



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:19 AM UTC

PDB ID : 4V4C / pdb_00004v4c
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici*
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.35 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)
Xtriage (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

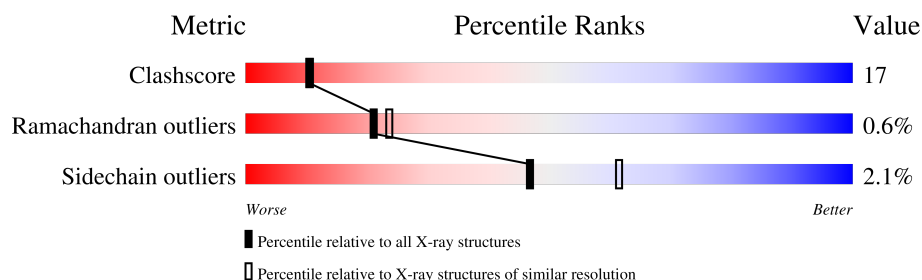
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

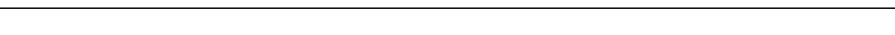
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	875	70% 27% .
1	C	875	66% 32% .
1	E	875	71% 27% .
1	G	875	69% 28% .
1	I	875	69% 29% .
1	K	875	70% 27% .
1	M	875	69% 28% .
1	O	875	68% 30% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	875	 70% 28% .
1	S	875	 69% 29% .
1	U	875	 67% 31% .
1	W	875	 64% 33% .
2	B	274	 64% 32% .
2	D	274	 63% 32% .
2	F	274	 64% 33% .
2	H	274	 62% 34% .
2	J	274	 65% 32% .
2	L	274	 56% 41% .
2	N	274	 65% 32% ..
2	P	274	 59% 38% .
2	R	274	 68% 29% .
2	T	274	 58% 38% .
2	V	274	 62% 35% .
2	X	274	 48% 48% .

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	ACT	C	901	-	-	X	-
3	ACT	E	901	-	-	X	-
3	ACT	G	901	-	-	X	-
3	ACT	I	901	-	-	X	-
3	ACT	K	901	-	-	X	-
3	ACT	O	901	-	-	X	-
3	ACT	W	901	-	-	X	-
7	SF4	B	303	-	-	X	-
7	SF4	D	303	-	-	X	-
7	SF4	D	304	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	H	304	-	-	X	-
7	SF4	J	303	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	L	304	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	302	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	P	304	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	R	304	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	T	304	-	-	X	-
7	SF4	V	303	-	-	X	-
7	SF4	X	302	-	-	X	-
7	SF4	X	303	-	-	X	-
7	SF4	X	304	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 122057 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 Pyrogallol hydroxytransferase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	C	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	E	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	G	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	I	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	K	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	M	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	O	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	Q	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	S	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	U	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	W	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P80563
C	1	MET	-	initiating methionine	UNP P80563
E	1	MET	-	initiating methionine	UNP P80563
G	1	MET	-	initiating methionine	UNP P80563
I	1	MET	-	initiating methionine	UNP P80563

Continued on next page...

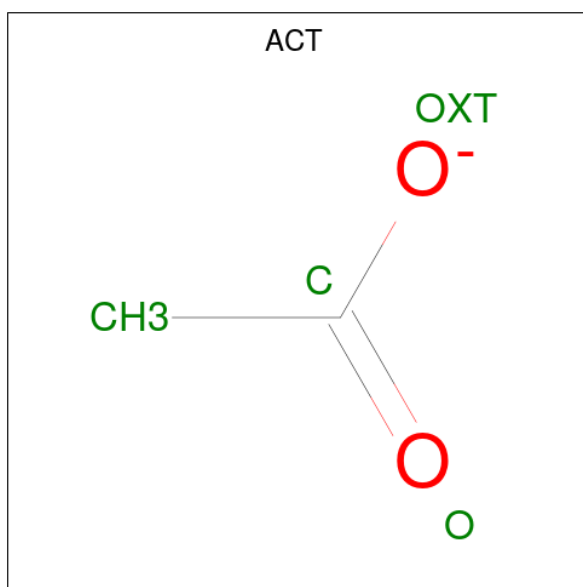
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	initiating methionine	UNP P80563
M	1	MET	-	initiating methionine	UNP P80563
O	1	MET	-	initiating methionine	UNP P80563
Q	1	MET	-	initiating methionine	UNP P80563
S	1	MET	-	initiating methionine	UNP P80563
U	1	MET	-	initiating methionine	UNP P80563
W	1	MET	-	initiating methionine	UNP P80563

- Molecule 2 is a protein called Pyrogallol hydroxytransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	D	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	F	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	H	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	J	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	L	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	N	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	P	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	R	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	T	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	V	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	X	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	M	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	S	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

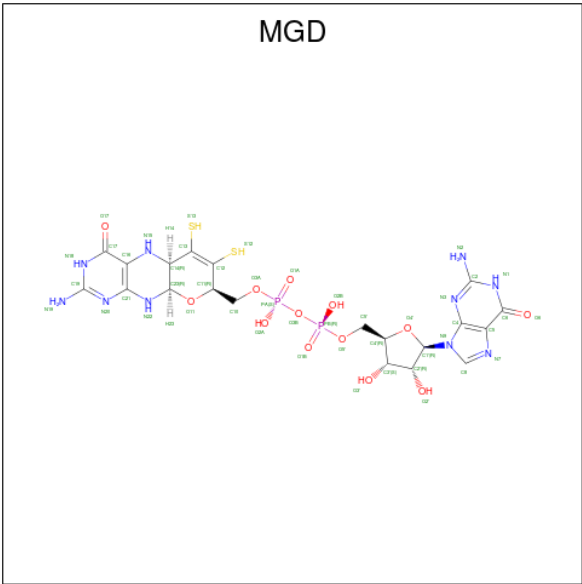
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0
4	N	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0
4	P	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	R	1	Total Ca 1 1	0	0
4	S	1	Total Ca 1 1	0	0
4	T	1	Total Ca 1 1	0	0
4	U	1	Total Ca 1 1	0	0
4	V	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	1	Total	Ca	0	0
			1	1		
4	X	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

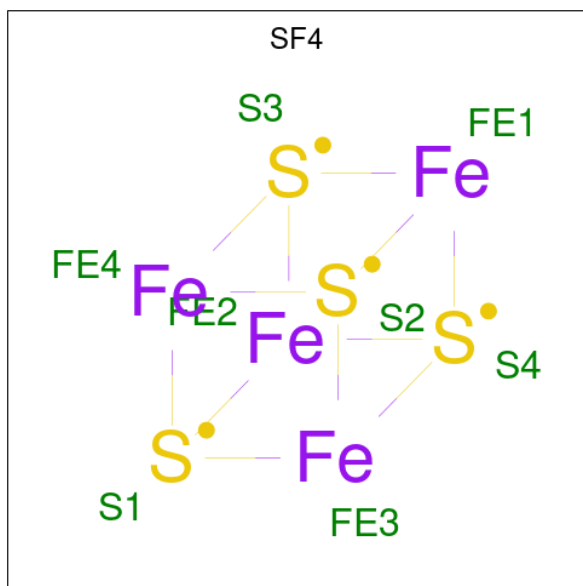
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Mo 1	0	0
6	C	1	Total 1	Mo 1	0	0
6	E	1	Total 1	Mo 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mo	0	0
			1	1		
6	I	1	Total	Mo	0	0
			1	1		
6	K	1	Total	Mo	0	0
			1	1		
6	M	1	Total	Mo	0	0
			1	1		
6	O	1	Total	Mo	0	0
			1	1		
6	Q	1	Total	Mo	0	0
			1	1		
6	S	1	Total	Mo	0	0
			1	1		
6	U	1	Total	Mo	0	0
			1	1		
6	W	1	Total	Mo	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	P	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	688	Total 688	O 688	0	0
8	B	167	Total 167	O 167	0	0
8	C	684	Total 684	O 684	0	0
8	D	167	Total 167	O 167	0	0
8	E	684	Total 684	O 684	0	0
8	F	167	Total 167	O 167	0	0

Continued on next page...

Continued from previous page...

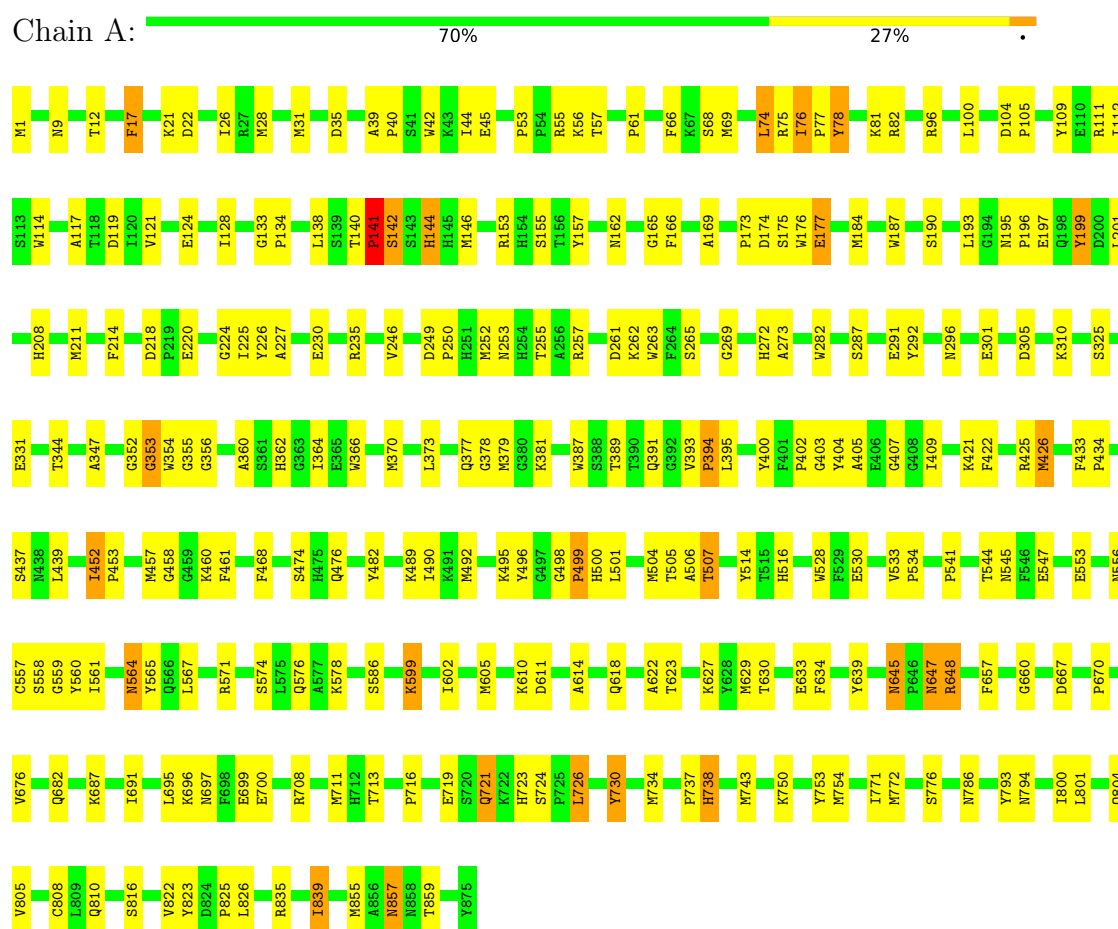
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	689	Total 689	O 689	0	0
8	H	162	Total 162	O 162	0	0
8	I	675	Total 675	O 675	0	0
8	J	170	Total 170	O 170	0	0
8	K	684	Total 684	O 684	0	0
8	L	168	Total 168	O 168	0	0
8	M	683	Total 683	O 683	0	0
8	N	163	Total 163	O 163	0	0
8	O	679	Total 679	O 679	0	0
8	P	163	Total 163	O 163	0	0
8	Q	692	Total 692	O 692	0	0
8	R	166	Total 166	O 166	0	0
8	S	675	Total 675	O 675	0	0
8	T	159	Total 159	O 159	0	0
8	U	667	Total 667	O 667	0	0
8	V	163	Total 163	O 163	0	0
8	W	677	Total 677	O 677	0	0
8	X	165	Total 165	O 165	0	0

3 Residue-property plots

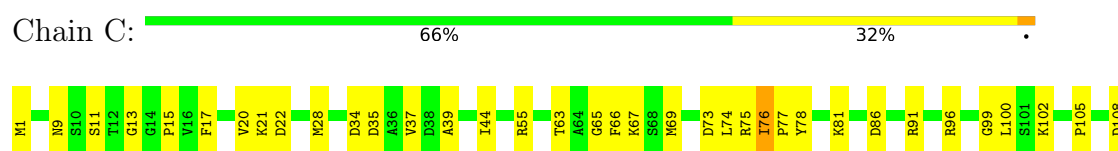
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

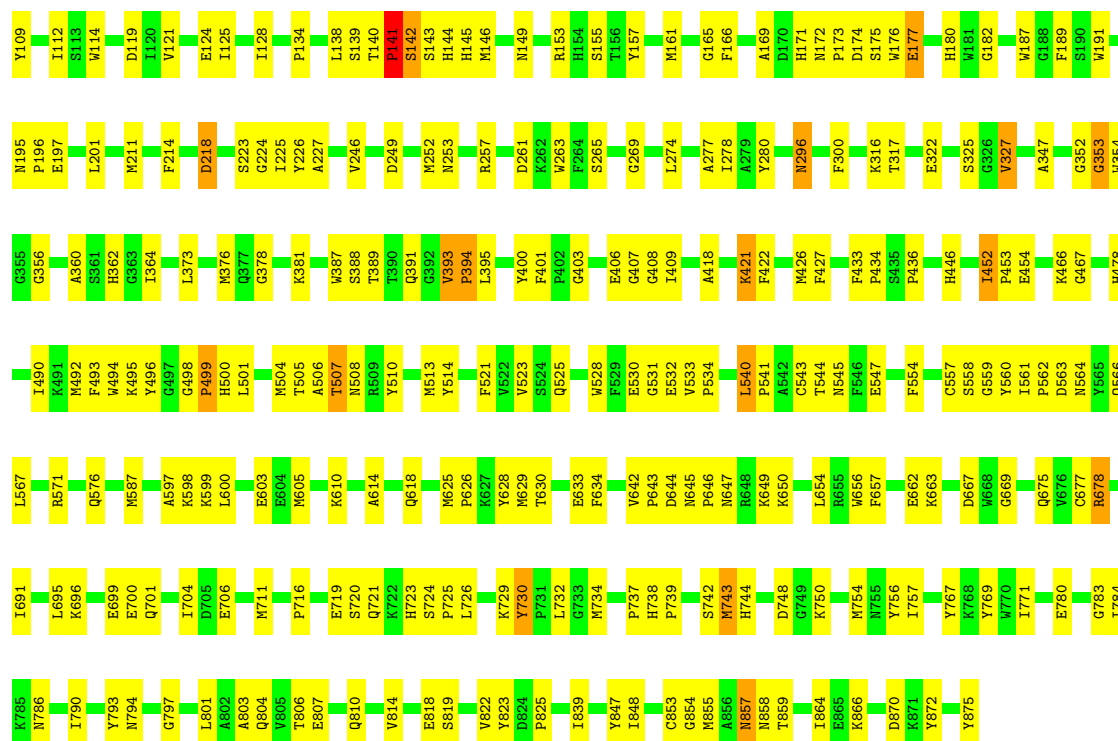
Note EDS was not executed.

• Molecule 1: Pyrogallol hydroxytransferase large subunit



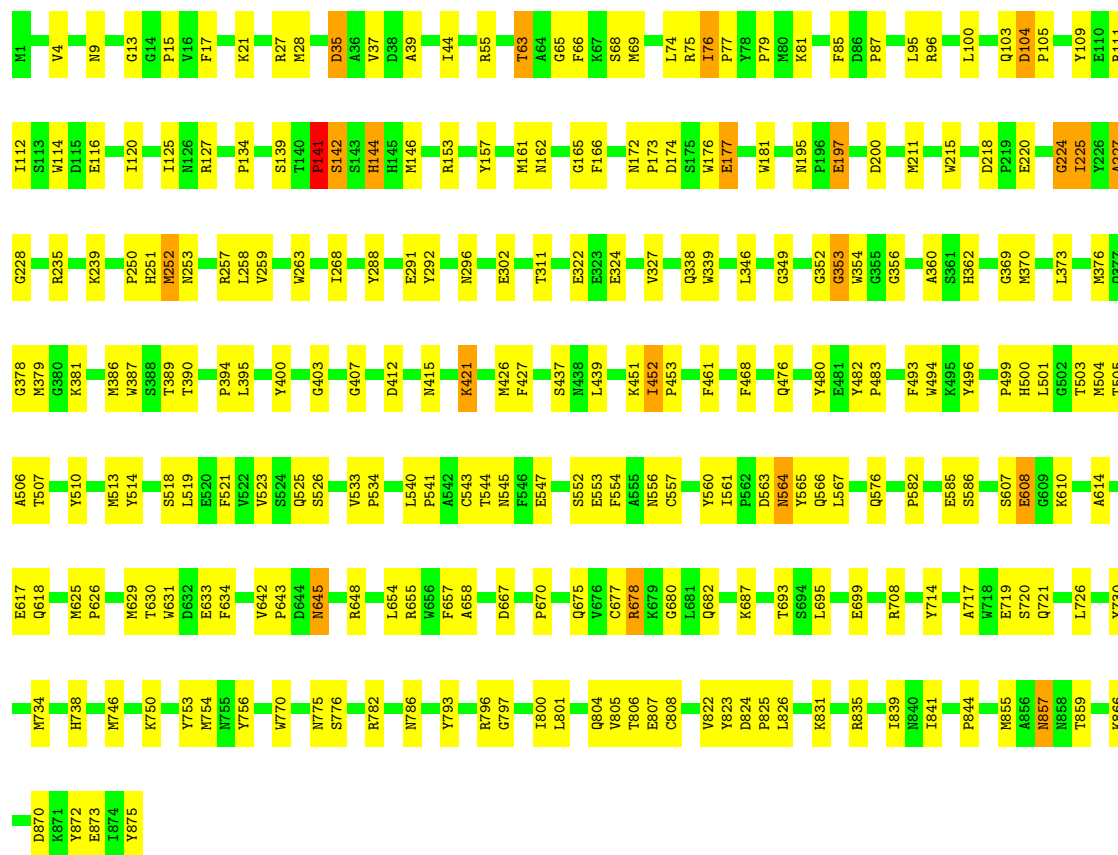
• Molecule 1: Pyrogallol hydroxytransferase large subunit



