



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 05:00 AM EDT

PDB ID : 1G63
Title : PEPTIDYL-CYSTEINE DECARBOXYLASE EPID
Authors : Blaesse, M.; Kupke, T.; Huber, R.; Steinbac, S.
Deposited on : 2000-11-03
Resolution : 2.50 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.36.2

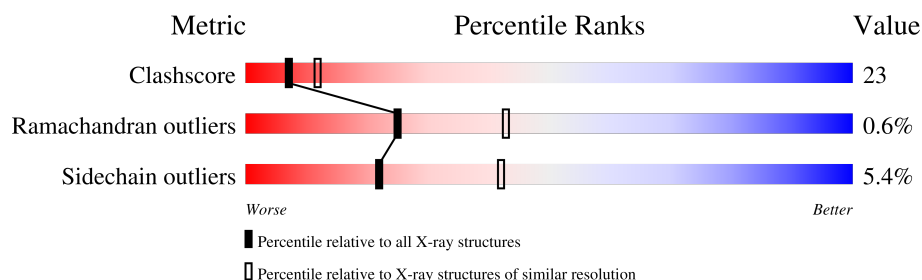
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)





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	181	59% 28% • 9%
1	B	181	61% 33% • •
1	C	181	59% 29% • 10%
1	D	181	55% 33% • 10%
1	E	181	55% 32% • 10%
1	F	181	65% 29% • •
1	G	181	54% 34% • 9%
1	H	181	60% 29% • 9%

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Mol	Chain	Length	Quality of chain
1	I	181	 62% 25% • 9%
1	J	181	 57% 30% • 9%
1	K	181	 59% 30% • 10%
1	L	181	 54% 33% • 9%

2 Entry composition

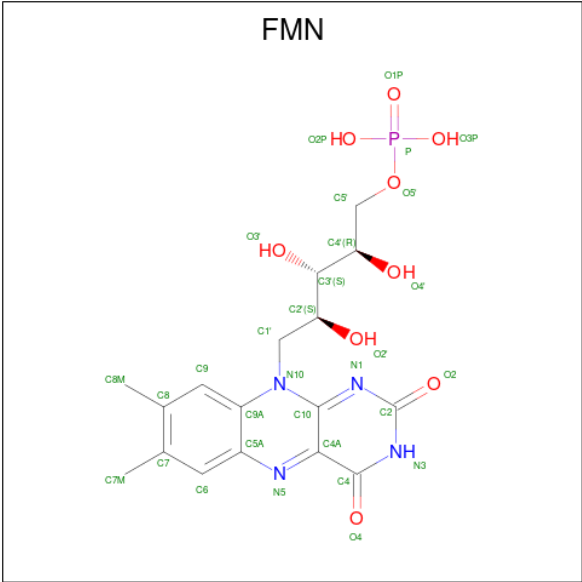
There are 3 unique types of molecules in this entry. The entry contains 16760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPIDERMIN MODIFYING ENZYME EPID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			
1	B	174	Total	C	N	O	S	0	0	0
			1403	904	231	259	9			
1	C	163	Total	C	N	O	S	0	0	0
			1312	846	215	242	9			
1	D	162	Total	C	N	O	S	0	0	0
			1304	842	213	240	9			
1	E	163	Total	C	N	O	S	0	0	0
			1312	846	215	242	9			
1	F	174	Total	C	N	O	S	0	0	0
			1403	904	231	259	9			
1	G	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			
1	H	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			
1	I	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			
1	J	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			
1	K	163	Total	C	N	O	S	0	0	0
			1312	846	215	242	9			
1	L	164	Total	C	N	O	S	0	0	0
			1321	852	217	243	9			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

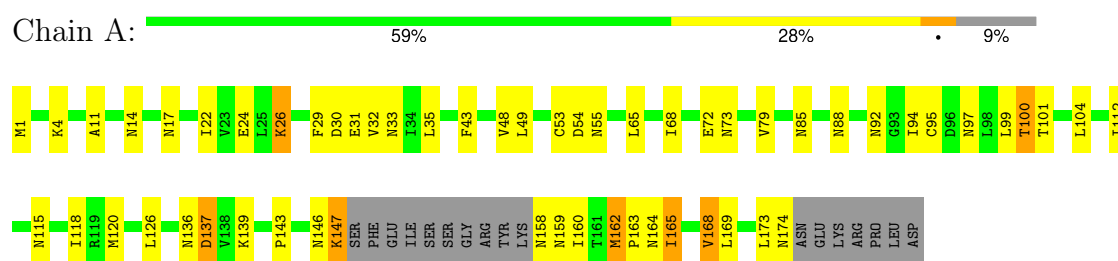
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	39	Total 39	O 39	0	0
3	C	28	Total 28	O 28	0	0
3	D	18	Total 18	O 18	0	0
3	E	30	Total 30	O 30	0	0
3	F	29	Total 29	O 29	0	0
3	G	24	Total 24	O 24	0	0
3	H	29	Total 29	O 29	0	0
3	I	30	Total 30	O 30	0	0
3	J	41	Total 41	O 41	0	0
3	K	33	Total 33	O 33	0	0
3	L	62	Total 62	O 62	0	0

3 Residue-property plots

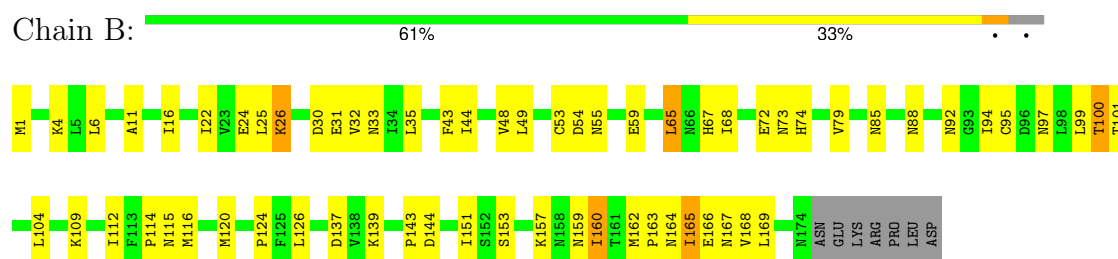
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

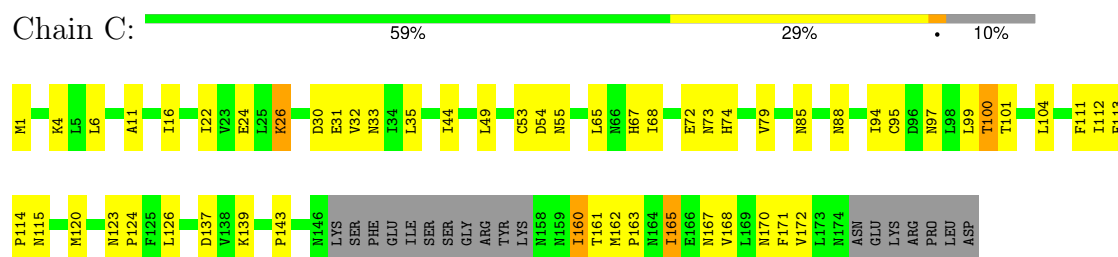
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID



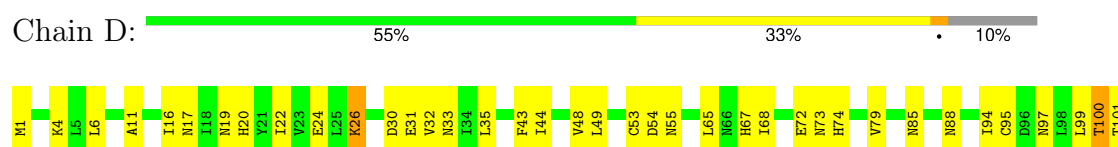
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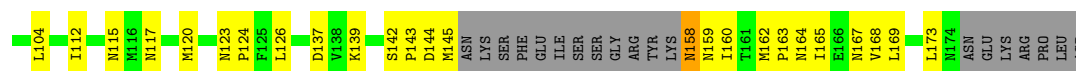


• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

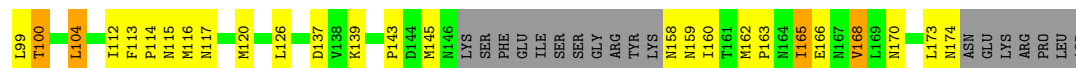


• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID





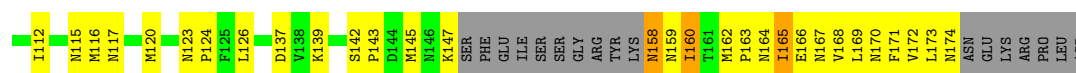
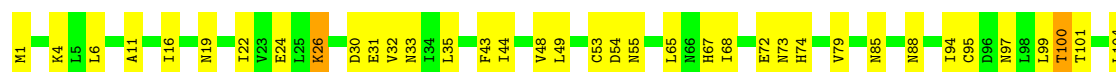
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID



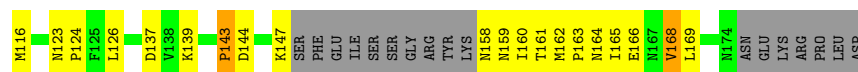
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID



• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

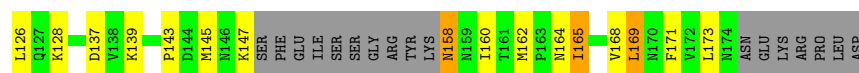


• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID



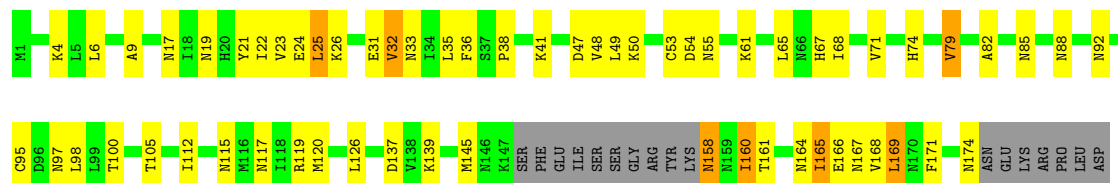
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID





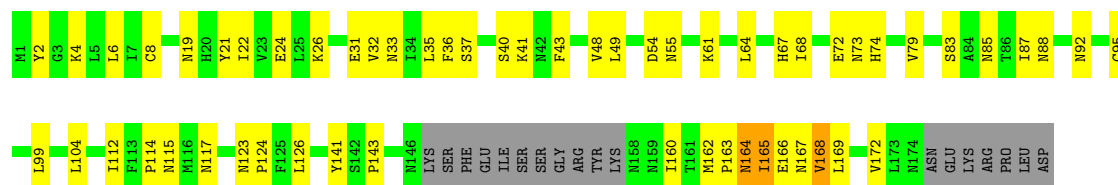
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain J: 57% 30% 9%



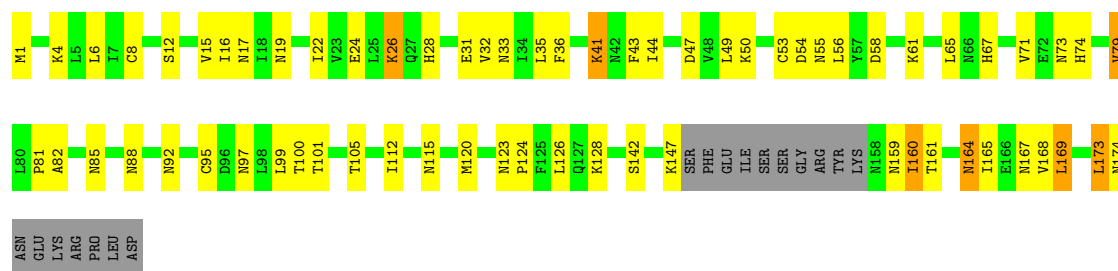
• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain K: 59% 30% 10%



• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain L: 54% 33% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.68Å 110.03Å 152.87Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	14.99 – 2.50	Depositor
% Data completeness (in resolution range)	87.1 (14.99-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	5.80	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16760	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: FMN

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	0/1346	0.61	0/1830
1	B	0.38	0/1431	0.61	0/1944
1	C	0.35	0/1337	0.61	0/1819
1	D	0.36	0/1329	0.61	0/1808
1	E	0.36	0/1337	0.61	0/1819
1	F	0.38	0/1431	0.92	3/1944 (0.2%)
1	G	0.36	0/1346	0.60	0/1830
1	H	0.36	0/1346	0.61	0/1830
1	I	0.36	0/1346	0.61	0/1830
1	J	0.43	0/1346	0.66	0/1830
1	K	0.39	0/1337	0.63	0/1819
1	L	0.44	0/1346	0.68	0/1830
All	All	0.38	0/16278	0.65	3/22133 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	ARG	NE-CZ-NH2	-21.12	109.74	120.30
1	F	119	ARG	NE-CZ-NH1	19.87	130.24	120.30
1	F	119	ARG	CD-NE-CZ	8.73	135.82	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1321	0	1337	67	0
1	B	1403	0	1417	76	0
1	C	1312	0	1324	60	0
1	D	1304	0	1318	67	0
1	E	1312	0	1324	69	0
1	F	1403	0	1417	65	0
1	G	1321	0	1337	75	0
1	H	1321	0	1337	68	0
1	I	1321	0	1337	68	0
1	J	1321	0	1337	61	0
1	K	1312	0	1324	69	0
1	L	1321	0	1337	76	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	1	0
2	K	31	0	19	0	0
2	L	31	0	19	0	0
3	A	53	0	0	6	0
3	B	39	0	0	4	0
3	C	28	0	0	0	0
3	D	18	0	0	0	0
3	E	30	0	0	0	0
3	F	29	0	0	0	0
3	G	24	0	0	1	0
3	H	29	0	0	1	0
3	I	30	0	0	3	0
3	J	41	0	0	4	0
3	K	33	0	0	1	0
3	L	62	0	0	2	0
All	All	16760	0	16374	741	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 23.

The worst 5 of 741 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:C:95:CYS:HA	1:C:100:THR:HG23	1.31	1.13
1:F:95:CYS:HA	1:F:100:THR:HG23	1.30	1.12
1:B:95:CYS:HA	1:B:100:THR:HG23	1.29	1.12
1:A:95:CYS:HA	1:A:100:THR:HG23	1.29	1.11
1:G:95:CYS:HA	1:G:100:THR:HG23	1.30	1.10

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	160/181 (88%)	156 (98%)	3 (2%)	1 (1%)	25	43
1	B	172/181 (95%)	168 (98%)	3 (2%)	1 (1%)	25	43
1	C	159/181 (88%)	156 (98%)	2 (1%)	1 (1%)	25	43
1	D	158/181 (87%)	154 (98%)	3 (2%)	1 (1%)	25	43
1	E	159/181 (88%)	154 (97%)	4 (2%)	1 (1%)	25	43
1	F	172/181 (95%)	167 (97%)	4 (2%)	1 (1%)	25	43
1	G	160/181 (88%)	154 (96%)	4 (2%)	2 (1%)	12	21
1	H	160/181 (88%)	154 (96%)	4 (2%)	2 (1%)	12	21
1	I	160/181 (88%)	155 (97%)	4 (2%)	1 (1%)	25	43
1	J	160/181 (88%)	154 (96%)	6 (4%)	0	100	100
1	K	159/181 (88%)	153 (96%)	5 (3%)	1 (1%)	25	43
1	L	160/181 (88%)	156 (98%)	4 (2%)	0	100	100
All	All	1939/2172 (89%)	1881 (97%)	46 (2%)	12 (1%)	25	43

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	160	ILE
1	H	143	PRO
1	H	11	ALA
1	A	11	ALA
1	C	11	ALA

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	155/171 (91%)	145 (94%)	10 (6%)	17	33
1	B	164/171 (96%)	155 (94%)	9 (6%)	21	41
1	C	154/171 (90%)	147 (96%)	7 (4%)	27	51
1	D	153/171 (90%)	147 (96%)	6 (4%)	32	57
1	E	154/171 (90%)	143 (93%)	11 (7%)	14	28
1	F	164/171 (96%)	156 (95%)	8 (5%)	25	47
1	G	155/171 (91%)	148 (96%)	7 (4%)	27	51
1	H	155/171 (91%)	149 (96%)	6 (4%)	32	57
1	I	155/171 (91%)	147 (95%)	8 (5%)	23	44
1	J	155/171 (91%)	141 (91%)	14 (9%)	9	19
1	K	154/171 (90%)	151 (98%)	3 (2%)	57	80
1	L	155/171 (91%)	143 (92%)	12 (8%)	13	25
All	All	1873/2052 (91%)	1772 (95%)	101 (5%)	22	42

