Full wwPDB EM Validation Report ⓘ

May 6, 2024 – 02:47 PM EDT

PDB ID	:	7JK9
EMDB ID	:	EMD-22364
Title	:	Helical filaments of plant light-dependent protochlorophyllide oxidoreductase (LPOR) bound to NADPH, Pchlide, and membrane
Authors	:	Nguyen, H.C.; Gabruk, M.; Frost, A.
Deposited on	:	2020-07-28
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

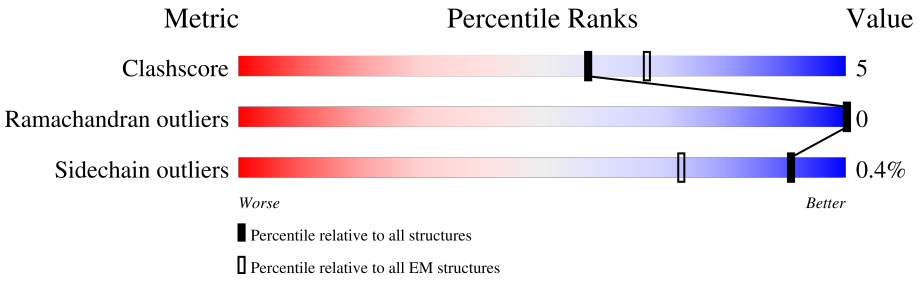
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	11% 70% 8% 21%
1	AA	401	11% 71% 8% 21%
1	B	401	10% 70% 8% 21%
1	BA	401	12% 71% 8% 21%
1	C	401	11% 70% 9% 21%
1	CA	401	12% 70% 9% 21%
1	D	401	12% 69% 9% 21%
1	DA	401	13% 70% 9% 21%

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Mol	Chain	Length	Quality of chain
1	E	401	12% 70% 8% 21%
1	EA	401	12% 70% 9% 21%
1	F	401	12% 71% 8% 21%
1	FA	401	11% 70% 8% 21%
1	G	401	10% 70% 9% 21%
1	GA	401	11% 71% 8% 21%
1	H	401	11% 71% 8% 21%
1	HA	401	11% 70% 9% 21%
1	I	401	10% 70% 9% 21%
1	IA	401	11% 70% 9% 21%
1	J	401	11% 71% 8% 21%
1	JA	401	10% 71% 8% 21%
1	K	401	11% 71% 7% 21%
1	KA	401	11% 70% 8% 21%
1	L	401	10% 68% 10% 21%
1	LA	401	11% 70% 9% 21%
1	M	401	12% 70% 9% 21%
1	MA	401	10% 70% 9% 21%
1	N	401	12% 71% 7% 21%
1	NA	401	10% 71% 8% 21%
1	O	401	12% 70% 9% 21%
1	OA	401	10% 70% 9% 21%
1	P	401	13% 71% 8% 21%
1	Q	401	11% 69% 9% 21%
1	R	401	11% 71% 8% 21%

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Mol	Chain	Length	Quality of chain
1	S	401	10% 70% 9% 21%
1	T	401	11% 70% 9% 21%
1	V	401	11% 70% 9% 21%
1	W	401	11% 71% 8% 21%
1	X	401	11% 70% 9% 21%
1	Y	401	10% 70% 8% 21%
1	Z	401	11% 70% 9% 21%

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
3	PMR	A	502	X	-	-	-
3	PMR	AA	502	X	-	-	-
3	PMR	B	502	X	-	-	-
3	PMR	BA	502	X	-	-	-
3	PMR	C	502	X	-	-	-
3	PMR	CA	502	X	-	-	-
3	PMR	D	502	X	-	-	-
3	PMR	DA	502	X	-	-	-
3	PMR	E	502	X	-	-	-
3	PMR	EA	502	X	-	-	-
3	PMR	F	502	X	-	-	-
3	PMR	FA	502	X	-	-	-
3	PMR	G	502	X	-	-	-
3	PMR	GA	502	X	-	-	-
3	PMR	H	502	X	-	-	-
3	PMR	HA	502	X	-	-	-
3	PMR	I	502	X	-	-	-
3	PMR	IA	502	X	-	-	-
3	PMR	J	502	X	-	-	-
3	PMR	JA	502	X	-	-	-
3	PMR	K	502	X	-	-	-
3	PMR	KA	502	X	-	-	-
3	PMR	L	502	X	-	-	-
3	PMR	LA	502	X	-	-	-
3	PMR	M	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PMR	MA	502	X	-	-	-
3	PMR	N	502	X	-	-	-
3	PMR	NA	502	X	-	-	-
3	PMR	O	502	X	-	-	-
3	PMR	OA	502	X	-	-	-
3	PMR	P	502	X	-	-	-
3	PMR	Q	502	X	-	-	-
3	PMR	R	502	X	-	-	-
3	PMR	S	502	X	-	-	-
3	PMR	T	502	X	-	-	-
3	PMR	V	502	X	-	-	-
3	PMR	W	502	X	-	-	-
3	PMR	X	502	X	-	-	-
3	PMR	Y	502	X	-	-	-
3	PMR	Z	502	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 197360 atoms, of which 95880 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protochlorophyllide reductase B, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	B	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	C	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	D	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	E	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	F	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	G	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	H	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	I	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	J	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	K	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	L	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	M	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	N	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	O	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	P	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	Q	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	S	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	T	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	V	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	W	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	X	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	Y	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	Z	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	AA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	BA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	CA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	DA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	EA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	FA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	GA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	HA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	IA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	JA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	KA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	LA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	MA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		

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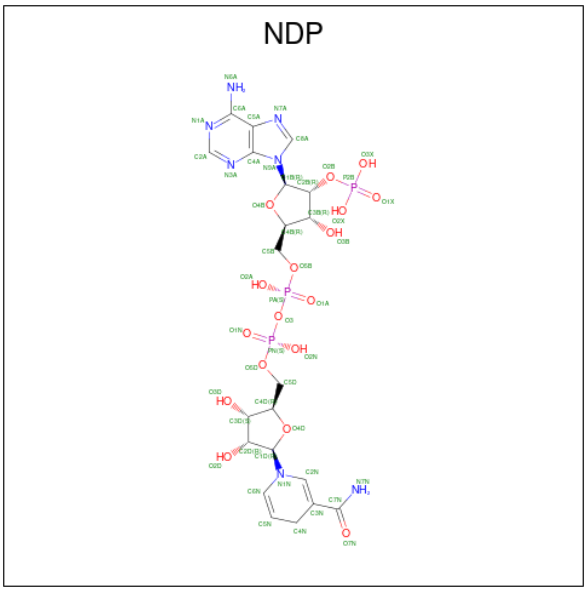
Mol	Chain	Residues	Atoms						AltConf	Trace
1	NA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		
1	OA	316	Total	C	H	N	O	S	0	0
			4818	1534	2397	418	459	10		

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	D	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	F	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	G	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	H	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	I	1	Total	C	N	O	P	0
			48	21	7	17	3	

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Mol	Chain	Residues	Atoms					AltConf
2	J	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	K	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	L	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	M	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	N	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	O	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	P	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	Q	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	R	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	S	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	T	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	V	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	W	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	X	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	Y	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	Z	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	AA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	BA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	CA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	DA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	EA	1	Total	C	N	O	P	0
			48	21	7	17	3	

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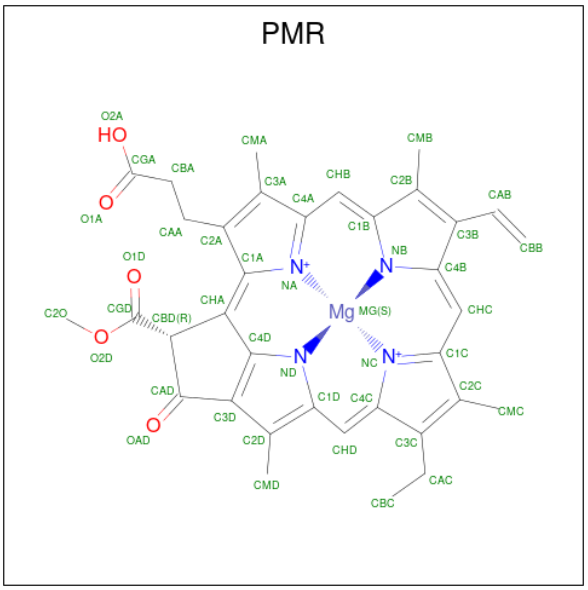
Mol	Chain	Residues	Atoms					AltConf
2	FA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	GA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	HA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	IA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	JA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	KA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	LA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	MA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	NA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	OA	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 is Protochlorophyllide (three-letter code: PMR) (formula: $C_{35}H_{32}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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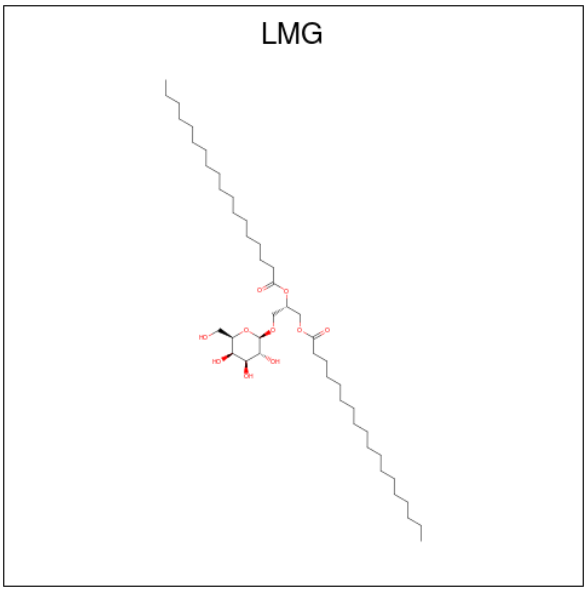
Mol	Chain	Residues	Atoms					AltConf
3	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	CA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	DA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	EA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	FA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	GA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	HA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	IA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	JA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	KA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	LA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	MA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	NA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	OA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 4 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			23	13	10	
4	B	1	Total	C	O	0
			23	13	10	
4	C	1	Total	C	O	0
			23	13	10	
4	D	1	Total	C	O	0
			23	13	10	
4	E	1	Total	C	O	0
			23	13	10	
4	F	1	Total	C	O	0
			23	13	10	
4	G	1	Total	C	O	0
			23	13	10	
4	H	1	Total	C	O	0
			23	13	10	
4	I	1	Total	C	O	0
			23	13	10	
4	J	1	Total	C	O	0
			23	13	10	
4	K	1	Total	C	O	0
			23	13	10	
4	L	1	Total	C	O	0
			23	13	10	
4	M	1	Total	C	O	0
			23	13	10	
4	N	1	Total	C	O	0
			23	13	10	

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Mol	Chain	Residues	Atoms	AltConf
4	O	1	Total C O 23 13 10	0
4	P	1	Total C O 23 13 10	0
4	Q	1	Total C O 23 13 10	0
4	R	1	Total C O 23 13 10	0
4	S	1	Total C O 23 13 10	0
4	T	1	Total C O 23 13 10	0
4	V	1	Total C O 23 13 10	0
4	W	1	Total C O 23 13 10	0
4	X	1	Total C O 23 13 10	0
4	Y	1	Total C O 23 13 10	0
4	Z	1	Total C O 23 13 10	0
4	AA	1	Total C O 23 13 10	0
4	BA	1	Total C O 23 13 10	0
4	CA	1	Total C O 23 13 10	0
4	DA	1	Total C O 23 13 10	0
4	EA	1	Total C O 23 13 10	0
4	FA	1	Total C O 23 13 10	0
4	GA	1	Total C O 23 13 10	0
4	HA	1	Total C O 23 13 10	0
4	IA	1	Total C O 23 13 10	0
4	JA	1	Total C O 23 13 10	0

Continued on next page...

Continued from previous page...

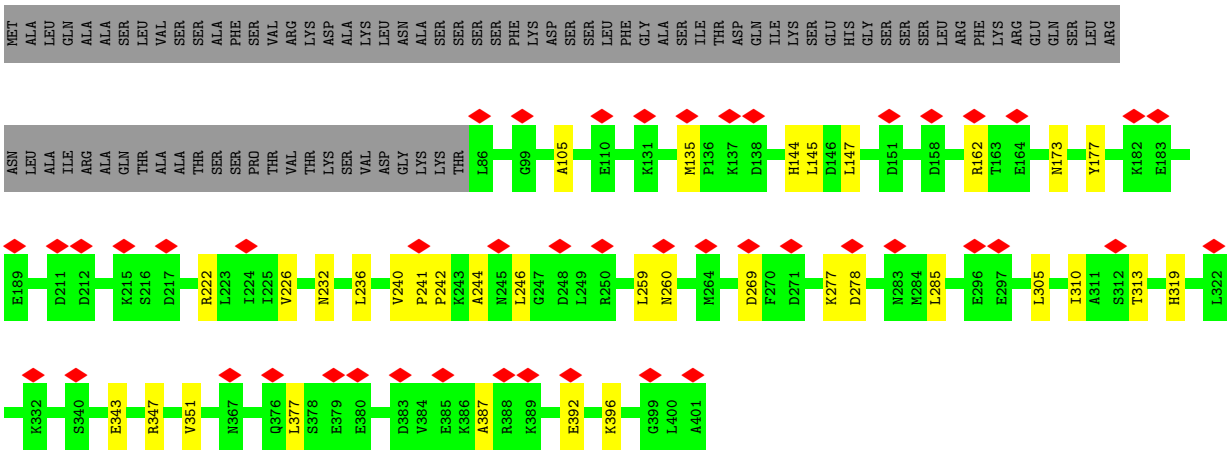
Mol	Chain	Residues	Atoms			AltConf
4	KA	1	Total	C	O	0
			23	13	10	
4	LA	1	Total	C	O	0
			23	13	10	
4	MA	1	Total	C	O	0
			23	13	10	
4	NA	1	Total	C	O	0
			23	13	10	
4	OA	1	Total	C	O	0
			23	13	10	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

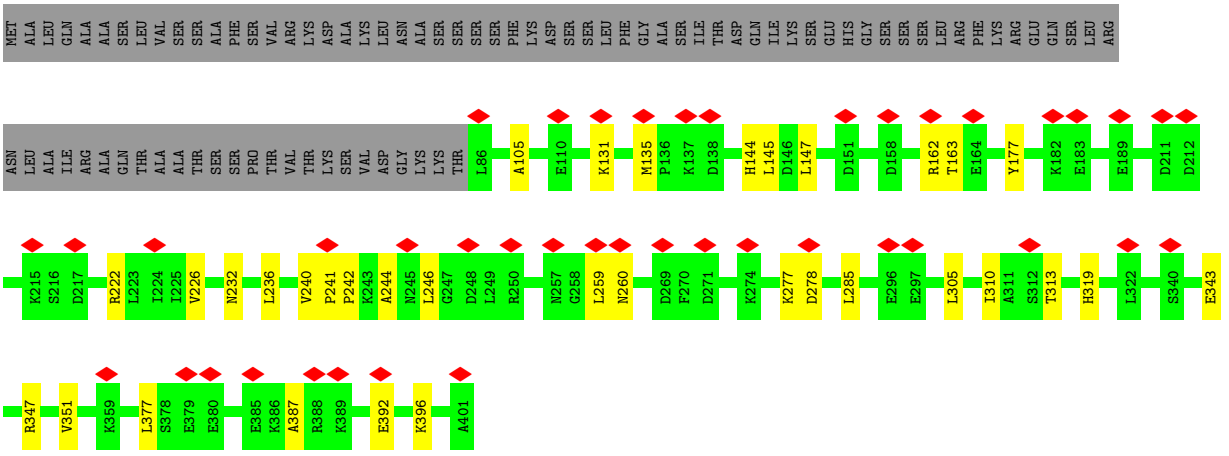
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain A:



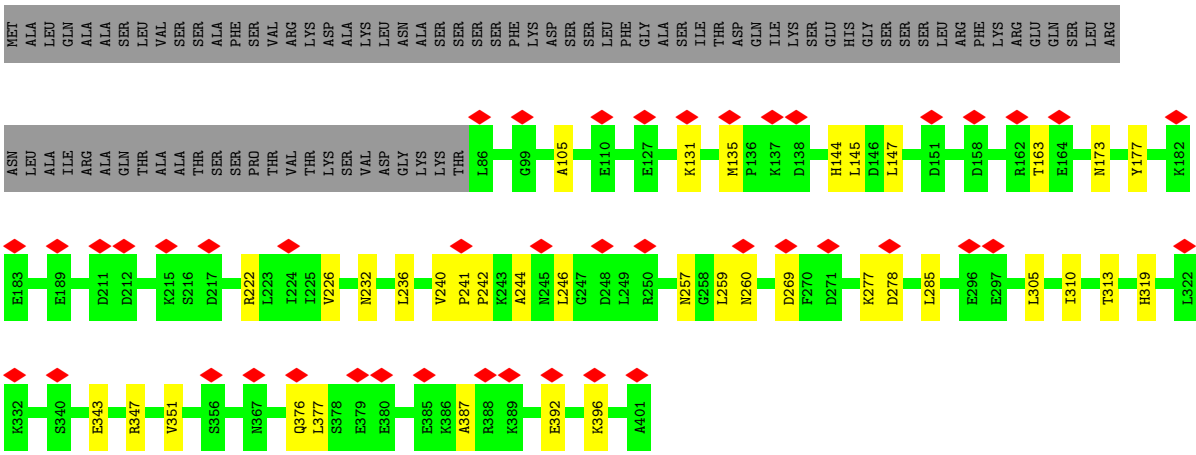
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain B:

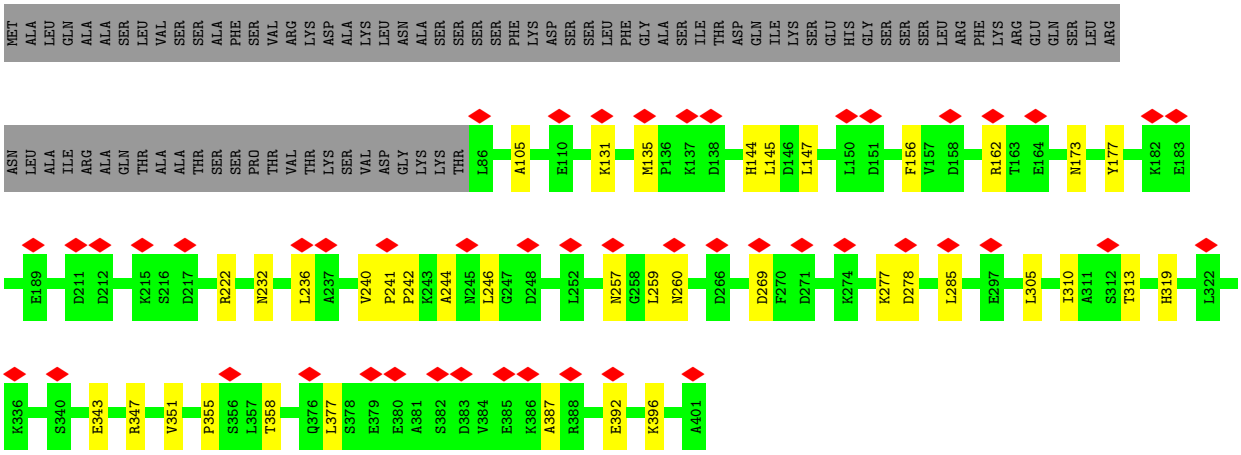


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

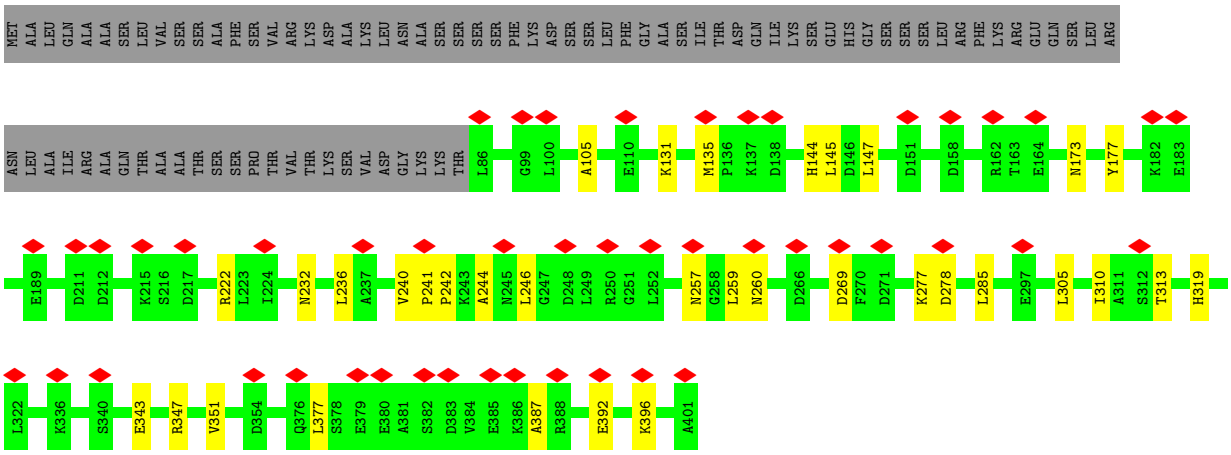
Chain C:



• Molecule 1: Protochlorophyllide reductase B, chloroplastic

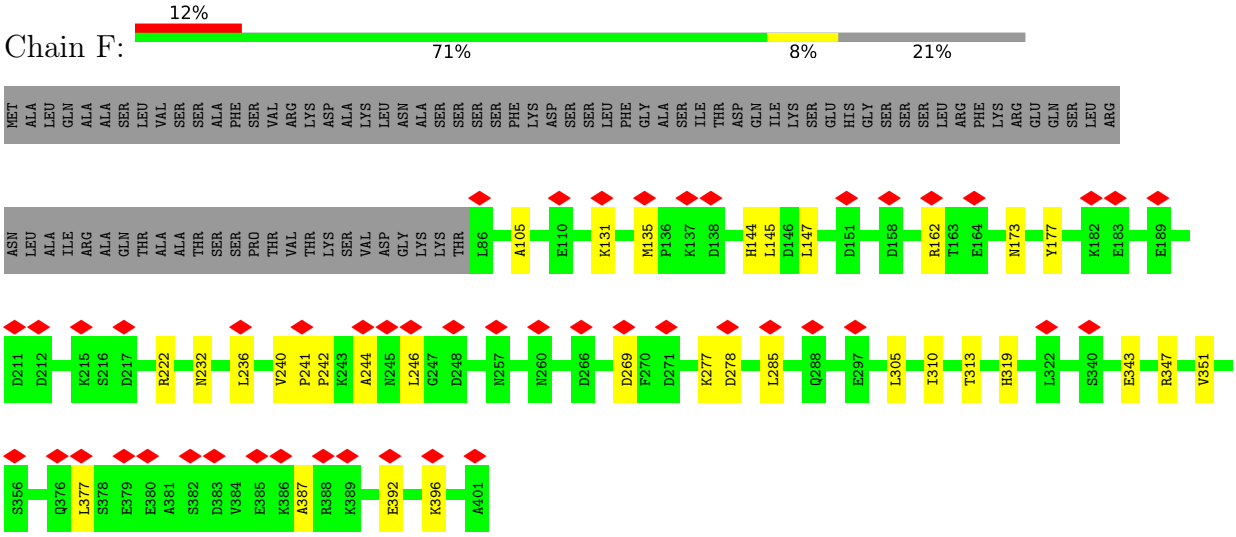


• Molecule 1: Protochlorophyllide reductase B, chloroplastic



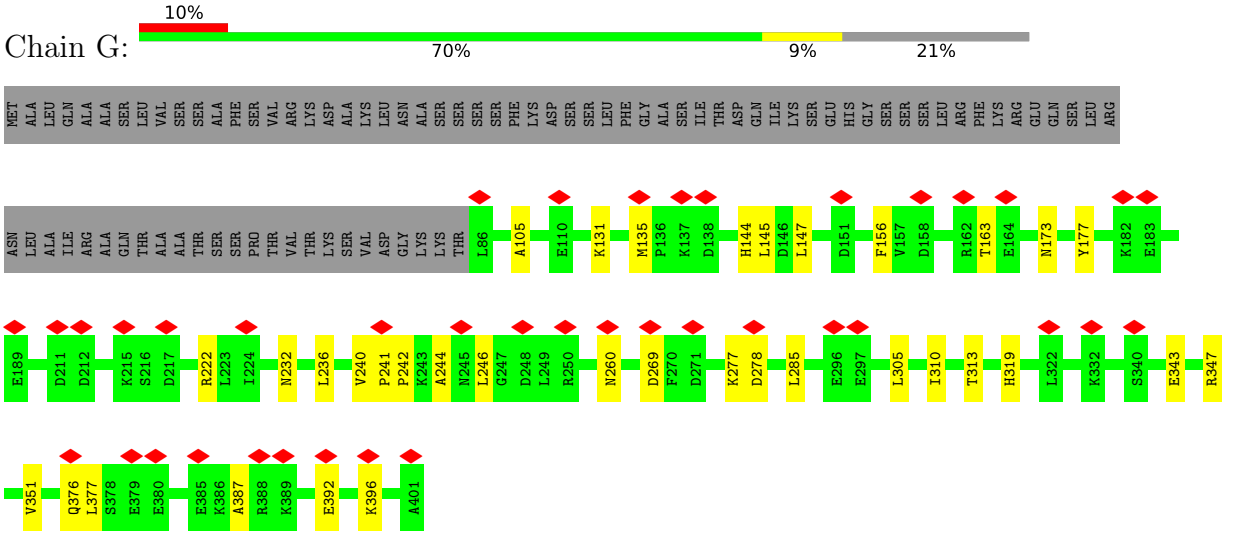
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain F:



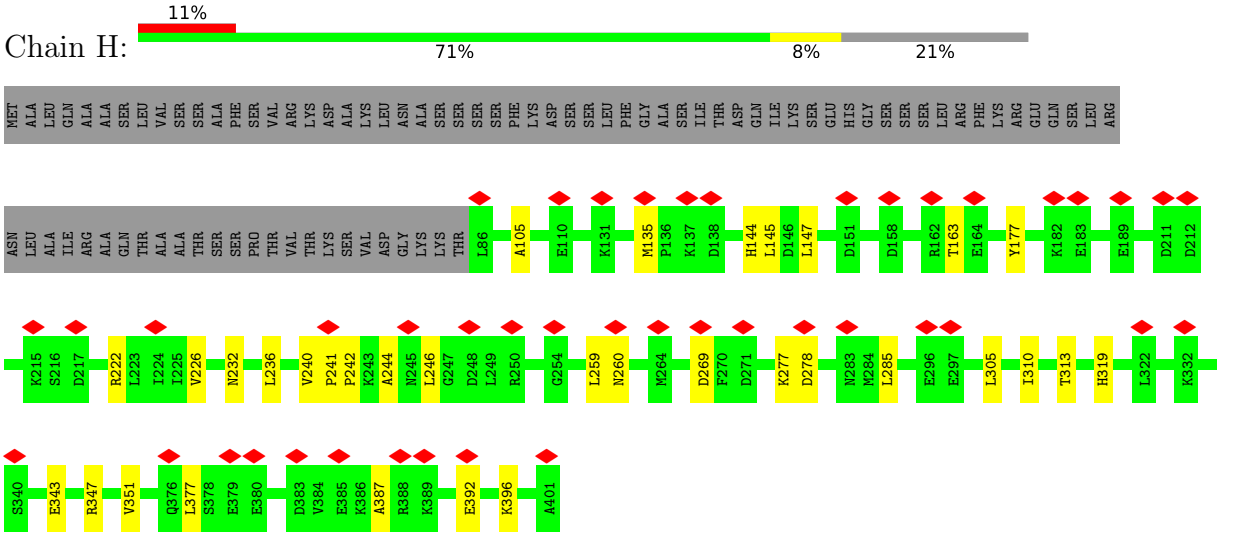
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain G:



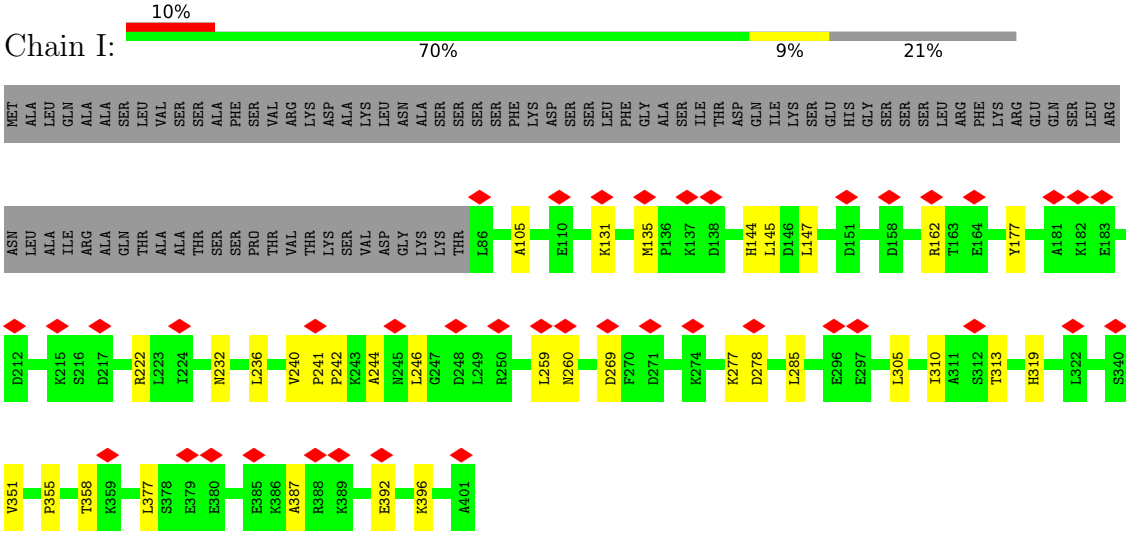
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain H:



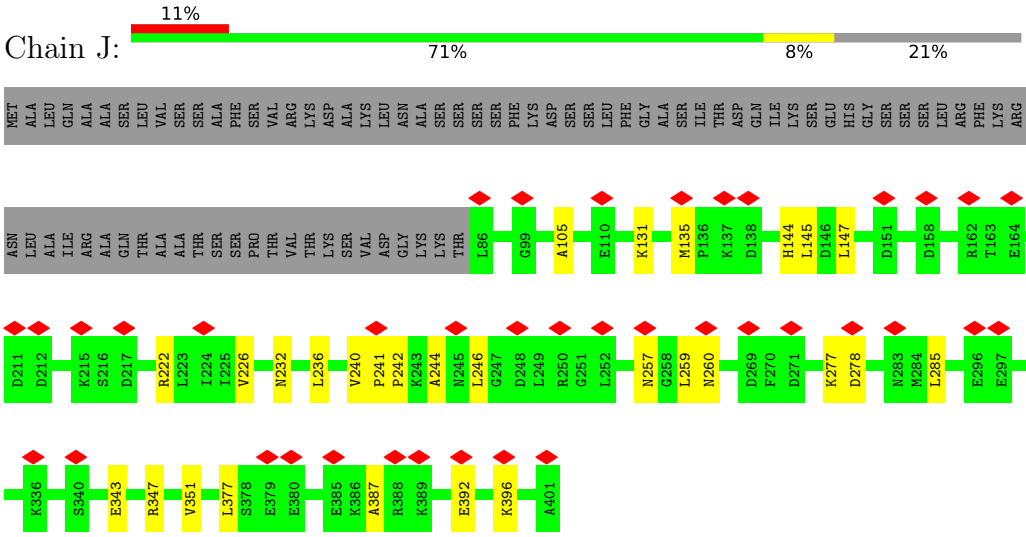
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain I:



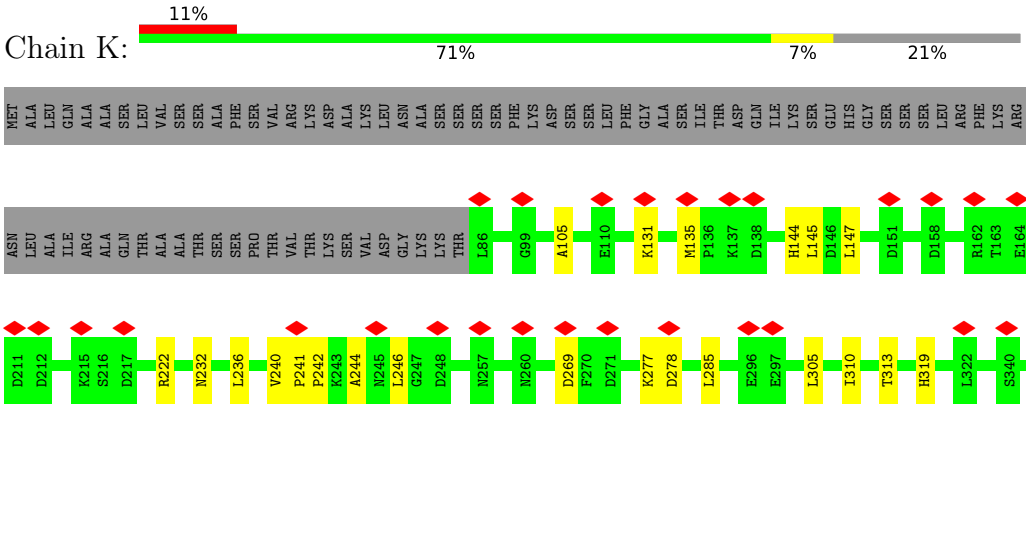
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

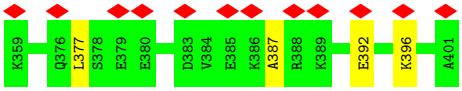
Chain J:



• Molecule 1: Protochlorophyllide reductase B, chloroplastic

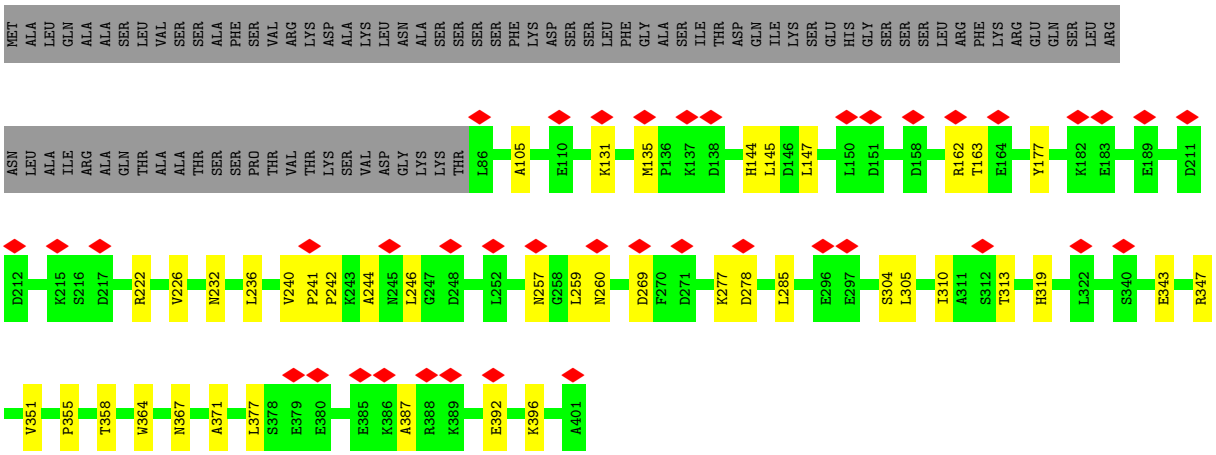
Chain K:





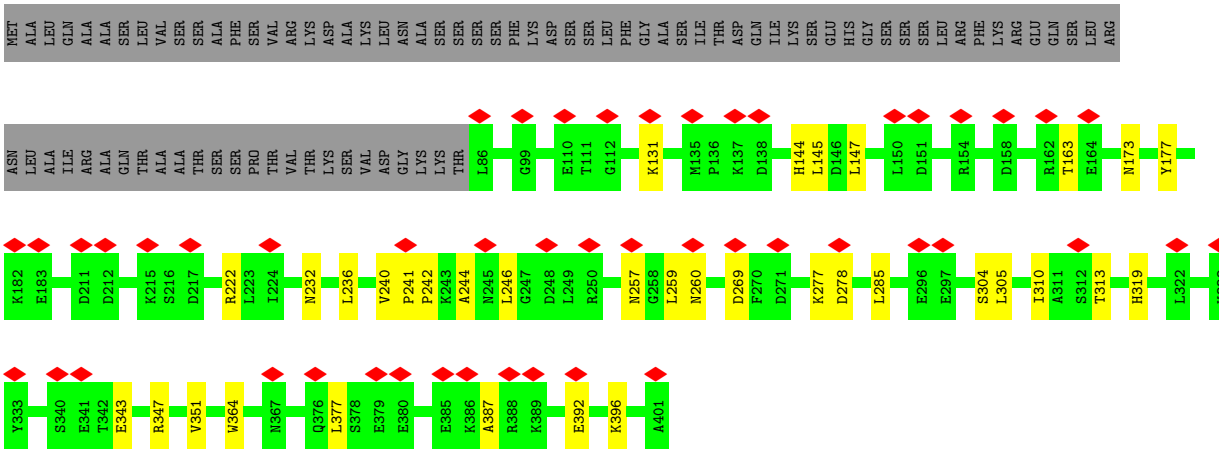
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain L:



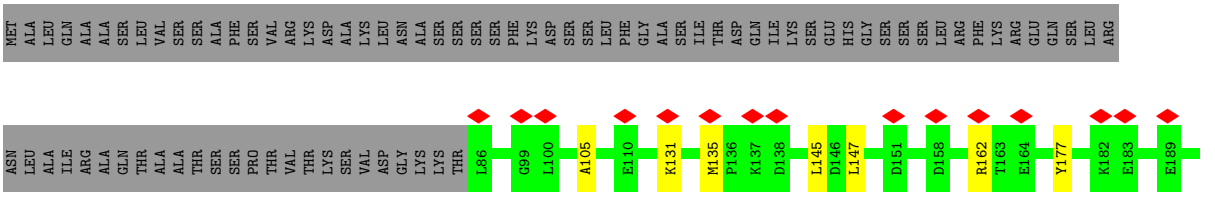
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

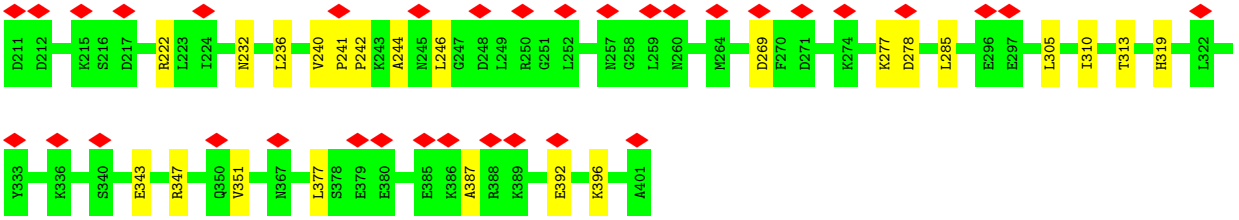
Chain M:



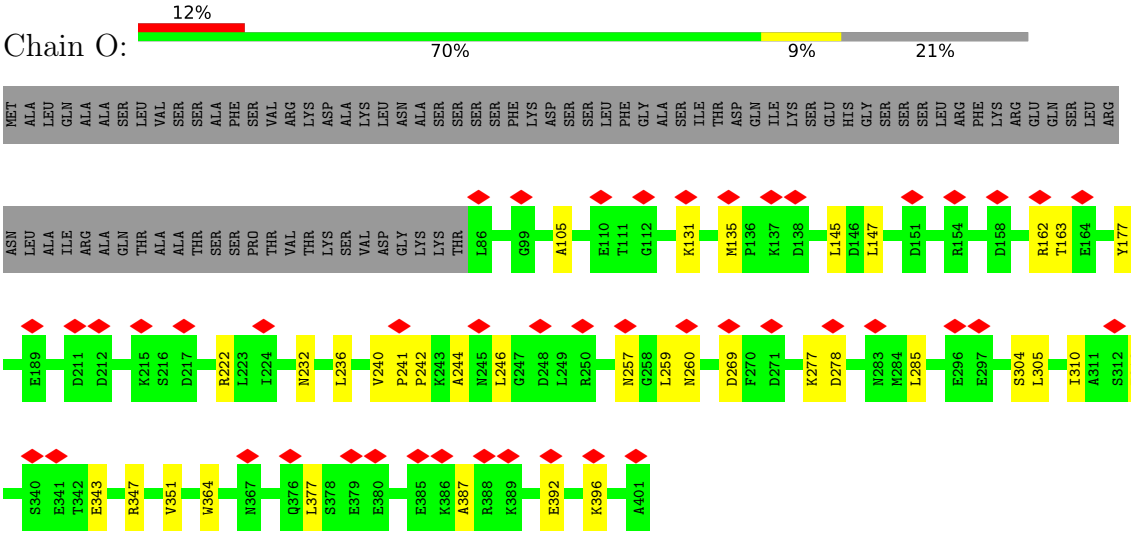
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain N:

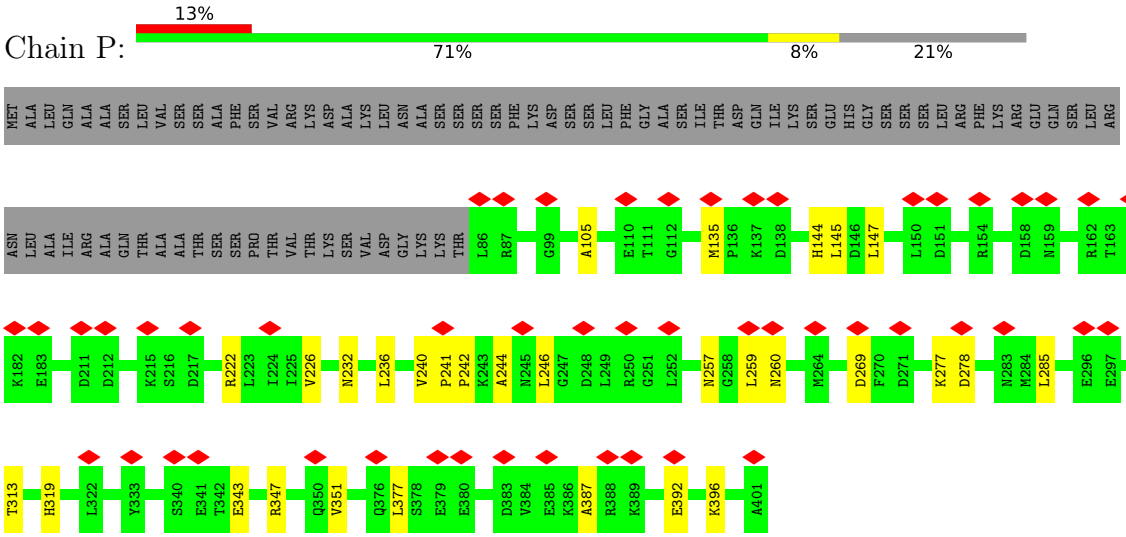




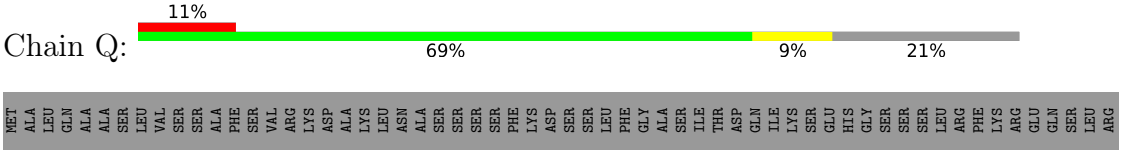
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

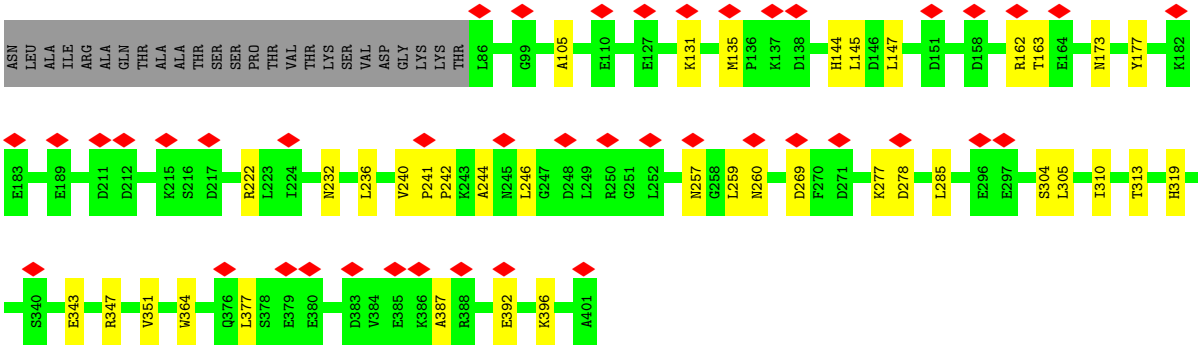


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

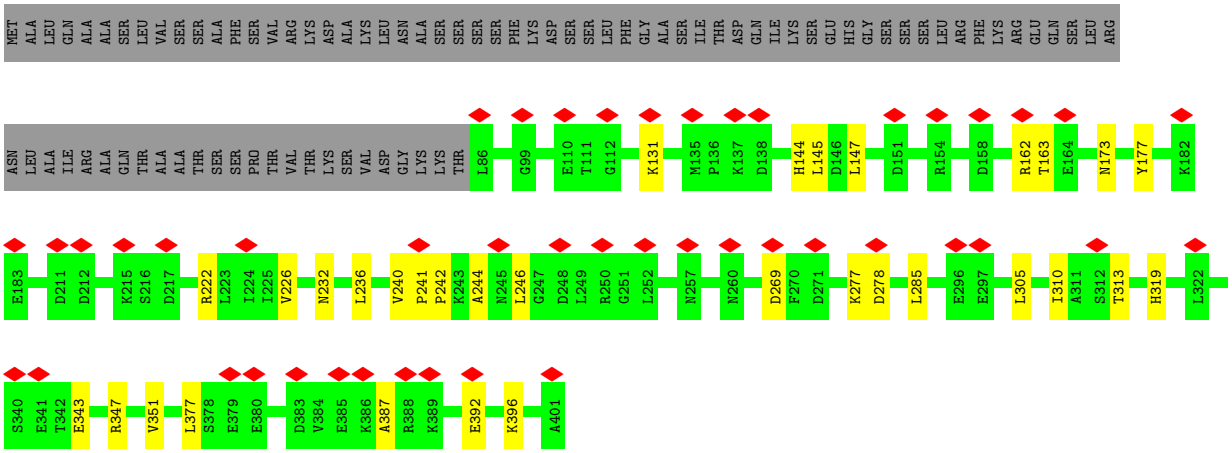


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

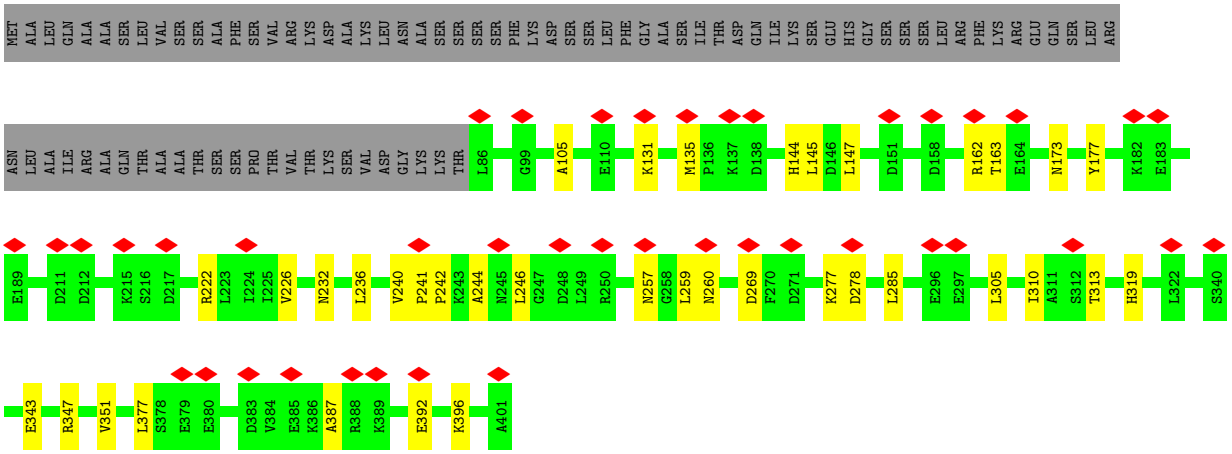




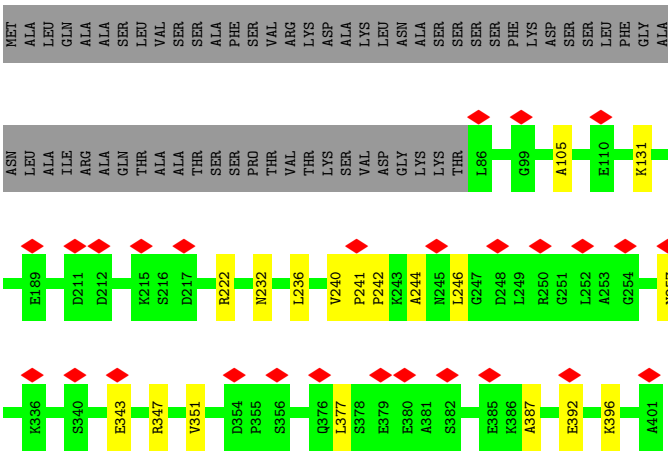
• Molecule 1: Protochlorophyllide reductase B, chloroplastic



• Molecule 1: Protochlorophyllide reductase B, chloroplastic

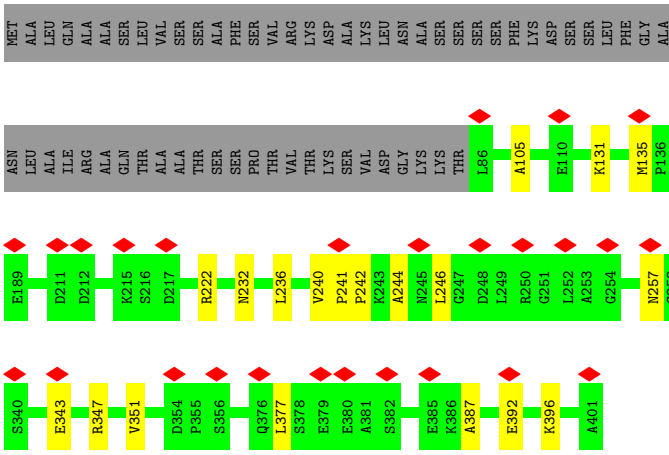


• Molecule 1: Protochlorophyllide reductase B, chloroplastic



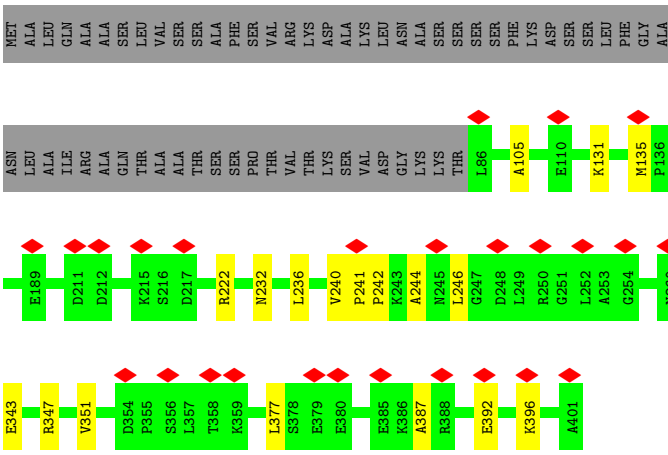
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain V:



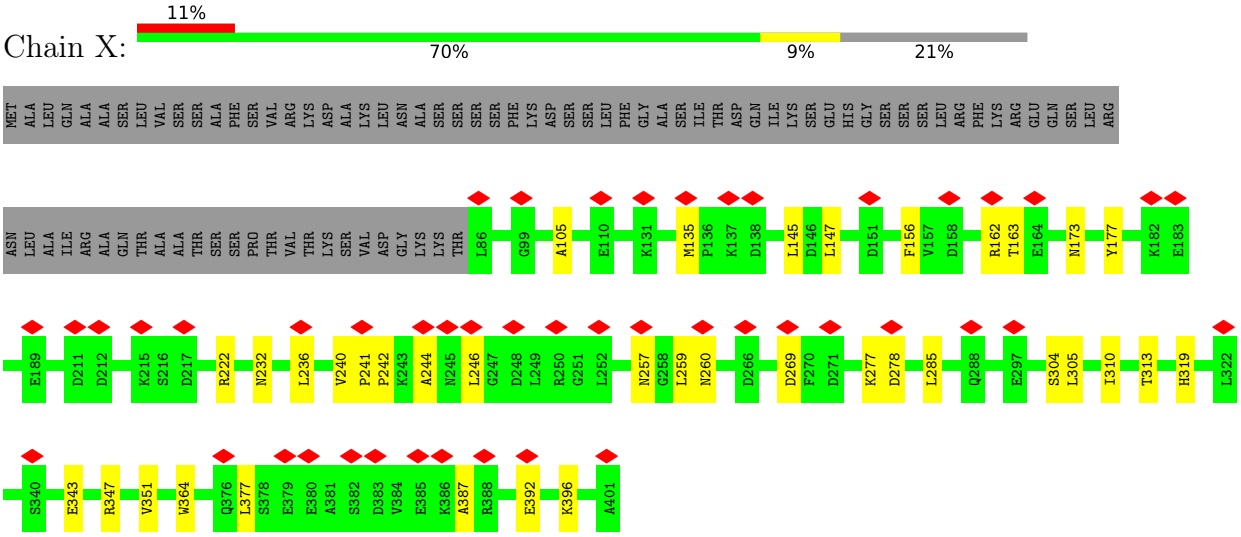
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain W:



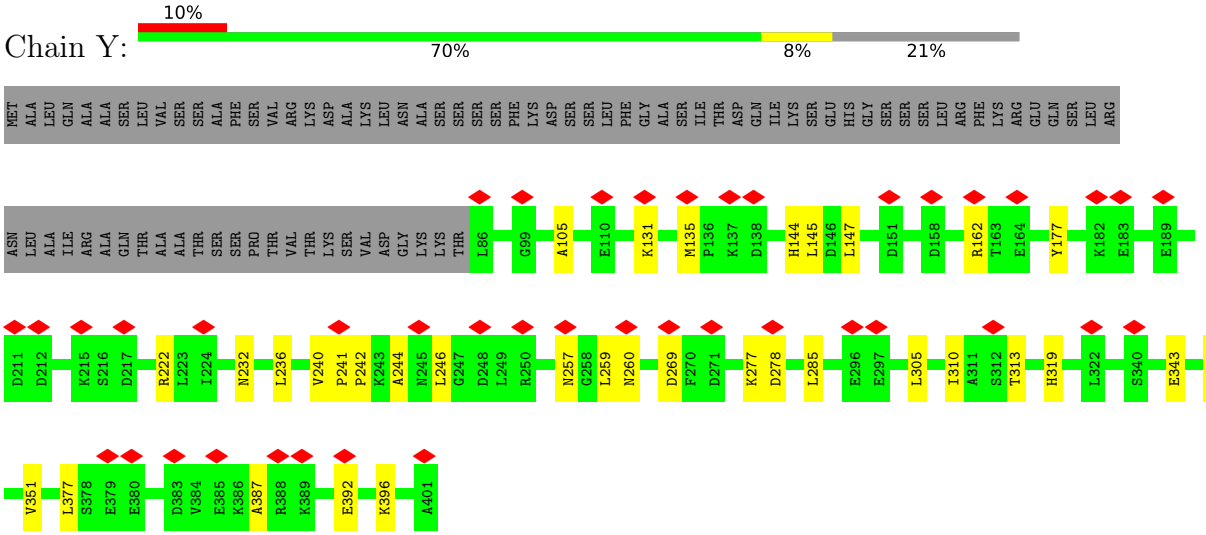
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain X:



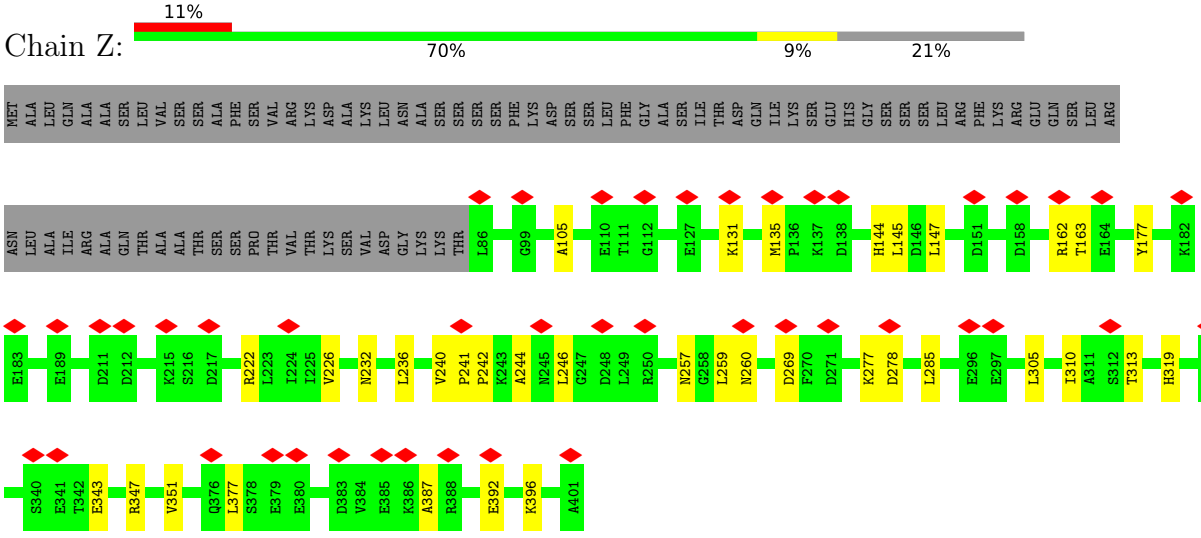
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain Y:



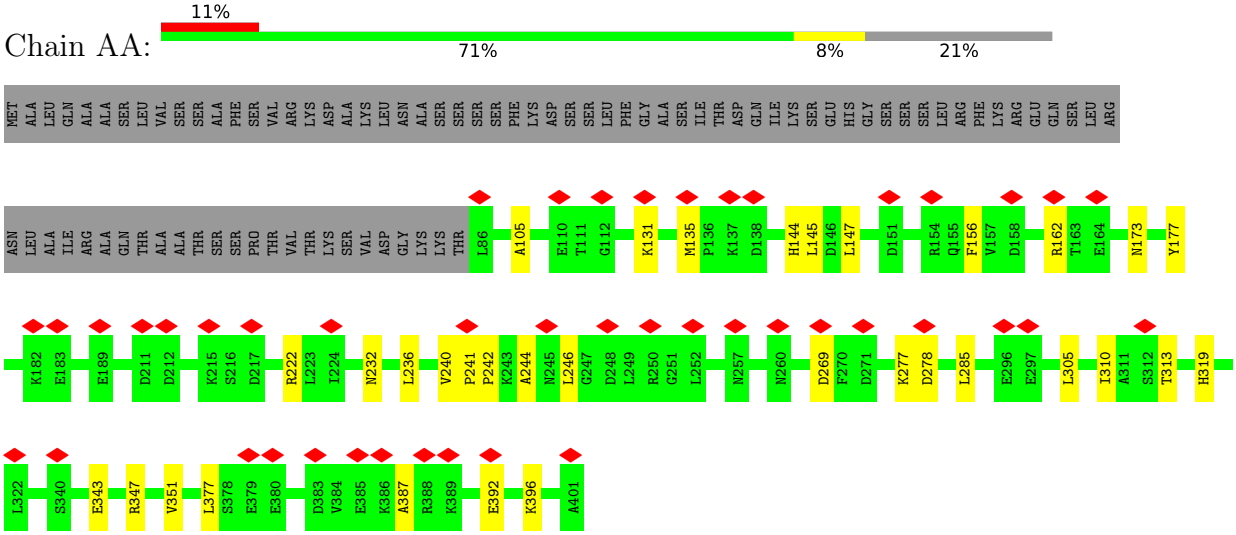
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain Z:



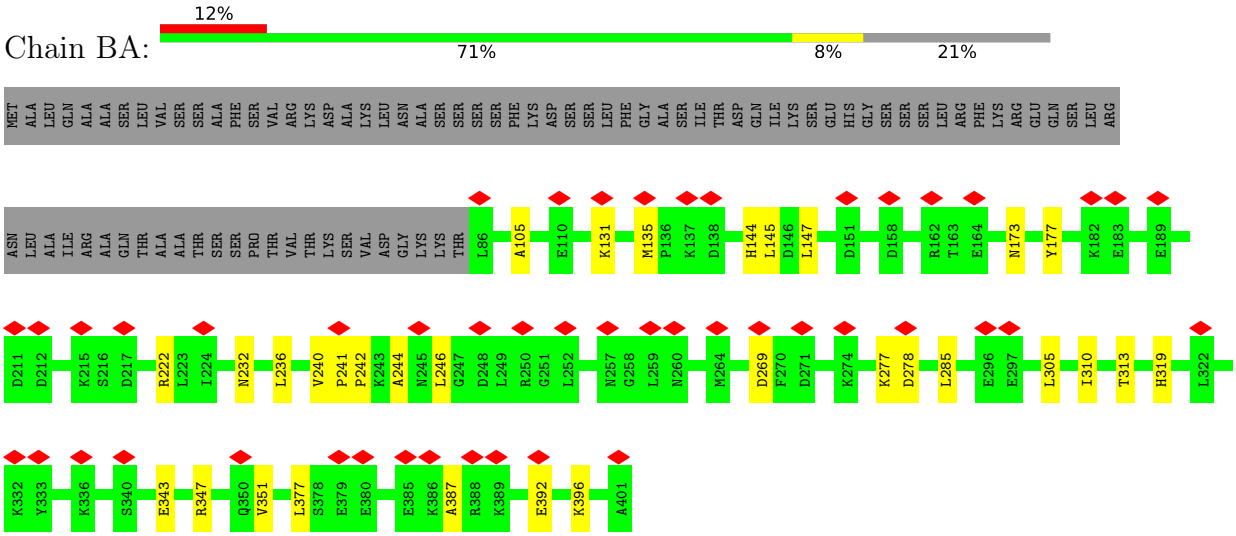
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AA:



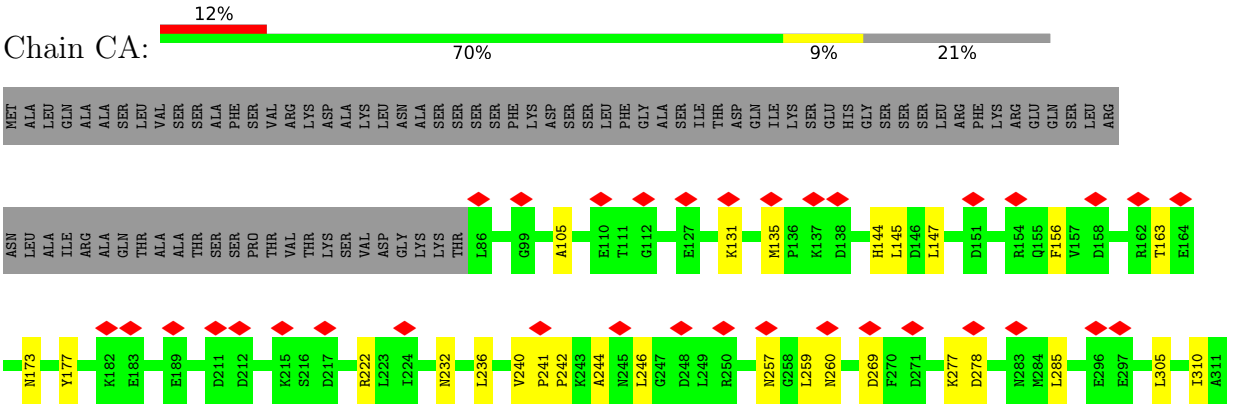
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

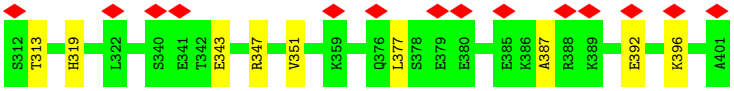
Chain BA:



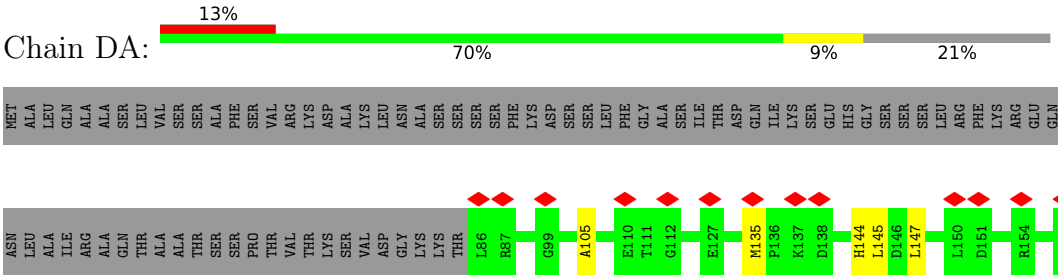
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CA:

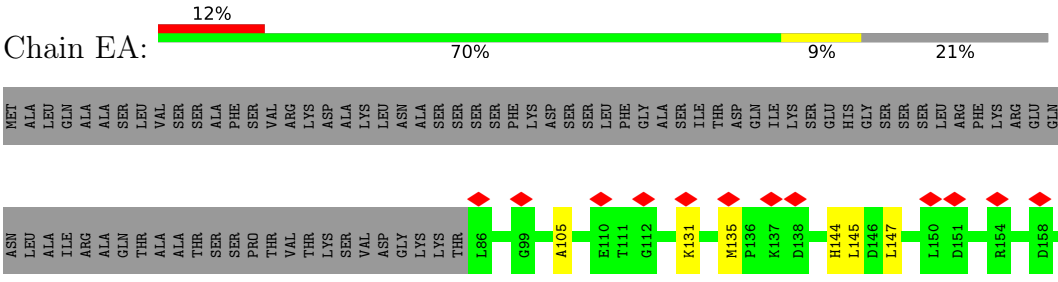




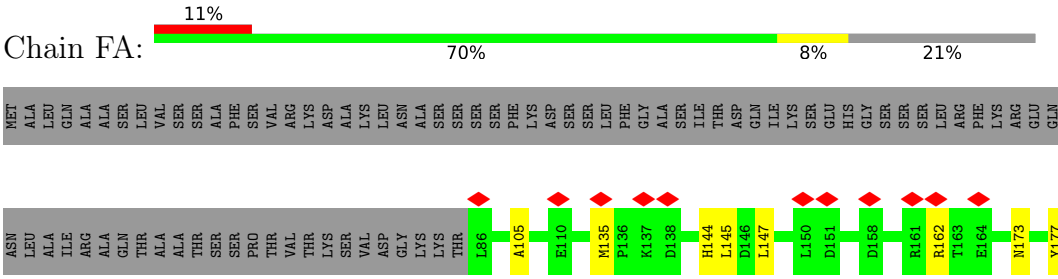
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

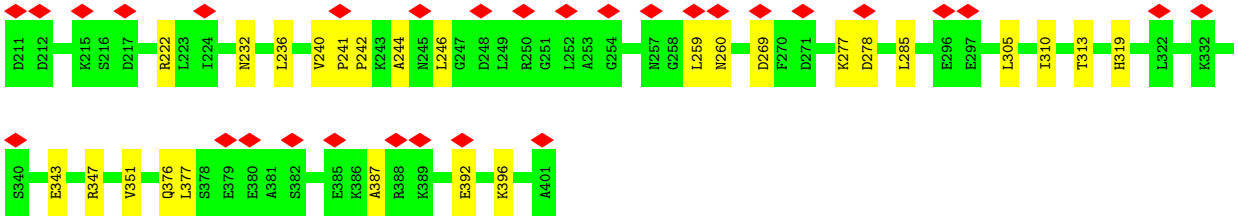


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

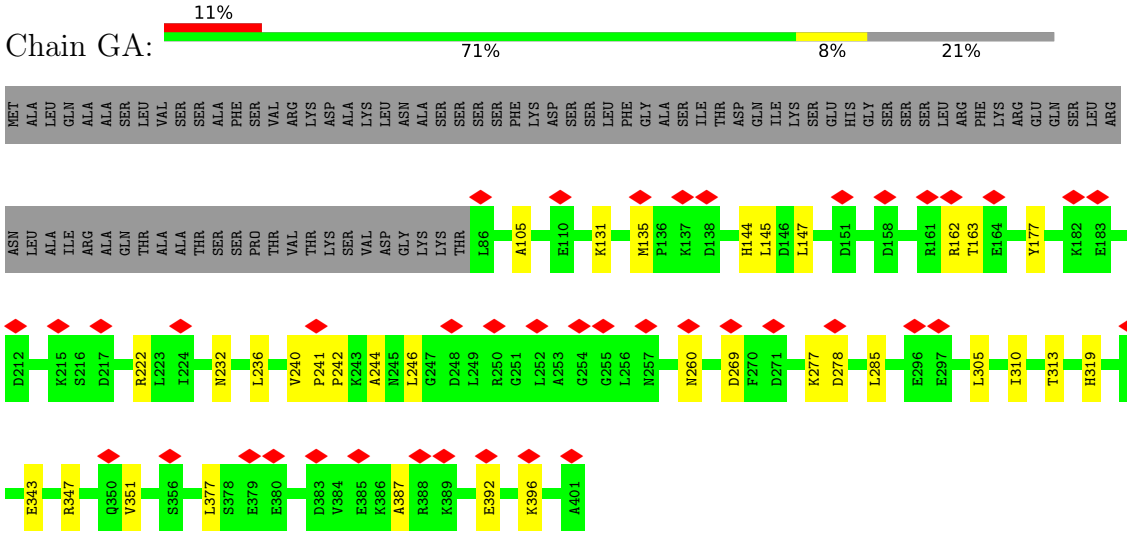


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

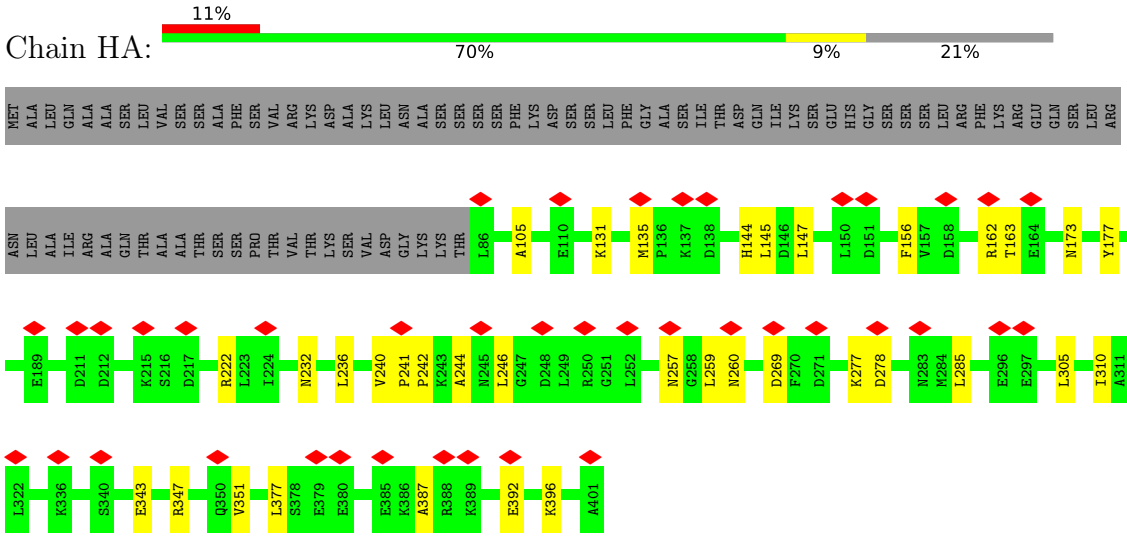




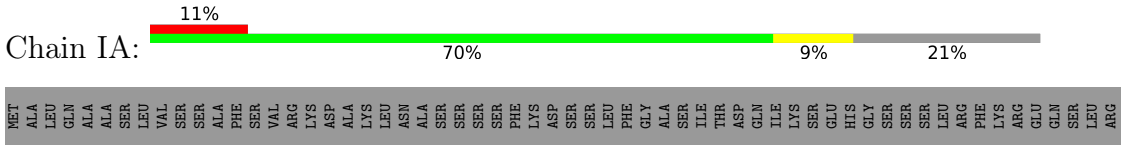
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

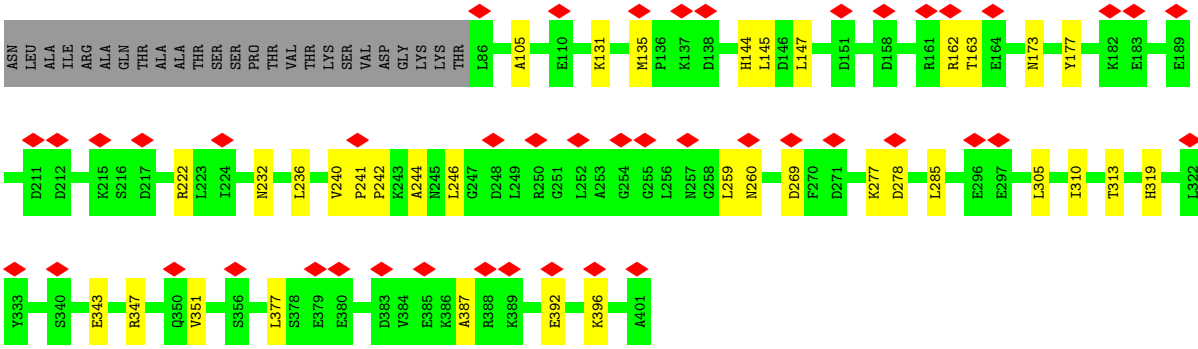


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

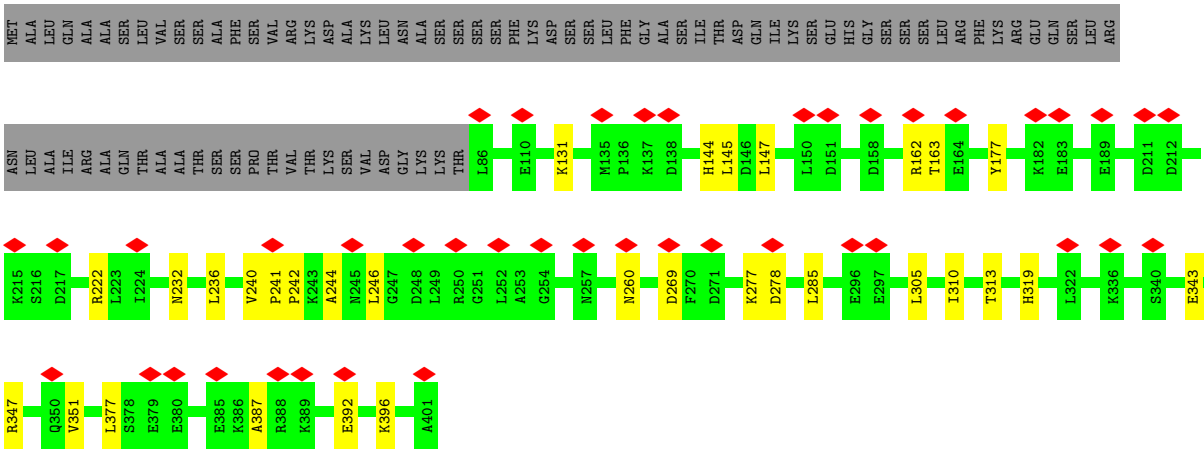


• Molecule 1: Protochlorophyllide reductase B, chloroplastic

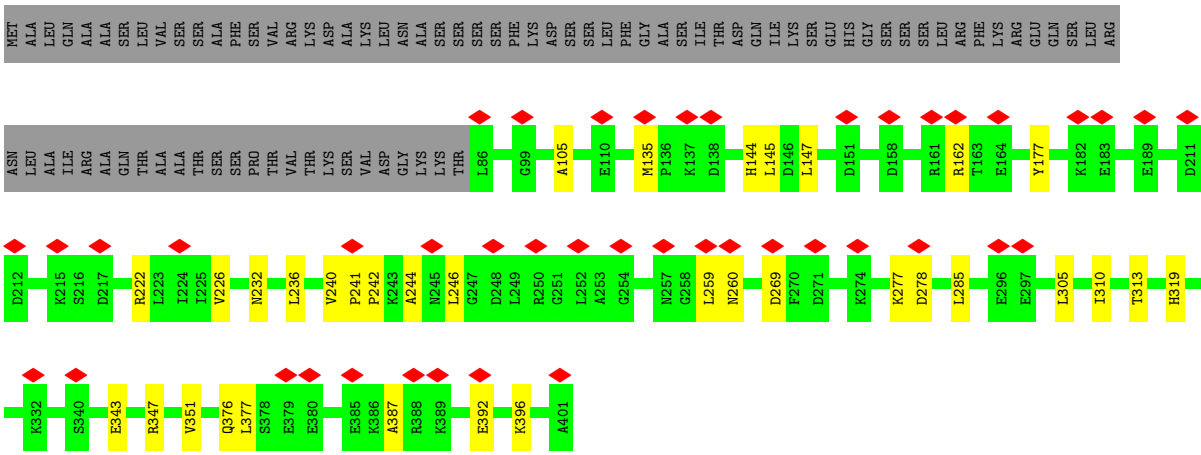




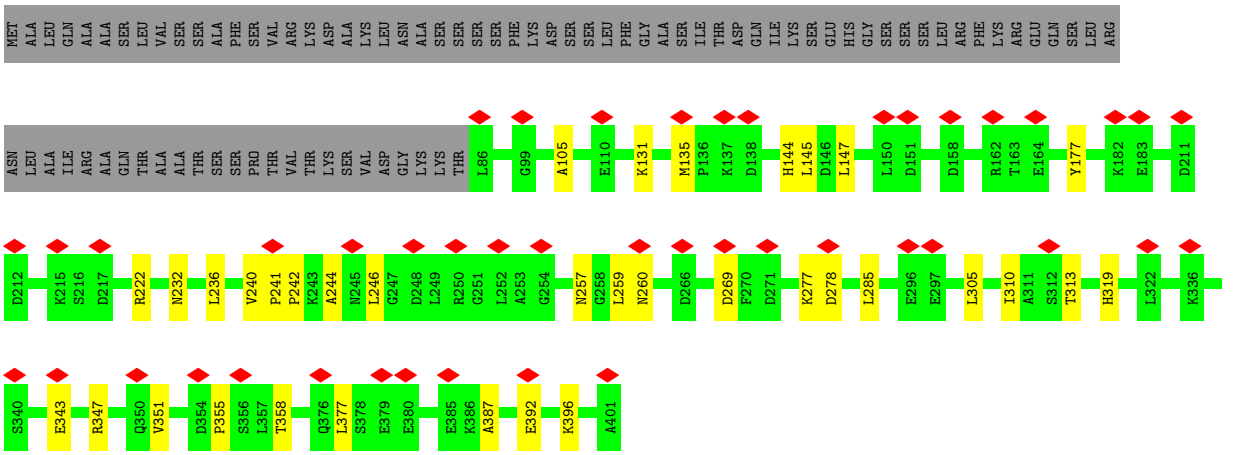
• Molecule 1: Protochlorophyllide reductase B, chloroplastic



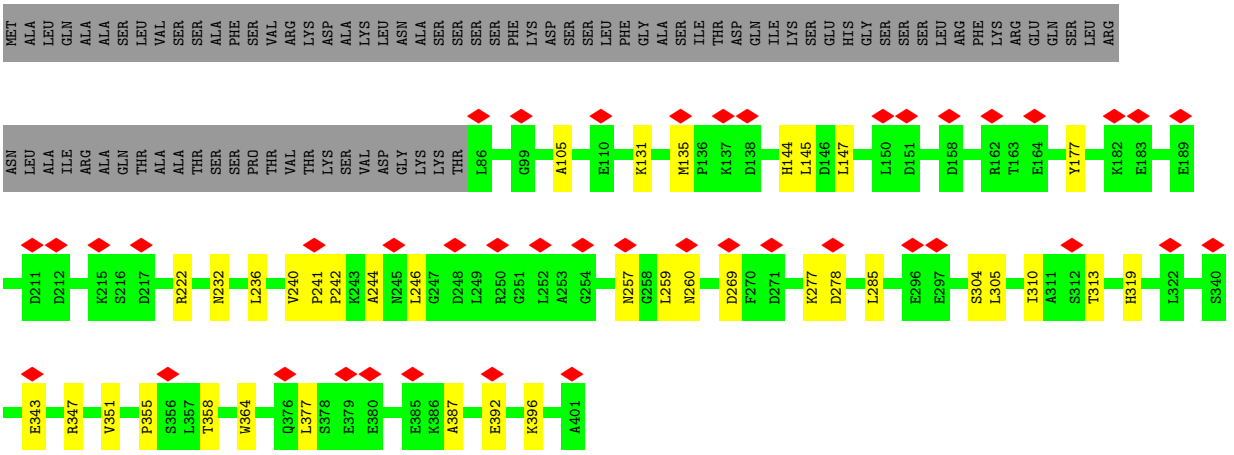
• Molecule 1: Protochlorophyllide reductase B, chloroplastic



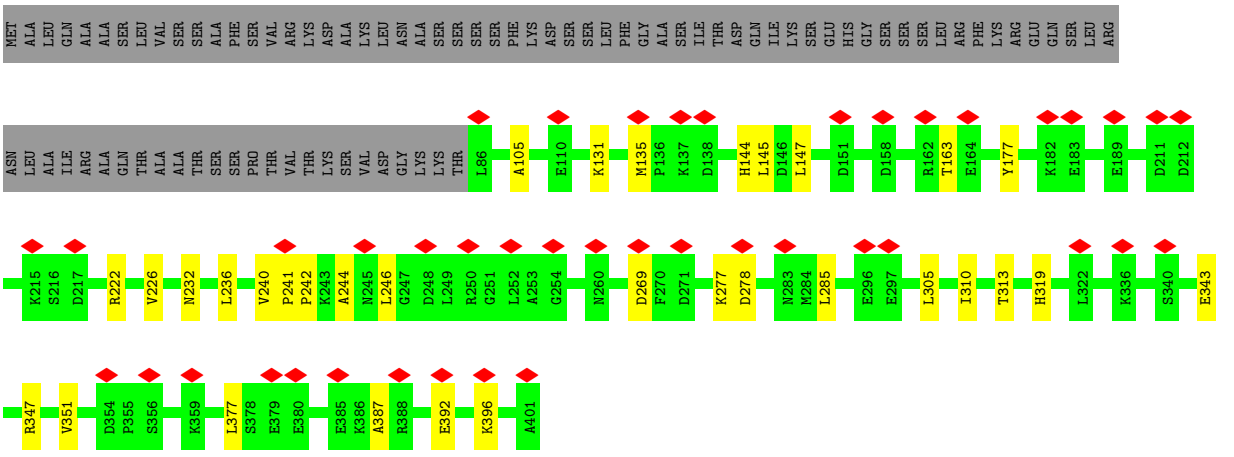
• Molecule 1: Protochlorophyllide reductase B, chloroplastic



• Molecule 1: Protochlorophyllide reductase B, chloroplastic

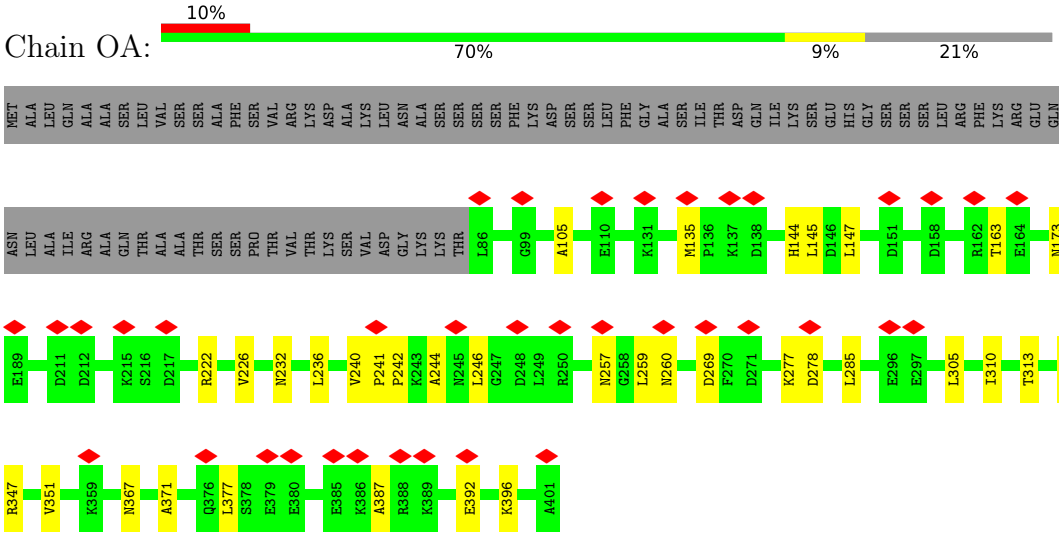


• Molecule 1: Protochlorophyllide reductase B, chloroplastic



• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain OA:


10%
70%
9%
21%
MET ALA LEU GLN ALA ALA SER LEU VAL SER SER ALA PHE SER VAL ARG LYS ASP ALA LYS LEU ASN ALA SER SER SER PHE LYS ASP SER SER LEU PHE GLY ALA SER ILE THR ASP GLN ILE LYS SER GLU HIS GLY SER SER SER LEU ARG PHE LYS ARG GLU GLN SER LEU ARG
ASN LEU ALA ILE ARG ALA GLN THR ALA ALA THR SER SER PRO THR VAL THR LYS SER VAL ASP GLY LYS LYS THR L86 G99 A105 E110 K131 M135 P136 K137 D138 H144 L145 D146 L147 D151 D158 R162 T163 E164 N173 Y177 K182 E183
E189 D211 D212 K215 S216 D217 R222 V226 N232 L236 V240 P241 P242 K243 A244 N245 L246 G247 D248 L249 R250 N257 G258 L259 N260 D269 P270 D271 K277 D278 L285 E296 E297 L305 I310 T313 H319 L322 S340 E343
R347 V351 K359 N367 A371 Q376 L377 S378 E379 E380 E385 K386 A387 R388 K389 E392 K396 A401

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=50.34°, rise=43.1 Å, axial sym=C2	Depositor
Number of segments used	17898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	73.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	427.51987, 427.51987, 427.51987	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113333, 1.113333, 1.113333	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PMR, NDP, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/2470	0.57	0/3342
1	AA	0.37	0/2470	0.57	0/3342
1	B	0.38	0/2470	0.57	0/3342
1	BA	0.37	0/2470	0.57	0/3342
1	C	0.37	0/2470	0.57	0/3342
1	CA	0.37	0/2470	0.57	0/3342
1	D	0.37	0/2470	0.57	0/3342
1	DA	0.37	0/2470	0.57	0/3342
1	E	0.37	0/2470	0.57	0/3342
1	EA	0.37	0/2470	0.57	0/3342
1	F	0.37	0/2470	0.57	0/3342
1	FA	0.37	0/2470	0.57	0/3342
1	G	0.37	0/2470	0.57	0/3342
1	GA	0.38	0/2470	0.57	0/3342
1	H	0.37	0/2470	0.57	0/3342
1	HA	0.37	0/2470	0.57	0/3342
1	I	0.37	0/2470	0.57	0/3342
1	IA	0.37	0/2470	0.57	0/3342
1	J	0.37	0/2470	0.57	0/3342
1	JA	0.37	0/2470	0.57	0/3342
1	K	0.37	0/2470	0.57	0/3342
1	KA	0.37	0/2470	0.57	0/3342
1	L	0.37	0/2470	0.57	0/3342
1	LA	0.37	0/2470	0.57	0/3342
1	M	0.37	0/2470	0.57	0/3342
1	MA	0.37	0/2470	0.57	0/3342
1	N	0.37	0/2470	0.57	0/3342
1	NA	0.37	0/2470	0.57	0/3342
1	O	0.37	0/2470	0.57	0/3342
1	OA	0.37	0/2470	0.57	0/3342
1	P	0.38	0/2470	0.57	0/3342
1	Q	0.37	0/2470	0.57	0/3342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	R	0.37	0/2470	0.57	0/3342
1	S	0.37	0/2470	0.57	0/3342
1	T	0.37	0/2470	0.57	0/3342
1	V	0.37	0/2470	0.57	0/3342
1	W	0.38	0/2470	0.57	0/3342
1	X	0.37	0/2470	0.57	0/3342
1	Y	0.37	0/2470	0.57	0/3342
1	Z	0.37	0/2470	0.57	0/3342
All	All	0.37	0/98800	0.57	0/133680