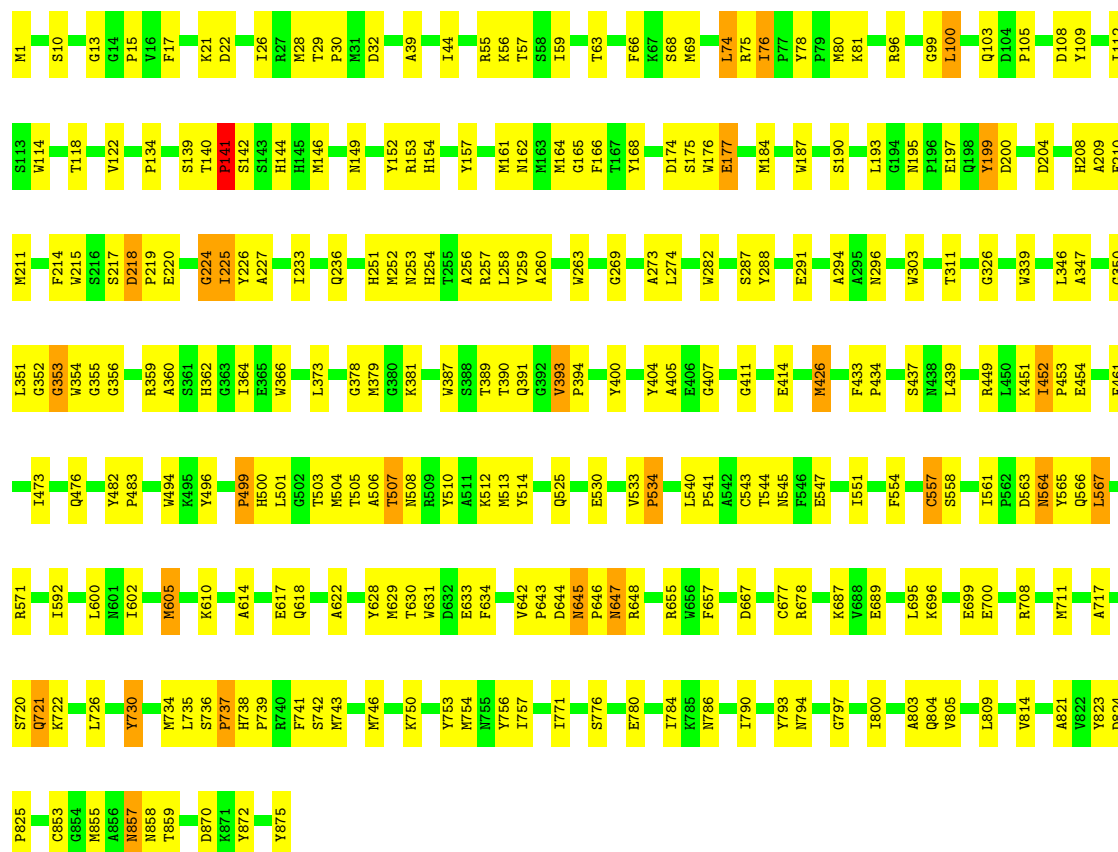


• Molecule 1: Pyrogallol hydroxytransferase large subunit

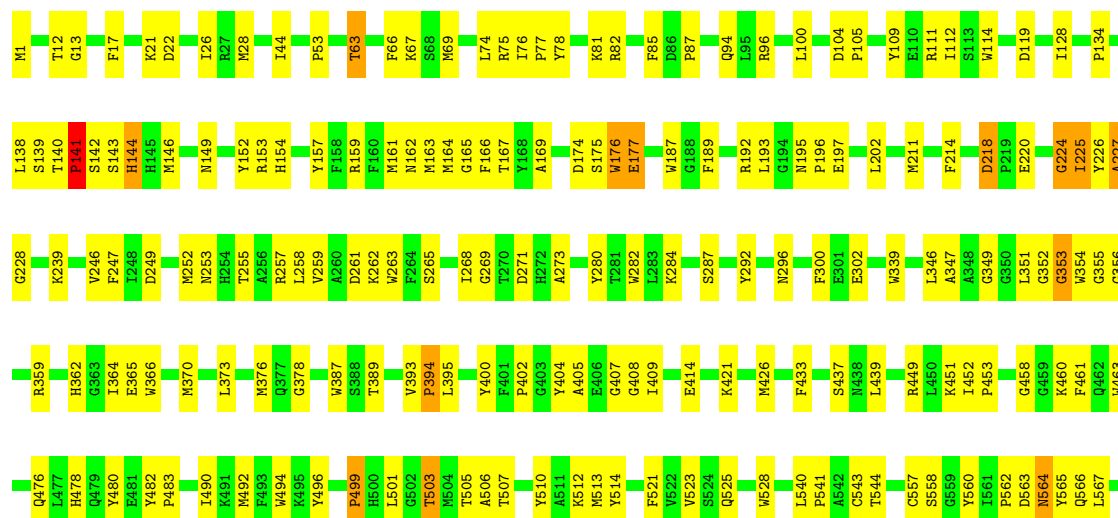
Chain E: 71% 27%

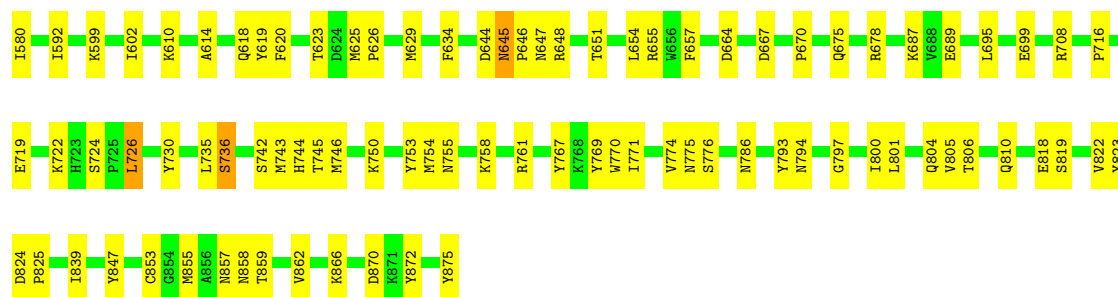


Chain G: 69% 28% .



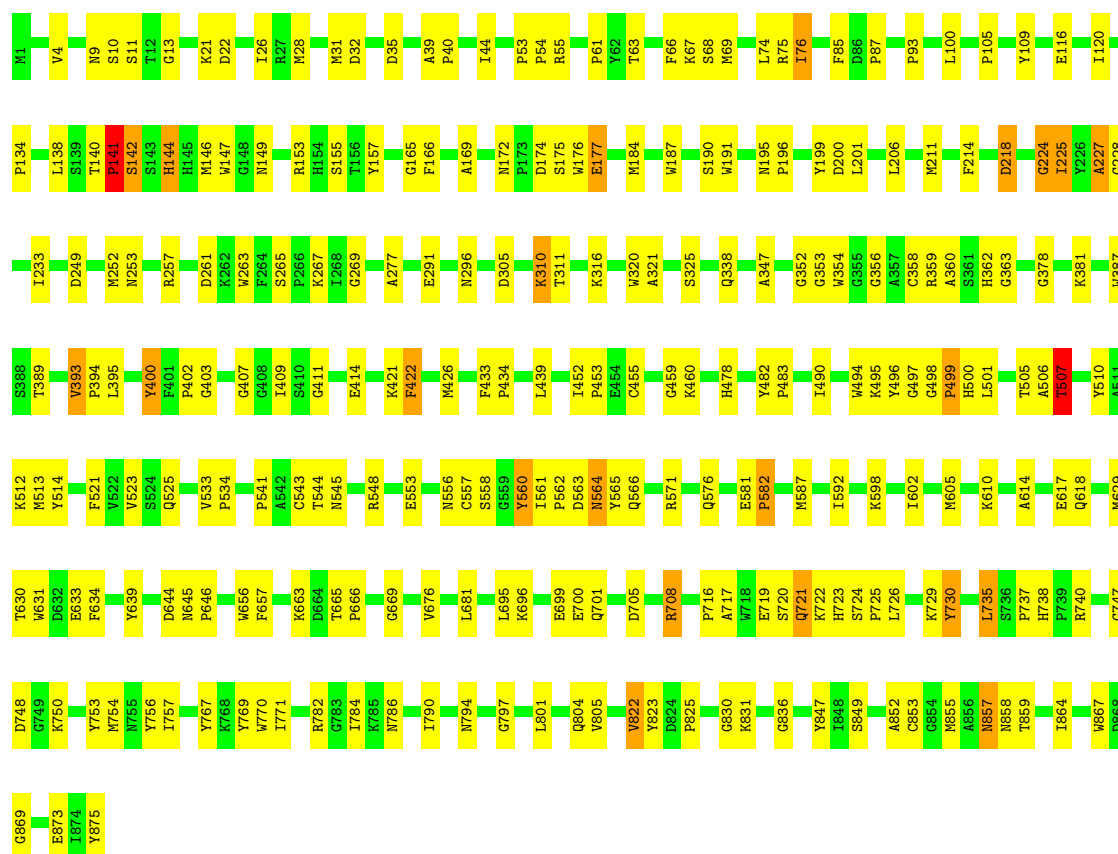
Chain I: 69% 29% .





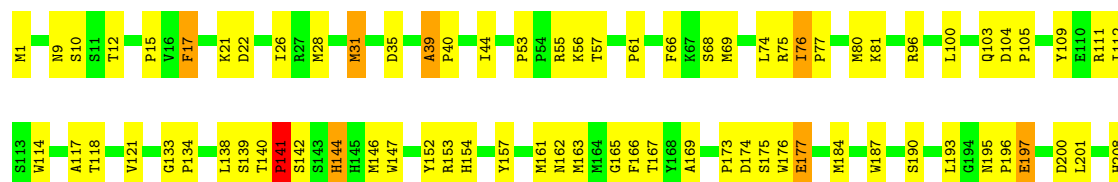
• Molecule 1: Pyrogallol hydroxytransferase large subunit

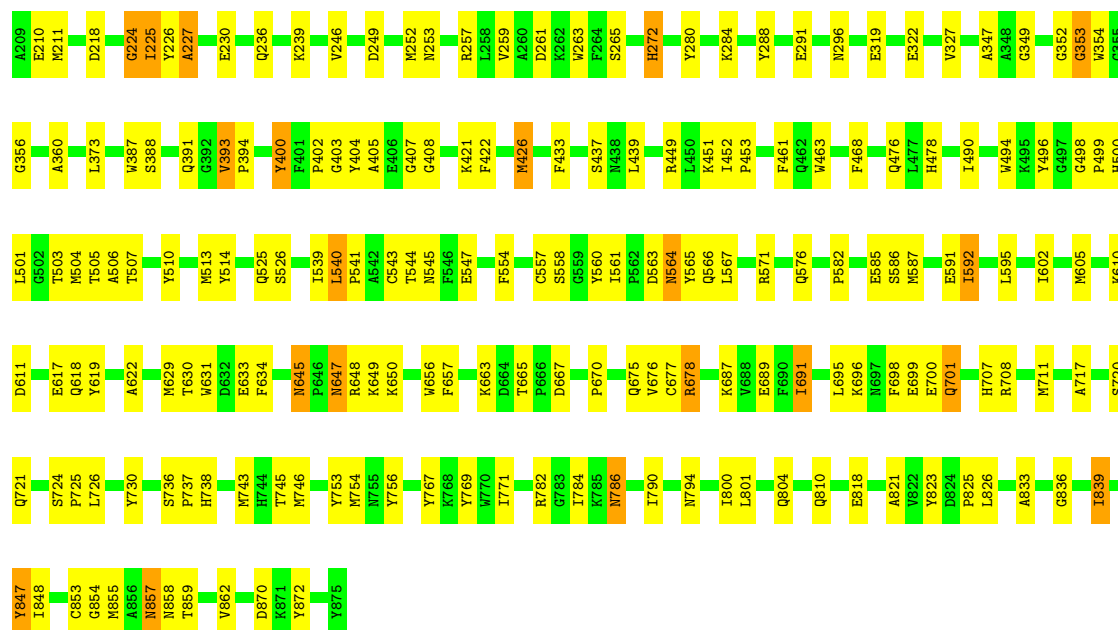
Chain K: 70% 27% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

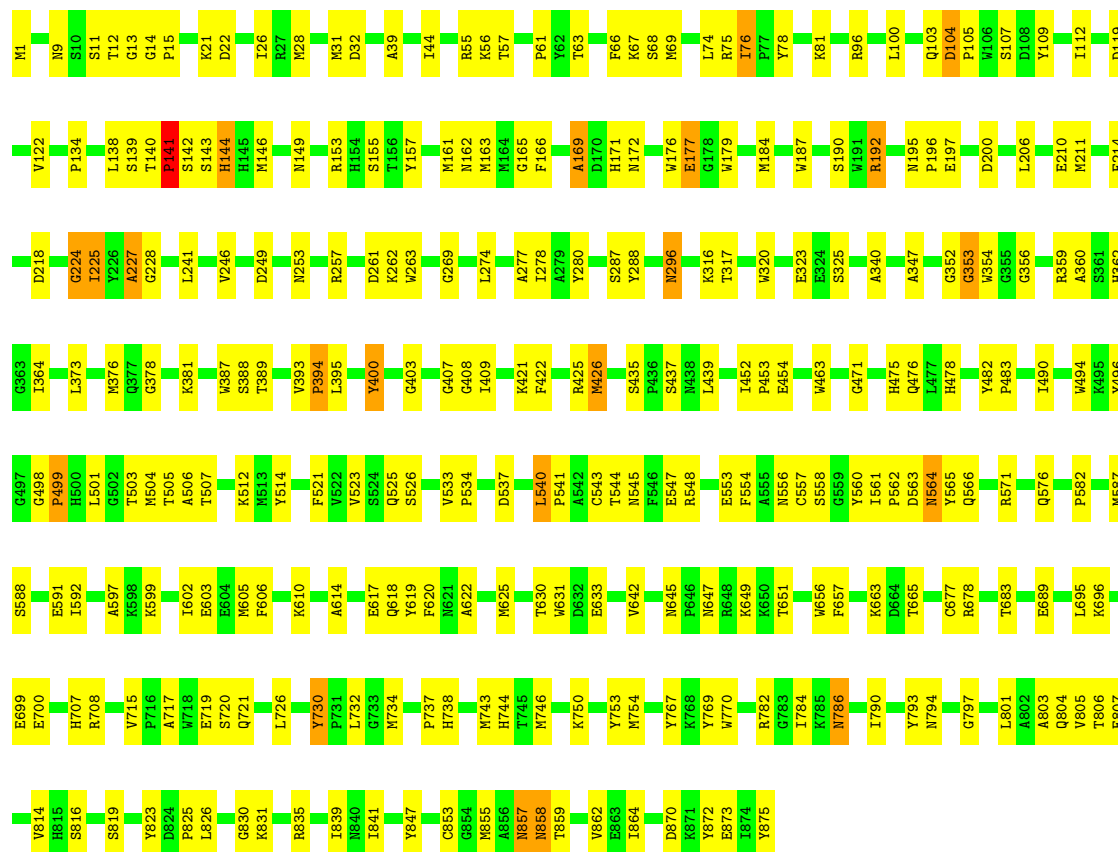
Chain M: 69% 28% .



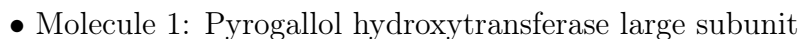


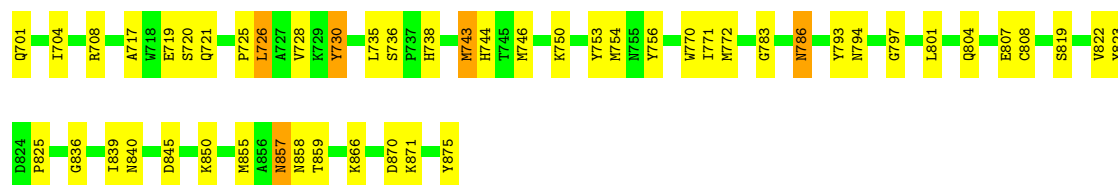
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O: 68% 30%



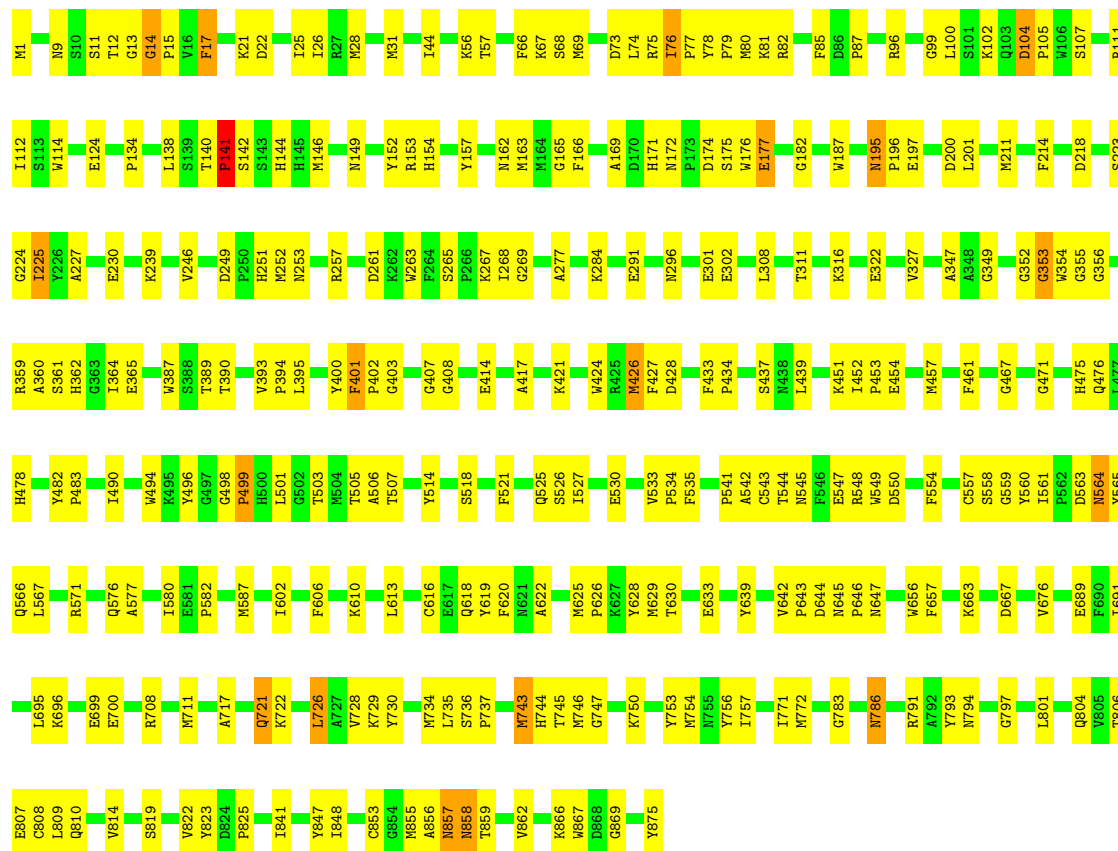
• Molecule 1: Pyrogallol hydroxytransferase large subunit





