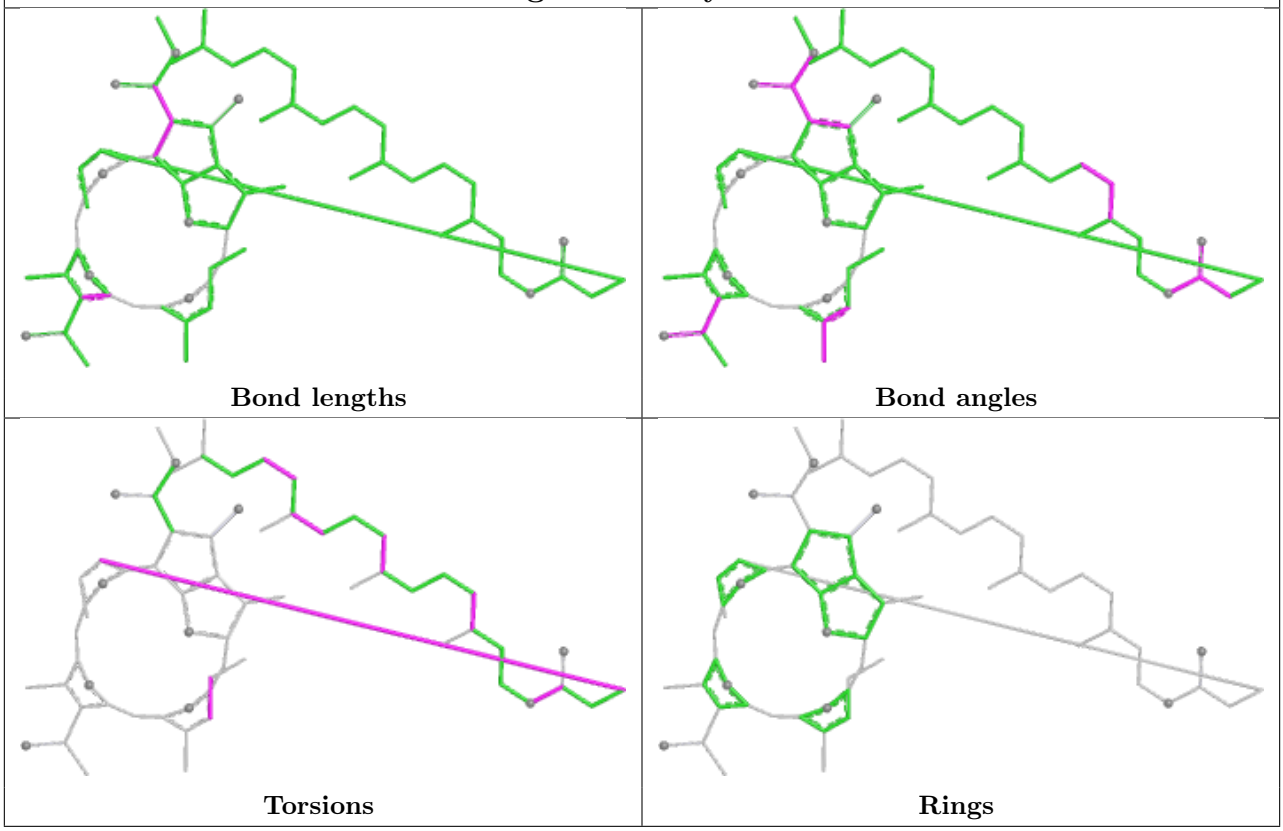


Torsions

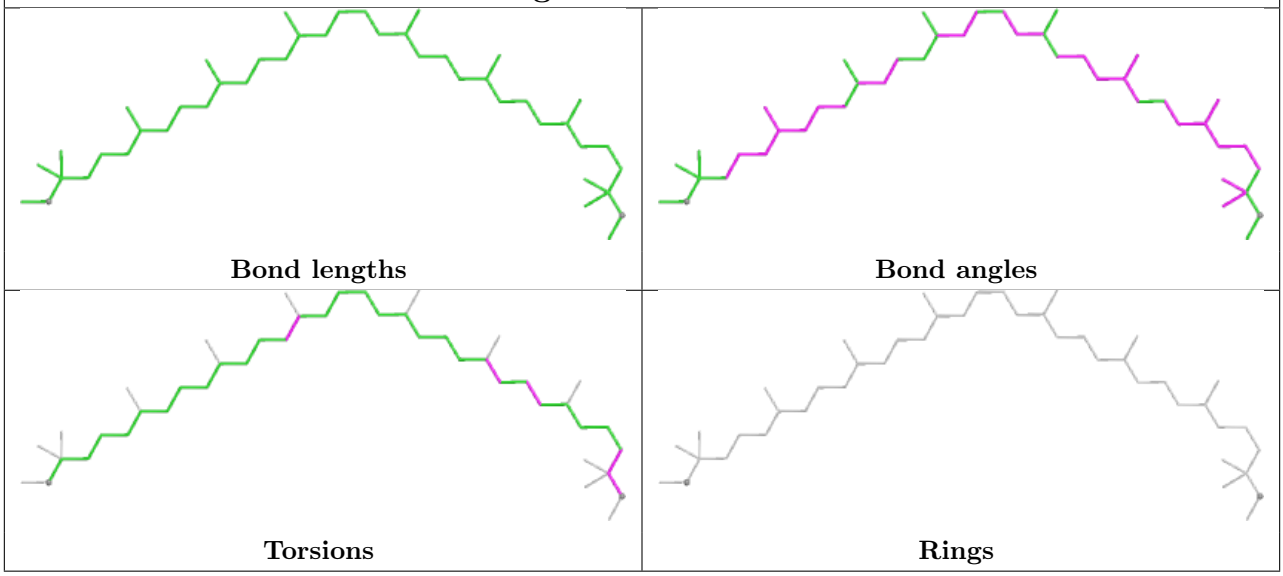


Rings

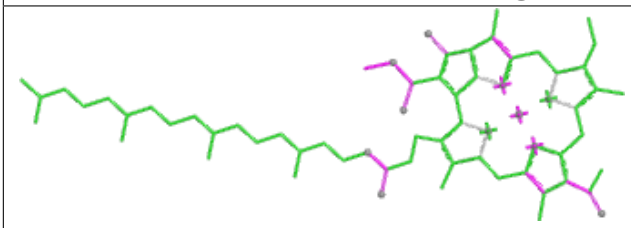
Ligand BPH y 402



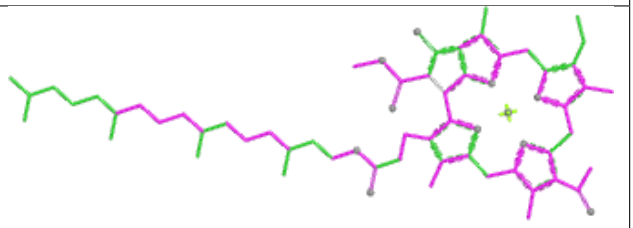
Ligand CRT i 101



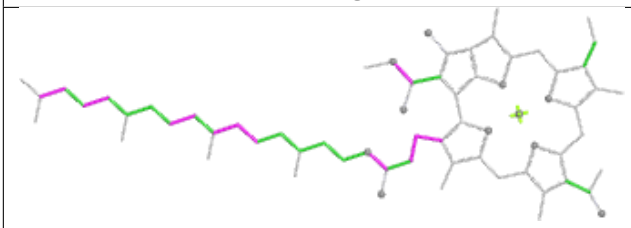
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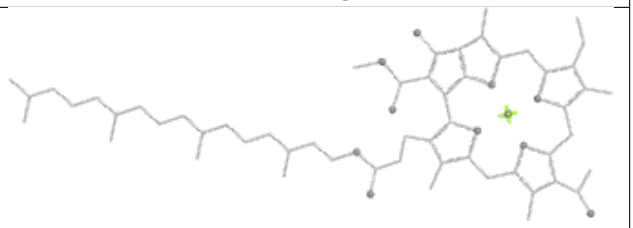
Bond lengths



Bond angles

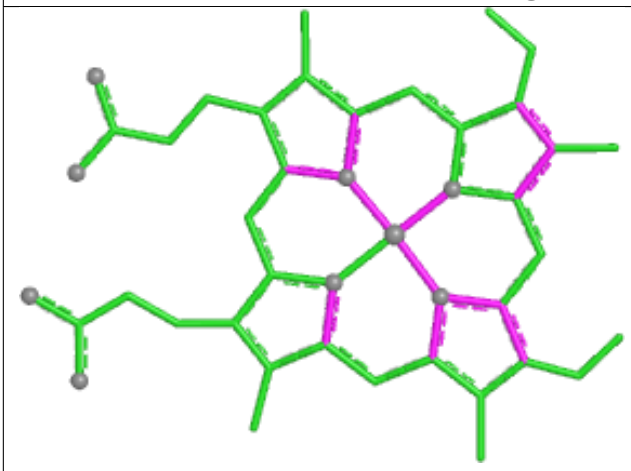


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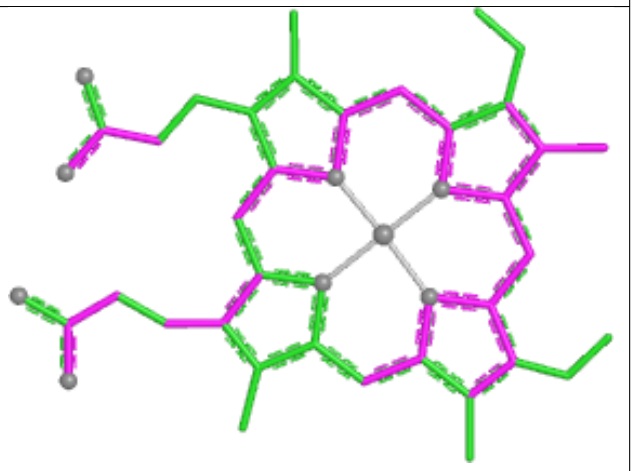


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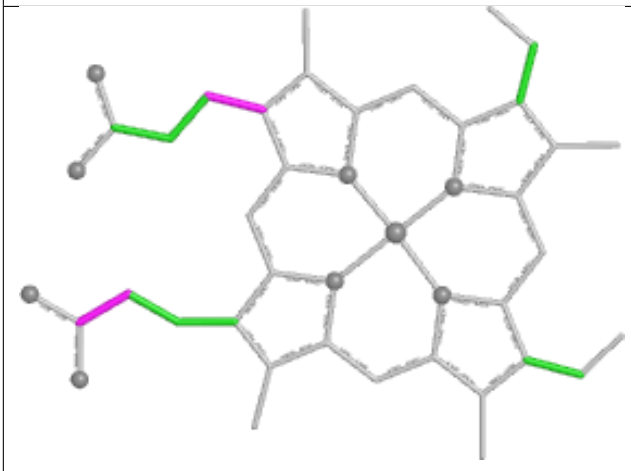
Ligand HEM o 504



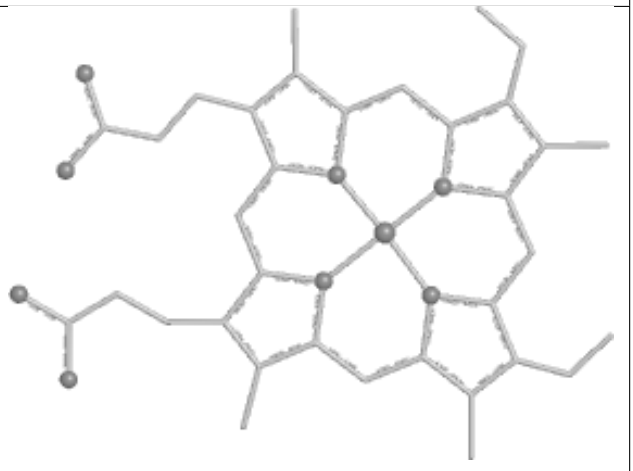
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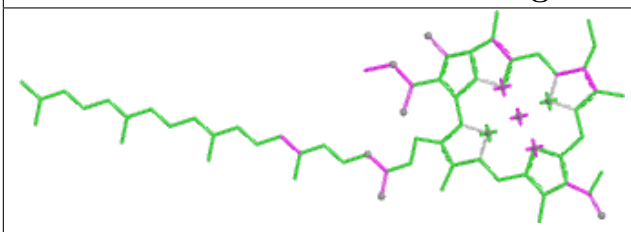


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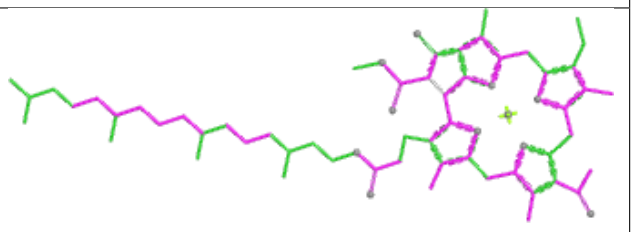


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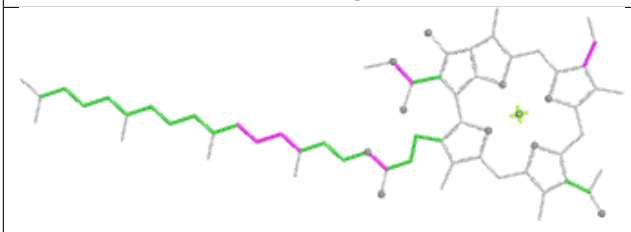
Ligand BCL I 101



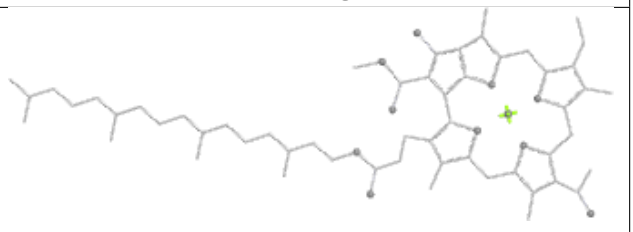
Bond lengths



Bond angles

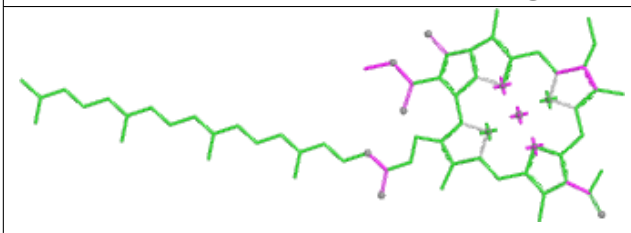


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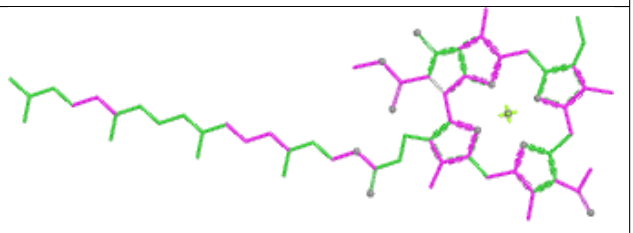


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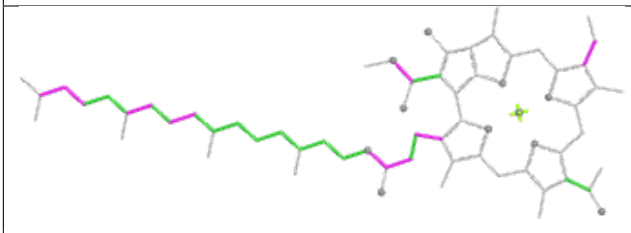
Ligand BCL Y 101



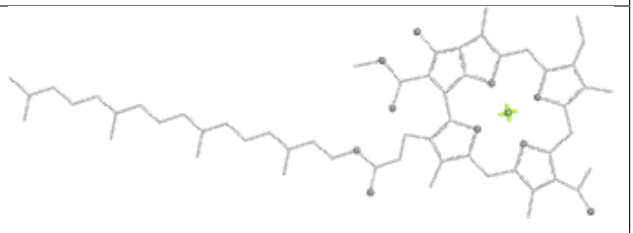
Bond lengths



Bond angles

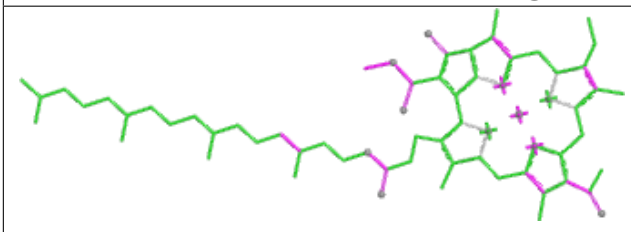


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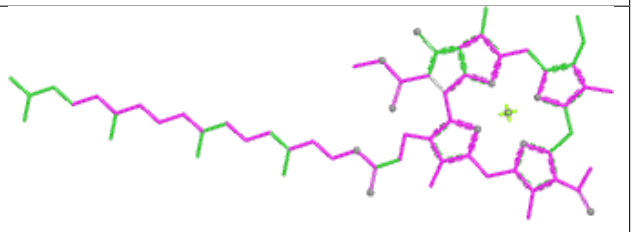


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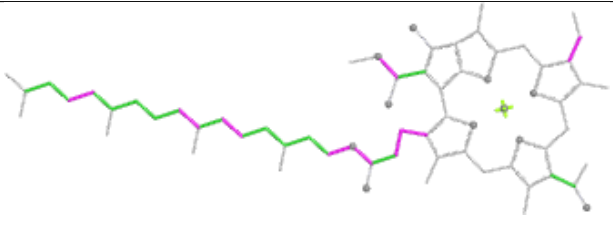
Ligand BCL T 102



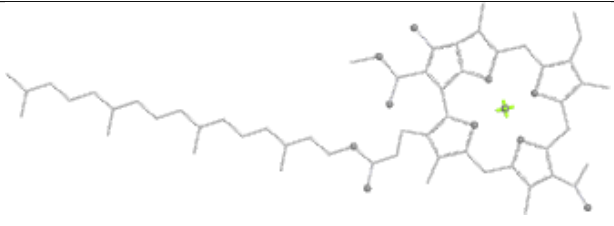
Bond lengths



Bond angles

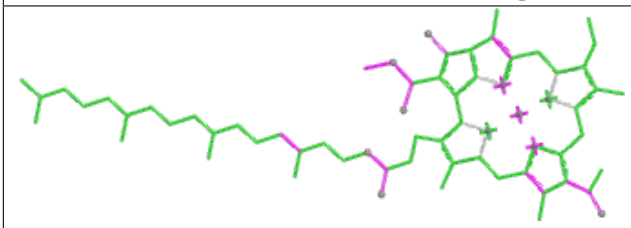


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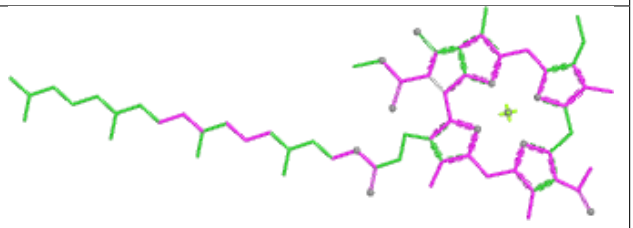


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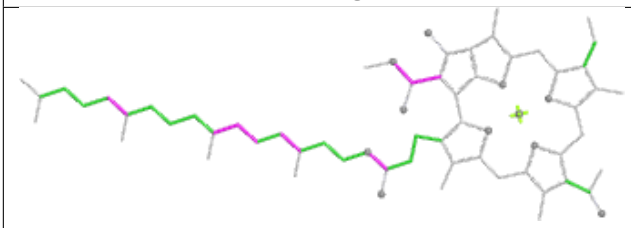
Ligand BCL AF 101



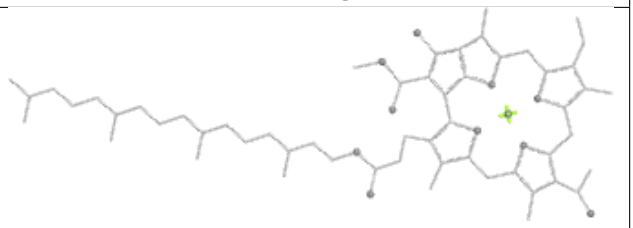
Bond lengths



Bond angles

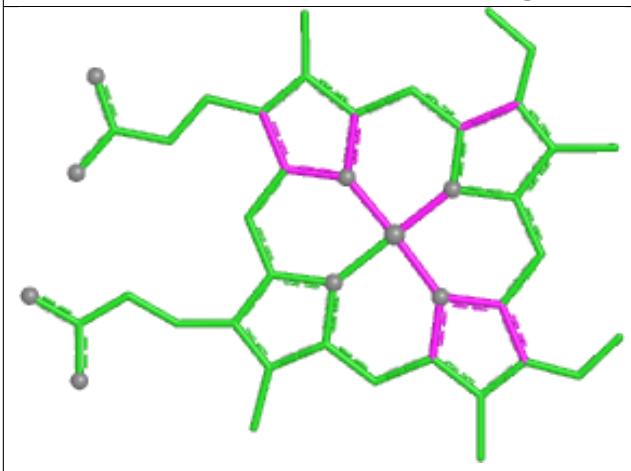


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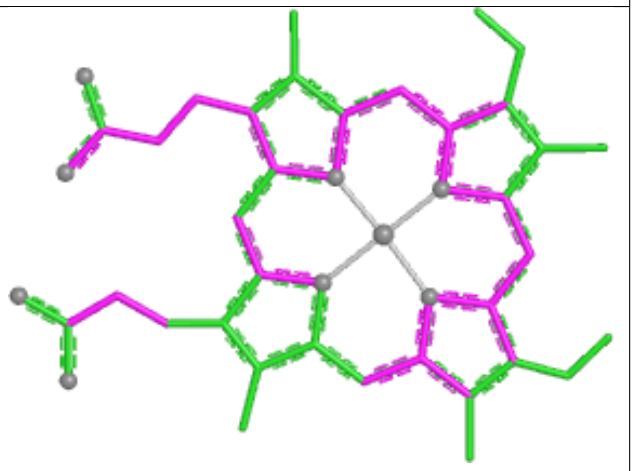


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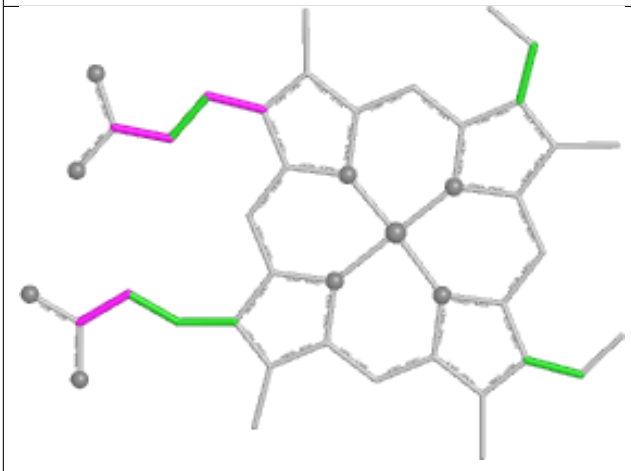
Ligand HEM C 504



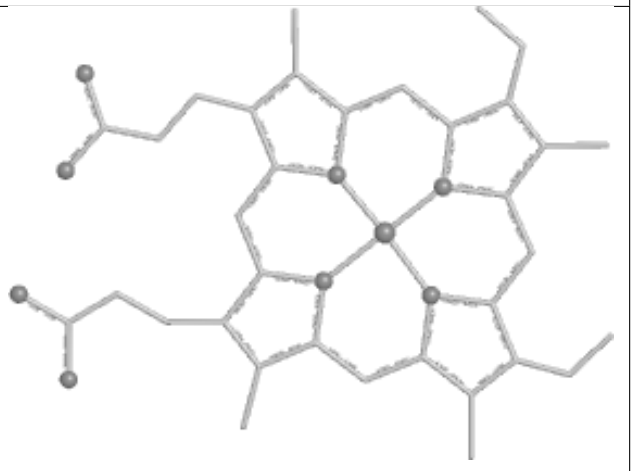
Bond lengths



Bond angles

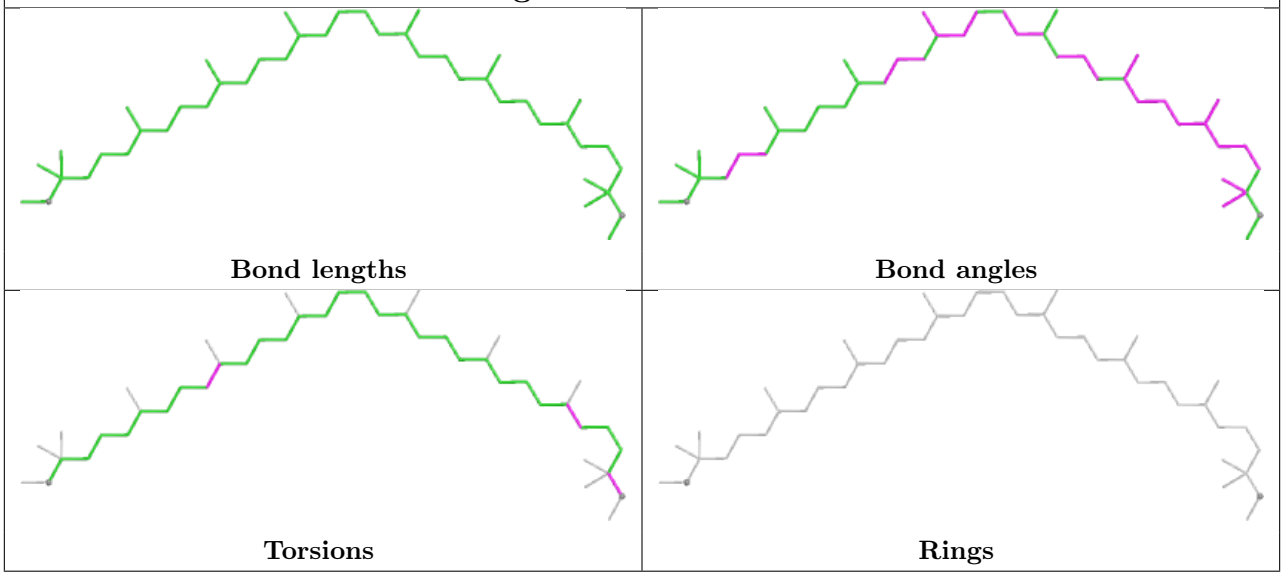


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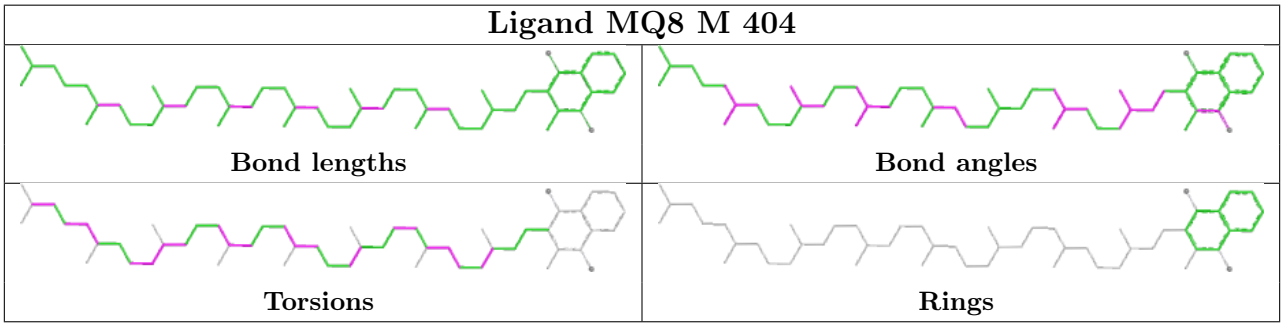


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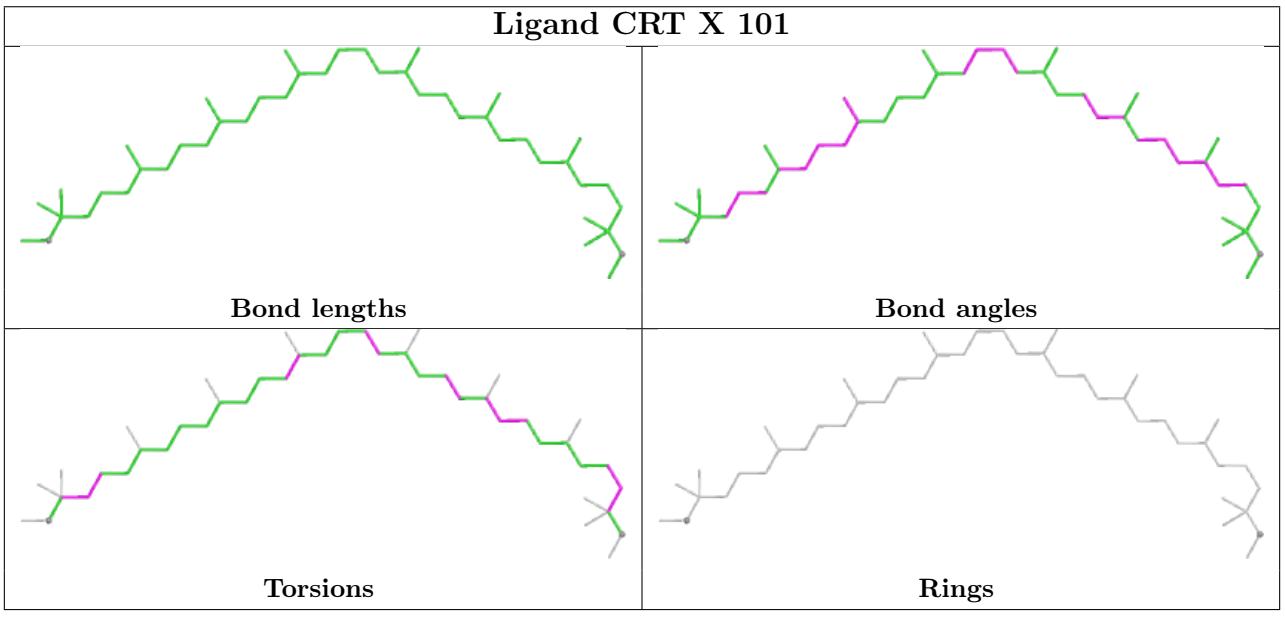
Ligand CRT AF 102



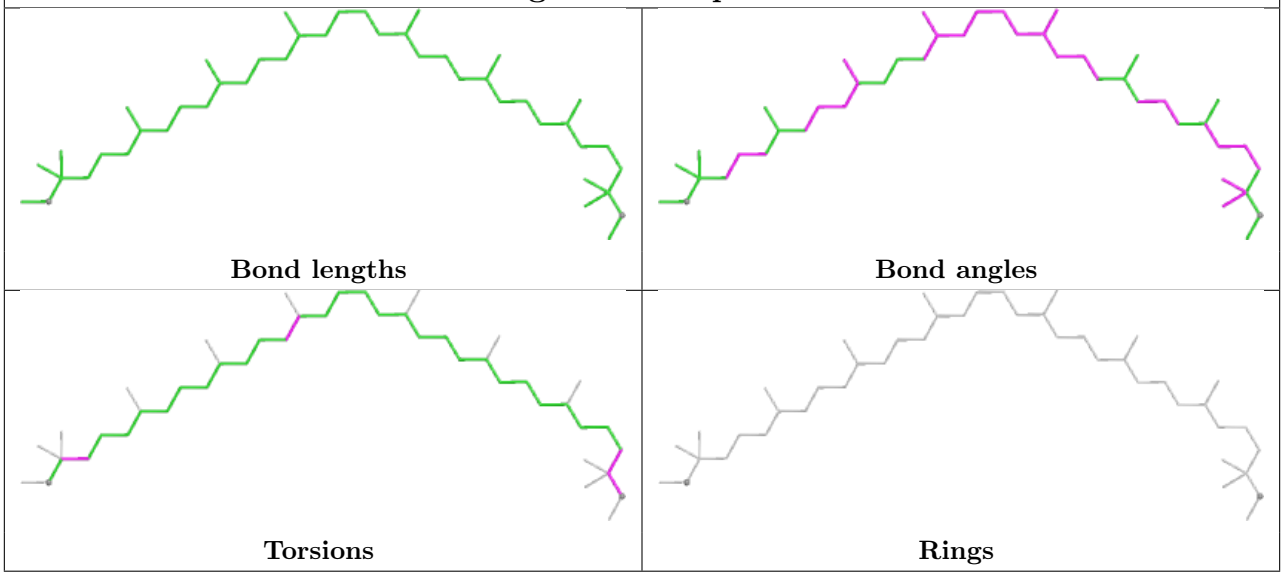
Ligand MQ8 M 404



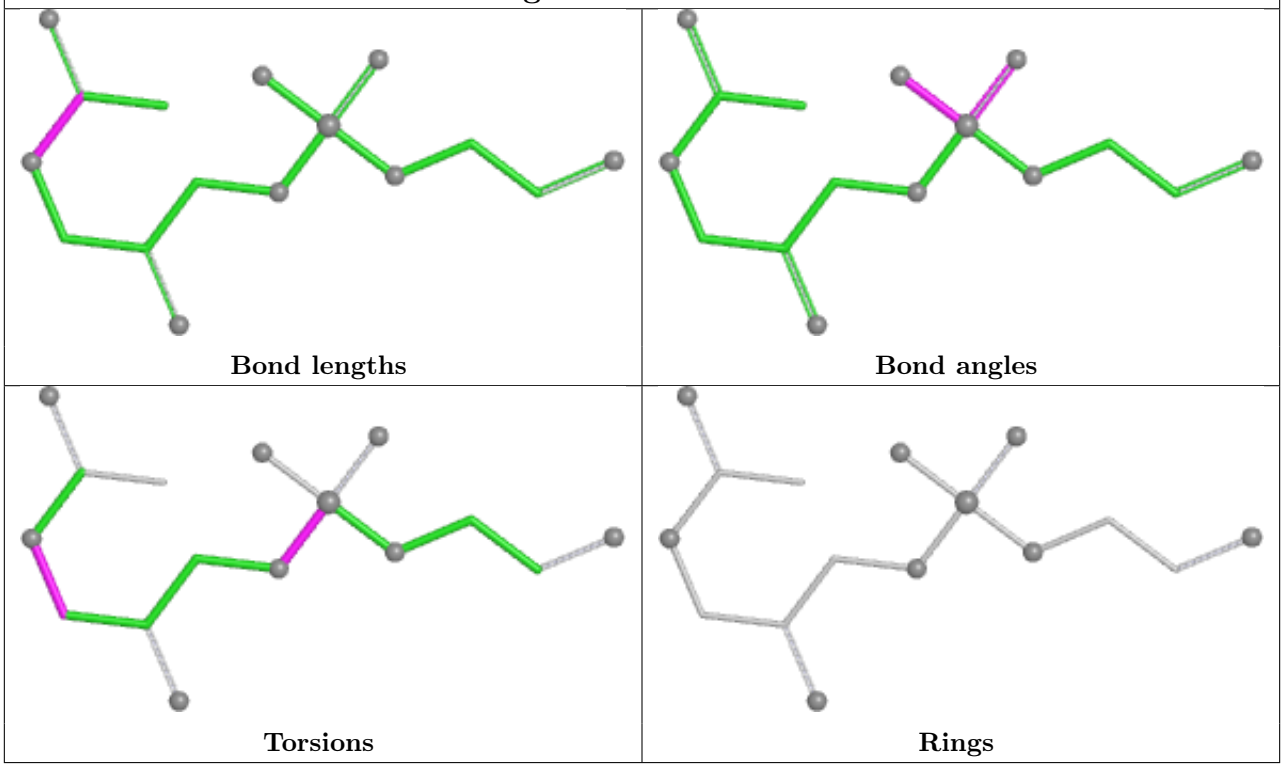
Ligand CRT X 101



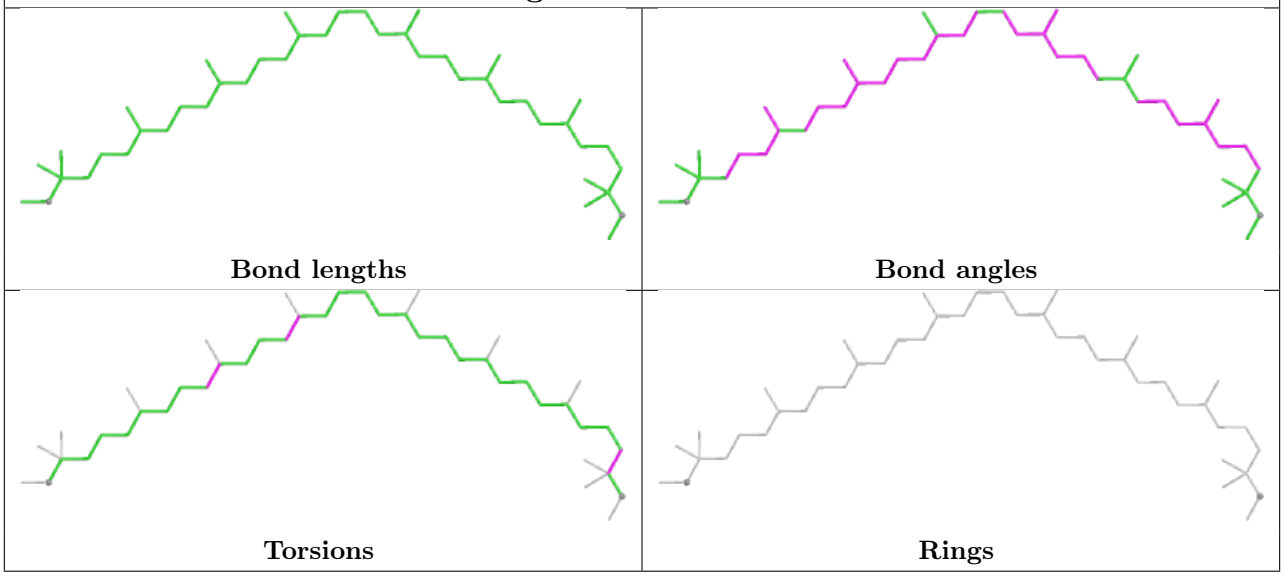
Ligand CRT q 101



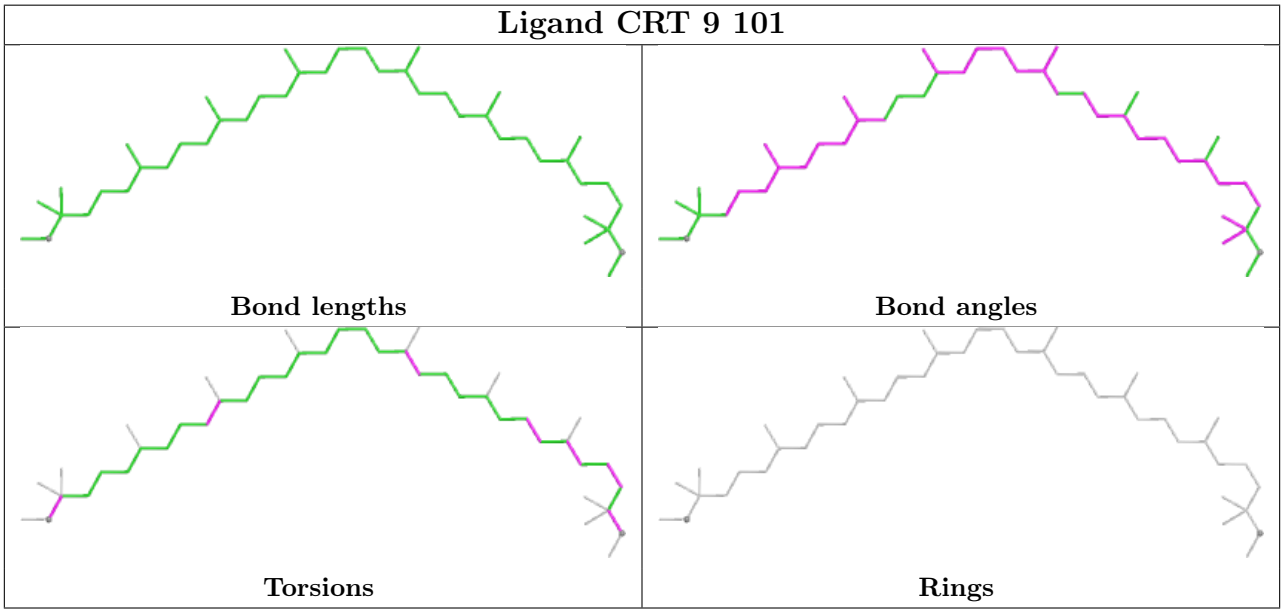
Ligand PEF M 407



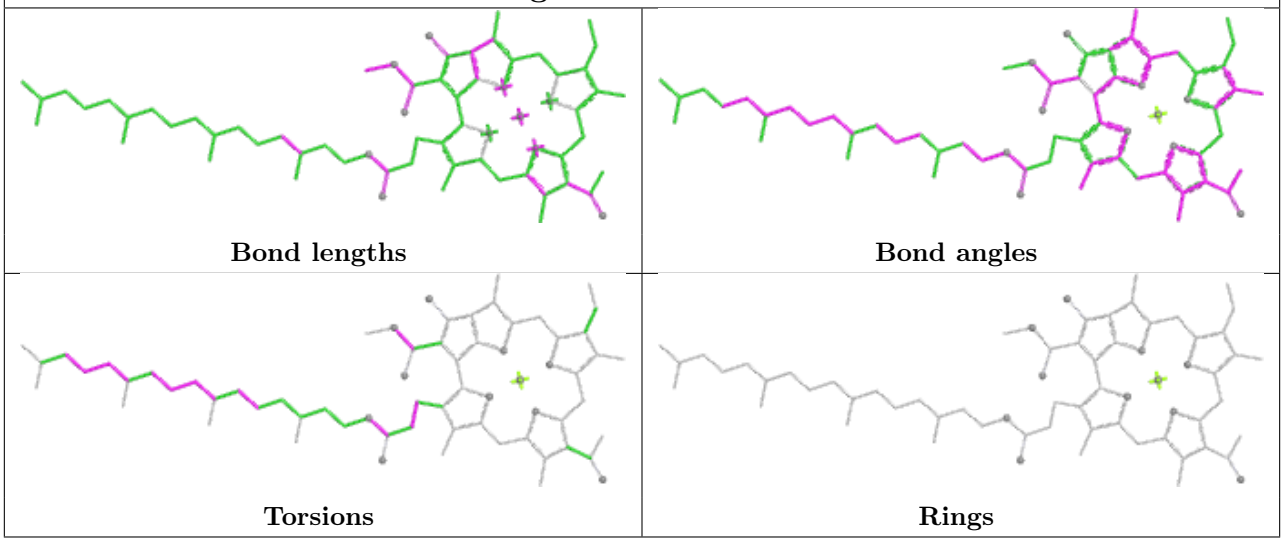
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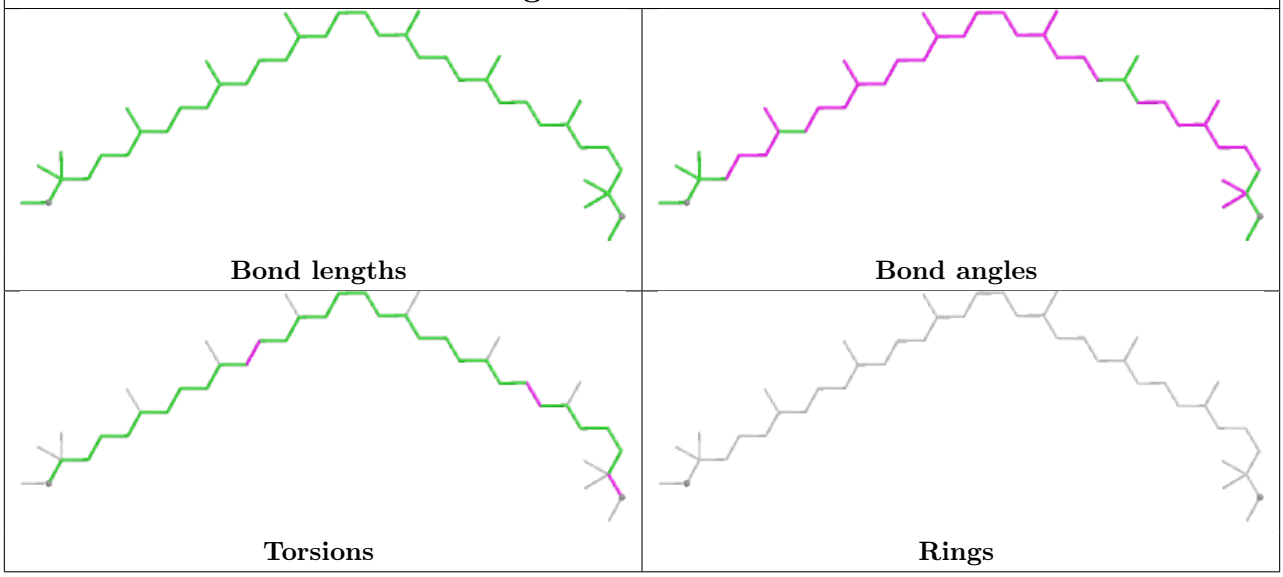
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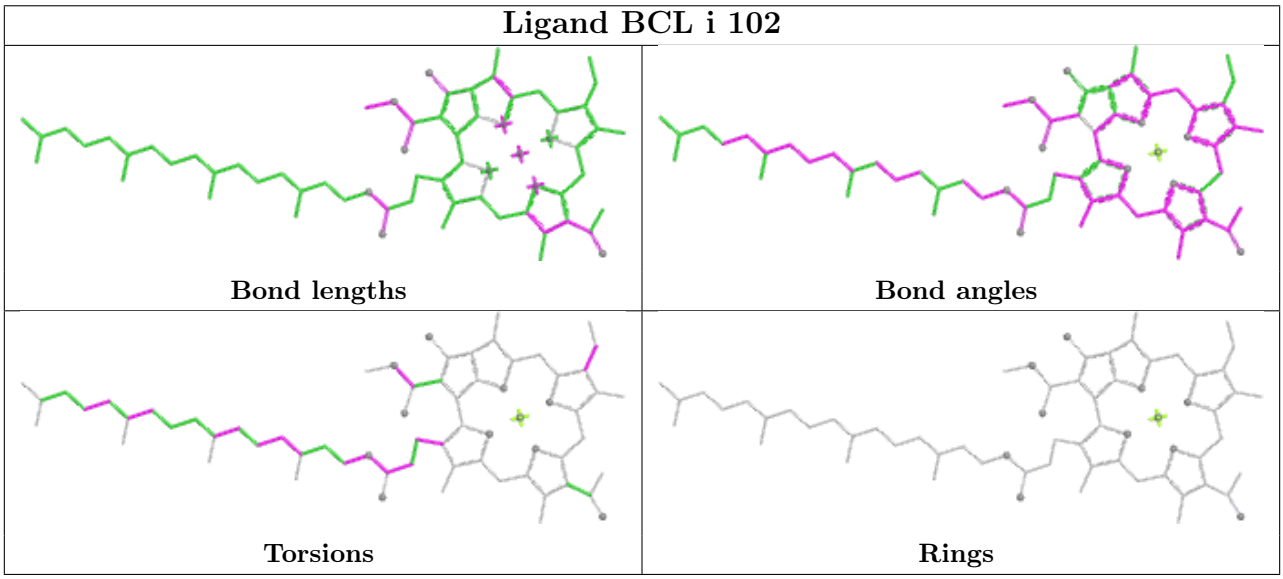
Ligand BCL 3 101