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2421	2397	2417	26	0
1	AA	2421	2397	2417	27	0
1	B	2421	2397	2417	27	0
1	BA	2421	2397	2417	24	0
1	C	2421	2397	2417	30	0
1	CA	2421	2397	2417	32	0
1	D	2421	2397	2417	32	0
1	DA	2421	2397	2417	27	0
1	E	2421	2397	2417	28	0
1	EA	2421	2397	2417	31	0
1	F	2421	2397	2417	24	0
1	FA	2421	2397	2417	27	0
1	G	2421	2397	2417	28	0
1	GA	2421	2397	2417	27	0
1	H	2421	2397	2417	25	0
1	HA	2421	2397	2417	32	0
1	I	2421	2397	2417	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IA	2421	2397	2417	29	0
1	J	2421	2397	2417	26	0
1	JA	2421	2397	2417	27	0
1	K	2421	2397	2417	23	0
1	KA	2421	2397	2417	27	0
1	L	2421	2397	2417	34	0
1	LA	2421	2397	2417	29	0
1	M	2421	2397	2417	30	0
1	MA	2421	2397	2417	30	0
1	N	2421	2397	2417	22	0
1	NA	2421	2397	2417	24	0
1	O	2421	2397	2417	31	0
1	OA	2421	2397	2417	30	0
1	P	2421	2397	2417	27	0
1	Q	2421	2397	2417	34	0
1	R	2421	2397	2417	26	0
1	S	2421	2397	2417	35	0
1	T	2421	2397	2417	31	0
1	V	2421	2397	2417	30	0
1	W	2421	2397	2417	26	0
1	X	2421	2397	2417	30	0
1	Y	2421	2397	2417	31	0
1	Z	2421	2397	2417	33	0
2	A	48	0	26	2	0
2	AA	48	0	26	1	0
2	B	48	0	26	1	0
2	BA	48	0	26	1	0
2	C	48	0	26	2	0
2	CA	48	0	26	1	0
2	D	48	0	26	1	0
2	DA	48	0	26	1	0
2	E	48	0	26	1	0
2	EA	48	0	26	1	0
2	F	48	0	26	1	0
2	FA	48	0	26	1	0
2	G	48	0	26	1	0
2	GA	48	0	26	0	0
2	H	48	0	26	1	0
2	HA	48	0	26	1	0
2	I	48	0	26	0	0
2	IA	48	0	26	1	0
2	J	48	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JA	48	0	26	0	0
2	K	48	0	26	0	0
2	KA	48	0	26	1	0
2	L	48	0	26	1	0
2	LA	48	0	26	0	0
2	M	48	0	26	1	0
2	MA	48	0	26	0	0
2	N	48	0	26	0	0
2	NA	48	0	26	1	0
2	O	48	0	26	0	0
2	OA	48	0	26	2	0
2	P	48	0	26	1	0
2	Q	48	0	26	1	0
2	R	48	0	26	2	0
2	S	48	0	26	2	0
2	T	48	0	26	1	0
2	V	48	0	26	1	0
2	W	48	0	26	1	0
2	X	48	0	26	1	0
2	Y	48	0	26	0	0
2	Z	48	0	26	1	0
3	A	45	0	31	4	0
3	AA	45	0	31	4	0
3	B	45	0	31	4	0
3	BA	45	0	31	4	0
3	C	45	0	31	4	0
3	CA	45	0	31	4	0
3	D	45	0	31	4	0
3	DA	45	0	31	4	0
3	E	45	0	31	4	0
3	EA	45	0	31	4	0
3	F	45	0	31	4	0
3	FA	45	0	31	4	0
3	G	45	0	31	4	0
3	GA	45	0	31	4	0
3	H	45	0	31	4	0
3	HA	45	0	31	4	0
3	I	45	0	31	4	0
3	IA	45	0	31	4	0
3	J	45	0	31	4	0
3	JA	45	0	31	4	0
3	K	45	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	KA	45	0	31	4	0
3	L	45	0	31	4	0
3	LA	45	0	31	4	0
3	M	45	0	31	4	0
3	MA	45	0	31	4	0
3	N	45	0	31	4	0
3	NA	45	0	31	4	0
3	O	45	0	31	4	0
3	OA	45	0	31	4	0
3	P	45	0	31	4	0
3	Q	45	0	31	4	0
3	R	45	0	31	4	0
3	S	45	0	31	4	0
3	T	45	0	31	4	0
3	V	45	0	31	4	0
3	W	45	0	31	4	0
3	X	45	0	31	4	0
3	Y	45	0	31	4	0
3	Z	45	0	31	4	0
4	A	23	0	16	1	0
4	AA	23	0	16	1	0
4	B	23	0	16	1	0
4	BA	23	0	16	1	0
4	C	23	0	16	1	0
4	CA	23	0	16	1	0
4	D	23	0	16	1	0
4	DA	23	0	16	1	0
4	E	23	0	16	1	0
4	EA	23	0	16	1	0
4	F	23	0	16	1	0
4	FA	23	0	16	1	0
4	G	23	0	16	1	0
4	GA	23	0	16	1	0
4	H	23	0	16	1	0
4	HA	23	0	16	1	0
4	I	23	0	16	1	0
4	IA	23	0	16	1	0
4	J	23	0	16	1	0
4	JA	23	0	16	1	0
4	K	23	0	16	1	0
4	KA	23	0	16	1	0
4	L	23	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	LA	23	0	16	1	0
4	M	23	0	16	1	0
4	MA	23	0	16	1	0
4	N	23	0	16	1	0
4	NA	23	0	16	1	0
4	O	23	0	16	1	0
4	OA	23	0	16	1	0
4	P	23	0	16	1	0
4	Q	23	0	16	1	0
4	R	23	0	16	1	0
4	S	23	0	16	1	0
4	T	23	0	16	1	0
4	V	23	0	16	1	0
4	W	23	0	16	1	0
4	X	23	0	16	1	0
4	Y	23	0	16	1	0
4	Z	23	0	16	1	0
All	All	101480	95880	99600	1013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1013) 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)
1:N:241:PRO:HG2	4:N:503:LMG:HC8	1.56	0.88
1:O:241:PRO:HG2	4:O:503:LMG:HC8	1.56	0.88
1:Z:241:PRO:HG2	4:Z:503:LMG:HC8	1.56	0.88
1:B:241:PRO:HG2	4:B:503:LMG:HC8	1.56	0.88
1:JA:241:PRO:HG2	4:JA:503:LMG:HC8	1.56	0.87
1:R:241:PRO:HG2	4:R:503:LMG:HC8	1.56	0.87
1:E:241:PRO:HG2	4:E:503:LMG:HC8	1.56	0.87
1:H:241:PRO:HG2	4:H:503:LMG:HC8	1.56	0.87
1:J:241:PRO:HG2	4:J:503:LMG:HC8	1.56	0.87
1:K:241:PRO:HG2	4:K:503:LMG:HC8	1.56	0.87
1:V:241:PRO:HG2	4:V:503:LMG:HC8	1.56	0.87
1:HA:241:PRO:HG2	4:HA:503:LMG:HC8	1.56	0.87
1:M:241:PRO:HG2	4:M:503:LMG:HC8	1.56	0.87
1:MA:241:PRO:HG2	4:MA:503:LMG:HC8	1.56	0.87
1:CA:241:PRO:HG2	4:CA:503:LMG:HC8	1.56	0.87
1:NA:241:PRO:HG2	4:NA:503:LMG:HC8	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:241:PRO:HG2	4:Q:503:LMG:HC8	1.56	0.87
1:I:241:PRO:HG2	4:I:503:LMG:HC8	1.56	0.87
1:OA:241:PRO:HG2	4:OA:503:LMG:HC8	1.56	0.87
1:P:241:PRO:HG2	4:P:503:LMG:HC8	1.56	0.86
1:W:241:PRO:HG2	4:W:503:LMG:HC8	1.56	0.86
1:X:241:PRO:HG2	4:X:503:LMG:HC8	1.56	0.86
1:A:241:PRO:HG2	4:A:503:LMG:HC8	1.56	0.86
1:C:241:PRO:HG2	4:C:503:LMG:HC8	1.56	0.86
1:F:241:PRO:HG2	4:F:503:LMG:HC8	1.56	0.86
1:BA:241:PRO:HG2	4:BA:503:LMG:HC8	1.56	0.86
1:FA:241:PRO:HG2	4:FA:503:LMG:HC8	1.56	0.86
1:KA:241:PRO:HG2	4:KA:503:LMG:HC8	1.56	0.86
1:L:241:PRO:HG2	4:L:503:LMG:HC8	1.56	0.86
1:GA:241:PRO:HG2	4:GA:503:LMG:HC8	1.56	0.86
1:IA:241:PRO:HG2	4:IA:503:LMG:HC8	1.56	0.86
1:S:241:PRO:HG2	4:S:503:LMG:HC8	1.56	0.86
1:AA:241:PRO:HG2	4:AA:503:LMG:HC8	1.56	0.86
1:Y:241:PRO:HG2	4:Y:503:LMG:HC8	1.56	0.85
1:LA:241:PRO:HG2	4:LA:503:LMG:HC8	1.56	0.85
1:EA:241:PRO:HG2	4:EA:503:LMG:HC8	1.56	0.85
1:DA:241:PRO:HG2	4:DA:503:LMG:HC8	1.56	0.85
1:D:241:PRO:HG2	4:D:503:LMG:HC8	1.56	0.84
1:T:241:PRO:HG2	4:T:503:LMG:HC8	1.56	0.84
1:G:241:PRO:HG2	4:G:503:LMG:HC8	1.56	0.84
1:GA:222:ARG:NH1	1:GA:351:VAL:O	2.24	0.71
1:JA:222:ARG:NH1	1:JA:351:VAL:O	2.24	0.71
1:Q:222:ARG:NH1	1:Q:351:VAL:O	2.24	0.71
1:NA:222:ARG:NH1	1:NA:351:VAL:O	2.24	0.71
1:L:222:ARG:NH1	1:L:351:VAL:O	2.24	0.70
1:B:222:ARG:NH1	1:B:351:VAL:O	2.24	0.70
1:C:222:ARG:NH1	1:C:351:VAL:O	2.24	0.70
1:E:222:ARG:NH1	1:E:351:VAL:O	2.24	0.70
1:BA:222:ARG:NH1	1:BA:351:VAL:O	2.24	0.70
1:MA:222:ARG:NH1	1:MA:351:VAL:O	2.24	0.70
1:H:222:ARG:NH1	1:H:351:VAL:O	2.24	0.70
1:M:222:ARG:NH1	1:M:351:VAL:O	2.24	0.70
1:O:222:ARG:NH1	1:O:351:VAL:O	2.24	0.70
1:EA:222:ARG:NH1	1:EA:351:VAL:O	2.24	0.70
1:OA:222:ARG:NH1	1:OA:351:VAL:O	2.24	0.70
1:K:222:ARG:NH1	1:K:351:VAL:O	2.24	0.70
1:S:222:ARG:NH1	1:S:351:VAL:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:222:ARG:NH1	1:Z:351:VAL:O	2.24	0.70
1:T:222:ARG:NH1	1:T:351:VAL:O	2.24	0.70
1:DA:222:ARG:NH1	1:DA:351:VAL:O	2.24	0.70
1:X:222:ARG:NH1	1:X:351:VAL:O	2.24	0.70
1:FA:222:ARG:NH1	1:FA:351:VAL:O	2.24	0.70
1:KA:222:ARG:NH1	1:KA:351:VAL:O	2.24	0.70
1:Y:222:ARG:NH1	1:Y:351:VAL:O	2.24	0.70
1:AA:222:ARG:NH1	1:AA:351:VAL:O	2.24	0.70
1:I:222:ARG:NH1	1:I:351:VAL:O	2.24	0.70
1:P:222:ARG:NH1	1:P:351:VAL:O	2.24	0.70
1:R:222:ARG:NH1	1:R:351:VAL:O	2.24	0.70
1:HA:222:ARG:NH1	1:HA:351:VAL:O	2.24	0.70
1:CA:222:ARG:NH1	1:CA:351:VAL:O	2.24	0.70
1:J:222:ARG:NH1	1:J:351:VAL:O	2.24	0.69
1:F:222:ARG:NH1	1:F:351:VAL:O	2.24	0.69
1:G:222:ARG:NH1	1:G:351:VAL:O	2.24	0.69
1:V:222:ARG:NH1	1:V:351:VAL:O	2.24	0.69
1:LA:222:ARG:NH1	1:LA:351:VAL:O	2.24	0.69
1:N:222:ARG:NH1	1:N:351:VAL:O	2.24	0.69
1:A:222:ARG:NH1	1:A:351:VAL:O	2.24	0.69
1:D:222:ARG:NH1	1:D:351:VAL:O	2.24	0.69
1:IA:222:ARG:NH1	1:IA:351:VAL:O	2.24	0.69
1:W:222:ARG:NH1	1:W:351:VAL:O	2.24	0.69
1:OA:285:LEU:HD23	1:OA:387:ALA:HA	1.83	0.61
1:Y:285:LEU:HD23	1:Y:387:ALA:HA	1.83	0.61
1:A:285:LEU:HD23	1:A:387:ALA:HA	1.83	0.60
1:K:285:LEU:HD23	1:K:387:ALA:HA	1.83	0.60
1:S:285:LEU:HD23	1:S:387:ALA:HA	1.83	0.60
1:Z:285:LEU:HD23	1:Z:387:ALA:HA	1.83	0.60
1:LA:285:LEU:HD23	1:LA:387:ALA:HA	1.83	0.60
1:MA:285:LEU:HD23	1:MA:387:ALA:HA	1.83	0.60
1:C:285:LEU:HD23	1:C:387:ALA:HA	1.83	0.60
1:H:285:LEU:HD23	1:H:387:ALA:HA	1.83	0.60
1:L:285:LEU:HD23	1:L:387:ALA:HA	1.83	0.60
1:R:285:LEU:HD23	1:R:387:ALA:HA	1.83	0.60
1:X:285:LEU:HD23	1:X:387:ALA:HA	1.84	0.60
1:NA:285:LEU:HD23	1:NA:387:ALA:HA	1.83	0.60
1:D:285:LEU:HD23	1:D:387:ALA:HA	1.83	0.60
1:G:285:LEU:HD23	1:G:387:ALA:HA	1.84	0.60
1:Q:285:LEU:HD23	1:Q:387:ALA:HA	1.83	0.60
1:AA:285:LEU:HD23	1:AA:387:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:285:LEU:HD23	1:EA:387:ALA:HA	1.83	0.60
1:E:285:LEU:HD23	1:E:387:ALA:HA	1.83	0.60
1:F:285:LEU:HD23	1:F:387:ALA:HA	1.84	0.60
1:M:285:LEU:HD23	1:M:387:ALA:HA	1.84	0.60
1:T:285:LEU:HD23	1:T:387:ALA:HA	1.84	0.60
1:V:285:LEU:HD23	1:V:387:ALA:HA	1.83	0.60
1:W:285:LEU:HD23	1:W:387:ALA:HA	1.83	0.60
1:GA:285:LEU:HD23	1:GA:387:ALA:HA	1.83	0.60
1:J:285:LEU:HD23	1:J:387:ALA:HA	1.83	0.60
1:FA:285:LEU:HD23	1:FA:387:ALA:HA	1.83	0.60
1:B:285:LEU:HD23	1:B:387:ALA:HA	1.83	0.60
1:O:285:LEU:HD23	1:O:387:ALA:HA	1.83	0.60
1:P:285:LEU:HD23	1:P:387:ALA:HA	1.83	0.60
1:JA:285:LEU:HD23	1:JA:387:ALA:HA	1.83	0.60
1:I:285:LEU:HD23	1:I:387:ALA:HA	1.83	0.60
1:N:285:LEU:HD23	1:N:387:ALA:HA	1.83	0.60
1:CA:285:LEU:HD23	1:CA:387:ALA:HA	1.83	0.60
1:DA:285:LEU:HD23	1:DA:387:ALA:HA	1.83	0.60
1:HA:285:LEU:HD23	1:HA:387:ALA:HA	1.84	0.60
1:IA:285:LEU:HD23	1:IA:387:ALA:HA	1.84	0.60
1:BA:285:LEU:HD23	1:BA:387:ALA:HA	1.83	0.60
1:KA:285:LEU:HD23	1:KA:387:ALA:HA	1.84	0.60
1:Q:232:ASN:HD21	1:Q:377:LEU:HD23	1.68	0.59
1:CA:232:ASN:HD21	1:CA:377:LEU:HD23	1.68	0.59
1:E:232:ASN:HD21	1:E:377:LEU:HD23	1.68	0.59
1:T:232:ASN:HD21	1:T:377:LEU:HD23	1.68	0.59
1:D:232:ASN:HD21	1:D:377:LEU:HD23	1.68	0.59
1:W:232:ASN:HD21	1:W:377:LEU:HD23	1.68	0.59
1:FA:232:ASN:HD21	1:FA:377:LEU:HD23	1.68	0.59
1:HA:232:ASN:HD21	1:HA:377:LEU:HD23	1.68	0.59
1:MA:232:ASN:HD21	1:MA:377:LEU:HD23	1.68	0.59
1:F:232:ASN:HD21	1:F:377:LEU:HD23	1.68	0.59
1:G:232:ASN:HD21	1:G:377:LEU:HD23	1.68	0.58
1:Y:232:ASN:HD21	1:Y:377:LEU:HD23	1.68	0.58
1:BA:232:ASN:HD21	1:BA:377:LEU:HD23	1.68	0.58
1:A:232:ASN:HD21	1:A:377:LEU:HD23	1.68	0.58
1:IA:232:ASN:HD21	1:IA:377:LEU:HD23	1.68	0.58
1:OA:232:ASN:HD21	1:OA:377:LEU:HD23	1.68	0.58
1:I:232:ASN:HD21	1:I:377:LEU:HD23	1.68	0.58
1:DA:232:ASN:HD21	1:DA:377:LEU:HD23	1.68	0.58
1:M:232:ASN:HD21	1:M:377:LEU:HD23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:232:ASN:HD21	1:X:377:LEU:HD23	1.68	0.58
1:P:232:ASN:HD21	1:P:377:LEU:HD23	1.68	0.58
1:R:232:ASN:HD21	1:R:377:LEU:HD23	1.68	0.58
1:EA:232:ASN:HD21	1:EA:377:LEU:HD23	1.68	0.58
1:S:232:ASN:HD21	1:S:377:LEU:HD23	1.68	0.58
1:J:232:ASN:HD21	1:J:377:LEU:HD23	1.68	0.58
1:NA:232:ASN:HD21	1:NA:377:LEU:HD23	1.68	0.58
1:C:232:ASN:HD21	1:C:377:LEU:HD23	1.68	0.57
1:GA:232:ASN:HD21	1:GA:377:LEU:HD23	1.68	0.57
1:KA:232:ASN:HD21	1:KA:377:LEU:HD23	1.68	0.57
1:B:232:ASN:HD21	1:B:377:LEU:HD23	1.68	0.57
1:JA:232:ASN:HD21	1:JA:377:LEU:HD23	1.68	0.57
1:H:232:ASN:HD21	1:H:377:LEU:HD23	1.68	0.57
1:K:232:ASN:HD21	1:K:377:LEU:HD23	1.68	0.57
1:O:232:ASN:HD21	1:O:377:LEU:HD23	1.68	0.57
1:V:232:ASN:HD21	1:V:377:LEU:HD23	1.68	0.57
1:AA:232:ASN:HD21	1:AA:377:LEU:HD23	1.68	0.57
1:N:232:ASN:HD21	1:N:377:LEU:HD23	1.68	0.57
1:J:236:LEU:HD21	3:J:502:PMR:HMCB	1.87	0.57
1:L:232:ASN:HD21	1:L:377:LEU:HD23	1.68	0.57
1:JA:236:LEU:HD21	3:JA:502:PMR:HMCB	1.87	0.57
1:B:236:LEU:HD21	3:B:502:PMR:HMCB	1.87	0.57
1:Z:232:ASN:HD21	1:Z:377:LEU:HD23	1.68	0.57
1:NA:236:LEU:HD21	3:NA:502:PMR:HMCB	1.87	0.57
1:O:236:LEU:HD21	3:O:502:PMR:HMCB	1.87	0.57
1:KA:236:LEU:HD21	3:KA:502:PMR:HMCB	1.87	0.57
1:Z:236:LEU:HD21	3:Z:502:PMR:HMCB	1.87	0.56
1:CA:236:LEU:HD21	3:CA:502:PMR:HMCB	1.87	0.56
1:R:236:LEU:HD21	3:R:502:PMR:HMCB	1.87	0.56
1:W:236:LEU:HD21	3:W:502:PMR:HMCB	1.87	0.56
1:BA:236:LEU:HD21	3:BA:502:PMR:HMCB	1.87	0.56
1:HA:236:LEU:HD21	3:HA:502:PMR:HMCB	1.87	0.56
1:A:236:LEU:HD21	3:A:502:PMR:HMCB	1.87	0.56
1:D:236:LEU:HD21	3:D:502:PMR:HMCB	1.87	0.56
1:E:236:LEU:HD21	3:E:502:PMR:HMCB	1.87	0.56
1:F:236:LEU:HD21	3:F:502:PMR:HMCB	1.87	0.56
1:I:236:LEU:HD21	3:I:502:PMR:HMCB	1.87	0.56
1:K:236:LEU:HD21	3:K:502:PMR:HMCB	1.86	0.56
1:L:236:LEU:HD21	3:L:502:PMR:HMCB	1.87	0.56
1:N:236:LEU:HD21	3:N:502:PMR:HMCB	1.87	0.56
1:P:236:LEU:HD21	3:P:502:PMR:HMCB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:236:LEU:HD21	3:V:502:PMR:HMCB	1.87	0.56
1:FA:236:LEU:HD21	3:FA:502:PMR:HMCB	1.87	0.56
1:LA:232:ASN:HD21	1:LA:377:LEU:HD23	1.68	0.56
1:MA:236:LEU:HD21	3:MA:502:PMR:HMCB	1.87	0.56
1:EA:236:LEU:HD21	3:EA:502:PMR:HMCB	1.87	0.56
1:H:236:LEU:HD21	3:H:502:PMR:HMCB	1.87	0.56
1:Q:236:LEU:HD21	3:Q:502:PMR:HMCB	1.87	0.56
1:DA:236:LEU:HD21	3:DA:502:PMR:HMCB	1.87	0.56
1:M:236:LEU:HD21	3:M:502:PMR:HMCB	1.87	0.56
1:S:236:LEU:HD21	3:S:502:PMR:HMCB	1.87	0.56
1:AA:236:LEU:HD21	3:AA:502:PMR:HMCB	1.87	0.56
1:C:236:LEU:HD21	3:C:502:PMR:HMCB	1.87	0.56
1:X:236:LEU:HD21	3:X:502:PMR:HMCB	1.87	0.56
1:GA:236:LEU:HD21	3:GA:502:PMR:HMCB	1.87	0.56
1:G:236:LEU:HD21	3:G:502:PMR:HMCB	1.87	0.55
1:T:236:LEU:HD21	3:T:502:PMR:HMCB	1.87	0.55
1:LA:236:LEU:HD21	3:LA:502:PMR:HMCB	1.87	0.55
1:OA:236:LEU:HD21	3:OA:502:PMR:HMCB	1.87	0.55
1:IA:236:LEU:HD21	3:IA:502:PMR:HMCB	1.87	0.55
1:Y:236:LEU:HD21	3:Y:502:PMR:HMCB	1.87	0.55
1:HA:131:LYS:HD3	1:MA:260:ASN:HB2	1.92	0.52
1:N:285:LEU:HD23	1:N:387:ALA:CA	2.41	0.51
1:O:285:LEU:HD23	1:O:387:ALA:CA	2.41	0.51
1:R:285:LEU:HD23	1:R:387:ALA:CA	2.41	0.51
1:S:285:LEU:HD23	1:S:387:ALA:CA	2.41	0.51
1:V:285:LEU:HD23	1:V:387:ALA:CA	2.41	0.51
1:B:285:LEU:HD23	1:B:387:ALA:CA	2.41	0.51
1:M:236:LEU:CD2	3:M:502:PMR:HMCB	2.41	0.51
1:GA:236:LEU:CD2	3:GA:502:PMR:HMCB	2.41	0.51
1:C:285:LEU:HD23	1:C:387:ALA:CA	2.41	0.51
1:P:285:LEU:HD23	1:P:387:ALA:CA	2.41	0.51
1:Y:236:LEU:CD2	3:Y:502:PMR:HMCB	2.41	0.51
1:Z:285:LEU:HD23	1:Z:387:ALA:CA	2.40	0.51
1:DA:236:LEU:CD2	3:DA:502:PMR:HMCB	2.41	0.51
1:LA:236:LEU:CD2	3:LA:502:PMR:HMCB	2.41	0.51
1:MA:236:LEU:CD2	3:MA:502:PMR:HMCB	2.41	0.51
1:OA:236:LEU:CD2	3:OA:502:PMR:HMCB	2.41	0.51
1:A:236:LEU:CD2	3:A:502:PMR:HMCB	2.41	0.51
1:E:236:LEU:CD2	3:E:502:PMR:HMCB	2.41	0.51
1:F:236:LEU:CD2	3:F:502:PMR:HMCB	2.41	0.51
1:M:285:LEU:HD23	1:M:387:ALA:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:260:ASN:HB2	1:JA:131:LYS:HD3	1.92	0.51
1:Y:285:LEU:HD23	1:Y:387:ALA:CA	2.41	0.51
1:Z:236:LEU:CD2	3:Z:502:PMR:HMCB	2.41	0.51
1:D:236:LEU:CD2	3:D:502:PMR:HMCB	2.41	0.51
1:CA:236:LEU:CD2	3:CA:502:PMR:HMCB	2.41	0.51
1:GA:131:LYS:HD3	1:LA:260:ASN:HB2	1.93	0.51
1:JA:285:LEU:HD23	1:JA:387:ALA:CA	2.41	0.51
1:L:236:LEU:CD2	3:L:502:PMR:HMCB	2.41	0.51
1:AA:236:LEU:CD2	3:AA:502:PMR:HMCB	2.41	0.51
1:FA:236:LEU:CD2	3:FA:502:PMR:HMCB	2.41	0.51
1:NA:236:LEU:CD2	3:NA:502:PMR:HMCB	2.41	0.51
1:NA:285:LEU:HD23	1:NA:387:ALA:CA	2.41	0.51
1:H:236:LEU:CD2	3:H:502:PMR:HMCB	2.41	0.51
1:K:236:LEU:CD2	3:K:502:PMR:HMCB	2.41	0.51
1:EA:236:LEU:CD2	3:EA:502:PMR:HMCB	2.41	0.51
1:HA:236:LEU:CD2	3:HA:502:PMR:HMCB	2.41	0.51
1:IA:236:LEU:CD2	3:IA:502:PMR:HMCB	2.41	0.51
1:H:285:LEU:HD23	1:H:387:ALA:CA	2.41	0.50
1:G:236:LEU:CD2	3:G:502:PMR:HMCB	2.41	0.50
1:J:236:LEU:CD2	3:J:502:PMR:HMCB	2.41	0.50
1:J:285:LEU:HD23	1:J:387:ALA:CA	2.41	0.50
1:Q:236:LEU:CD2	3:Q:502:PMR:HMCB	2.41	0.50
1:X:236:LEU:CD2	3:X:502:PMR:HMCB	2.41	0.50
1:EA:285:LEU:HD23	1:EA:387:ALA:CA	2.41	0.50
1:K:285:LEU:HD23	1:K:387:ALA:CA	2.41	0.50
1:FA:285:LEU:HD23	1:FA:387:ALA:CA	2.41	0.50
1:A:285:LEU:HD23	1:A:387:ALA:CA	2.41	0.50
1:BA:236:LEU:CD2	3:BA:502:PMR:HMCB	2.41	0.50
1:GA:285:LEU:HD23	1:GA:387:ALA:CA	2.41	0.50
1:LA:285:LEU:HD23	1:LA:387:ALA:CA	2.41	0.50
1:I:236:LEU:CD2	3:I:502:PMR:HMCB	2.41	0.50
1:L:285:LEU:HD23	1:L:387:ALA:CA	2.41	0.50
1:T:236:LEU:CD2	3:T:502:PMR:HMCB	2.41	0.50
1:W:236:LEU:CD2	3:W:502:PMR:HMCB	2.41	0.50
1:BA:285:LEU:HD23	1:BA:387:ALA:CA	2.41	0.50
1:JA:236:LEU:CD2	3:JA:502:PMR:HMCB	2.41	0.50
1:KA:236:LEU:CD2	3:KA:502:PMR:HMCB	2.41	0.50
1:KA:285:LEU:HD23	1:KA:387:ALA:CA	2.41	0.50
1:F:285:LEU:HD23	1:F:387:ALA:CA	2.41	0.50
1:G:285:LEU:HD23	1:G:387:ALA:CA	2.41	0.50
1:AA:285:LEU:HD23	1:AA:387:ALA:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:310:ILE:HG22	1:JA:313:THR:HG23	1.94	0.50
1:D:305:LEU:HD22	1:D:351:VAL:HG21	1.94	0.50
1:E:285:LEU:HD23	1:E:387:ALA:CA	2.41	0.50
1:H:310:ILE:HG22	1:H:313:THR:HG23	1.94	0.50
1:K:310:ILE:HG22	1:K:313:THR:HG23	1.94	0.50
1:O:236:LEU:CD2	3:O:502:PMR:HMCB	2.41	0.50
1:O:310:ILE:HG22	1:O:313:THR:HG23	1.94	0.50
1:Q:285:LEU:HD23	1:Q:387:ALA:CA	2.41	0.50
1:X:285:LEU:HD23	1:X:387:ALA:CA	2.41	0.50
1:HA:285:LEU:HD23	1:HA:387:ALA:CA	2.41	0.50
1:N:310:ILE:HG22	1:N:313:THR:HG23	1.94	0.50
1:X:310:ILE:HG22	1:X:313:THR:HG23	1.94	0.50
1:CA:285:LEU:HD23	1:CA:387:ALA:CA	2.41	0.50
1:FA:305:LEU:HD22	1:FA:351:VAL:HG21	1.94	0.50
1:IA:305:LEU:HD22	1:IA:351:VAL:HG21	1.94	0.50
1:IA:310:ILE:HG22	1:IA:313:THR:HG23	1.94	0.50
1:OA:285:LEU:HD23	1:OA:387:ALA:CA	2.41	0.50
1:D:285:LEU:HD23	1:D:387:ALA:CA	2.41	0.50
1:E:305:LEU:HD22	1:E:351:VAL:HG21	1.94	0.50
1:G:310:ILE:HG22	1:G:313:THR:HG23	1.94	0.50
1:I:285:LEU:HD23	1:I:387:ALA:CA	2.41	0.50
1:J:305:LEU:HD22	1:J:351:VAL:HG21	1.94	0.50
1:J:310:ILE:HG22	1:J:313:THR:HG23	1.94	0.50
1:K:305:LEU:HD22	1:K:351:VAL:HG21	1.94	0.50
1:M:310:ILE:HG22	1:M:313:THR:HG23	1.94	0.50
1:Q:259:LEU:HD11	1:LA:257:ASN:HB3	1.93	0.50
1:T:305:LEU:HD22	1:T:351:VAL:HG21	1.94	0.50
1:W:305:LEU:HD22	1:W:351:VAL:HG21	1.94	0.50
1:Y:310:ILE:HG22	1:Y:313:THR:HG23	1.94	0.50
1:Z:305:LEU:HD22	1:Z:351:VAL:HG21	1.94	0.50
1:IA:285:LEU:HD23	1:IA:387:ALA:CA	2.41	0.50
1:JA:305:LEU:HD22	1:JA:351:VAL:HG21	1.94	0.50
1:KA:310:ILE:HG22	1:KA:313:THR:HG23	1.94	0.50
1:MA:285:LEU:HD23	1:MA:387:ALA:CA	2.41	0.50
1:C:236:LEU:CD2	3:C:502:PMR:HMCB	2.41	0.49
1:D:177:TYR:CE1	3:D:502:PMR:H2O	2.47	0.49
1:H:305:LEU:HD22	1:H:351:VAL:HG21	1.94	0.49
1:V:177:TYR:CE1	3:V:502:PMR:H2O	2.47	0.49
1:V:305:LEU:HD22	1:V:351:VAL:HG21	1.94	0.49
1:W:285:LEU:HD23	1:W:387:ALA:CA	2.41	0.49
1:DA:285:LEU:HD23	1:DA:387:ALA:CA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:177:TYR:CE1	3:JA:502:PMR:H2O	2.47	0.49
1:B:236:LEU:CD2	3:B:502:PMR:HMCB	2.41	0.49
1:B:310:ILE:HG22	1:B:313:THR:HG23	1.94	0.49
1:G:305:LEU:HD22	1:G:351:VAL:HG21	1.94	0.49
1:J:177:TYR:CE1	3:J:502:PMR:H2O	2.47	0.49
1:N:236:LEU:CD2	3:N:502:PMR:HMCB	2.41	0.49
1:O:305:LEU:HD22	1:O:351:VAL:HG21	1.94	0.49
1:T:177:TYR:CE1	3:T:502:PMR:H2O	2.47	0.49
1:T:310:ILE:HG22	1:T:313:THR:HG23	1.94	0.49
1:V:236:LEU:CD2	3:V:502:PMR:HMCB	2.41	0.49
1:V:310:ILE:HG22	1:V:313:THR:HG23	1.94	0.49
1:X:177:TYR:CE1	3:X:502:PMR:H2O	2.48	0.49
1:X:305:LEU:HD22	1:X:351:VAL:HG21	1.94	0.49
1:Z:310:ILE:HG22	1:Z:313:THR:HG23	1.94	0.49
1:DA:305:LEU:HD22	1:DA:351:VAL:HG21	1.94	0.49
1:FA:177:TYR:CE1	3:FA:502:PMR:H2O	2.47	0.49
1:NA:305:LEU:HD22	1:NA:351:VAL:HG21	1.94	0.49
1:NA:310:ILE:HG22	1:NA:313:THR:HG23	1.94	0.49
1:D:310:ILE:HG22	1:D:313:THR:HG23	1.94	0.49
1:M:305:LEU:HD22	1:M:351:VAL:HG21	1.94	0.49
1:O:131:LYS:HD3	1:Z:260:ASN:HB2	1.94	0.49
1:Y:305:LEU:HD22	1:Y:351:VAL:HG21	1.94	0.49
1:HA:305:LEU:HD22	1:HA:351:VAL:HG21	1.94	0.49
1:KA:177:TYR:CE1	3:KA:502:PMR:H2O	2.47	0.49
1:H:260:ASN:HB2	1:Z:131:LYS:HD3	1.93	0.49
1:K:177:TYR:CE1	3:K:502:PMR:H2O	2.47	0.49
1:P:236:LEU:CD2	3:P:502:PMR:HMCB	2.41	0.49
1:P:310:ILE:HG22	1:P:313:THR:HG23	1.94	0.49
1:T:285:LEU:HD23	1:T:387:ALA:CA	2.41	0.49
1:AA:310:ILE:HG22	1:AA:313:THR:HG23	1.94	0.49
1:IA:177:TYR:CE1	3:IA:502:PMR:H2O	2.48	0.49
1:KA:305:LEU:HD22	1:KA:351:VAL:HG21	1.94	0.49
1:LA:177:TYR:CE1	3:LA:502:PMR:H2O	2.47	0.49
1:A:305:LEU:HD22	1:A:351:VAL:HG21	1.94	0.49
1:H:177:TYR:CE1	3:H:502:PMR:H2O	2.47	0.49
1:P:305:LEU:HD22	1:P:351:VAL:HG21	1.94	0.49
1:Q:177:TYR:CE1	3:Q:502:PMR:H2O	2.47	0.49
1:Q:260:ASN:HB2	1:CA:131:LYS:HD3	1.95	0.49
1:Q:305:LEU:HD22	1:Q:351:VAL:HG21	1.94	0.49
1:S:236:LEU:CD2	3:S:502:PMR:HMCB	2.41	0.49
1:W:177:TYR:CE1	3:W:502:PMR:H2O	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:177:TYR:CE1	3:EA:502:PMR:H2O	2.48	0.49
1:HA:177:TYR:CE1	3:HA:502:PMR:H2O	2.47	0.49
1:B:305:LEU:HD22	1:B:351:VAL:HG21	1.94	0.49
1:E:177:TYR:CE1	3:E:502:PMR:H2O	2.47	0.49
1:I:305:LEU:HD22	1:I:351:VAL:HG21	1.94	0.49
1:L:305:LEU:HD22	1:L:351:VAL:HG21	1.94	0.49
1:L:310:ILE:HG22	1:L:313:THR:HG23	1.94	0.49
1:N:305:LEU:HD22	1:N:351:VAL:HG21	1.94	0.49
1:R:177:TYR:CE1	3:R:502:PMR:H2O	2.47	0.49
1:R:236:LEU:CD2	3:R:502:PMR:HMCB	2.41	0.49
1:T:260:ASN:HB2	1:IA:131:LYS:HD3	1.93	0.49
1:BA:177:TYR:CE1	3:BA:502:PMR:H2O	2.47	0.49
1:CA:305:LEU:HD22	1:CA:351:VAL:HG21	1.94	0.49
1:GA:305:LEU:HD22	1:GA:351:VAL:HG21	1.94	0.49
1:MA:305:LEU:HD22	1:MA:351:VAL:HG21	1.94	0.49
1:F:177:TYR:CE1	3:F:502:PMR:H2O	2.47	0.49
1:F:305:LEU:HD22	1:F:351:VAL:HG21	1.94	0.49
1:I:310:ILE:HG22	1:I:313:THR:HG23	1.94	0.49
1:P:177:TYR:CE1	3:P:502:PMR:H2O	2.48	0.49
1:R:310:ILE:HG22	1:R:313:THR:HG23	1.94	0.49
1:S:257:ASN:HB3	1:MA:259:LEU:HD11	1.94	0.49
1:Z:177:TYR:CE1	3:Z:502:PMR:H2O	2.47	0.49
1:KA:241:PRO:HB2	1:KA:242:PRO:HD3	1.95	0.49
1:LA:305:LEU:HD22	1:LA:351:VAL:HG21	1.94	0.49
1:NA:177:TYR:CE1	3:NA:502:PMR:H2O	2.47	0.49
1:NA:241:PRO:HB2	1:NA:242:PRO:HD3	1.95	0.49
1:C:177:TYR:CE1	3:C:502:PMR:H2O	2.47	0.49
1:DA:177:TYR:CE1	3:DA:502:PMR:H2O	2.47	0.49
1:DA:310:ILE:HG22	1:DA:313:THR:HG23	1.94	0.49
1:LA:241:PRO:HB2	1:LA:242:PRO:HD3	1.95	0.49
1:A:177:TYR:CE1	3:A:502:PMR:H2O	2.48	0.49
1:L:177:TYR:CE1	3:L:502:PMR:H2O	2.48	0.49
1:M:177:TYR:CE1	3:M:502:PMR:H2O	2.47	0.49
1:T:259:LEU:HD11	1:Z:257:ASN:HB3	1.95	0.49
1:AA:305:LEU:HD22	1:AA:351:VAL:HG21	1.94	0.49
1:OA:177:TYR:CE1	3:OA:502:PMR:H2O	2.48	0.49
1:OA:305:LEU:HD22	1:OA:351:VAL:HG21	1.94	0.49
1:B:241:PRO:HB2	1:B:242:PRO:HD3	1.95	0.49
1:C:241:PRO:HB2	1:C:242:PRO:HD3	1.95	0.49
1:C:305:LEU:HD22	1:C:351:VAL:HG21	1.94	0.49
1:C:310:ILE:HG22	1:C:313:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:310:ILE:HG22	1:W:313:THR:HG23	1.94	0.49
1:Y:177:TYR:CE1	3:Y:502:PMR:H2O	2.47	0.49
1:Z:241:PRO:HB2	1:Z:242:PRO:HD3	1.95	0.49
1:LA:310:ILE:HG22	1:LA:313:THR:HG23	1.94	0.49
1:MA:241:PRO:HB2	1:MA:242:PRO:HD3	1.95	0.49
1:A:241:PRO:HB2	1:A:242:PRO:HD3	1.95	0.48
1:C:260:ASN:HB2	1:S:131:LYS:HD3	1.95	0.48
1:F:241:PRO:HB2	1:F:242:PRO:HD3	1.95	0.48
1:G:177:TYR:CE1	3:G:502:PMR:H2O	2.47	0.48
1:O:177:TYR:CE1	3:O:502:PMR:H2O	2.47	0.48
1:S:305:LEU:HD22	1:S:351:VAL:HG21	1.94	0.48
1:FA:310:ILE:HG22	1:FA:313:THR:HG23	1.94	0.48
1:JA:241:PRO:HB2	1:JA:242:PRO:HD3	1.95	0.48
1:B:177:TYR:CE1	3:B:502:PMR:H2O	2.47	0.48
1:M:131:LYS:HD3	1:Y:260:ASN:HB2	1.94	0.48
1:R:241:PRO:HB2	1:R:242:PRO:HD3	1.95	0.48
1:CA:177:TYR:CE1	3:CA:502:PMR:H2O	2.47	0.48
1:EA:310:ILE:HG22	1:EA:313:THR:HG23	1.94	0.48
1:N:241:PRO:HB2	1:N:242:PRO:HD3	1.95	0.48
1:Q:257:ASN:HB3	1:LA:259:LEU:HD11	1.94	0.48
1:R:305:LEU:HD22	1:R:351:VAL:HG21	1.94	0.48
1:AA:177:TYR:CE1	3:AA:502:PMR:H2O	2.47	0.48
1:EA:305:LEU:HD22	1:EA:351:VAL:HG21	1.94	0.48
1:GA:310:ILE:HG22	1:GA:313:THR:HG23	1.94	0.48
1:MA:177:TYR:CE1	3:MA:502:PMR:H2O	2.47	0.48
1:E:310:ILE:HG22	1:E:313:THR:HG23	1.94	0.48
1:I:177:TYR:CE1	3:I:502:PMR:H2O	2.47	0.48
1:S:241:PRO:HB2	1:S:242:PRO:HD3	1.95	0.48
1:GA:177:TYR:CE1	3:GA:502:PMR:H2O	2.47	0.48
1:S:177:TYR:CE1	3:S:502:PMR:H2O	2.47	0.48
1:S:260:ASN:HB2	1:EA:131:LYS:HD3	1.96	0.48
1:BA:241:PRO:HB2	1:BA:242:PRO:HD3	1.95	0.48
1:BA:305:LEU:HD22	1:BA:351:VAL:HG21	1.94	0.48
1:CA:310:ILE:HG22	1:CA:313:THR:HG23	1.94	0.48
1:OA:310:ILE:HG22	1:OA:313:THR:HG23	1.94	0.48
1:N:177:TYR:CE1	3:N:502:PMR:H2O	2.47	0.48
1:O:241:PRO:HB2	1:O:242:PRO:HD3	1.95	0.48
1:O:244:ALA:HB2	1:O:277:LYS:HB3	1.96	0.48
1:BA:310:ILE:HG22	1:BA:313:THR:HG23	1.94	0.48
1:HA:310:ILE:HG22	1:HA:313:THR:HG23	1.94	0.48
1:A:310:ILE:HG22	1:A:313:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:244:ALA:HB2	1:J:277:LYS:HB3	1.96	0.48
1:P:241:PRO:HB2	1:P:242:PRO:HD3	1.95	0.48
1:Q:241:PRO:HB2	1:Q:242:PRO:HD3	1.95	0.48
1:S:310:ILE:HG22	1:S:313:THR:HG23	1.94	0.48
1:V:241:PRO:HB2	1:V:242:PRO:HD3	1.95	0.48
1:Y:241:PRO:HB2	1:Y:242:PRO:HD3	1.95	0.48
1:EA:241:PRO:HB2	1:EA:242:PRO:HD3	1.95	0.48
1:JA:244:ALA:HB2	1:JA:277:LYS:HB3	1.96	0.48
1:B:244:ALA:HB2	1:B:277:LYS:HB3	1.96	0.48
1:F:310:ILE:HG22	1:F:313:THR:HG23	1.94	0.48
1:L:241:PRO:HB2	1:L:242:PRO:HD3	1.95	0.48
1:Q:310:ILE:HG22	1:Q:313:THR:HG23	1.94	0.48
1:V:244:ALA:HB2	1:V:277:LYS:HB3	1.96	0.48
1:X:244:ALA:HB2	1:X:277:LYS:HB3	1.96	0.48
1:Z:244:ALA:HB2	1:Z:277:LYS:HB3	1.96	0.48
1:NA:244:ALA:HB2	1:NA:277:LYS:HB3	1.96	0.48
1:OA:241:PRO:HB2	1:OA:242:PRO:HD3	1.95	0.48
1:L:131:LYS:HD3	1:KA:260:ASN:HB2	1.95	0.48
1:IA:244:ALA:HB2	1:IA:277:LYS:HB3	1.96	0.48
1:E:241:PRO:HB2	1:E:242:PRO:HD3	1.95	0.48
1:H:244:ALA:HB2	1:H:277:LYS:HB3	1.96	0.48
1:I:131:LYS:HD3	1:CA:260:ASN:HB2	1.95	0.48
1:J:241:PRO:HB2	1:J:242:PRO:HD3	1.95	0.48
1:K:244:ALA:HB2	1:K:277:LYS:HB3	1.96	0.48
1:R:244:ALA:HB2	1:R:277:LYS:HB3	1.96	0.48
1:IA:241:PRO:HB2	1:IA:242:PRO:HD3	1.95	0.48
1:KA:244:ALA:HB2	1:KA:277:LYS:HB3	1.96	0.48
1:MA:310:ILE:HG22	1:MA:313:THR:HG23	1.94	0.48
1:N:244:ALA:HB2	1:N:277:LYS:HB3	1.96	0.47
1:S:259:LEU:HD11	1:MA:257:ASN:HB3	1.95	0.47
1:T:257:ASN:HB3	1:Z:259:LEU:HD11	1.96	0.47
1:W:241:PRO:HB2	1:W:242:PRO:HD3	1.95	0.47
1:Q:244:ALA:HB2	1:Q:277:LYS:HB3	1.96	0.47
1:T:244:ALA:HB2	1:T:277:LYS:HB3	1.96	0.47
1:Y:244:ALA:HB2	1:Y:277:LYS:HB3	1.96	0.47
1:BA:131:LYS:HD3	1:EA:260:ASN:HB2	1.96	0.47
1:C:144:HIS:CE1	1:E:144:HIS:CE1	3.03	0.47
1:I:241:PRO:HB2	1:I:242:PRO:HD3	1.95	0.47
1:M:244:ALA:HB2	1:M:277:LYS:HB3	1.96	0.47
1:T:241:PRO:HB2	1:T:242:PRO:HD3	1.95	0.47
1:BA:244:ALA:HB2	1:BA:277:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:244:ALA:HB2	1:CA:277:LYS:HB3	1.96	0.47
1:GA:241:PRO:HB2	1:GA:242:PRO:HD3	1.95	0.47
1:E:259:LEU:HD11	1:P:257:ASN:HB3	1.95	0.47
1:M:241:PRO:HB2	1:M:242:PRO:HD3	1.95	0.47
1:P:244:ALA:HB2	1:P:277:LYS:HB3	1.96	0.47
1:HA:244:ALA:HB2	1:HA:277:LYS:HB3	1.96	0.47
1:MA:244:ALA:HB2	1:MA:277:LYS:HB3	1.96	0.47
1:A:244:ALA:HB2	1:A:277:LYS:HB3	1.96	0.47
1:A:260:ASN:HB2	1:Q:131:LYS:HD3	1.96	0.47
1:G:244:ALA:HB2	1:G:277:LYS:HB3	1.96	0.47
1:H:241:PRO:HB2	1:H:242:PRO:HD3	1.95	0.47
1:K:241:PRO:HB2	1:K:242:PRO:HD3	1.95	0.47
1:AA:241:PRO:HB2	1:AA:242:PRO:HD3	1.95	0.47
1:D:244:ALA:HB2	1:D:277:LYS:HB3	1.96	0.47
1:G:241:PRO:HB2	1:G:242:PRO:HD3	1.95	0.47
1:HA:241:PRO:HB2	1:HA:242:PRO:HD3	1.95	0.47
1:D:241:PRO:HB2	1:D:242:PRO:HD3	1.95	0.47
1:E:244:ALA:HB2	1:E:277:LYS:HB3	1.96	0.47
1:F:244:ALA:HB2	1:F:277:LYS:HB3	1.96	0.47
1:I:244:ALA:HB2	1:I:277:LYS:HB3	1.96	0.47
1:L:244:ALA:HB2	1:L:277:LYS:HB3	1.96	0.47
1:CA:241:PRO:HB2	1:CA:242:PRO:HD3	1.95	0.47
1:DA:241:PRO:HB2	1:DA:242:PRO:HD3	1.95	0.47
1:FA:241:PRO:HB2	1:FA:242:PRO:HD3	1.95	0.47
1:OA:244:ALA:HB2	1:OA:277:LYS:HB3	1.96	0.47
1:X:241:PRO:HB2	1:X:242:PRO:HD3	1.95	0.47
1:DA:244:ALA:HB2	1:DA:277:LYS:HB3	1.96	0.47
1:EA:244:ALA:HB2	1:EA:277:LYS:HB3	1.96	0.47
1:B:260:ASN:HB2	1:R:131:LYS:HD3	1.97	0.47
1:G:131:LYS:HD3	1:DA:260:ASN:HB2	1.95	0.47
1:KA:177:TYR:CZ	3:KA:502:PMR:H2O	2.50	0.47
1:O:177:TYR:CZ	3:O:502:PMR:H2O	2.50	0.47
1:GA:177:TYR:CZ	3:GA:502:PMR:H2O	2.50	0.47
1:GA:244:ALA:HB2	1:GA:277:LYS:HB3	1.96	0.47
1:NA:177:TYR:CZ	3:NA:502:PMR:H2O	2.50	0.47
1:D:177:TYR:CZ	3:D:502:PMR:H2O	2.50	0.46
1:I:260:ASN:HB2	1:AA:131:LYS:HD3	1.96	0.46
1:J:259:LEU:HD11	1:DA:257:ASN:HB3	1.97	0.46
1:S:177:TYR:CZ	3:S:502:PMR:H2O	2.50	0.46
1:MA:177:TYR:CZ	3:MA:502:PMR:H2O	2.50	0.46
1:C:177:TYR:CZ	3:C:502:PMR:H2O	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ALA:HB2	1:C:277:LYS:HB3	1.96	0.46
1:J:177:TYR:CZ	3:J:502:PMR:H2O	2.50	0.46
1:M:260:ASN:HB2	1:N:131:LYS:HD3	1.97	0.46
1:T:177:TYR:CZ	3:T:502:PMR:H2O	2.50	0.46
1:V:257:ASN:HB3	1:Y:259:LEU:HD11	1.98	0.46
1:W:244:ALA:HB2	1:W:277:LYS:HB3	1.96	0.46
1:FA:177:TYR:CZ	3:FA:502:PMR:H2O	2.50	0.46
1:OA:177:TYR:CZ	3:OA:502:PMR:H2O	2.50	0.46
1:F:177:TYR:CZ	3:F:502:PMR:H2O	2.50	0.46
1:N:177:TYR:CZ	3:N:502:PMR:H2O	2.50	0.46
1:AA:244:ALA:HB2	1:AA:277:LYS:HB3	1.96	0.46
1:FA:244:ALA:HB2	1:FA:277:LYS:HB3	1.96	0.46
1:B:177:TYR:CZ	3:B:502:PMR:H2O	2.50	0.46
1:X:177:TYR:CZ	3:X:502:PMR:H2O	2.50	0.46
1:Z:145:LEU:HD21	1:Z:147:LEU:HD23	1.98	0.46
1:FA:145:LEU:HD21	1:FA:147:LEU:HD23	1.98	0.46
1:IA:177:TYR:CZ	3:IA:502:PMR:H2O	2.50	0.46
1:A:177:TYR:CZ	3:A:502:PMR:H2O	2.50	0.46
1:F:145:LEU:HD21	1:F:147:LEU:HD23	1.98	0.46
1:L:177:TYR:CZ	3:L:502:PMR:H2O	2.50	0.46
1:R:177:TYR:CZ	3:R:502:PMR:H2O	2.50	0.46
1:S:244:ALA:HB2	1:S:277:LYS:HB3	1.96	0.46
1:W:177:TYR:CZ	3:W:502:PMR:H2O	2.50	0.46
1:BA:145:LEU:HD21	1:BA:147:LEU:HD23	1.98	0.46
1:CA:145:LEU:HD21	1:CA:147:LEU:HD23	1.98	0.46
1:HA:145:LEU:HD21	1:HA:147:LEU:HD23	1.98	0.46
1:JA:145:LEU:HD21	1:JA:147:LEU:HD23	1.98	0.46
1:NA:145:LEU:HD21	1:NA:147:LEU:HD23	1.98	0.46
1:C:131:LYS:HD3	1:P:260:ASN:HB2	1.98	0.46
1:D:131:LYS:HD3	1:FA:260:ASN:HB2	1.97	0.46
1:E:145:LEU:HD21	1:E:147:LEU:HD23	1.98	0.46
1:E:260:ASN:HB2	1:W:131:LYS:HD3	1.98	0.46
1:G:260:ASN:HB2	1:Y:131:LYS:HD3	1.97	0.46
1:M:145:LEU:HD21	1:M:147:LEU:HD23	1.98	0.46
1:W:145:LEU:HD21	1:W:147:LEU:HD23	1.98	0.46
1:Z:177:TYR:CZ	3:Z:502:PMR:H2O	2.50	0.46
1:AA:145:LEU:HD21	1:AA:147:LEU:HD23	1.98	0.46
1:DA:145:LEU:HD21	1:DA:147:LEU:HD23	1.98	0.46
1:DA:177:TYR:CZ	3:DA:502:PMR:H2O	2.50	0.46
1:LA:177:TYR:CZ	3:LA:502:PMR:H2O	2.50	0.46
1:A:145:LEU:HD21	1:A:147:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD21	1:B:147:LEU:HD23	1.98	0.46
1:E:177:TYR:CZ	3:E:502:PMR:H2O	2.50	0.46
1:G:177:TYR:CZ	3:G:502:PMR:H2O	2.50	0.46
1:J:145:LEU:HD21	1:J:147:LEU:HD23	1.98	0.46
1:L:145:LEU:HD21	1:L:147:LEU:HD23	1.98	0.46
1:N:145:LEU:HD21	1:N:147:LEU:HD23	1.98	0.46
1:O:145:LEU:HD21	1:O:147:LEU:HD23	1.98	0.46
1:S:145:LEU:HD21	1:S:147:LEU:HD23	1.98	0.46
1:V:145:LEU:HD21	1:V:147:LEU:HD23	1.98	0.46
1:Y:145:LEU:HD21	1:Y:147:LEU:HD23	1.98	0.46
1:EA:145:LEU:HD21	1:EA:147:LEU:HD23	1.98	0.46
1:MA:145:LEU:HD21	1:MA:147:LEU:HD23	1.98	0.46
1:P:145:LEU:HD21	1:P:147:LEU:HD23	1.98	0.46
1:Q:145:LEU:HD21	1:Q:147:LEU:HD23	1.98	0.46
1:T:145:LEU:HD21	1:T:147:LEU:HD23	1.98	0.46
1:V:177:TYR:CZ	3:V:502:PMR:H2O	2.50	0.46
1:X:145:LEU:HD21	1:X:147:LEU:HD23	1.98	0.46
1:IA:145:LEU:HD21	1:IA:147:LEU:HD23	1.98	0.46
1:LA:244:ALA:HB2	1:LA:277:LYS:HB3	1.96	0.46
1:I:177:TYR:CZ	3:I:502:PMR:H2O	2.50	0.46
1:K:177:TYR:CZ	3:K:502:PMR:H2O	2.50	0.46
1:GA:145:LEU:HD21	1:GA:147:LEU:HD23	1.98	0.46
1:KA:145:LEU:HD21	1:KA:147:LEU:HD23	1.98	0.46
1:D:145:LEU:HD21	1:D:147:LEU:HD23	1.98	0.46
1:G:145:LEU:HD21	1:G:147:LEU:HD23	1.98	0.46
1:H:145:LEU:HD21	1:H:147:LEU:HD23	1.98	0.46
1:H:177:TYR:CZ	3:H:502:PMR:H2O	2.50	0.46
1:I:145:LEU:HD21	1:I:147:LEU:HD23	1.98	0.46
1:K:145:LEU:HD21	1:K:147:LEU:HD23	1.98	0.46
1:AA:177:TYR:CZ	3:AA:502:PMR:H2O	2.50	0.46
1:EA:177:TYR:CZ	3:EA:502:PMR:H2O	2.51	0.46
1:HA:177:TYR:CZ	3:HA:502:PMR:H2O	2.50	0.46
1:LA:145:LEU:HD21	1:LA:147:LEU:HD23	1.98	0.46
1:K:131:LYS:HD3	1:IA:260:ASN:HB2	1.98	0.45
1:P:177:TYR:CZ	3:P:502:PMR:H2O	2.50	0.45
1:R:145:LEU:HD21	1:R:147:LEU:HD23	1.98	0.45
1:Y:177:TYR:CZ	3:Y:502:PMR:H2O	2.50	0.45
1:Z:162:ARG:HD3	1:IA:162:ARG:HE	1.81	0.45
1:CA:177:TYR:CZ	3:CA:502:PMR:H2O	2.50	0.45
1:C:145:LEU:HD21	1:C:147:LEU:HD23	1.98	0.45
1:D:260:ASN:HB2	1:T:131:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:ASN:HB2	1:NA:131:LYS:HD3	1.99	0.45
1:BA:177:TYR:CZ	3:BA:502:PMR:H2O	2.50	0.45
1:HA:131:LYS:HE2	1:MA:259:LEU:O	2.17	0.45
1:OA:145:LEU:HD21	1:OA:147:LEU:HD23	1.98	0.45
1:M:177:TYR:CZ	3:M:502:PMR:H2O	2.50	0.45
1:Z:162:ARG:HE	1:IA:162:ARG:HD3	1.81	0.45
1:JA:177:TYR:CZ	3:JA:502:PMR:H2O	2.50	0.45
1:E:257:ASN:HB3	1:P:259:LEU:HD11	1.98	0.45
1:L:259:LEU:HD11	1:CA:257:ASN:HB3	1.98	0.45
1:Q:259:LEU:HD21	1:LA:257:ASN:O	2.17	0.45
1:B:131:LYS:HD3	1:O:260:ASN:HB2	1.99	0.45
1:Q:257:ASN:O	1:LA:259:LEU:HD21	2.17	0.45
1:S:144:HIS:CE1	1:HA:144:HIS:CE1	3.05	0.45
1:Q:177:TYR:CZ	3:Q:502:PMR:H2O	2.50	0.45
1:V:259:LEU:HD11	1:Y:257:ASN:HB3	1.98	0.45
1:L:260:ASN:HB2	1:LA:131:LYS:HD3	1.99	0.45
1:S:162:ARG:HD3	1:HA:162:ARG:HE	1.81	0.45
1:EA:257:ASN:HB3	1:OA:259:LEU:HD11	1.99	0.45
1:J:257:ASN:HB3	1:DA:259:LEU:HD11	1.99	0.45
1:T:259:LEU:HD21	1:Z:257:ASN:O	2.17	0.45
1:Y:162:ARG:HD3	1:JA:162:ARG:HE	1.80	0.45
1:G:144:HIS:CE1	1:J:144:HIS:CE1	3.05	0.44
1:A:144:HIS:CE1	1:F:144:HIS:CE1	3.05	0.44
1:H:343:GLU:O	1:H:347:ARG:HG3	2.18	0.44
1:K:343:GLU:O	1:K:347:ARG:HG3	2.18	0.44
1:X:343:GLU:O	1:X:347:ARG:HG3	2.18	0.44
1:CA:343:GLU:O	1:CA:347:ARG:HG3	2.18	0.44
1:F:131:LYS:HD3	1:GA:260:ASN:HB2	1.99	0.44
1:M:343:GLU:O	1:M:347:ARG:HG3	2.18	0.44
1:N:343:GLU:O	1:N:347:ARG:HG3	2.18	0.44
1:HA:343:GLU:O	1:HA:347:ARG:HG3	2.18	0.44
1:E:343:GLU:O	1:E:347:ARG:HG3	2.18	0.44
1:R:144:HIS:CE1	1:FA:144:HIS:CE1	3.05	0.44
1:V:343:GLU:O	1:V:347:ARG:HG3	2.18	0.44
1:IA:343:GLU:O	1:IA:347:ARG:HG3	2.18	0.44
1:D:259:LEU:HD11	1:O:257:ASN:HB3	1.99	0.44
1:E:131:LYS:HD3	1:HA:260:ASN:HB2	1.99	0.44
1:I:343:GLU:O	1:I:347:ARG:HG3	2.18	0.44
1:M:257:ASN:HB3	1:X:259:LEU:HD11	1.99	0.44
1:S:257:ASN:O	1:MA:259:LEU:HD21	2.17	0.44
1:W:343:GLU:O	1:W:347:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:343:GLU:O	1:Y:347:ARG:HG3	2.18	0.44
1:Q:343:GLU:O	1:Q:347:ARG:HG3	2.18	0.44
1:O:162:ARG:HE	1:T:162:ARG:HD3	1.82	0.44
1:O:343:GLU:O	1:O:347:ARG:HG3	2.18	0.44
1:S:259:LEU:HD21	1:MA:257:ASN:O	2.18	0.44
1:V:259:LEU:O	1:JA:131:LYS:HE2	2.16	0.44
1:Z:343:GLU:O	1:Z:347:ARG:HG3	2.18	0.44
1:MA:131:LYS:HD3	1:OA:260:ASN:HB2	2.00	0.44
1:MA:343:GLU:O	1:MA:347:ARG:HG3	2.18	0.44
1:B:162:ARG:HE	1:D:162:ARG:HD3	1.82	0.44
1:GA:131:LYS:HE2	1:LA:259:LEU:O	2.18	0.44
1:JA:343:GLU:O	1:JA:347:ARG:HG3	2.18	0.44
1:M:259:LEU:HD11	1:X:257:ASN:HB3	1.99	0.44
1:Y:162:ARG:HE	1:JA:162:ARG:HD3	1.83	0.44
1:BA:144:HIS:CE1	1:OA:144:HIS:CE1	3.06	0.44
1:BA:343:GLU:O	1:BA:347:ARG:HG3	2.18	0.44
1:FA:343:GLU:O	1:FA:347:ARG:HG3	2.18	0.44
1:A:343:GLU:O	1:A:347:ARG:HG3	2.18	0.43
1:H:144:HIS:CE1	1:K:144:HIS:CE1	3.06	0.43
1:L:257:ASN:HB3	1:CA:259:LEU:HD11	2.00	0.43
1:T:257:ASN:O	1:Z:259:LEU:HD21	2.18	0.43
1:T:343:GLU:O	1:T:347:ARG:HG3	2.18	0.43
1:X:246:LEU:HD21	1:X:278:ASP:HB3	2.00	0.43
1:AA:343:GLU:O	1:AA:347:ARG:HG3	2.18	0.43
1:DA:246:LEU:HD21	1:DA:278:ASP:HB3	2.00	0.43
1:OA:343:GLU:O	1:OA:347:ARG:HG3	2.18	0.43
1:B:343:GLU:O	1:B:347:ARG:HG3	2.18	0.43
1:E:259:LEU:HD21	1:P:257:ASN:O	2.18	0.43
1:F:343:GLU:O	1:F:347:ARG:HG3	2.18	0.43
1:H:246:LEU:HD21	1:H:278:ASP:HB3	2.00	0.43
1:J:131:LYS:HD3	1:JA:260:ASN:HB2	1.99	0.43
1:Q:246:LEU:HD21	1:Q:278:ASP:HB3	2.01	0.43
1:T:246:LEU:HD21	1:T:278:ASP:HB3	2.01	0.43
1:AA:144:HIS:CE1	1:KA:144:HIS:CE1	3.06	0.43
1:BA:246:LEU:HD21	1:BA:278:ASP:HB3	2.01	0.43
1:EA:246:LEU:HD21	1:EA:278:ASP:HB3	2.01	0.43
1:HA:246:LEU:HD21	1:HA:278:ASP:HB3	2.00	0.43
1:E:246:LEU:HD21	1:E:278:ASP:HB3	2.01	0.43
1:G:246:LEU:HD21	1:G:278:ASP:HB3	2.01	0.43
1:H:259:LEU:O	1:Z:131:LYS:HE2	2.17	0.43
1:I:246:LEU:HD21	1:I:278:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:LEU:HD21	1:K:278:ASP:HB3	2.01	0.43
1:MA:246:LEU:HD21	1:MA:278:ASP:HB3	2.01	0.43
1:A:246:LEU:HD21	1:A:278:ASP:HB3	2.00	0.43
1:G:343:GLU:O	1:G:347:ARG:HG3	2.18	0.43
1:J:343:GLU:O	1:J:347:ARG:HG3	2.18	0.43
1:M:246:LEU:HD21	1:M:278:ASP:HB3	2.01	0.43
1:R:343:GLU:O	1:R:347:ARG:HG3	2.18	0.43
1:S:246:LEU:HD21	1:S:278:ASP:HB3	2.01	0.43
1:Y:246:LEU:HD21	1:Y:278:ASP:HB3	2.01	0.43
1:AA:246:LEU:HD21	1:AA:278:ASP:HB3	2.01	0.43
1:CA:246:LEU:HD21	1:CA:278:ASP:HB3	2.00	0.43
1:DA:343:GLU:O	1:DA:347:ARG:HG3	2.18	0.43
1:EA:343:GLU:O	1:EA:347:ARG:HG3	2.18	0.43
1:FA:246:LEU:HD21	1:FA:278:ASP:HB3	2.01	0.43
1:GA:246:LEU:HD21	1:GA:278:ASP:HB3	2.01	0.43
1:GA:343:GLU:O	1:GA:347:ARG:HG3	2.18	0.43
1:OA:246:LEU:HD21	1:OA:278:ASP:HB3	2.00	0.43
1:F:246:LEU:HD21	1:F:278:ASP:HB3	2.01	0.43
1:V:246:LEU:HD21	1:V:278:ASP:HB3	2.01	0.43
1:IA:246:LEU:HD21	1:IA:278:ASP:HB3	2.01	0.43
1:D:246:LEU:HD21	1:D:278:ASP:HB3	2.01	0.43
1:P:246:LEU:HD21	1:P:278:ASP:HB3	2.00	0.43
1:T:259:LEU:O	1:IA:131:LYS:HE2	2.18	0.43
1:AA:162:ARG:HD3	1:KA:162:ARG:HE	1.83	0.43
1:JA:240:VAL:HG23	1:JA:242:PRO:O	2.19	0.43
1:JA:246:LEU:HD21	1:JA:278:ASP:HB3	2.01	0.43
1:NA:343:GLU:O	1:NA:347:ARG:HG3	2.18	0.43
1:C:246:LEU:HD21	1:C:278:ASP:HB3	2.01	0.43
1:L:246:LEU:HD21	1:L:278:ASP:HB3	2.01	0.43
1:M:240:VAL:HG23	1:M:242:PRO:O	2.19	0.43
1:O:246:LEU:HD21	1:O:278:ASP:HB3	2.00	0.43
1:P:343:GLU:O	1:P:347:ARG:HG3	2.18	0.43
1:Z:144:HIS:CE1	1:IA:144:HIS:CE1	3.06	0.43
1:EA:259:LEU:HD11	1:OA:257:ASN:HB3	2.00	0.43
1:D:343:GLU:O	1:D:347:ARG:HG3	2.18	0.43
1:E:240:VAL:HG23	1:E:242:PRO:O	2.19	0.43
1:I:144:HIS:CE1	1:L:144:HIS:CE1	3.06	0.43
1:J:246:LEU:HD21	1:J:278:ASP:HB3	2.01	0.43
1:S:392:GLU:O	1:S:396:LYS:HG2	2.19	0.43
1:W:246:LEU:HD21	1:W:278:ASP:HB3	2.01	0.43
1:AA:392:GLU:O	1:AA:396:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:392:GLU:O	1:FA:396:LYS:HG2	2.19	0.43
1:LA:343:GLU:O	1:LA:347:ARG:HG3	2.18	0.43
1:A:240:VAL:HG23	1:A:242:PRO:O	2.19	0.43
1:F:240:VAL:HG23	1:F:242:PRO:O	2.19	0.43
1:H:240:VAL:HG23	1:H:242:PRO:O	2.19	0.43
1:L:343:GLU:O	1:L:347:ARG:HG3	2.18	0.43
1:N:246:LEU:HD21	1:N:278:ASP:HB3	2.01	0.43
1:Q:392:GLU:O	1:Q:396:LYS:HG2	2.19	0.43
1:X:240:VAL:HG23	1:X:242:PRO:O	2.19	0.43
1:Z:240:VAL:HG23	1:Z:242:PRO:O	2.19	0.43
1:Z:246:LEU:HD21	1:Z:278:ASP:HB3	2.01	0.43
1:CA:392:GLU:O	1:CA:396:LYS:HG2	2.19	0.43
1:HA:240:VAL:HG23	1:HA:242:PRO:O	2.19	0.43
1:KA:246:LEU:HD21	1:KA:278:ASP:HB3	2.01	0.43
1:KA:343:GLU:O	1:KA:347:ARG:HG3	2.18	0.43
1:MA:392:GLU:O	1:MA:396:LYS:HG2	2.19	0.43
1:A:392:GLU:O	1:A:396:LYS:HG2	2.19	0.43
1:B:246:LEU:HD21	1:B:278:ASP:HB3	2.01	0.43
1:C:343:GLU:O	1:C:347:ARG:HG3	2.18	0.43
1:E:392:GLU:O	1:E:396:LYS:HG2	2.19	0.43
1:Q:240:VAL:HG23	1:Q:242:PRO:O	2.19	0.43
1:R:246:LEU:HD21	1:R:278:ASP:HB3	2.01	0.43
1:S:343:GLU:O	1:S:347:ARG:HG3	2.18	0.43
1:T:392:GLU:O	1:T:396:LYS:HG2	2.19	0.43
1:BA:392:GLU:O	1:BA:396:LYS:HG2	2.19	0.43
1:EA:392:GLU:O	1:EA:396:LYS:HG2	2.19	0.43
1:LA:246:LEU:HD21	1:LA:278:ASP:HB3	2.01	0.43
1:NA:246:LEU:HD21	1:NA:278:ASP:HB3	2.00	0.43
1:B:240:VAL:HG23	1:B:242:PRO:O	2.19	0.42
1:F:392:GLU:O	1:F:396:LYS:HG2	2.19	0.42
1:I:392:GLU:O	1:I:396:LYS:HG2	2.19	0.42
1:S:240:VAL:HG23	1:S:242:PRO:O	2.19	0.42
1:DA:392:GLU:O	1:DA:396:LYS:HG2	2.19	0.42
1:FA:240:VAL:HG23	1:FA:242:PRO:O	2.19	0.42
1:GA:392:GLU:O	1:GA:396:LYS:HG2	2.19	0.42
1:NA:240:VAL:HG23	1:NA:242:PRO:O	2.19	0.42
1:C:259:LEU:HD11	1:HA:257:ASN:HB3	2.00	0.42
1:C:392:GLU:O	1:C:396:LYS:HG2	2.19	0.42
1:G:376:GLN:HE22	1:KA:376:GLN:HE22	1.67	0.42
1:K:240:VAL:HG23	1:K:242:PRO:O	2.19	0.42
1:L:240:VAL:HG23	1:L:242:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:144:HIS:CE1	1:GA:144:HIS:CE1	3.07	0.42
1:V:240:VAL:HG23	1:V:242:PRO:O	2.19	0.42
1:W:240:VAL:HG23	1:W:242:PRO:O	2.19	0.42
1:W:392:GLU:O	1:W:396:LYS:HG2	2.19	0.42
1:EA:240:VAL:HG23	1:EA:242:PRO:O	2.19	0.42
1:GA:240:VAL:HG23	1:GA:242:PRO:O	2.19	0.42
1:MA:240:VAL:HG23	1:MA:242:PRO:O	2.19	0.42
1:C:240:VAL:HG23	1:C:242:PRO:O	2.19	0.42
1:G:240:VAL:HG23	1:G:242:PRO:O	2.19	0.42
1:L:392:GLU:O	1:L:396:LYS:HG2	2.19	0.42
1:O:240:VAL:HG23	1:O:242:PRO:O	2.19	0.42
1:P:392:GLU:O	1:P:396:LYS:HG2	2.19	0.42
1:T:240:VAL:HG23	1:T:242:PRO:O	2.19	0.42
1:CA:240:VAL:HG23	1:CA:242:PRO:O	2.19	0.42
1:IA:240:VAL:HG23	1:IA:242:PRO:O	2.19	0.42
1:B:392:GLU:O	1:B:396:LYS:HG2	2.19	0.42
1:D:240:VAL:HG23	1:D:242:PRO:O	2.19	0.42
1:X:392:GLU:O	1:X:396:LYS:HG2	2.19	0.42
1:HA:392:GLU:O	1:HA:396:LYS:HG2	2.19	0.42
1:KA:240:VAL:HG23	1:KA:242:PRO:O	2.19	0.42
1:E:257:ASN:O	1:P:259:LEU:HD21	2.20	0.42
1:G:392:GLU:O	1:G:396:LYS:HG2	2.19	0.42
1:I:162:ARG:HE	1:L:162:ARG:HD3	1.84	0.42
1:J:240:VAL:HG23	1:J:242:PRO:O	2.19	0.42
1:L:131:LYS:HE2	1:KA:259:LEU:O	2.19	0.42
1:R:162:ARG:HD3	1:FA:162:ARG:HE	1.84	0.42
1:BA:240:VAL:HG23	1:BA:242:PRO:O	2.19	0.42
1:LA:392:GLU:O	1:LA:396:LYS:HG2	2.19	0.42
1:D:257:ASN:HB3	1:O:259:LEU:HD11	2.02	0.42
1:D:392:GLU:O	1:D:396:LYS:HG2	2.19	0.42
1:M:392:GLU:O	1:M:396:LYS:HG2	2.19	0.42
1:Q:162:ARG:HD3	1:GA:162:ARG:HE	1.83	0.42
1:R:392:GLU:O	1:R:396:LYS:HG2	2.19	0.42
1:AA:240:VAL:HG23	1:AA:242:PRO:O	2.19	0.42
1:JA:392:GLU:O	1:JA:396:LYS:HG2	2.19	0.42
1:R:240:VAL:HG23	1:R:242:PRO:O	2.19	0.42
1:V:131:LYS:HD3	1:X:260:ASN:HB2	2.01	0.42
1:LA:240:VAL:HG23	1:LA:242:PRO:O	2.19	0.42
1:C:259:LEU:O	1:S:131:LYS:HE2	2.20	0.42
1:H:392:GLU:O	1:H:396:LYS:HG2	2.19	0.42
1:I:240:VAL:HG23	1:I:242:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:240:VAL:HG23	1:P:242:PRO:O	2.19	0.42
1:NA:392:GLU:O	1:NA:396:LYS:HG2	2.19	0.42
1:OA:240:VAL:HG23	1:OA:242:PRO:O	2.19	0.42
1:B:162:ARG:HD3	1:D:162:ARG:HE	1.84	0.42
1:B:259:LEU:O	1:R:131:LYS:HE2	2.20	0.42
1:L:304:SER:O	1:L:364:TRP:N	2.50	0.42
1:M:257:ASN:O	1:X:259:LEU:HD21	2.20	0.42
1:O:131:LYS:HE2	1:Z:259:LEU:O	2.20	0.42
1:Y:240:VAL:HG23	1:Y:242:PRO:O	2.19	0.42
1:Y:392:GLU:O	1:Y:396:LYS:HG2	2.19	0.42
1:Z:392:GLU:O	1:Z:396:LYS:HG2	2.19	0.42
1:DA:240:VAL:HG23	1:DA:242:PRO:O	2.19	0.42
1:EA:257:ASN:O	1:OA:259:LEU:HD21	2.20	0.42
1:IA:392:GLU:O	1:IA:396:LYS:HG2	2.19	0.42
1:I:131:LYS:HE2	1:CA:259:LEU:O	2.19	0.41
1:K:392:GLU:O	1:K:396:LYS:HG2	2.19	0.41
1:N:240:VAL:HG23	1:N:242:PRO:O	2.19	0.41
1:N:269:ASP:OD1	1:N:269:ASP:N	2.54	0.41
1:P:269:ASP:OD1	1:P:269:ASP:N	2.53	0.41
1:V:269:ASP:OD1	1:V:269:ASP:N	2.53	0.41
1:M:304:SER:O	1:M:364:TRP:N	2.50	0.41
1:Y:269:ASP:OD1	1:Y:269:ASP:N	2.53	0.41
1:NA:269:ASP:N	1:NA:269:ASP:OD1	2.54	0.41
1:J:392:GLU:O	1:J:396:LYS:HG2	2.19	0.41
1:K:269:ASP:OD1	1:K:269:ASP:N	2.53	0.41
1:L:259:LEU:HD21	1:CA:257:ASN:O	2.20	0.41
1:O:392:GLU:O	1:O:396:LYS:HG2	2.19	0.41
1:R:269:ASP:OD1	1:R:269:ASP:N	2.53	0.41
1:Y:144:HIS:CE1	1:JA:144:HIS:CE1	3.08	0.41
1:Z:269:ASP:N	1:Z:269:ASP:OD1	2.54	0.41
1:KA:269:ASP:OD1	1:KA:269:ASP:N	2.53	0.41
1:OA:392:GLU:O	1:OA:396:LYS:HG2	2.19	0.41
1:D:259:LEU:HD21	1:O:257:ASN:O	2.20	0.41
1:H:269:ASP:OD1	1:H:269:ASP:N	2.53	0.41
1:N:392:GLU:O	1:N:396:LYS:HG2	2.19	0.41
1:O:269:ASP:OD1	1:O:269:ASP:N	2.54	0.41
1:X:304:SER:O	1:X:364:TRP:N	2.50	0.41
1:LA:269:ASP:OD1	1:LA:269:ASP:N	2.53	0.41
1:M:259:LEU:HD21	1:X:257:ASN:O	2.20	0.41
1:N:162:ARG:HD3	1:X:162:ARG:HE	1.85	0.41
1:Q:304:SER:O	1:Q:364:TRP:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:144:HIS:CE1	1:LA:144:HIS:CE1	3.09	0.41
1:DA:144:HIS:CE1	1:NA:144:HIS:CE1	3.08	0.41
1:MA:304:SER:O	1:MA:364:TRP:N	2.50	0.41
1:S:269:ASP:OD1	1:S:269:ASP:N	2.53	0.41
1:IA:269:ASP:OD1	1:IA:269:ASP:N	2.53	0.41
1:E:105:ALA:HB1	1:E:135:MET:SD	2.61	0.41
1:O:304:SER:O	1:O:364:TRP:N	2.50	0.41
1:P:144:HIS:CE1	1:W:144:HIS:CE1	3.08	0.41
1:Q:259:LEU:O	1:CA:131:LYS:HE2	2.21	0.41
1:S:162:ARG:HE	1:HA:162:ARG:HD3	1.84	0.41
1:T:269:ASP:OD1	1:T:269:ASP:N	2.53	0.41
1:DA:269:ASP:N	1:DA:269:ASP:OD1	2.53	0.41
1:DA:304:SER:O	1:DA:364:TRP:N	2.50	0.41
1:IA:105:ALA:HB1	1:IA:135:MET:SD	2.61	0.41
1:D:131:LYS:HE2	1:FA:259:LEU:O	2.21	0.41
1:L:269:ASP:OD1	1:L:269:ASP:N	2.54	0.41
1:M:144:HIS:CE1	1:V:144:HIS:CE1	3.09	0.41
1:S:163:THR:HG22	1:S:163:THR:O	2.21	0.41
1:V:392:GLU:O	1:V:396:LYS:HG2	2.19	0.41
1:X:105:ALA:HB1	1:X:135:MET:SD	2.61	0.41
1:GA:105:ALA:HB1	1:GA:135:MET:SD	2.61	0.41
1:HA:105:ALA:HB1	1:HA:135:MET:SD	2.61	0.41
1:LA:105:ALA:HB1	1:LA:135:MET:SD	2.61	0.41
1:MA:105:ALA:HB1	1:MA:135:MET:SD	2.61	0.41
1:OA:105:ALA:HB1	1:OA:135:MET:SD	2.61	0.41
1:A:105:ALA:HB1	1:A:135:MET:SD	2.61	0.41
1:A:259:LEU:O	1:Q:131:LYS:HE2	2.20	0.41
1:B:144:HIS:CE1	1:D:144:HIS:CE1	3.09	0.41
1:C:163:THR:O	1:C:163:THR:HG22	2.21	0.41
1:C:376:GLN:HE22	1:FA:376:GLN:HE22	1.68	0.41
1:F:105:ALA:HB1	1:F:135:MET:SD	2.61	0.41
1:G:105:ALA:HB1	1:G:135:MET:SD	2.61	0.41
1:G:131:LYS:HE2	1:DA:259:LEU:O	2.20	0.41
1:J:105:ALA:HB1	1:J:135:MET:SD	2.61	0.41
1:L:163:THR:O	1:L:163:THR:HG22	2.21	0.41
1:L:257:ASN:O	1:CA:259:LEU:HD21	2.21	0.41
1:M:131:LYS:HE2	1:Y:259:LEU:O	2.19	0.41
1:M:163:THR:O	1:M:163:THR:HG22	2.21	0.41
1:N:105:ALA:HB1	1:N:135:MET:SD	2.61	0.41
1:O:105:ALA:HB1	1:O:135:MET:SD	2.61	0.41
1:Q:105:ALA:HB1	1:Q:135:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:163:THR:HG22	1:R:163:THR:O	2.21	0.41
1:S:259:LEU:O	1:EA:131:LYS:HE2	2.21	0.41
1:V:105:ALA:HB1	1:V:135:MET:SD	2.61	0.41
1:V:257:ASN:O	1:Y:259:LEU:HD21	2.21	0.41
1:V:259:LEU:HD21	1:Y:257:ASN:O	2.21	0.41
1:W:105:ALA:HB1	1:W:135:MET:SD	2.61	0.41
1:X:163:THR:HG22	1:X:163:THR:O	2.21	0.41
1:Y:105:ALA:HB1	1:Y:135:MET:SD	2.61	0.41
1:EA:144:HIS:CE1	1:MA:144:HIS:CE1	3.08	0.41
1:HA:173:ASN:O	2:HA:501:NDP:H52N	2.21	0.41
1:JA:163:THR:O	1:JA:163:THR:HG22	2.21	0.41
1:KA:105:ALA:HB1	1:KA:135:MET:SD	2.61	0.41
1:KA:392:GLU:O	1:KA:396:LYS:HG2	2.19	0.41
1:MA:269:ASP:OD1	1:MA:269:ASP:N	2.53	0.41
1:NA:163:THR:O	1:NA:163:THR:HG22	2.21	0.41
1:B:163:THR:O	1:B:163:THR:HG22	2.21	0.41
1:F:269:ASP:OD1	1:F:269:ASP:N	2.53	0.41
1:G:173:ASN:O	2:G:501:NDP:H52N	2.21	0.41
1:K:131:LYS:HE2	1:IA:259:LEU:O	2.21	0.41
1:L:105:ALA:HB1	1:L:135:MET:SD	2.61	0.41
1:Q:269:ASP:N	1:Q:269:ASP:OD1	2.53	0.41
1:T:173:ASN:O	2:T:501:NDP:H52N	2.21	0.41
1:Z:163:THR:O	1:Z:163:THR:HG22	2.21	0.41
1:AA:269:ASP:OD1	1:AA:269:ASP:N	2.53	0.41
1:CA:105:ALA:HB1	1:CA:135:MET:SD	2.61	0.41
1:CA:269:ASP:OD1	1:CA:269:ASP:N	2.53	0.41
1:EA:173:ASN:O	2:EA:501:NDP:H52N	2.21	0.41
1:FA:105:ALA:HB1	1:FA:135:MET:SD	2.61	0.41
1:FA:269:ASP:OD1	1:FA:269:ASP:N	2.53	0.41
1:GA:163:THR:O	1:GA:163:THR:HG22	2.21	0.41
1:GA:269:ASP:N	1:GA:269:ASP:OD1	2.53	0.41
1:JA:269:ASP:OD1	1:JA:269:ASP:N	2.53	0.41
1:NA:105:ALA:HB1	1:NA:135:MET:SD	2.61	0.41
1:OA:163:THR:O	1:OA:163:THR:HG22	2.21	0.41
1:A:173:ASN:O	2:A:501:NDP:H52N	2.22	0.40
1:A:269:ASP:OD1	1:A:269:ASP:N	2.53	0.40
1:C:105:ALA:HB1	1:C:135:MET:SD	2.61	0.40
1:D:105:ALA:HB1	1:D:135:MET:SD	2.61	0.40
1:D:173:ASN:O	2:D:501:NDP:H52N	2.22	0.40
1:D:269:ASP:OD1	1:D:269:ASP:N	2.53	0.40
1:E:269:ASP:OD1	1:E:269:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:ASN:O	2:F:501:NDP:H52N	2.21	0.40
1:I:259:LEU:O	1:AA:131:LYS:HE2	2.20	0.40
1:O:162:ARG:HD3	1:T:162:ARG:HE	1.85	0.40
1:Q:173:ASN:O	2:Q:501:NDP:H52N	2.22	0.40
1:R:226:VAL:HG11	2:R:501:NDP:H1D	2.04	0.40
1:S:173:ASN:O	2:S:501:NDP:H52N	2.22	0.40
1:T:105:ALA:HB1	1:T:135:MET:SD	2.61	0.40
1:V:163:THR:HG22	1:V:163:THR:O	2.21	0.40
1:W:173:ASN:O	2:W:501:NDP:H52N	2.22	0.40
1:W:269:ASP:N	1:W:269:ASP:OD1	2.53	0.40
1:Z:105:ALA:HB1	1:Z:135:MET:SD	2.61	0.40
1:AA:162:ARG:HE	1:KA:162:ARG:HD3	1.86	0.40
1:BA:131:LYS:HE2	1:EA:259:LEU:O	2.20	0.40
1:DA:173:ASN:O	2:DA:501:NDP:H52N	2.21	0.40
1:EA:163:THR:O	1:EA:163:THR:HG22	2.21	0.40
1:HA:269:ASP:N	1:HA:269:ASP:OD1	2.53	0.40
1:B:105:ALA:HB1	1:B:135:MET:SD	2.61	0.40
1:C:173:ASN:O	2:C:501:NDP:H52N	2.21	0.40
1:E:173:ASN:O	2:E:501:NDP:H52N	2.21	0.40
1:I:269:ASP:OD1	1:I:269:ASP:N	2.53	0.40
1:L:226:VAL:HG11	2:L:501:NDP:H1D	2.04	0.40
1:P:105:ALA:HB1	1:P:135:MET:SD	2.61	0.40
1:Q:163:THR:HG22	1:Q:163:THR:O	2.21	0.40
1:T:163:THR:HG22	1:T:163:THR:O	2.21	0.40
1:W:145:LEU:HD12	1:W:156:PHE:CG	2.57	0.40
1:X:173:ASN:O	2:X:501:NDP:H52N	2.22	0.40
1:BA:269:ASP:OD1	1:BA:269:ASP:N	2.53	0.40
1:CA:173:ASN:O	2:CA:501:NDP:H52N	2.21	0.40
1:OA:173:ASN:O	2:OA:501:NDP:H52N	2.21	0.40
1:C:226:VAL:HG11	2:C:501:NDP:H1D	2.04	0.40
1:C:269:ASP:OD1	1:C:269:ASP:N	2.53	0.40
1:G:145:LEU:HD12	1:G:156:PHE:CG	2.57	0.40
1:H:163:THR:O	1:H:163:THR:HG22	2.21	0.40
1:I:105:ALA:HB1	1:I:135:MET:SD	2.61	0.40
1:J:226:VAL:HG11	2:J:501:NDP:H1D	2.04	0.40
1:K:105:ALA:HB1	1:K:135:MET:SD	2.61	0.40
1:O:347:ARG:O	1:O:351:VAL:HG23	2.22	0.40
1:V:173:ASN:O	2:V:501:NDP:H52N	2.22	0.40
1:W:347:ARG:O	1:W:351:VAL:HG23	2.22	0.40
1:AA:105:ALA:HB1	1:AA:135:MET:SD	2.61	0.40
1:AA:173:ASN:O	2:AA:501:NDP:H52N	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:259:LEU:HD21	1:OA:257:ASN:O	2.21	0.40
1:FA:173:ASN:O	2:FA:501:NDP:H52N	2.21	0.40
1:IA:163:THR:HG22	1:IA:163:THR:O	2.21	0.40
1:JA:347:ARG:O	1:JA:351:VAL:HG23	2.22	0.40
1:KA:226:VAL:HG11	2:KA:501:NDP:H1D	2.04	0.40
1:NA:226:VAL:HG11	2:NA:501:NDP:H1D	2.04	0.40
1:B:226:VAL:HG11	2:B:501:NDP:H1D	2.04	0.40
1:C:257:ASN:HB3	1:HA:259:LEU:HD11	2.03	0.40
1:G:163:THR:O	1:G:163:THR:HG22	2.21	0.40
1:H:105:ALA:HB1	1:H:135:MET:SD	2.61	0.40
1:L:355:PRO:O	1:L:358:THR:HG23	2.22	0.40
1:L:367:ASN:HB3	1:L:371:ALA:HB3	2.04	0.40
1:M:269:ASP:OD1	1:M:269:ASP:N	2.53	0.40
1:O:163:THR:O	1:O:163:THR:HG22	2.21	0.40
1:Q:347:ARG:O	1:Q:351:VAL:HG23	2.22	0.40
1:R:173:ASN:O	2:R:501:NDP:H52N	2.22	0.40
1:S:105:ALA:HB1	1:S:135:MET:SD	2.61	0.40
1:S:347:ARG:O	1:S:351:VAL:HG23	2.22	0.40
1:W:163:THR:HG22	1:W:163:THR:O	2.21	0.40
1:X:145:LEU:HD12	1:X:156:PHE:CG	2.57	0.40
1:X:269:ASP:OD1	1:X:269:ASP:N	2.53	0.40
1:Y:347:ARG:O	1:Y:351:VAL:HG23	2.22	0.40
1:Z:226:VAL:HG11	2:Z:501:NDP:H1D	2.04	0.40
1:BA:105:ALA:HB1	1:BA:135:MET:SD	2.61	0.40
1:BA:173:ASN:O	2:BA:501:NDP:H52N	2.22	0.40
1:DA:105:ALA:HB1	1:DA:135:MET:SD	2.61	0.40
1:FA:347:ARG:O	1:FA:351:VAL:HG23	2.22	0.40
1:GA:347:ARG:O	1:GA:351:VAL:HG23	2.22	0.40
1:HA:347:ARG:O	1:HA:351:VAL:HG23	2.22	0.40
1:IA:173:ASN:O	2:IA:501:NDP:H52N	2.22	0.40
1:OA:226:VAL:HG11	2:OA:501:NDP:H1D	2.04	0.40
1:OA:269:ASP:OD1	1:OA:269:ASP:N	2.53	0.40
1:A:162:ARG:HE	1:F:162:ARG:HD3	1.85	0.40
1:A:226:VAL:HG11	2:A:501:NDP:H1D	2.04	0.40
1:D:145:LEU:HD12	1:D:156:PHE:CG	2.57	0.40
1:D:355:PRO:O	1:D:358:THR:HG23	2.22	0.40
1:G:269:ASP:OD1	1:G:269:ASP:N	2.53	0.40
1:H:226:VAL:HG11	2:H:501:NDP:H1D	2.04	0.40
1:I:347:ARG:O	1:I:351:VAL:HG23	2.22	0.40
1:I:355:PRO:O	1:I:358:THR:HG23	2.22	0.40
1:J:347:ARG:O	1:J:351:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:173:ASN:O	2:M:501:NDP:H52N	2.21	0.40
1:P:226:VAL:HG11	2:P:501:NDP:H1D	2.04	0.40
1:S:226:VAL:HG11	2:S:501:NDP:H1D	2.04	0.40
1:AA:145:LEU:HD12	1:AA:156:PHE:CG	2.57	0.40
1:CA:145:LEU:HD12	1:CA:156:PHE:CG	2.57	0.40
1:CA:163:THR:HG22	1:CA:163:THR:O	2.21	0.40
1:EA:105:ALA:HB1	1:EA:135:MET:SD	2.61	0.40
1:EA:269:ASP:N	1:EA:269:ASP:OD1	2.53	0.40
1:HA:145:LEU:HD12	1:HA:156:PHE:CG	2.57	0.40
1:HA:163:THR:O	1:HA:163:THR:HG22	2.21	0.40
1:LA:355:PRO:O	1:LA:358:THR:HG23	2.22	0.40
1:MA:355:PRO:O	1:MA:358:THR:HG23	2.22	0.40
1:OA:367:ASN:HB3	1:OA:371:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	AA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	B	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	BA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	C	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	CA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	D	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	DA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	E	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	EA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	FA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	G	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	GA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	H	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	HA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	I	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	IA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	J	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	JA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	K	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	KA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	L	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	LA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	M	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	MA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	N	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	NA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	O	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	OA	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	P	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	Q	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	R	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	S	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	T	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	V	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	W	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	X	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	Y	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
1	Z	314/401 (78%)	308 (98%)	6 (2%)	0	100	100
All	All	12560/16040 (78%)	12320 (98%)	240 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	AA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	B	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	BA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	C	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	CA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	D	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	DA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	E	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	EA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	F	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	FA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	G	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	GA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	H	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	HA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	I	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	IA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	J	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	JA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	K	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	KA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	L	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	LA	259/330 (78%)	258 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	MA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	N	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	NA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	O	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	OA	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	P	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	Q	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	R	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	S	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	T	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	V	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	W	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	X	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	Y	259/330 (78%)	258 (100%)	1 (0%)	91	96
1	Z	259/330 (78%)	258 (100%)	1 (0%)	91	96
All	All	10360/13200 (78%)	10320 (100%)	40 (0%)	91	96

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	B	319	HIS
1	C	319	HIS
1	D	319	HIS
1	E	319	HIS
1	F	319	HIS
1	G	319	HIS
1	H	319	HIS
1	I	319	HIS
1	J	319	HIS
1	K	319	HIS
1	L	319	HIS
1	M	319	HIS
1	N	319	HIS
1	O	319	HIS

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Mol	Chain	Res	Type
1	P	319	HIS
1	Q	319	HIS
1	R	319	HIS
1	S	319	HIS
1	T	319	HIS
1	V	319	HIS
1	W	319	HIS
1	X	319	HIS
1	Y	319	HIS
1	Z	319	HIS
1	AA	319	HIS
1	BA	319	HIS
1	CA	319	HIS
1	DA	319	HIS
1	EA	319	HIS
1	FA	319	HIS
1	GA	319	HIS
1	HA	319	HIS
1	IA	319	HIS
1	JA	319	HIS
1	KA	319	HIS
1	LA	319	HIS
1	MA	319	HIS
1	NA	319	HIS
1	OA	319	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	291	HIS
1	B	232	ASN
1	B	291	HIS
1	C	232	ASN
1	C	291	HIS
1	C	376	GLN
1	D	232	ASN
1	D	291	HIS
1	D	376	GLN
1	E	232	ASN
1	E	291	HIS
1	F	232	ASN

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Mol	Chain	Res	Type
1	F	291	HIS
1	G	232	ASN
1	G	291	HIS
1	H	232	ASN
1	H	291	HIS
1	H	376	GLN
1	I	232	ASN
1	I	291	HIS
1	J	232	ASN
1	J	291	HIS
1	K	232	ASN
1	K	291	HIS
1	L	232	ASN
1	L	291	HIS
1	L	376	GLN
1	M	232	ASN
1	M	291	HIS
1	N	232	ASN
1	N	291	HIS
1	O	232	ASN
1	O	291	HIS
1	P	232	ASN
1	P	291	HIS
1	Q	232	ASN
1	Q	291	HIS
1	Q	376	GLN
1	R	232	ASN
1	R	291	HIS
1	S	232	ASN
1	S	291	HIS
1	T	232	ASN
1	T	291	HIS
1	V	232	ASN
1	V	291	HIS
1	W	232	ASN
1	W	291	HIS
1	X	232	ASN
1	X	291	HIS
1	X	376	GLN
1	Y	232	ASN
1	Y	291	HIS
1	Z	232	ASN

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Mol	Chain	Res	Type
1	Z	291	HIS
1	AA	232	ASN
1	AA	291	HIS
1	BA	232	ASN
1	BA	291	HIS
1	CA	232	ASN
1	CA	291	HIS
1	CA	376	GLN
1	DA	232	ASN
1	DA	291	HIS
1	EA	232	ASN
1	EA	291	HIS
1	FA	232	ASN
1	FA	291	HIS
1	GA	232	ASN
1	GA	291	HIS
1	HA	232	ASN
1	HA	291	HIS
1	HA	376	GLN
1	IA	232	ASN
1	IA	291	HIS
1	JA	232	ASN
1	JA	291	HIS
1	KA	232	ASN
1	KA	291	HIS
1	KA	376	GLN
1	LA	232	ASN
1	LA	291	HIS
1	MA	232	ASN
1	MA	291	HIS
1	NA	232	ASN
1	NA	291	HIS
1	OA	232	ASN
1	OA	291	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

120 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	NDP	HA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	HA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	NA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	X	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	B	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	Y	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	D	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
2	NDP	P	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	IA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	LA	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
3	PMR	O	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	Z	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	F	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.26	18 (33%)
2	NDP	GA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.51	7 (13%)
3	PMR	NA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	GA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	FA	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
2	NDP	H	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	H	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	J	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	N	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	E	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PMR	IA	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
3	PMR	W	502	-	48,53,53	6.40	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	D	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	JA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	L	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	K	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	FA	503	-	23,23,55	1.02	0	31,31,63	1.30	5 (16%)
2	NDP	A	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
3	PMR	R	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	KA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
2	NDP	X	501	-	45,52,52	1.07	4 (8%)	53,80,80	1.50	7 (13%)
4	LMG	LA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	Y	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	Z	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	S	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
4	LMG	V	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	I	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.28	18 (33%)
3	PMR	DA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	P	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	E	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	K	503	-	23,23,55	1.02	0	31,31,63	1.30	5 (16%)
4	LMG	KA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	M	503	-	23,23,55	1.02	0	31,31,63	1.31	5 (16%)
3	PMR	Y	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	E	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	Z	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
4	LMG	OA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	G	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	B	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	DA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.51	7 (13%)
4	LMG	N	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	OA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	FA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	C	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	A	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.26	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PMR	B	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
2	NDP	V	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	X	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.26	18 (33%)
3	PMR	N	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
2	NDP	C	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
2	NDP	EA	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
4	LMG	EA	503	-	23,23,55	1.04	0	31,31,63	1.30	5 (16%)
3	PMR	H	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	G	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
3	PMR	T	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.28	18 (33%)
2	NDP	T	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
3	PMR	KA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	JA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	R	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	R	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	OA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	T	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	G	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	D	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	L	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.26	18 (33%)
3	PMR	Q	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	EA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	AA	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
4	LMG	F	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
4	LMG	A	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	NA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	BA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	CA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.51	7 (13%)
4	LMG	CA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	V	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	F	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
2	NDP	BA	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
2	NDP	IA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	M	502	-	48,53,53	6.41	7 (14%)	54,89,89	2.27	18 (33%)
4	LMG	MA	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NDP	L	501	-	45,52,52	1.07	4 (8%)	53,80,80	1.51	7 (13%)
2	NDP	AA	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	C	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	AA	503	-	23,23,55	1.03	0	31,31,63	1.29	5 (16%)
2	NDP	S	501	-	45,52,52	1.07	4 (8%)	53,80,80	1.51	7 (13%)
2	NDP	O	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	W	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	LA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
3	PMR	CA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	Q	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	J	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	MA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
4	LMG	J	503	-	23,23,55	1.04	0	31,31,63	1.30	5 (16%)
4	LMG	S	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
2	NDP	MA	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.50	7 (13%)
3	PMR	HA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.27	18 (33%)
2	NDP	M	501	-	45,52,52	1.07	4 (8%)	53,80,80	1.50	7 (13%)
2	NDP	W	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.50	7 (13%)
2	NDP	JA	501	-	45,52,52	1.06	4 (8%)	53,80,80	1.50	7 (13%)
4	LMG	BA	503	-	23,23,55	1.02	0	31,31,63	1.30	5 (16%)
2	NDP	I	501	-	45,52,52	1.07	3 (6%)	53,80,80	1.51	7 (13%)
2	NDP	Q	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.51	7 (13%)
4	LMG	I	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)
3	PMR	GA	502	-	48,53,53	6.41	8 (16%)	54,89,89	2.26	18 (33%)
2	NDP	K	501	-	45,52,52	1.06	3 (6%)	53,80,80	1.50	7 (13%)
4	LMG	O	503	-	23,23,55	1.03	0	31,31,63	1.29	5 (16%)
4	LMG	DA	503	-	23,23,55	1.04	0	31,31,63	1.30	5 (16%)
4	LMG	P	503	-	23,23,55	1.03	0	31,31,63	1.30	5 (16%)

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
2	NDP	HA	501	-	-	15/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMG	HA	503	-	-	8/16/36/70	0/1/1/1
4	LMG	NA	503	-	-	8/16/36/70	0/1/1/1
4	LMG	X	503	-	-	8/16/36/70	0/1/1/1
2	NDP	B	501	-	-	15/30/77/77	0/5/5/5
4	LMG	Y	503	-	-	8/16/36/70	0/1/1/1
2	NDP	D	501	-	-	15/30/77/77	0/5/5/5
2	NDP	P	501	-	-	15/30/77/77	0/5/5/5
4	LMG	IA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	LA	501	-	-	15/30/77/77	0/5/5/5
3	PMR	O	502	-	3/3/16/20	4/15/111/111	-
4	LMG	Z	503	-	-	8/16/36/70	0/1/1/1
3	PMR	F	502	-	3/3/16/20	4/15/111/111	-
3	PMR	NA	502	-	3/3/16/20	4/15/111/111	-
2	NDP	GA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	GA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	FA	501	-	-	15/30/77/77	0/5/5/5
2	NDP	H	501	-	-	15/30/77/77	0/5/5/5
4	LMG	H	503	-	-	8/16/36/70	0/1/1/1
3	PMR	J	502	-	3/3/16/20	4/15/111/111	-
3	PMR	E	502	-	3/3/16/20	4/15/111/111	-
2	NDP	N	501	-	-	15/30/77/77	0/5/5/5
3	PMR	IA	502	-	3/3/16/20	4/15/111/111	-
3	PMR	W	502	-	3/3/16/20	4/15/111/111	-
4	LMG	D	503	-	-	8/16/36/70	0/1/1/1
3	PMR	JA	502	-	3/3/16/20	4/15/111/111	-
4	LMG	L	503	-	-	8/16/36/70	0/1/1/1
3	PMR	K	502	-	3/3/16/20	4/15/111/111	-
4	LMG	FA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	A	501	-	-	15/30/77/77	0/5/5/5
3	PMR	R	502	-	3/3/16/20	4/15/111/111	-
2	NDP	KA	501	-	-	15/30/77/77	0/5/5/5
2	NDP	X	501	-	-	15/30/77/77	0/5/5/5
4	LMG	LA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	Y	501	-	-	15/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMR	Z	502	-	3/3/16/20	4/15/111/111	-
3	PMR	S	502	-	3/3/16/20	4/15/111/111	-
4	LMG	V	503	-	-	8/16/36/70	0/1/1/1
3	PMR	I	502	-	3/3/16/20	4/15/111/111	-
3	PMR	DA	502	-	3/3/16/20	4/15/111/111	-
3	PMR	P	502	-	3/3/16/20	4/15/111/111	-
2	NDP	E	501	-	-	15/30/77/77	0/5/5/5
4	LMG	K	503	-	-	8/16/36/70	0/1/1/1
4	LMG	KA	503	-	-	8/16/36/70	0/1/1/1
4	LMG	M	503	-	-	8/16/36/70	0/1/1/1
3	PMR	Y	502	-	3/3/16/20	4/15/111/111	-
4	LMG	E	503	-	-	8/16/36/70	0/1/1/1
2	NDP	Z	501	-	-	15/30/77/77	0/5/5/5
4	LMG	OA	503	-	-	8/16/36/70	0/1/1/1
4	LMG	G	503	-	-	8/16/36/70	0/1/1/1
4	LMG	B	503	-	-	8/16/36/70	0/1/1/1
2	NDP	DA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	N	503	-	-	8/16/36/70	0/1/1/1
3	PMR	OA	502	-	3/3/16/20	4/15/111/111	-
3	PMR	FA	502	-	3/3/16/20	4/15/111/111	-
4	LMG	C	503	-	-	8/16/36/70	0/1/1/1
3	PMR	A	502	-	3/3/16/20	4/15/111/111	-
3	PMR	B	502	-	3/3/16/20	4/15/111/111	-
3	PMR	X	502	-	3/3/16/20	4/15/111/111	-
2	NDP	V	501	-	-	15/30/77/77	0/5/5/5
3	PMR	N	502	-	3/3/16/20	4/15/111/111	-
2	NDP	C	501	-	-	15/30/77/77	0/5/5/5
2	NDP	EA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	EA	503	-	-	8/16/36/70	0/1/1/1
3	PMR	H	502	-	3/3/16/20	4/15/111/111	-
2	NDP	G	501	-	-	15/30/77/77	0/5/5/5
3	PMR	T	502	-	3/3/16/20	4/15/111/111	-
2	NDP	T	501	-	-	15/30/77/77	0/5/5/5
3	PMR	KA	502	-	3/3/16/20	4/15/111/111	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMG	JA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	R	501	-	-	15/30/77/77	0/5/5/5
4	LMG	R	503	-	-	8/16/36/70	0/1/1/1
2	NDP	OA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	T	503	-	-	8/16/36/70	0/1/1/1
3	PMR	G	502	-	3/3/16/20	4/15/111/111	-
3	PMR	D	502	-	3/3/16/20	4/15/111/111	-
3	PMR	Q	502	-	3/3/16/20	4/15/111/111	-
3	PMR	L	502	-	3/3/16/20	4/15/111/111	-
3	PMR	EA	502	-	3/3/16/20	4/15/111/111	-
3	PMR	AA	502	-	3/3/16/20	4/15/111/111	-
4	LMG	F	503	-	-	8/16/36/70	0/1/1/1
4	LMG	A	503	-	-	8/16/36/70	0/1/1/1
2	NDP	NA	501	-	-	15/30/77/77	0/5/5/5
3	PMR	BA	502	-	3/3/16/20	4/15/111/111	-
2	NDP	CA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	CA	503	-	-	8/16/36/70	0/1/1/1
3	PMR	V	502	-	3/3/16/20	4/15/111/111	-
2	NDP	F	501	-	-	15/30/77/77	0/5/5/5
2	NDP	BA	501	-	-	15/30/77/77	0/5/5/5
2	NDP	IA	501	-	-	15/30/77/77	0/5/5/5
3	PMR	M	502	-	3/3/16/20	4/15/111/111	-
4	LMG	MA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	L	501	-	-	15/30/77/77	0/5/5/5
3	PMR	C	502	-	3/3/16/20	4/15/111/111	-
2	NDP	AA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	AA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	S	501	-	-	15/30/77/77	0/5/5/5
2	NDP	O	501	-	-	15/30/77/77	0/5/5/5
4	LMG	W	503	-	-	8/16/36/70	0/1/1/1
3	PMR	LA	502	-	3/3/16/20	4/15/111/111	-
3	PMR	CA	502	-	3/3/16/20	4/15/111/111	-
4	LMG	Q	503	-	-	8/16/36/70	0/1/1/1
2	NDP	J	501	-	-	15/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMR	MA	502	-	3/3/16/20	4/15/111/111	-
4	LMG	J	503	-	-	8/16/36/70	0/1/1/1
4	LMG	S	503	-	-	8/16/36/70	0/1/1/1
2	NDP	MA	501	-	-	15/30/77/77	0/5/5/5
3	PMR	HA	502	-	3/3/16/20	4/15/111/111	-
2	NDP	M	501	-	-	15/30/77/77	0/5/5/5
2	NDP	W	501	-	-	15/30/77/77	0/5/5/5
2	NDP	JA	501	-	-	15/30/77/77	0/5/5/5
4	LMG	BA	503	-	-	8/16/36/70	0/1/1/1
2	NDP	I	501	-	-	15/30/77/77	0/5/5/5
2	NDP	Q	501	-	-	15/30/77/77	0/5/5/5
4	LMG	I	503	-	-	8/16/36/70	0/1/1/1
3	PMR	GA	502	-	3/3/16/20	4/15/111/111	-
2	NDP	K	501	-	-	15/30/77/77	0/5/5/5
4	LMG	O	503	-	-	8/16/36/70	0/1/1/1
4	LMG	DA	503	-	-	8/16/36/70	0/1/1/1
4	LMG	P	503	-	-	8/16/36/70	0/1/1/1