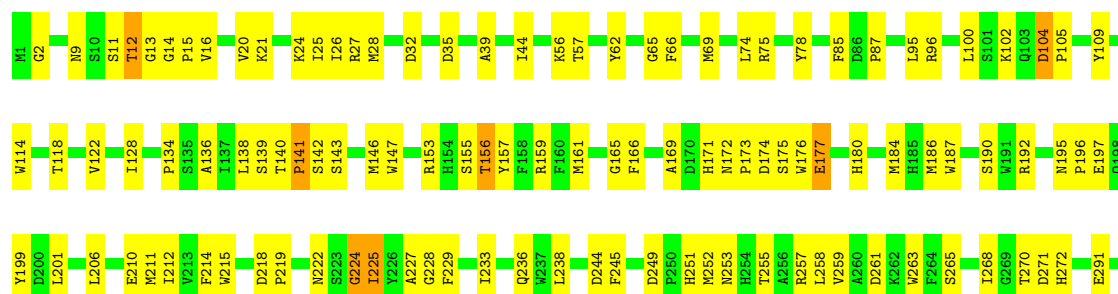
• Molecule 1: Pyrogallol hydroxytransferase large subunit

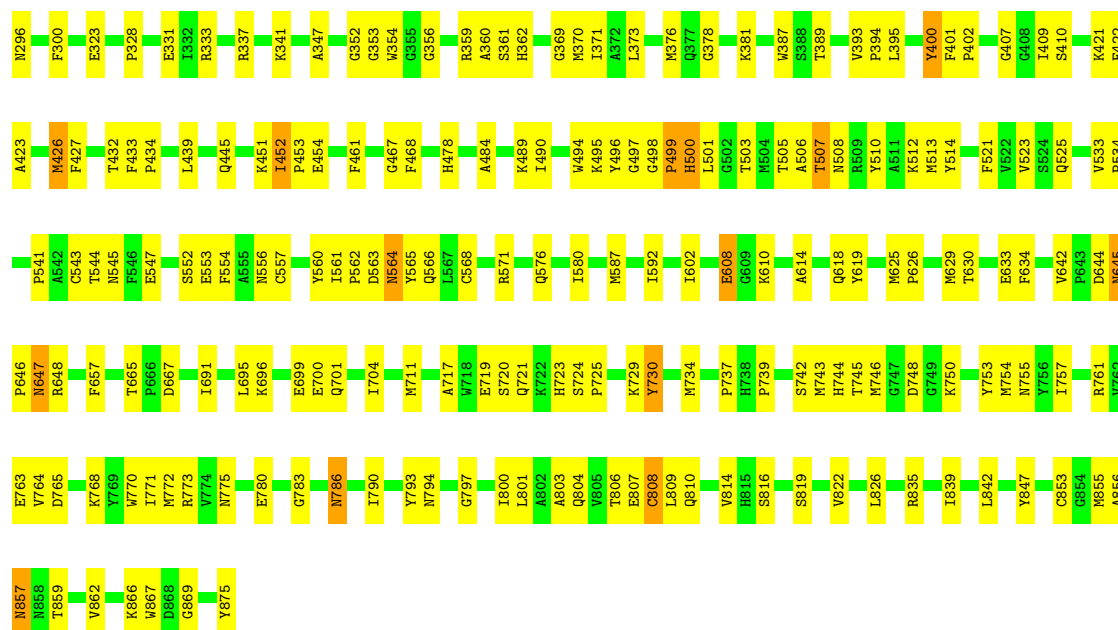
Chain U: 67% 31% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

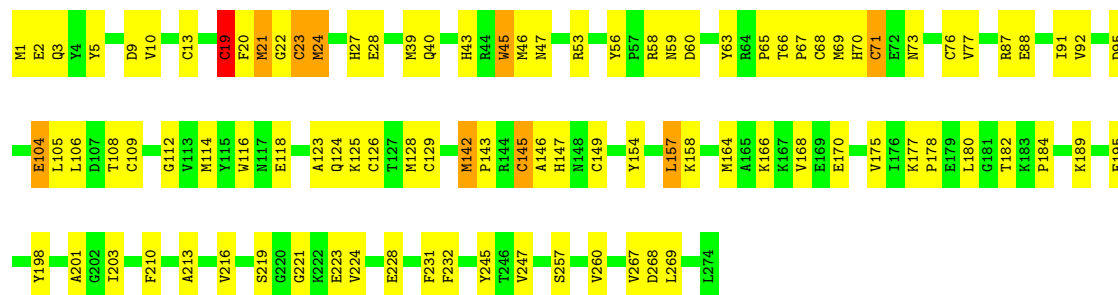
Chain W: 64% 33% .





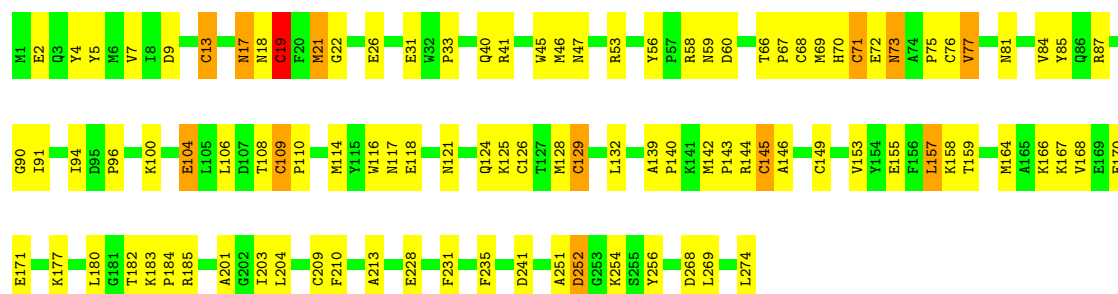
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B: 64% 32%



• Molecule 2: Pyrogallol hydroxytransferase small subunit

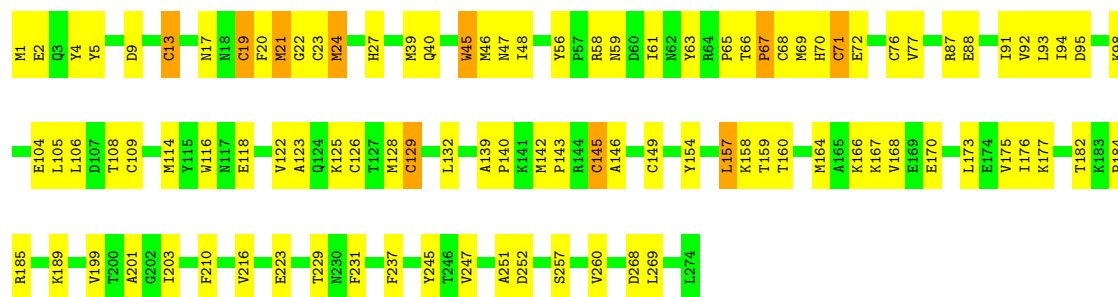
Chain D: 63% 32%



• Molecule 2: Pyrogallol hydroxytransferase small subunit

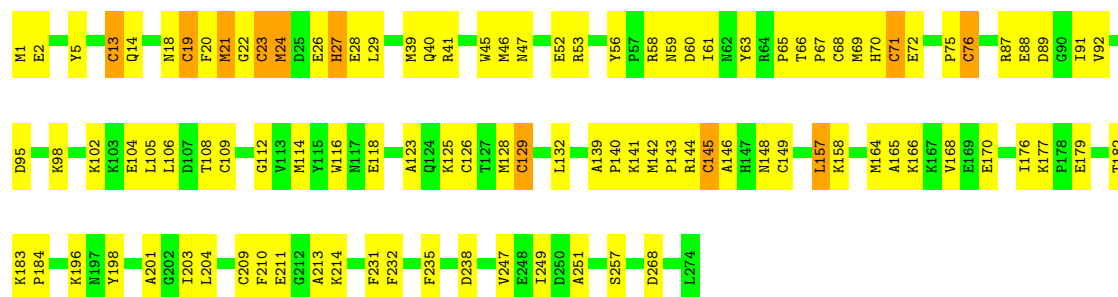
Chain F: 64% 33%





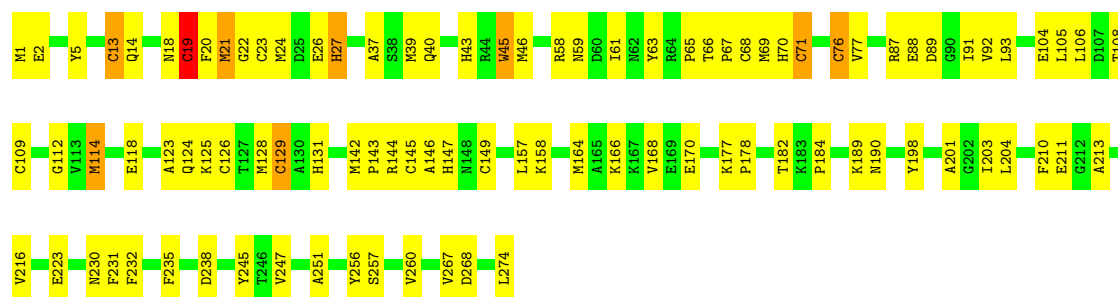
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H: 62% 34%



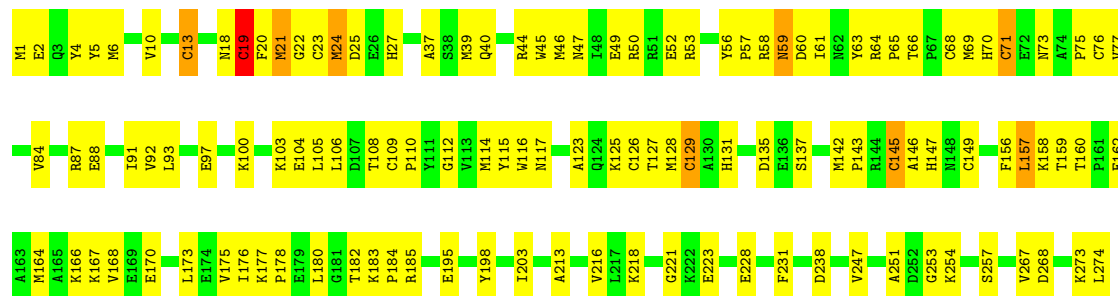
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J: 65% 32%



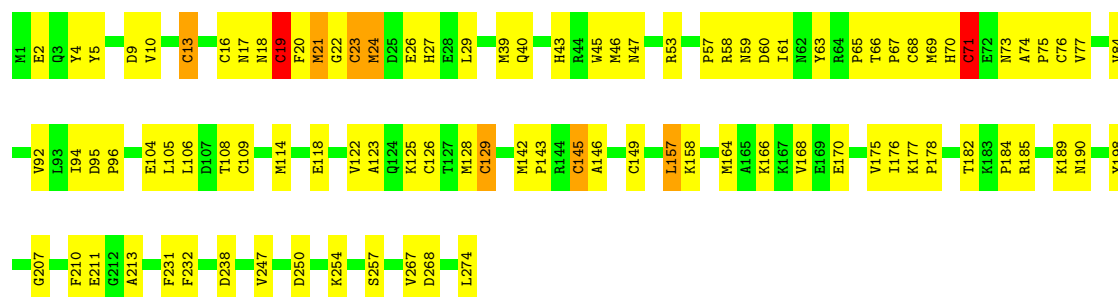
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L: 56% 41%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N:  65% 32% ..



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:  59% 38% .



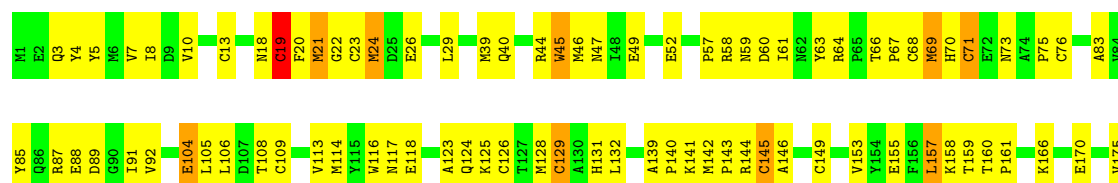
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:  68% 29% .



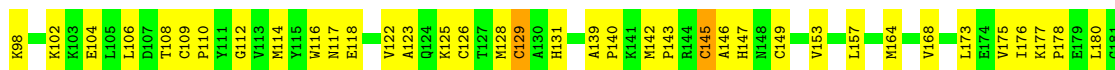
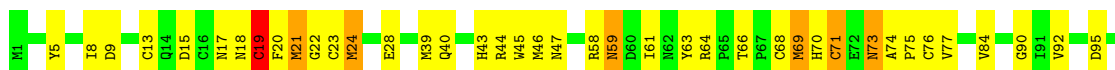
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T:  58% 38% .

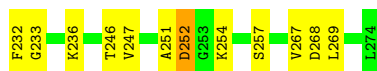
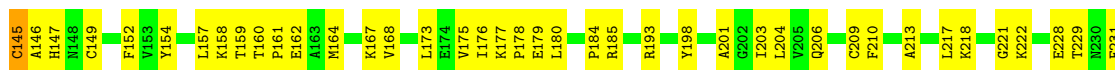
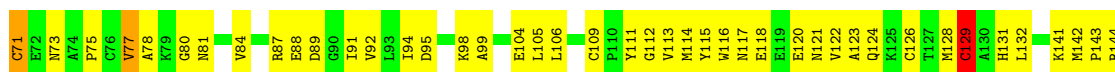
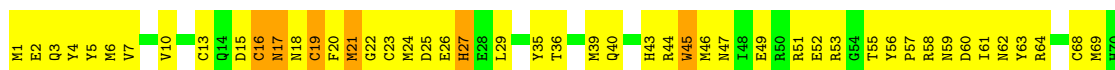




• Molecule 2: Pyrogallol hydroxytransferase small subunit



• Molecule 2: Pyrogallol hydroxytransferase small subunit



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	174.02Å 179.64Å 181.22Å 63.69° 63.98° 64.90°	Depositor
Resolution (Å)	24.98 – 2.35	Depositor
% Data completeness (in resolution range)	86.0 (24.98-2.35)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	122057	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: 4MO, CA, MGD, SF4, ACT

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	0.41	0/7240	0.98	47/9815 (0.5%)
1	C	0.39	0/7240	0.97	44/9815 (0.4%)
1	E	0.39	0/7240	0.97	34/9815 (0.3%)
1	G	0.40	0/7240	0.97	46/9815 (0.5%)
1	I	0.40	0/7240	0.96	39/9815 (0.4%)
1	K	0.41	0/7240	0.97	35/9815 (0.4%)
1	M	0.41	0/7240	0.98	51/9815 (0.5%)
1	O	0.40	0/7240	0.97	44/9815 (0.4%)
1	Q	0.41	0/7240	0.98	44/9815 (0.4%)
1	S	0.39	0/7240	0.96	34/9815 (0.3%)
1	U	0.39	0/7240	0.96	38/9815 (0.4%)
1	W	0.37	0/7240	0.95	32/9815 (0.3%)
2	B	0.45	1/2231 (0.0%)	0.97	10/3009 (0.3%)
2	D	0.37	0/2231	0.90	5/3009 (0.2%)
2	F	0.41	0/2231	0.91	5/3009 (0.2%)
2	H	0.41	0/2231	0.93	4/3009 (0.1%)
2	J	0.45	0/2231	0.94	6/3009 (0.2%)
2	L	0.40	0/2231	0.89	5/3009 (0.2%)
2	N	0.45	0/2231	0.96	10/3009 (0.3%)
2	P	0.40	0/2231	0.92	4/3009 (0.1%)
2	R	0.45	0/2231	0.98	9/3009 (0.3%)
2	T	0.37	0/2231	0.89	5/3009 (0.2%)
2	V	0.38	0/2231	0.92	7/3009 (0.2%)
2	X	0.34	0/2231	0.90	6/3009 (0.2%)
All	All	0.40	1/113652 (0.0%)	0.96	564/153888 (0.4%)

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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	MET	SD-CE	-5.90	1.64	1.79

The worst 5 of 564 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	353	GLY	N-CA-C	-9.95	99.91	111.85
1	Q	76	ILE	CA-C-N	9.88	129.52	119.24
1	Q	76	ILE	C-N-CA	9.88	129.52	119.24
2	P	77	VAL	N-CA-C	-9.37	102.73	111.45
1	C	353	GLY	N-CA-C	-9.33	100.66	111.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	847	TYR	Sidechain

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	7018	0	6645	201	0
1	C	7018	0	6645	217	0
1	E	7018	0	6645	188	0
1	G	7018	0	6645	216	0
1	I	7018	0	6645	199	0
1	K	7018	0	6645	208	0
1	M	7018	0	6645	203	0
1	O	7018	0	6645	215	0
1	Q	7018	0	6645	195	0
1	S	7018	0	6645	223	0
1	U	7018	0	6645	251	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	7018	0	6645	254	0
2	B	2182	0	2077	85	0
2	D	2182	0	2077	96	0
2	F	2182	0	2077	88	0
2	H	2182	0	2077	97	0
2	J	2182	0	2077	87	0
2	L	2182	0	2077	108	0
2	N	2182	0	2077	88	0
2	P	2182	0	2077	114	0
2	R	2182	0	2077	80	0
2	T	2182	0	2077	110	0
2	V	2182	0	2077	96	0
2	X	2182	0	2077	146	0
3	A	4	0	3	1	0
3	C	4	0	3	3	0
3	E	4	0	3	2	0
3	G	4	0	3	3	0
3	I	4	0	3	3	0
3	K	4	0	3	3	0
3	M	4	0	3	1	0
3	O	4	0	3	2	0
3	Q	4	0	3	1	0
3	S	4	0	3	1	0
3	U	4	0	3	1	0
3	W	4	0	3	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
5	A	94	0	44	12	0
5	C	94	0	44	11	0
5	E	94	0	44	8	0
5	G	94	0	44	10	0
5	I	94	0	44	12	0
5	K	94	0	44	10	0
5	M	94	0	44	11	0
5	O	94	0	44	10	0
5	Q	94	0	44	9	0
5	S	94	0	44	11	0
5	U	94	0	44	14	0
5	W	94	0	44	13	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	Q	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	1	0	0	0	0
7	B	24	0	0	3	0
7	D	24	0	0	5	0
7	F	24	0	0	3	0
7	H	24	0	0	5	0
7	J	24	0	0	3	0
7	L	24	0	0	6	0
7	N	24	0	0	4	0
7	P	24	0	0	6	0
7	R	24	0	0	5	0
7	T	24	0	0	7	0
7	V	24	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	24	0	0	7	0
8	A	688	0	0	20	0
8	B	167	0	0	5	0
8	C	684	0	0	18	0
8	D	167	0	0	4	0
8	E	684	0	0	22	0
8	F	167	0	0	1	0
8	G	689	0	0	19	0
8	H	162	0	0	6	0
8	I	675	0	0	20	0
8	J	170	0	0	3	0
8	K	684	0	0	25	0
8	L	168	0	0	9	0
8	M	683	0	0	16	0
8	N	163	0	0	6	0
8	O	679	0	0	21	0
8	P	163	0	0	6	0
8	Q	692	0	0	20	0
8	R	166	0	0	3	0
8	S	675	0	0	21	0
8	T	159	0	0	4	0
8	U	667	0	0	26	0
8	V	163	0	0	6	0
8	W	677	0	0	27	0
8	X	165	0	0	12	0
All	All	122057	0	105228	3673	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 17.

