



wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 03:46 PM UTC

PDB ID : 1MT5 / pdb_00001mt5
Title : CRYSTAL STRUCTURE OF FATTY ACID AMIDE HYDROLASE
Authors : Bracey, M.H.; Hanson, M.A.; Masuda, K.R.; Stevens, R.C.; Cravatt, B.F.
Deposited on : 2002-09-20
Resolution : 2.80 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

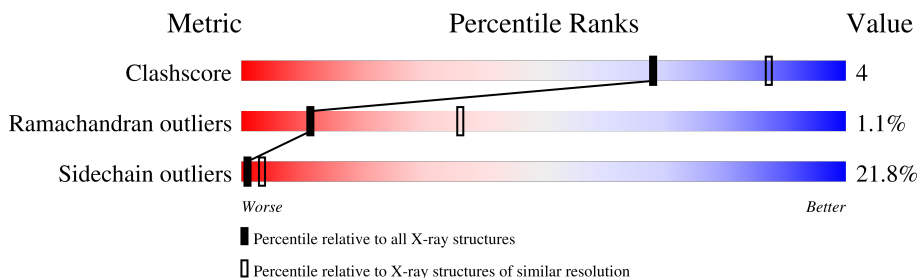
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	537	74% 23% .
1	B	537	75% 20% . .
1	C	537	75% 20% 5%
1	D	537	75% 20% . .
1	E	537	74% 21% . .
1	F	537	73% 21% 6%
1	G	537	74% 22% . .
1	H	537	73% 22% .

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Mol	Chain	Length	Quality of chain
1	I	537	 74% 21% .
1	J	537	 74% 21% 5%
1	K	537	 74% 22% . .
1	L	537	 74% 22% .
1	M	537	 64% 30% . .
1	N	537	 70% 23% 6% .
1	O	537	 72% 24% . .
1	P	537	 73% 22% .

2 Entry composition [i](#)

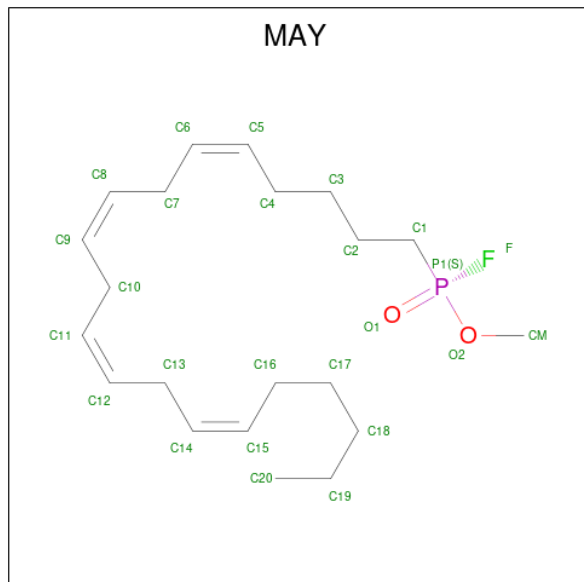
There are 2 unique types of molecules in this entry. The entry contains 64524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty-acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4010	2568	669	744	29	0	0	0
1	B	537	4008	2568	669	742	29	0	0	0
1	C	537	4008	2568	669	742	29	0	0	0
1	D	537	4008	2568	669	742	29	0	0	0
1	E	537	4008	2568	669	742	29	0	0	0
1	F	537	4008	2568	669	742	29	0	0	0
1	G	537	4010	2568	669	744	29	0	0	0
1	H	537	4008	2568	669	742	29	0	0	0
1	I	537	4010	2568	669	744	29	0	0	0
1	J	537	4008	2568	669	742	29	0	0	0
1	K	537	4008	2568	669	742	29	0	0	0
1	L	537	4010	2568	669	744	29	0	0	0
1	M	537	4010	2568	669	744	29	0	0	0
1	N	537	4008	2568	669	742	29	0	0	0
1	O	537	4010	2568	669	744	29	0	0	0
1	P	537	4008	2568	669	742	29	0	0	0

- Molecule 2 is METHYL ARACHIDONYL FLUOROPHOSPHONATE (CCD ID: MAY) (formula: $C_{21}H_{36}FO_2P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	24	21	2	1	0	0
2	B	1	24	21	2	1	0	0
2	C	1	24	21	2	1	0	0
2	D	1	24	21	2	1	0	0
2	E	1	24	21	2	1	0	0
2	F	1	24	21	2	1	0	0
2	G	1	24	21	2	1	0	0
2	H	1	24	21	2	1	0	0
2	I	1	24	21	2	1	0	0
2	J	1	24	21	2	1	0	0
2	K	1	24	21	2	1	0	0
2	L	1	24	21	2	1	0	0

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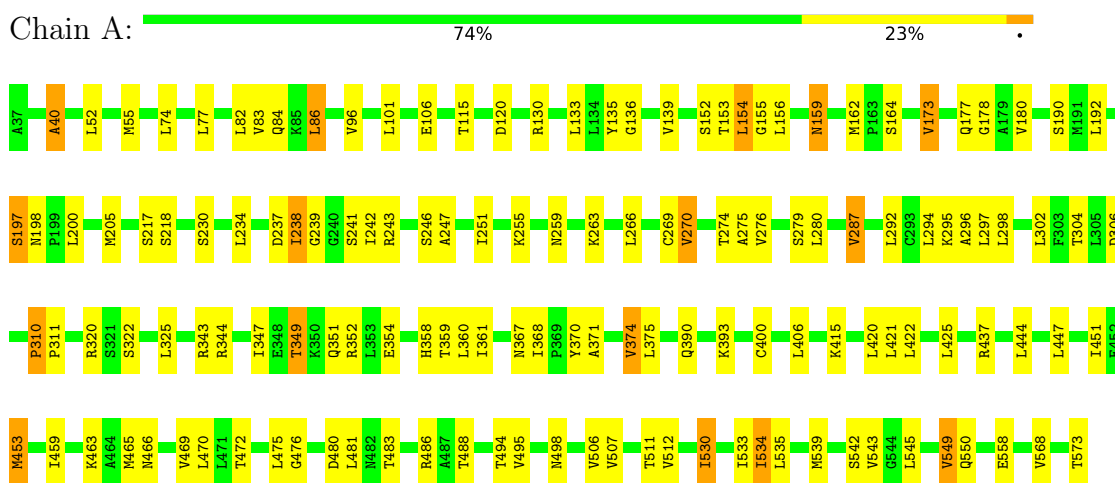
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	M	1	Total 24	C 21	O 2	P 1	0	0
2	N	1	Total 24	C 21	O 2	P 1	0	0
2	O	1	Total 24	C 21	O 2	P 1	0	0
2	P	1	Total 24	C 21	O 2	P 1	0	0

3 Residue-property plots

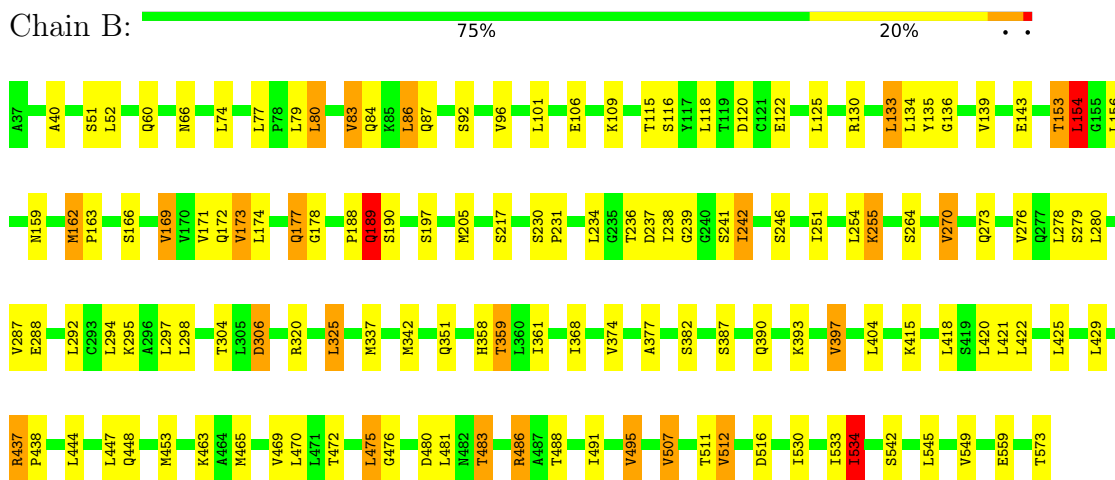
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

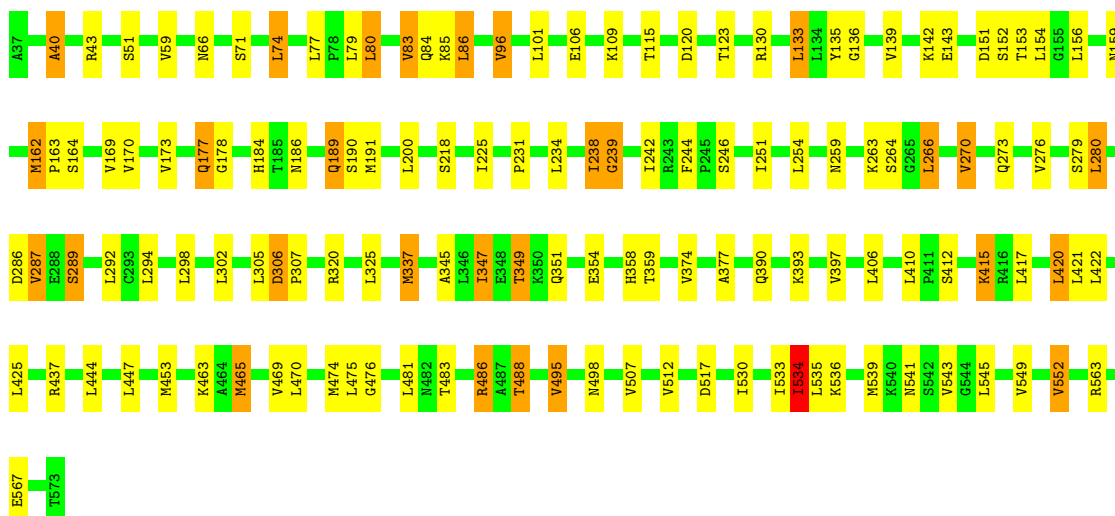


- Molecule 1: Fatty-acid amide hydrolase



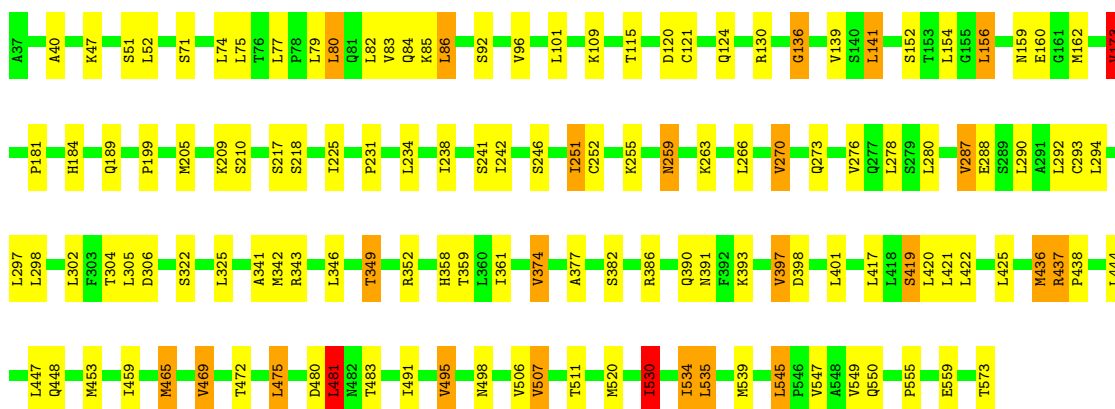
- Molecule 1: Fatty-acid amide hydrolase