All (436) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	502	PMR	MG-NA	31.52	2.81	2.06
3	OA	502	PMR	MG-NA	31.52	2.81	2.06
3	K	502	PMR	MG-NA	31.52	2.81	2.06
3	G	502	PMR	MG-NA	31.51	2.81	2.06
3	MA	502	PMR	MG-NA	31.51	2.81	2.06
3	O	502	PMR	MG-NA	31.51	2.81	2.06
3	DA	502	PMR	MG-NA	31.50	2.81	2.06
3	EA	502	PMR	MG-NA	31.50	2.81	2.06
3	AA	502	PMR	MG-NA	31.49	2.81	2.06
3	E	502	PMR	MG-NA	31.49	2.81	2.06
3	T	502	PMR	MG-NA	31.49	2.81	2.06
3	LA	502	PMR	MG-NA	31.49	2.81	2.06
3	BA	502	PMR	MG-NA	31.49	2.81	2.06
3	CA	502	PMR	MG-NA	31.49	2.81	2.06
3	IA	502	PMR	MG-NA	31.49	2.81	2.06
3	KA	502	PMR	MG-NA	31.49	2.81	2.06
3	A	502	PMR	MG-NA	31.49	2.81	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	PMR	MG-NA	31.49	2.81	2.06
3	W	502	PMR	MG-NA	31.49	2.81	2.06
3	X	502	PMR	MG-NA	31.49	2.81	2.06
3	V	502	PMR	MG-NA	31.48	2.81	2.06
3	J	502	PMR	MG-NA	31.48	2.81	2.06
3	JA	502	PMR	MG-NA	31.48	2.81	2.06
3	B	502	PMR	MG-NA	31.48	2.81	2.06
3	I	502	PMR	MG-NA	31.48	2.81	2.06
3	HA	502	PMR	MG-NA	31.48	2.81	2.06
3	NA	502	PMR	MG-NA	31.48	2.81	2.06
3	M	502	PMR	MG-NA	31.48	2.81	2.06
3	GA	502	PMR	MG-NA	31.48	2.81	2.06
3	P	502	PMR	MG-NA	31.48	2.81	2.06
3	F	502	PMR	MG-NA	31.48	2.81	2.06
3	S	502	PMR	MG-NA	31.47	2.81	2.06
3	N	502	PMR	MG-NA	31.47	2.81	2.06
3	Z	502	PMR	MG-NA	31.47	2.81	2.06
3	FA	502	PMR	MG-NA	31.47	2.81	2.06
3	C	502	PMR	MG-NA	31.47	2.81	2.06
3	Q	502	PMR	MG-NA	31.46	2.81	2.06
3	L	502	PMR	MG-NA	31.46	2.81	2.06
3	Y	502	PMR	MG-NA	31.46	2.81	2.06
3	D	502	PMR	MG-NA	31.46	2.81	2.06
3	Y	502	PMR	MG-NC	30.26	2.78	2.06
3	C	502	PMR	MG-NC	30.26	2.78	2.06
3	Q	502	PMR	MG-NC	30.26	2.78	2.06
3	F	502	PMR	MG-NC	30.25	2.78	2.06
3	H	502	PMR	MG-NC	30.25	2.78	2.06
3	L	502	PMR	MG-NC	30.25	2.78	2.06
3	CA	502	PMR	MG-NC	30.25	2.78	2.06
3	HA	502	PMR	MG-NC	30.24	2.78	2.06
3	N	502	PMR	MG-NC	30.24	2.78	2.06
3	BA	502	PMR	MG-NC	30.24	2.78	2.06
3	B	502	PMR	MG-NC	30.24	2.78	2.06
3	OA	502	PMR	MG-NC	30.24	2.78	2.06
3	IA	502	PMR	MG-NC	30.23	2.78	2.06
3	AA	502	PMR	MG-NC	30.23	2.78	2.06
3	V	502	PMR	MG-NC	30.23	2.78	2.06
3	D	502	PMR	MG-NC	30.23	2.78	2.06
3	S	502	PMR	MG-NC	30.23	2.78	2.06
3	T	502	PMR	MG-NC	30.23	2.78	2.06
3	J	502	PMR	MG-NC	30.23	2.78	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	502	PMR	MG-NC	30.23	2.78	2.06
3	NA	502	PMR	MG-NC	30.23	2.78	2.06
3	G	502	PMR	MG-NC	30.23	2.78	2.06
3	P	502	PMR	MG-NC	30.22	2.78	2.06
3	Z	502	PMR	MG-NC	30.22	2.78	2.06
3	EA	502	PMR	MG-NC	30.22	2.78	2.06
3	KA	502	PMR	MG-NC	30.22	2.78	2.06
3	M	502	PMR	MG-NC	30.22	2.78	2.06
3	FA	502	PMR	MG-NC	30.22	2.78	2.06
3	MA	502	PMR	MG-NC	30.21	2.78	2.06
3	K	502	PMR	MG-NC	30.21	2.78	2.06
3	R	502	PMR	MG-NC	30.21	2.78	2.06
3	E	502	PMR	MG-NC	30.21	2.78	2.06
3	JA	502	PMR	MG-NC	30.21	2.78	2.06
3	A	502	PMR	MG-NC	30.21	2.78	2.06
3	O	502	PMR	MG-NC	30.21	2.78	2.06
3	DA	502	PMR	MG-NC	30.21	2.78	2.06
3	GA	502	PMR	MG-NC	30.20	2.78	2.06
3	LA	502	PMR	MG-NC	30.20	2.78	2.06
3	I	502	PMR	MG-NC	30.20	2.78	2.06
3	W	502	PMR	MG-NC	30.19	2.78	2.06
2	LA	501	NDP	C7N-C3N	-3.32	1.41	1.48
2	N	501	NDP	C7N-C3N	-3.31	1.41	1.48
2	MA	501	NDP	C7N-C3N	-3.31	1.41	1.48
2	EA	501	NDP	C7N-C3N	-3.31	1.41	1.48
2	L	501	NDP	C7N-C3N	-3.30	1.41	1.48
2	F	501	NDP	C7N-C3N	-3.30	1.41	1.48
2	GA	501	NDP	C7N-C3N	-3.30	1.41	1.48
2	AA	501	NDP	C7N-C3N	-3.30	1.41	1.48
2	T	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	FA	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	C	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	B	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	G	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	I	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	S	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	Y	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	W	501	NDP	C7N-C3N	-3.29	1.41	1.48
2	CA	501	NDP	C7N-C3N	-3.28	1.41	1.48
2	A	501	NDP	C7N-C3N	-3.28	1.41	1.48
2	H	501	NDP	C7N-C3N	-3.28	1.41	1.48
2	R	501	NDP	C7N-C3N	-3.28	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	501	NDP	C7N-C3N	-3.27	1.41	1.48
2	O	501	NDP	C7N-C3N	-3.27	1.41	1.48
2	IA	501	NDP	C7N-C3N	-3.27	1.41	1.48
2	M	501	NDP	C7N-C3N	-3.27	1.41	1.48
2	J	501	NDP	C7N-C3N	-3.27	1.41	1.48
2	BA	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	P	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	DA	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	X	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	OA	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	KA	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	Q	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	Z	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	D	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	NA	501	NDP	C7N-C3N	-3.26	1.41	1.48
2	HA	501	NDP	C7N-C3N	-3.25	1.41	1.48
2	JA	501	NDP	C7N-C3N	-3.25	1.41	1.48
2	K	501	NDP	C7N-C3N	-3.24	1.41	1.48
2	E	501	NDP	C7N-C3N	-3.24	1.41	1.48
3	M	502	PMR	C1D-ND	3.23	1.38	1.35
3	EA	502	PMR	C1D-ND	3.23	1.38	1.35
3	F	502	PMR	C1D-ND	3.22	1.38	1.35
3	R	502	PMR	C1D-ND	3.22	1.38	1.35
3	A	502	PMR	C1D-ND	3.21	1.38	1.35
3	Z	502	PMR	C1D-ND	3.21	1.38	1.35
3	GA	502	PMR	C1D-ND	3.21	1.38	1.35
3	B	502	PMR	C1D-ND	3.21	1.38	1.35
3	OA	502	PMR	C1D-ND	3.19	1.38	1.35
3	AA	502	PMR	C1D-ND	3.19	1.38	1.35
3	CA	502	PMR	C1D-ND	3.19	1.38	1.35
3	BA	502	PMR	C1D-ND	3.18	1.38	1.35
3	C	502	PMR	C1D-ND	3.17	1.38	1.35
3	KA	502	PMR	C1D-ND	3.17	1.38	1.35
3	H	502	PMR	C1D-ND	3.17	1.38	1.35
3	L	502	PMR	C1D-ND	3.17	1.38	1.35
3	T	502	PMR	C1D-ND	3.16	1.38	1.35
3	LA	502	PMR	C1D-ND	3.16	1.38	1.35
3	JA	502	PMR	C1D-ND	3.16	1.38	1.35
3	NA	502	PMR	C1D-ND	3.15	1.38	1.35
3	I	502	PMR	C1D-ND	3.15	1.38	1.35
3	E	502	PMR	C1D-ND	3.15	1.38	1.35
3	J	502	PMR	C1D-ND	3.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	PMR	C1D-ND	3.14	1.38	1.35
3	V	502	PMR	C1D-ND	3.14	1.38	1.35
3	MA	502	PMR	C1D-ND	3.14	1.38	1.35
3	S	502	PMR	C1D-ND	3.14	1.38	1.35
3	Y	502	PMR	C1D-ND	3.14	1.38	1.35
3	IA	502	PMR	C1D-ND	3.14	1.38	1.35
3	O	502	PMR	C1D-ND	3.14	1.38	1.35
3	W	502	PMR	C1D-ND	3.13	1.38	1.35
3	K	502	PMR	C1D-ND	3.13	1.38	1.35
3	P	502	PMR	C1D-ND	3.10	1.38	1.35
3	DA	502	PMR	C1D-ND	3.10	1.38	1.35
3	X	502	PMR	C1D-ND	3.10	1.38	1.35
3	Q	502	PMR	C1D-ND	3.10	1.38	1.35
3	FA	502	PMR	C1D-ND	3.09	1.38	1.35
3	N	502	PMR	C1D-ND	3.07	1.37	1.35
3	G	502	PMR	C1D-ND	3.07	1.37	1.35
3	HA	502	PMR	C1D-ND	3.05	1.37	1.35
3	R	502	PMR	CHD-C4C	2.90	1.42	1.35
3	F	502	PMR	CHD-C4C	2.90	1.42	1.35
3	CA	502	PMR	CHD-C4C	2.89	1.42	1.35
3	A	502	PMR	CHD-C4C	2.88	1.42	1.35
3	C	502	PMR	CHD-C4C	2.88	1.42	1.35
3	AA	502	PMR	CHD-C4C	2.88	1.42	1.35
3	M	502	PMR	CHD-C4C	2.88	1.42	1.35
3	Z	502	PMR	CHD-C4C	2.88	1.42	1.35
3	IA	502	PMR	CHD-C4C	2.88	1.42	1.35
3	O	502	PMR	CHD-C4C	2.87	1.42	1.35
3	KA	502	PMR	CHD-C4C	2.87	1.42	1.35
3	L	502	PMR	CHD-C4C	2.87	1.42	1.35
3	K	502	PMR	CHD-C4C	2.87	1.42	1.35
3	D	502	PMR	CHD-C4C	2.87	1.42	1.35
3	N	502	PMR	CHD-C4C	2.87	1.42	1.35
3	V	502	PMR	CHD-C4C	2.87	1.42	1.35
3	MA	502	PMR	CHD-C4C	2.87	1.42	1.35
3	NA	502	PMR	CHD-C4C	2.87	1.42	1.35
3	X	502	PMR	CHD-C4C	2.86	1.42	1.35
3	OA	502	PMR	CHD-C4C	2.86	1.42	1.35
3	T	502	PMR	CHD-C4C	2.86	1.42	1.35
3	JA	502	PMR	CHD-C4C	2.86	1.42	1.35
3	LA	502	PMR	CHD-C4C	2.86	1.42	1.35
3	E	502	PMR	CHD-C4C	2.86	1.42	1.35
3	J	502	PMR	CHD-C4C	2.86	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	502	PMR	CHD-C4C	2.86	1.42	1.35
3	HA	502	PMR	CHD-C4C	2.86	1.42	1.35
3	P	502	PMR	CHD-C4C	2.86	1.42	1.35
3	G	502	PMR	CHD-C4C	2.85	1.42	1.35
3	H	502	PMR	CHD-C4C	2.85	1.42	1.35
3	S	502	PMR	CHD-C4C	2.85	1.42	1.35
3	Y	502	PMR	CHD-C4C	2.85	1.42	1.35
3	EA	502	PMR	CHD-C4C	2.85	1.42	1.35
3	B	502	PMR	CHD-C4C	2.85	1.42	1.35
3	I	502	PMR	CHD-C4C	2.85	1.42	1.35
3	GA	502	PMR	CHD-C4C	2.84	1.42	1.35
3	W	502	PMR	CHD-C4C	2.84	1.42	1.35
3	FA	502	PMR	CHD-C4C	2.84	1.42	1.35
3	DA	502	PMR	CHD-C4C	2.83	1.42	1.35
3	BA	502	PMR	CHD-C4C	2.83	1.42	1.35
3	T	502	PMR	CBA-CGA	2.66	1.56	1.50
3	NA	502	PMR	CBA-CGA	2.65	1.56	1.50
3	R	502	PMR	CBA-CGA	2.65	1.56	1.50
3	S	502	PMR	CBA-CGA	2.64	1.56	1.50
3	W	502	PMR	CBA-CGA	2.64	1.56	1.50
3	Q	502	PMR	CBA-CGA	2.64	1.56	1.50
3	LA	502	PMR	CBA-CGA	2.64	1.56	1.50
3	D	502	PMR	CBA-CGA	2.64	1.56	1.50
3	Y	502	PMR	CBA-CGA	2.64	1.56	1.50
3	I	502	PMR	CBA-CGA	2.64	1.56	1.50
3	O	502	PMR	CBA-CGA	2.64	1.56	1.50
3	AA	502	PMR	CBA-CGA	2.64	1.56	1.50
3	H	502	PMR	CBA-CGA	2.64	1.56	1.50
3	K	502	PMR	CBA-CGA	2.63	1.56	1.50
3	C	502	PMR	CBA-CGA	2.63	1.56	1.50
3	G	502	PMR	CBA-CGA	2.63	1.56	1.50
3	X	502	PMR	CBA-CGA	2.63	1.56	1.50
3	OA	502	PMR	CBA-CGA	2.63	1.56	1.50
3	N	502	PMR	CBA-CGA	2.63	1.56	1.50
3	BA	502	PMR	CBA-CGA	2.63	1.56	1.50
3	V	502	PMR	CBA-CGA	2.63	1.56	1.50
3	JA	502	PMR	CBA-CGA	2.63	1.56	1.50
3	IA	502	PMR	CBA-CGA	2.63	1.56	1.50
3	FA	502	PMR	CBA-CGA	2.62	1.56	1.50
3	KA	502	PMR	CBA-CGA	2.62	1.56	1.50
3	P	502	PMR	CBA-CGA	2.62	1.56	1.50
3	DA	502	PMR	CBA-CGA	2.62	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CA	502	PMR	CBA-CGA	2.62	1.56	1.50
3	J	502	PMR	CBA-CGA	2.62	1.56	1.50
3	B	502	PMR	CBA-CGA	2.62	1.56	1.50
3	L	502	PMR	CBA-CGA	2.62	1.56	1.50
3	A	502	PMR	CBA-CGA	2.62	1.56	1.50
3	F	502	PMR	CBA-CGA	2.62	1.56	1.50
3	Z	502	PMR	CBA-CGA	2.62	1.56	1.50
3	HA	502	PMR	CBA-CGA	2.61	1.56	1.50
3	GA	502	PMR	CBA-CGA	2.61	1.56	1.50
3	M	502	PMR	CBA-CGA	2.61	1.56	1.50
3	E	502	PMR	CBA-CGA	2.61	1.56	1.50
3	EA	502	PMR	CBA-CGA	2.60	1.56	1.50
3	MA	502	PMR	CBA-CGA	2.59	1.56	1.50
2	T	501	NDP	C8A-N7A	-2.50	1.30	1.34
2	Z	501	NDP	C8A-N7A	-2.49	1.30	1.34
2	NA	501	NDP	C8A-N7A	-2.48	1.30	1.34
2	IA	501	NDP	C8A-N7A	-2.47	1.30	1.34
2	P	501	NDP	C8A-N7A	-2.47	1.30	1.34
2	G	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	X	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	OA	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	EA	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	C	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	I	501	NDP	C8A-N7A	-2.46	1.30	1.34
2	O	501	NDP	C8A-N7A	-2.45	1.30	1.34
2	CA	501	NDP	C8A-N7A	-2.45	1.30	1.34
2	S	501	NDP	C8A-N7A	-2.45	1.30	1.34
2	Y	501	NDP	C8A-N7A	-2.45	1.30	1.34
2	MA	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	FA	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	W	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	D	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	L	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	V	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	M	501	NDP	C8A-N7A	-2.44	1.30	1.34
2	JA	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	H	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	GA	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	LA	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	F	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	R	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	AA	501	NDP	C8A-N7A	-2.43	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	BA	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	HA	501	NDP	C8A-N7A	-2.43	1.30	1.34
3	J	502	PMR	C4D-CHA	-2.43	1.42	1.45
2	E	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	J	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	N	501	NDP	C8A-N7A	-2.43	1.30	1.34
2	DA	501	NDP	C8A-N7A	-2.43	1.30	1.34
3	B	502	PMR	C4D-CHA	-2.43	1.42	1.45
3	HA	502	PMR	C4D-CHA	-2.43	1.42	1.45
3	JA	502	PMR	C4D-CHA	-2.43	1.42	1.45
2	Q	501	NDP	C8A-N7A	-2.43	1.30	1.34
3	K	502	PMR	C4D-CHA	-2.43	1.42	1.45
3	FA	502	PMR	C4D-CHA	-2.42	1.42	1.45
3	Q	502	PMR	C4D-CHA	-2.42	1.42	1.45
3	Y	502	PMR	C4D-CHA	-2.42	1.42	1.45
3	NA	502	PMR	C4D-CHA	-2.41	1.42	1.45
2	A	501	NDP	C8A-N7A	-2.41	1.30	1.34
3	O	502	PMR	C4D-CHA	-2.41	1.42	1.45
2	K	501	NDP	C8A-N7A	-2.41	1.30	1.34
2	KA	501	NDP	C8A-N7A	-2.41	1.30	1.34
3	E	502	PMR	C4D-CHA	-2.40	1.42	1.45
3	EA	502	PMR	C4D-CHA	-2.40	1.42	1.45
3	MA	502	PMR	C4D-CHA	-2.40	1.42	1.45
3	H	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	IA	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	Z	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	DA	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	W	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	A	502	PMR	C4D-CHA	-2.39	1.42	1.45
3	V	502	PMR	C4D-CHA	-2.38	1.42	1.45
3	C	502	PMR	C4D-CHA	-2.38	1.42	1.45
3	G	502	PMR	C4D-CHA	-2.38	1.42	1.45
3	CA	502	PMR	C4D-CHA	-2.38	1.42	1.45
3	LA	502	PMR	C4D-CHA	-2.38	1.42	1.45
3	M	502	PMR	C4D-CHA	-2.38	1.42	1.45
2	X	501	NDP	C4A-N3A	-2.37	1.32	1.35
2	Z	501	NDP	C4A-N3A	-2.37	1.32	1.35
2	C	501	NDP	C4A-N3A	-2.37	1.32	1.35
3	R	502	PMR	C4D-CHA	-2.37	1.42	1.45
3	N	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	X	502	PMR	C4D-CHA	-2.36	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	OA	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	F	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	D	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	L	502	PMR	C4D-CHA	-2.36	1.42	1.45
3	I	502	PMR	C4D-CHA	-2.35	1.42	1.45
2	NA	501	NDP	C4A-N3A	-2.35	1.32	1.35
3	GA	502	PMR	C4D-CHA	-2.35	1.42	1.45
2	K	501	NDP	C4A-N3A	-2.35	1.32	1.35
3	KA	502	PMR	C4D-CHA	-2.35	1.42	1.45
2	L	501	NDP	C4A-N3A	-2.35	1.32	1.35
2	LA	501	NDP	C4A-N3A	-2.35	1.32	1.35
2	T	501	NDP	C4A-N3A	-2.34	1.32	1.35
2	JA	501	NDP	C4A-N3A	-2.34	1.32	1.35
2	O	501	NDP	C4A-N3A	-2.34	1.32	1.35
2	KA	501	NDP	C4A-N3A	-2.34	1.32	1.35
3	S	502	PMR	C4D-CHA	-2.34	1.42	1.45
3	T	502	PMR	C4D-CHA	-2.34	1.42	1.45
2	BA	501	NDP	C4A-N3A	-2.34	1.32	1.35
3	AA	502	PMR	C4D-CHA	-2.33	1.42	1.45
2	M	501	NDP	C4A-N3A	-2.33	1.32	1.35
2	J	501	NDP	C4A-N3A	-2.33	1.32	1.35
2	DA	501	NDP	C4A-N3A	-2.33	1.32	1.35
2	A	501	NDP	C4A-N3A	-2.33	1.32	1.35
2	H	501	NDP	C4A-N3A	-2.33	1.32	1.35
3	P	502	PMR	C4D-CHA	-2.32	1.42	1.45
2	OA	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	P	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	I	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	FA	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	V	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	MA	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	W	501	NDP	C4A-N3A	-2.32	1.32	1.35
2	R	501	NDP	C4A-N3A	-2.31	1.32	1.35
2	AA	501	NDP	C4A-N3A	-2.31	1.32	1.35
3	J	502	PMR	C3D-C4D	2.31	1.42	1.40
3	CA	502	PMR	C3D-C4D	2.31	1.42	1.40
2	E	501	NDP	C4A-N3A	-2.31	1.32	1.35
2	Q	501	NDP	C4A-N3A	-2.30	1.32	1.35
2	F	501	NDP	C4A-N3A	-2.30	1.32	1.35
2	G	501	NDP	C4A-N3A	-2.30	1.32	1.35
2	GA	501	NDP	C4A-N3A	-2.30	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	IA	501	NDP	C4A-N3A	-2.30	1.32	1.35
2	B	501	NDP	C4A-N3A	-2.29	1.32	1.35
2	CA	501	NDP	C4A-N3A	-2.28	1.32	1.35
3	N	502	PMR	C3D-C4D	2.28	1.42	1.40
2	EA	501	NDP	C4A-N3A	-2.28	1.32	1.35
3	LA	502	PMR	C3D-C4D	2.28	1.42	1.40
2	S	501	NDP	C4A-N3A	-2.28	1.32	1.35
2	Y	501	NDP	C4A-N3A	-2.28	1.32	1.35
3	B	502	PMR	C3D-C4D	2.27	1.42	1.40
2	HA	501	NDP	C4A-N3A	-2.27	1.32	1.35
2	D	501	NDP	C4A-N3A	-2.27	1.32	1.35
3	H	502	PMR	C3D-C4D	2.25	1.42	1.40
2	N	501	NDP	C4A-N3A	-2.25	1.32	1.35
3	HA	502	PMR	C3D-C4D	2.25	1.42	1.40
3	BA	502	PMR	C3D-C4D	2.25	1.42	1.40
3	R	502	PMR	C3D-C4D	2.24	1.42	1.40
3	Y	502	PMR	C3D-C4D	2.24	1.42	1.40
3	F	502	PMR	C3D-C4D	2.23	1.42	1.40
3	I	502	PMR	C3D-C4D	2.23	1.42	1.40
3	P	502	PMR	C3D-C4D	2.23	1.42	1.40
3	Q	502	PMR	C3D-C4D	2.23	1.42	1.40
3	DA	502	PMR	C3D-C4D	2.23	1.42	1.40
3	IA	502	PMR	C3D-C4D	2.23	1.42	1.40
3	C	502	PMR	C3D-C4D	2.23	1.42	1.40
3	NA	502	PMR	C3D-C4D	2.22	1.42	1.40
3	D	502	PMR	C3D-C4D	2.22	1.42	1.40
3	X	502	PMR	C3D-C4D	2.22	1.42	1.40
3	EA	502	PMR	C3D-C4D	2.22	1.42	1.40
3	OA	502	PMR	C3D-C4D	2.22	1.42	1.40
3	E	502	PMR	C3D-C4D	2.22	1.42	1.40
3	K	502	PMR	C3D-C4D	2.21	1.42	1.40
3	V	502	PMR	C3D-C4D	2.21	1.42	1.40
3	Z	502	PMR	C3D-C4D	2.21	1.42	1.40
3	M	502	PMR	C3D-C4D	2.21	1.42	1.40
3	FA	502	PMR	C3D-C4D	2.21	1.42	1.40
3	GA	502	PMR	C3D-C4D	2.21	1.42	1.40
3	G	502	PMR	C3D-C4D	2.21	1.42	1.40
3	JA	502	PMR	C3D-C4D	2.21	1.42	1.40
3	T	502	PMR	C3D-C4D	2.19	1.42	1.40
3	W	502	PMR	C3D-C4D	2.19	1.42	1.40
3	AA	502	PMR	C3D-C4D	2.18	1.42	1.40
3	A	502	PMR	C3D-C4D	2.18	1.42	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	KA	502	PMR	C3D-C4D	2.18	1.42	1.40
3	O	502	PMR	C3D-C4D	2.17	1.42	1.40
3	MA	502	PMR	C3D-C4D	2.16	1.42	1.40
3	S	502	PMR	C3D-C4D	2.16	1.42	1.40
3	L	502	PMR	C3D-C4D	2.15	1.42	1.40
3	JA	502	PMR	O2A-CGA	-2.04	1.23	1.30
3	LA	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	NA	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	O	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	OA	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	KA	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	R	502	PMR	O2A-CGA	-2.03	1.23	1.30
3	K	502	PMR	O2A-CGA	-2.02	1.23	1.30
3	T	502	PMR	O2A-CGA	-2.02	1.23	1.30
3	W	502	PMR	O2A-CGA	-2.02	1.23	1.30
3	Y	502	PMR	O2A-CGA	-2.02	1.24	1.30
3	EA	502	PMR	O2A-CGA	-2.02	1.24	1.30
3	GA	502	PMR	O2A-CGA	-2.02	1.24	1.30
3	C	502	PMR	O2A-CGA	-2.02	1.24	1.30
3	G	502	PMR	O2A-CGA	-2.02	1.24	1.30
2	S	501	NDP	O4B-C1B	2.01	1.43	1.41
2	L	501	NDP	O4B-C1B	2.01	1.43	1.41
3	P	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	FA	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	CA	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	DA	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	V	502	PMR	O2A-CGA	-2.01	1.24	1.30
2	M	501	NDP	O4B-C1B	2.01	1.43	1.41
3	H	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	I	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	HA	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	X	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	Q	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	Z	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	BA	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	L	502	PMR	O2A-CGA	-2.01	1.24	1.30
3	D	502	PMR	O2A-CGA	-2.00	1.24	1.30
2	JA	501	NDP	O4B-C1B	2.00	1.43	1.41
3	MA	502	PMR	O2A-CGA	-2.00	1.24	1.30
2	X	501	NDP	O4B-C1B	2.00	1.43	1.41
3	J	502	PMR	O2A-CGA	-2.00	1.24	1.30

All (1200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	IA	502	PMR	C1A-NA-C4A	-7.78	103.21	106.71
3	I	502	PMR	C1A-NA-C4A	-7.75	103.22	106.71
3	AA	502	PMR	C1A-NA-C4A	-7.73	103.23	106.71
3	C	502	PMR	C1A-NA-C4A	-7.72	103.23	106.71
3	T	502	PMR	C1A-NA-C4A	-7.72	103.23	106.71
3	CA	502	PMR	C1A-NA-C4A	-7.72	103.23	106.71
3	P	502	PMR	C1A-NA-C4A	-7.71	103.24	106.71
3	D	502	PMR	C1A-NA-C4A	-7.71	103.24	106.71
3	K	502	PMR	C1A-NA-C4A	-7.70	103.24	106.71
3	M	502	PMR	C1A-NA-C4A	-7.70	103.25	106.71
3	FA	502	PMR	C1A-NA-C4A	-7.69	103.25	106.71
3	B	502	PMR	C1A-NA-C4A	-7.68	103.25	106.71
3	N	502	PMR	C1A-NA-C4A	-7.67	103.26	106.71
3	EA	502	PMR	C1A-NA-C4A	-7.67	103.26	106.71
3	V	502	PMR	C1A-NA-C4A	-7.66	103.26	106.71
3	KA	502	PMR	C1A-NA-C4A	-7.66	103.26	106.71
3	MA	502	PMR	C1A-NA-C4A	-7.66	103.26	106.71
3	W	502	PMR	C1A-NA-C4A	-7.66	103.26	106.71
3	G	502	PMR	C1A-NA-C4A	-7.66	103.26	106.71
3	HA	502	PMR	C1A-NA-C4A	-7.65	103.27	106.71
3	JA	502	PMR	C1A-NA-C4A	-7.65	103.27	106.71
3	R	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	S	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	J	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	O	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	A	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	H	502	PMR	C1A-NA-C4A	-7.64	103.27	106.71
3	LA	502	PMR	C1A-NA-C4A	-7.63	103.28	106.71
3	DA	502	PMR	C1A-NA-C4A	-7.62	103.28	106.71
3	Q	502	PMR	C1A-NA-C4A	-7.60	103.29	106.71
3	L	502	PMR	C1A-NA-C4A	-7.60	103.29	106.71
3	E	502	PMR	C1A-NA-C4A	-7.60	103.29	106.71
3	Z	502	PMR	C1A-NA-C4A	-7.59	103.29	106.71
3	Y	502	PMR	C1A-NA-C4A	-7.58	103.30	106.71
3	OA	502	PMR	C1A-NA-C4A	-7.58	103.30	106.71
3	X	502	PMR	C1A-NA-C4A	-7.57	103.30	106.71
3	NA	502	PMR	C1A-NA-C4A	-7.56	103.31	106.71
3	BA	502	PMR	C1A-NA-C4A	-7.55	103.31	106.71
3	F	502	PMR	C1A-NA-C4A	-7.53	103.32	106.71
3	GA	502	PMR	C1A-NA-C4A	-7.53	103.32	106.71
3	J	502	PMR	C2O-O2D-CGD	5.50	128.37	115.94
3	R	502	PMR	C2O-O2D-CGD	5.50	128.37	115.94
3	FA	502	PMR	C2O-O2D-CGD	5.50	128.37	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	502	PMR	C2O-O2D-CGD	5.49	128.37	115.94
3	BA	502	PMR	C2O-O2D-CGD	5.49	128.36	115.94
3	HA	502	PMR	C2O-O2D-CGD	5.49	128.35	115.94
3	NA	502	PMR	C2O-O2D-CGD	5.49	128.35	115.94
3	G	502	PMR	C2O-O2D-CGD	5.49	128.35	115.94
3	F	502	PMR	C2O-O2D-CGD	5.49	128.35	115.94
3	GA	502	PMR	C2O-O2D-CGD	5.49	128.34	115.94
3	LA	502	PMR	C2O-O2D-CGD	5.49	128.34	115.94
3	X	502	PMR	C2O-O2D-CGD	5.48	128.34	115.94
3	O	502	PMR	C2O-O2D-CGD	5.48	128.34	115.94
3	W	502	PMR	C2O-O2D-CGD	5.48	128.34	115.94
3	H	502	PMR	C2O-O2D-CGD	5.48	128.33	115.94
3	Z	502	PMR	C2O-O2D-CGD	5.48	128.33	115.94
3	V	502	PMR	C2O-O2D-CGD	5.48	128.33	115.94
3	DA	502	PMR	C2O-O2D-CGD	5.48	128.33	115.94
3	CA	502	PMR	C2O-O2D-CGD	5.48	128.33	115.94
3	K	502	PMR	C2O-O2D-CGD	5.48	128.32	115.94
3	Y	502	PMR	C2O-O2D-CGD	5.48	128.32	115.94
3	C	502	PMR	C2O-O2D-CGD	5.48	128.32	115.94
3	M	502	PMR	C2O-O2D-CGD	5.48	128.32	115.94
3	AA	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	P	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	KA	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	E	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	IA	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	MA	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	B	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	JA	502	PMR	C2O-O2D-CGD	5.47	128.31	115.94
3	L	502	PMR	C2O-O2D-CGD	5.47	128.30	115.94
3	EA	502	PMR	C2O-O2D-CGD	5.47	128.30	115.94
3	N	502	PMR	C2O-O2D-CGD	5.46	128.29	115.94
3	I	502	PMR	C2O-O2D-CGD	5.46	128.29	115.94
3	A	502	PMR	C2O-O2D-CGD	5.46	128.29	115.94
3	D	502	PMR	C2O-O2D-CGD	5.46	128.29	115.94
3	Q	502	PMR	C2O-O2D-CGD	5.46	128.28	115.94
3	OA	502	PMR	C2O-O2D-CGD	5.46	128.28	115.94
3	S	502	PMR	C2O-O2D-CGD	5.45	128.27	115.94
2	D	501	NDP	PN-O3-PA	-5.36	114.43	132.83
2	FA	501	NDP	PN-O3-PA	-5.36	114.44	132.83
2	C	501	NDP	PN-O3-PA	-5.36	114.44	132.83
2	Q	501	NDP	PN-O3-PA	-5.36	114.44	132.83
2	O	501	NDP	PN-O3-PA	-5.36	114.45	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	501	NDP	PN-O3-PA	-5.36	114.45	132.83
2	LA	501	NDP	PN-O3-PA	-5.36	114.45	132.83
2	G	501	NDP	PN-O3-PA	-5.35	114.45	132.83
2	B	501	NDP	PN-O3-PA	-5.35	114.45	132.83
2	NA	501	NDP	PN-O3-PA	-5.35	114.45	132.83
2	CA	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	AA	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	EA	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	A	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	MA	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	R	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	P	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	DA	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	N	501	NDP	PN-O3-PA	-5.35	114.46	132.83
2	HA	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	X	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	E	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	J	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	V	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	IA	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	W	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	KA	501	NDP	PN-O3-PA	-5.35	114.47	132.83
2	JA	501	NDP	PN-O3-PA	-5.35	114.48	132.83
2	F	501	NDP	PN-O3-PA	-5.35	114.48	132.83
2	Z	501	NDP	PN-O3-PA	-5.35	114.48	132.83
2	S	501	NDP	PN-O3-PA	-5.34	114.49	132.83
2	K	501	NDP	PN-O3-PA	-5.34	114.49	132.83
2	H	501	NDP	PN-O3-PA	-5.34	114.50	132.83
2	GA	501	NDP	PN-O3-PA	-5.34	114.50	132.83
2	OA	501	NDP	PN-O3-PA	-5.34	114.50	132.83
2	BA	501	NDP	PN-O3-PA	-5.34	114.50	132.83
2	M	501	NDP	PN-O3-PA	-5.34	114.51	132.83
2	L	501	NDP	PN-O3-PA	-5.34	114.51	132.83
2	Y	501	NDP	PN-O3-PA	-5.34	114.51	132.83
2	I	501	NDP	PN-O3-PA	-5.34	114.51	132.83
3	S	502	PMR	C3C-C4C-NC	-4.79	105.36	109.88
3	EA	502	PMR	C3C-C4C-NC	-4.77	105.38	109.88
3	BA	502	PMR	C3C-C4C-NC	-4.77	105.39	109.88
3	OA	502	PMR	C3C-C4C-NC	-4.76	105.39	109.88
3	Q	502	PMR	C3C-C4C-NC	-4.76	105.39	109.88
3	G	502	PMR	C3C-C4C-NC	-4.76	105.39	109.88
3	FA	502	PMR	C3C-C4C-NC	-4.75	105.40	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	502	PMR	C3C-C4C-NC	-4.75	105.40	109.88
3	DA	502	PMR	C3C-C4C-NC	-4.75	105.41	109.88
3	GA	502	PMR	C3C-C4C-NC	-4.75	105.41	109.88
3	H	502	PMR	C3C-C4C-NC	-4.75	105.41	109.88
3	MA	502	PMR	C3C-C4C-NC	-4.75	105.41	109.88
3	K	502	PMR	C3C-C4C-NC	-4.74	105.41	109.88
3	Y	502	PMR	C3C-C4C-NC	-4.74	105.41	109.88
3	T	502	PMR	C3C-C4C-NC	-4.74	105.41	109.88
3	W	502	PMR	C3C-C4C-NC	-4.74	105.41	109.88
3	J	502	PMR	C3C-C4C-NC	-4.74	105.42	109.88
3	I	502	PMR	C3C-C4C-NC	-4.74	105.42	109.88
3	C	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	V	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	HA	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	B	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	LA	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	A	502	PMR	C3C-C4C-NC	-4.73	105.42	109.88
3	X	502	PMR	C3C-C4C-NC	-4.72	105.43	109.88
3	NA	502	PMR	C3C-C4C-NC	-4.72	105.43	109.88
3	E	502	PMR	C3C-C4C-NC	-4.72	105.43	109.88
3	JA	502	PMR	C3C-C4C-NC	-4.72	105.43	109.88
3	KA	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	P	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	IA	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	D	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	R	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	AA	502	PMR	C3C-C4C-NC	-4.71	105.44	109.88
3	O	502	PMR	C3C-C4C-NC	-4.70	105.45	109.88
3	F	502	PMR	C3C-C4C-NC	-4.70	105.45	109.88
3	M	502	PMR	C3C-C4C-NC	-4.69	105.46	109.88
3	L	502	PMR	C3C-C4C-NC	-4.69	105.46	109.88
3	Z	502	PMR	C3C-C4C-NC	-4.68	105.47	109.88
3	CA	502	PMR	C3C-C4C-NC	-4.68	105.47	109.88
2	DA	501	NDP	N3A-C2A-N1A	-4.42	121.77	128.68
2	JA	501	NDP	N3A-C2A-N1A	-4.41	121.78	128.68
2	A	501	NDP	N3A-C2A-N1A	-4.41	121.79	128.68
2	S	501	NDP	N3A-C2A-N1A	-4.41	121.79	128.68
2	BA	501	NDP	N3A-C2A-N1A	-4.41	121.79	128.68
2	I	501	NDP	N3A-C2A-N1A	-4.40	121.80	128.68
2	N	501	NDP	N3A-C2A-N1A	-4.40	121.80	128.68
2	G	501	NDP	N3A-C2A-N1A	-4.40	121.80	128.68
2	T	501	NDP	N3A-C2A-N1A	-4.40	121.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	501	NDP	N3A-C2A-N1A	-4.40	121.81	128.68
2	L	501	NDP	N3A-C2A-N1A	-4.39	121.81	128.68
2	Q	501	NDP	N3A-C2A-N1A	-4.39	121.81	128.68
2	F	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	LA	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	C	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	EA	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	O	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	CA	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	V	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	Z	501	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
2	R	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	KA	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	Y	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	M	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	GA	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	OA	501	NDP	N3A-C2A-N1A	-4.38	121.83	128.68
2	K	501	NDP	N3A-C2A-N1A	-4.38	121.84	128.68
2	HA	501	NDP	N3A-C2A-N1A	-4.38	121.84	128.68
2	NA	501	NDP	N3A-C2A-N1A	-4.38	121.84	128.68
2	MA	501	NDP	N3A-C2A-N1A	-4.37	121.84	128.68
2	X	501	NDP	N3A-C2A-N1A	-4.37	121.84	128.68
2	J	501	NDP	N3A-C2A-N1A	-4.37	121.84	128.68
2	W	501	NDP	N3A-C2A-N1A	-4.37	121.84	128.68
2	FA	501	NDP	N3A-C2A-N1A	-4.37	121.85	128.68
2	E	501	NDP	N3A-C2A-N1A	-4.37	121.85	128.68
2	D	501	NDP	N3A-C2A-N1A	-4.36	121.86	128.68
2	H	501	NDP	N3A-C2A-N1A	-4.36	121.86	128.68
2	B	501	NDP	N3A-C2A-N1A	-4.36	121.86	128.68
2	P	501	NDP	N3A-C2A-N1A	-4.36	121.86	128.68
2	IA	501	NDP	N3A-C2A-N1A	-4.35	121.87	128.68
3	NA	502	PMR	C3A-C4A-NA	-4.27	105.91	110.57
3	E	502	PMR	C3A-C4A-NA	-4.26	105.92	110.57
3	O	502	PMR	C3A-C4A-NA	-4.26	105.92	110.57
3	LA	502	PMR	C3A-C4A-NA	-4.26	105.92	110.57
3	OA	502	PMR	C3A-C4A-NA	-4.26	105.92	110.57
3	GA	502	PMR	C3A-C4A-NA	-4.25	105.93	110.57
3	Z	502	PMR	C3A-C4A-NA	-4.25	105.94	110.57
3	A	502	PMR	C3A-C4A-NA	-4.24	105.94	110.57
3	HA	502	PMR	C3A-C4A-NA	-4.24	105.94	110.57
3	Y	502	PMR	C3A-C4A-NA	-4.24	105.94	110.57
3	BA	502	PMR	C3A-C4A-NA	-4.24	105.94	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	502	PMR	C3A-C4A-NA	-4.24	105.95	110.57
3	Q	502	PMR	C3A-C4A-NA	-4.23	105.95	110.57
3	EA	502	PMR	C3A-C4A-NA	-4.23	105.95	110.57
3	DA	502	PMR	C3A-C4A-NA	-4.23	105.95	110.57
3	KA	502	PMR	C3A-C4A-NA	-4.23	105.95	110.57
3	MA	502	PMR	C3A-C4A-NA	-4.23	105.96	110.57
3	K	502	PMR	C3A-C4A-NA	-4.22	105.96	110.57
3	B	502	PMR	C3A-C4A-NA	-4.22	105.96	110.57
3	G	502	PMR	C3A-C4A-NA	-4.22	105.97	110.57
3	V	502	PMR	C3A-C4A-NA	-4.22	105.97	110.57
3	J	502	PMR	C3A-C4A-NA	-4.22	105.97	110.57
3	AA	502	PMR	C2C-C1C-NC	-4.22	105.97	110.57
3	H	502	PMR	C3A-C4A-NA	-4.21	105.97	110.57
3	X	502	PMR	C3A-C4A-NA	-4.21	105.97	110.57
3	JA	502	PMR	C3A-C4A-NA	-4.21	105.97	110.57
3	C	502	PMR	C2C-C1C-NC	-4.21	105.97	110.57
3	F	502	PMR	C2C-C1C-NC	-4.21	105.97	110.57
3	F	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	Y	502	PMR	C2C-C1C-NC	-4.21	105.98	110.57
3	CA	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	Q	502	PMR	C2C-C1C-NC	-4.21	105.98	110.57
3	R	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	S	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	N	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	D	502	PMR	C3A-C4A-NA	-4.21	105.98	110.57
3	I	502	PMR	C3A-C4A-NA	-4.20	105.99	110.57
3	M	502	PMR	C3A-C4A-NA	-4.20	105.99	110.57
3	T	502	PMR	C3A-C4A-NA	-4.20	105.99	110.57
3	LA	502	PMR	C2C-C1C-NC	-4.19	106.00	110.57
3	AA	502	PMR	C3A-C4A-NA	-4.19	106.00	110.57
3	D	502	PMR	C2C-C1C-NC	-4.19	106.00	110.57
3	P	502	PMR	C3A-C4A-NA	-4.19	106.00	110.57
3	W	502	PMR	C3A-C4A-NA	-4.19	106.00	110.57
3	M	502	PMR	C2C-C1C-NC	-4.19	106.00	110.57
3	FA	502	PMR	C3A-C4A-NA	-4.19	106.00	110.57
3	OA	502	PMR	C2C-C1C-NC	-4.19	106.00	110.57
3	CA	502	PMR	C2C-C1C-NC	-4.19	106.00	110.57
3	IA	502	PMR	C3A-C4A-NA	-4.19	106.00	110.57
3	C	502	PMR	C3A-C4A-NA	-4.18	106.00	110.57
3	R	502	PMR	C2C-C1C-NC	-4.18	106.01	110.57
3	K	502	PMR	C2C-C1C-NC	-4.18	106.01	110.57
3	BA	502	PMR	C2C-C1C-NC	-4.18	106.01	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DA	502	PMR	C2C-C1C-NC	-4.17	106.01	110.57
3	MA	502	PMR	C2C-C1C-NC	-4.17	106.01	110.57
3	L	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	T	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	Z	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	V	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	EA	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	KA	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	G	502	PMR	C2C-C1C-NC	-4.17	106.02	110.57
3	GA	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	X	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	HA	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	NA	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	B	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	S	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	N	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	J	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	JA	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	O	502	PMR	C2C-C1C-NC	-4.16	106.03	110.57
3	H	502	PMR	C2C-C1C-NC	-4.15	106.04	110.57
3	P	502	PMR	C2C-C1C-NC	-4.15	106.04	110.57
3	W	502	PMR	C2C-C1C-NC	-4.15	106.05	110.57
3	E	502	PMR	C2C-C1C-NC	-4.14	106.05	110.57
3	I	502	PMR	C2C-C1C-NC	-4.14	106.06	110.57
3	IA	502	PMR	C2C-C1C-NC	-4.13	106.06	110.57
3	FA	502	PMR	C2C-C1C-NC	-4.13	106.06	110.57
3	A	502	PMR	C2C-C1C-NC	-4.12	106.08	110.57
3	CA	502	PMR	O2D-CGD-CBD	3.86	118.13	111.27
3	J	502	PMR	O2D-CGD-CBD	3.86	118.12	111.27
3	F	502	PMR	O2D-CGD-CBD	3.85	118.12	111.27
3	T	502	PMR	O2D-CGD-CBD	3.85	118.11	111.27
3	BA	502	PMR	O2D-CGD-CBD	3.85	118.11	111.27
3	HA	502	PMR	O2D-CGD-CBD	3.85	118.11	111.27
3	Z	502	PMR	O2D-CGD-CBD	3.85	118.11	111.27
3	NA	502	PMR	O2D-CGD-CBD	3.85	118.11	111.27
3	FA	502	PMR	O2D-CGD-CBD	3.85	118.10	111.27
3	K	502	PMR	O2D-CGD-CBD	3.85	118.10	111.27
3	X	502	PMR	O2D-CGD-CBD	3.84	118.10	111.27
3	O	502	PMR	O2D-CGD-CBD	3.84	118.10	111.27
3	GA	502	PMR	O2D-CGD-CBD	3.84	118.10	111.27
3	R	502	PMR	O2D-CGD-CBD	3.84	118.10	111.27
3	N	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27
3	M	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27
3	V	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27
3	IA	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27
3	I	502	PMR	O2D-CGD-CBD	3.84	118.09	111.27
3	LA	502	PMR	O2D-CGD-CBD	3.84	118.08	111.27
3	Y	502	PMR	O2D-CGD-CBD	3.84	118.08	111.27
3	H	502	PMR	O2D-CGD-CBD	3.83	118.08	111.27
3	MA	502	PMR	O2D-CGD-CBD	3.83	118.08	111.27
3	AA	502	PMR	O2D-CGD-CBD	3.83	118.08	111.27
3	KA	502	PMR	O2D-CGD-CBD	3.83	118.08	111.27
3	E	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	C	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	Q	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	P	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	S	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	A	502	PMR	O2D-CGD-CBD	3.83	118.07	111.27
3	OA	502	PMR	O2D-CGD-CBD	3.82	118.06	111.27
3	W	502	PMR	O2D-CGD-CBD	3.82	118.06	111.27
3	EA	502	PMR	O2D-CGD-CBD	3.82	118.06	111.27
3	DA	502	PMR	O2D-CGD-CBD	3.82	118.06	111.27
3	B	502	PMR	O2D-CGD-CBD	3.82	118.05	111.27
3	L	502	PMR	O2D-CGD-CBD	3.82	118.05	111.27
3	JA	502	PMR	O2D-CGD-CBD	3.81	118.04	111.27
3	D	502	PMR	O2D-CGD-CBD	3.80	118.02	111.27
3	Y	502	PMR	CHC-C1C-NC	3.55	129.79	124.20
3	Z	502	PMR	CHC-C1C-NC	3.54	129.78	124.20
3	JA	502	PMR	CHC-C1C-NC	3.54	129.78	124.20
3	EA	502	PMR	CHC-C1C-NC	3.54	129.78	124.20
3	HA	502	PMR	CHC-C1C-NC	3.54	129.78	124.20
3	S	502	PMR	CHC-C1C-NC	3.54	129.77	124.20
3	CA	502	PMR	CHC-C1C-NC	3.54	129.77	124.20
3	H	502	PMR	CHC-C1C-NC	3.53	129.77	124.20
3	B	502	PMR	CHC-C1C-NC	3.53	129.77	124.20
3	C	502	PMR	CHC-C1C-NC	3.53	129.76	124.20
3	D	502	PMR	CHC-C1C-NC	3.53	129.76	124.20
3	E	502	PMR	CHC-C1C-NC	3.53	129.76	124.20
3	Q	502	PMR	CHC-C1C-NC	3.53	129.76	124.20
3	R	502	PMR	CHC-C1C-NC	3.53	129.76	124.20
3	OA	502	PMR	CHC-C1C-NC	3.52	129.76	124.20
3	F	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	L	502	PMR	CHC-C1C-NC	3.52	129.75	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	T	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	W	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	DA	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	LA	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	V	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	I	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	X	502	PMR	CHC-C1C-NC	3.52	129.75	124.20
3	AA	502	PMR	CHC-C1C-NC	3.52	129.74	124.20
3	J	502	PMR	CHC-C1C-NC	3.51	129.74	124.20
3	KA	502	PMR	CHC-C1C-NC	3.51	129.74	124.20
3	O	502	PMR	CHC-C1C-NC	3.51	129.73	124.20
3	IA	502	PMR	CHC-C1C-NC	3.51	129.73	124.20
3	A	502	PMR	CHC-C1C-NC	3.51	129.73	124.20
3	P	502	PMR	CHC-C1C-NC	3.51	129.73	124.20
3	N	502	PMR	CHC-C1C-NC	3.51	129.73	124.20
3	BA	502	PMR	CHC-C1C-NC	3.50	129.72	124.20
3	GA	502	PMR	CHC-C1C-NC	3.50	129.72	124.20
3	K	502	PMR	CHC-C1C-NC	3.50	129.72	124.20
3	M	502	PMR	CHC-C1C-NC	3.50	129.72	124.20
3	NA	502	PMR	CHC-C1C-NC	3.50	129.71	124.20
3	MA	502	PMR	CHC-C1C-NC	3.49	129.71	124.20
3	FA	502	PMR	CHC-C1C-NC	3.49	129.70	124.20
3	R	502	PMR	C2B-C1B-NB	-3.43	107.57	110.10
3	DA	502	PMR	C2B-C1B-NB	-3.40	107.60	110.10
3	BA	502	PMR	C2B-C1B-NB	-3.40	107.60	110.10
3	CA	502	PMR	C2B-C1B-NB	-3.40	107.60	110.10
3	F	502	PMR	C2B-C1B-NB	-3.40	107.60	110.10
3	Y	502	PMR	C2B-C1B-NB	-3.40	107.60	110.10
3	J	502	PMR	C2B-C1B-NB	-3.39	107.60	110.10
3	O	502	PMR	C2B-C1B-NB	-3.39	107.61	110.10
3	I	502	PMR	C2B-C1B-NB	-3.38	107.61	110.10
3	K	502	PMR	C2B-C1B-NB	-3.38	107.61	110.10
3	NA	502	PMR	C2B-C1B-NB	-3.38	107.61	110.10
3	FA	502	PMR	C2B-C1B-NB	-3.37	107.62	110.10
3	H	502	PMR	C2B-C1B-NB	-3.37	107.62	110.10
3	Z	502	PMR	C2B-C1B-NB	-3.37	107.62	110.10
3	KA	502	PMR	C2B-C1B-NB	-3.37	107.62	110.10
3	Q	502	PMR	C2B-C1B-NB	-3.36	107.63	110.10
3	B	502	PMR	C2B-C1B-NB	-3.36	107.63	110.10
3	D	502	PMR	C2B-C1B-NB	-3.36	107.63	110.10
3	EA	502	PMR	C2B-C1B-NB	-3.35	107.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	502	PMR	C2B-C1B-NB	-3.35	107.63	110.10
3	AA	502	PMR	C2B-C1B-NB	-3.35	107.64	110.10
3	N	502	PMR	C2B-C1B-NB	-3.34	107.64	110.10
3	V	502	PMR	C2B-C1B-NB	-3.34	107.64	110.10
3	T	502	PMR	C2B-C1B-NB	-3.34	107.64	110.10
3	JA	502	PMR	C2B-C1B-NB	-3.33	107.65	110.10
3	S	502	PMR	C2B-C1B-NB	-3.33	107.65	110.10
3	P	502	PMR	C2B-C1B-NB	-3.32	107.66	110.10
3	GA	502	PMR	C2B-C1B-NB	-3.32	107.66	110.10
3	LA	502	PMR	C2B-C1B-NB	-3.32	107.66	110.10
3	A	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	W	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	X	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	OA	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	C	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	G	502	PMR	C2B-C1B-NB	-3.31	107.66	110.10
3	M	502	PMR	C2B-C1B-NB	-3.30	107.67	110.10
3	E	502	PMR	C2B-C1B-NB	-3.29	107.68	110.10
3	HA	502	PMR	C2B-C1B-NB	-3.29	107.68	110.10
3	MA	502	PMR	C2B-C1B-NB	-3.29	107.68	110.10
3	IA	502	PMR	C2B-C1B-NB	-3.25	107.71	110.10
2	LA	501	NDP	PA-O5B-C5B	-3.00	104.09	121.68
2	D	501	NDP	PA-O5B-C5B	-3.00	104.10	121.68
2	G	501	NDP	PA-O5B-C5B	-3.00	104.10	121.68
2	W	501	NDP	PA-O5B-C5B	-3.00	104.10	121.68
2	JA	501	NDP	PA-O5B-C5B	-3.00	104.11	121.68
2	R	501	NDP	PA-O5B-C5B	-3.00	104.11	121.68
2	OA	501	NDP	PA-O5B-C5B	-3.00	104.11	121.68
2	C	501	NDP	PA-O5B-C5B	-3.00	104.11	121.68
2	L	501	NDP	PA-O5B-C5B	-3.00	104.11	121.68
2	KA	501	NDP	PA-O5B-C5B	-3.00	104.12	121.68
2	M	501	NDP	PA-O5B-C5B	-2.99	104.12	121.68
2	P	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	B	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	J	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	MA	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	S	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	Y	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	I	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
2	V	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	A	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	H	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	NA	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	BA	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	EA	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	IA	501	NDP	PA-O5B-C5B	-2.99	104.14	121.68
2	F	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	HA	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	K	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	N	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	Q	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	T	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	GA	501	NDP	PA-O5B-C5B	-2.99	104.15	121.68
2	O	501	NDP	PA-O5B-C5B	-2.99	104.16	121.68
2	CA	501	NDP	PA-O5B-C5B	-2.99	104.16	121.68
2	DA	501	NDP	PA-O5B-C5B	-2.99	104.16	121.68
2	E	501	NDP	PA-O5B-C5B	-2.99	104.17	121.68
2	Z	501	NDP	PA-O5B-C5B	-2.99	104.17	121.68
2	AA	501	NDP	PA-O5B-C5B	-2.99	104.17	121.68
2	FA	501	NDP	PA-O5B-C5B	-2.99	104.17	121.68
3	F	502	PMR	O2D-CGD-O1D	-2.83	118.30	123.84
3	FA	502	PMR	O2D-CGD-O1D	-2.83	118.31	123.84
3	H	502	PMR	O2D-CGD-O1D	-2.82	118.31	123.84
3	R	502	PMR	O2D-CGD-O1D	-2.82	118.31	123.84
3	LA	502	PMR	O2D-CGD-O1D	-2.82	118.32	123.84
3	NA	502	PMR	O2D-CGD-O1D	-2.82	118.33	123.84
2	N	501	NDP	PN-O5D-C5D	-2.82	105.16	121.68
3	IA	502	PMR	O2D-CGD-O1D	-2.82	118.33	123.84
2	R	501	NDP	PN-O5D-C5D	-2.82	105.16	121.68
2	X	501	NDP	PN-O5D-C5D	-2.82	105.16	121.68
2	MA	501	NDP	PN-O5D-C5D	-2.82	105.17	121.68
2	S	501	NDP	PN-O5D-C5D	-2.82	105.17	121.68
2	L	501	NDP	PN-O5D-C5D	-2.82	105.17	121.68
2	IA	501	NDP	PN-O5D-C5D	-2.82	105.17	121.68
2	J	501	NDP	PN-O5D-C5D	-2.81	105.17	121.68
3	OA	502	PMR	O2D-CGD-O1D	-2.81	118.33	123.84
2	G	501	NDP	PN-O5D-C5D	-2.81	105.18	121.68
2	HA	501	NDP	PN-O5D-C5D	-2.81	105.18	121.68
2	Q	501	NDP	PN-O5D-C5D	-2.81	105.18	121.68
2	GA	501	NDP	PN-O5D-C5D	-2.81	105.18	121.68
2	I	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	W	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	DA	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	NA	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	JA	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	A	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	BA	501	NDP	PN-O5D-C5D	-2.81	105.19	121.68
2	F	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
3	G	502	PMR	O2D-CGD-O1D	-2.81	118.34	123.84
2	Y	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	E	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	T	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	LA	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	V	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	K	501	NDP	PN-O5D-C5D	-2.81	105.20	121.68
2	H	501	NDP	PN-O5D-C5D	-2.81	105.21	121.68
2	P	501	NDP	PN-O5D-C5D	-2.81	105.21	121.68
2	CA	501	NDP	PN-O5D-C5D	-2.81	105.21	121.68
2	B	501	NDP	PN-O5D-C5D	-2.81	105.21	121.68
2	O	501	NDP	PN-O5D-C5D	-2.81	105.22	121.68
3	J	502	PMR	O2D-CGD-O1D	-2.81	118.35	123.84
3	DA	502	PMR	O2D-CGD-O1D	-2.81	118.35	123.84
3	P	502	PMR	O2D-CGD-O1D	-2.81	118.35	123.84
2	OA	501	NDP	PN-O5D-C5D	-2.81	105.23	121.68
2	KA	501	NDP	PN-O5D-C5D	-2.81	105.23	121.68
3	HA	502	PMR	O2D-CGD-O1D	-2.81	118.35	123.84
2	C	501	NDP	PN-O5D-C5D	-2.81	105.23	121.68
2	D	501	NDP	PN-O5D-C5D	-2.81	105.23	121.68
2	Z	501	NDP	PN-O5D-C5D	-2.80	105.23	121.68
3	EA	502	PMR	O2D-CGD-O1D	-2.80	118.36	123.84
3	GA	502	PMR	O2D-CGD-O1D	-2.80	118.36	123.84
2	FA	501	NDP	PN-O5D-C5D	-2.80	105.24	121.68
3	MA	502	PMR	O2D-CGD-O1D	-2.80	118.36	123.84
2	EA	501	NDP	PN-O5D-C5D	-2.80	105.25	121.68
3	I	502	PMR	O2D-CGD-O1D	-2.80	118.36	123.84
2	AA	501	NDP	PN-O5D-C5D	-2.80	105.26	121.68
2	M	501	NDP	PN-O5D-C5D	-2.80	105.26	121.68
3	V	502	PMR	O2D-CGD-O1D	-2.80	118.36	123.84
3	Y	502	PMR	O2D-CGD-O1D	-2.80	118.37	123.84
3	S	502	PMR	O2D-CGD-O1D	-2.80	118.37	123.84
3	BA	502	PMR	O2D-CGD-O1D	-2.80	118.37	123.84
3	T	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	Q	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	L	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	A	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	M	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	N	502	PMR	O2D-CGD-O1D	-2.79	118.38	123.84
3	W	502	PMR	O2D-CGD-O1D	-2.79	118.39	123.84
3	X	502	PMR	O2D-CGD-O1D	-2.79	118.39	123.84
3	Z	502	PMR	O2D-CGD-O1D	-2.79	118.39	123.84
3	JA	502	PMR	O2D-CGD-O1D	-2.79	118.39	123.84
3	C	502	PMR	O2D-CGD-O1D	-2.79	118.39	123.84
3	O	502	PMR	O2D-CGD-O1D	-2.78	118.39	123.84
3	K	502	PMR	O2D-CGD-O1D	-2.78	118.40	123.84
3	CA	502	PMR	O2D-CGD-O1D	-2.78	118.40	123.84
3	D	502	PMR	O2D-CGD-O1D	-2.78	118.40	123.84
3	KA	502	PMR	O2D-CGD-O1D	-2.78	118.41	123.84
3	AA	502	PMR	O2D-CGD-O1D	-2.77	118.42	123.84
3	B	502	PMR	O2D-CGD-O1D	-2.77	118.43	123.84
3	T	502	PMR	O1A-CGA-CBA	-2.76	114.20	123.08
3	X	502	PMR	O1A-CGA-CBA	-2.76	114.21	123.08
3	K	502	PMR	O1A-CGA-CBA	-2.76	114.22	123.08
3	Q	502	PMR	O1A-CGA-CBA	-2.76	114.22	123.08
3	R	502	PMR	O1A-CGA-CBA	-2.76	114.23	123.08
3	FA	502	PMR	O1A-CGA-CBA	-2.76	114.23	123.08
3	N	502	PMR	O1A-CGA-CBA	-2.76	114.23	123.08
3	BA	502	PMR	O1A-CGA-CBA	-2.76	114.23	123.08
3	LA	502	PMR	O1A-CGA-CBA	-2.76	114.23	123.08
3	NA	502	PMR	O1A-CGA-CBA	-2.75	114.23	123.08
3	W	502	PMR	O1A-CGA-CBA	-2.75	114.23	123.08
3	JA	502	PMR	O1A-CGA-CBA	-2.75	114.24	123.08
3	C	502	PMR	O1A-CGA-CBA	-2.75	114.24	123.08
3	I	502	PMR	O1A-CGA-CBA	-2.75	114.24	123.08
3	EA	502	PMR	O1A-CGA-CBA	-2.75	114.24	123.08
3	OA	502	PMR	O1A-CGA-CBA	-2.75	114.24	123.08
3	O	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	S	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	AA	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	Z	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	D	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	F	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	H	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	KA	502	PMR	O1A-CGA-CBA	-2.75	114.25	123.08
3	V	502	PMR	O1A-CGA-CBA	-2.75	114.26	123.08
3	P	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08
3	DA	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08
3	IA	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08
3	L	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08
3	OA	502	PMR	CHD-C4C-NC	2.74	128.36	124.20
3	CA	502	PMR	O1A-CGA-CBA	-2.74	114.27	123.08
3	HA	502	PMR	O1A-CGA-CBA	-2.74	114.28	123.08
3	J	502	PMR	O1A-CGA-CBA	-2.74	114.28	123.08
3	GA	502	PMR	O1A-CGA-CBA	-2.74	114.29	123.08
3	Y	502	PMR	O1A-CGA-CBA	-2.74	114.29	123.08
3	A	502	PMR	O1A-CGA-CBA	-2.74	114.29	123.08
3	E	502	PMR	O1A-CGA-CBA	-2.74	114.29	123.08
3	M	502	PMR	O1A-CGA-CBA	-2.74	114.29	123.08
3	E	502	PMR	CHD-C4C-NC	2.73	128.35	124.20
3	B	502	PMR	O1A-CGA-CBA	-2.73	114.31	123.08
3	MA	502	PMR	O1A-CGA-CBA	-2.73	114.31	123.08
3	N	502	PMR	CHD-C4C-NC	2.73	128.34	124.20
3	Q	502	PMR	CHD-C4C-NC	2.73	128.34	124.20
3	S	502	PMR	CHD-C4C-NC	2.72	128.34	124.20
3	GA	502	PMR	CHD-C4C-NC	2.72	128.33	124.20
3	T	502	PMR	CHD-C4C-NC	2.72	128.33	124.20
3	G	502	PMR	CHD-C4C-NC	2.72	128.32	124.20
3	I	502	PMR	CHD-C4C-NC	2.72	128.32	124.20
3	X	502	PMR	CHD-C4C-NC	2.72	128.32	124.20
3	D	502	PMR	CHD-C4C-NC	2.71	128.32	124.20
3	K	502	PMR	CHD-C4C-NC	2.71	128.32	124.20
3	IA	502	PMR	CHD-C4C-NC	2.71	128.32	124.20
3	W	502	PMR	CHD-C4C-NC	2.71	128.32	124.20
3	LA	502	PMR	CHD-C4C-NC	2.71	128.32	124.20
3	JA	502	PMR	CHD-C4C-NC	2.71	128.31	124.20
3	B	502	PMR	CHD-C4C-NC	2.71	128.31	124.20
3	BA	502	PMR	CHD-C4C-NC	2.71	128.31	124.20
3	J	502	PMR	CHD-C4C-NC	2.71	128.31	124.20
3	MA	502	PMR	CHD-C4C-NC	2.71	128.31	124.20
3	EA	502	PMR	CHD-C4C-NC	2.70	128.31	124.20
3	KA	502	PMR	CHD-C4C-NC	2.70	128.30	124.20
3	C	502	PMR	CHD-C4C-NC	2.70	128.30	124.20
3	H	502	PMR	CHD-C4C-NC	2.70	128.30	124.20
3	DA	502	PMR	CHD-C4C-NC	2.70	128.30	124.20
3	NA	502	PMR	CHD-C4C-NC	2.70	128.30	124.20
3	Y	502	PMR	CHD-C4C-NC	2.70	128.29	124.20
3	V	502	PMR	CHD-C4C-NC	2.70	128.29	124.20
3	M	502	PMR	CHD-C4C-NC	2.70	128.29	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	502	PMR	CHD-C4C-NC	2.69	128.29	124.20
3	F	502	PMR	CHD-C4C-NC	2.69	128.28	124.20
3	L	502	PMR	CHD-C4C-NC	2.69	128.28	124.20
3	FA	502	PMR	CHD-C4C-NC	2.69	128.28	124.20
3	O	502	PMR	CHD-C4C-NC	2.69	128.28	124.20
3	AA	502	PMR	CHD-C4C-NC	2.68	128.27	124.20
3	R	502	PMR	CHD-C4C-NC	2.68	128.27	124.20
3	A	502	PMR	CHD-C4C-NC	2.68	128.26	124.20
3	Z	502	PMR	CHD-C4C-NC	2.67	128.26	124.20
3	HA	502	PMR	CHD-C4C-NC	2.67	128.26	124.20
3	CA	502	PMR	CHD-C4C-NC	2.66	128.24	124.20
4	CA	503	LMG	O6-C1-O1	-2.42	104.24	109.97
4	X	503	LMG	O6-C1-O1	-2.42	104.25	109.97
4	E	503	LMG	O6-C1-O1	-2.42	104.25	109.97
4	M	503	LMG	O6-C1-O1	-2.42	104.25	109.97
4	I	503	LMG	O6-C1-O1	-2.41	104.26	109.97
4	MA	503	LMG	O6-C1-O1	-2.41	104.26	109.97
4	NA	503	LMG	O6-C1-O1	-2.41	104.26	109.97
4	BA	503	LMG	O6-C1-O1	-2.41	104.26	109.97
4	D	503	LMG	O6-C1-O1	-2.41	104.27	109.97
4	A	503	LMG	O6-C1-O1	-2.41	104.27	109.97
4	JA	503	LMG	O6-C1-O1	-2.41	104.27	109.97
4	DA	503	LMG	O6-C1-O1	-2.41	104.27	109.97
4	R	503	LMG	O6-C1-O1	-2.41	104.27	109.97
4	OA	503	LMG	O6-C1-O1	-2.40	104.28	109.97
4	T	503	LMG	O6-C1-O1	-2.40	104.28	109.97
4	V	503	LMG	O6-C1-O1	-2.40	104.28	109.97
4	KA	503	LMG	O6-C1-O1	-2.40	104.28	109.97
4	S	503	LMG	O6-C1-O1	-2.40	104.29	109.97
4	Z	503	LMG	O6-C1-O1	-2.40	104.29	109.97
4	W	503	LMG	O6-C1-O1	-2.40	104.29	109.97
4	F	503	LMG	O6-C1-O1	-2.40	104.29	109.97
4	P	503	LMG	O6-C1-O1	-2.40	104.30	109.97
4	HA	503	LMG	O6-C1-O1	-2.40	104.30	109.97
4	G	503	LMG	O6-C1-O1	-2.40	104.30	109.97
4	GA	503	LMG	O6-C1-O1	-2.40	104.30	109.97
4	J	503	LMG	O6-C1-O1	-2.40	104.30	109.97
4	IA	503	LMG	O6-C1-O1	-2.39	104.30	109.97
4	K	503	LMG	O6-C1-O1	-2.39	104.31	109.97
4	FA	503	LMG	O6-C1-O1	-2.39	104.31	109.97
4	Q	503	LMG	O6-C1-O1	-2.39	104.31	109.97
2	EA	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75
4	C	503	LMG	O6-C1-O1	-2.39	104.31	109.97
4	LA	503	LMG	O6-C1-O1	-2.39	104.31	109.97
4	Y	503	LMG	O6-C1-O1	-2.39	104.31	109.97
2	J	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75
2	L	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75
4	AA	503	LMG	O6-C1-O1	-2.39	104.32	109.97
4	N	503	LMG	O6-C1-O1	-2.39	104.32	109.97
2	S	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75
2	Y	501	NDP	C2A-N1A-C6A	2.39	122.84	118.75
4	L	503	LMG	O6-C1-O1	-2.39	104.32	109.97
4	O	503	LMG	O6-C1-O1	-2.39	104.32	109.97
4	EA	503	LMG	O6-C1-O1	-2.39	104.32	109.97
4	B	503	LMG	O6-C1-O1	-2.38	104.33	109.97
4	H	503	LMG	O6-C1-O1	-2.38	104.33	109.97
2	BA	501	NDP	C2A-N1A-C6A	2.38	122.83	118.75
2	AA	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	GA	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	I	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	G	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	CA	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	N	501	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	Q	501	NDP	C2A-N1A-C6A	2.37	122.82	118.75
2	F	501	NDP	C2A-N1A-C6A	2.37	122.81	118.75
3	M	502	PMR	C1A-C2A-C3A	-2.37	103.48	106.61
2	Z	501	NDP	C2A-N1A-C6A	2.37	122.81	118.75
2	JA	501	NDP	C2A-N1A-C6A	2.37	122.81	118.75
2	C	501	NDP	C2A-N1A-C6A	2.37	122.81	118.75
2	EA	501	NDP	C3B-C2B-C1B	-2.37	98.43	102.89
3	N	502	PMR	C1A-C2A-C3A	-2.37	103.49	106.61
2	GA	501	NDP	C3B-C2B-C1B	-2.37	98.44	102.89
2	DA	501	NDP	C2A-N1A-C6A	2.37	122.81	118.75
2	V	501	NDP	C2A-N1A-C6A	2.37	122.80	118.75
2	MA	501	NDP	C2A-N1A-C6A	2.37	122.80	118.75
2	CA	501	NDP	C3B-C2B-C1B	-2.37	98.44	102.89
3	EA	502	PMR	C1A-C2A-C3A	-2.37	103.49	106.61
3	FA	502	PMR	C1A-C2A-C3A	-2.37	103.49	106.61
3	Y	502	PMR	C1A-C2A-C3A	-2.37	103.49	106.61
2	HA	501	NDP	C2A-N1A-C6A	2.37	122.80	118.75
3	E	502	PMR	C1A-C2A-C3A	-2.36	103.50	106.61
2	O	501	NDP	C2A-N1A-C6A	2.36	122.80	118.75
3	AA	502	PMR	C1A-C2A-C3A	-2.36	103.50	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	OA	501	NDP	C2A-N1A-C6A	2.36	122.80	118.75
2	G	501	NDP	C3B-C2B-C1B	-2.36	98.45	102.89
2	W	501	NDP	C2A-N1A-C6A	2.36	122.80	118.75
2	D	501	NDP	C2A-N1A-C6A	2.36	122.80	118.75
2	M	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
2	NA	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
2	LA	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
3	T	502	PMR	C1A-C2A-C3A	-2.36	103.50	106.61
2	H	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
3	HA	502	PMR	C1A-C2A-C3A	-2.36	103.50	106.61
2	E	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
2	FA	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
2	KA	501	NDP	C2A-N1A-C6A	2.36	122.79	118.75
2	I	501	NDP	C3B-C2B-C1B	-2.36	98.46	102.89
3	O	502	PMR	C1A-C2A-C3A	-2.36	103.51	106.61
3	D	502	PMR	C1A-C2A-C3A	-2.36	103.51	106.61
3	P	502	PMR	C1A-C2A-C3A	-2.36	103.51	106.61
2	A	501	NDP	C3B-C2B-C1B	-2.36	98.46	102.89
2	R	501	NDP	C3B-C2B-C1B	-2.36	98.46	102.89
2	E	501	NDP	C3B-C2B-C1B	-2.35	98.46	102.89
2	T	501	NDP	C2A-N1A-C6A	2.35	122.78	118.75
2	X	501	NDP	C3B-C2B-C1B	-2.35	98.46	102.89
2	R	501	NDP	C2A-N1A-C6A	2.35	122.78	118.75
2	S	501	NDP	C3B-C2B-C1B	-2.35	98.46	102.89
3	G	502	PMR	C1A-C2A-C3A	-2.35	103.51	106.61
3	W	502	PMR	C1A-C2A-C3A	-2.35	103.51	106.61
3	R	502	PMR	C1A-C2A-C3A	-2.35	103.51	106.61
2	HA	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	NA	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	LA	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	N	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	K	501	NDP	C2A-N1A-C6A	2.35	122.77	118.75
2	J	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	L	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
3	CA	502	PMR	C1A-C2A-C3A	-2.35	103.52	106.61
2	H	501	NDP	C3B-C2B-C1B	-2.35	98.47	102.89
2	OA	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
2	B	501	NDP	C2A-N1A-C6A	2.35	122.77	118.75
2	AA	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
3	JA	502	PMR	C1A-C2A-C3A	-2.35	103.52	106.61
2	X	501	NDP	C2A-N1A-C6A	2.35	122.77	118.75
2	KA	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
2	V	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
2	P	501	NDP	C2A-N1A-C6A	2.35	122.77	118.75
3	S	502	PMR	C1A-C2A-C3A	-2.35	103.52	106.61
2	O	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
2	P	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
2	DA	501	NDP	C3B-C2B-C1B	-2.35	98.48	102.89
3	L	502	PMR	C1A-C2A-C3A	-2.35	103.52	106.61
3	KA	502	PMR	C1A-C2A-C3A	-2.35	103.52	106.61
2	JA	501	NDP	C3B-C2B-C1B	-2.34	98.48	102.89
2	IA	501	NDP	C2A-N1A-C6A	2.34	122.76	118.75
3	K	502	PMR	C1A-C2A-C3A	-2.34	103.52	106.61
3	LA	502	PMR	C1A-C2A-C3A	-2.34	103.52	106.61
2	IA	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
3	I	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
2	BA	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
2	Z	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
2	Q	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
2	T	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
2	MA	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
3	Q	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
2	Y	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
2	B	501	NDP	C3B-C2B-C1B	-2.34	98.49	102.89
3	V	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
3	BA	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
3	A	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
2	D	501	NDP	C3B-C2B-C1B	-2.34	98.50	102.89
3	GA	502	PMR	C1A-C2A-C3A	-2.34	103.53	106.61
2	F	501	NDP	C3B-C2B-C1B	-2.34	98.50	102.89
3	F	502	PMR	CAA-C2A-C1A	-2.33	121.66	128.29
3	I	502	PMR	CAA-C2A-C1A	-2.33	121.66	128.29
3	Z	502	PMR	C1A-C2A-C3A	-2.33	103.54	106.61
3	NA	502	PMR	C1A-C2A-C3A	-2.33	103.54	106.61
2	M	501	NDP	C3B-C2B-C1B	-2.33	98.51	102.89
3	BA	502	PMR	CAA-C2A-C1A	-2.33	121.67	128.29
3	IA	502	PMR	CAA-C2A-C1A	-2.33	121.67	128.29
2	FA	501	NDP	C3B-C2B-C1B	-2.33	98.51	102.89
3	IA	502	PMR	C1A-C2A-C3A	-2.33	103.54	106.61
3	J	502	PMR	CAA-C2A-C1A	-2.33	121.67	128.29
2	K	501	NDP	C3B-C2B-C1B	-2.33	98.51	102.89
3	N	502	PMR	CAA-C2A-C1A	-2.33	121.68	128.29
3	X	502	PMR	C1A-C2A-C3A	-2.33	103.55	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	OA	502	PMR	C1A-C2A-C3A	-2.33	103.55	106.61
3	LA	502	PMR	CAA-C2A-C1A	-2.33	121.68	128.29
3	D	502	PMR	CAA-C2A-C1A	-2.33	121.68	128.29
3	F	502	PMR	C1A-C2A-C3A	-2.32	103.55	106.61
3	DA	502	PMR	C1A-C2A-C3A	-2.32	103.55	106.61
3	GA	502	PMR	CAA-C2A-C1A	-2.32	121.69	128.29
3	W	502	PMR	CAA-C2A-C1A	-2.32	121.69	128.29
3	J	502	PMR	C1A-C2A-C3A	-2.32	103.55	106.61
3	B	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	E	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	HA	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	Z	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	R	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	CA	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	H	502	PMR	C1A-C2A-C3A	-2.32	103.56	106.61
2	C	501	NDP	C3B-C2B-C1B	-2.32	98.53	102.89
3	H	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	K	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	V	502	PMR	CAA-C2A-C1A	-2.32	121.70	128.29
3	C	502	PMR	CAA-C2A-C1A	-2.32	121.71	128.29
3	A	502	PMR	CAA-C2A-C1A	-2.32	121.71	128.29
3	FA	502	PMR	CAA-C2A-C1A	-2.32	121.71	128.29
3	X	502	PMR	CAA-C2A-C1A	-2.32	121.71	128.29
3	MA	502	PMR	C1A-C2A-C3A	-2.32	103.56	106.61
3	Q	502	PMR	CAA-C2A-C1A	-2.32	121.71	128.29
3	B	502	PMR	C1A-C2A-C3A	-2.31	103.56	106.61
3	T	502	PMR	CAA-C2A-C1A	-2.31	121.71	128.29
3	Y	502	PMR	CAA-C2A-C1A	-2.31	121.71	128.29
3	EA	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	KA	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	AA	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	O	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	G	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	S	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	M	502	PMR	CAA-C2A-C1A	-2.31	121.72	128.29
3	L	502	PMR	CAA-C2A-C1A	-2.31	121.73	128.29
3	OA	502	PMR	CAA-C2A-C1A	-2.31	121.73	128.29
3	JA	502	PMR	CAA-C2A-C1A	-2.31	121.74	128.29
3	DA	502	PMR	CAA-C2A-C1A	-2.30	121.74	128.29
3	CA	502	PMR	O1D-CGD-CBD	-2.30	119.77	124.48
3	MA	502	PMR	CAA-C2A-C1A	-2.30	121.75	128.29
3	NA	502	PMR	CAA-C2A-C1A	-2.30	121.75	128.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	502	PMR	CAA-C2A-C1A	-2.30	121.75	128.29
3	N	502	PMR	O1D-CGD-CBD	-2.30	119.78	124.48
3	C	502	PMR	C1A-C2A-C3A	-2.30	103.59	106.61
3	AA	502	PMR	O1D-CGD-CBD	-2.29	119.80	124.48
3	Z	502	PMR	O1D-CGD-CBD	-2.29	119.80	124.48
4	LA	503	LMG	O2-C2-C1	-2.29	104.49	110.05
3	K	502	PMR	O1D-CGD-CBD	-2.29	119.81	124.48
4	I	503	LMG	O2-C2-C1	-2.29	104.49	110.05
3	O	502	PMR	O1D-CGD-CBD	-2.29	119.81	124.48
4	L	503	LMG	O2-C2-C1	-2.28	104.50	110.05
4	M	503	LMG	O2-C2-C1	-2.28	104.50	110.05
3	X	502	PMR	O1D-CGD-CBD	-2.28	119.82	124.48
3	T	502	PMR	O1D-CGD-CBD	-2.28	119.82	124.48
3	M	502	PMR	O1D-CGD-CBD	-2.28	119.82	124.48
3	HA	502	PMR	O1D-CGD-CBD	-2.28	119.82	124.48
4	CA	503	LMG	O2-C2-C1	-2.28	104.51	110.05
4	B	503	LMG	O2-C2-C1	-2.28	104.51	110.05
4	JA	503	LMG	O2-C2-C1	-2.28	104.51	110.05
4	R	503	LMG	O2-C2-C1	-2.28	104.52	110.05
3	I	502	PMR	O1D-CGD-CBD	-2.28	119.83	124.48
3	J	502	PMR	O1D-CGD-CBD	-2.28	119.83	124.48
3	GA	502	PMR	O1D-CGD-CBD	-2.27	119.83	124.48
3	KA	502	PMR	O1D-CGD-CBD	-2.27	119.83	124.48
3	B	502	PMR	O1D-CGD-CBD	-2.27	119.83	124.48
4	H	503	LMG	O2-C2-C1	-2.27	104.53	110.05
4	E	503	LMG	O2-C2-C1	-2.27	104.53	110.05
4	A	503	LMG	O2-C2-C1	-2.27	104.53	110.05
4	F	503	LMG	O2-C2-C1	-2.27	104.53	110.05
3	BA	502	PMR	O1D-CGD-CBD	-2.27	119.84	124.48
3	V	502	PMR	O1D-CGD-CBD	-2.27	119.84	124.48
4	D	503	LMG	O2-C2-C1	-2.27	104.53	110.05
4	BA	503	LMG	O2-C2-C1	-2.27	104.53	110.05
3	C	502	PMR	CMC-C2C-C1C	-2.27	121.58	125.04
4	MA	503	LMG	O2-C2-C1	-2.27	104.54	110.05
3	Q	502	PMR	O1D-CGD-CBD	-2.27	119.84	124.48
3	KA	502	PMR	CMC-C2C-C1C	-2.27	121.59	125.04
3	Y	502	PMR	O1D-CGD-CBD	-2.27	119.85	124.48
3	D	502	PMR	O1D-CGD-CBD	-2.27	119.85	124.48
3	DA	502	PMR	CMC-C2C-C1C	-2.27	121.59	125.04
4	G	503	LMG	O2-C2-C1	-2.27	104.54	110.05
3	G	502	PMR	O1D-CGD-CBD	-2.26	119.85	124.48
4	OA	503	LMG	O2-C2-C1	-2.26	104.55	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	502	PMR	O1D-CGD-CBD	-2.26	119.85	124.48
4	GA	503	LMG	O2-C2-C1	-2.26	104.55	110.05
3	LA	502	PMR	CMC-C2C-C1C	-2.26	121.59	125.04
3	C	502	PMR	O1D-CGD-CBD	-2.26	119.85	124.48
3	P	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
4	V	503	LMG	O2-C2-C1	-2.26	104.55	110.05
4	EA	503	LMG	O2-C2-C1	-2.26	104.55	110.05
3	L	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
3	E	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
3	W	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
2	NA	501	NDP	C4D-O4D-C1D	-2.26	104.48	109.47
3	AA	502	PMR	CMC-C2C-C1C	-2.26	121.60	125.04
4	X	503	LMG	O2-C2-C1	-2.26	104.56	110.05
4	Z	503	LMG	O2-C2-C1	-2.26	104.56	110.05
4	KA	503	LMG	O2-C2-C1	-2.26	104.56	110.05
3	A	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
3	EA	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
4	HA	503	LMG	O2-C2-C1	-2.26	104.56	110.05
4	M	503	LMG	O3-C3-C2	-2.26	105.13	110.35
3	F	502	PMR	O1D-CGD-CBD	-2.26	119.86	124.48
4	Q	503	LMG	O2-C2-C1	-2.26	104.56	110.05
3	FA	502	PMR	O1D-CGD-CBD	-2.26	119.87	124.48
4	K	503	LMG	O2-C2-C1	-2.26	104.56	110.05
4	S	503	LMG	O2-C2-C1	-2.26	104.56	110.05
4	Y	503	LMG	O2-C2-C1	-2.26	104.56	110.05
3	M	502	PMR	CMC-C2C-C1C	-2.26	121.60	125.04
3	JA	502	PMR	O1D-CGD-CBD	-2.26	119.87	124.48
4	W	503	LMG	O2-C2-C1	-2.26	104.57	110.05
4	BA	503	LMG	O3-C3-C2	-2.25	105.14	110.35
2	M	501	NDP	C4D-O4D-C1D	-2.25	104.50	109.47
3	H	502	PMR	O1D-CGD-CBD	-2.25	119.87	124.48
2	N	501	NDP	C4D-O4D-C1D	-2.25	104.50	109.47
2	BA	501	NDP	C4D-O4D-C1D	-2.25	104.50	109.47
4	AA	503	LMG	O2-C2-C1	-2.25	104.57	110.05
3	NA	502	PMR	O1D-CGD-CBD	-2.25	119.87	124.48
3	MA	502	PMR	O1D-CGD-CBD	-2.25	119.87	124.48
4	NA	503	LMG	O2-C2-C1	-2.25	104.57	110.05
2	EA	501	NDP	C4D-O4D-C1D	-2.25	104.50	109.47
4	P	503	LMG	O2-C2-C1	-2.25	104.57	110.05
4	DA	503	LMG	O2-C2-C1	-2.25	104.57	110.05
4	J	503	LMG	O2-C2-C1	-2.25	104.58	110.05
2	L	501	NDP	C4D-O4D-C1D	-2.25	104.50	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	LA	502	PMR	O1D-CGD-CBD	-2.25	119.88	124.48
4	T	503	LMG	O2-C2-C1	-2.25	104.58	110.05
4	O	503	LMG	O2-C2-C1	-2.25	104.58	110.05
3	N	502	PMR	CMC-C2C-C1C	-2.25	121.61	125.04
3	BA	502	PMR	CMC-C2C-C1C	-2.25	121.61	125.04
4	N	503	LMG	O2-C2-C1	-2.25	104.58	110.05
4	IA	503	LMG	O2-C2-C1	-2.25	104.58	110.05
2	D	501	NDP	C4D-O4D-C1D	-2.25	104.51	109.47
4	FA	503	LMG	O2-C2-C1	-2.25	104.59	110.05
3	R	502	PMR	O1D-CGD-CBD	-2.25	119.89	124.48
3	IA	502	PMR	O1D-CGD-CBD	-2.25	119.89	124.48
2	HA	501	NDP	C4D-O4D-C1D	-2.25	104.51	109.47
3	MA	502	PMR	CMC-C2C-C1C	-2.25	121.62	125.04
3	FA	502	PMR	CMC-C2C-C1C	-2.25	121.62	125.04
4	F	503	LMG	O3-C3-C2	-2.25	105.16	110.35
4	X	503	LMG	O3-C3-C2	-2.25	105.16	110.35
2	MA	501	NDP	C4D-O4D-C1D	-2.25	104.52	109.47
4	P	503	LMG	O3-C3-C2	-2.25	105.16	110.35
4	HA	503	LMG	O3-C3-C2	-2.25	105.16	110.35
4	K	503	LMG	O3-C3-C2	-2.24	105.16	110.35
4	Z	503	LMG	O3-C3-C2	-2.24	105.16	110.35
2	T	501	NDP	C4D-O4D-C1D	-2.24	104.52	109.47
4	B	503	LMG	O3-C3-C2	-2.24	105.16	110.35
4	D	503	LMG	O3-C3-C2	-2.24	105.16	110.35
4	JA	503	LMG	O3-C3-C2	-2.24	105.16	110.35
4	C	503	LMG	O2-C2-C1	-2.24	104.60	110.05
2	OA	501	NDP	C4D-O4D-C1D	-2.24	104.52	109.47
3	OA	502	PMR	O1D-CGD-CBD	-2.24	119.89	124.48
3	O	502	PMR	CMC-C2C-C1C	-2.24	121.62	125.04
2	F	501	NDP	C4D-O4D-C1D	-2.24	104.52	109.47
4	E	503	LMG	O3-C3-C2	-2.24	105.16	110.35
2	B	501	NDP	C4D-O4D-C1D	-2.24	104.52	109.47
3	OA	502	PMR	CMC-C2C-C1C	-2.24	121.62	125.04
4	S	503	LMG	O3-C3-C2	-2.24	105.17	110.35
3	DA	502	PMR	O1D-CGD-CBD	-2.24	119.90	124.48
2	Y	501	NDP	C4D-O4D-C1D	-2.24	104.53	109.47
3	R	502	PMR	CMC-C2C-C1C	-2.24	121.62	125.04
3	Y	502	PMR	CMC-C2C-C1C	-2.24	121.62	125.04
3	EA	502	PMR	CMC-C2C-C1C	-2.24	121.62	125.04
4	H	503	LMG	O3-C3-C2	-2.24	105.17	110.35
4	N	503	LMG	O3-C3-C2	-2.24	105.17	110.35
4	FA	503	LMG	O3-C3-C2	-2.24	105.17	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	502	PMR	CMC-C2C-C1C	-2.24	121.63	125.04
3	S	502	PMR	CMC-C2C-C1C	-2.24	121.63	125.04
2	Q	501	NDP	C4D-O4D-C1D	-2.24	104.53	109.47
4	T	503	LMG	O3-C3-C2	-2.24	105.17	110.35
2	V	501	NDP	C4D-O4D-C1D	-2.24	104.53	109.47
4	A	503	LMG	O3-C3-C2	-2.24	105.17	110.35
2	I	501	NDP	C4D-O4D-C1D	-2.24	104.53	109.47
4	LA	503	LMG	O3-C3-C2	-2.24	105.17	110.35
4	MA	503	LMG	O3-C3-C2	-2.24	105.17	110.35
3	I	502	PMR	CMC-C2C-C1C	-2.24	121.63	125.04
4	R	503	LMG	O3-C3-C2	-2.24	105.18	110.35
4	KA	503	LMG	O3-C3-C2	-2.24	105.18	110.35
4	OA	503	LMG	O3-C3-C2	-2.24	105.18	110.35
2	W	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	X	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	Z	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
3	IA	502	PMR	CMC-C2C-C1C	-2.24	121.63	125.04
4	V	503	LMG	O3-C3-C2	-2.24	105.18	110.35
4	GA	503	LMG	O3-C3-C2	-2.24	105.18	110.35
2	C	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	S	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	FA	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	AA	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
2	KA	501	NDP	C4D-O4D-C1D	-2.24	104.54	109.47
3	V	502	PMR	CMC-C2C-C1C	-2.24	121.64	125.04
2	K	501	NDP	C4D-O4D-C1D	-2.23	104.54	109.47
2	O	501	NDP	C4D-O4D-C1D	-2.23	104.54	109.47
4	I	503	LMG	O3-C3-C2	-2.23	105.19	110.35
3	L	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04
4	W	503	LMG	O3-C3-C2	-2.23	105.19	110.35
4	DA	503	LMG	O3-C3-C2	-2.23	105.19	110.35
4	AA	503	LMG	O3-C3-C2	-2.23	105.19	110.35
3	A	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04
3	T	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04
2	GA	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
4	O	503	LMG	O3-C3-C2	-2.23	105.19	110.35
2	CA	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
3	Q	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04
2	R	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
2	JA	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
2	LA	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
3	Z	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	IA	501	NDP	C4D-O4D-C1D	-2.23	104.55	109.47
4	Y	503	LMG	O3-C3-C2	-2.23	105.19	110.35
3	B	502	PMR	CMC-C2C-C1C	-2.23	121.64	125.04
4	L	503	LMG	O3-C3-C2	-2.23	105.20	110.35
4	CA	503	LMG	O3-C3-C2	-2.23	105.20	110.35
2	P	501	NDP	C4D-O4D-C1D	-2.23	104.56	109.47
2	A	501	NDP	C4D-O4D-C1D	-2.23	104.56	109.47
2	H	501	NDP	C4D-O4D-C1D	-2.23	104.56	109.47
4	EA	503	LMG	O3-C3-C2	-2.23	105.20	110.35
4	C	503	LMG	O3-C3-C2	-2.23	105.20	110.35
3	H	502	PMR	CMC-C2C-C1C	-2.22	121.65	125.04
3	NA	502	PMR	CMC-C2C-C1C	-2.22	121.65	125.04
2	E	501	NDP	C4D-O4D-C1D	-2.22	104.56	109.47
2	J	501	NDP	C4D-O4D-C1D	-2.22	104.57	109.47
3	GA	502	PMR	CMC-C2C-C1C	-2.22	121.65	125.04
2	G	501	NDP	C4D-O4D-C1D	-2.22	104.57	109.47
3	W	502	PMR	CMC-C2C-C1C	-2.22	121.66	125.04
4	G	503	LMG	O3-C3-C2	-2.22	105.22	110.35
2	DA	501	NDP	C4D-O4D-C1D	-2.22	104.58	109.47
4	J	503	LMG	O3-C3-C2	-2.22	105.22	110.35
4	Q	503	LMG	O3-C3-C2	-2.22	105.22	110.35
3	HA	502	PMR	CMC-C2C-C1C	-2.22	121.67	125.04
4	IA	503	LMG	O3-C3-C2	-2.22	105.23	110.35
3	G	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
3	J	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
3	X	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
3	JA	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
4	NA	503	LMG	O3-C3-C2	-2.21	105.23	110.35
3	F	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
3	D	502	PMR	CMC-C2C-C1C	-2.21	121.67	125.04
3	P	502	PMR	CMC-C2C-C1C	-2.21	121.68	125.04
3	E	502	PMR	CMC-C2C-C1C	-2.21	121.68	125.04
3	CA	502	PMR	CMC-C2C-C1C	-2.20	121.69	125.04
3	W	502	PMR	C1B-CHB-C4A	2.19	130.78	126.06
3	F	502	PMR	C1B-CHB-C4A	2.18	130.77	126.06
3	CA	502	PMR	C1B-CHB-C4A	2.18	130.76	126.06
3	T	502	PMR	C1B-CHB-C4A	2.18	130.76	126.06
3	B	502	PMR	C1B-CHB-C4A	2.18	130.75	126.06
3	E	502	PMR	C1B-CHB-C4A	2.18	130.75	126.06
3	N	502	PMR	C1B-CHB-C4A	2.18	130.75	126.06
3	EA	502	PMR	C1B-CHB-C4A	2.17	130.75	126.06
3	D	502	PMR	C1B-CHB-C4A	2.17	130.75	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	FA	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	KA	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	LA	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	K	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	Q	502	PMR	C1B-CHB-C4A	2.17	130.74	126.06
3	Y	502	PMR	C1B-CHB-C4A	2.17	130.73	126.06
3	X	502	PMR	C1B-CHB-C4A	2.17	130.73	126.06
3	M	502	PMR	C1B-CHB-C4A	2.16	130.73	126.06
3	BA	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	I	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	J	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	L	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	P	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	V	502	PMR	C1B-CHB-C4A	2.16	130.72	126.06
3	GA	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	O	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	AA	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	NA	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	R	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	S	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	H	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	Z	502	PMR	C1B-CHB-C4A	2.16	130.71	126.06
3	G	502	PMR	C1B-CHB-C4A	2.15	130.71	126.06
3	MA	502	PMR	C1B-CHB-C4A	2.15	130.70	126.06
3	HA	502	PMR	C1B-CHB-C4A	2.15	130.70	126.06
3	A	502	PMR	C1B-CHB-C4A	2.15	130.69	126.06
3	JA	502	PMR	C1B-CHB-C4A	2.15	130.69	126.06
3	DA	502	PMR	C1B-CHB-C4A	2.15	130.69	126.06
3	OA	502	PMR	C1B-CHB-C4A	2.15	130.69	126.06
3	IA	502	PMR	C1B-CHB-C4A	2.15	130.69	126.06
3	N	502	PMR	C4B-CHC-C1C	2.13	130.66	126.06
3	KA	502	PMR	C4B-CHC-C1C	2.13	130.65	126.06
3	BA	502	PMR	C4B-CHC-C1C	2.13	130.65	126.06
3	F	502	PMR	C4B-CHC-C1C	2.13	130.65	126.06
4	M	503	LMG	C1-C2-C3	-2.13	105.57	110.00
3	FA	502	PMR	C4B-CHC-C1C	2.13	130.64	126.06
4	X	503	LMG	C1-C2-C3	-2.13	105.57	110.00
3	Q	502	PMR	C4B-CHC-C1C	2.13	130.64	126.06
3	M	502	PMR	C4B-CHC-C1C	2.12	130.64	126.06
3	NA	502	PMR	C4B-CHC-C1C	2.12	130.64	126.06
3	J	502	PMR	C4B-CHC-C1C	2.12	130.64	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	503	LMG	C1-C2-C3	-2.12	105.57	110.00
3	GA	502	PMR	C4B-CHC-C1C	2.12	130.64	126.06
4	HA	503	LMG	C1-C2-C3	-2.12	105.58	110.00
4	MA	503	LMG	C1-C2-C3	-2.12	105.58	110.00
4	D	503	LMG	C1-C2-C3	-2.12	105.58	110.00
3	OA	502	PMR	C4B-CHC-C1C	2.12	130.63	126.06
3	NA	502	PMR	CAA-C2A-C3A	-2.12	123.93	127.88
4	BA	503	LMG	C1-C2-C3	-2.12	105.59	110.00
4	F	503	LMG	C1-C2-C3	-2.12	105.59	110.00
4	OA	503	LMG	C1-C2-C3	-2.12	105.59	110.00
4	R	503	LMG	C1-C2-C3	-2.12	105.59	110.00
4	Z	503	LMG	C1-C2-C3	-2.11	105.59	110.00
4	KA	503	LMG	C1-C2-C3	-2.11	105.59	110.00
3	P	502	PMR	C4B-CHC-C1C	2.11	130.62	126.06
3	MA	502	PMR	C4B-CHC-C1C	2.11	130.62	126.06
3	A	502	PMR	C4B-CHC-C1C	2.11	130.62	126.06
3	AA	502	PMR	C4B-CHC-C1C	2.11	130.62	126.06
4	N	503	LMG	C1-C2-C3	-2.11	105.60	110.00
4	P	503	LMG	C1-C2-C3	-2.11	105.60	110.00
4	DA	503	LMG	C1-C2-C3	-2.11	105.60	110.00
3	S	502	PMR	C4B-CHC-C1C	2.11	130.61	126.06
4	B	503	LMG	C1-C2-C3	-2.11	105.60	110.00
4	FA	503	LMG	C1-C2-C3	-2.11	105.60	110.00
3	V	502	PMR	C4B-CHC-C1C	2.11	130.61	126.06
4	E	503	LMG	C1-C2-C3	-2.11	105.60	110.00
4	T	503	LMG	C1-C2-C3	-2.11	105.60	110.00
3	K	502	PMR	C4B-CHC-C1C	2.11	130.61	126.06
3	T	502	PMR	C4B-CHC-C1C	2.11	130.61	126.06
3	X	502	PMR	C4B-CHC-C1C	2.11	130.61	126.06
4	V	503	LMG	C1-C2-C3	-2.11	105.60	110.00
3	C	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
4	J	503	LMG	C1-C2-C3	-2.11	105.61	110.00
4	K	503	LMG	C1-C2-C3	-2.11	105.61	110.00
4	IA	503	LMG	C1-C2-C3	-2.11	105.61	110.00
4	NA	503	LMG	C1-C2-C3	-2.11	105.61	110.00
3	G	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
3	W	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
3	O	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
3	H	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
4	C	503	LMG	C1-C2-C3	-2.11	105.61	110.00
3	D	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
3	L	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DA	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
4	CA	503	LMG	C1-C2-C3	-2.11	105.61	110.00
3	CA	502	PMR	C4B-CHC-C1C	2.11	130.60	126.06
4	I	503	LMG	C1-C2-C3	-2.11	105.61	110.00
4	JA	503	LMG	C1-C2-C3	-2.11	105.61	110.00
3	HA	502	PMR	C4B-CHC-C1C	2.10	130.60	126.06
4	GA	503	LMG	C1-C2-C3	-2.10	105.61	110.00
3	C	502	PMR	CAA-C2A-C3A	-2.10	123.96	127.88
3	EA	502	PMR	C4B-CHC-C1C	2.10	130.59	126.06
4	H	503	LMG	C1-C2-C3	-2.10	105.62	110.00
4	LA	503	LMG	C1-C2-C3	-2.10	105.62	110.00
3	Y	502	PMR	C4B-CHC-C1C	2.10	130.59	126.06
3	LA	502	PMR	C4B-CHC-C1C	2.10	130.59	126.06
4	A	503	LMG	C1-C2-C3	-2.10	105.62	110.00
3	H	502	PMR	CAA-C2A-C3A	-2.10	123.97	127.88
4	S	503	LMG	C1-C2-C3	-2.10	105.62	110.00
4	EA	503	LMG	C1-C2-C3	-2.10	105.62	110.00
3	I	502	PMR	C4B-CHC-C1C	2.10	130.58	126.06
4	O	503	LMG	C1-C2-C3	-2.10	105.63	110.00
4	AA	503	LMG	C1-C2-C3	-2.10	105.63	110.00
3	E	502	PMR	C4B-CHC-C1C	2.10	130.58	126.06
4	DA	503	LMG	C6-C5-C4	-2.10	108.09	113.00
3	MA	502	PMR	CAA-C2A-C3A	-2.10	123.97	127.88
3	AA	502	PMR	CAA-C2A-C3A	-2.09	123.98	127.88
3	IA	502	PMR	C4B-CHC-C1C	2.09	130.57	126.06
4	L	503	LMG	C1-C2-C3	-2.09	105.64	110.00
3	Z	502	PMR	C4B-CHC-C1C	2.09	130.57	126.06
4	G	503	LMG	C1-C2-C3	-2.09	105.64	110.00
3	B	502	PMR	C4B-CHC-C1C	2.09	130.57	126.06
3	OA	502	PMR	CAA-C2A-C3A	-2.09	123.98	127.88
3	P	502	PMR	CAA-C2A-C3A	-2.09	123.98	127.88
3	JA	502	PMR	CAA-C2A-C3A	-2.09	123.98	127.88
4	Z	503	LMG	C6-C5-C4	-2.09	108.11	113.00
3	CA	502	PMR	CAA-C2A-C3A	-2.09	123.99	127.88
3	G	502	PMR	CAA-C2A-C3A	-2.09	123.99	127.88
3	L	502	PMR	CAA-C2A-C3A	-2.09	123.99	127.88
3	R	502	PMR	C4B-CHC-C1C	2.09	130.56	126.06
4	KA	503	LMG	C6-C5-C4	-2.09	108.11	113.00
3	A	502	PMR	CAA-C2A-C3A	-2.09	123.99	127.88
4	HA	503	LMG	C6-C5-C4	-2.09	108.12	113.00
4	JA	503	LMG	C6-C5-C4	-2.09	108.12	113.00
3	T	502	PMR	CAA-C2A-C3A	-2.09	123.99	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	503	LMG	C1-C2-C3	-2.09	105.65	110.00
4	Q	503	LMG	C1-C2-C3	-2.08	105.65	110.00
4	S	503	LMG	C6-C5-C4	-2.08	108.12	113.00
4	NA	503	LMG	C6-C5-C4	-2.08	108.12	113.00
3	K	502	PMR	CAA-C2A-C3A	-2.08	124.00	127.88
4	K	503	LMG	C6-C5-C4	-2.08	108.12	113.00
4	R	503	LMG	C6-C5-C4	-2.08	108.12	113.00
4	EA	503	LMG	C6-C5-C4	-2.08	108.12	113.00
4	F	503	LMG	C6-C5-C4	-2.08	108.12	113.00
3	JA	502	PMR	C4B-CHC-C1C	2.08	130.55	126.06
4	N	503	LMG	C6-C5-C4	-2.08	108.13	113.00
3	Q	502	PMR	CAA-C2A-C3A	-2.08	124.00	127.88
3	V	502	PMR	CAA-C2A-C3A	-2.08	124.00	127.88
4	H	503	LMG	C6-C5-C4	-2.08	108.13	113.00
4	Y	503	LMG	C6-C5-C4	-2.08	108.13	113.00
4	FA	503	LMG	C6-C5-C4	-2.08	108.13	113.00
3	S	502	PMR	CAA-C2A-C3A	-2.08	124.00	127.88
4	J	503	LMG	C6-C5-C4	-2.08	108.13	113.00
4	B	503	LMG	C6-C5-C4	-2.08	108.13	113.00
4	I	503	LMG	C6-C5-C4	-2.08	108.13	113.00
4	E	503	LMG	C6-C5-C4	-2.08	108.13	113.00
3	GA	502	PMR	CAA-C2A-C3A	-2.08	124.01	127.88
3	O	502	PMR	CAA-C2A-C3A	-2.08	124.01	127.88
4	X	503	LMG	C6-C5-C4	-2.08	108.14	113.00
3	Y	502	PMR	CAA-C2A-C3A	-2.08	124.01	127.88
4	G	503	LMG	C6-C5-C4	-2.08	108.14	113.00
4	V	503	LMG	C6-C5-C4	-2.08	108.14	113.00
3	DA	502	PMR	CAA-C2A-C3A	-2.07	124.01	127.88
3	I	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
4	Q	503	LMG	C6-C5-C4	-2.07	108.15	113.00
4	M	503	LMG	C6-C5-C4	-2.07	108.15	113.00
3	BA	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	IA	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
4	AA	503	LMG	C6-C5-C4	-2.07	108.15	113.00
3	B	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	J	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
4	A	503	LMG	C6-C5-C4	-2.07	108.15	113.00
4	O	503	LMG	C6-C5-C4	-2.07	108.15	113.00
3	M	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	Z	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
4	IA	503	LMG	C6-C5-C4	-2.07	108.15	113.00
4	C	503	LMG	C6-C5-C4	-2.07	108.15	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	503	LMG	C6-C5-C4	-2.07	108.15	113.00
3	X	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	EA	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
4	GA	503	LMG	C6-C5-C4	-2.07	108.16	113.00
3	D	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	HA	502	PMR	CAA-C2A-C3A	-2.07	124.02	127.88
3	W	502	PMR	CAA-C2A-C3A	-2.07	124.03	127.88
4	P	503	LMG	C6-C5-C4	-2.07	108.16	113.00
3	F	502	PMR	CAA-C2A-C3A	-2.07	124.03	127.88
4	L	503	LMG	C6-C5-C4	-2.07	108.16	113.00
4	T	503	LMG	C6-C5-C4	-2.07	108.16	113.00
4	LA	503	LMG	C6-C5-C4	-2.07	108.16	113.00
4	MA	503	LMG	C6-C5-C4	-2.07	108.16	113.00
4	OA	503	LMG	C6-C5-C4	-2.07	108.16	113.00
3	R	502	PMR	CAA-C2A-C3A	-2.07	124.03	127.88
4	D	503	LMG	C6-C5-C4	-2.07	108.16	113.00
3	KA	502	PMR	CAA-C2A-C3A	-2.06	124.03	127.88
3	FA	502	PMR	CAA-C2A-C3A	-2.06	124.04	127.88
3	E	502	PMR	CAA-C2A-C3A	-2.06	124.04	127.88
3	LA	502	PMR	CAA-C2A-C3A	-2.06	124.05	127.88
3	N	502	PMR	CAA-C2A-C3A	-2.05	124.05	127.88
4	CA	503	LMG	C6-C5-C4	-2.05	108.20	113.00
4	BA	503	LMG	C6-C5-C4	-2.05	108.20	113.00

All (120) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	502	PMR	NB
3	A	502	PMR	NA
3	A	502	PMR	NC
3	B	502	PMR	NB
3	B	502	PMR	NA
3	B	502	PMR	NC
3	C	502	PMR	NB
3	C	502	PMR	NA
3	C	502	PMR	NC
3	D	502	PMR	NB
3	D	502	PMR	NA
3	D	502	PMR	NC
3	E	502	PMR	NB
3	E	502	PMR	NA
3	E	502	PMR	NC

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Mol	Chain	Res	Type	Atom
3	F	502	PMR	NB
3	F	502	PMR	NA
3	F	502	PMR	NC
3	G	502	PMR	NB
3	G	502	PMR	NA
3	G	502	PMR	NC
3	H	502	PMR	NB
3	H	502	PMR	NA
3	H	502	PMR	NC
3	I	502	PMR	NB
3	I	502	PMR	NA
3	I	502	PMR	NC
3	J	502	PMR	NB
3	J	502	PMR	NA
3	J	502	PMR	NC
3	K	502	PMR	NB
3	K	502	PMR	NA
3	K	502	PMR	NC
3	L	502	PMR	NB
3	L	502	PMR	NA
3	L	502	PMR	NC
3	M	502	PMR	NB
3	M	502	PMR	NA
3	M	502	PMR	NC
3	N	502	PMR	NB
3	N	502	PMR	NA
3	N	502	PMR	NC
3	O	502	PMR	NB
3	O	502	PMR	NA
3	O	502	PMR	NC
3	P	502	PMR	NB
3	P	502	PMR	NA
3	P	502	PMR	NC
3	Q	502	PMR	NB
3	Q	502	PMR	NA
3	Q	502	PMR	NC
3	R	502	PMR	NB
3	R	502	PMR	NA
3	R	502	PMR	NC
3	S	502	PMR	NB
3	S	502	PMR	NA
3	S	502	PMR	NC

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Mol	Chain	Res	Type	Atom
3	T	502	PMR	NB
3	T	502	PMR	NA
3	T	502	PMR	NC
3	V	502	PMR	NB
3	V	502	PMR	NA
3	V	502	PMR	NC
3	W	502	PMR	NB
3	W	502	PMR	NA
3	W	502	PMR	NC
3	X	502	PMR	NB
3	X	502	PMR	NA
3	X	502	PMR	NC
3	Y	502	PMR	NB
3	Y	502	PMR	NA
3	Y	502	PMR	NC
3	Z	502	PMR	NB
3	Z	502	PMR	NA
3	Z	502	PMR	NC
3	AA	502	PMR	NB
3	AA	502	PMR	NA
3	AA	502	PMR	NC
3	BA	502	PMR	NB
3	BA	502	PMR	NA
3	BA	502	PMR	NC
3	CA	502	PMR	NB
3	CA	502	PMR	NA
3	CA	502	PMR	NC
3	DA	502	PMR	NB
3	DA	502	PMR	NA
3	DA	502	PMR	NC
3	EA	502	PMR	NB
3	EA	502	PMR	NA
3	EA	502	PMR	NC
3	FA	502	PMR	NB
3	FA	502	PMR	NA
3	FA	502	PMR	NC
3	GA	502	PMR	NB
3	GA	502	PMR	NA
3	GA	502	PMR	NC
3	HA	502	PMR	NB
3	HA	502	PMR	NA
3	HA	502	PMR	NC

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Mol	Chain	Res	Type	Atom
3	IA	502	PMR	NB
3	IA	502	PMR	NA
3	IA	502	PMR	NC
3	JA	502	PMR	NB
3	JA	502	PMR	NA
3	JA	502	PMR	NC
3	KA	502	PMR	NB
3	KA	502	PMR	NA
3	KA	502	PMR	NC
3	LA	502	PMR	NB
3	LA	502	PMR	NA
3	LA	502	PMR	NC
3	MA	502	PMR	NB
3	MA	502	PMR	NA
3	MA	502	PMR	NC
3	NA	502	PMR	NB
3	NA	502	PMR	NA
3	NA	502	PMR	NC
3	OA	502	PMR	NB
3	OA	502	PMR	NA
3	OA	502	PMR	NC