The worst 5 of 3673 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)
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.19	1.09
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.37	1.03
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.40	1.02
1:A:557:CYS:H	1:A:564:ASN:HD21	1.07	1.02
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.40	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	875/875 (100%)	821 (94%)	49 (6%)	5 (1%)	21	24
1	C	875/875 (100%)	804 (92%)	65 (7%)	6 (1%)	18	20
1	E	875/875 (100%)	807 (92%)	61 (7%)	7 (1%)	16	17
1	G	875/875 (100%)	820 (94%)	50 (6%)	5 (1%)	21	24
1	I	875/875 (100%)	816 (93%)	54 (6%)	5 (1%)	21	24
1	K	875/875 (100%)	813 (93%)	57 (6%)	5 (1%)	21	24
1	M	875/875 (100%)	814 (93%)	57 (6%)	4 (0%)	24	27
1	O	875/875 (100%)	819 (94%)	51 (6%)	5 (1%)	21	24
1	Q	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	14	14
1	S	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	14	14
1	U	875/875 (100%)	808 (92%)	63 (7%)	4 (0%)	24	27
1	W	875/875 (100%)	803 (92%)	65 (7%)	7 (1%)	16	17
2	B	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	30	34
2	D	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	30	34
2	F	272/274 (99%)	249 (92%)	22 (8%)	1 (0%)	30	34
2	H	272/274 (99%)	255 (94%)	16 (6%)	1 (0%)	30	34
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	L	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	N	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	34
2	P	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	30	34
2	R	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	30	34
2	T	272/274 (99%)	251 (92%)	20 (7%)	1 (0%)	30	34
2	V	272/274 (99%)	257 (94%)	13 (5%)	2 (1%)	18	20
2	X	272/274 (99%)	239 (88%)	30 (11%)	3 (1%)	11	11
All	All	13764/13788 (100%)	12807 (93%)	873 (6%)	84 (1%)	21	24

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU
1	G	177	GLU
1	G	225	ILE

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	731/729 (100%)	716 (98%)	15 (2%)	47	61
1	C	731/729 (100%)	722 (99%)	9 (1%)	63	77
1	E	731/729 (100%)	723 (99%)	8 (1%)	65	79
1	G	731/729 (100%)	719 (98%)	12 (2%)	55	70
1	I	731/729 (100%)	721 (99%)	10 (1%)	59	73
1	K	731/729 (100%)	721 (99%)	10 (1%)	59	73
1	M	731/729 (100%)	720 (98%)	11 (2%)	57	72
1	O	731/729 (100%)	718 (98%)	13 (2%)	51	66
1	Q	731/729 (100%)	718 (98%)	13 (2%)	51	66
1	S	731/729 (100%)	722 (99%)	9 (1%)	63	77
1	U	731/729 (100%)	723 (99%)	8 (1%)	65	79
1	W	731/729 (100%)	724 (99%)	7 (1%)	68	81
2	B	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	D	235/235 (100%)	222 (94%)	13 (6%)	19	24
2	F	235/235 (100%)	223 (95%)	12 (5%)	21	26
2	H	235/235 (100%)	222 (94%)	13 (6%)	19	24
2	J	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	L	235/235 (100%)	224 (95%)	11 (5%)	23	30
2	N	235/235 (100%)	223 (95%)	12 (5%)	21	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	235/235 (100%)	226 (96%)	9 (4%)	29	39
2	R	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	T	235/235 (100%)	223 (95%)	12 (5%)	21	26
2	V	235/235 (100%)	224 (95%)	11 (5%)	23	30
2	X	235/235 (100%)	225 (96%)	10 (4%)	26	34
All	All	11592/11568 (100%)	11334 (98%)	258 (2%)	47	59

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	19	CYS
2	V	129	CYS
1	I	564	ASN
1	I	499	PRO
1	W	560[A]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 278 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	162	ASN
1	U	525	GLN
1	W	478	HIS
1	I	415	ASN
1	I	154	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 108 ligands modelled in this entry, 36 are monoatomic - leaving 72 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	S	901	6	3,3,3	1.27	0	3,3,3	1.02	0
7	SF4	R	304	2	0,12,12	-	-	-		
3	ACT	I	901	6	3,3,3	1.18	0	3,3,3	0.97	0
5	MGD	E	904	6	47,52,52	2.40	14 (29%)	58,81,81	1.10	2 (3%)
5	MGD	Q	904	6	47,52,52	2.21	14 (29%)	58,81,81	1.23	3 (5%)
3	ACT	E	901	6	3,3,3	1.17	0	3,3,3	1.17	0
5	MGD	W	904	6	47,52,52	2.25	14 (29%)	58,81,81	1.12	3 (5%)
5	MGD	M	904	6	47,52,52	2.30	14 (29%)	58,81,81	1.27	2 (3%)
7	SF4	X	303	2	0,12,12	-	-	-		
3	ACT	U	901	6	3,3,3	1.31	0	3,3,3	0.95	0
7	SF4	R	302	2	0,12,12	-	-	-		
5	MGD	C	904	6	47,52,52	2.34	14 (29%)	58,81,81	1.09	3 (5%)
5	MGD	G	903	6	47,52,52	2.18	14 (29%)	58,81,81	2.14	9 (15%)
5	MGD	I	904	6	47,52,52	2.19	13 (27%)	58,81,81	1.66	5 (8%)
3	ACT	W	901	6	3,3,3	1.31	0	3,3,3	0.82	0
7	SF4	F	304	2	0,12,12	-	-	-		
7	SF4	V	303	2	0,12,12	-	-	-		
7	SF4	H	304	2	0,12,12	-	-	-		
7	SF4	N	304	2	0,12,12	-	-	-		
7	SF4	V	304	2	0,12,12	-	-	-		
7	SF4	N	302	2	0,12,12	-	-	-		
7	SF4	B	304	2	0,12,12	-	-	-		
7	SF4	J	304	2	0,12,12	-	-	-		
7	SF4	L	303	2	0,12,12	-	-	-		
7	SF4	T	304	2	0,12,12	-	-	-		
7	SF4	X	304	2	0,12,12	-	-	-		
3	ACT	A	901	6	3,3,3	1.28	0	3,3,3	0.85	0
7	SF4	L	304	2	0,12,12	-	-	-		
5	MGD	O	903	6	47,52,52	2.13	16 (34%)	58,81,81	2.14	7 (12%)
7	SF4	D	302	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	E	903	6	47,52,52	2.20	15 (31%)	58,81,81	2.07	8 (13%)
5	MGD	G	904	6	47,52,52	2.15	14 (29%)	58,81,81	1.14	4 (6%)
7	SF4	B	302	2	0,12,12	-	-	-		
5	MGD	K	903	6	47,52,52	1.82	12 (25%)	58,81,81	2.06	7 (12%)
5	MGD	U	903	6	47,52,52	2.19	13 (27%)	58,81,81	2.14	9 (15%)
3	ACT	M	901	6	3,3,3	1.17	0	3,3,3	1.18	0
7	SF4	F	302	2	0,12,12	-	-	-		
3	ACT	C	901	6	3,3,3	1.11	0	3,3,3	1.07	0
7	SF4	H	302	2	0,12,12	-	-	-		
7	SF4	T	303	2	0,12,12	-	-	-		
7	SF4	D	304	2	0,12,12	-	-	-		
5	MGD	A	904	6	47,52,52	2.37	12 (25%)	58,81,81	1.21	4 (6%)
7	SF4	J	302	2	0,12,12	-	-	-		
5	MGD	S	903	6	47,52,52	1.95	13 (27%)	58,81,81	2.23	9 (15%)
7	SF4	P	303	2	0,12,12	-	-	-		
3	ACT	K	901	6	3,3,3	1.24	0	3,3,3	1.07	0
7	SF4	T	302	2	0,12,12	-	-	-		
7	SF4	X	302	2	0,12,12	-	-	-		
5	MGD	O	904	6	47,52,52	2.30	14 (29%)	58,81,81	1.19	3 (5%)
3	ACT	O	901	6	3,3,3	1.22	0	3,3,3	1.03	0
5	MGD	Q	903	6	47,52,52	2.14	15 (31%)	58,81,81	2.19	8 (13%)
5	MGD	I	903	6	47,52,52	2.30	11 (23%)	58,81,81	2.14	8 (13%)
5	MGD	U	904	6	47,52,52	2.34	14 (29%)	58,81,81	1.09	3 (5%)
7	SF4	F	303	2	0,12,12	-	-	-		
5	MGD	K	904	6	47,52,52	2.28	15 (31%)	58,81,81	1.16	3 (5%)
5	MGD	M	903	6	47,52,52	2.11	13 (27%)	58,81,81	2.17	9 (15%)
5	MGD	W	903	6	47,52,52	2.35	13 (27%)	58,81,81	1.98	7 (12%)
7	SF4	J	303	2	0,12,12	-	-	-		
3	ACT	G	901	6	3,3,3	1.20	0	3,3,3	1.05	0
7	SF4	V	302	2	0,12,12	-	-	-		
5	MGD	C	903	6	47,52,52	2.14	15 (31%)	58,81,81	2.09	7 (12%)
7	SF4	B	303	2	0,12,12	-	-	-		
7	SF4	L	302	2	0,12,12	-	-	-		
7	SF4	P	302	2	0,12,12	-	-	-		
7	SF4	P	304	2	0,12,12	-	-	-		
7	SF4	D	303	2	0,12,12	-	-	-		
5	MGD	S	904	6	47,52,52	2.31	14 (29%)	58,81,81	1.12	4 (6%)
7	SF4	H	303	2	0,12,12	-	-	-		
7	SF4	N	303	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	R	303	2	0,12,12	-	-	-		
5	MGD	A	903	6	47,52,52	1.88	11 (23%)	58,81,81	2.09	7 (12%)
3	ACT	Q	901	6	3,3,3	1.23	0	3,3,3	0.93	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
7	SF4	R	304	2	-	-	0/6/5/5
5	MGD	E	904	6	-	5/22/66/66	0/6/6/6
5	MGD	Q	904	6	-	5/22/66/66	0/6/6/6
5	MGD	W	904	6	-	5/22/66/66	0/6/6/6
7	SF4	X	303	2	-	-	0/6/5/5
5	MGD	M	904	6	-	5/22/66/66	0/6/6/6
7	SF4	R	302	2	-	-	0/6/5/5
5	MGD	C	904	6	-	4/22/66/66	0/6/6/6
5	MGD	G	903	6	-	10/22/66/66	0/6/6/6
5	MGD	I	904	6	-	3/22/66/66	0/6/6/6
7	SF4	F	304	2	-	-	0/6/5/5
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	H	304	2	-	-	0/6/5/5
7	SF4	N	304	2	-	-	0/6/5/5
7	SF4	V	304	2	-	-	0/6/5/5
7	SF4	N	302	2	-	-	0/6/5/5
7	SF4	B	304	2	-	-	0/6/5/5
7	SF4	J	304	2	-	-	0/6/5/5
7	SF4	L	303	2	-	-	0/6/5/5
7	SF4	T	304	2	-	-	0/6/5/5
7	SF4	X	304	2	-	-	0/6/5/5
7	SF4	L	304	2	-	-	0/6/5/5
5	MGD	O	903	6	-	9/22/66/66	0/6/6/6
7	SF4	D	302	2	-	-	0/6/5/5
5	MGD	E	903	6	-	9/22/66/66	0/6/6/6
5	MGD	G	904	6	-	5/22/66/66	0/6/6/6
7	SF4	B	302	2	-	-	0/6/5/5
5	MGD	K	903	6	-	7/22/66/66	0/6/6/6
5	MGD	U	903	6	-	9/22/66/66	0/6/6/6
7	SF4	F	302	2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	H	302	2	-	-	0/6/5/5
7	SF4	T	303	2	-	-	0/6/5/5
7	SF4	D	304	2	-	-	0/6/5/5
5	MGD	A	904	6	-	5/22/66/66	0/6/6/6
7	SF4	J	302	2	-	-	0/6/5/5
5	MGD	S	903	6	-	11/22/66/66	0/6/6/6
7	SF4	P	303	2	-	-	0/6/5/5
7	SF4	T	302	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
5	MGD	O	904	6	-	4/22/66/66	0/6/6/6
5	MGD	Q	903	6	-	7/22/66/66	0/6/6/6
5	MGD	U	904	6	-	4/22/66/66	0/6/6/6
5	MGD	I	903	6	-	7/22/66/66	0/6/6/6
7	SF4	F	303	2	-	-	0/6/5/5
5	MGD	K	904	6	-	4/22/66/66	0/6/6/6
5	MGD	M	903	6	-	8/22/66/66	0/6/6/6
5	MGD	W	903	6	-	10/22/66/66	0/6/6/6
7	SF4	J	303	2	-	-	0/6/5/5
7	SF4	V	302	2	-	-	0/6/5/5
5	MGD	C	903	6	-	7/22/66/66	0/6/6/6
7	SF4	B	303	2	-	-	0/6/5/5
7	SF4	L	302	2	-	-	0/6/5/5
7	SF4	P	302	2	-	-	0/6/5/5
7	SF4	P	304	2	-	-	0/6/5/5
7	SF4	D	303	2	-	-	0/6/5/5
5	MGD	S	904	6	-	4/22/66/66	0/6/6/6
7	SF4	H	303	2	-	-	0/6/5/5
7	SF4	N	303	2	-	-	0/6/5/5
7	SF4	R	303	2	-	-	0/6/5/5
5	MGD	A	903	6	-	7/22/66/66	0/6/6/6

The worst 5 of 327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	904	MGD	C23-C14	7.21	1.59	1.53
5	U	904	MGD	C14-N15	7.16	1.54	1.46
5	S	904	MGD	C14-N15	7.06	1.54	1.46
5	K	904	MGD	C14-N15	7.04	1.54	1.46
5	I	903	MGD	C14-N15	6.97	1.54	1.46

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	903	MGD	O2A-PA-O3B	-10.89	77.85	107.27
5	O	903	MGD	O2A-PA-O3B	-10.77	78.16	107.27
5	S	903	MGD	O2A-PA-O3B	-10.57	78.71	107.27
5	M	903	MGD	O2A-PA-O3B	-10.53	78.82	107.27
5	G	903	MGD	O2A-PA-O3B	-10.42	79.12	107.27

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	MGD	C5'-O5'-PB-O1B
5	A	903	MGD	C5'-O5'-PB-O2B
5	A	903	MGD	C5'-O5'-PB-O3B
5	A	903	MGD	C10-O3A-PA-O2A
5	A	903	MGD	O3A-C10-C11-O11

There are no ring outliers.

69 monomers are involved in 212 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	901	ACT	1	0
7	R	304	SF4	2	0
3	I	901	ACT	3	0
5	E	904	MGD	3	0
5	Q	904	MGD	4	0
3	E	901	ACT	2	0
5	W	904	MGD	7	0
5	M	904	MGD	7	0
7	X	303	SF4	2	0
3	U	901	ACT	1	0
7	R	302	SF4	1	0
5	C	904	MGD	6	0
5	G	903	MGD	6	0
5	I	904	MGD	7	0
3	W	901	ACT	2	0
7	F	304	SF4	1	0
7	V	303	SF4	2	0
7	H	304	SF4	2	0
7	N	304	SF4	1	0
7	V	304	SF4	1	0
7	N	302	SF4	1	0

Continued on next page...

Continued from previous page...

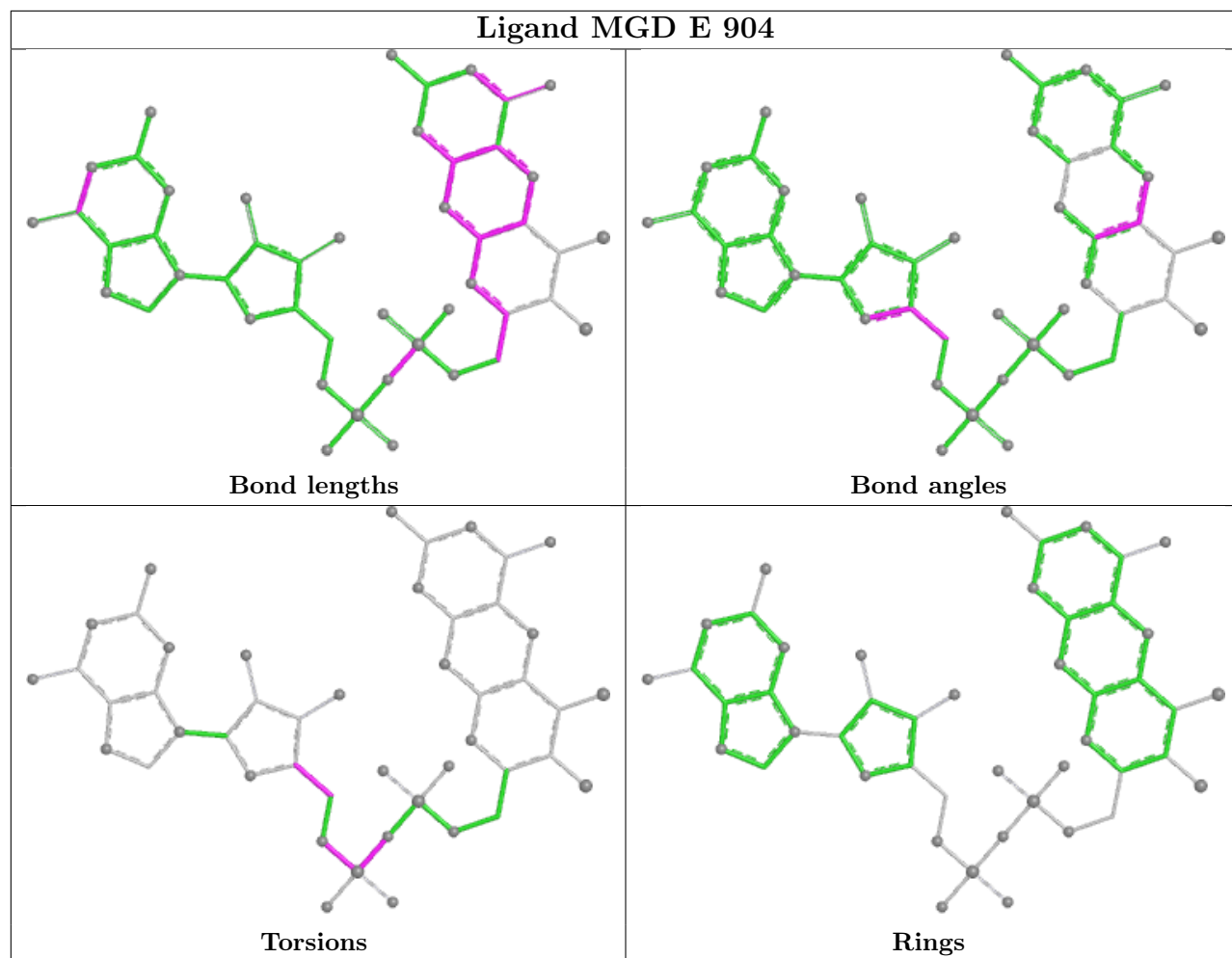
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	304	SF4	1	0
7	L	303	SF4	2	0
7	T	304	SF4	4	0
7	X	304	SF4	3	0
3	A	901	ACT	1	0
7	L	304	SF4	3	0
5	O	903	MGD	5	0
7	D	302	SF4	1	0
5	E	903	MGD	5	0
5	G	904	MGD	4	0
5	K	903	MGD	6	0
5	U	903	MGD	7	0
3	M	901	ACT	1	0
3	C	901	ACT	3	0
7	H	302	SF4	1	0
7	T	303	SF4	2	0
7	D	304	SF4	2	0
5	A	904	MGD	6	0
7	J	302	SF4	1	0
5	S	903	MGD	6	0
7	P	303	SF4	2	0
3	K	901	ACT	3	0
7	T	302	SF4	1	0
7	X	302	SF4	2	0
5	O	904	MGD	5	0
3	O	901	ACT	2	0
5	Q	903	MGD	5	0
5	I	903	MGD	5	0
5	U	904	MGD	7	0
7	F	303	SF4	2	0
5	K	904	MGD	4	0
5	M	903	MGD	4	0
5	W	903	MGD	6	0
7	J	303	SF4	2	0
3	G	901	ACT	3	0
7	V	302	SF4	1	0
5	C	903	MGD	5	0
7	B	303	SF4	2	0
7	L	302	SF4	1	0
7	P	302	SF4	2	0
7	P	304	SF4	2	0
7	D	303	SF4	2	0