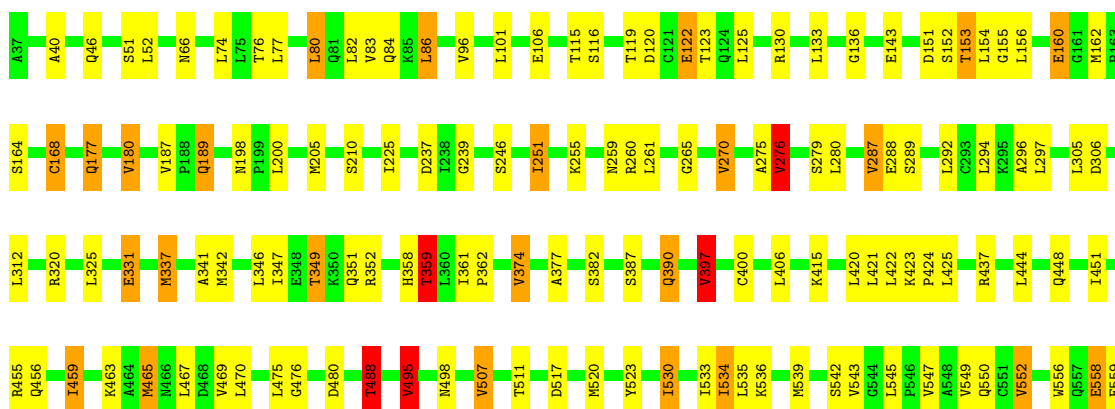
- Molecule 1: Fatty-acid amide hydrolase

Chain D: 75% 20%



- Molecule 1: Fatty-acid amide hydrolase

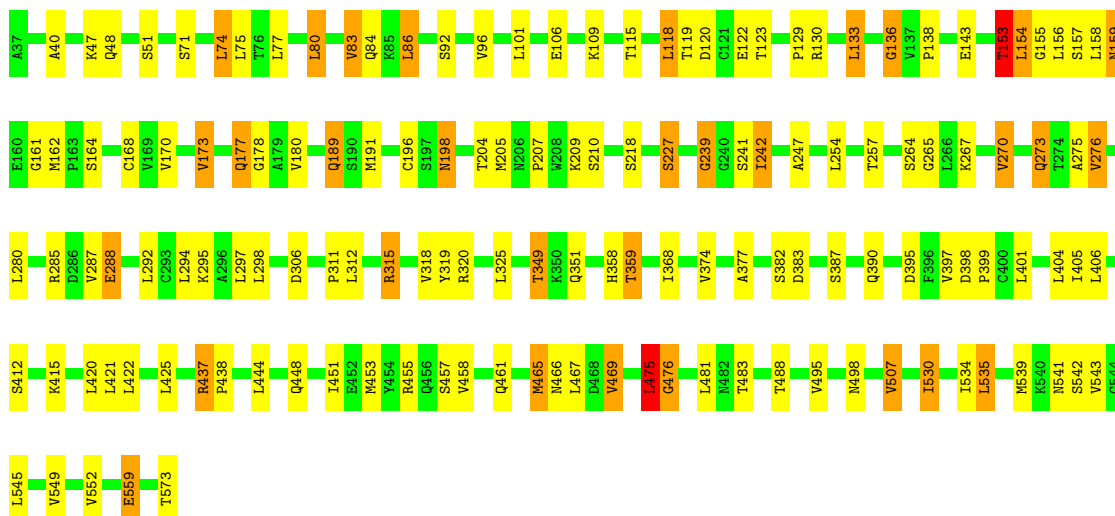
Chain E: 74% 21%





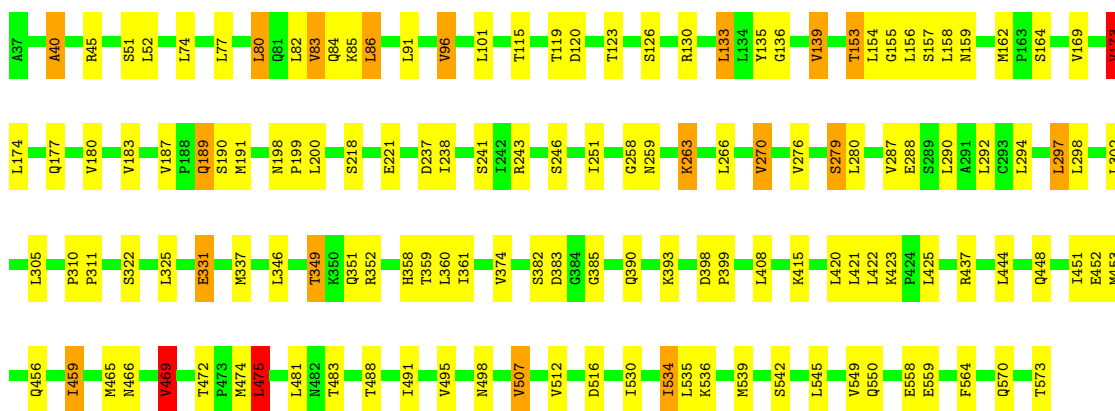
- Molecule 1: Fatty-acid amide hydrolase

Chain F: 73% 21% 6%



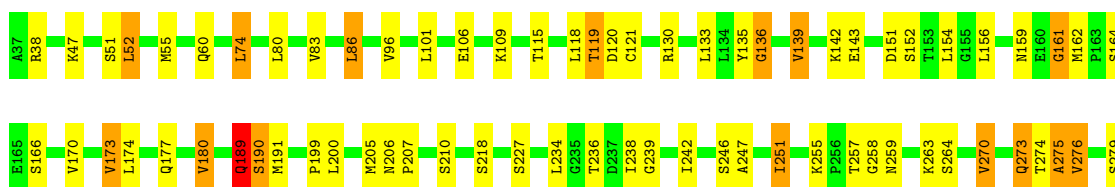
- Molecule 1: Fatty-acid amide hydrolase

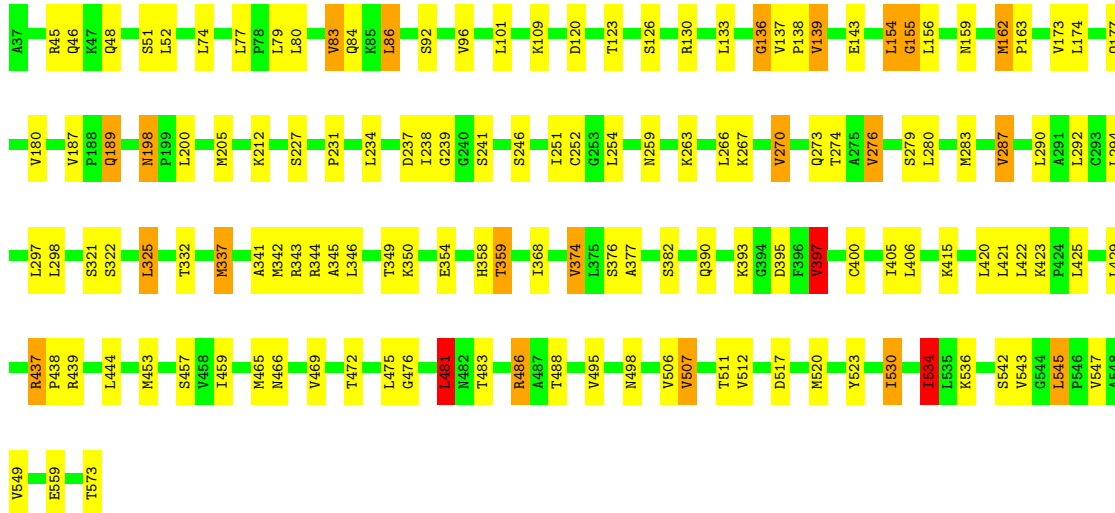
Chain G: 74% 22%



- Molecule 1: Fatty-acid amide hydrolase

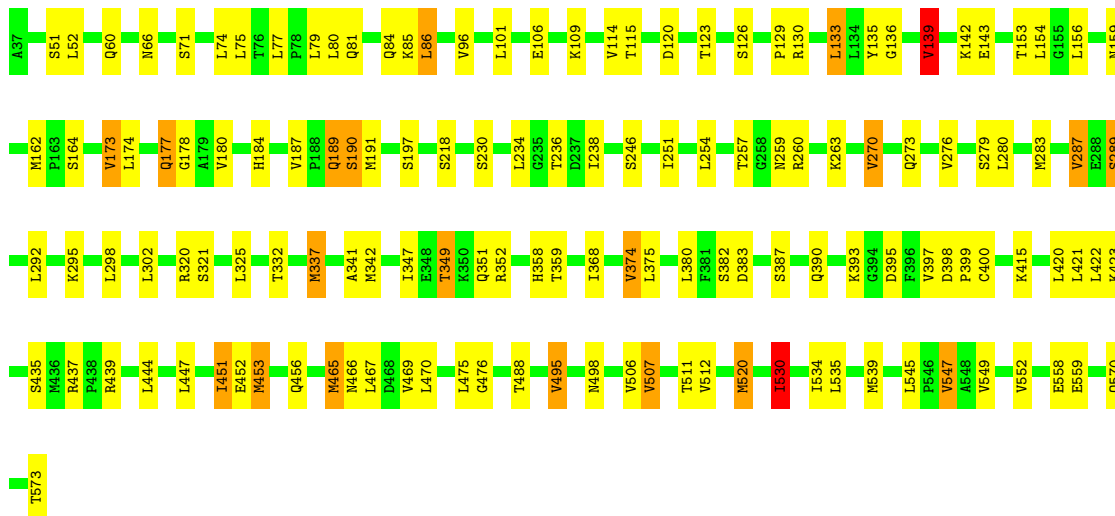
Chain H: 73% 22%





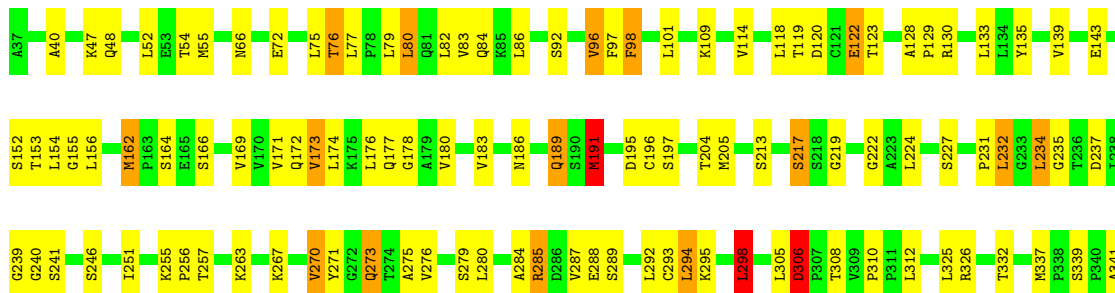
- Molecule 1: Fatty-acid amide hydrolase

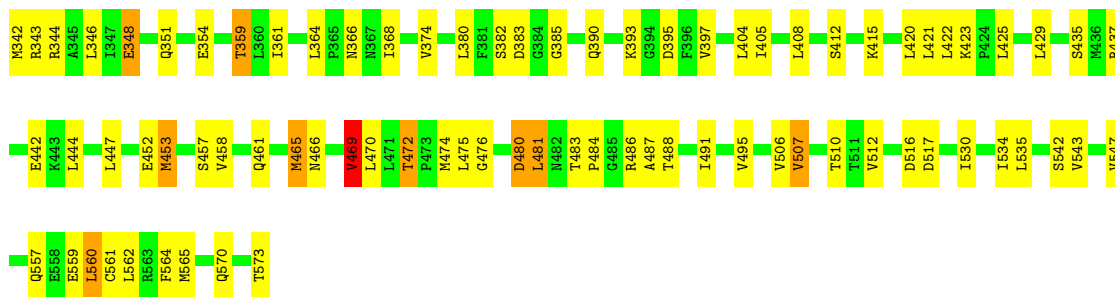
Chain L: 74% 22%



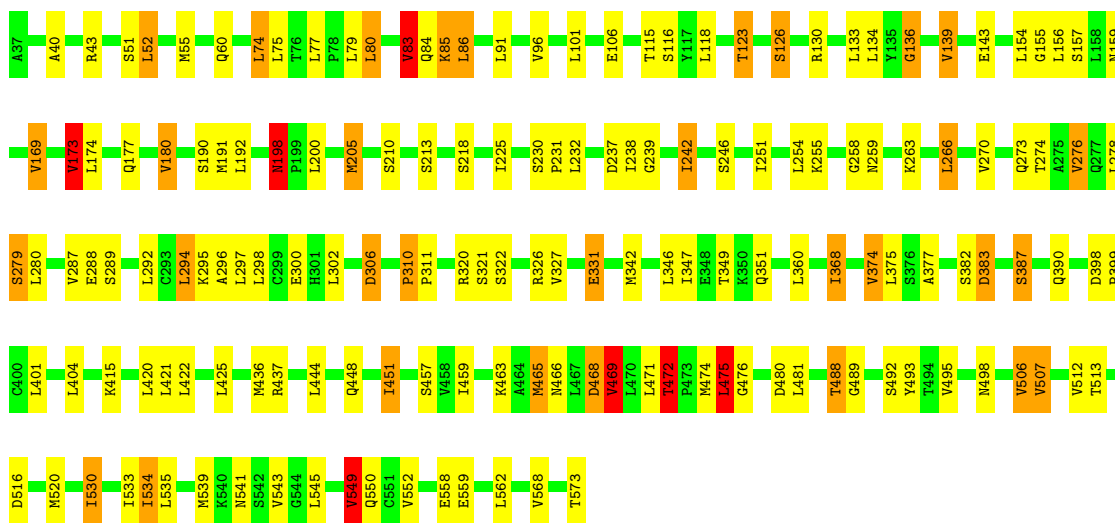
- Molecule 1: Fatty-acid amide hydrolase