All (1080) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	C5B-O5B-PA-O2A
2	A	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O2A
2	B	501	NDP	C5D-O5D-PN-O1N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	C	501	NDP	C5B-O5B-PA-O1A
2	C	501	NDP	C5B-O5B-PA-O2A
2	C	501	NDP	C5D-O5D-PN-O1N
2	C	501	NDP	O4D-C1D-N1N-C6N
2	D	501	NDP	C5B-O5B-PA-O1A
2	D	501	NDP	C5B-O5B-PA-O2A
2	D	501	NDP	C5D-O5D-PN-O1N
2	D	501	NDP	O4D-C1D-N1N-C6N
2	E	501	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	E	501	NDP	C5B-O5B-PA-O2A
2	E	501	NDP	C5D-O5D-PN-O1N
2	E	501	NDP	O4D-C1D-N1N-C6N
2	F	501	NDP	C5B-O5B-PA-O1A
2	F	501	NDP	C5B-O5B-PA-O2A
2	F	501	NDP	C5D-O5D-PN-O1N
2	F	501	NDP	O4D-C1D-N1N-C6N
2	G	501	NDP	C5B-O5B-PA-O1A
2	G	501	NDP	C5B-O5B-PA-O2A
2	G	501	NDP	C5D-O5D-PN-O1N
2	G	501	NDP	O4D-C1D-N1N-C6N
2	H	501	NDP	C5B-O5B-PA-O1A
2	H	501	NDP	C5B-O5B-PA-O2A
2	H	501	NDP	C5D-O5D-PN-O1N
2	H	501	NDP	O4D-C1D-N1N-C6N
2	I	501	NDP	C5B-O5B-PA-O1A
2	I	501	NDP	C5B-O5B-PA-O2A
2	I	501	NDP	C5D-O5D-PN-O1N
2	I	501	NDP	O4D-C1D-N1N-C6N
2	J	501	NDP	C5B-O5B-PA-O1A
2	J	501	NDP	C5B-O5B-PA-O2A
2	J	501	NDP	C5D-O5D-PN-O1N
2	J	501	NDP	O4D-C1D-N1N-C6N
2	K	501	NDP	C5B-O5B-PA-O1A
2	K	501	NDP	C5B-O5B-PA-O2A
2	K	501	NDP	C5D-O5D-PN-O1N
2	K	501	NDP	O4D-C1D-N1N-C6N
2	L	501	NDP	C5B-O5B-PA-O1A
2	L	501	NDP	C5B-O5B-PA-O2A
2	L	501	NDP	C5D-O5D-PN-O1N
2	L	501	NDP	O4D-C1D-N1N-C6N
2	M	501	NDP	C5B-O5B-PA-O1A
2	M	501	NDP	C5B-O5B-PA-O2A
2	M	501	NDP	C5D-O5D-PN-O1N
2	M	501	NDP	O4D-C1D-N1N-C6N
2	N	501	NDP	C5B-O5B-PA-O1A
2	N	501	NDP	C5B-O5B-PA-O2A
2	N	501	NDP	C5D-O5D-PN-O1N
2	N	501	NDP	O4D-C1D-N1N-C6N
2	O	501	NDP	C5B-O5B-PA-O1A
2	O	501	NDP	C5B-O5B-PA-O2A
2	O	501	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	O	501	NDP	O4D-C1D-N1N-C6N
2	P	501	NDP	C5B-O5B-PA-O1A
2	P	501	NDP	C5B-O5B-PA-O2A
2	P	501	NDP	C5D-O5D-PN-O1N
2	P	501	NDP	O4D-C1D-N1N-C6N
2	Q	501	NDP	C5B-O5B-PA-O1A
2	Q	501	NDP	C5B-O5B-PA-O2A
2	Q	501	NDP	C5D-O5D-PN-O1N
2	Q	501	NDP	O4D-C1D-N1N-C6N
2	R	501	NDP	C5B-O5B-PA-O1A
2	R	501	NDP	C5B-O5B-PA-O2A
2	R	501	NDP	C5D-O5D-PN-O1N
2	R	501	NDP	O4D-C1D-N1N-C6N
2	S	501	NDP	C5B-O5B-PA-O1A
2	S	501	NDP	C5B-O5B-PA-O2A
2	S	501	NDP	C5D-O5D-PN-O1N
2	S	501	NDP	O4D-C1D-N1N-C6N
2	T	501	NDP	C5B-O5B-PA-O1A
2	T	501	NDP	C5B-O5B-PA-O2A
2	T	501	NDP	C5D-O5D-PN-O1N
2	T	501	NDP	O4D-C1D-N1N-C6N
2	V	501	NDP	C5B-O5B-PA-O1A
2	V	501	NDP	C5B-O5B-PA-O2A
2	V	501	NDP	C5D-O5D-PN-O1N
2	V	501	NDP	O4D-C1D-N1N-C6N
2	W	501	NDP	C5B-O5B-PA-O1A
2	W	501	NDP	C5B-O5B-PA-O2A
2	W	501	NDP	C5D-O5D-PN-O1N
2	W	501	NDP	O4D-C1D-N1N-C6N
2	X	501	NDP	C5B-O5B-PA-O1A
2	X	501	NDP	C5B-O5B-PA-O2A
2	X	501	NDP	C5D-O5D-PN-O1N
2	X	501	NDP	O4D-C1D-N1N-C6N
2	Y	501	NDP	C5B-O5B-PA-O1A
2	Y	501	NDP	C5B-O5B-PA-O2A
2	Y	501	NDP	C5D-O5D-PN-O1N
2	Y	501	NDP	O4D-C1D-N1N-C6N
2	Z	501	NDP	C5B-O5B-PA-O1A
2	Z	501	NDP	C5B-O5B-PA-O2A
2	Z	501	NDP	C5D-O5D-PN-O1N
2	Z	501	NDP	O4D-C1D-N1N-C6N
2	AA	501	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	AA	501	NDP	C5B-O5B-PA-O2A
2	AA	501	NDP	C5D-O5D-PN-O1N
2	AA	501	NDP	O4D-C1D-N1N-C6N
2	BA	501	NDP	C5B-O5B-PA-O1A
2	BA	501	NDP	C5B-O5B-PA-O2A
2	BA	501	NDP	C5D-O5D-PN-O1N
2	BA	501	NDP	O4D-C1D-N1N-C6N
2	CA	501	NDP	C5B-O5B-PA-O1A
2	CA	501	NDP	C5B-O5B-PA-O2A
2	CA	501	NDP	C5D-O5D-PN-O1N
2	CA	501	NDP	O4D-C1D-N1N-C6N
2	DA	501	NDP	C5B-O5B-PA-O1A
2	DA	501	NDP	C5B-O5B-PA-O2A
2	DA	501	NDP	C5D-O5D-PN-O1N
2	DA	501	NDP	O4D-C1D-N1N-C6N
2	EA	501	NDP	C5B-O5B-PA-O1A
2	EA	501	NDP	C5B-O5B-PA-O2A
2	EA	501	NDP	C5D-O5D-PN-O1N
2	EA	501	NDP	O4D-C1D-N1N-C6N
2	FA	501	NDP	C5B-O5B-PA-O1A
2	FA	501	NDP	C5B-O5B-PA-O2A
2	FA	501	NDP	C5D-O5D-PN-O1N
2	FA	501	NDP	O4D-C1D-N1N-C6N
2	GA	501	NDP	C5B-O5B-PA-O1A
2	GA	501	NDP	C5B-O5B-PA-O2A
2	GA	501	NDP	C5D-O5D-PN-O1N
2	GA	501	NDP	O4D-C1D-N1N-C6N
2	HA	501	NDP	C5B-O5B-PA-O1A
2	HA	501	NDP	C5B-O5B-PA-O2A
2	HA	501	NDP	C5D-O5D-PN-O1N
2	HA	501	NDP	O4D-C1D-N1N-C6N
2	IA	501	NDP	C5B-O5B-PA-O1A
2	IA	501	NDP	C5B-O5B-PA-O2A
2	IA	501	NDP	C5D-O5D-PN-O1N
2	IA	501	NDP	O4D-C1D-N1N-C6N
2	JA	501	NDP	C5B-O5B-PA-O1A
2	JA	501	NDP	C5B-O5B-PA-O2A
2	JA	501	NDP	C5D-O5D-PN-O1N
2	JA	501	NDP	O4D-C1D-N1N-C6N
2	KA	501	NDP	C5B-O5B-PA-O1A
2	KA	501	NDP	C5B-O5B-PA-O2A
2	KA	501	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	KA	501	NDP	O4D-C1D-N1N-C6N
2	LA	501	NDP	C5B-O5B-PA-O1A
2	LA	501	NDP	C5B-O5B-PA-O2A
2	LA	501	NDP	C5D-O5D-PN-O1N
2	LA	501	NDP	O4D-C1D-N1N-C6N
2	MA	501	NDP	C5B-O5B-PA-O1A
2	MA	501	NDP	C5B-O5B-PA-O2A
2	MA	501	NDP	C5D-O5D-PN-O1N
2	MA	501	NDP	O4D-C1D-N1N-C6N
2	NA	501	NDP	C5B-O5B-PA-O1A
2	NA	501	NDP	C5B-O5B-PA-O2A
2	NA	501	NDP	C5D-O5D-PN-O1N
2	NA	501	NDP	O4D-C1D-N1N-C6N
2	OA	501	NDP	C5B-O5B-PA-O1A
2	OA	501	NDP	C5B-O5B-PA-O2A
2	OA	501	NDP	C5D-O5D-PN-O1N
2	OA	501	NDP	O4D-C1D-N1N-C6N
4	A	503	LMG	C2-C1-O1-C7
4	A	503	LMG	O6-C1-O1-C7
4	A	503	LMG	O9-C10-O7-C8
4	A	503	LMG	C11-C10-O7-C8
4	B	503	LMG	C2-C1-O1-C7
4	B	503	LMG	O6-C1-O1-C7
4	B	503	LMG	O9-C10-O7-C8
4	B	503	LMG	C11-C10-O7-C8
4	C	503	LMG	C2-C1-O1-C7
4	C	503	LMG	O6-C1-O1-C7
4	C	503	LMG	O9-C10-O7-C8
4	C	503	LMG	C11-C10-O7-C8
4	D	503	LMG	C2-C1-O1-C7
4	D	503	LMG	O6-C1-O1-C7
4	D	503	LMG	O9-C10-O7-C8
4	D	503	LMG	C11-C10-O7-C8
4	E	503	LMG	C2-C1-O1-C7
4	E	503	LMG	O6-C1-O1-C7
4	E	503	LMG	O9-C10-O7-C8
4	E	503	LMG	C11-C10-O7-C8
4	F	503	LMG	C2-C1-O1-C7
4	F	503	LMG	O6-C1-O1-C7
4	F	503	LMG	O9-C10-O7-C8
4	F	503	LMG	C11-C10-O7-C8
4	G	503	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
4	G	503	LMG	O6-C1-O1-C7
4	G	503	LMG	O9-C10-O7-C8
4	G	503	LMG	C11-C10-O7-C8
4	H	503	LMG	C2-C1-O1-C7
4	H	503	LMG	O6-C1-O1-C7
4	H	503	LMG	O9-C10-O7-C8
4	H	503	LMG	C11-C10-O7-C8
4	I	503	LMG	C2-C1-O1-C7
4	I	503	LMG	O6-C1-O1-C7
4	I	503	LMG	O9-C10-O7-C8
4	I	503	LMG	C11-C10-O7-C8
4	J	503	LMG	C2-C1-O1-C7
4	J	503	LMG	O6-C1-O1-C7
4	J	503	LMG	O9-C10-O7-C8
4	J	503	LMG	C11-C10-O7-C8
4	K	503	LMG	C2-C1-O1-C7
4	K	503	LMG	O6-C1-O1-C7
4	K	503	LMG	O9-C10-O7-C8
4	K	503	LMG	C11-C10-O7-C8
4	L	503	LMG	C2-C1-O1-C7
4	L	503	LMG	O6-C1-O1-C7
4	L	503	LMG	O9-C10-O7-C8
4	L	503	LMG	C11-C10-O7-C8
4	M	503	LMG	C2-C1-O1-C7
4	M	503	LMG	O6-C1-O1-C7
4	M	503	LMG	O9-C10-O7-C8
4	M	503	LMG	C11-C10-O7-C8
4	N	503	LMG	C2-C1-O1-C7
4	N	503	LMG	O6-C1-O1-C7
4	N	503	LMG	O9-C10-O7-C8
4	N	503	LMG	C11-C10-O7-C8
4	O	503	LMG	C2-C1-O1-C7
4	O	503	LMG	O6-C1-O1-C7
4	O	503	LMG	O9-C10-O7-C8
4	O	503	LMG	C11-C10-O7-C8
4	P	503	LMG	C2-C1-O1-C7
4	P	503	LMG	O6-C1-O1-C7
4	P	503	LMG	O9-C10-O7-C8
4	P	503	LMG	C11-C10-O7-C8
4	Q	503	LMG	C2-C1-O1-C7
4	Q	503	LMG	O6-C1-O1-C7
4	Q	503	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
4	Q	503	LMG	C11-C10-O7-C8
4	R	503	LMG	C2-C1-O1-C7
4	R	503	LMG	O6-C1-O1-C7
4	R	503	LMG	O9-C10-O7-C8
4	R	503	LMG	C11-C10-O7-C8
4	S	503	LMG	C2-C1-O1-C7
4	S	503	LMG	O6-C1-O1-C7
4	S	503	LMG	O9-C10-O7-C8
4	S	503	LMG	C11-C10-O7-C8
4	T	503	LMG	C2-C1-O1-C7
4	T	503	LMG	O6-C1-O1-C7
4	T	503	LMG	O9-C10-O7-C8
4	T	503	LMG	C11-C10-O7-C8
4	V	503	LMG	C2-C1-O1-C7
4	V	503	LMG	O6-C1-O1-C7
4	V	503	LMG	O9-C10-O7-C8
4	V	503	LMG	C11-C10-O7-C8
4	W	503	LMG	C2-C1-O1-C7
4	W	503	LMG	O6-C1-O1-C7
4	W	503	LMG	O9-C10-O7-C8
4	W	503	LMG	C11-C10-O7-C8
4	X	503	LMG	C2-C1-O1-C7
4	X	503	LMG	O6-C1-O1-C7
4	X	503	LMG	O9-C10-O7-C8
4	X	503	LMG	C11-C10-O7-C8
4	Y	503	LMG	C2-C1-O1-C7
4	Y	503	LMG	O6-C1-O1-C7
4	Y	503	LMG	O9-C10-O7-C8
4	Y	503	LMG	C11-C10-O7-C8
4	Z	503	LMG	C2-C1-O1-C7
4	Z	503	LMG	O6-C1-O1-C7
4	Z	503	LMG	O9-C10-O7-C8
4	Z	503	LMG	C11-C10-O7-C8
4	AA	503	LMG	C2-C1-O1-C7
4	AA	503	LMG	O6-C1-O1-C7
4	AA	503	LMG	O9-C10-O7-C8
4	AA	503	LMG	C11-C10-O7-C8
4	BA	503	LMG	C2-C1-O1-C7
4	BA	503	LMG	O6-C1-O1-C7
4	BA	503	LMG	O9-C10-O7-C8
4	BA	503	LMG	C11-C10-O7-C8
4	CA	503	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
4	CA	503	LMG	O6-C1-O1-C7
4	CA	503	LMG	O9-C10-O7-C8
4	CA	503	LMG	C11-C10-O7-C8
4	DA	503	LMG	C2-C1-O1-C7
4	DA	503	LMG	O6-C1-O1-C7
4	DA	503	LMG	O9-C10-O7-C8
4	DA	503	LMG	C11-C10-O7-C8
4	EA	503	LMG	C2-C1-O1-C7
4	EA	503	LMG	O6-C1-O1-C7
4	EA	503	LMG	O9-C10-O7-C8
4	EA	503	LMG	C11-C10-O7-C8
4	FA	503	LMG	C2-C1-O1-C7
4	FA	503	LMG	O6-C1-O1-C7
4	FA	503	LMG	O9-C10-O7-C8
4	FA	503	LMG	C11-C10-O7-C8
4	GA	503	LMG	C2-C1-O1-C7
4	GA	503	LMG	O6-C1-O1-C7
4	GA	503	LMG	O9-C10-O7-C8
4	GA	503	LMG	C11-C10-O7-C8
4	HA	503	LMG	C2-C1-O1-C7
4	HA	503	LMG	O6-C1-O1-C7
4	HA	503	LMG	O9-C10-O7-C8
4	HA	503	LMG	C11-C10-O7-C8
4	IA	503	LMG	C2-C1-O1-C7
4	IA	503	LMG	O6-C1-O1-C7
4	IA	503	LMG	O9-C10-O7-C8
4	IA	503	LMG	C11-C10-O7-C8
4	JA	503	LMG	C2-C1-O1-C7
4	JA	503	LMG	O6-C1-O1-C7
4	JA	503	LMG	O9-C10-O7-C8
4	JA	503	LMG	C11-C10-O7-C8
4	KA	503	LMG	C2-C1-O1-C7
4	KA	503	LMG	O6-C1-O1-C7
4	KA	503	LMG	O9-C10-O7-C8
4	KA	503	LMG	C11-C10-O7-C8
4	LA	503	LMG	C2-C1-O1-C7
4	LA	503	LMG	O6-C1-O1-C7
4	LA	503	LMG	O9-C10-O7-C8
4	LA	503	LMG	C11-C10-O7-C8
4	MA	503	LMG	C2-C1-O1-C7
4	MA	503	LMG	O6-C1-O1-C7
4	MA	503	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
4	MA	503	LMG	C11-C10-O7-C8
4	NA	503	LMG	C2-C1-O1-C7
4	NA	503	LMG	O6-C1-O1-C7
4	NA	503	LMG	O9-C10-O7-C8
4	NA	503	LMG	C11-C10-O7-C8
4	OA	503	LMG	C2-C1-O1-C7
4	OA	503	LMG	O6-C1-O1-C7
4	OA	503	LMG	O9-C10-O7-C8
4	OA	503	LMG	C11-C10-O7-C8
3	A	502	PMR	O1D-CGD-O2D-C2O
3	B	502	PMR	O1D-CGD-O2D-C2O
3	C	502	PMR	O1D-CGD-O2D-C2O
3	D	502	PMR	O1D-CGD-O2D-C2O
3	E	502	PMR	O1D-CGD-O2D-C2O
3	F	502	PMR	O1D-CGD-O2D-C2O
3	G	502	PMR	O1D-CGD-O2D-C2O
3	H	502	PMR	O1D-CGD-O2D-C2O
3	I	502	PMR	O1D-CGD-O2D-C2O
3	J	502	PMR	O1D-CGD-O2D-C2O
3	K	502	PMR	O1D-CGD-O2D-C2O
3	L	502	PMR	O1D-CGD-O2D-C2O
3	M	502	PMR	O1D-CGD-O2D-C2O
3	N	502	PMR	O1D-CGD-O2D-C2O
3	O	502	PMR	O1D-CGD-O2D-C2O
3	P	502	PMR	O1D-CGD-O2D-C2O
3	Q	502	PMR	O1D-CGD-O2D-C2O
3	R	502	PMR	O1D-CGD-O2D-C2O
3	S	502	PMR	O1D-CGD-O2D-C2O
3	T	502	PMR	O1D-CGD-O2D-C2O
3	V	502	PMR	O1D-CGD-O2D-C2O
3	W	502	PMR	O1D-CGD-O2D-C2O
3	X	502	PMR	O1D-CGD-O2D-C2O
3	Y	502	PMR	O1D-CGD-O2D-C2O
3	Z	502	PMR	O1D-CGD-O2D-C2O
3	AA	502	PMR	O1D-CGD-O2D-C2O
3	BA	502	PMR	O1D-CGD-O2D-C2O
3	CA	502	PMR	O1D-CGD-O2D-C2O
3	DA	502	PMR	O1D-CGD-O2D-C2O
3	EA	502	PMR	O1D-CGD-O2D-C2O
3	FA	502	PMR	O1D-CGD-O2D-C2O
3	GA	502	PMR	O1D-CGD-O2D-C2O
3	HA	502	PMR	O1D-CGD-O2D-C2O

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Mol	Chain	Res	Type	Atoms
3	IA	502	PMR	O1D-CGD-O2D-C2O
3	JA	502	PMR	O1D-CGD-O2D-C2O
3	KA	502	PMR	O1D-CGD-O2D-C2O
3	LA	502	PMR	O1D-CGD-O2D-C2O
3	MA	502	PMR	O1D-CGD-O2D-C2O
3	NA	502	PMR	O1D-CGD-O2D-C2O
3	OA	502	PMR	O1D-CGD-O2D-C2O
4	A	503	LMG	C29-C28-O8-C9
4	B	503	LMG	C29-C28-O8-C9
4	C	503	LMG	C29-C28-O8-C9
4	D	503	LMG	C29-C28-O8-C9
4	E	503	LMG	C29-C28-O8-C9
4	F	503	LMG	C29-C28-O8-C9
4	G	503	LMG	C29-C28-O8-C9
4	H	503	LMG	C29-C28-O8-C9
4	I	503	LMG	C29-C28-O8-C9
4	J	503	LMG	C29-C28-O8-C9
4	K	503	LMG	C29-C28-O8-C9
4	L	503	LMG	C29-C28-O8-C9
4	M	503	LMG	C29-C28-O8-C9
4	N	503	LMG	C29-C28-O8-C9
4	O	503	LMG	C29-C28-O8-C9
4	P	503	LMG	C29-C28-O8-C9
4	Q	503	LMG	C29-C28-O8-C9
4	R	503	LMG	C29-C28-O8-C9
4	S	503	LMG	C29-C28-O8-C9
4	T	503	LMG	C29-C28-O8-C9
4	V	503	LMG	C29-C28-O8-C9
4	W	503	LMG	C29-C28-O8-C9
4	X	503	LMG	C29-C28-O8-C9
4	Y	503	LMG	C29-C28-O8-C9
4	Z	503	LMG	C29-C28-O8-C9
4	AA	503	LMG	C29-C28-O8-C9
4	BA	503	LMG	C29-C28-O8-C9
4	CA	503	LMG	C29-C28-O8-C9
4	DA	503	LMG	C29-C28-O8-C9
4	EA	503	LMG	C29-C28-O8-C9
4	FA	503	LMG	C29-C28-O8-C9
4	GA	503	LMG	C29-C28-O8-C9
4	HA	503	LMG	C29-C28-O8-C9
4	IA	503	LMG	C29-C28-O8-C9
4	JA	503	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
4	KA	503	LMG	C29-C28-O8-C9
4	LA	503	LMG	C29-C28-O8-C9
4	MA	503	LMG	C29-C28-O8-C9
4	NA	503	LMG	C29-C28-O8-C9
4	OA	503	LMG	C29-C28-O8-C9
3	B	502	PMR	CBD-CGD-O2D-C2O
3	F	502	PMR	CBD-CGD-O2D-C2O
3	G	502	PMR	CBD-CGD-O2D-C2O
3	H	502	PMR	CBD-CGD-O2D-C2O
3	O	502	PMR	CBD-CGD-O2D-C2O
3	P	502	PMR	CBD-CGD-O2D-C2O
3	Q	502	PMR	CBD-CGD-O2D-C2O
3	R	502	PMR	CBD-CGD-O2D-C2O
3	T	502	PMR	CBD-CGD-O2D-C2O
3	V	502	PMR	CBD-CGD-O2D-C2O
3	W	502	PMR	CBD-CGD-O2D-C2O
3	DA	502	PMR	CBD-CGD-O2D-C2O
3	FA	502	PMR	CBD-CGD-O2D-C2O
3	HA	502	PMR	CBD-CGD-O2D-C2O
3	KA	502	PMR	CBD-CGD-O2D-C2O
3	LA	502	PMR	CBD-CGD-O2D-C2O
3	MA	502	PMR	CBD-CGD-O2D-C2O
3	OA	502	PMR	CBD-CGD-O2D-C2O
3	A	502	PMR	CBD-CGD-O2D-C2O
3	C	502	PMR	CBD-CGD-O2D-C2O
3	D	502	PMR	CBD-CGD-O2D-C2O
3	E	502	PMR	CBD-CGD-O2D-C2O
3	I	502	PMR	CBD-CGD-O2D-C2O
3	J	502	PMR	CBD-CGD-O2D-C2O
3	K	502	PMR	CBD-CGD-O2D-C2O
3	L	502	PMR	CBD-CGD-O2D-C2O
3	M	502	PMR	CBD-CGD-O2D-C2O
3	N	502	PMR	CBD-CGD-O2D-C2O
3	S	502	PMR	CBD-CGD-O2D-C2O
3	X	502	PMR	CBD-CGD-O2D-C2O
3	Y	502	PMR	CBD-CGD-O2D-C2O
3	Z	502	PMR	CBD-CGD-O2D-C2O
3	AA	502	PMR	CBD-CGD-O2D-C2O
3	BA	502	PMR	CBD-CGD-O2D-C2O
3	CA	502	PMR	CBD-CGD-O2D-C2O
3	EA	502	PMR	CBD-CGD-O2D-C2O
3	GA	502	PMR	CBD-CGD-O2D-C2O

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Mol	Chain	Res	Type	Atoms
3	IA	502	PMR	CBD-CGD-O2D-C2O
3	JA	502	PMR	CBD-CGD-O2D-C2O
3	NA	502	PMR	CBD-CGD-O2D-C2O
4	B	503	LMG	O10-C28-O8-C9
4	F	503	LMG	O10-C28-O8-C9
4	M	503	LMG	O10-C28-O8-C9
4	O	503	LMG	O10-C28-O8-C9
4	S	503	LMG	O10-C28-O8-C9
4	T	503	LMG	O10-C28-O8-C9
4	W	503	LMG	O10-C28-O8-C9
4	BA	503	LMG	O10-C28-O8-C9
4	FA	503	LMG	O10-C28-O8-C9
4	IA	503	LMG	O10-C28-O8-C9
4	LA	503	LMG	O10-C28-O8-C9
4	A	503	LMG	O10-C28-O8-C9
4	C	503	LMG	O10-C28-O8-C9
4	D	503	LMG	O10-C28-O8-C9
4	E	503	LMG	O10-C28-O8-C9
4	G	503	LMG	O10-C28-O8-C9
4	H	503	LMG	O10-C28-O8-C9
4	I	503	LMG	O10-C28-O8-C9
4	J	503	LMG	O10-C28-O8-C9
4	K	503	LMG	O10-C28-O8-C9
4	L	503	LMG	O10-C28-O8-C9
4	N	503	LMG	O10-C28-O8-C9
4	P	503	LMG	O10-C28-O8-C9
4	Q	503	LMG	O10-C28-O8-C9
4	R	503	LMG	O10-C28-O8-C9
4	V	503	LMG	O10-C28-O8-C9
4	X	503	LMG	O10-C28-O8-C9
4	Y	503	LMG	O10-C28-O8-C9
4	Z	503	LMG	O10-C28-O8-C9
4	AA	503	LMG	O10-C28-O8-C9
4	CA	503	LMG	O10-C28-O8-C9
4	DA	503	LMG	O10-C28-O8-C9
4	EA	503	LMG	O10-C28-O8-C9
4	GA	503	LMG	O10-C28-O8-C9
4	HA	503	LMG	O10-C28-O8-C9
4	KA	503	LMG	O10-C28-O8-C9
4	MA	503	LMG	O10-C28-O8-C9
4	NA	503	LMG	O10-C28-O8-C9
4	JA	503	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
4	OA	503	LMG	O10-C28-O8-C9
2	A	501	NDP	C1B-C2B-O2B-P2B
2	B	501	NDP	C1B-C2B-O2B-P2B
2	C	501	NDP	C1B-C2B-O2B-P2B
2	D	501	NDP	C1B-C2B-O2B-P2B
2	E	501	NDP	C1B-C2B-O2B-P2B
2	F	501	NDP	C1B-C2B-O2B-P2B
2	G	501	NDP	C1B-C2B-O2B-P2B
2	H	501	NDP	C1B-C2B-O2B-P2B
2	I	501	NDP	C1B-C2B-O2B-P2B
2	J	501	NDP	C1B-C2B-O2B-P2B
2	K	501	NDP	C1B-C2B-O2B-P2B
2	L	501	NDP	C1B-C2B-O2B-P2B
2	M	501	NDP	C1B-C2B-O2B-P2B
2	N	501	NDP	C1B-C2B-O2B-P2B
2	O	501	NDP	C1B-C2B-O2B-P2B
2	P	501	NDP	C1B-C2B-O2B-P2B
2	Q	501	NDP	C1B-C2B-O2B-P2B
2	R	501	NDP	C1B-C2B-O2B-P2B
2	S	501	NDP	C1B-C2B-O2B-P2B
2	T	501	NDP	C1B-C2B-O2B-P2B
2	V	501	NDP	C1B-C2B-O2B-P2B
2	W	501	NDP	C1B-C2B-O2B-P2B
2	X	501	NDP	C1B-C2B-O2B-P2B
2	Y	501	NDP	C1B-C2B-O2B-P2B
2	Z	501	NDP	C1B-C2B-O2B-P2B
2	AA	501	NDP	C1B-C2B-O2B-P2B
2	BA	501	NDP	C1B-C2B-O2B-P2B
2	CA	501	NDP	C1B-C2B-O2B-P2B
2	DA	501	NDP	C1B-C2B-O2B-P2B
2	EA	501	NDP	C1B-C2B-O2B-P2B
2	FA	501	NDP	C1B-C2B-O2B-P2B
2	GA	501	NDP	C1B-C2B-O2B-P2B
2	HA	501	NDP	C1B-C2B-O2B-P2B
2	IA	501	NDP	C1B-C2B-O2B-P2B
2	JA	501	NDP	C1B-C2B-O2B-P2B
2	KA	501	NDP	C1B-C2B-O2B-P2B
2	LA	501	NDP	C1B-C2B-O2B-P2B
2	MA	501	NDP	C1B-C2B-O2B-P2B
2	NA	501	NDP	C1B-C2B-O2B-P2B
2	OA	501	NDP	C1B-C2B-O2B-P2B
3	H	502	PMR	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	K	502	PMR	C2A-CAA-CBA-CGA
3	L	502	PMR	C2A-CAA-CBA-CGA
3	O	502	PMR	C2A-CAA-CBA-CGA
3	P	502	PMR	C2A-CAA-CBA-CGA
3	JA	502	PMR	C2A-CAA-CBA-CGA
3	MA	502	PMR	C2A-CAA-CBA-CGA
3	NA	502	PMR	C2A-CAA-CBA-CGA
3	OA	502	PMR	C2A-CAA-CBA-CGA
3	A	502	PMR	C2A-CAA-CBA-CGA
3	B	502	PMR	C2A-CAA-CBA-CGA
3	C	502	PMR	C2A-CAA-CBA-CGA
3	D	502	PMR	C2A-CAA-CBA-CGA
3	E	502	PMR	C2A-CAA-CBA-CGA
3	F	502	PMR	C2A-CAA-CBA-CGA
3	G	502	PMR	C2A-CAA-CBA-CGA
3	I	502	PMR	C2A-CAA-CBA-CGA
3	J	502	PMR	C2A-CAA-CBA-CGA
3	M	502	PMR	C2A-CAA-CBA-CGA
3	N	502	PMR	C2A-CAA-CBA-CGA
3	Q	502	PMR	C2A-CAA-CBA-CGA
3	R	502	PMR	C2A-CAA-CBA-CGA
3	S	502	PMR	C2A-CAA-CBA-CGA
3	T	502	PMR	C2A-CAA-CBA-CGA
3	V	502	PMR	C2A-CAA-CBA-CGA
3	W	502	PMR	C2A-CAA-CBA-CGA
3	X	502	PMR	C2A-CAA-CBA-CGA
3	Y	502	PMR	C2A-CAA-CBA-CGA
3	Z	502	PMR	C2A-CAA-CBA-CGA
3	AA	502	PMR	C2A-CAA-CBA-CGA
3	BA	502	PMR	C2A-CAA-CBA-CGA
3	CA	502	PMR	C2A-CAA-CBA-CGA
3	DA	502	PMR	C2A-CAA-CBA-CGA
3	EA	502	PMR	C2A-CAA-CBA-CGA
3	FA	502	PMR	C2A-CAA-CBA-CGA
3	GA	502	PMR	C2A-CAA-CBA-CGA
3	HA	502	PMR	C2A-CAA-CBA-CGA
3	IA	502	PMR	C2A-CAA-CBA-CGA
3	KA	502	PMR	C2A-CAA-CBA-CGA
3	LA	502	PMR	C2A-CAA-CBA-CGA
2	A	501	NDP	PN-O3-PA-O5B
2	B	501	NDP	PN-O3-PA-O5B
2	C	501	NDP	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	D	501	NDP	PN-O3-PA-O5B
2	E	501	NDP	PN-O3-PA-O5B
2	F	501	NDP	PN-O3-PA-O5B
2	G	501	NDP	PN-O3-PA-O5B
2	H	501	NDP	PN-O3-PA-O5B
2	I	501	NDP	PN-O3-PA-O5B
2	J	501	NDP	PN-O3-PA-O5B
2	K	501	NDP	PN-O3-PA-O5B
2	L	501	NDP	PN-O3-PA-O5B
2	M	501	NDP	PN-O3-PA-O5B
2	N	501	NDP	PN-O3-PA-O5B
2	O	501	NDP	PN-O3-PA-O5B
2	P	501	NDP	PN-O3-PA-O5B
2	Q	501	NDP	PN-O3-PA-O5B
2	R	501	NDP	PN-O3-PA-O5B
2	S	501	NDP	PN-O3-PA-O5B
2	T	501	NDP	PN-O3-PA-O5B
2	V	501	NDP	PN-O3-PA-O5B
2	W	501	NDP	PN-O3-PA-O5B
2	X	501	NDP	PN-O3-PA-O5B
2	Y	501	NDP	PN-O3-PA-O5B
2	Z	501	NDP	PN-O3-PA-O5B
2	AA	501	NDP	PN-O3-PA-O5B
2	BA	501	NDP	PN-O3-PA-O5B
2	CA	501	NDP	PN-O3-PA-O5B
2	DA	501	NDP	PN-O3-PA-O5B
2	EA	501	NDP	PN-O3-PA-O5B
2	FA	501	NDP	PN-O3-PA-O5B
2	GA	501	NDP	PN-O3-PA-O5B
2	HA	501	NDP	PN-O3-PA-O5B
2	IA	501	NDP	PN-O3-PA-O5B
2	JA	501	NDP	PN-O3-PA-O5B
2	KA	501	NDP	PN-O3-PA-O5B
2	LA	501	NDP	PN-O3-PA-O5B
2	MA	501	NDP	PN-O3-PA-O5B
2	NA	501	NDP	PN-O3-PA-O5B
2	OA	501	NDP	PN-O3-PA-O5B
2	B	501	NDP	C3B-C2B-O2B-P2B
2	C	501	NDP	C3B-C2B-O2B-P2B
2	D	501	NDP	C3B-C2B-O2B-P2B
2	E	501	NDP	C3B-C2B-O2B-P2B
2	F	501	NDP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
2	G	501	NDP	C3B-C2B-O2B-P2B
2	H	501	NDP	C3B-C2B-O2B-P2B
2	I	501	NDP	C3B-C2B-O2B-P2B
2	J	501	NDP	C3B-C2B-O2B-P2B
2	K	501	NDP	C3B-C2B-O2B-P2B
2	L	501	NDP	C3B-C2B-O2B-P2B
2	M	501	NDP	C3B-C2B-O2B-P2B
2	N	501	NDP	C3B-C2B-O2B-P2B
2	O	501	NDP	C3B-C2B-O2B-P2B
2	P	501	NDP	C3B-C2B-O2B-P2B
2	Q	501	NDP	C3B-C2B-O2B-P2B
2	R	501	NDP	C3B-C2B-O2B-P2B
2	T	501	NDP	C3B-C2B-O2B-P2B
2	V	501	NDP	C3B-C2B-O2B-P2B
2	W	501	NDP	C3B-C2B-O2B-P2B
2	X	501	NDP	C3B-C2B-O2B-P2B
2	Y	501	NDP	C3B-C2B-O2B-P2B
2	Z	501	NDP	C3B-C2B-O2B-P2B
2	BA	501	NDP	C3B-C2B-O2B-P2B
2	CA	501	NDP	C3B-C2B-O2B-P2B
2	DA	501	NDP	C3B-C2B-O2B-P2B
2	EA	501	NDP	C3B-C2B-O2B-P2B
2	FA	501	NDP	C3B-C2B-O2B-P2B
2	HA	501	NDP	C3B-C2B-O2B-P2B
2	IA	501	NDP	C3B-C2B-O2B-P2B
2	JA	501	NDP	C3B-C2B-O2B-P2B
2	LA	501	NDP	C3B-C2B-O2B-P2B
2	MA	501	NDP	C3B-C2B-O2B-P2B
2	NA	501	NDP	C3B-C2B-O2B-P2B
2	OA	501	NDP	C3B-C2B-O2B-P2B
4	A	503	LMG	O1-C7-C8-C9
4	B	503	LMG	O1-C7-C8-C9
4	C	503	LMG	O1-C7-C8-C9
4	D	503	LMG	O1-C7-C8-C9
4	E	503	LMG	O1-C7-C8-C9
4	F	503	LMG	O1-C7-C8-C9
4	G	503	LMG	O1-C7-C8-C9
4	H	503	LMG	O1-C7-C8-C9
4	I	503	LMG	O1-C7-C8-C9
4	J	503	LMG	O1-C7-C8-C9
4	K	503	LMG	O1-C7-C8-C9
4	L	503	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	M	503	LMG	O1-C7-C8-C9
4	N	503	LMG	O1-C7-C8-C9
4	O	503	LMG	O1-C7-C8-C9
4	P	503	LMG	O1-C7-C8-C9
4	Q	503	LMG	O1-C7-C8-C9
4	R	503	LMG	O1-C7-C8-C9
4	S	503	LMG	O1-C7-C8-C9
4	T	503	LMG	O1-C7-C8-C9
4	V	503	LMG	O1-C7-C8-C9
4	W	503	LMG	O1-C7-C8-C9
4	X	503	LMG	O1-C7-C8-C9
4	Y	503	LMG	O1-C7-C8-C9
4	Z	503	LMG	O1-C7-C8-C9
4	AA	503	LMG	O1-C7-C8-C9
4	BA	503	LMG	O1-C7-C8-C9
4	CA	503	LMG	O1-C7-C8-C9
4	DA	503	LMG	O1-C7-C8-C9
4	EA	503	LMG	O1-C7-C8-C9
4	FA	503	LMG	O1-C7-C8-C9
4	GA	503	LMG	O1-C7-C8-C9
4	HA	503	LMG	O1-C7-C8-C9
4	IA	503	LMG	O1-C7-C8-C9
4	JA	503	LMG	O1-C7-C8-C9
4	KA	503	LMG	O1-C7-C8-C9
4	LA	503	LMG	O1-C7-C8-C9
4	MA	503	LMG	O1-C7-C8-C9
4	NA	503	LMG	O1-C7-C8-C9
4	OA	503	LMG	O1-C7-C8-C9
2	A	501	NDP	C3B-C2B-O2B-P2B
2	S	501	NDP	C3B-C2B-O2B-P2B
2	AA	501	NDP	C3B-C2B-O2B-P2B
2	GA	501	NDP	C3B-C2B-O2B-P2B
2	KA	501	NDP	C3B-C2B-O2B-P2B
4	A	503	LMG	O1-C7-C8-O7
4	B	503	LMG	O1-C7-C8-O7
4	C	503	LMG	O1-C7-C8-O7
4	D	503	LMG	O1-C7-C8-O7
4	E	503	LMG	O1-C7-C8-O7
4	F	503	LMG	O1-C7-C8-O7
4	G	503	LMG	O1-C7-C8-O7
4	H	503	LMG	O1-C7-C8-O7
4	I	503	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
4	J	503	LMG	O1-C7-C8-O7
4	K	503	LMG	O1-C7-C8-O7
4	L	503	LMG	O1-C7-C8-O7
4	M	503	LMG	O1-C7-C8-O7
4	N	503	LMG	O1-C7-C8-O7
4	O	503	LMG	O1-C7-C8-O7
4	P	503	LMG	O1-C7-C8-O7
4	Q	503	LMG	O1-C7-C8-O7
4	R	503	LMG	O1-C7-C8-O7
4	S	503	LMG	O1-C7-C8-O7
4	T	503	LMG	O1-C7-C8-O7
4	V	503	LMG	O1-C7-C8-O7
4	W	503	LMG	O1-C7-C8-O7
4	X	503	LMG	O1-C7-C8-O7
4	Y	503	LMG	O1-C7-C8-O7
4	Z	503	LMG	O1-C7-C8-O7
4	AA	503	LMG	O1-C7-C8-O7
4	BA	503	LMG	O1-C7-C8-O7
4	CA	503	LMG	O1-C7-C8-O7
4	DA	503	LMG	O1-C7-C8-O7
4	EA	503	LMG	O1-C7-C8-O7
4	FA	503	LMG	O1-C7-C8-O7
4	GA	503	LMG	O1-C7-C8-O7
4	HA	503	LMG	O1-C7-C8-O7
4	IA	503	LMG	O1-C7-C8-O7
4	JA	503	LMG	O1-C7-C8-O7
4	KA	503	LMG	O1-C7-C8-O7
4	LA	503	LMG	O1-C7-C8-O7
4	MA	503	LMG	O1-C7-C8-O7
4	NA	503	LMG	O1-C7-C8-O7
4	OA	503	LMG	O1-C7-C8-O7
2	A	501	NDP	PN-O3-PA-O1A
2	B	501	NDP	PN-O3-PA-O1A
2	C	501	NDP	PN-O3-PA-O1A
2	D	501	NDP	PN-O3-PA-O1A
2	E	501	NDP	PN-O3-PA-O1A
2	F	501	NDP	PN-O3-PA-O1A
2	G	501	NDP	PN-O3-PA-O1A
2	J	501	NDP	PN-O3-PA-O1A
2	K	501	NDP	PN-O3-PA-O1A
2	L	501	NDP	PN-O3-PA-O1A
2	N	501	NDP	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	O	501	NDP	PN-O3-PA-O1A
2	P	501	NDP	PN-O3-PA-O1A
2	Q	501	NDP	PN-O3-PA-O1A
2	R	501	NDP	PN-O3-PA-O1A
2	S	501	NDP	PN-O3-PA-O1A
2	T	501	NDP	PN-O3-PA-O1A
2	V	501	NDP	PN-O3-PA-O1A
2	W	501	NDP	PN-O3-PA-O1A
2	BA	501	NDP	PN-O3-PA-O1A
2	CA	501	NDP	PN-O3-PA-O1A
2	DA	501	NDP	PN-O3-PA-O1A
2	EA	501	NDP	PN-O3-PA-O1A
2	FA	501	NDP	PN-O3-PA-O1A
2	HA	501	NDP	PN-O3-PA-O1A
2	IA	501	NDP	PN-O3-PA-O1A
2	JA	501	NDP	PN-O3-PA-O1A
2	KA	501	NDP	PN-O3-PA-O1A
2	LA	501	NDP	PN-O3-PA-O1A
2	OA	501	NDP	PN-O3-PA-O1A
2	A	501	NDP	C2B-O2B-P2B-O1X
2	B	501	NDP	C2B-O2B-P2B-O1X
2	C	501	NDP	C2B-O2B-P2B-O1X
2	D	501	NDP	C2B-O2B-P2B-O1X
2	E	501	NDP	C2B-O2B-P2B-O1X
2	F	501	NDP	C2B-O2B-P2B-O1X
2	G	501	NDP	C2B-O2B-P2B-O1X
2	H	501	NDP	C2B-O2B-P2B-O1X
2	I	501	NDP	C2B-O2B-P2B-O1X
2	J	501	NDP	C2B-O2B-P2B-O1X
2	K	501	NDP	C2B-O2B-P2B-O1X
2	L	501	NDP	C2B-O2B-P2B-O1X
2	M	501	NDP	C2B-O2B-P2B-O1X
2	N	501	NDP	C2B-O2B-P2B-O1X
2	O	501	NDP	C2B-O2B-P2B-O1X
2	P	501	NDP	C2B-O2B-P2B-O1X
2	Q	501	NDP	C2B-O2B-P2B-O1X
2	R	501	NDP	C2B-O2B-P2B-O1X
2	S	501	NDP	C2B-O2B-P2B-O1X
2	T	501	NDP	C2B-O2B-P2B-O1X
2	V	501	NDP	C2B-O2B-P2B-O1X
2	W	501	NDP	C2B-O2B-P2B-O1X
2	X	501	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
2	Y	501	NDP	C2B-O2B-P2B-O1X
2	Z	501	NDP	C2B-O2B-P2B-O1X
2	AA	501	NDP	C2B-O2B-P2B-O1X
2	BA	501	NDP	C2B-O2B-P2B-O1X
2	CA	501	NDP	C2B-O2B-P2B-O1X
2	DA	501	NDP	C2B-O2B-P2B-O1X
2	EA	501	NDP	C2B-O2B-P2B-O1X
2	FA	501	NDP	C2B-O2B-P2B-O1X
2	GA	501	NDP	C2B-O2B-P2B-O1X
2	HA	501	NDP	C2B-O2B-P2B-O1X
2	IA	501	NDP	C2B-O2B-P2B-O1X
2	JA	501	NDP	C2B-O2B-P2B-O1X
2	KA	501	NDP	C2B-O2B-P2B-O1X
2	LA	501	NDP	C2B-O2B-P2B-O1X
2	MA	501	NDP	C2B-O2B-P2B-O1X
2	NA	501	NDP	C2B-O2B-P2B-O1X
2	OA	501	NDP	C2B-O2B-P2B-O1X
3	A	502	PMR	CAD-CBD-CGD-O2D
3	B	502	PMR	CAD-CBD-CGD-O2D
3	C	502	PMR	CAD-CBD-CGD-O2D
3	D	502	PMR	CAD-CBD-CGD-O2D
3	E	502	PMR	CAD-CBD-CGD-O2D
3	F	502	PMR	CAD-CBD-CGD-O2D
3	G	502	PMR	CAD-CBD-CGD-O2D
3	H	502	PMR	CAD-CBD-CGD-O2D
3	I	502	PMR	CAD-CBD-CGD-O2D
3	J	502	PMR	CAD-CBD-CGD-O2D
3	K	502	PMR	CAD-CBD-CGD-O2D
3	L	502	PMR	CAD-CBD-CGD-O2D
3	M	502	PMR	CAD-CBD-CGD-O2D
3	N	502	PMR	CAD-CBD-CGD-O2D
3	O	502	PMR	CAD-CBD-CGD-O2D
3	P	502	PMR	CAD-CBD-CGD-O2D
3	Q	502	PMR	CAD-CBD-CGD-O2D
3	R	502	PMR	CAD-CBD-CGD-O2D
3	S	502	PMR	CAD-CBD-CGD-O2D
3	T	502	PMR	CAD-CBD-CGD-O2D
3	V	502	PMR	CAD-CBD-CGD-O2D
3	W	502	PMR	CAD-CBD-CGD-O2D
3	X	502	PMR	CAD-CBD-CGD-O2D
3	Y	502	PMR	CAD-CBD-CGD-O2D
3	Z	502	PMR	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	AA	502	PMR	CAD-CBD-CGD-O2D
3	BA	502	PMR	CAD-CBD-CGD-O2D
3	CA	502	PMR	CAD-CBD-CGD-O2D
3	DA	502	PMR	CAD-CBD-CGD-O2D
3	EA	502	PMR	CAD-CBD-CGD-O2D
3	FA	502	PMR	CAD-CBD-CGD-O2D
3	GA	502	PMR	CAD-CBD-CGD-O2D
3	HA	502	PMR	CAD-CBD-CGD-O2D
3	IA	502	PMR	CAD-CBD-CGD-O2D
3	JA	502	PMR	CAD-CBD-CGD-O2D
3	KA	502	PMR	CAD-CBD-CGD-O2D
3	LA	502	PMR	CAD-CBD-CGD-O2D
3	MA	502	PMR	CAD-CBD-CGD-O2D
3	NA	502	PMR	CAD-CBD-CGD-O2D
3	OA	502	PMR	CAD-CBD-CGD-O2D
2	A	501	NDP	C5B-O5B-PA-O3
2	A	501	NDP	C2B-O2B-P2B-O2X
2	A	501	NDP	C2B-O2B-P2B-O3X
2	A	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C2B-O2B-P2B-O2X
2	B	501	NDP	C2B-O2B-P2B-O3X
2	B	501	NDP	C5D-O5D-PN-O3
2	C	501	NDP	C5B-O5B-PA-O3
2	C	501	NDP	C2B-O2B-P2B-O2X
2	C	501	NDP	C2B-O2B-P2B-O3X
2	C	501	NDP	C5D-O5D-PN-O3
2	D	501	NDP	C5B-O5B-PA-O3
2	D	501	NDP	C2B-O2B-P2B-O2X
2	D	501	NDP	C2B-O2B-P2B-O3X
2	D	501	NDP	C5D-O5D-PN-O3
2	E	501	NDP	C5B-O5B-PA-O3
2	E	501	NDP	C2B-O2B-P2B-O2X
2	E	501	NDP	C2B-O2B-P2B-O3X
2	E	501	NDP	C5D-O5D-PN-O3
2	F	501	NDP	C5B-O5B-PA-O3
2	F	501	NDP	C2B-O2B-P2B-O2X
2	F	501	NDP	C2B-O2B-P2B-O3X
2	F	501	NDP	C5D-O5D-PN-O3
2	G	501	NDP	C5B-O5B-PA-O3
2	G	501	NDP	C2B-O2B-P2B-O2X
2	G	501	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
2	G	501	NDP	C5D-O5D-PN-O3
2	H	501	NDP	C5B-O5B-PA-O3
2	H	501	NDP	C2B-O2B-P2B-O2X
2	H	501	NDP	C2B-O2B-P2B-O3X
2	H	501	NDP	C5D-O5D-PN-O3
2	I	501	NDP	C5B-O5B-PA-O3
2	I	501	NDP	C2B-O2B-P2B-O2X
2	I	501	NDP	C2B-O2B-P2B-O3X
2	I	501	NDP	C5D-O5D-PN-O3
2	J	501	NDP	C5B-O5B-PA-O3
2	J	501	NDP	C2B-O2B-P2B-O2X
2	J	501	NDP	C2B-O2B-P2B-O3X
2	J	501	NDP	C5D-O5D-PN-O3
2	K	501	NDP	C5B-O5B-PA-O3
2	K	501	NDP	C2B-O2B-P2B-O2X
2	K	501	NDP	C2B-O2B-P2B-O3X
2	K	501	NDP	C5D-O5D-PN-O3
2	L	501	NDP	C5B-O5B-PA-O3
2	L	501	NDP	C2B-O2B-P2B-O2X
2	L	501	NDP	C2B-O2B-P2B-O3X
2	L	501	NDP	C5D-O5D-PN-O3
2	M	501	NDP	C5B-O5B-PA-O3
2	M	501	NDP	C2B-O2B-P2B-O2X
2	M	501	NDP	C2B-O2B-P2B-O3X
2	M	501	NDP	C5D-O5D-PN-O3
2	N	501	NDP	C5B-O5B-PA-O3
2	N	501	NDP	C2B-O2B-P2B-O2X
2	N	501	NDP	C2B-O2B-P2B-O3X
2	N	501	NDP	C5D-O5D-PN-O3
2	O	501	NDP	C5B-O5B-PA-O3
2	O	501	NDP	C2B-O2B-P2B-O2X
2	O	501	NDP	C2B-O2B-P2B-O3X
2	O	501	NDP	C5D-O5D-PN-O3
2	P	501	NDP	C5B-O5B-PA-O3
2	P	501	NDP	C2B-O2B-P2B-O2X
2	P	501	NDP	C2B-O2B-P2B-O3X
2	P	501	NDP	C5D-O5D-PN-O3
2	Q	501	NDP	C5B-O5B-PA-O3
2	Q	501	NDP	C2B-O2B-P2B-O2X
2	Q	501	NDP	C2B-O2B-P2B-O3X
2	Q	501	NDP	C5D-O5D-PN-O3
2	R	501	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	R	501	NDP	C2B-O2B-P2B-O2X
2	R	501	NDP	C2B-O2B-P2B-O3X
2	R	501	NDP	C5D-O5D-PN-O3
2	S	501	NDP	C5B-O5B-PA-O3
2	S	501	NDP	C2B-O2B-P2B-O2X
2	S	501	NDP	C2B-O2B-P2B-O3X
2	S	501	NDP	C5D-O5D-PN-O3
2	T	501	NDP	C5B-O5B-PA-O3
2	T	501	NDP	C2B-O2B-P2B-O2X
2	T	501	NDP	C2B-O2B-P2B-O3X
2	T	501	NDP	C5D-O5D-PN-O3
2	V	501	NDP	C5B-O5B-PA-O3
2	V	501	NDP	C2B-O2B-P2B-O2X
2	V	501	NDP	C2B-O2B-P2B-O3X
2	V	501	NDP	C5D-O5D-PN-O3
2	W	501	NDP	C5B-O5B-PA-O3
2	W	501	NDP	C2B-O2B-P2B-O2X
2	W	501	NDP	C2B-O2B-P2B-O3X
2	W	501	NDP	C5D-O5D-PN-O3
2	X	501	NDP	C5B-O5B-PA-O3
2	X	501	NDP	C2B-O2B-P2B-O2X
2	X	501	NDP	C2B-O2B-P2B-O3X
2	X	501	NDP	C5D-O5D-PN-O3
2	Y	501	NDP	C5B-O5B-PA-O3
2	Y	501	NDP	C2B-O2B-P2B-O2X
2	Y	501	NDP	C2B-O2B-P2B-O3X
2	Y	501	NDP	C5D-O5D-PN-O3
2	Z	501	NDP	C5B-O5B-PA-O3
2	Z	501	NDP	C2B-O2B-P2B-O2X
2	Z	501	NDP	C2B-O2B-P2B-O3X
2	Z	501	NDP	C5D-O5D-PN-O3
2	AA	501	NDP	C5B-O5B-PA-O3
2	AA	501	NDP	C2B-O2B-P2B-O2X
2	AA	501	NDP	C2B-O2B-P2B-O3X
2	AA	501	NDP	C5D-O5D-PN-O3
2	BA	501	NDP	C5B-O5B-PA-O3
2	BA	501	NDP	C2B-O2B-P2B-O2X
2	BA	501	NDP	C2B-O2B-P2B-O3X
2	BA	501	NDP	C5D-O5D-PN-O3
2	CA	501	NDP	C5B-O5B-PA-O3
2	CA	501	NDP	C2B-O2B-P2B-O2X
2	CA	501	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
2	CA	501	NDP	C5D-O5D-PN-O3
2	DA	501	NDP	C5B-O5B-PA-O3
2	DA	501	NDP	C2B-O2B-P2B-O2X
2	DA	501	NDP	C2B-O2B-P2B-O3X
2	DA	501	NDP	C5D-O5D-PN-O3
2	EA	501	NDP	C5B-O5B-PA-O3
2	EA	501	NDP	C2B-O2B-P2B-O2X
2	EA	501	NDP	C2B-O2B-P2B-O3X
2	EA	501	NDP	C5D-O5D-PN-O3
2	FA	501	NDP	C5B-O5B-PA-O3
2	FA	501	NDP	C2B-O2B-P2B-O2X
2	FA	501	NDP	C2B-O2B-P2B-O3X
2	FA	501	NDP	C5D-O5D-PN-O3
2	GA	501	NDP	C5B-O5B-PA-O3
2	GA	501	NDP	C2B-O2B-P2B-O2X
2	GA	501	NDP	C2B-O2B-P2B-O3X
2	GA	501	NDP	C5D-O5D-PN-O3
2	HA	501	NDP	C5B-O5B-PA-O3
2	HA	501	NDP	C2B-O2B-P2B-O2X
2	HA	501	NDP	C2B-O2B-P2B-O3X
2	HA	501	NDP	C5D-O5D-PN-O3
2	IA	501	NDP	C5B-O5B-PA-O3
2	IA	501	NDP	C2B-O2B-P2B-O2X
2	IA	501	NDP	C2B-O2B-P2B-O3X
2	IA	501	NDP	C5D-O5D-PN-O3
2	JA	501	NDP	C5B-O5B-PA-O3
2	JA	501	NDP	C2B-O2B-P2B-O2X
2	JA	501	NDP	C2B-O2B-P2B-O3X
2	JA	501	NDP	C5D-O5D-PN-O3
2	KA	501	NDP	C5B-O5B-PA-O3
2	KA	501	NDP	C2B-O2B-P2B-O2X
2	KA	501	NDP	C2B-O2B-P2B-O3X
2	KA	501	NDP	C5D-O5D-PN-O3
2	LA	501	NDP	C5B-O5B-PA-O3
2	LA	501	NDP	C2B-O2B-P2B-O2X
2	LA	501	NDP	C2B-O2B-P2B-O3X
2	LA	501	NDP	C5D-O5D-PN-O3
2	MA	501	NDP	C5B-O5B-PA-O3
2	MA	501	NDP	C2B-O2B-P2B-O2X
2	MA	501	NDP	C2B-O2B-P2B-O3X
2	MA	501	NDP	C5D-O5D-PN-O3
2	NA	501	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	NA	501	NDP	C2B-O2B-P2B-O2X
2	NA	501	NDP	C2B-O2B-P2B-O3X
2	NA	501	NDP	C5D-O5D-PN-O3
2	OA	501	NDP	C5B-O5B-PA-O3
2	OA	501	NDP	C2B-O2B-P2B-O2X
2	OA	501	NDP	C2B-O2B-P2B-O3X
2	OA	501	NDP	C5D-O5D-PN-O3
2	A	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	O4B-C4B-C5B-O5B
2	C	501	NDP	O4B-C4B-C5B-O5B
2	D	501	NDP	O4B-C4B-C5B-O5B
2	E	501	NDP	O4B-C4B-C5B-O5B
2	F	501	NDP	O4B-C4B-C5B-O5B
2	G	501	NDP	O4B-C4B-C5B-O5B
2	H	501	NDP	O4B-C4B-C5B-O5B
2	I	501	NDP	O4B-C4B-C5B-O5B
2	J	501	NDP	O4B-C4B-C5B-O5B
2	K	501	NDP	O4B-C4B-C5B-O5B
2	L	501	NDP	O4B-C4B-C5B-O5B
2	M	501	NDP	O4B-C4B-C5B-O5B
2	N	501	NDP	O4B-C4B-C5B-O5B
2	O	501	NDP	O4B-C4B-C5B-O5B
2	P	501	NDP	O4B-C4B-C5B-O5B
2	Q	501	NDP	O4B-C4B-C5B-O5B
2	R	501	NDP	O4B-C4B-C5B-O5B
2	S	501	NDP	O4B-C4B-C5B-O5B
2	T	501	NDP	O4B-C4B-C5B-O5B
2	V	501	NDP	O4B-C4B-C5B-O5B
2	W	501	NDP	O4B-C4B-C5B-O5B
2	X	501	NDP	O4B-C4B-C5B-O5B
2	Y	501	NDP	O4B-C4B-C5B-O5B
2	Z	501	NDP	O4B-C4B-C5B-O5B
2	AA	501	NDP	O4B-C4B-C5B-O5B
2	BA	501	NDP	O4B-C4B-C5B-O5B
2	CA	501	NDP	O4B-C4B-C5B-O5B
2	DA	501	NDP	O4B-C4B-C5B-O5B
2	EA	501	NDP	O4B-C4B-C5B-O5B
2	FA	501	NDP	O4B-C4B-C5B-O5B
2	GA	501	NDP	O4B-C4B-C5B-O5B
2	HA	501	NDP	O4B-C4B-C5B-O5B
2	IA	501	NDP	O4B-C4B-C5B-O5B
2	JA	501	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	KA	501	NDP	O4B-C4B-C5B-O5B
2	LA	501	NDP	O4B-C4B-C5B-O5B
2	MA	501	NDP	O4B-C4B-C5B-O5B
2	NA	501	NDP	O4B-C4B-C5B-O5B
2	OA	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	PN-O3-PA-O2A
2	B	501	NDP	PN-O3-PA-O2A
2	C	501	NDP	PN-O3-PA-O2A
2	D	501	NDP	PN-O3-PA-O2A
2	E	501	NDP	PN-O3-PA-O2A
2	F	501	NDP	PN-O3-PA-O2A
2	G	501	NDP	PN-O3-PA-O2A
2	H	501	NDP	PN-O3-PA-O1A
2	H	501	NDP	PN-O3-PA-O2A
2	I	501	NDP	PN-O3-PA-O1A
2	I	501	NDP	PN-O3-PA-O2A
2	J	501	NDP	PN-O3-PA-O2A
2	K	501	NDP	PN-O3-PA-O2A
2	L	501	NDP	PN-O3-PA-O2A
2	M	501	NDP	PN-O3-PA-O1A
2	M	501	NDP	PN-O3-PA-O2A
2	N	501	NDP	PN-O3-PA-O2A
2	O	501	NDP	PN-O3-PA-O2A
2	P	501	NDP	PN-O3-PA-O2A
2	Q	501	NDP	PN-O3-PA-O2A
2	R	501	NDP	PN-O3-PA-O2A
2	S	501	NDP	PN-O3-PA-O2A
2	T	501	NDP	PN-O3-PA-O2A
2	V	501	NDP	PN-O3-PA-O2A
2	W	501	NDP	PN-O3-PA-O2A
2	X	501	NDP	PN-O3-PA-O1A
2	X	501	NDP	PN-O3-PA-O2A
2	Y	501	NDP	PN-O3-PA-O1A
2	Y	501	NDP	PN-O3-PA-O2A
2	Z	501	NDP	PN-O3-PA-O1A
2	Z	501	NDP	PN-O3-PA-O2A
2	AA	501	NDP	PN-O3-PA-O1A
2	AA	501	NDP	PN-O3-PA-O2A
2	BA	501	NDP	PN-O3-PA-O2A
2	CA	501	NDP	PN-O3-PA-O2A
2	DA	501	NDP	PN-O3-PA-O2A
2	EA	501	NDP	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	FA	501	NDP	PN-O3-PA-O2A
2	GA	501	NDP	PN-O3-PA-O1A
2	GA	501	NDP	PN-O3-PA-O2A
2	HA	501	NDP	PN-O3-PA-O2A
2	IA	501	NDP	PN-O3-PA-O2A
2	JA	501	NDP	PN-O3-PA-O2A
2	KA	501	NDP	PN-O3-PA-O2A
2	LA	501	NDP	PN-O3-PA-O2A
2	MA	501	NDP	PN-O3-PA-O1A
2	MA	501	NDP	PN-O3-PA-O2A
2	NA	501	NDP	PN-O3-PA-O1A
2	NA	501	NDP	PN-O3-PA-O2A
2	OA	501	NDP	PN-O3-PA-O2A

There are no ring outliers.

111 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	HA	501	NDP	1	0
4	HA	503	LMG	1	0
4	NA	503	LMG	1	0
4	X	503	LMG	1	0
2	B	501	NDP	1	0
4	Y	503	LMG	1	0
2	D	501	NDP	1	0
2	P	501	NDP	1	0
4	IA	503	LMG	1	0
3	O	502	PMR	4	0
4	Z	503	LMG	1	0
3	F	502	PMR	4	0
3	NA	502	PMR	4	0
4	GA	503	LMG	1	0
2	FA	501	NDP	1	0
2	H	501	NDP	1	0
4	H	503	LMG	1	0
3	J	502	PMR	4	0
3	E	502	PMR	4	0
3	IA	502	PMR	4	0
3	W	502	PMR	4	0
4	D	503	LMG	1	0
3	JA	502	PMR	4	0
4	L	503	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	502	PMR	4	0
4	FA	503	LMG	1	0
2	A	501	NDP	2	0
3	R	502	PMR	4	0
2	KA	501	NDP	1	0
2	X	501	NDP	1	0
4	LA	503	LMG	1	0
3	Z	502	PMR	4	0
3	S	502	PMR	4	0
4	V	503	LMG	1	0
3	I	502	PMR	4	0
3	DA	502	PMR	4	0
3	P	502	PMR	4	0
2	E	501	NDP	1	0
4	K	503	LMG	1	0
4	KA	503	LMG	1	0
4	M	503	LMG	1	0
3	Y	502	PMR	4	0
4	E	503	LMG	1	0
2	Z	501	NDP	1	0
4	OA	503	LMG	1	0
4	G	503	LMG	1	0
4	B	503	LMG	1	0
2	DA	501	NDP	1	0
4	N	503	LMG	1	0
3	OA	502	PMR	4	0
3	FA	502	PMR	4	0
4	C	503	LMG	1	0
3	A	502	PMR	4	0
3	B	502	PMR	4	0
2	V	501	NDP	1	0
3	X	502	PMR	4	0
3	N	502	PMR	4	0
2	C	501	NDP	2	0
2	EA	501	NDP	1	0
4	EA	503	LMG	1	0
3	H	502	PMR	4	0
2	G	501	NDP	1	0
3	T	502	PMR	4	0
2	T	501	NDP	1	0
3	KA	502	PMR	4	0
4	JA	503	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	501	NDP	2	0
4	R	503	LMG	1	0
2	OA	501	NDP	2	0
4	T	503	LMG	1	0
3	G	502	PMR	4	0
3	D	502	PMR	4	0
3	L	502	PMR	4	0
3	Q	502	PMR	4	0
3	EA	502	PMR	4	0
3	AA	502	PMR	4	0
4	F	503	LMG	1	0
4	A	503	LMG	1	0
2	NA	501	NDP	1	0
3	BA	502	PMR	4	0
2	CA	501	NDP	1	0
4	CA	503	LMG	1	0
3	V	502	PMR	4	0
2	F	501	NDP	1	0
2	BA	501	NDP	1	0
2	IA	501	NDP	1	0
3	M	502	PMR	4	0
4	MA	503	LMG	1	0
2	L	501	NDP	1	0
2	AA	501	NDP	1	0
3	C	502	PMR	4	0
4	AA	503	LMG	1	0
2	S	501	NDP	2	0
4	W	503	LMG	1	0
3	LA	502	PMR	4	0
3	CA	502	PMR	4	0
4	Q	503	LMG	1	0
2	J	501	NDP	1	0
3	MA	502	PMR	4	0
4	J	503	LMG	1	0
4	S	503	LMG	1	0
3	HA	502	PMR	4	0
2	M	501	NDP	1	0
2	W	501	NDP	1	0
4	BA	503	LMG	1	0
2	Q	501	NDP	1	0
4	I	503	LMG	1	0
3	GA	502	PMR	4	0

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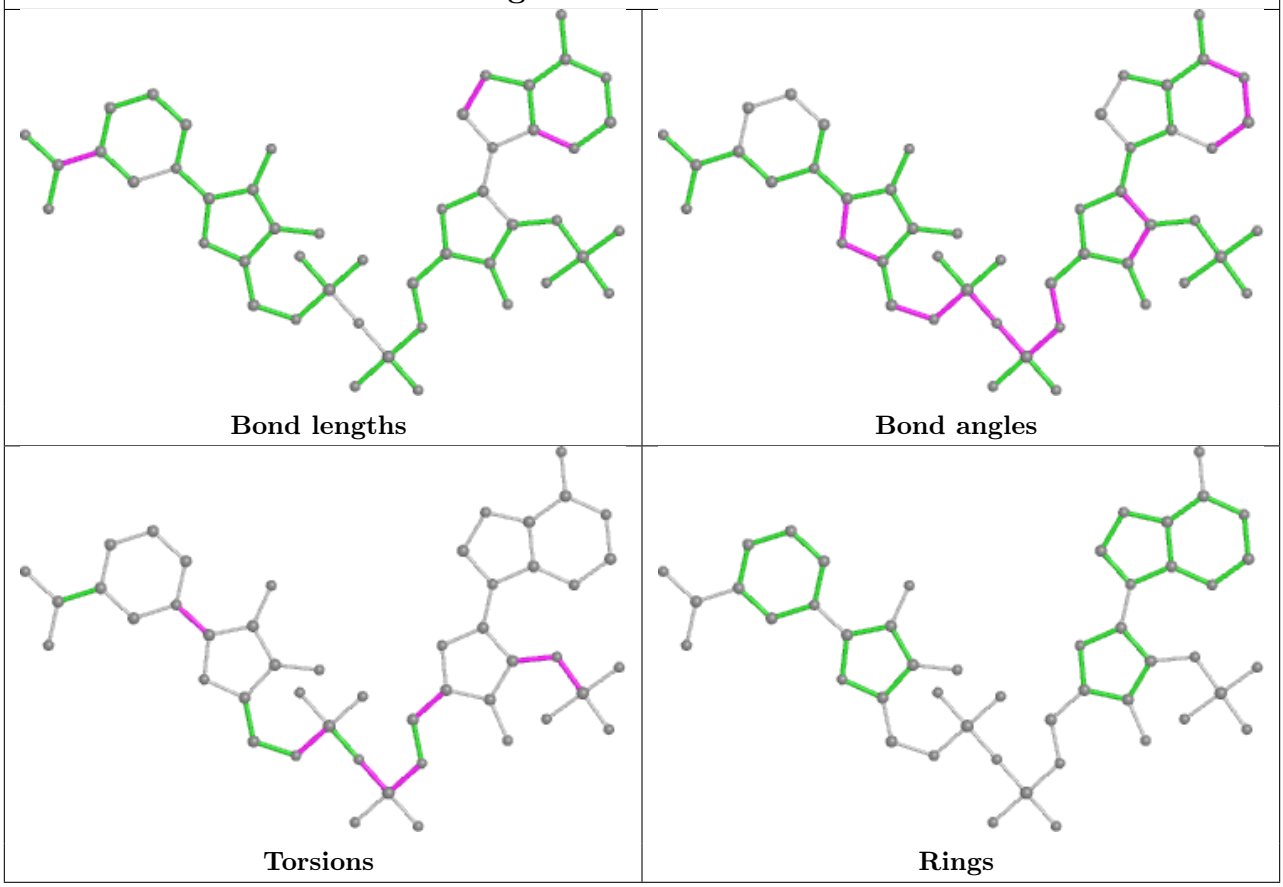
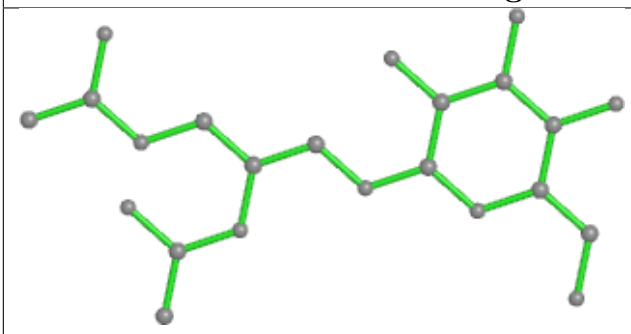
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	503	LMG	1	0
4	DA	503	LMG	1	0
4	P	503	LMG	1	0

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.

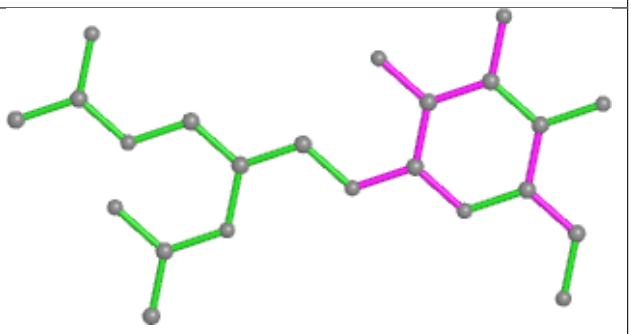
Ligand NDP HA 501



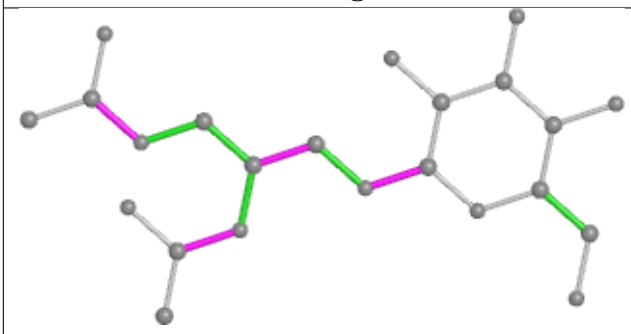
Ligand LMG HA 503



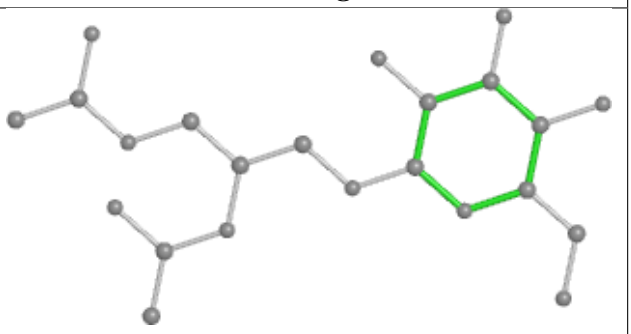
Bond lengths



Bond angles

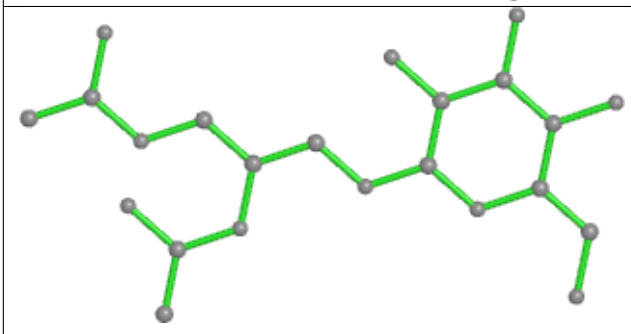


Torsions

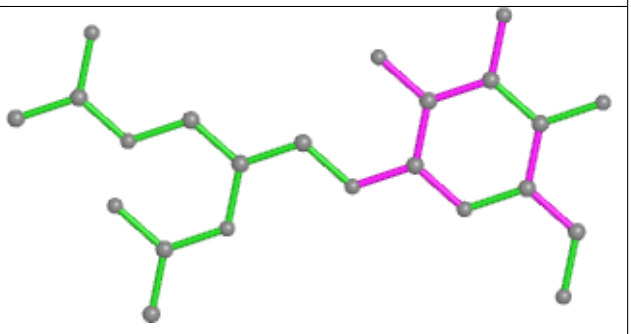


Rings

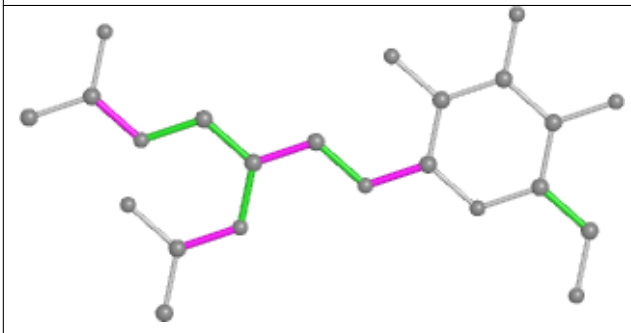
Ligand LMG NA 503



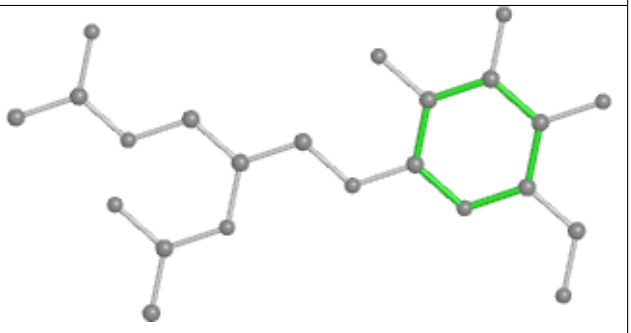
Bond lengths



Bond angles

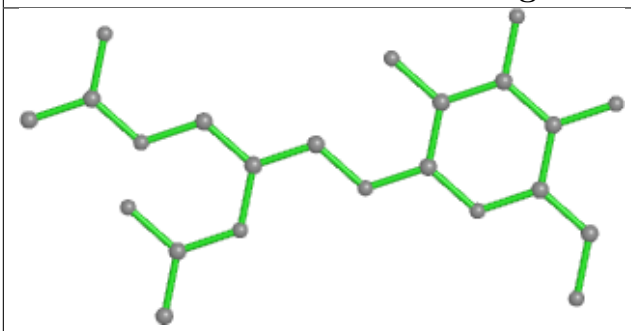


Torsions

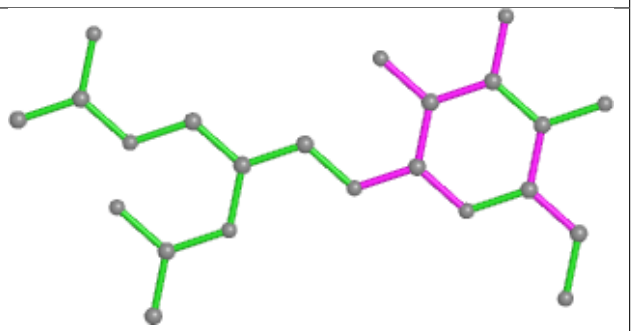


Rings

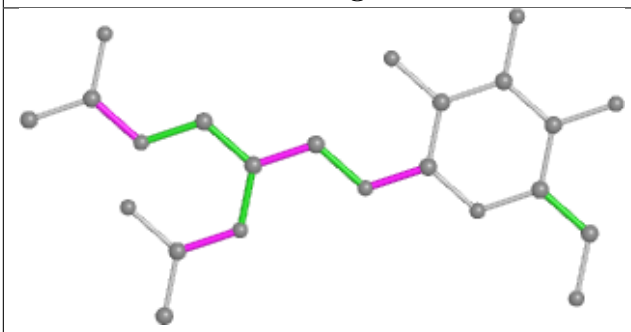
Ligand LMG X 503



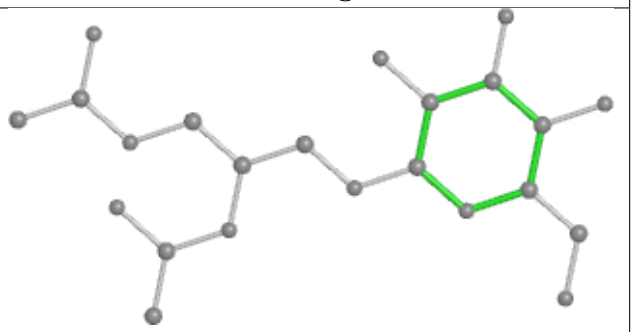
Bond lengths



Bond angles

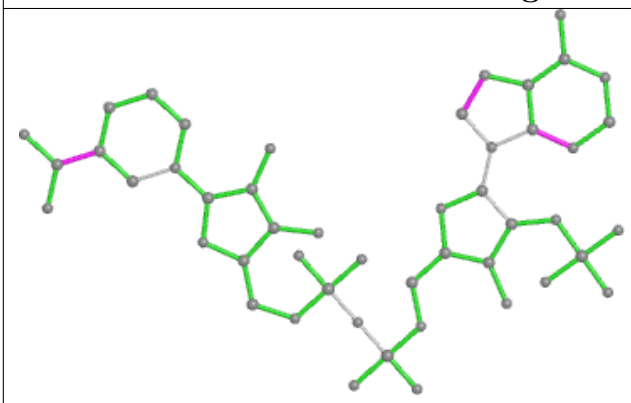


Torsions

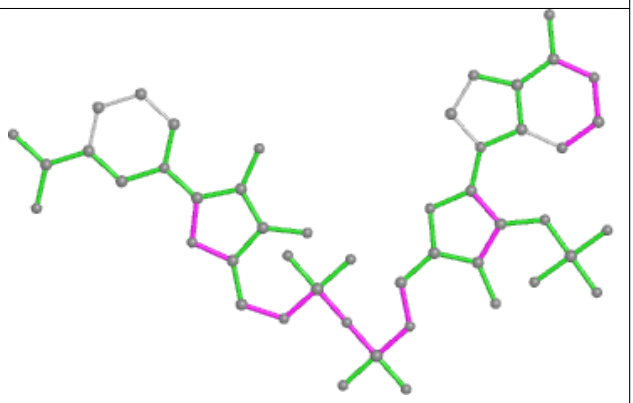


Rings

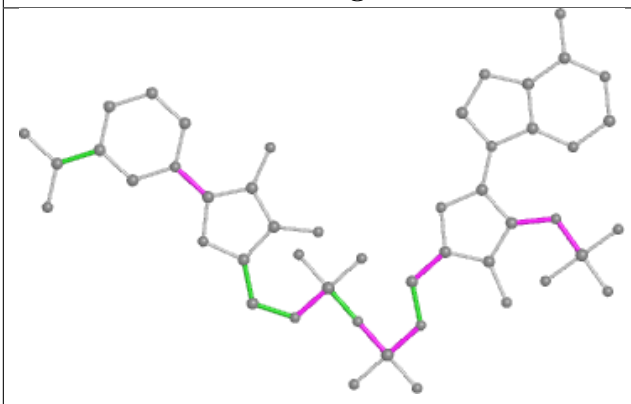
Ligand NDP B 501



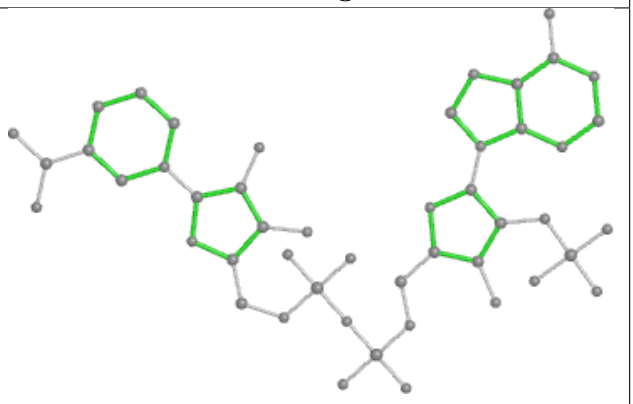
Bond lengths



Bond angles

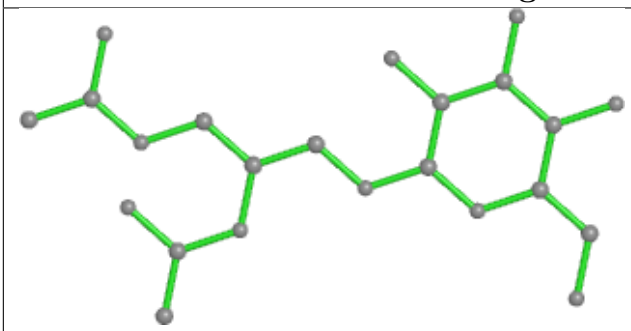


Torsions

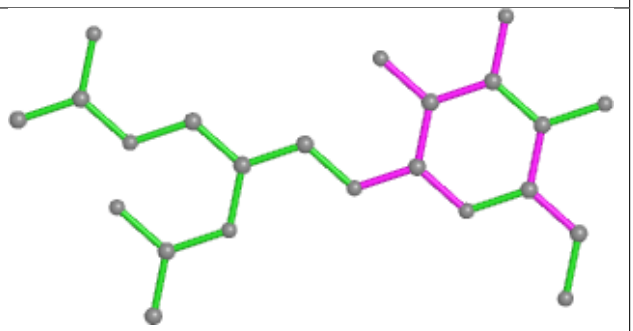


Rings

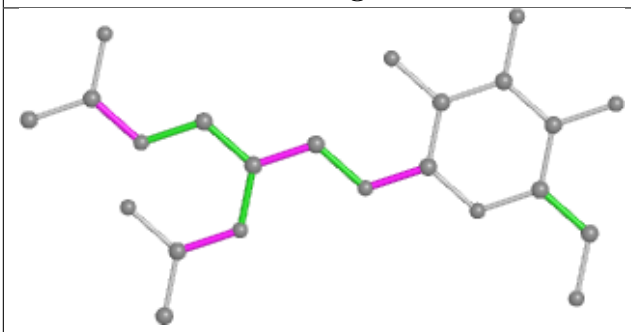
Ligand LMG Y 503



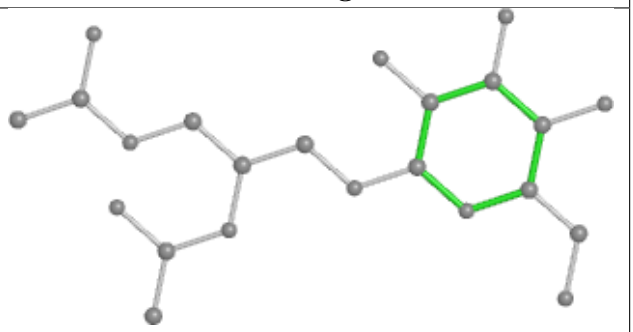
Bond lengths



Bond angles

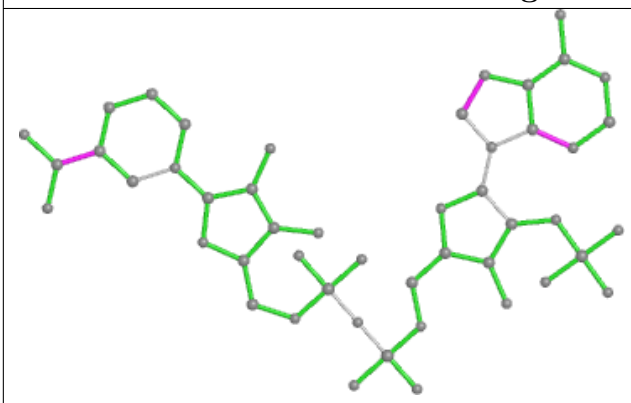


Torsions

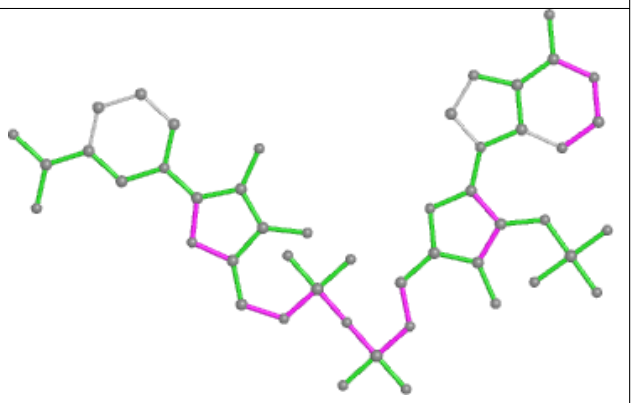


Rings

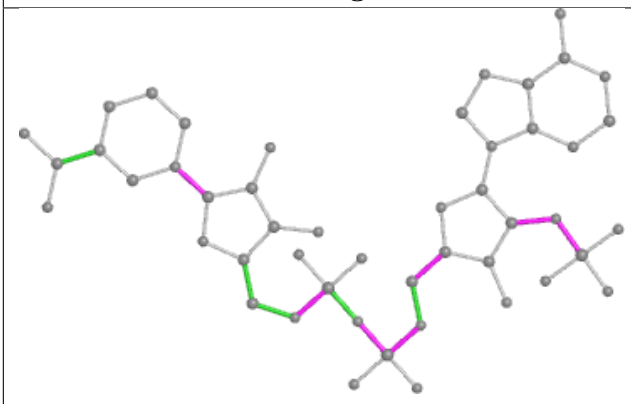
Ligand NDP D 501



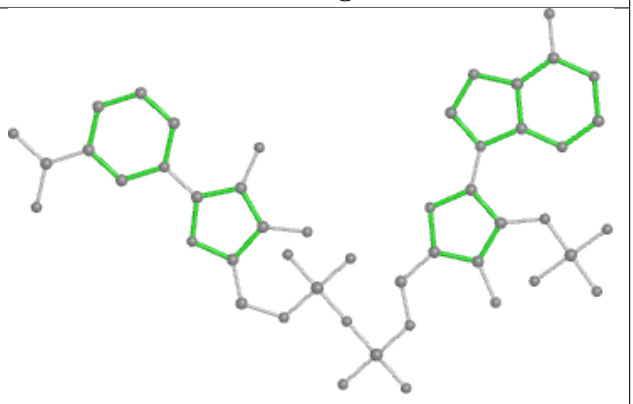
Bond lengths



Bond angles

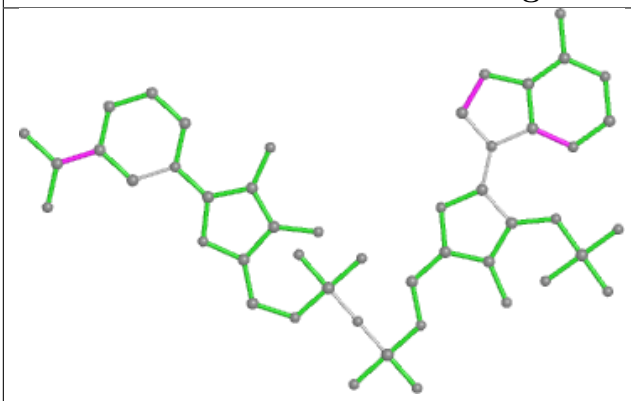


Torsions

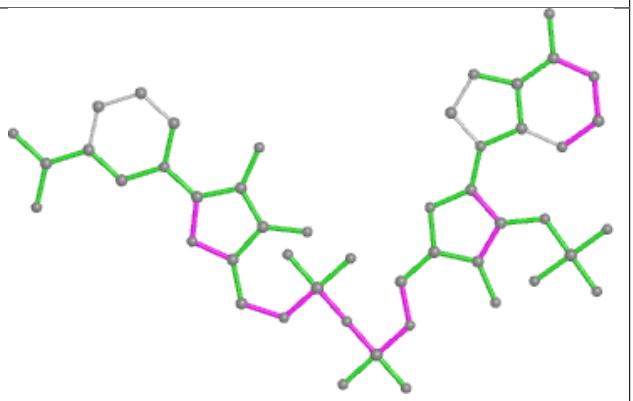


Rings

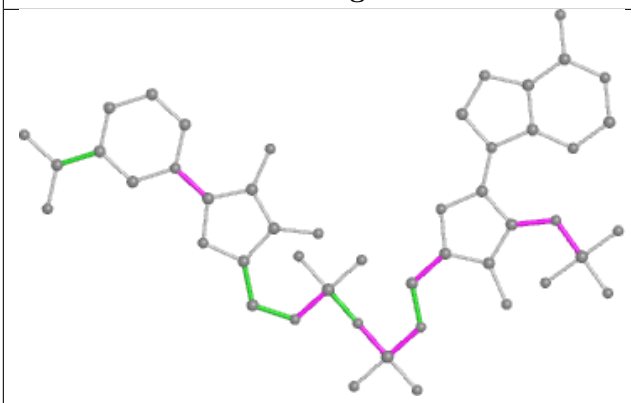
Ligand NDP P 501



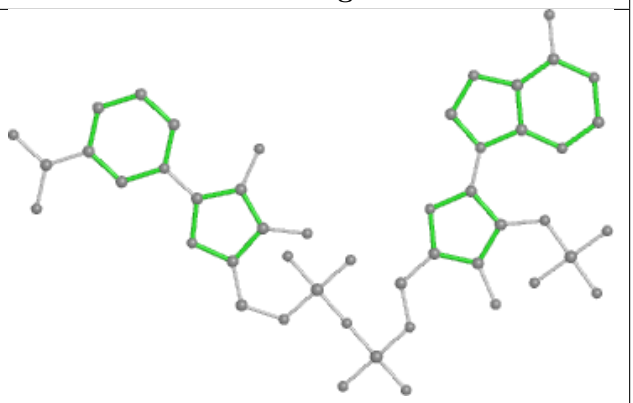
Bond lengths



Bond angles

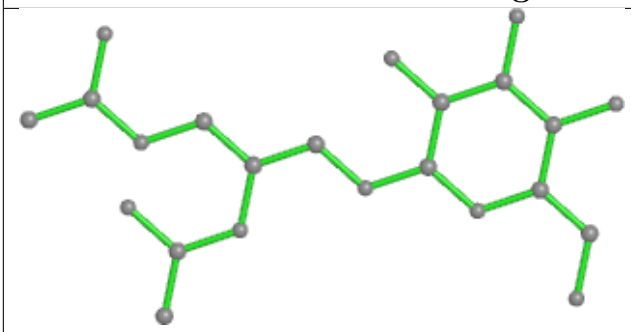


Torsions



Rings

Ligand LMG IA 503



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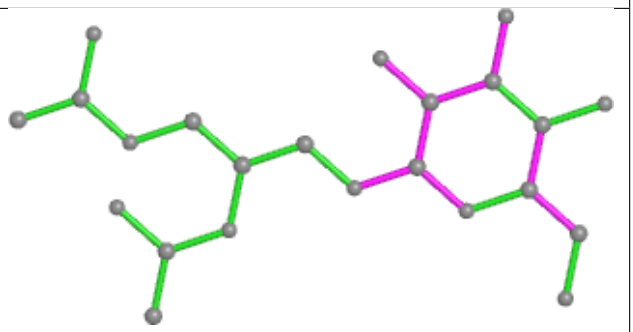

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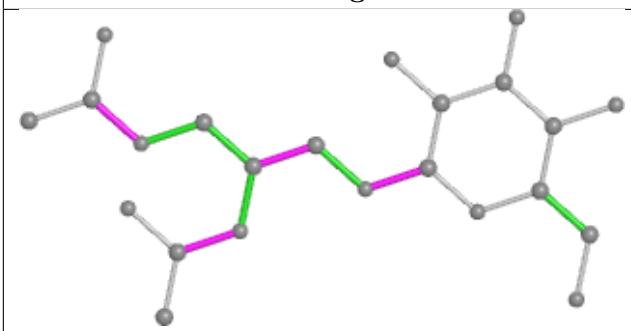

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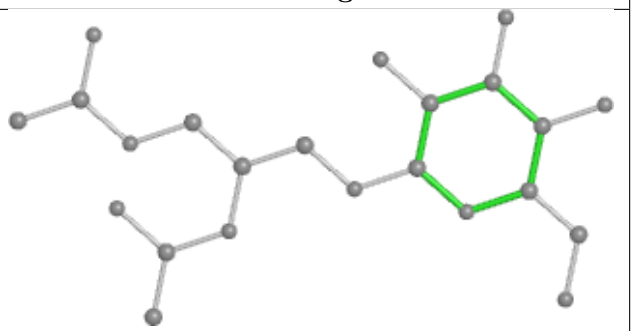
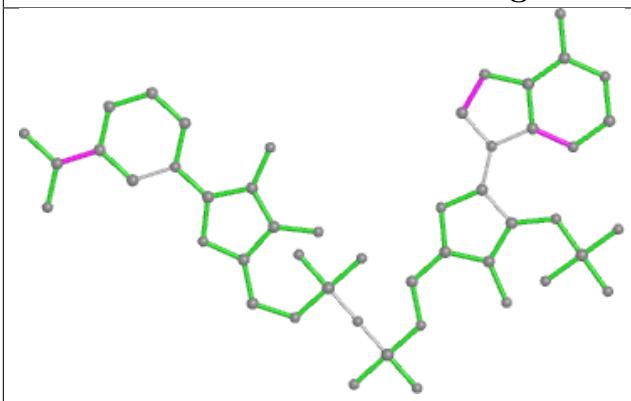


Rings

Ligand NDP LA 501



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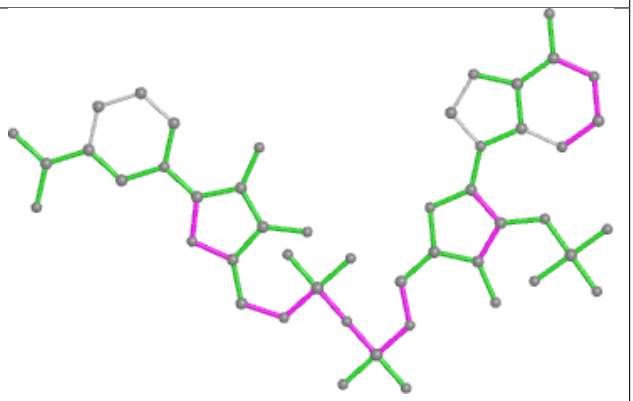

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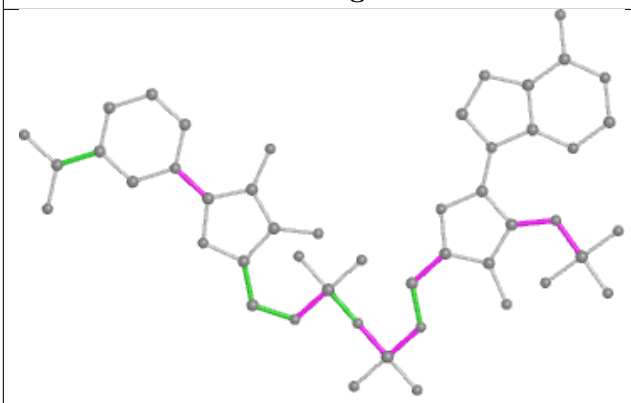

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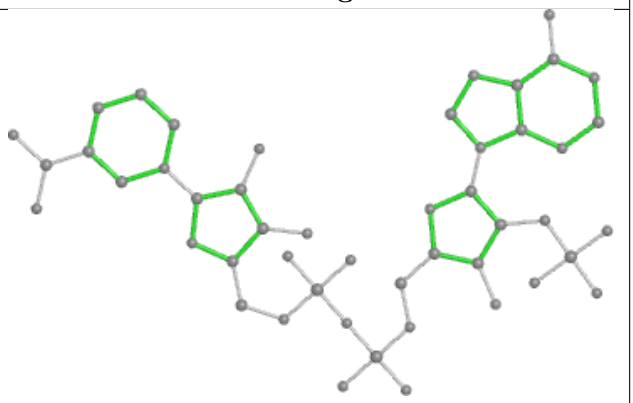

Rings

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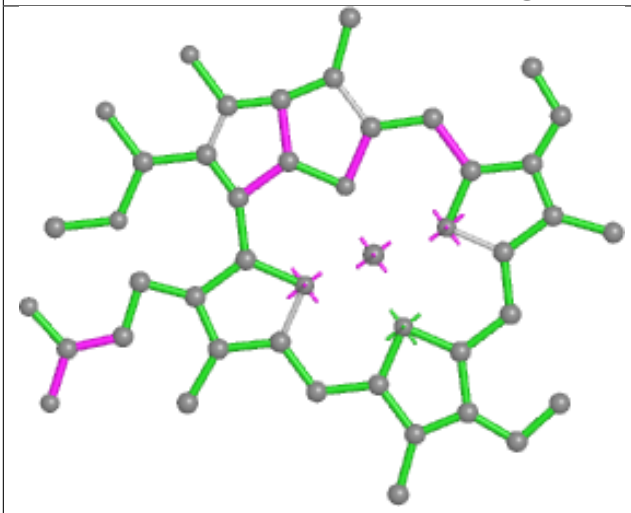

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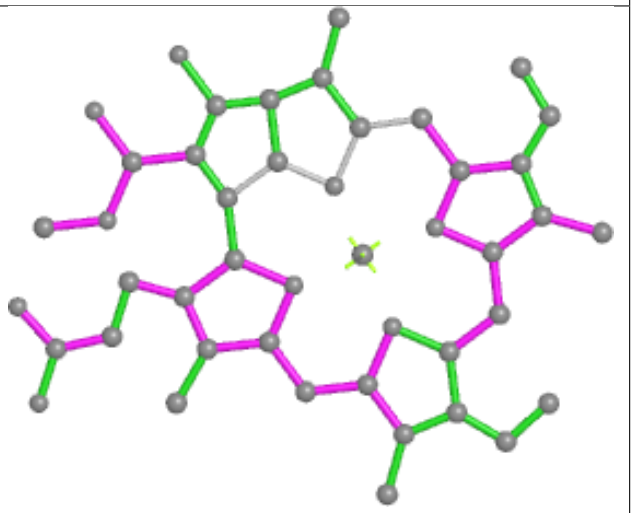

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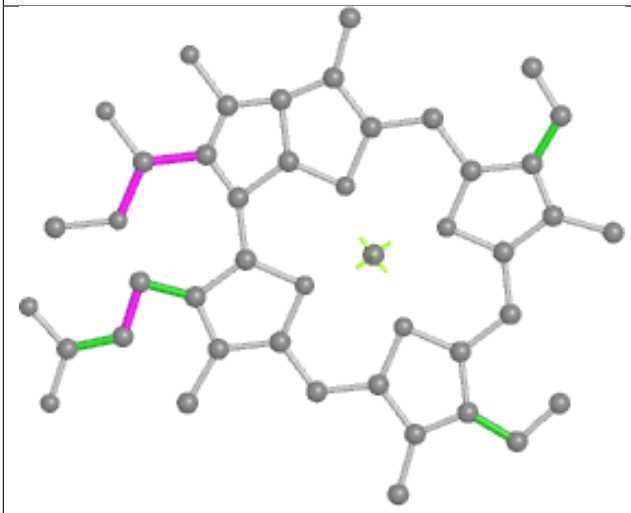

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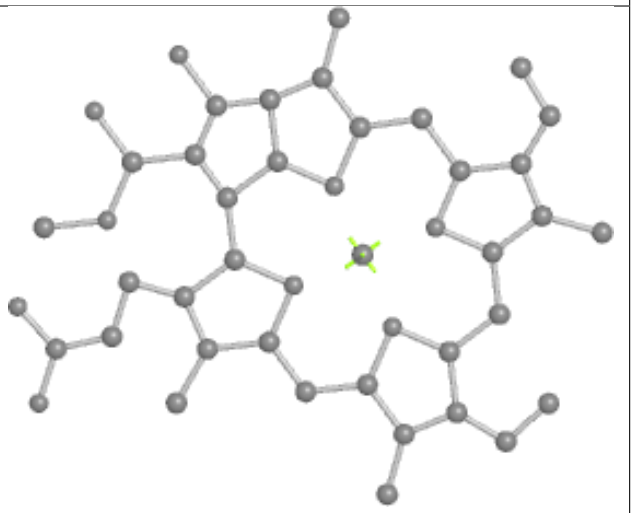
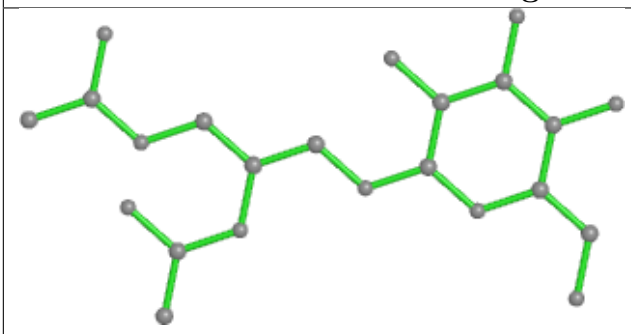


Rings

Ligand LMG Z 503



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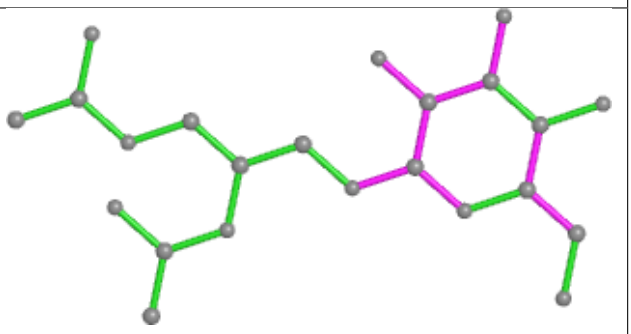

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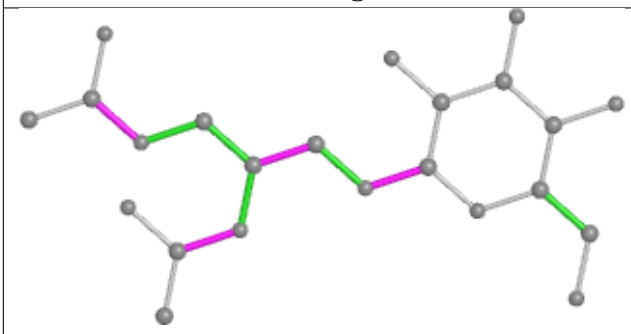

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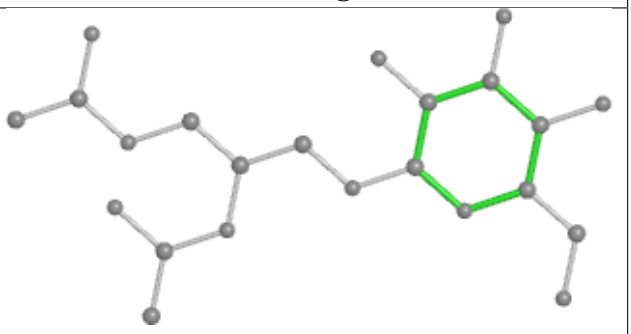

Rings

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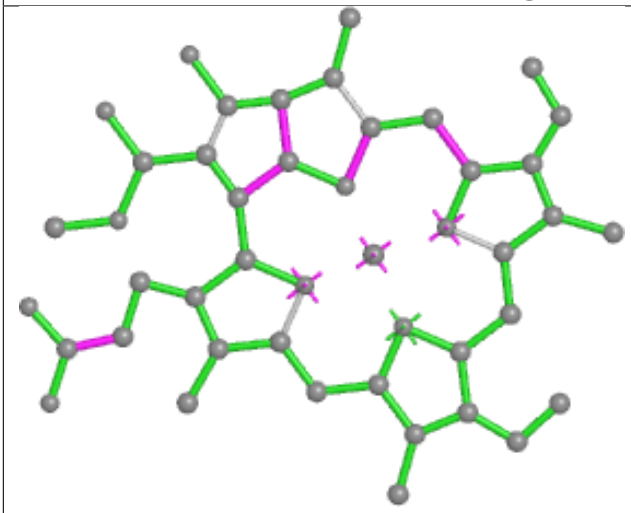

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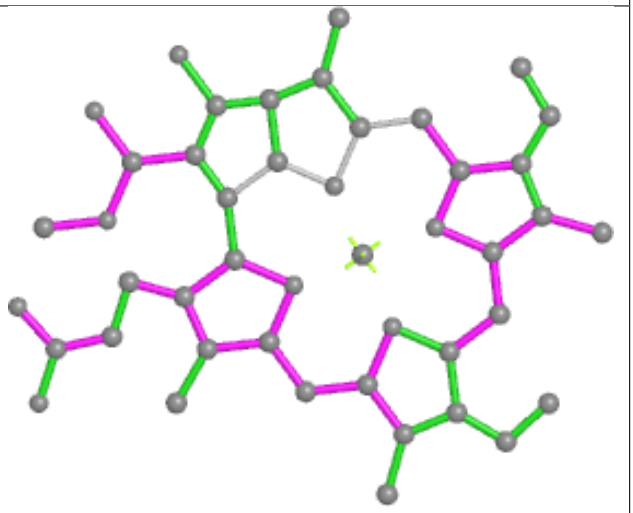

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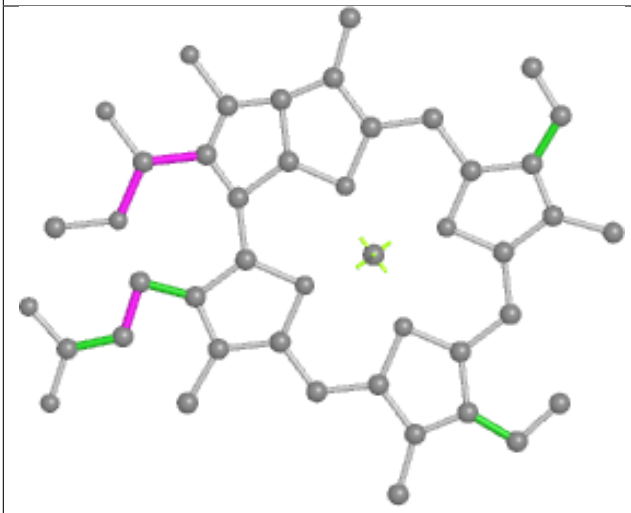