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	165	ILE
1	I	169	LEU
1	L	173	LEU
1	H	65	LEU
1	I	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	42	ASN
1	I	167	ASN
1	H	73	ASN
1	I	17	ASN
1	J	88	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	FMN	F	505	-	33,33,33	1.48	4 (12%)	48,50,50	1.09	3 (6%)
2	FMN	A	500	-	33,33,33	1.49	4 (12%)	48,50,50	1.09	4 (8%)
2	FMN	B	501	-	33,33,33	1.54	5 (15%)	48,50,50	1.06	3 (6%)
2	FMN	I	508	-	33,33,33	1.53	5 (15%)	48,50,50	1.05	3 (6%)
2	FMN	C	502	-	33,33,33	1.52	5 (15%)	48,50,50	1.05	3 (6%)
2	FMN	H	507	-	33,33,33	1.55	5 (15%)	48,50,50	1.08	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	G	506	-	33,33,33	1.53	4 (12%)	48,50,50	1.06	3 (6%)
2	FMN	J	509	-	33,33,33	1.46	4 (12%)	48,50,50	1.11	3 (6%)
2	FMN	D	503	-	33,33,33	1.49	4 (12%)	48,50,50	1.09	3 (6%)
2	FMN	L	511	-	33,33,33	1.51	4 (12%)	48,50,50	1.04	3 (6%)
2	FMN	E	504	-	33,33,33	1.54	5 (15%)	48,50,50	1.07	3 (6%)
2	FMN	K	510	-	33,33,33	1.53	7 (21%)	48,50,50	1.09	4 (8%)

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	FMN	F	505	-	-	0/18/18/18	0/3/3/3
2	FMN	A	500	-	-	0/18/18/18	0/3/3/3
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
2	FMN	I	508	-	-	0/18/18/18	0/3/3/3
2	FMN	C	502	-	-	0/18/18/18	0/3/3/3
2	FMN	H	507	-	-	0/18/18/18	0/3/3/3
2	FMN	G	506	-	-	0/18/18/18	0/3/3/3
2	FMN	J	509	-	-	0/18/18/18	0/3/3/3
2	FMN	D	503	-	-	0/18/18/18	0/3/3/3
2	FMN	L	511	-	-	0/18/18/18	0/3/3/3
2	FMN	E	504	-	-	0/18/18/18	0/3/3/3
2	FMN	K	510	-	-	0/18/18/18	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	506	FMN	C6-C5A	4.45	1.46	1.40
2	B	501	FMN	C6-C5A	4.42	1.46	1.40
2	D	503	FMN	C6-C5A	4.41	1.46	1.40
2	E	504	FMN	C6-C5A	4.41	1.46	1.40
2	F	505	FMN	C6-C5A	4.40	1.46	1.40

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	FMN	C5A-C9A-N10	-2.97	115.28	117.97
2	J	509	FMN	C5A-C9A-N10	-2.95	115.30	117.97
2	K	510	FMN	C5A-C9A-N10	-2.92	115.33	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FMN	C5A-C9A-N10	-2.89	115.35	117.97
2	B	501	FMN	C5A-C9A-N10	-2.85	115.39	117.97

There are no chirality outliers.

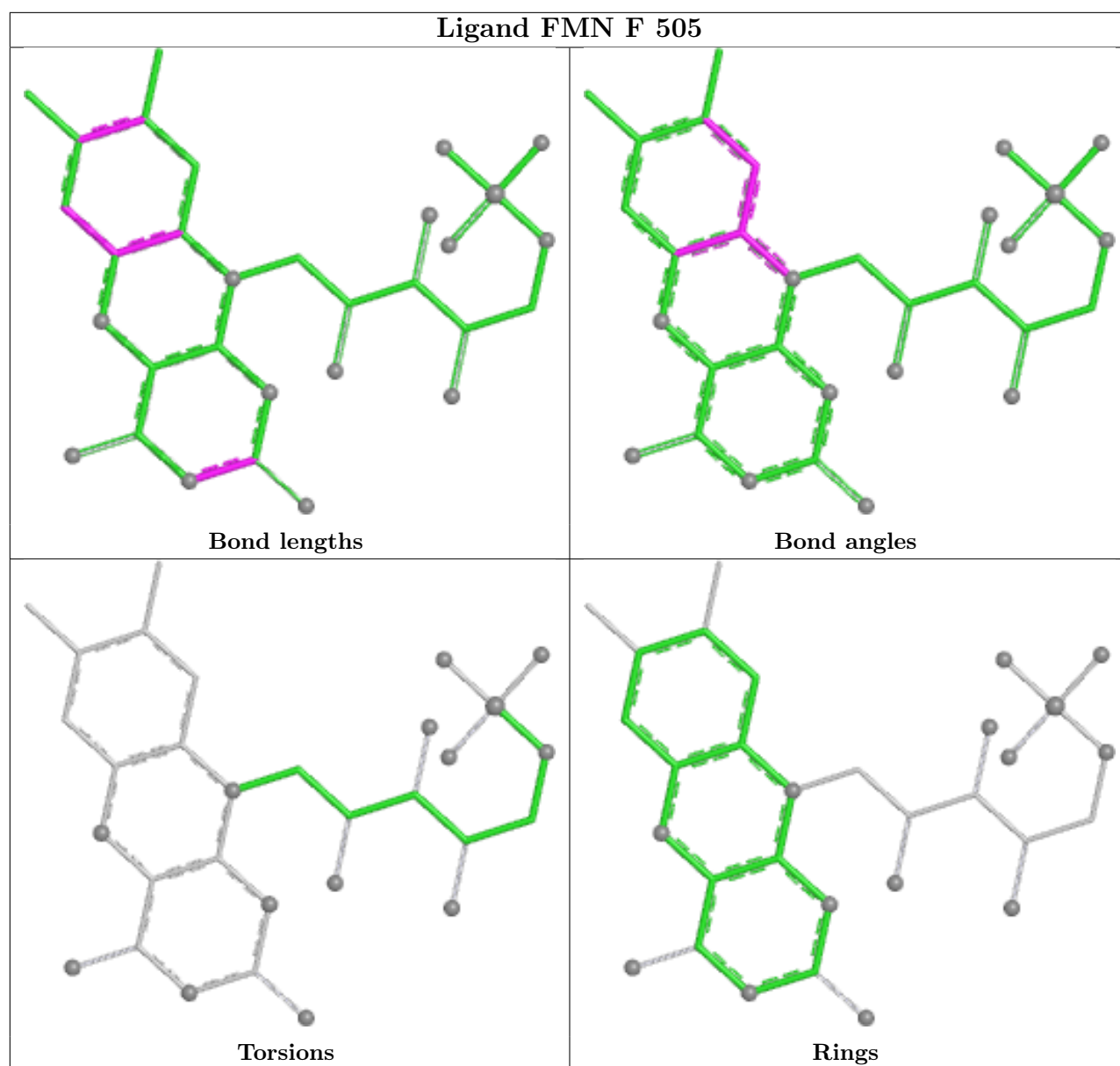
There are no torsion outliers.