Chain M: 64% 30%

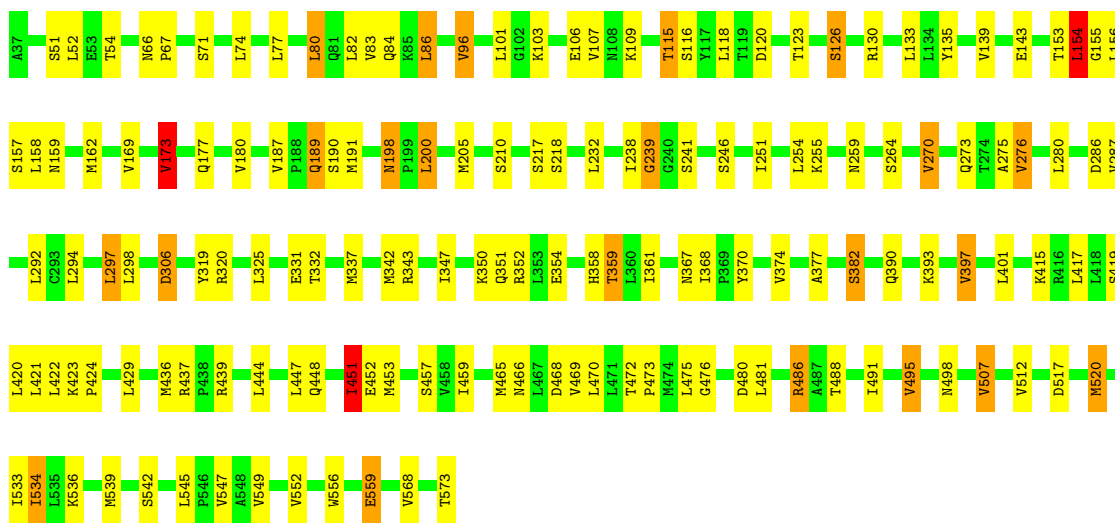




• Molecule 1: Fatty-acid amide hydrolase

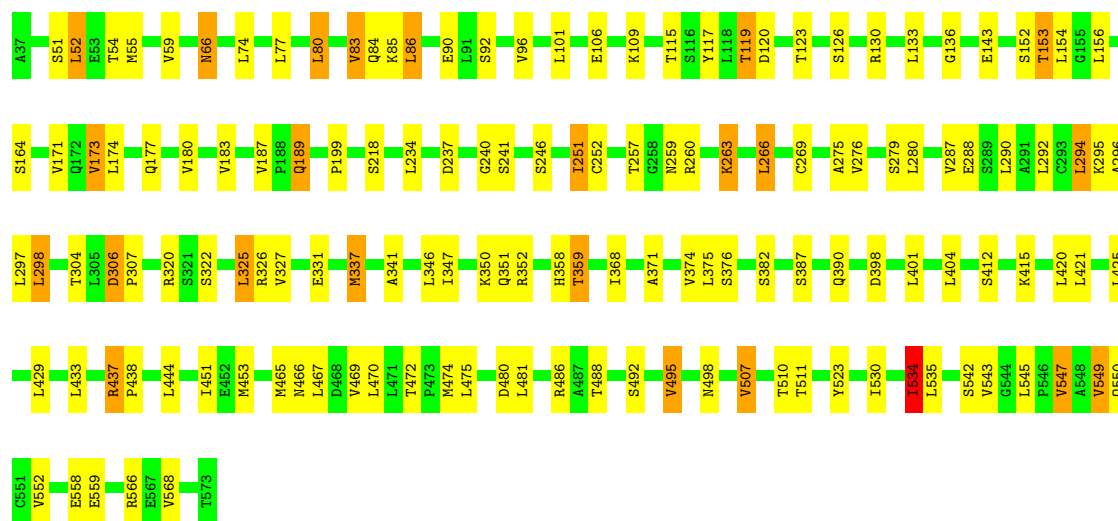


• Molecule 1: Fatty-acid amide hydrolase



• Molecule 1: Fatty-acid amide hydrolase

Chain P:  73% 22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.11Å 272.02Å 147.22Å 90.00° 115.21° 90.00°	Depositor
Resolution (Å)	141.42 – 2.80	Depositor
% Data completeness (in resolution range)	71.4 (141.42-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.218 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	64524	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	1.25	23/4102 (0.6%)	1.15	0/5589
1	B	1.28	21/4100 (0.5%)	1.14	0/5586
1	C	1.25	21/4100 (0.5%)	1.15	5/5586 (0.1%)
1	D	1.25	19/4100 (0.5%)	1.15	3/5586 (0.1%)
1	E	1.30	27/4100 (0.7%)	1.12	1/5586 (0.0%)
1	F	1.29	22/4100 (0.5%)	1.16	5/5586 (0.1%)
1	G	1.26	20/4102 (0.5%)	1.14	6/5589 (0.1%)
1	H	1.22	17/4100 (0.4%)	1.14	5/5586 (0.1%)
1	I	1.27	24/4102 (0.6%)	1.13	4/5589 (0.1%)
1	J	1.27	21/4100 (0.5%)	1.14	2/5586 (0.0%)
1	K	1.29	23/4100 (0.6%)	1.15	2/5586 (0.0%)
1	L	1.31	20/4102 (0.5%)	1.16	4/5589 (0.1%)
1	M	1.47	34/4102 (0.8%)	1.18	7/5589 (0.1%)
1	N	1.40	34/4100 (0.8%)	1.16	1/5586 (0.0%)
1	O	1.26	23/4102 (0.6%)	1.15	4/5589 (0.1%)
1	P	1.32	20/4100 (0.5%)	1.15	2/5586 (0.0%)
All	All	1.29	369/65612 (0.6%)	1.15	51/89394 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	4
1	F	0	6
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	6
1	I	0	5
1	J	0	4
1	K	0	3
1	L	0	1
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	2
All	All	0	57

The worst 5 of 369 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	368	ILE	CA-CB	12.93	1.60	1.54
1	P	507	VAL	CA-CB	11.90	1.63	1.54
1	F	368	ILE	CA-CB	11.68	1.59	1.54
1	B	368	ILE	CA-CB	11.51	1.59	1.54
1	L	287	VAL	CA-CB	10.26	1.66	1.54

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLN	N-CA-C	7.94	120.64	111.11
1	M	139	VAL	N-CA-C	6.86	118.35	108.48
1	L	374	VAL	N-CA-C	6.55	118.14	111.00
1	C	169	VAL	N-CA-C	6.47	116.63	110.42
1	I	137	VAL	N-CA-C	6.19	113.95	108.63

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ASP	Peptide
1	A	197	SER	Peptide
1	B	120	ASP	Peptide
1	B	40	ALA	Peptide
1	B	475	LEU	Peptide

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	4010	0	3953	31	0
1	B	4008	0	3953	28	0
1	C	4008	0	3953	28	0
1	D	4008	0	3953	32	0
1	E	4008	0	3953	30	0
1	F	4008	0	3953	30	0
1	G	4010	0	3953	30	0
1	H	4008	0	3953	27	0
1	I	4010	0	3953	22	0
1	J	4008	0	3953	28	0
1	K	4008	0	3953	28	0
1	L	4010	0	3953	25	0
1	M	4010	0	3953	30	0
1	N	4008	0	3953	39	0
1	O	4010	0	3953	27	0
1	P	4008	0	3953	30	0
2	A	24	0	36	5	0
2	B	24	0	36	3	0
2	C	24	0	36	3	0
2	D	24	0	36	4	0
2	E	24	0	36	3	0
2	F	24	0	36	4	0
2	G	24	0	36	1	0
2	H	24	0	36	4	0
2	I	24	0	36	2	0
2	J	24	0	36	2	0
2	K	24	0	36	3	0
2	L	24	0	36	1	0
2	M	24	0	36	2	0
2	N	24	0	36	4	0
2	O	24	0	36	3	0
2	P	24	0	36	2	0
All	All	64524	0	63824	463	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 4.

The worst 5 of 463 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:L:453:MET:SD	1:L:453:MET:CE	2.02	1.48
1:D:325:LEU:H	1:D:358:HIS:HD2	1.18	0.90
1:A:155:GLY:HA3	1:A:198:ASN:HD21	1.38	0.87
1:C:325:LEU:H	1:C:358:HIS:HD2	1.27	0.81
1:D:86:LEU:HG	1:D:136:GLY:HA3	1.64	0.80

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	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	11	36
1	B	535/537 (100%)	503 (94%)	24 (4%)	8 (2%)	8	28
1	C	535/537 (100%)	507 (95%)	23 (4%)	5 (1%)	14	41
1	D	535/537 (100%)	499 (93%)	31 (6%)	5 (1%)	14	41
1	E	535/537 (100%)	491 (92%)	36 (7%)	8 (2%)	8	28
1	F	535/537 (100%)	502 (94%)	27 (5%)	6 (1%)	11	36
1	G	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	21	51
1	H	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	11	36
1	I	535/537 (100%)	496 (93%)	37 (7%)	2 (0%)	30	60
1	J	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	21	51
1	K	535/537 (100%)	497 (93%)	32 (6%)	6 (1%)	11	36
1	L	535/537 (100%)	494 (92%)	36 (7%)	5 (1%)	14	41
1	M	535/537 (100%)	466 (87%)	57 (11%)	12 (2%)	5	19
1	N	535/537 (100%)	494 (92%)	33 (6%)	8 (2%)	8	28
1	O	535/537 (100%)	499 (93%)	30 (6%)	6 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	535/537 (100%)	497 (93%)	34 (6%)	4 (1%)	18	47
All	All	8560/8592 (100%)	7953 (93%)	514 (6%)	93 (1%)	11	36

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	480	ASP
1	E	189	GLN
1	E	480	ASP
1	E	488	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/455 (94%)	345 (81%)	81 (19%)	1	5
1	B	425/455 (93%)	336 (79%)	89 (21%)	1	4
1	C	425/455 (93%)	338 (80%)	87 (20%)	1	4
1	D	425/455 (93%)	341 (80%)	84 (20%)	1	5
1	E	425/455 (93%)	337 (79%)	88 (21%)	1	4
1	F	425/455 (93%)	329 (77%)	96 (23%)	1	3
1	G	426/455 (94%)	340 (80%)	86 (20%)	1	4
1	H	425/455 (93%)	330 (78%)	95 (22%)	1	3
1	I	426/455 (94%)	332 (78%)	94 (22%)	1	3
1	J	425/455 (93%)	337 (79%)	88 (21%)	1	4
1	K	425/455 (93%)	335 (79%)	90 (21%)	1	4
1	L	426/455 (94%)	330 (78%)	96 (22%)	1	3
1	M	426/455 (94%)	310 (73%)	116 (27%)	0	1
1	N	425/455 (93%)	326 (77%)	99 (23%)	1	3
1	O	426/455 (94%)	324 (76%)	102 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	425/455 (93%)	333 (78%)	92 (22%)	1 3
All	All	6806/7280 (94%)	5323 (78%)	1483 (22%)	1 3

