



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 04:24 PM EDT

PDB ID : 1C2Y
Title : CRYSTAL STRUCTURES OF A PENTAMERIC FUNGAL AND AN ICOSAHERAL PLANT LUMAZINE SYNTHASE REVEALS THE STRUCTURAL BASIS FOR DIFFERENCES IN ASSEMBLY
Authors : Persson, K.; Schneider, G.; Jordan, D.B.; Viitanen, P.V.; Sandalova, T.
Deposited on : 1999-07-27
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

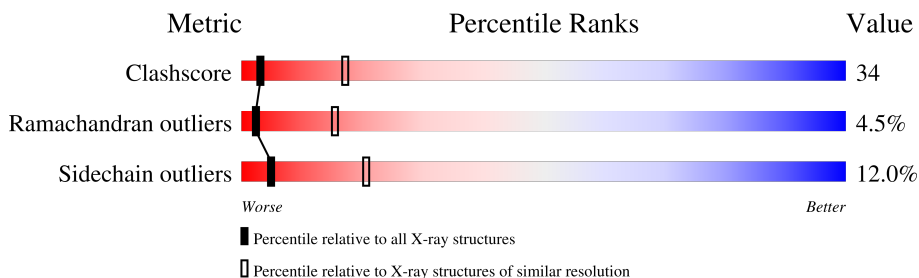
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)




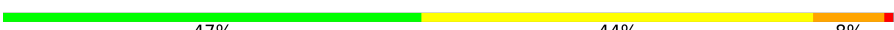
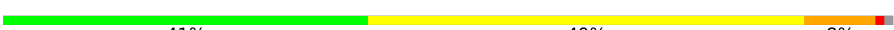
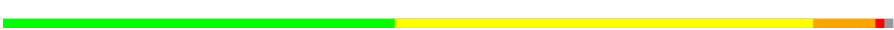




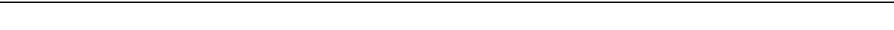

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	44% 48% 6% ..
1	B	156	47% 45% 6% ..
1	C	156	40% 51% 7% ..
1	D	156	42% 49% 7% ..
1	E	156	43% 48% 7% ..
1	F	156	42% 49% 7% ..
1	G	156	42% 49% 8% ..
1	H	156	40% 51% 6% ..

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Mol	Chain	Length	Quality of chain
1	I	156	 49% 42% 7% ..
1	J	156	 40% 51% 7% ..
1	K	156	 44% 47% 6% ..
1	L	156	 47% 44% 8% ..
1	M	156	 41% 49% 8% ..
1	N	156	 44% 47% 7% ..
1	O	156	 44% 48% 6% ..
1	P	156	 48% 43% 7% ..
1	Q	156	 45% 46% 8% ..
1	R	156	 49% 42% 8% ..
1	S	156	 46% 45% 7% ..
1	T	156	 42% 49% 6% ..

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
2	LMZ	A	201	-	X	-	-
2	LMZ	B	202	-	X	-	-
2	LMZ	C	203	-	X	-	-
2	LMZ	D	204	-	X	-	-
2	LMZ	E	205	-	X	X	-
2	LMZ	F	206	-	X	-	-
2	LMZ	G	207	-	X	X	-
2	LMZ	H	208	-	X	-	-
2	LMZ	I	209	-	X	X	-
2	LMZ	J	210	-	X	-	-
2	LMZ	K	211	-	X	X	-
2	LMZ	L	212	-	X	-	-
2	LMZ	M	213	-	X	-	-
2	LMZ	N	214	-	X	-	-
2	LMZ	O	215	-	X	-	-
2	LMZ	P	216	-	X	-	-
2	LMZ	Q	217	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMZ	R	218	-	X	-	-
2	LMZ	S	219	-	X	-	-
2	LMZ	T	220	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (LUMAZINE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	B	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	C	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	D	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	E	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	F	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	G	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	H	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	I	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	J	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	K	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	L	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	M	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	N	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	O	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	P	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	R	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	S	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			
1	T	155	Total	C	N	O	S	0	0	0
			1155	728	199	221	7			

There are 40 discrepancies between the modelled and reference sequences:

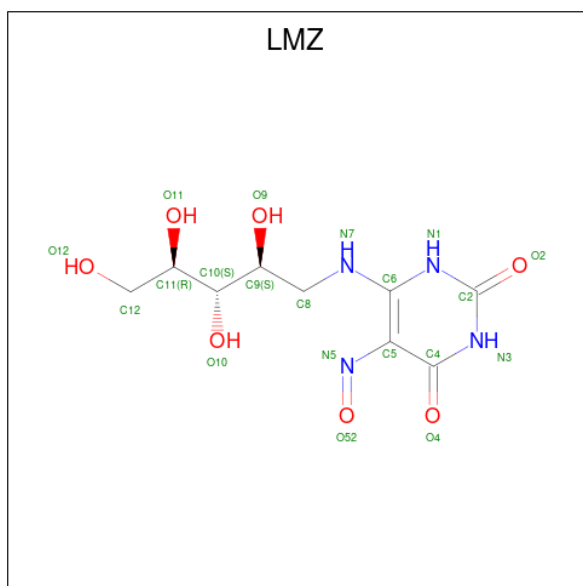
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	VAL	engineered mutation	UNP Q9XH32
A	2	ASN	ARG	engineered mutation	UNP Q9XH32
B	1	MET	VAL	engineered mutation	UNP Q9XH32
B	2	ASN	ARG	engineered mutation	UNP Q9XH32
C	1	MET	VAL	engineered mutation	UNP Q9XH32
C	2	ASN	ARG	engineered mutation	UNP Q9XH32
D	1	MET	VAL	engineered mutation	UNP Q9XH32
D	2	ASN	ARG	engineered mutation	UNP Q9XH32
E	1	MET	VAL	engineered mutation	UNP Q9XH32
E	2	ASN	ARG	engineered mutation	UNP Q9XH32
F	1	MET	VAL	engineered mutation	UNP Q9XH32
F	2	ASN	ARG	engineered mutation	UNP Q9XH32
G	1	MET	VAL	engineered mutation	UNP Q9XH32
G	2	ASN	ARG	engineered mutation	UNP Q9XH32
H	1	MET	VAL	engineered mutation	UNP Q9XH32
H	2	ASN	ARG	engineered mutation	UNP Q9XH32
I	1	MET	VAL	engineered mutation	UNP Q9XH32
I	2	ASN	ARG	engineered mutation	UNP Q9XH32
J	1	MET	VAL	engineered mutation	UNP Q9XH32
J	2	ASN	ARG	engineered mutation	UNP Q9XH32
K	1	MET	VAL	engineered mutation	UNP Q9XH32
K	2	ASN	ARG	engineered mutation	UNP Q9XH32
L	1	MET	VAL	engineered mutation	UNP Q9XH32
L	2	ASN	ARG	engineered mutation	UNP Q9XH32
M	1	MET	VAL	engineered mutation	UNP Q9XH32
M	2	ASN	ARG	engineered mutation	UNP Q9XH32
N	1	MET	VAL	engineered mutation	UNP Q9XH32
N	2	ASN	ARG	engineered mutation	UNP Q9XH32
O	1	MET	VAL	engineered mutation	UNP Q9XH32
O	2	ASN	ARG	engineered mutation	UNP Q9XH32
P	1	MET	VAL	engineered mutation	UNP Q9XH32

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Chain	Residue	Modelled	Actual	Comment	Reference
P	2	ASN	ARG	engineered mutation	UNP Q9XH32
Q	1	MET	VAL	engineered mutation	UNP Q9XH32
Q	2	ASN	ARG	engineered mutation	UNP Q9XH32
R	1	MET	VAL	engineered mutation	UNP Q9XH32
R	2	ASN	ARG	engineered mutation	UNP Q9XH32
S	1	MET	VAL	engineered mutation	UNP Q9XH32
S	2	ASN	ARG	engineered mutation	UNP Q9XH32
T	1	MET	VAL	engineered mutation	UNP Q9XH32
T	2	ASN	ARG	engineered mutation	UNP Q9XH32

- Molecule 2 is 5-NITROSO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: LMZ) (formula: C₉H₁₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	9	4	7		
2	B	1	Total	C	N	O	0	0
			20	9	4	7		
2	C	1	Total	C	N	O	0	0
			20	9	4	7		
2	D	1	Total	C	N	O	0	0
			20	9	4	7		
2	E	1	Total	C	N	O	0	0
			20	9	4	7		
2	F	1	Total	C	N	O	0	0
			20	9	4	7		

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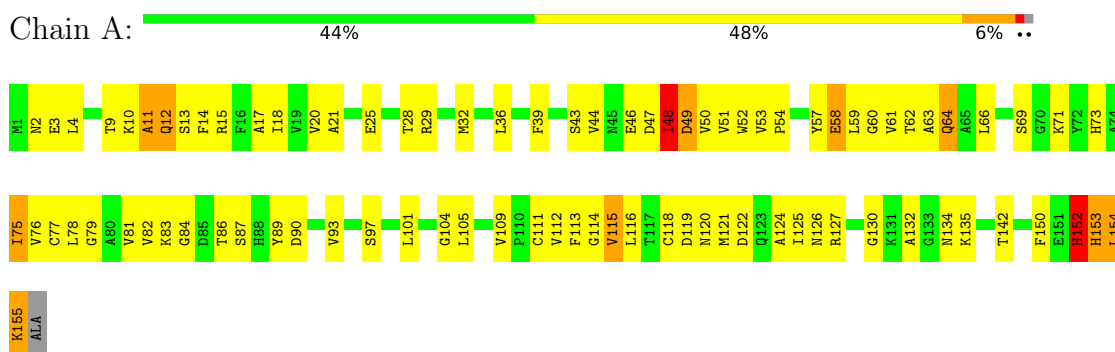
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			20	9	4	7		
2	H	1	Total	C	N	O	0	0
			20	9	4	7		
2	I	1	Total	C	N	O	0	0
			20	9	4	7		
2	J	1	Total	C	N	O	0	0
			20	9	4	7		
2	K	1	Total	C	N	O	0	0
			20	9	4	7		
2	L	1	Total	C	N	O	0	0
			20	9	4	7		
2	M	1	Total	C	N	O	0	0
			20	9	4	7		
2	N	1	Total	C	N	O	0	0
			20	9	4	7		
2	O	1	Total	C	N	O	0	0
			20	9	4	7		
2	P	1	Total	C	N	O	0	0
			20	9	4	7		
2	Q	1	Total	C	N	O	0	0
			20	9	4	7		
2	R	1	Total	C	N	O	0	0
			20	9	4	7		
2	S	1	Total	C	N	O	0	0
			20	9	4	7		
2	T	1	Total	C	N	O	0	0
			20	9	4	7		

3 Residue-property plots [i](#)

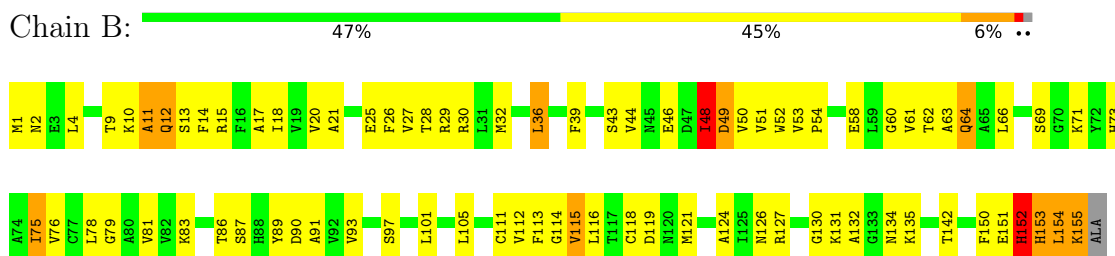
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

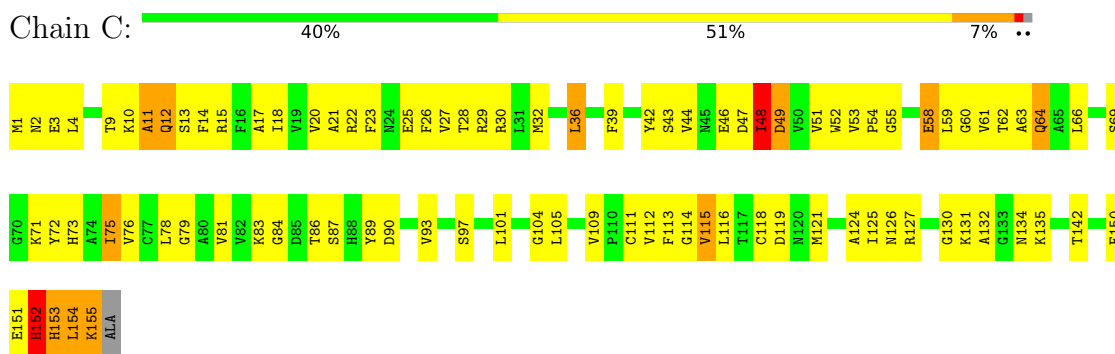
- Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



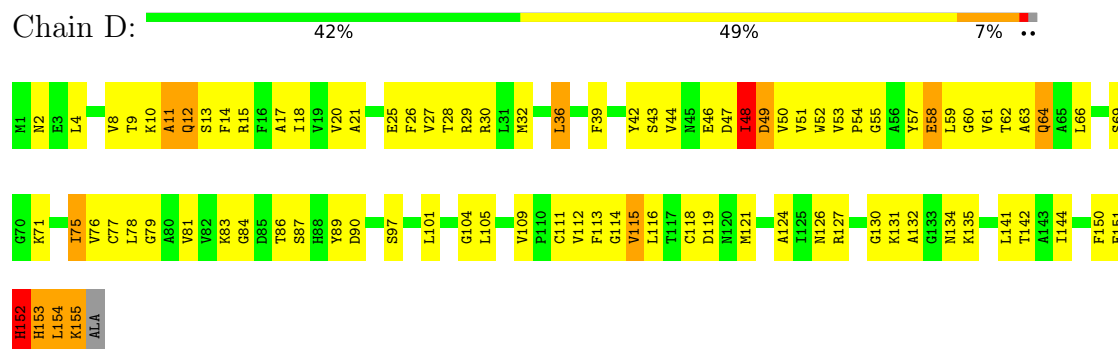
- Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