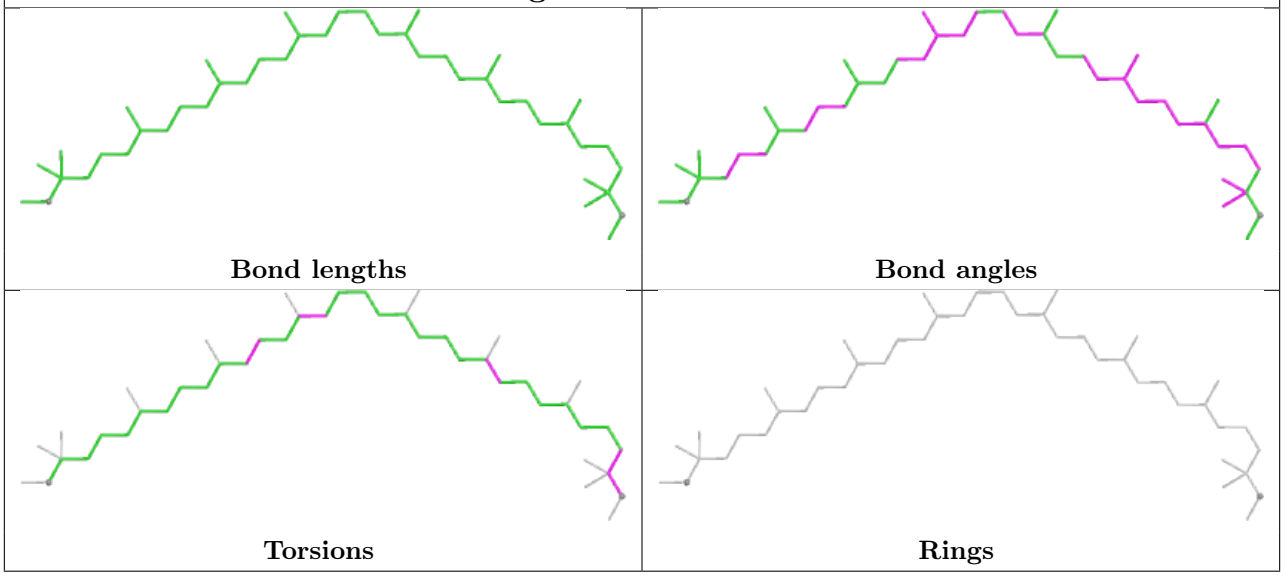
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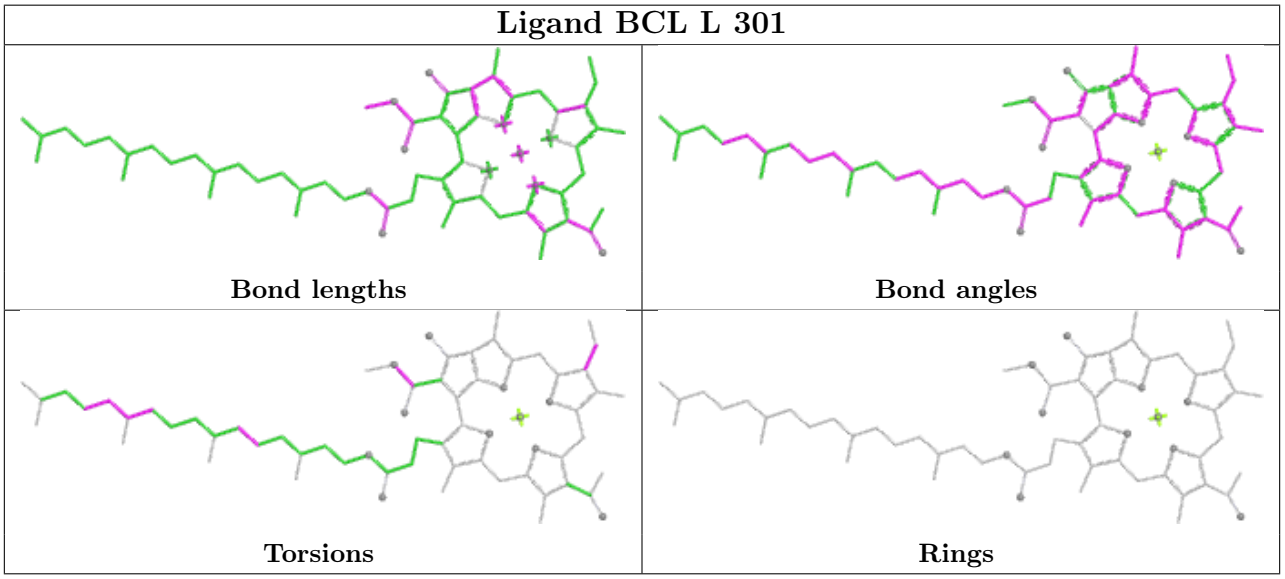
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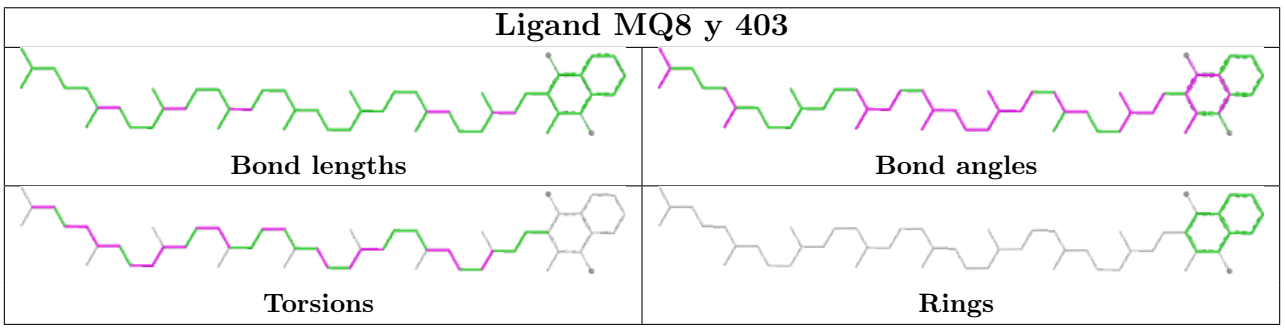
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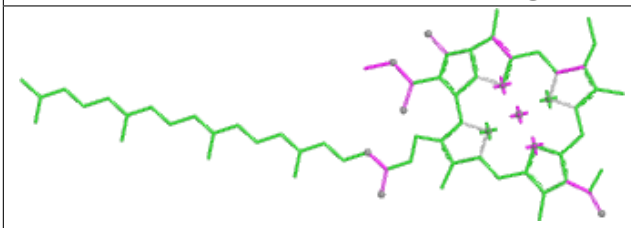
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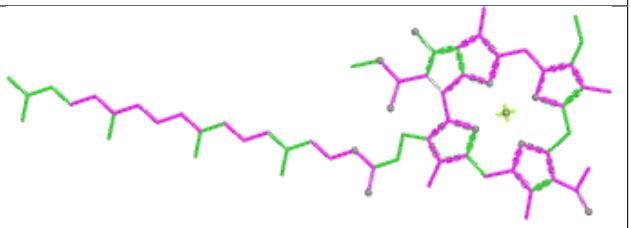
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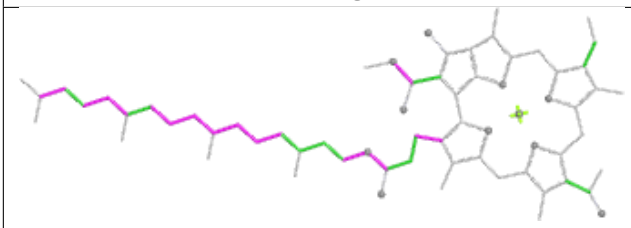
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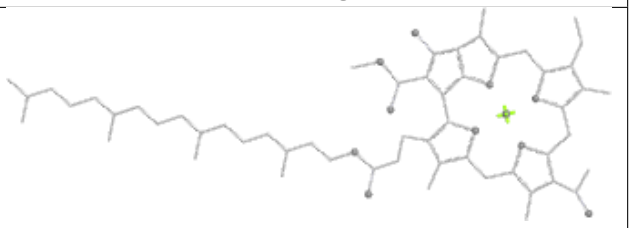
Bond lengths



Bond angles

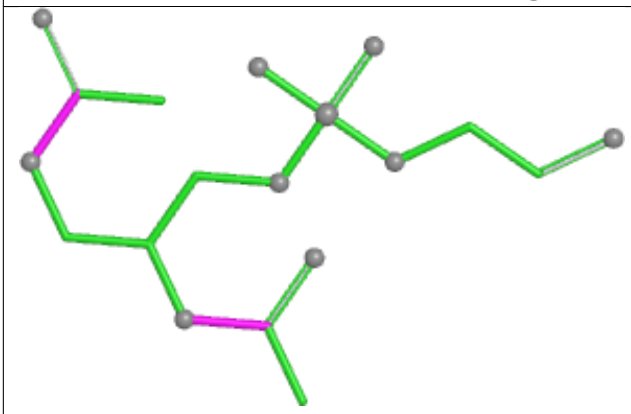


Torsions

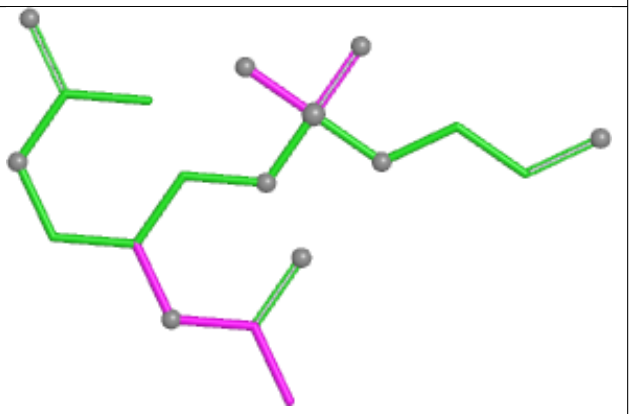


Rings

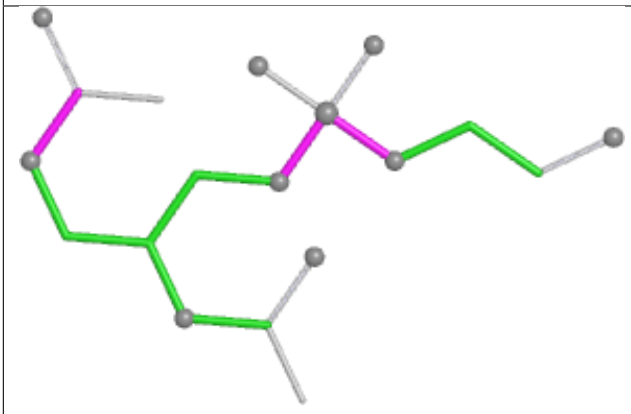
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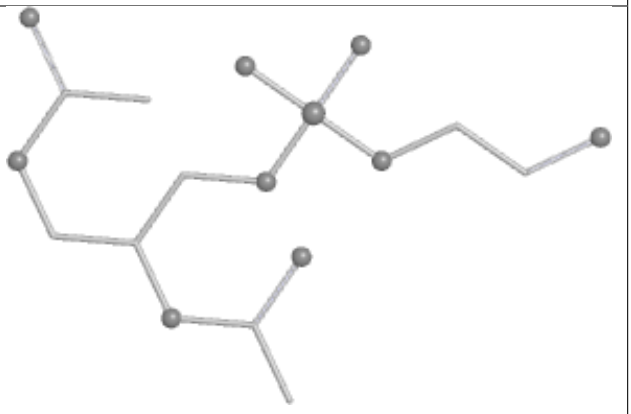
Bond lengths



Bond angles

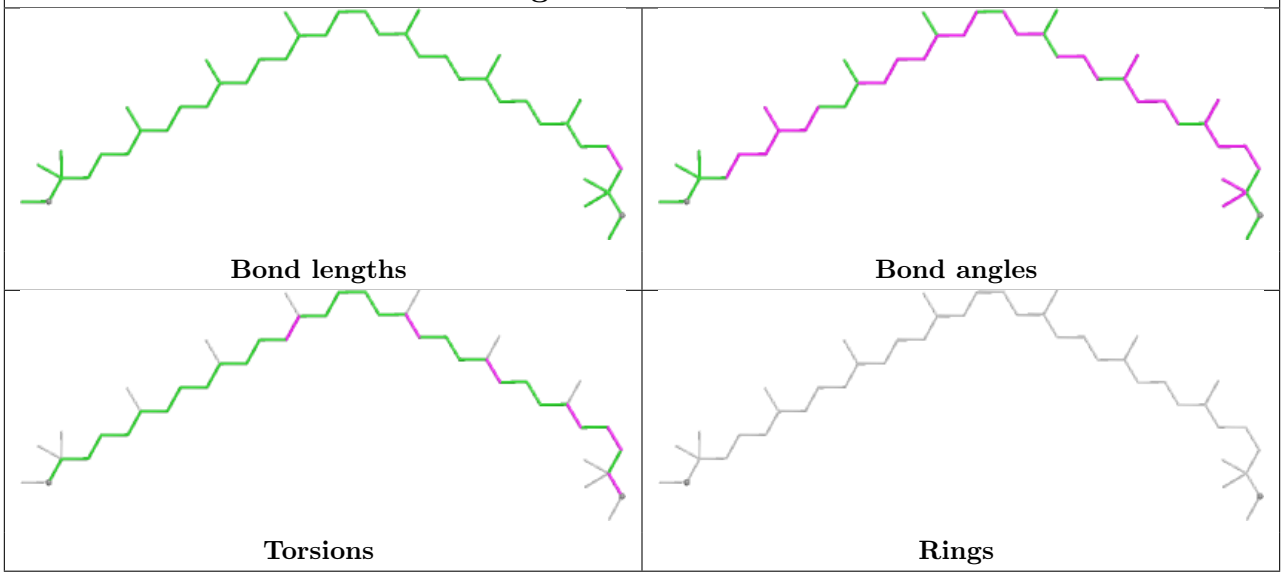


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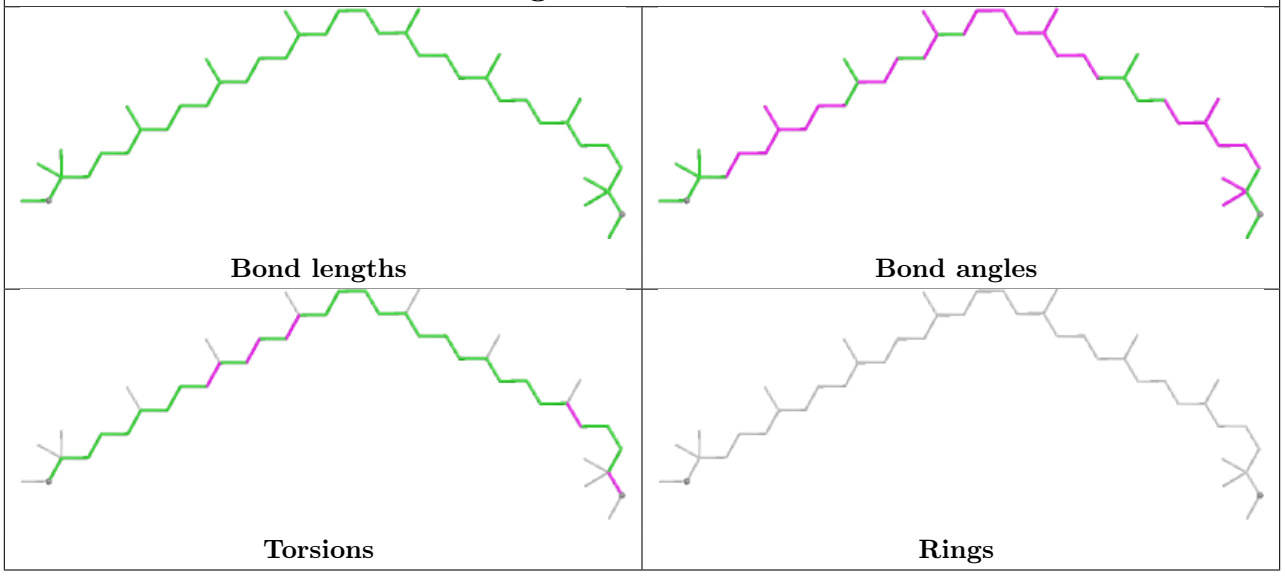


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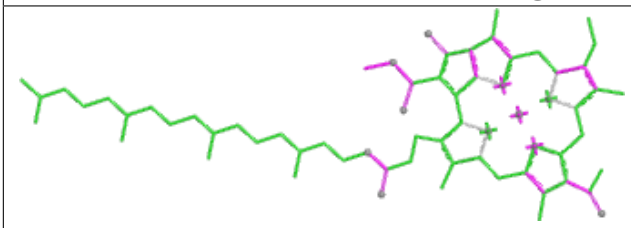
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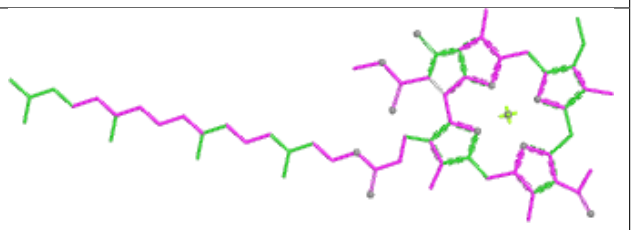
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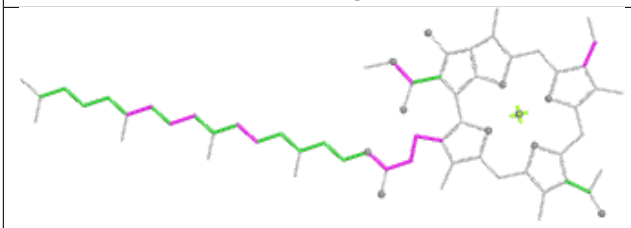
Ligand BCL 4 102



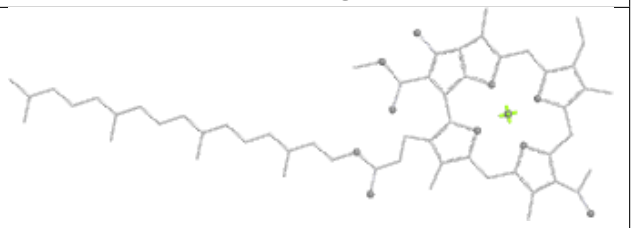
Bond lengths



Bond angles

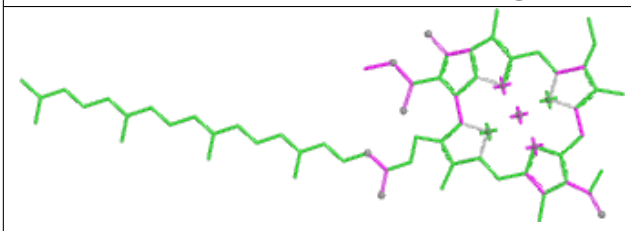


Torsions

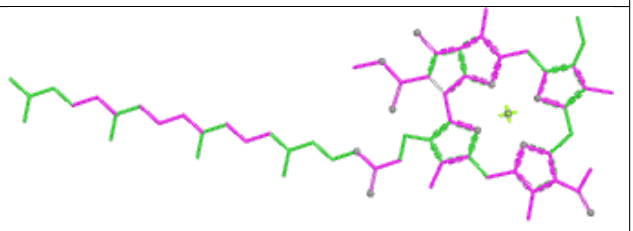


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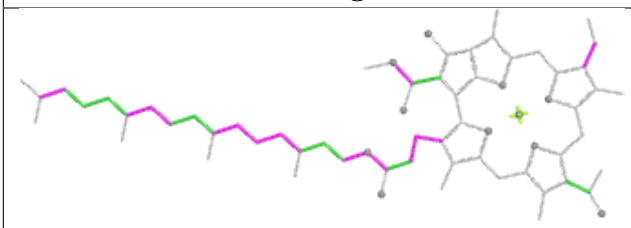
Ligand BCL AH 101



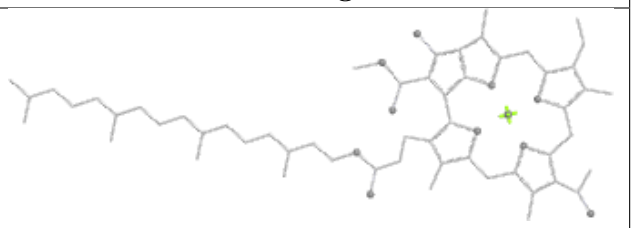
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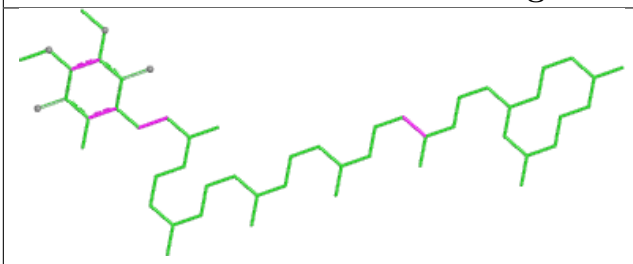


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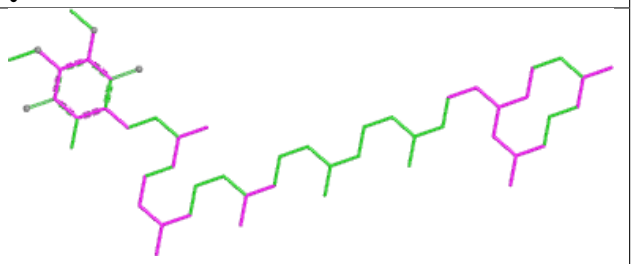


Rings

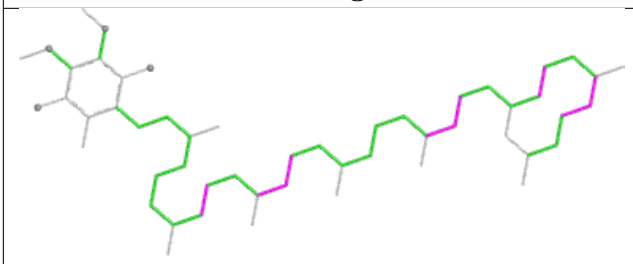
Ligand UQ8 L 304



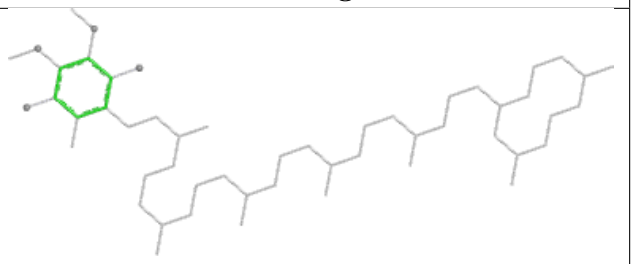
Bond lengths



Bond angles

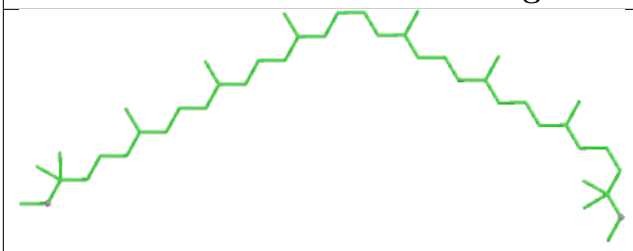


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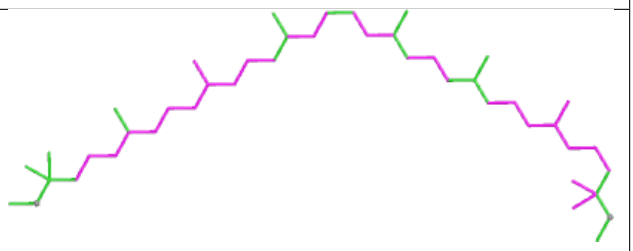


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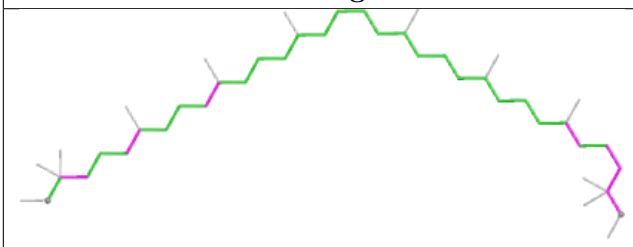
Ligand CRT G 101



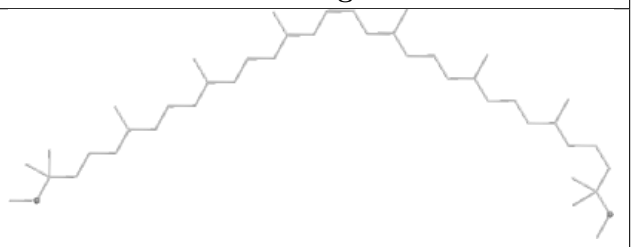
Bond lengths



Bond angles

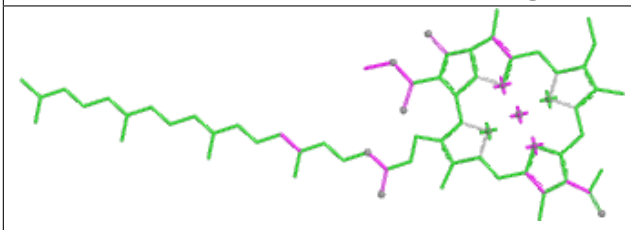


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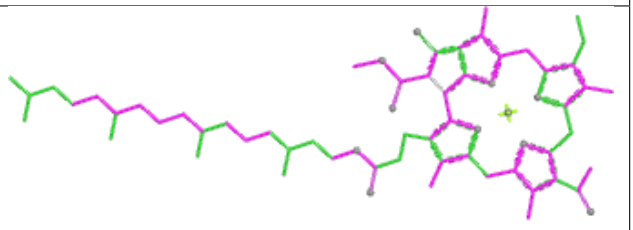


Rings

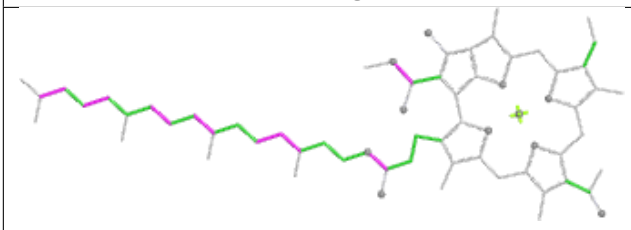
Ligand BCL K 101



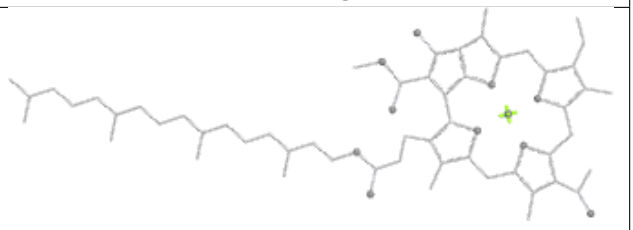
Bond lengths



Bond angles

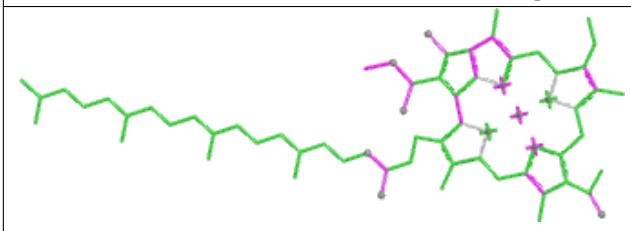


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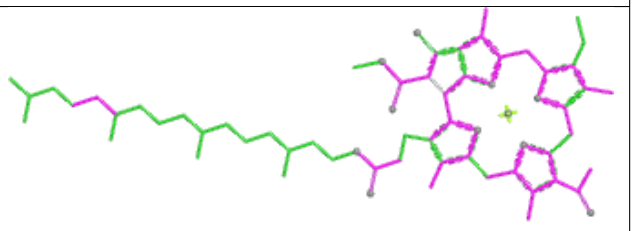


Rings

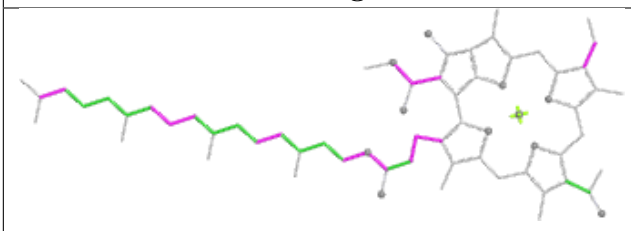
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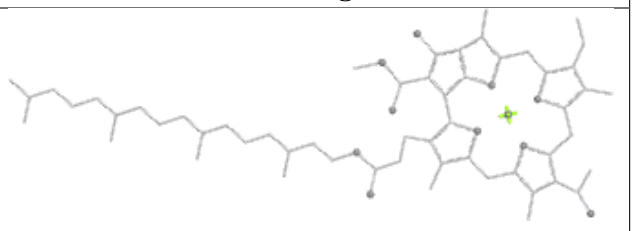
Bond lengths



Bond angles

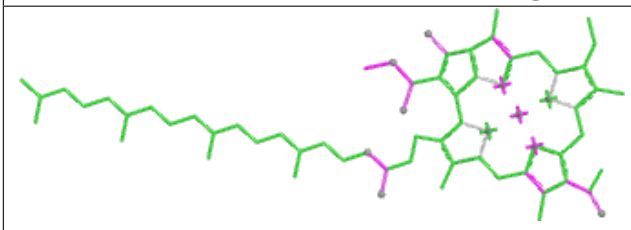


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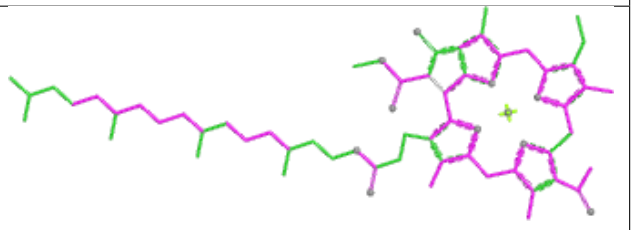


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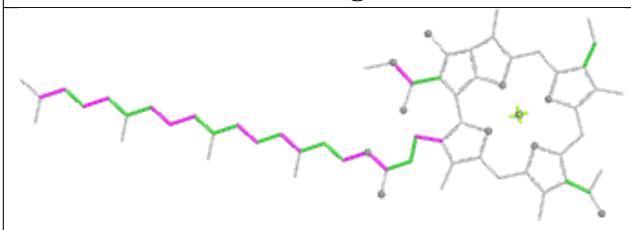
Ligand BCL Z 102



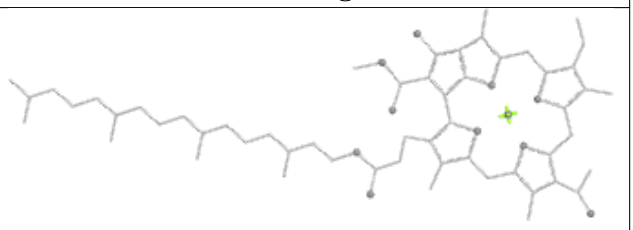
Bond lengths



Bond angles

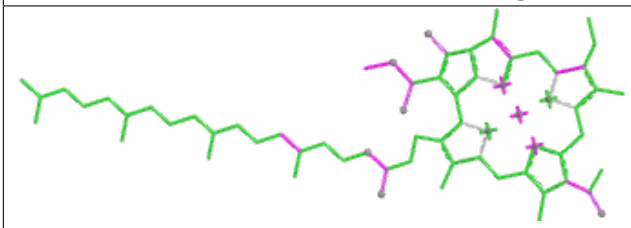


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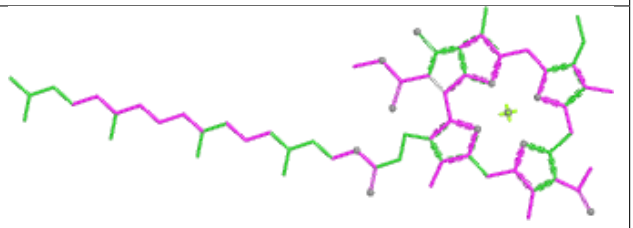


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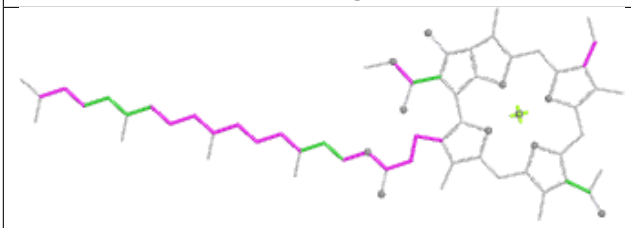
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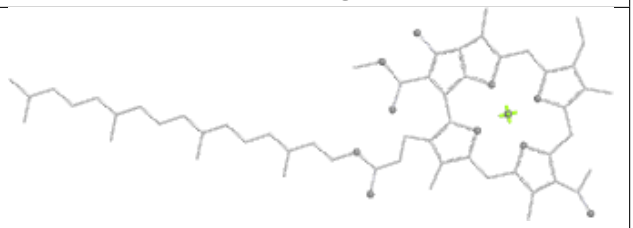
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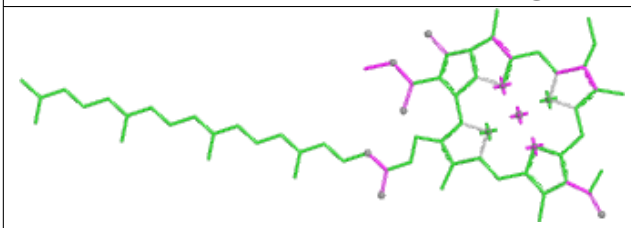


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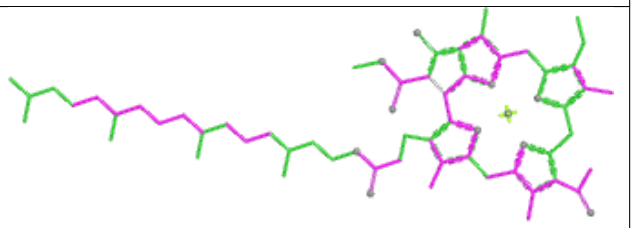


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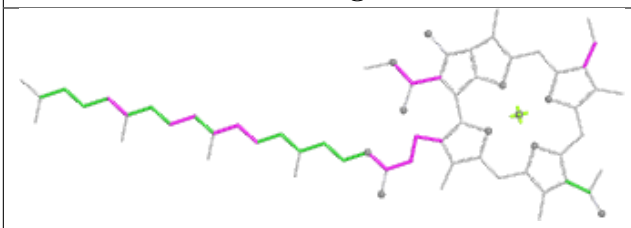
Ligand BCL S 102



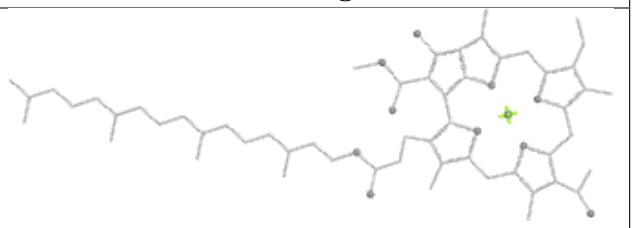
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Bond angles

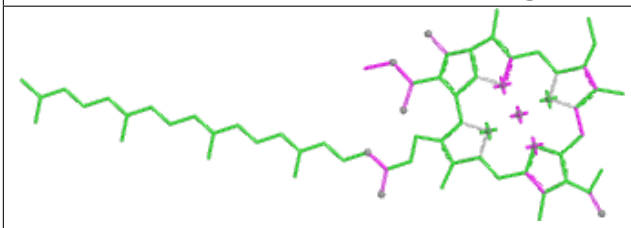


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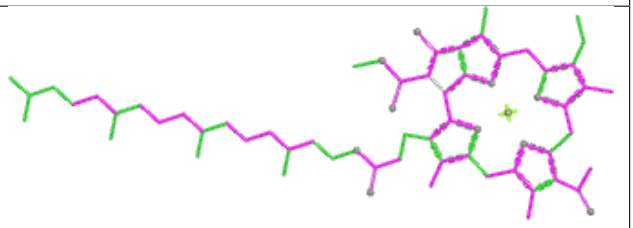


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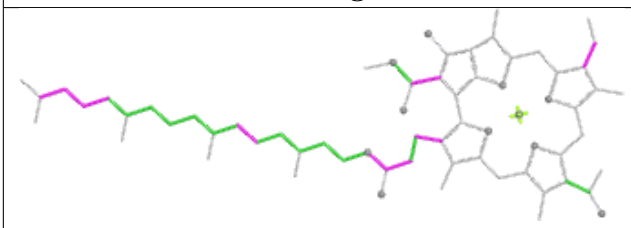
Ligand BCL M 402



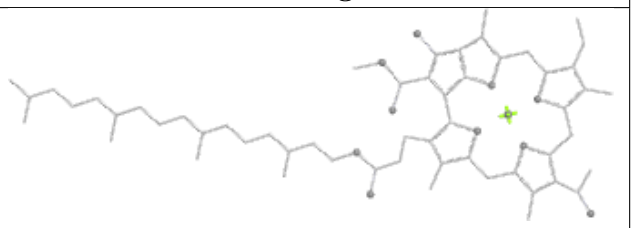
Bond lengths



Bond angles

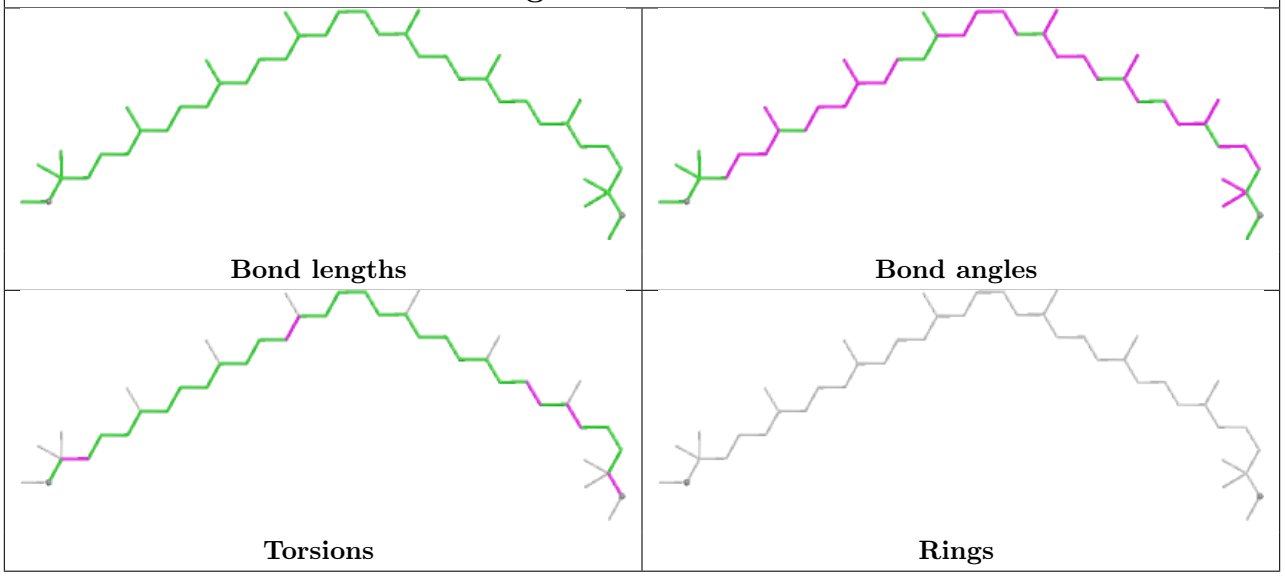


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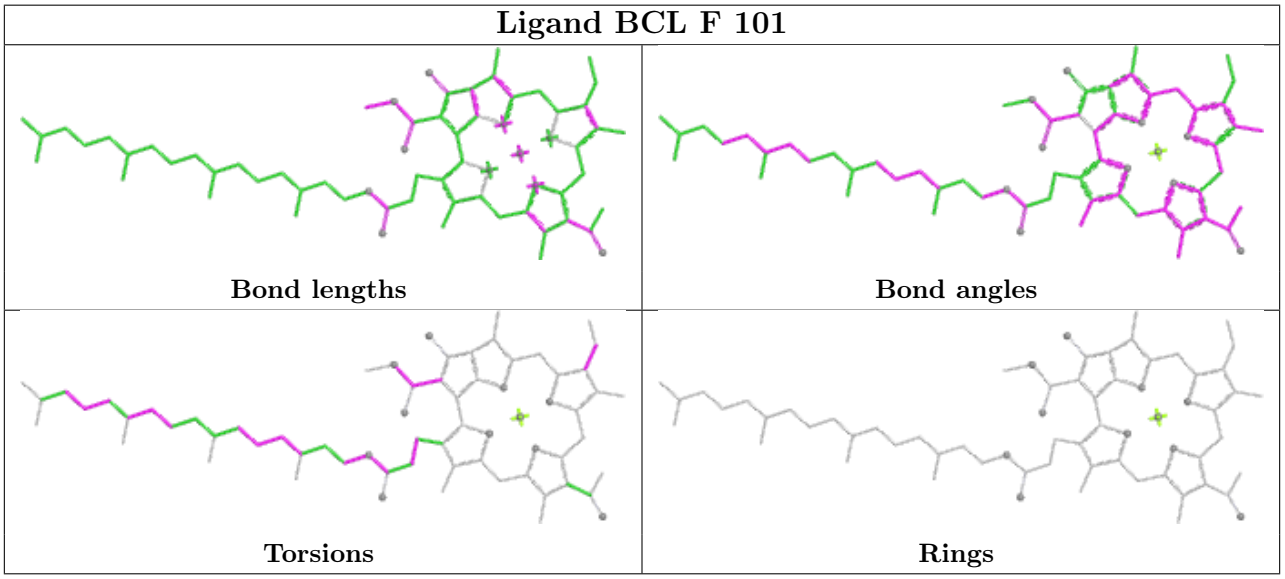


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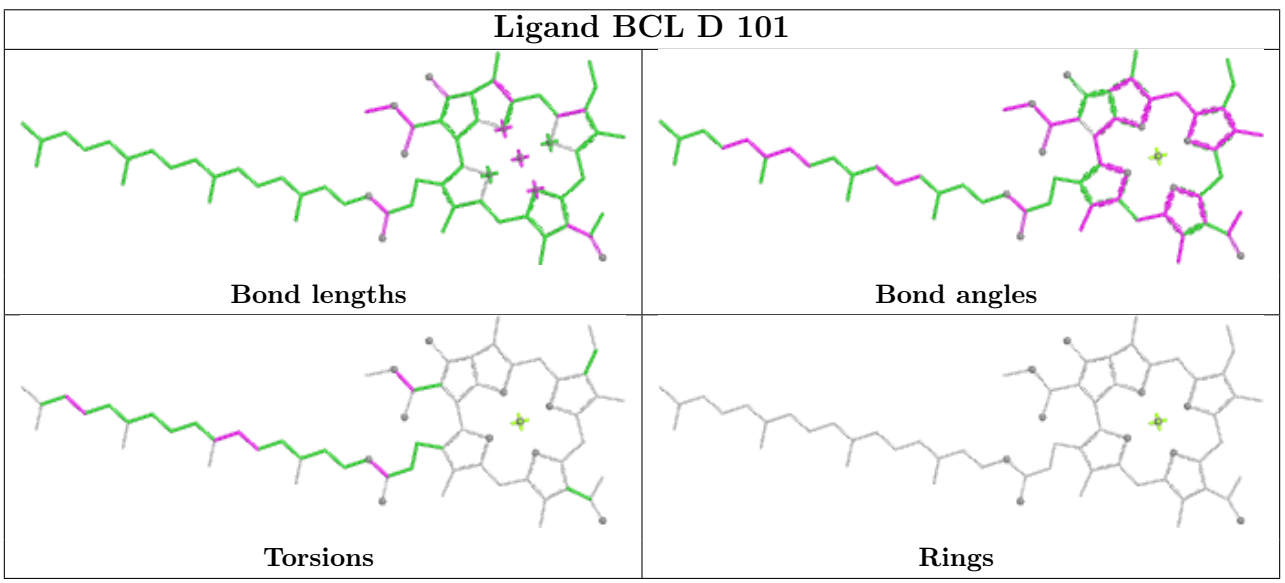
Ligand CRT E 101



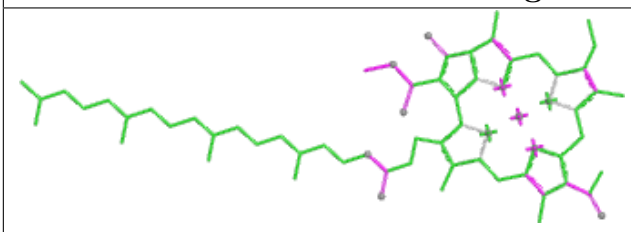
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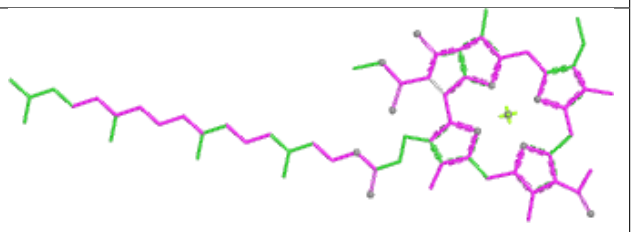
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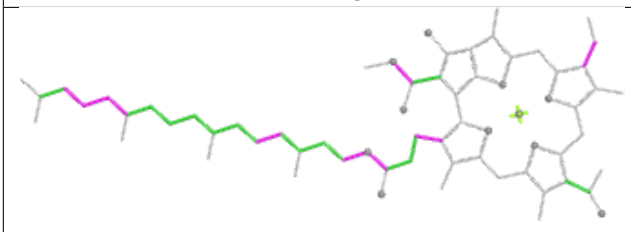
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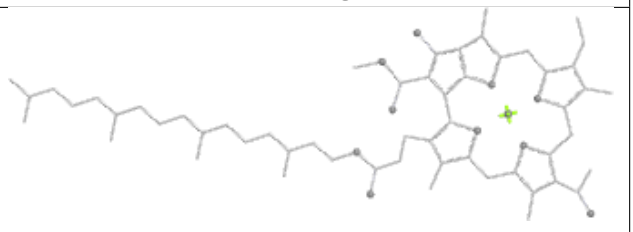
Bond lengths



Bond angles

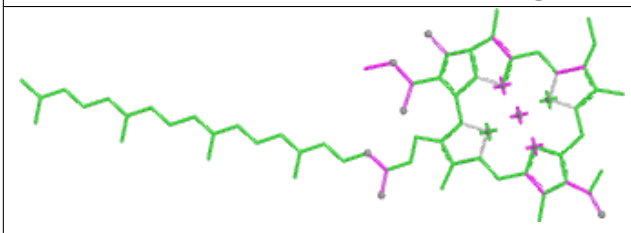


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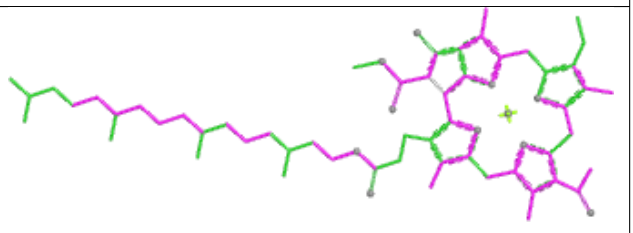