5 of 1483 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	287	VAL
1	M	380	LEU
1	K	425	LEU
1	K	283	MET
1	L	387	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	81	GLN
1	N	48	GLN
1	K	259	ASN
1	L	366	ASN
1	N	334	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	MAY	G	600	1	20,23,24	0.34	0	18,23,26	0.65	0
2	MAY	N	600	1	20,23,24	0.45	0	18,23,26	0.57	0
2	MAY	B	600	1	20,23,24	0.46	0	18,23,26	0.57	0
2	MAY	K	600	1	20,23,24	0.44	0	18,23,26	0.53	0
2	MAY	C	600	1	20,23,24	0.33	0	18,23,26	0.57	0
2	MAY	E	600	1	20,23,24	0.44	0	18,23,26	0.58	0
2	MAY	A	600	1	20,23,24	0.38	0	18,23,26	0.63	0
2	MAY	M	600	1	20,23,24	0.34	0	18,23,26	0.60	0
2	MAY	L	600	1	20,23,24	0.44	0	18,23,26	0.64	0
2	MAY	P	600	1	20,23,24	0.40	0	18,23,26	0.52	0
2	MAY	O	600	1	20,23,24	0.46	0	18,23,26	0.50	0
2	MAY	H	600	1	20,23,24	0.44	0	18,23,26	0.61	0
2	MAY	F	600	1	20,23,24	0.44	0	18,23,26	0.46	0
2	MAY	J	600	1	20,23,24	0.46	0	18,23,26	0.55	0
2	MAY	I	600	1	20,23,24	0.34	0	18,23,26	0.60	0
2	MAY	D	600	1	20,23,24	0.37	0	18,23,26	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAY	G	600	1	-	8/18/22/24	-
2	MAY	N	600	1	-	8/18/22/24	-
2	MAY	B	600	1	-	9/18/22/24	-
2	MAY	K	600	1	-	8/18/22/24	-
2	MAY	C	600	1	-	8/18/22/24	-
2	MAY	E	600	1	-	7/18/22/24	-
2	MAY	A	600	1	-	7/18/22/24	-
2	MAY	M	600	1	-	7/18/22/24	-
2	MAY	L	600	1	-	9/18/22/24	-
2	MAY	P	600	1	-	7/18/22/24	-
2	MAY	O	600	1	-	8/18/22/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAY	H	600	1	-	9/18/22/24	-
2	MAY	F	600	1	-	8/18/22/24	-
2	MAY	J	600	1	-	8/18/22/24	-
2	MAY	I	600	1	-	7/18/22/24	-
2	MAY	D	600	1	-	9/18/22/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	MAY	P1-C1-C2-C3
2	K	600	MAY	P1-C1-C2-C3
2	M	600	MAY	P1-C1-C2-C3
2	O	600	MAY	C1-C2-C3-C4
2	D	600	MAY	C1-C2-C3-C4

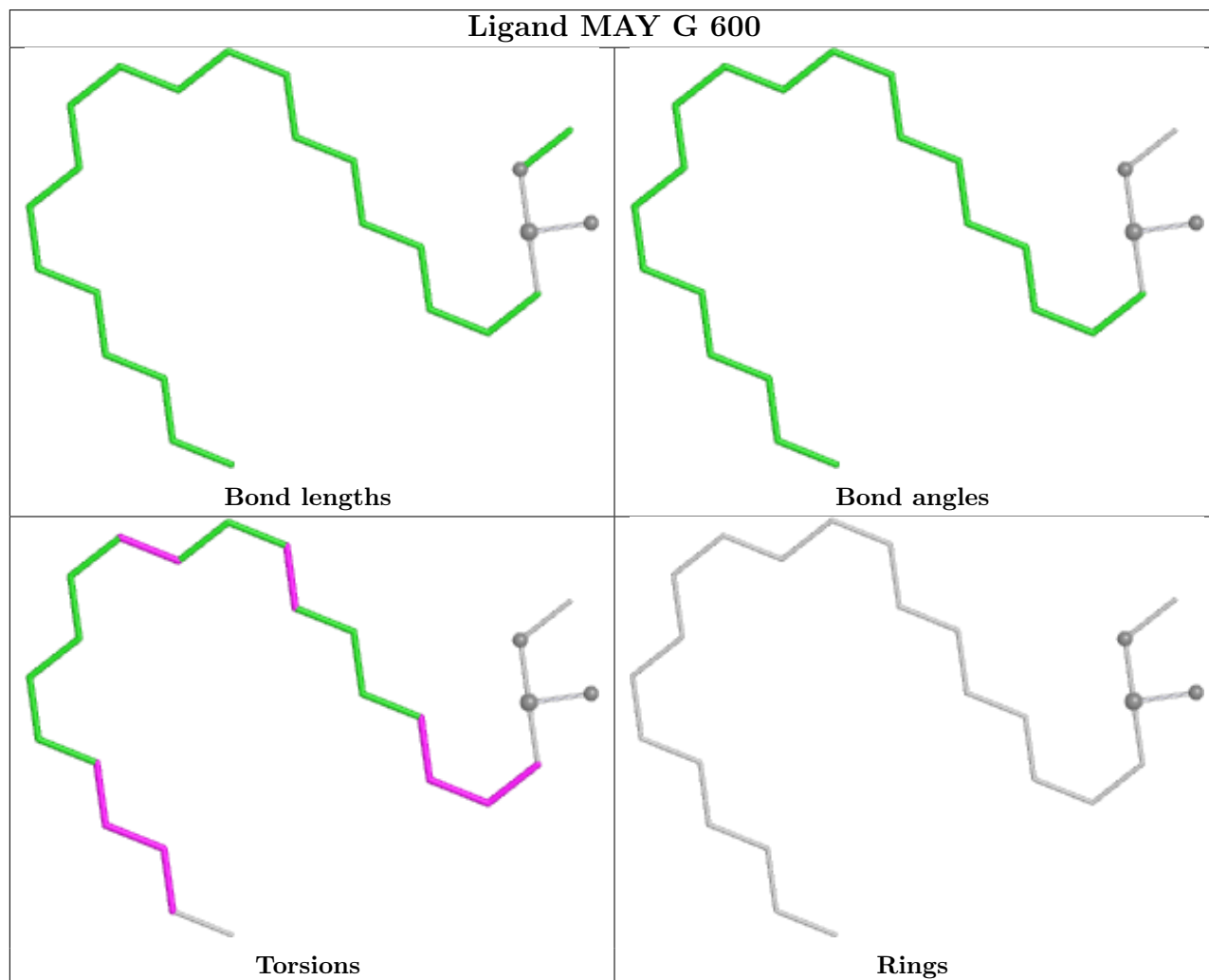
There are no ring outliers.

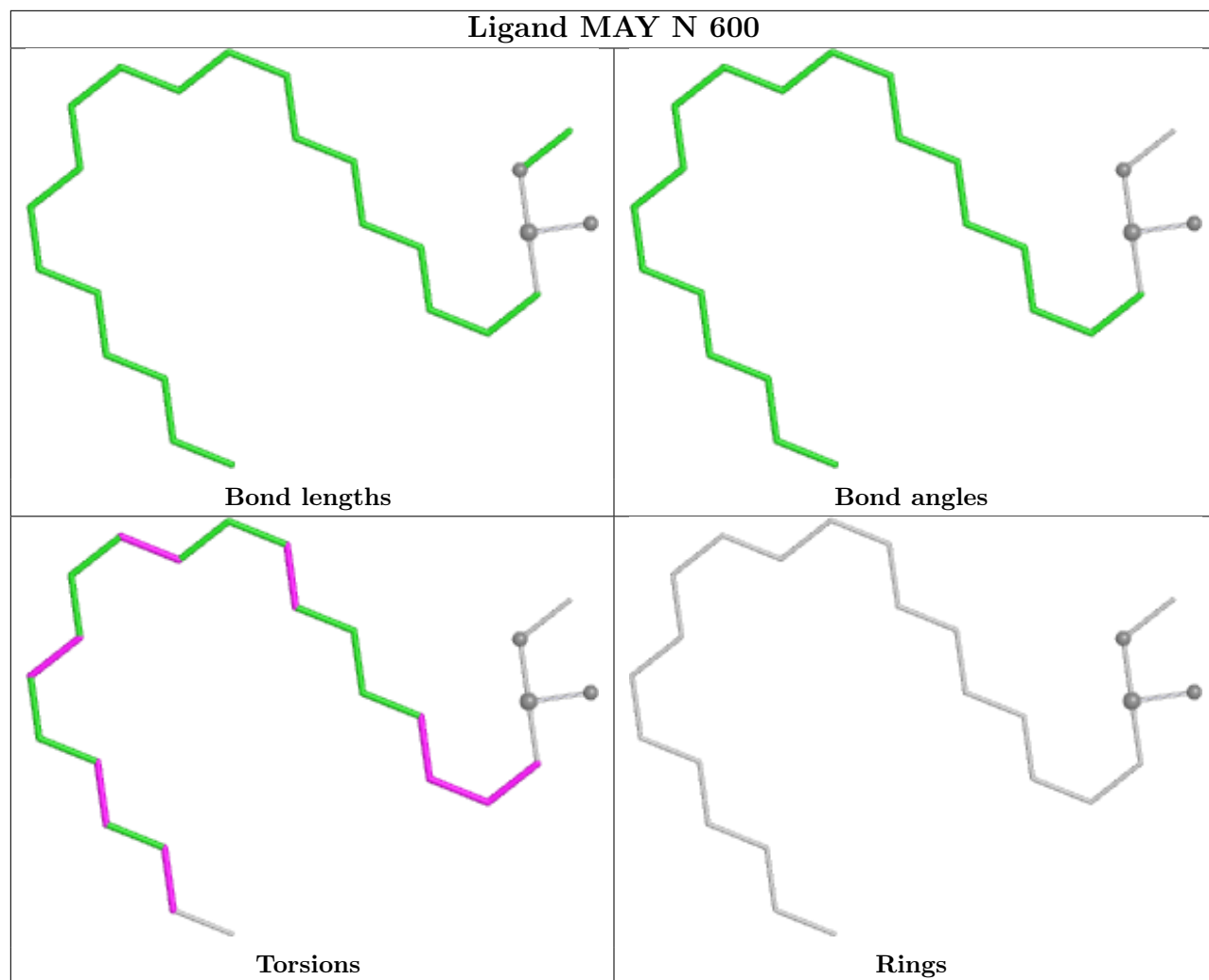
16 monomers are involved in 46 short contacts:

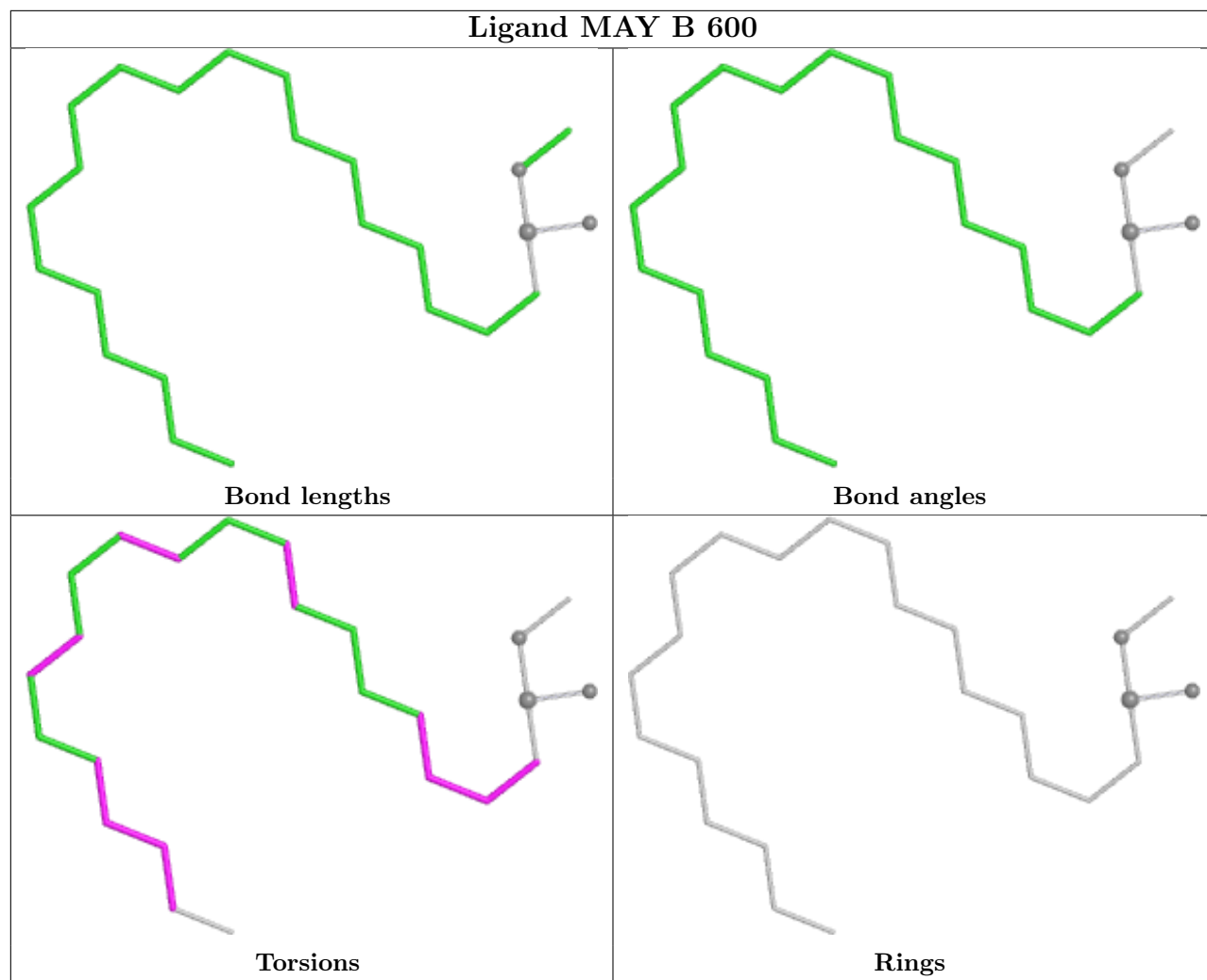
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	600	MAY	1	0
2	N	600	MAY	4	0
2	B	600	MAY	3	0
2	K	600	MAY	3	0
2	C	600	MAY	3	0
2	E	600	MAY	3	0
2	A	600	MAY	5	0
2	M	600	MAY	2	0
2	L	600	MAY	1	0
2	P	600	MAY	2	0
2	O	600	MAY	3	0
2	H	600	MAY	4	0
2	F	600	MAY	4	0
2	J	600	MAY	2	0
2	I	600	MAY	2	0
2	D	600	MAY	4	0