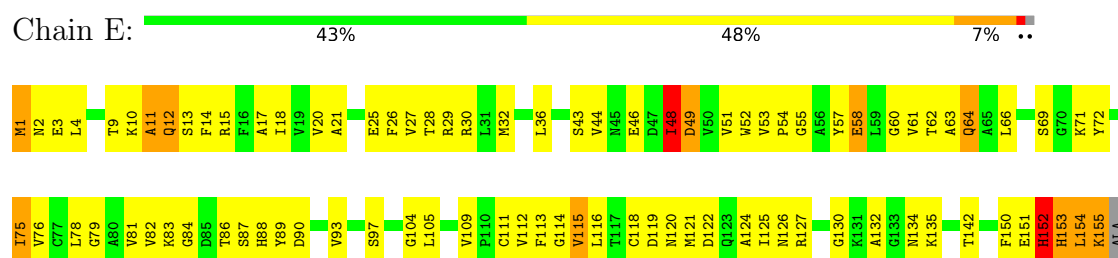
- Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



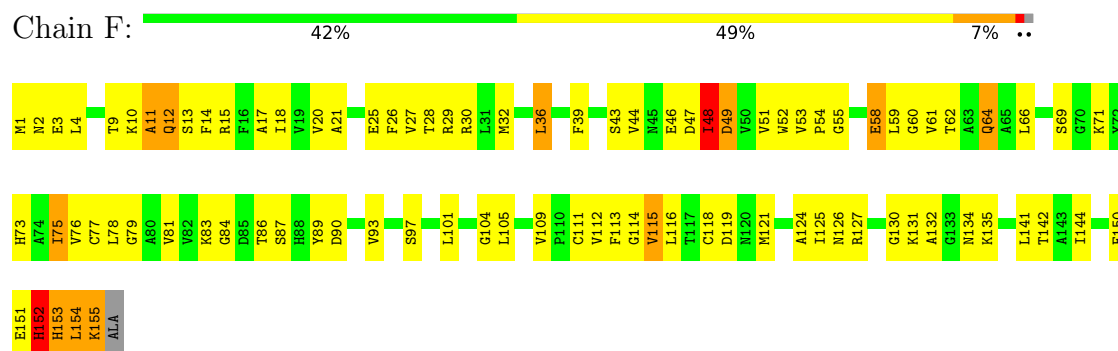
- Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



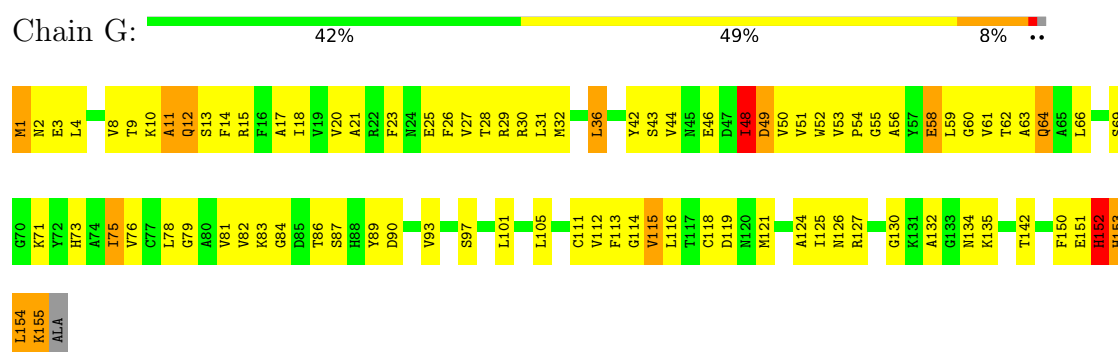
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

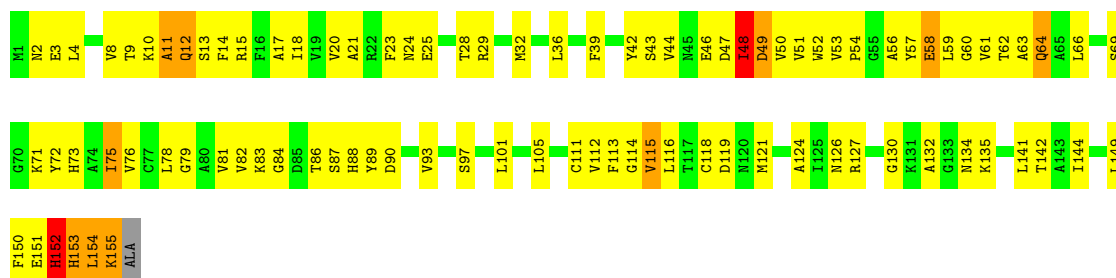


• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



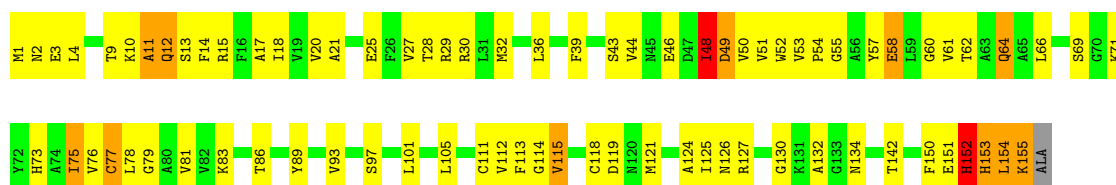
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)





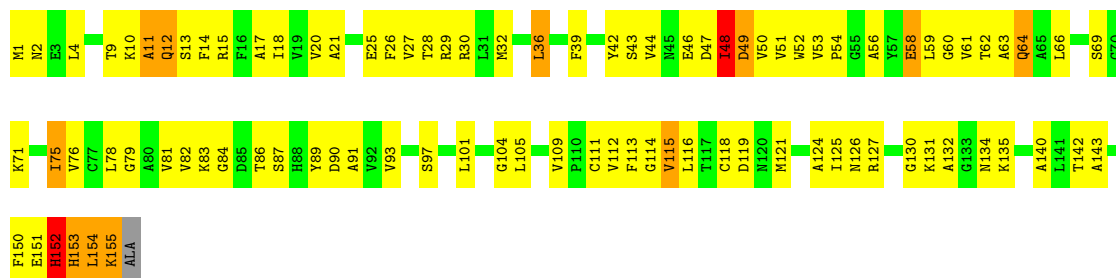
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain I: 49% 42% 7% ..



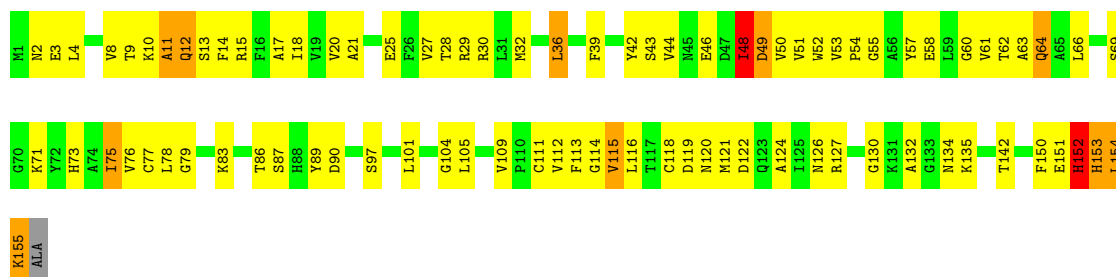
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain J: 40% 51% 7% ..



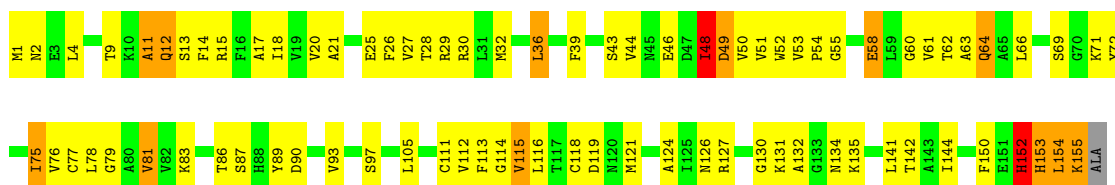
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain K: 44% 47% 6% ..

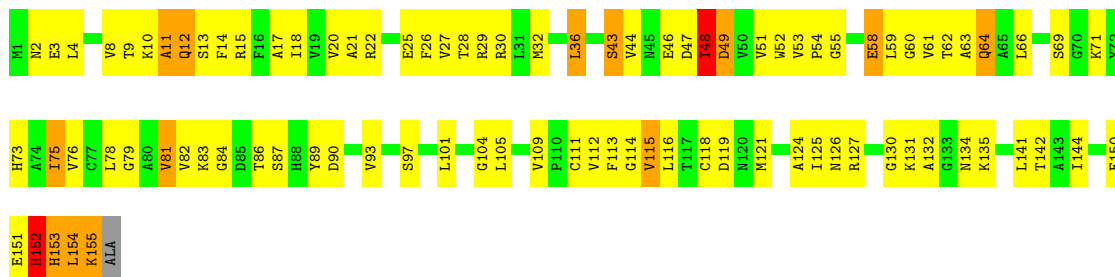


• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

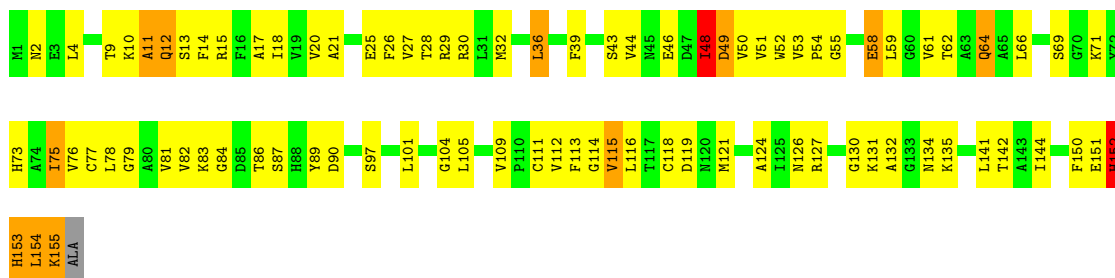
Chain L: 47% 44% 8% ..



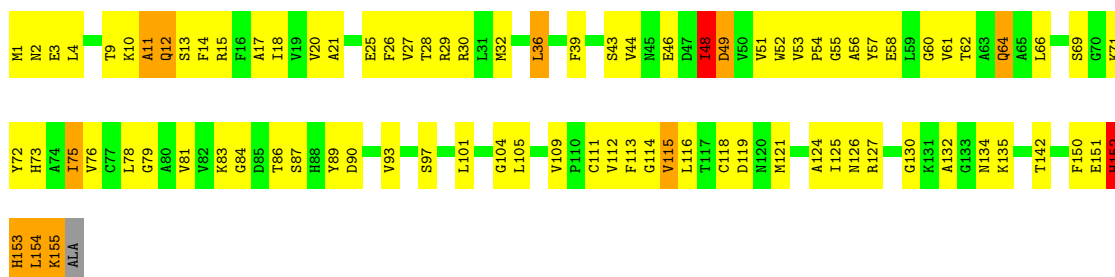
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

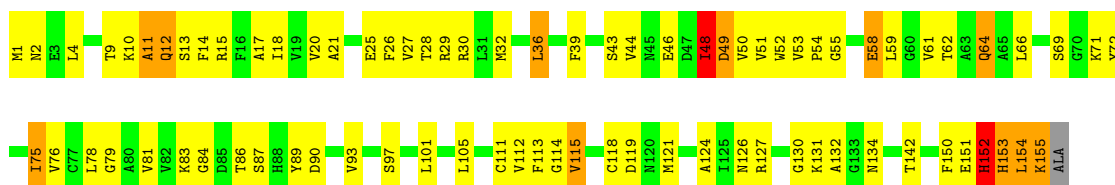


• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)



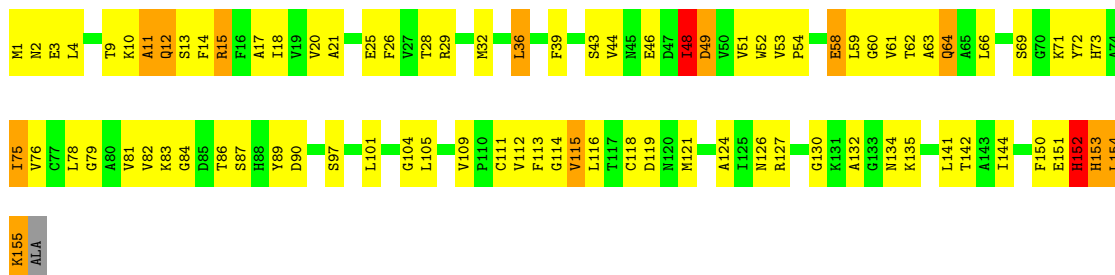
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)





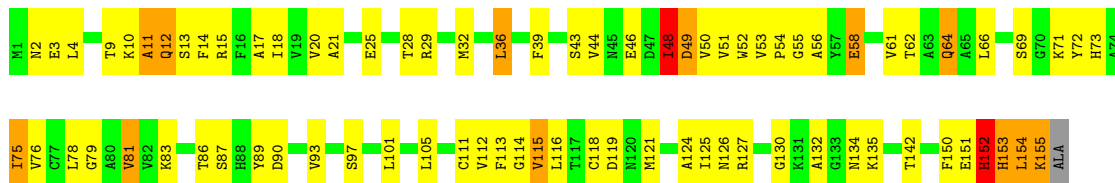
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain Q: 45% 46% 8% ..