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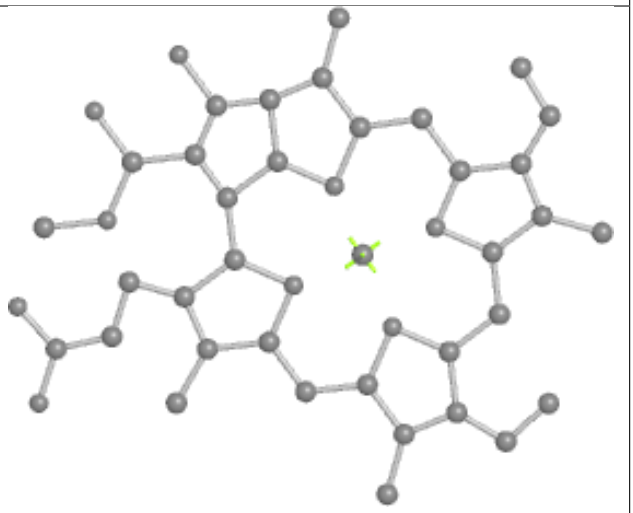
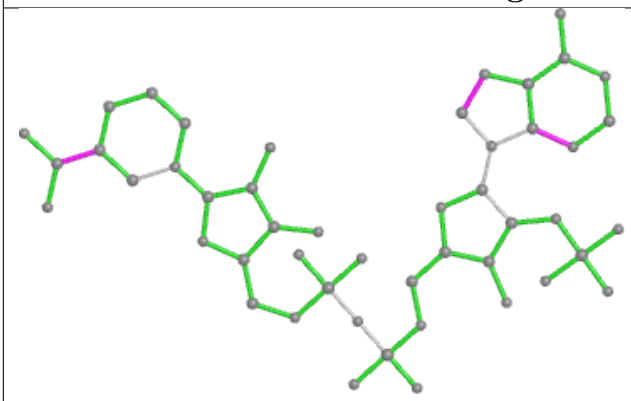


Rings

Ligand NDP GA 501



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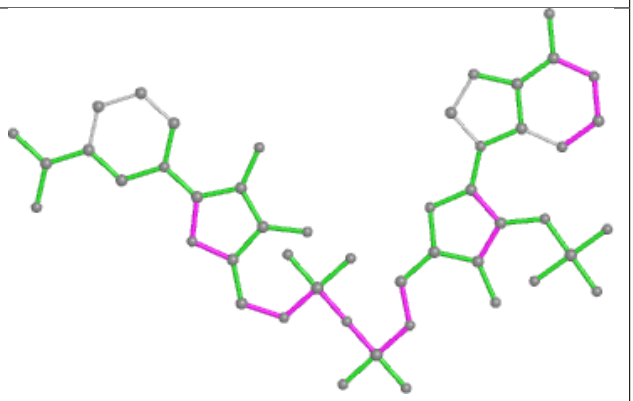

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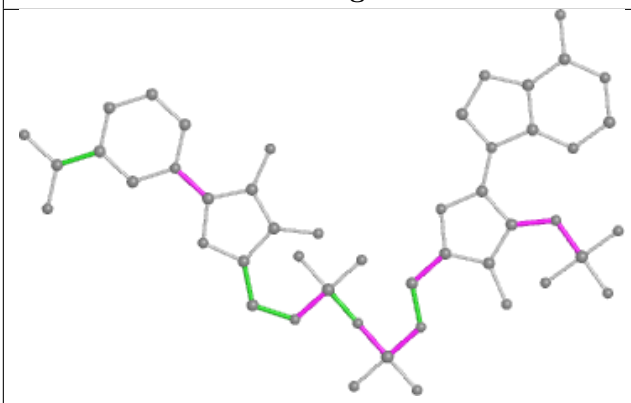

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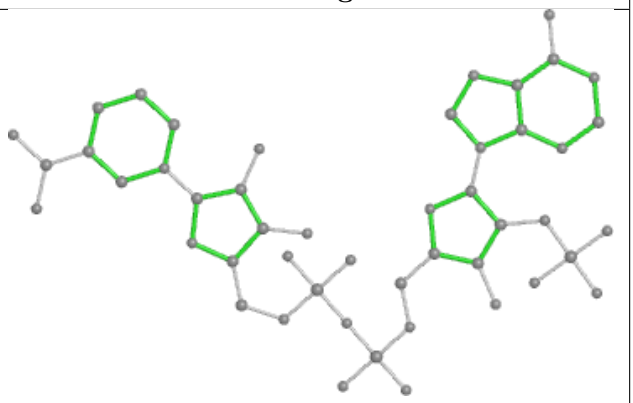

Rings

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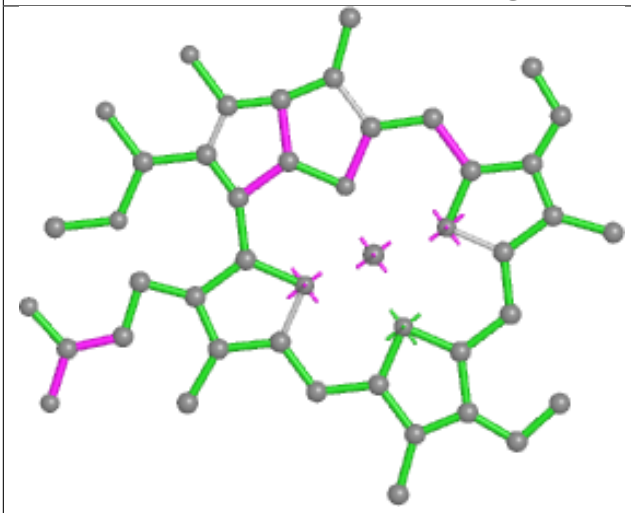

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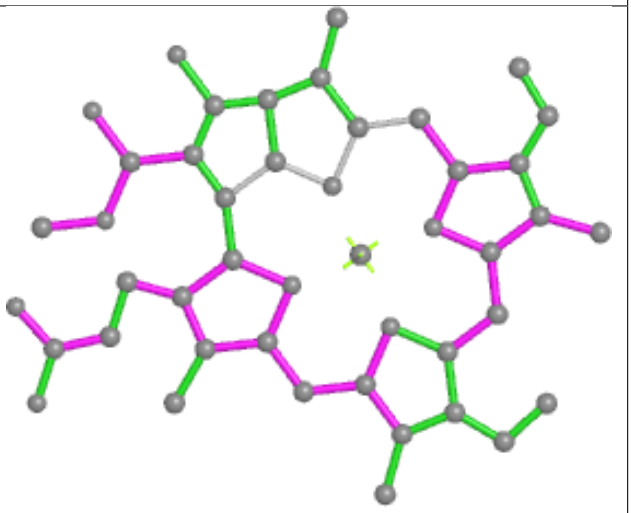

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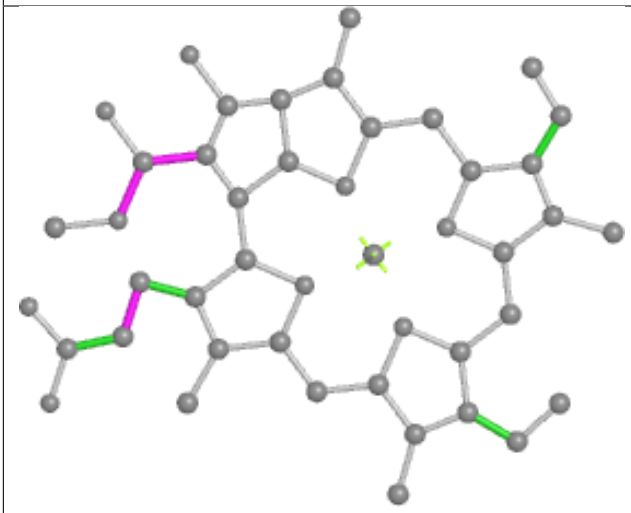

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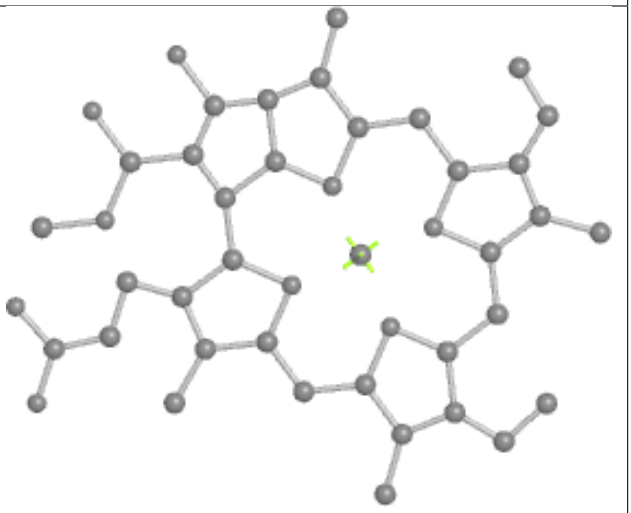
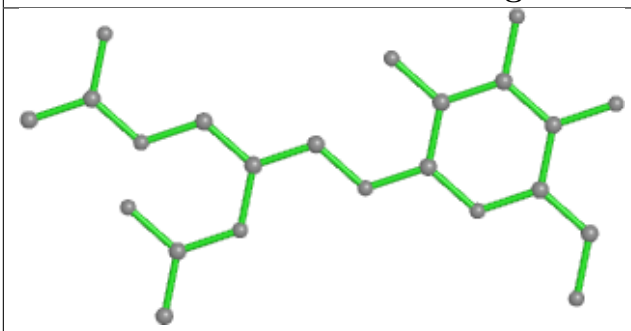


Rings

Ligand LMG GA 503



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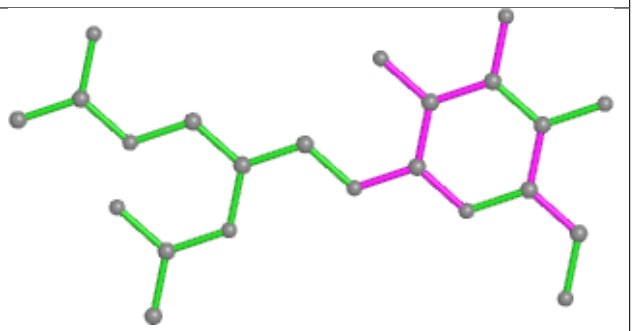

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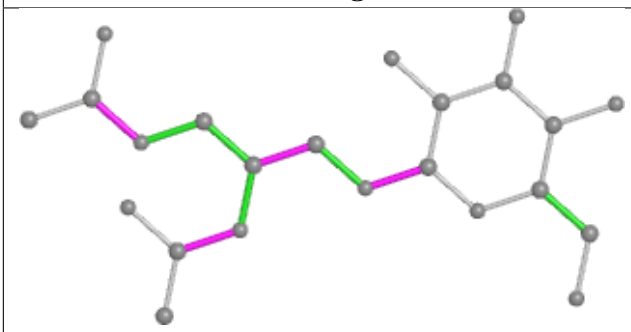

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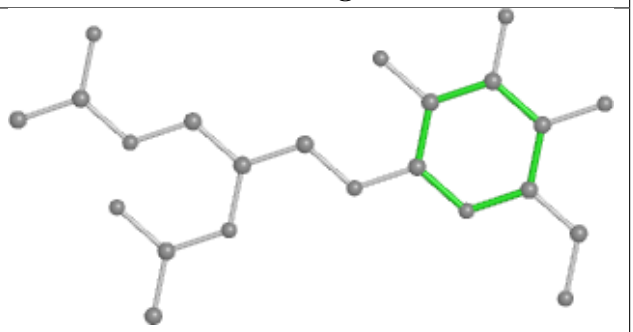
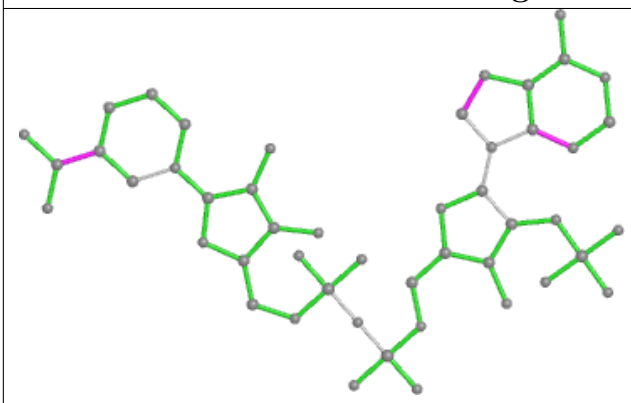


Rings

Ligand NDP FA 501



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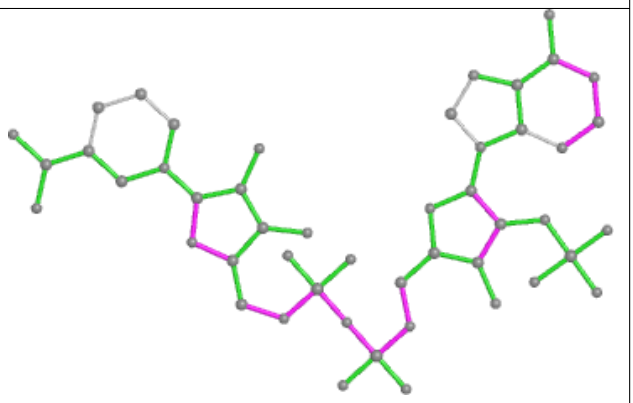

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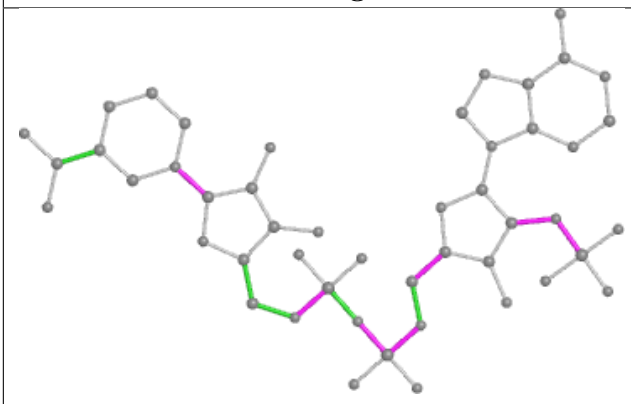

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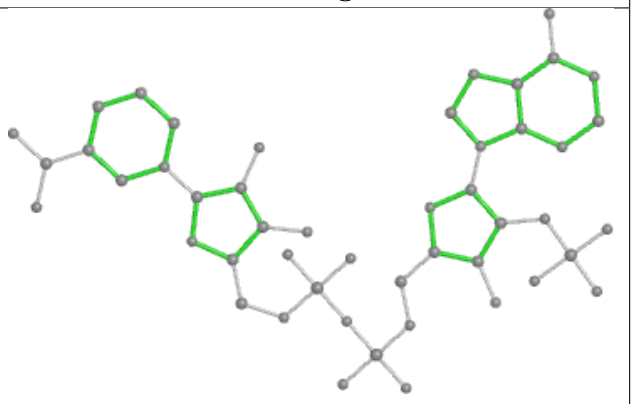

Rings

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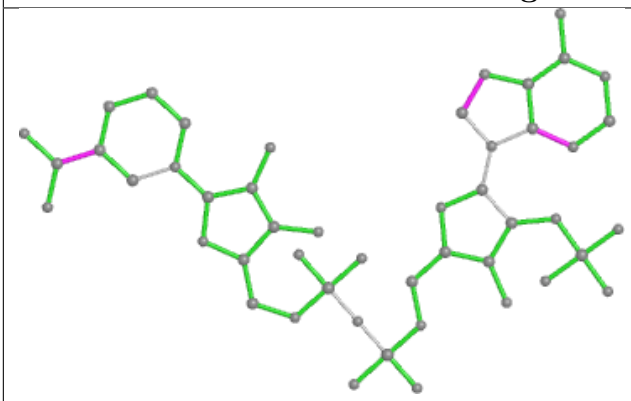

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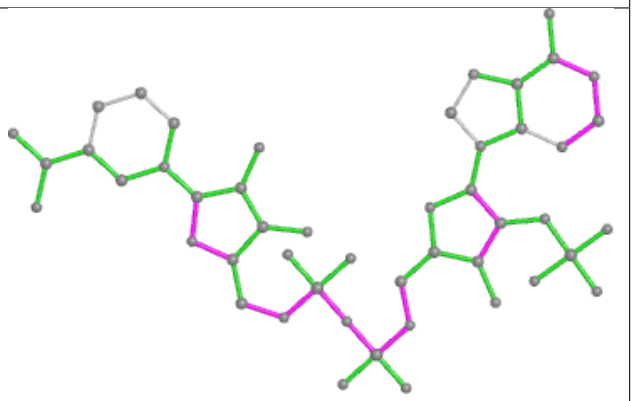

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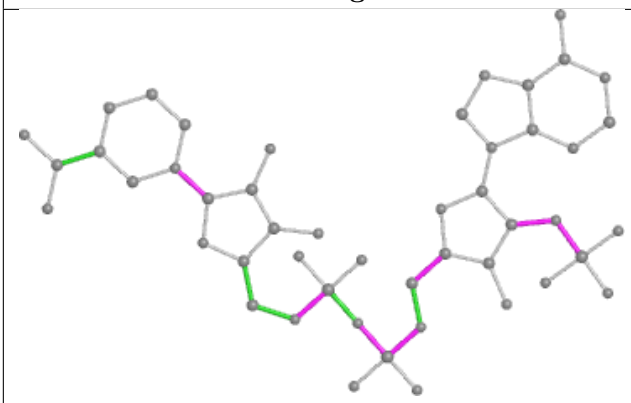

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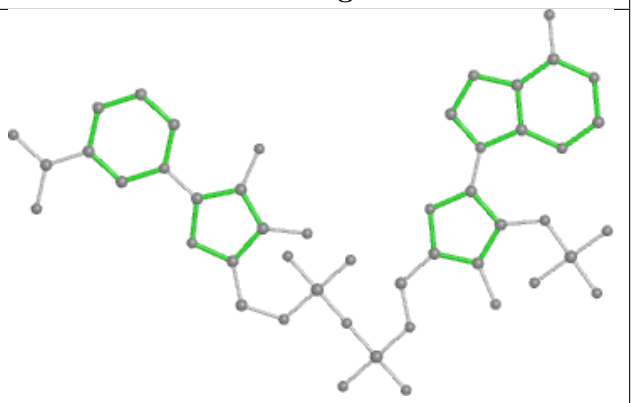
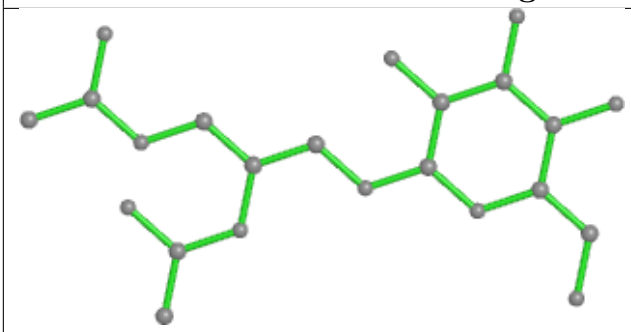


Rings

Ligand LMG H 503



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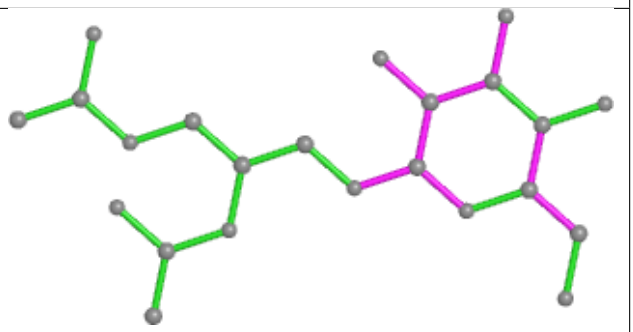

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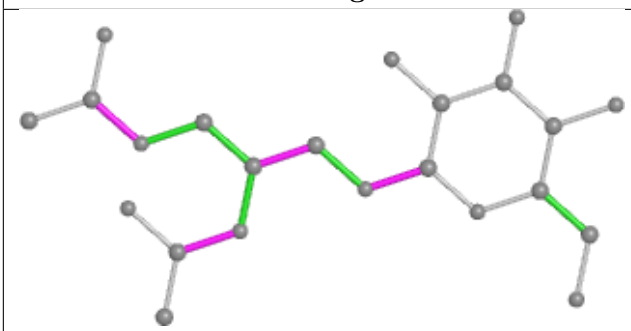

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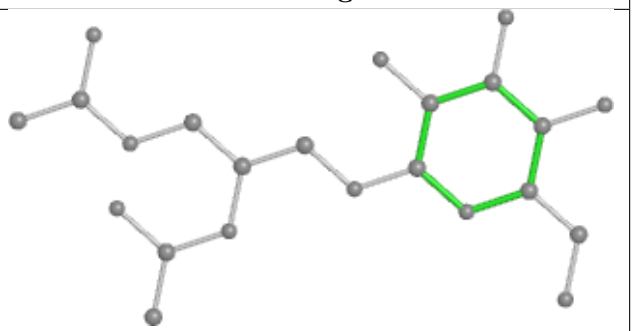
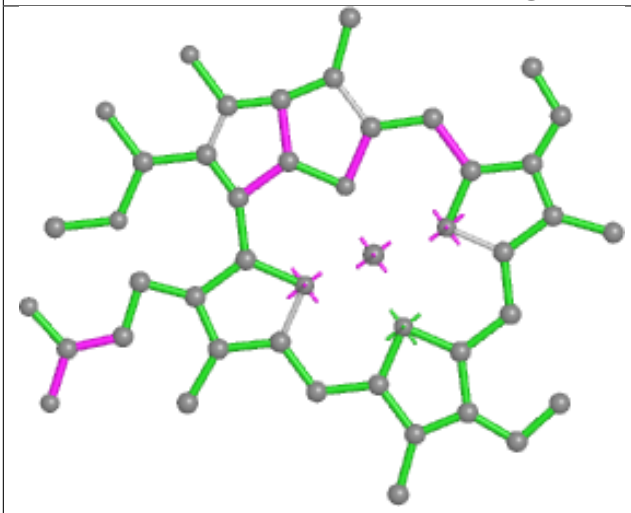


Rings

Ligand PMR J 502



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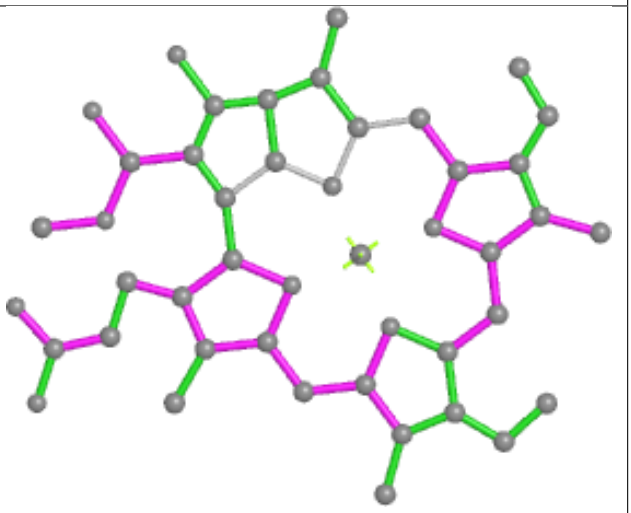

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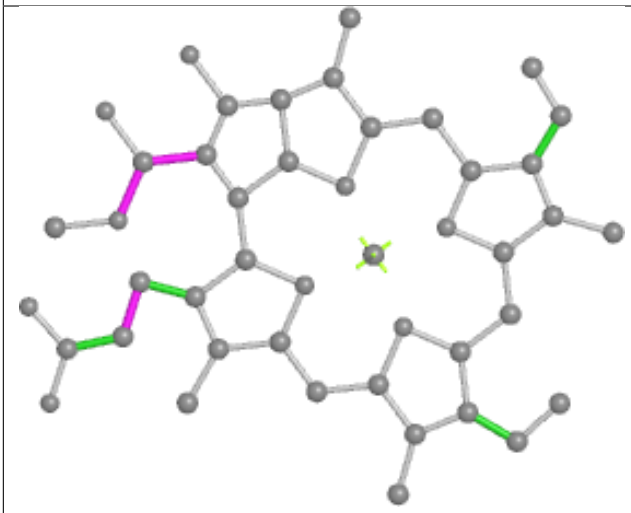

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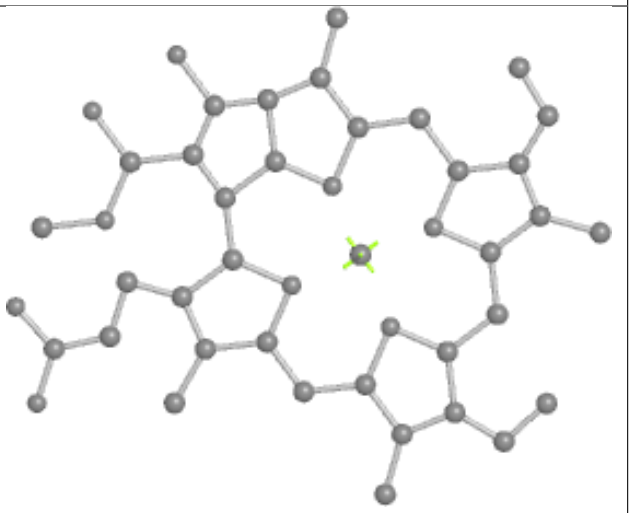
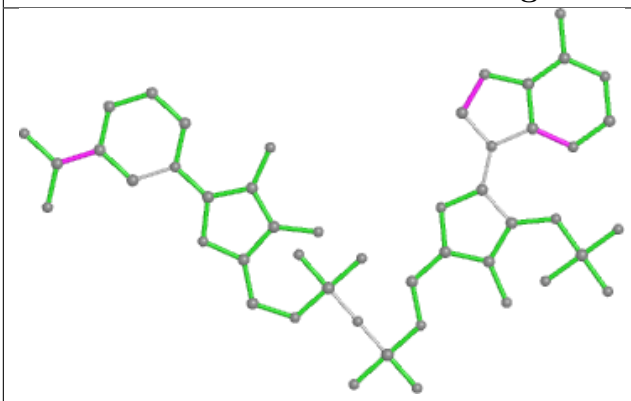


Rings

Ligand NDP N 501



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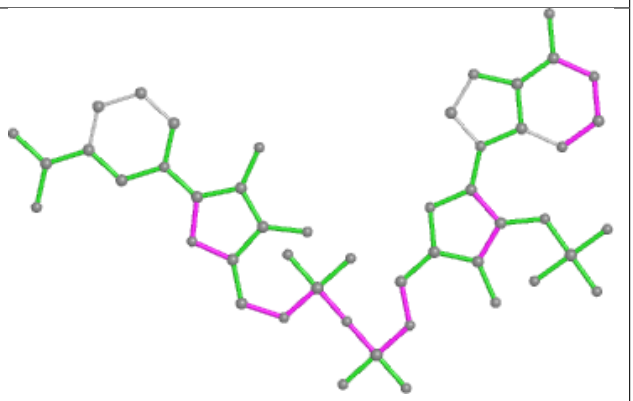
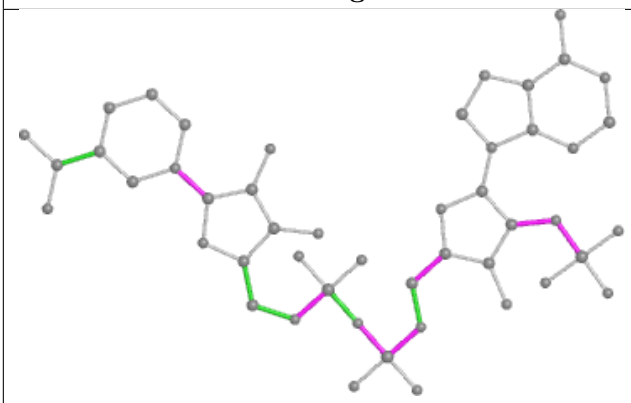


Bond angles



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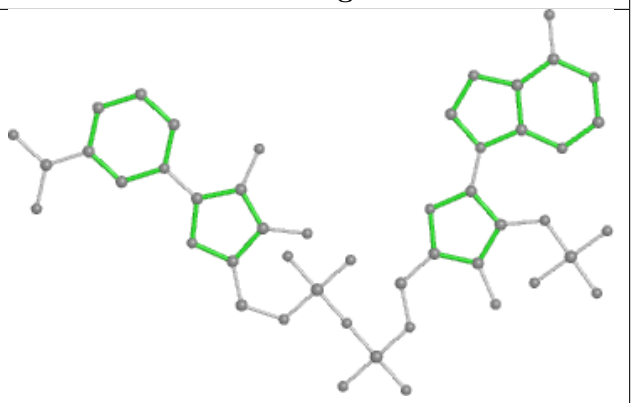
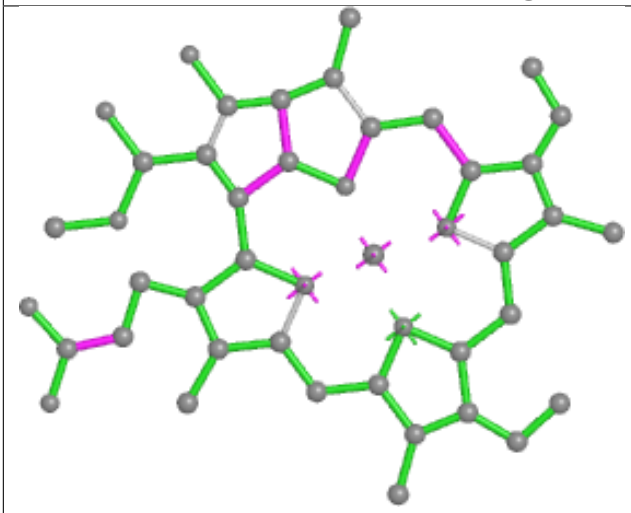


Rings

Ligand PMR E 502



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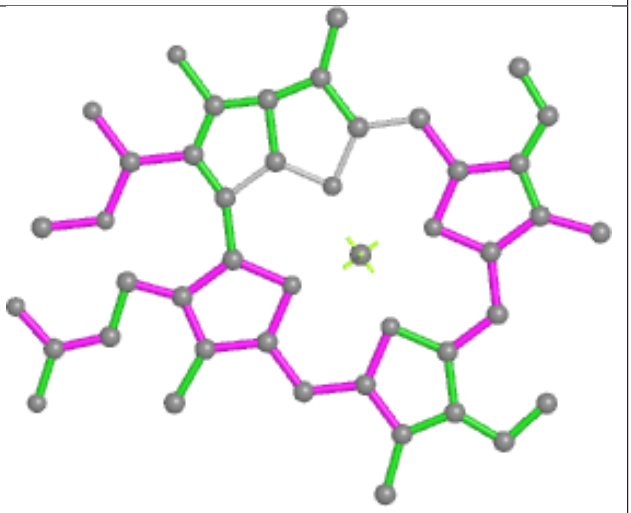
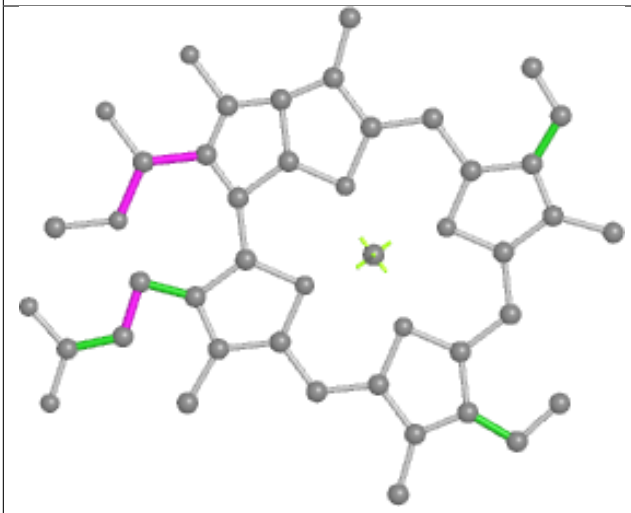
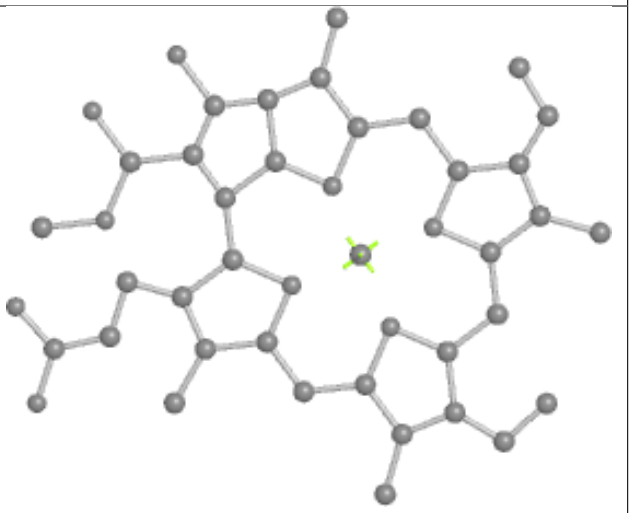


Bond angles

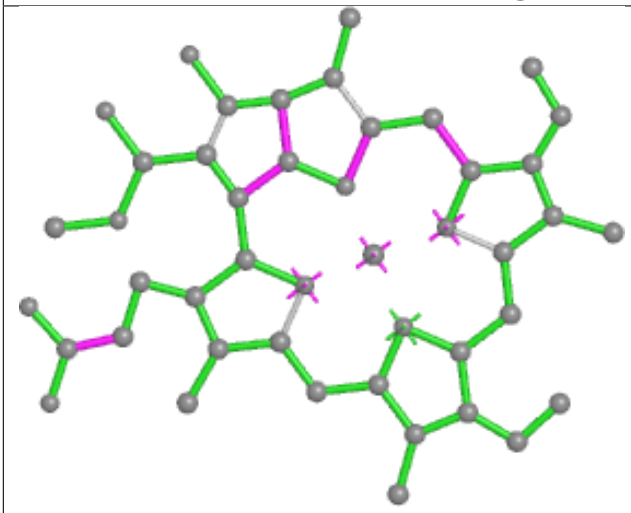


Torsions



Rings

Ligand PMR IA 502



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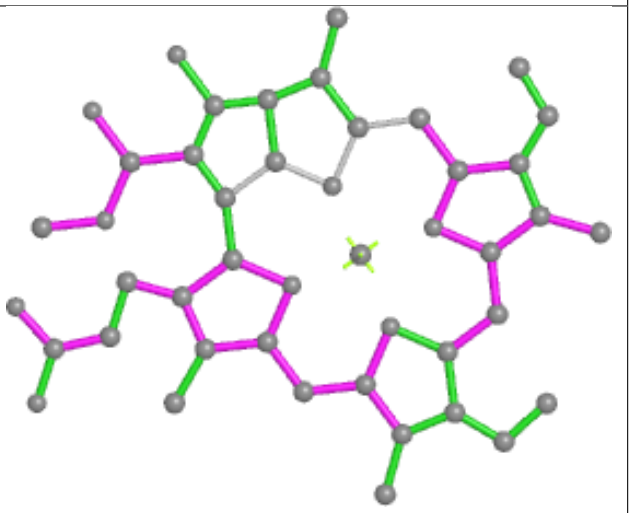

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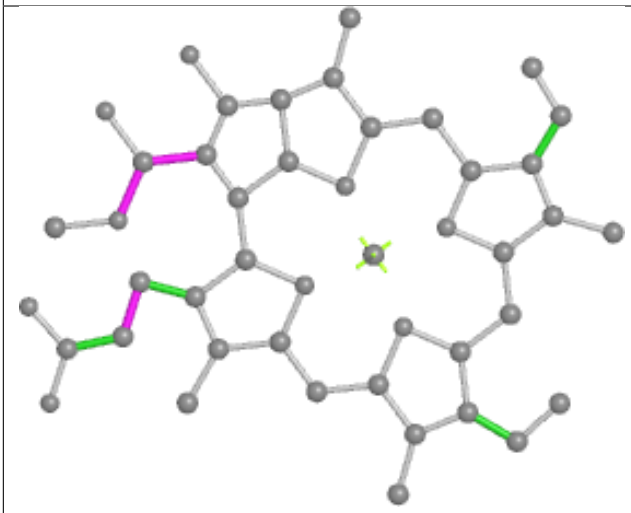

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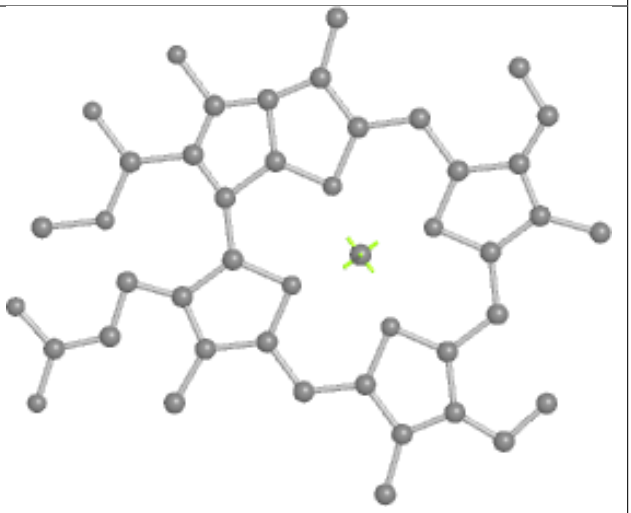

Rings

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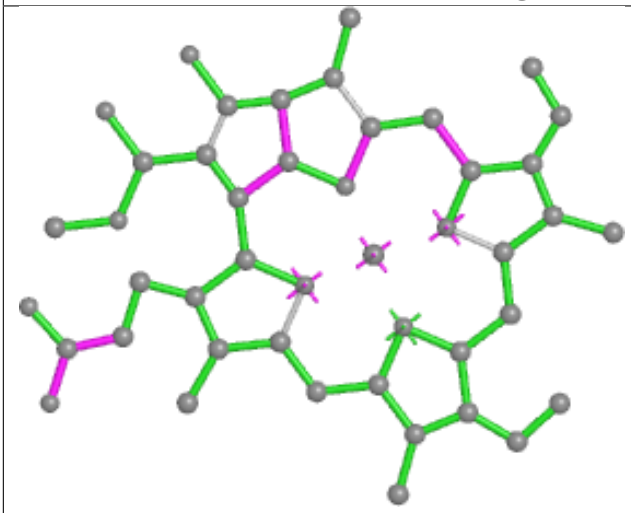

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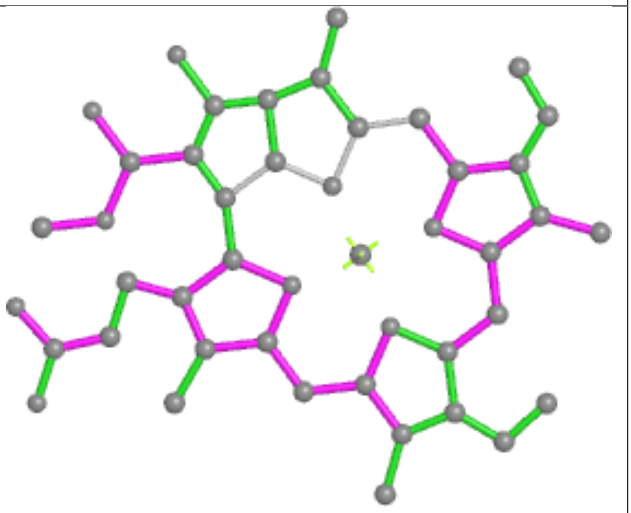

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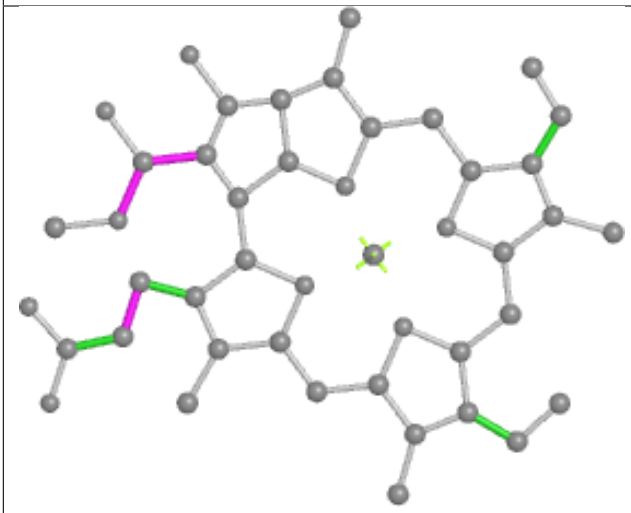

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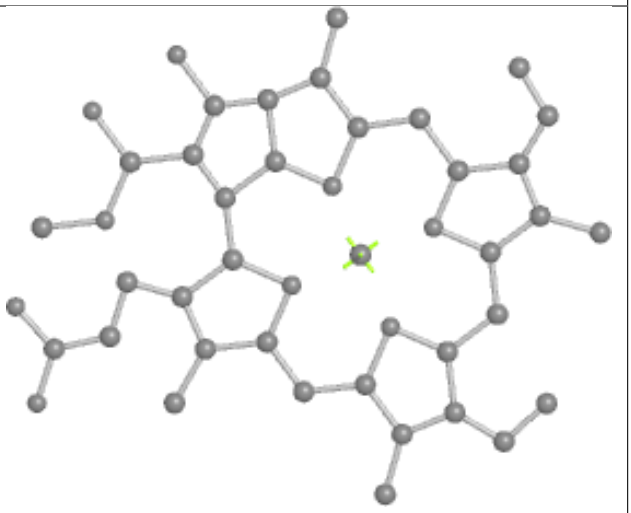

Rings

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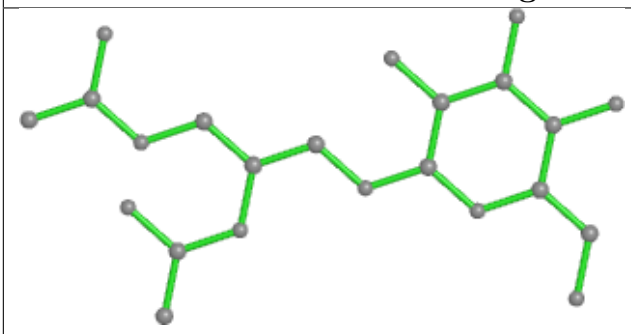

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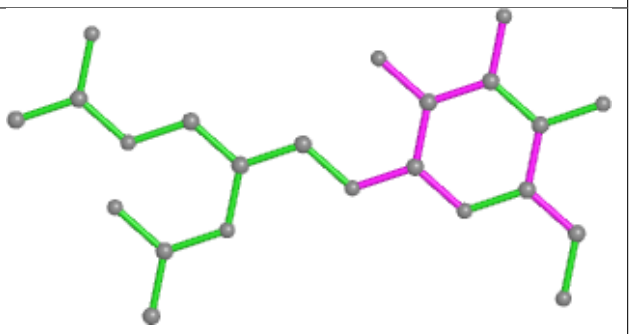

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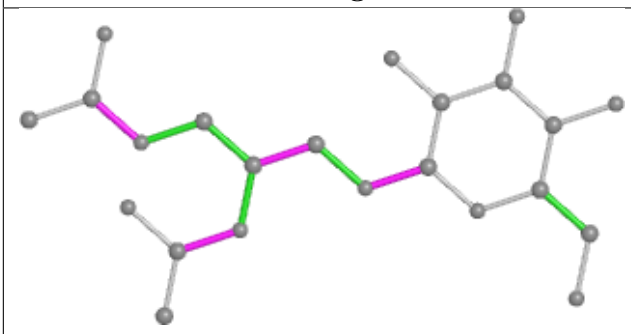

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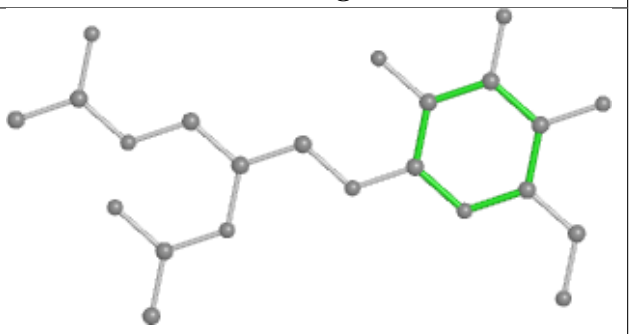

Rings

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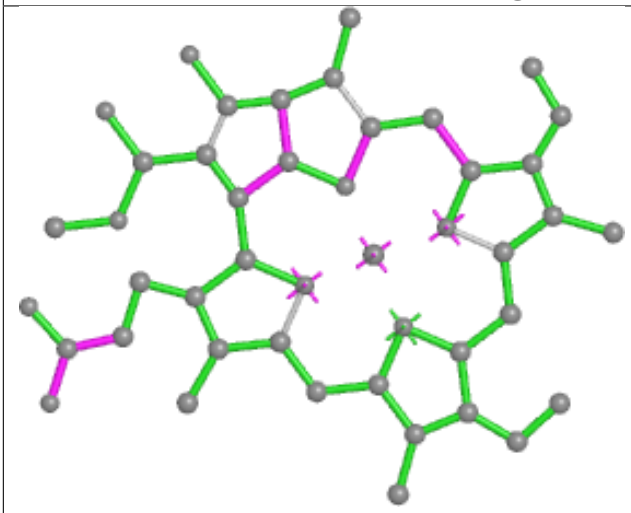

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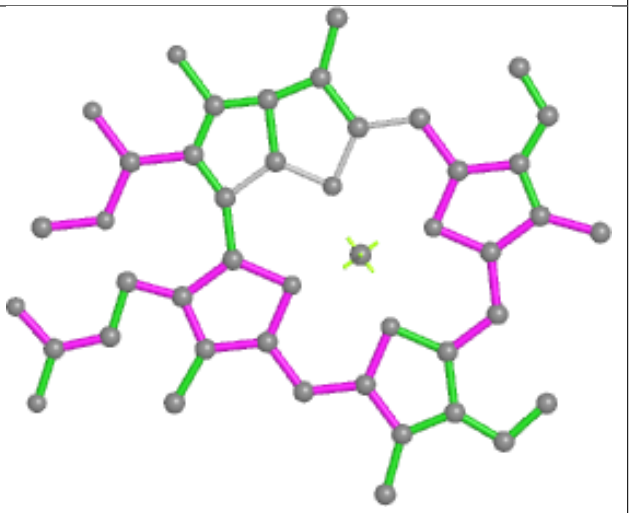

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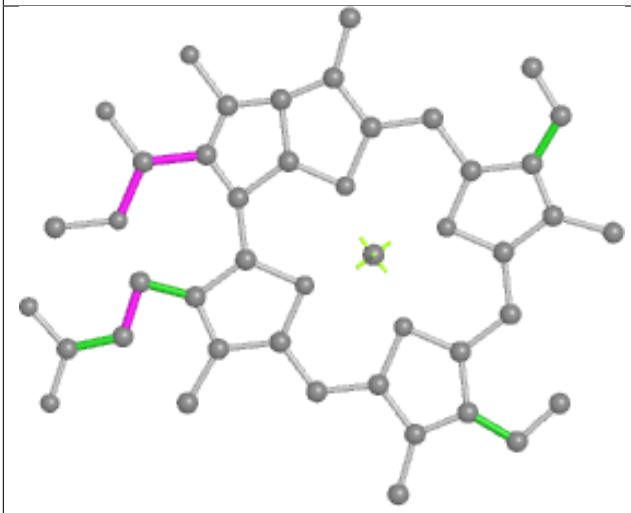

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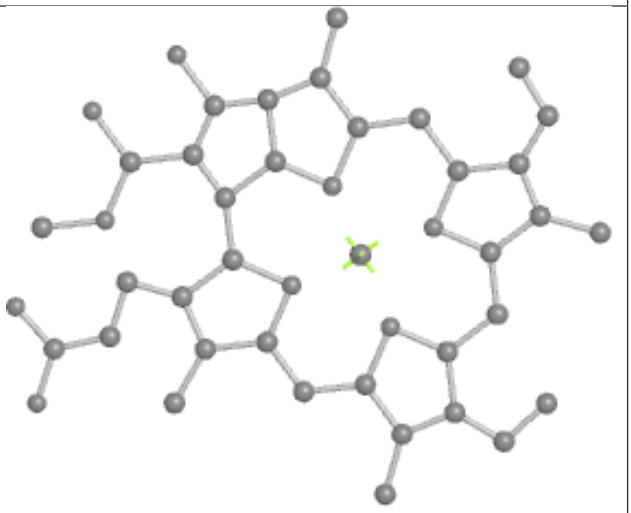
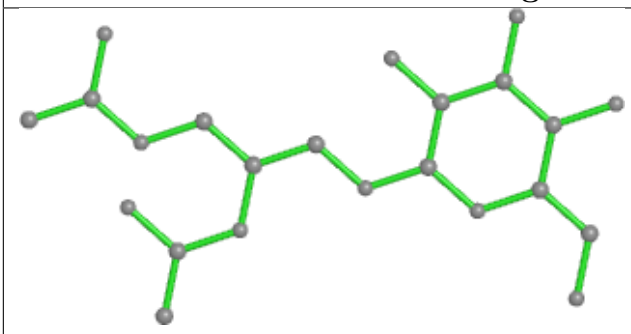


Rings

Ligand LMG L 503



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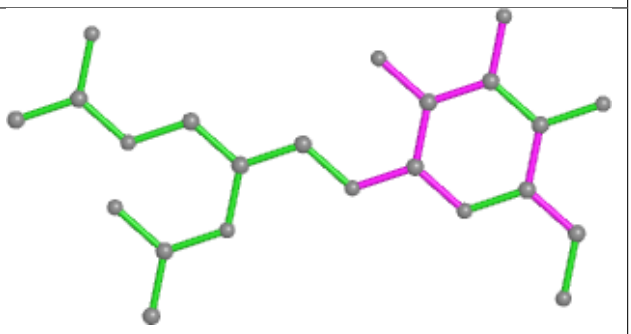

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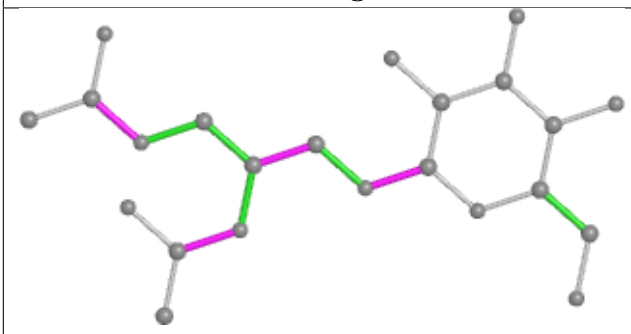

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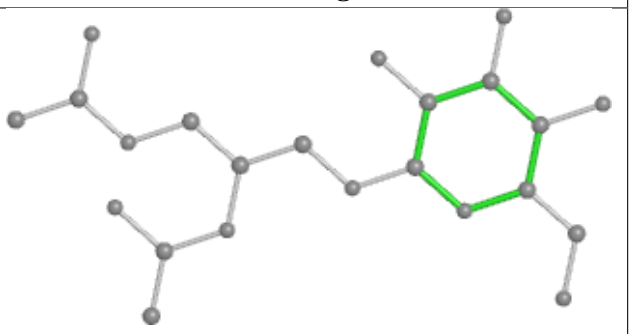

Rings

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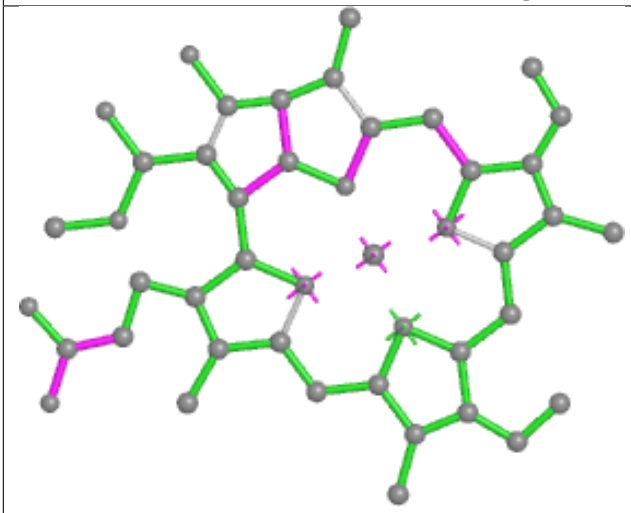

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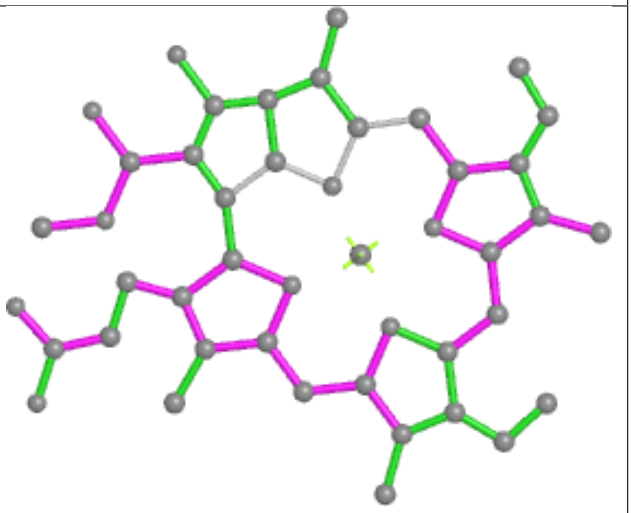

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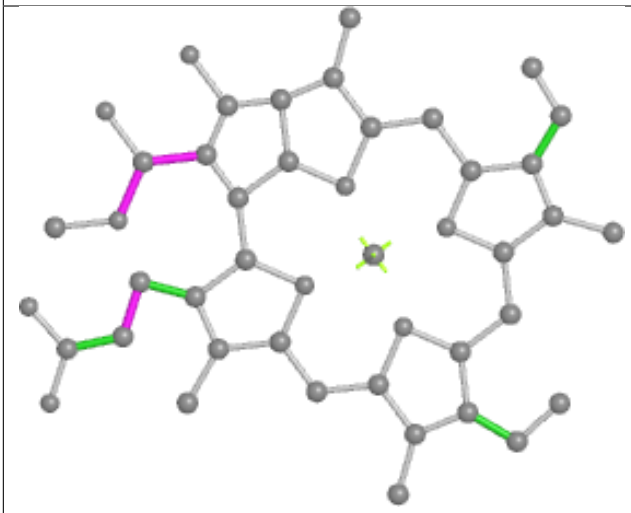

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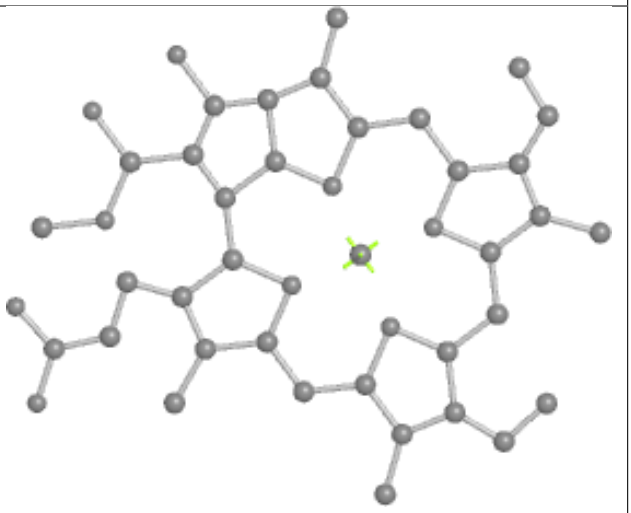
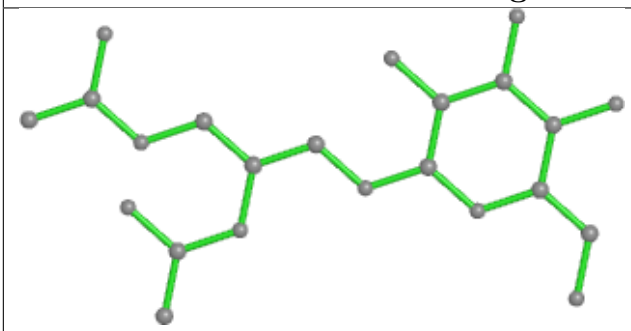


Rings

Ligand LMG FA 503



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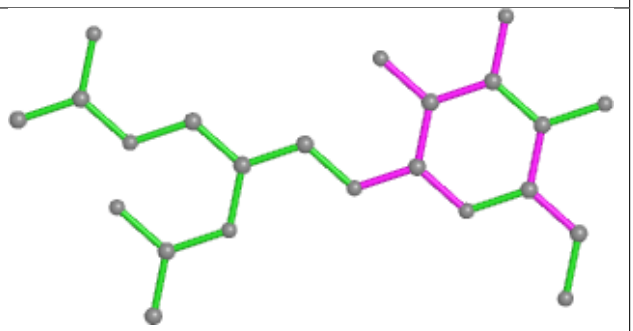

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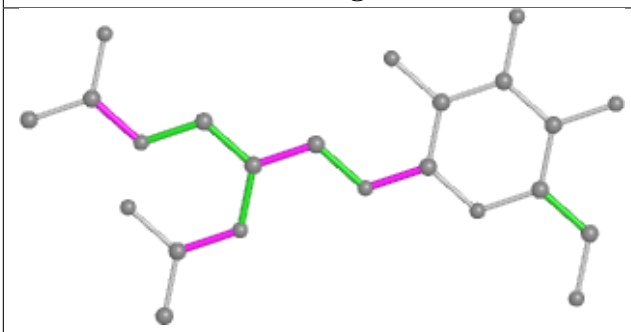

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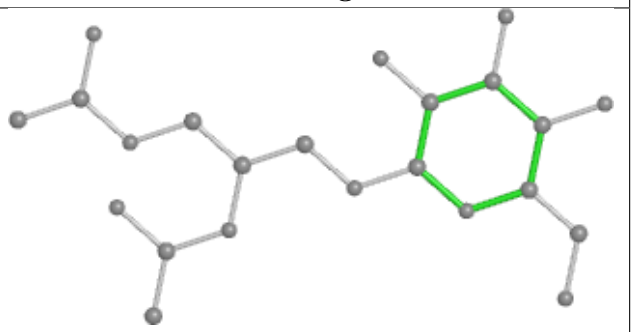

Rings

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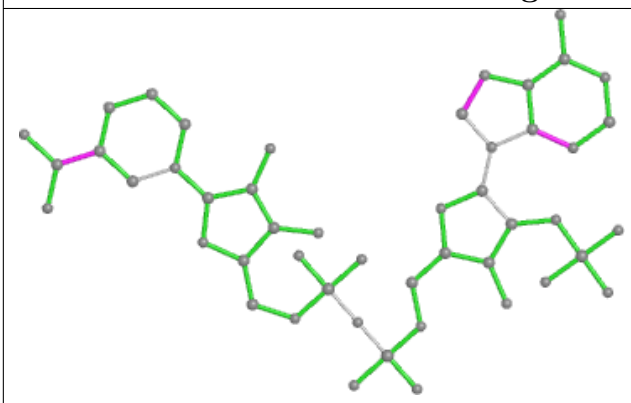

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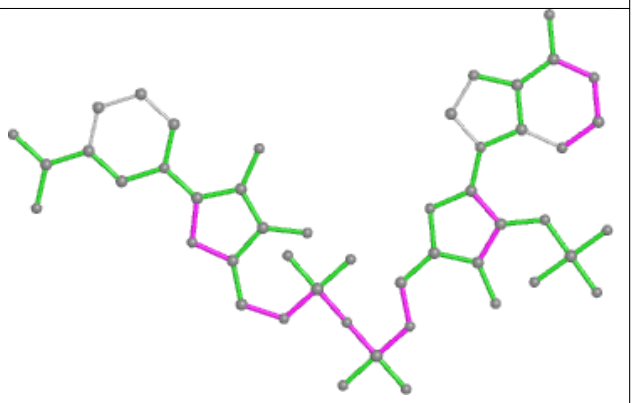

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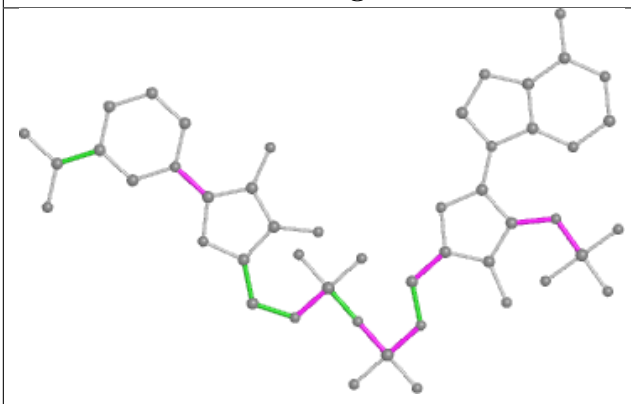

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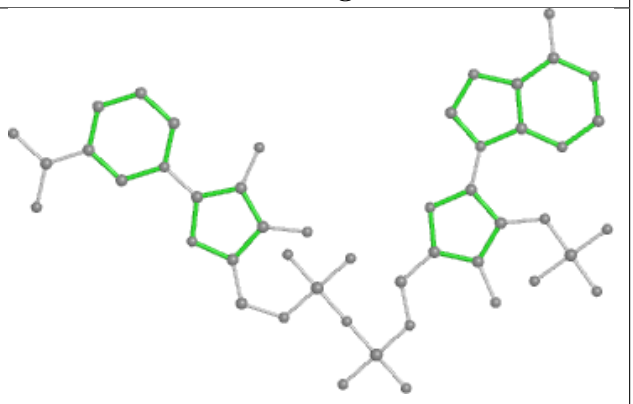

Rings

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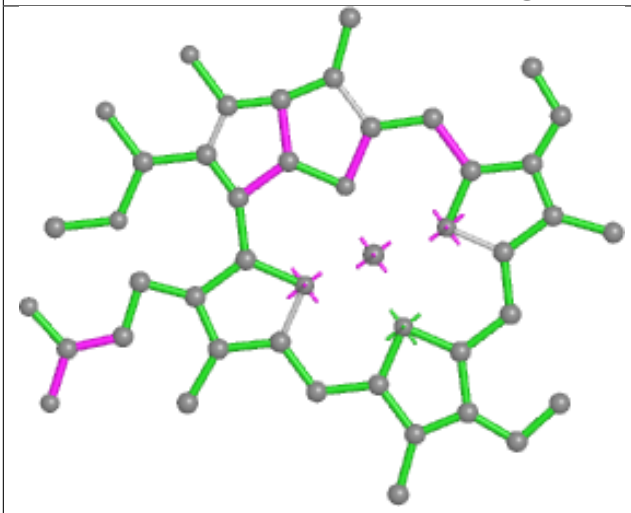

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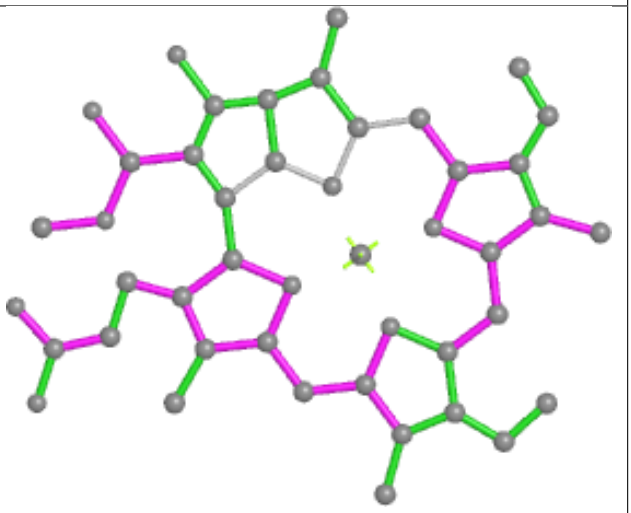

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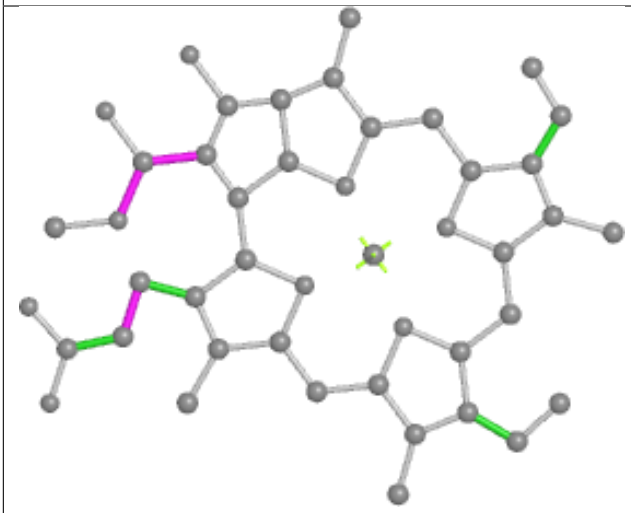

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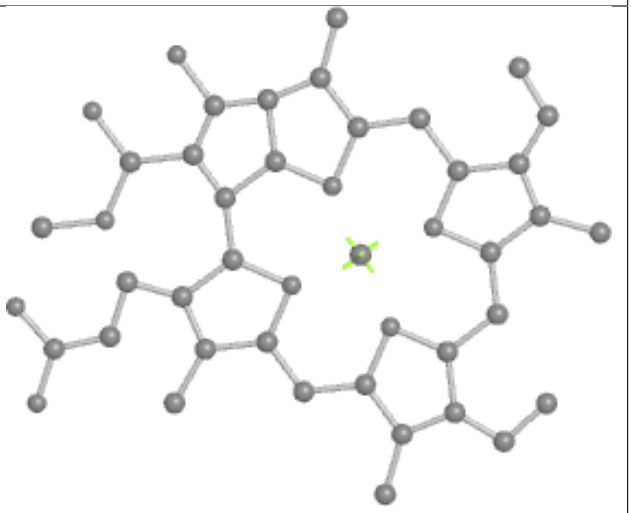

Rings

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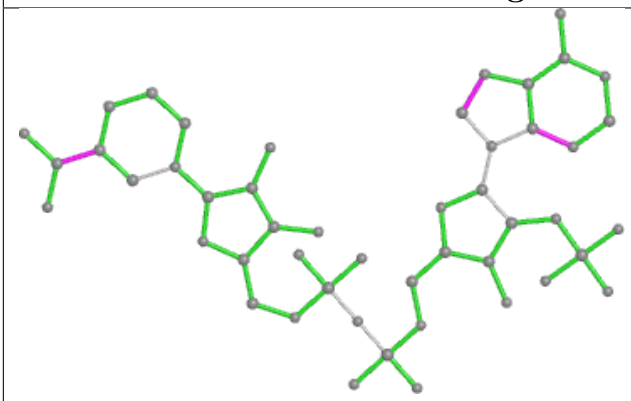

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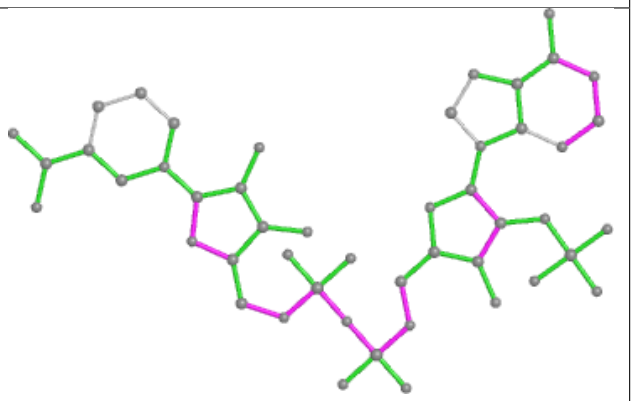

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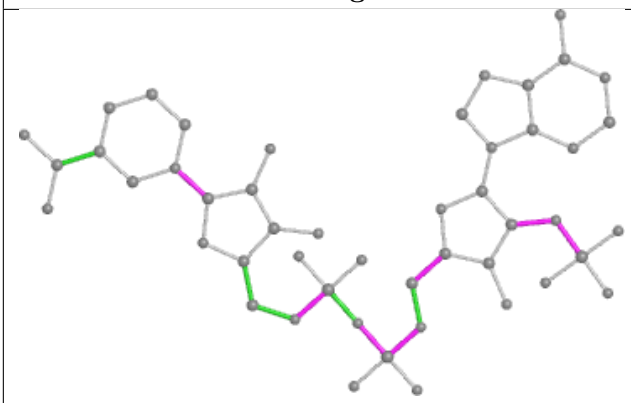

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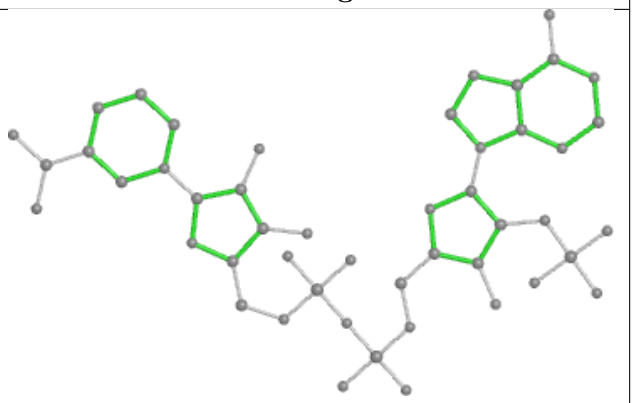

Rings

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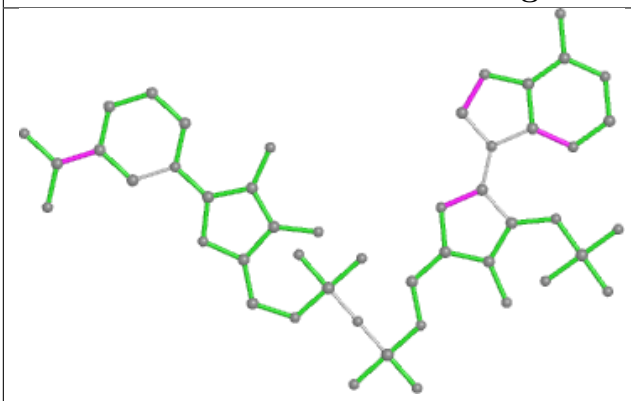

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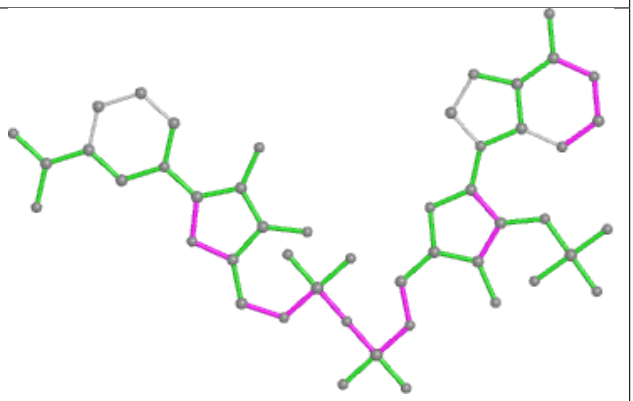

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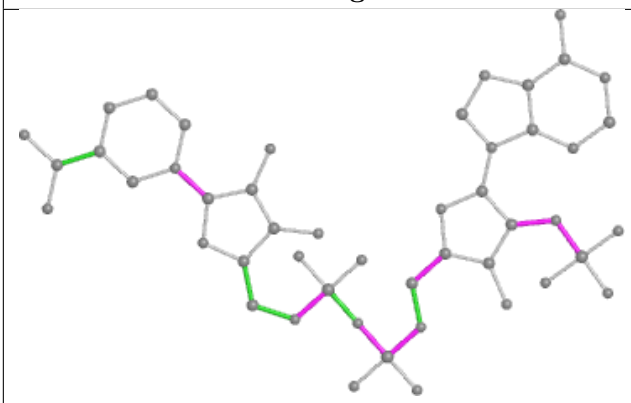

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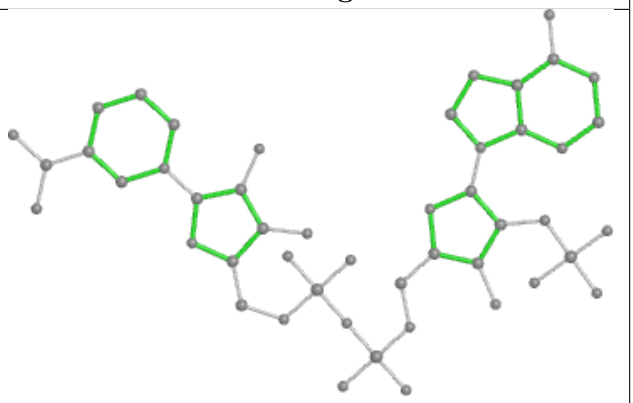
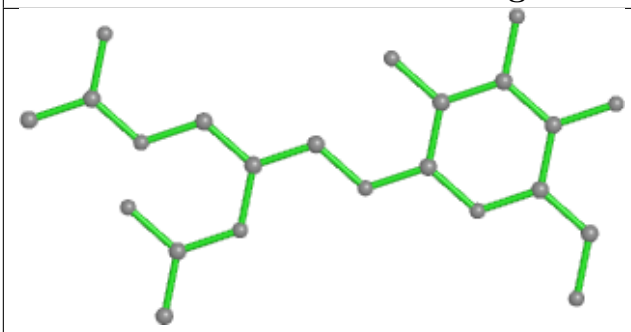


Rings

Ligand LMG LA 503



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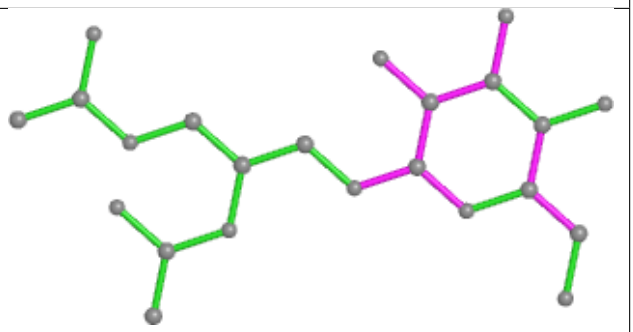

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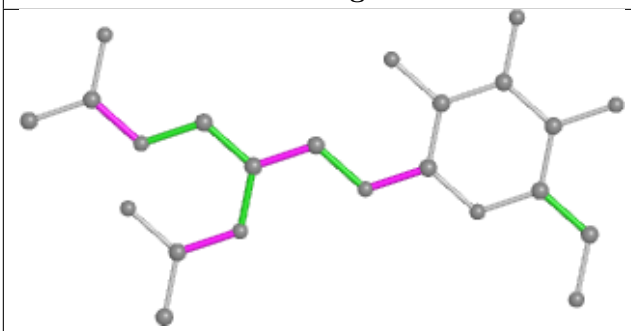

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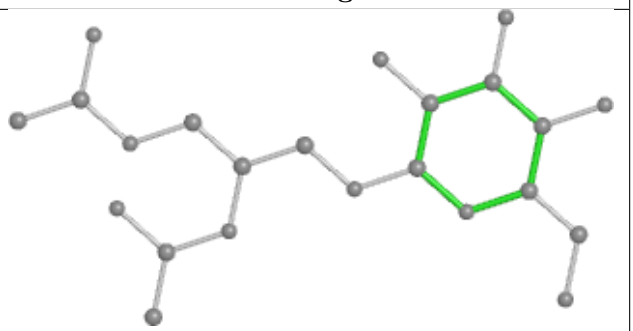

Rings

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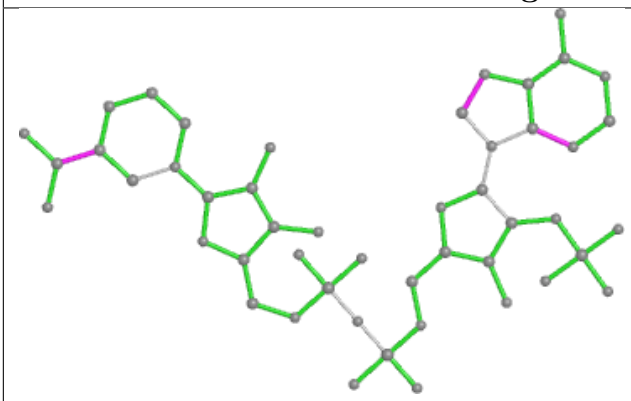

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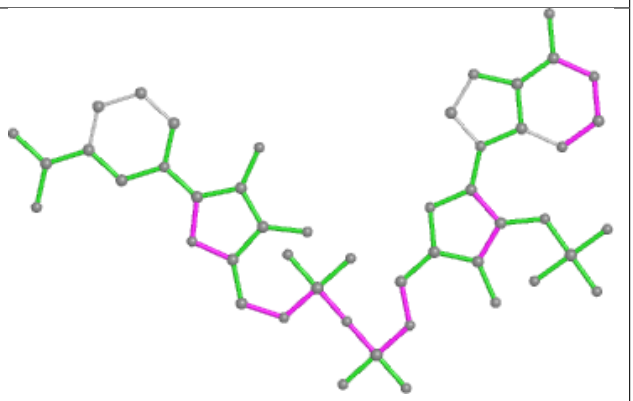

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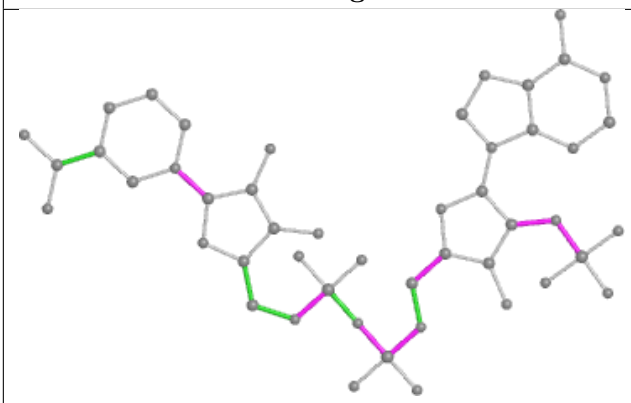

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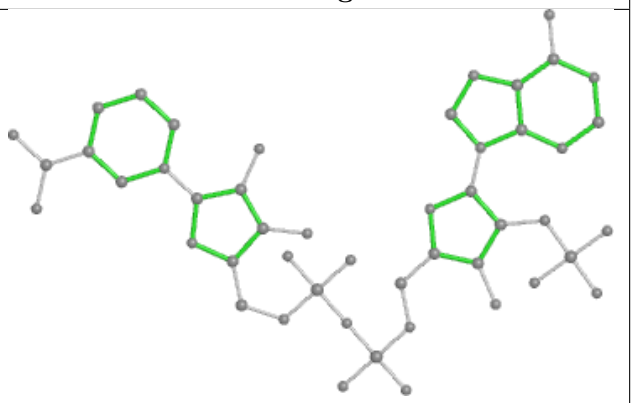
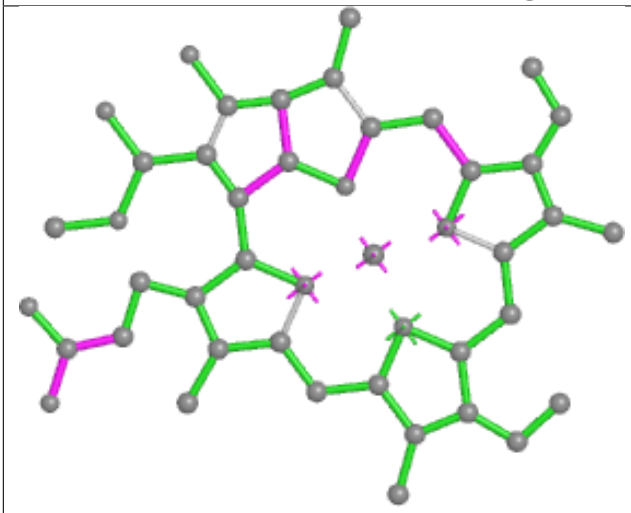


Rings

Ligand PMR Z 502



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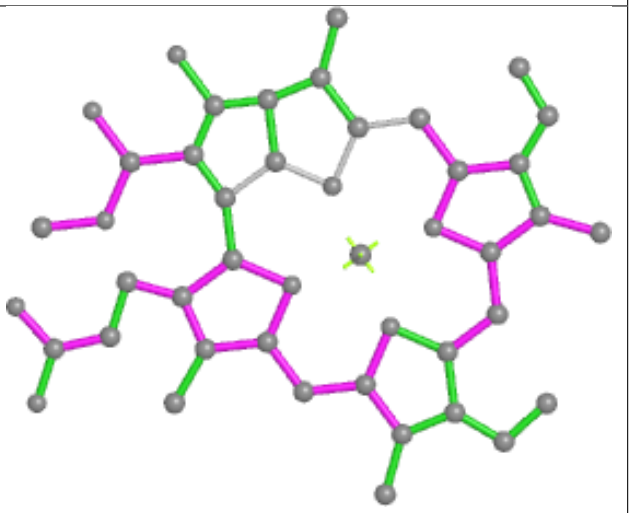

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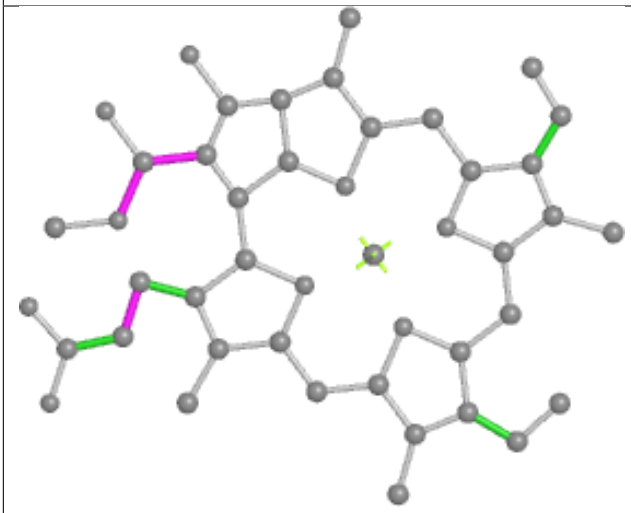

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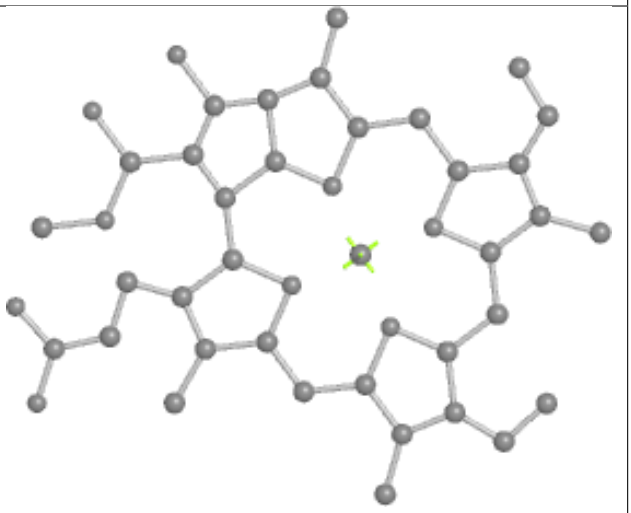
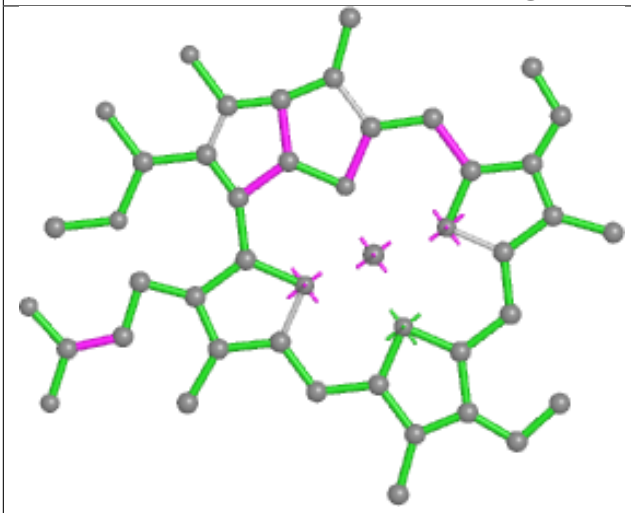


Rings

Ligand PMR S 502



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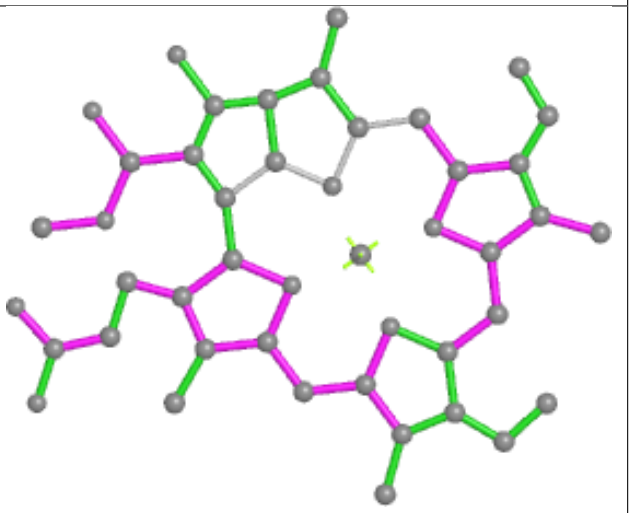

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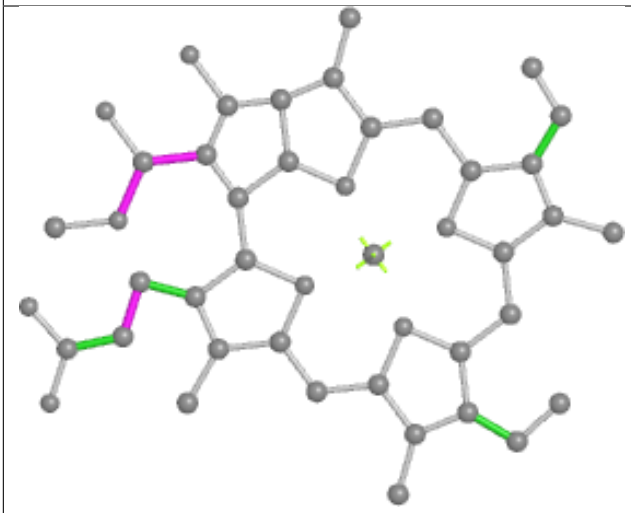

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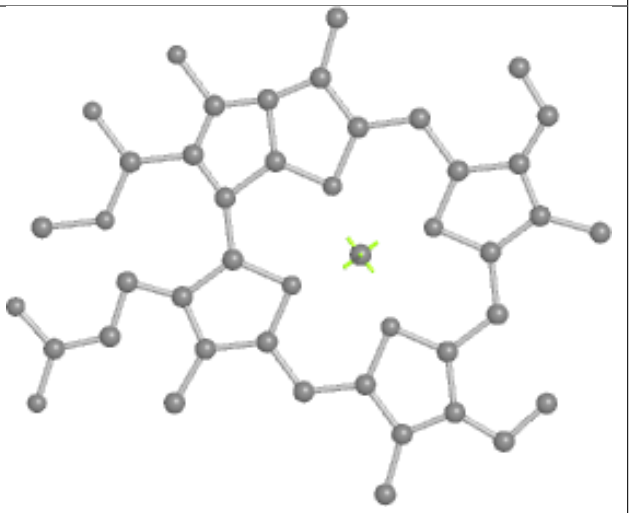
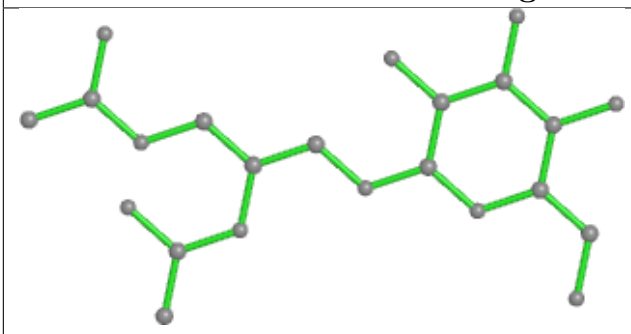


Rings

Ligand LMG V 503



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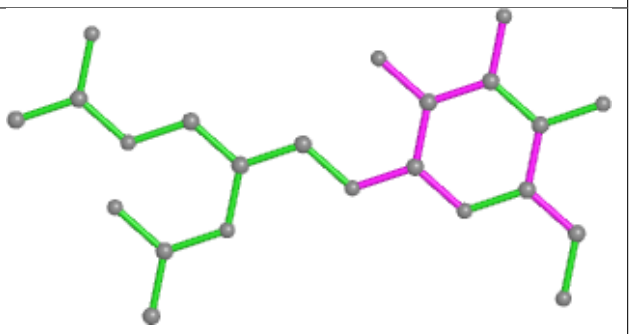

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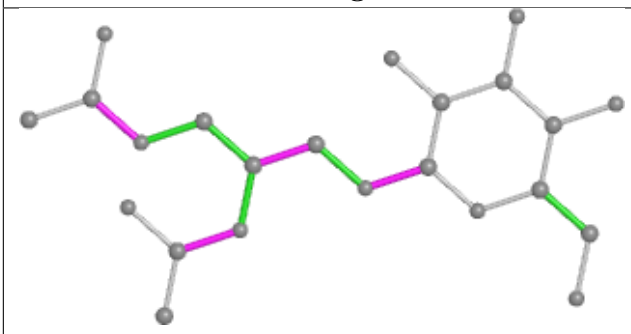

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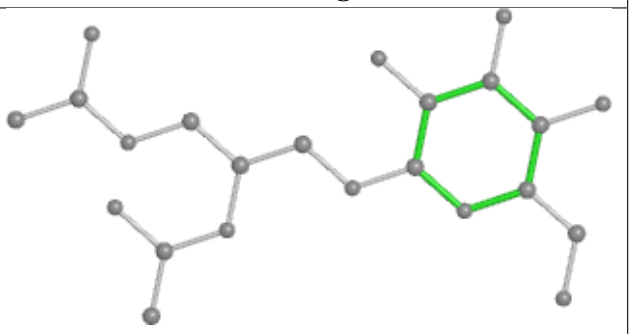
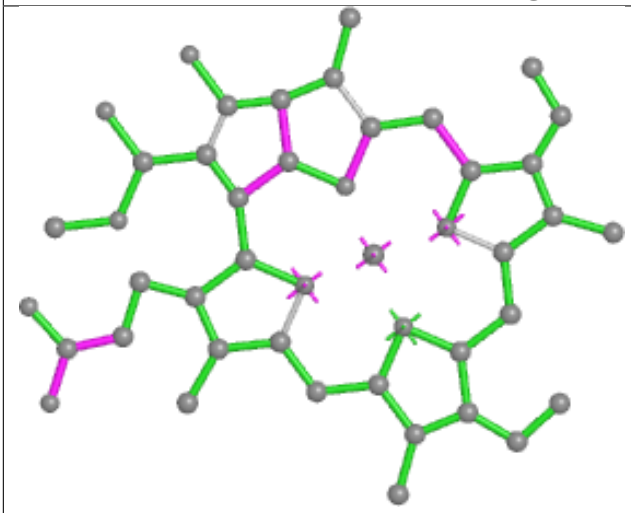


Rings

Ligand PMR I 502



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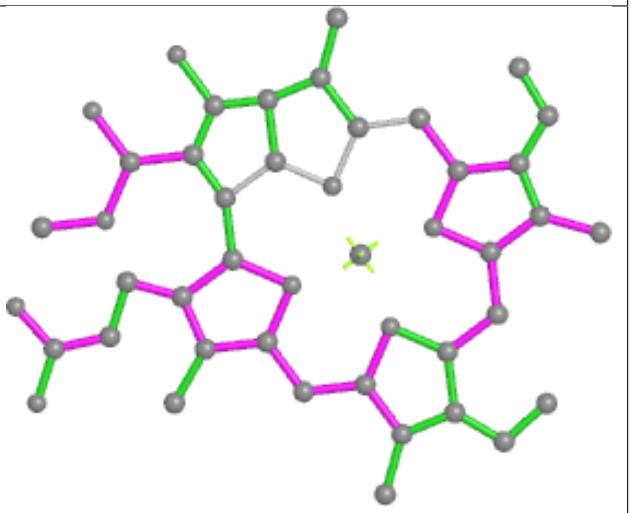

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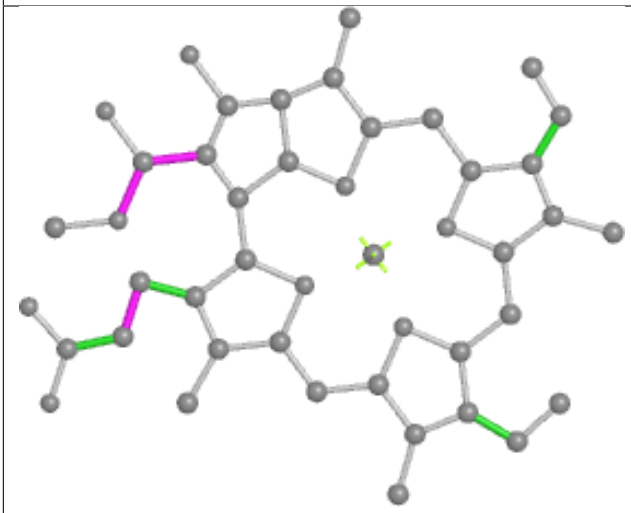

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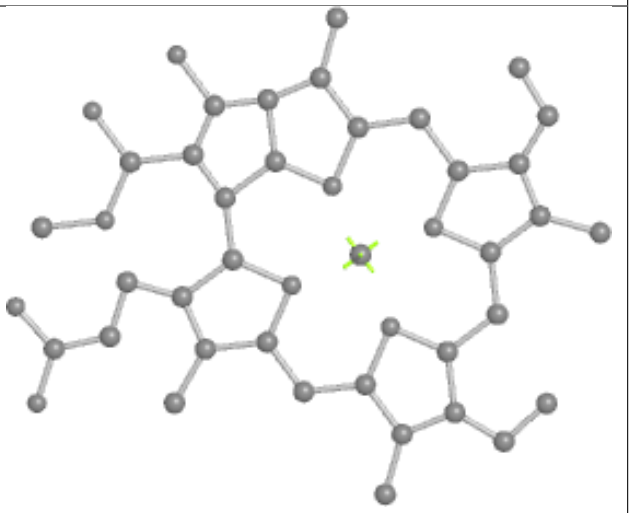

Rings

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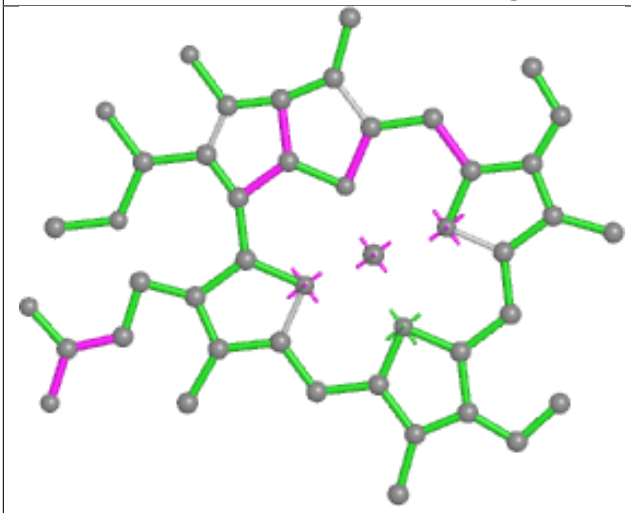

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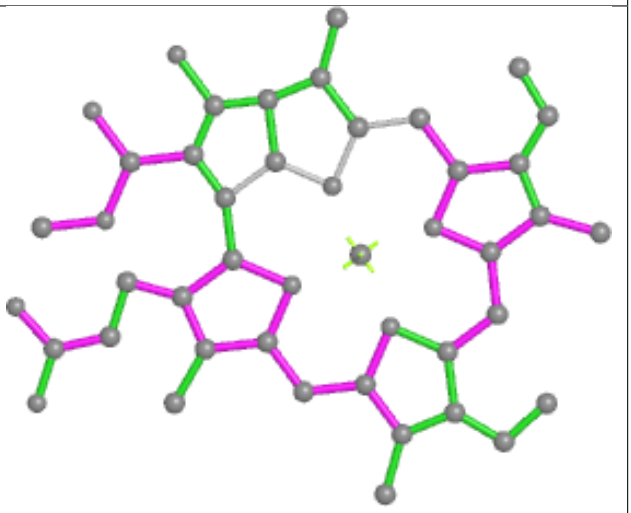

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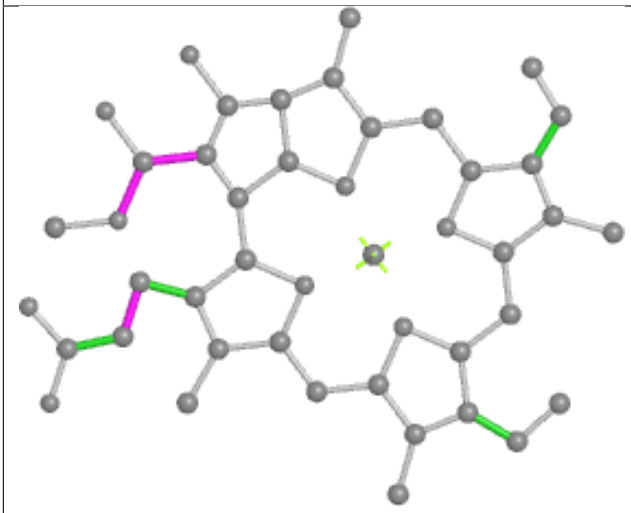

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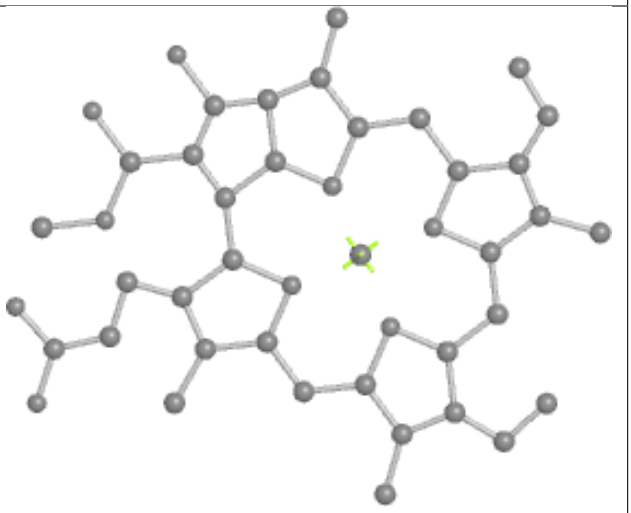
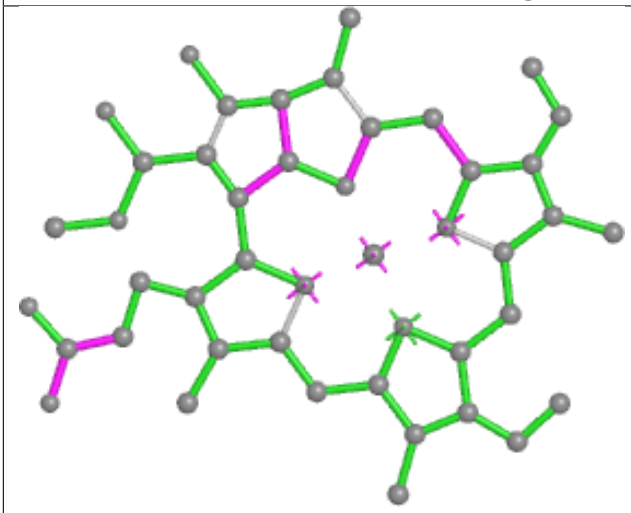


Rings

Ligand PMR P 502



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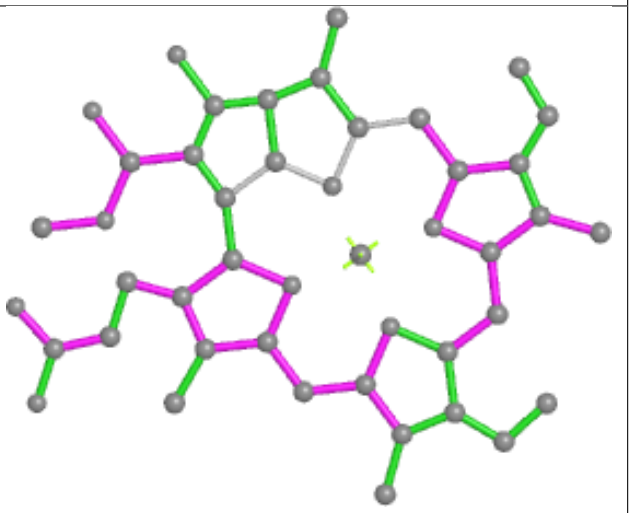

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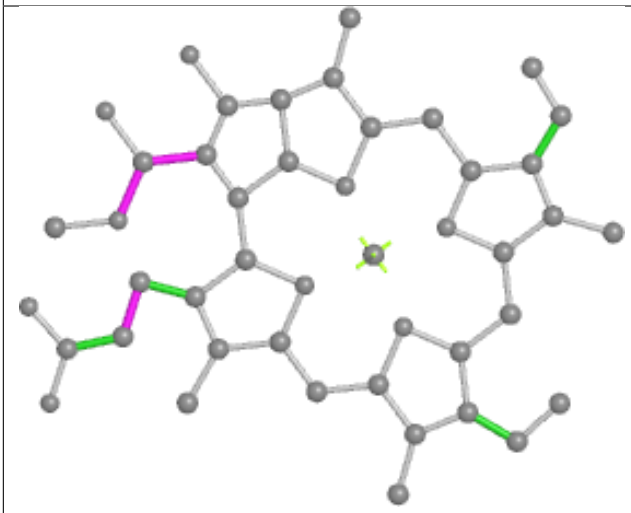

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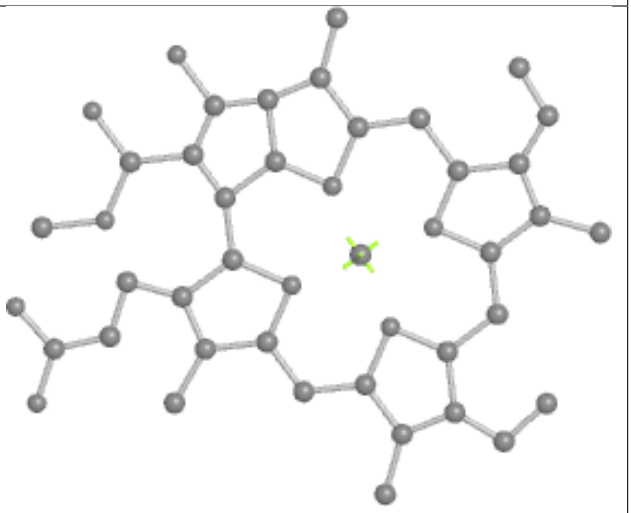
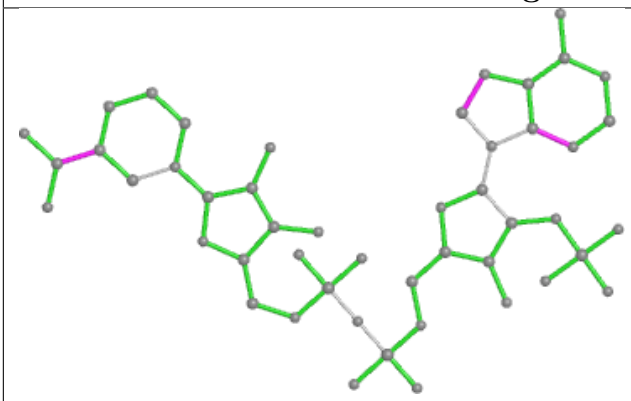


Rings

Ligand NDP E 501



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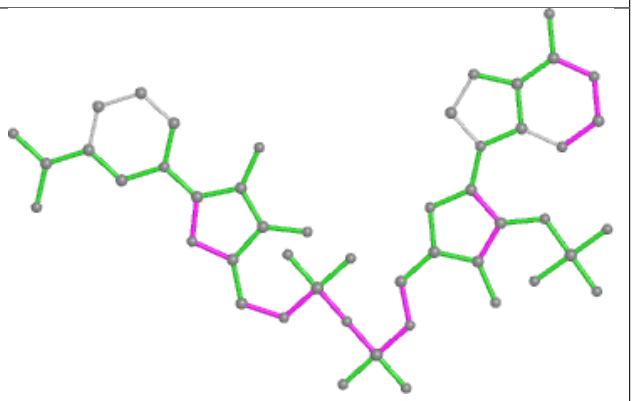