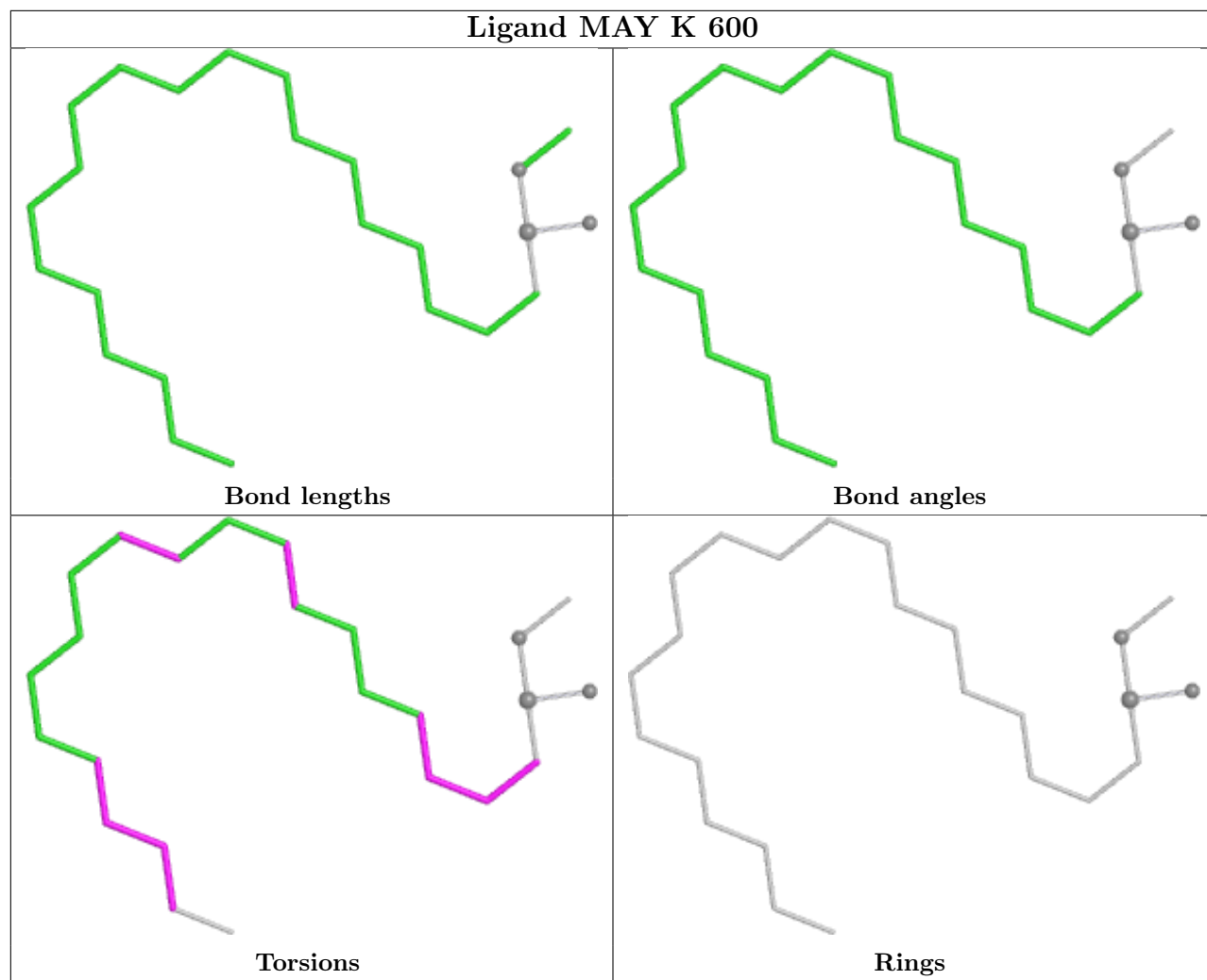
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

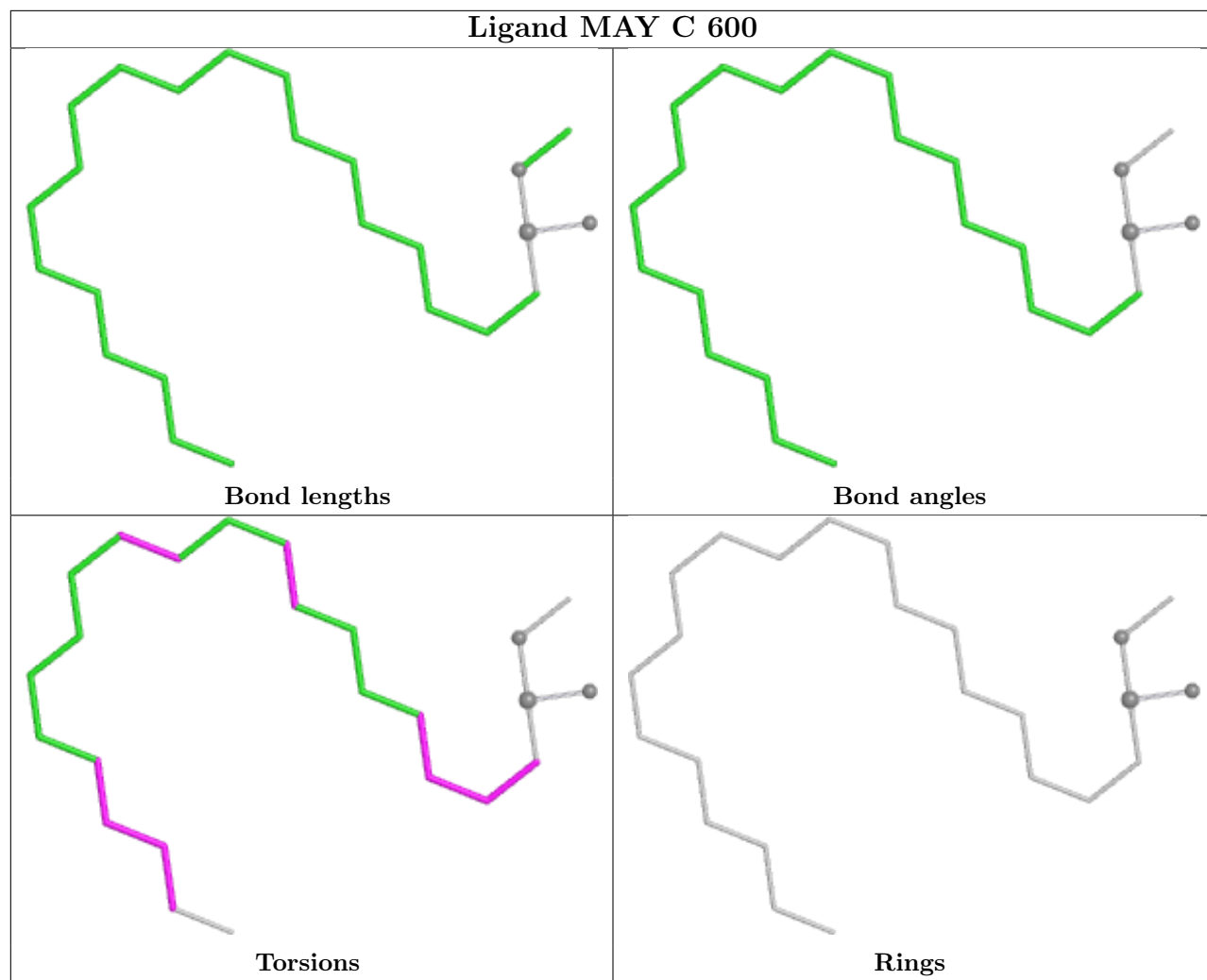
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