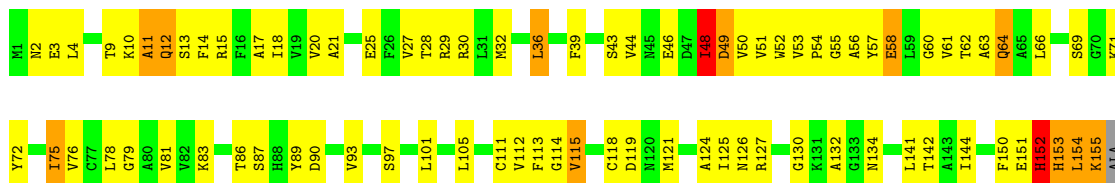
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain R: 49% 42% 8% ..



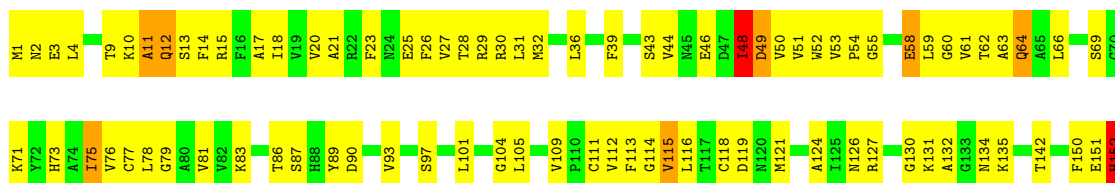
• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain S: 46% 45% 7% ..



• Molecule 1: PROTEIN (LUMAZINE SYNTHASE)

Chain T: 42% 49% 6% ..



H153
L154
K155
ALA

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	218.24Å 218.24Å 218.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	11.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.310 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23500	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMZ

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	0.73	0/1174	0.76	0/1586
1	B	0.75	0/1174	0.76	0/1586
1	C	0.74	0/1174	0.76	0/1586
1	D	0.73	0/1174	0.77	0/1586
1	E	0.74	0/1174	0.76	0/1586
1	F	0.72	0/1174	0.76	0/1586
1	G	0.72	0/1174	0.76	0/1586
1	H	0.72	0/1174	0.76	0/1586
1	I	0.72	0/1174	0.77	0/1586
1	J	0.73	0/1174	0.76	0/1586
1	K	0.70	0/1174	0.76	0/1586
1	L	0.71	0/1174	0.76	0/1586
1	M	0.72	0/1174	0.76	0/1586
1	N	0.72	0/1174	0.77	0/1586
1	O	0.74	0/1174	0.75	0/1586
1	P	0.73	0/1174	0.76	0/1586
1	Q	0.74	0/1174	0.76	0/1586
1	R	0.73	0/1174	0.76	0/1586
1	S	0.74	0/1174	0.75	0/1586
1	T	0.73	0/1174	0.76	0/1586
All	All	0.73	0/23480	0.76	0/31720

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	1155	0	1145	87	0
1	B	1155	0	1145	84	0
1	C	1155	0	1145	98	0
1	D	1155	0	1145	96	0
1	E	1155	0	1145	90	0
1	F	1155	0	1145	95	0
1	G	1155	0	1145	92	0
1	H	1155	0	1145	99	0
1	I	1155	0	1145	87	0
1	J	1155	0	1145	95	0
1	K	1155	0	1145	84	0
1	L	1155	0	1145	89	0
1	M	1155	0	1145	99	0
1	N	1155	0	1145	88	0
1	O	1155	0	1145	90	0
1	P	1155	0	1145	88	0
1	Q	1155	0	1145	90	0
1	R	1155	0	1145	83	0
1	S	1155	0	1145	85	0
1	T	1155	0	1145	88	0
2	A	20	0	14	5	0
2	B	20	0	14	4	0
2	C	20	0	14	4	0
2	D	20	0	14	4	0
2	E	20	0	14	7	0
2	F	20	0	14	4	0
2	G	20	0	14	7	0
2	H	20	0	14	4	0
2	I	20	0	14	7	0
2	J	20	0	14	5	0
2	K	20	0	14	7	0
2	L	20	0	14	5	0
2	M	20	0	14	5	0
2	N	20	0	14	3	0
2	O	20	0	14	5	0
2	P	20	0	14	5	0
2	Q	20	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	20	0	14	4	0
2	S	20	0	14	4	0
2	T	20	0	14	3	0
All	All	23500	0	23180	1573	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 34.

The worst 5 of 1573 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:K:12:GLN:HA	1:K:44:VAL:HA	1.47	0.97
1:N:12:GLN:HA	1:N:44:VAL:HA	1.46	0.97
1:E:12:GLN:HA	1:E:44:VAL:HA	1.48	0.96
1:H:12:GLN:HA	1:H:44:VAL:HA	1.48	0.96
1:F:86:THR:HG21	1:J:118:CYS:HA	1.48	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	2	15
1	B	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	2	15
1	C	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	D	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	E	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	2	15
1	F	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	2	15
1	G	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	153/156 (98%)	120 (78%)	26 (17%)	7 (5%)	2	15
1	I	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	J	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	K	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	2	15
1	L	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	M	153/156 (98%)	119 (78%)	27 (18%)	7 (5%)	2	15
1	N	153/156 (98%)	118 (77%)	29 (19%)	6 (4%)	3	18
1	O	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	P	153/156 (98%)	121 (79%)	26 (17%)	6 (4%)	3	18
1	Q	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	R	153/156 (98%)	119 (78%)	28 (18%)	6 (4%)	3	18
1	S	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
1	T	153/156 (98%)	118 (77%)	28 (18%)	7 (5%)	2	15
All	All	3060/3120 (98%)	2373 (78%)	550 (18%)	137 (4%)	2	15

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	48	ILE
1	B	12	GLN
1	B	48	ILE
1	C	12	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	B	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	C	120/120 (100%)	106 (88%)	14 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	E	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	F	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	G	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	H	120/120 (100%)	107 (89%)	13 (11%)	6	24
1	I	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	J	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	K	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	L	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	M	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	N	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	O	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	P	120/120 (100%)	105 (88%)	15 (12%)	4	19
1	Q	120/120 (100%)	104 (87%)	16 (13%)	4	17
1	R	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	S	120/120 (100%)	106 (88%)	14 (12%)	5	21
1	T	120/120 (100%)	105 (88%)	15 (12%)	4	19
All	All	2400/2400 (100%)	2111 (88%)	289 (12%)	5	20

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	9	THR
1	T	152	HIS
1	Q	58	GLU
1	S	9	THR
1	G	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	153	HIS
1	P	153	HIS
1	N	12	GLN
1	O	153	HIS

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Mol	Chain	Res	Type
1	Q	153	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	LMZ	B	202	-	18,20,20	2.55	8 (44%)	22,27,27	4.44	13 (59%)
2	LMZ	E	205	-	18,20,20	3.06	10 (55%)	22,27,27	4.32	12 (54%)
2	LMZ	S	219	-	18,20,20	2.59	9 (50%)	22,27,27	4.38	12 (54%)
2	LMZ	Q	217	-	18,20,20	2.83	8 (44%)	22,27,27	4.42	13 (59%)
2	LMZ	K	211	-	18,20,20	3.21	11 (61%)	22,27,27	4.61	13 (59%)
2	LMZ	L	212	-	18,20,20	2.55	7 (38%)	22,27,27	4.35	13 (59%)
2	LMZ	J	210	-	18,20,20	3.22	9 (50%)	22,27,27	4.47	12 (54%)
2	LMZ	M	213	-	18,20,20	3.40	8 (44%)	22,27,27	4.48	12 (54%)
2	LMZ	D	204	-	18,20,20	2.88	9 (50%)	22,27,27	4.56	12 (54%)
2	LMZ	I	209	-	18,20,20	3.24	11 (61%)	22,27,27	4.24	12 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMZ	O	215	-	18,20,20	2.99	7 (38%)	22,27,27	4.49	13 (59%)
2	LMZ	C	203	-	18,20,20	3.05	8 (44%)	22,27,27	4.44	12 (54%)
2	LMZ	T	220	-	18,20,20	3.19	9 (50%)	22,27,27	4.57	12 (54%)
2	LMZ	H	208	-	18,20,20	2.67	10 (55%)	22,27,27	4.39	12 (54%)
2	LMZ	P	216	-	18,20,20	2.81	9 (50%)	22,27,27	4.22	12 (54%)
2	LMZ	A	201	-	18,20,20	2.50	8 (44%)	22,27,27	4.42	12 (54%)
2	LMZ	G	207	-	18,20,20	2.88	10 (55%)	22,27,27	4.41	12 (54%)
2	LMZ	N	214	-	18,20,20	3.20	10 (55%)	22,27,27	4.43	12 (54%)
2	LMZ	F	206	-	18,20,20	2.93	8 (44%)	22,27,27	4.45	11 (50%)
2	LMZ	R	218	-	18,20,20	2.84	10 (55%)	22,27,27	4.35	12 (54%)

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	LMZ	B	202	-	-	12/17/17/17	0/1/1/1
2	LMZ	E	205	-	-	10/17/17/17	0/1/1/1
2	LMZ	S	219	-	-	10/17/17/17	0/1/1/1
2	LMZ	Q	217	-	-	9/17/17/17	0/1/1/1
2	LMZ	K	211	-	-	9/17/17/17	0/1/1/1
2	LMZ	L	212	-	-	8/17/17/17	0/1/1/1
2	LMZ	J	210	-	-	9/17/17/17	0/1/1/1
2	LMZ	M	213	-	-	9/17/17/17	0/1/1/1
2	LMZ	D	204	-	-	7/17/17/17	0/1/1/1
2	LMZ	I	209	-	-	8/17/17/17	0/1/1/1
2	LMZ	O	215	-	-	11/17/17/17	0/1/1/1
2	LMZ	C	203	-	-	10/17/17/17	0/1/1/1
2	LMZ	T	220	-	-	13/17/17/17	0/1/1/1
2	LMZ	H	208	-	-	11/17/17/17	0/1/1/1
2	LMZ	P	216	-	-	10/17/17/17	0/1/1/1
2	LMZ	A	201	-	-	10/17/17/17	0/1/1/1
2	LMZ	G	207	-	-	11/17/17/17	0/1/1/1
2	LMZ	N	214	-	-	7/17/17/17	0/1/1/1
2	LMZ	F	206	-	-	9/17/17/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMZ	R	218	-	-	9/17/17/17	0/1/1/1

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	213	LMZ	C11-C10	7.76	1.68	1.53
2	E	205	LMZ	C11-C10	7.27	1.67	1.53
2	O	215	LMZ	C11-C10	7.06	1.66	1.53
2	J	210	LMZ	C8-C9	6.69	1.61	1.52
2	N	214	LMZ	C8-C9	6.59	1.61	1.52

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	205	LMZ	C4-N3-C2	12.29	125.52	115.14
2	T	220	LMZ	C4-N3-C2	12.24	125.48	115.14
2	I	209	LMZ	C4-N3-C2	12.24	125.47	115.14
2	G	207	LMZ	C4-N3-C2	12.13	125.38	115.14
2	P	216	LMZ	C4-N3-C2	11.75	125.06	115.14

There are no chirality outliers.

5 of 192 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	LMZ	N1-C6-N7-C8
2	A	201	LMZ	C5-C6-N7-C8
2	A	201	LMZ	C9-C10-C11-O11
2	A	201	LMZ	C9-C10-C11-C12
2	A	201	LMZ	O10-C10-C11-O11

There are no ring outliers.

20 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	202	LMZ	4	0
2	E	205	LMZ	7	0
2	S	219	LMZ	4	0
2	Q	217	LMZ	4	0
2	K	211	LMZ	7	0
2	L	212	LMZ	5	0
2	J	210	LMZ	5	0