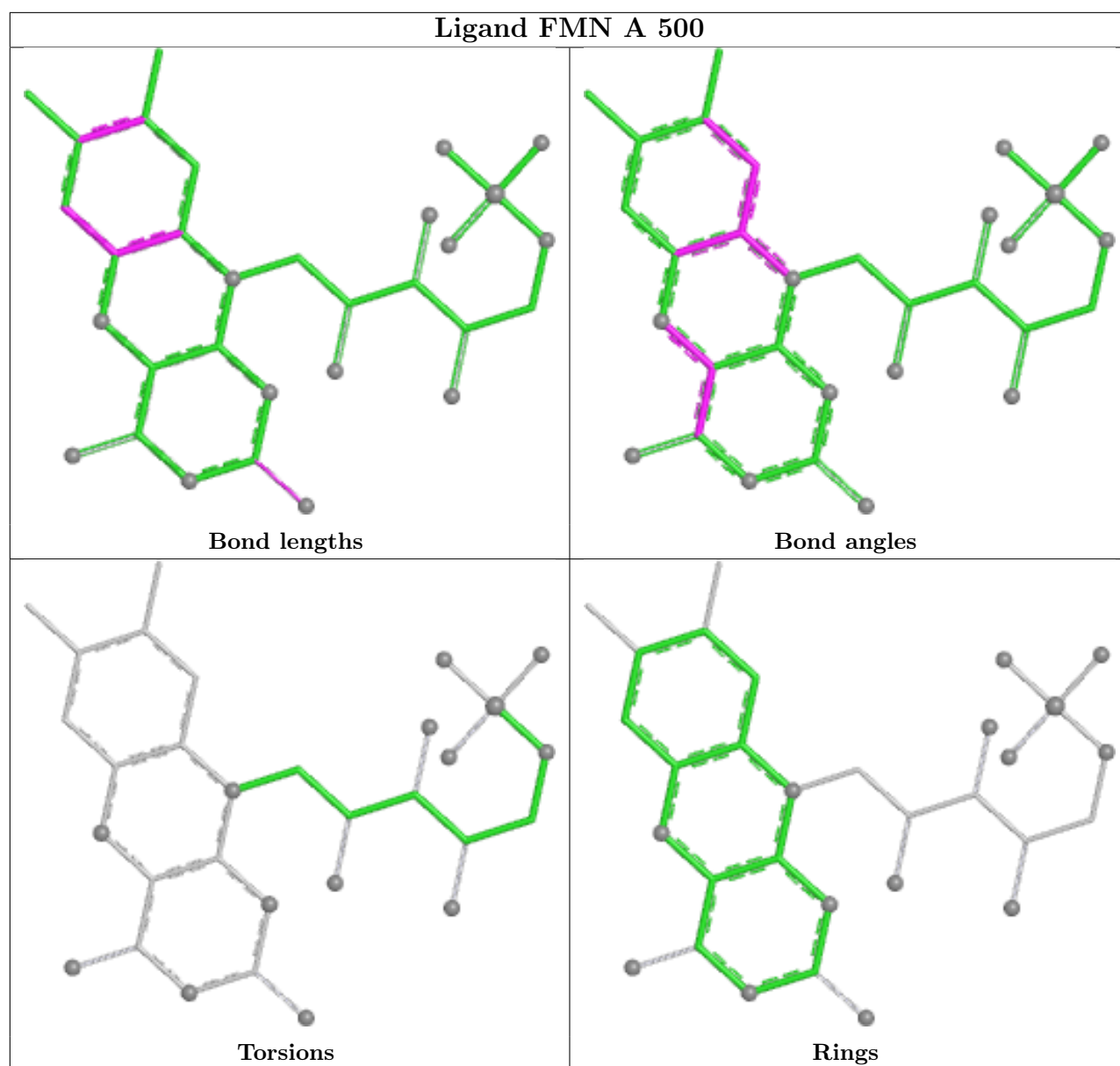
There are no ring outliers.

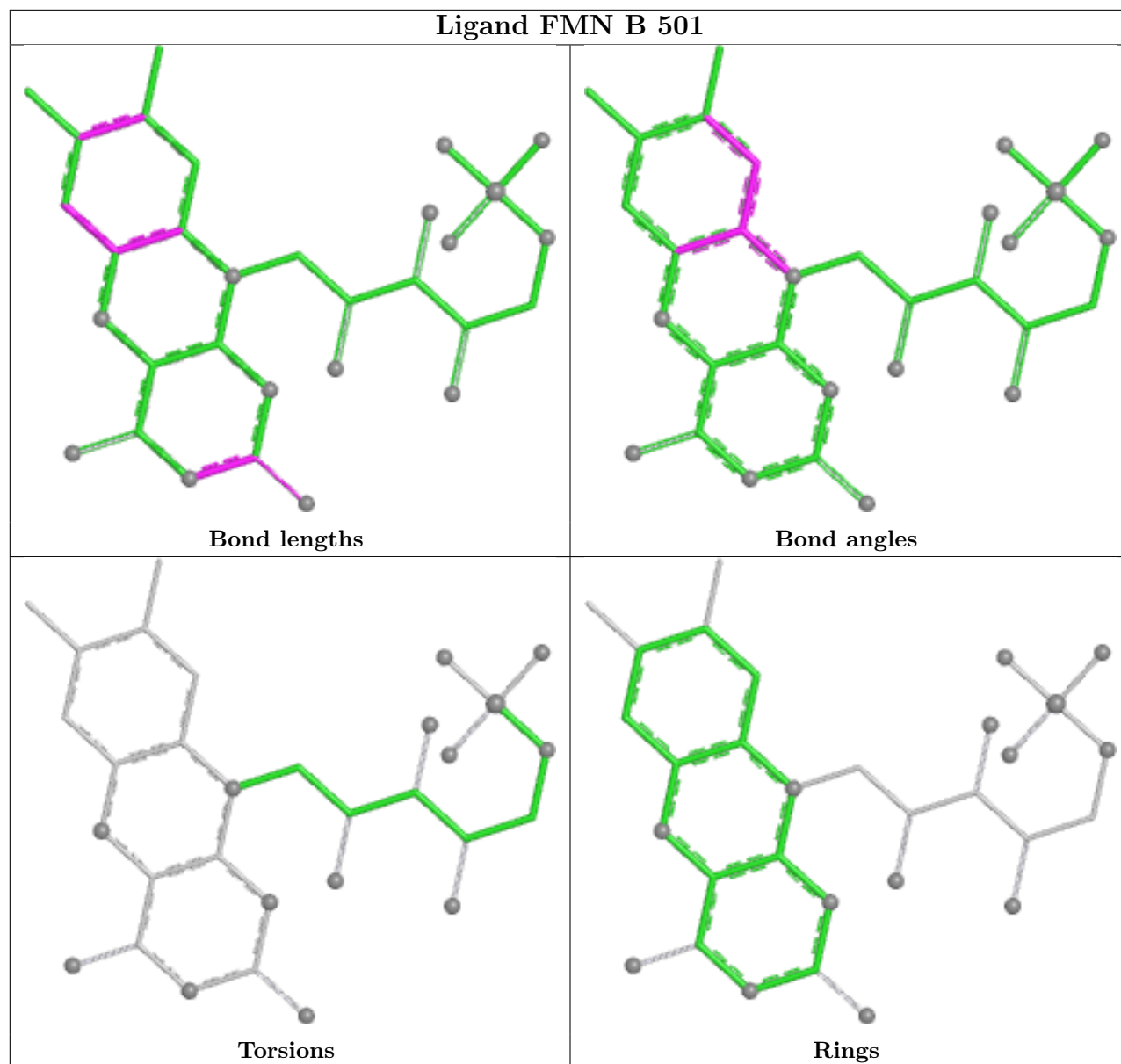
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	509	FMN	1	0