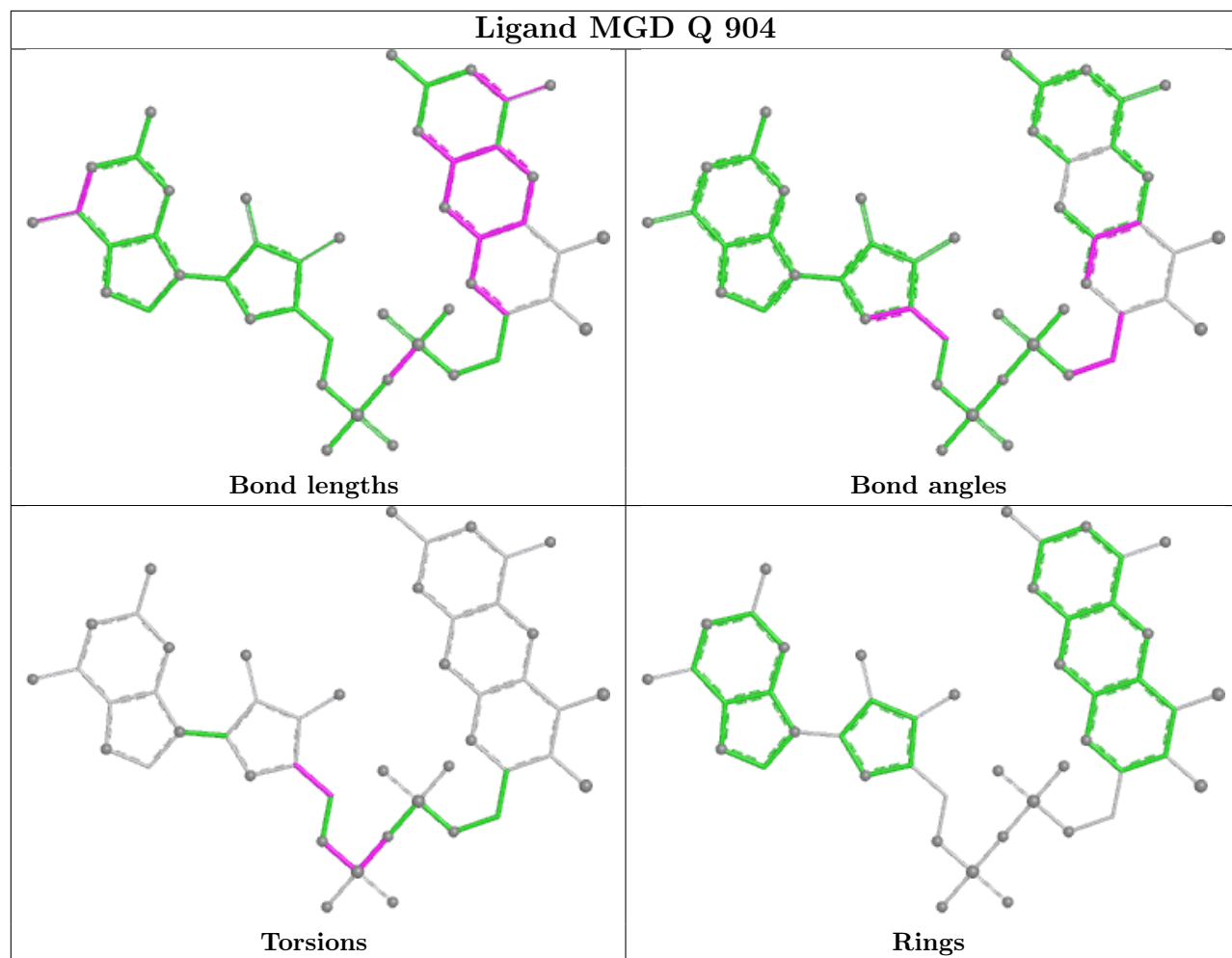
Continued on next page...

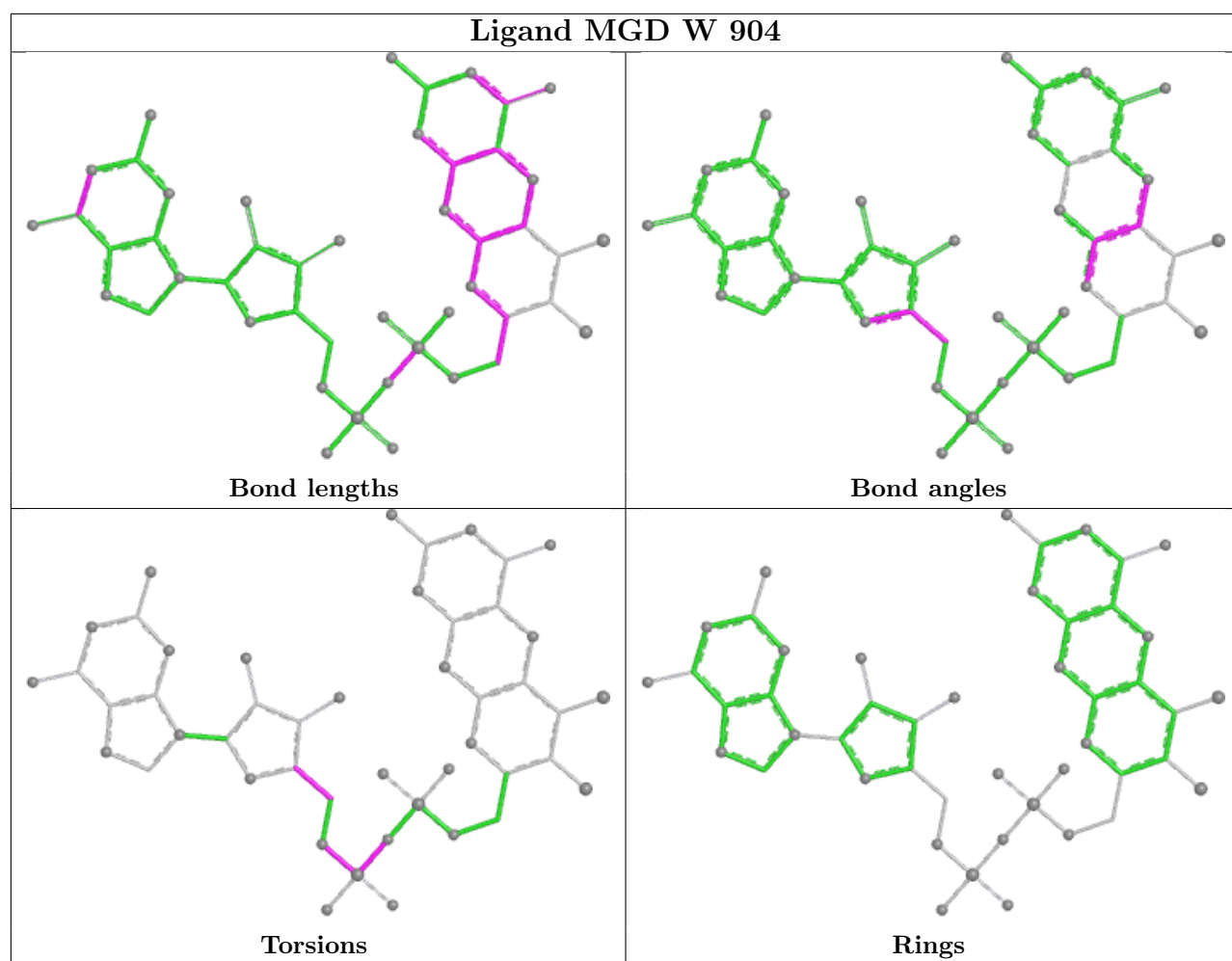
Continued from previous page...

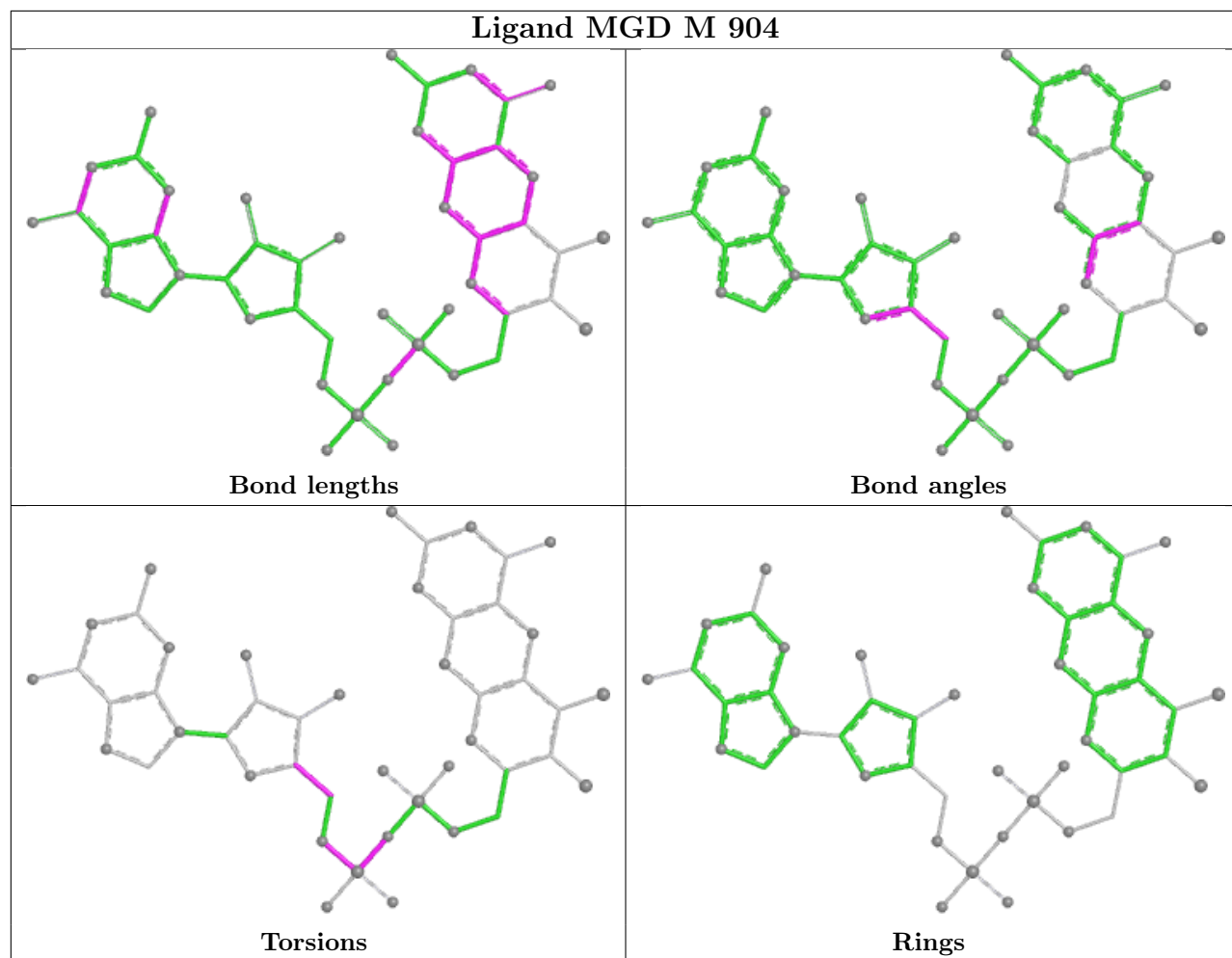
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	904	MGD	5	0
7	H	303	SF4	2	0
7	N	303	SF4	2	0
7	R	303	SF4	2	0
5	A	903	MGD	6	0
3	Q	901	ACT	1	0

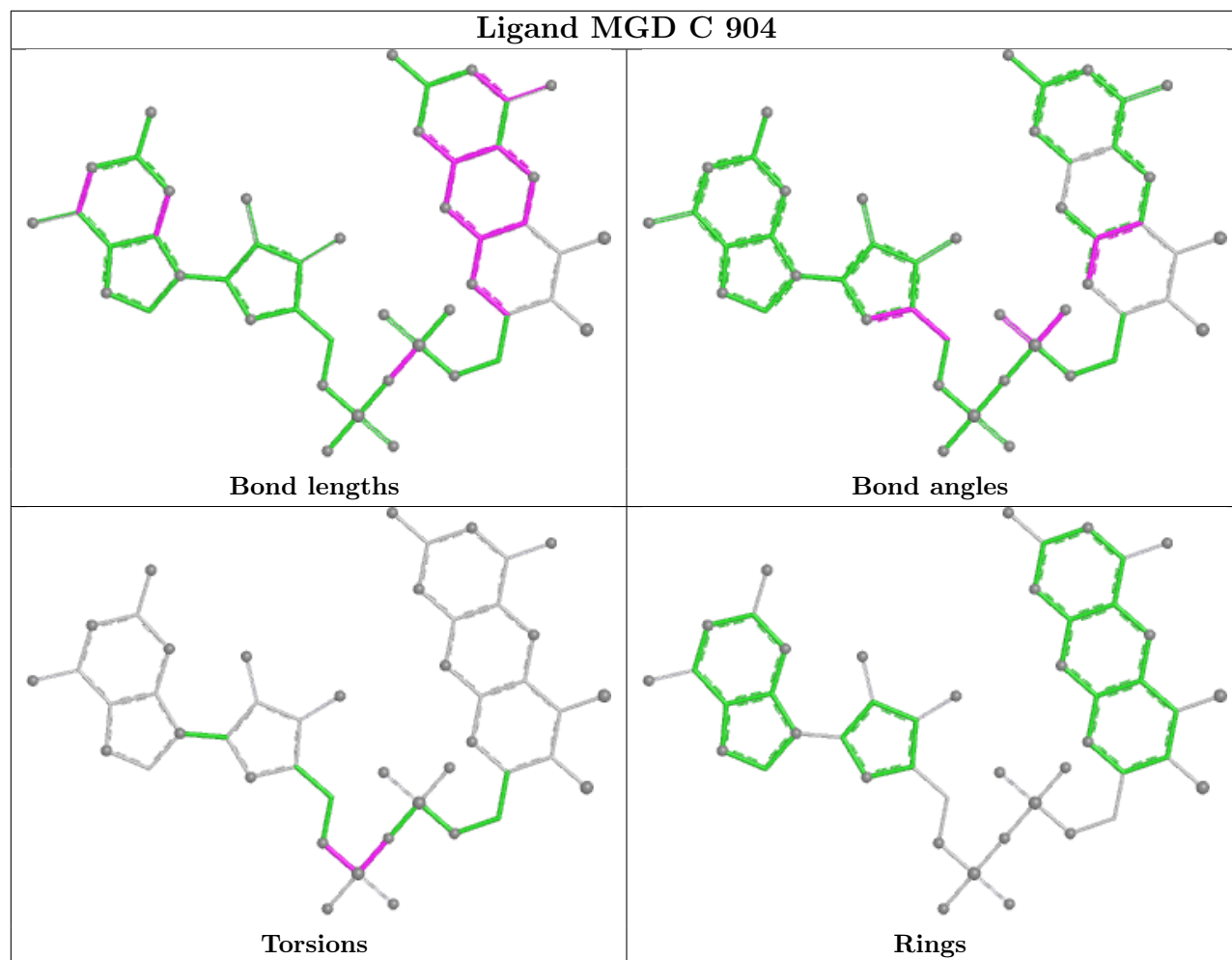
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