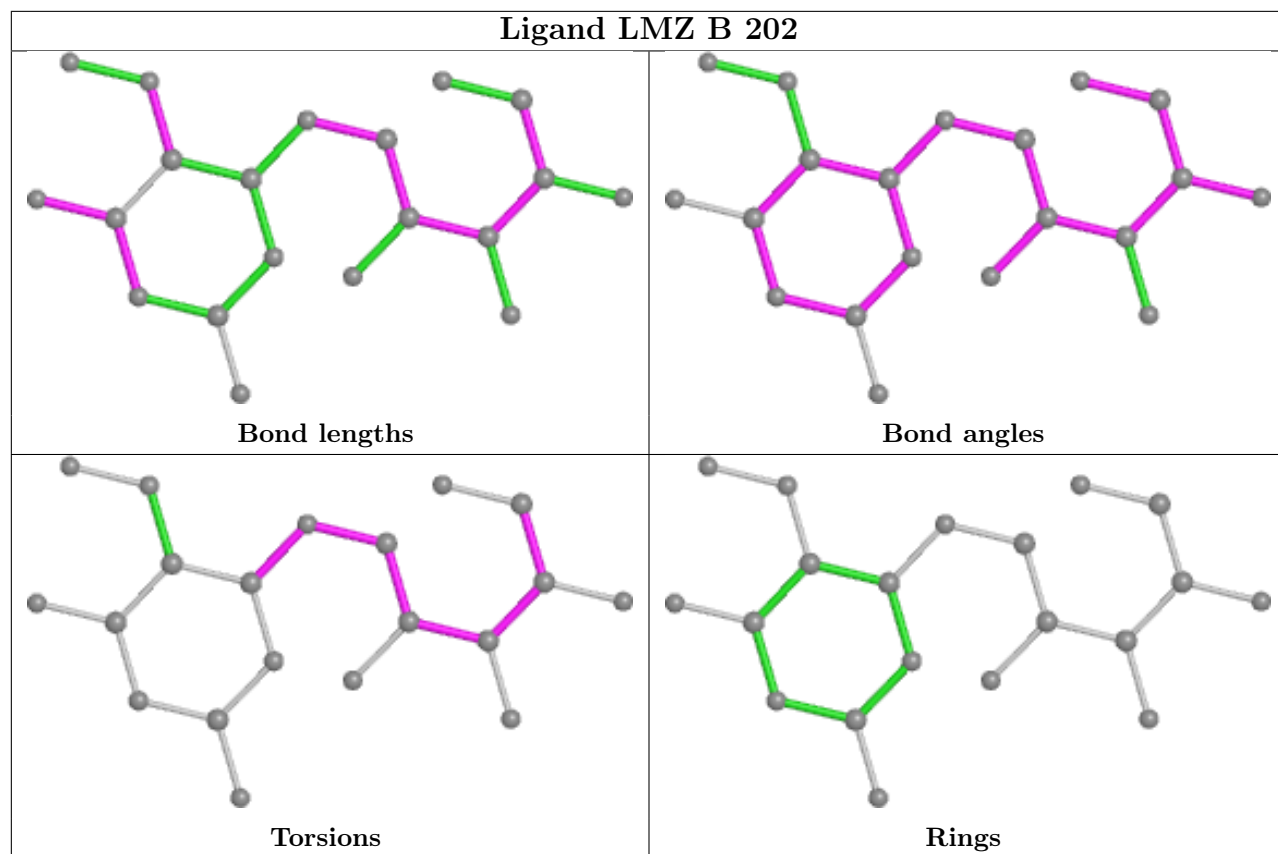
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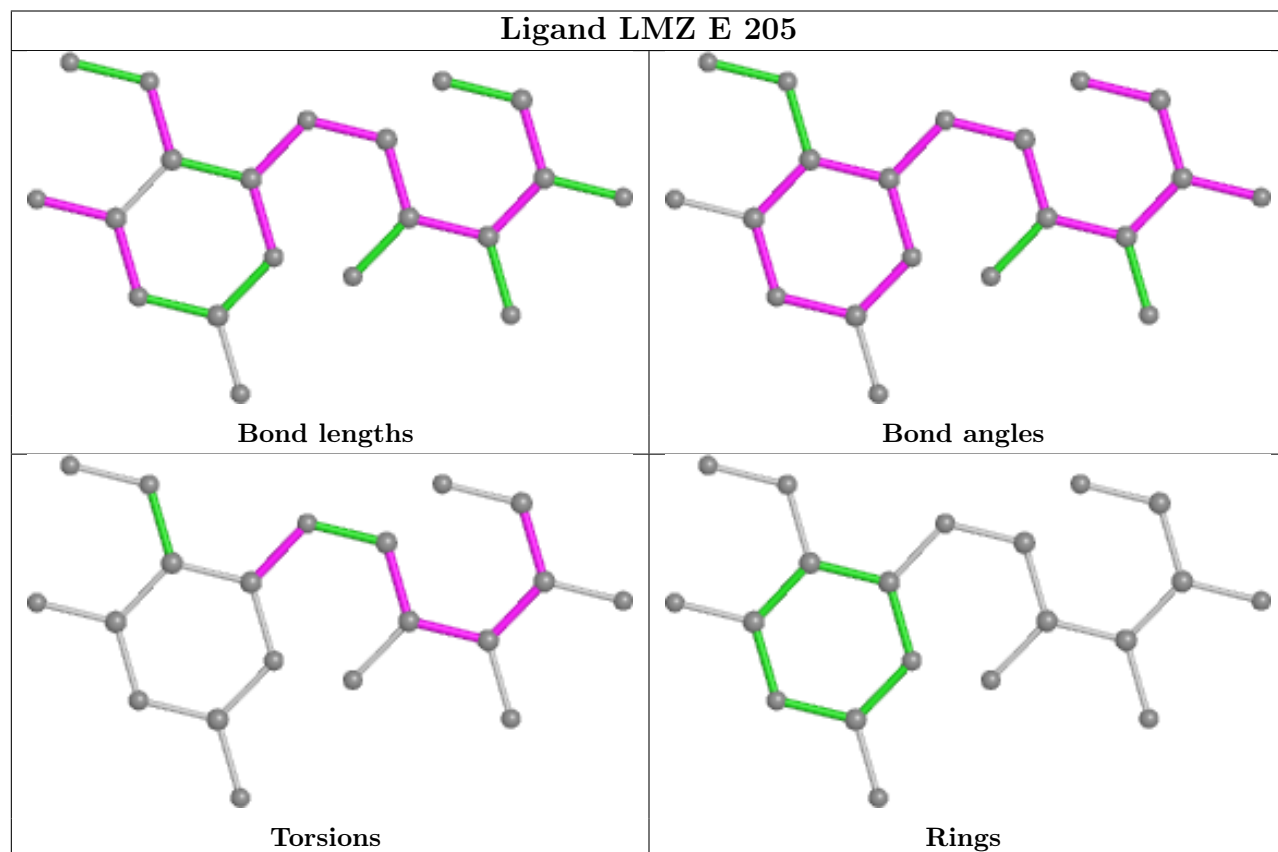
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	213	LMZ	5	0
2	D	204	LMZ	4	0
2	I	209	LMZ	7	0
2	O	215	LMZ	5	0
2	C	203	LMZ	4	0
2	T	220	LMZ	3	0
2	H	208	LMZ	4	0
2	P	216	LMZ	5	0
2	A	201	LMZ	5	0
2	G	207	LMZ	7	0
2	N	214	LMZ	3	0
2	F	206	LMZ	4	0
2	R	218	LMZ	4	0

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

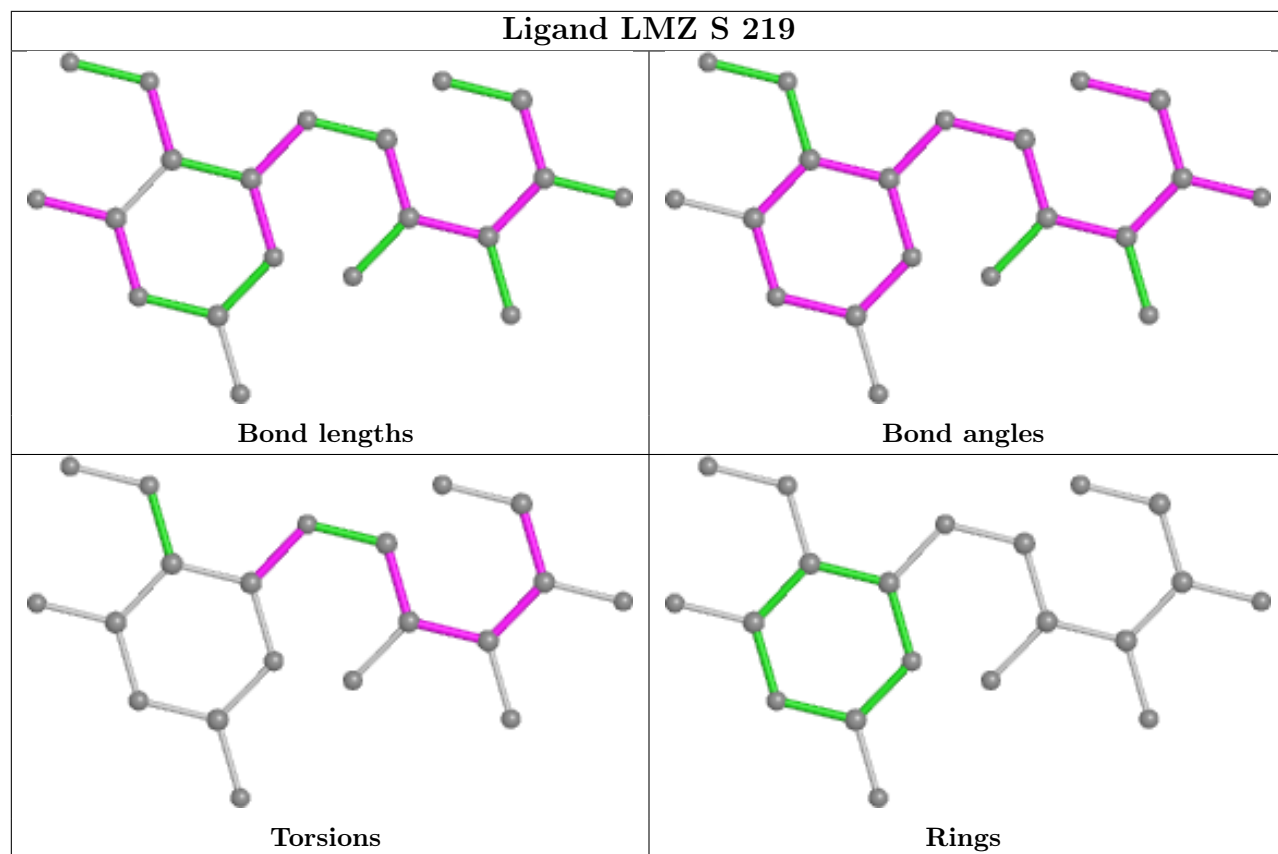
Ligand LMZ B 202



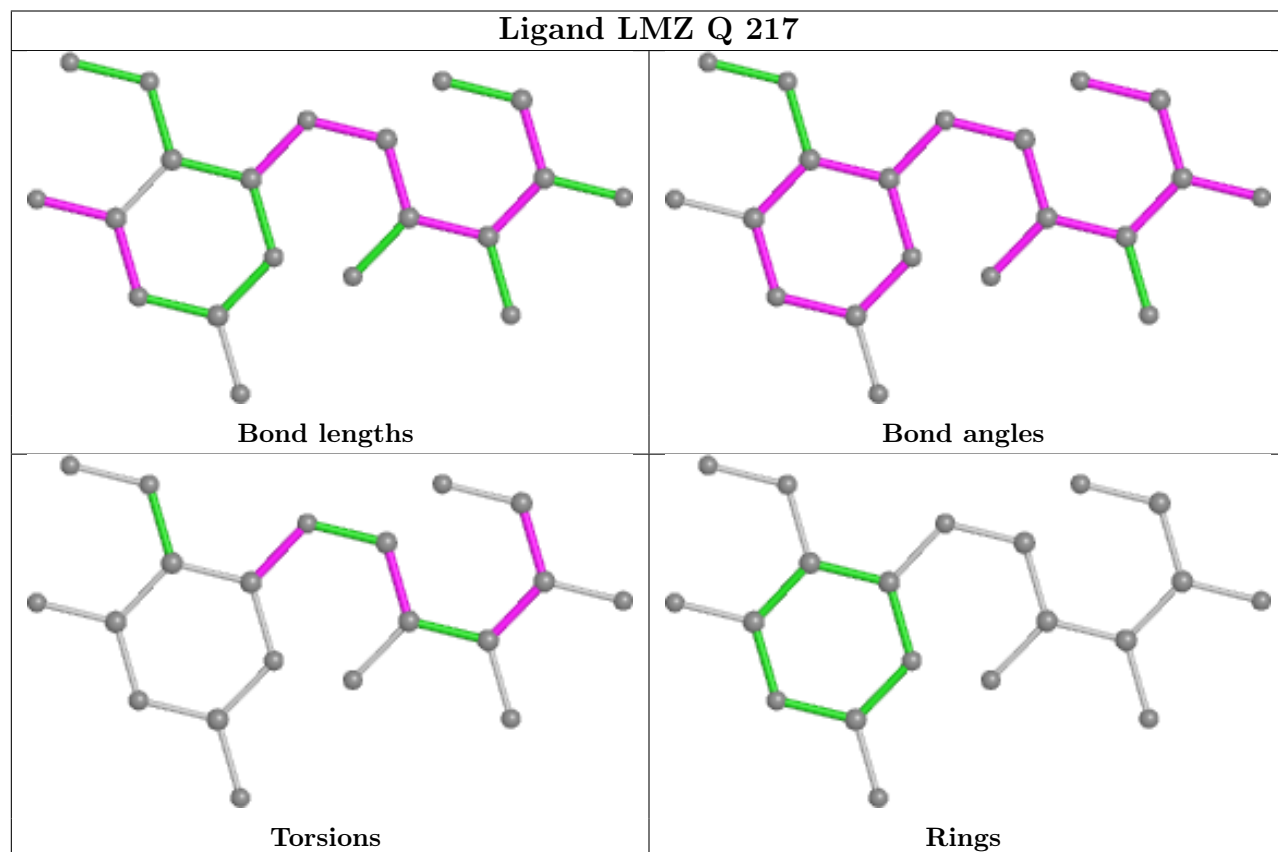
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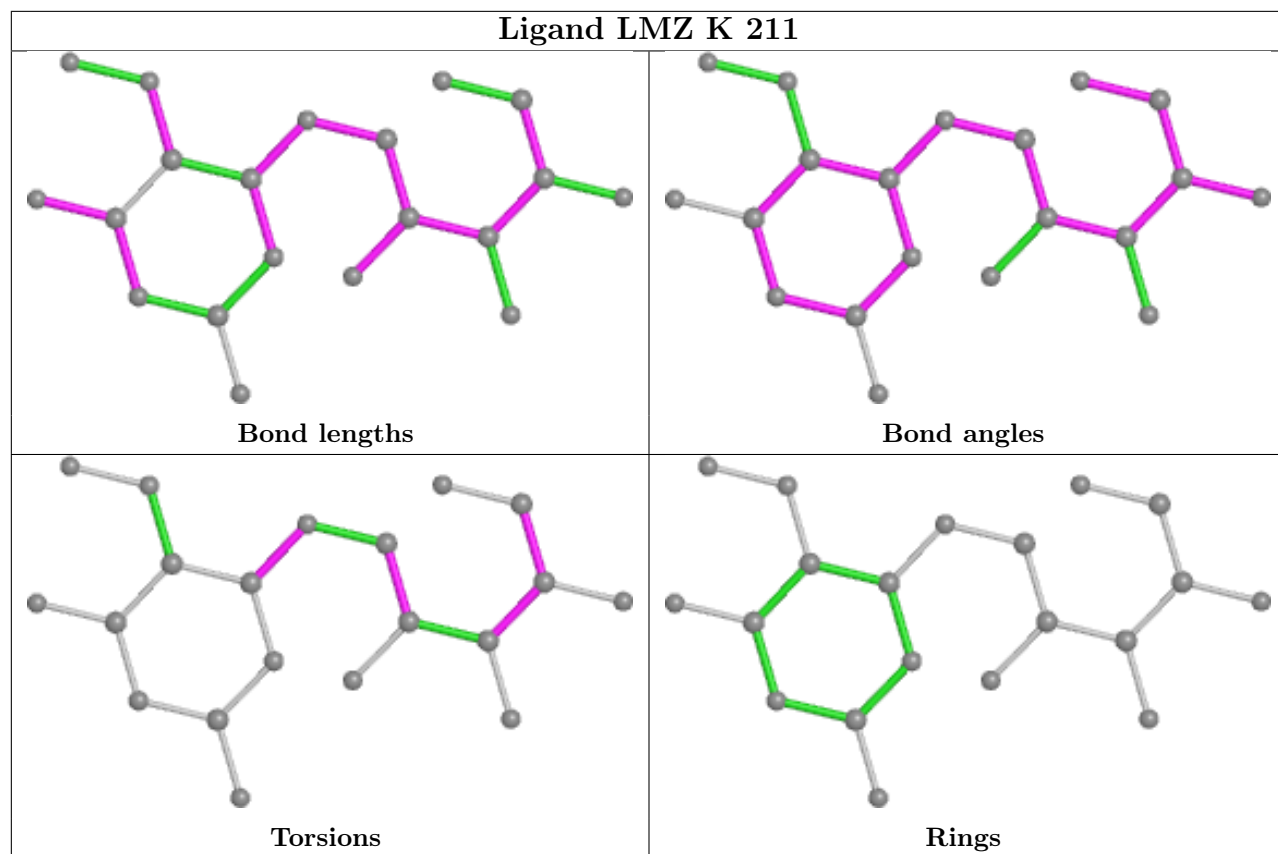
Ligand LMZ S 219