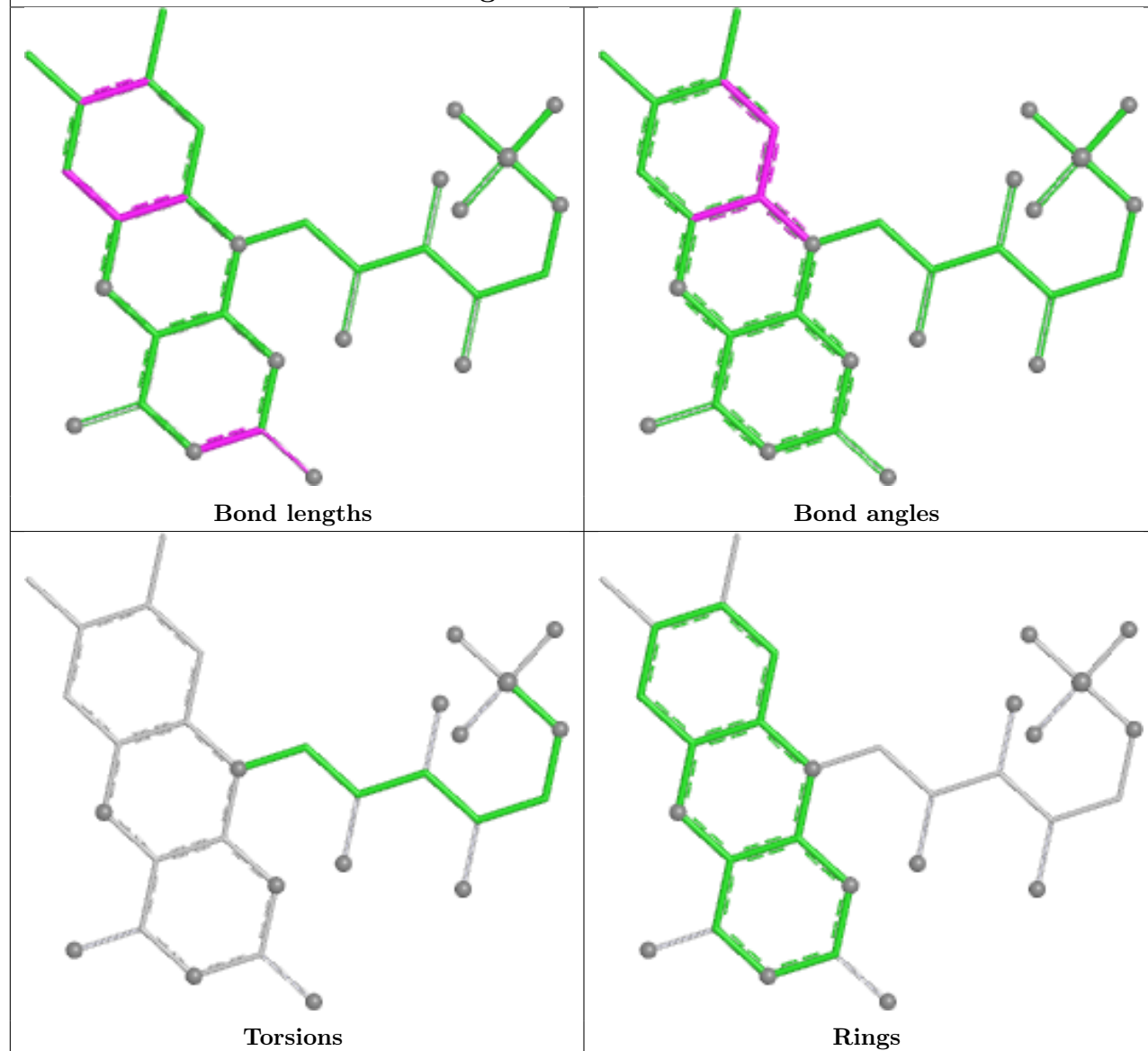
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