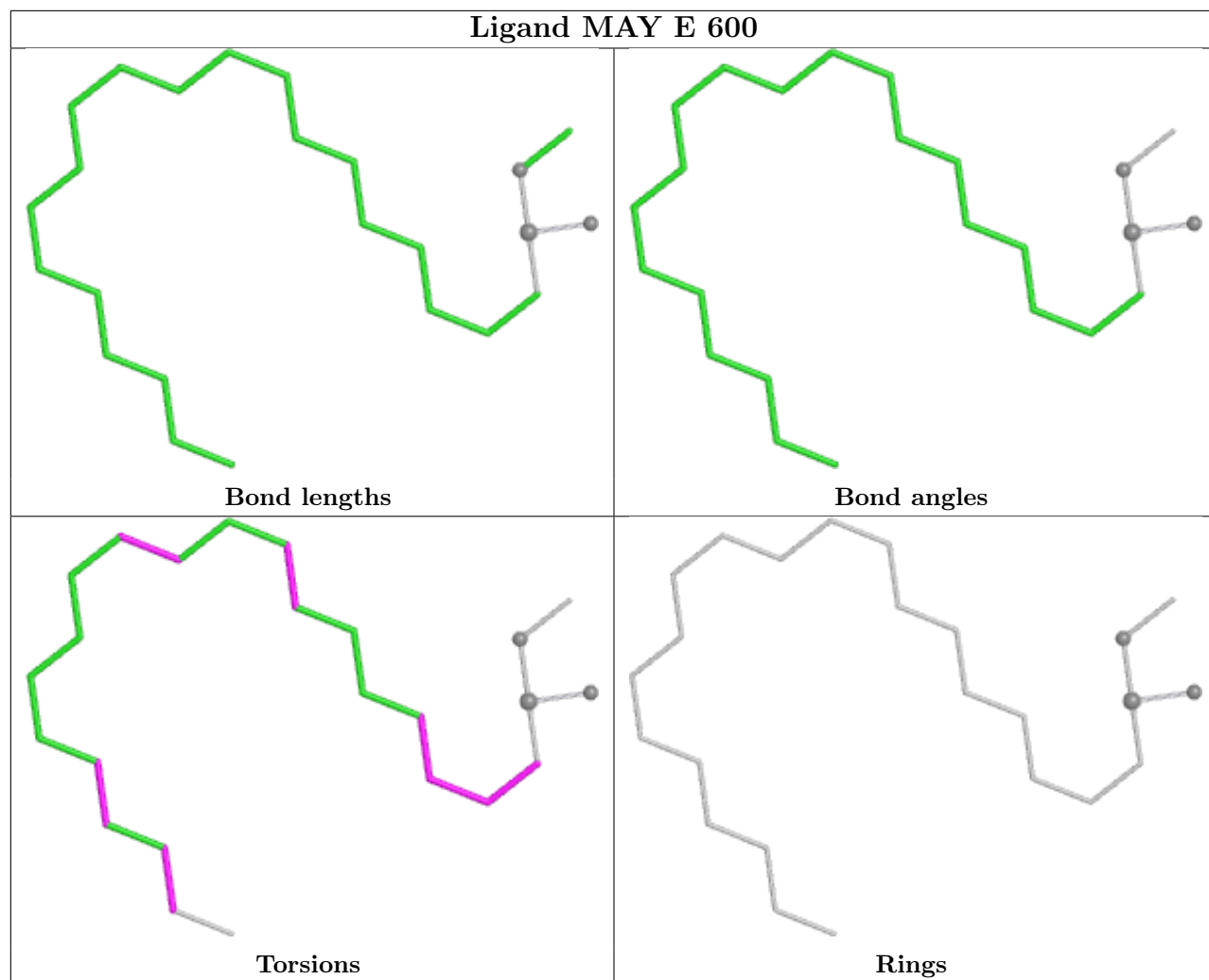


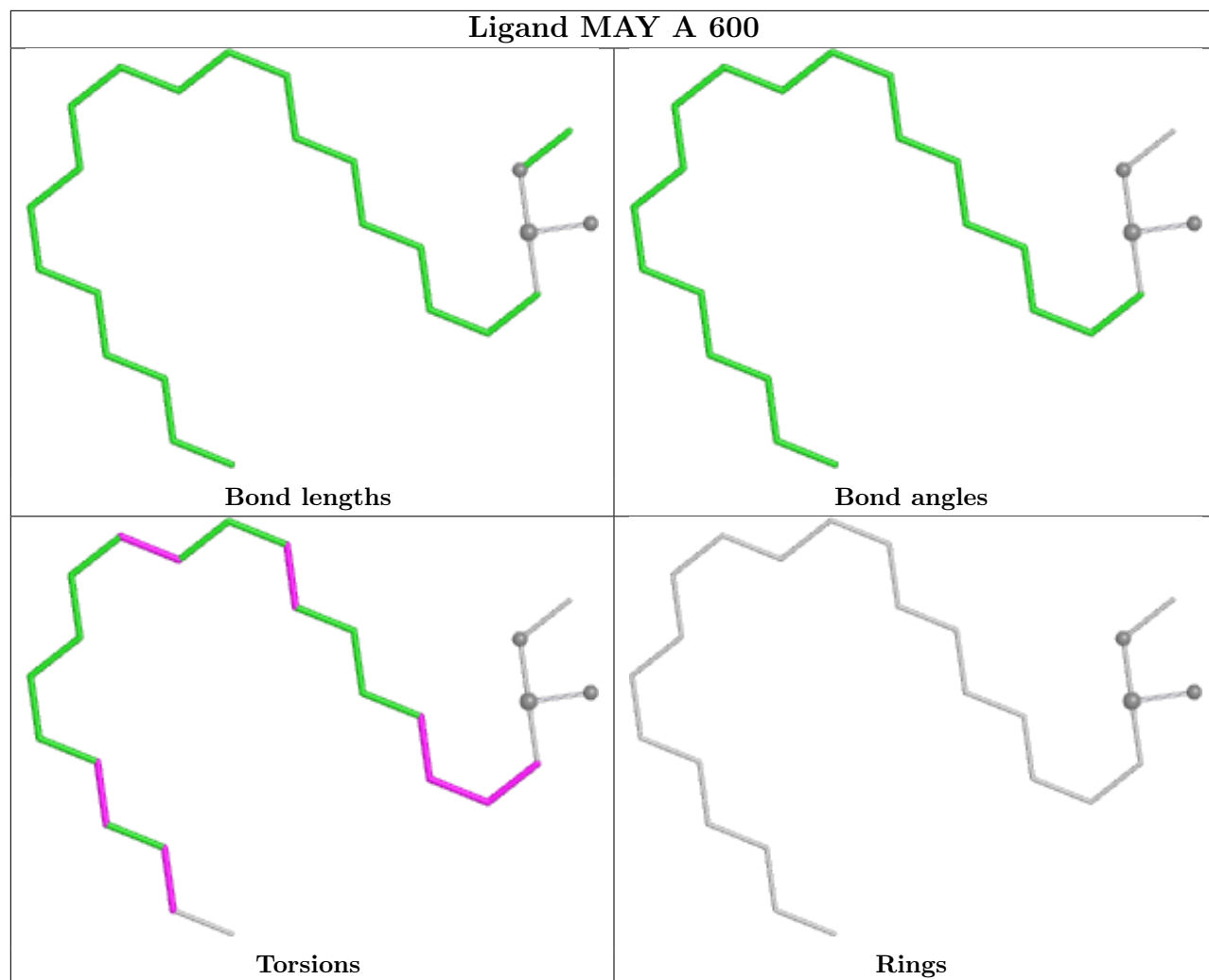


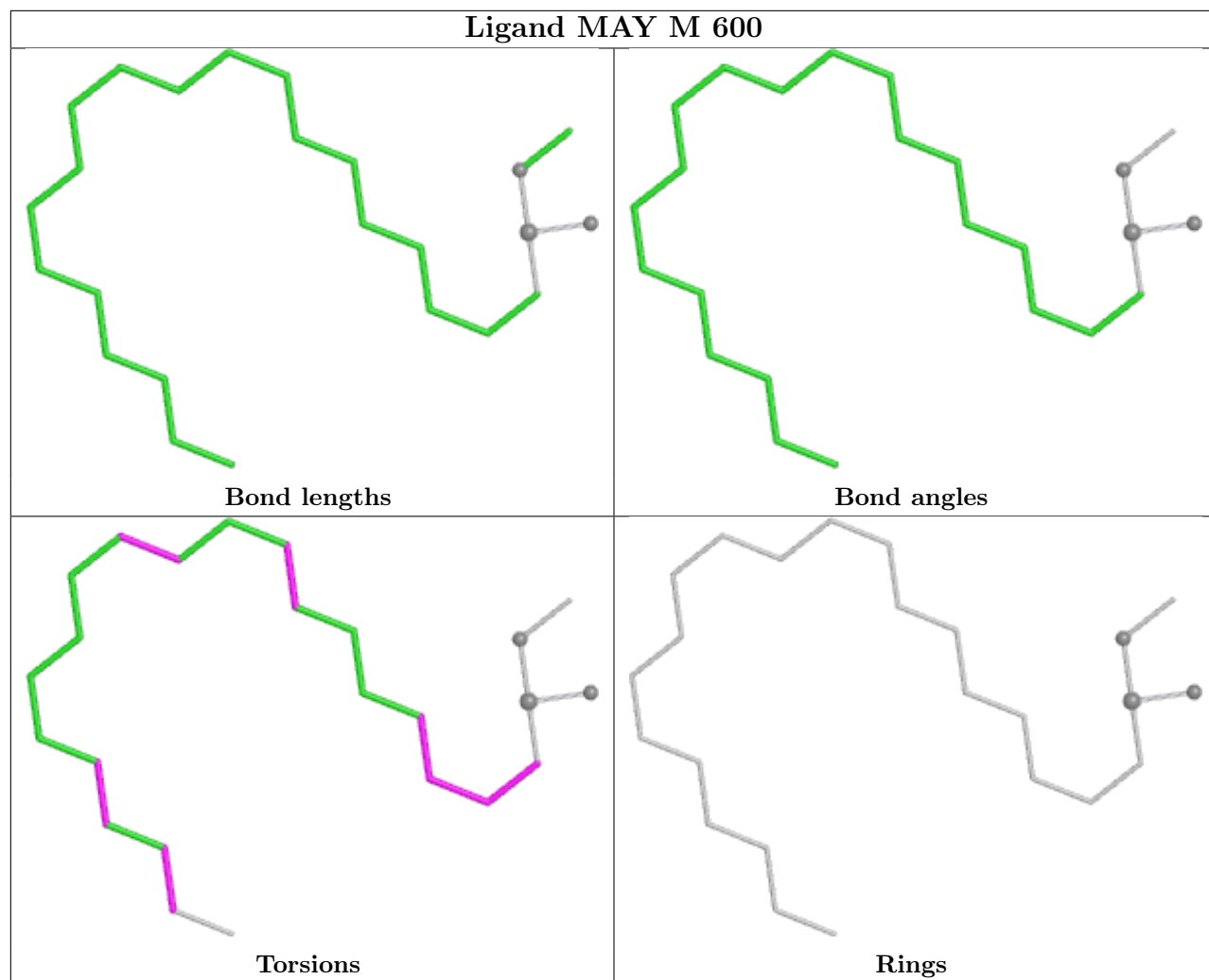


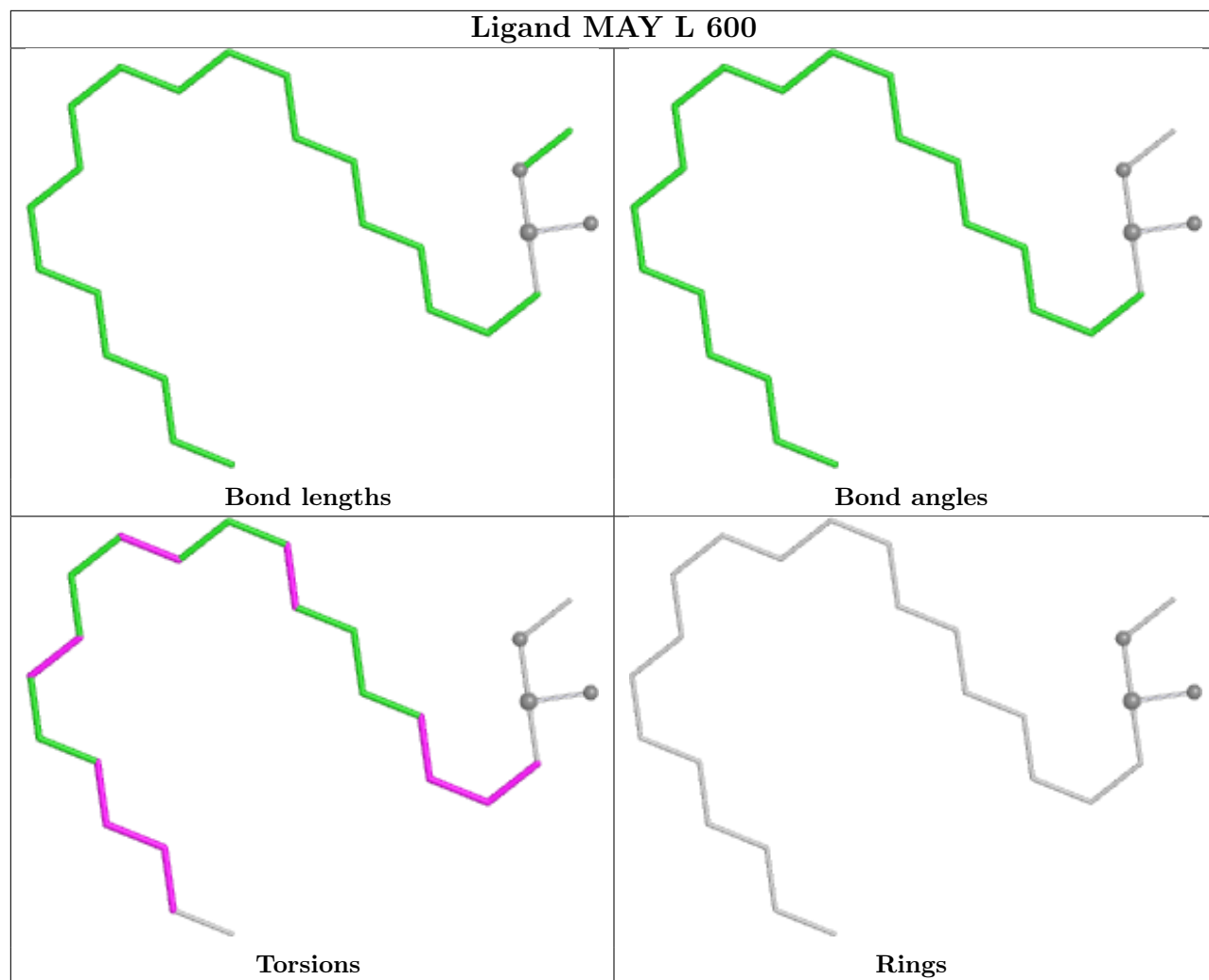