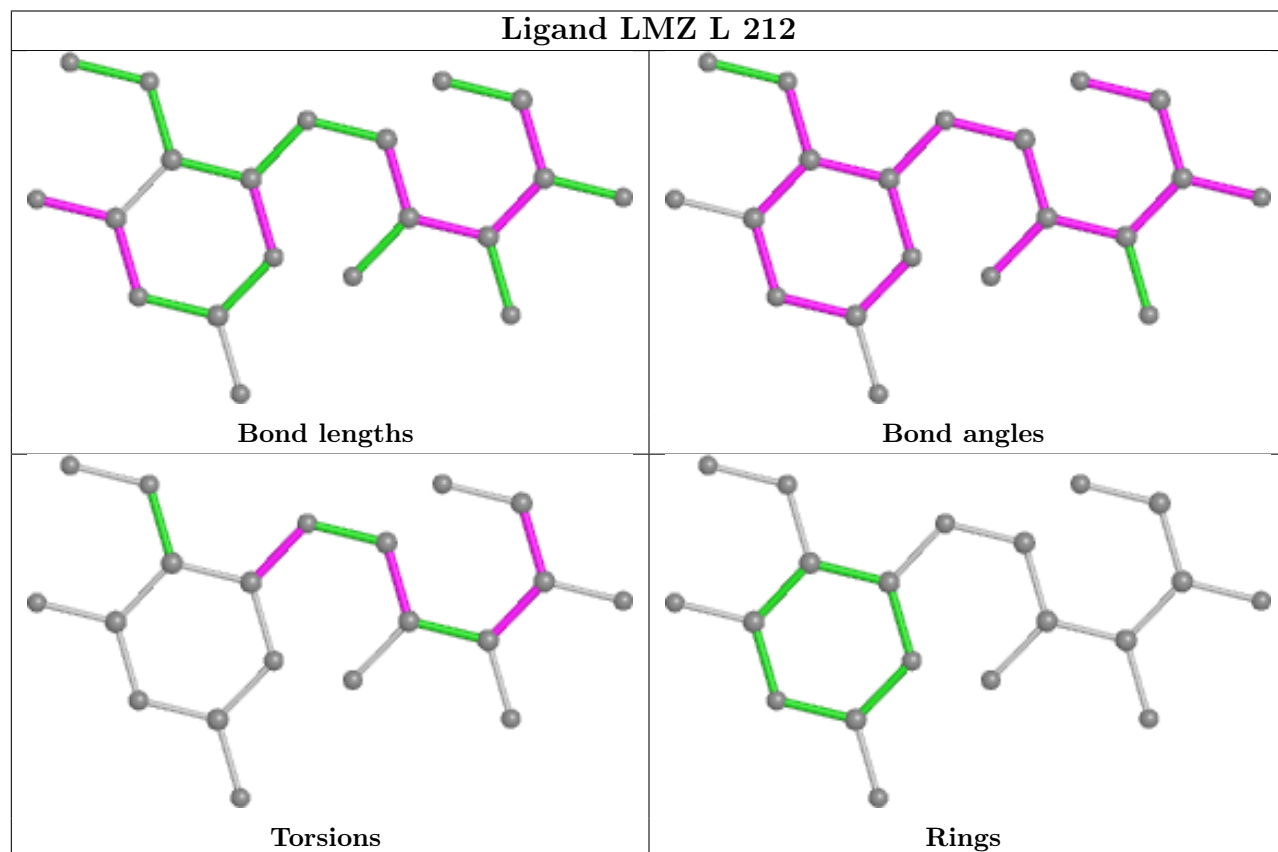
Ligand LMZ Q 217



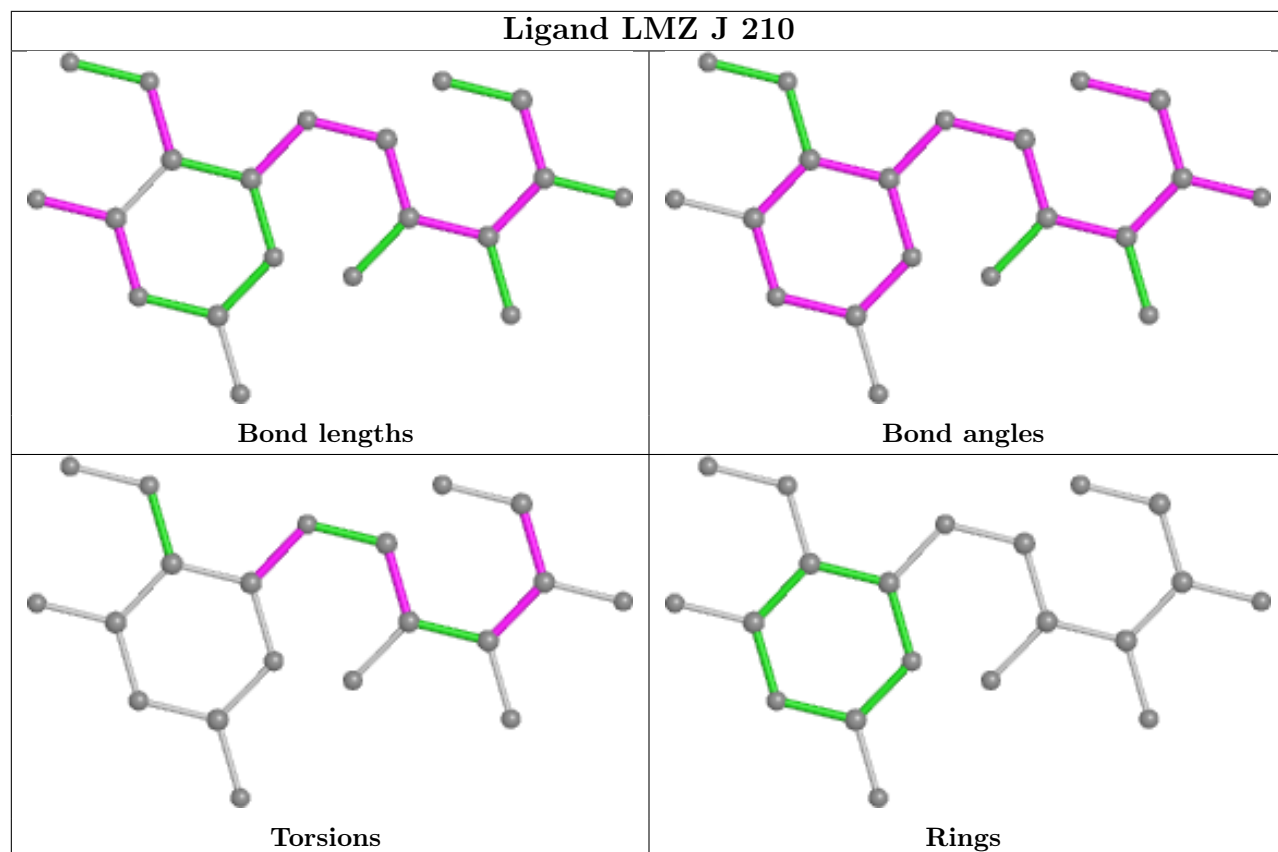
Ligand LMZ K 211



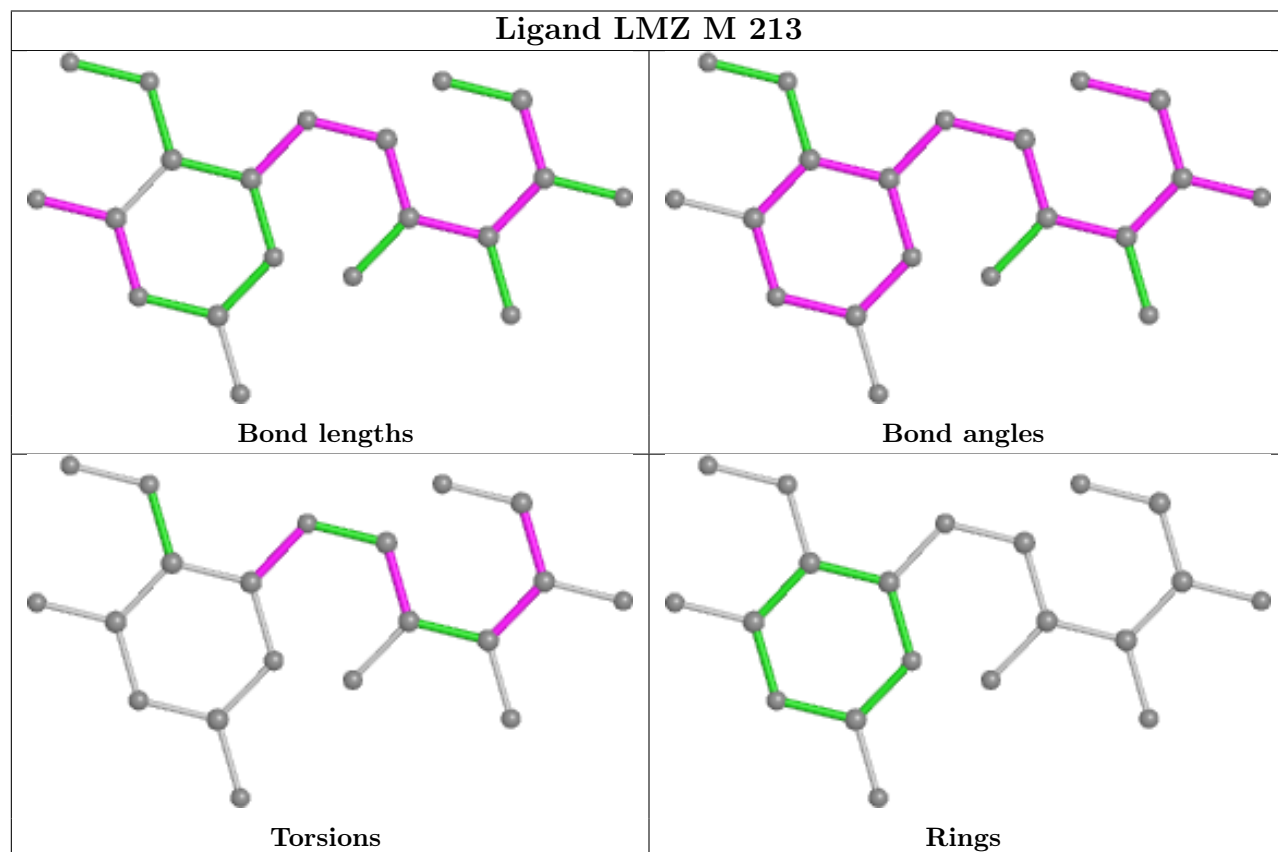
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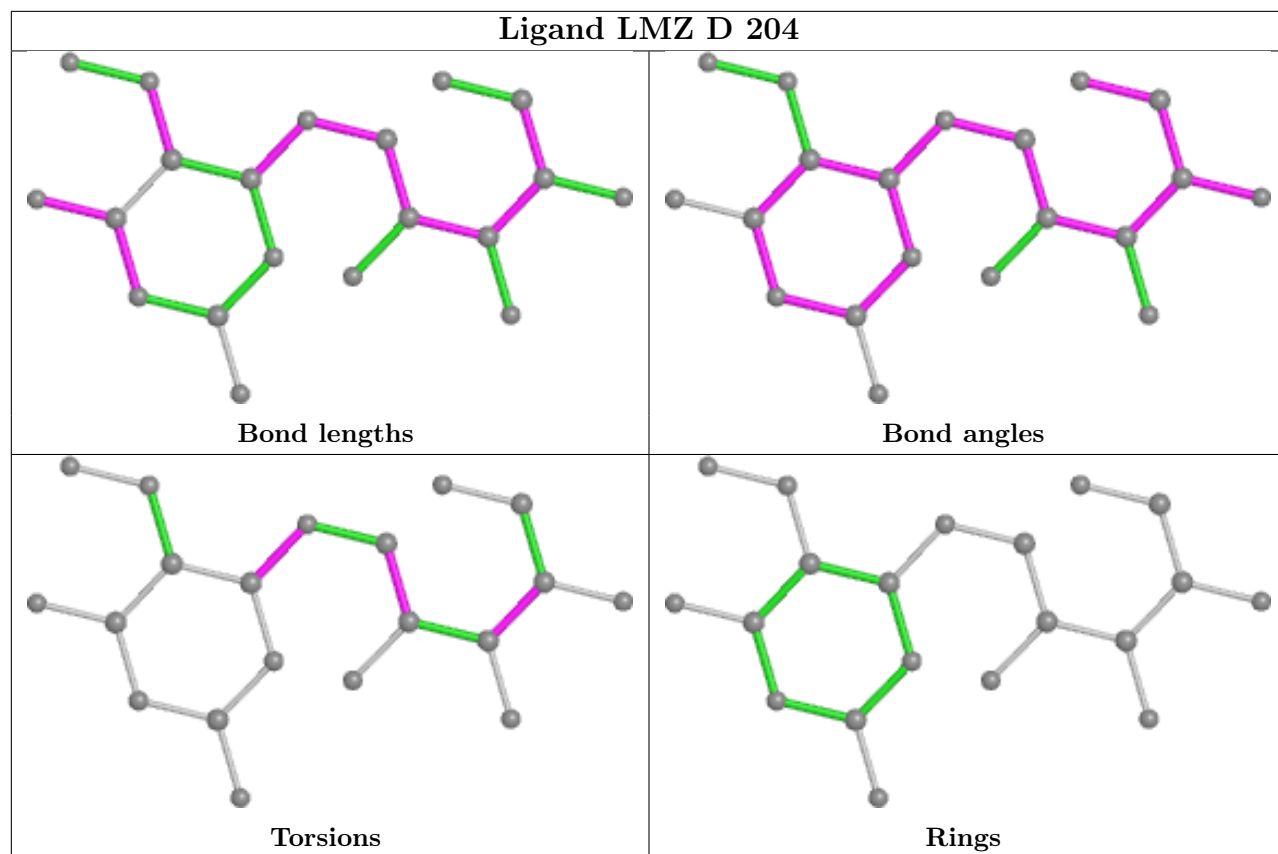