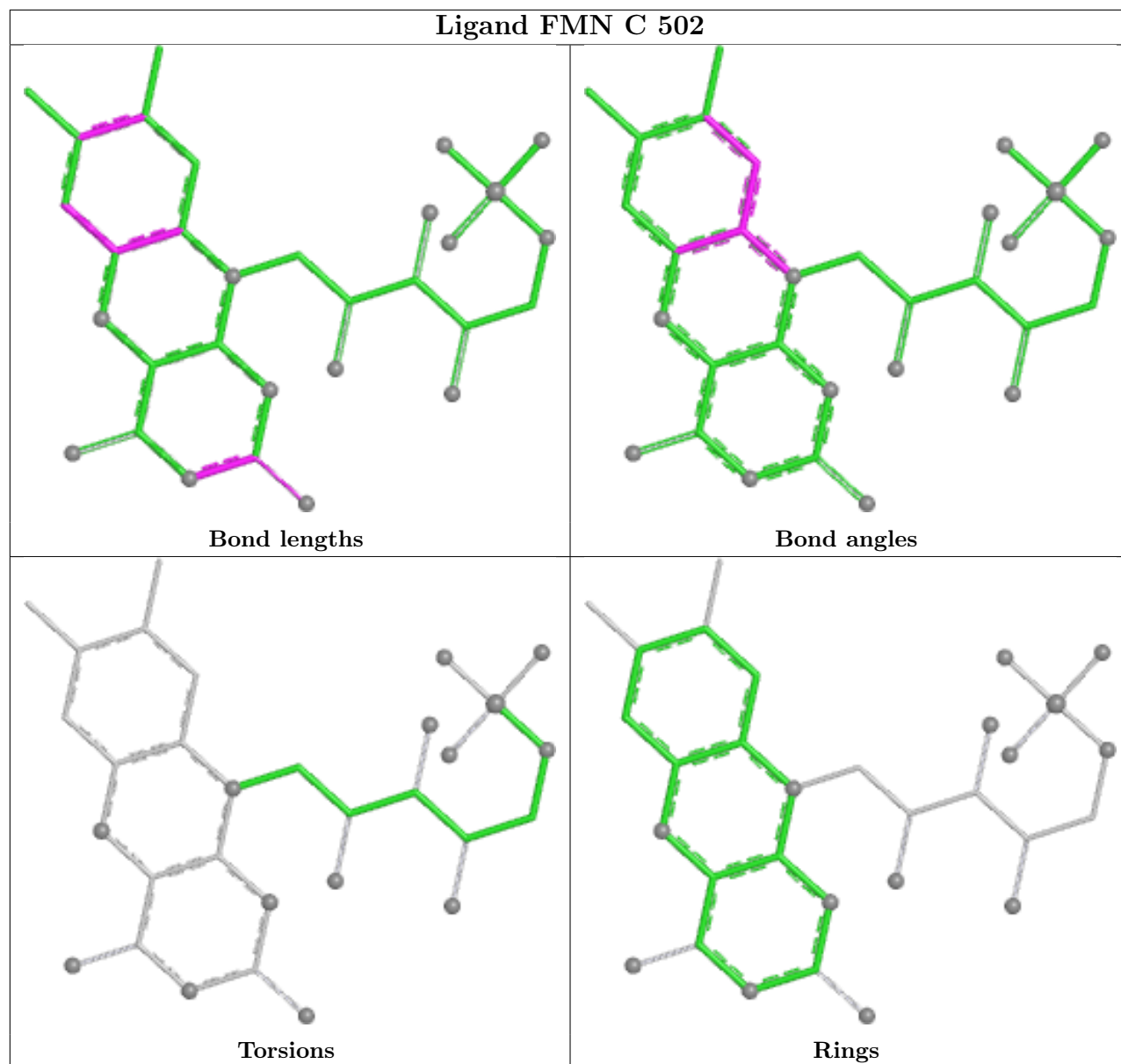


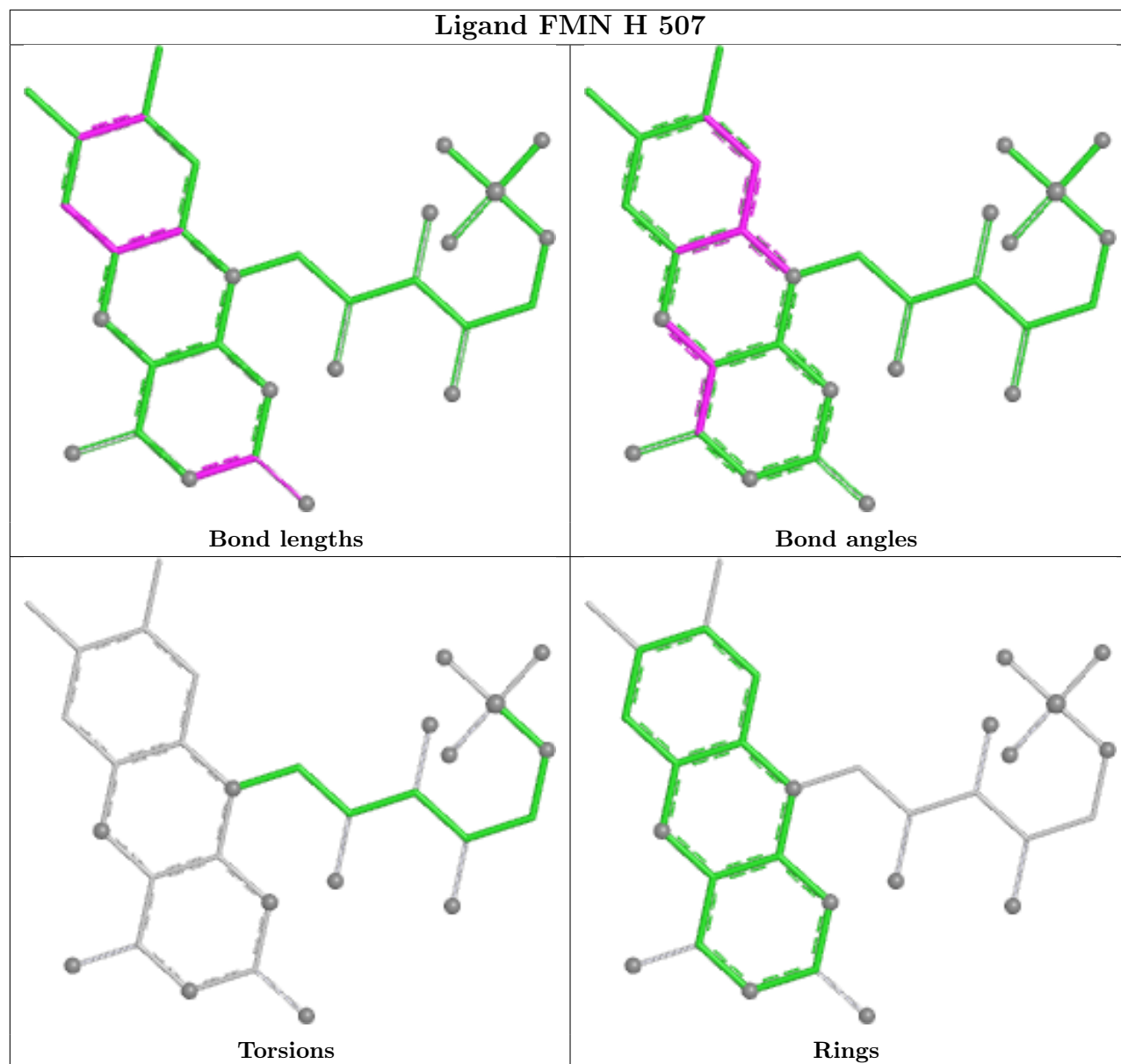


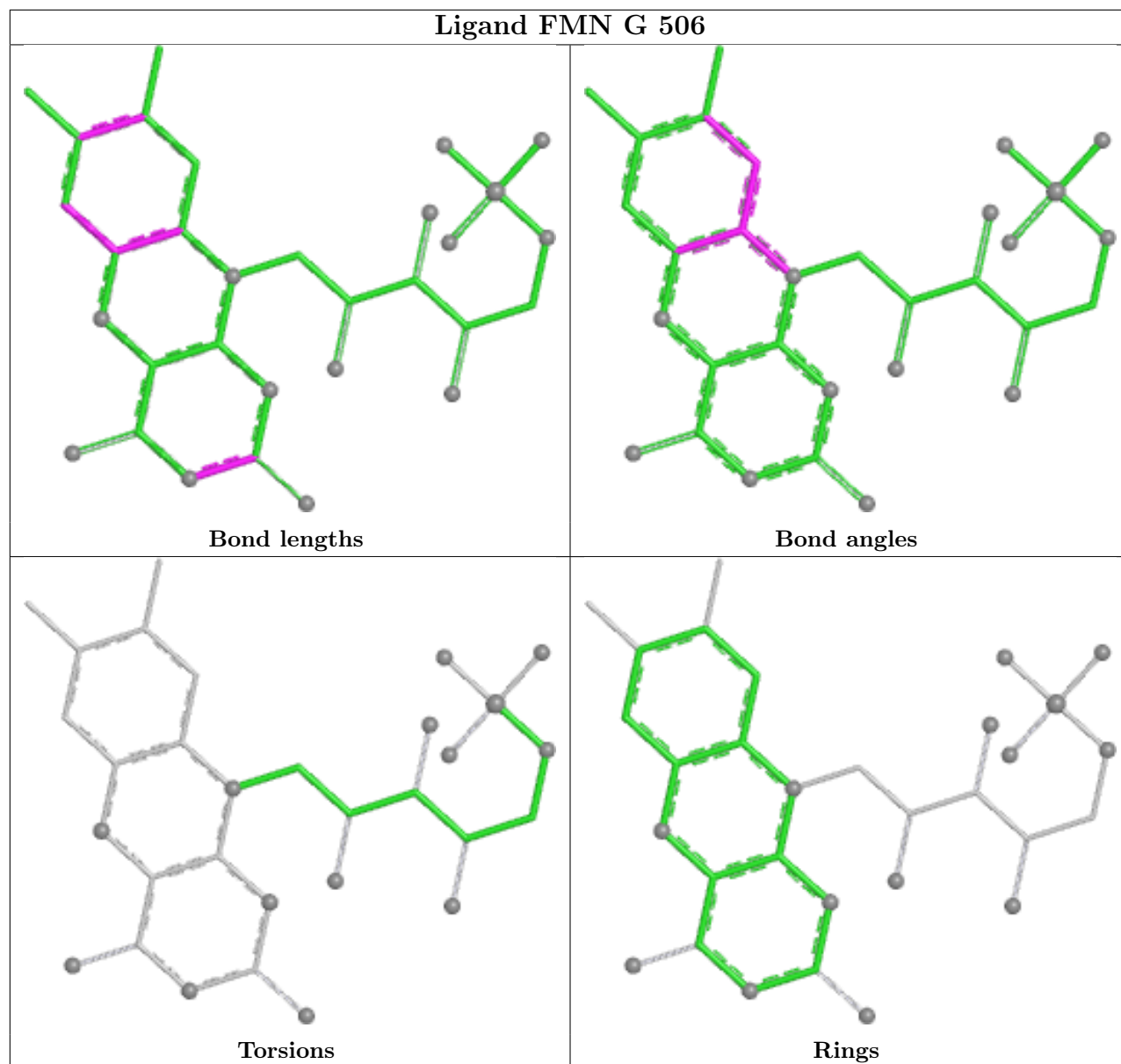


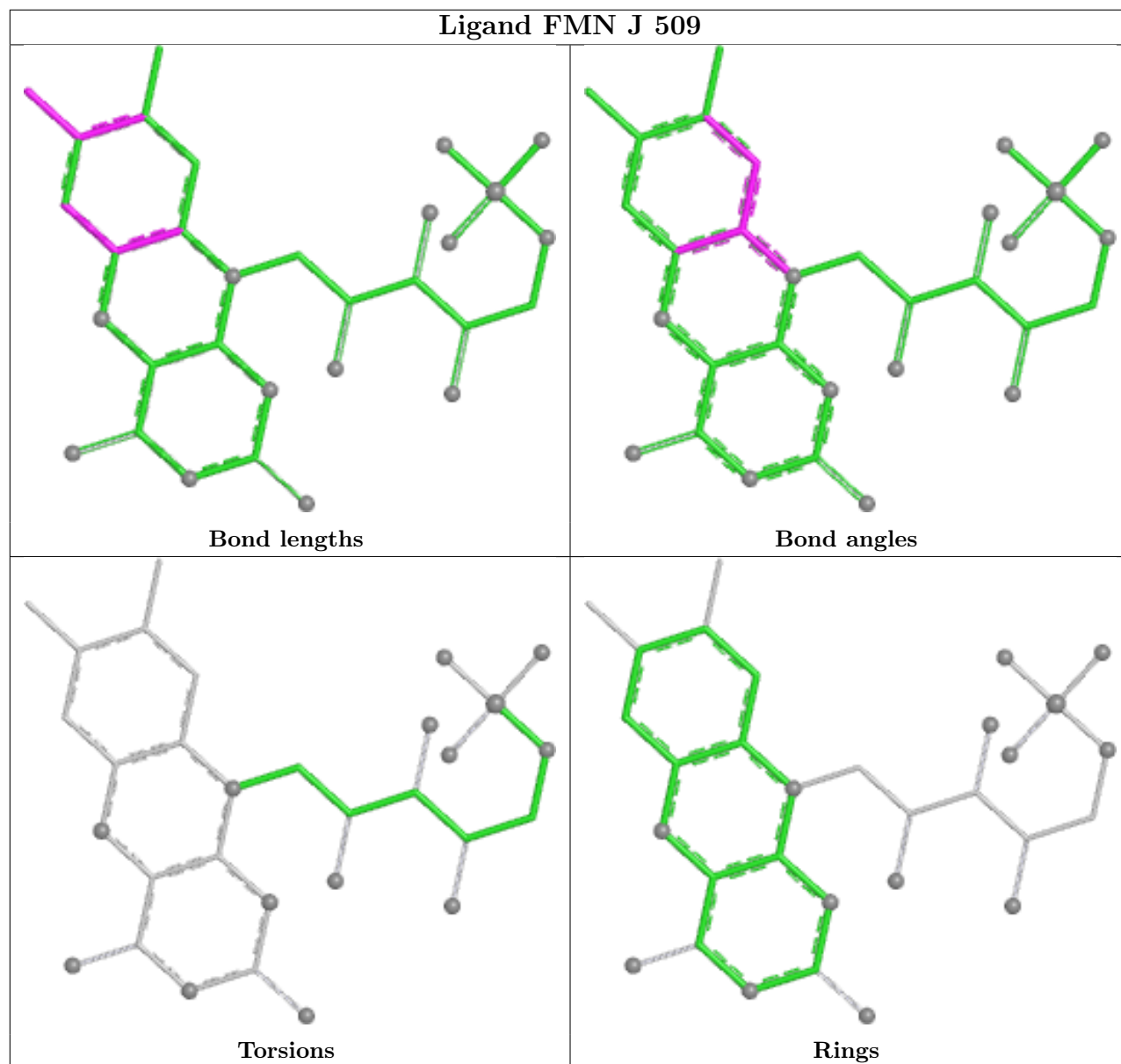