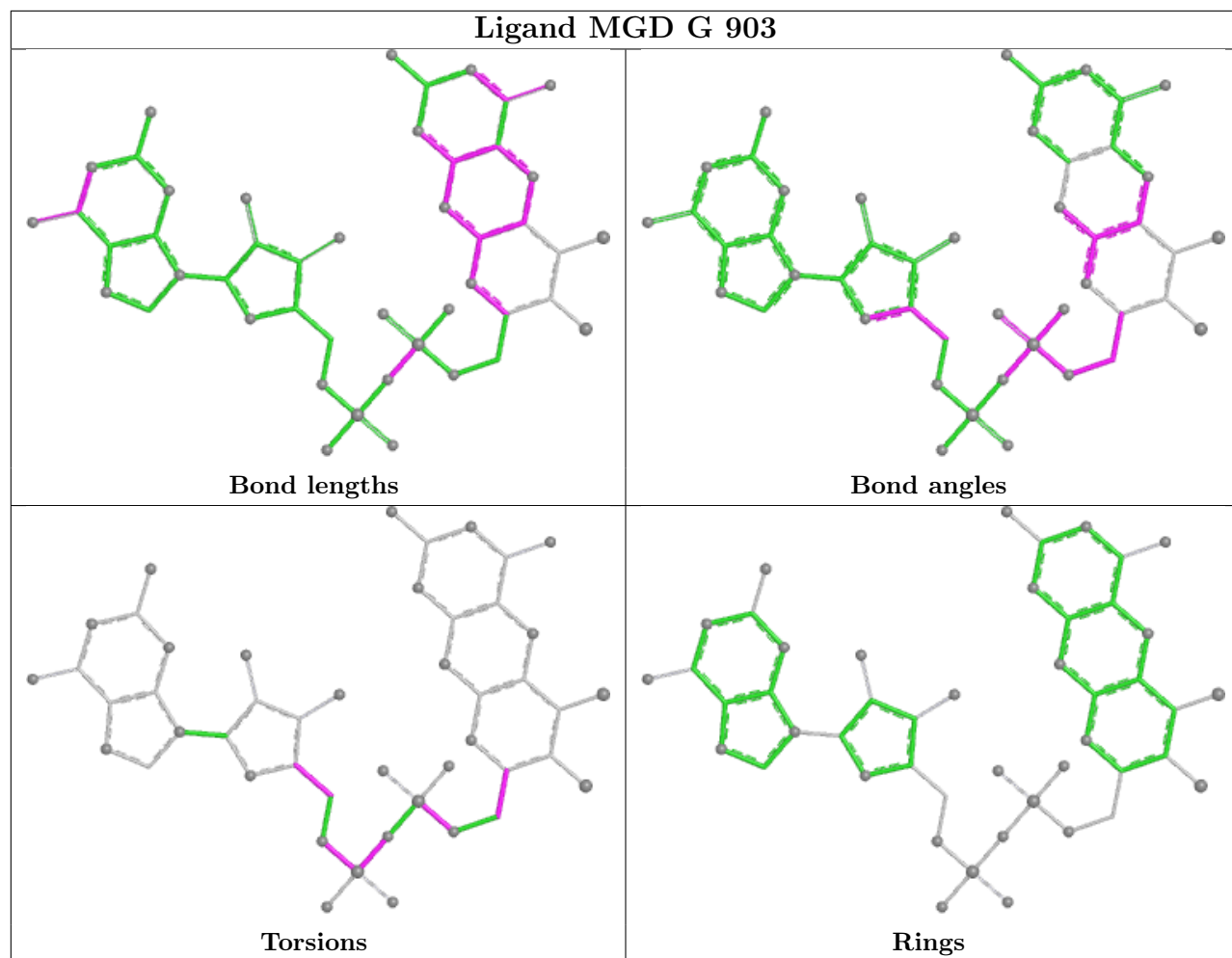


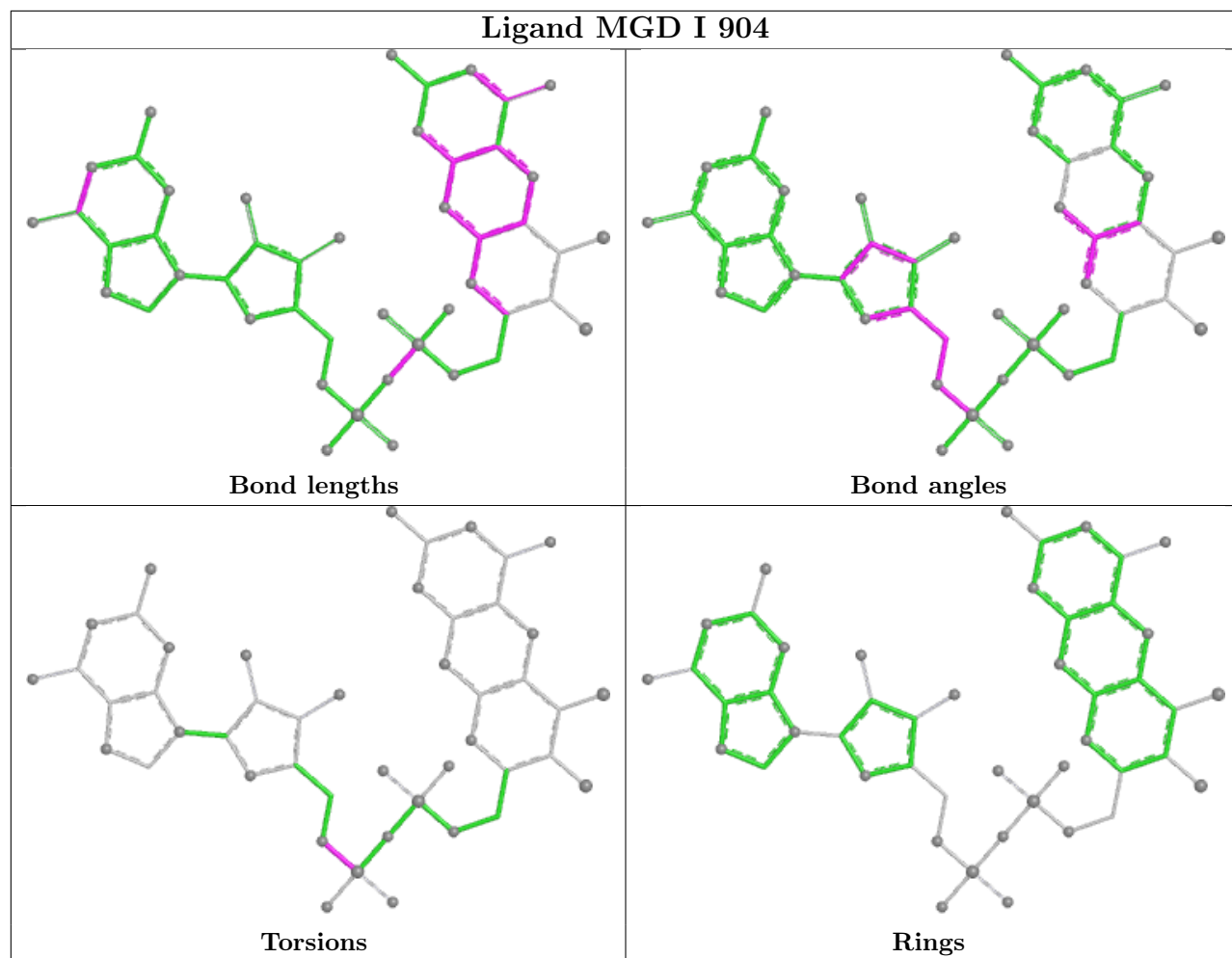


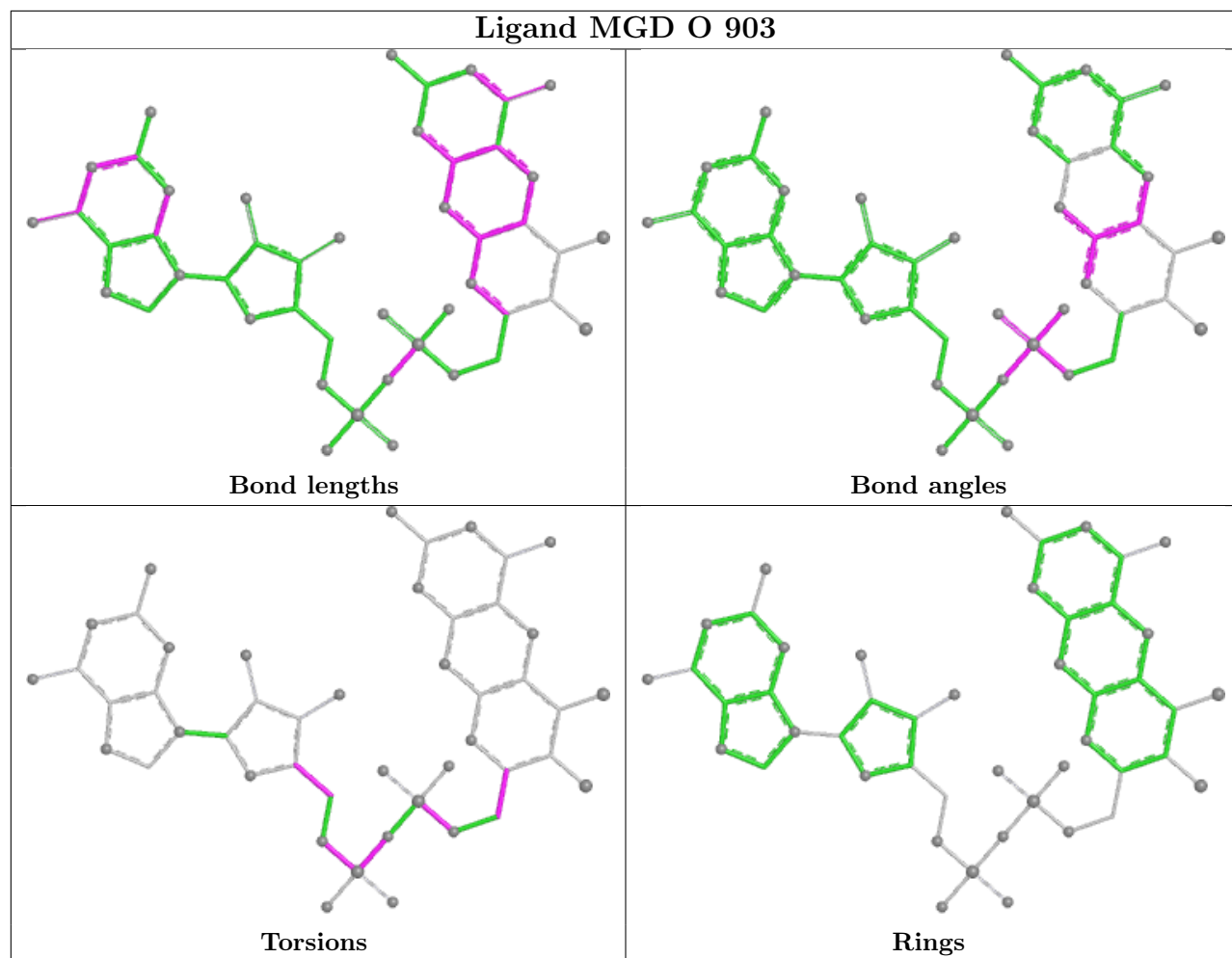


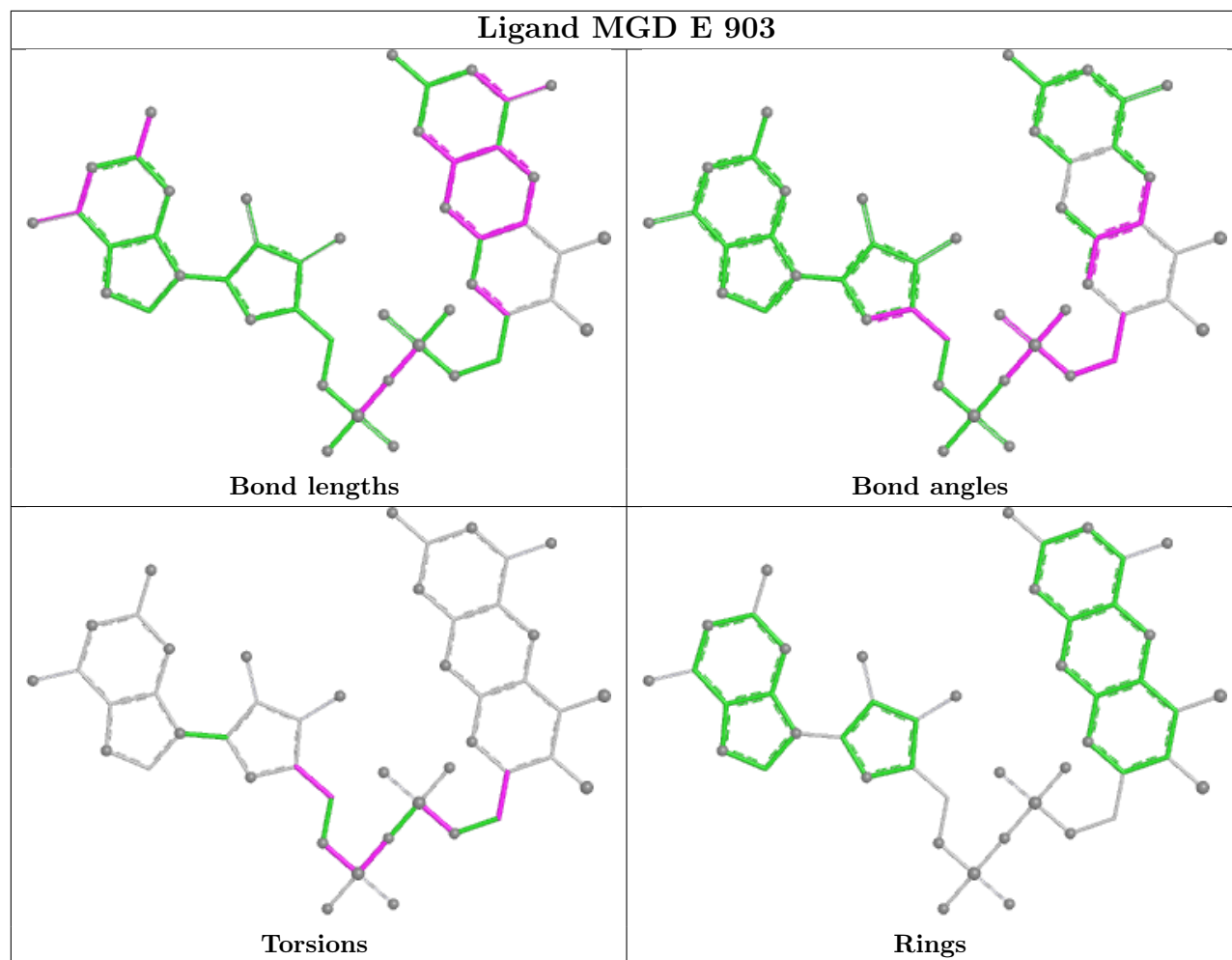


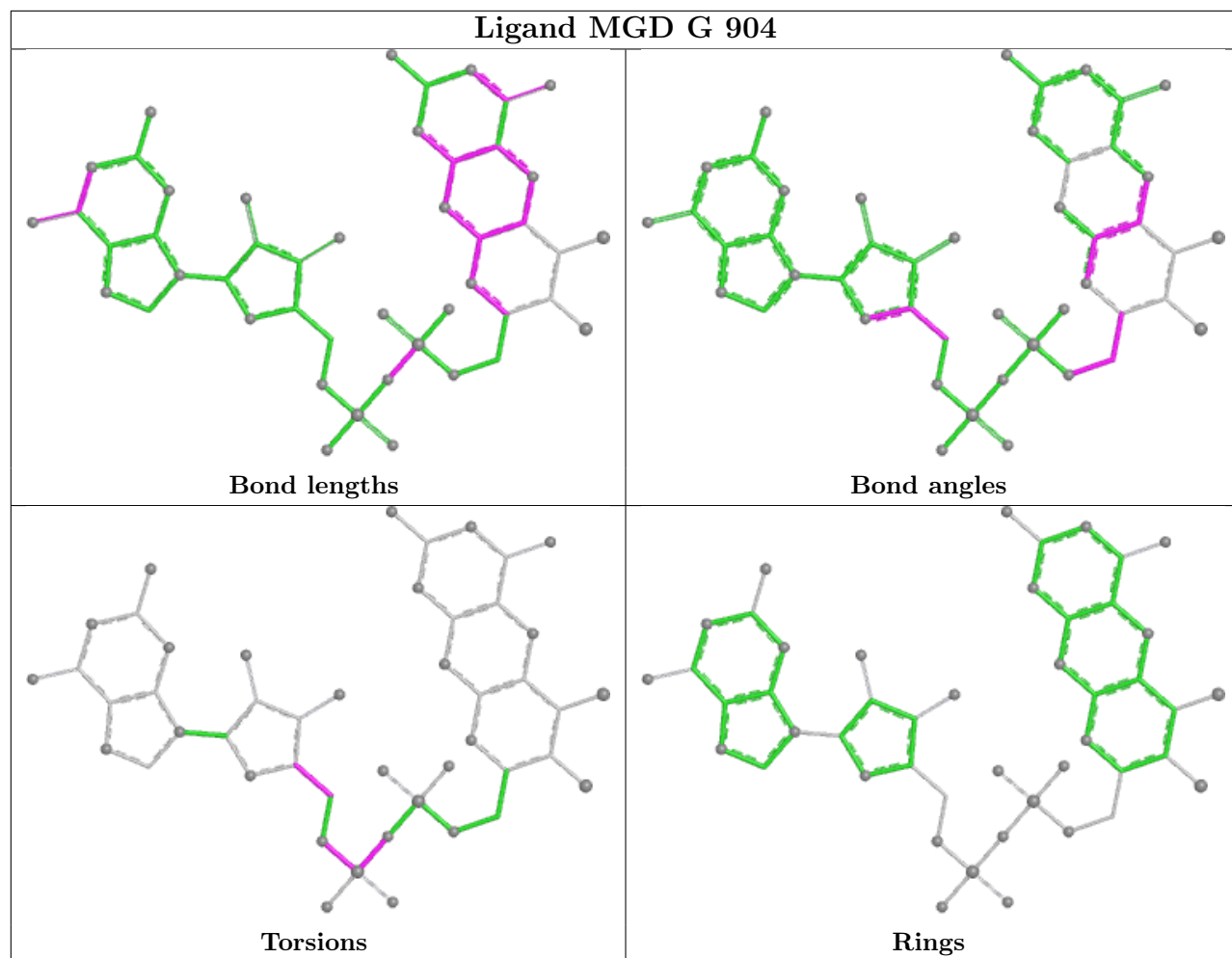