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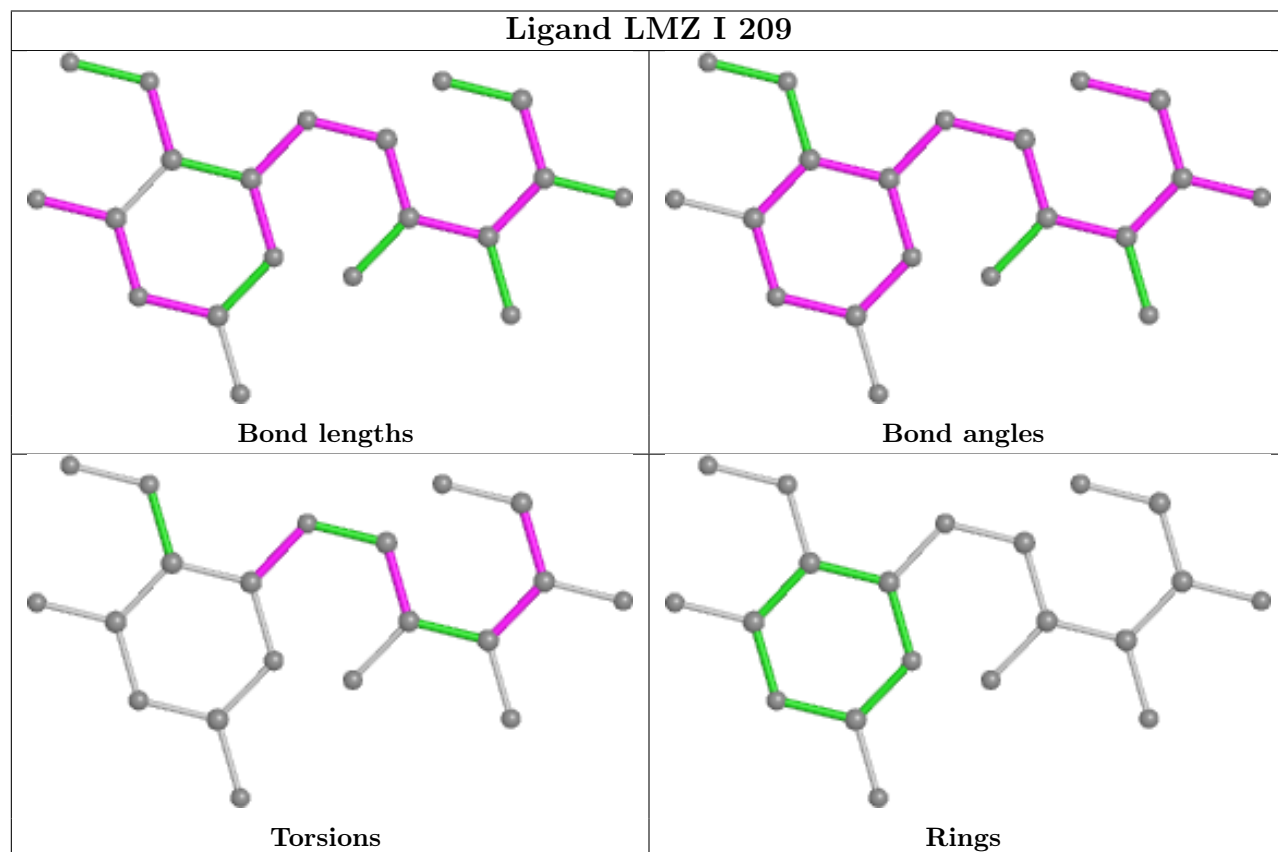
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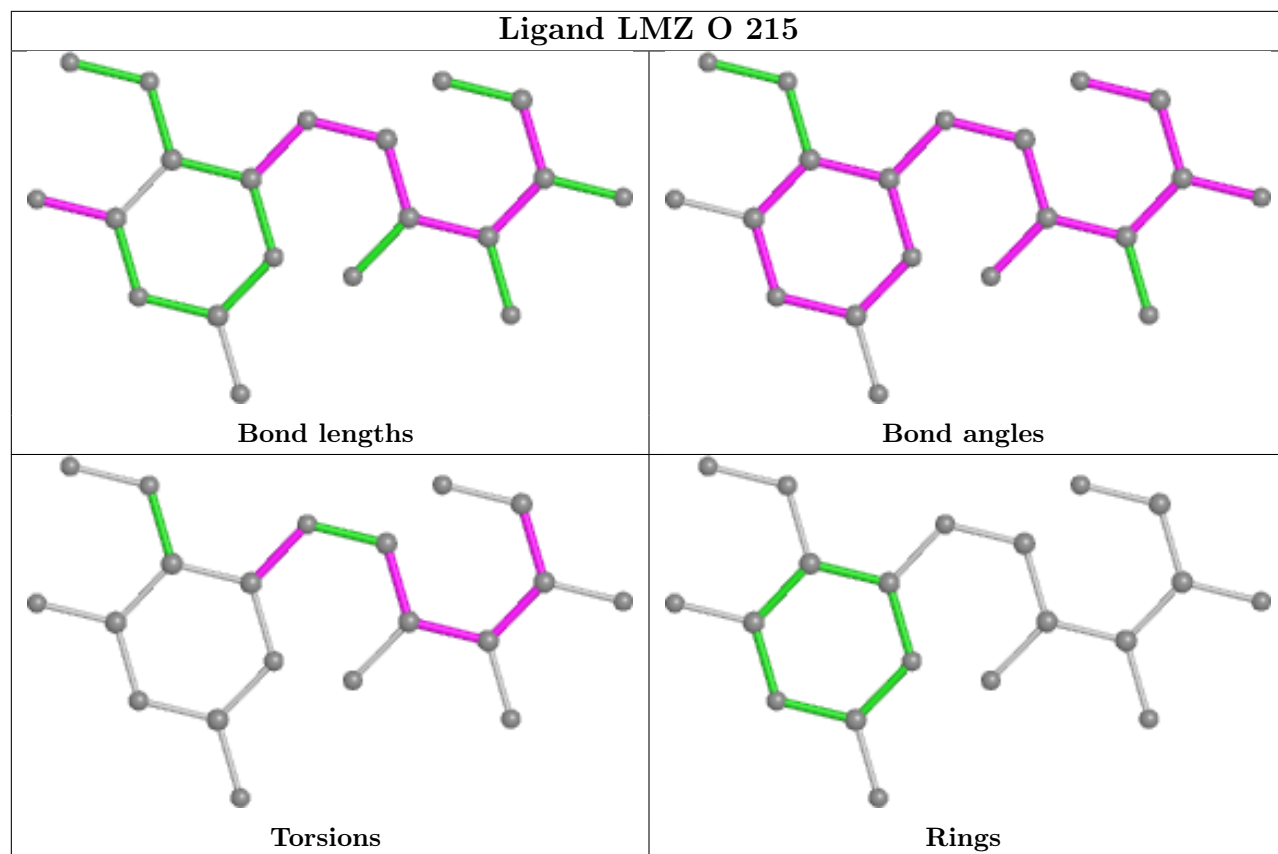
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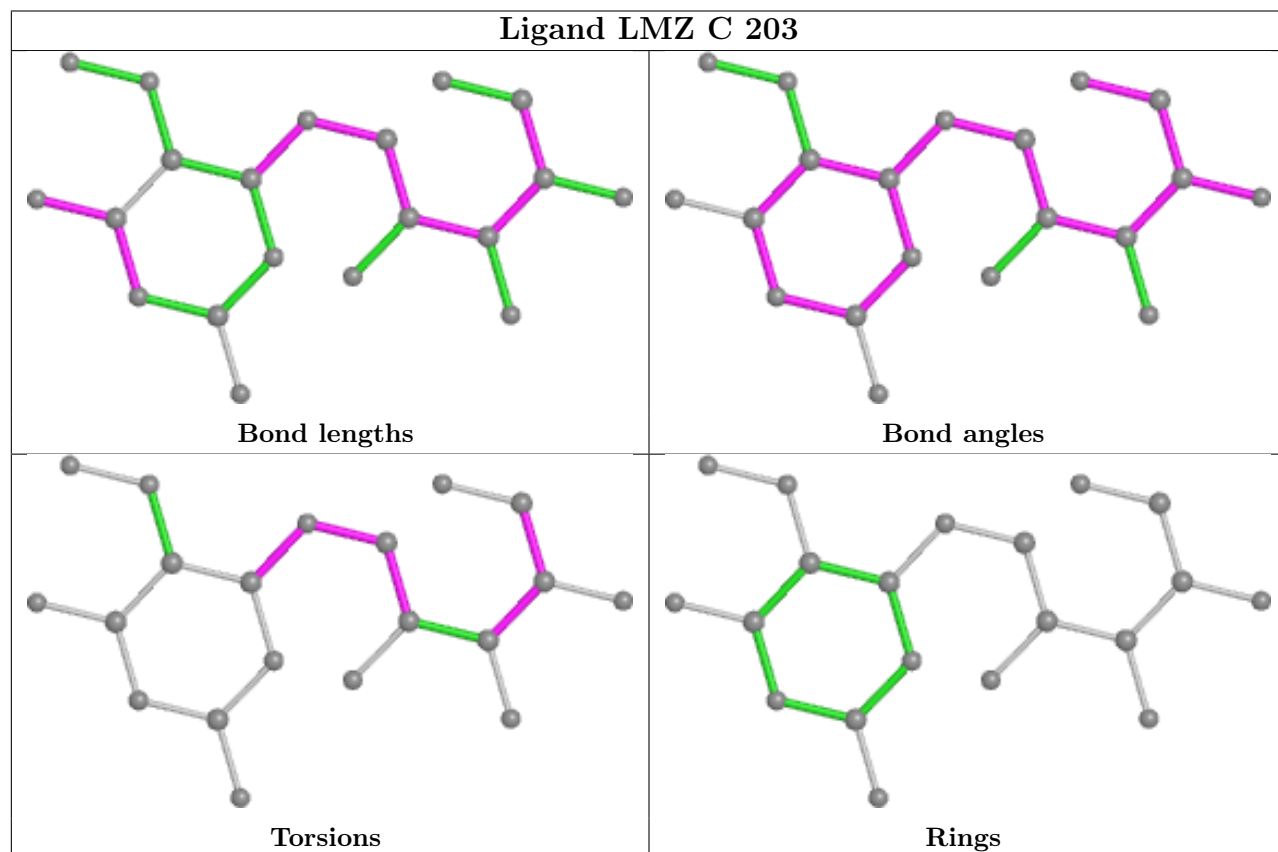
Ligand LMZ I 209