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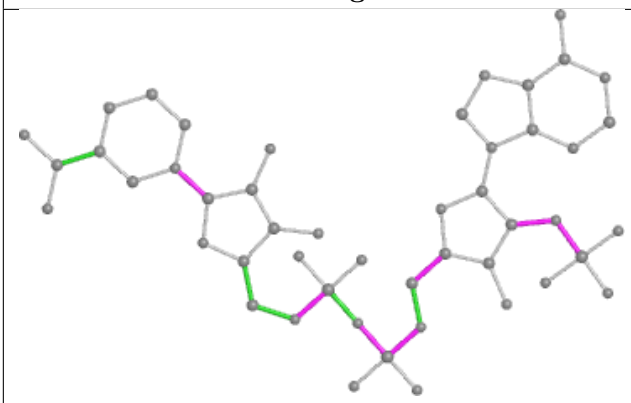

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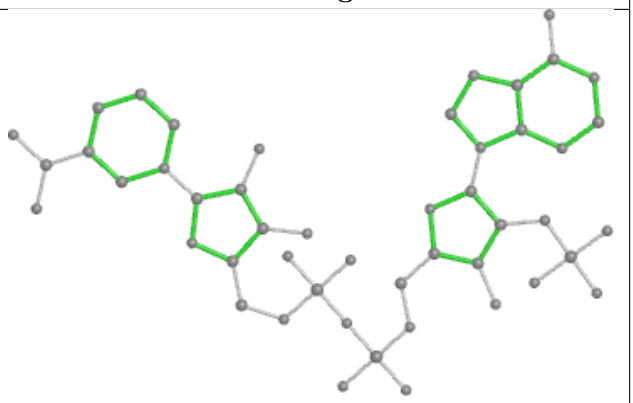
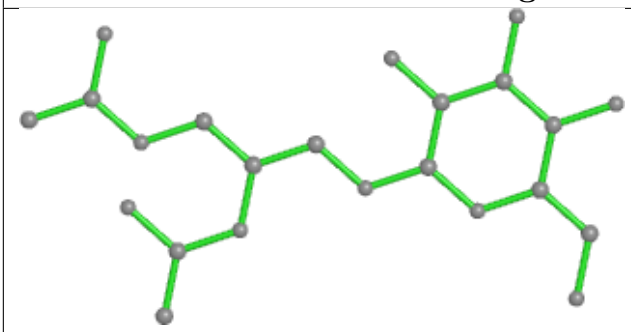


Rings

Ligand LMG K 503



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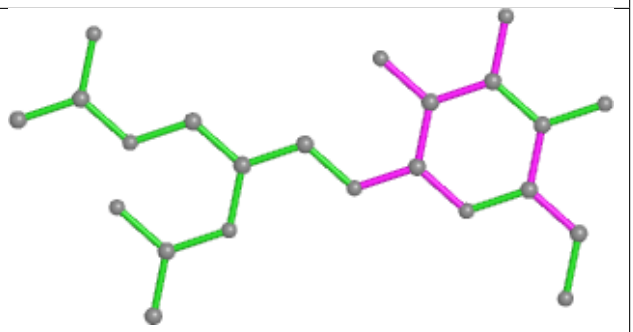

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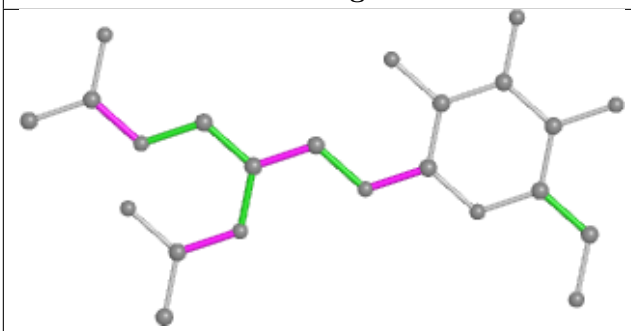

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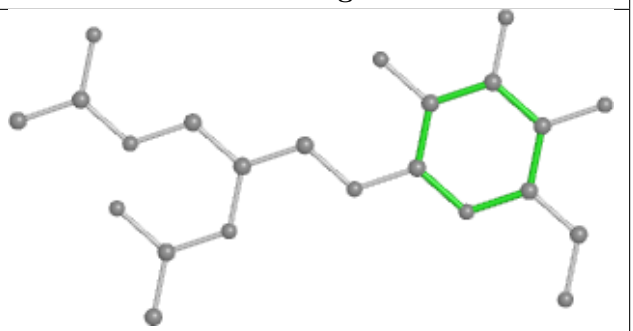
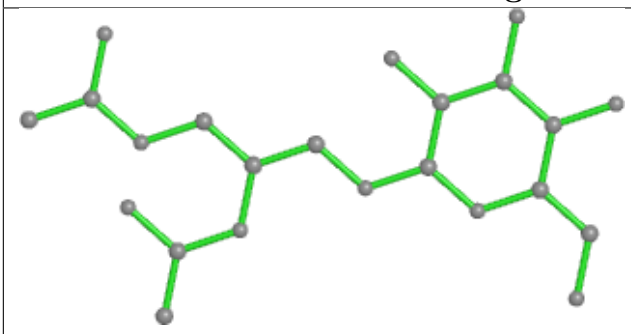


Rings

Ligand LMG KA 503



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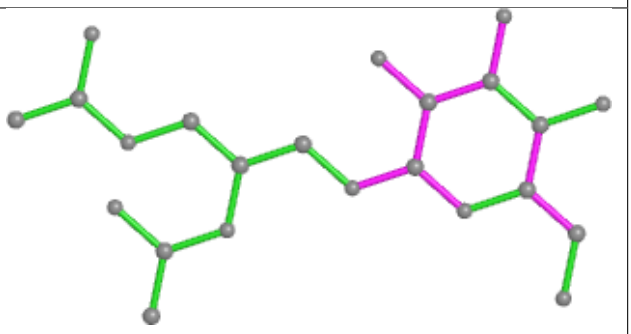

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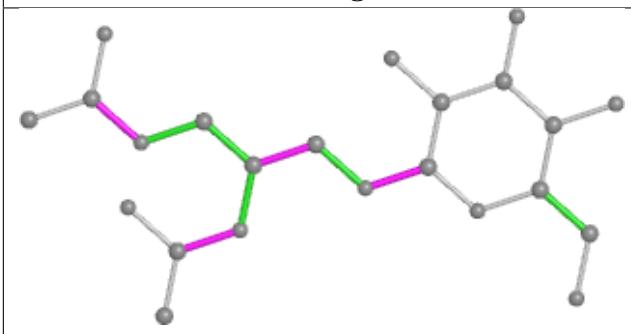

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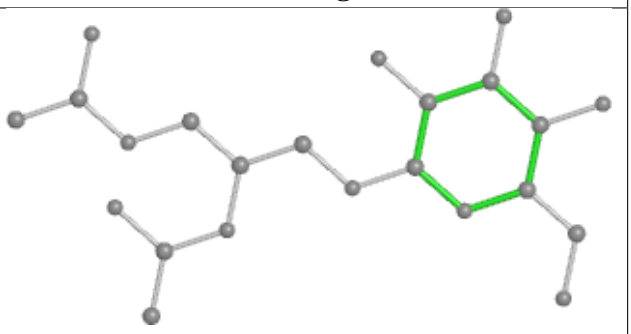
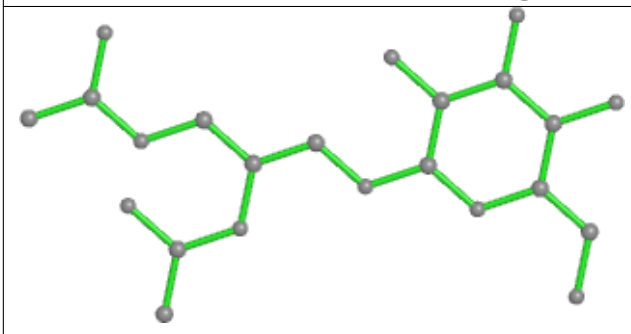


Rings

Ligand LMG M 503



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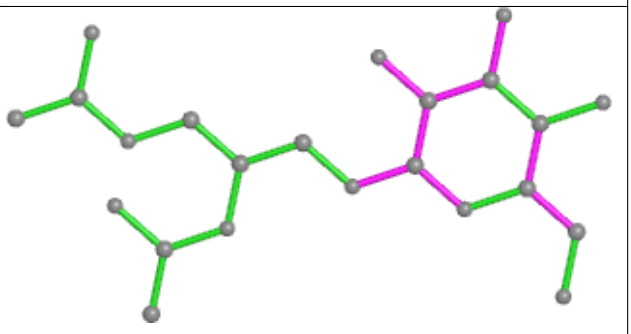

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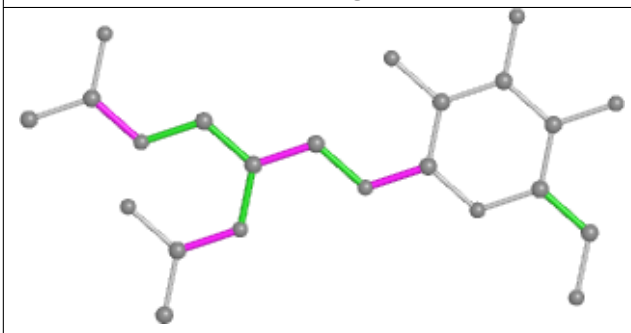

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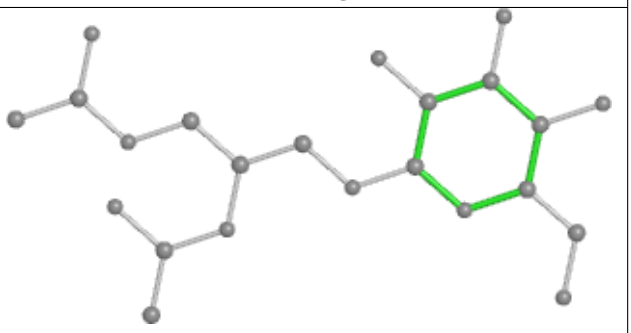
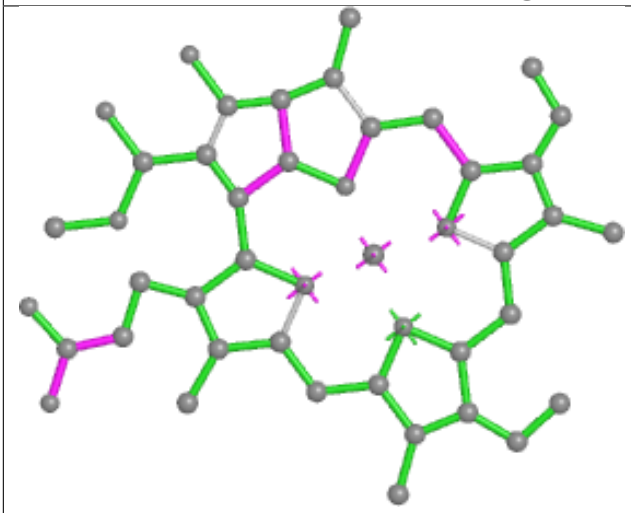


Rings

Ligand PMR Y 502



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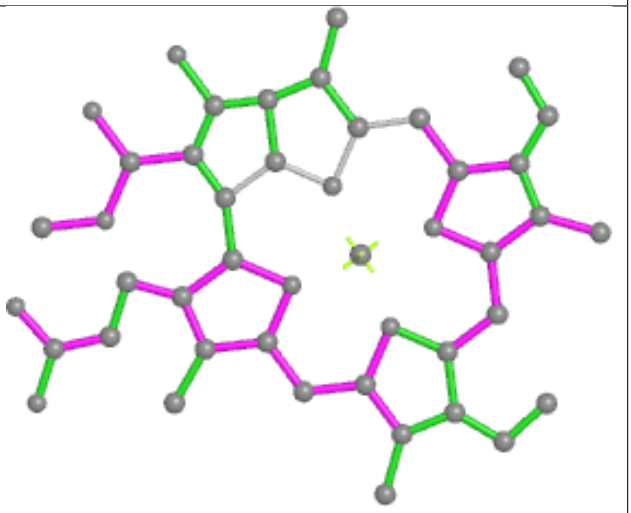

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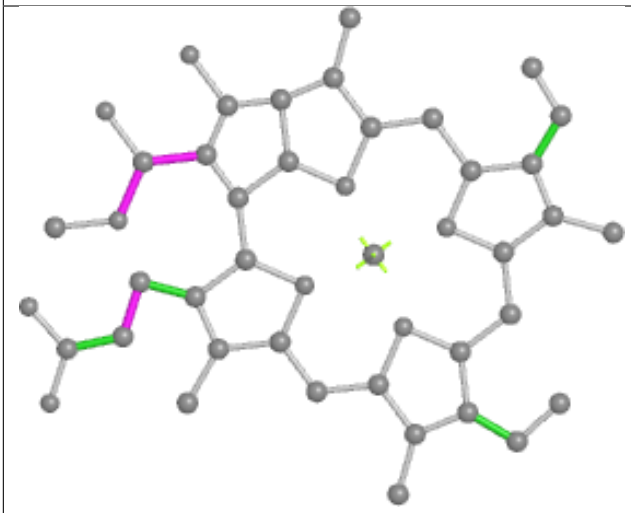

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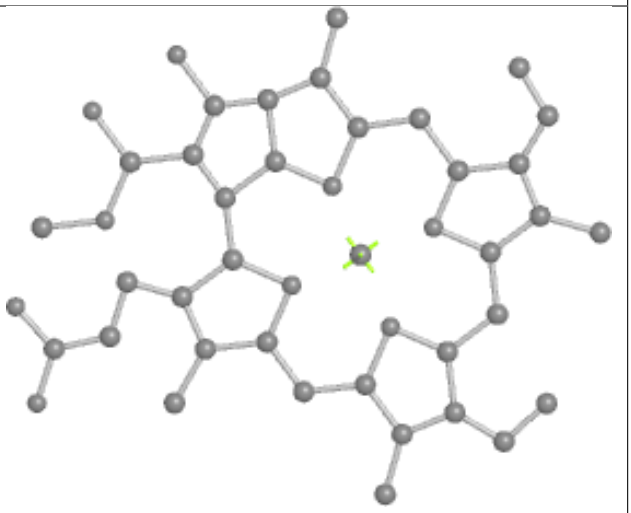
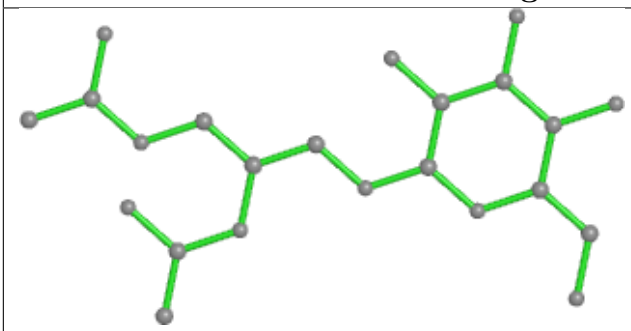


Rings

Ligand LMG E 503



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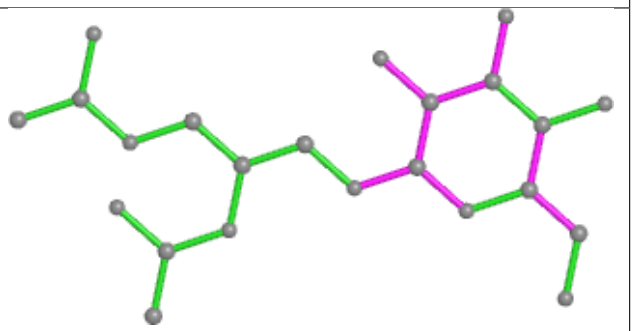

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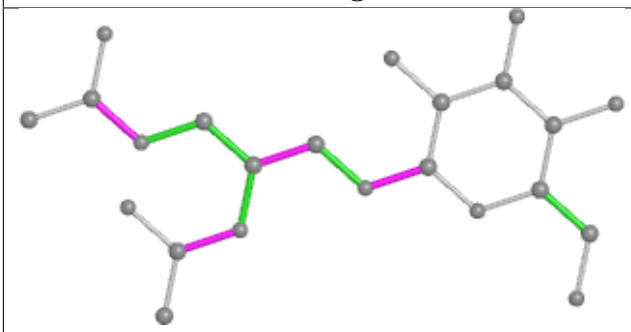

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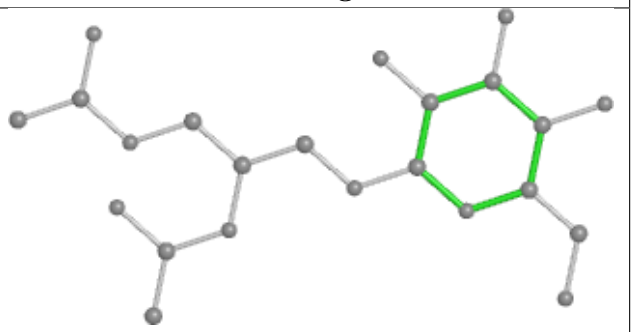
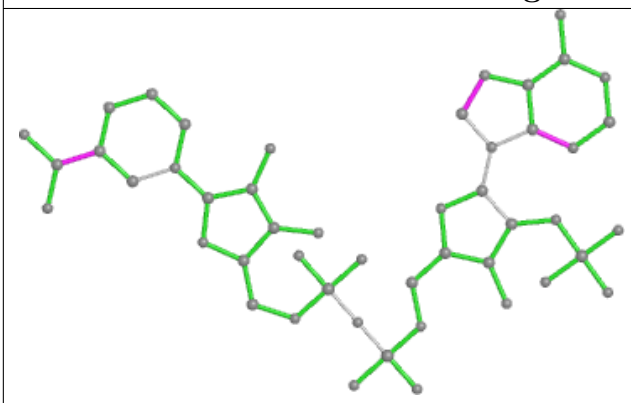


Rings

Ligand NDP Z 501



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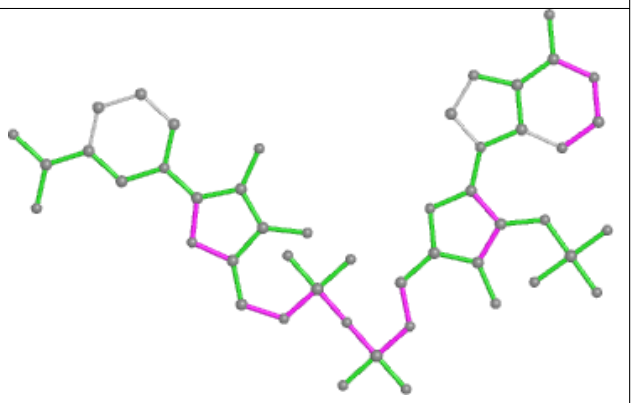

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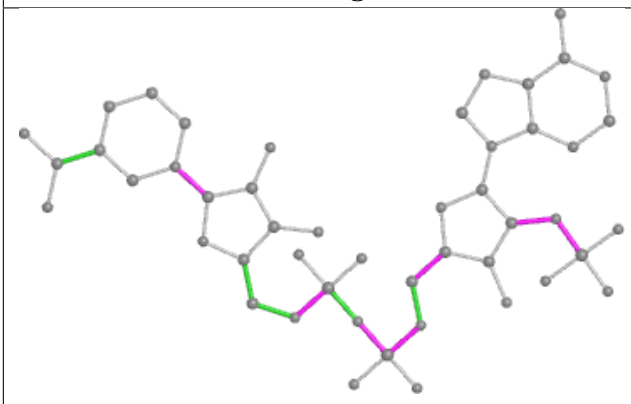

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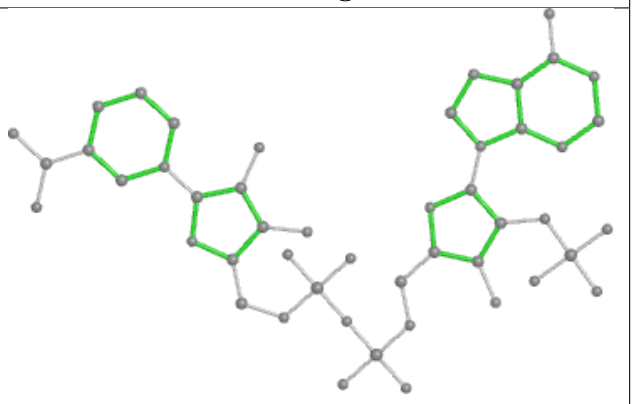
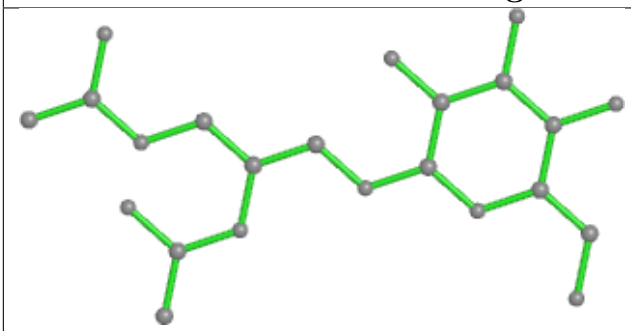


Rings

Ligand LMG OA 503



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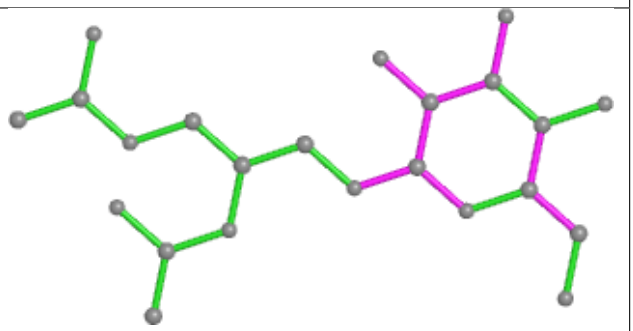

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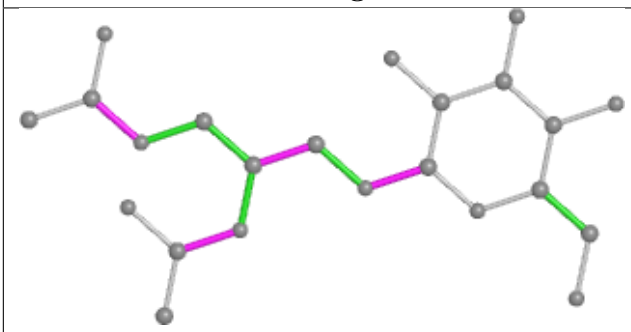

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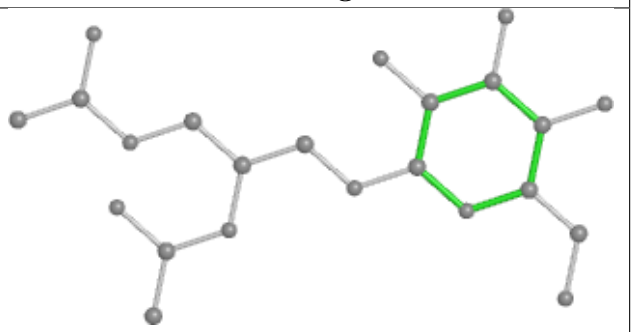
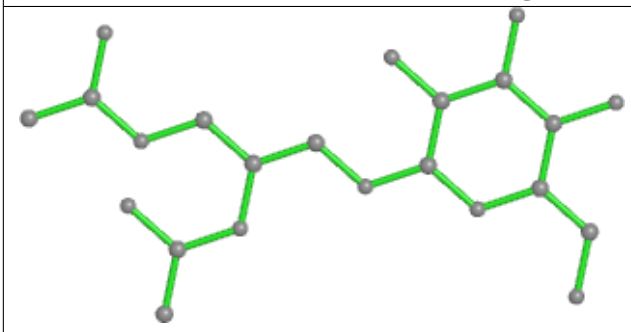


Rings

Ligand LMG G 503



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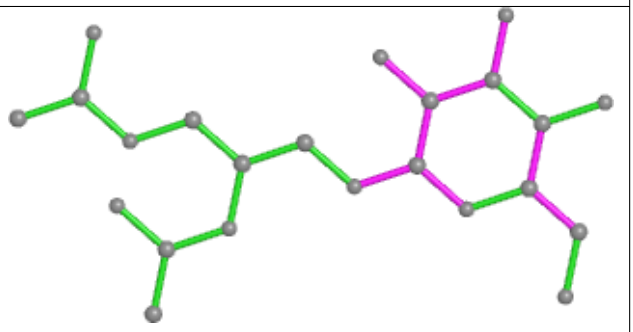
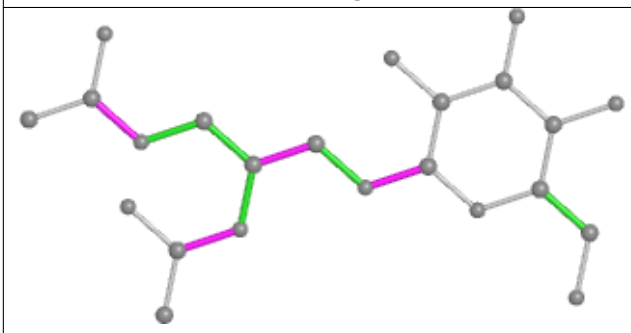


Bond angles



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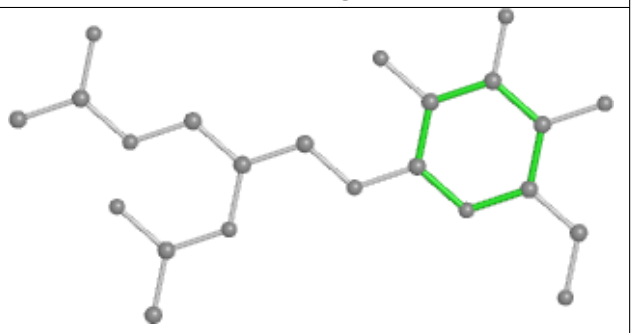
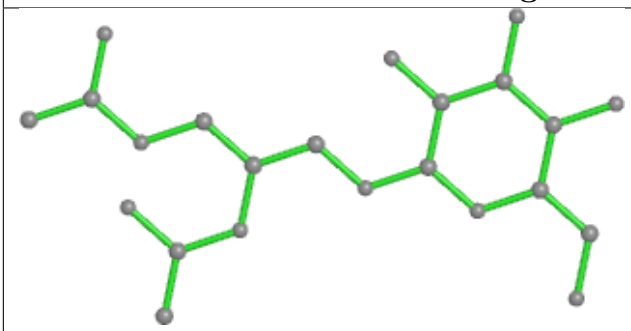


Rings

Ligand LMG B 503



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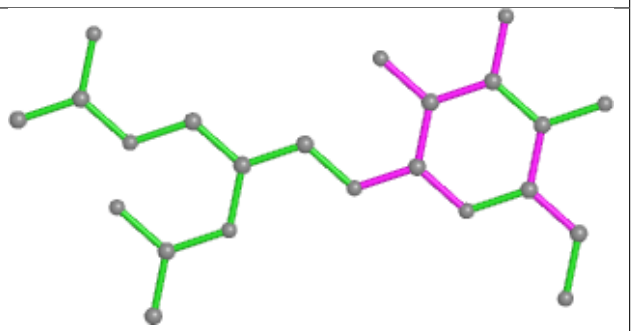
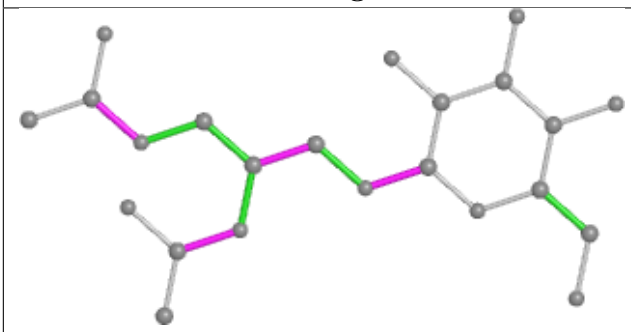
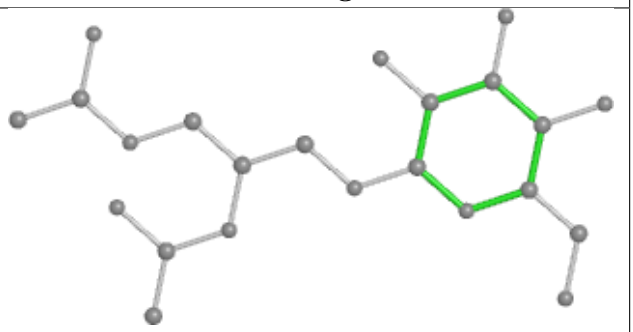


Bond angles

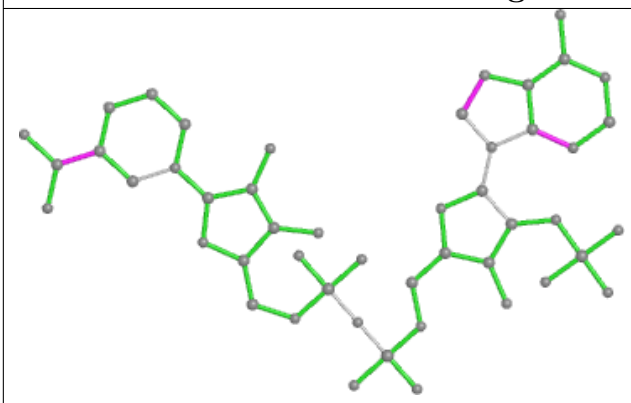


Torsions



Rings

Ligand NDP DA 501



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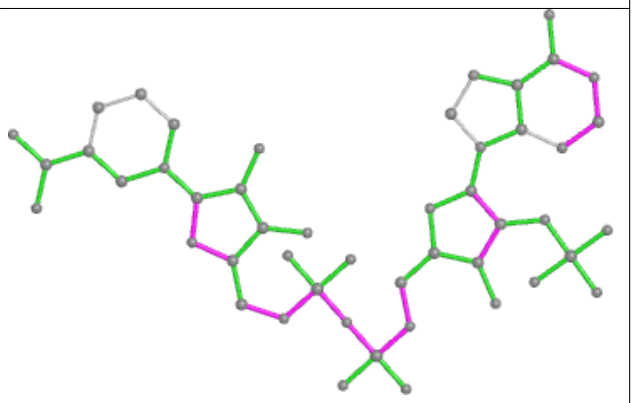

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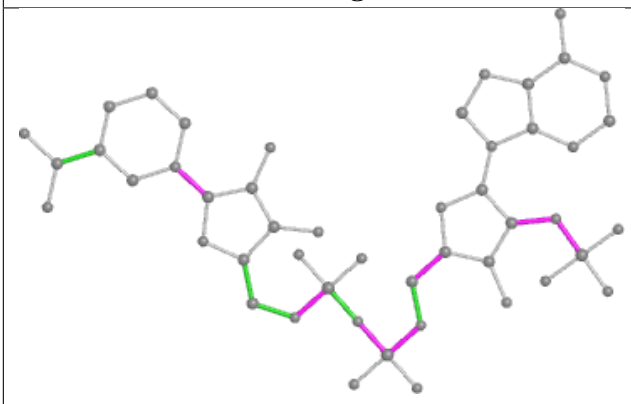

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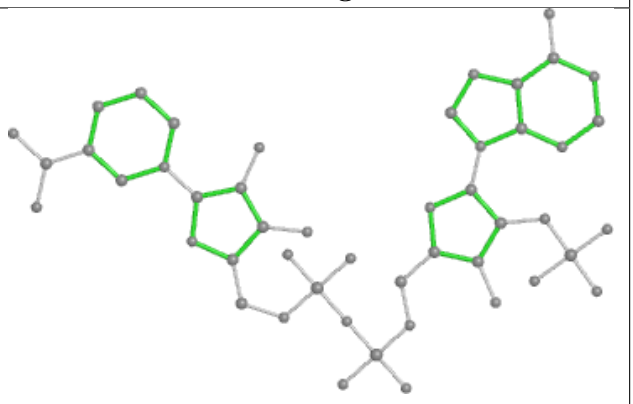
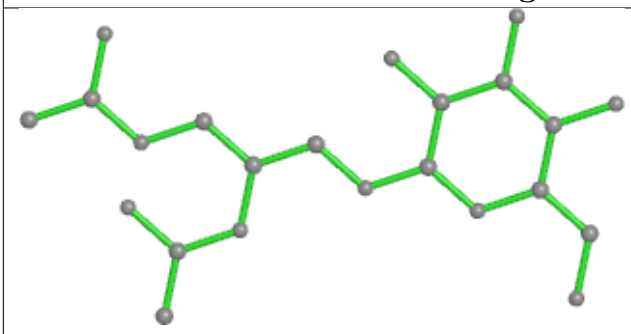


Rings

Ligand LMG N 503



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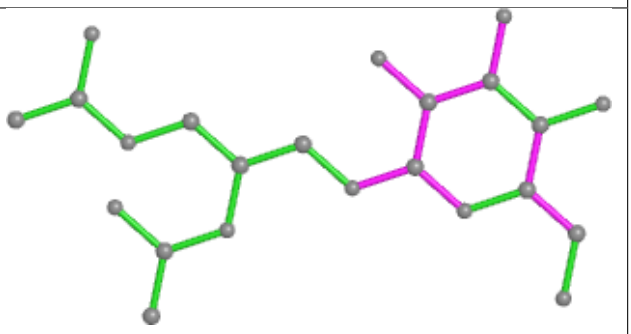

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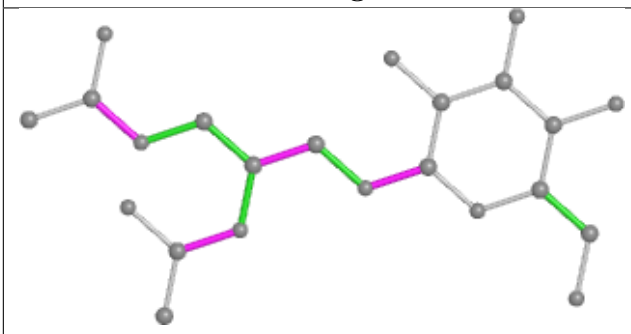

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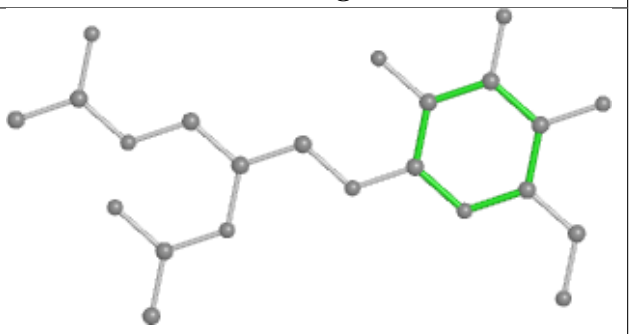
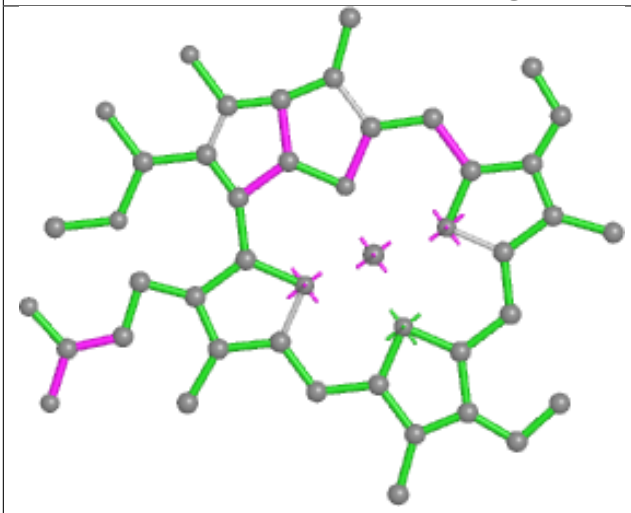


Rings

Ligand PMR OA 502



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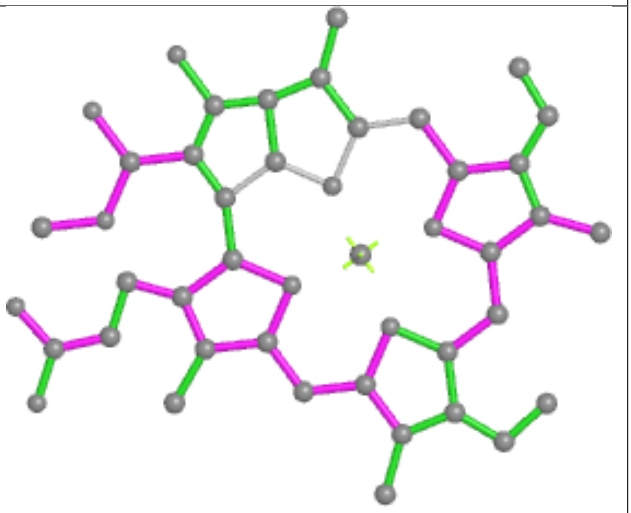

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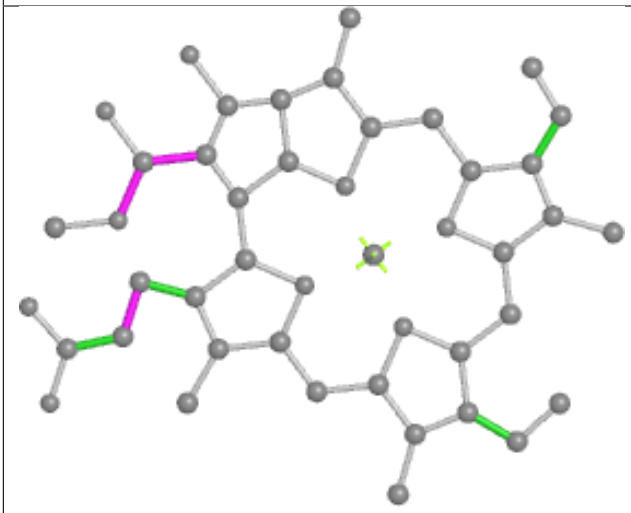

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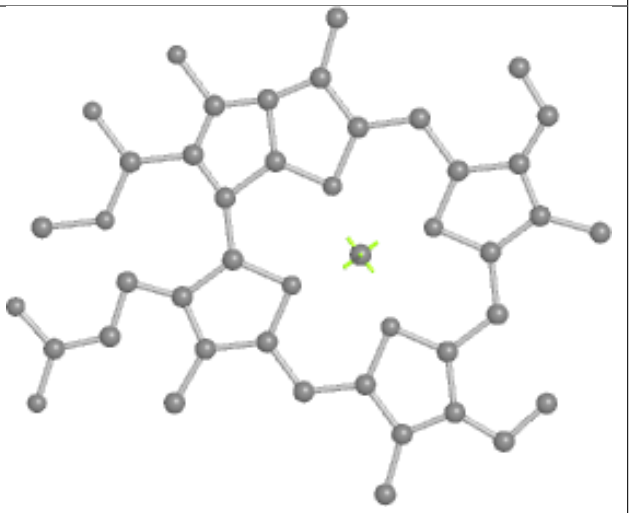
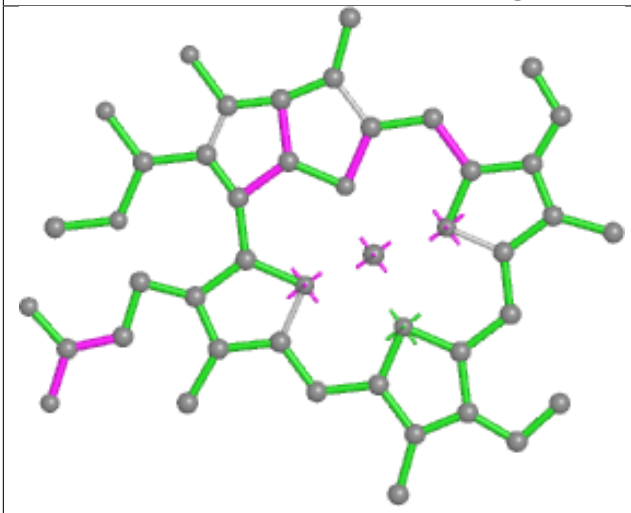


Rings

Ligand PMR FA 502



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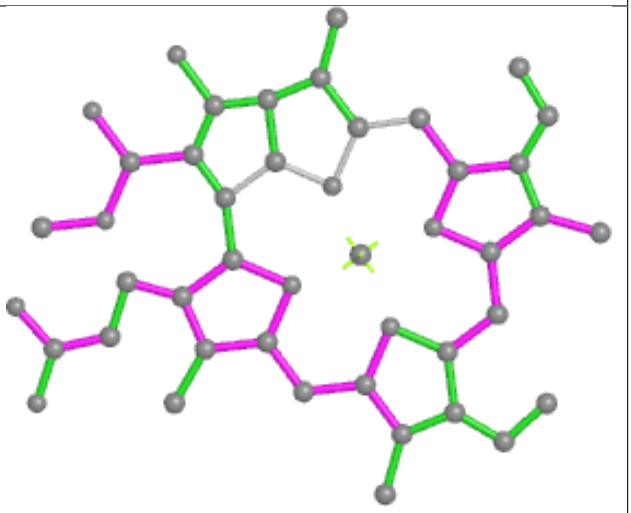

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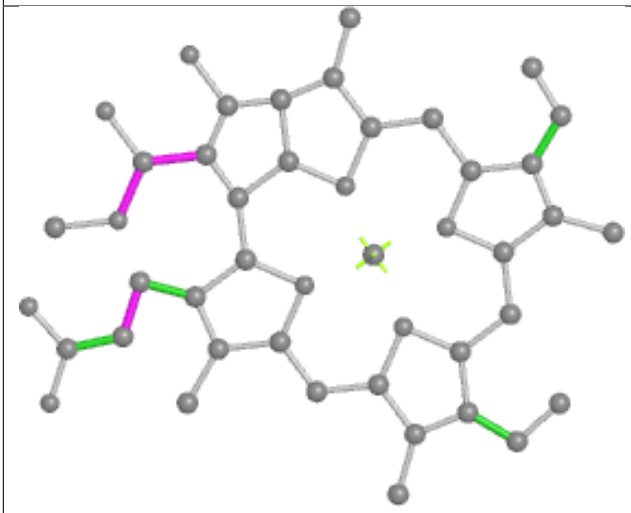

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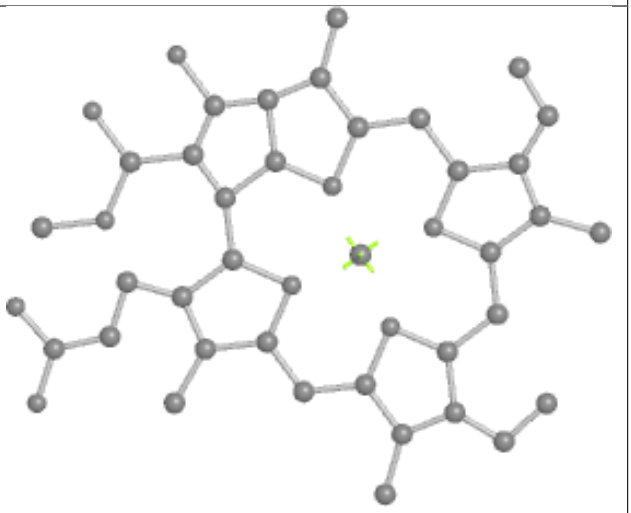
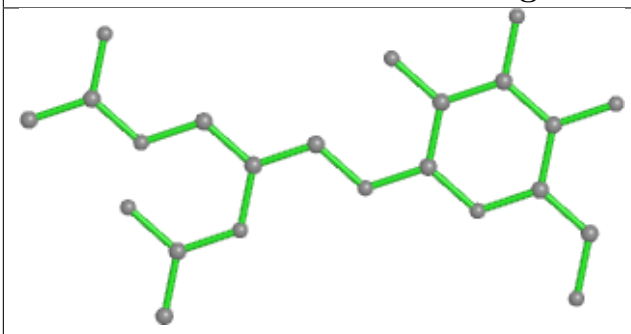


Rings

Ligand LMG C 503



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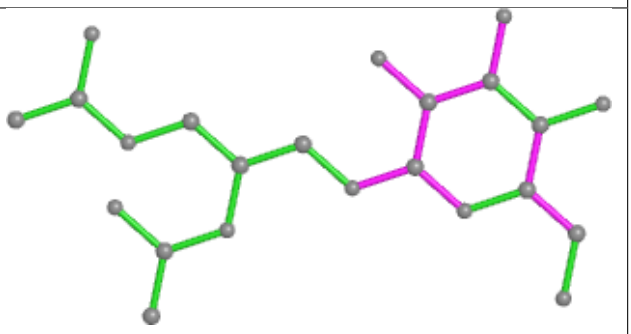

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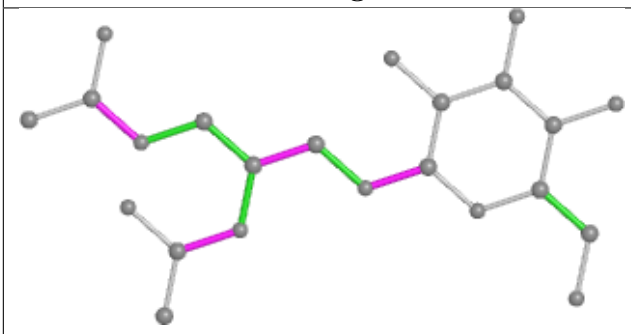

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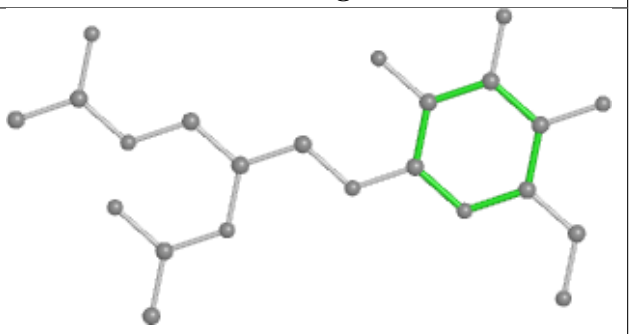
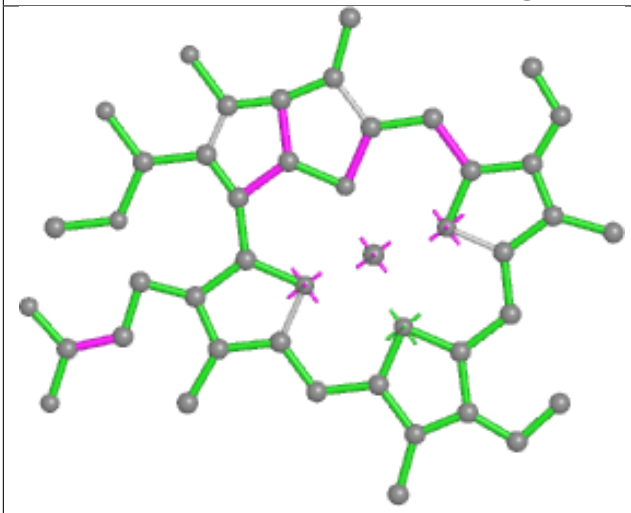


Rings

Ligand PMR A 502



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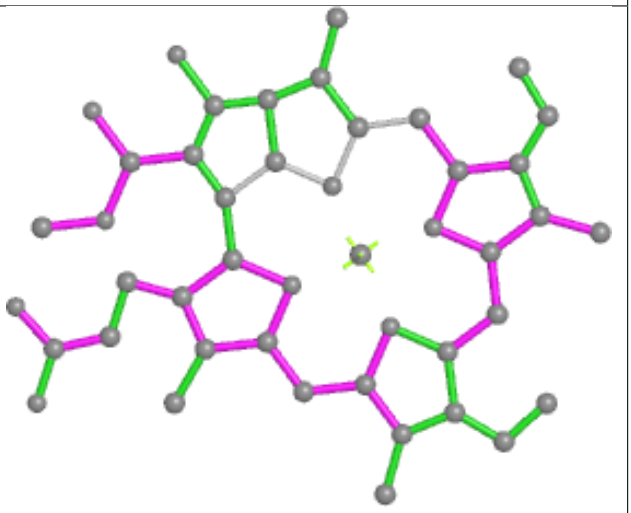

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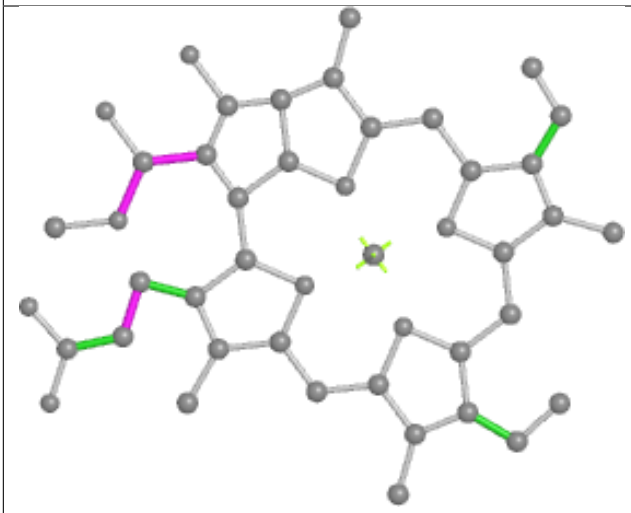

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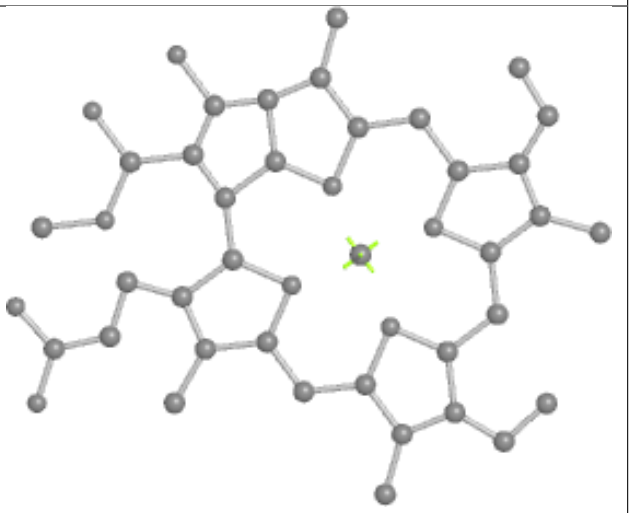
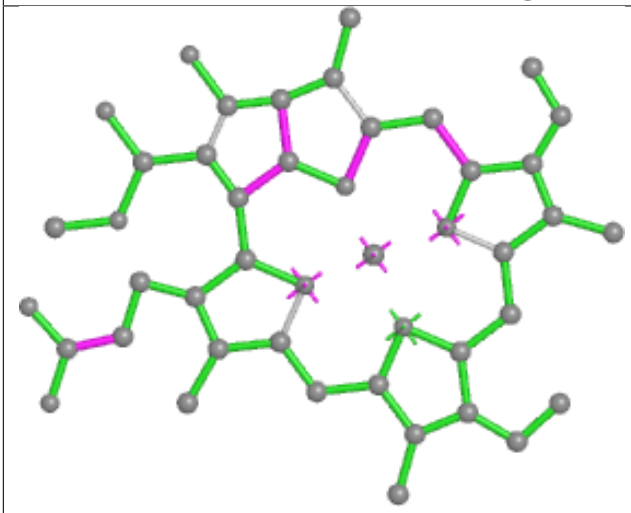


Rings

Ligand PMR B 502



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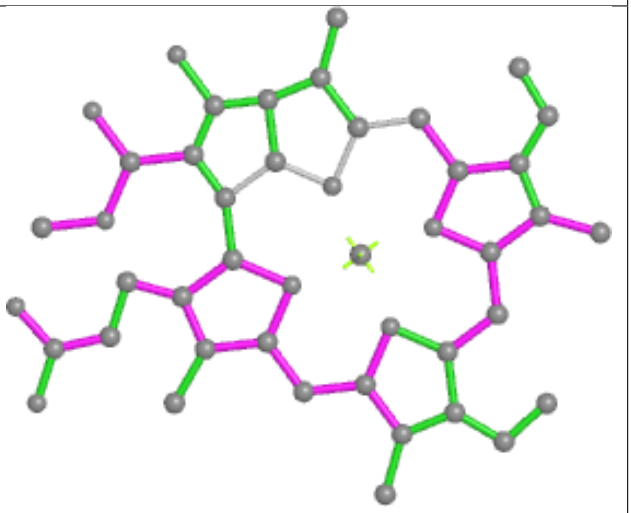

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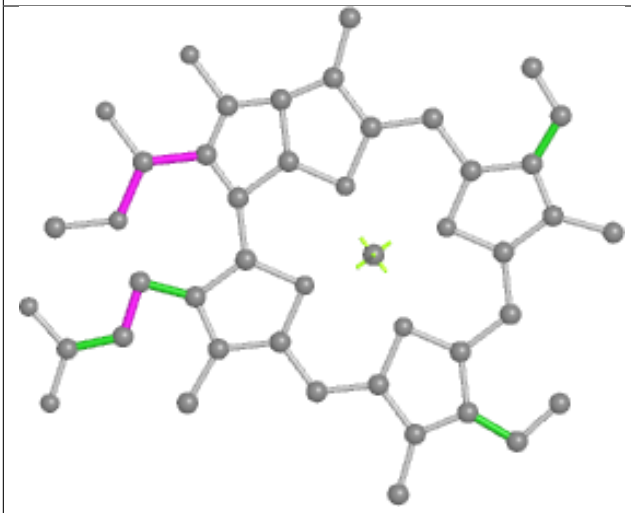

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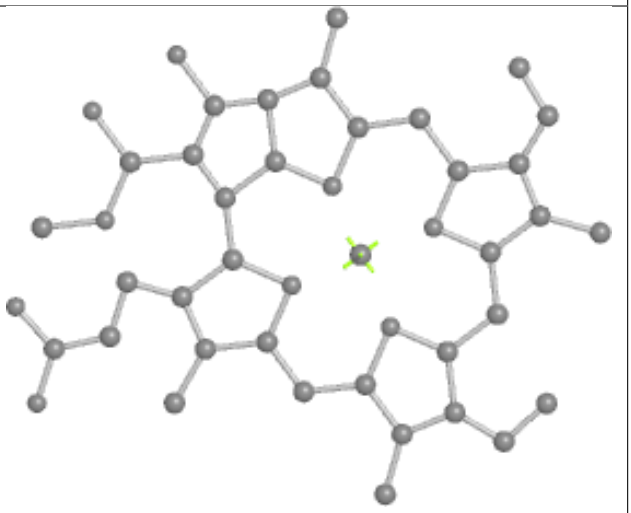
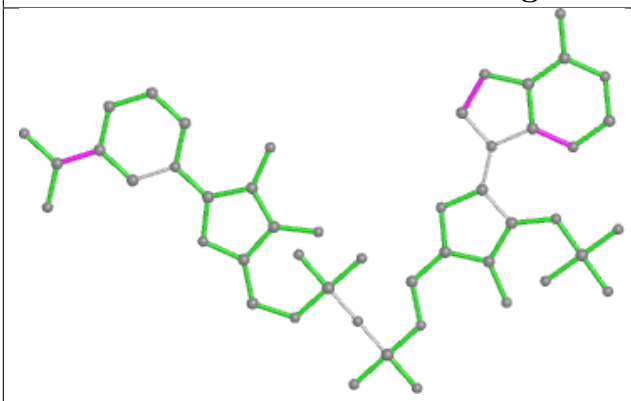


Rings

Ligand NDP V 501



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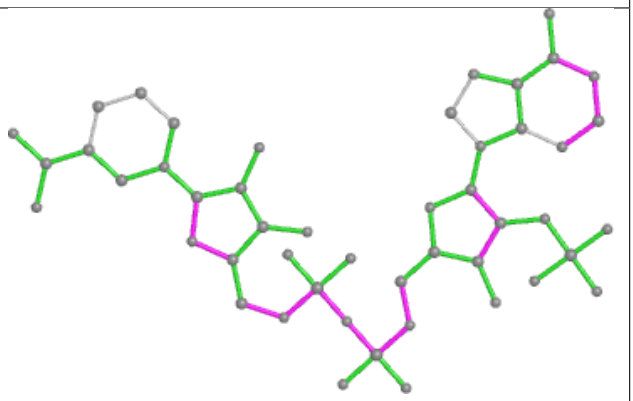
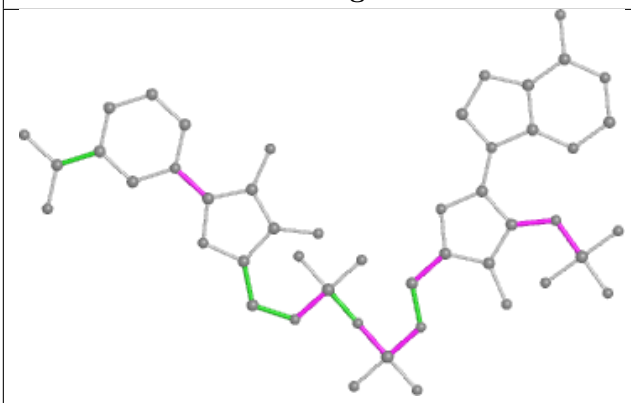


Bond angles



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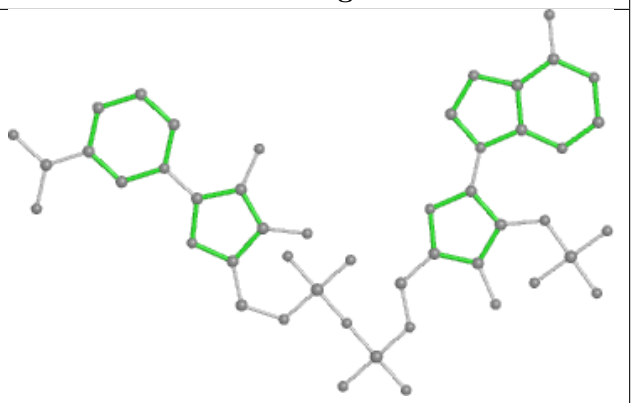
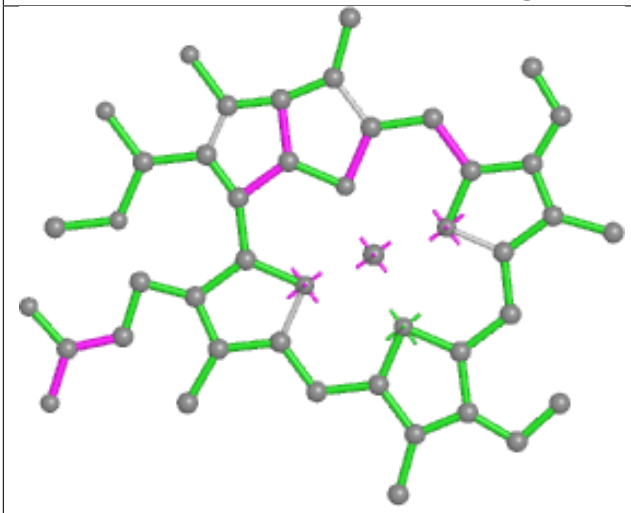


Rings

Ligand PMR X 502



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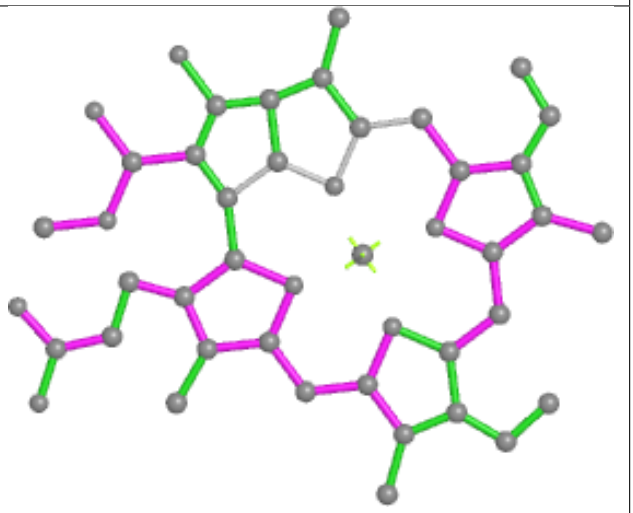
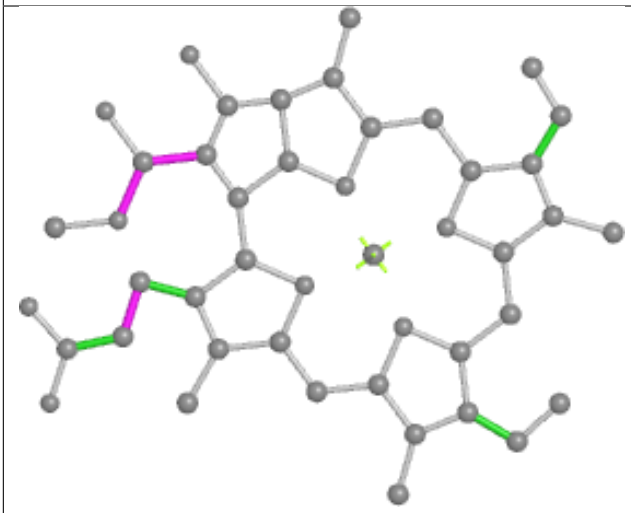


Bond angles



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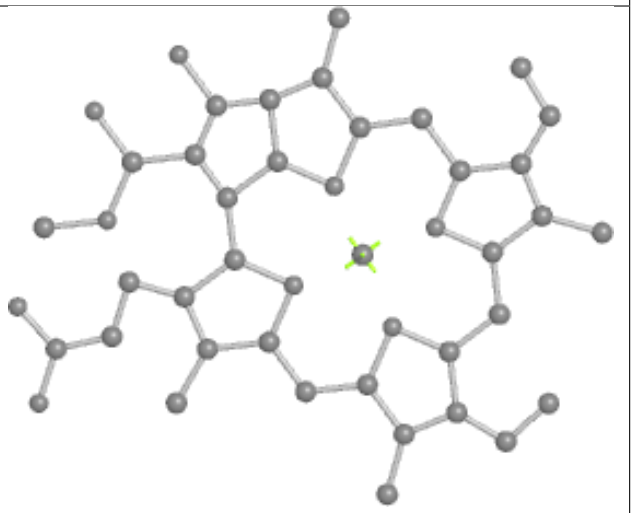
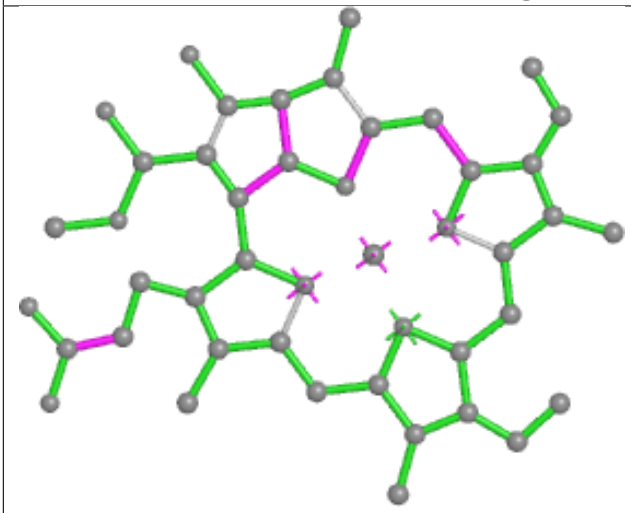


Rings

Ligand PMR N 502



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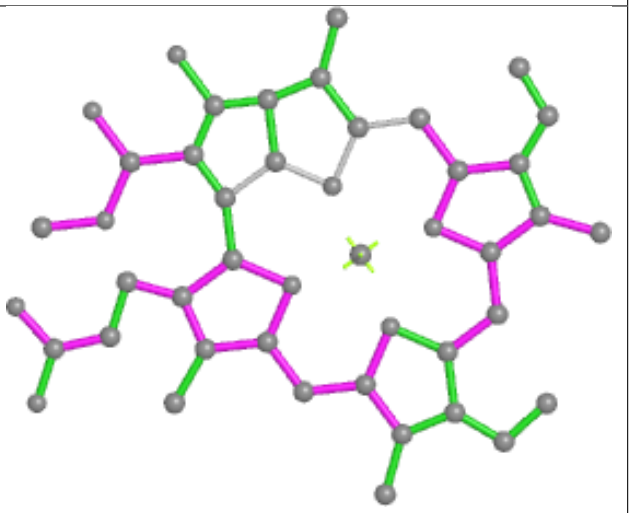
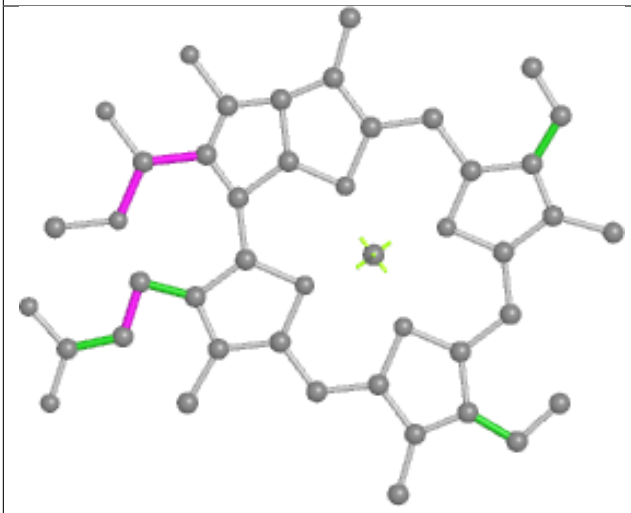


Bond angles



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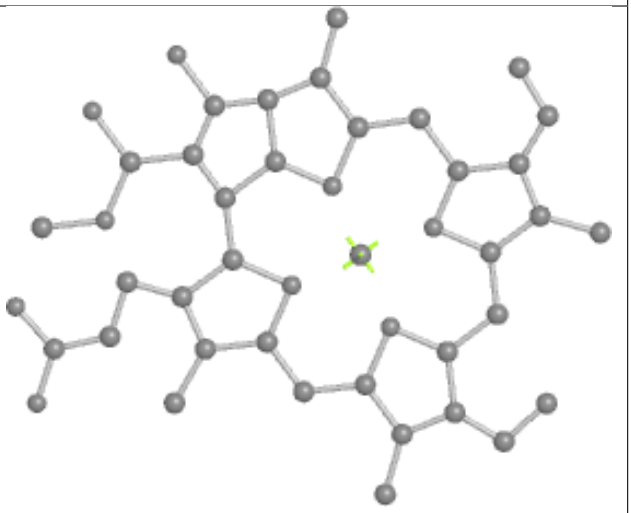
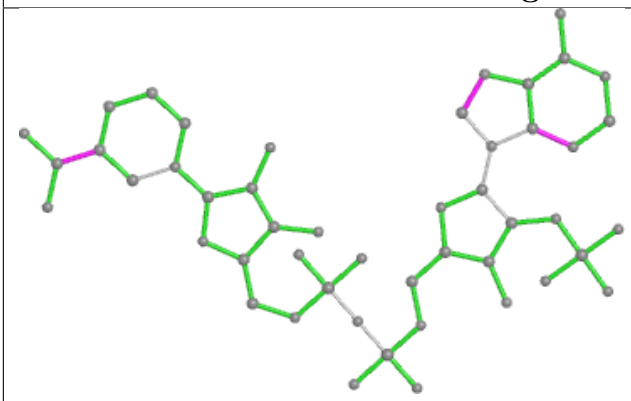


Rings

Ligand NDP C 501



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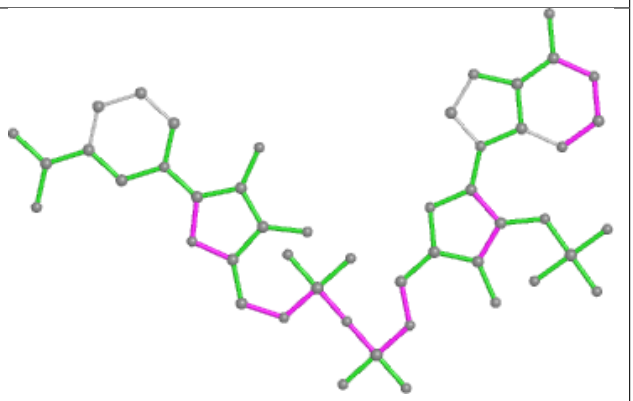

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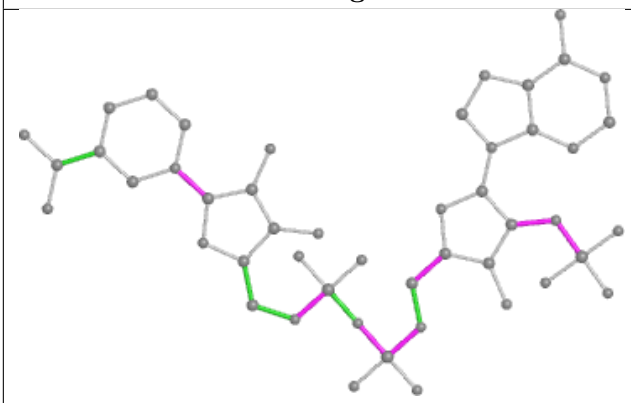

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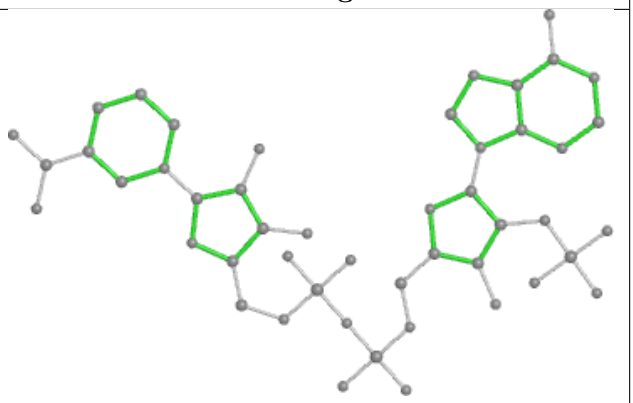
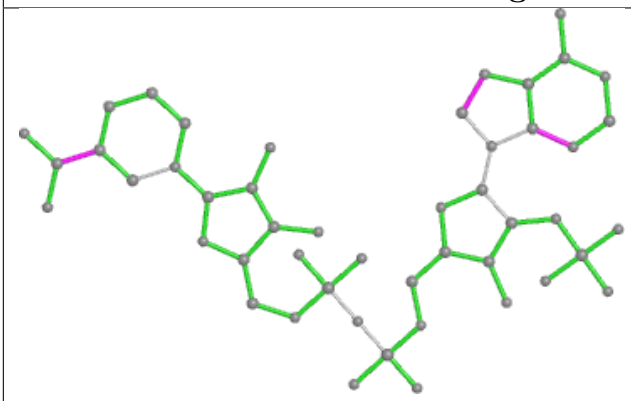


Rings

Ligand NDP EA 501



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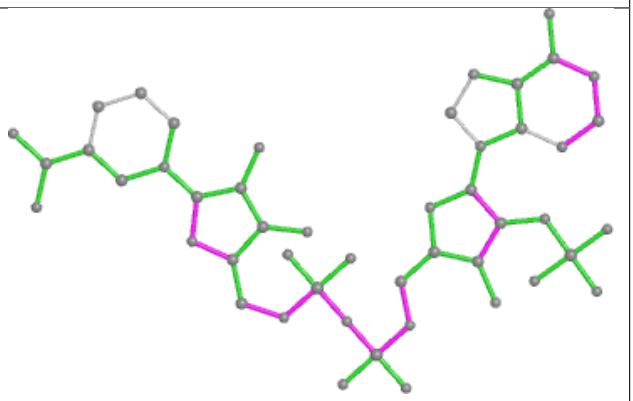
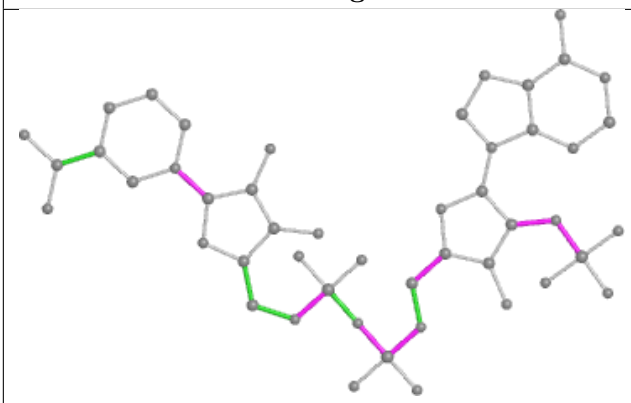


Bond angles



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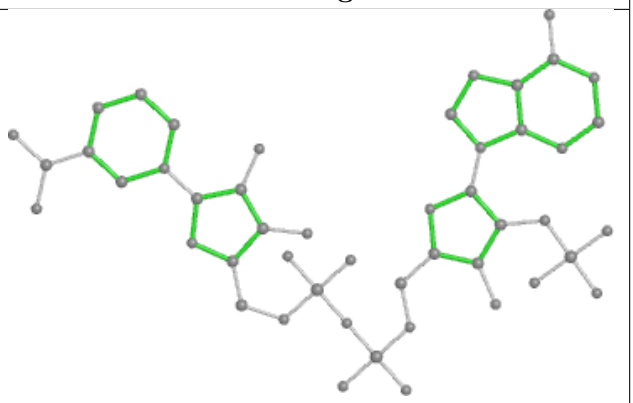
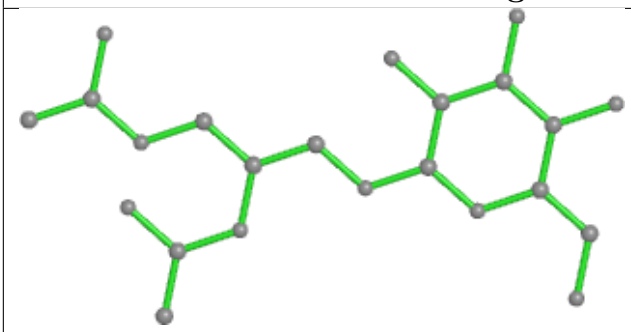


Rings

Ligand LMG EA 503



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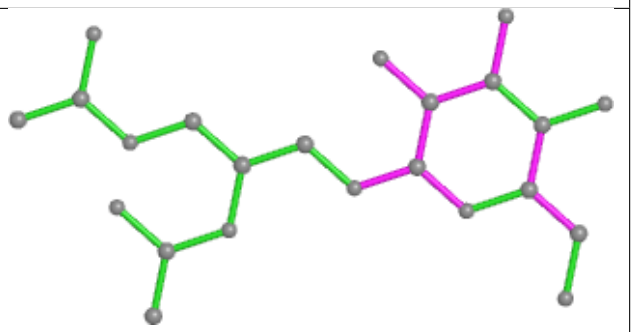

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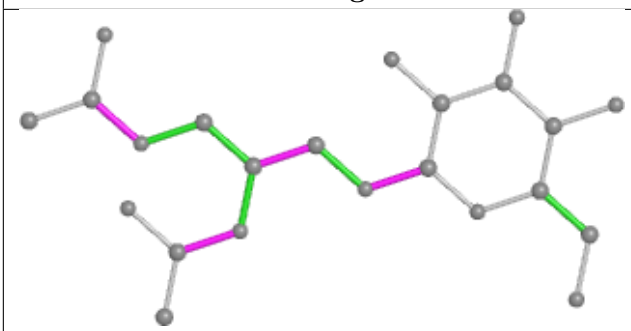

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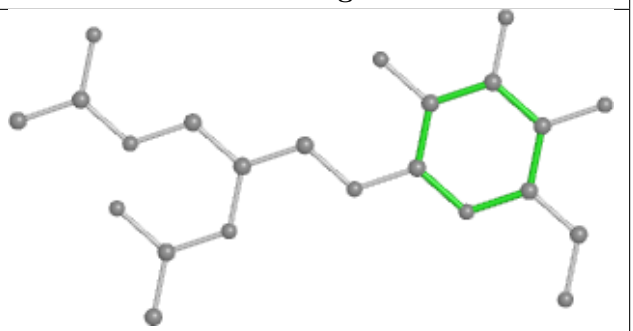
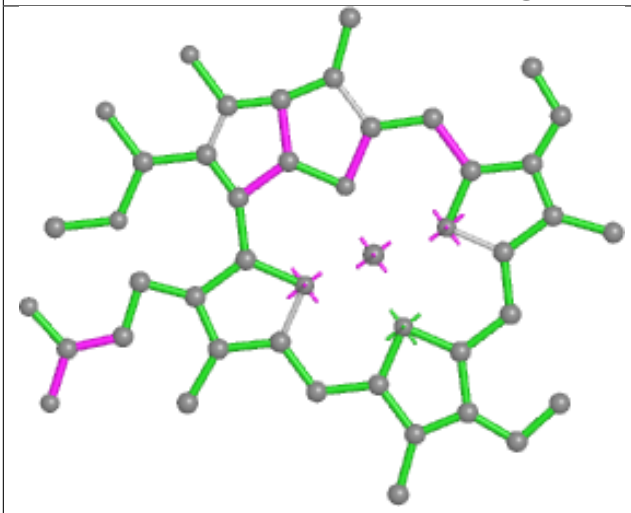


Rings

Ligand PMR H 502



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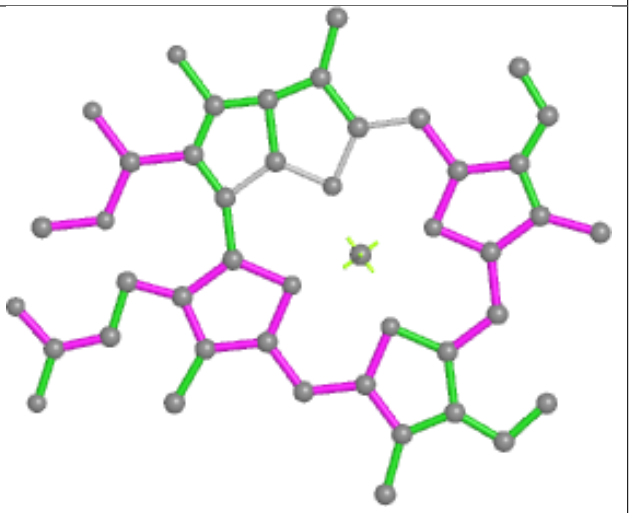
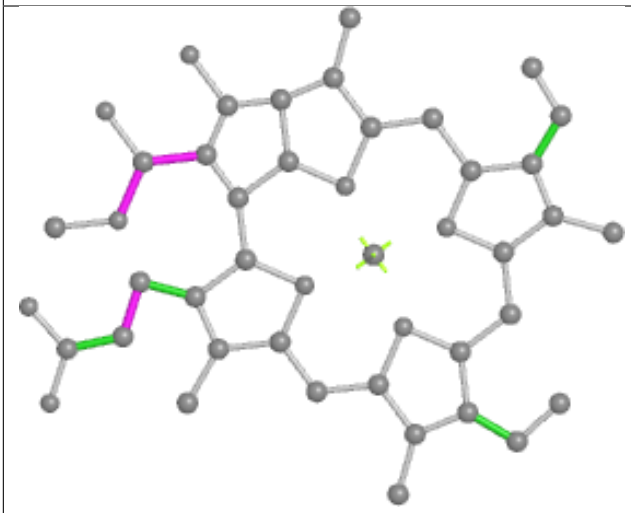
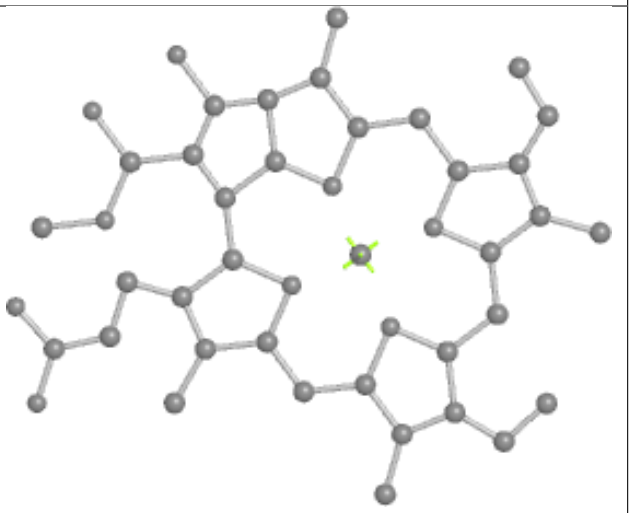


Bond angles

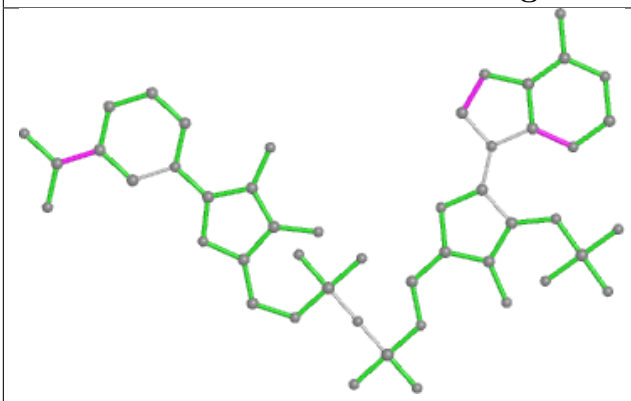


Torsions



Rings

Ligand NDP G 501



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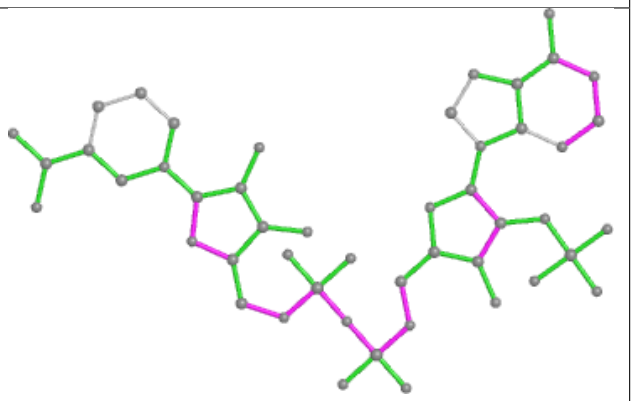

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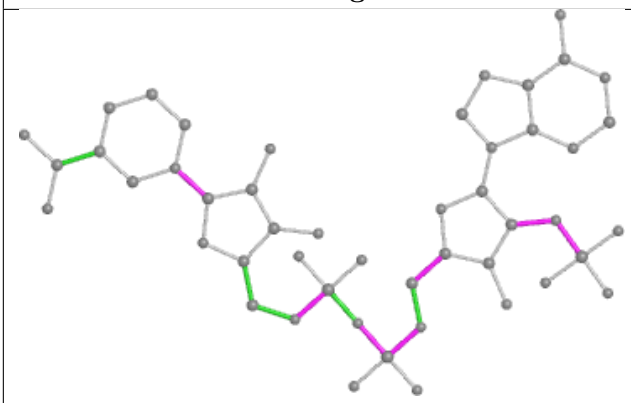

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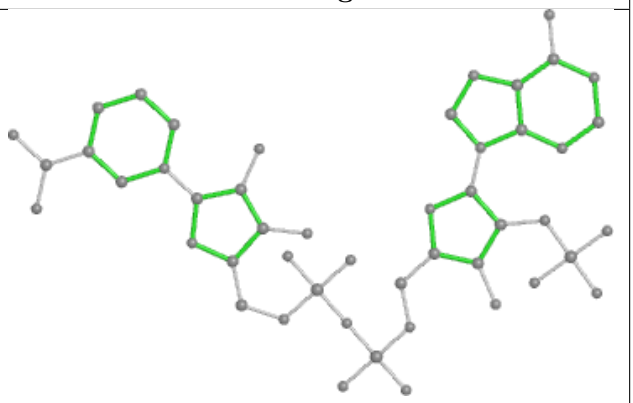

Rings

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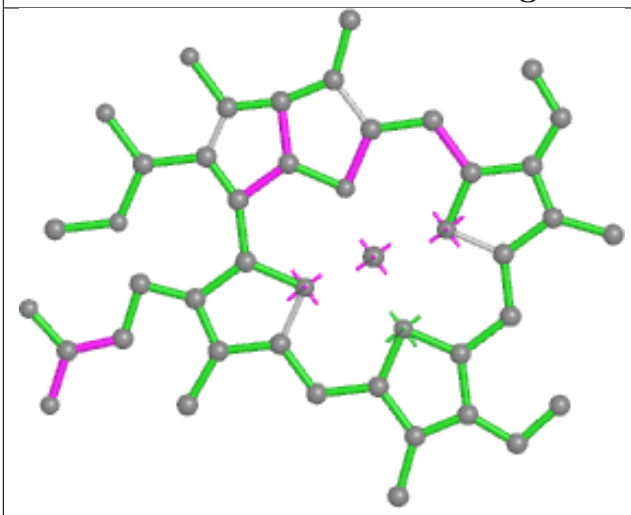

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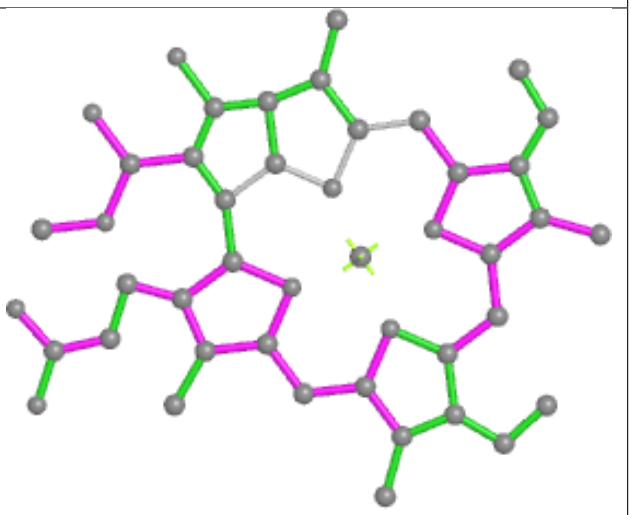

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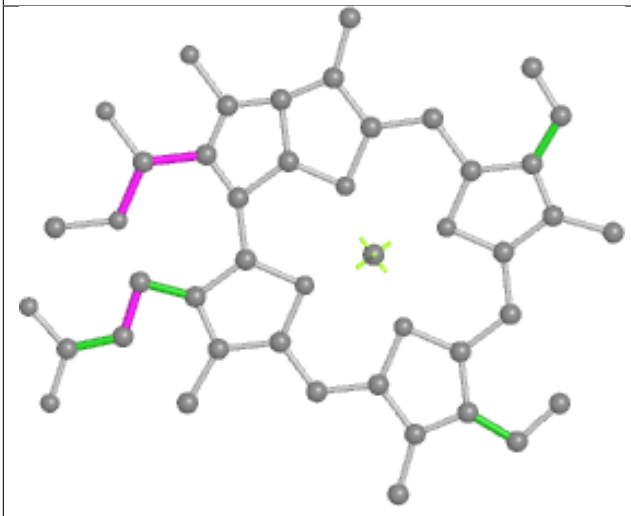

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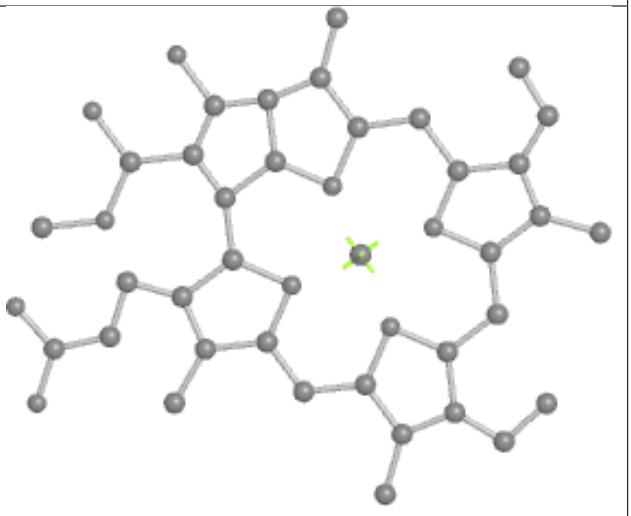

Rings

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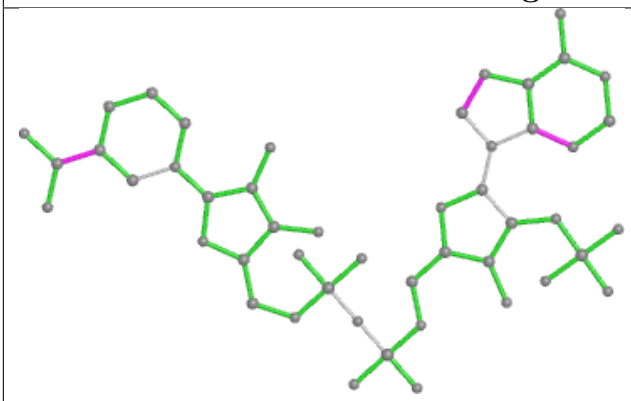

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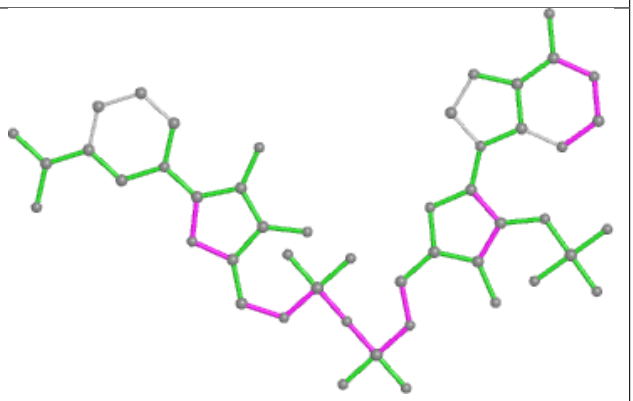

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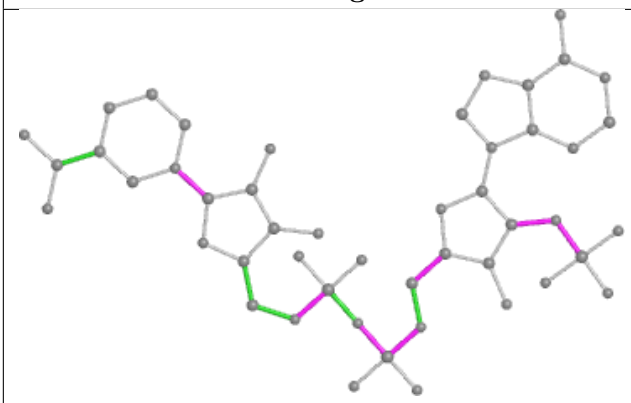

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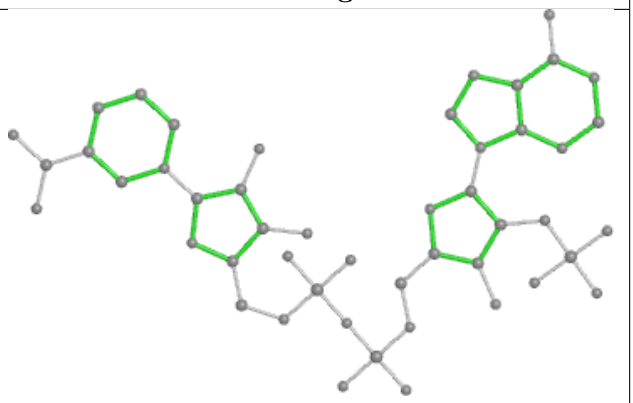

Rings

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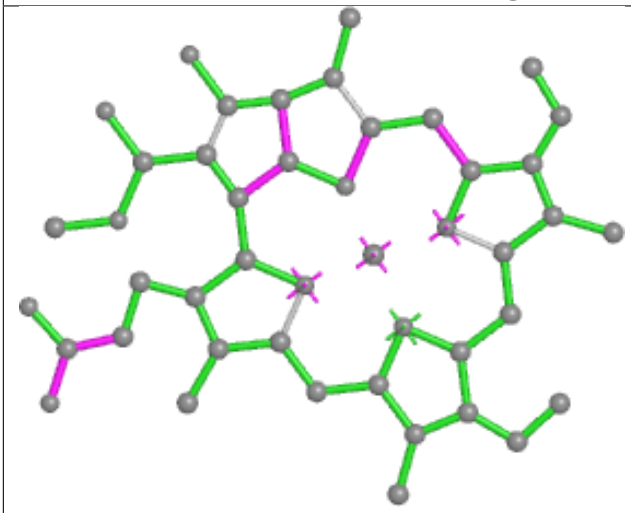

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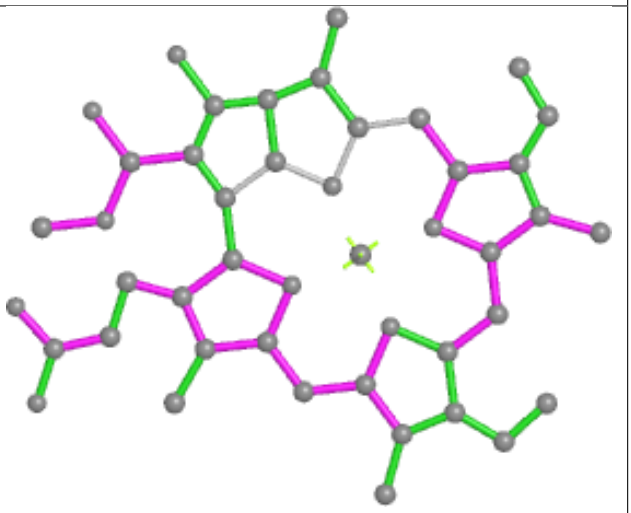

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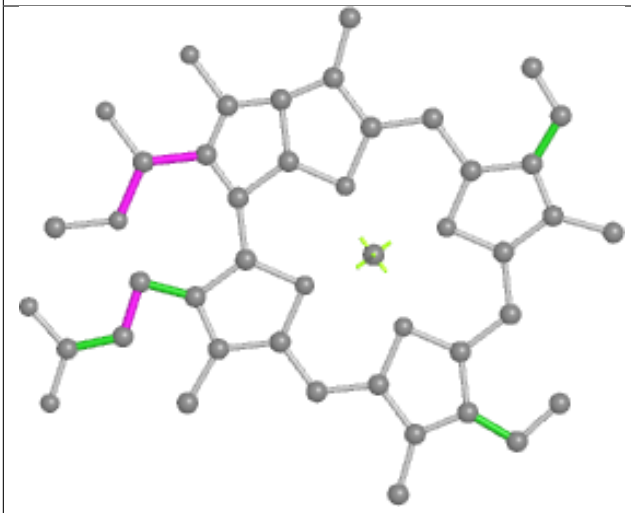

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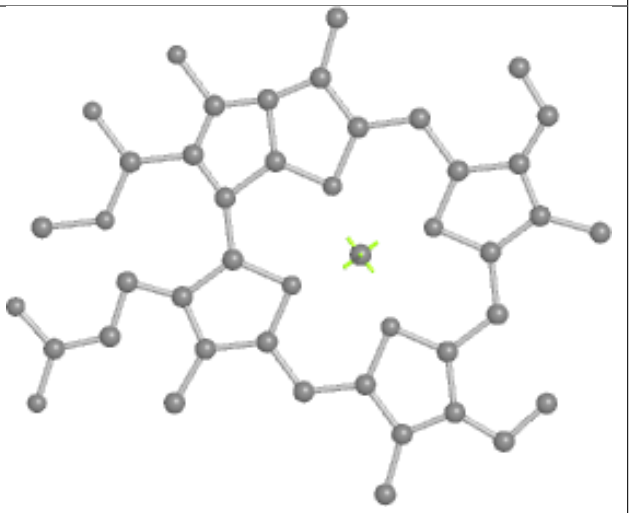
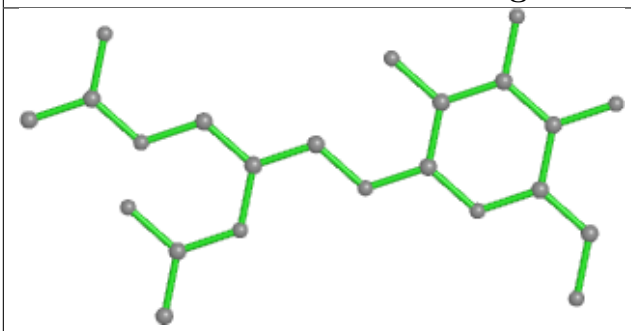


Rings

Ligand LMG JA 503



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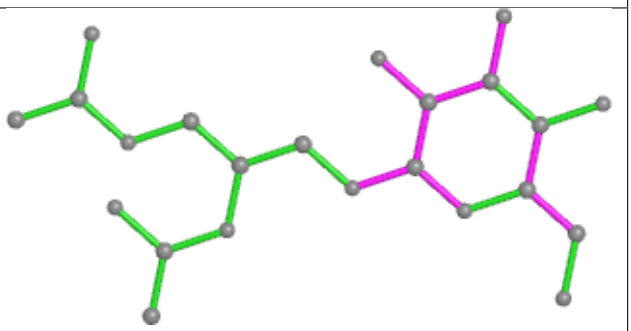

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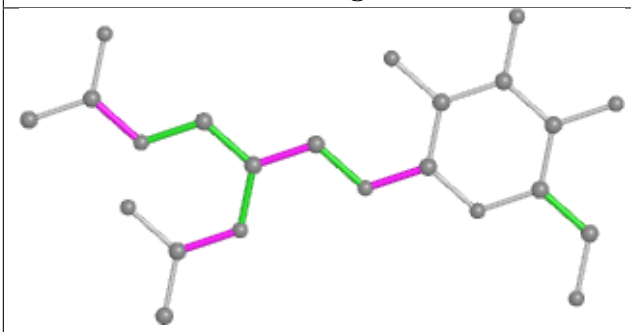

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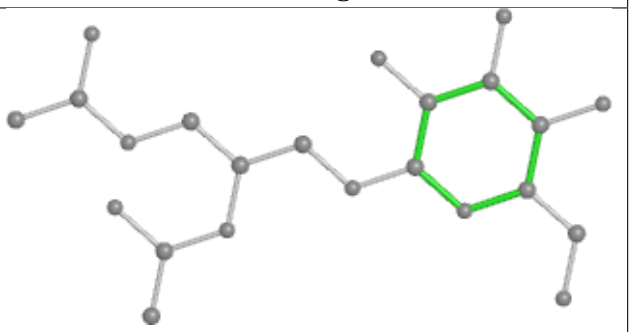
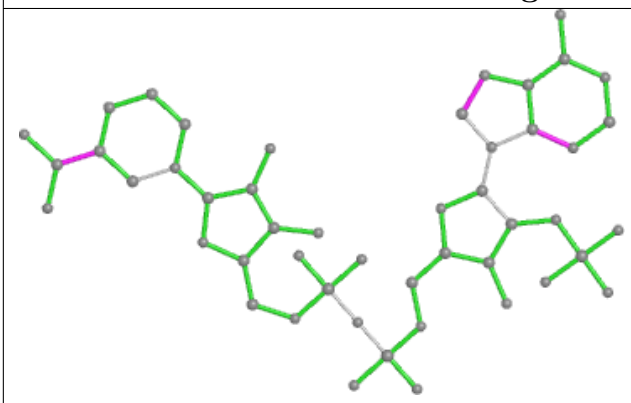


Rings

Ligand NDP R 501



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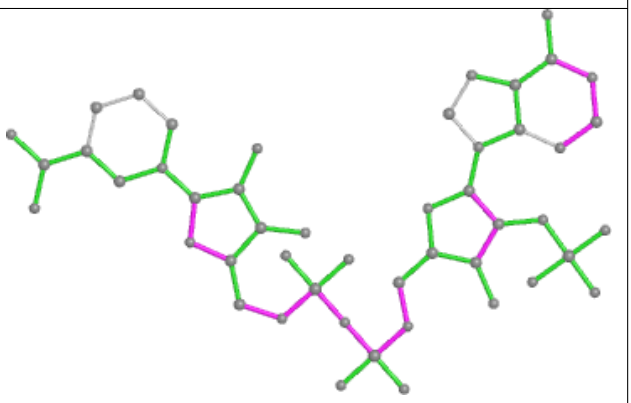

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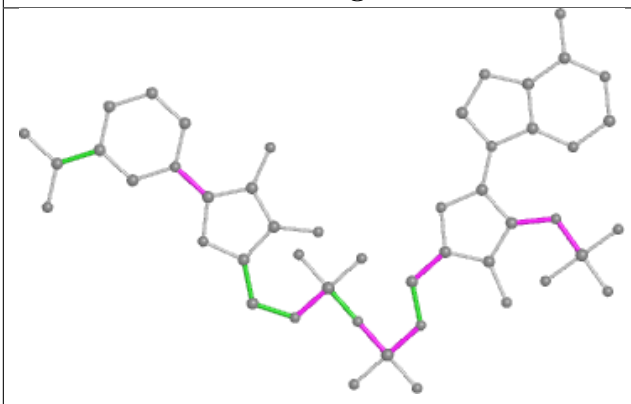

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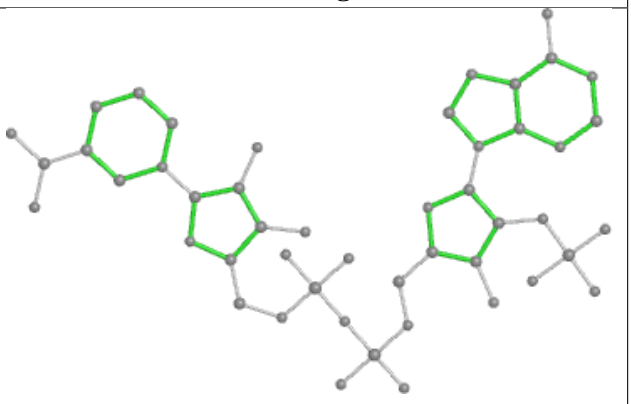
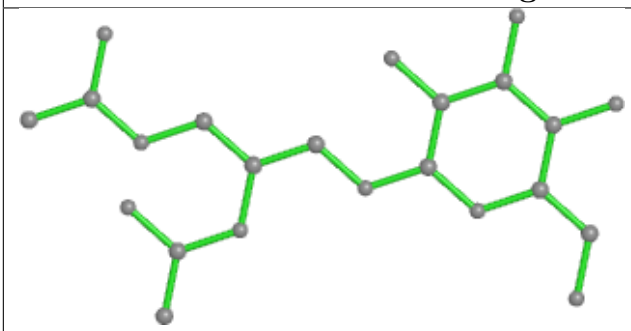


Rings

Ligand LMG R 503



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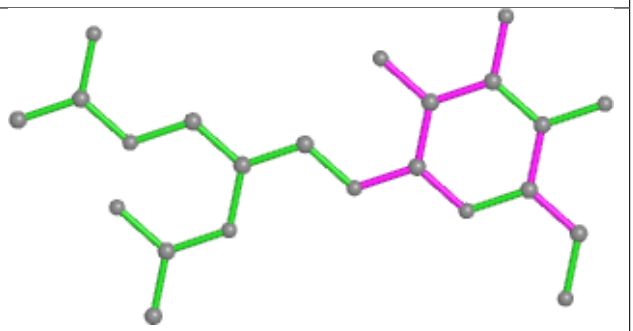

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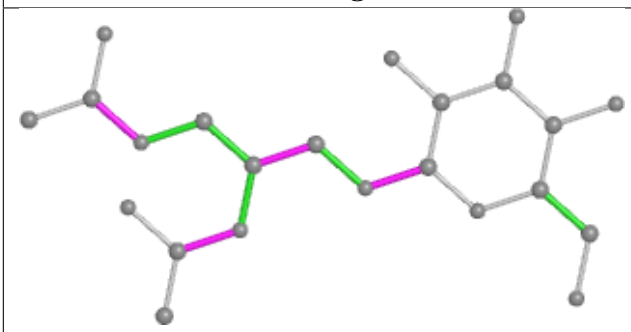

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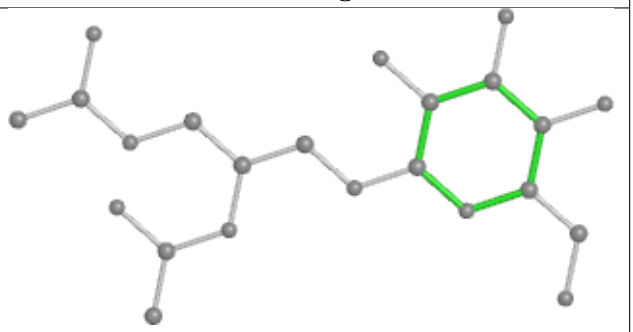