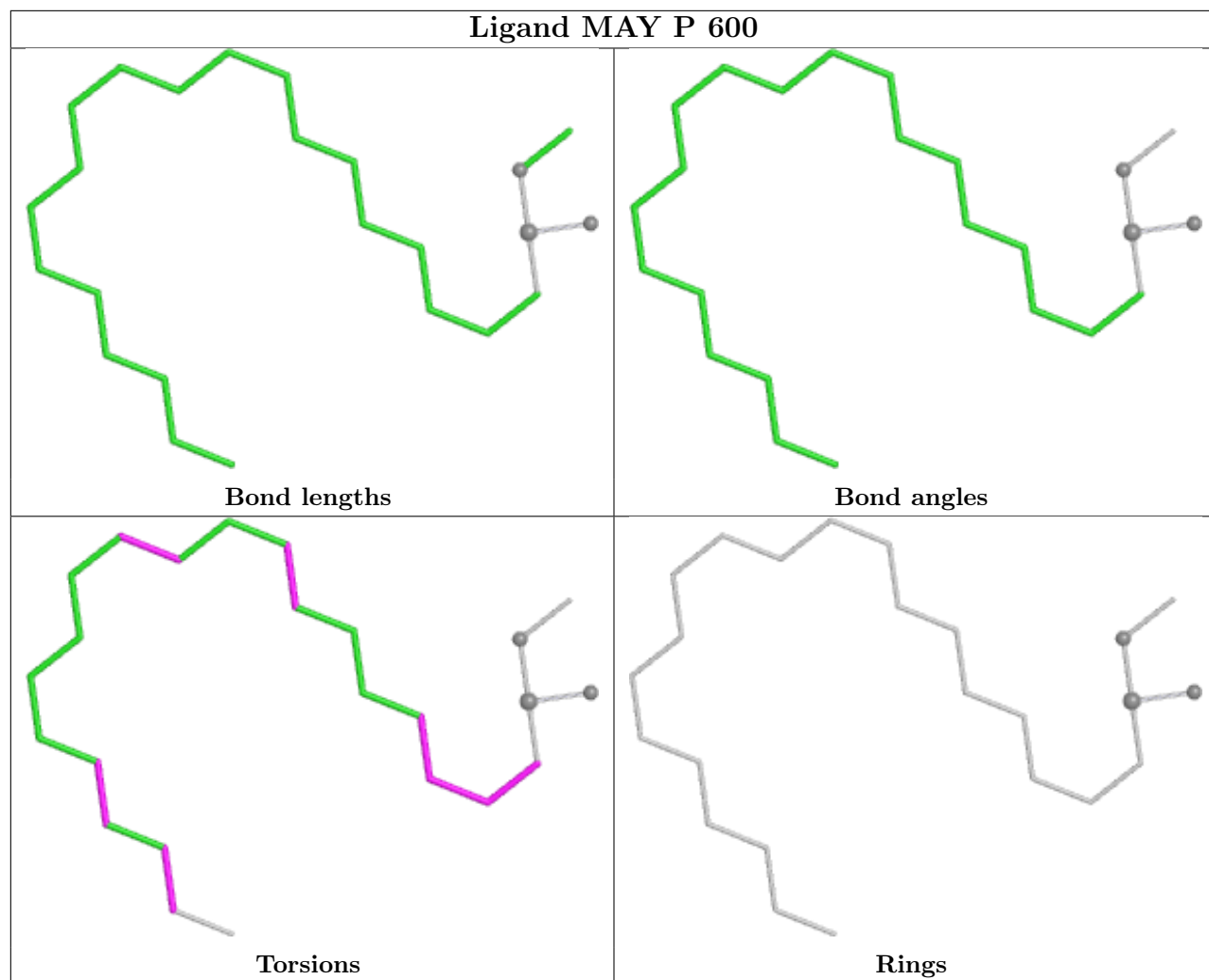


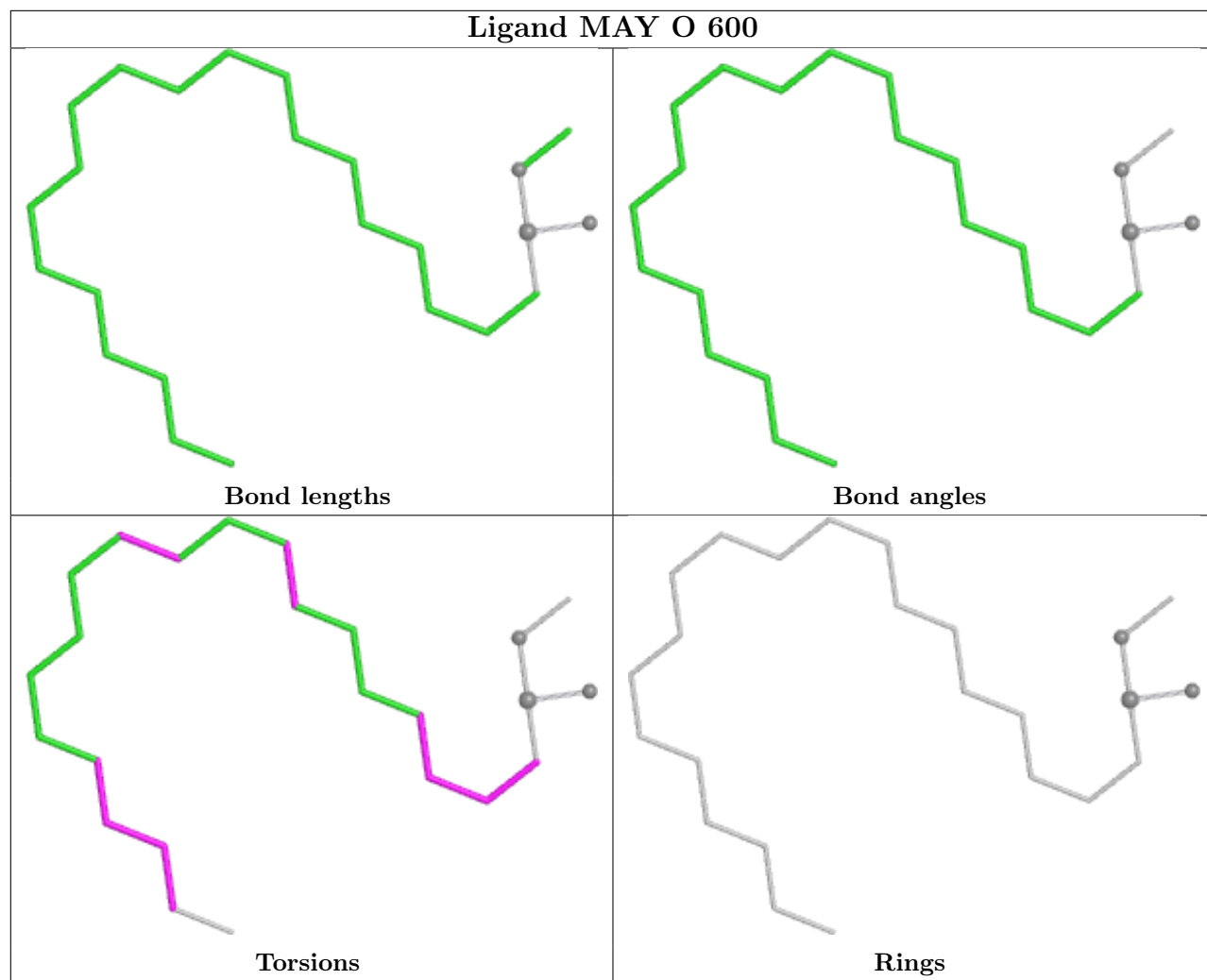


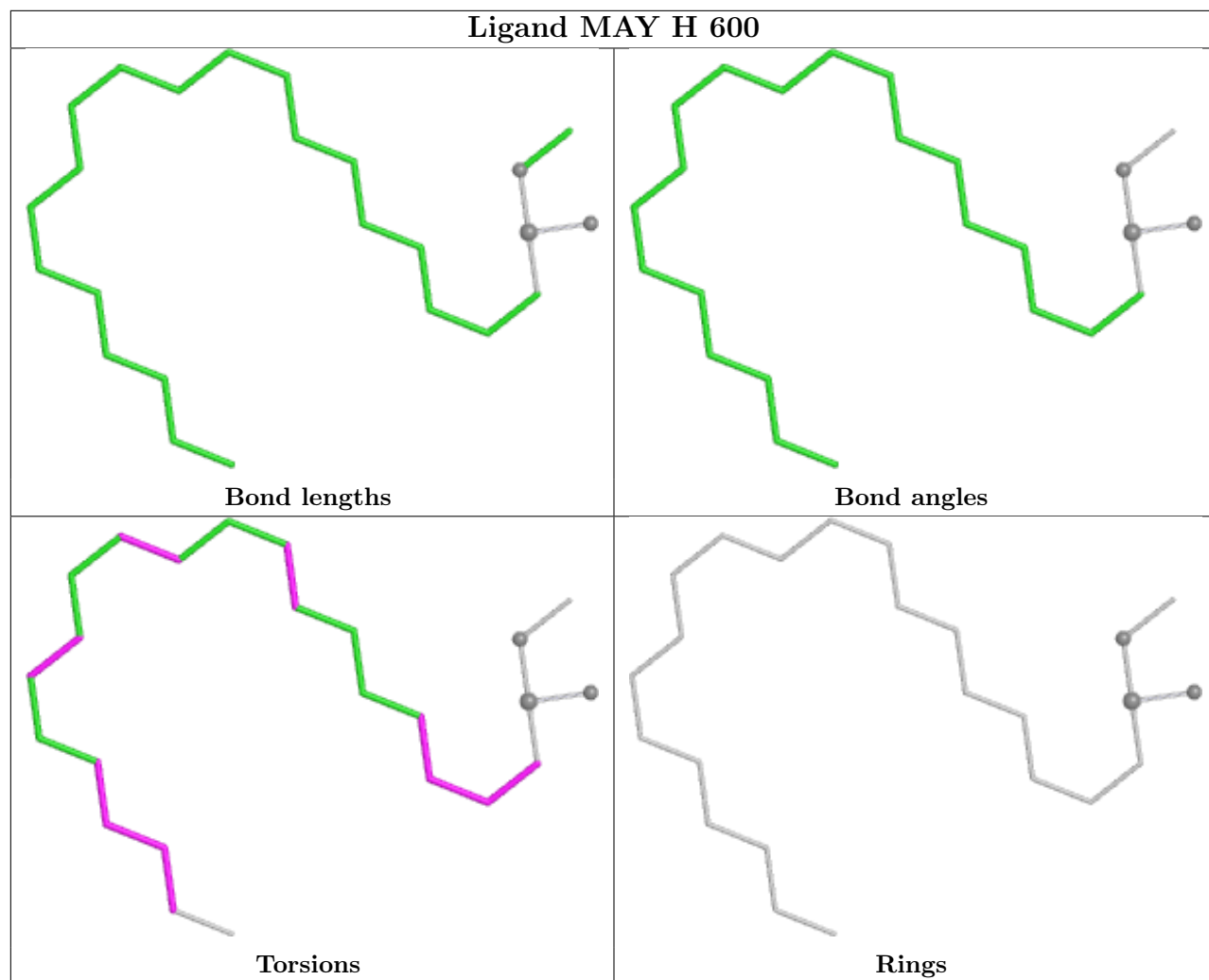


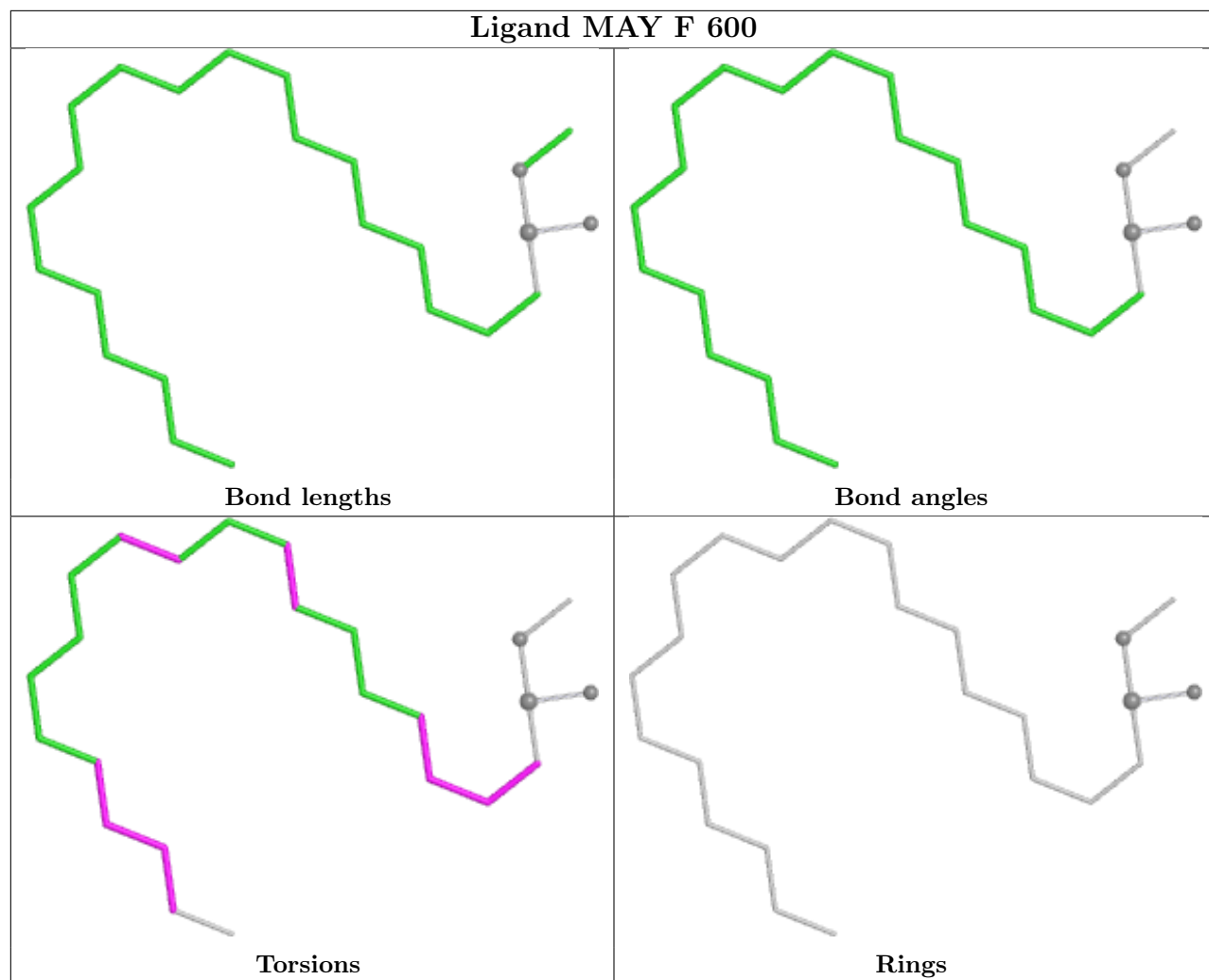


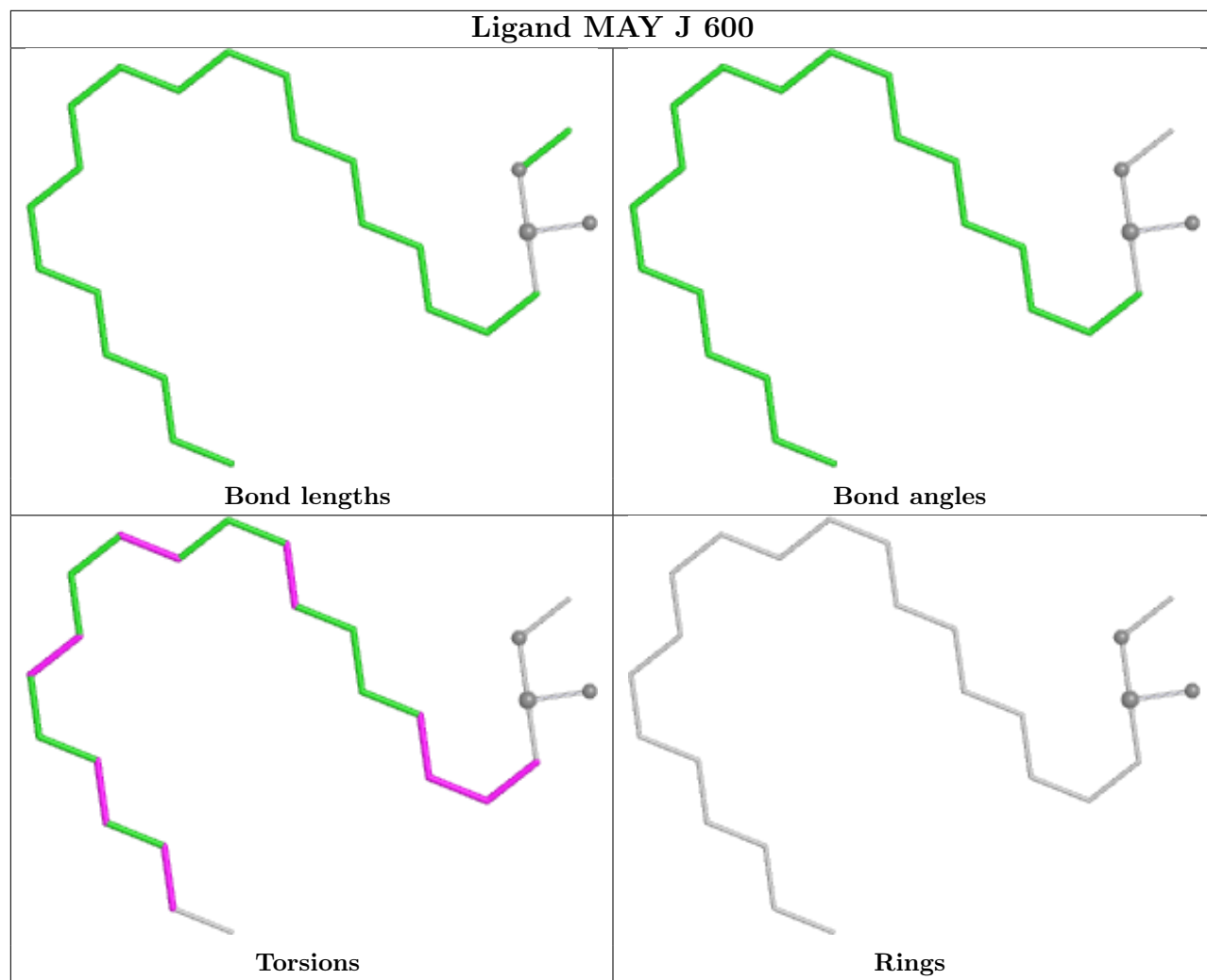