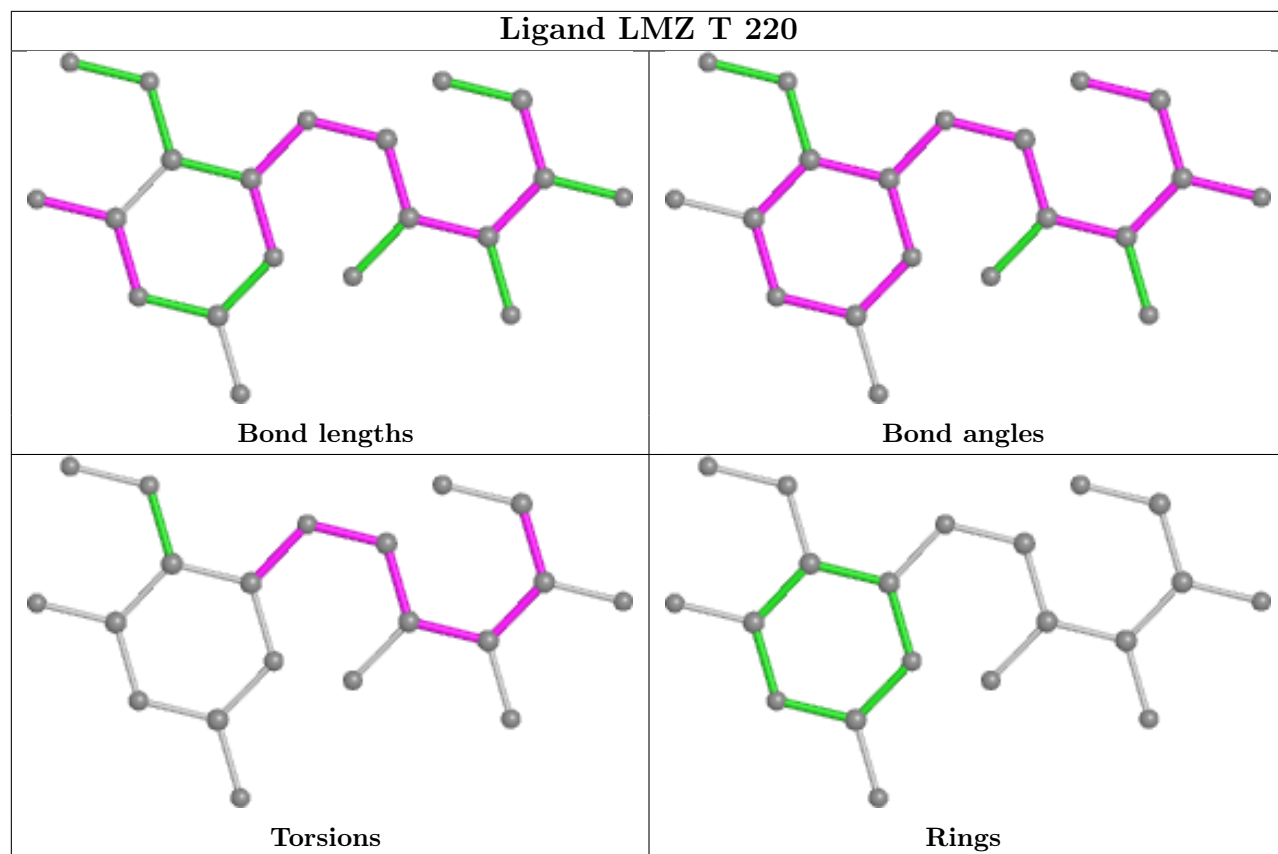
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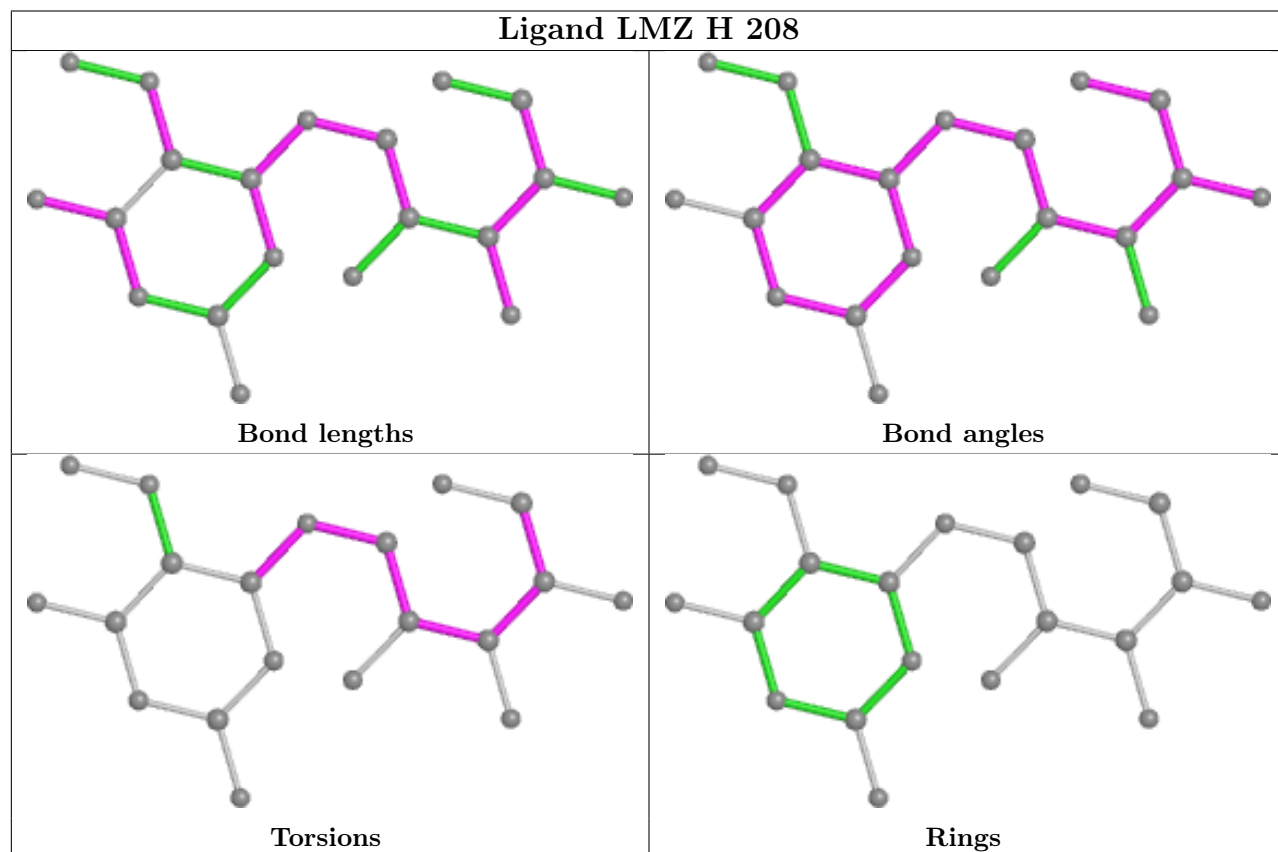
Ligand LMZ C 203



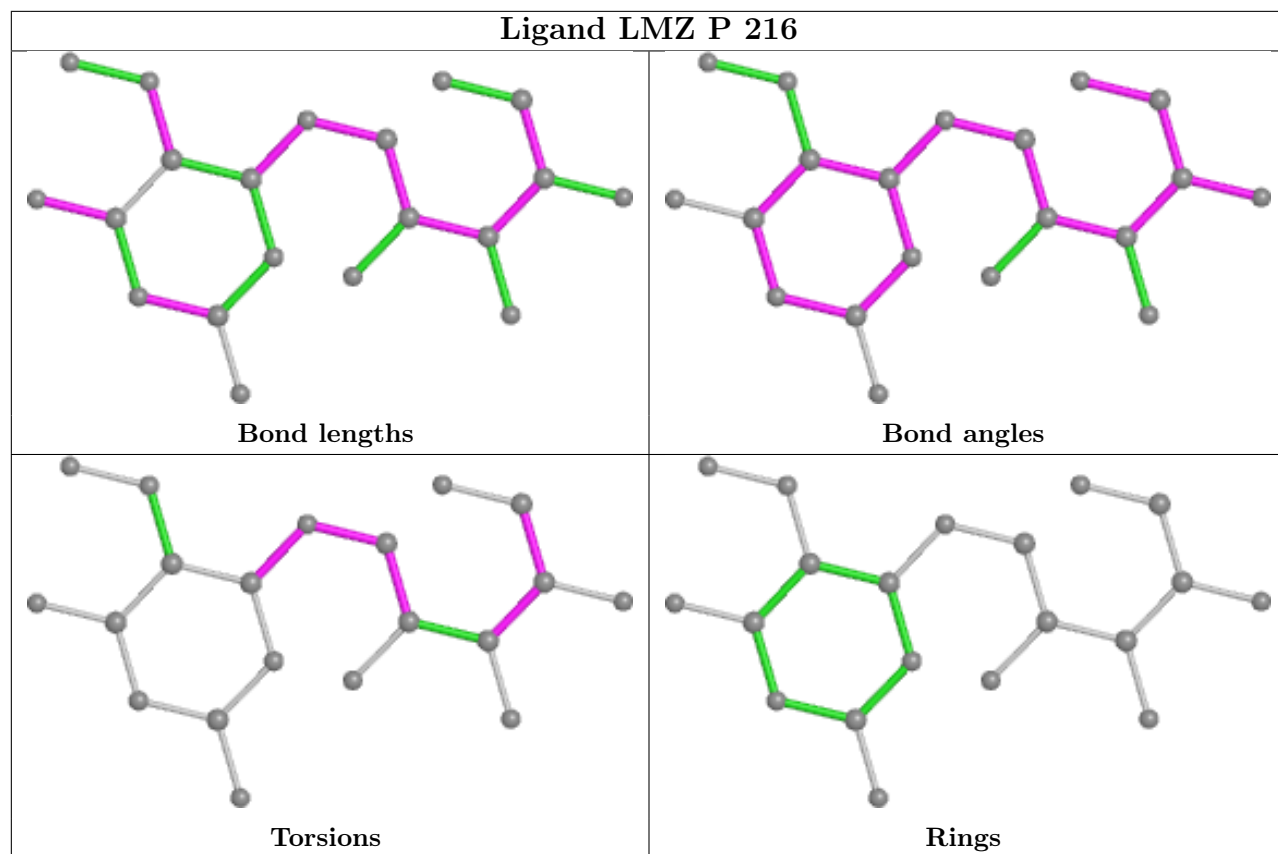
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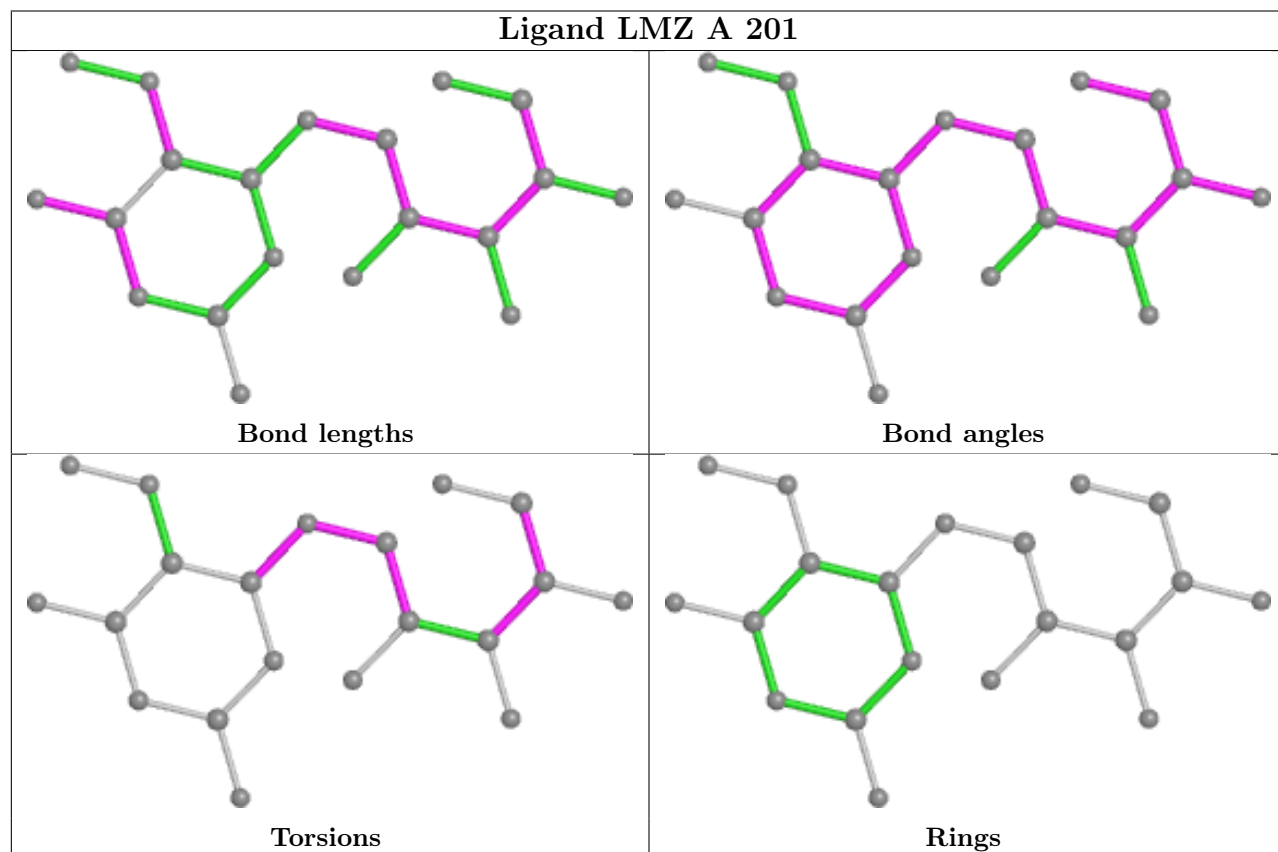
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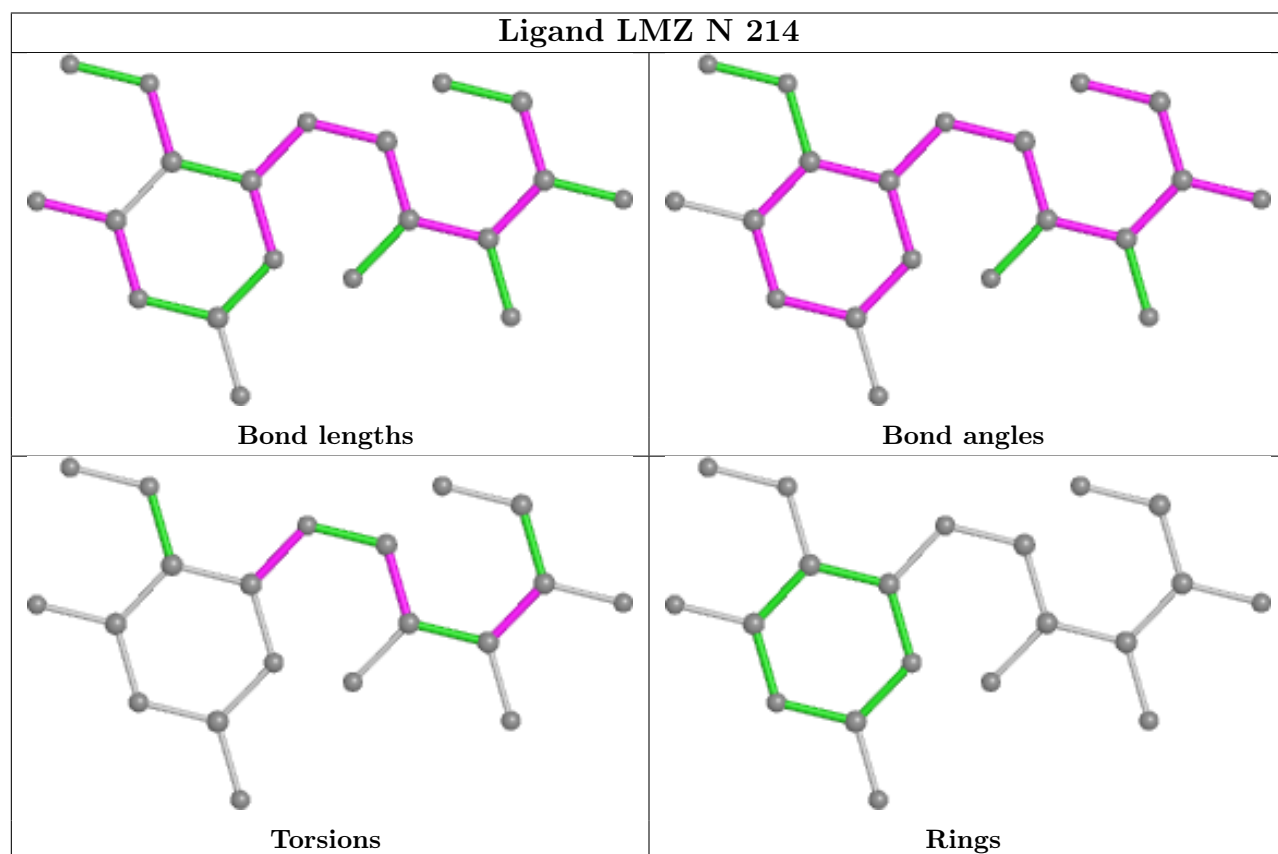
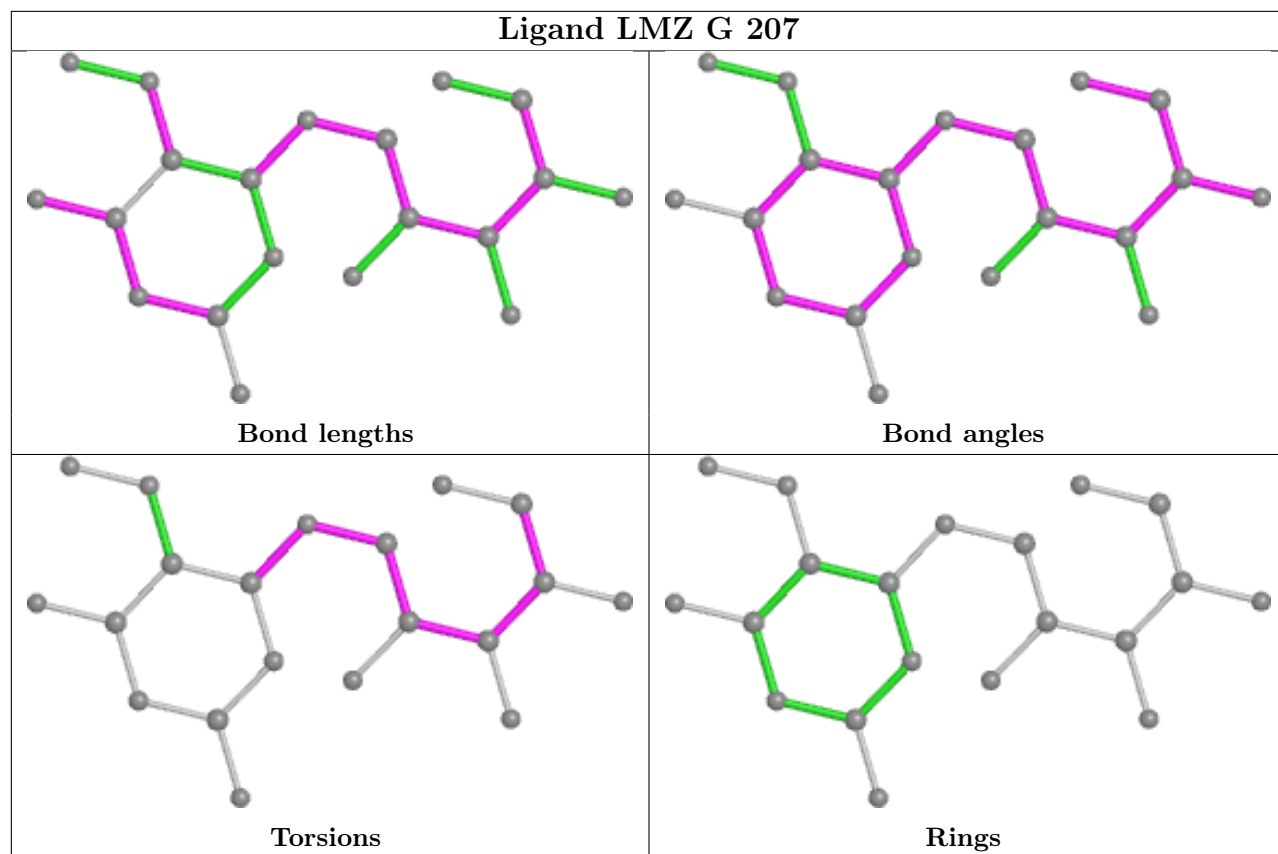