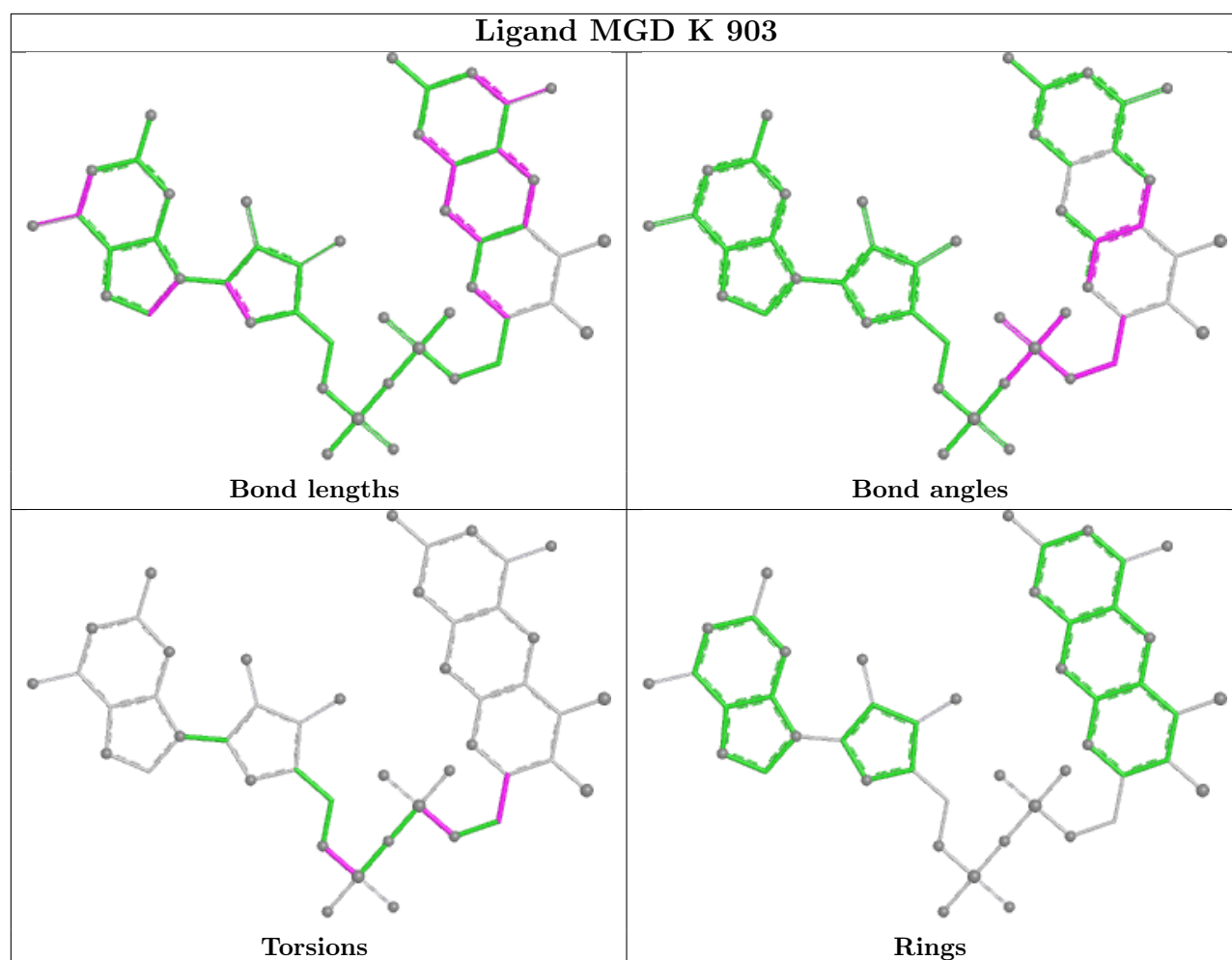


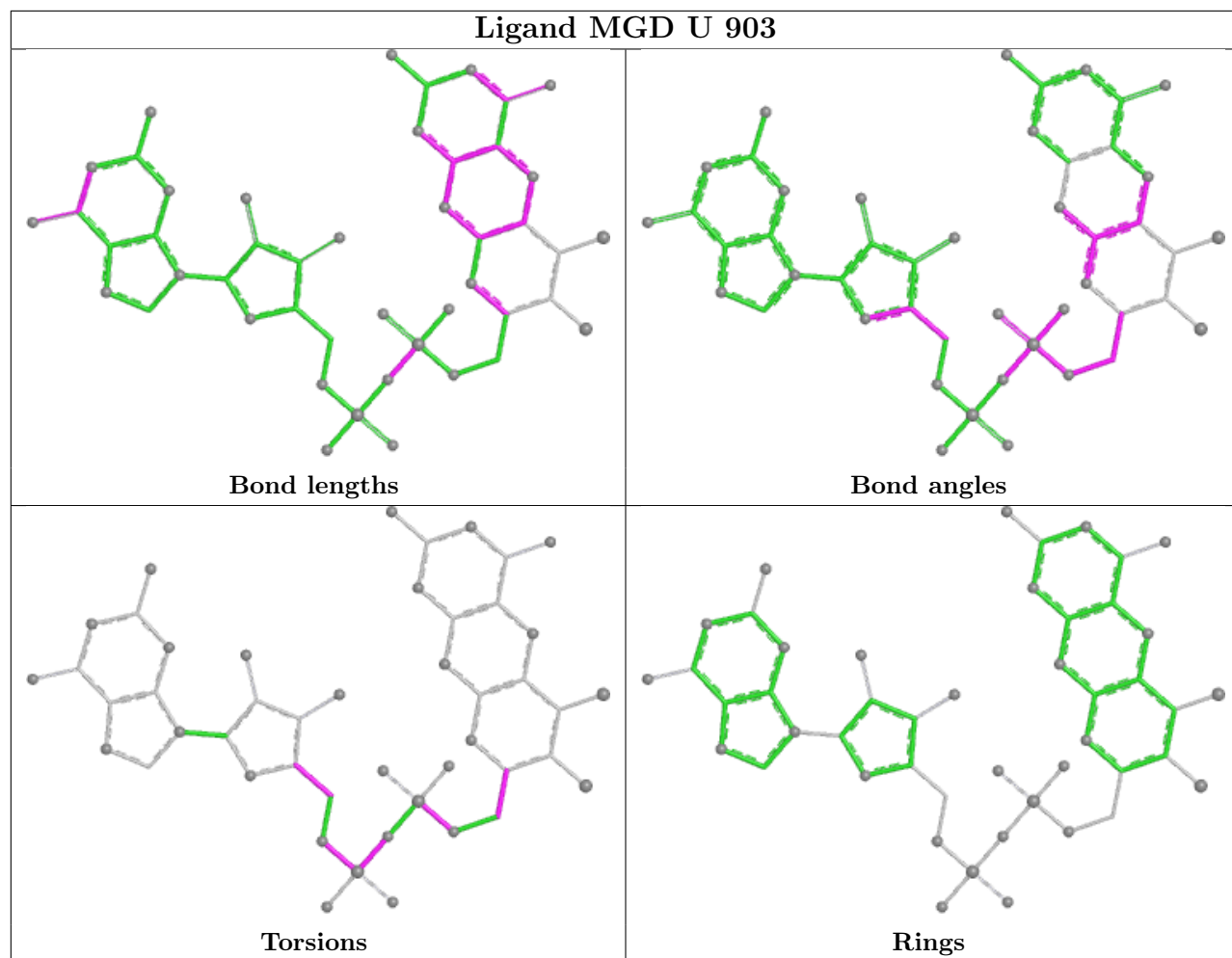


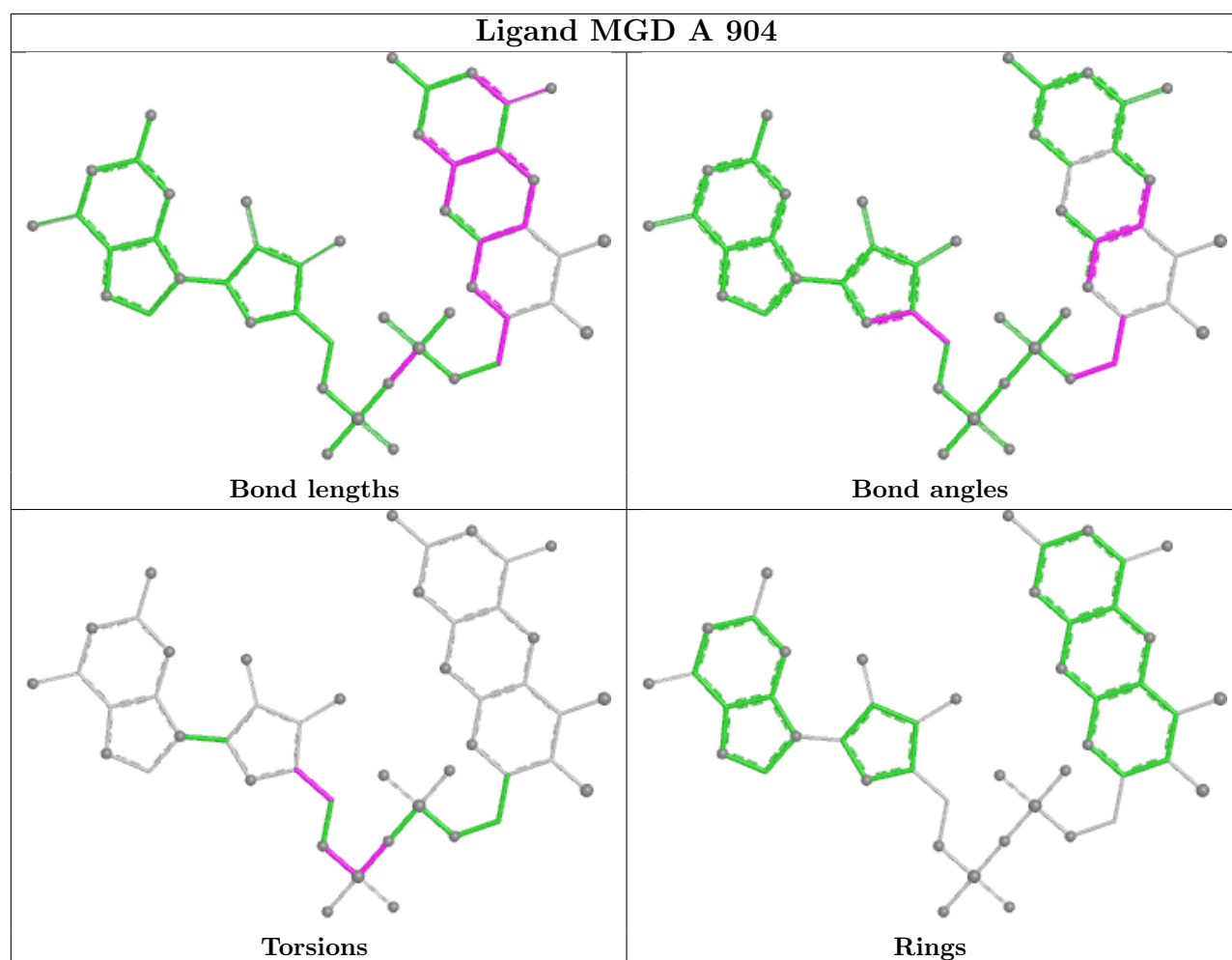


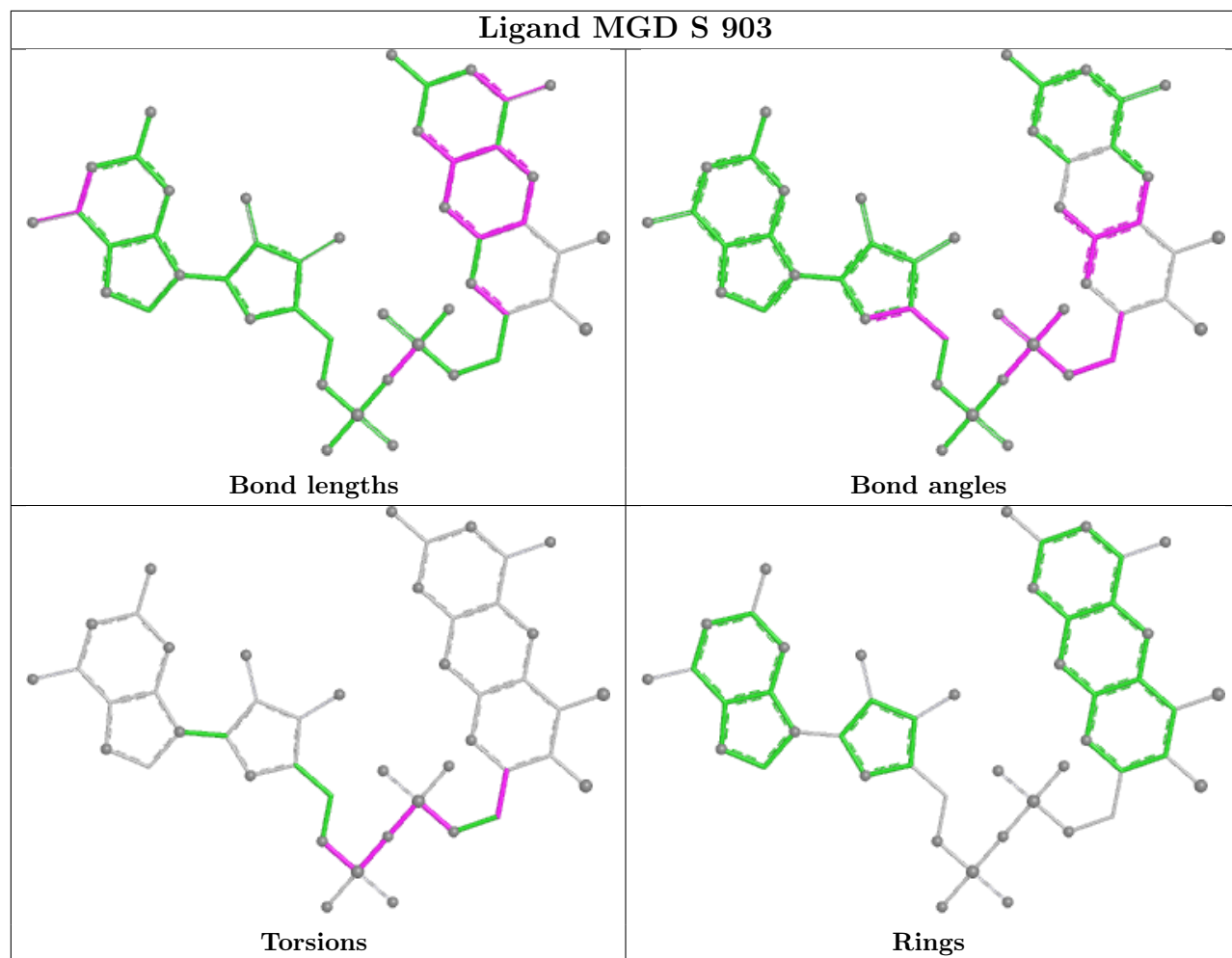


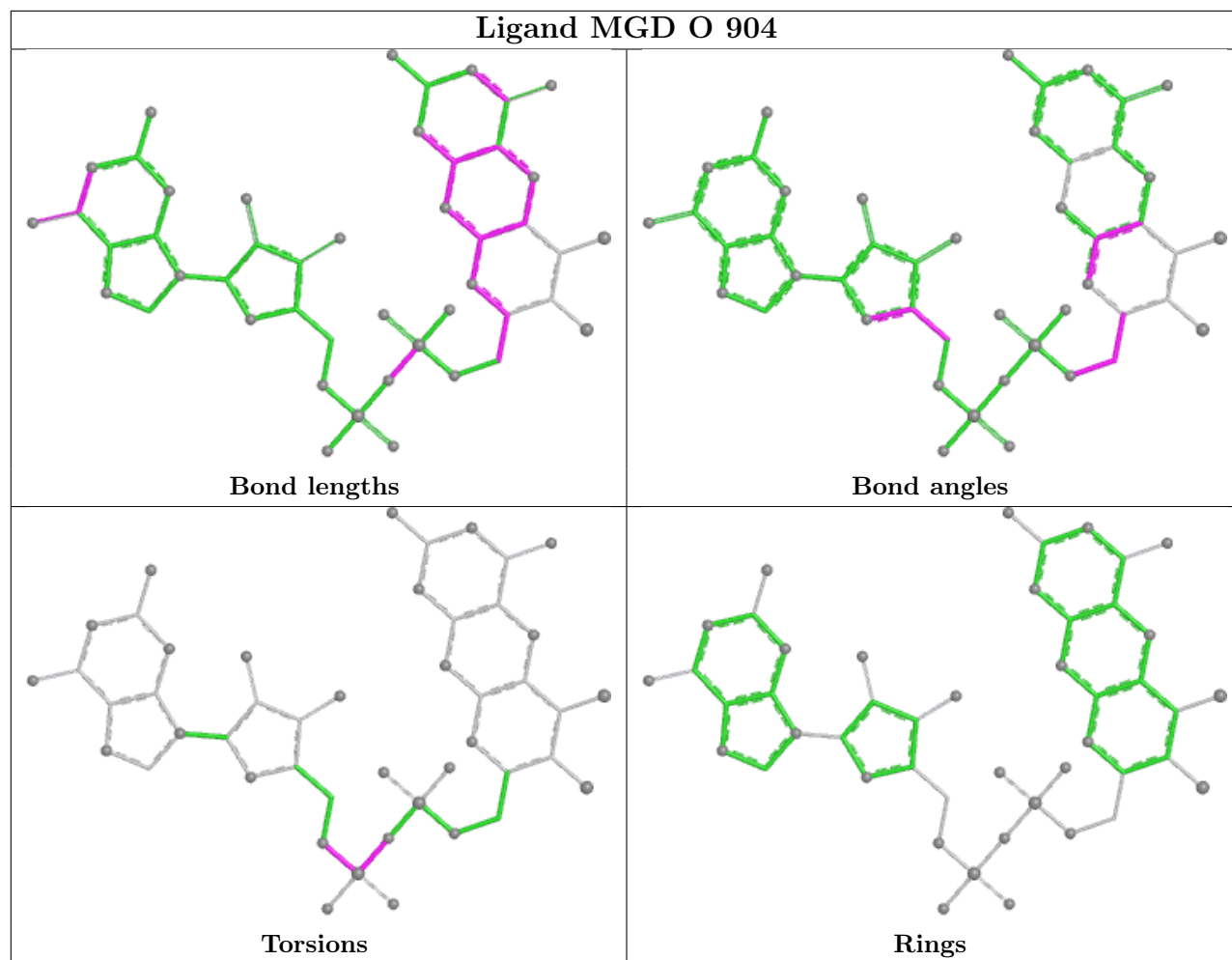


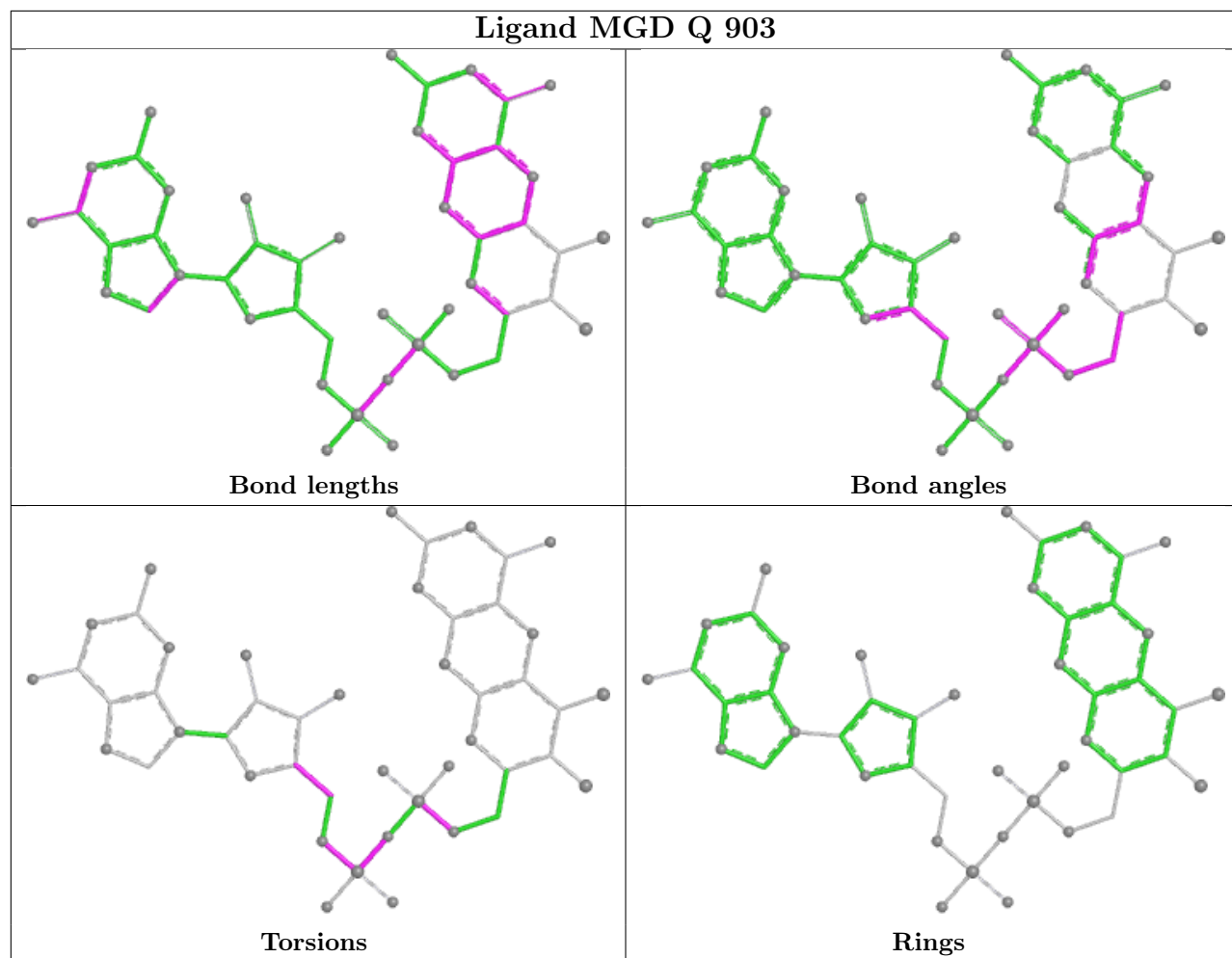