Ligand FMN I 508

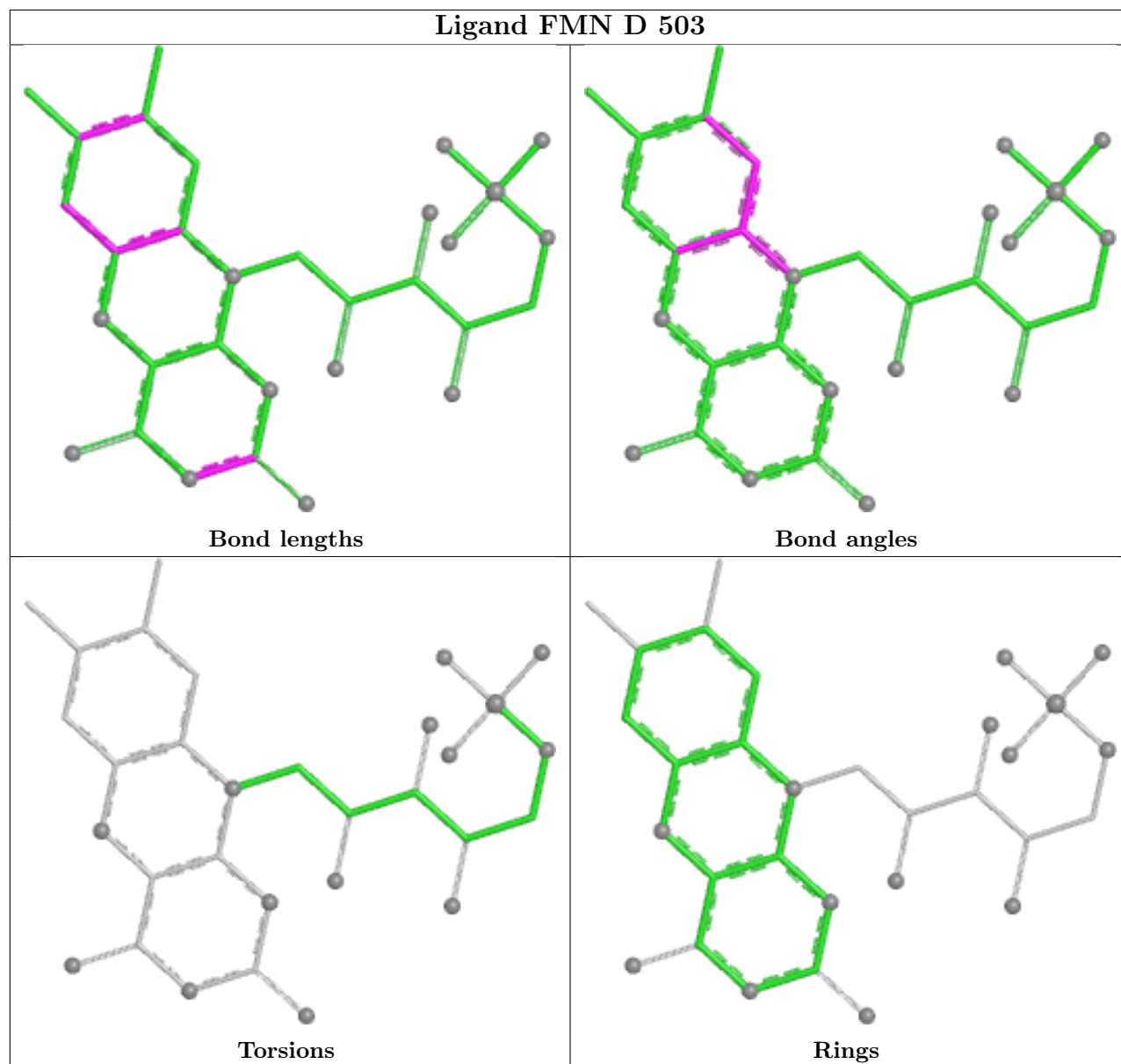


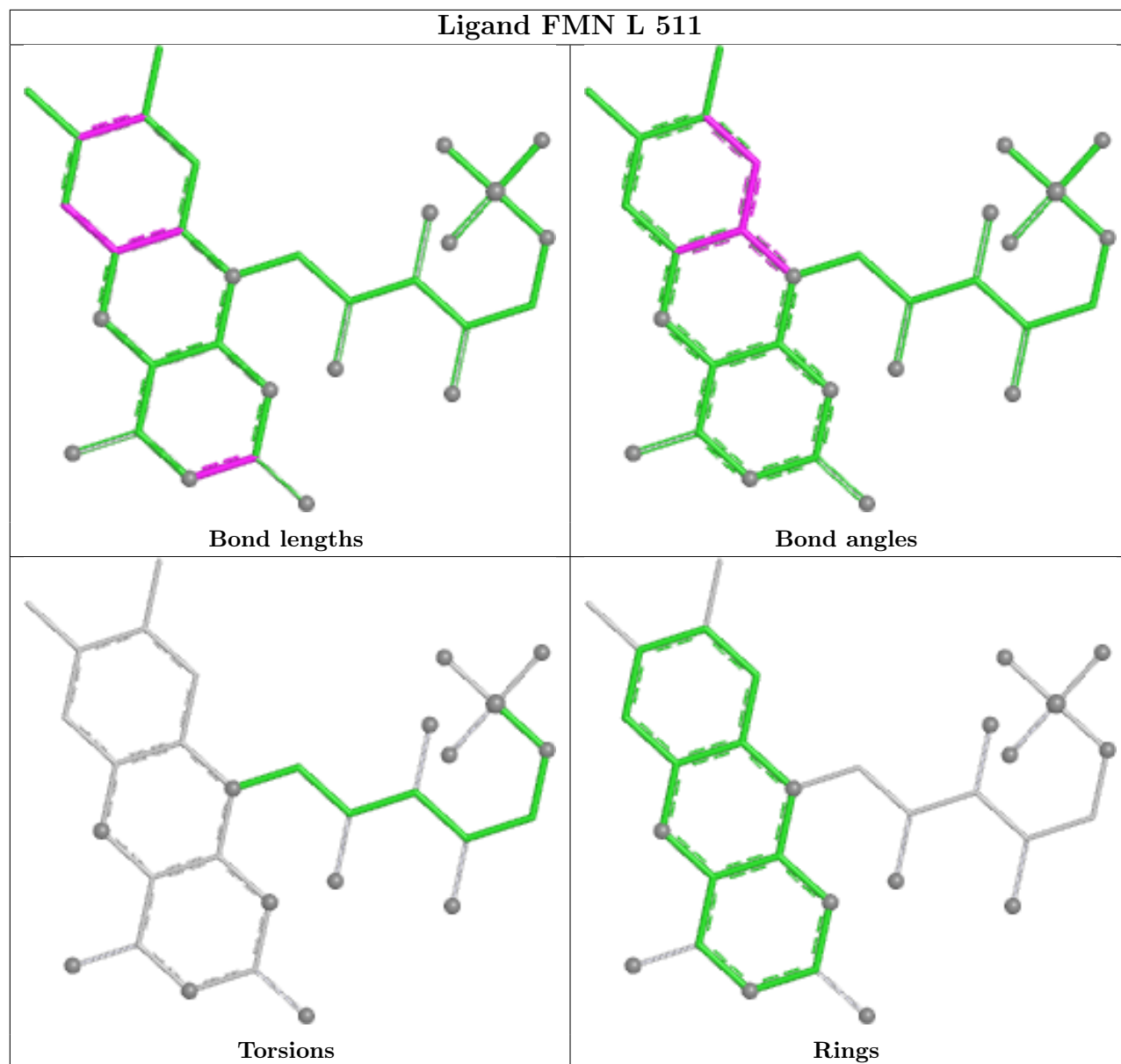


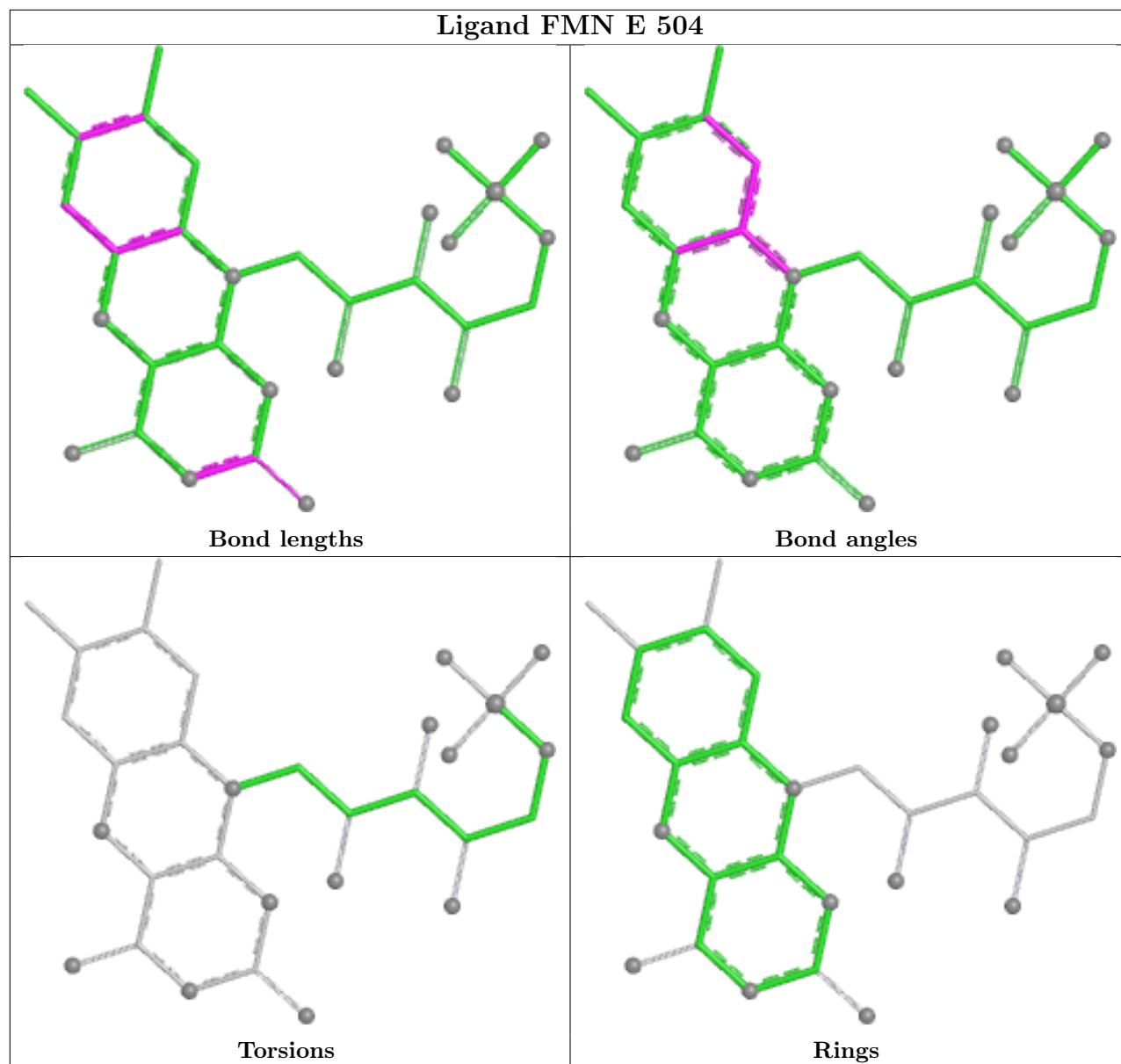