Ligand LMZ P 216

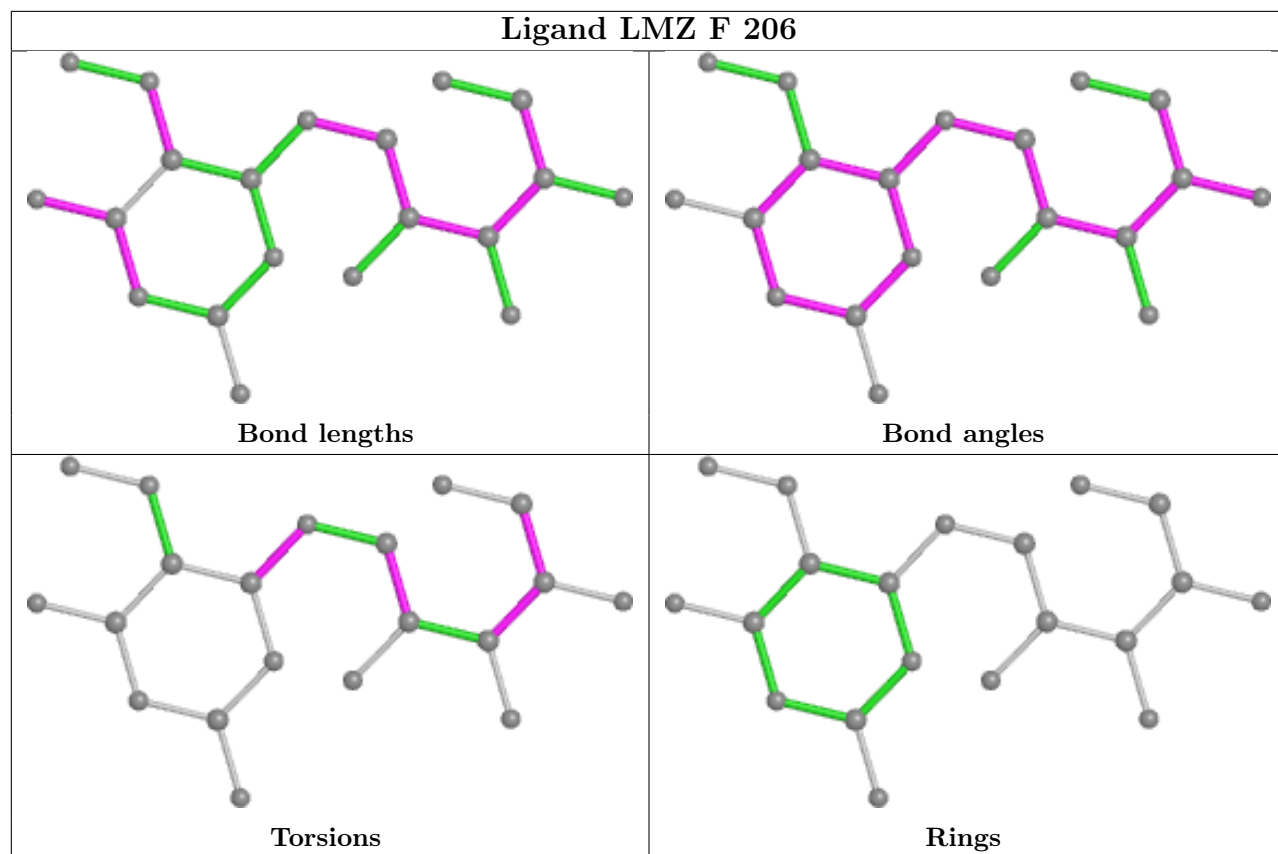


Ligand LMZ A 201

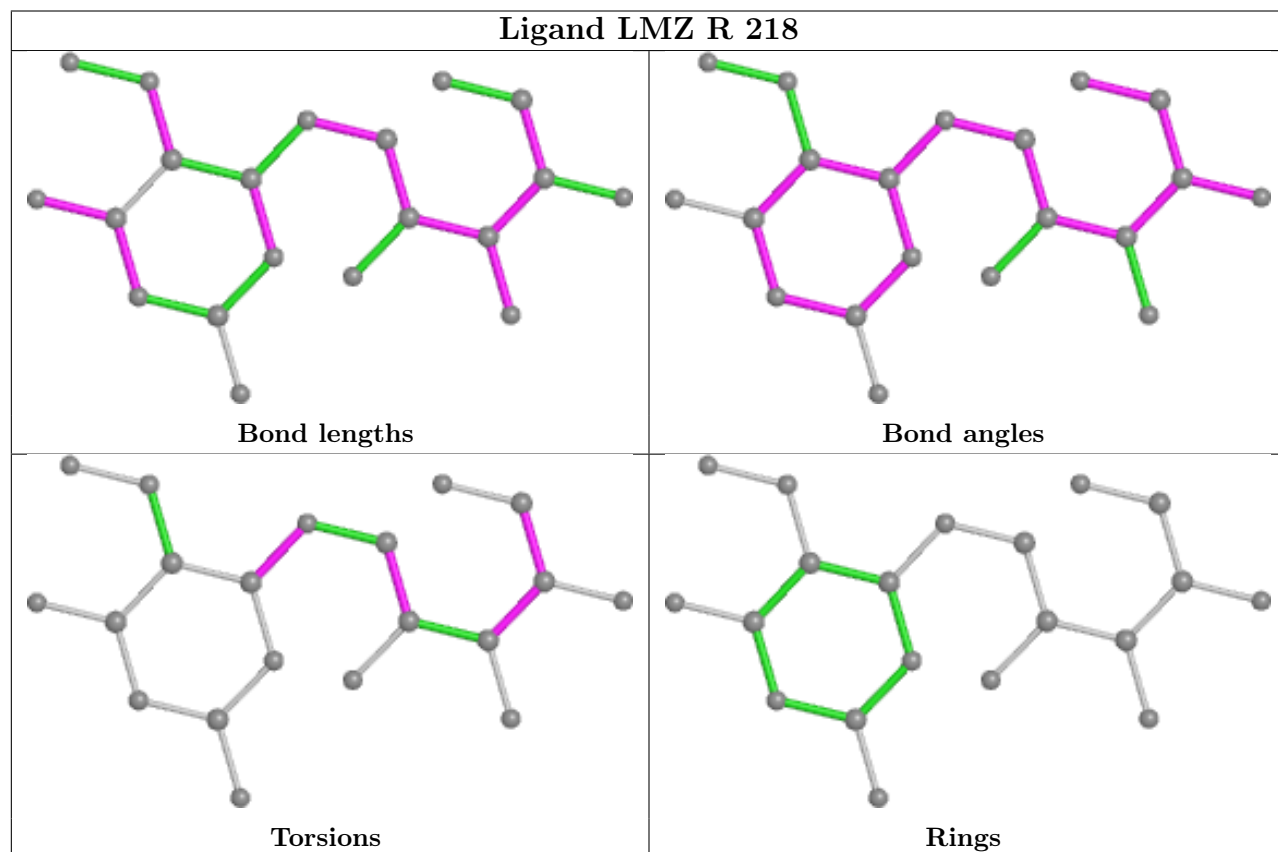




Ligand LMZ F 206



Ligand LMZ R 218



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.