Rings

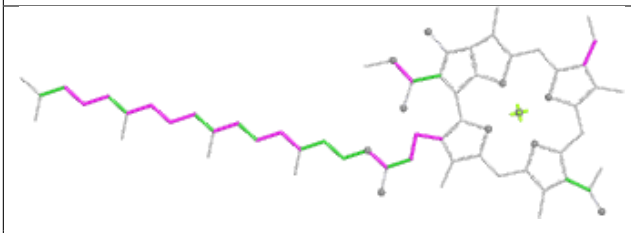
Ligand BCL c 101



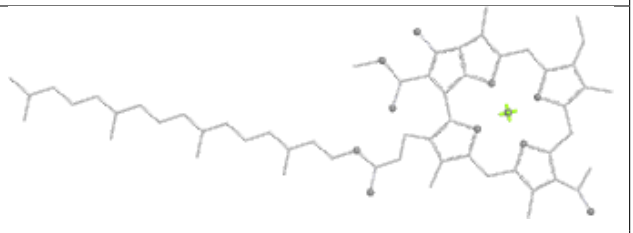
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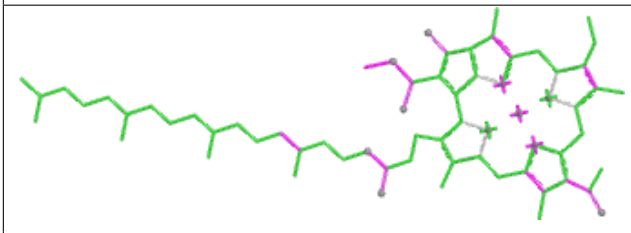


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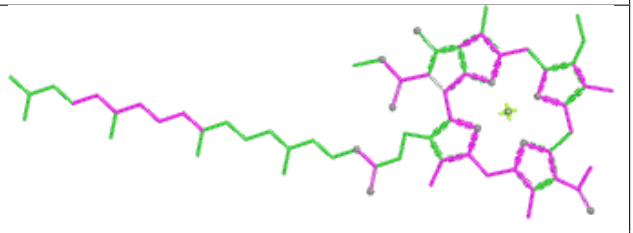


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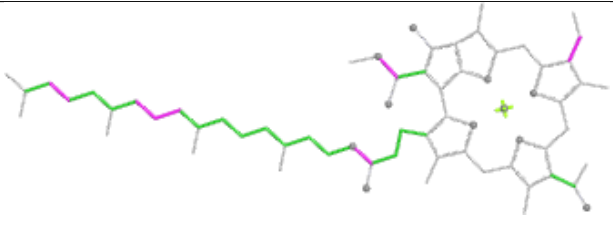
Ligand BCL 5 101



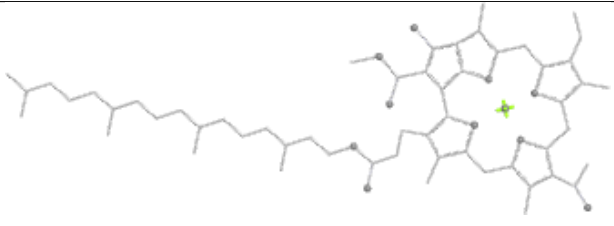
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Bond angles

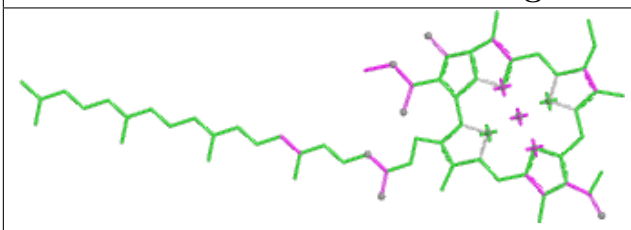


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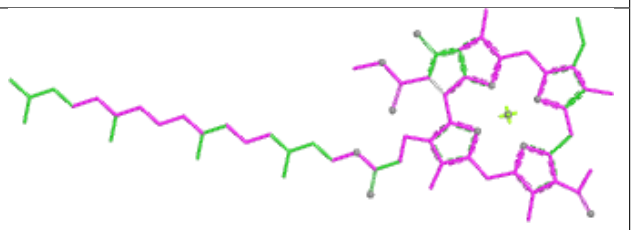


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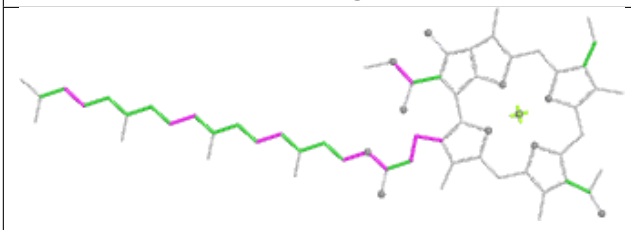
Ligand BCL V 102



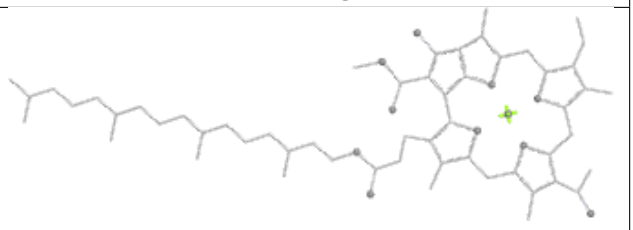
Bond lengths



Bond angles

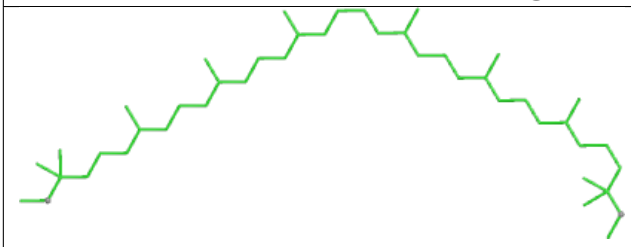


Torsions

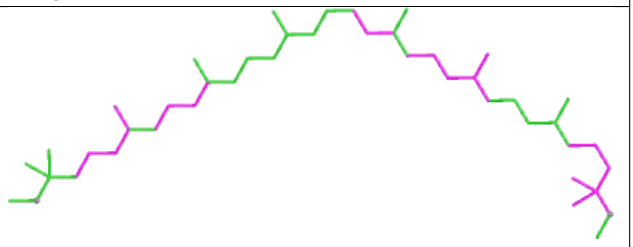


Rings

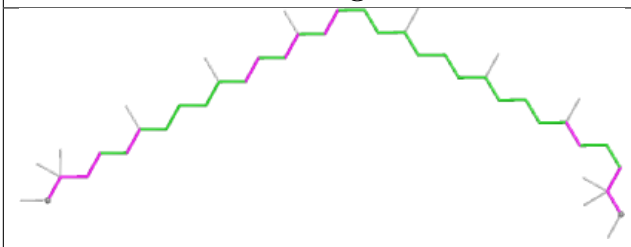
Ligand CRT y 404



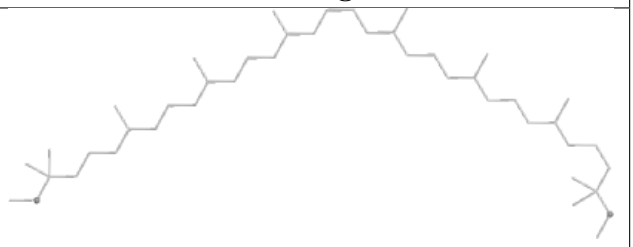
Bond lengths



Bond angles

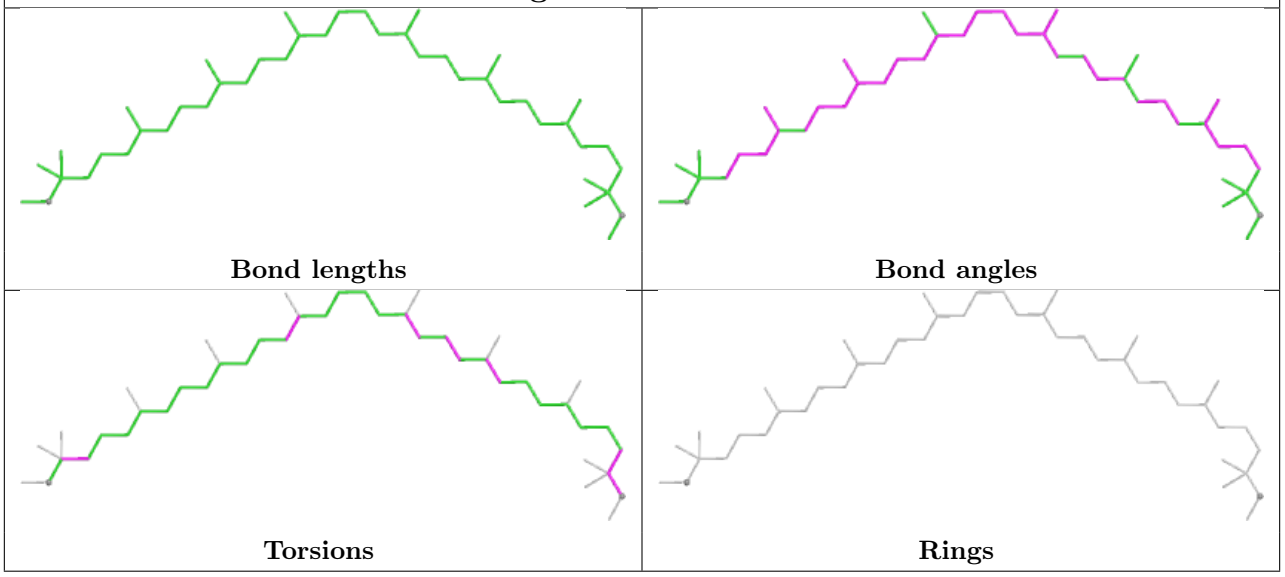


Torsions

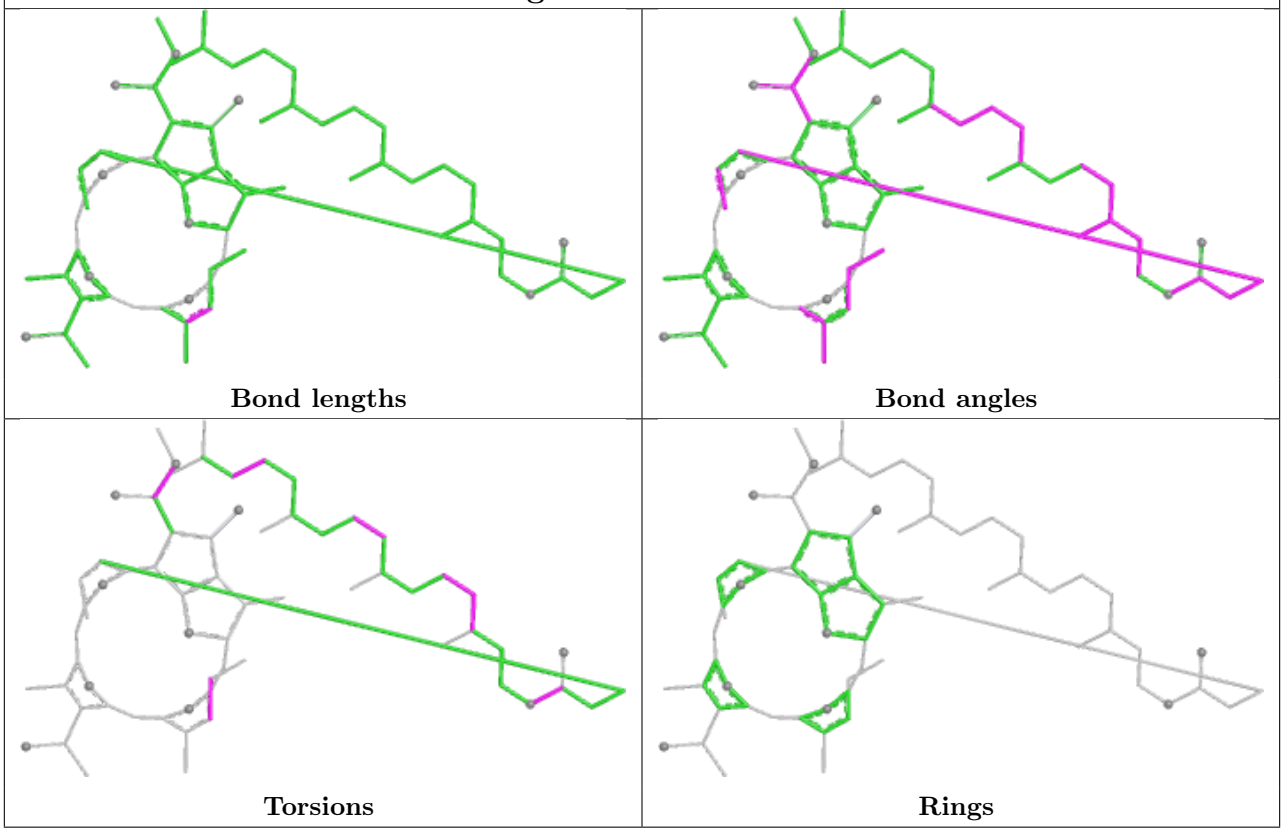


Rings

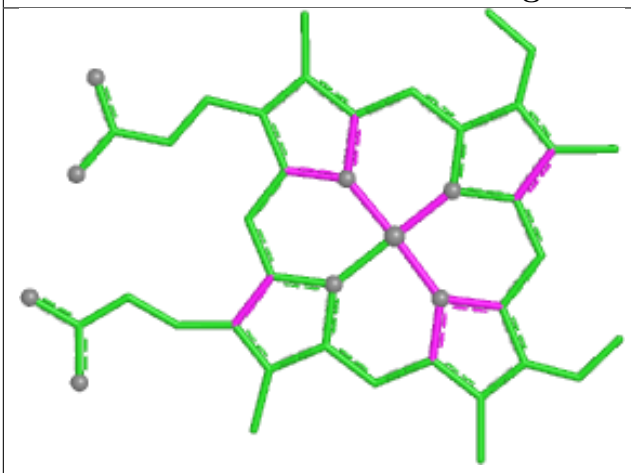
Ligand CRT e 101



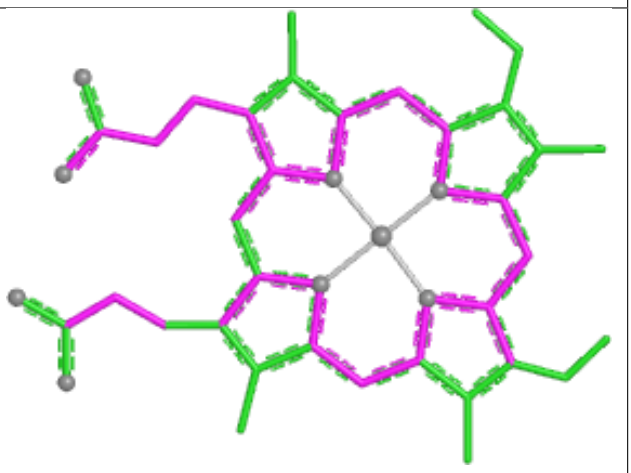
Ligand BPH x 302



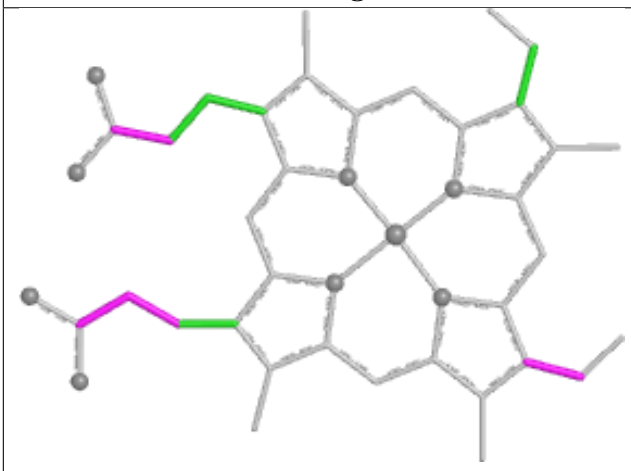
Ligand HEM o 501



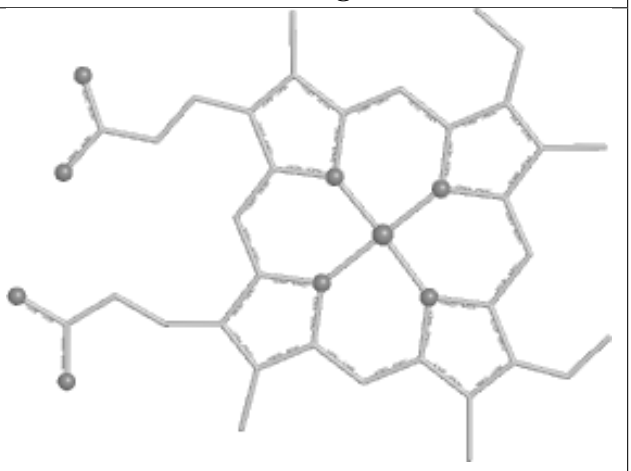
Bond lengths



Bond angles

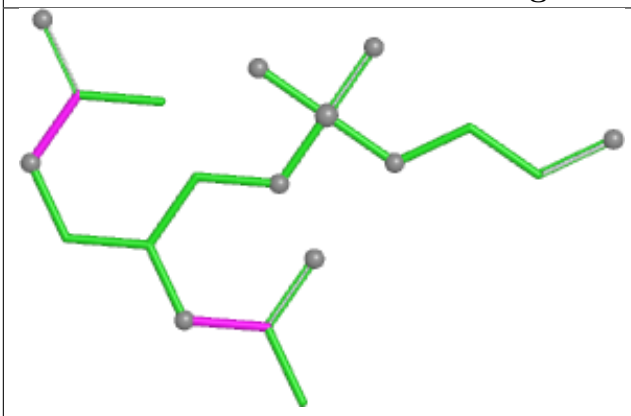


Torsions

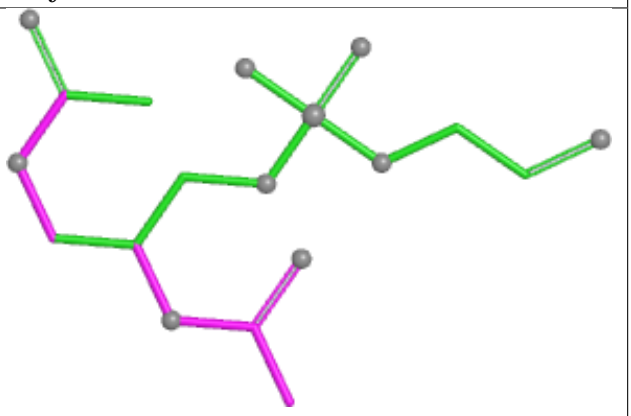


Rings

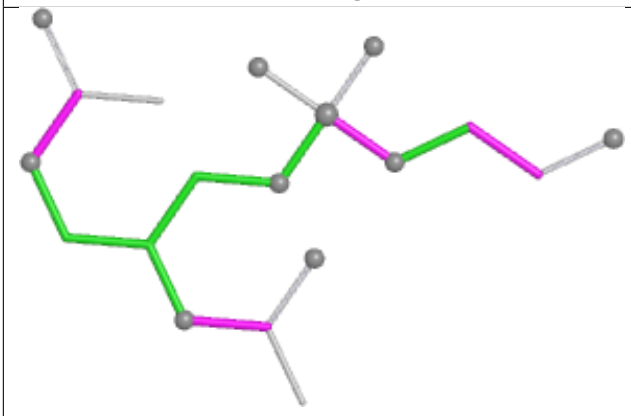
Ligand PEF y 406



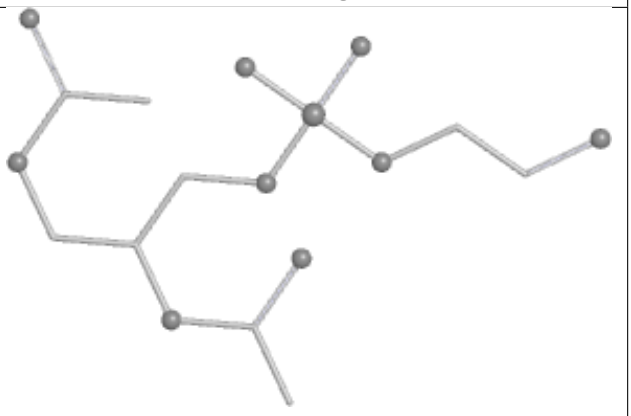
Bond lengths



Bond angles

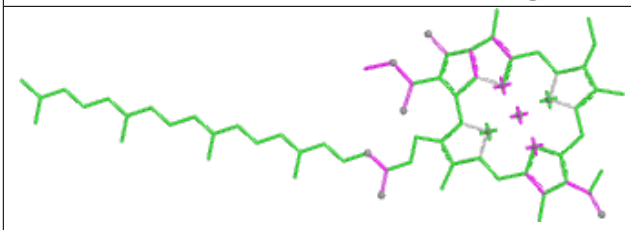


Torsions

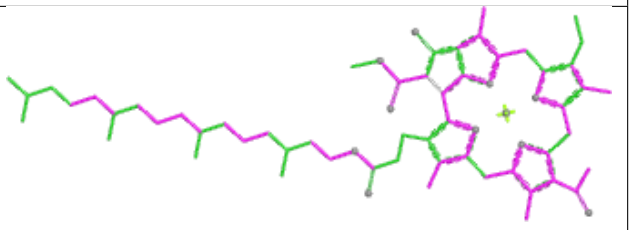


Rings

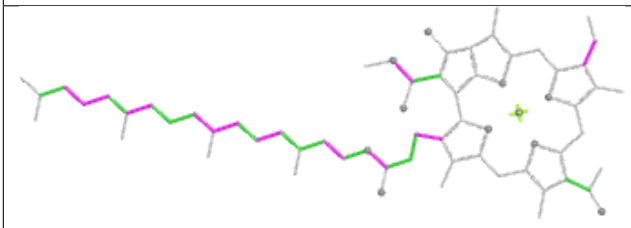
Ligand BCL N 101



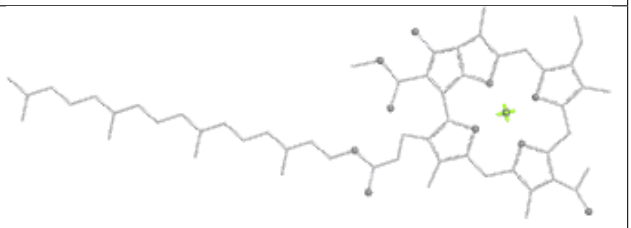
Bond lengths



Bond angles

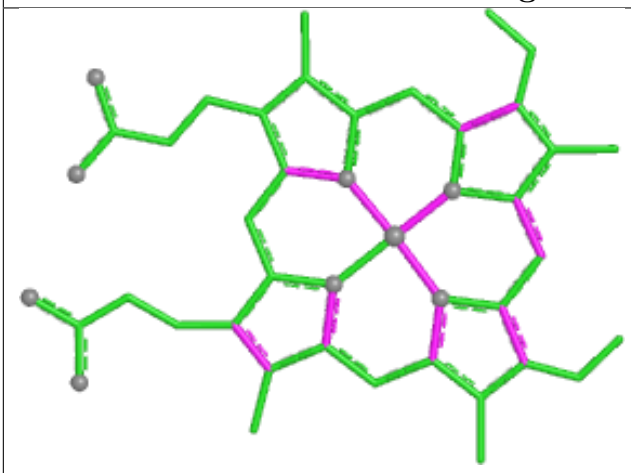


Torsions

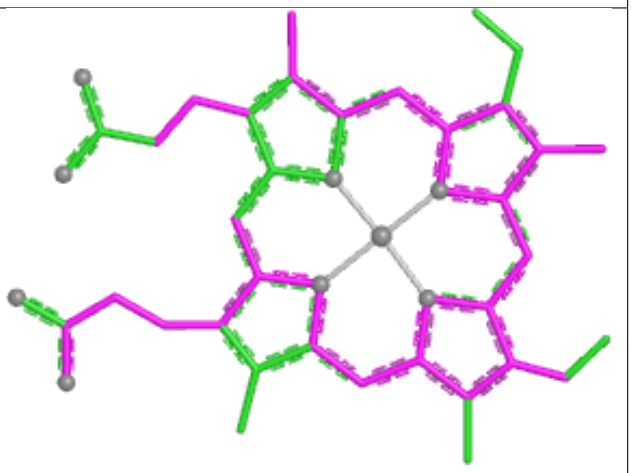


Rings

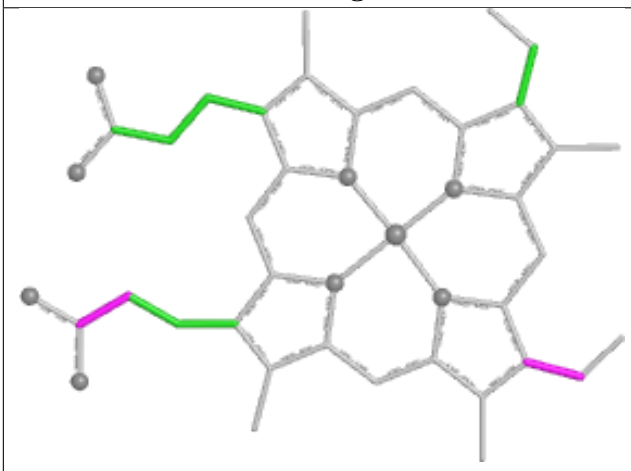
Ligand HEM C 503



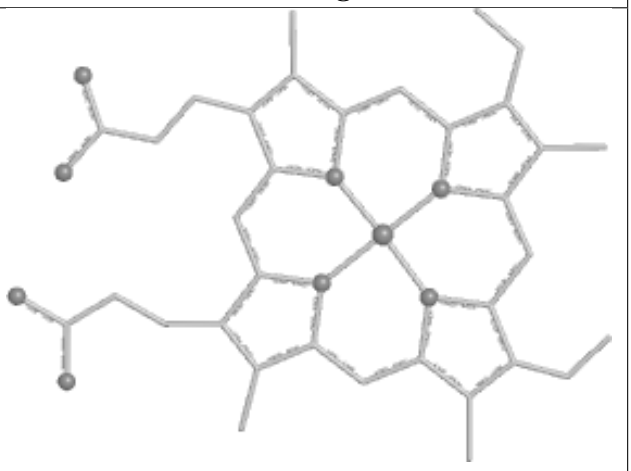
Bond lengths



Bond angles

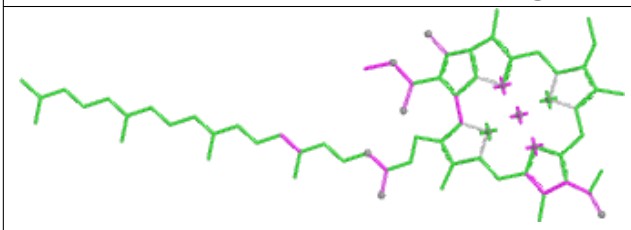


Torsions

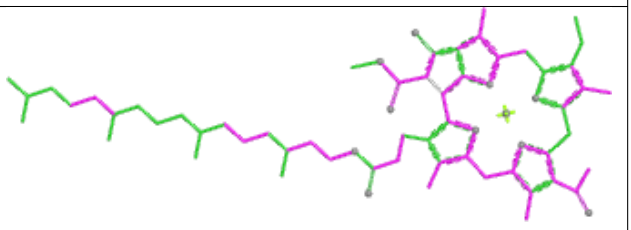


Rings

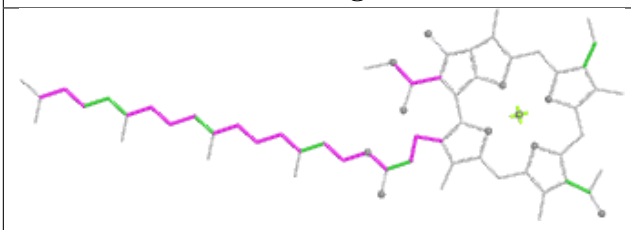
Ligand BCL 8 101



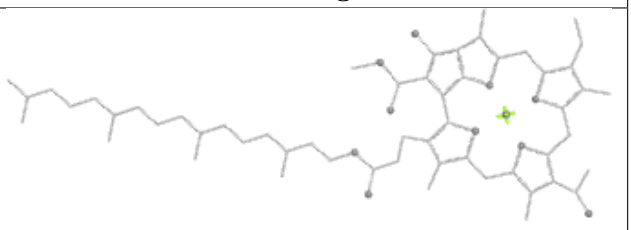
Bond lengths



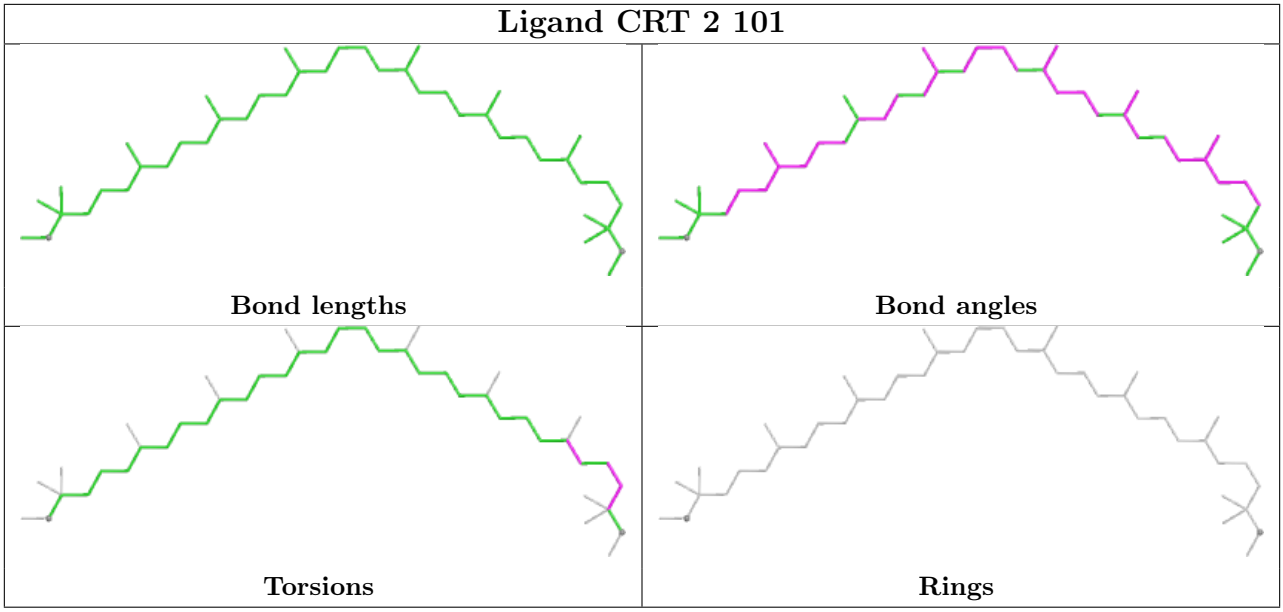
Bond angles

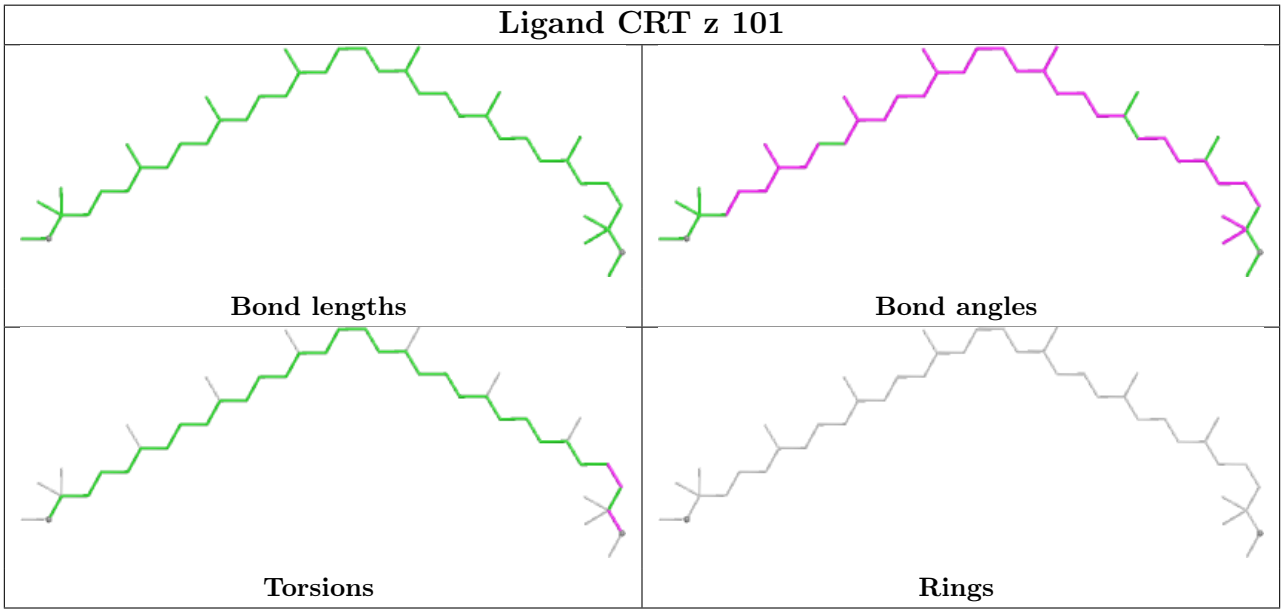


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.34	20 (6%)	26	17	89, 118, 143, 160	0
1	o	317/333 (95%)	0.36	18 (5%)	29	20	97, 126, 153, 166	0
2	L	280/281 (99%)	0.26	15 (5%)	31	21	73, 99, 149, 173	0
2	x	280/281 (99%)	0.26	11 (3%)	43	29	75, 98, 145, 174	0
3	M	318/319 (99%)	0.20	15 (4%)	36	24	73, 105, 141, 160	0
3	y	318/319 (99%)	0.34	16 (5%)	34	23	73, 110, 148, 173	0
4	H	258/259 (99%)	0.03	4 (1%)	70	52	78, 105, 162, 245	0
4	t	258/259 (99%)	0.06	7 (2%)	56	37	84, 107, 140, 240	0
5	1	60/61 (98%)	0.37	3 (5%)	34	23	134, 157, 202, 223	0
5	3	60/61 (98%)	0.61	7 (11%)	9	8	137, 157, 204, 216	0
5	5	60/61 (98%)	0.70	7 (11%)	9	8	142, 169, 243, 251	0
5	7	60/61 (98%)	0.52	2 (3%)	49	33	155, 180, 257, 271	0
5	9	60/61 (98%)	0.19	2 (3%)	49	33	156, 191, 228, 241	0
5	A	60/61 (98%)	0.37	3 (5%)	34	23	165, 198, 248, 252	0
5	AA	60/61 (98%)	0.52	4 (6%)	24	16	157, 202, 261, 269	0
5	AC	60/61 (98%)	0.65	6 (10%)	12	10	161, 205, 258, 265	0
5	AE	60/61 (98%)	0.56	4 (6%)	24	16	88, 207, 255, 264	1 (1%)
5	AG	60/61 (98%)	0.36	3 (5%)	34	23	161, 192, 245, 246	0
5	AI	60/61 (98%)	0.35	6 (10%)	12	10	145, 177, 226, 231	0
5	AK	60/61 (98%)	0.36	7 (11%)	9	8	139, 163, 219, 236	0
5	D	60/61 (98%)	0.37	2 (3%)	49	33	161, 206, 256, 265	0
5	F	60/61 (98%)	0.42	3 (5%)	34	23	169, 210, 255, 258	0
5	I	60/61 (98%)	0.31	2 (3%)	49	33	178, 209, 255, 264	0
5	K	60/61 (98%)	0.50	6 (10%)	12	10	162, 203, 269, 278	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	O	60/61 (98%)	0.27	4 (6%) 24 16	140, 193, 265, 272	0
5	Q	60/61 (98%)	0.53	7 (11%) 9 8	142, 180, 254, 258	0
5	S	60/61 (98%)	0.34	1 (1%) 69 50	81, 189, 247, 254	1 (1%)
5	U	60/61 (98%)	0.60	7 (11%) 9 8	145, 178, 238, 244	0
5	W	60/61 (98%)	0.39	3 (5%) 34 23	131, 159, 215, 220	0
5	Y	60/61 (98%)	0.42	5 (8%) 17 13	128, 156, 220, 249	0
5	d	60/61 (98%)	0.38	3 (5%) 34 23	134, 165, 216, 223	0
5	f	60/61 (98%)	0.37	5 (8%) 17 13	143, 161, 217, 229	0
5	h	60/61 (98%)	0.48	5 (8%) 17 13	140, 170, 234, 249	0
5	j	60/61 (98%)	0.09	1 (1%) 69 50	149, 179, 230, 245	0
5	l	60/61 (98%)	0.60	7 (11%) 9 8	141, 174, 222, 231	0
5	m	60/61 (98%)	0.45	5 (8%) 17 13	142, 178, 239, 244	0
5	p	60/61 (98%)	0.66	6 (10%) 12 10	136, 182, 239, 240	0
5	r	60/61 (98%)	0.20	5 (8%) 17 13	143, 184, 248, 251	0
5	u	60/61 (98%)	0.59	7 (11%) 9 8	162, 195, 251, 260	0
5	w	60/61 (98%)	0.24	1 (1%) 69 50	165, 204, 259, 265	0
6	0	40/47 (85%)	0.09	1 (2%) 58 39	166, 222, 247, 250	0
6	2	40/47 (85%)	-0.10	0 100 100	164, 179, 206, 212	0
6	4	40/47 (85%)	-0.31	1 (2%) 58 39	162, 176, 195, 200	0
6	6	40/47 (85%)	-0.14	0 100 100	174, 192, 206, 209	0
6	8	40/47 (85%)	0.15	2 (5%) 34 23	186, 217, 229, 232	0
6	AB	40/47 (85%)	0.25	3 (7%) 20 15	177, 217, 249, 252	0
6	AD	40/47 (85%)	0.21	1 (2%) 58 39	196, 226, 250, 256	0
6	AF	40/47 (85%)	0.15	1 (2%) 58 39	211, 233, 245, 251	0
6	AH	40/47 (85%)	0.21	4 (10%) 12 10	201, 219, 238, 242	0
6	AJ	40/47 (85%)	0.03	1 (2%) 58 39	180, 200, 220, 224	0
6	AL	40/47 (85%)	0.17	2 (5%) 34 23	169, 183, 204, 214	0
6	B	40/47 (85%)	0.07	2 (5%) 34 23	180, 225, 250, 252	0
6	E	40/47 (85%)	0.32	3 (7%) 20 15	186, 222, 253, 255	0
6	G	40/47 (85%)	0.13	2 (5%) 34 23	182, 227, 257, 259	0
6	J	40/47 (85%)	0.30	2 (5%) 34 23	187, 227, 259, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
6	N	40/47 (85%)	0.28	2 (5%)	34	23	167, 212, 250, 252	0
6	P	40/47 (85%)	0.14	3 (7%)	20	15	166, 212, 248, 255	0
6	R	40/47 (85%)	0.15	3 (7%)	20	15	164, 208, 240, 243	0
6	T	40/47 (85%)	-0.06	2 (5%)	34	23	178, 211, 230, 241	0
6	V	40/47 (85%)	-0.34	0	100	100	172, 198, 213, 222	0
6	X	40/47 (85%)	0.00	0	100	100	162, 182, 195, 198	0
6	Z	40/47 (85%)	-0.13	0	100	100	161, 175, 196, 201	0
6	c	40/47 (85%)	0.23	3 (7%)	20	15	151, 202, 239, 250	0
6	e	40/47 (85%)	-0.04	1 (2%)	58	39	172, 185, 215, 220	0
6	g	40/47 (85%)	-0.15	1 (2%)	58	39	180, 190, 212, 218	0
6	i	40/47 (85%)	-0.07	1 (2%)	58	39	182, 201, 214, 214	0
6	k	40/47 (85%)	-0.14	1 (2%)	58	39	175, 212, 229, 243	0
6	n	40/47 (85%)	0.23	1 (2%)	58	39	146, 196, 239, 246	0
6	q	40/47 (85%)	-0.07	2 (5%)	34	23	152, 190, 235, 243	0
6	s	40/47 (85%)	-0.01	1 (2%)	58	39	156, 194, 238, 243	0
6	v	40/47 (85%)	0.19	1 (2%)	58	39	175, 201, 247, 250	0
6	z	40/47 (85%)	0.05	0	100	100	176, 210, 255, 256	0
All	All	5546/5840 (94%)	0.26	292 (5%)	32	22	73, 162, 243, 278	2 (0%)

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	f	54	SER	10.3
5	3	46	TRP	6.9
1	o	321	ALA	6.6
4	t	56	VAL	6.5
5	m	37	MET	6.2
3	M	191	ILE	6.1
5	l	40	LEU	6.0
5	p	54	SER	5.9
5	5	33	LEU	5.7
5	AC	54	SER	5.6
5	j	37	MET	5.1
1	C	303	LEU	5.1
1	o	162	PRO	5.0
3	y	117	MET	5.0

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Mol	Chain	Res	Type	RSRZ
5	U	54	SER	4.9
1	o	154	THR	4.9
5	u	51	ILE	4.6
1	o	161	VAL	4.5
5	3	44	LEU	4.4
5	K	8	LEU	4.3
5	l	37	MET	4.3
5	K	57	ALA	4.3
3	y	83	VAL	4.3
1	o	233	PHE	4.2
3	M	101	GLN	4.2
5	AE	54	SER	4.1
5	AA	52	PRO	4.1
5	p	47	LEU	4.0
5	AK	46	TRP	4.0
3	M	198	TYR	4.0
5	l	47	LEU	4.0
5	U	58	LEU	3.9
5	F	42	THR	3.9
5	AK	51	ILE	3.9
6	c	17	PHE	3.8
6	J	41	LEU	3.8
5	AA	48	ASP	3.8
1	o	76	TYR	3.8
2	L	15	GLY	3.8
5	l	44	LEU	3.8
1	C	321	ALA	3.8
5	AE	53	VAL	3.8
1	C	59	VAL	3.7
1	o	72	ALA	3.7
2	L	223	THR	3.7
5	AK	47	LEU	3.7
6	R	17	PHE	3.6
5	U	45	ASN	3.6
5	Q	11	ILE	3.6
6	q	39	ALA	3.6
1	o	97	VAL	3.6
6	n	17	PHE	3.6
5	u	47	LEU	3.5
5	AG	54	SER	3.5
5	l	41	SER	3.5
3	M	287	SER	3.4