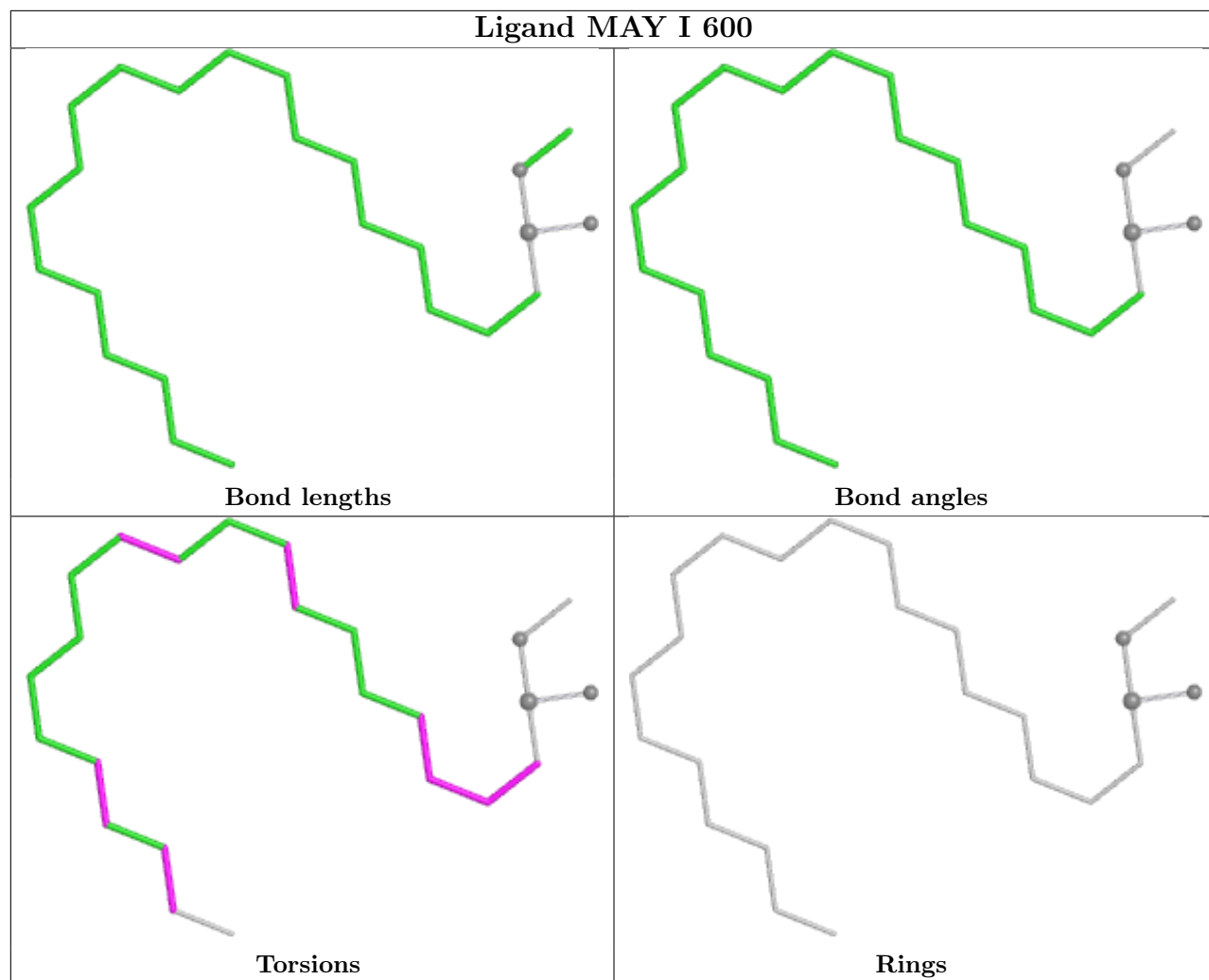


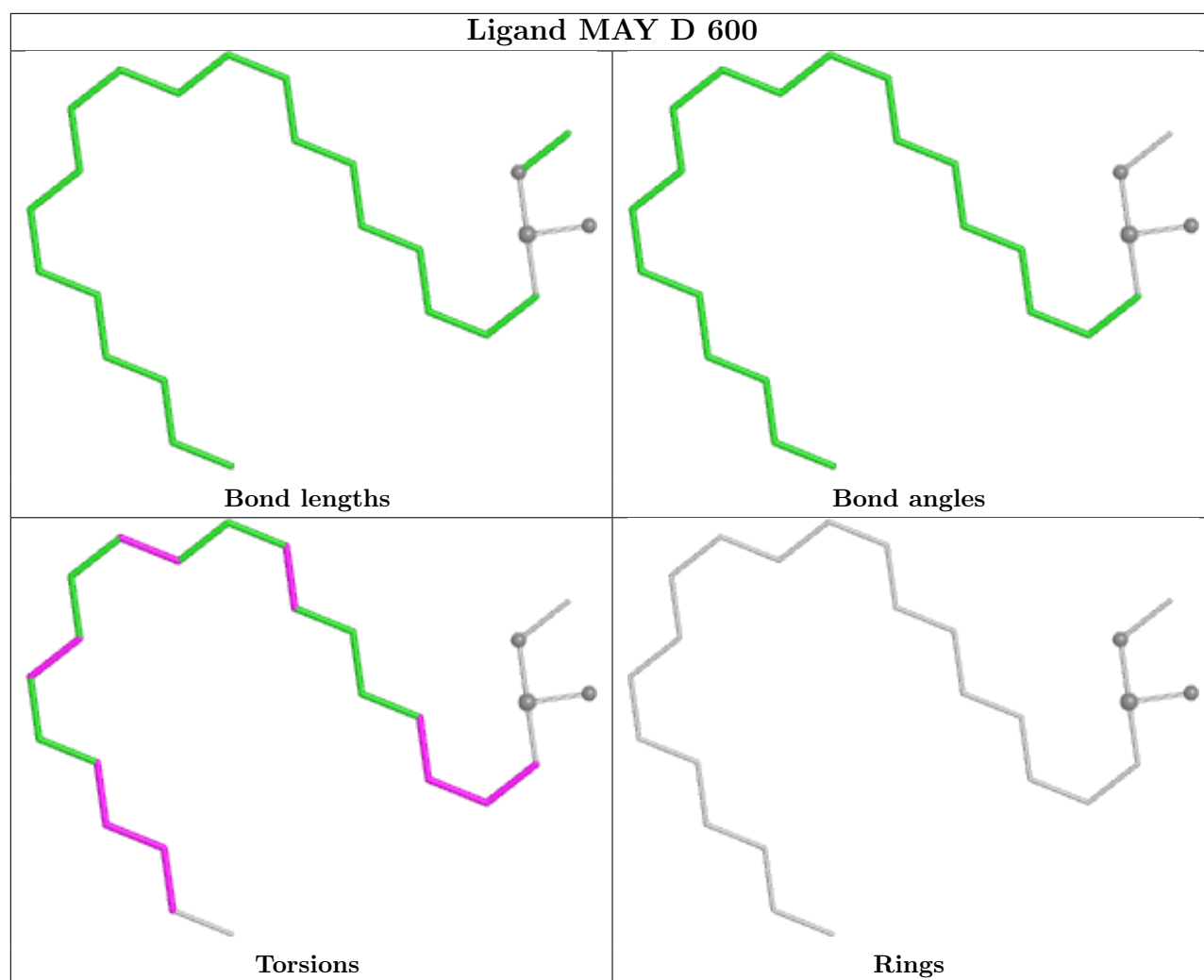












5.7 Other polymers [i](#)

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.