Rings

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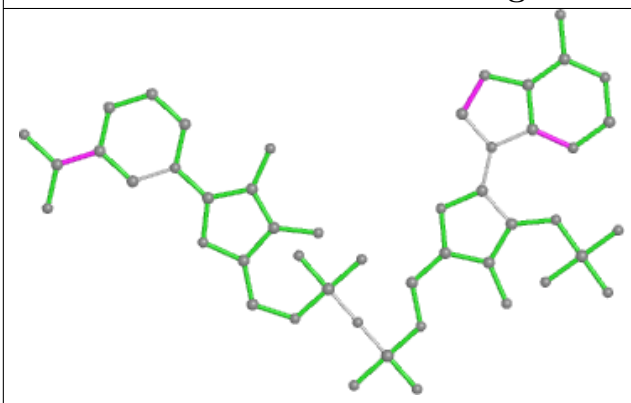

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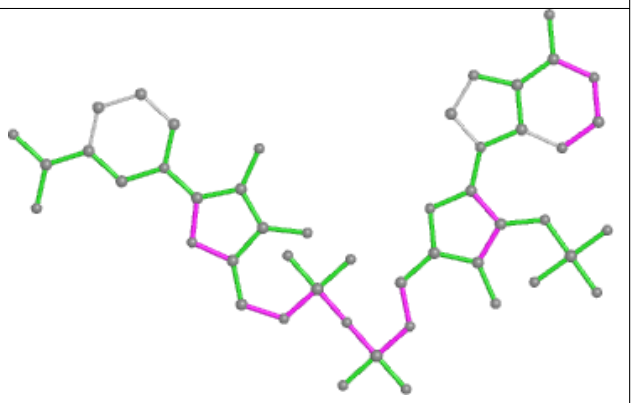

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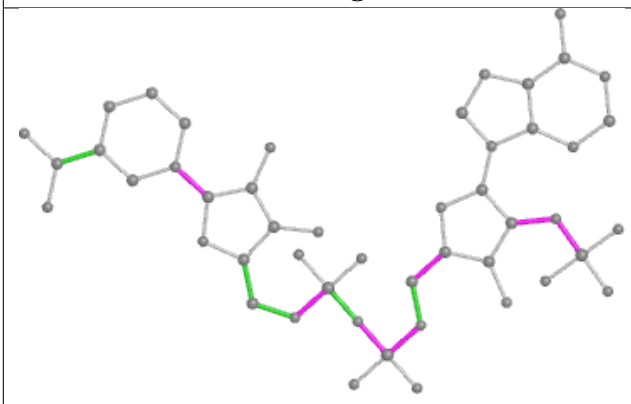

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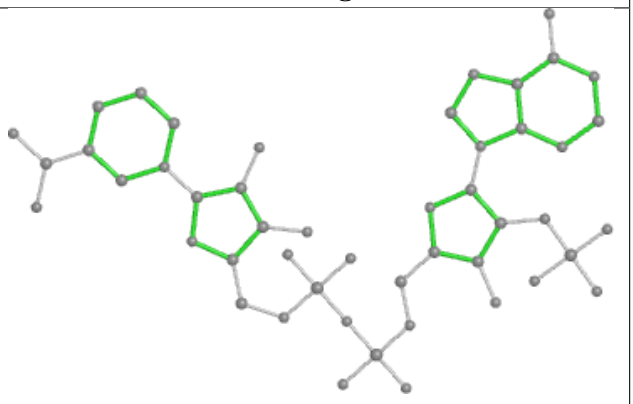

Rings

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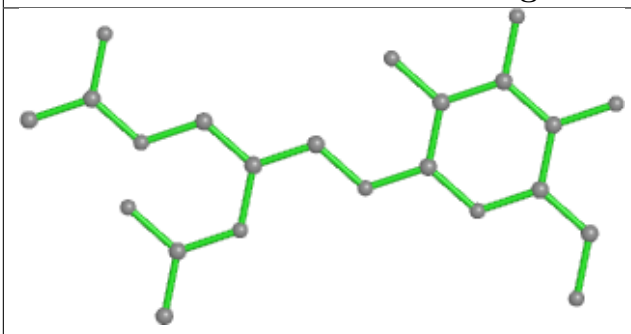

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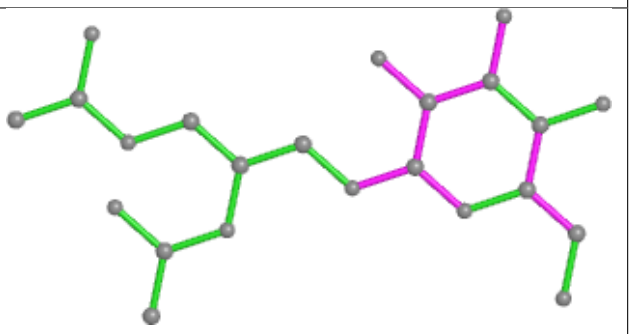

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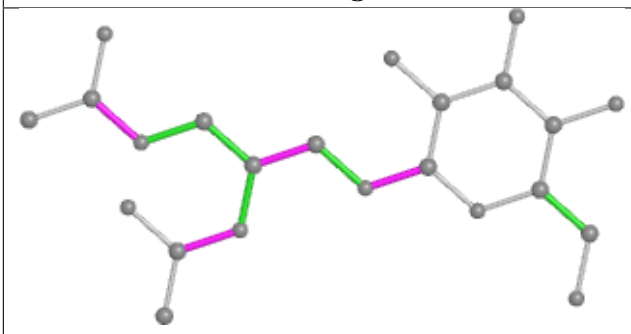

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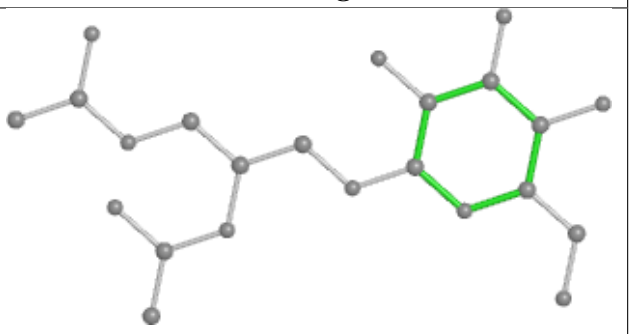

Rings

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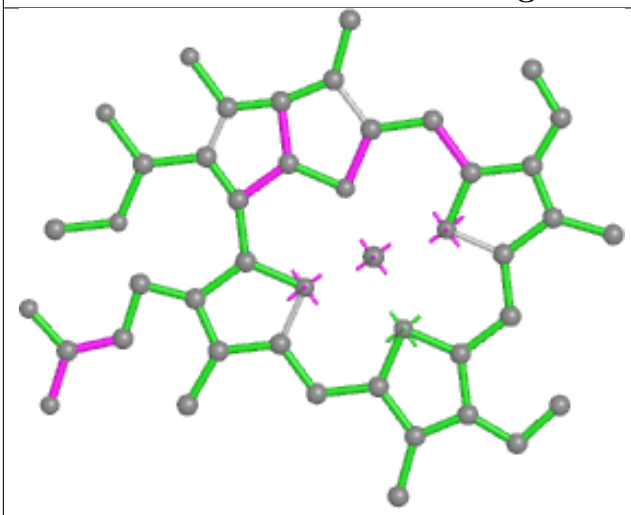

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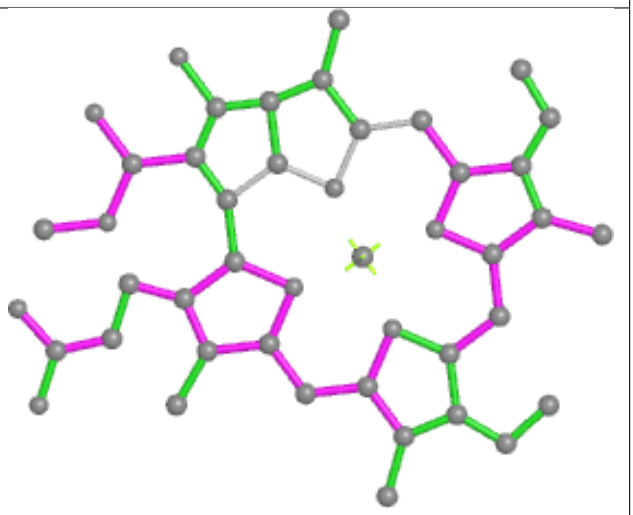

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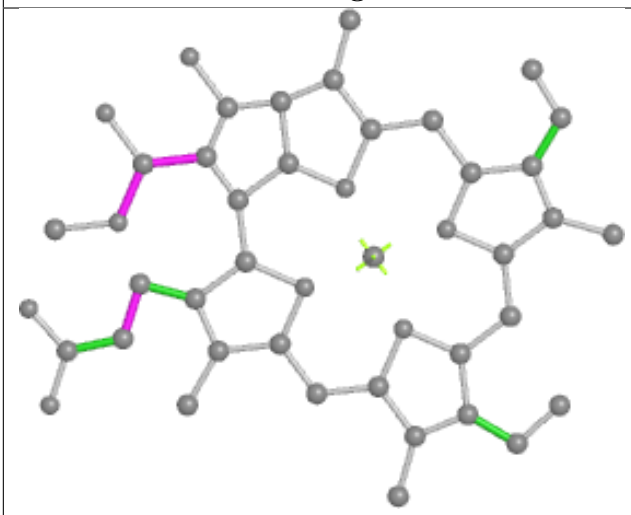

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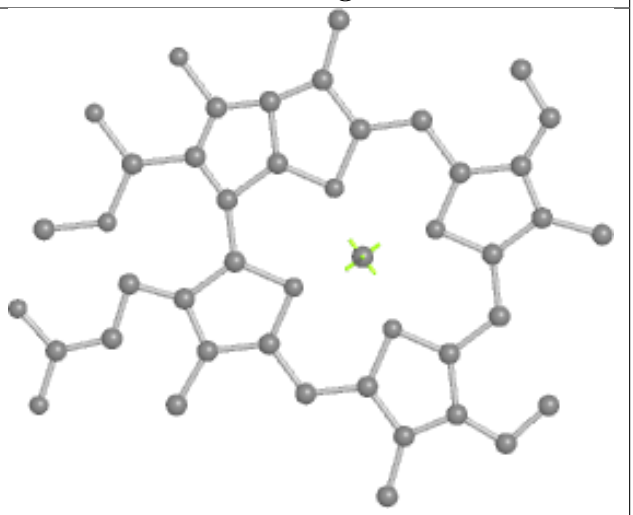
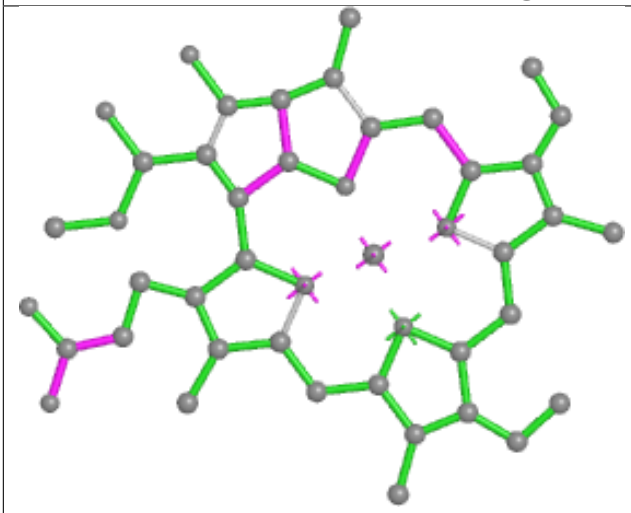


Rings

Ligand PMR D 502



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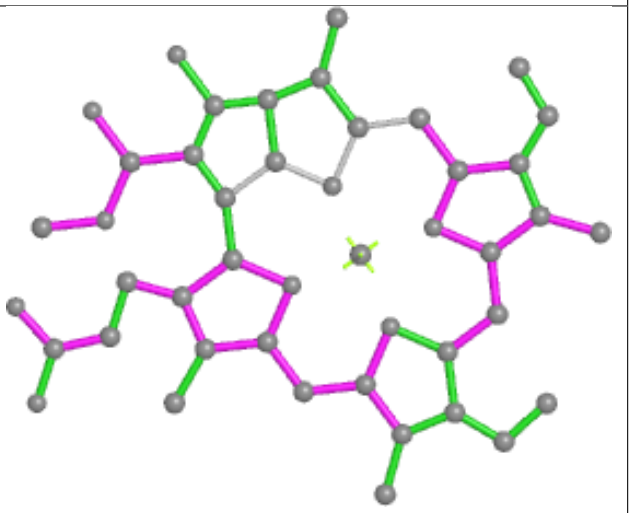

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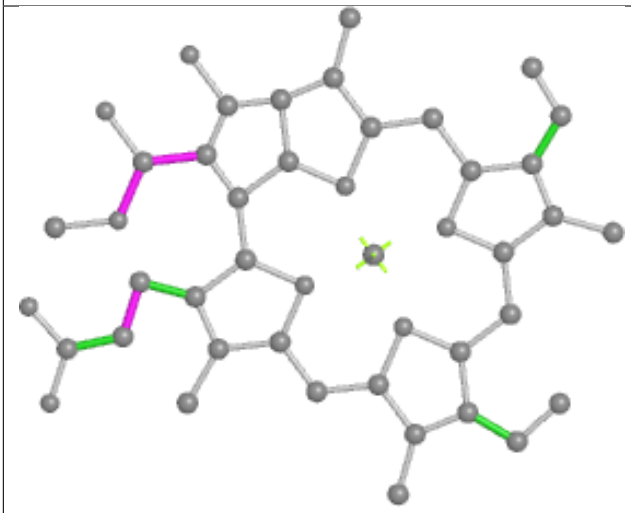

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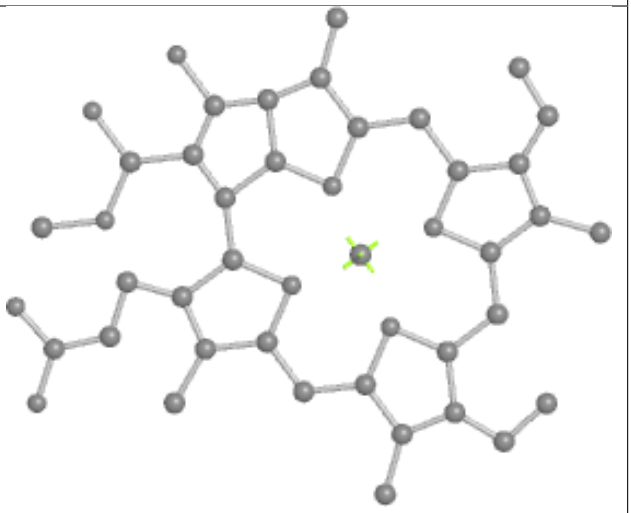
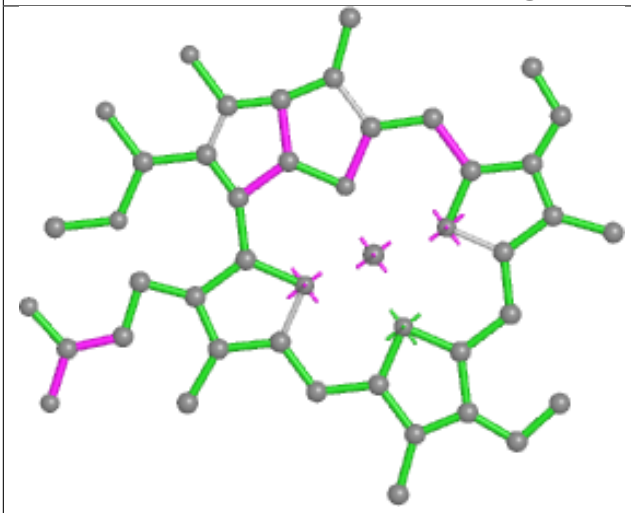


Rings

Ligand PMR L 502



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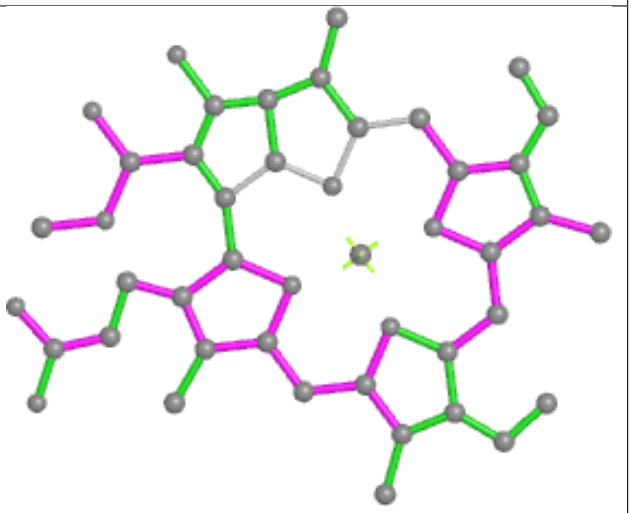

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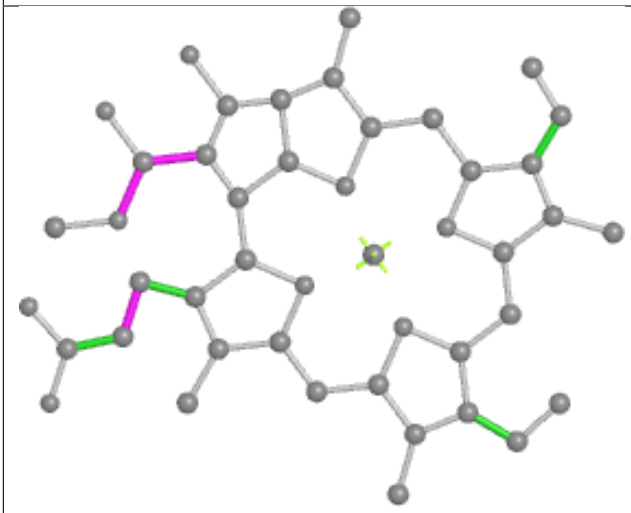

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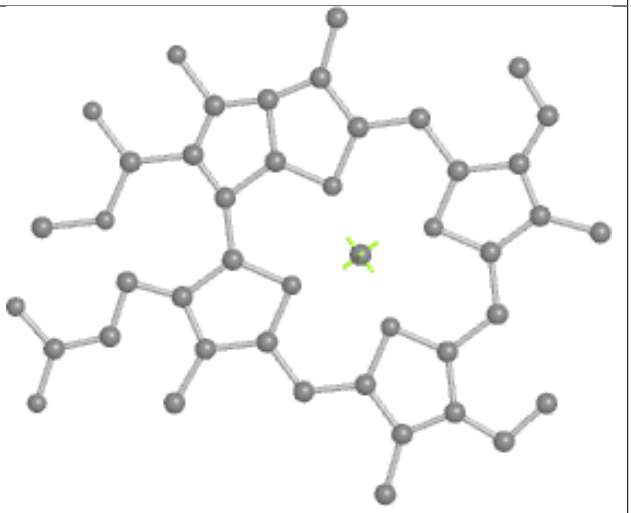
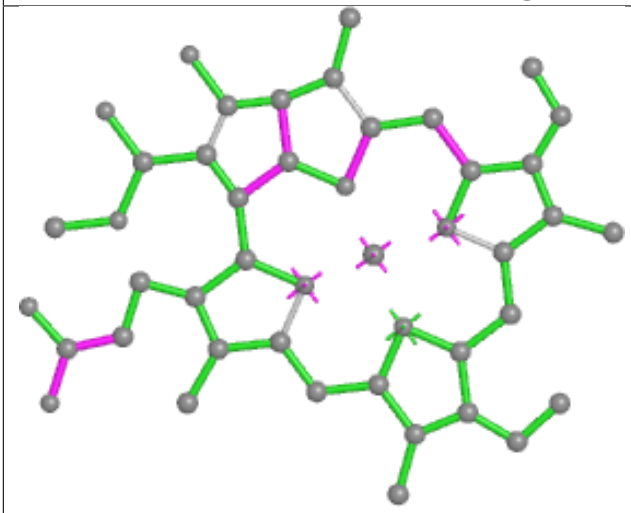


Rings

Ligand PMR Q 502



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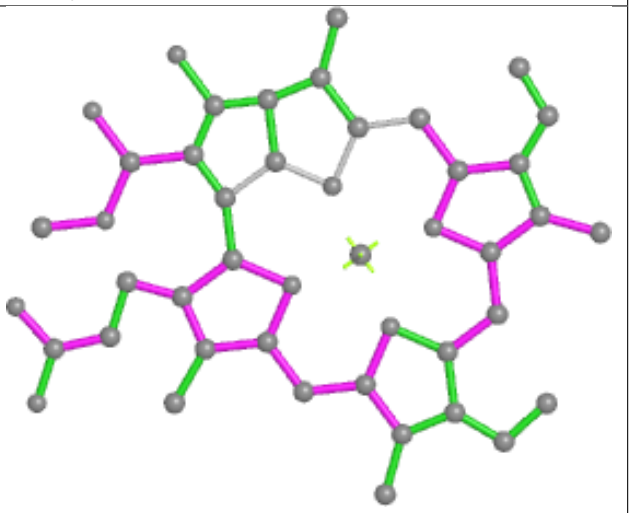

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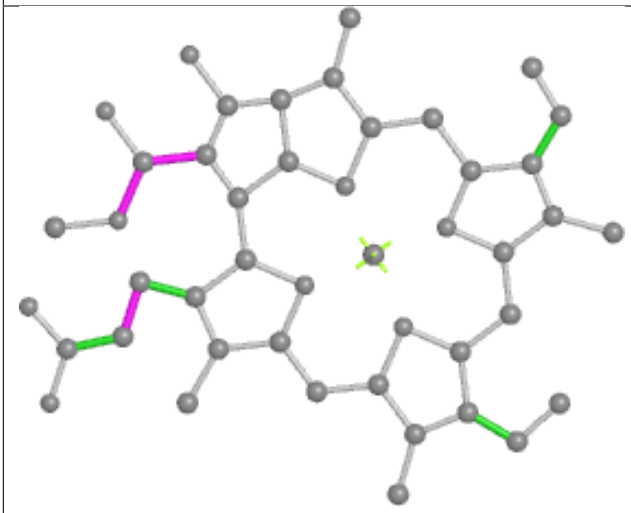

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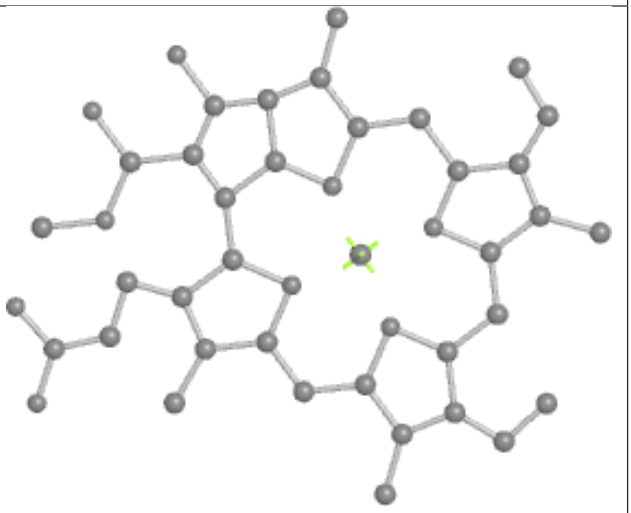
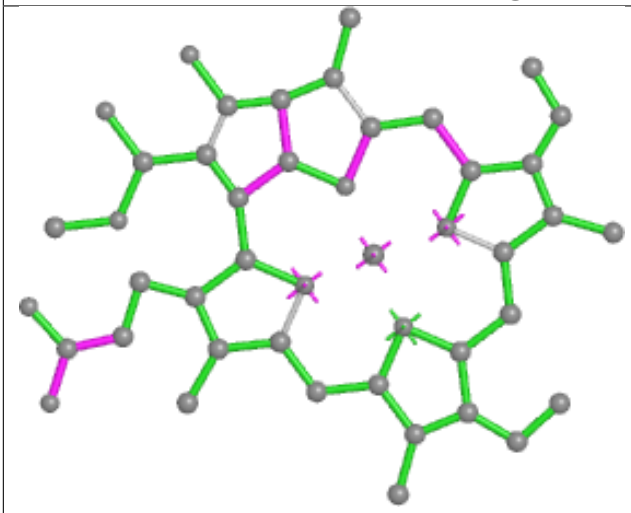


Rings

Ligand PMR EA 502



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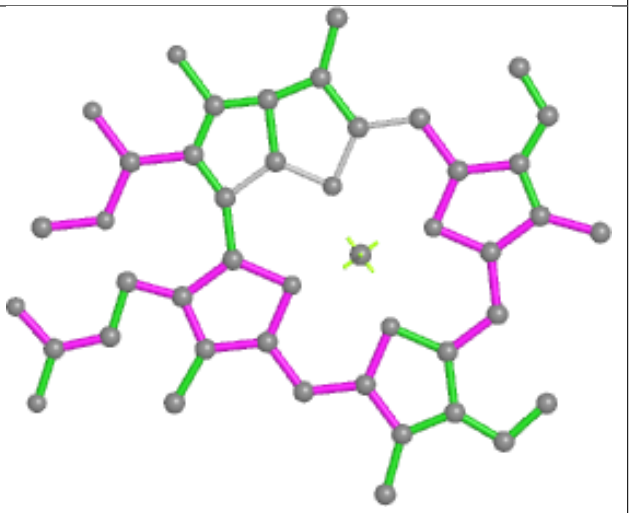
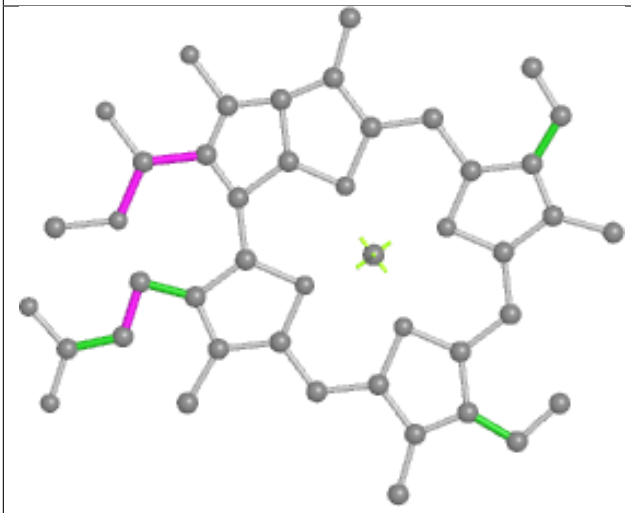


Bond angles



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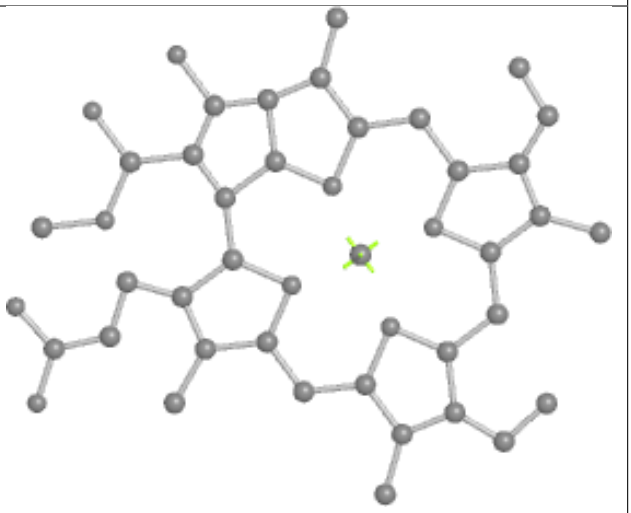
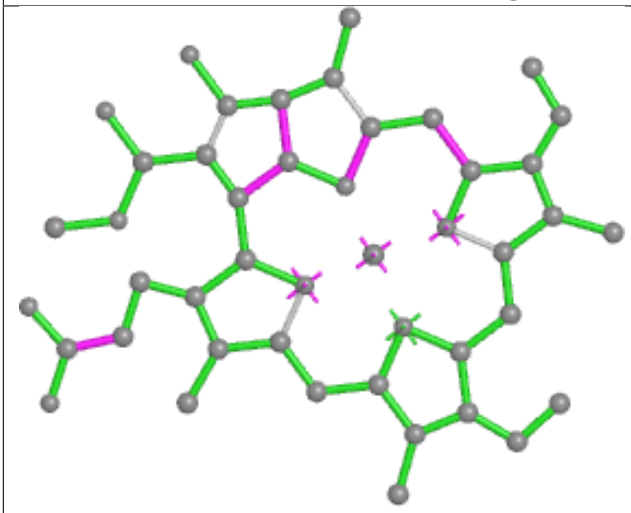


Rings

Ligand PMR AA 502



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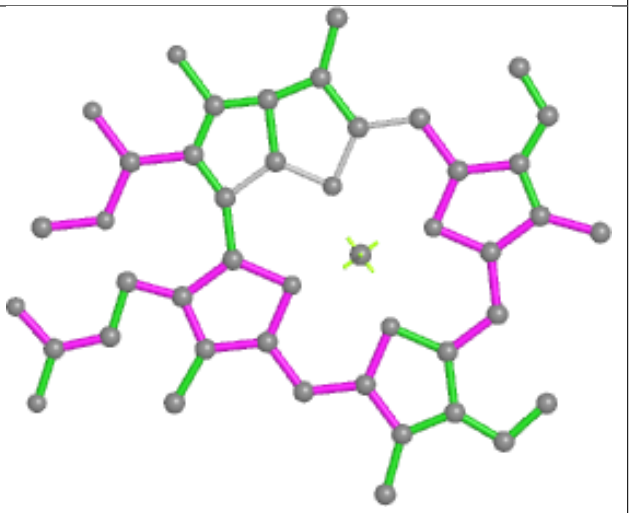

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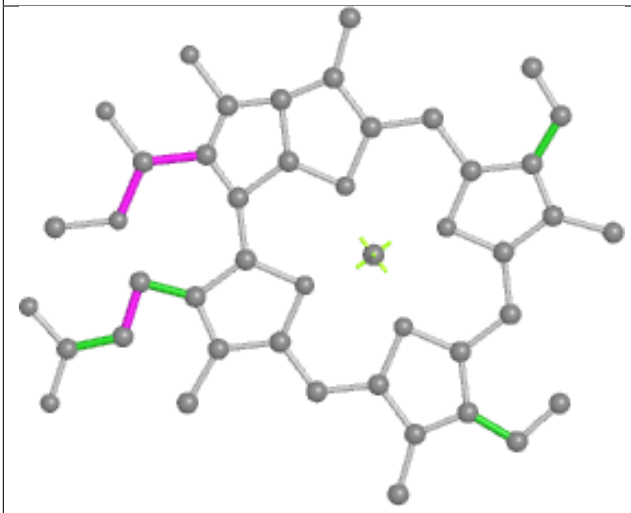
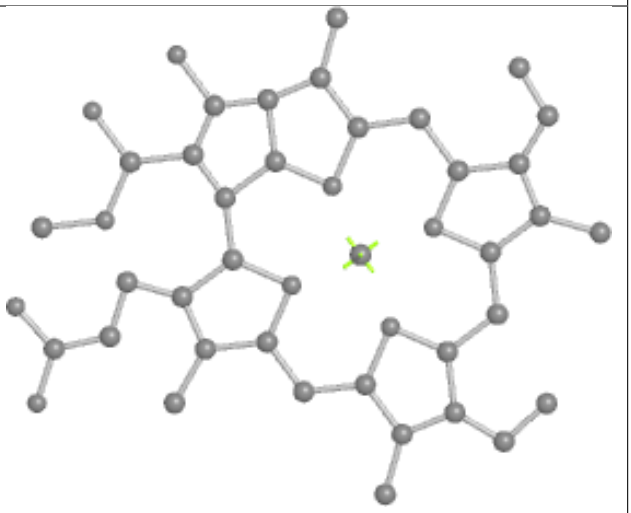
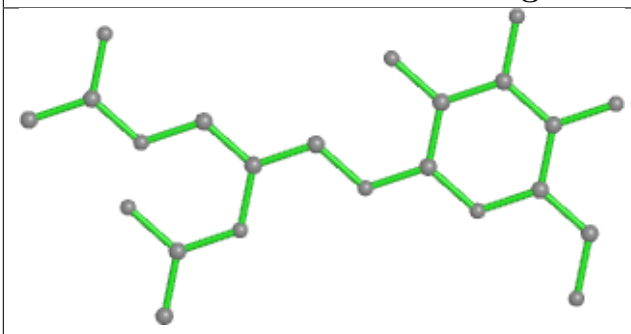


Torsions



Rings

Ligand LMG F 503



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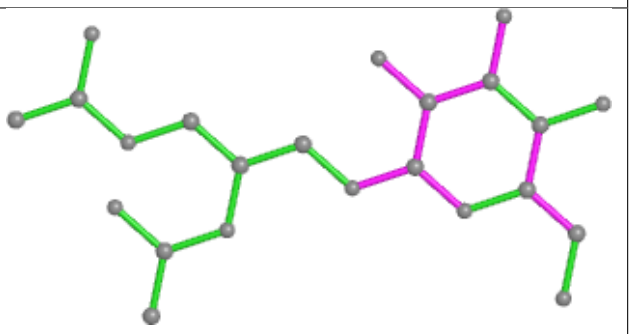

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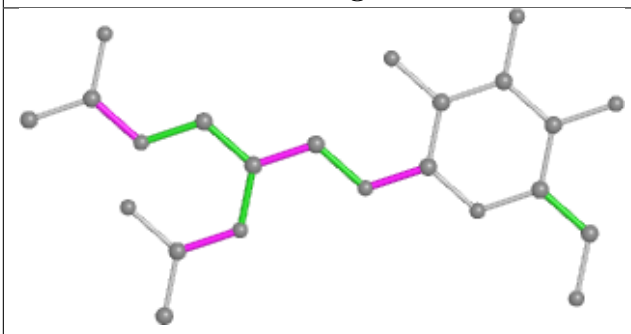

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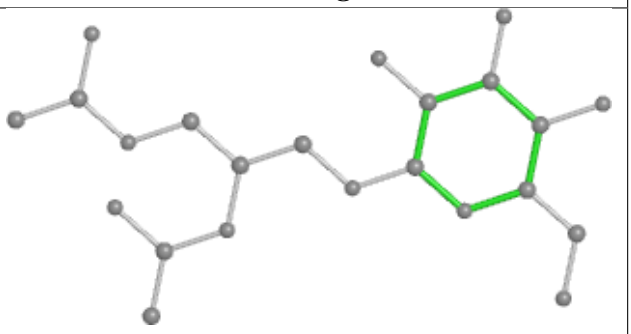
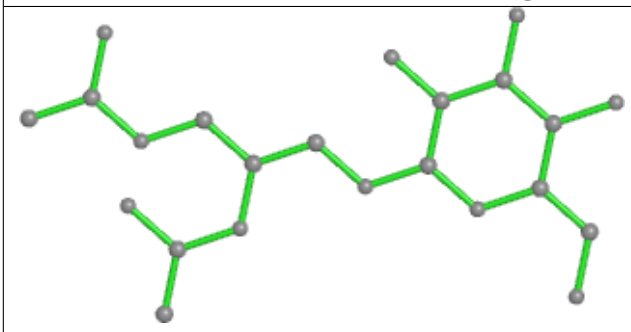


Rings

Ligand LMG A 503



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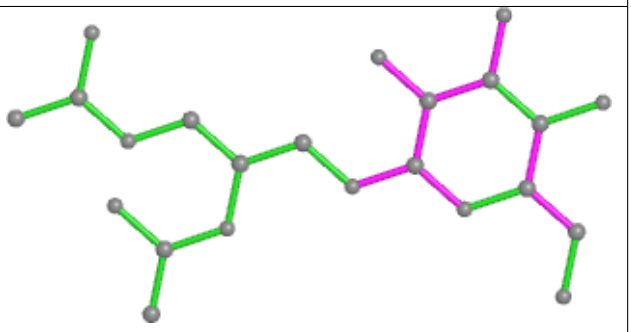

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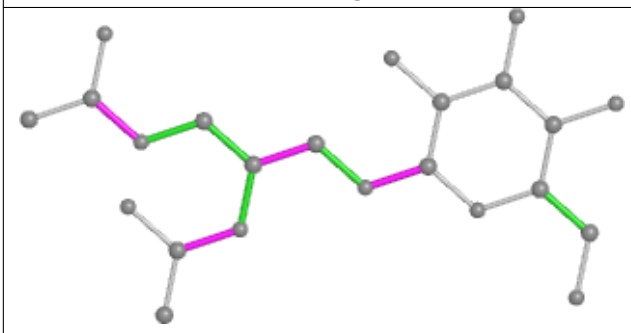

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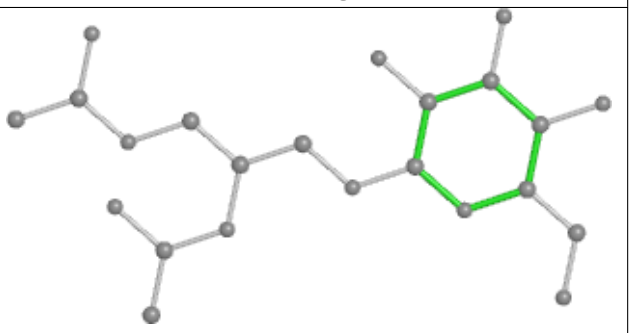
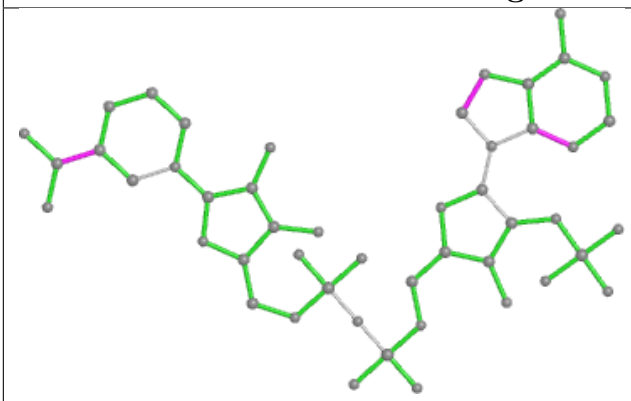


Rings

Ligand NDP NA 501



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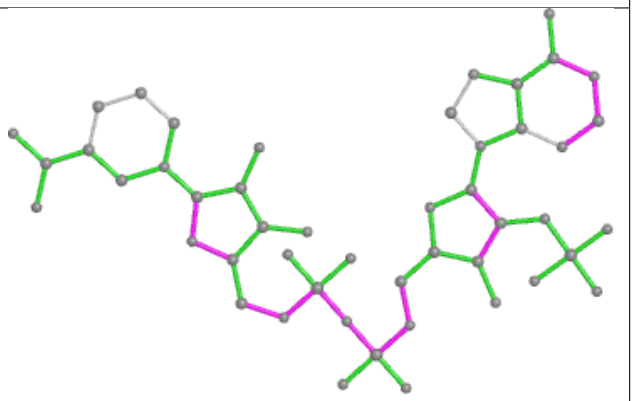

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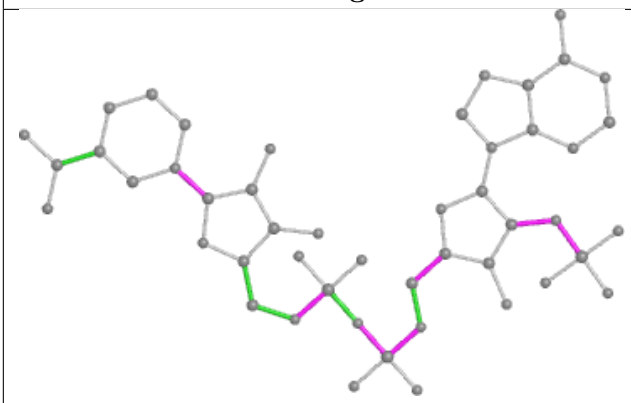

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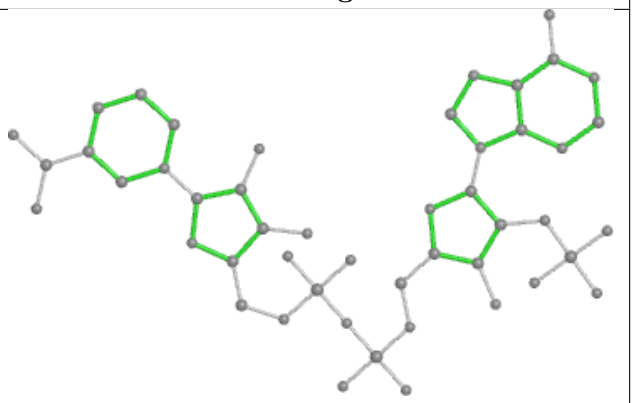
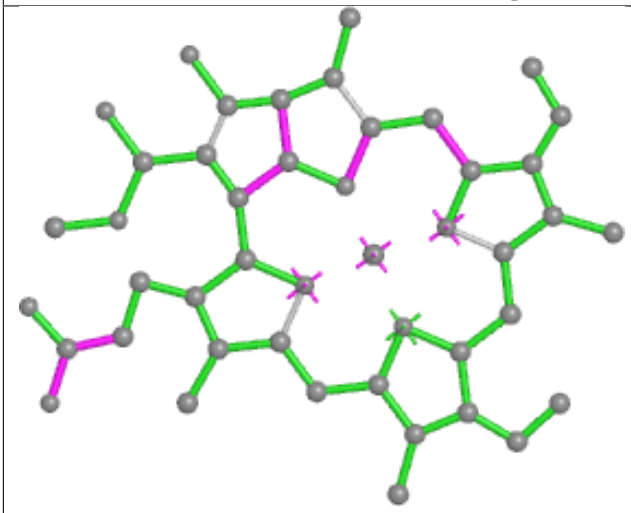


Rings

Ligand PMR BA 502



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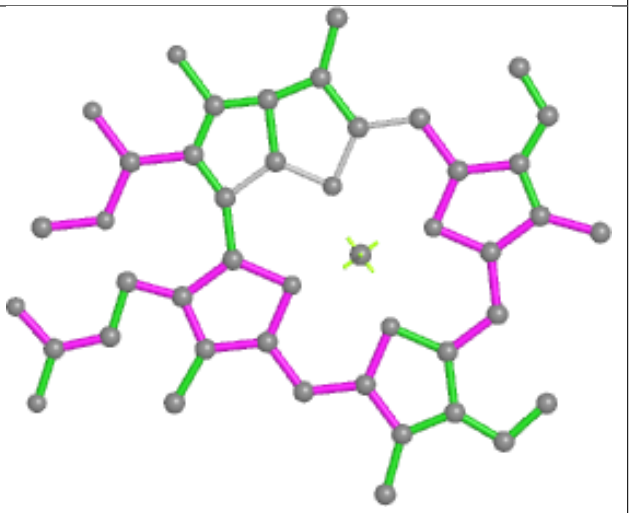

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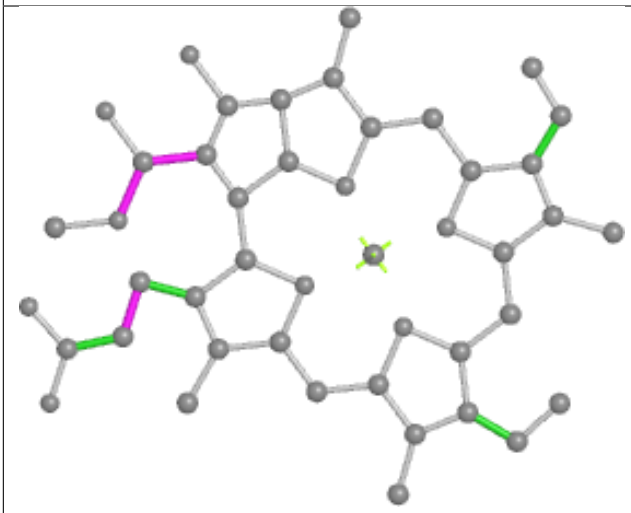

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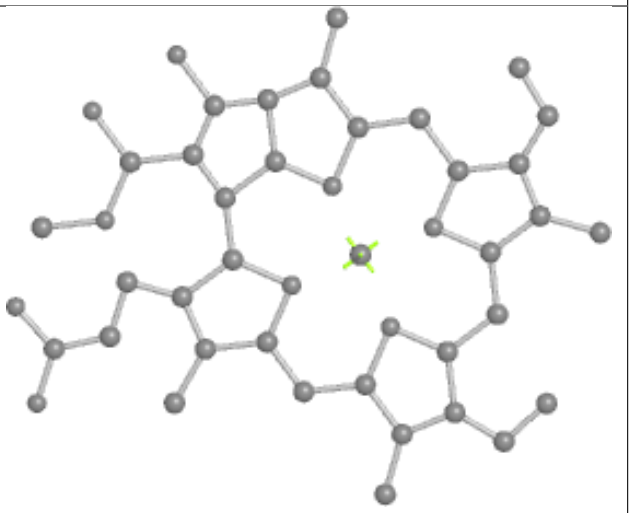
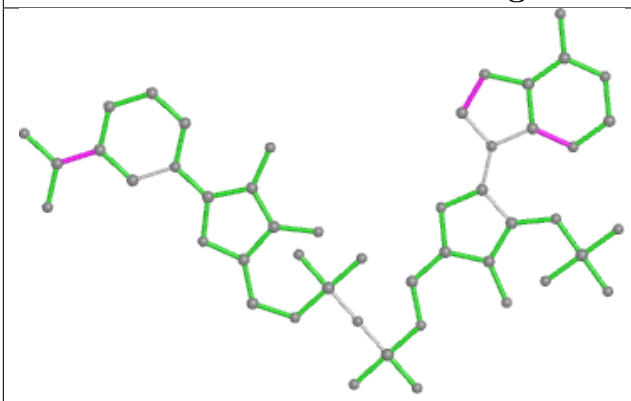


Rings

Ligand NDP CA 501



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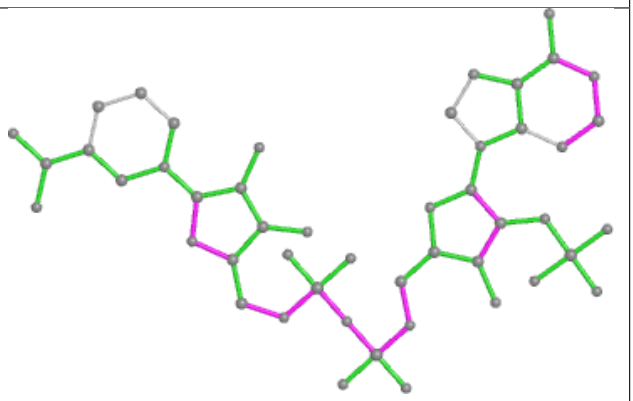

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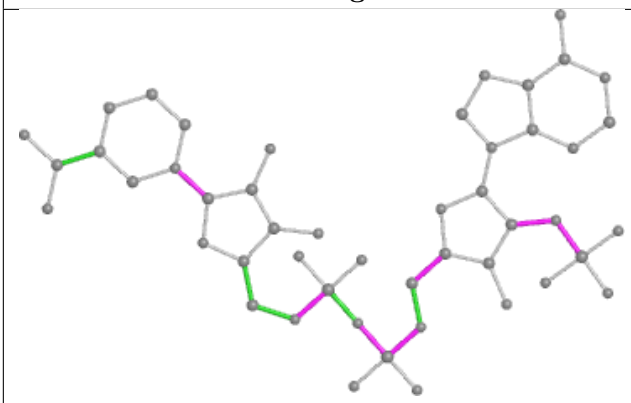

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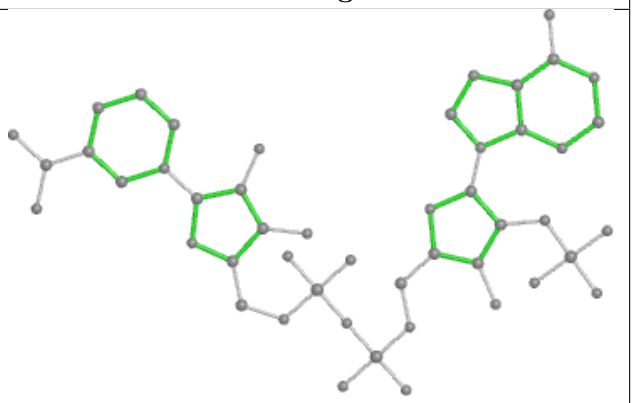
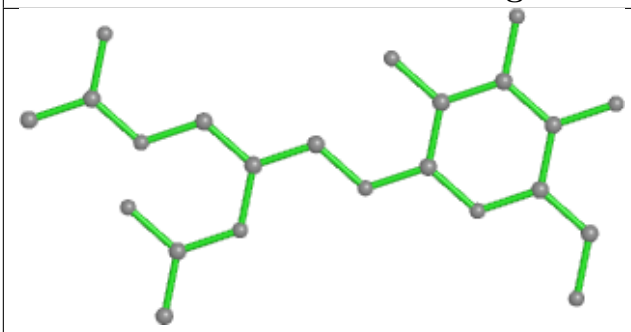


Rings

Ligand LMG CA 503



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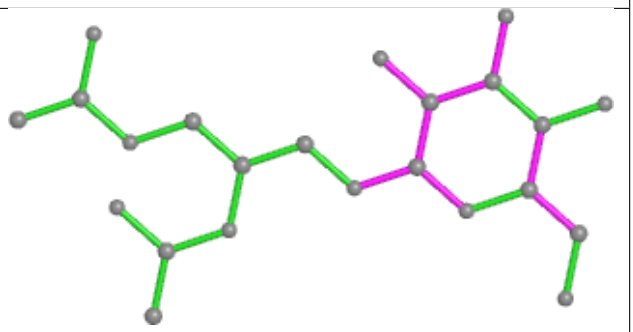

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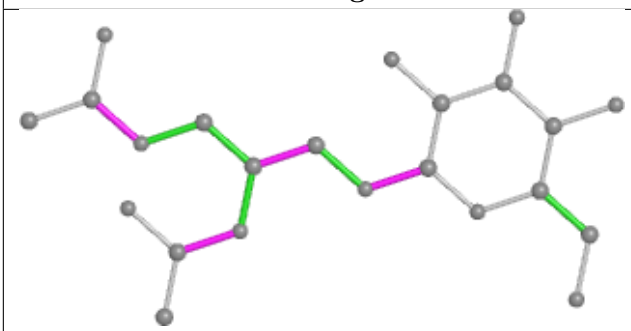

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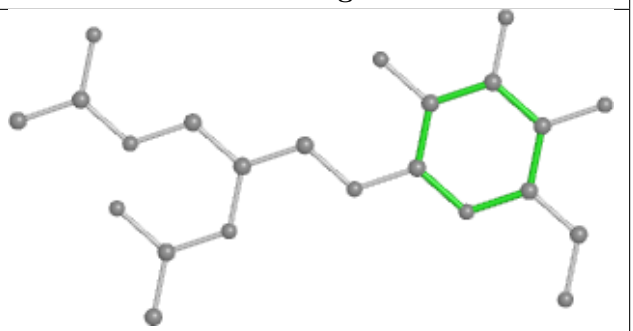
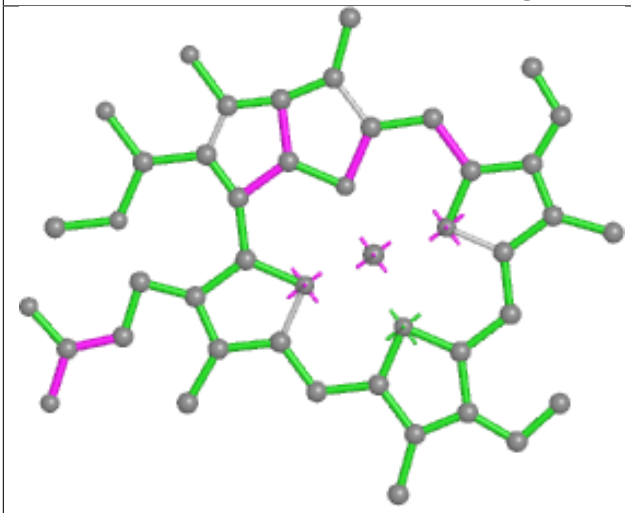


Rings

Ligand PMR V 502



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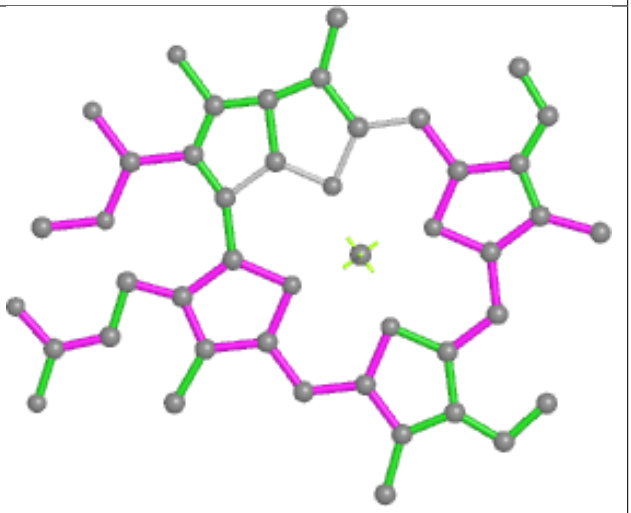

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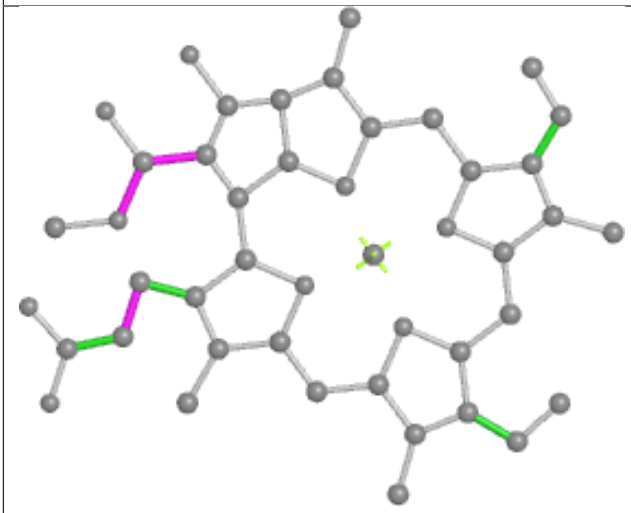

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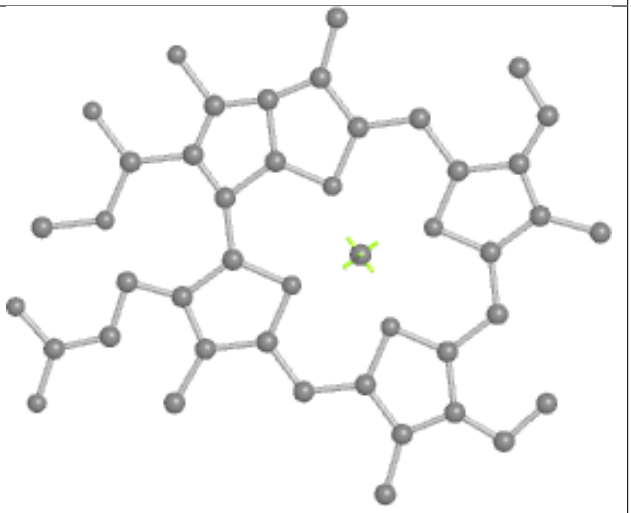
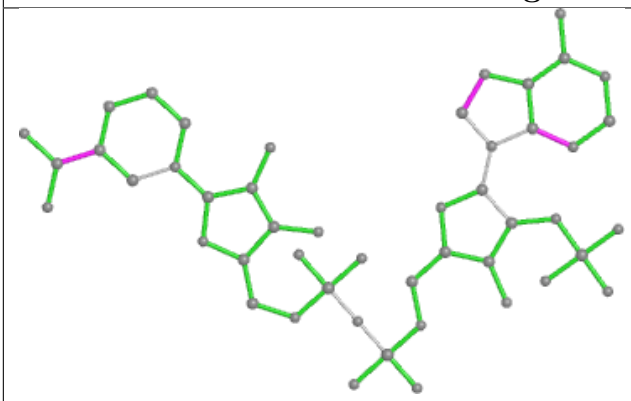


Rings

Ligand NDP F 501



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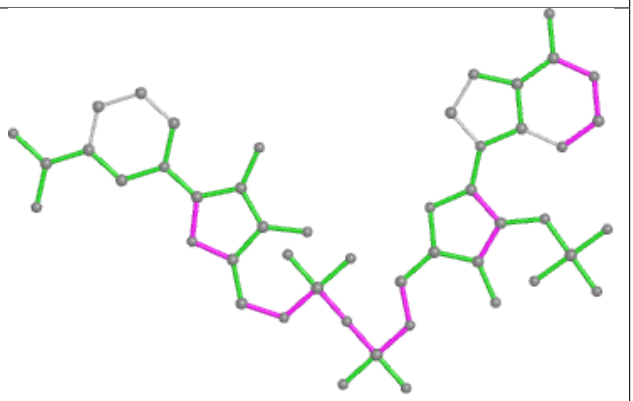

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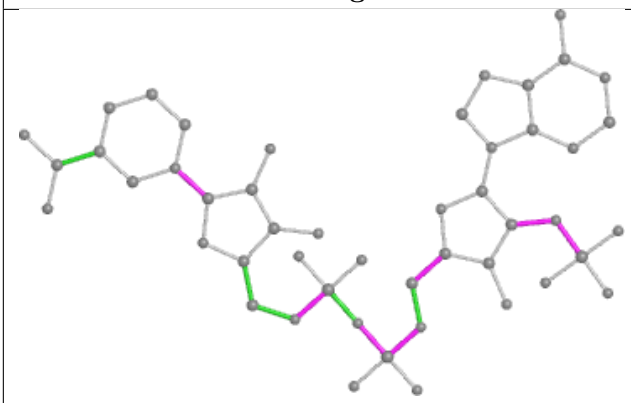

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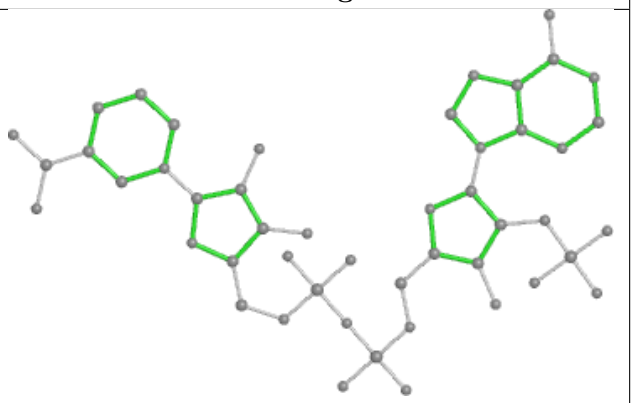
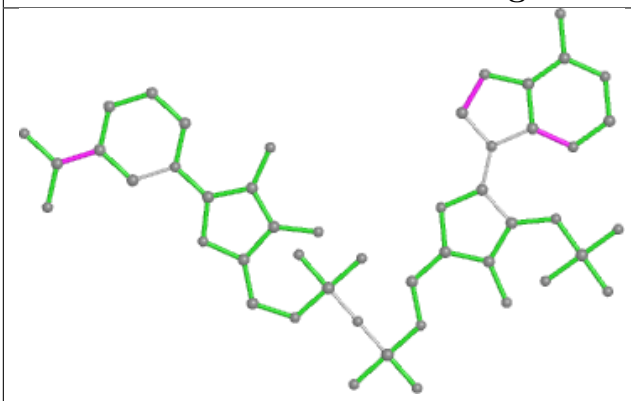


Rings

Ligand NDP BA 501



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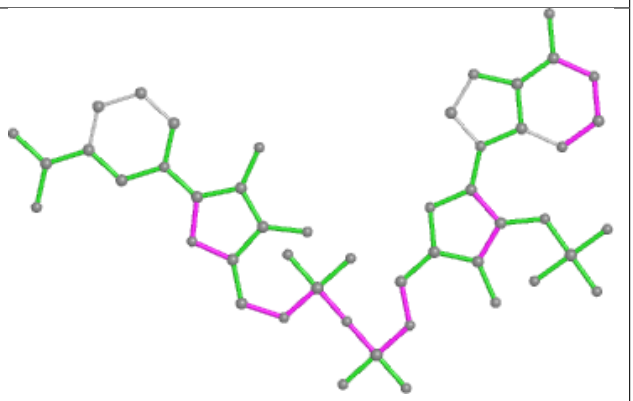

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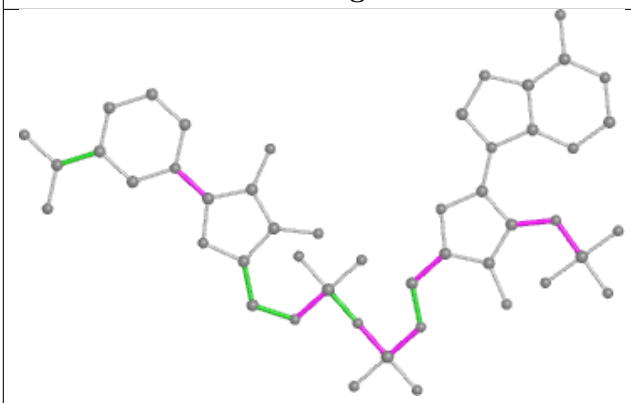

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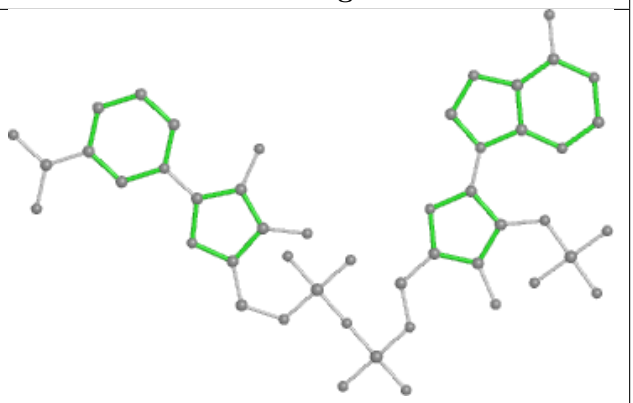
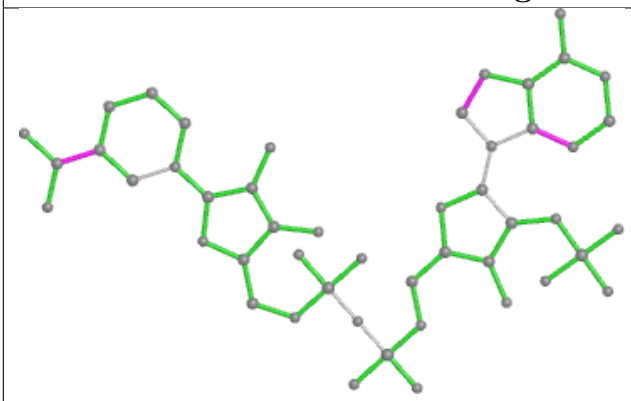


Rings

Ligand NDP IA 501



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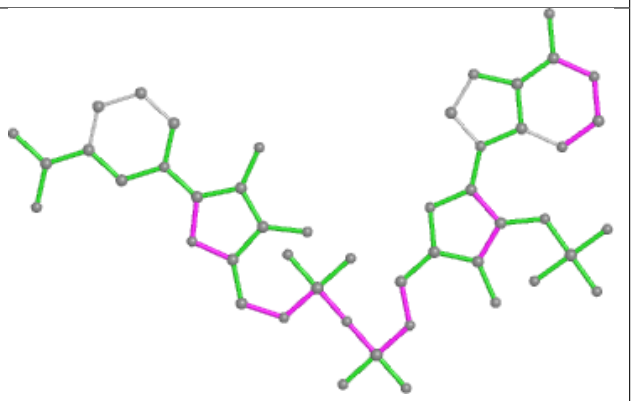

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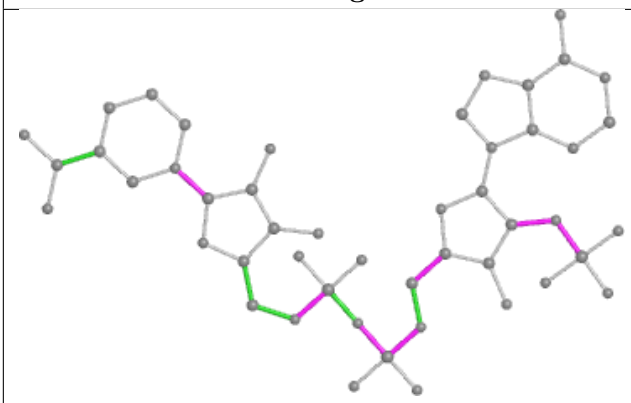

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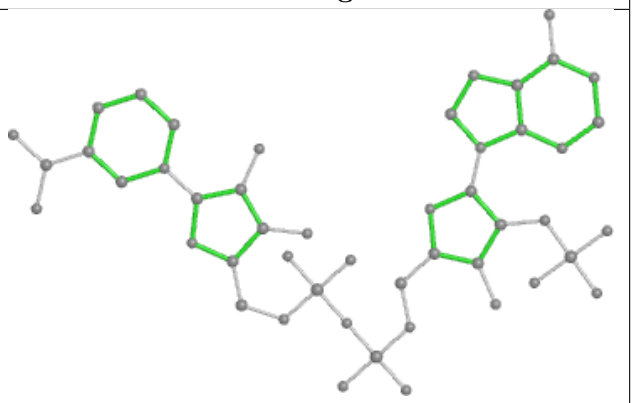
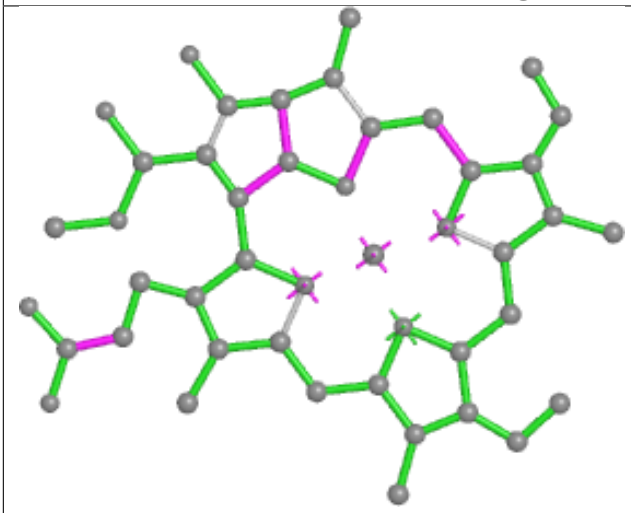


Rings

Ligand PMR M 502



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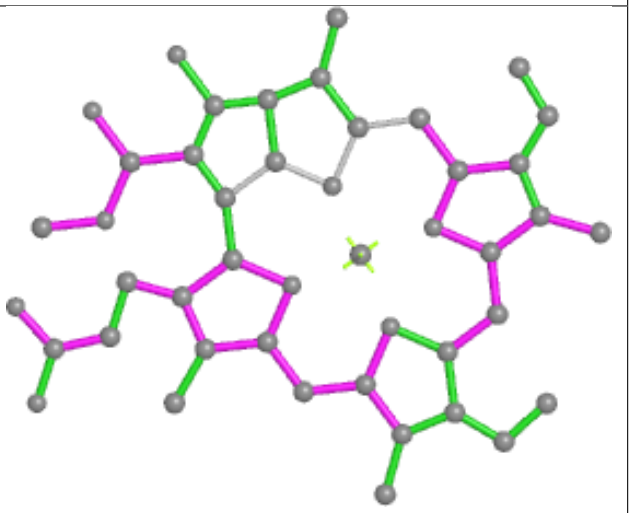

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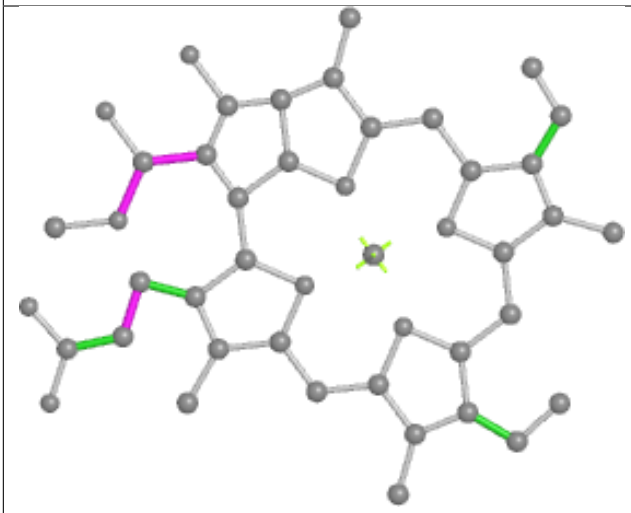

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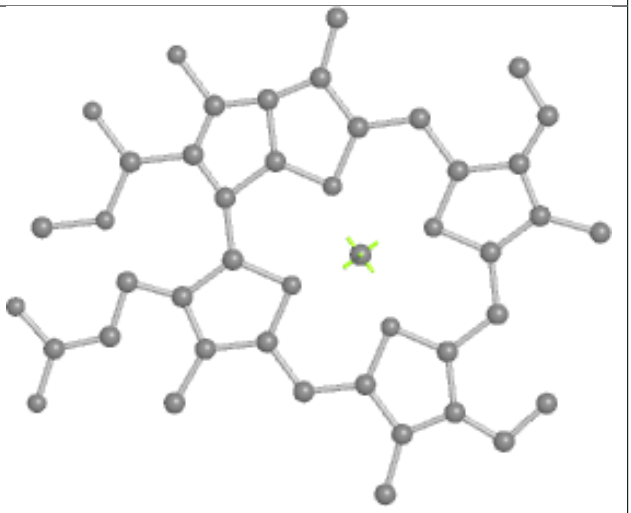
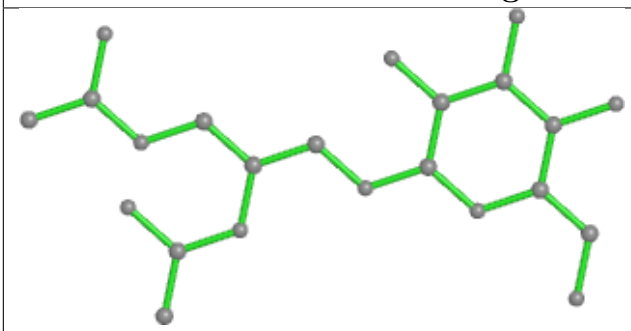


Rings

Ligand LMG MA 503



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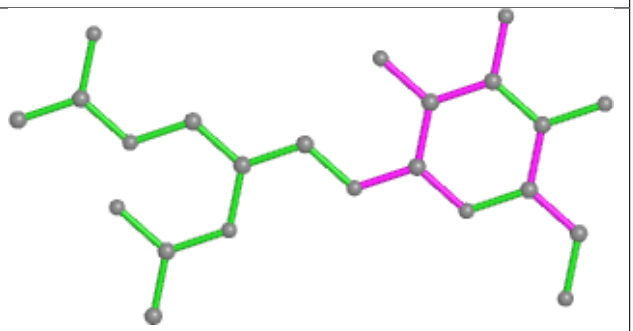

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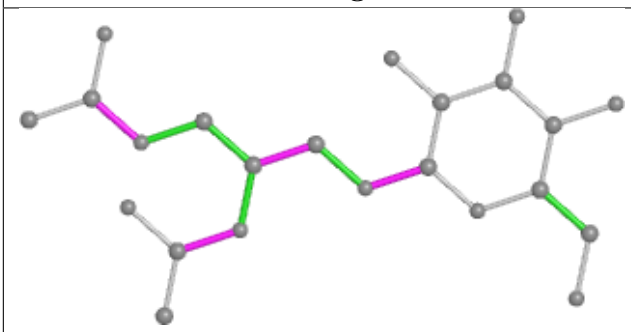

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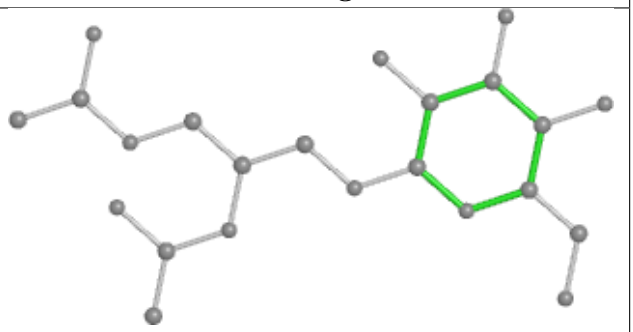
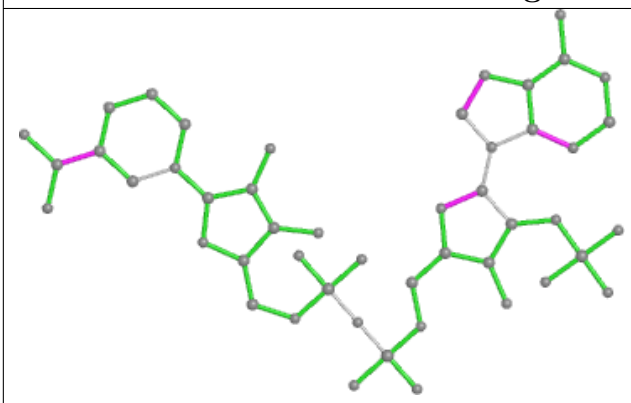


Rings

Ligand NDP L 501



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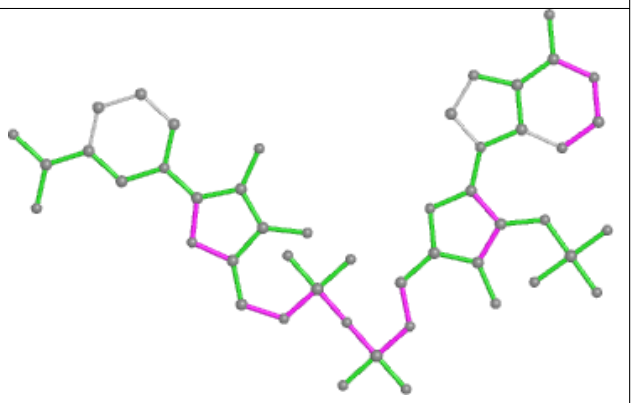
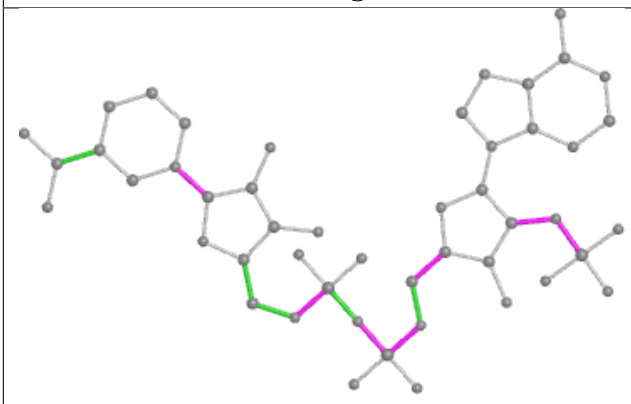


Bond angles



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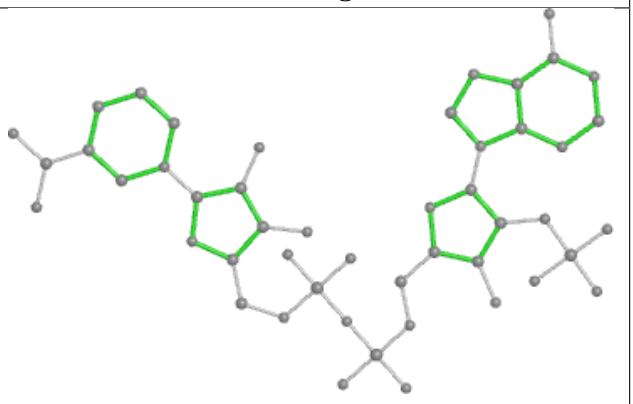
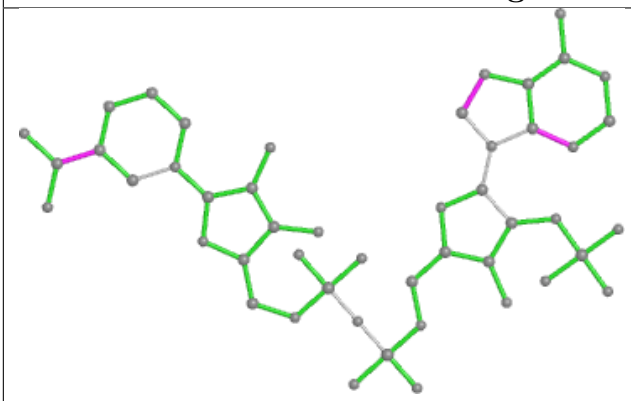


Rings

Ligand NDP AA 501



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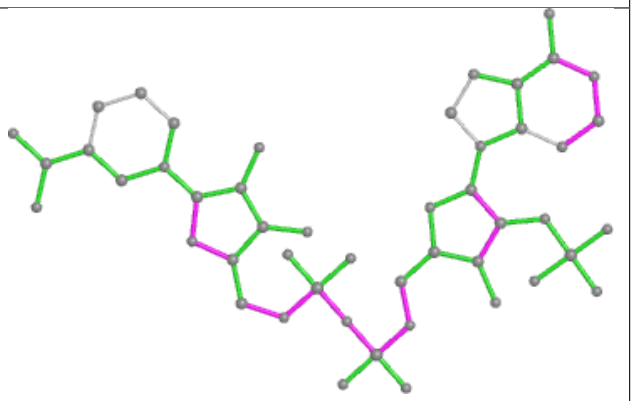
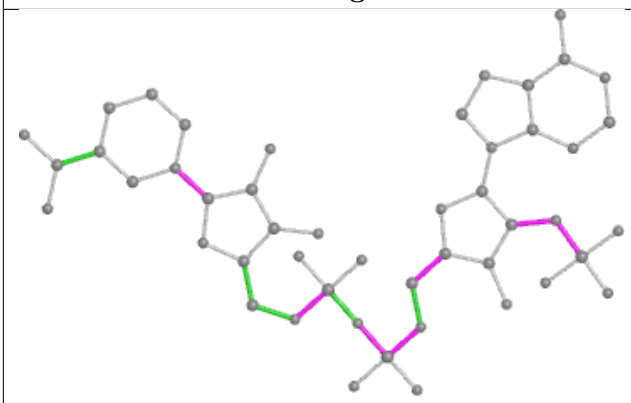
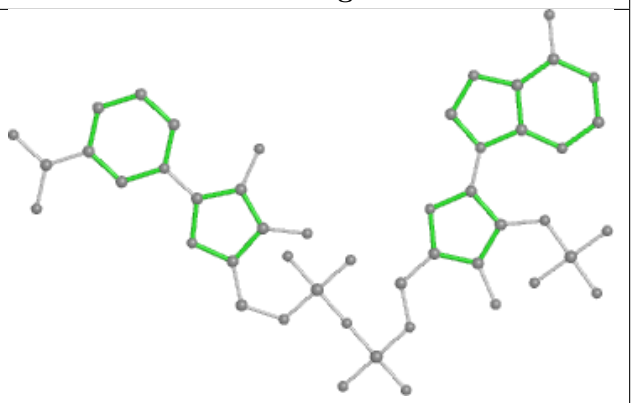


Bond angles

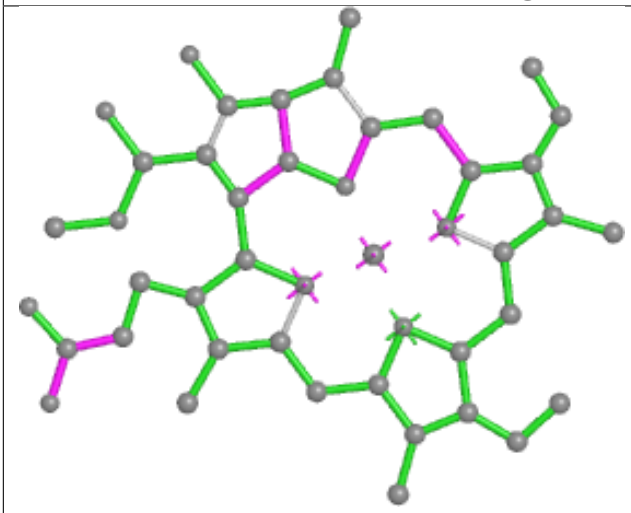


Torsions



Rings

Ligand PMR C 502



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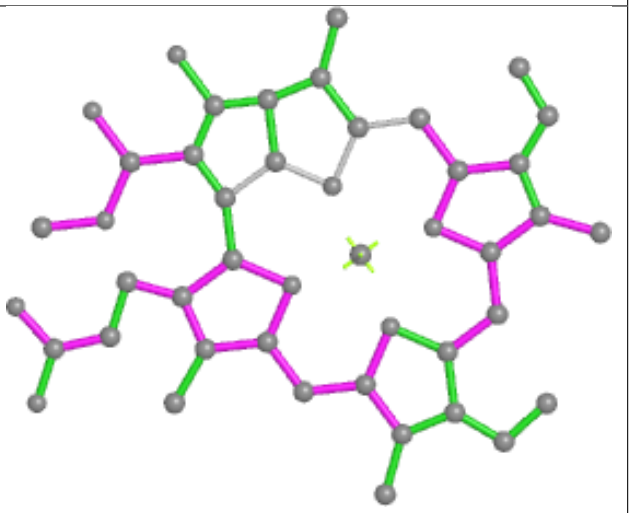

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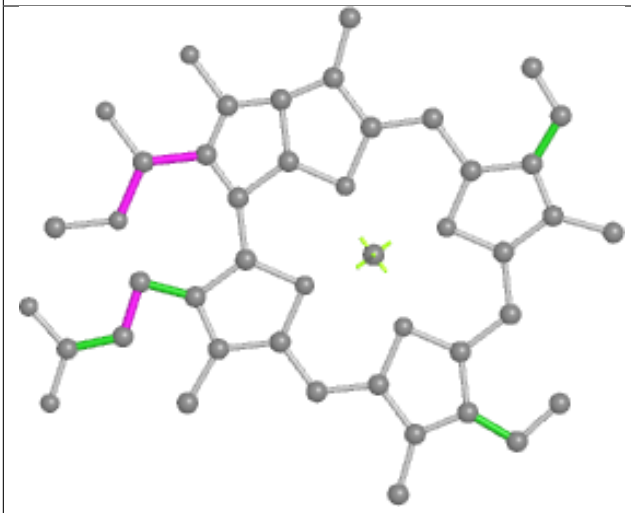

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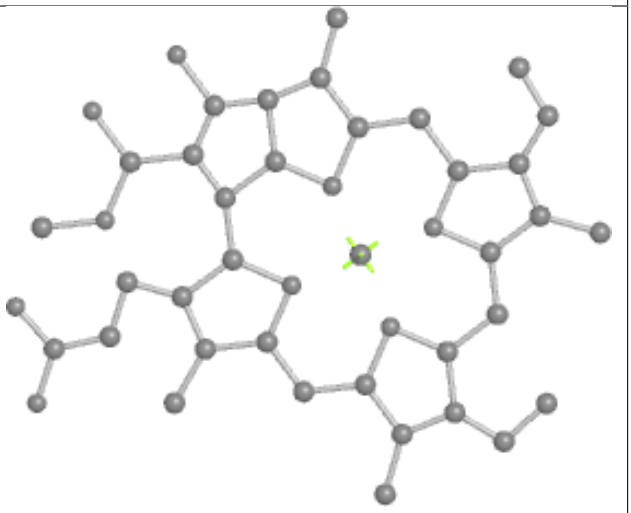
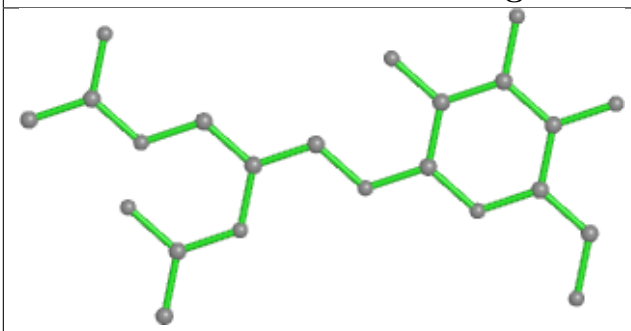


Rings

Ligand LMG AA 503



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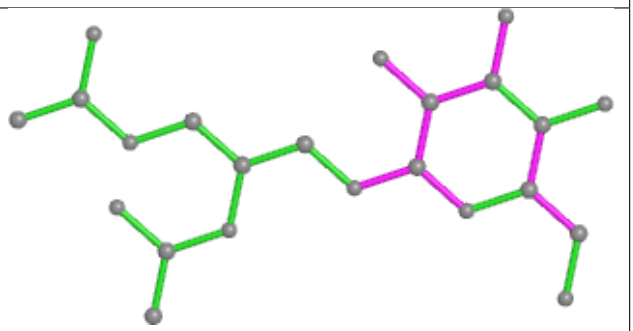

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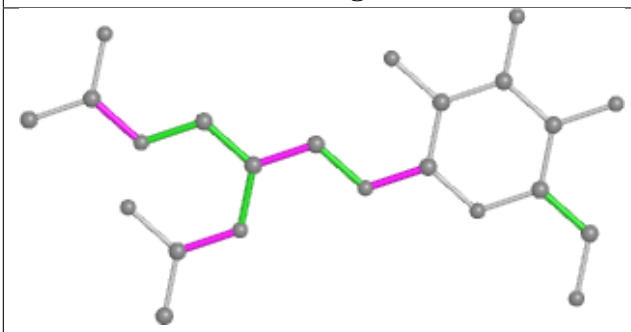

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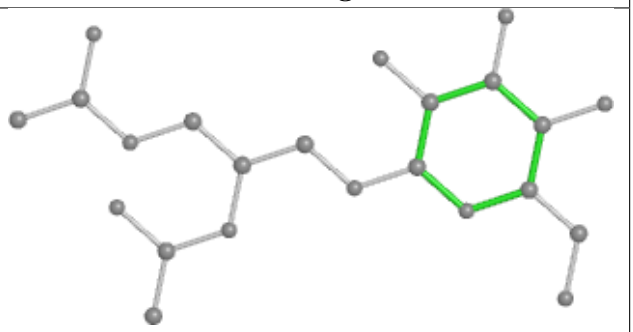

Rings

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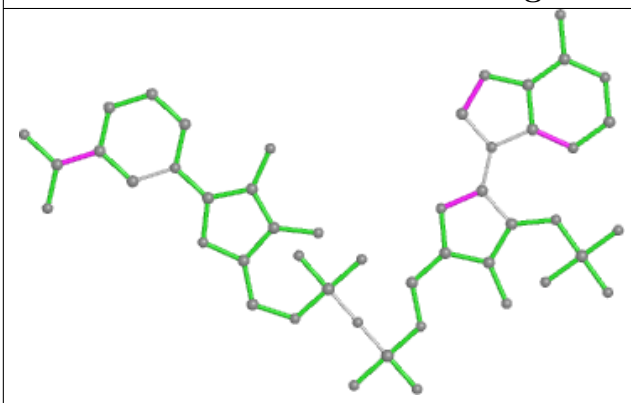

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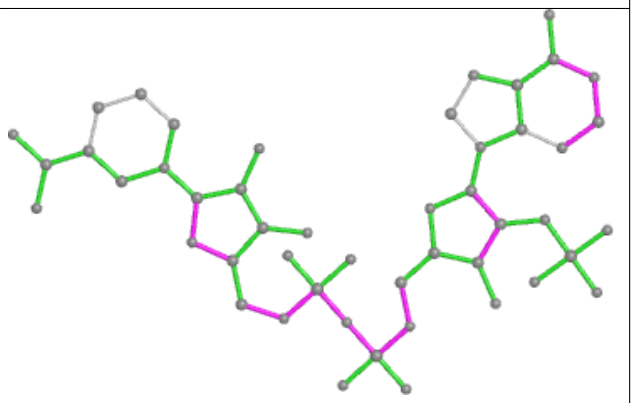

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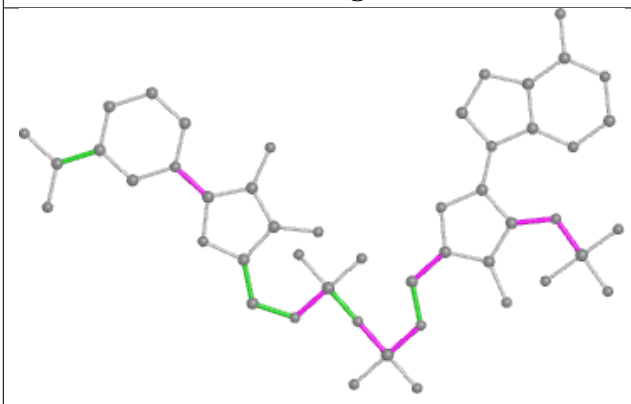

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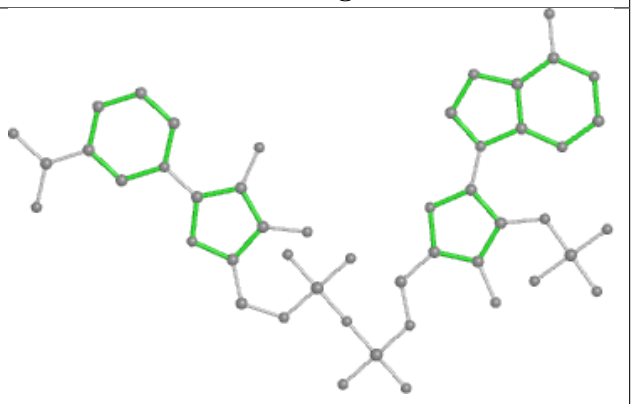

Rings

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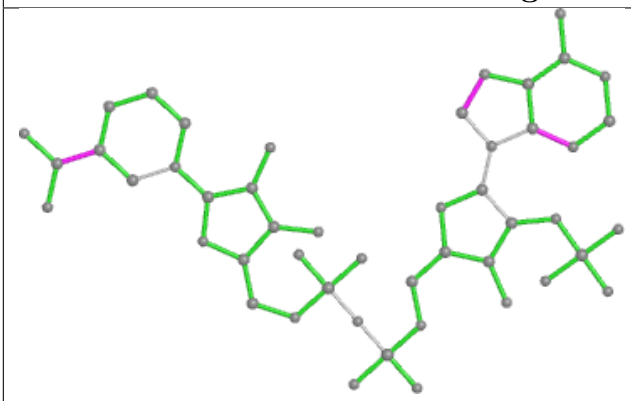

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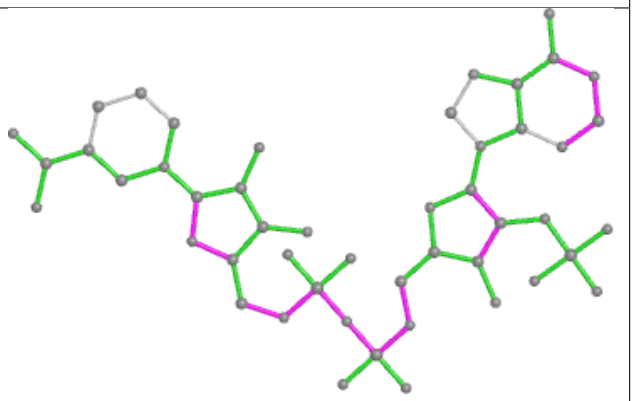

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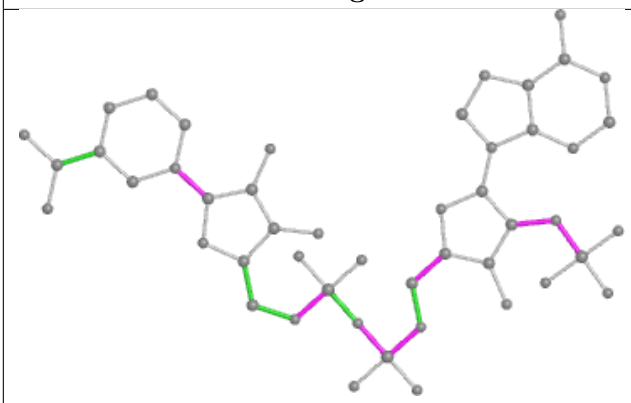

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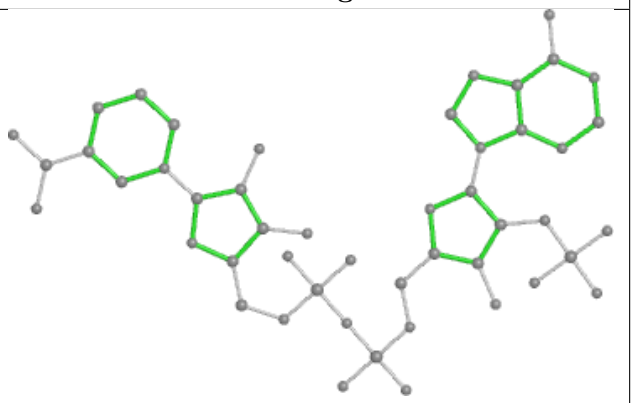
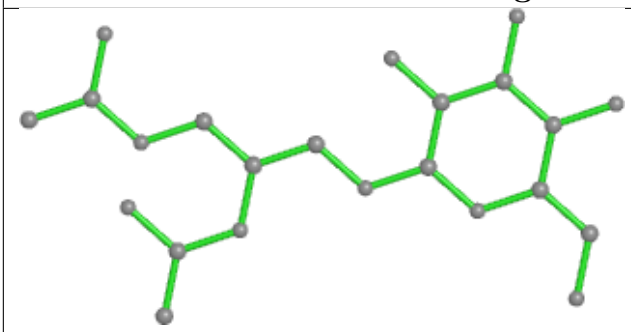


Rings

Ligand LMG W 503



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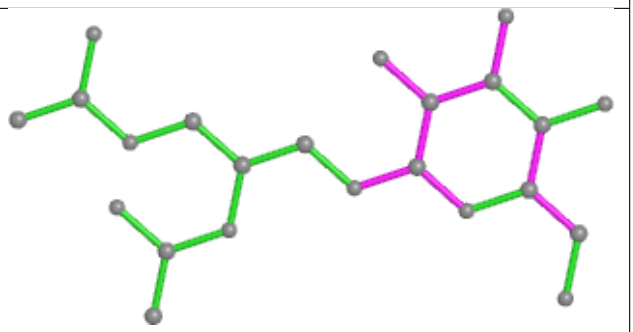

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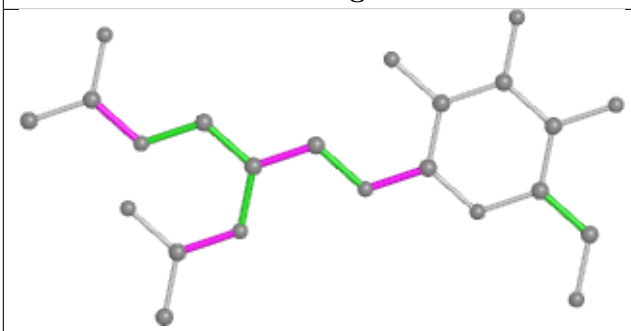

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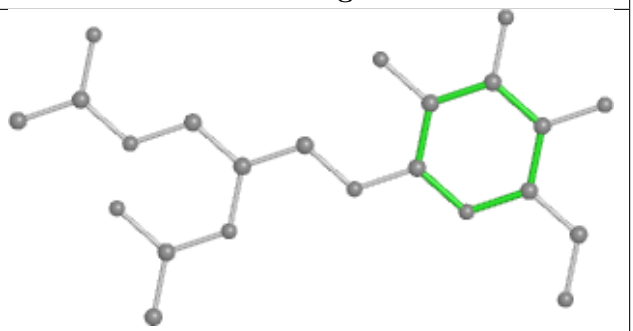

Rings

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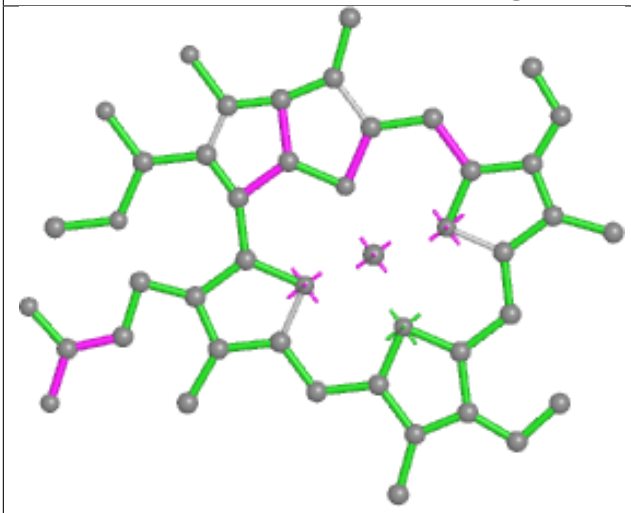

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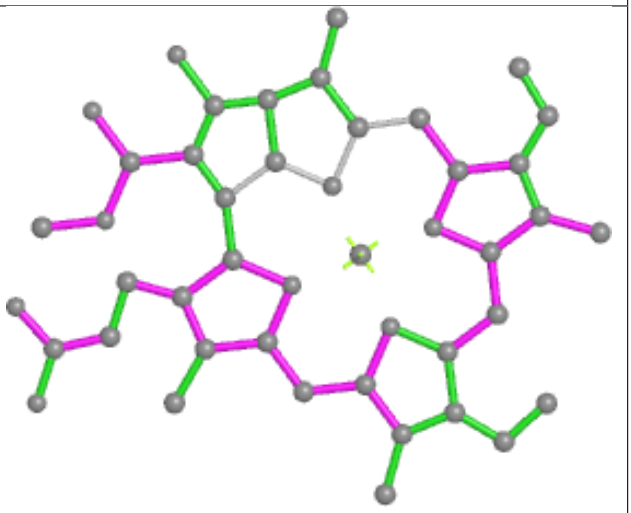

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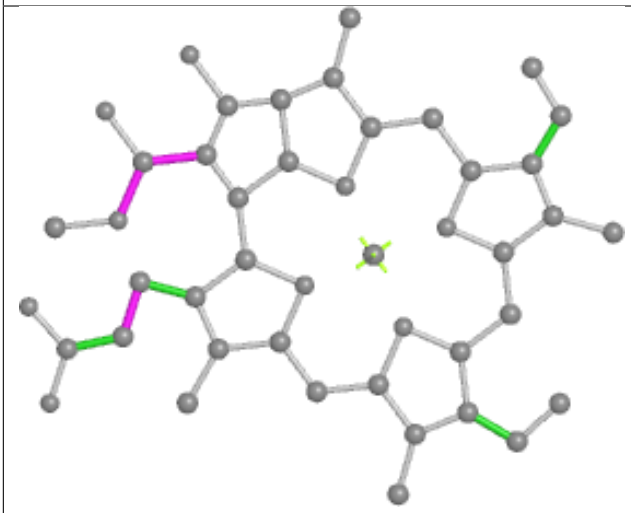

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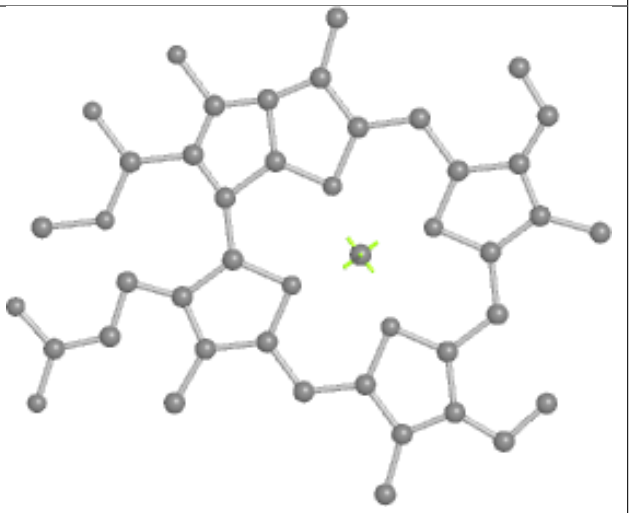

Rings

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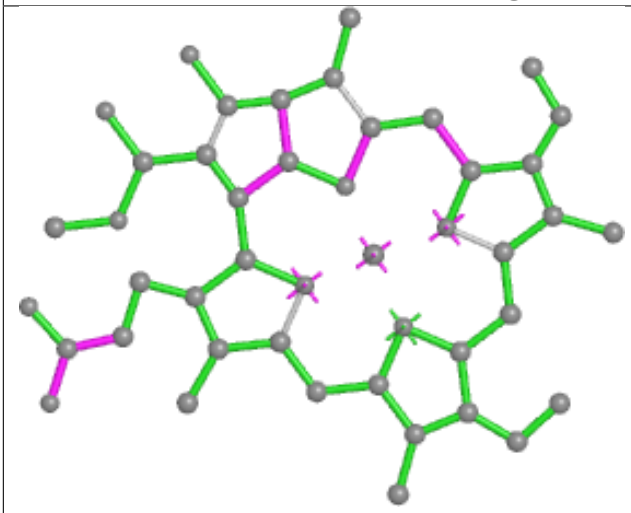

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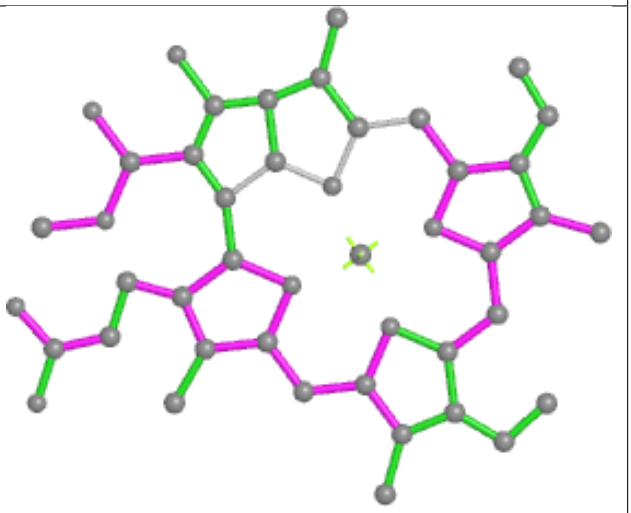

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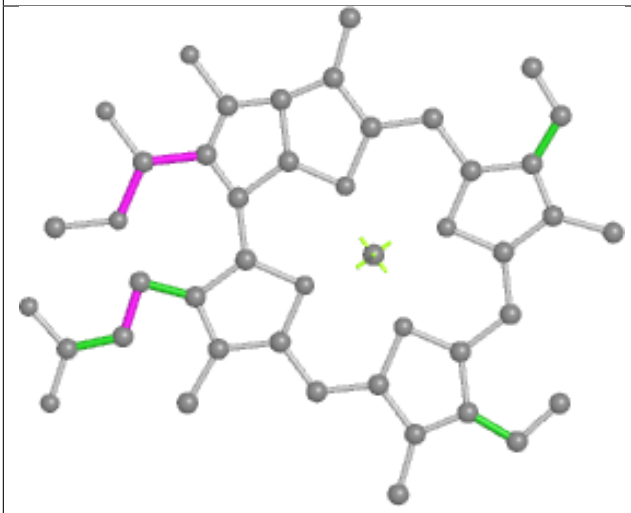

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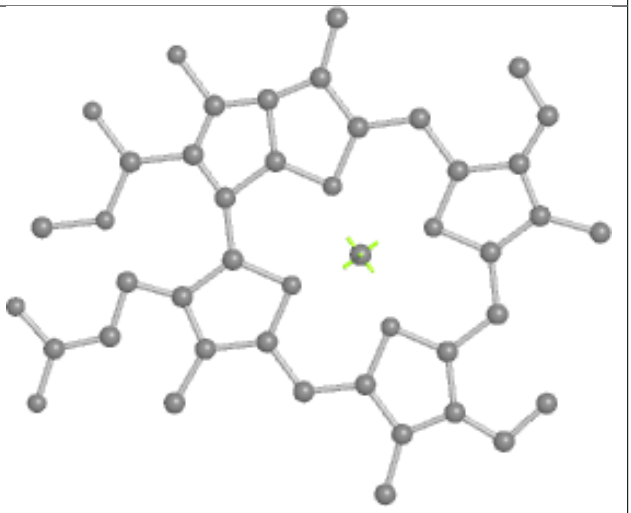