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Mol	Chain	Res	Type	RSRZ
5	AI	51	ILE	3.4
4	t	124	ASP	3.4
2	x	89	LEU	3.4
3	y	169	GLY	3.4
6	AH	30	GLY	3.4
2	L	176	PHE	3.4
2	x	111	LEU	3.4
1	C	72	ALA	3.4
1	C	125	VAL	3.4
5	5	44	LEU	3.4
5	3	51	ILE	3.4
5	Q	51	ILE	3.3
3	y	86	PHE	3.3
5	5	8	LEU	3.3
3	y	198	TYR	3.3
5	f	53	VAL	3.3
5	f	47	LEU	3.3
1	o	37	GLY	3.3
5	O	52	PRO	3.2
5	D	5	ASN	3.2
6	s	45	TRP	3.2
5	u	46	TRP	3.2
3	M	6	ASN	3.2
5	Q	54	SER	3.2
5	m	54	SER	3.2
2	x	54	ALA	3.2
1	C	28	PRO	3.1
4	t	55	VAL	3.1
2	x	51	VAL	3.1
6	g	39	ALA	3.1
6	E	9	LEU	3.1
5	Y	3	THR	3.0
6	i	21	PHE	3.0
6	G	12	ASP	3.0
2	L	14	GLY	3.0
1	o	125	VAL	3.0
2	L	228	ILE	3.0
2	x	120	LEU	3.0
2	L	171	TYR	3.0
5	O	44	LEU	2.9
5	f	55	TYR	2.9
3	y	106	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
5	AI	47	LEU	2.9
1	C	305	VAL	2.9
2	L	67	THR	2.9
4	t	145	ALA	2.9
5	f	46	TRP	2.9
1	C	329	GLY	2.9
5	u	59	GLY	2.9
2	L	224	PHE	2.9
5	F	44	LEU	2.9
4	t	138	VAL	2.9
5	Q	57	ALA	2.8
1	C	284	ILE	2.8
3	y	210	TYR	2.8
5	5	58	LEU	2.8
5	5	46	TRP	2.8
1	C	61	SER	2.8
5	A	52	PRO	2.8
5	U	53	VAL	2.8
5	Y	54	SER	2.8
3	y	59	LEU	2.8
3	y	189	PHE	2.8
5	l	51	ILE	2.8
6	c	21	PHE	2.8
3	y	85	GLN	2.8
5	W	53	VAL	2.8
6	J	37	LEU	2.8
2	x	268	TRP	2.7
5	AE	61	LYS	2.7
2	L	229	VAL	2.7
5	7	3	THR	2.7
5	AK	3	THR	2.7
6	AH	45	TRP	2.7
2	x	35	PHE	2.7
5	9	41	SER	2.7
6	e	45	TRP	2.7
6	v	26	TYR	2.7
6	8	41	LEU	2.7
3	M	288	GLY	2.7
5	S	61	LYS	2.7
5	AC	36	HIS	2.7
5	AG	53	VAL	2.7
2	x	15	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
5	u	41	SER	2.7
5	A	55	TYR	2.7
5	K	58	LEU	2.6
5	3	53	VAL	2.6
5	5	55	TYR	2.6
6	P	36	HIS	2.6
6	E	10	THR	2.6
5	m	13	LEU	2.6
5	AI	46	TRP	2.6
5	AC	41	SER	2.6
5	W	23	SER	2.6
4	H	182	LEU	2.6
3	y	303	MET	2.5
2	x	173	PHE	2.5
5	r	54	SER	2.5
5	A	39	VAL	2.5
6	AD	14	ALA	2.5
2	L	265	THR	2.5
6	T	28	TRP	2.5
1	C	70	PRO	2.5
5	I	55	TYR	2.5
5	W	55	TYR	2.5
2	L	174	LEU	2.5
5	AG	55	TYR	2.5
3	M	95	LEU	2.5
6	B	9	LEU	2.5
6	R	43	ARG	2.5
6	R	39	ALA	2.5
1	C	239	ILE	2.5
1	C	151	THR	2.5
5	AC	46	TRP	2.5
3	M	140	LEU	2.5
3	M	160	LEU	2.5
3	y	113	GLY	2.5
5	m	53	VAL	2.5
4	t	237	ASP	2.4
2	x	45	LEU	2.4
6	P	37	LEU	2.4
5	K	59	GLY	2.4
5	AA	53	VAL	2.4
5	p	26	ALA	2.4
1	o	121	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
5	7	54	SER	2.4
1	o	318	LEU	2.4
4	H	195	LEU	2.4
5	AI	44	LEU	2.4
5	K	46	TRP	2.4
5	1	46	TRP	2.4
5	U	48	ASP	2.4
3	M	102	TYR	2.4
5	r	53	VAL	2.4
6	AL	43	ARG	2.4
2	x	14	GLY	2.4
5	3	60	LYS	2.4
5	u	2	PHE	2.4
3	y	116	LEU	2.4
6	B	37	LEU	2.4
6	AJ	41	LEU	2.4
6	AL	45	TRP	2.4
2	L	267	GLY	2.3
1	C	165	ALA	2.3
1	o	252	ASN	2.3
1	C	241	ASP	2.3
5	AI	40	LEU	2.3
6	8	46	LEU	2.3
5	Y	5	ASN	2.3
5	h	37	MET	2.3
6	N	42	TYR	2.3
5	1	44	LEU	2.3
6	E	14	ALA	2.3
6	AH	39	ALA	2.3
2	L	17	LEU	2.3
2	L	84	LEU	2.3
5	3	47	LEU	2.3
5	AA	34	LEU	2.3
5	AK	2	PHE	2.3
6	T	21	PHE	2.3
5	AC	48	ASP	2.3
5	U	39	VAL	2.3
3	M	188	ALA	2.3
5	h	6	ALA	2.3
6	N	8	GLY	2.3
3	y	144	GLN	2.3
5	m	10	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
5	1	53	VAL	2.3
3	y	138	GLU	2.2
4	H	133	ILE	2.2
5	AC	17	PRO	2.2
6	0	44	PRO	2.2
3	y	62	PHE	2.2
2	L	27	VAL	2.2
1	C	60	GLU	2.2
1	o	193	ALA	2.2
5	r	18	ARG	2.2
1	o	73	SER	2.2
5	3	54	SER	2.2
3	M	106	ILE	2.2
5	Q	47	LEU	2.2
5	p	57	ALA	2.2
5	r	52	PRO	2.2
5	AK	44	LEU	2.2
6	AB	11	ASP	2.2
5	D	55	TYR	2.2
6	q	45	TRP	2.2
6	AH	34	ILE	2.2
5	p	13	LEU	2.2
5	AI	2	PHE	2.2
6	c	45	TRP	2.2
5	w	39	VAL	2.1
5	d	29	ILE	2.1
5	h	34	LEU	2.1
3	M	231	GLY	2.1
3	M	189	PHE	2.1
5	5	2	PHE	2.1
6	4	26	TYR	2.1
1	C	39	GLY	2.1
5	Y	41	SER	2.1
5	d	59	GLY	2.1
5	l	46	TRP	2.1
6	P	45	TRP	2.1
5	I	61	LYS	2.1
5	Y	14	ILE	2.1
6	AB	20	ILE	2.1
1	o	317	PRO	2.1
1	C	121	ILE	2.1
5	p	35	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
5	AK	21	LEU	2.1
1	o	329	GLY	2.1
5	U	59	GLY	2.1
1	C	233	PHE	2.1
5	K	39	VAL	2.1
5	O	42	THR	2.1
5	O	21	LEU	2.0
5	AE	24	ILE	2.0
5	h	12	TRP	2.0
5	9	55	TYR	2.0
5	r	48	ASP	2.0
6	G	7	THR	2.0
6	AF	11	ASP	2.0
4	H	92	PHE	2.0
5	F	53	VAL	2.0
5	d	13	LEU	2.0
6	AB	46	LEU	2.0
6	k	37	LEU	2.0
1	C	86	SER	2.0
3	M	227	SER	2.0
5	Q	6	ALA	2.0
1	o	22	GLY	2.0
5	Q	53	VAL	2.0
5	h	15	LEU	2.0
4	t	5	ILE	2.0
5	u	14	ILE	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, 95^{th} 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
17	PGW	AE	101	21/51	0.60	0.13	141,155,167,171	0
12	PEF	y	406	19/47	0.61	0.12	116,122,128,131	0
17	PGW	S	101	21/51	0.62	0.14	122,133,142,147	0
12	PEF	H	304	19/47	0.65	0.14	160,166,175,180	0
16	PO4	y	405	5/5	0.66	0.12	134,136,141,141	0
12	PEF	m	101	19/47	0.68	0.19	119,125,133,136	0
12	PEF	A	101	19/47	0.68	0.17	142,147,157,161	0
12	PEF	x	306	19/47	0.69	0.11	97,102,107,107	0
16	PO4	H	303	5/5	0.72	0.09	158,160,164,166	0
12	PEF	y	408	19/47	0.75	0.11	102,108,116,118	0
16	PO4	t	302	5/5	0.78	0.13	142,142,144,149	0
12	PEF	M	408	19/47	0.78	0.11	95,99,103,105	0
12	PEF	y	407	19/47	0.78	0.12	97,101,106,108	0
12	PEF	L	305	12/47	0.79	0.12	113,118,123,123	0
9	BCL	I	103	66/66	0.82	0.16	200,223,264,273	0
15	CRT	T	101	44/44	0.82	0.20	154,186,198,199	0
15	CRT	7	103	44/44	0.82	0.22	171,193,205,208	0
12	PEF	H	301	19/47	0.82	0.10	108,115,119,121	0
15	CRT	m	104	44/44	0.83	0.18	171,183,189,191	0
15	CRT	v	101	44/44	0.83	0.18	170,189,194,196	0
15	CRT	AC	101	44/44	0.83	0.18	180,197,200,202	0
15	CRT	AL	101	44/44	0.83	0.24	130,168,200,203	0
9	BCL	D	102	66/66	0.83	0.15	194,218,258,259	0
9	BCL	AC	103	66/66	0.83	0.18	188,211,257,265	0
15	CRT	O	101	44/44	0.83	0.18	179,194,202,205	0
9	BCL	AG	101	66/66	0.83	0.20	179,190,215,226	0
9	BCL	d	101	66/66	0.83	0.15	131,157,168,173	0
12	PEF	H	302	19/47	0.84	0.13	139,156,167,170	0
9	BCL	p	102	66/66	0.84	0.16	128,189,203,208	0
12	PEF	p	101	16/47	0.84	0.15	131,142,148,151	0
15	CRT	I	102	44/44	0.84	0.20	194,205,211,214	0
9	BCL	u	102	66/66	0.85	0.15	181,205,248,268	0
15	CRT	e	101	44/44	0.85	0.25	140,173,206,210	0
12	PEF	M	407	16/47	0.85	0.10	86,89,91,92	0
9	BCL	1	101	66/66	0.85	0.12	123,149,159,163	0
9	BCL	m	103	66/66	0.85	0.13	173,198,219,230	0
9	BCL	D	101	66/66	0.85	0.15	153,209,226,231	0
15	CRT	AH	102	44/44	0.85	0.17	155,198,229,231	0
9	BCL	AB	102	66/66	0.86	0.14	187,214,258,267	0
9	BCL	f	101	66/66	0.86	0.15	144,163,174,180	0
9	BCL	w	101	66/66	0.86	0.16	176,199,217,222	0
15	CRT	i	101	44/44	0.86	0.19	156,180,197,201	0
12	PEF	t	303	19/47	0.86	0.10	94,97,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CRT	0	101	44/44	0.86	0.19	175,197,206,206	0
9	BCL	AE	102	66/66	0.86	0.11	188,207,244,262	0
9	BCL	z	102	66/66	0.86	0.13	183,211,253,269	0
15	CRT	G	101	44/44	0.86	0.19	187,209,215,218	0
9	BCL	AC	102	66/66	0.87	0.13	181,205,218,228	0
9	BCL	N	101	66/66	0.87	0.14	189,213,255,262	0
15	CRT	AJ	101	44/44	0.87	0.17	139,182,214,217	0
15	CRT	R	101	44/44	0.87	0.19	159,181,189,191	0
9	BCL	k	102	66/66	0.87	0.15	171,195,223,234	0
15	CRT	4	101	44/44	0.87	0.19	141,166,185,190	0
15	CRT	k	101	44/44	0.87	0.17	166,186,199,202	0
11	UQ8	x	304	53/53	0.87	0.14	80,87,90,91	0
12	PEF	H	305	19/47	0.87	0.11	93,97,104,105	0
9	BCL	P	101	66/66	0.87	0.14	173,201,216,221	0
15	CRT	n	101	44/44	0.87	0.19	166,179,185,189	0
9	BCL	G	102	66/66	0.87	0.13	197,220,264,265	0
9	BCL	u	101	66/66	0.88	0.14	133,196,212,216	0
15	CRT	M	405	44/44	0.88	0.15	90,108,139,148	0
15	CRT	g	101	44/44	0.88	0.19	145,172,198,202	0
9	BCL	m	102	66/66	0.88	0.16	157,190,207,214	0
9	BCL	V	102	66/66	0.88	0.14	162,177,208,223	0
15	CRT	q	101	44/44	0.88	0.15	159,174,179,182	0
9	BCL	g	102	66/66	0.88	0.17	153,171,206,215	0
8	BA	A	105	1/1	0.88	0.17	243,243,243,243	0
11	UQ8	L	304	53/53	0.88	0.13	81,86,88,89	0
9	BCL	AF	101	66/66	0.88	0.15	161,205,215,225	0
9	BCL	c	101	66/66	0.89	0.12	173,199,243,258	0
15	CRT	AF	102	44/44	0.89	0.15	170,212,229,231	0
9	BCL	U	101	66/66	0.89	0.16	153,176,186,191	0
8	BA	7	104	1/1	0.89	0.19	215,215,215,215	0
7	HEM	o	501	43/43	0.89	0.17	129,137,145,148	0
9	BCL	2	102	66/66	0.89	0.13	145,156,185,195	0
12	PEF	t	301	19/47	0.89	0.10	100,104,107,108	0
9	BCL	e	102	66/66	0.89	0.14	152,164,191,197	0
15	CRT	y	404	44/44	0.89	0.16	99,115,146,154	0
9	BCL	O	102	66/66	0.89	0.14	179,206,250,251	0
9	BCL	I	101	66/66	0.89	0.12	149,216,231,234	0
9	BCL	h	101	66/66	0.89	0.14	155,171,185,187	0
9	BCL	T	102	66/66	0.89	0.14	166,185,223,243	0
15	CRT	z	101	44/44	0.89	0.20	176,193,197,198	0
15	CRT	s	101	44/44	0.90	0.14	163,178,182,183	0
9	BCL	AI	102	66/66	0.90	0.13	163,172,197,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	AL	102	66/66	0.90	0.16	152,161,183,190	0
15	CRT	P	102	44/44	0.90	0.15	170,186,189,190	0
15	CRT	AD	101	44/44	0.90	0.19	175,204,211,213	0
9	BCL	K	101	66/66	0.90	0.16	183,209,225,229	0
9	BCL	Q	101	66/66	0.90	0.15	166,193,205,211	0
15	CRT	V	101	44/44	0.90	0.16	140,179,197,198	0
15	CRT	2	101	44/44	0.90	0.16	136,165,190,194	0
9	BCL	6	101	66/66	0.90	0.17	154,174,210,221	0
15	CRT	7	101	44/44	0.90	0.19	155,177,191,193	0
9	BCL	7	102	66/66	0.90	0.15	163,180,195,200	0
15	CRT	9	101	44/44	0.90	0.15	181,205,211,215	0
9	BCL	0	102	66/66	0.90	0.12	183,208,254,257	0
9	BCL	j	101	66/66	0.90	0.13	166,183,198,203	0
9	BCL	S	102	66/66	0.90	0.16	136,186,197,205	0
15	CRT	E	101	44/44	0.90	0.13	179,205,211,213	0
9	BCL	AI	101	66/66	0.90	0.14	167,179,190,196	0
9	BCL	s	102	66/66	0.91	0.12	174,198,247,260	0
15	CRT	Z	101	44/44	0.91	0.14	127,160,186,189	0
9	BCL	8	101	66/66	0.91	0.11	173,196,221,230	0
9	BCL	9	102	66/66	0.91	0.12	165,191,211,216	0
9	BCL	X	102	66/66	0.91	0.11	148,159,180,192	0
14	MQ8	M	404	53/53	0.91	0.13	82,100,144,151	0
14	MQ8	y	403	53/53	0.91	0.15	79,93,131,138	0
9	BCL	AH	101	66/66	0.91	0.13	182,196,206,212	0
9	BCL	3	101	66/66	0.91	0.13	138,153,165,168	0
9	BCL	l	101	66/66	0.91	0.11	157,189,205,210	0
16	PO4	M	406	5/5	0.91	0.09	121,126,127,128	0
9	BCL	AB	101	66/66	0.91	0.12	176,202,220,226	0
10	BPH	M	403	65/65	0.91	0.13	84,88,117,126	0
10	BPH	y	402	65/65	0.91	0.15	87,95,132,142	0
9	BCL	Z	102	66/66	0.91	0.13	143,151,174,182	0
9	BCL	R	102	66/66	0.91	0.11	170,194,236,245	0
9	BCL	x	305	66/66	0.92	0.14	83,90,98,105	0
9	BCL	y	401	66/66	0.92	0.16	86,93,102,106	0
9	BCL	A	102	66/66	0.92	0.12	182,205,221,225	0
15	CRT	X	101	44/44	0.92	0.15	129,166,188,191	0
8	BA	I	104	1/1	0.92	0.14	276,276,276,276	0
8	BA	U	102	1/1	0.92	0.22	224,224,224,224	0
9	BCL	q	102	66/66	0.92	0.15	170,194,226,241	0
9	BCL	r	101	66/66	0.92	0.12	160,190,204,208	0
9	BCL	F	101	66/66	0.92	0.14	183,211,226,232	0
9	BCL	AK	101	66/66	0.92	0.14	152,162,177,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BA	3	102	1/1	0.92	0.16	191,191,191,191	0
7	HEM	C	501	43/43	0.92	0.14	118,126,133,136	0
8	BA	u	103	1/1	0.92	0.17	264,264,264,264	0
8	BA	w	102	1/1	0.92	0.09	271,271,271,271	0
8	BA	AE	103	1/1	0.92	0.10	248,248,248,248	0
9	BCL	x	301	66/66	0.92	0.18	81,86,92,97	0
9	BCL	i	102	66/66	0.92	0.12	161,181,218,232	0
9	BCL	M	401	66/66	0.93	0.13	86,94,107,114	0
9	BCL	W	101	66/66	0.93	0.14	152,165,171,179	0
9	BCL	L	303	66/66	0.93	0.16	79,86,91,96	0
9	BCL	Y	101	66/66	0.93	0.13	142,152,162,174	0
9	BCL	A	103	66/66	0.93	0.12	190,213,242,251	0
9	BCL	5	101	66/66	0.94	0.14	147,166,178,183	0
8	BA	x	308	1/1	0.94	0.07	175,175,175,175	0
9	BCL	M	402	66/66	0.94	0.12	83,90,96,99	0
9	BCL	x	303	66/66	0.94	0.14	82,89,97,98	0
10	BPH	x	302	65/65	0.94	0.15	78,84,104,106	0
8	BA	m	106	1/1	0.94	0.06	242,242,242,242	0
7	HEM	o	503	43/43	0.95	0.16	98,109,122,124	0
8	BA	O	103	1/1	0.95	0.14	244,244,244,244	0
10	BPH	L	302	65/65	0.95	0.11	79,88,109,114	0
7	HEM	o	504	43/43	0.95	0.16	111,114,119,122	0
8	BA	W	102	1/1	0.95	0.12	209,209,209,209	0
8	BA	A	104	1/1	0.95	0.11	247,247,247,247	0
8	BA	AI	103	1/1	0.95	0.13	210,210,210,210	0
8	BA	f	102	1/1	0.95	0.08	205,205,205,205	0
9	BCL	L	301	66/66	0.95	0.13	79,84,98,103	0
7	HEM	C	502	43/43	0.95	0.18	108,114,120,121	0
9	BCL	4	102	66/66	0.95	0.10	144,159,189,198	0
8	BA	D	103	1/1	0.96	0.16	252,252,252,252	0
8	BA	F	102	1/1	0.96	0.11	271,271,271,271	0
8	BA	AK	102	1/1	0.96	0.09	186,186,186,186	0
8	BA	L	306	1/1	0.96	0.05	185,185,185,185	0
8	BA	K	102	1/1	0.96	0.14	265,265,265,265	0
7	HEM	C	504	43/43	0.96	0.16	105,106,110,111	0
8	BA	p	103	1/1	0.96	0.11	257,257,257,257	0
8	BA	Q	102	1/1	0.96	0.12	245,245,245,245	0
7	HEM	o	502	43/43	0.96	0.15	119,124,128,129	0
8	BA	AC	104	1/1	0.96	0.10	257,257,257,257	0
8	BA	d	102	1/1	0.97	0.07	174,174,174,174	0
8	BA	5	102	1/1	0.97	0.16	212,212,212,212	0
8	BA	m	105	1/1	0.97	0.08	226,226,226,226	0

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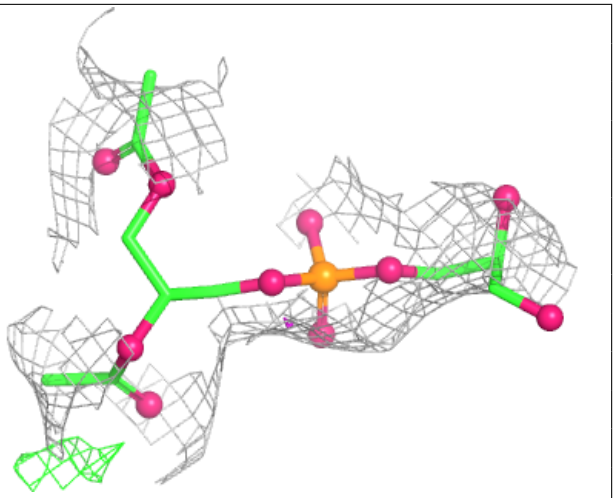
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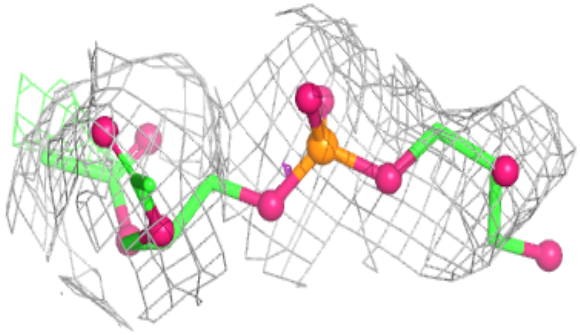
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BA	AG	102	1/1	0.97	0.08	225,225,225,225	0
7	HEM	C	503	43/43	0.97	0.17	96,107,121,123	0
8	BA	AA	101	1/1	0.97	0.06	260,260,260,260	0
8	BA	r	102	1/1	0.98	0.08	250,250,250,250	0
8	BA	j	102	1/1	0.98	0.04	228,228,228,228	0
8	BA	C	505	1/1	0.98	0.09	93,93,93,93	0
8	BA	L	307	1/1	0.98	0.03	160,160,160,160	0
8	BA	1	102	1/1	0.98	0.09	177,177,177,177	0
8	BA	x	307	1/1	0.98	0.04	186,186,186,186	0
8	BA	o	505	1/1	0.99	0.10	100,100,100,100	0
8	BA	S	103	1/1	0.99	0.10	227,227,227,227	0
13	FE	x	309	1/1	0.99	0.07	76,76,76,76	0
8	BA	h	102	1/1	0.99	0.13	210,210,210,210	0
8	BA	Y	102	1/1	0.99	0.14	181,181,181,181	0
13	FE	L	308	1/1	1.00	0.06	76,76,76,76	0

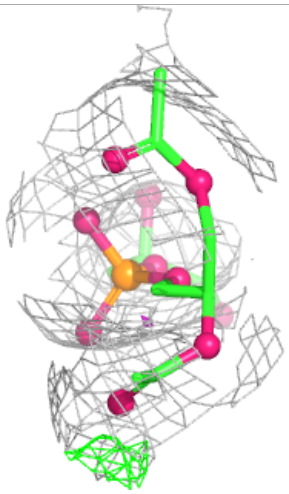
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW AE 101:

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

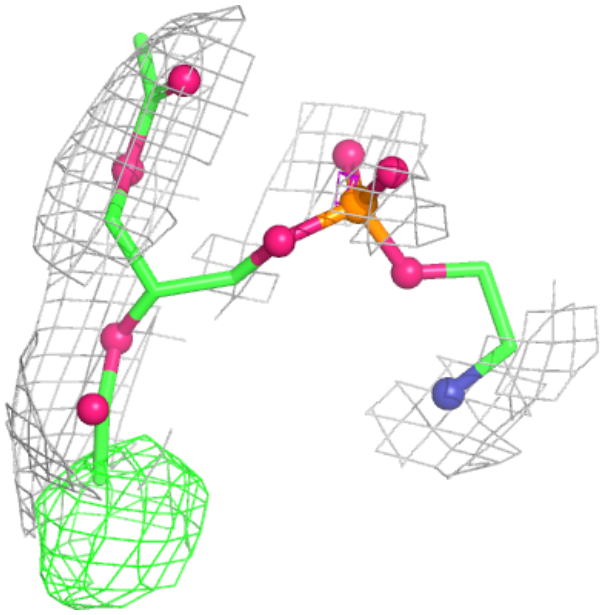


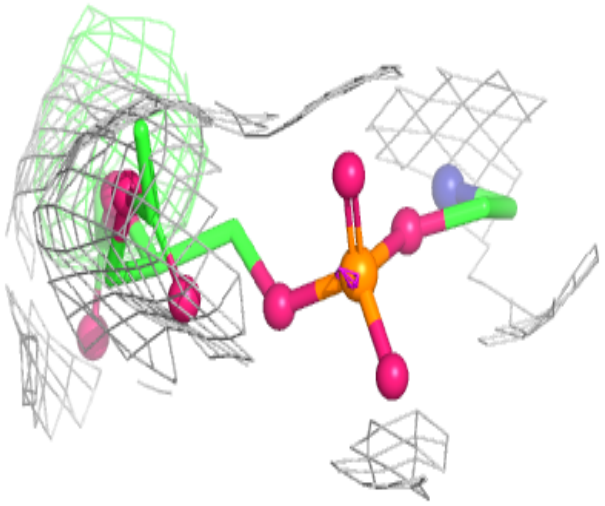


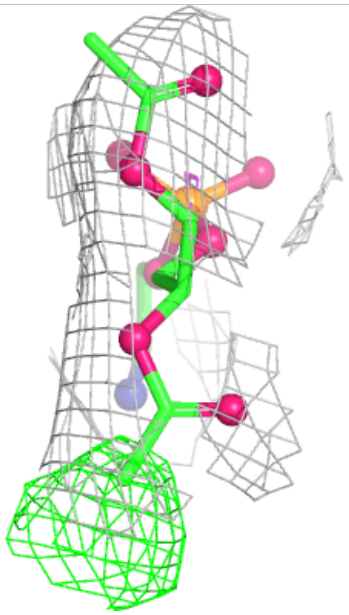


Electron density around PEF y 406:

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

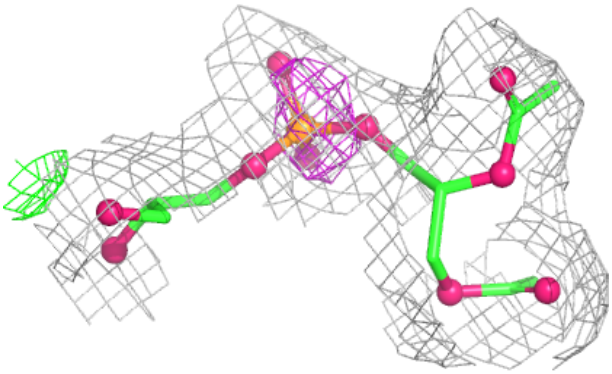


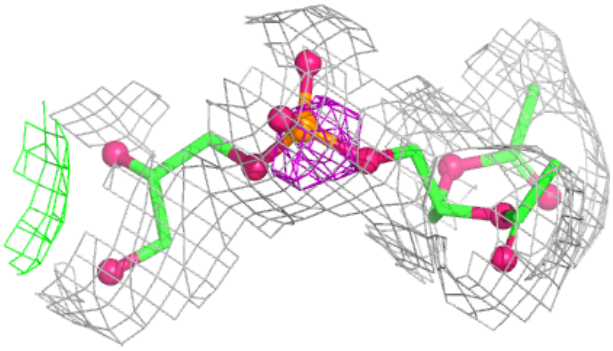


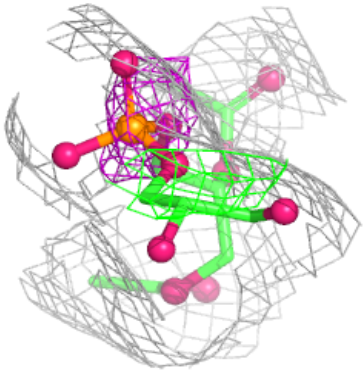


Electron density around PGW S 101:

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

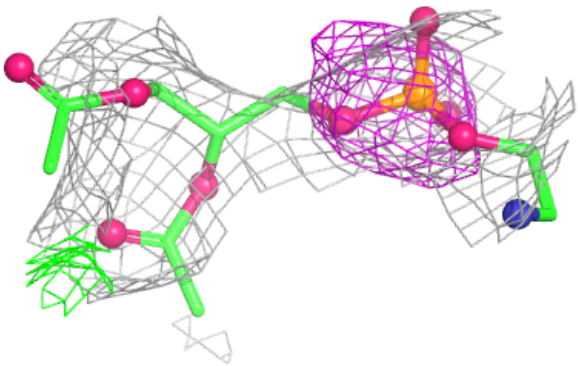


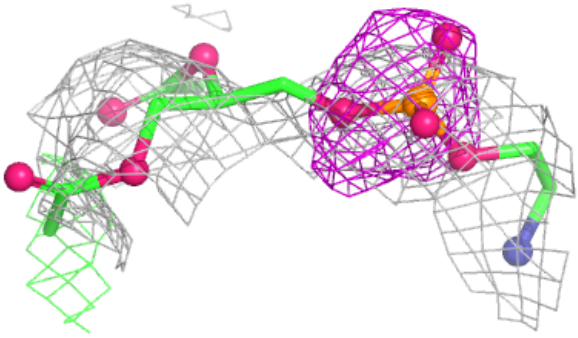


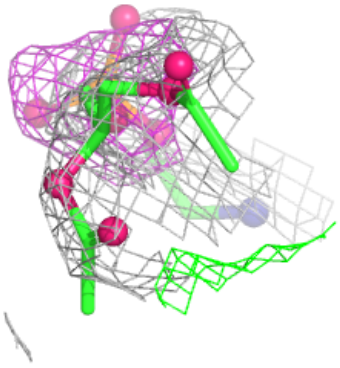


Electron density around PEF H 304:

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

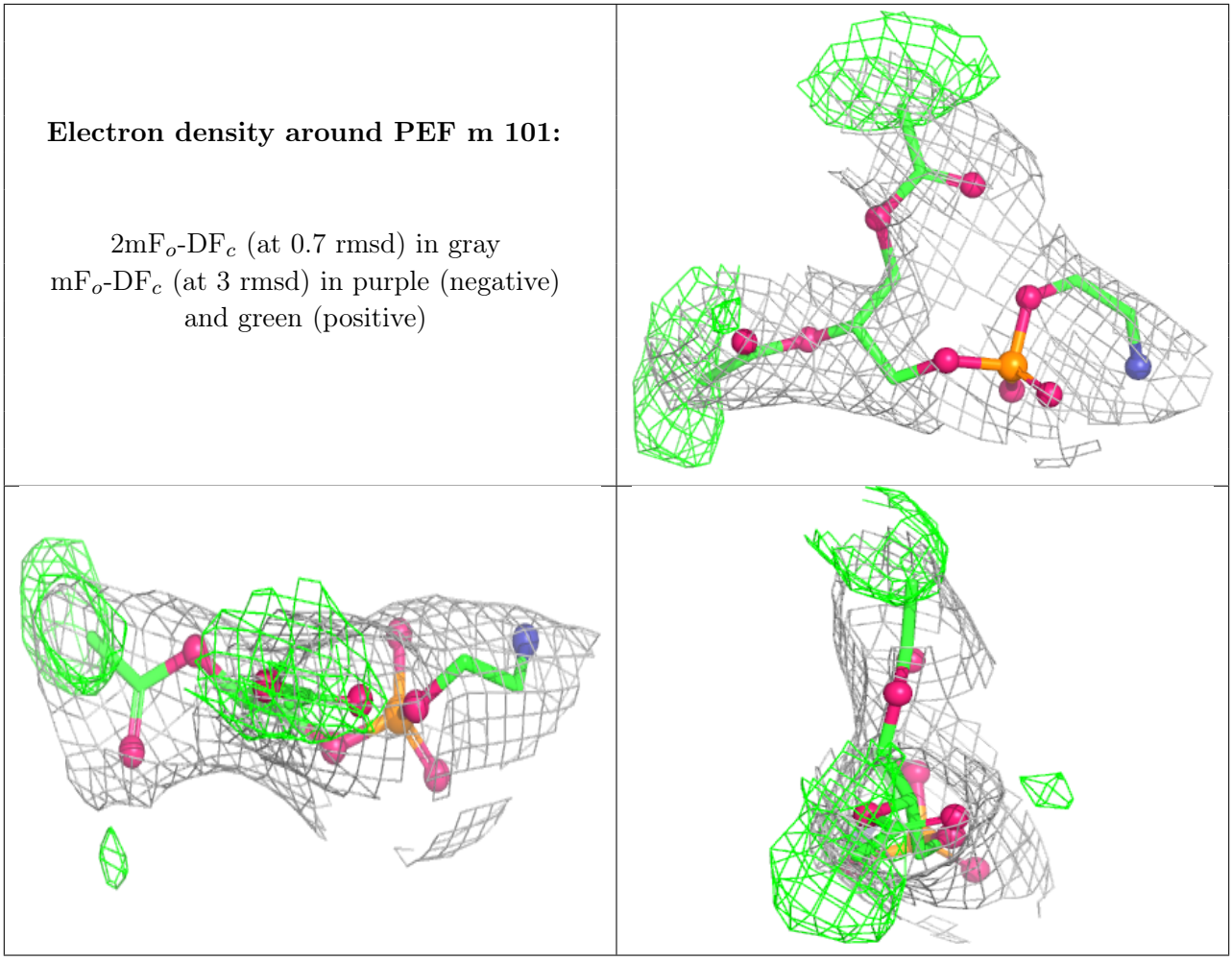






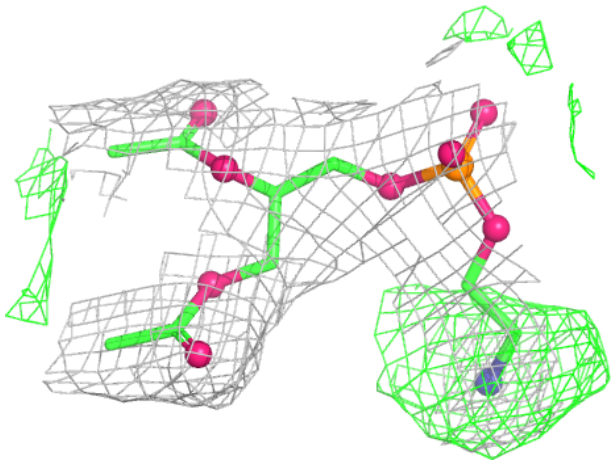
Electron density around PEF m 101:

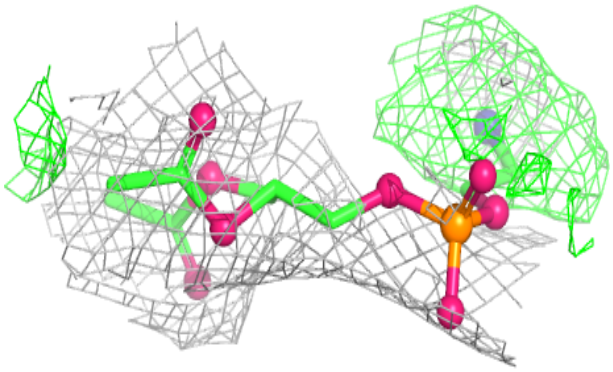
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

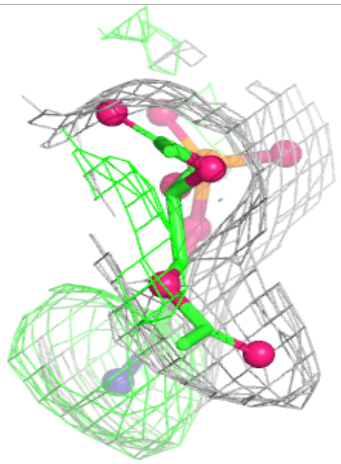


Electron density around PEF A 101:

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

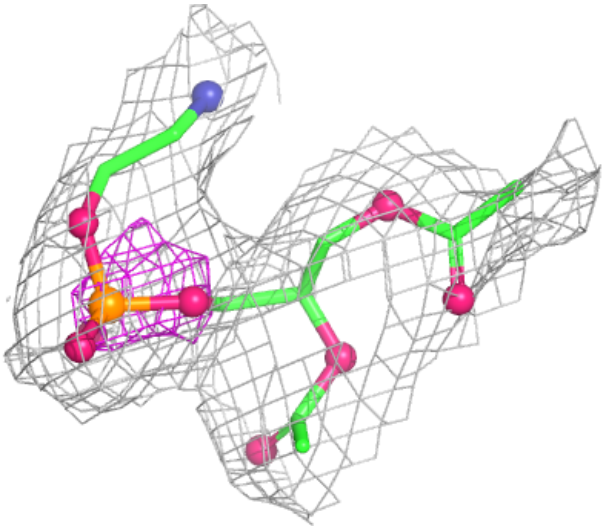


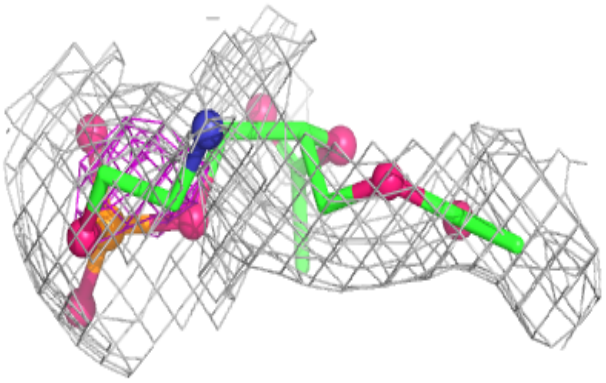


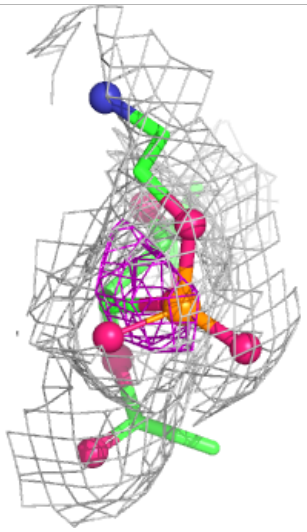


Electron density around PEF x 306:

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

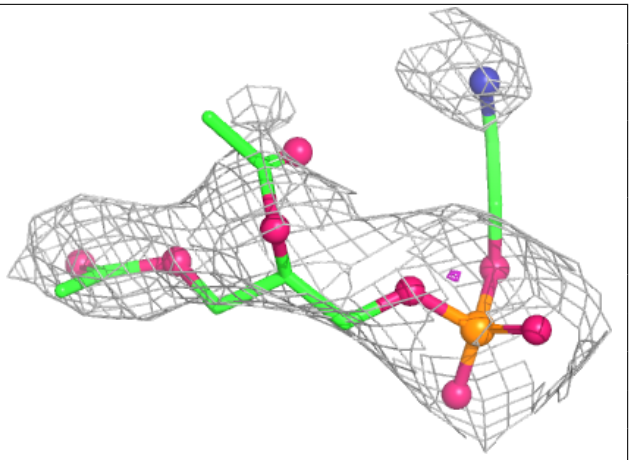


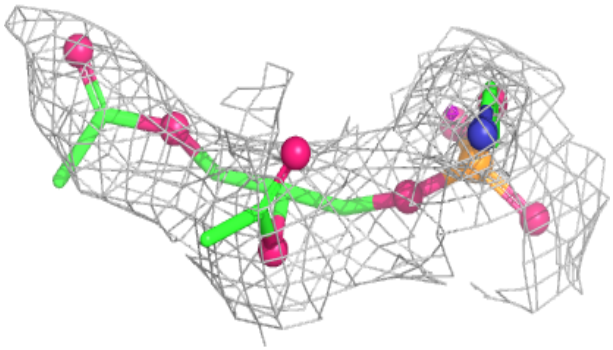


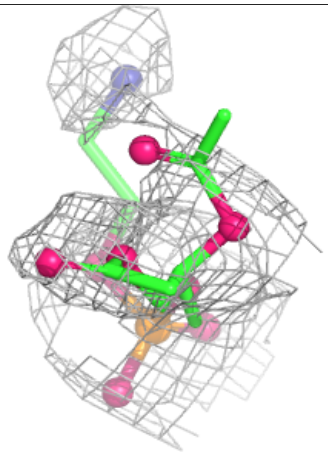


Electron density around PEF y 408:

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

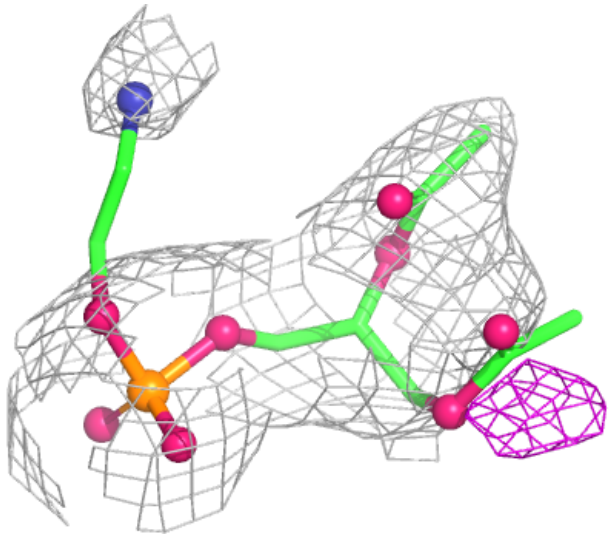


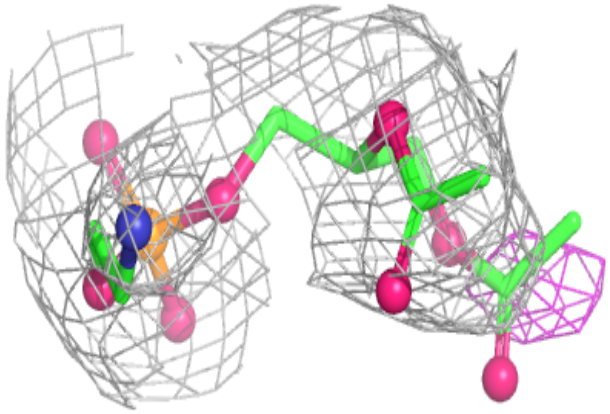


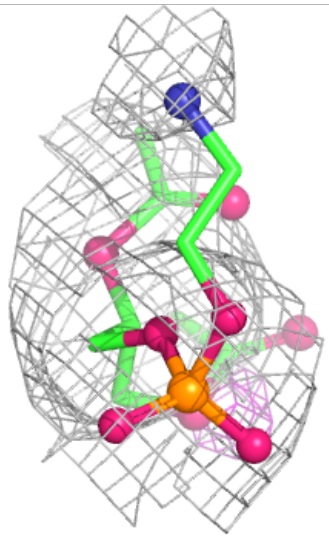


Electron density around PEF M 408:

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

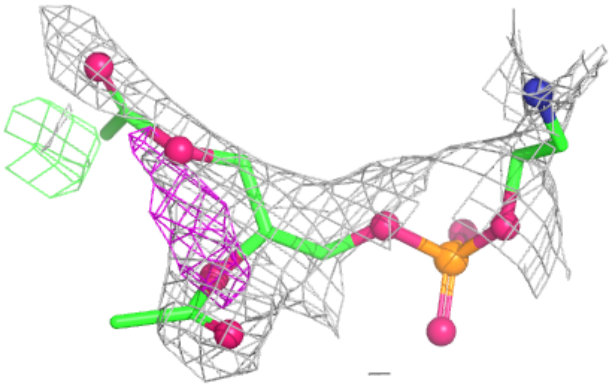


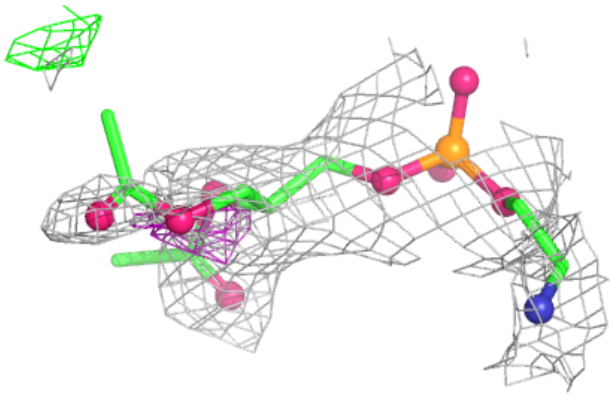


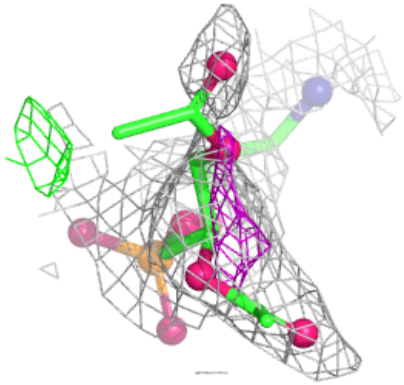


Electron density around PEF y 407:

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

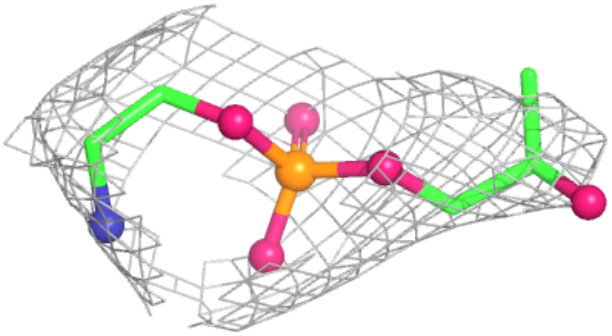


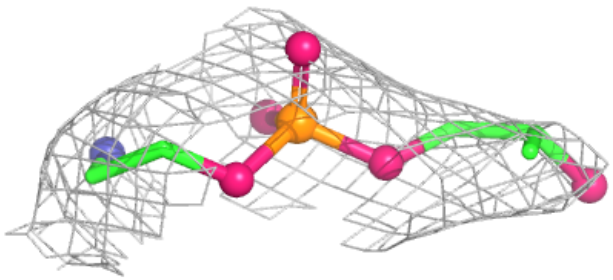


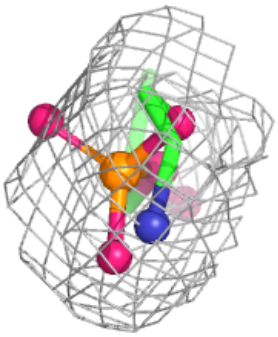


Electron density around PEF L 305:

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

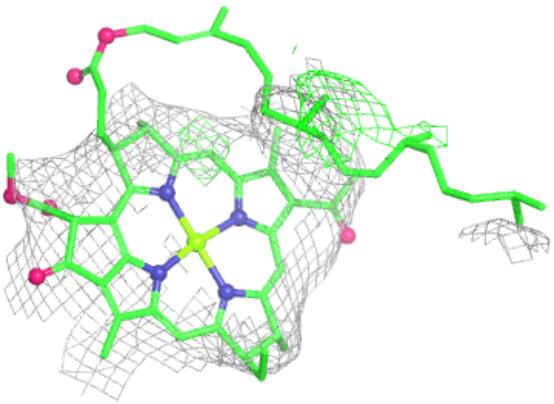


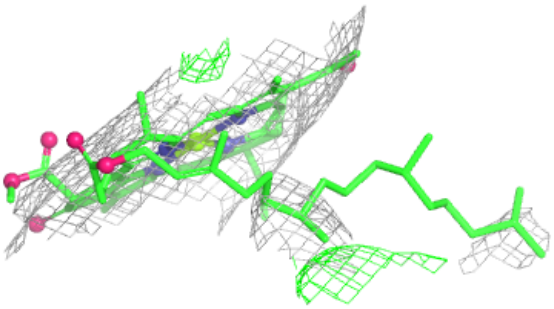


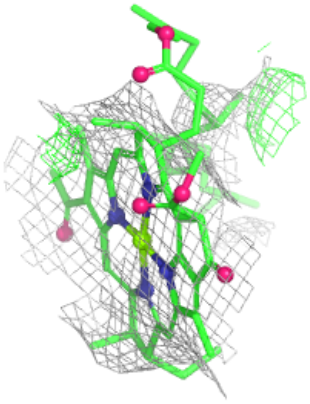


Electron density around BCL I 103:

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

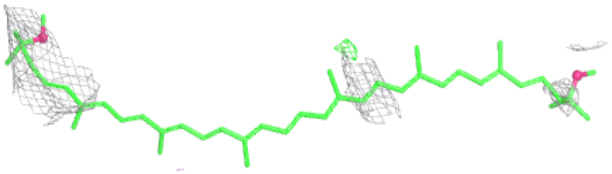


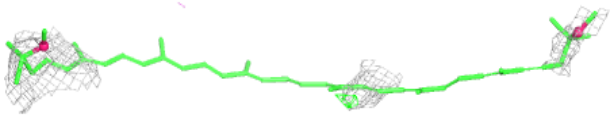




Electron density around CRT T 101:

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

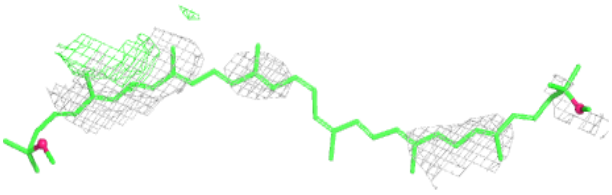


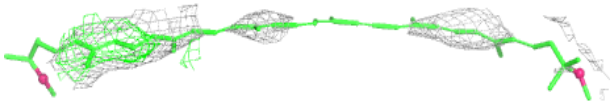


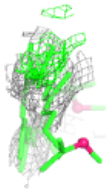


Electron density around CRT 7 103:

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

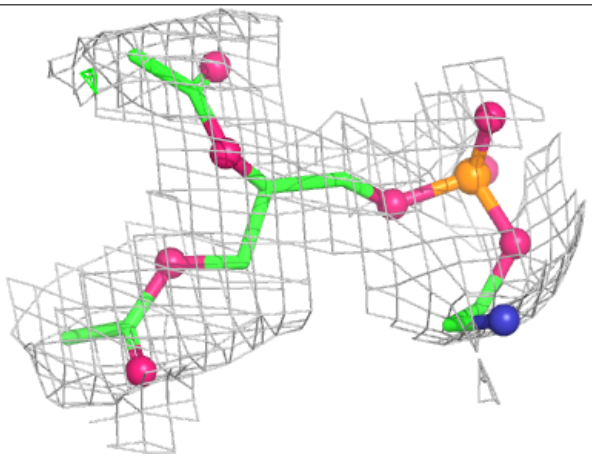


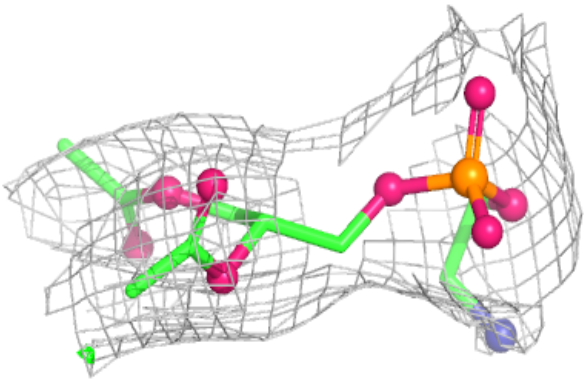


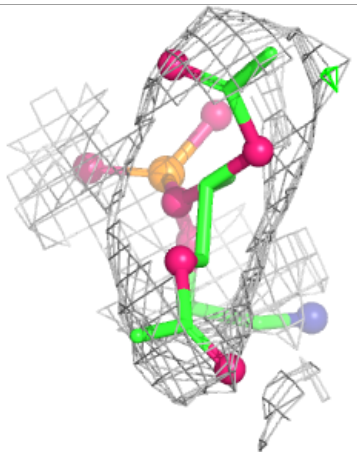


Electron density around PEF H 301:

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

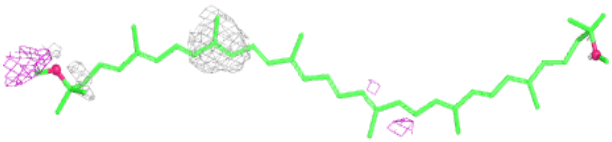


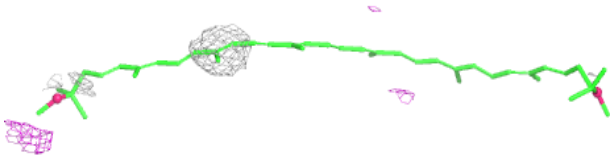


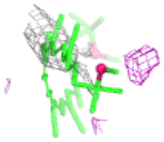


Electron density around CRT m 104:

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

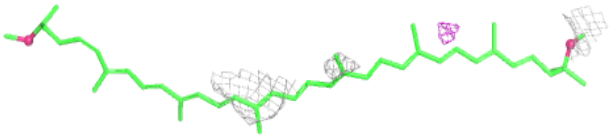


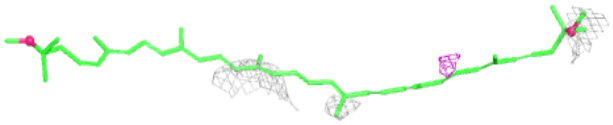


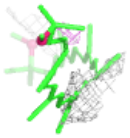


Electron density around CRT v 101:

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

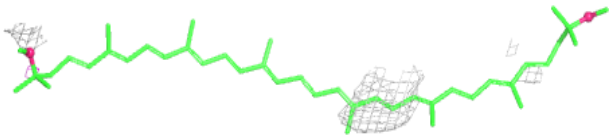


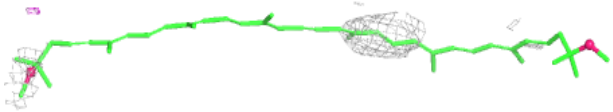




Electron density around CRT AC 101:

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

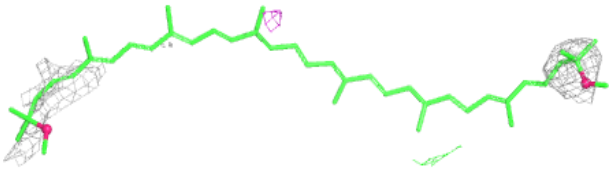


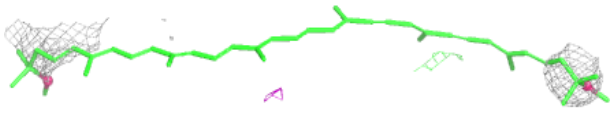


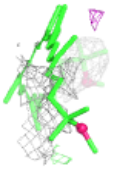


Electron density around CRT AL 101:

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

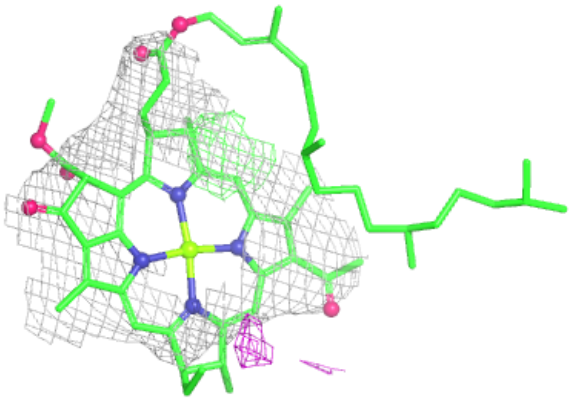


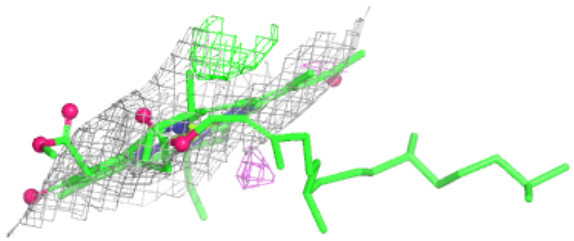


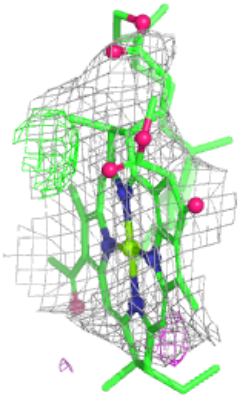


Electron density around BCL D 102:

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

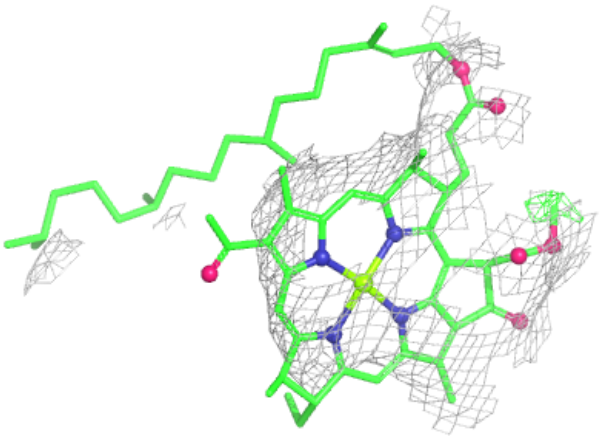


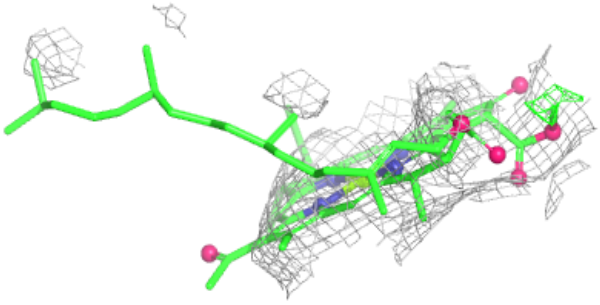




Electron density around BCL AC 103:

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

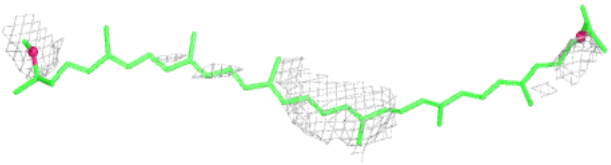


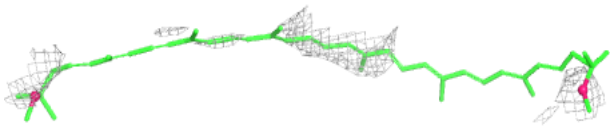


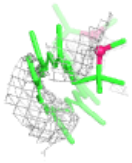


Electron density around CRT O 101:

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

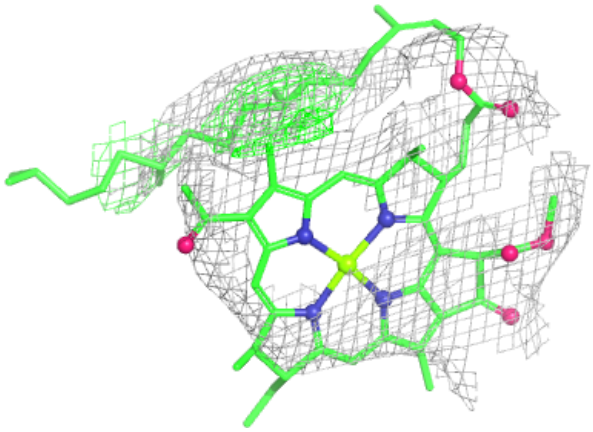


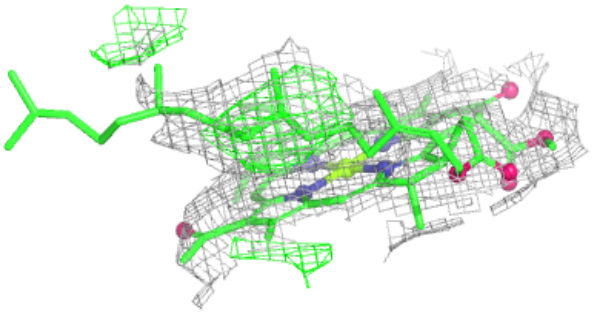


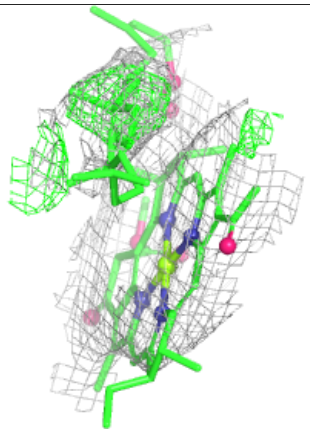


Electron density around BCL AG 101:

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

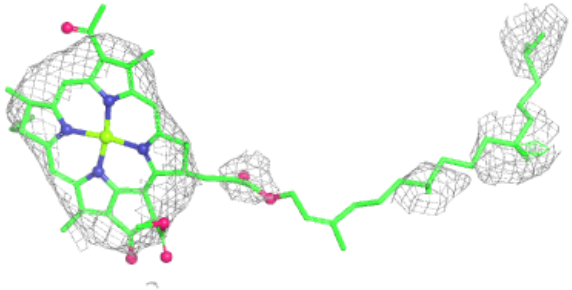


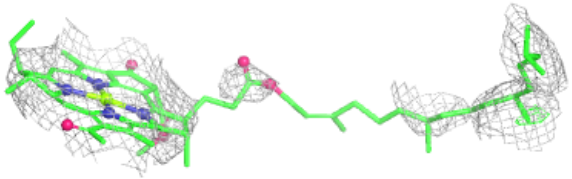


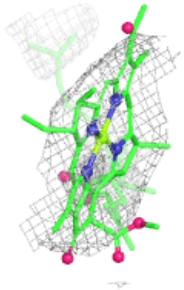


Electron density around BCL d 101:

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

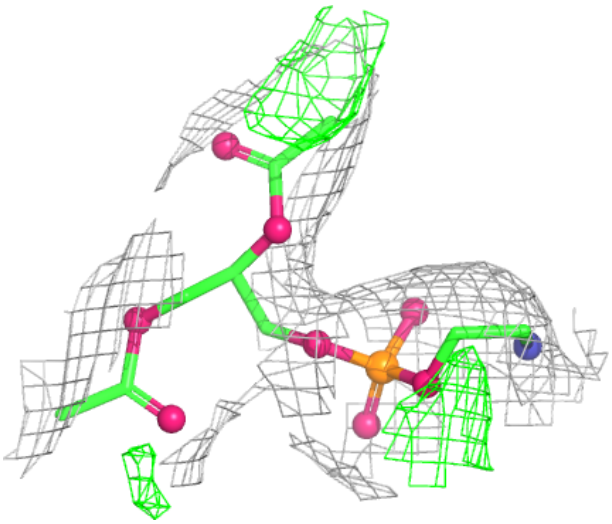


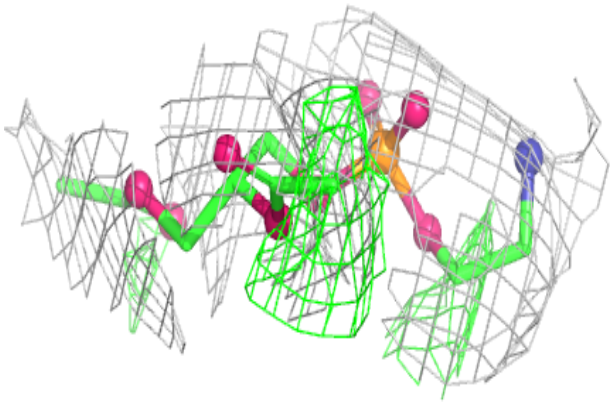




Electron density around PEF H 302:

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

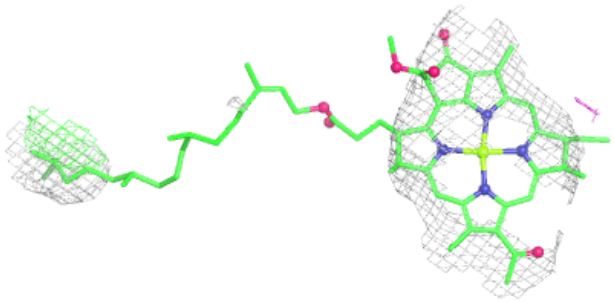


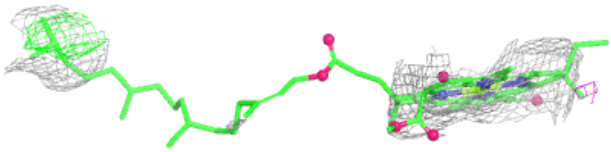


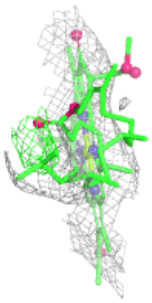


Electron density around BCL p 102:

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

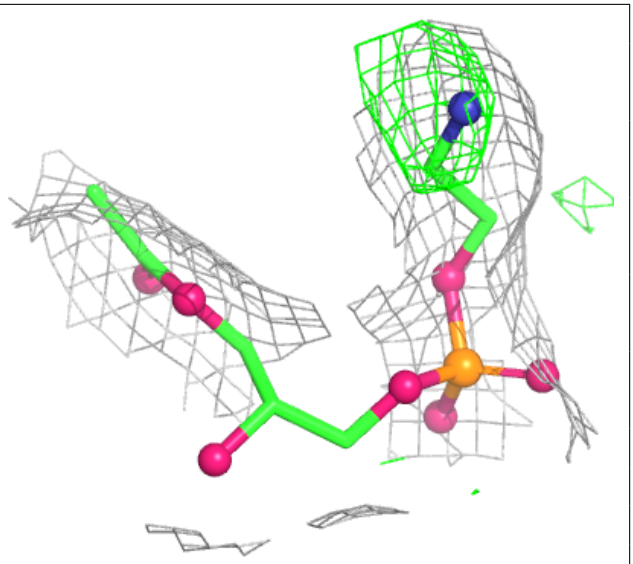


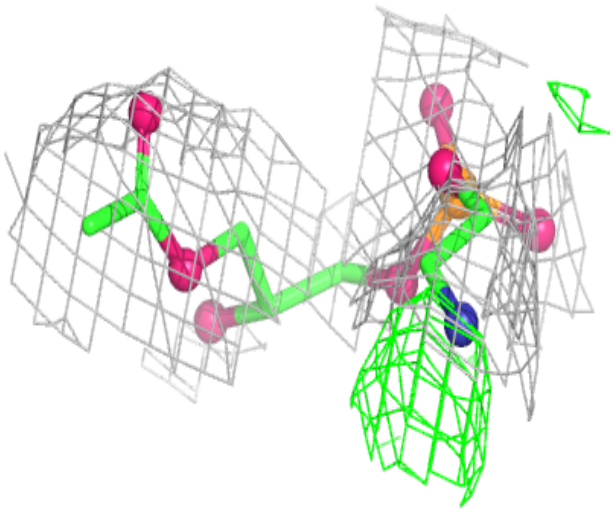


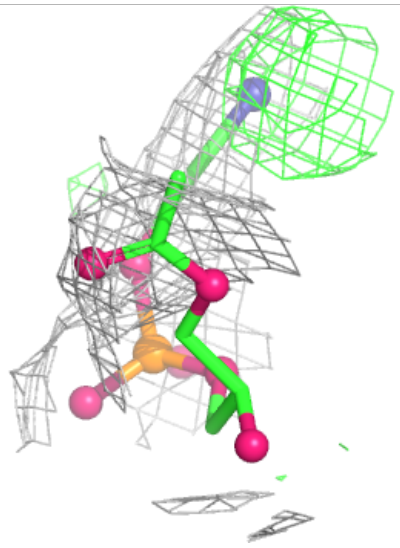


Electron density around PEF p 101:

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

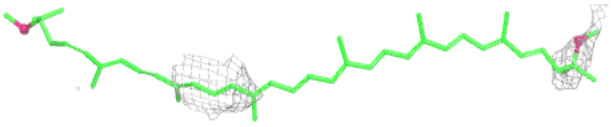


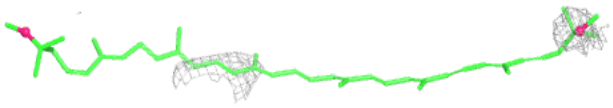


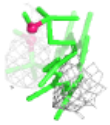


Electron density around CRT I 102:

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

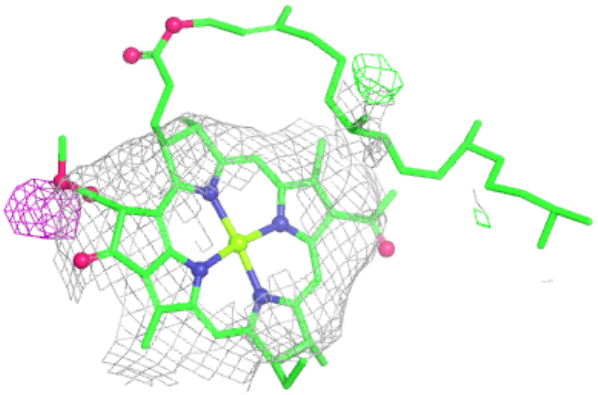


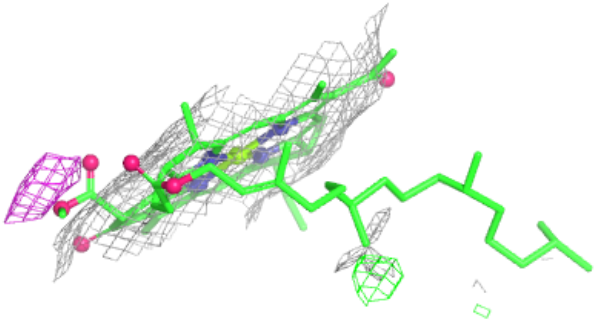


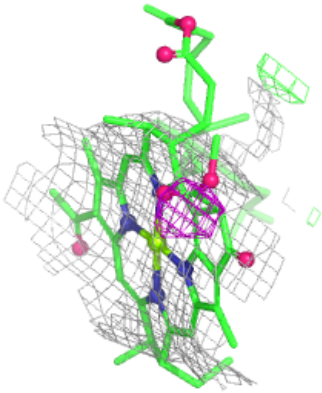


Electron density around BCL u 102:

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

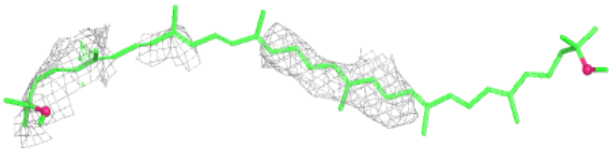


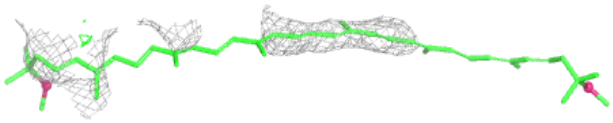




Electron density around CRT e 101:

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

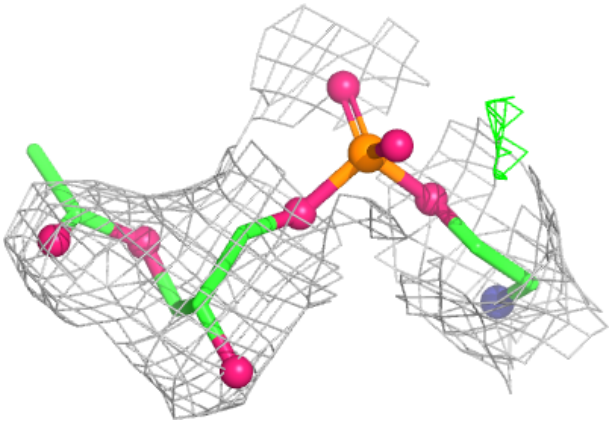


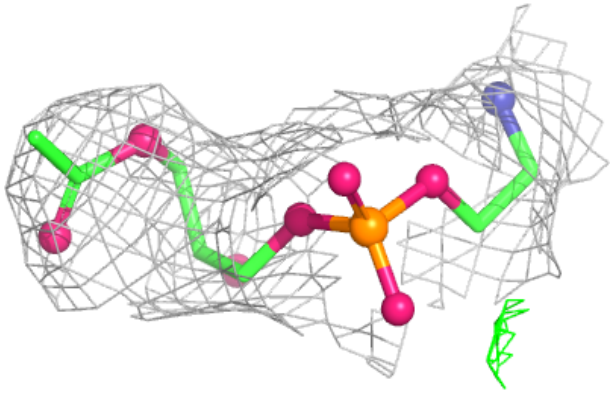


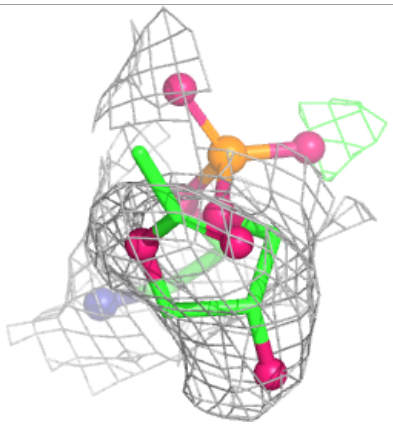


Electron density around PEF M 407:

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

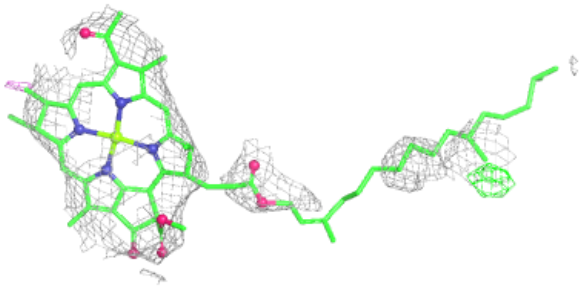


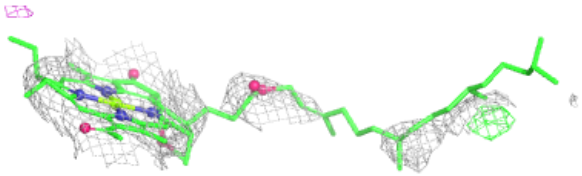


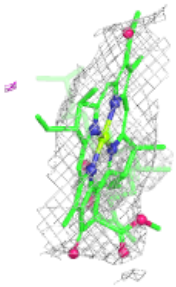


Electron density around BCL 1 101:

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

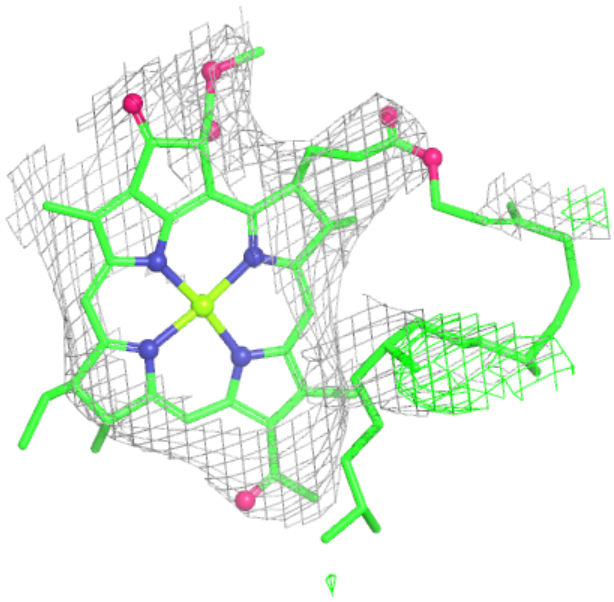


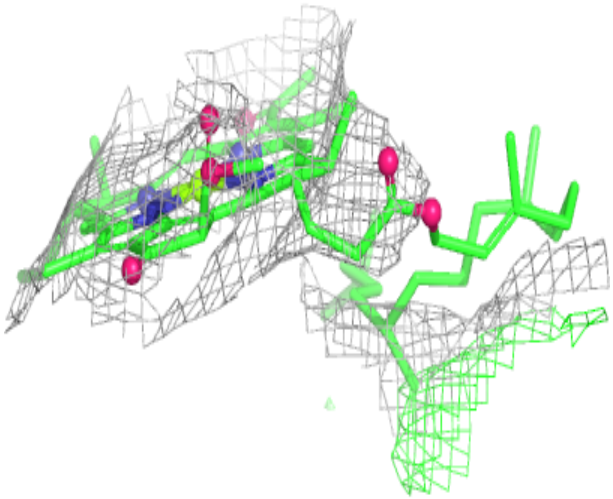


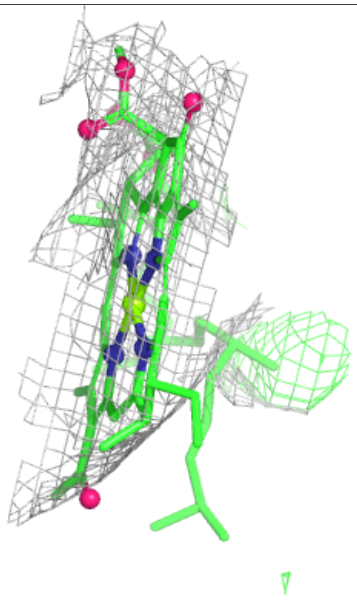


Electron density around BCL m 103:

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

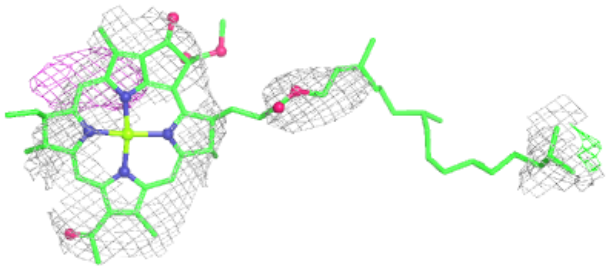


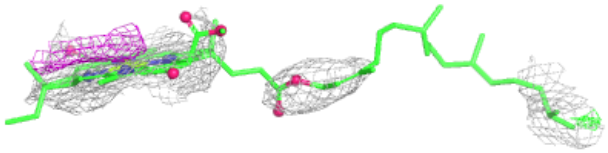


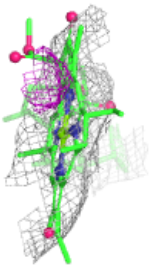


Electron density around BCL D 101:

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

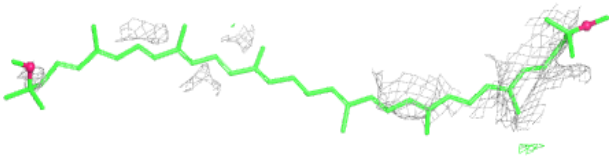


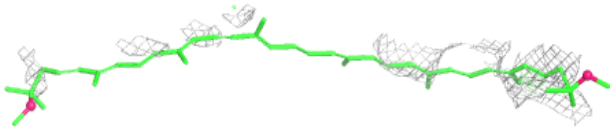


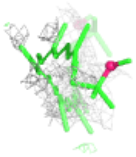


Electron density around CRT AH 102:

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

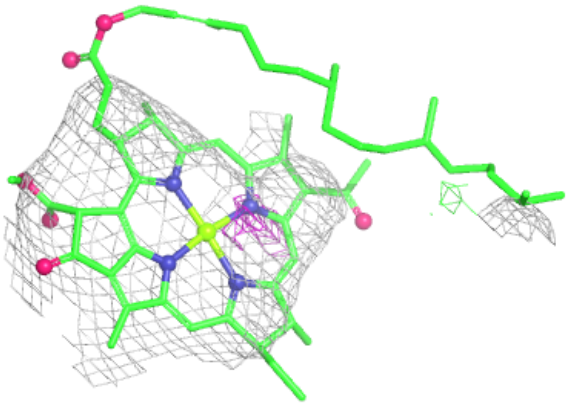


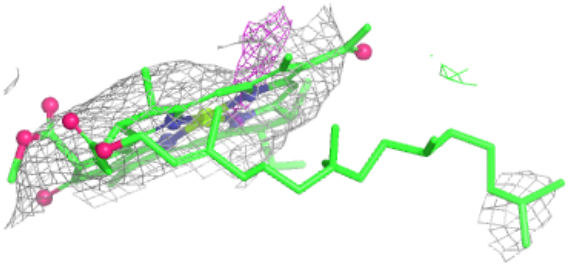


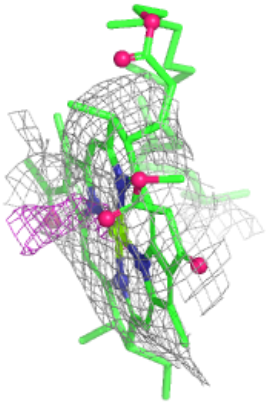


Electron density around BCL AB 102:

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

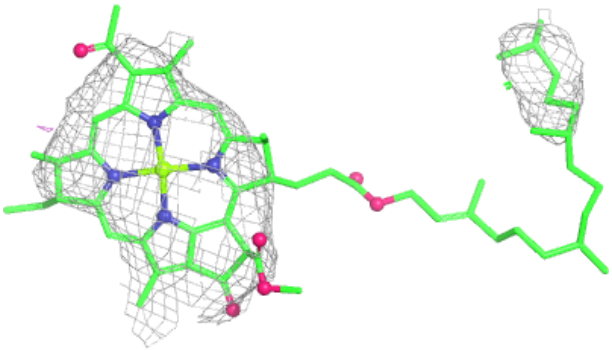


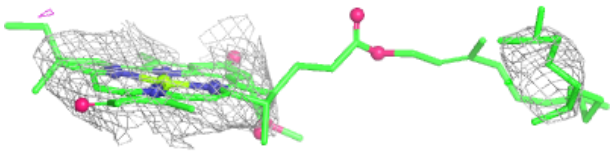


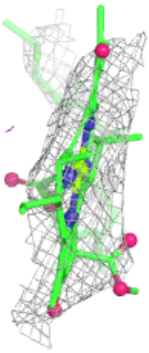


Electron density around BCL f 101:

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

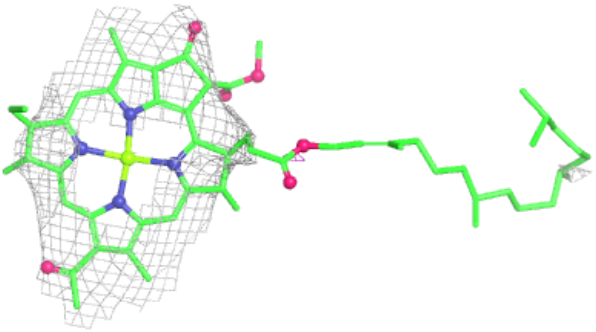


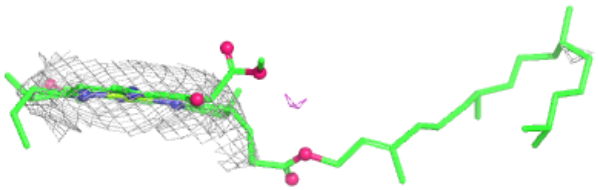


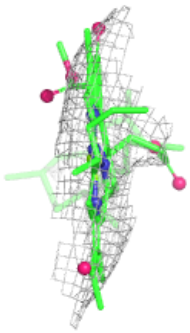


Electron density around BCL w 101:

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

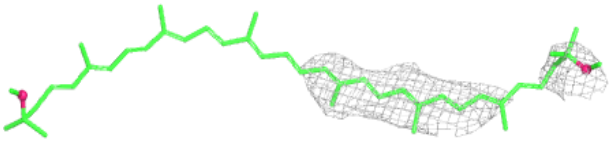


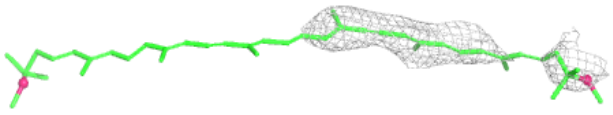




Electron density around CRT i 101:

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

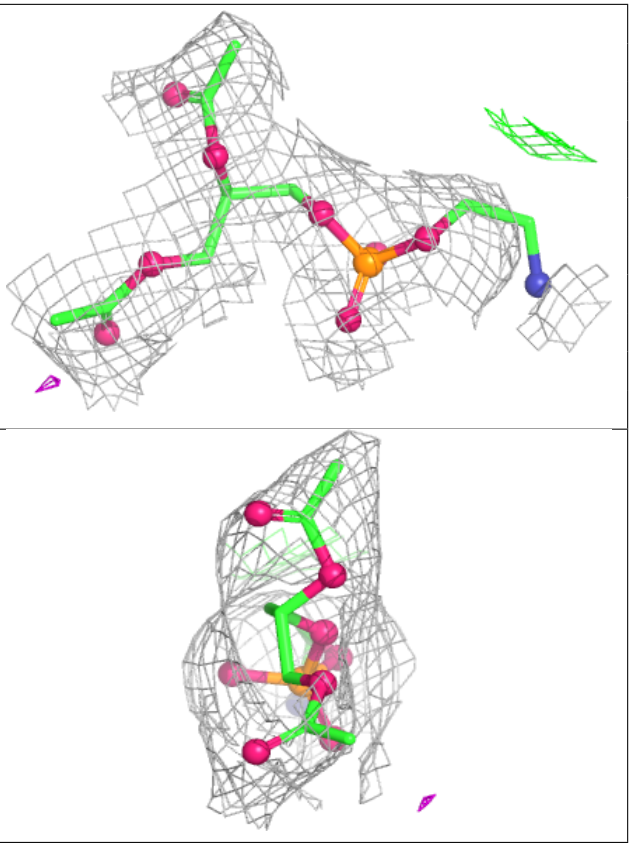


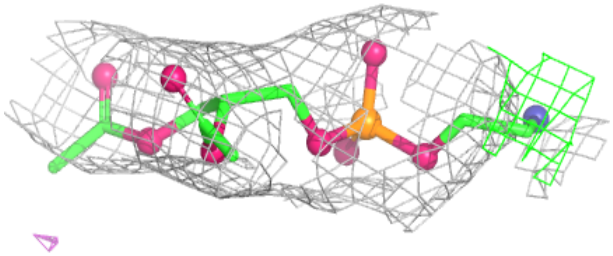




Electron density around PEF t 303:

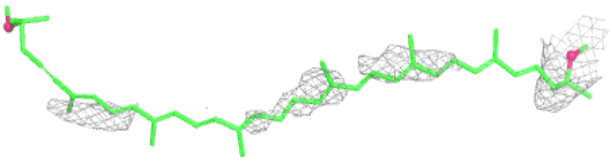
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

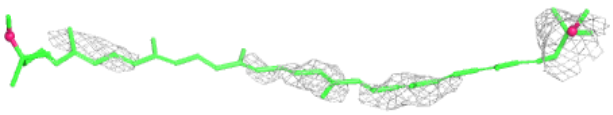




Electron density around CRT 0 101:

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

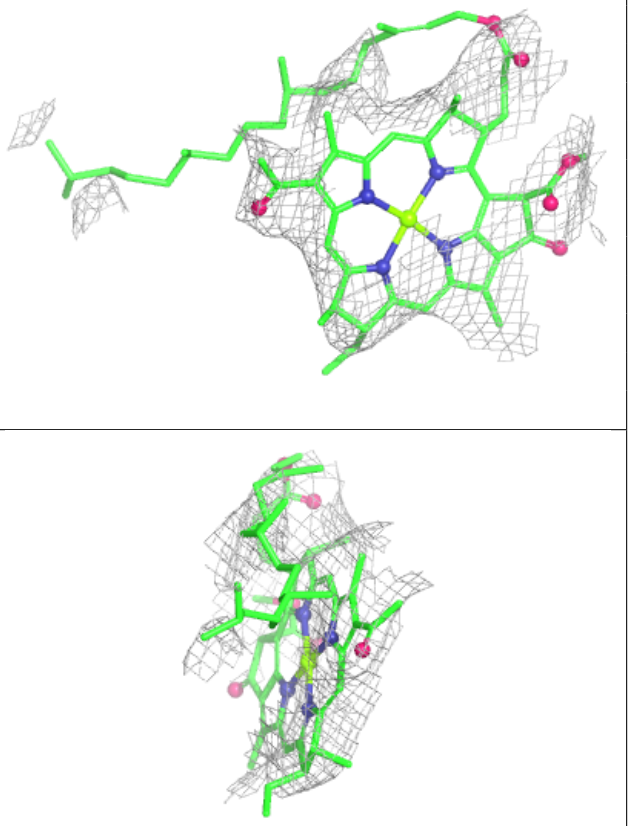


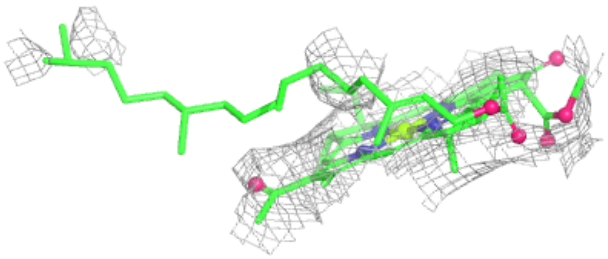




Electron density around BCL AE 102:

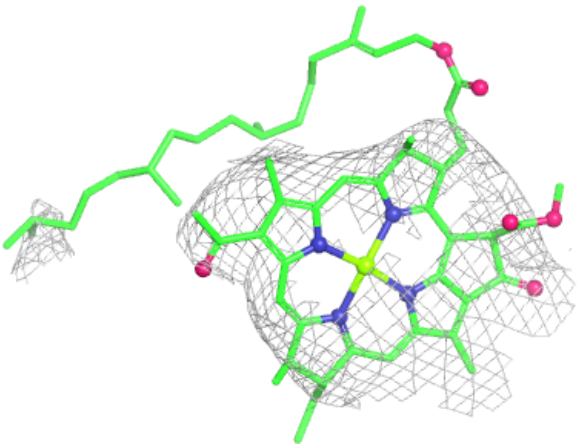
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

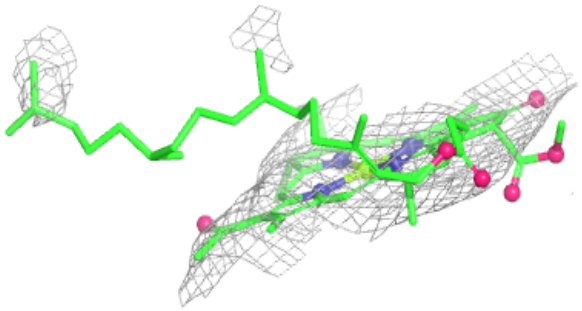


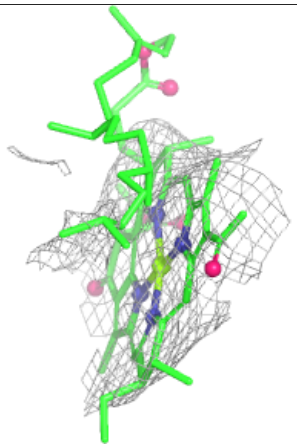


Electron density around BCL z 102:

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

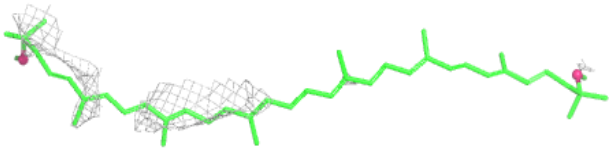


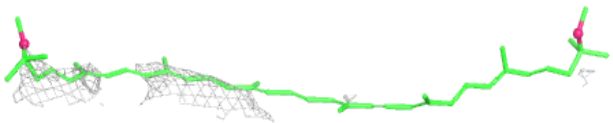


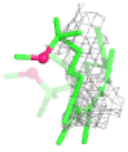


Electron density around CRT G 101:

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

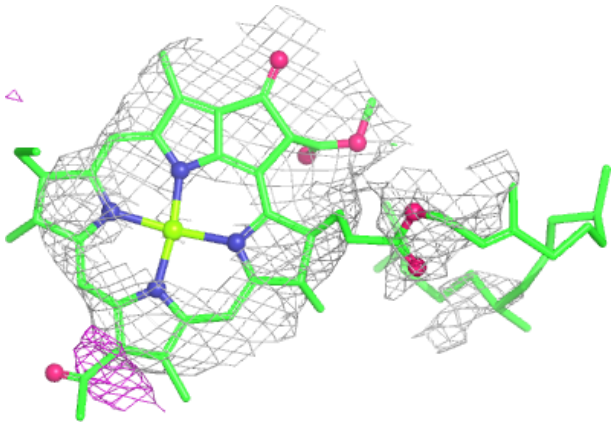


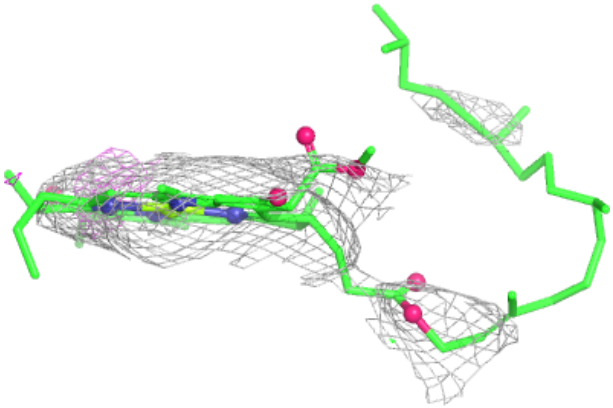


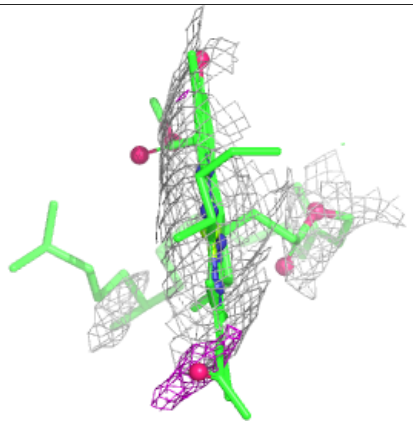


Electron density around BCL AC 102:

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

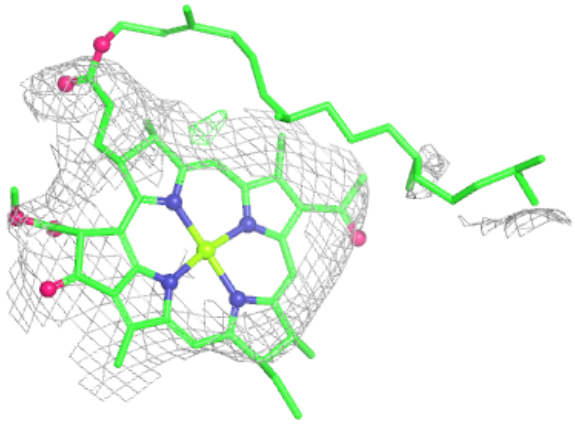


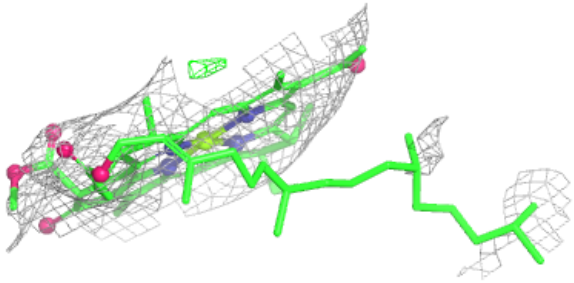


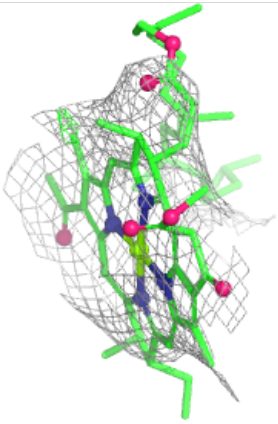


Electron density around BCL N 101:

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

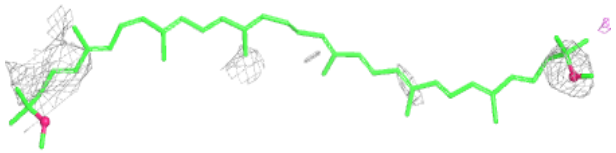


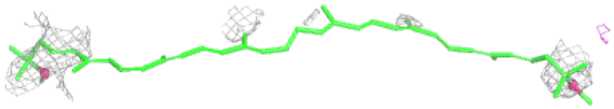


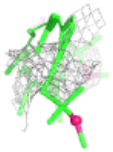


Electron density around CRT AJ 101:

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

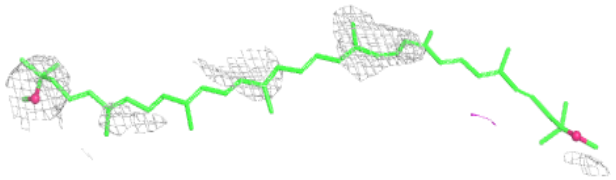


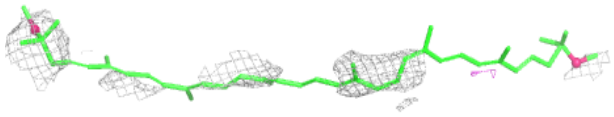


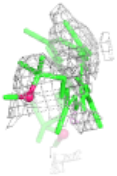


Electron density around CRT R 101:

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

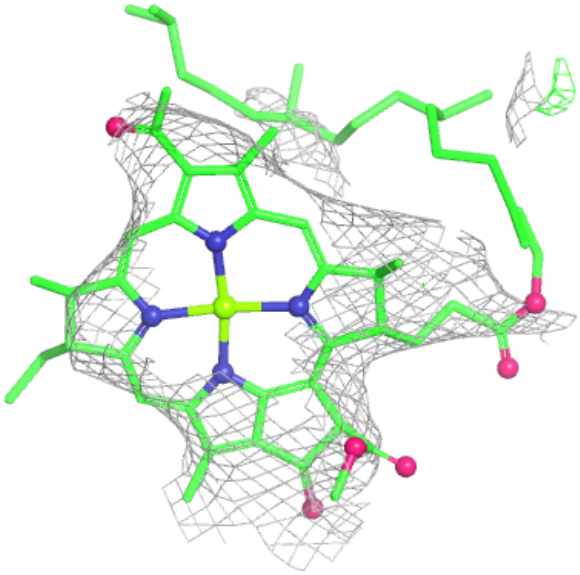


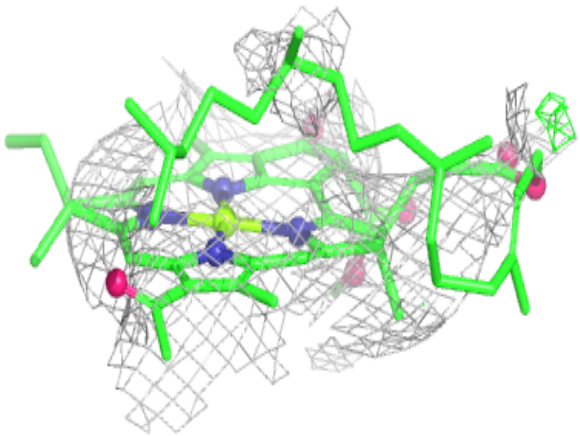


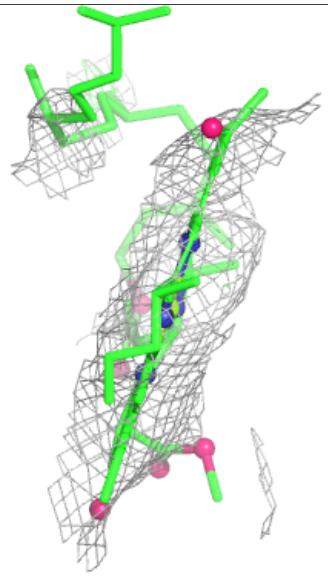


Electron density around BCL k 102:

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

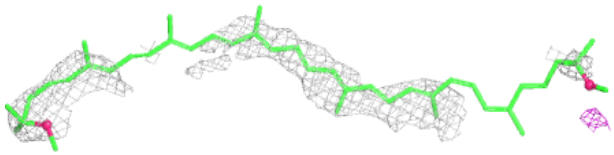


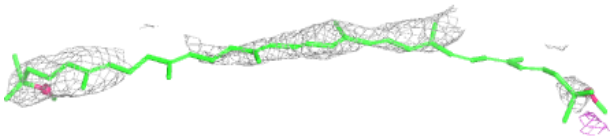


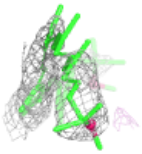


Electron density around CRT 4 101:

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

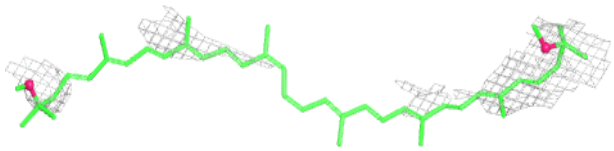


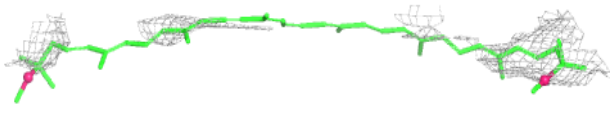




Electron density around CRT k 101:

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

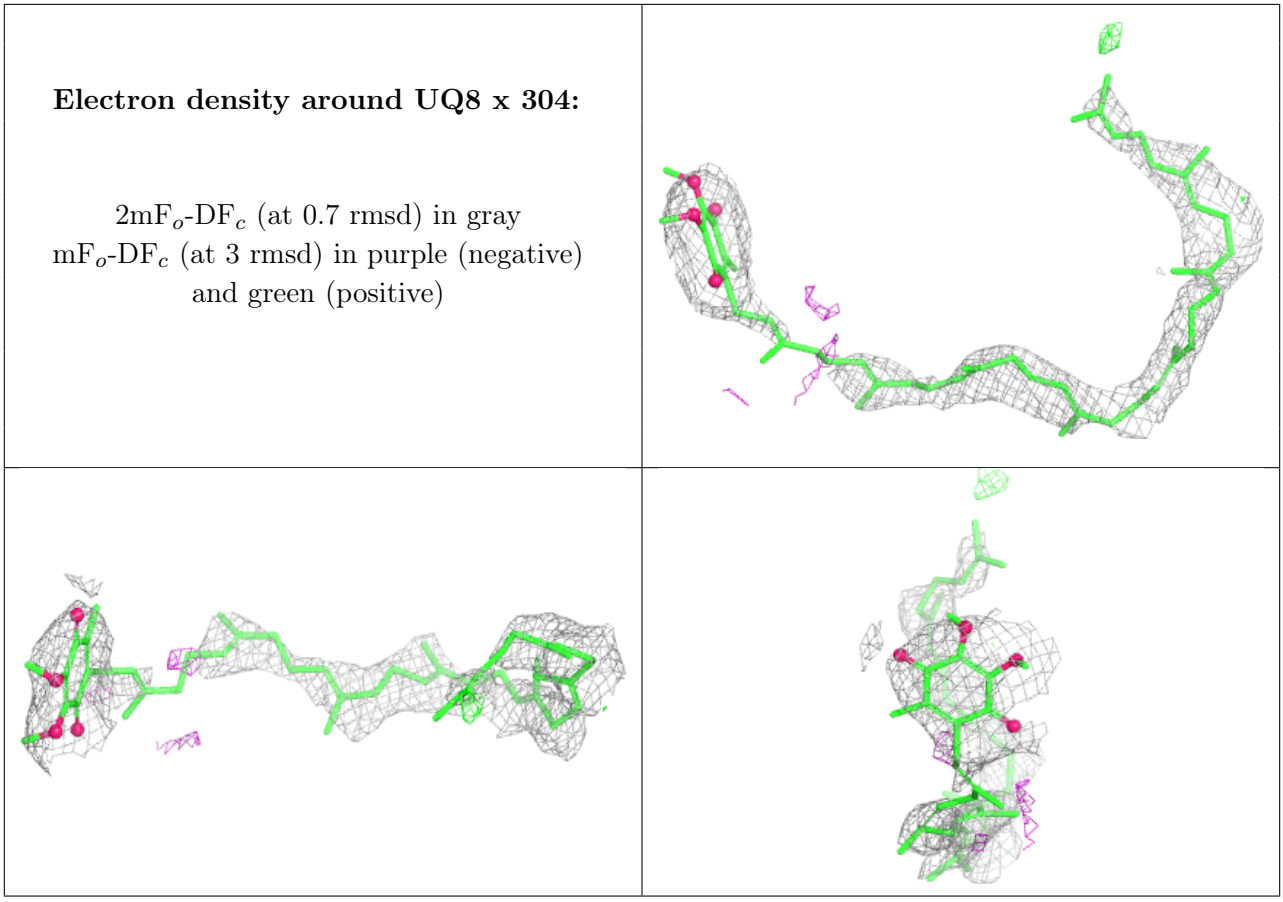






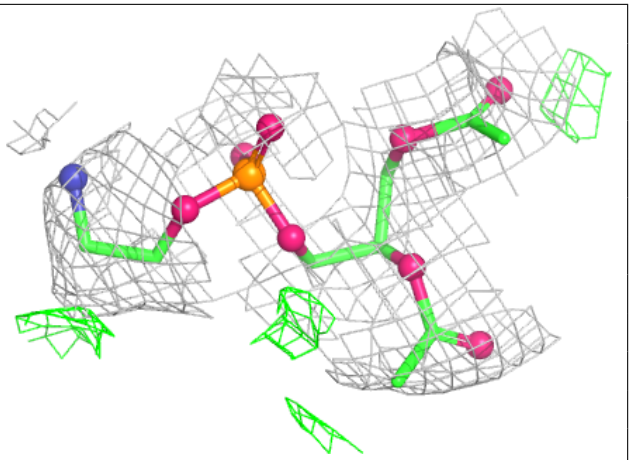
Electron density around UQ8 x 304:

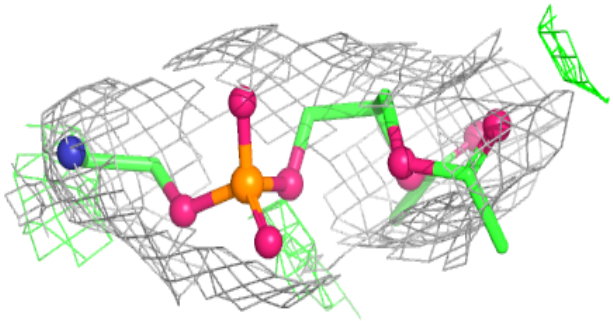
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

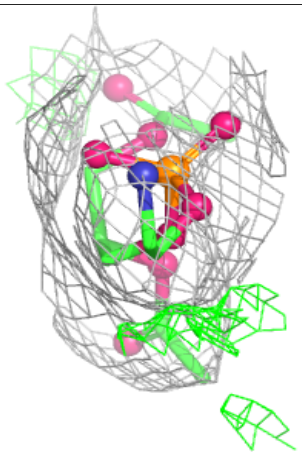


Electron density around PEF H 305:

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

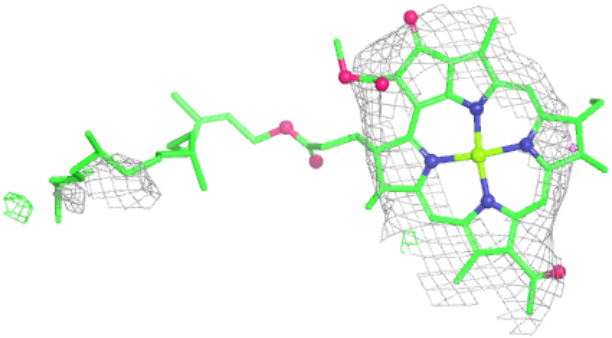


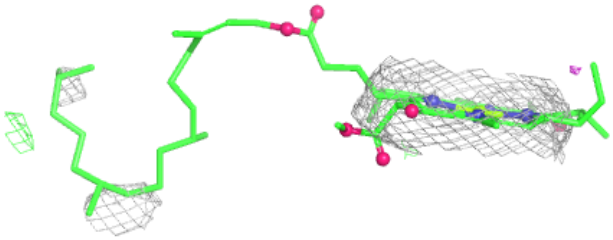


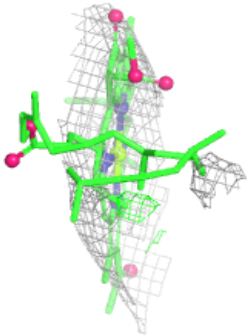


Electron density around BCL P 101:

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

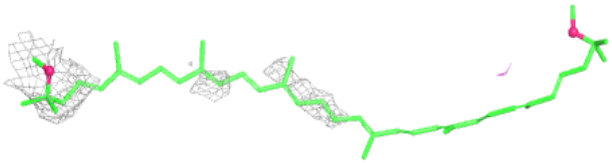


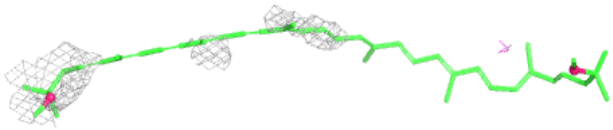


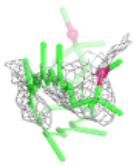


Electron density around CRT n 101:

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

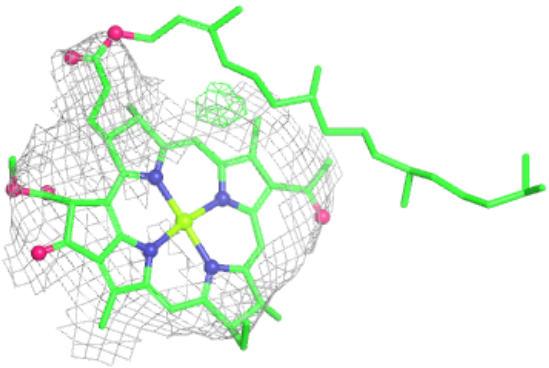


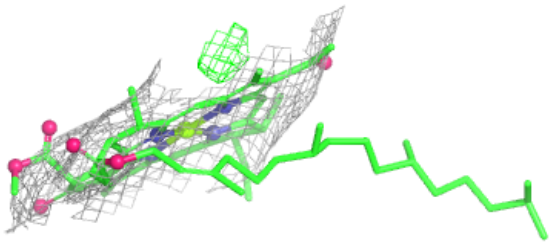


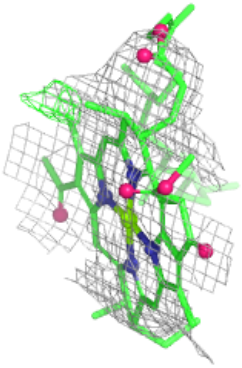


Electron density around BCL G 102:

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

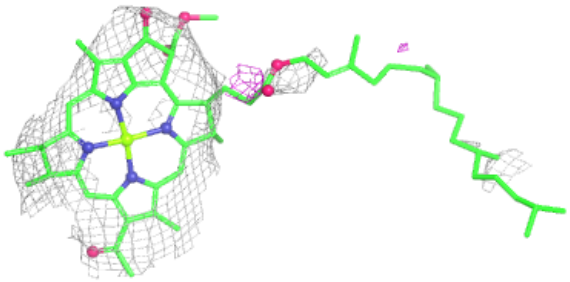


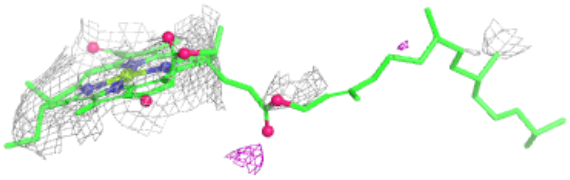


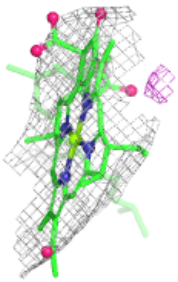


Electron density around BCL u 101:

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

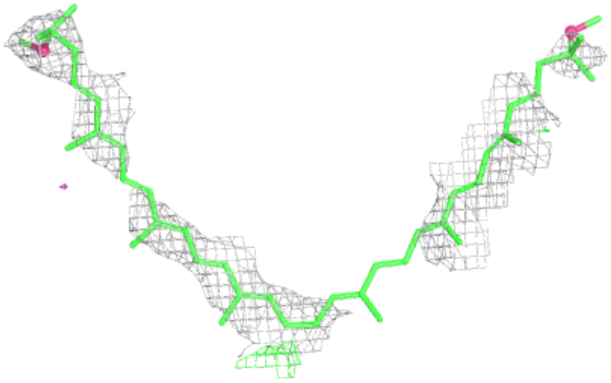


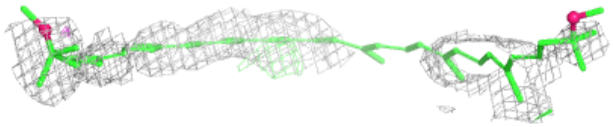


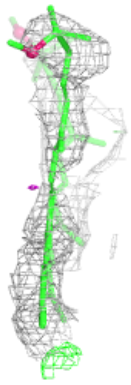


Electron density around CRT M 405:

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

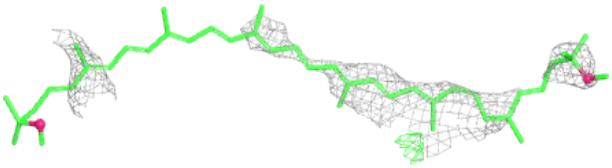


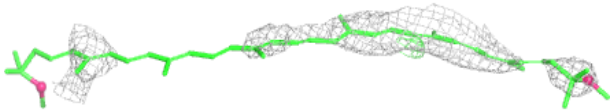




Electron density around CRT g 101:

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

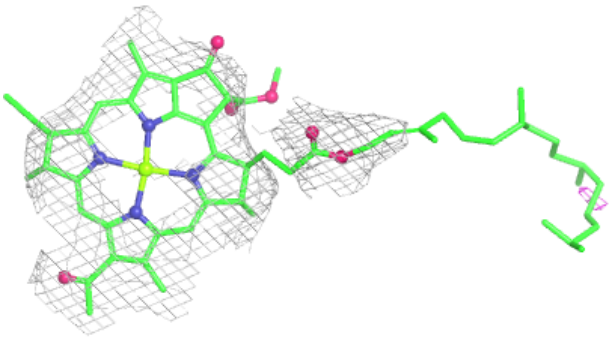


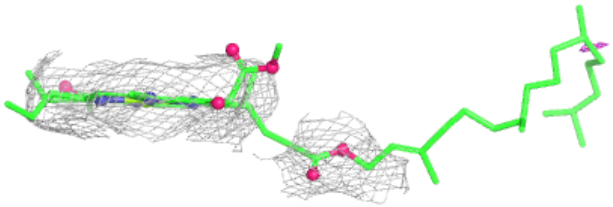


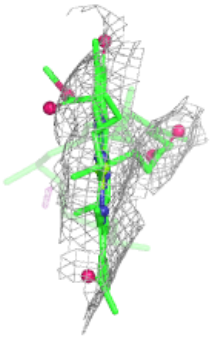


Electron density around BCL m 102:

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

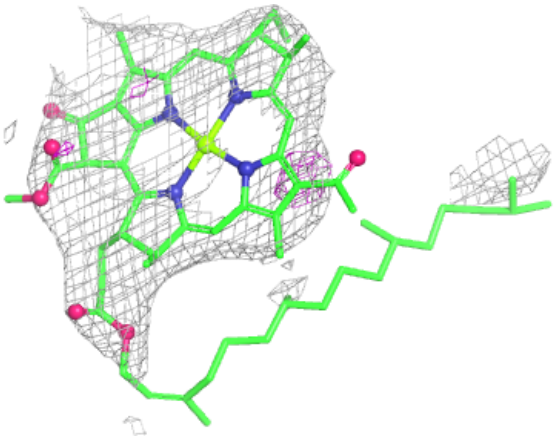


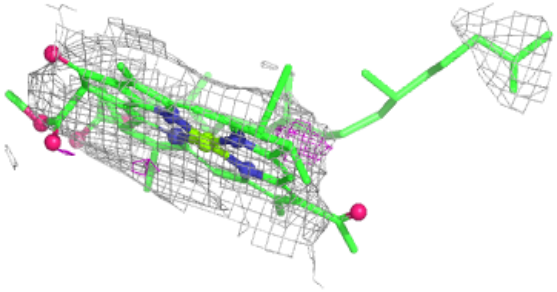


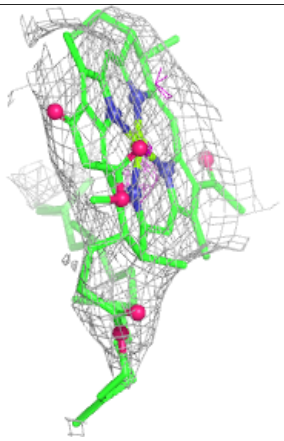


Electron density around BCL V 102:

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

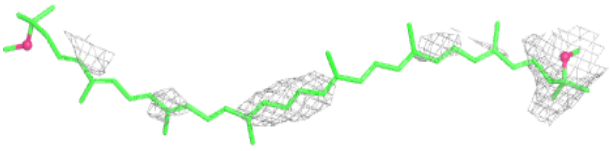


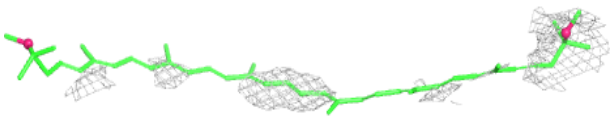


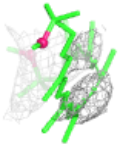


Electron density around CRT q 101:

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

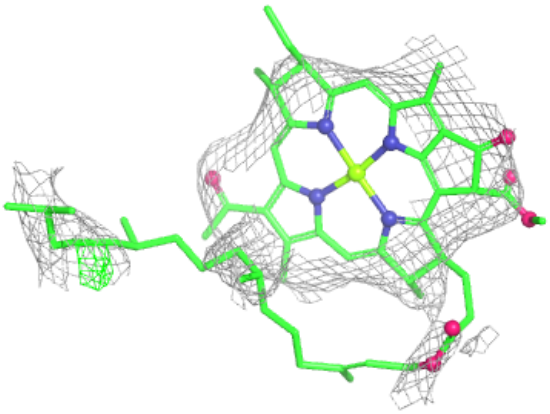


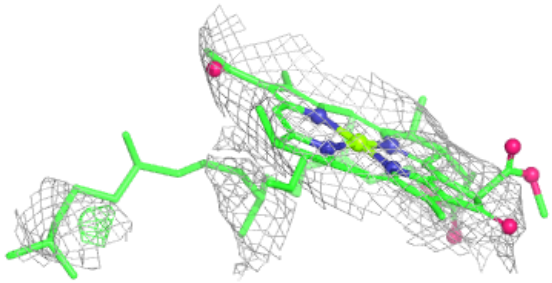


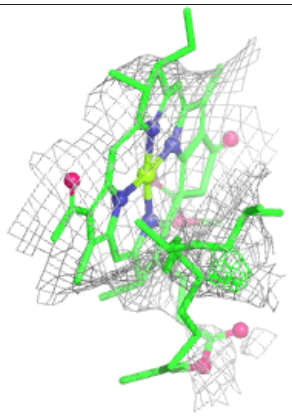


Electron density around BCL g 102:

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

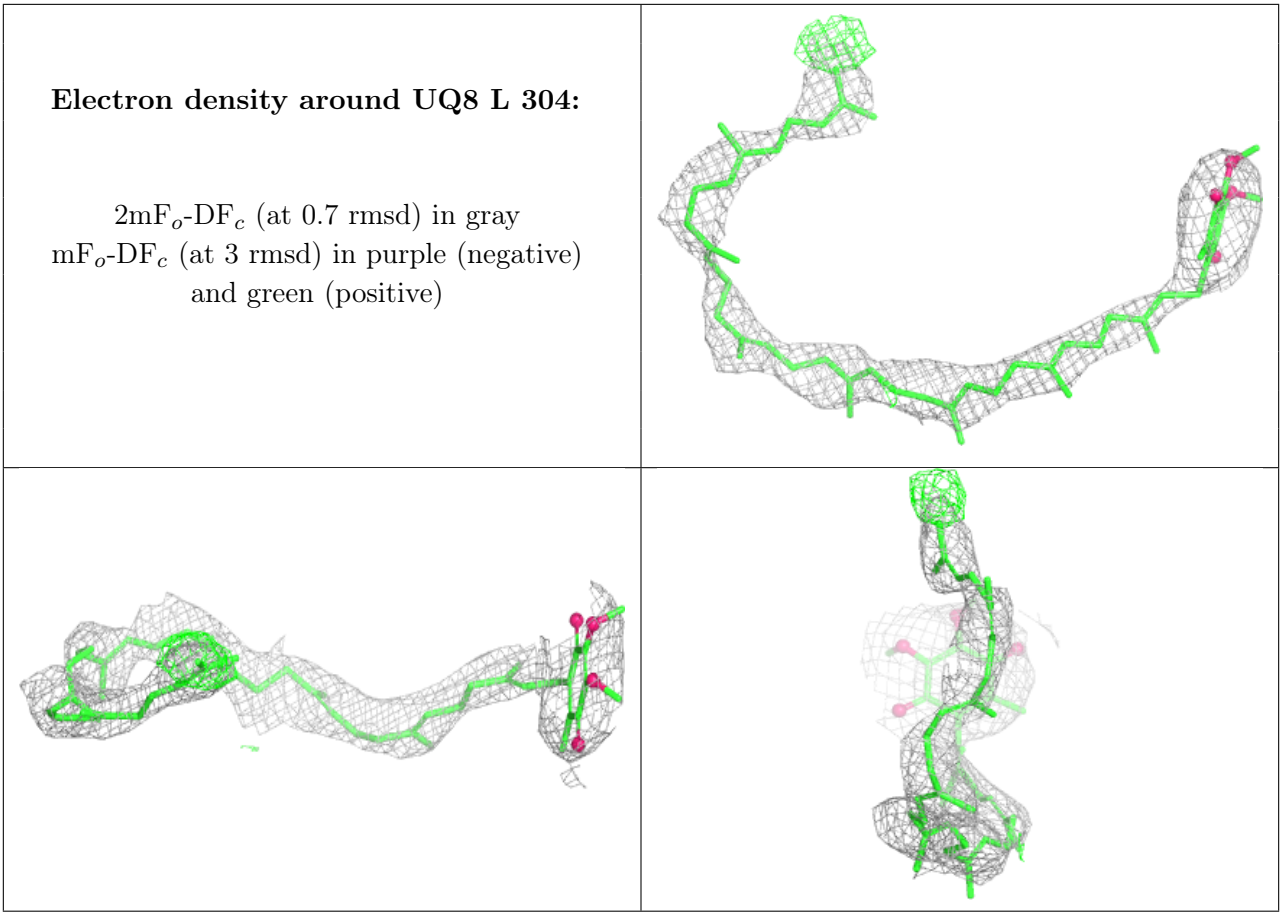






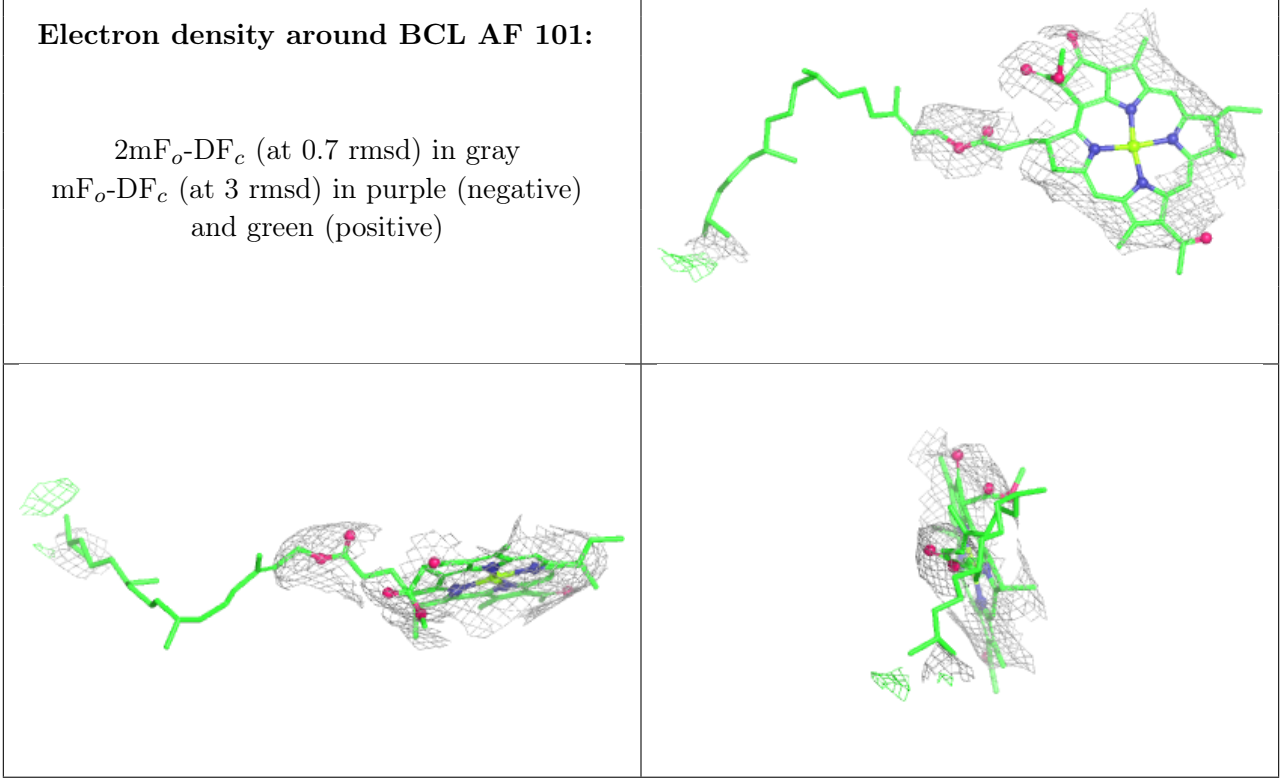
Electron density around UQ8 L 304:

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



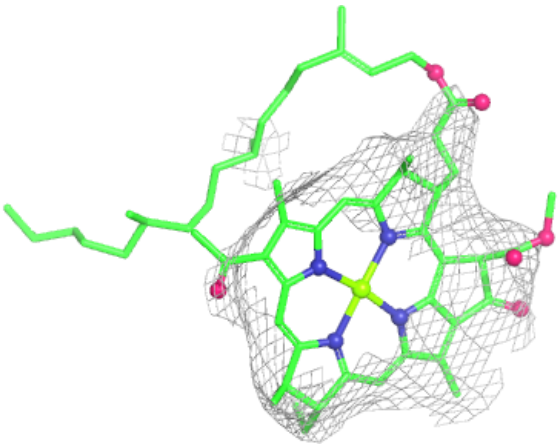
Electron density around BCL AF 101:

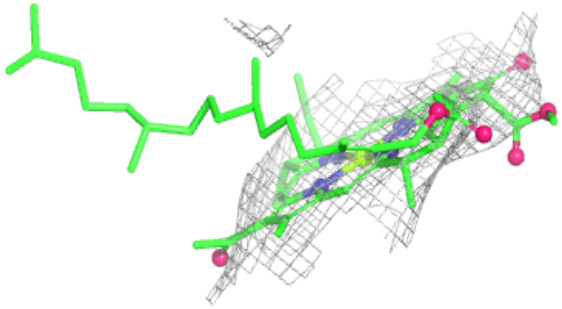
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

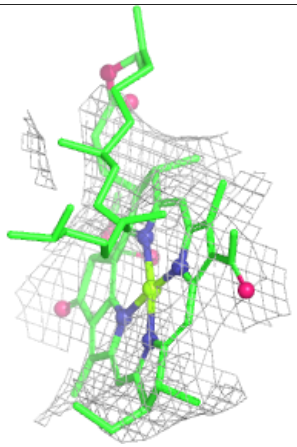


Electron density around BCL c 101:

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

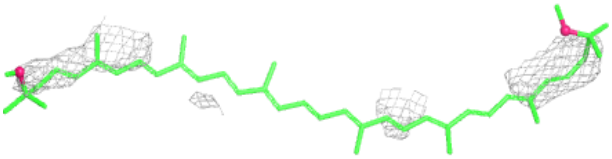


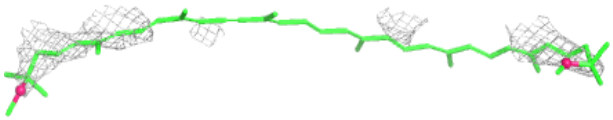


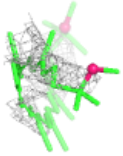


Electron density around CRT AF 102:

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

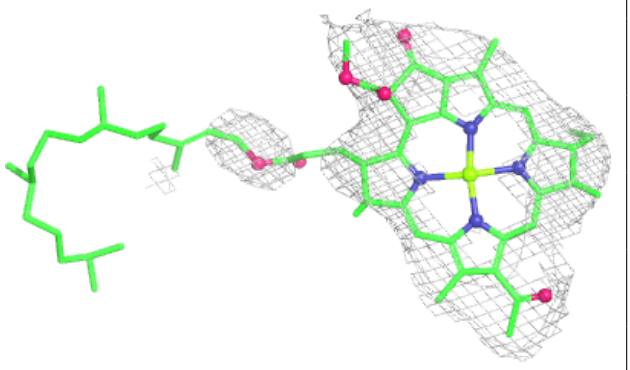


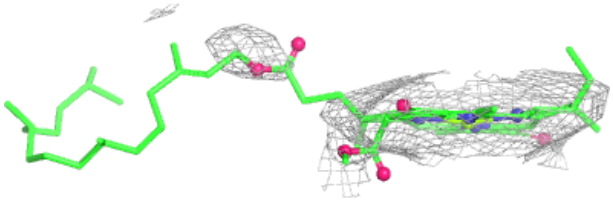


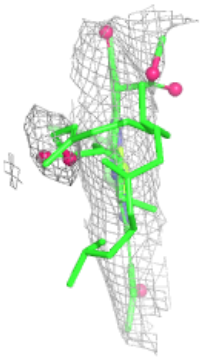


Electron density around BCL U 101:

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

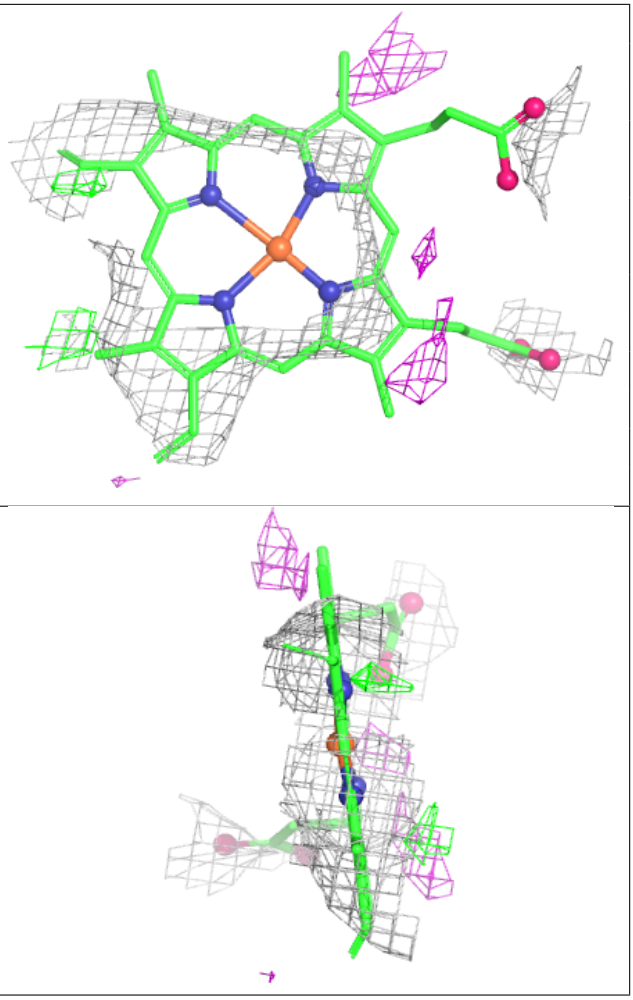






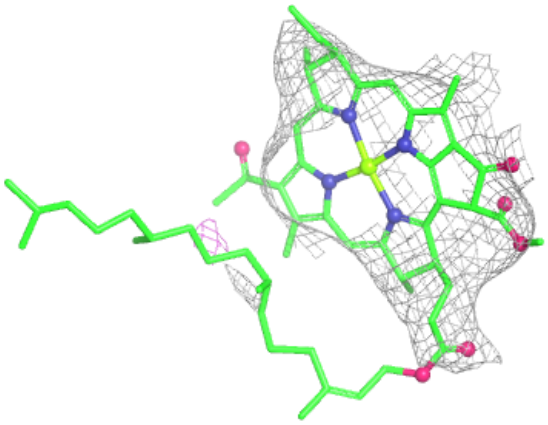
Electron density around HEM o 501:

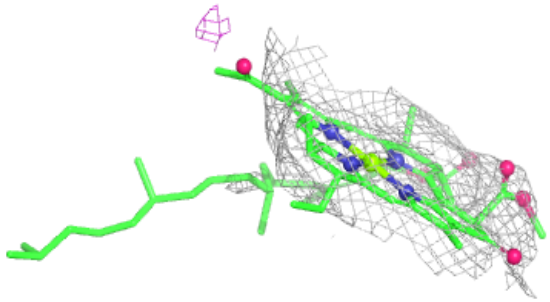
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

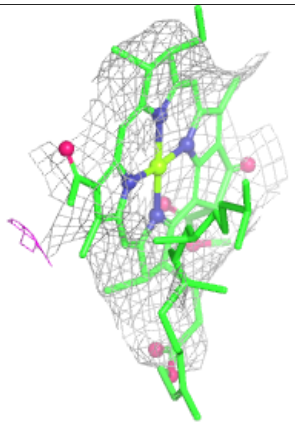


Electron density around BCL 2 102:

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

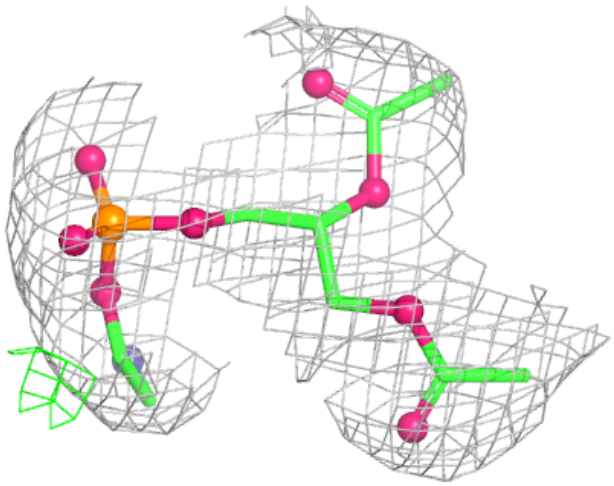


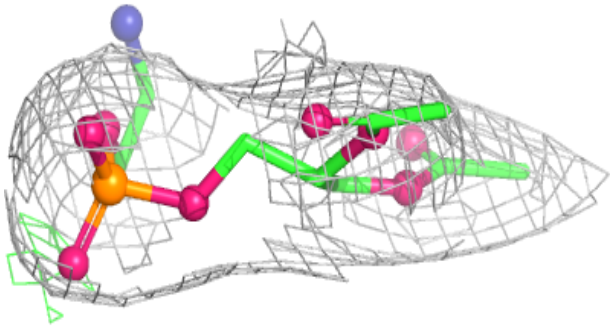


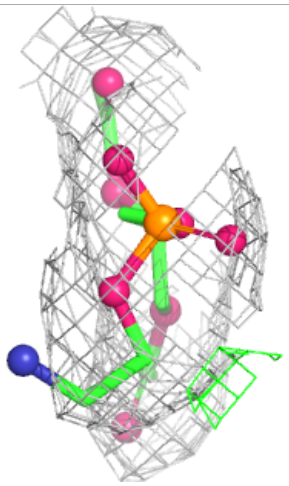


Electron density around PEF t 301:

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

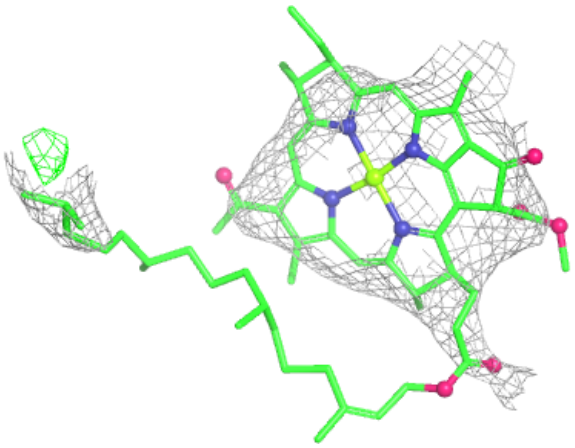


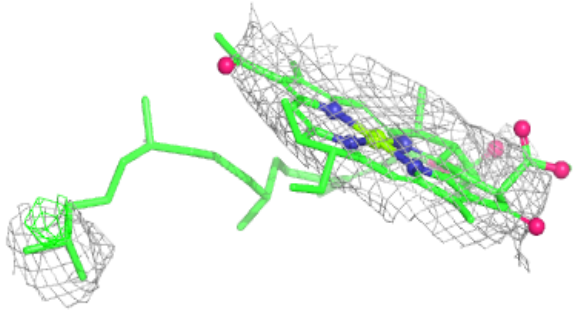




Electron density around BCL e 102:

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

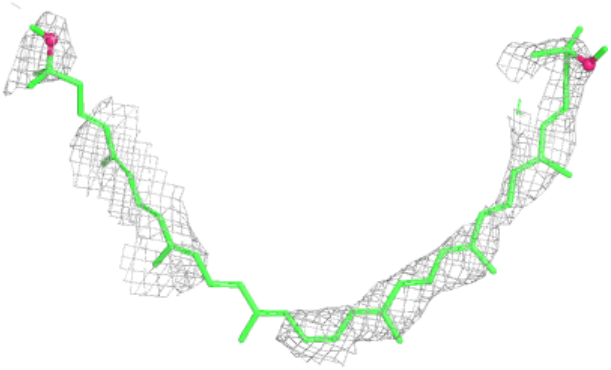


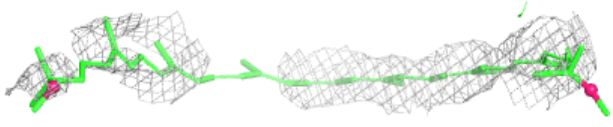




Electron density around CRT y 404:

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

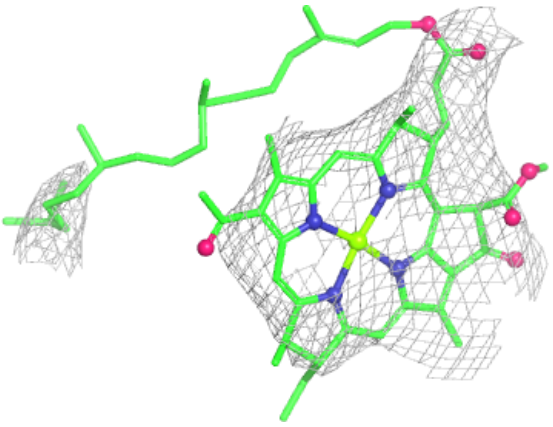


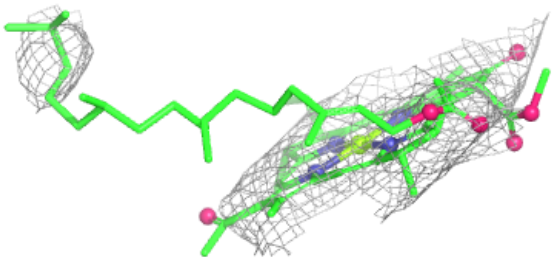




Electron density around BCL O 102:

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

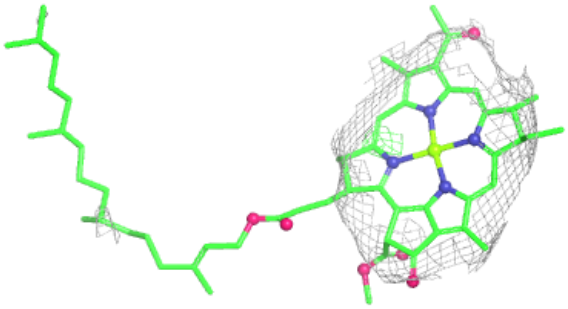


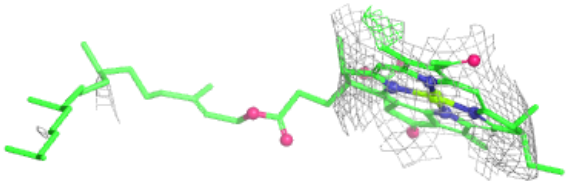


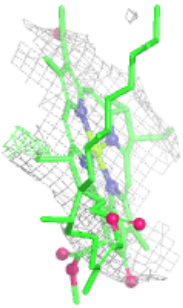


Electron density around BCL I 101:

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

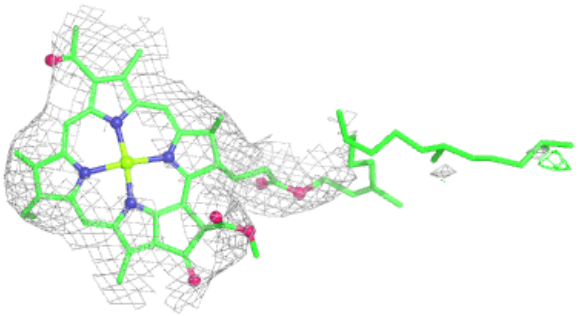


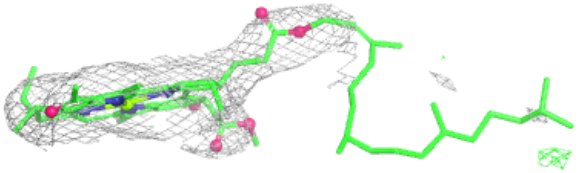


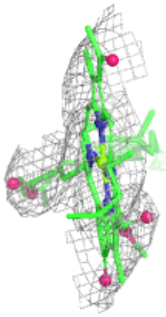


Electron density around BCL h 101:

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

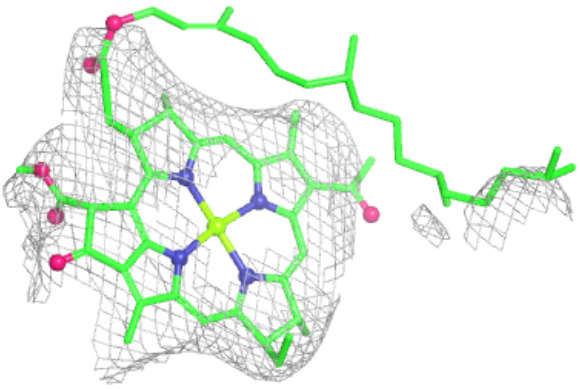


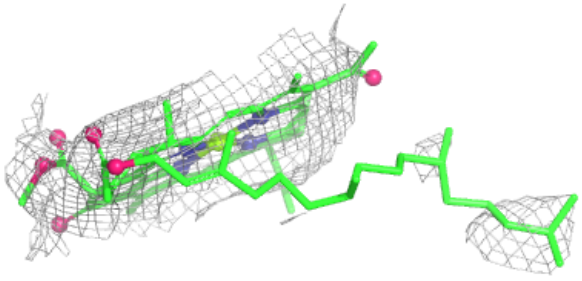


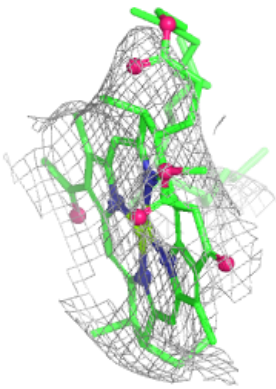


Electron density around BCL T 102:

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

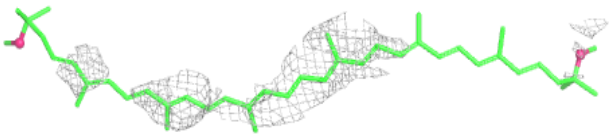


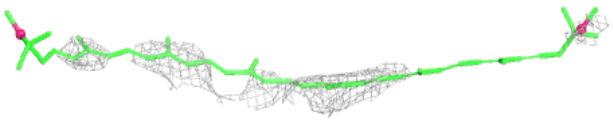


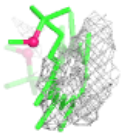


Electron density around CRT z 101:

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

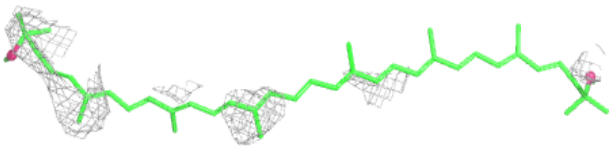


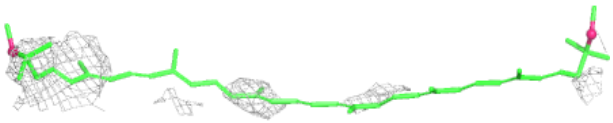


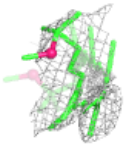


Electron density around CRT s 101:

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

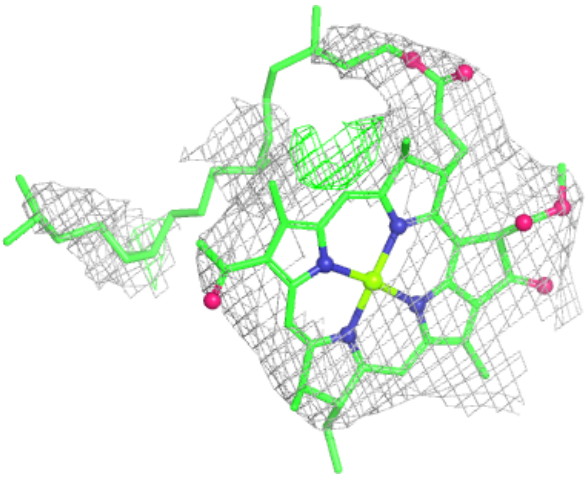


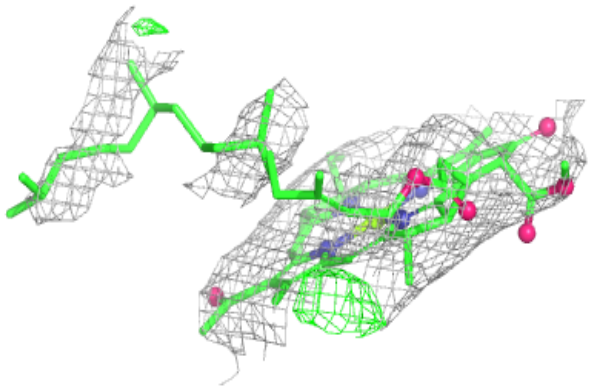


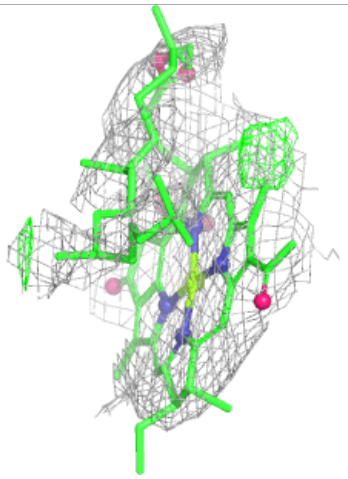


Electron density around BCL AI 102:

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

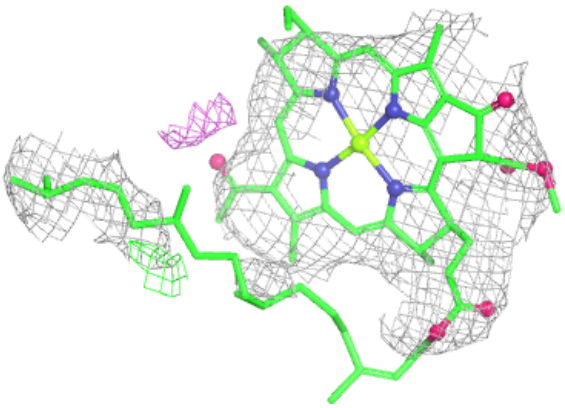


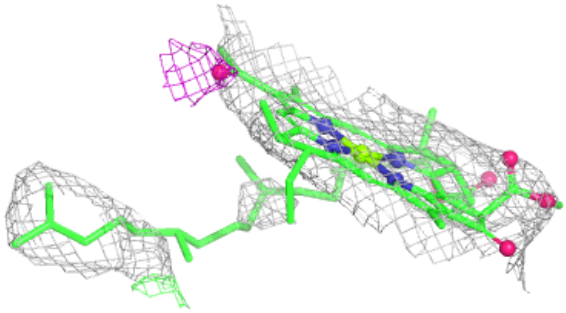


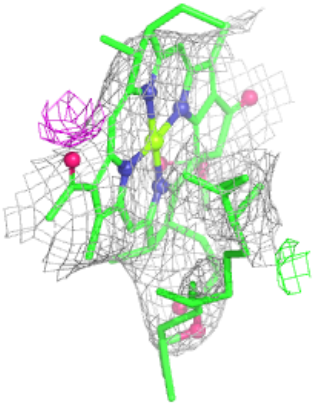


Electron density around BCL AL 102:

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

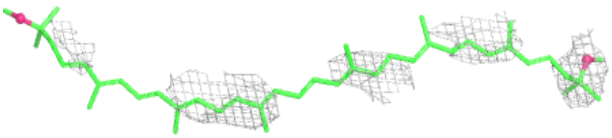






Electron density around CRT P 102:

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

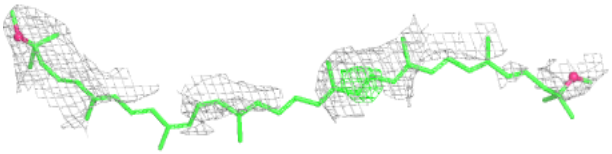


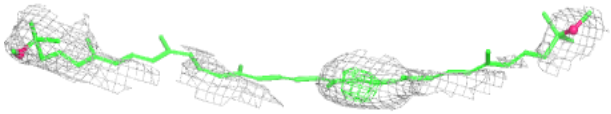


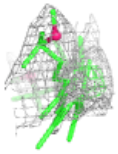


Electron density around CRT AD 101:

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

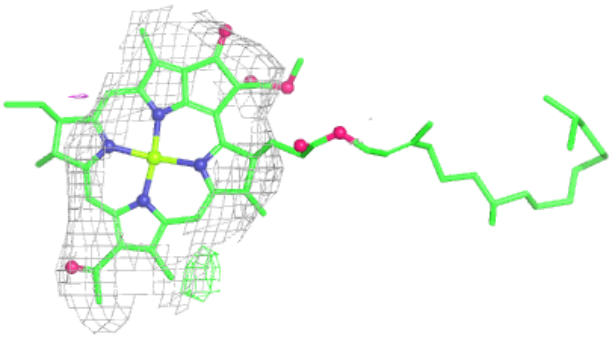


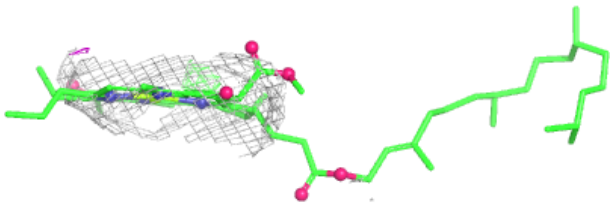


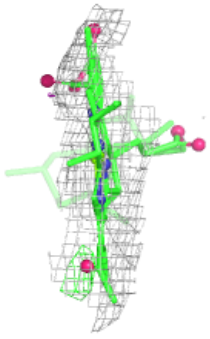


Electron density around BCL K 101:

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

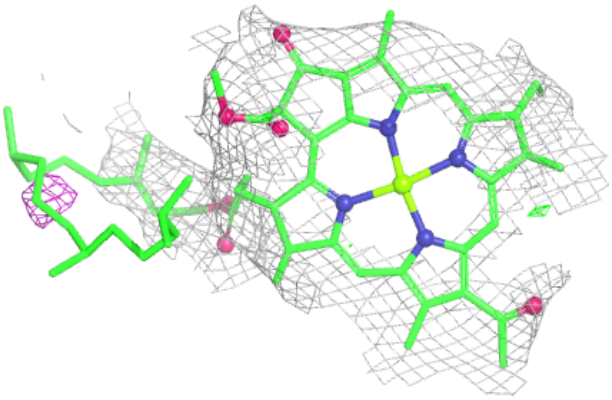


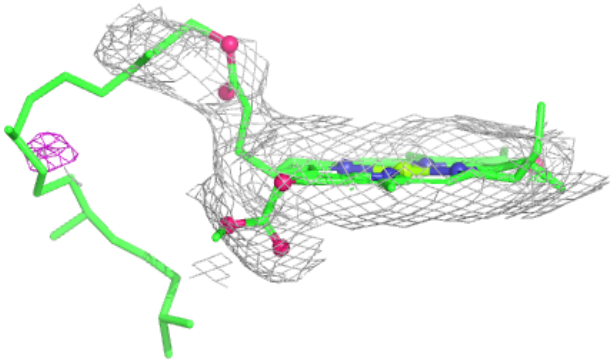


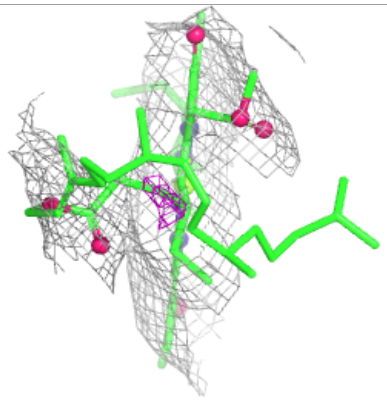


Electron density around BCL Q 101:

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

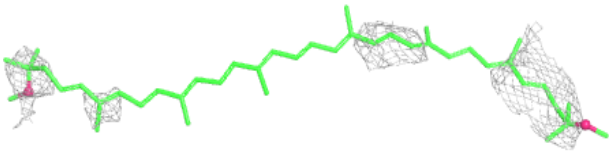


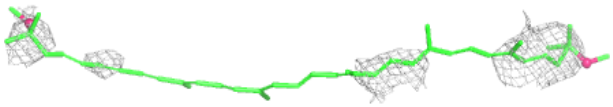


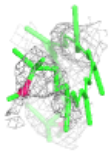


Electron density around CRT V 101:

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

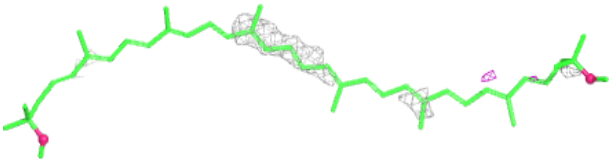


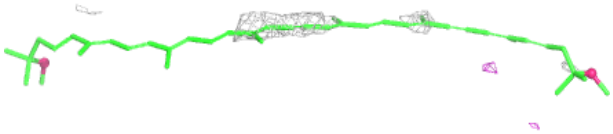




Electron density around CRT 2 101:

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

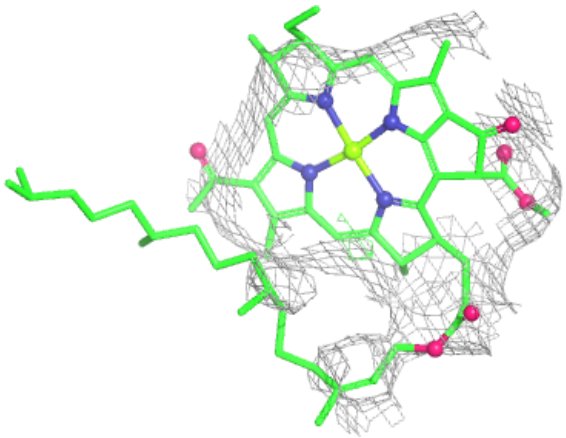


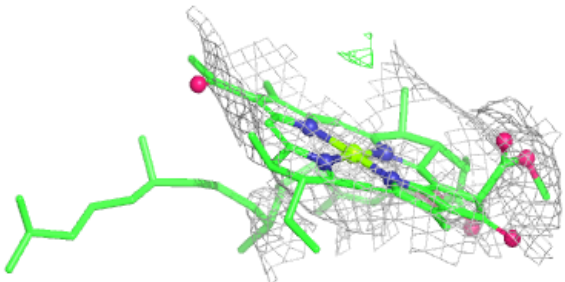




Electron density around BCL 6 101:

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

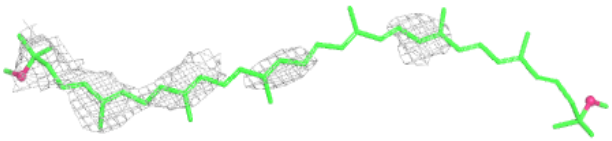


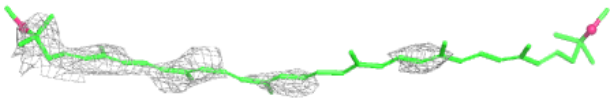


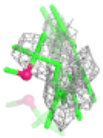


Electron density around CRT 7 101:

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

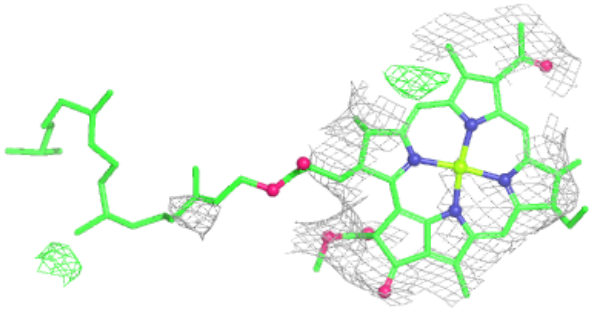


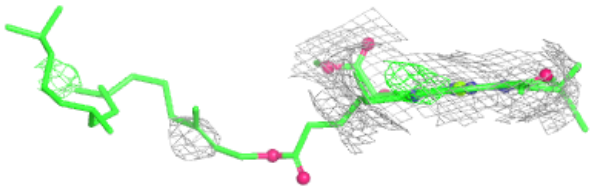


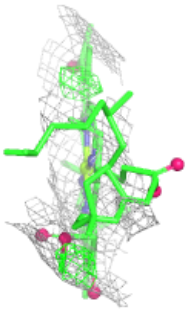


Electron density around BCL 7 102:

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

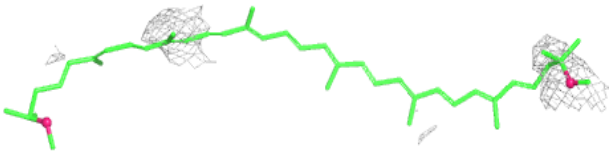


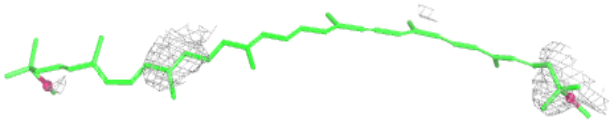




Electron density around CRT 9 101:

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

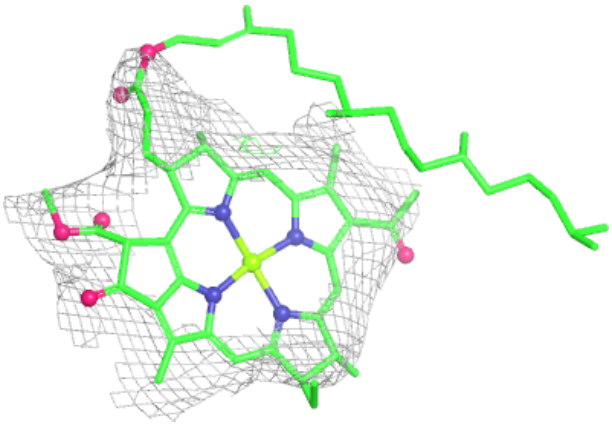


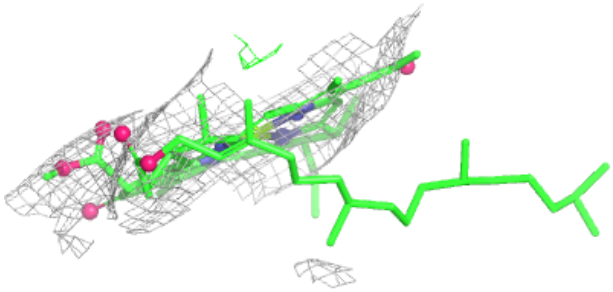


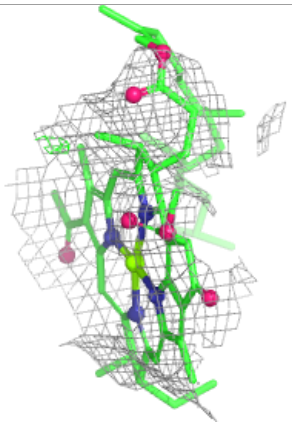


Electron density around BCL 0 102:

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

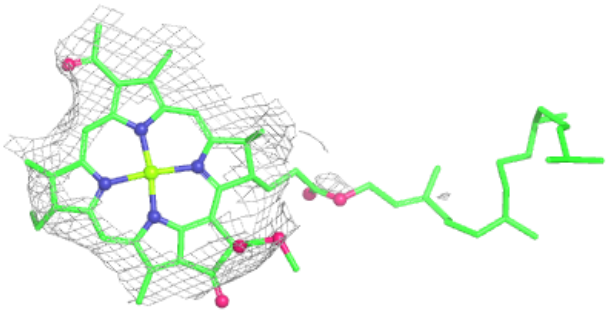


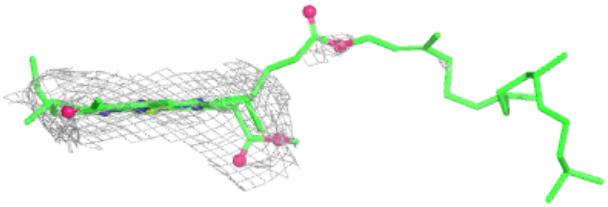




Electron density around BCL j 101:

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

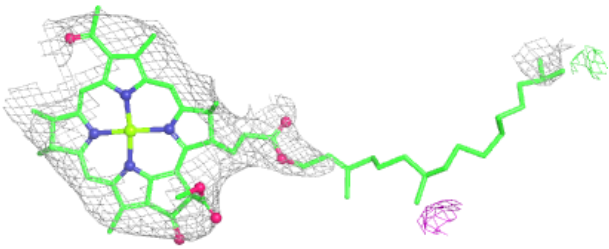


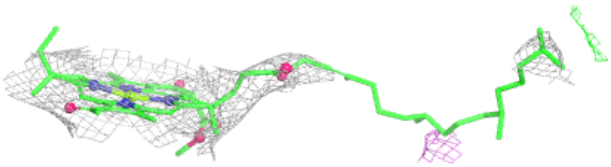




Electron density around BCL S 102:

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

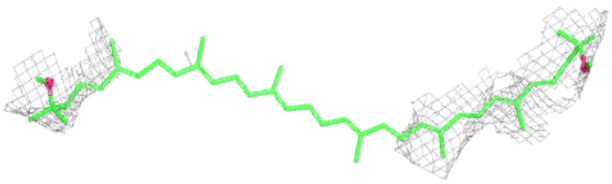


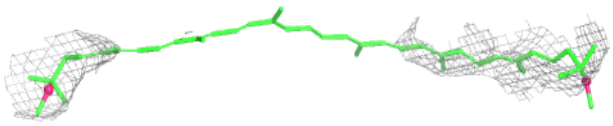


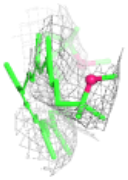


Electron density around CRT E 101:

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

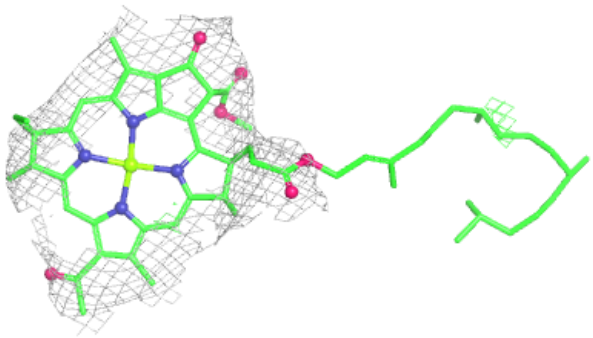


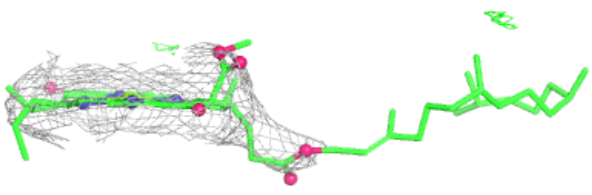


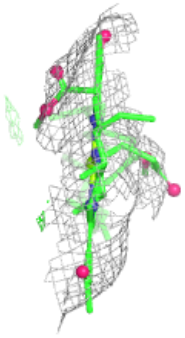


Electron density around BCL AI 101:

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

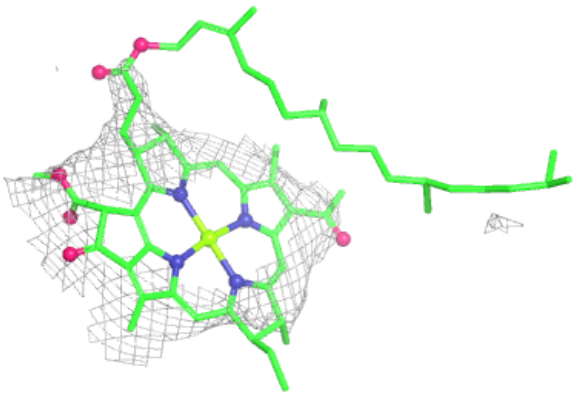


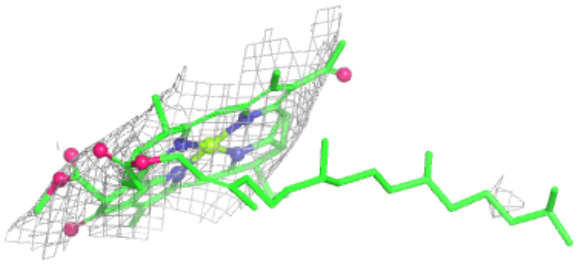


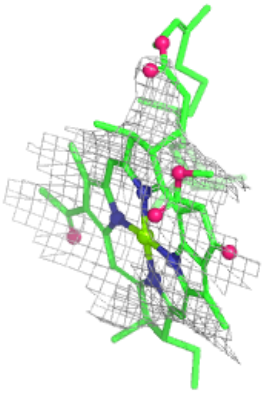


Electron density around BCL s 102:

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

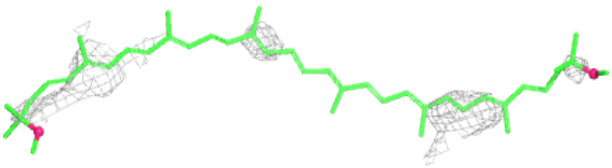


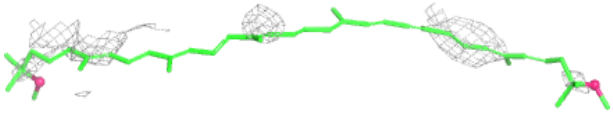


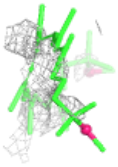


Electron density around CRT Z 101:

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

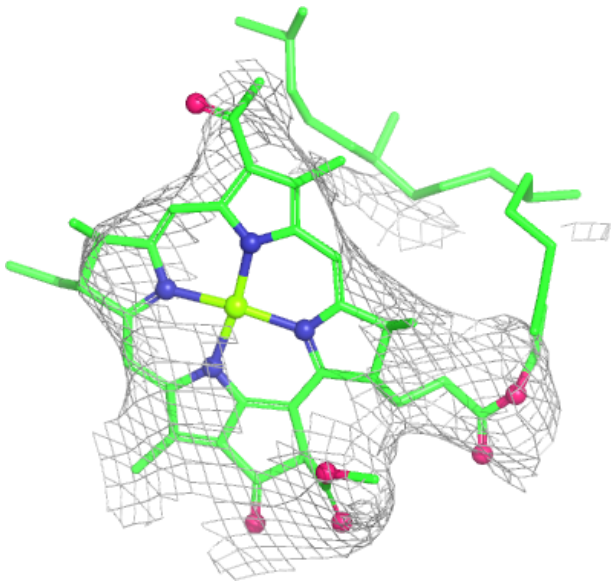


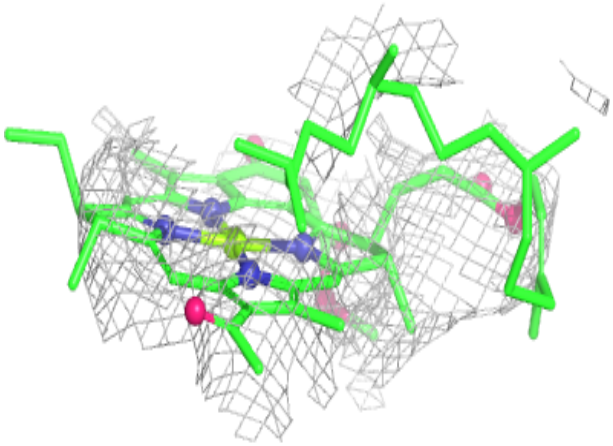


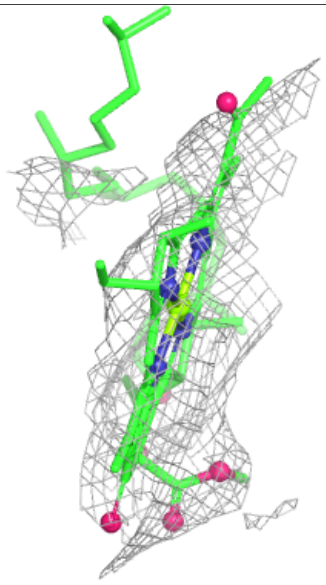


Electron density around BCL 8 101:

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

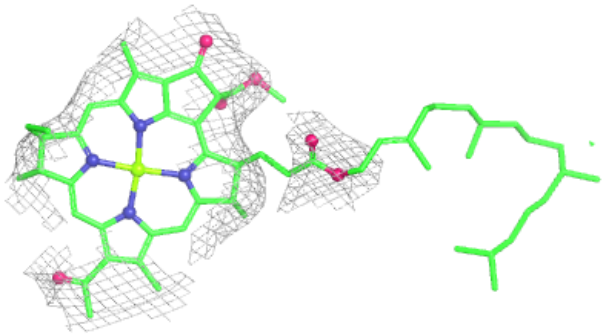


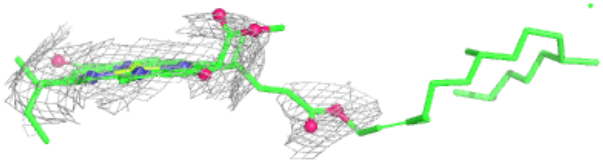


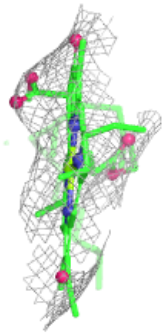


Electron density around BCL 9 102:

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

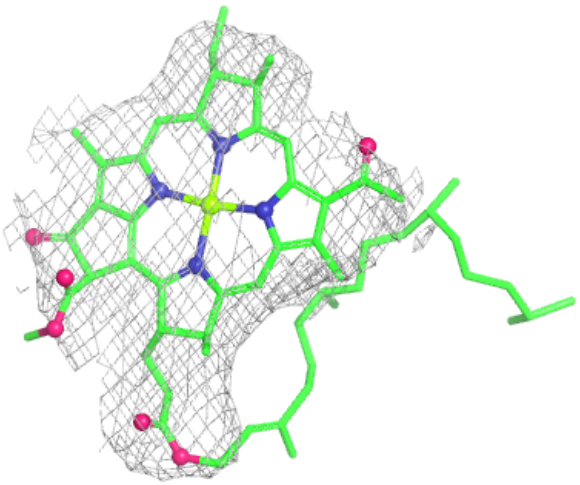


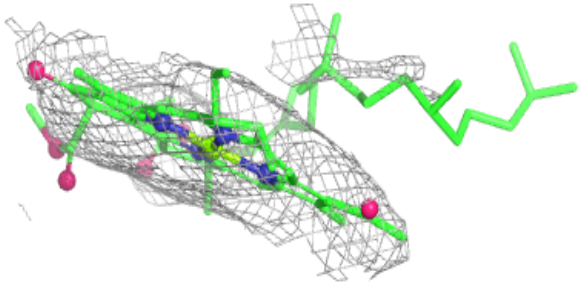


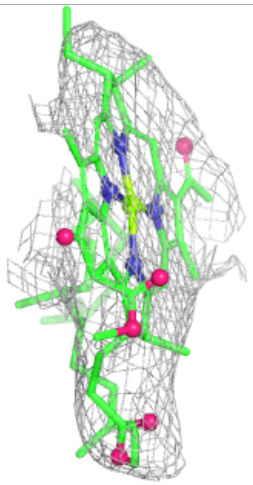


Electron density around BCL X 102:

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

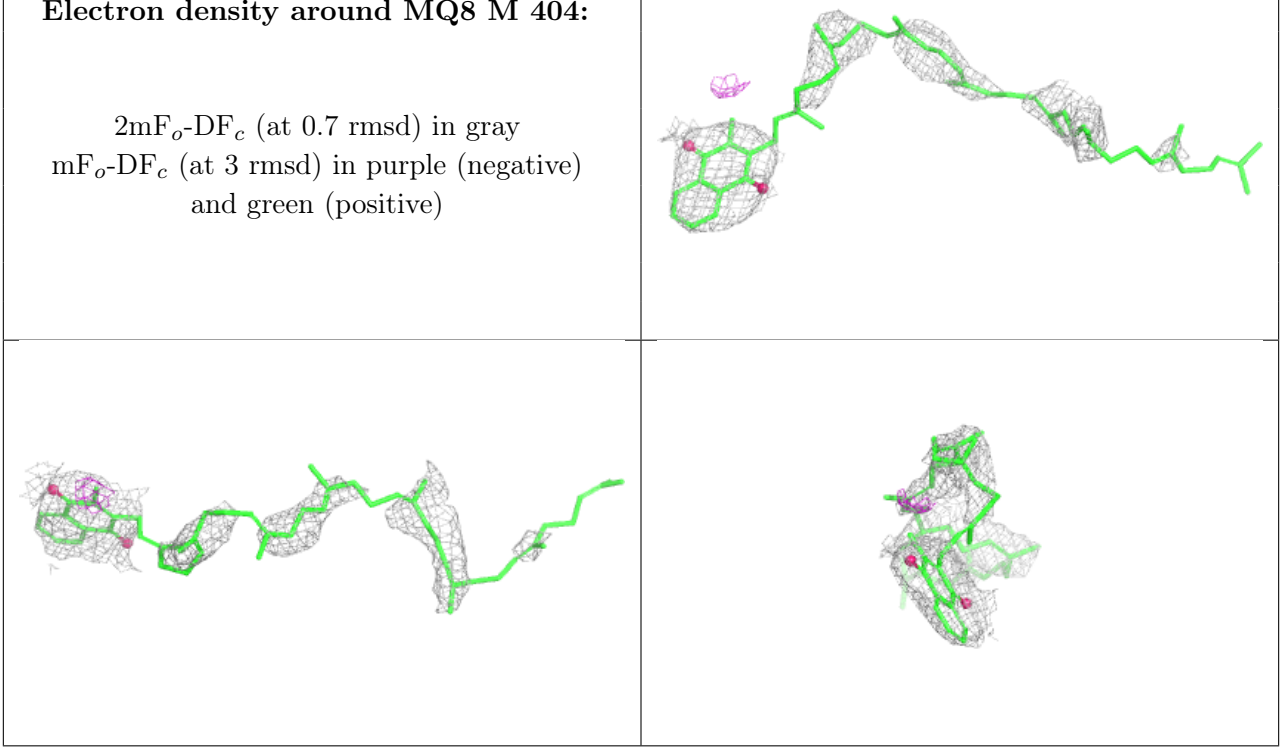






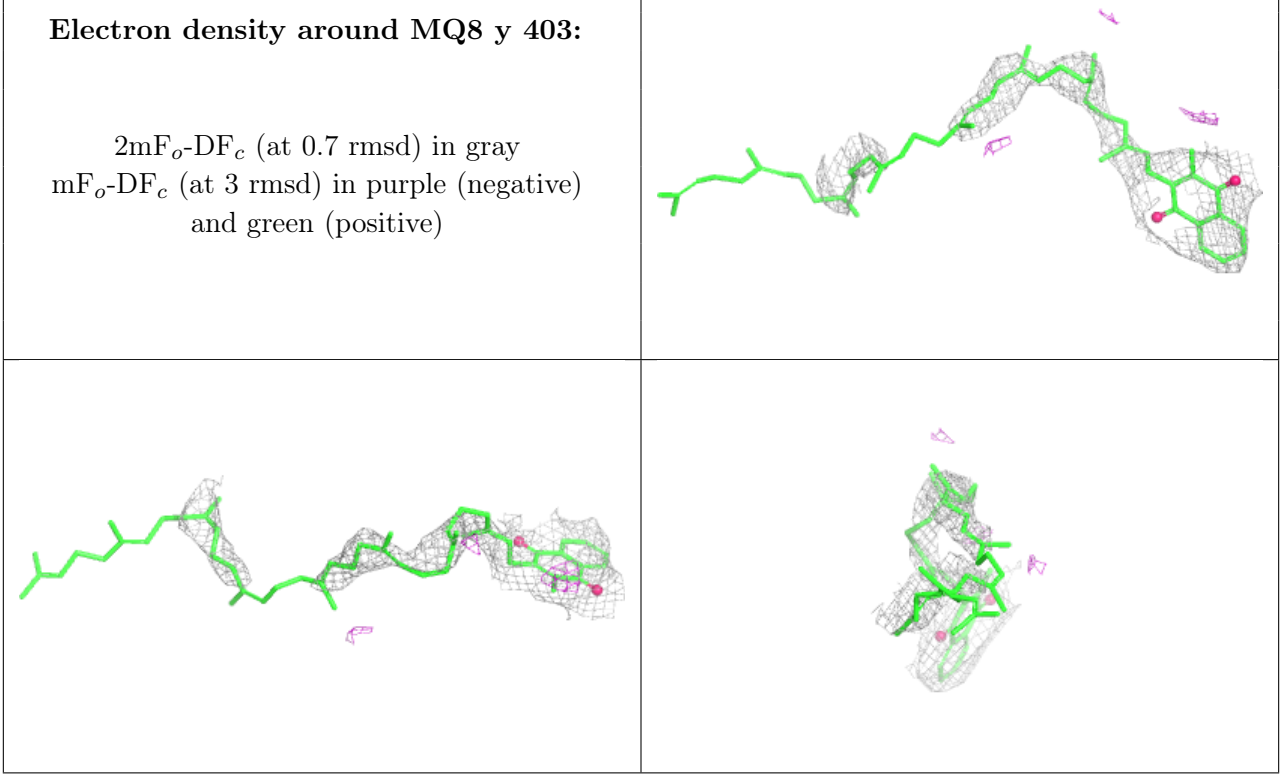
Electron density around MQ8 M 404:

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



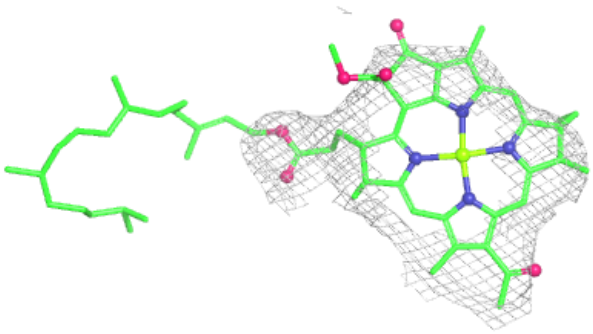
Electron density around MQ8 y 403:

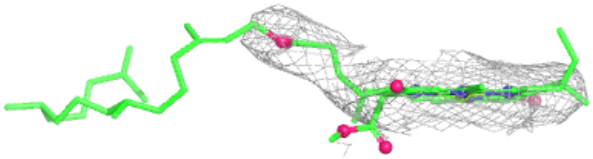
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

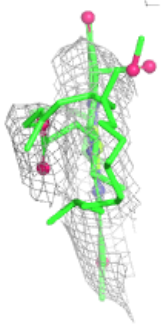


Electron density around BCL AH 101:

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

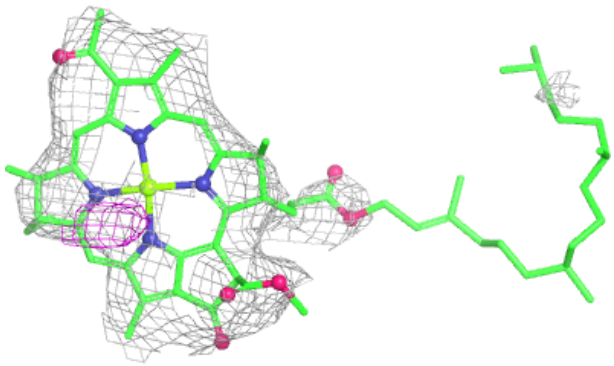


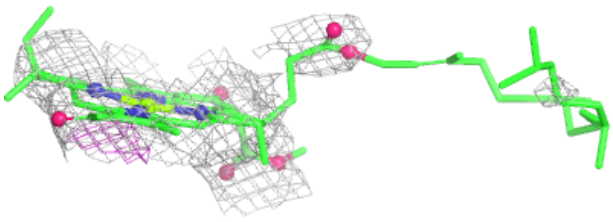


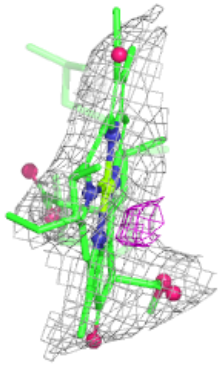


Electron density around BCL 3 101:

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

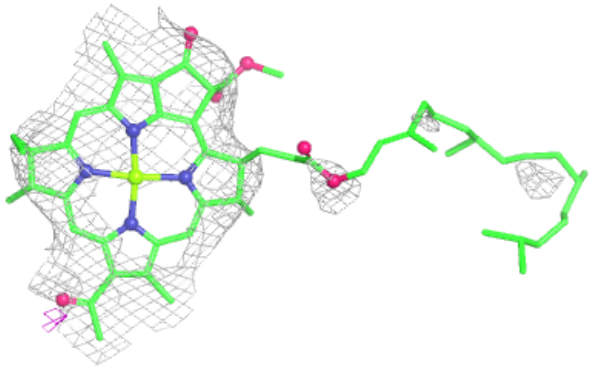


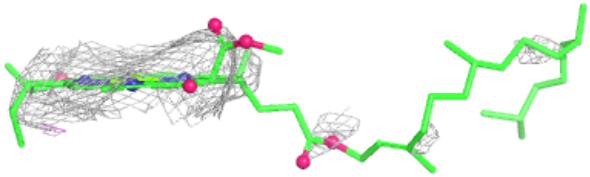


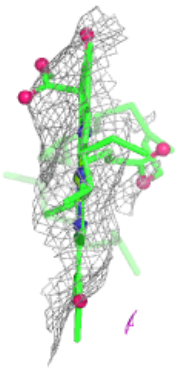


Electron density around BCL l 101:

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

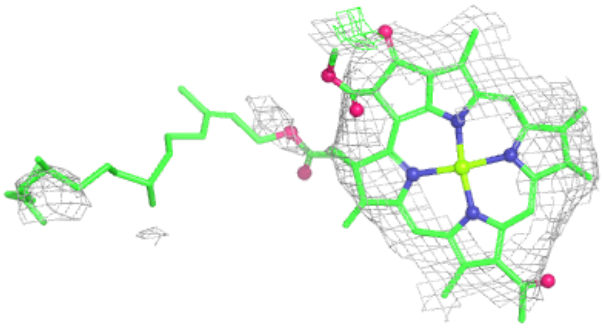


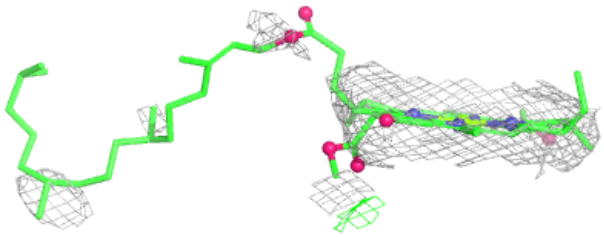


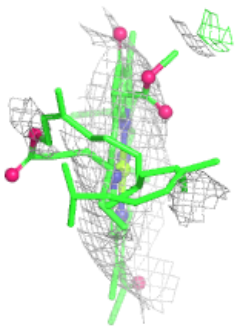


Electron density around BCL AB 101:

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

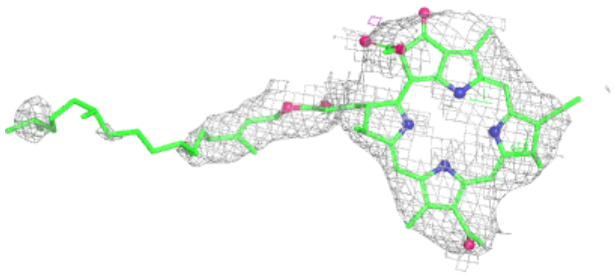






Electron density around BPH M 403:

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

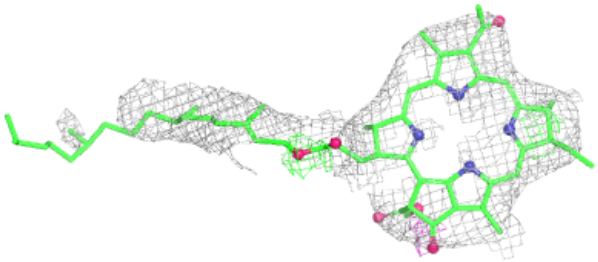


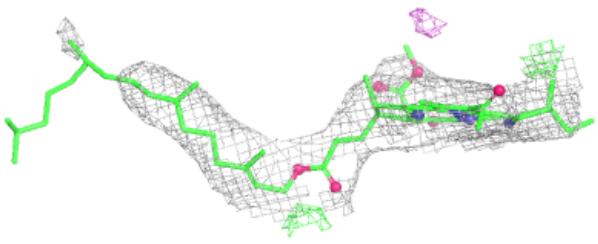


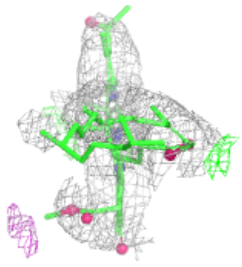


Electron density around BPH y 402:

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

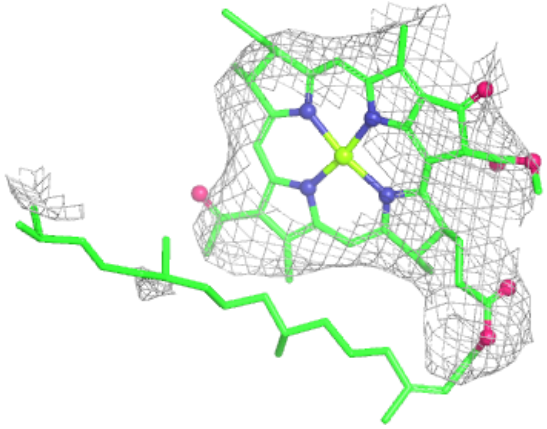


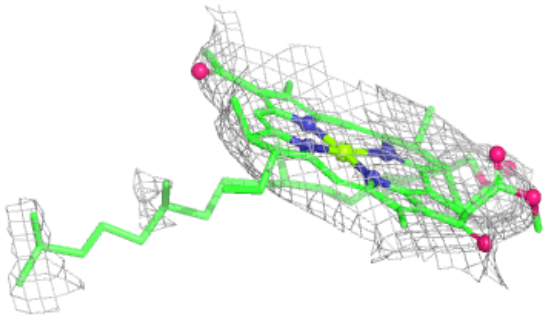




Electron density around BCL Z 102:

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

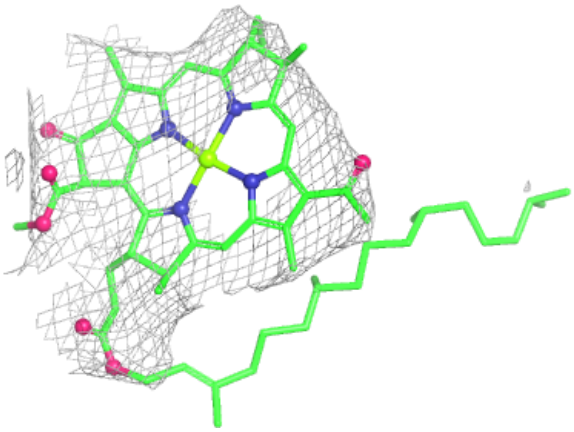


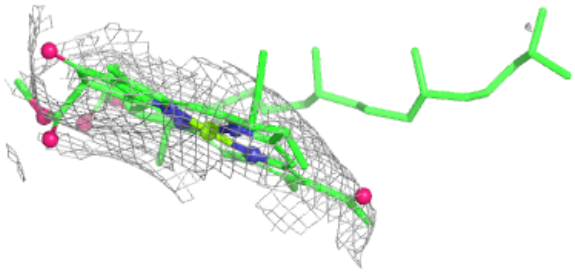


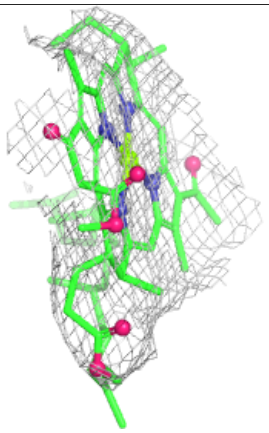


Electron density around BCL R 102:

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

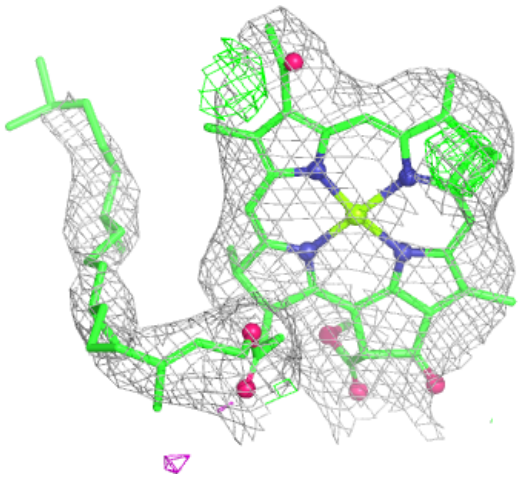


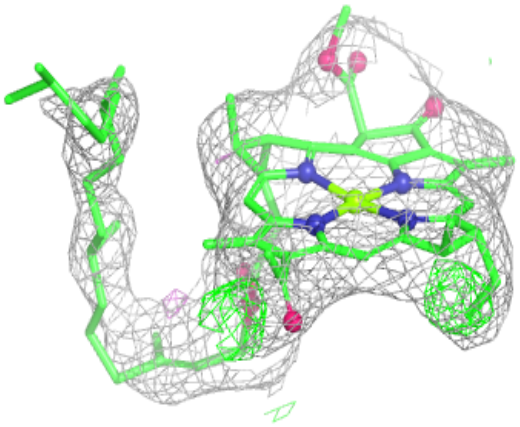


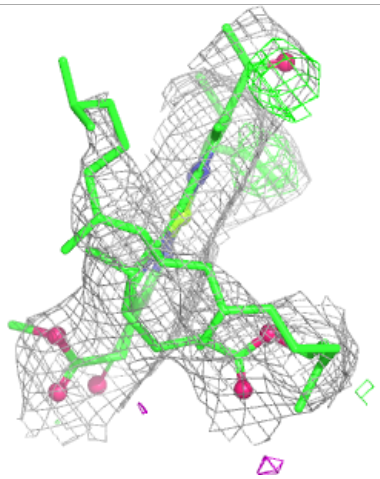


Electron density around BCL x 305:

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

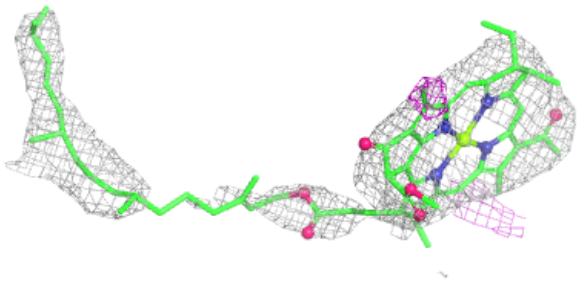


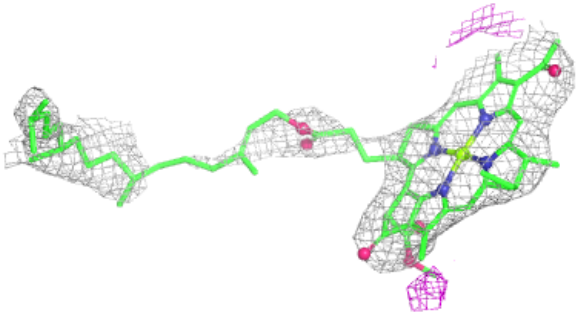


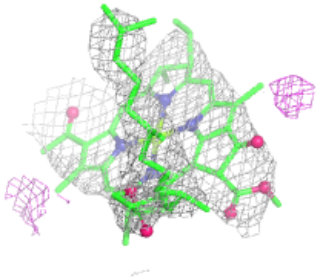


Electron density around BCL y 401:

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

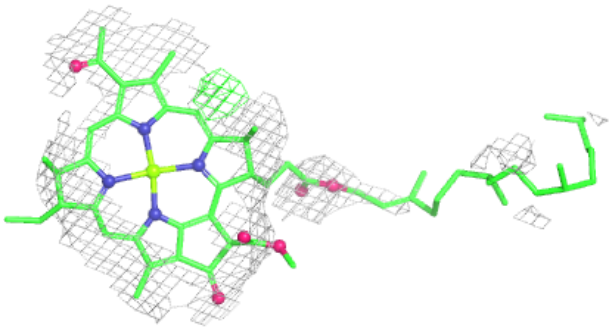


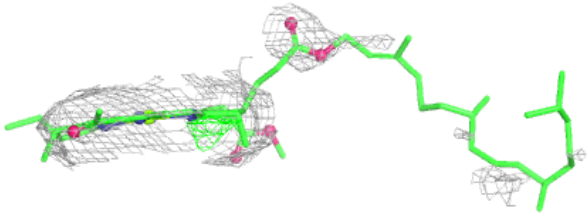


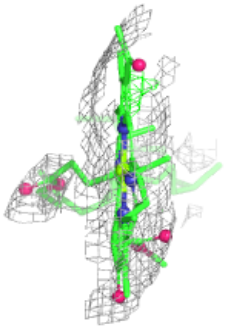


Electron density around BCL A 102:

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

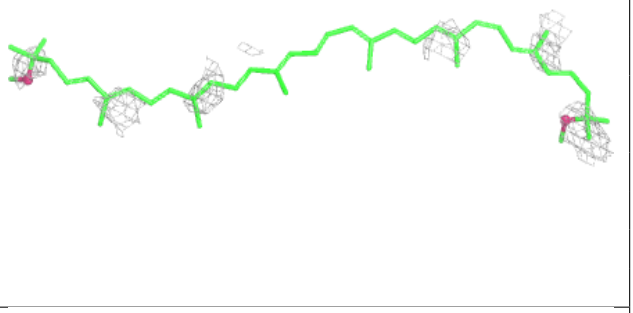


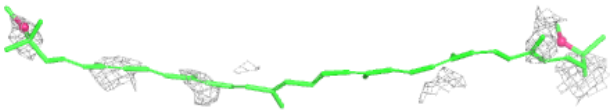


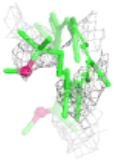


Electron density around CRT X 101:

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

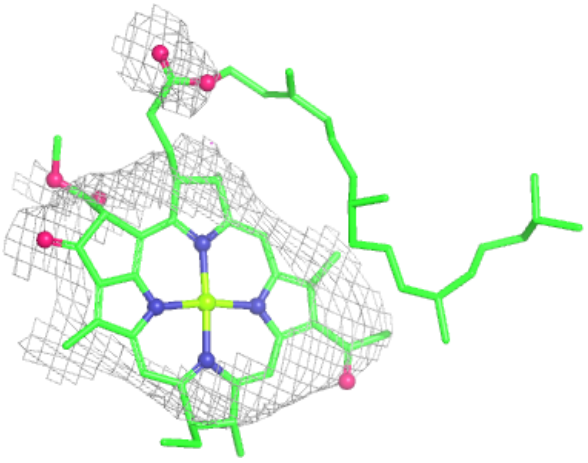


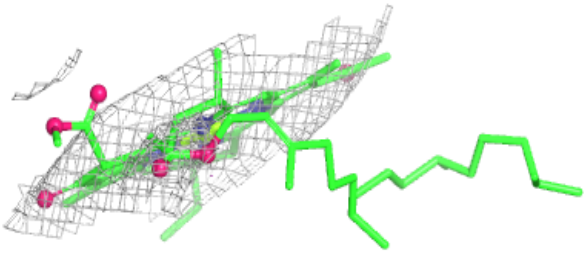


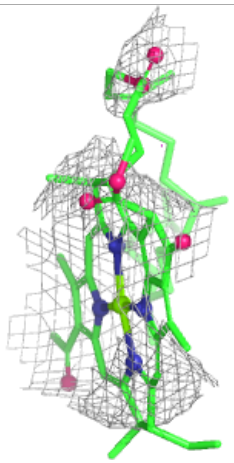


Electron density around BCL q 102:

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

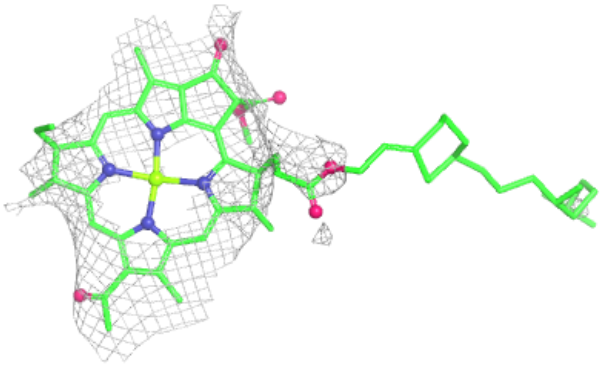


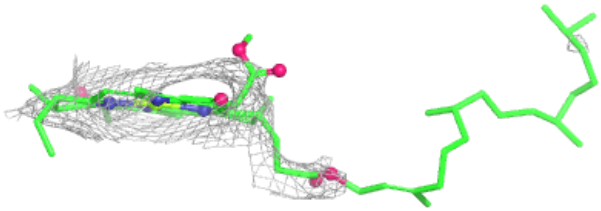


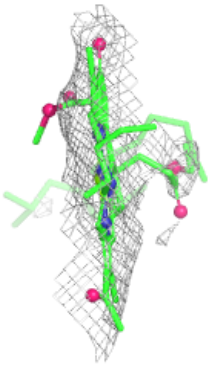


Electron density around BCL r 101:

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

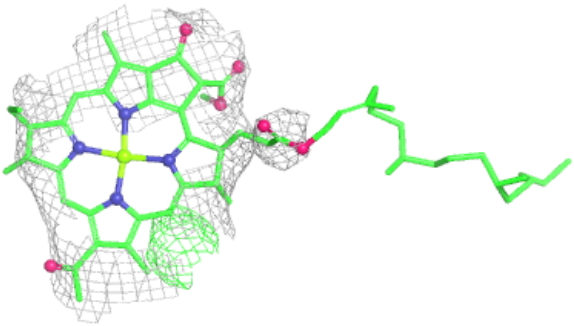


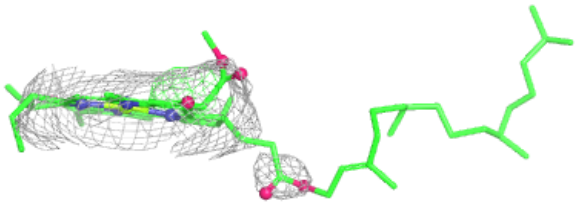




Electron density around BCL F 101:

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

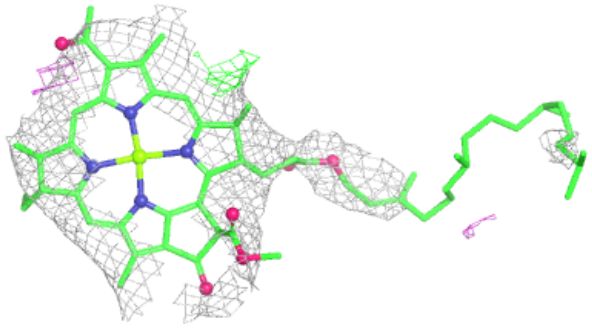


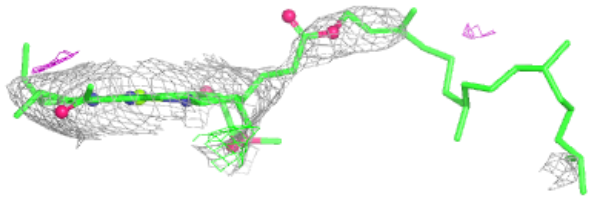


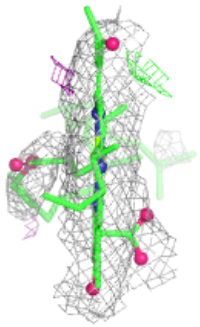


Electron density around BCL AK 101:

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

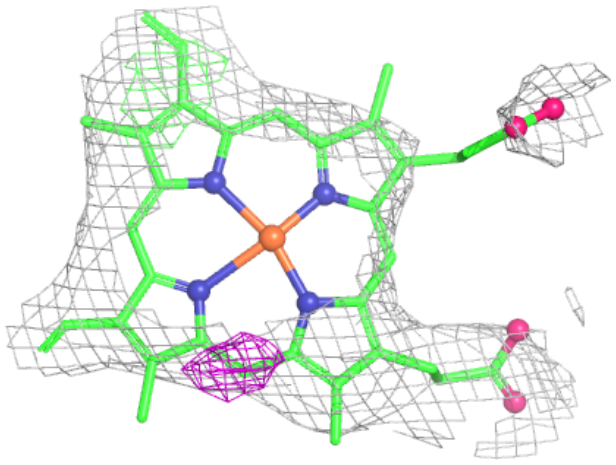


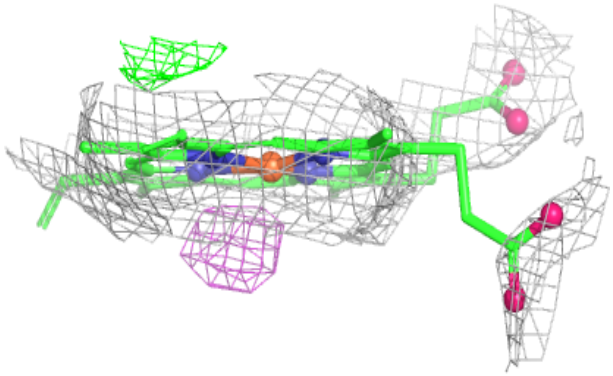


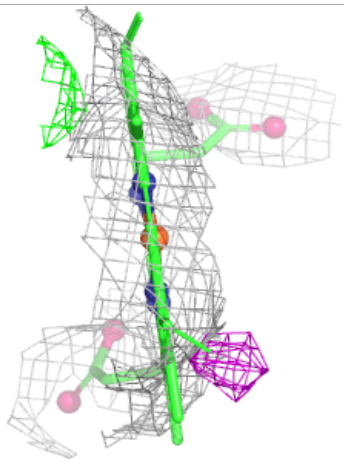


Electron density around HEM C 501:

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

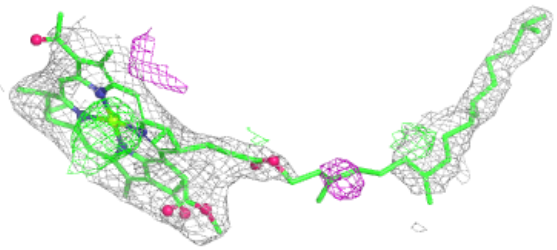


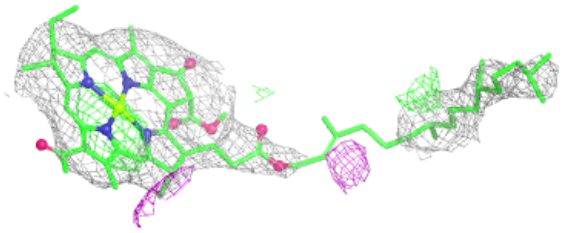


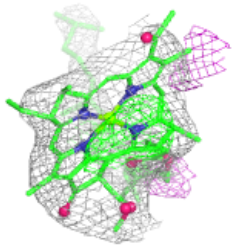


Electron density around BCL x 301:

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

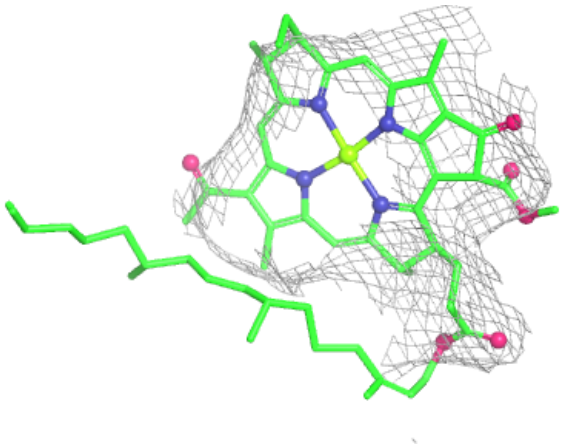


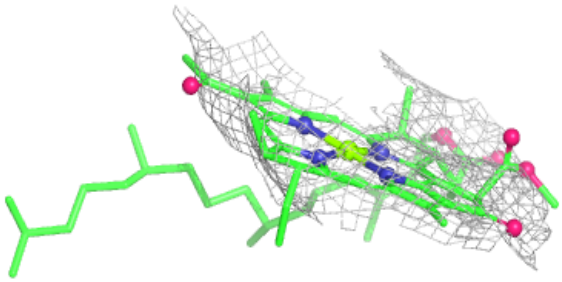


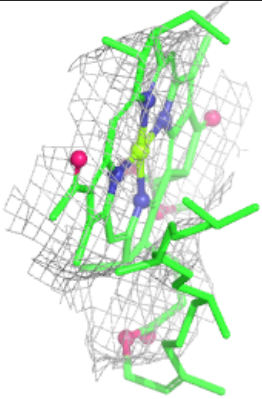


Electron density around BCL i 102:

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

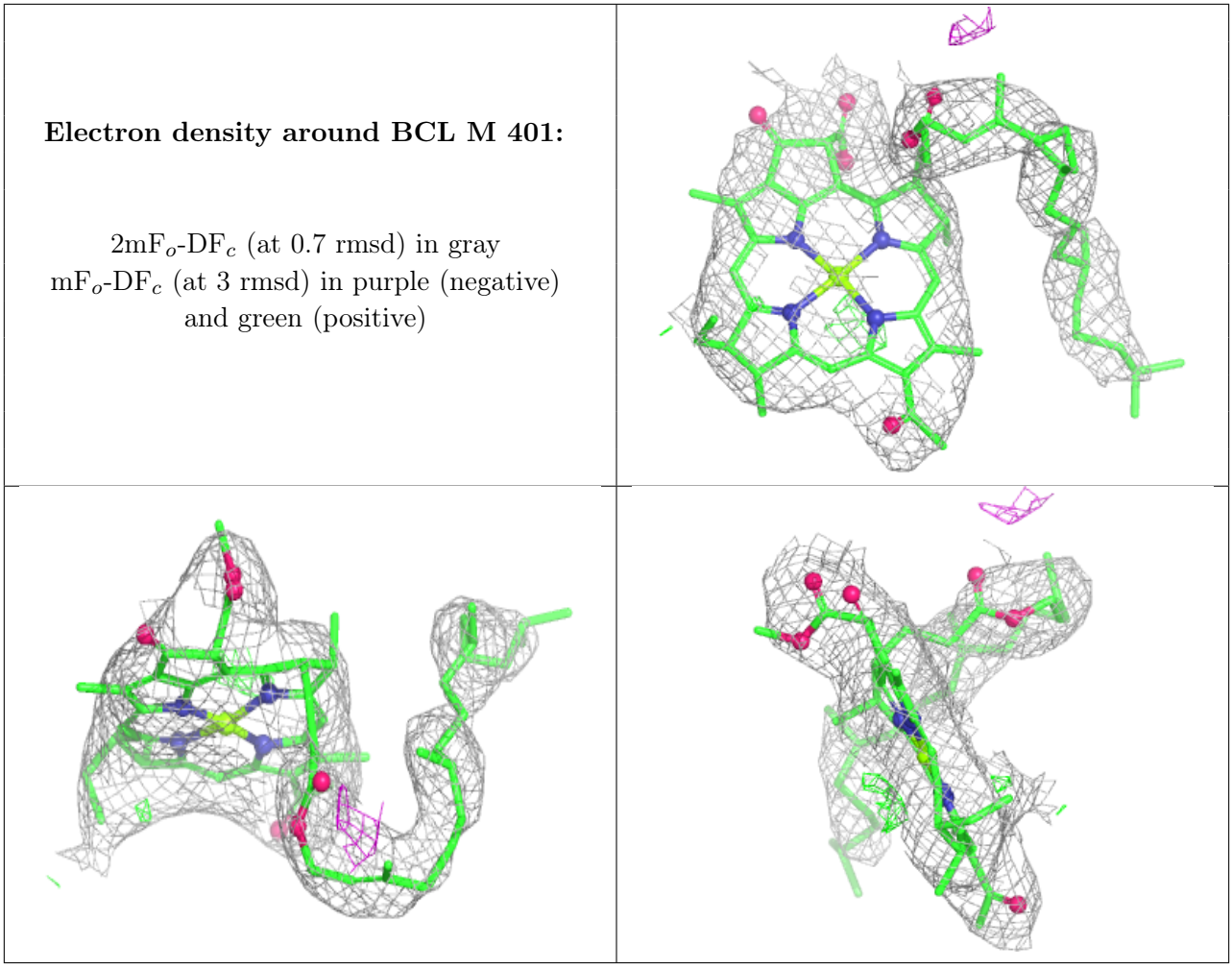






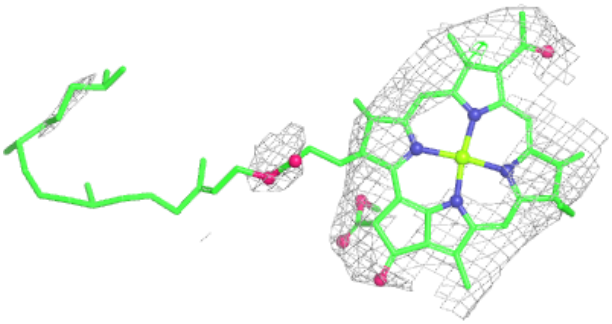
Electron density around BCL M 401:

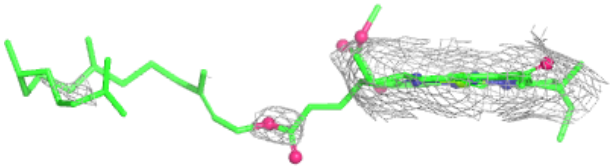
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

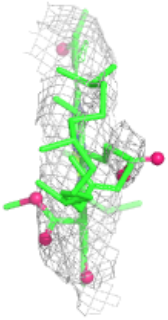


Electron density around BCL W 101:

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

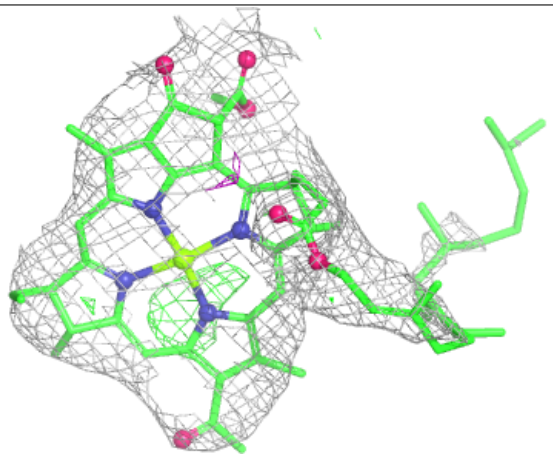


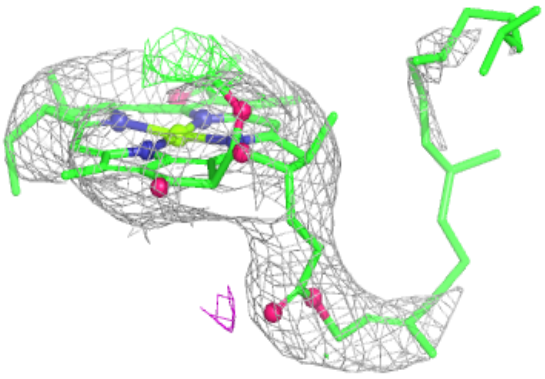




Electron density around BCL L 303:

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

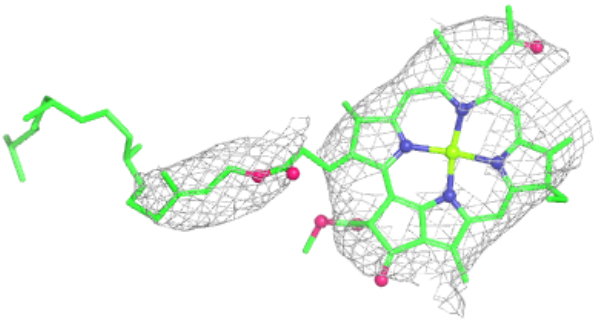


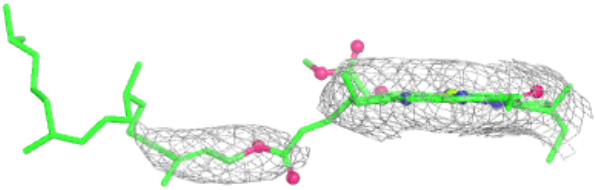




Electron density around BCL Y 101:

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

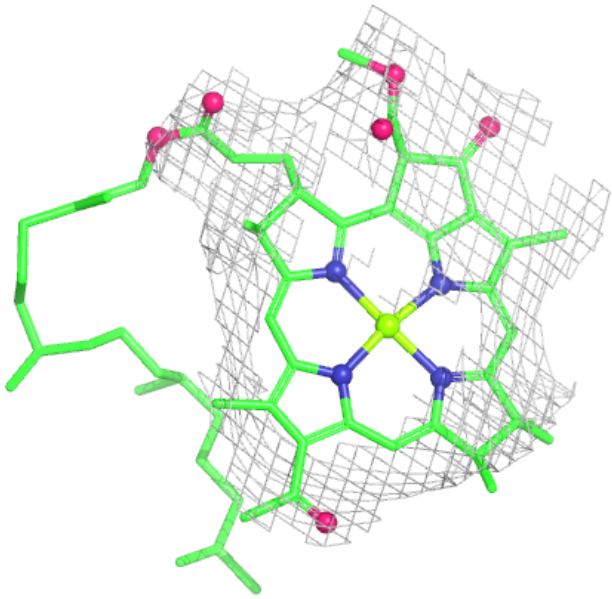


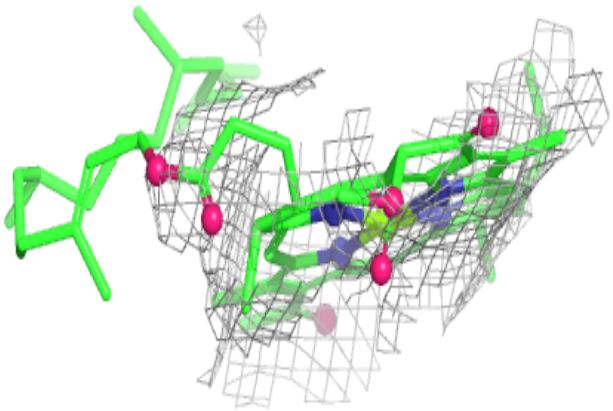


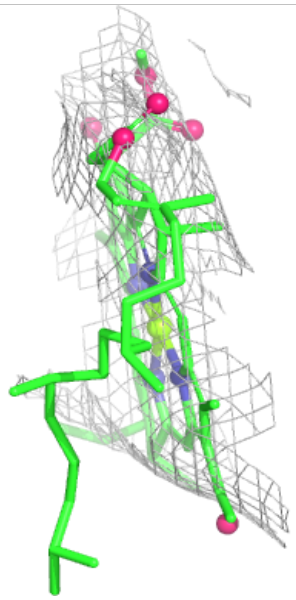


Electron density around BCL A 103:

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

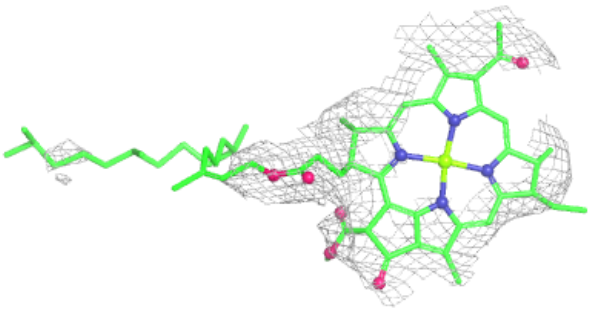


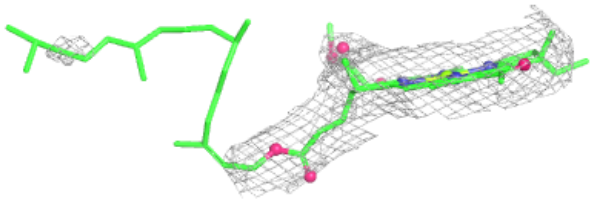


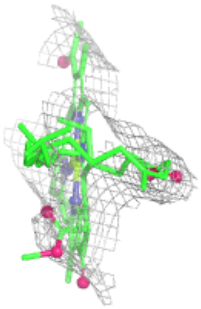


Electron density around BCL 5 101:

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



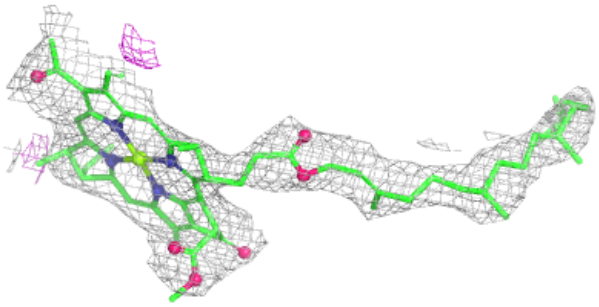


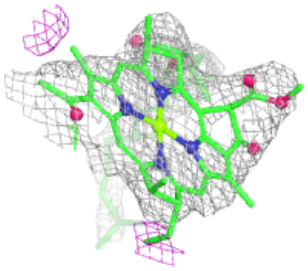


Electron density around BCL M 402:

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

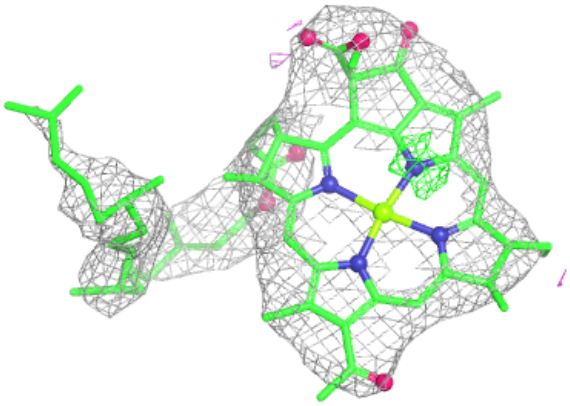


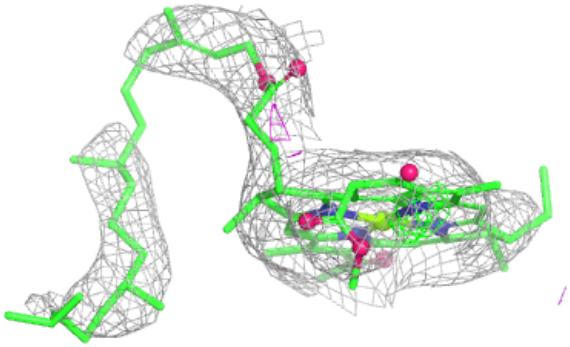


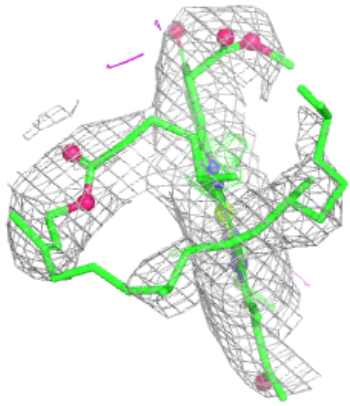


Electron density around BCL x 303:

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

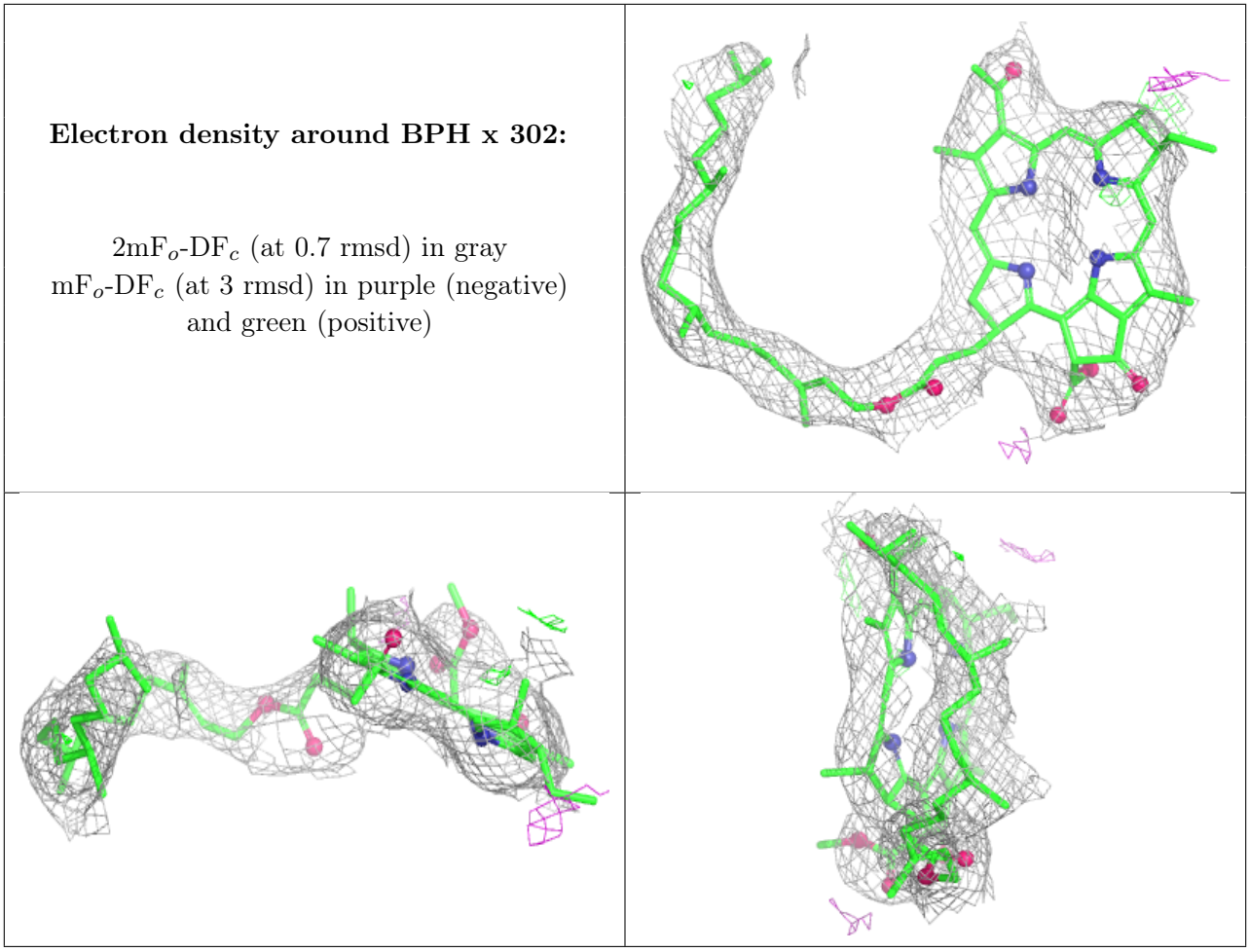






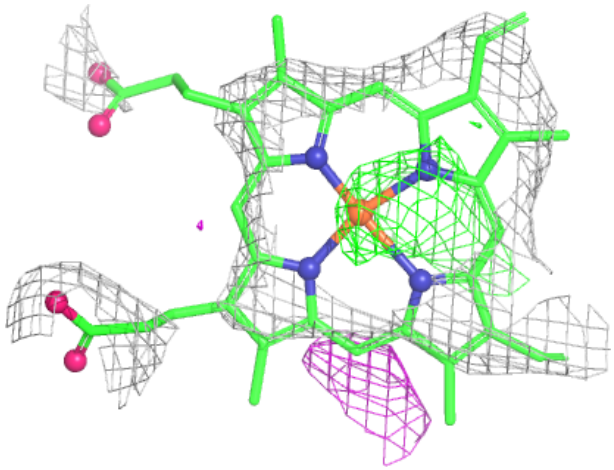
Electron density around BPH x 302:

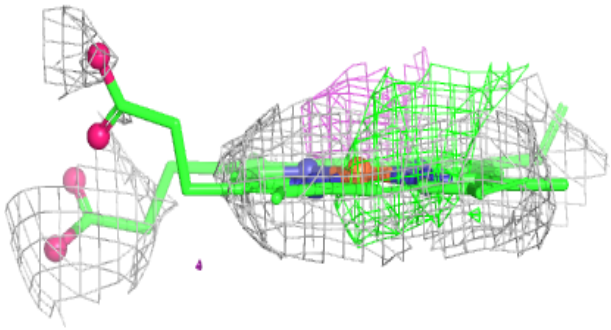
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

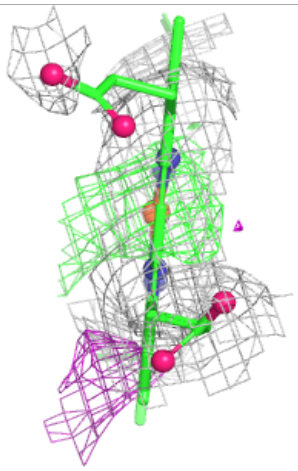


Electron density around HEM o 503:

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

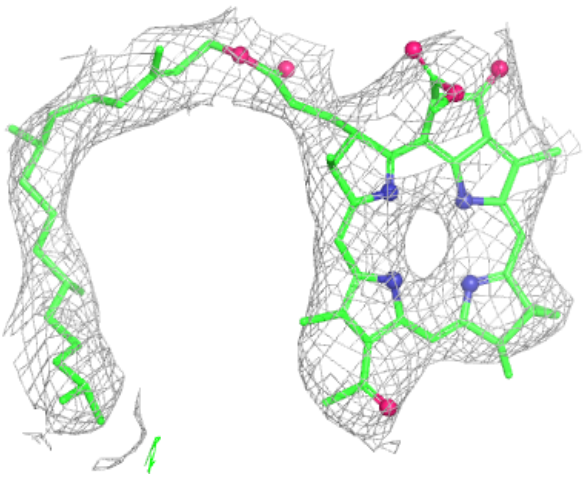


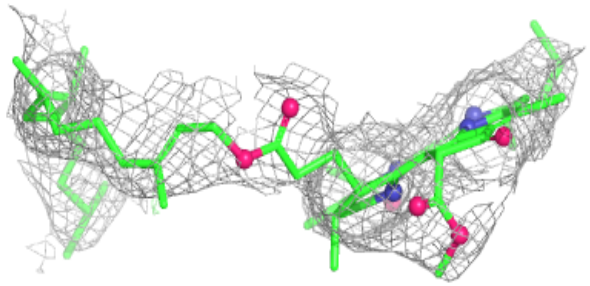


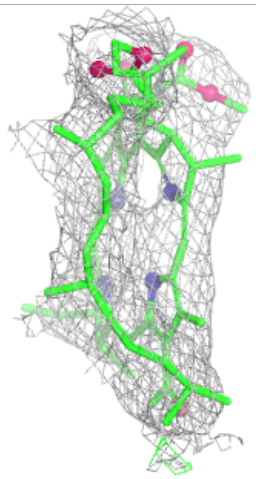


Electron density around BPH L 302:

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

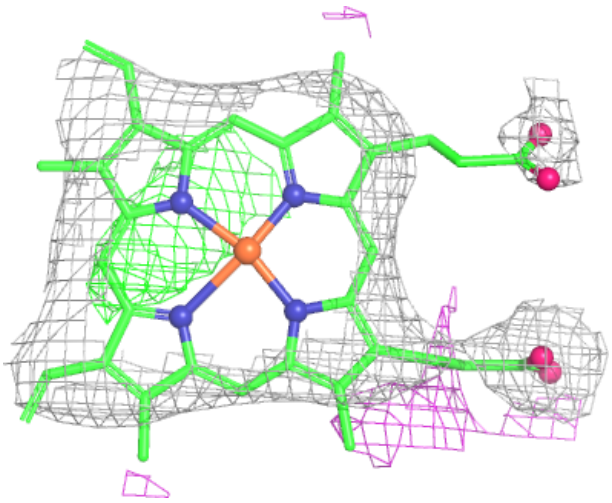


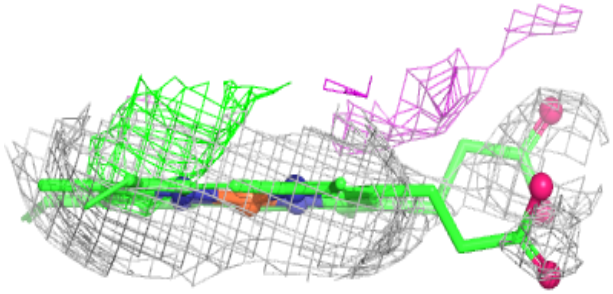


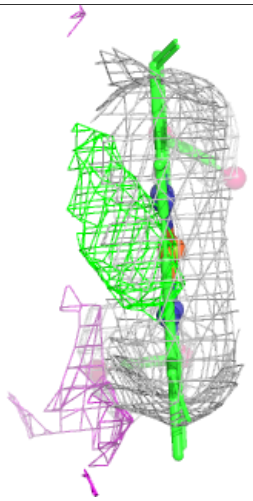


Electron density around HEM o 504:

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

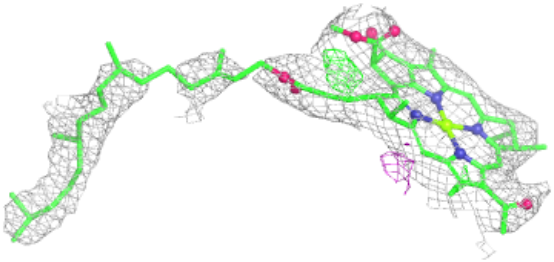


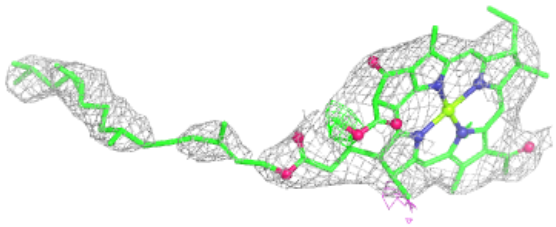


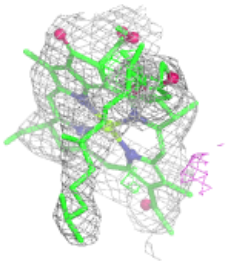


Electron density around BCL L 301:

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

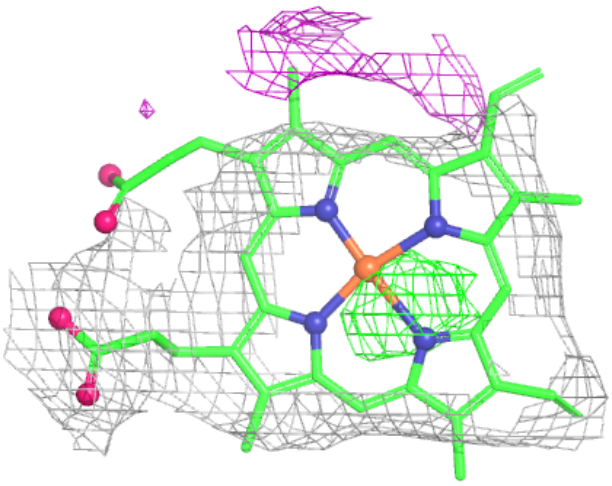


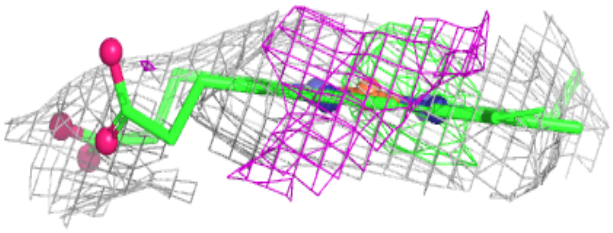


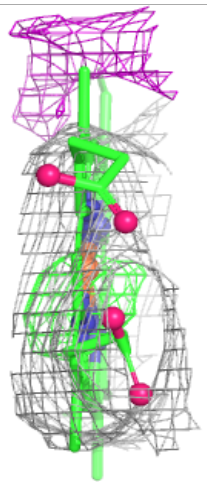


Electron density around HEM C 502:

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

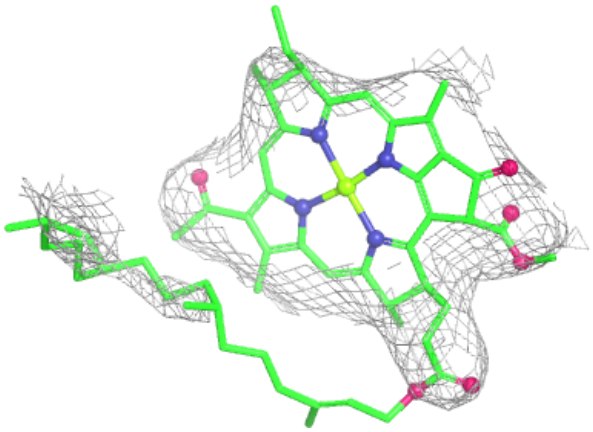


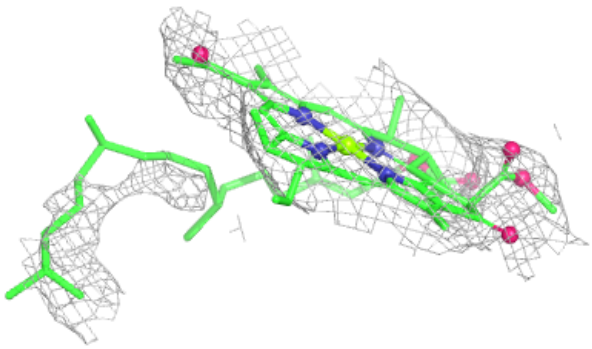




Electron density around BCL 4 102:

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

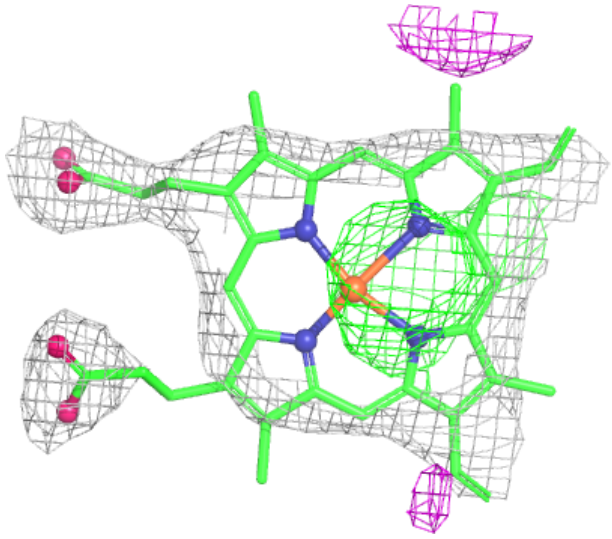


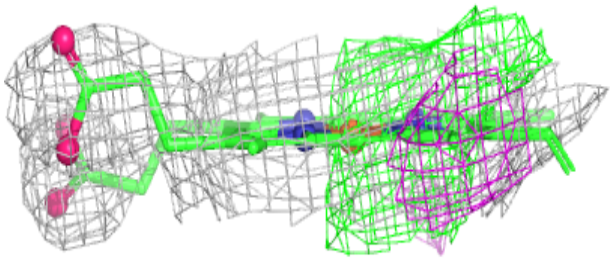


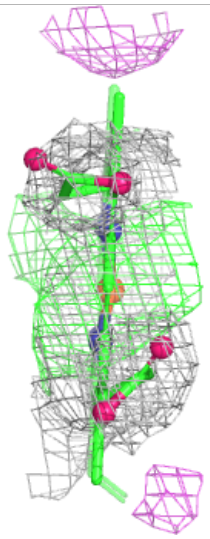


Electron density around HEM C 504:

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

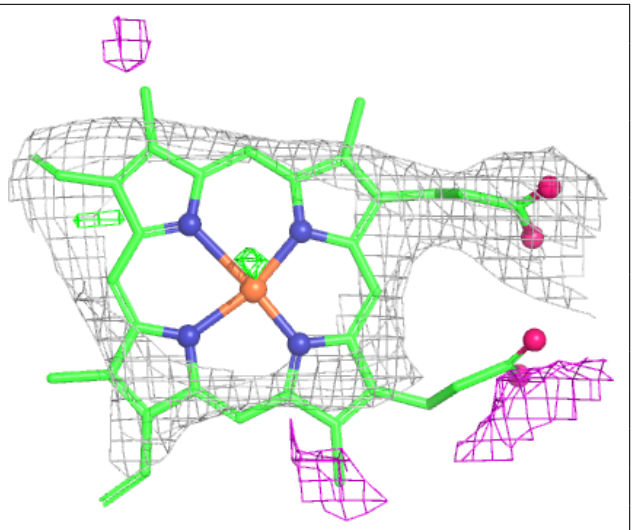


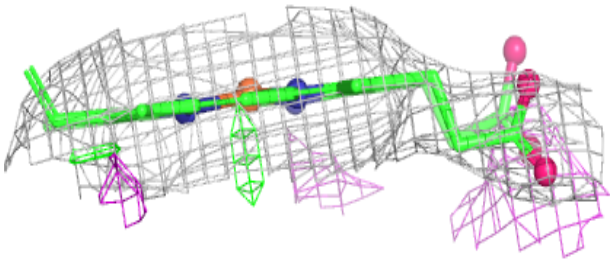


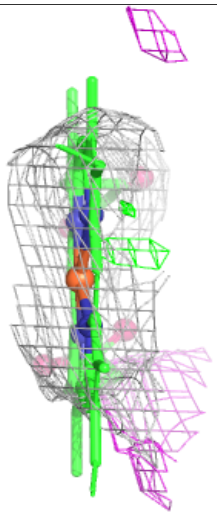


Electron density around HEM o 502:

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

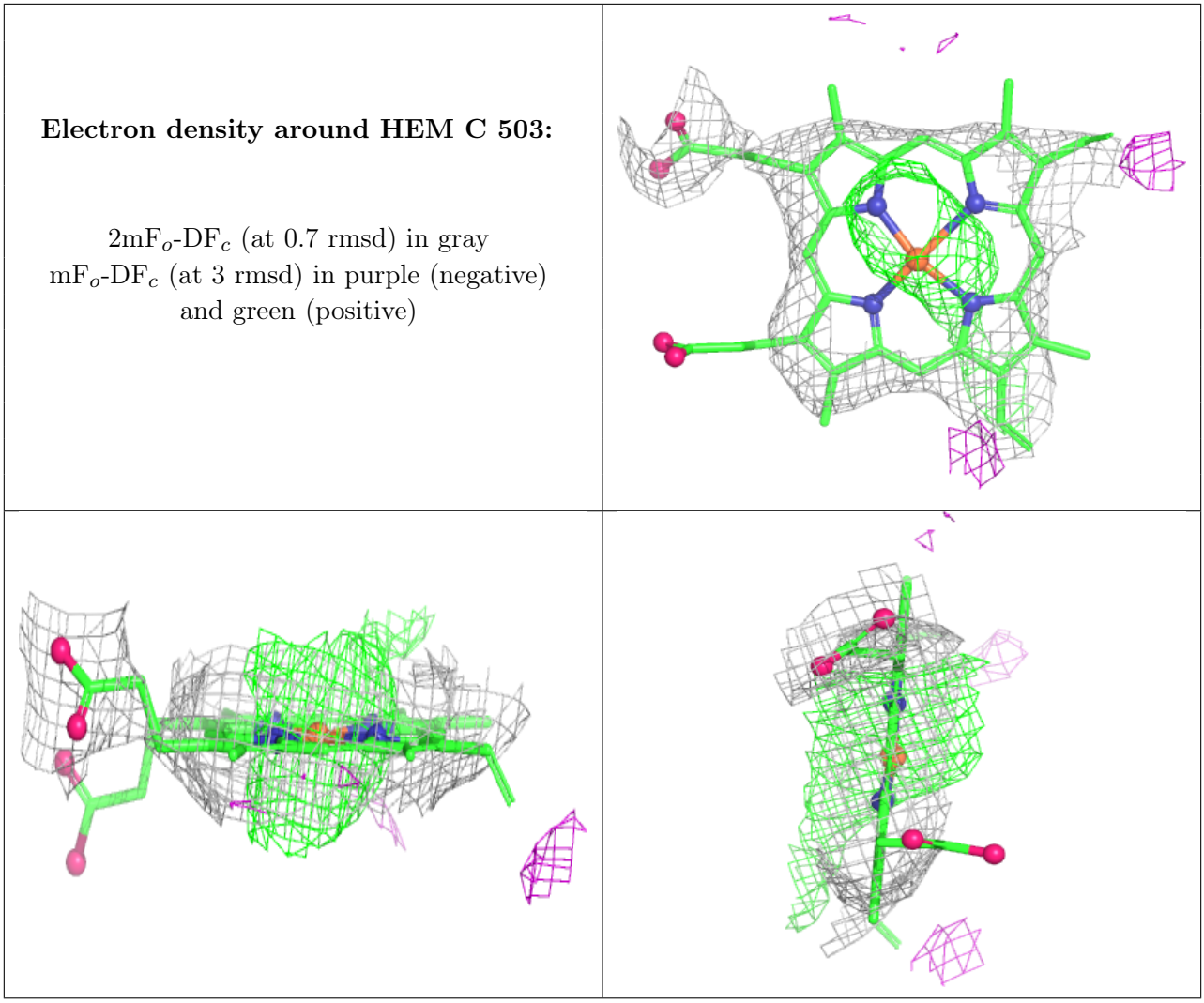






Electron density around HEM C 503:

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



6.5 Other polymers (i)

There are no such residues in this entry.