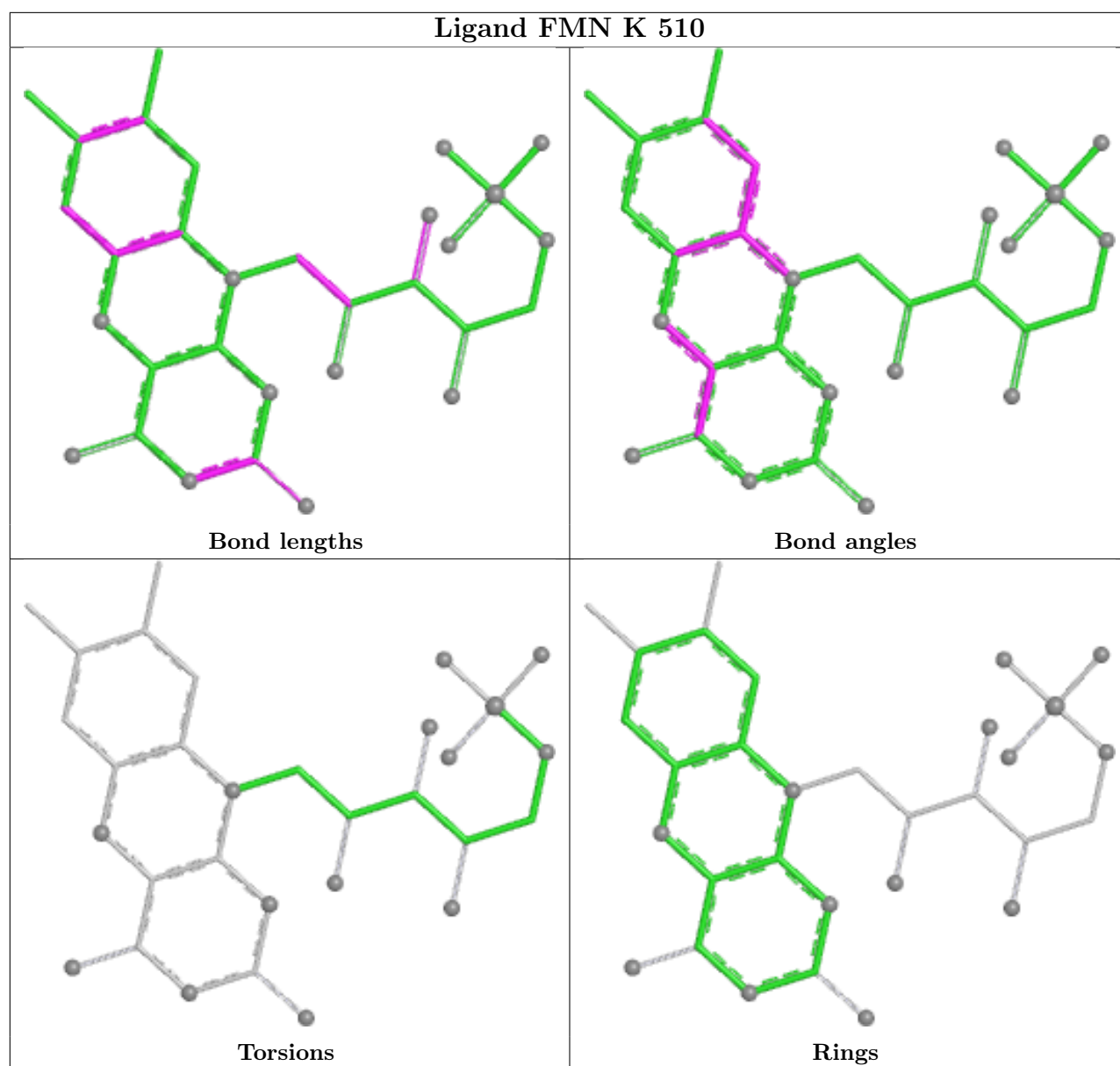












5.7 Other polymers [i](#)

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.