Rings

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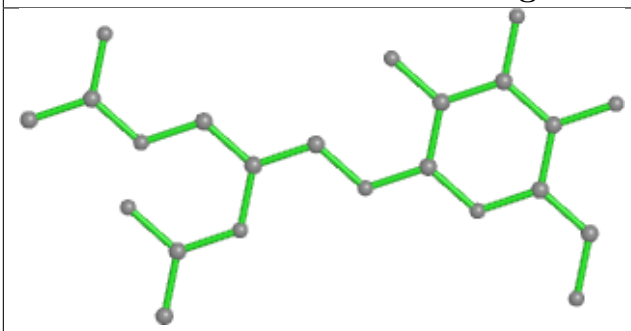

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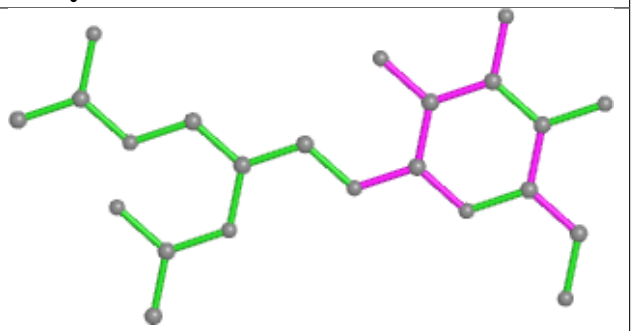

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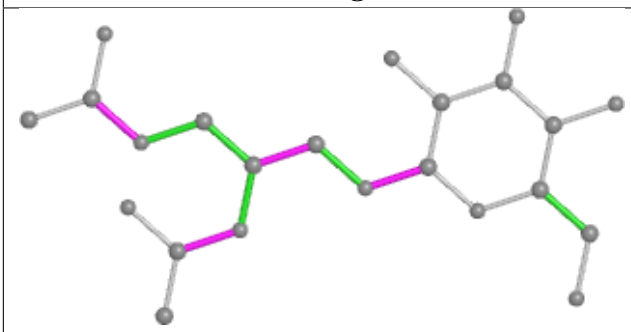

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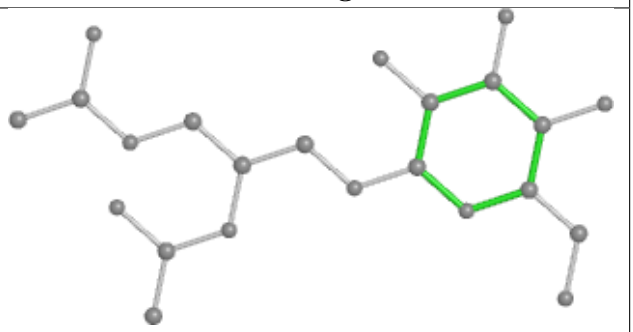
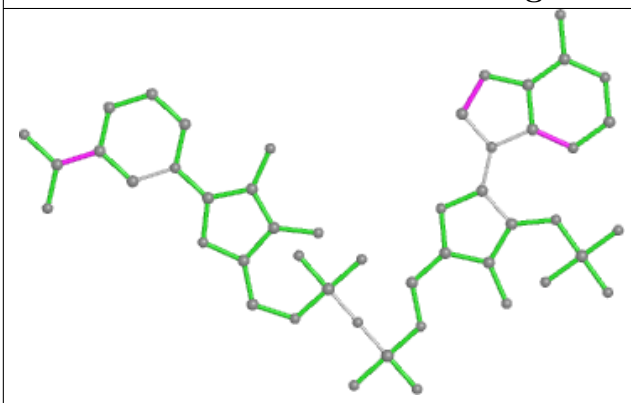


Rings

Ligand NDP J 501



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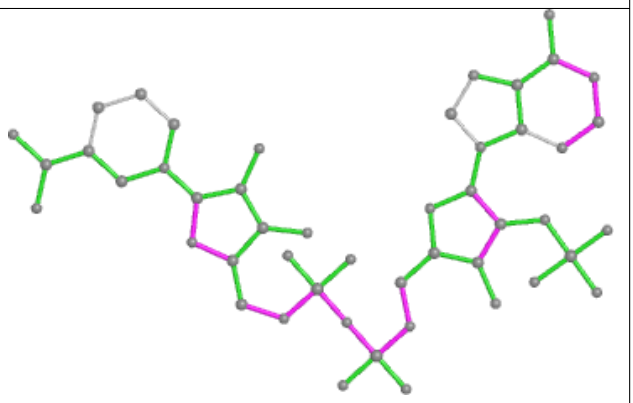

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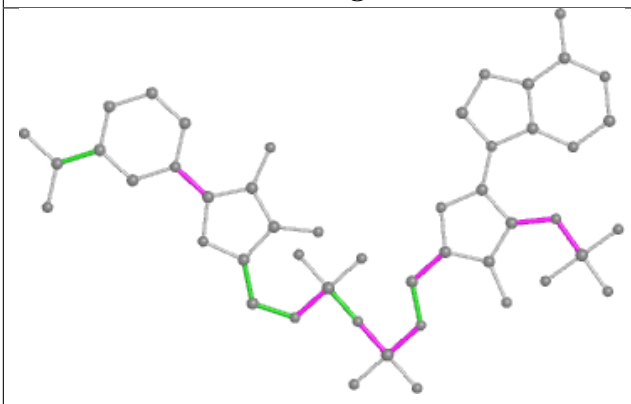

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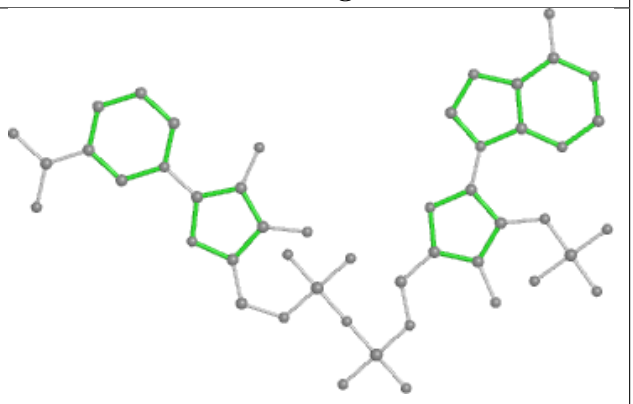
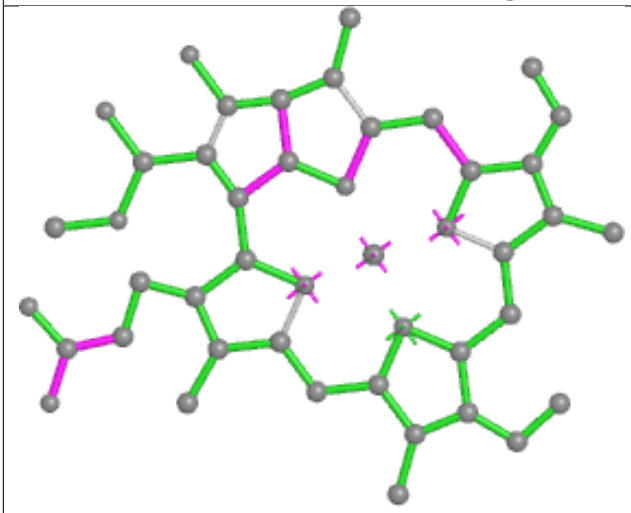


Rings

Ligand PMR MA 502



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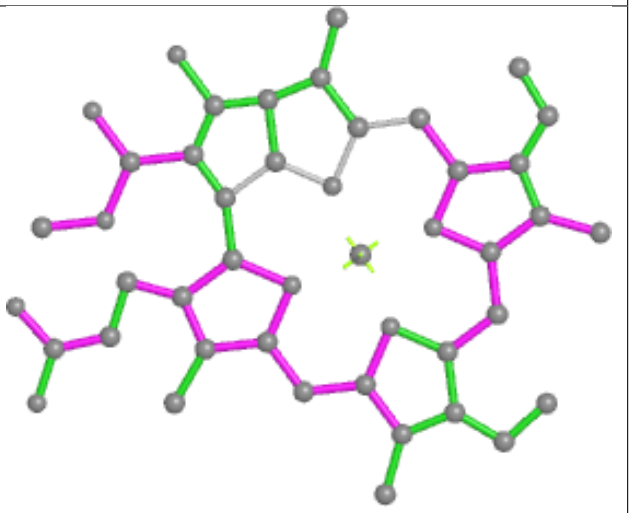

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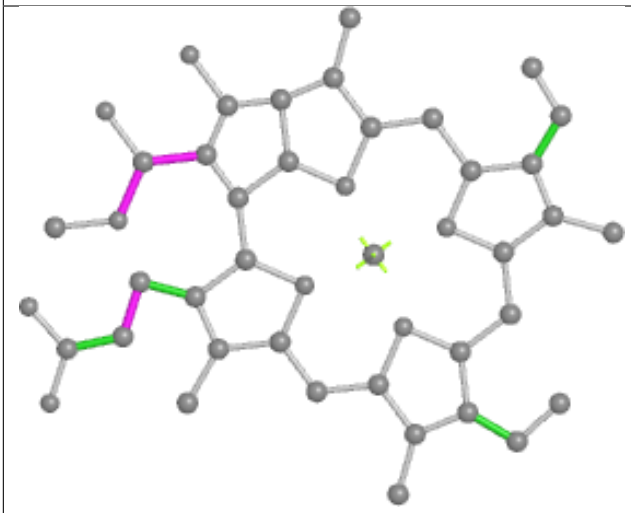

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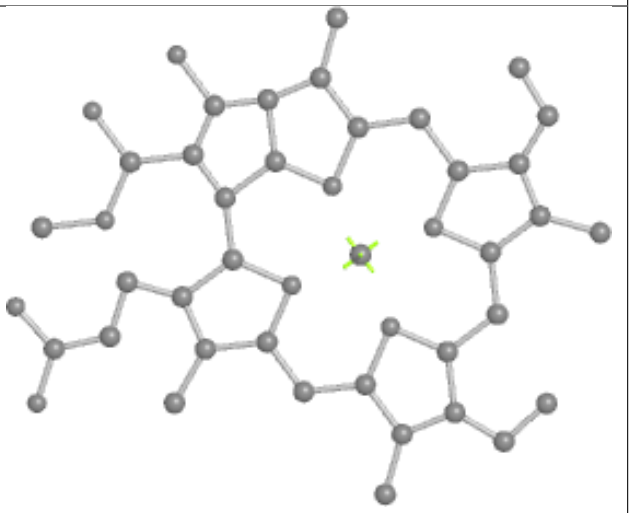
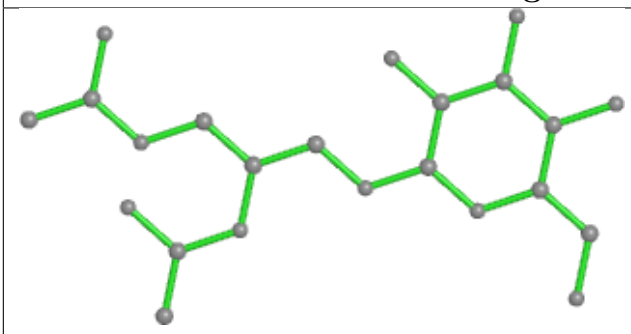


Rings

Ligand LMG J 503



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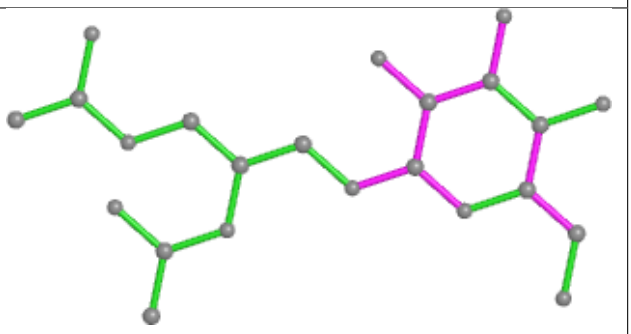

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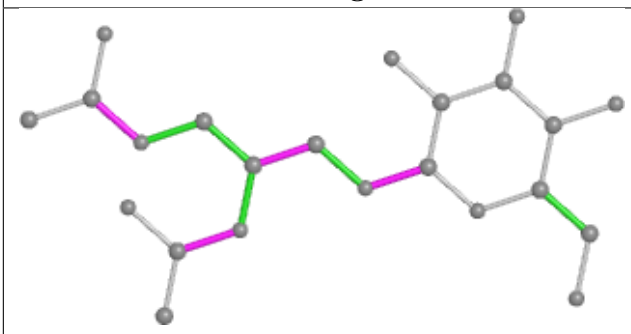

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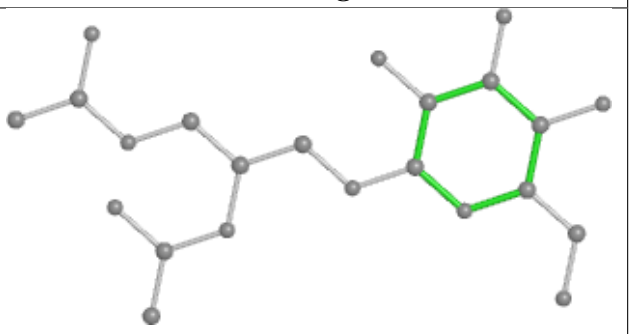
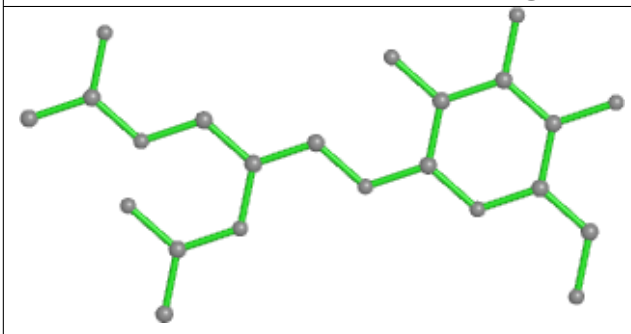


Rings

Ligand LMG S 503



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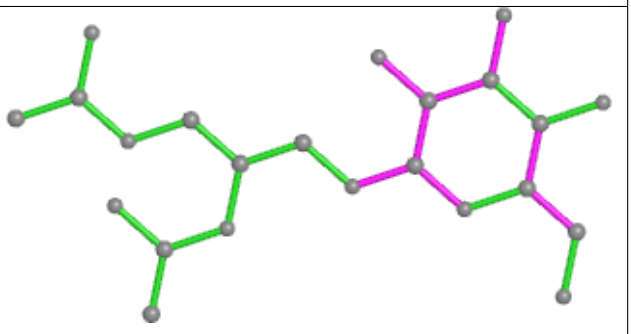

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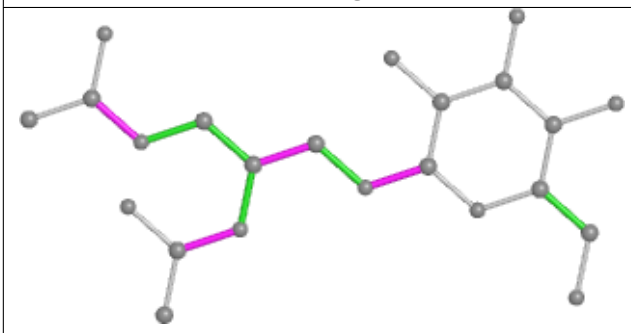

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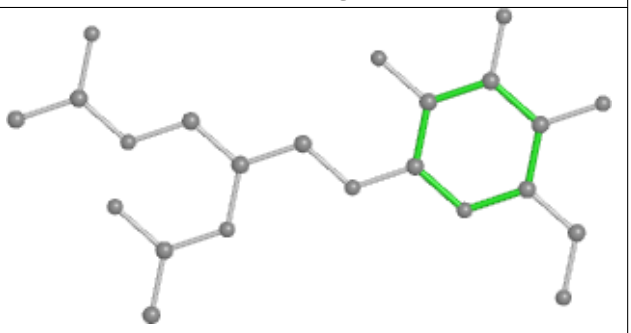
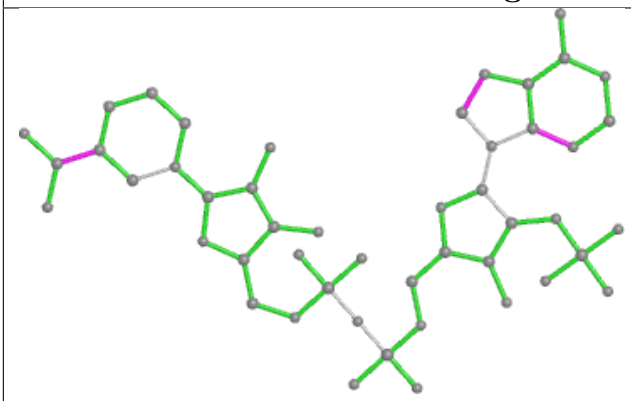


Rings

Ligand NDP MA 501



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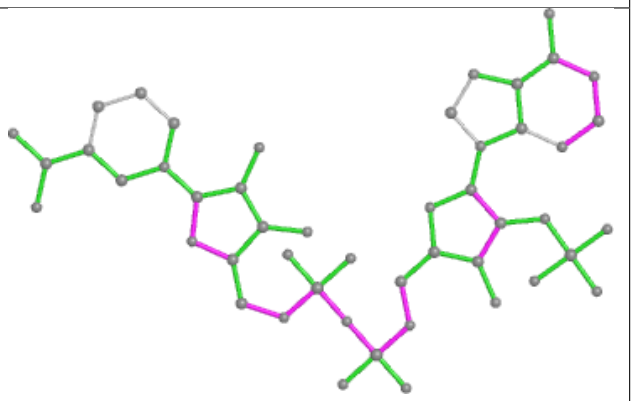

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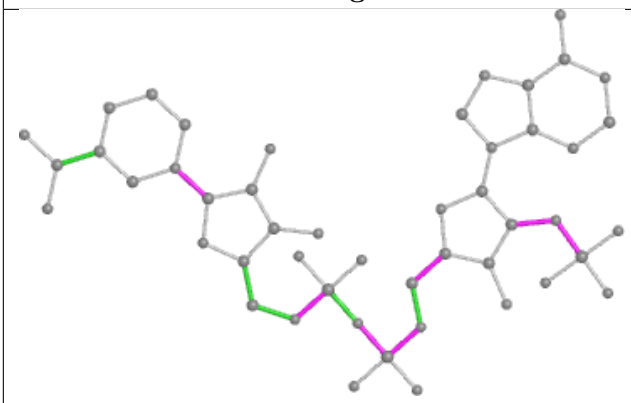

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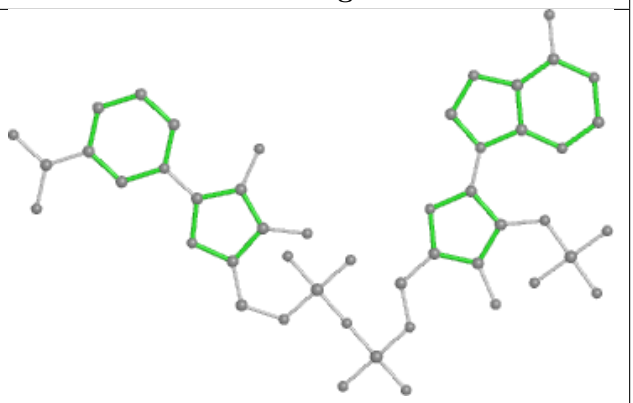
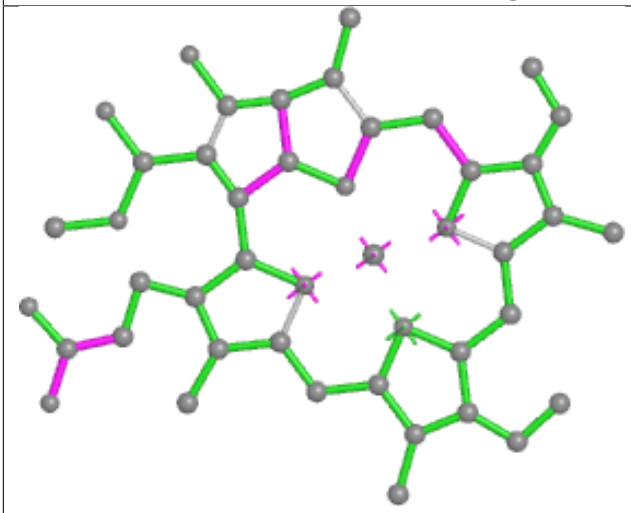


Rings

Ligand PMR HA 502



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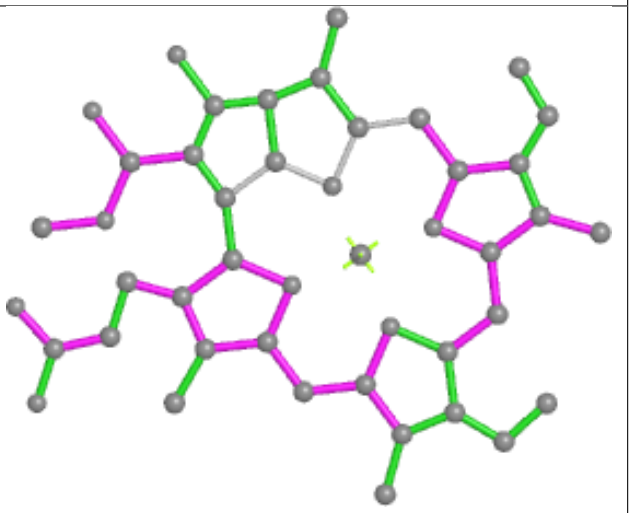
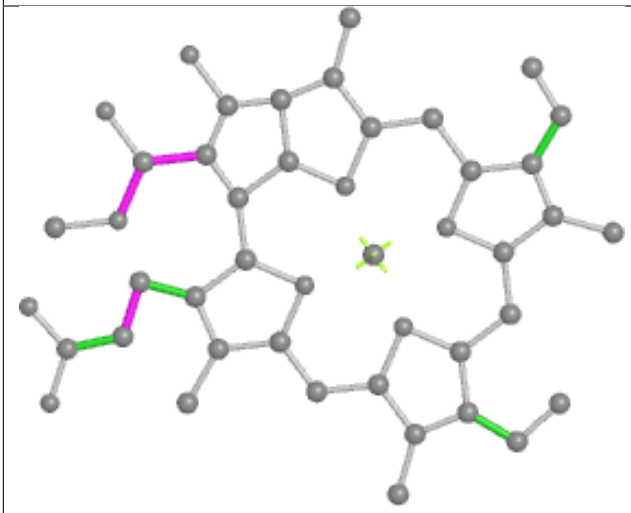
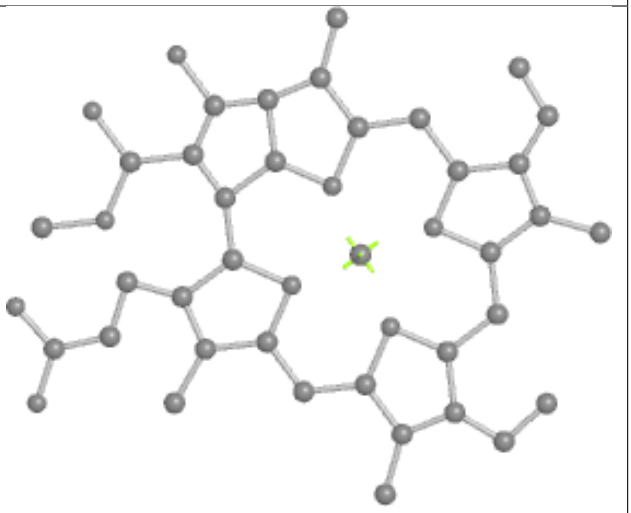


Bond angles

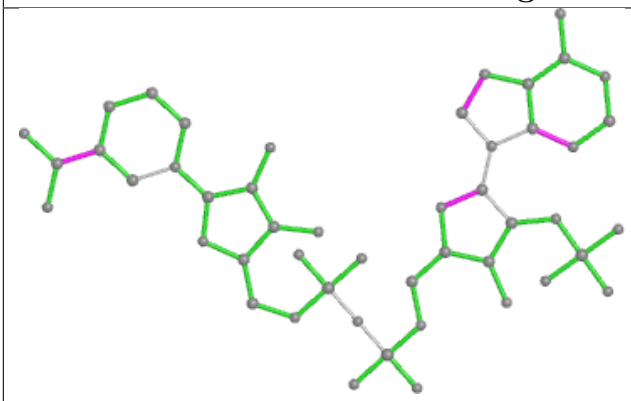


Torsions

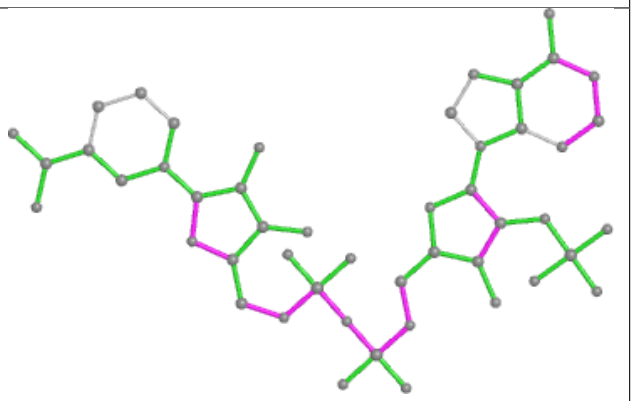


Rings

Ligand NDP M 501



Bond lengths



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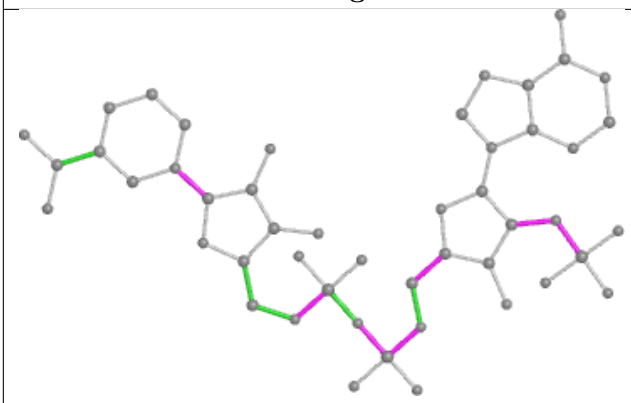
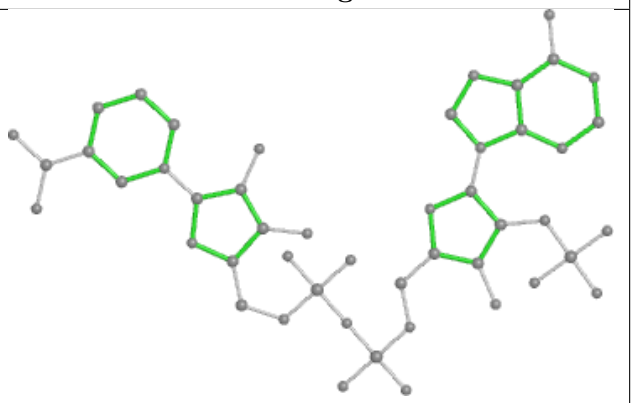
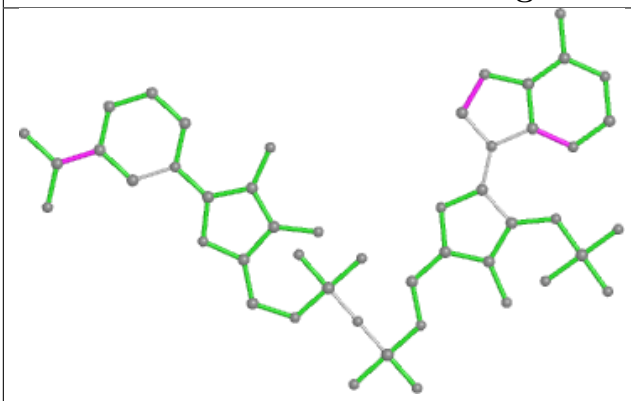


Torsions



Rings

Ligand NDP W 501



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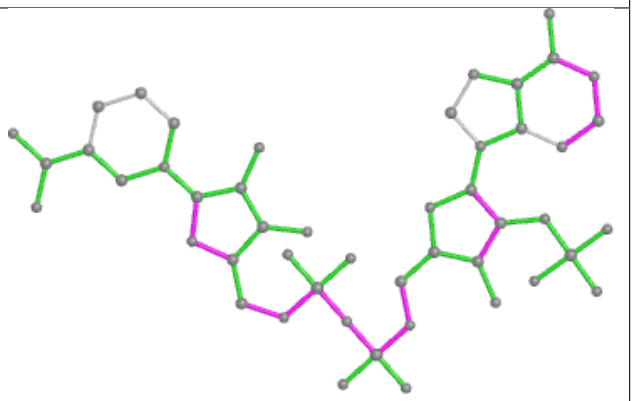
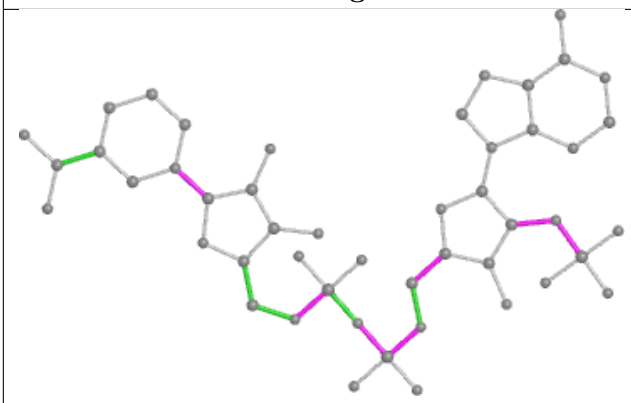


Bond angles



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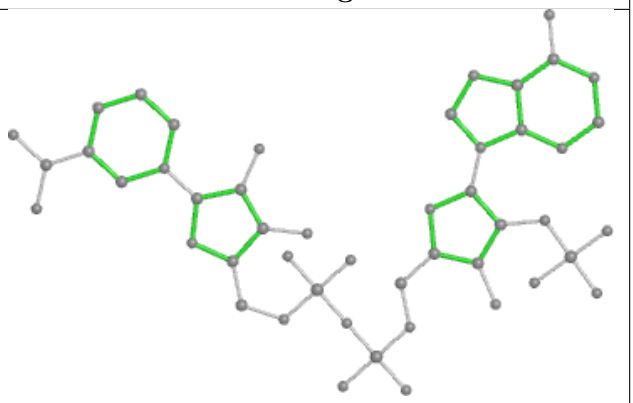
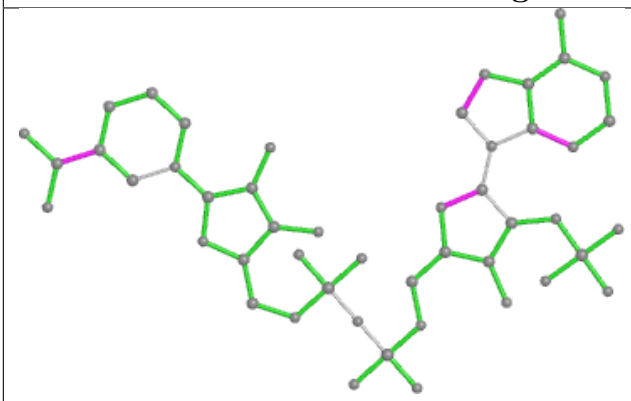
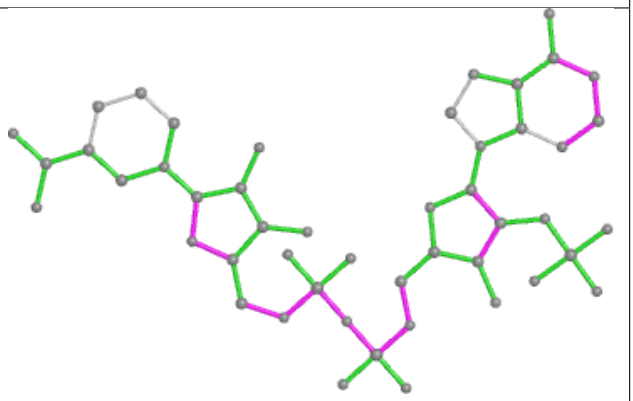


Rings

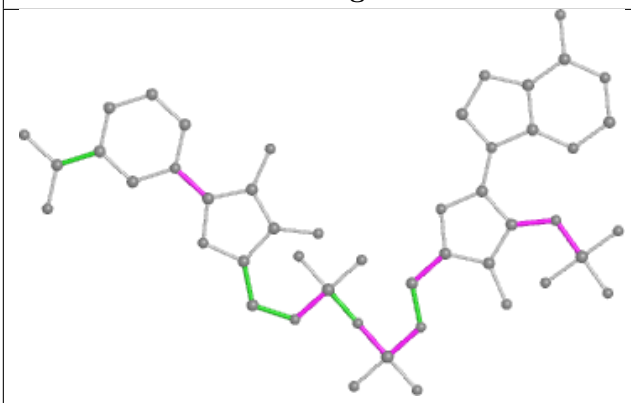
Ligand NDP JA 501



Bond lengths



Bond angles



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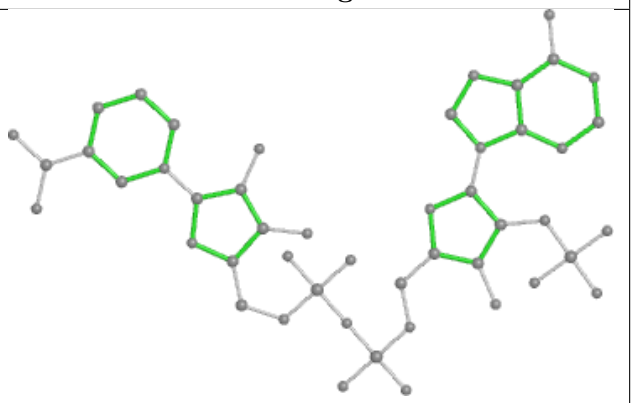
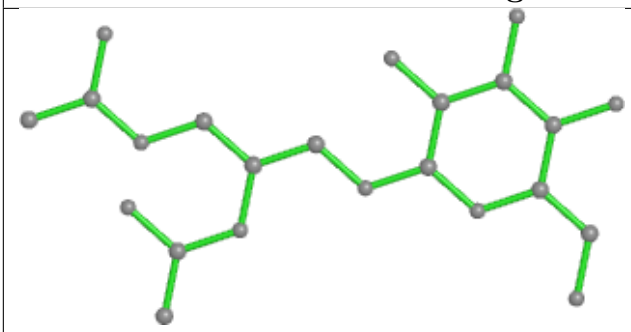


Rings

Ligand LMG BA 503



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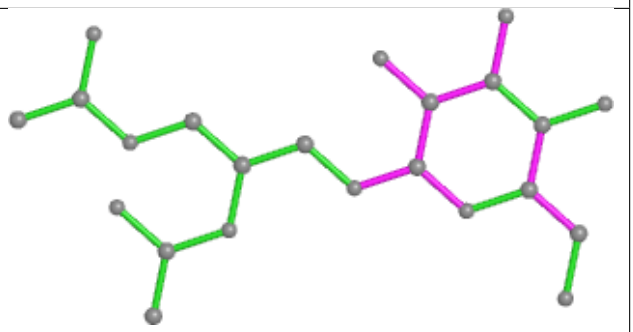
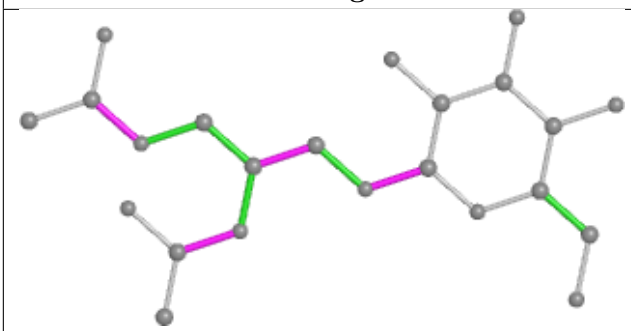
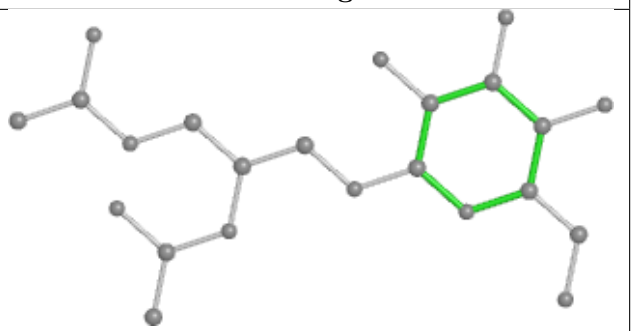


Bond angles

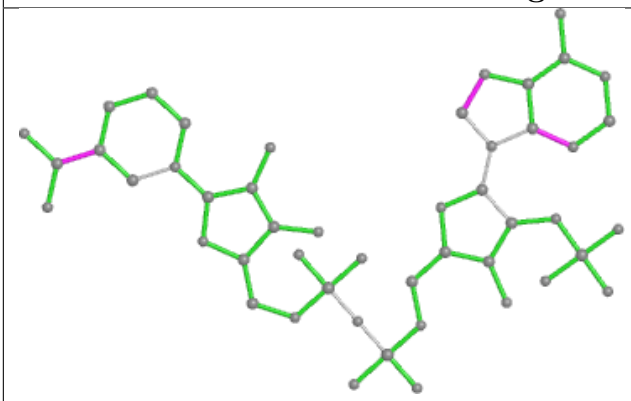


Torsions



Rings

Ligand NDP I 501



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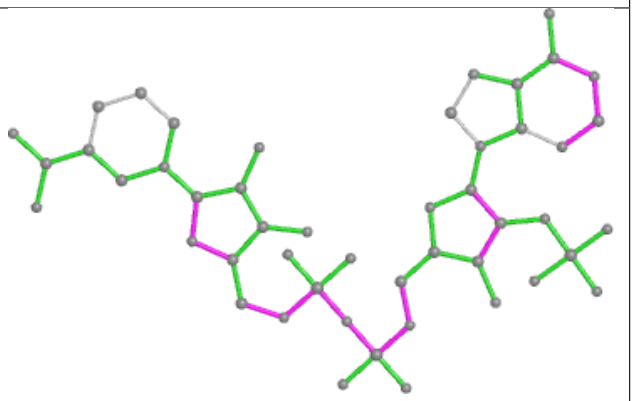
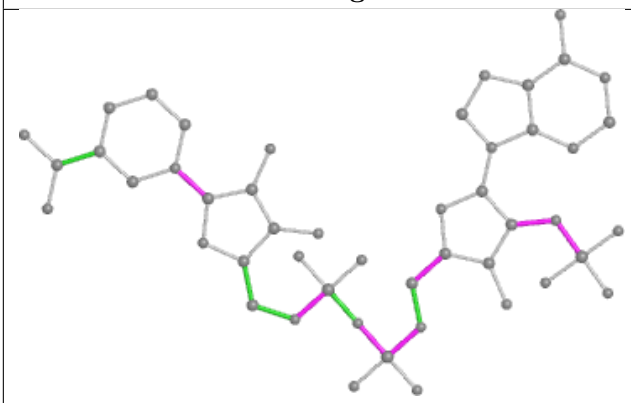


Bond angles



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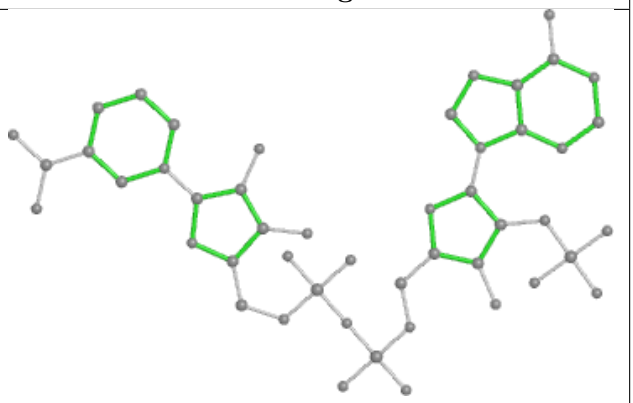
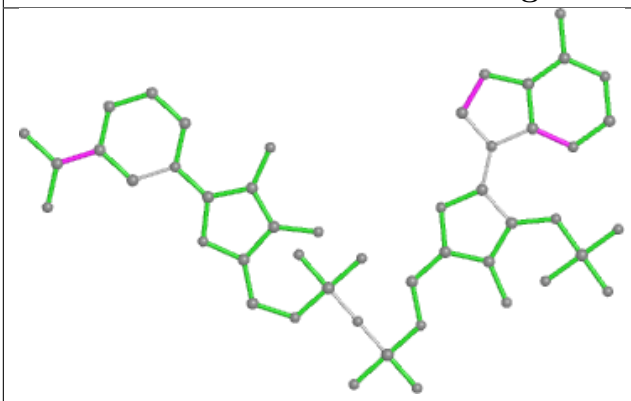


Rings

Ligand NDP Q 501



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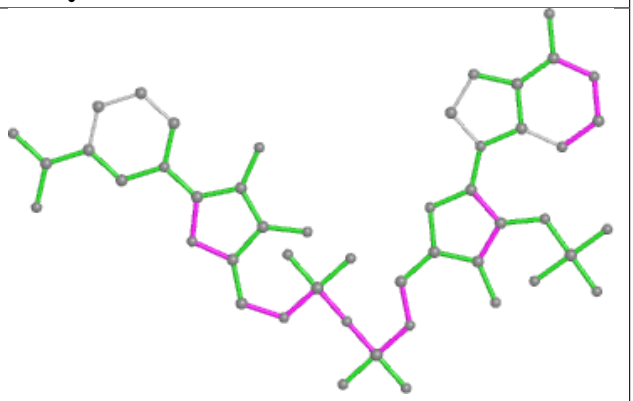
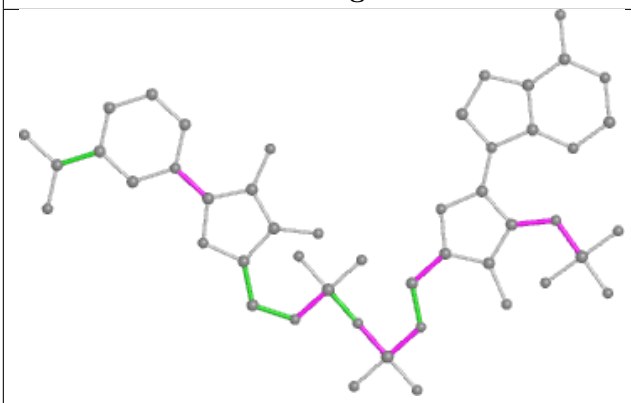
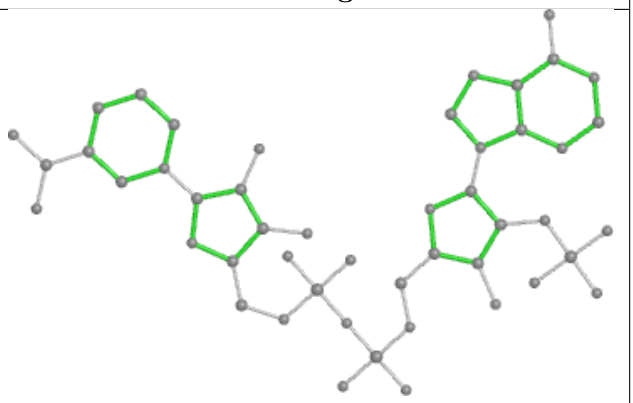


Bond angles

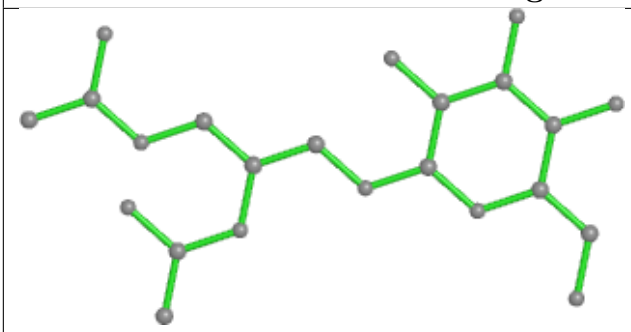


Torsions



Rings

Ligand LMG I 503



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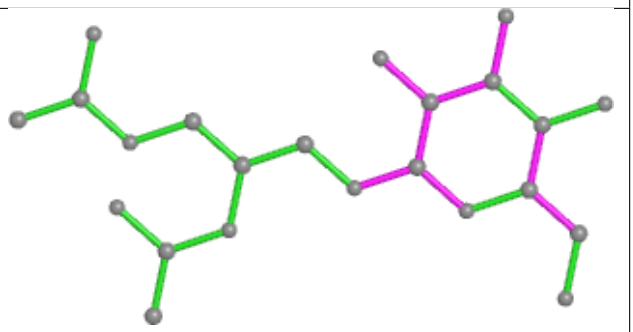
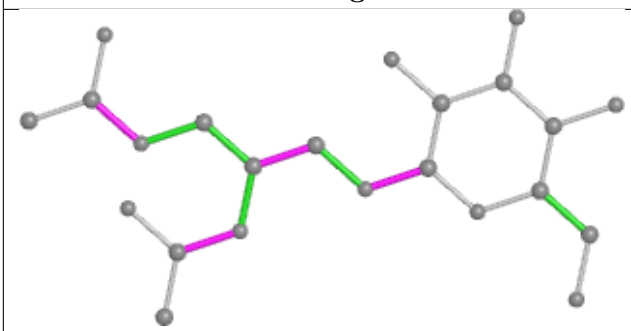


Bond angles



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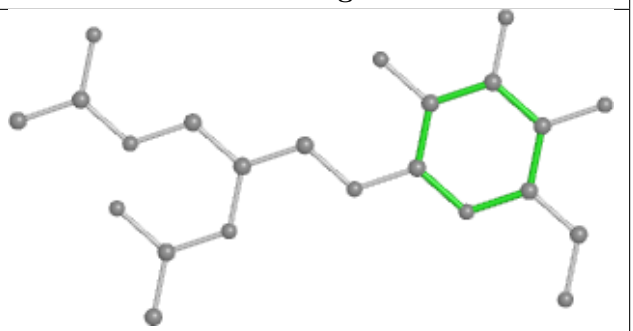
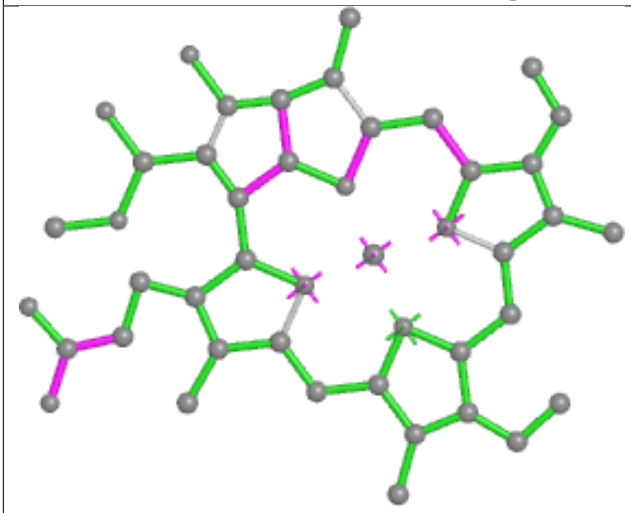
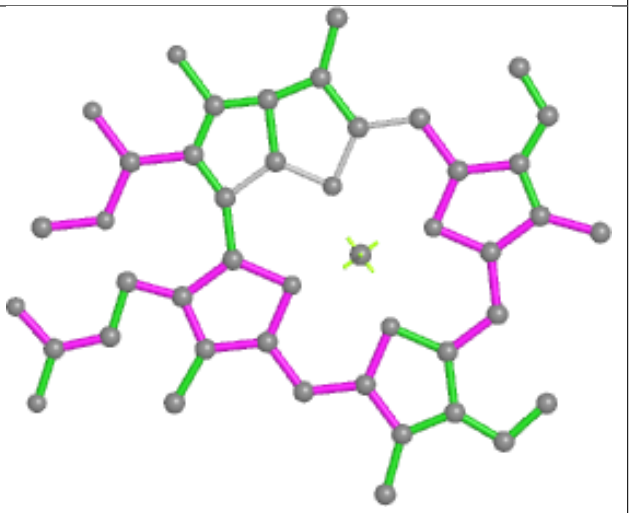


Rings

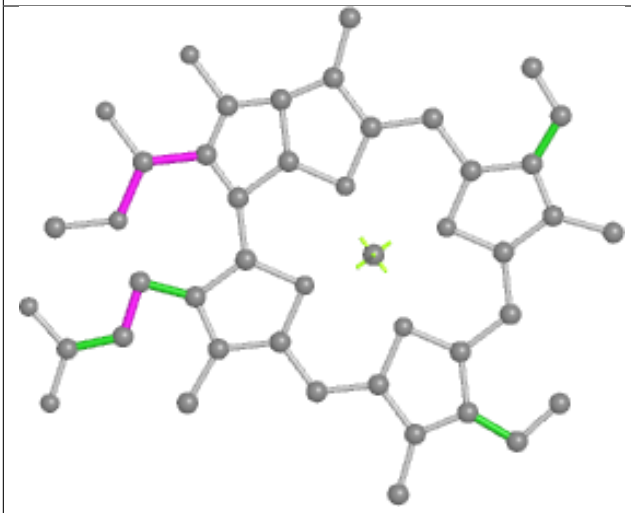
Ligand PMR GA 502



Bond lengths



Bond angles



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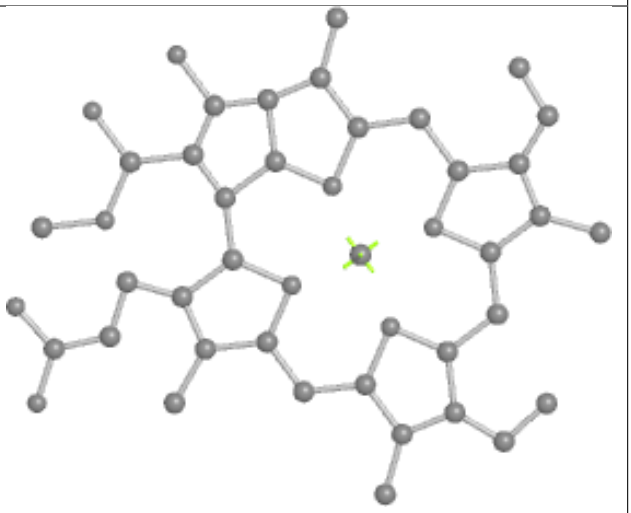
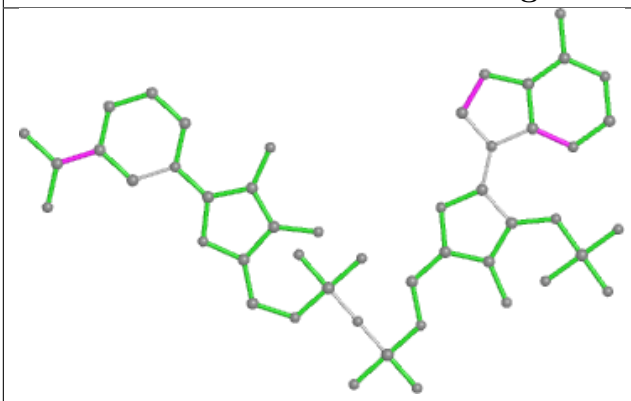
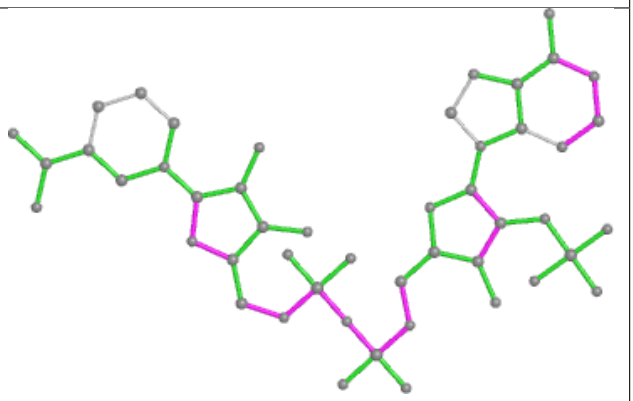


Rings

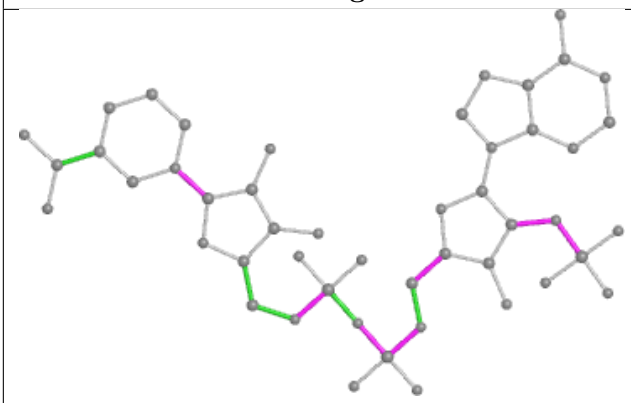
Ligand NDP K 501



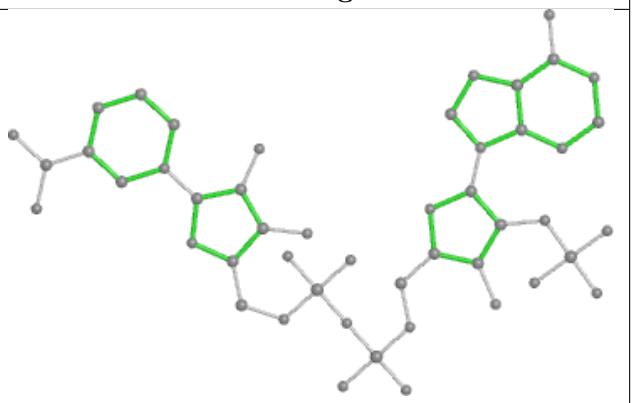
Bond lengths



Bond angles

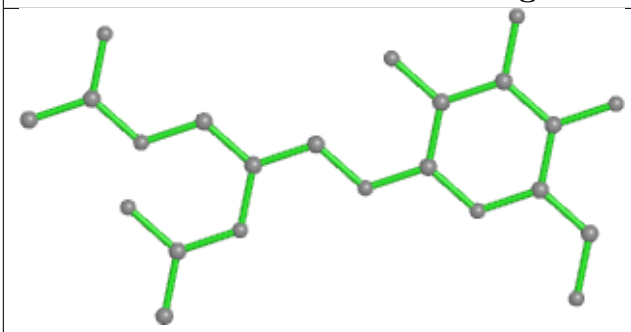


Torsions



Rings

Ligand LMG O 503



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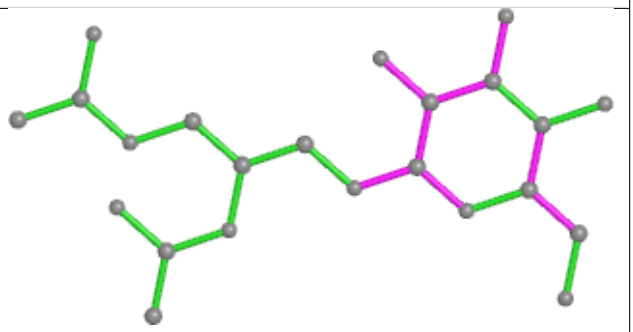
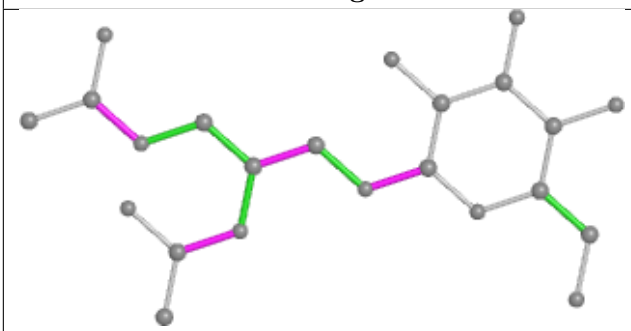


Bond angles



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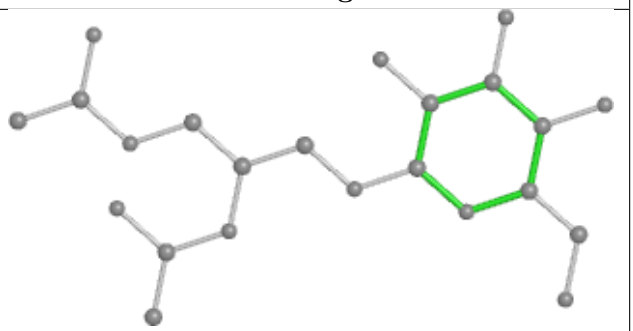
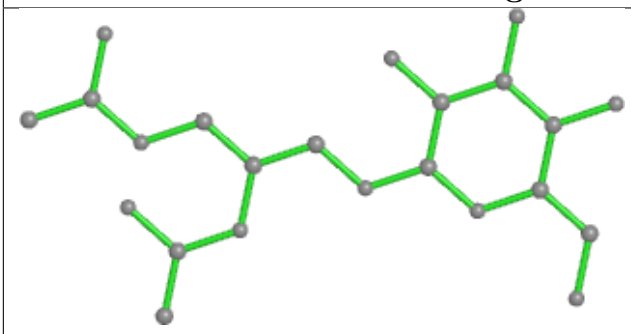


Rings

Ligand LMG DA 503



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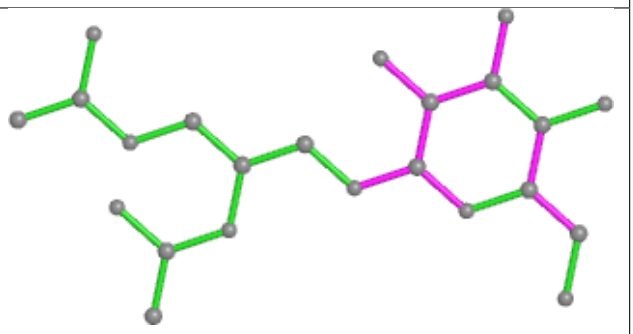
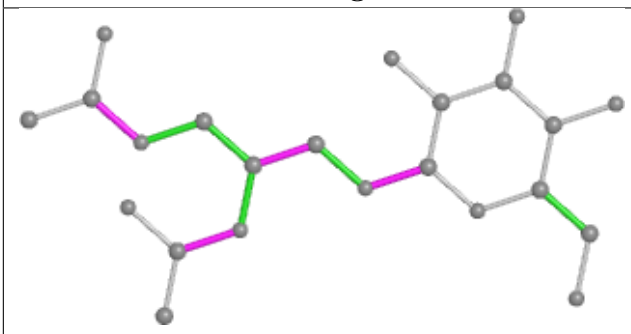
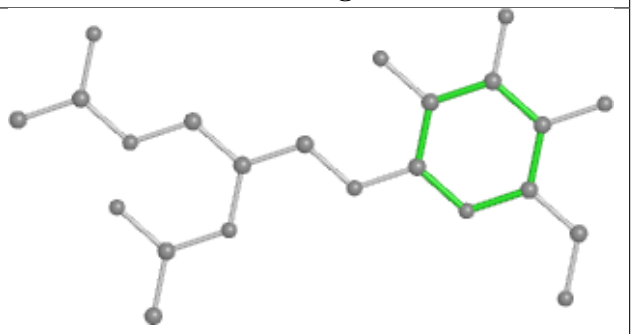


Bond angles

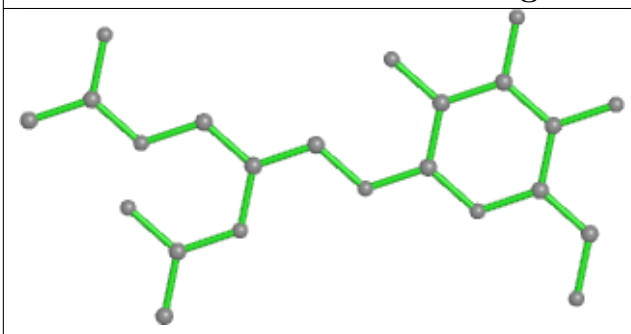


Torsions

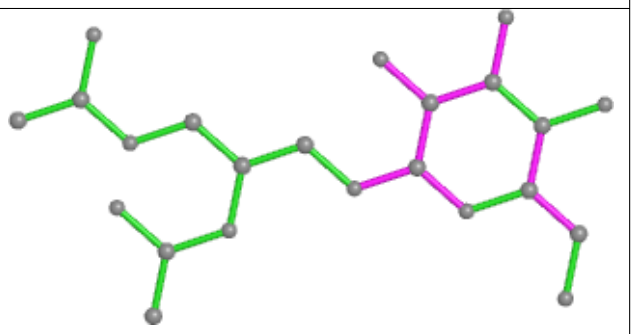


Rings

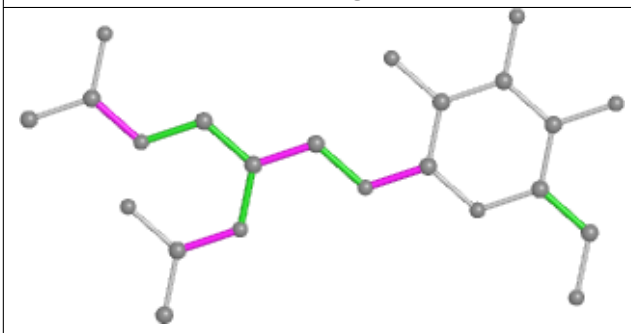
Ligand LMG P 503



Bond lengths



Bond angles



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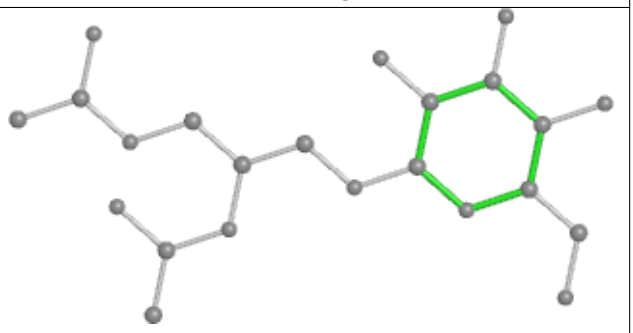


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

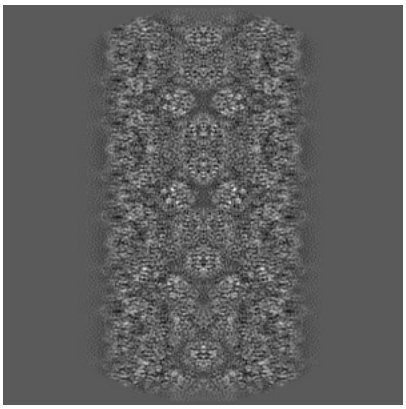
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22364. These allow visual inspection of the internal detail of the map and identification of artifacts.

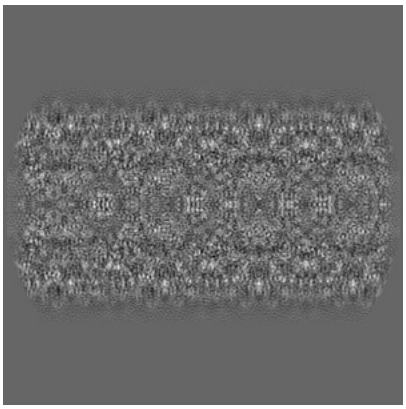
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

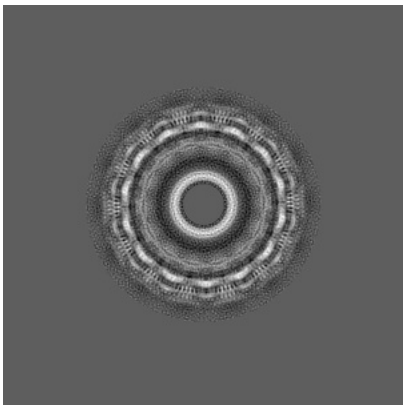
6.1.1 Primary map



X

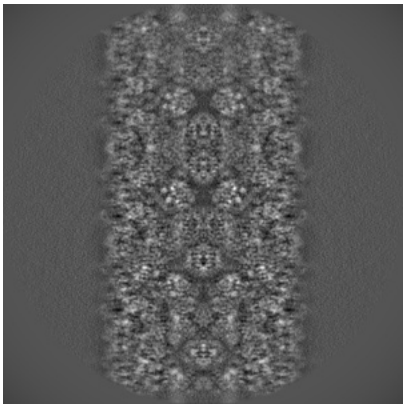


Y

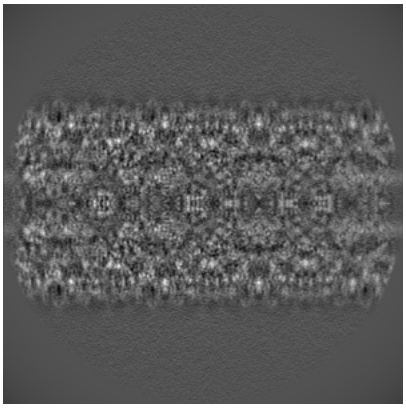


Z

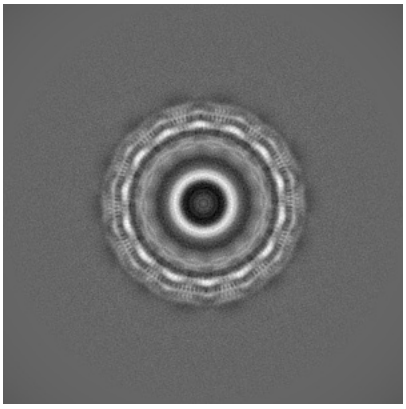
6.1.2 Raw map



X



Y

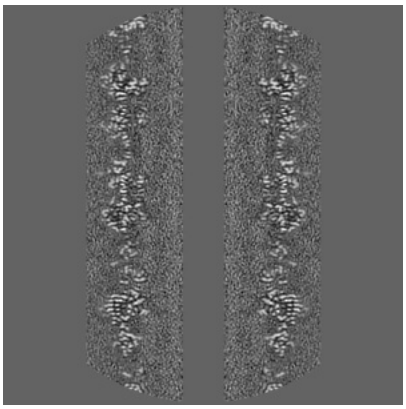


Z

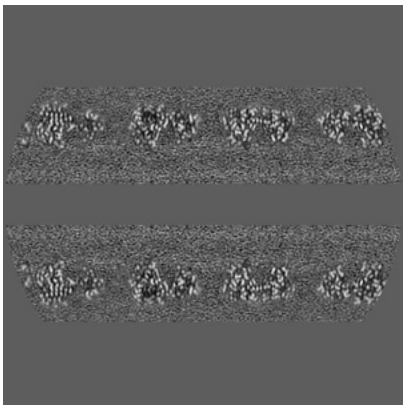
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

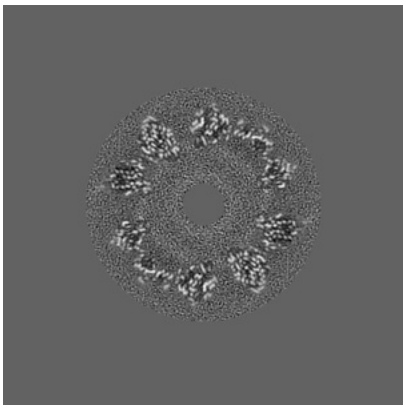
6.2.1 Primary map



X Index: 192

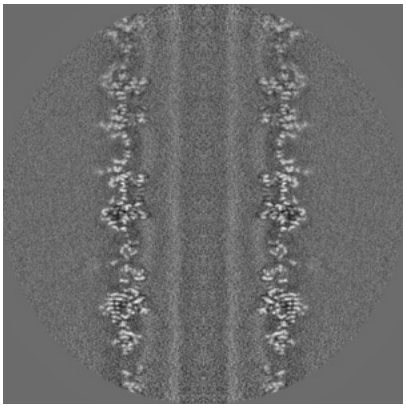


Y Index: 192

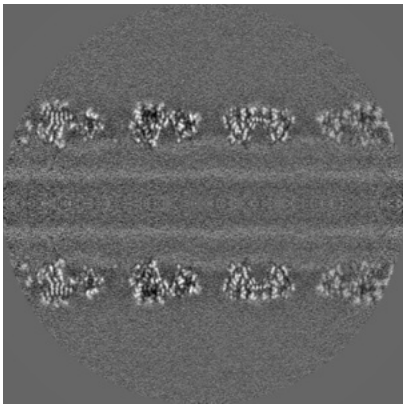


Z Index: 192

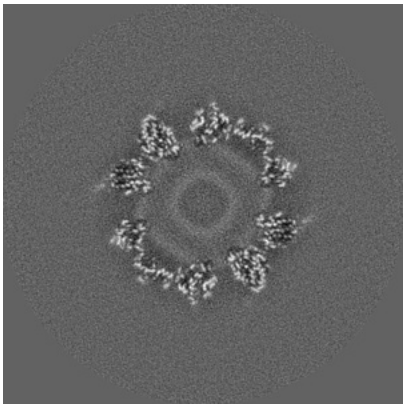
6.2.2 Raw map



X Index: 192



Y Index: 192

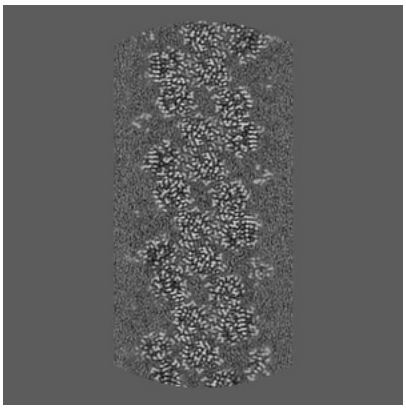


Z Index: 192

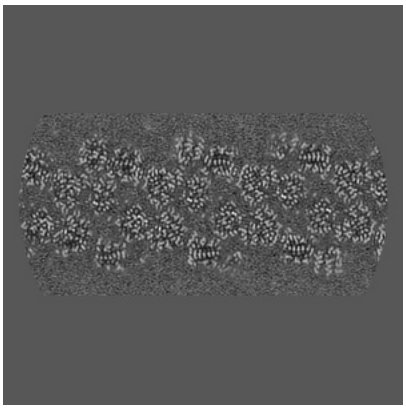
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

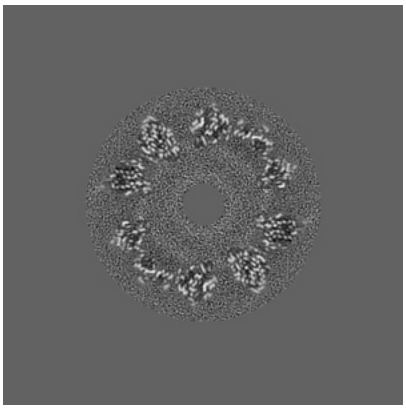
6.3.1 Primary map



X Index: 119

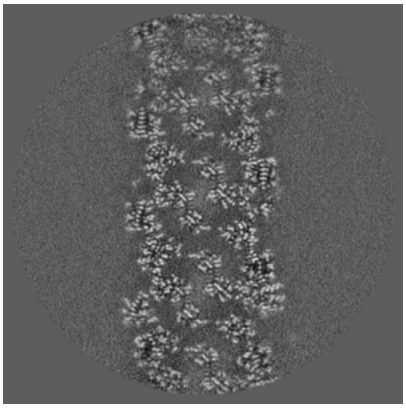


Y Index: 263

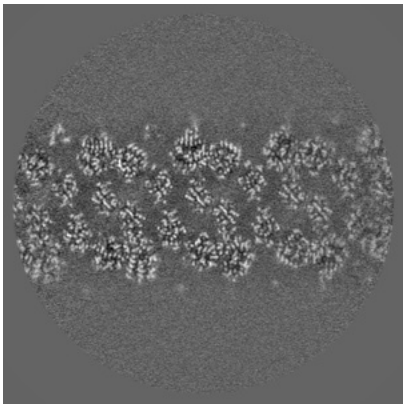


Z Index: 192

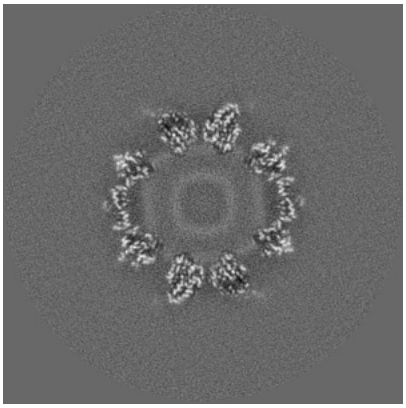
6.3.2 Raw map



X Index: 131



Y Index: 256

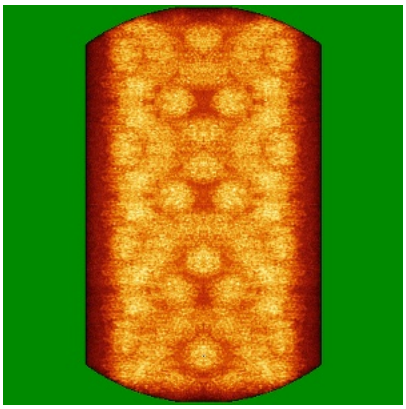


Z Index: 154

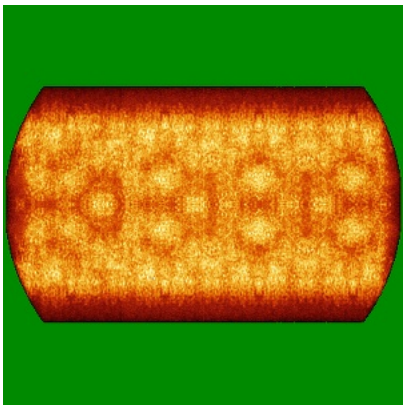
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

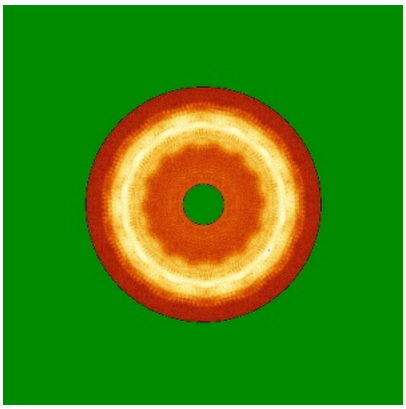
6.4.1 Primary map



X

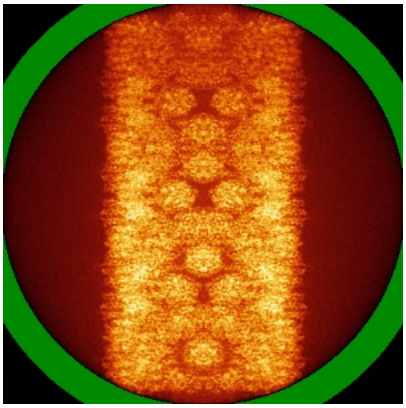


Y

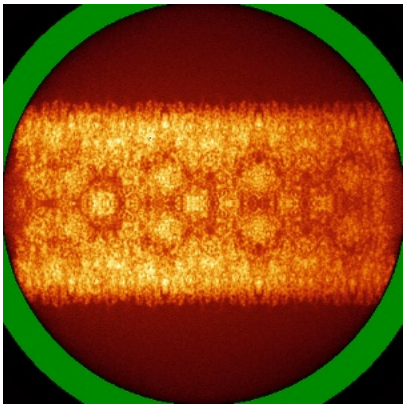


Z

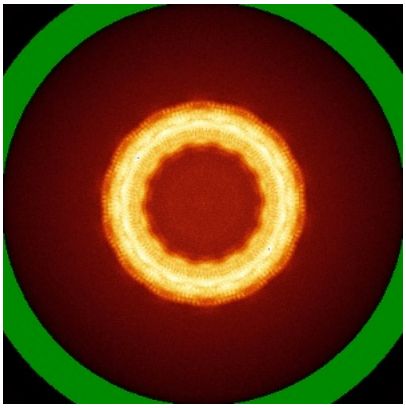
6.4.2 Raw map



X



Y

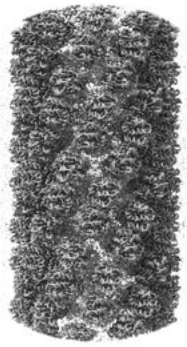


Z

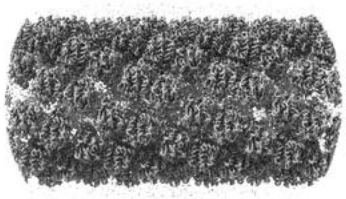
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

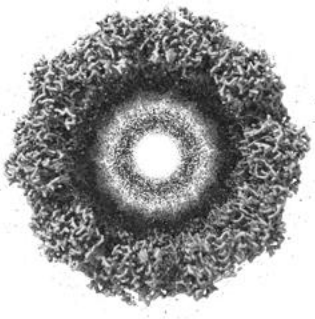
6.5.1 Primary map



X



Y

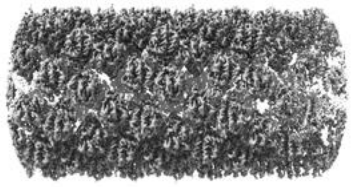


Z

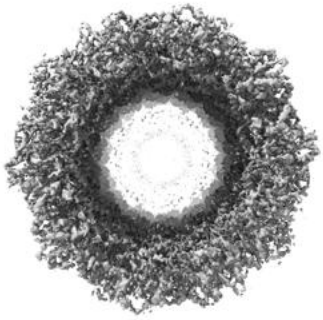
The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

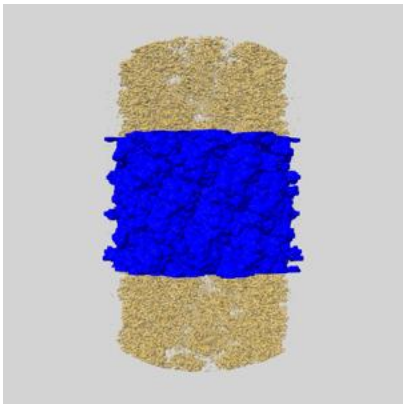
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

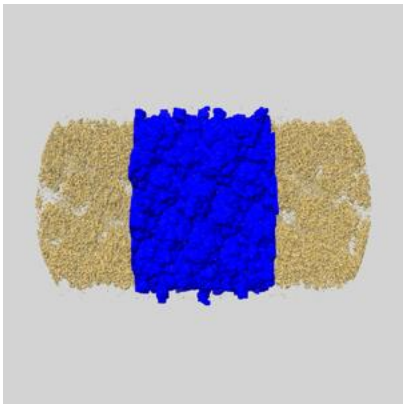
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

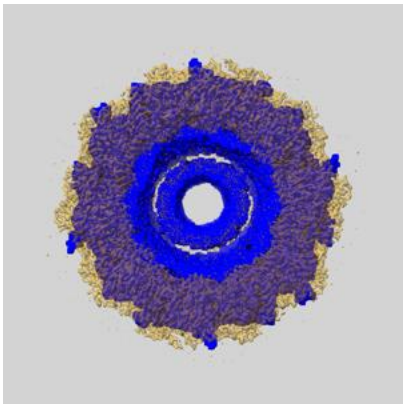
6.6.1 emd_22364_msk_1.map



X



Y

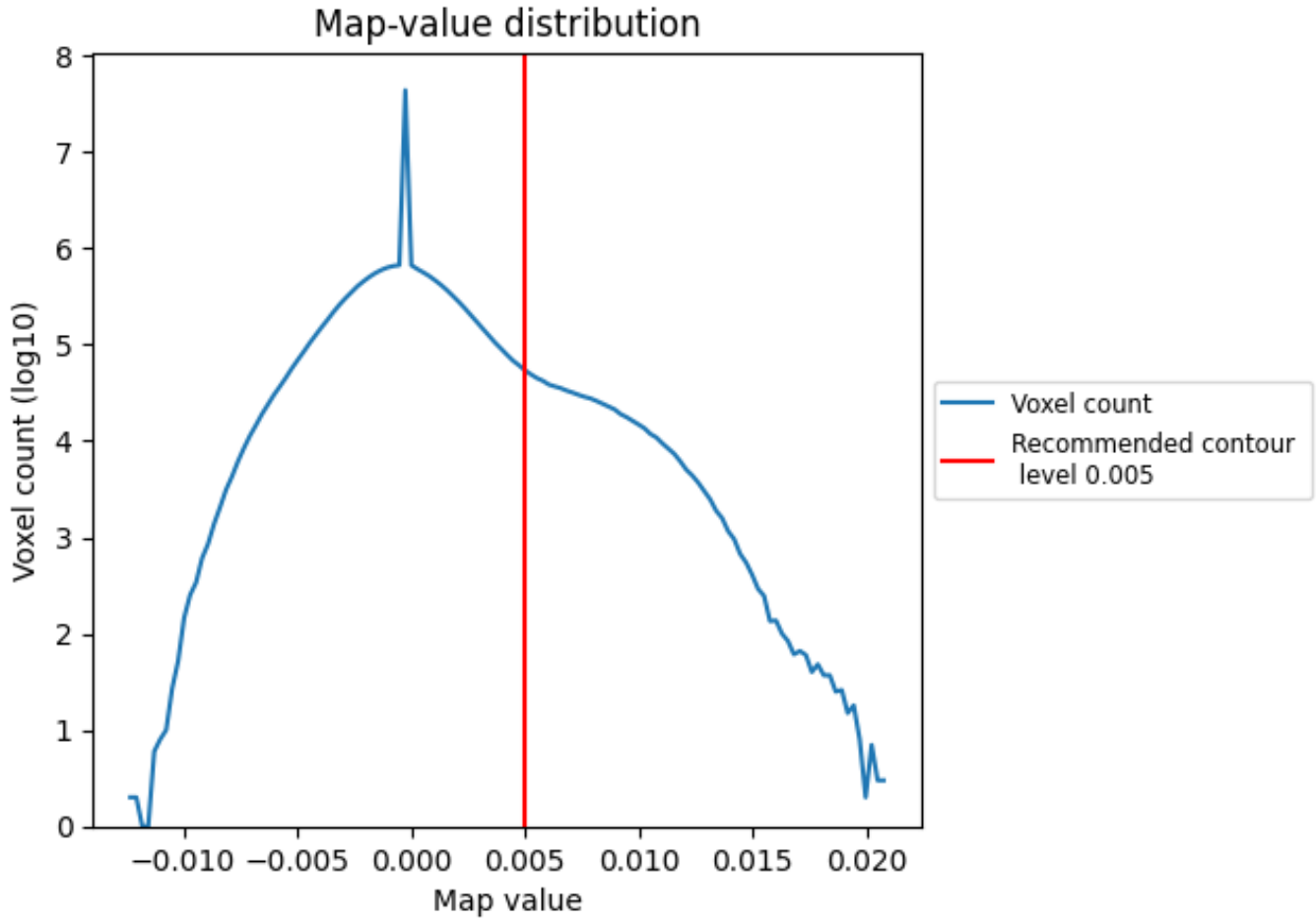


Z

7 Map analysis

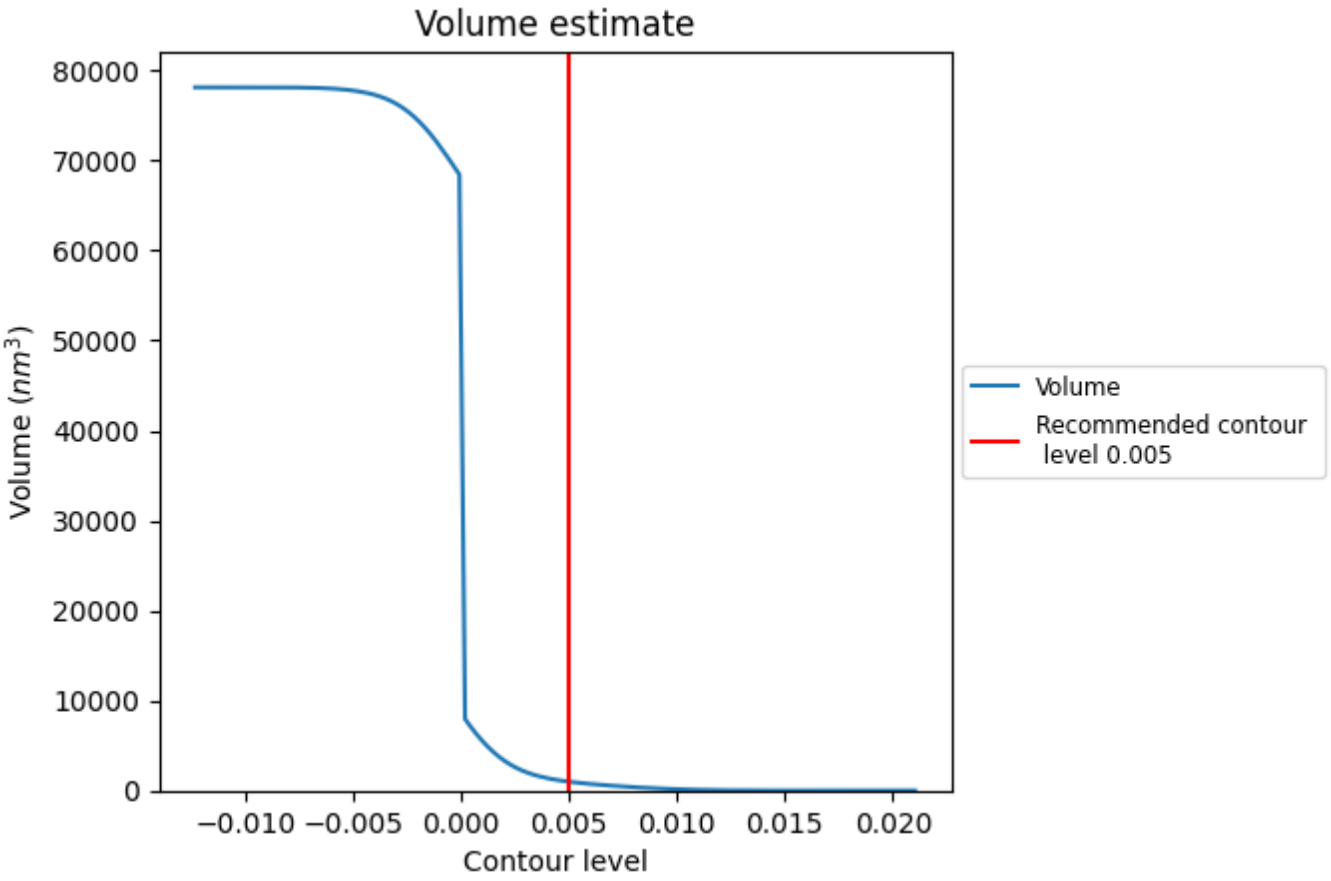
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

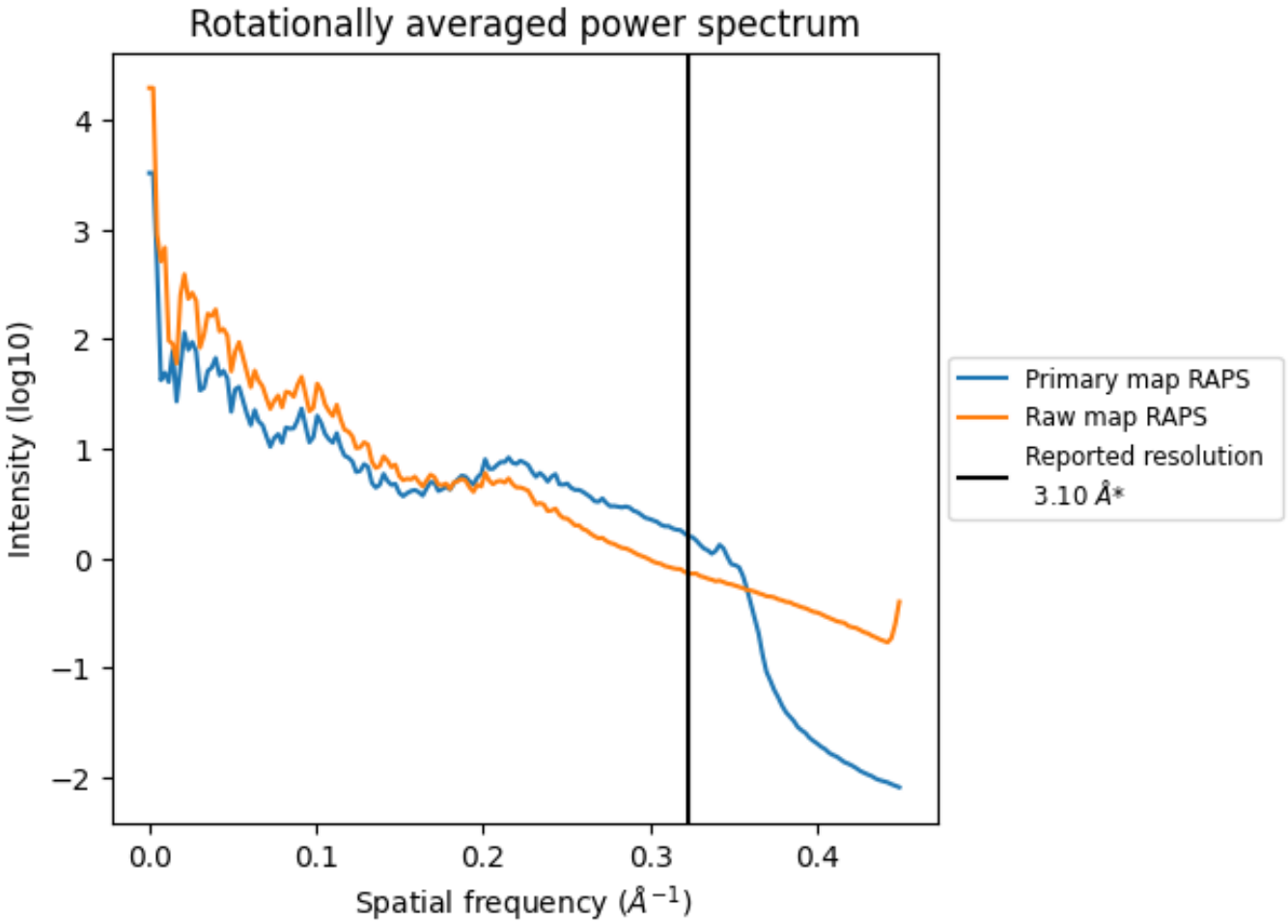
7.2 Volume estimate



The volume at the recommended contour level is 983 nm^3; this corresponds to an approximate mass of 888 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

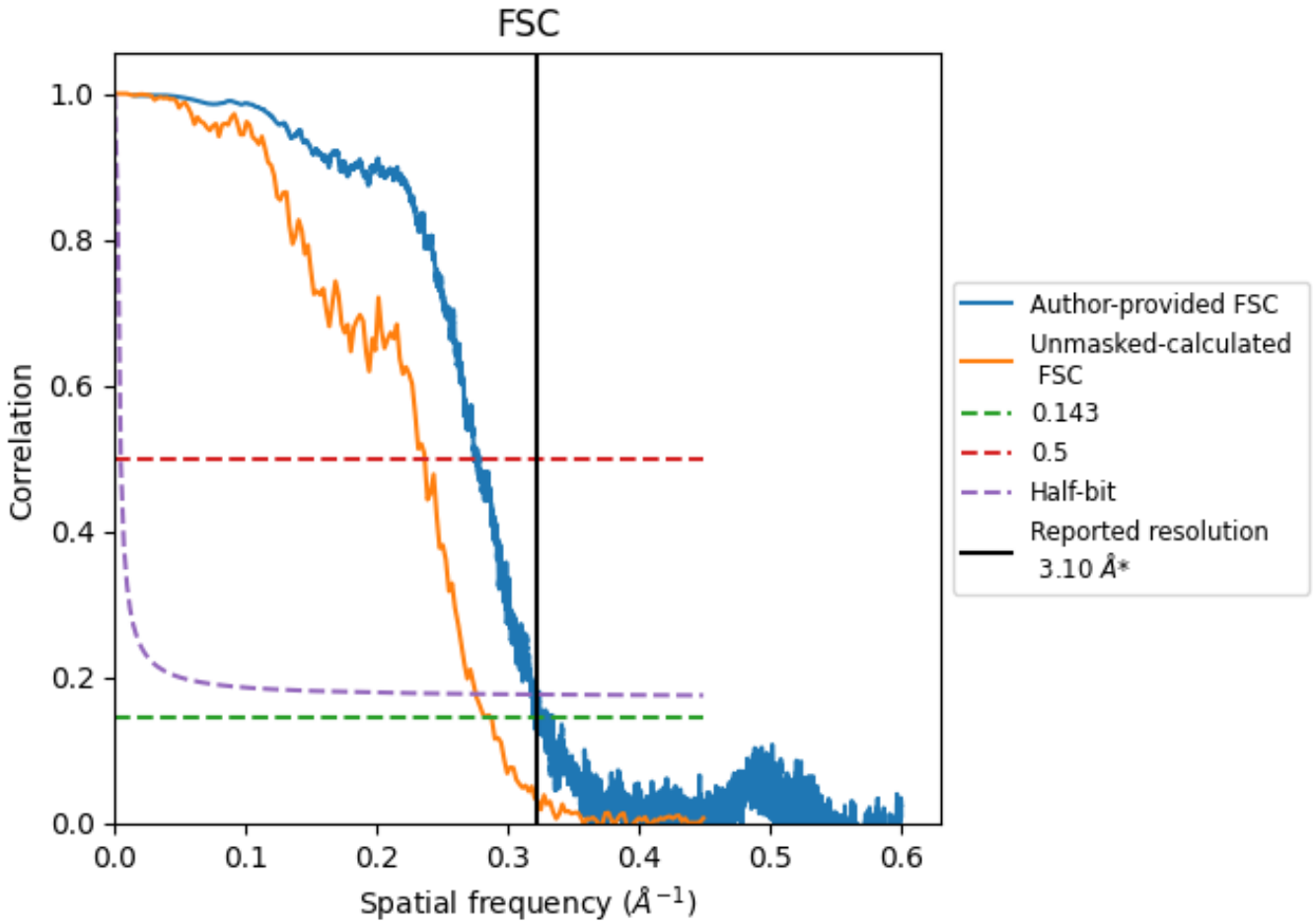


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

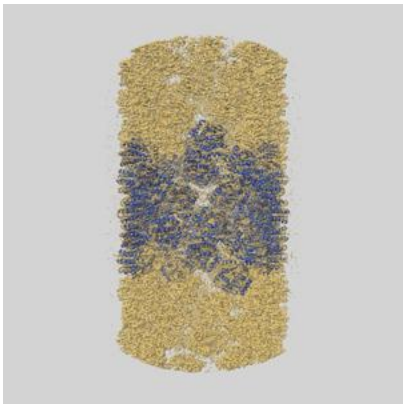
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.64	3.14
Unmasked-calculated*	3.48	4.23	3.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 3.1 by more than 10 %

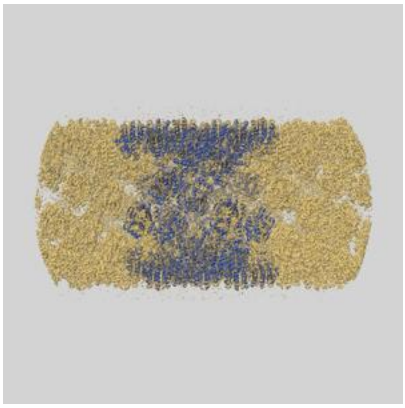
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22364 and PDB model 7JK9. Per-residue inclusion information can be found in section 3 on page 16.

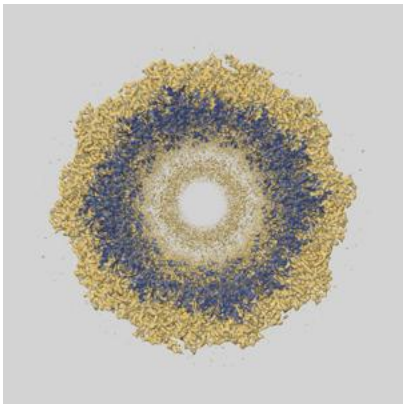
9.1 Map-model overlay



X



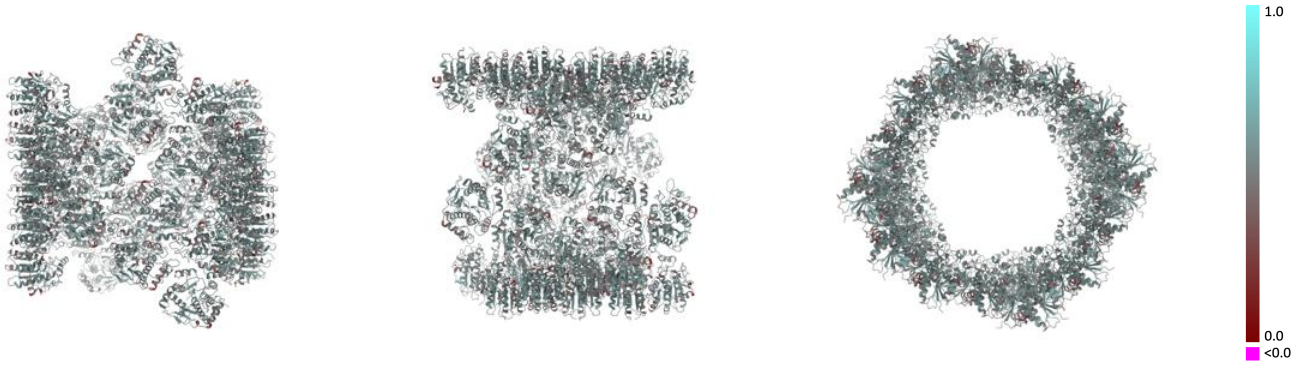
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

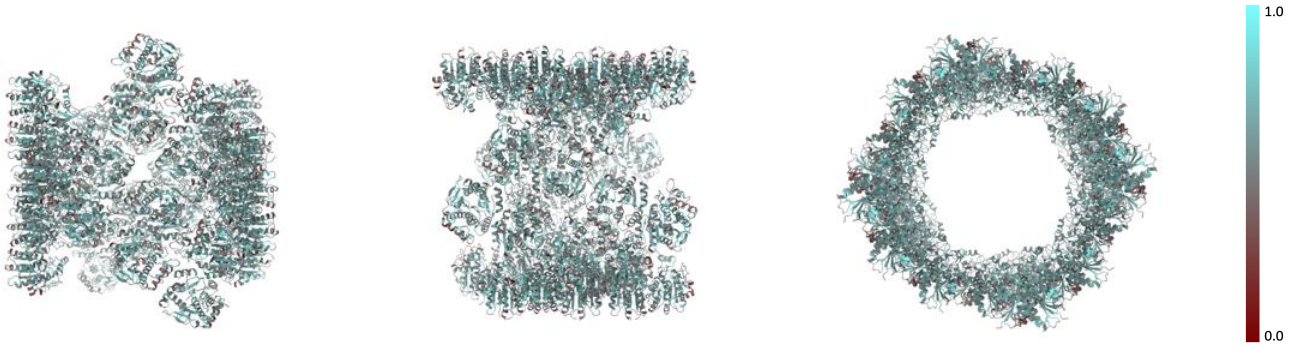
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

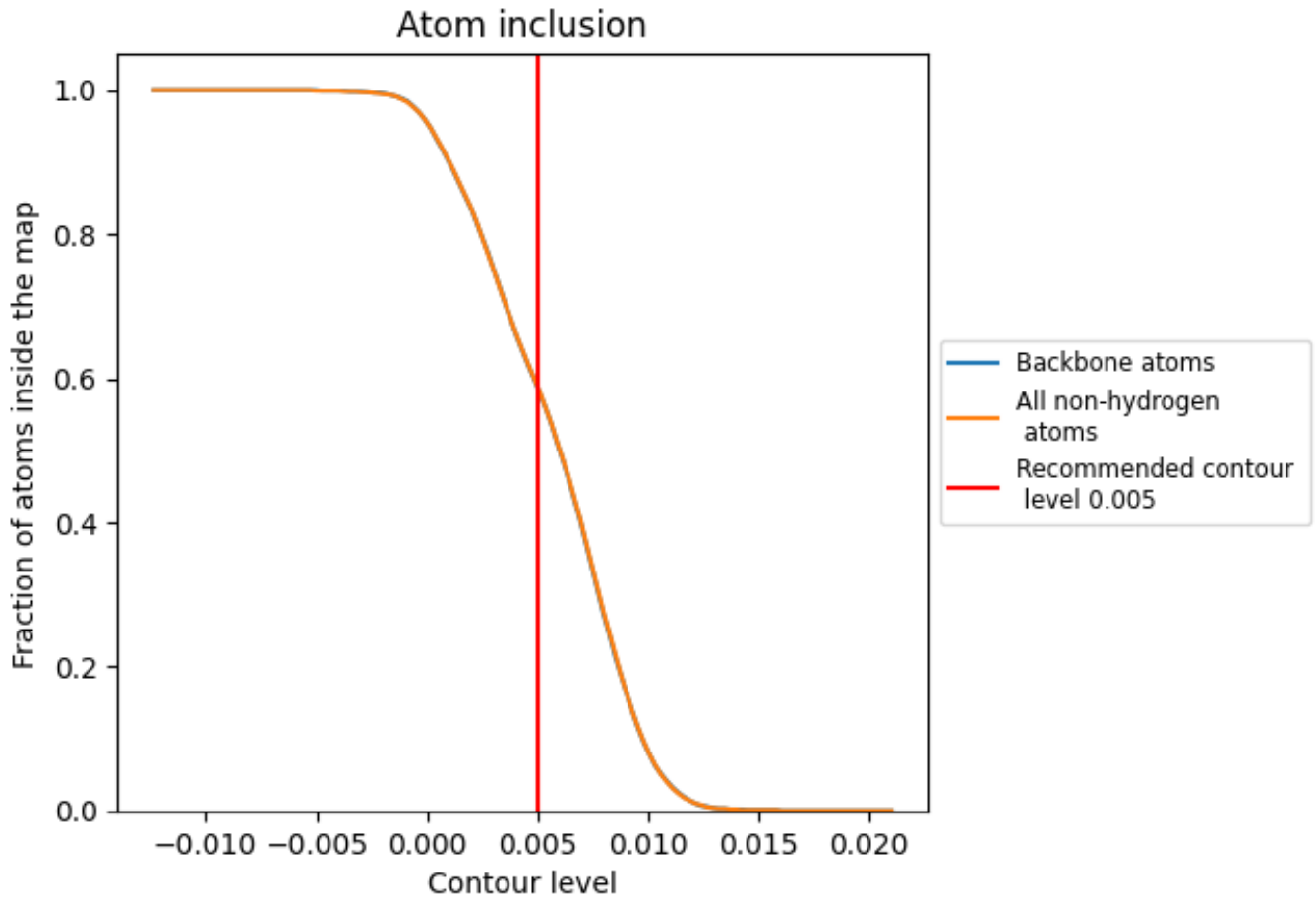
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.5180
A	0.5910	0.5170
AA	0.6030	0.5140
B	0.6020	0.5190
BA	0.5850	0.5190
C	0.5970	0.5220
CA	0.5930	0.5150
D	0.5920	0.5180
DA	0.5890	0.5060
E	0.5860	0.5190
EA	0.5920	0.5080
F	0.5900	0.5190
FA	0.5940	0.5220
G	0.6010	0.5240
GA	0.5940	0.5220
H	0.5920	0.5190
HA	0.5920	0.5190
I	0.6020	0.5220
IA	0.5900	0.5230
J	0.5940	0.5170
JA	0.5900	0.5200
K	0.5980	0.5190
KA	0.5930	0.5210
L	0.6030	0.5160
LA	0.5950	0.5190
M	0.5920	0.5060
MA	0.6030	0.5210
N	0.5800	0.5160
NA	0.6050	0.5220
O	0.5930	0.5140
OA	0.6060	0.5210
P	0.5890	0.5080
Q	0.6030	0.5220
R	0.6020	0.5120
S	0.6140	0.5230

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	0.5950	0.5180
V	0.6010	0.5200
W	0.6060	0.5240
X	0.5940	0.5220
Y	0.6120	0.5210
Z	0.6020	0.5200