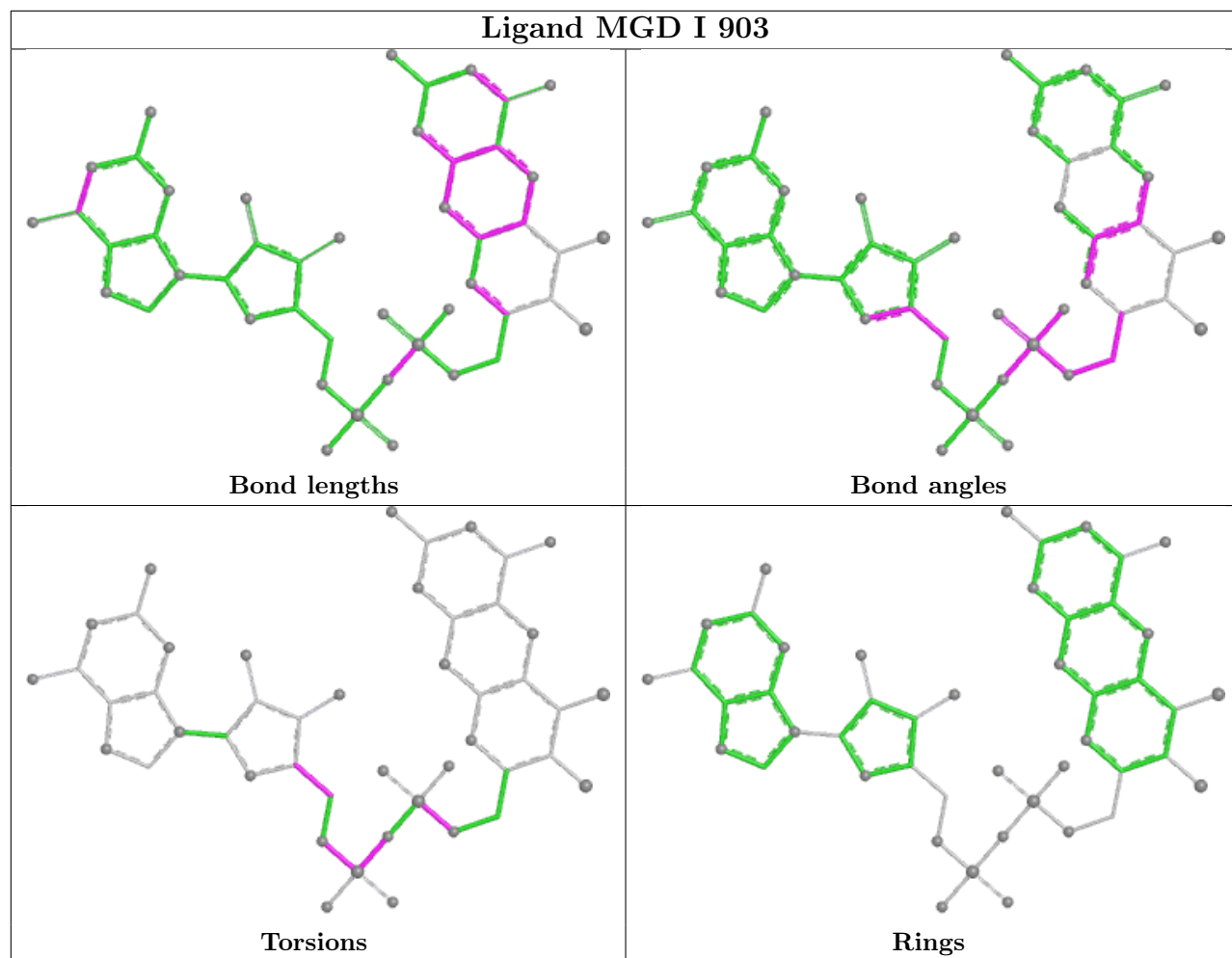


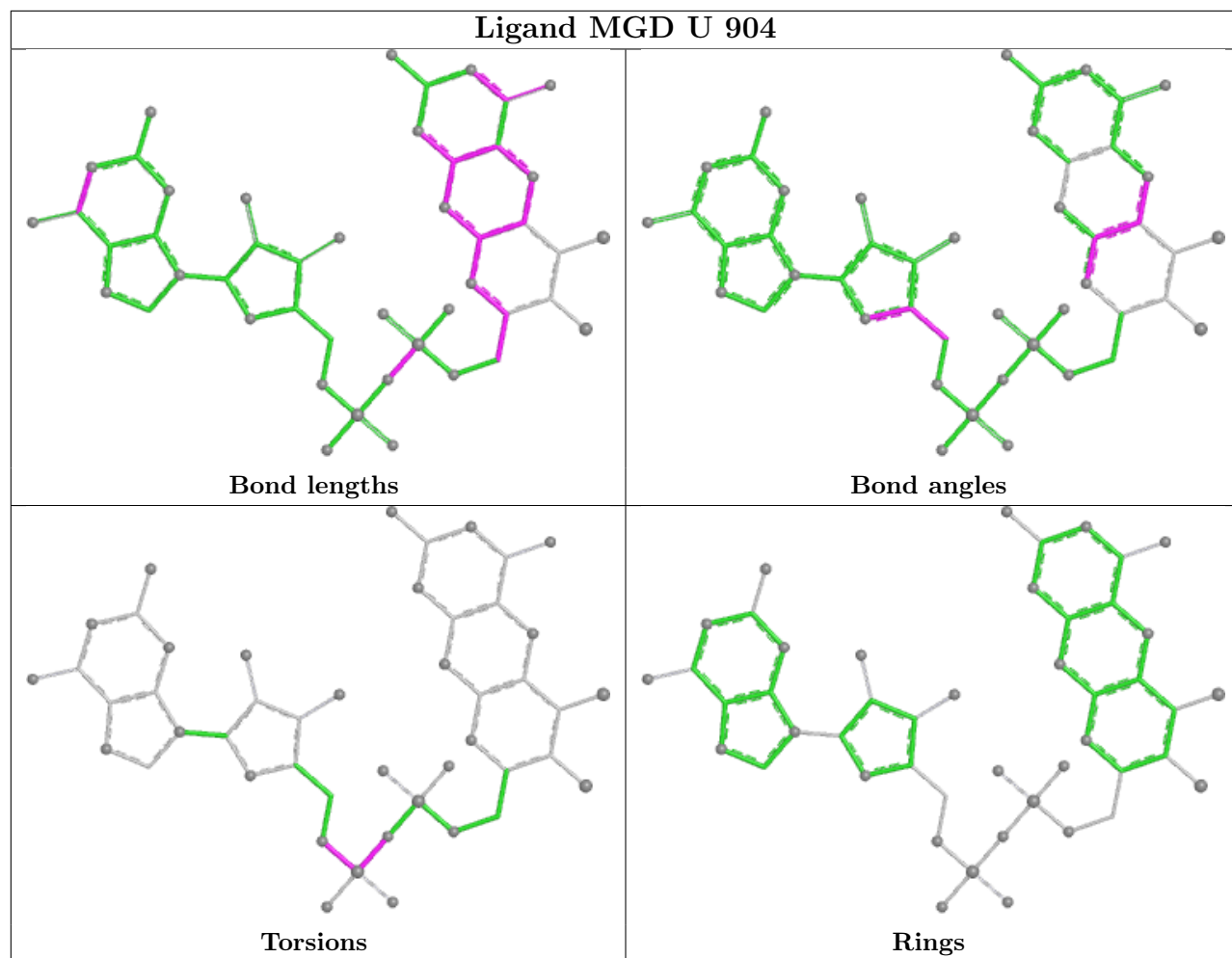


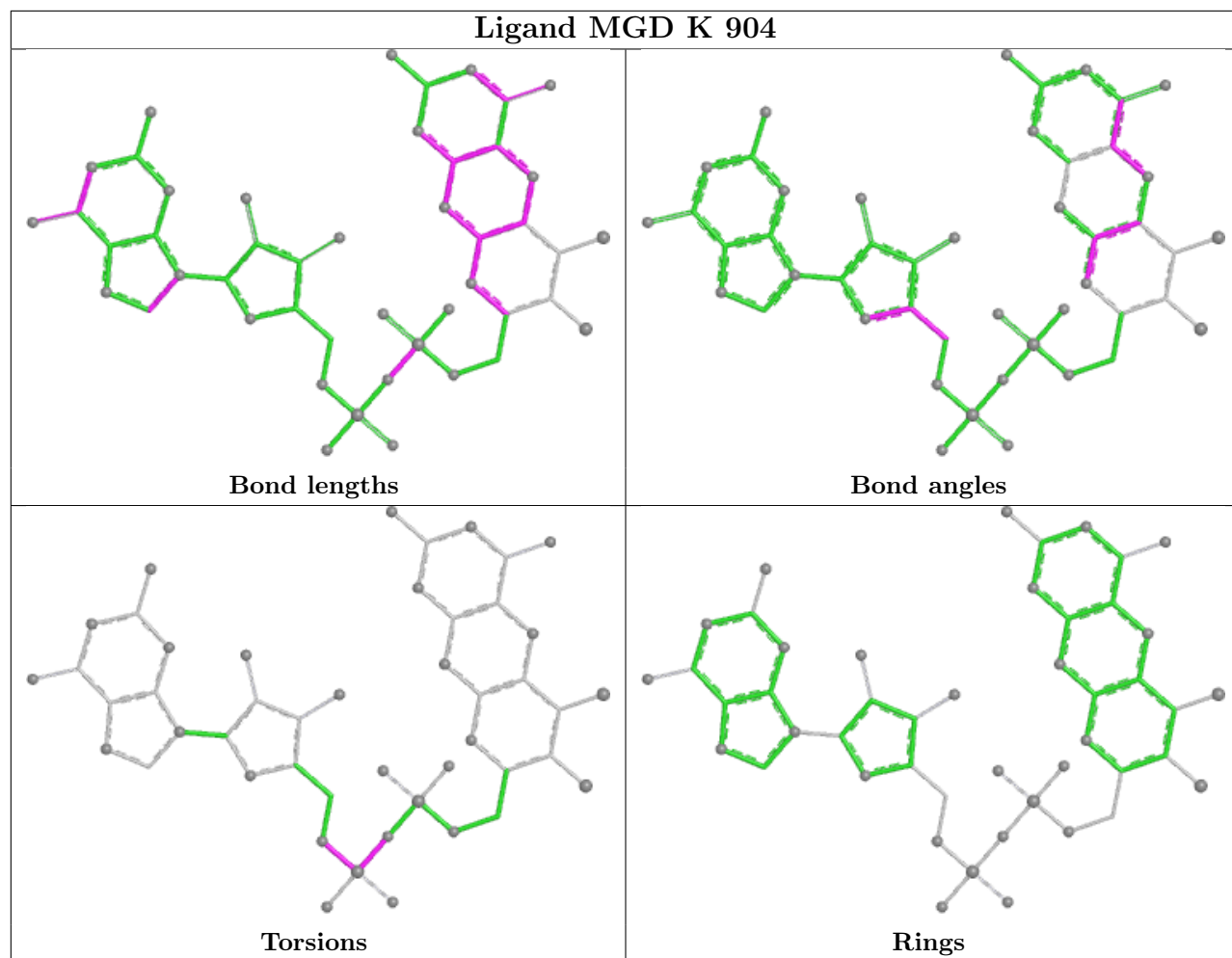


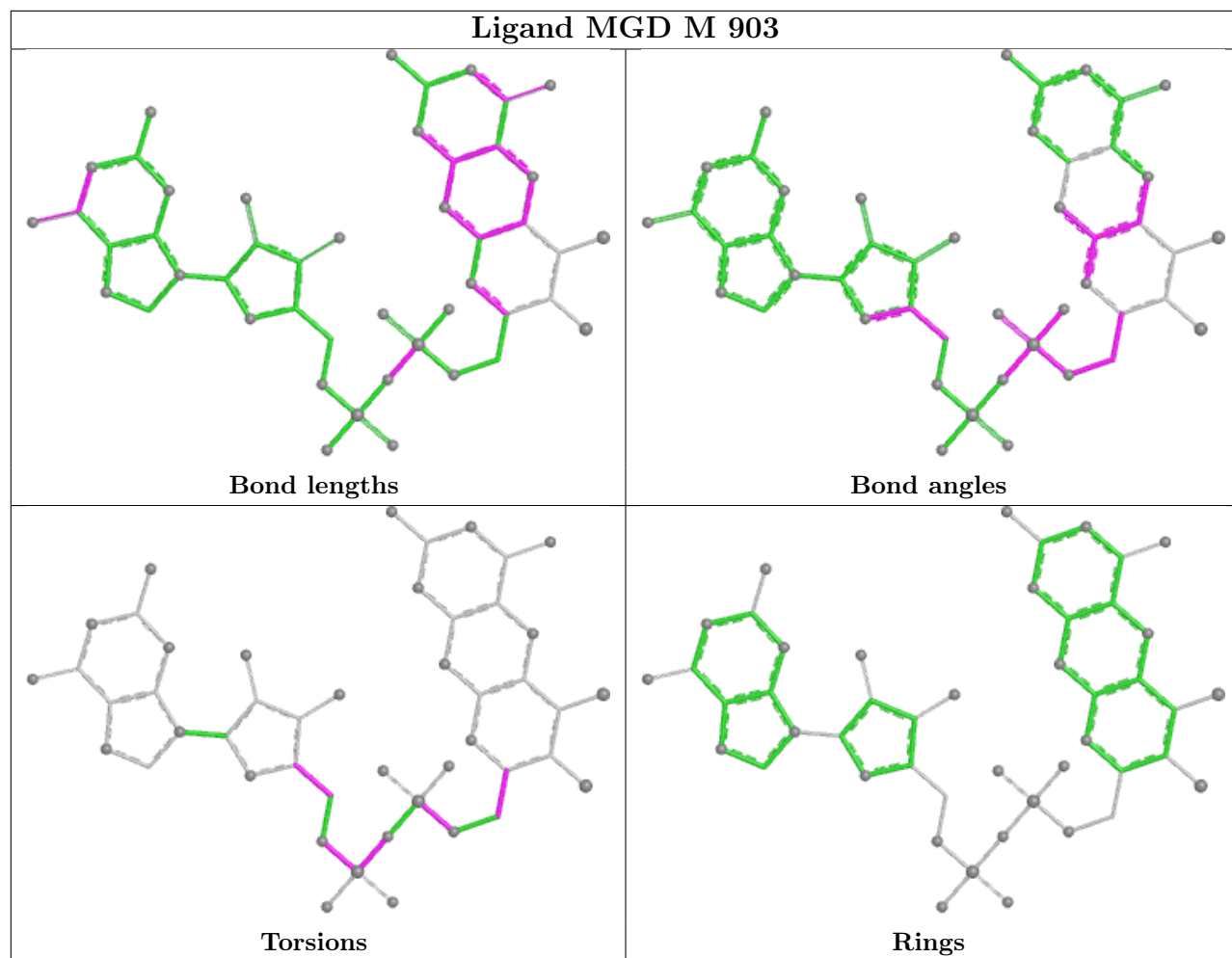


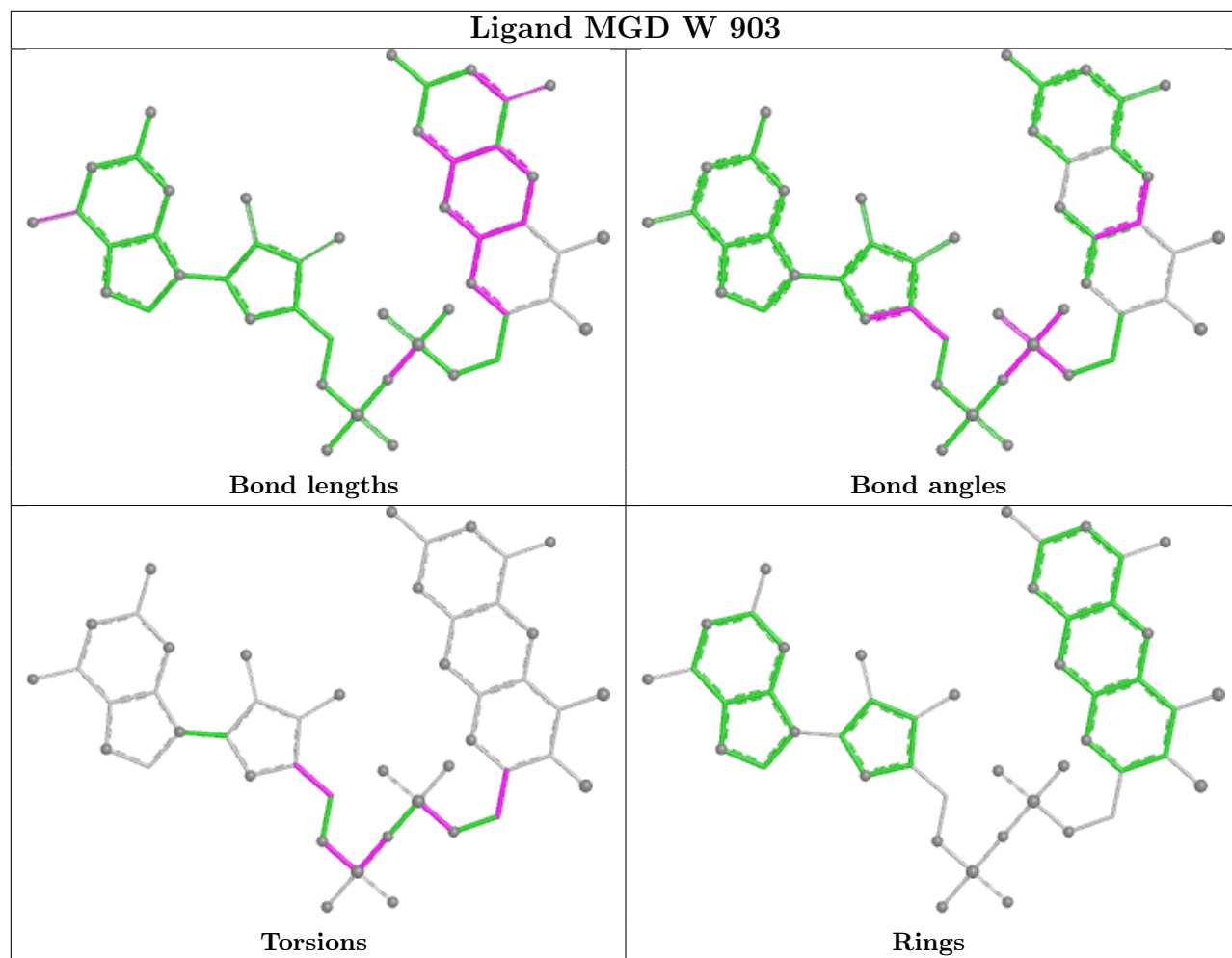


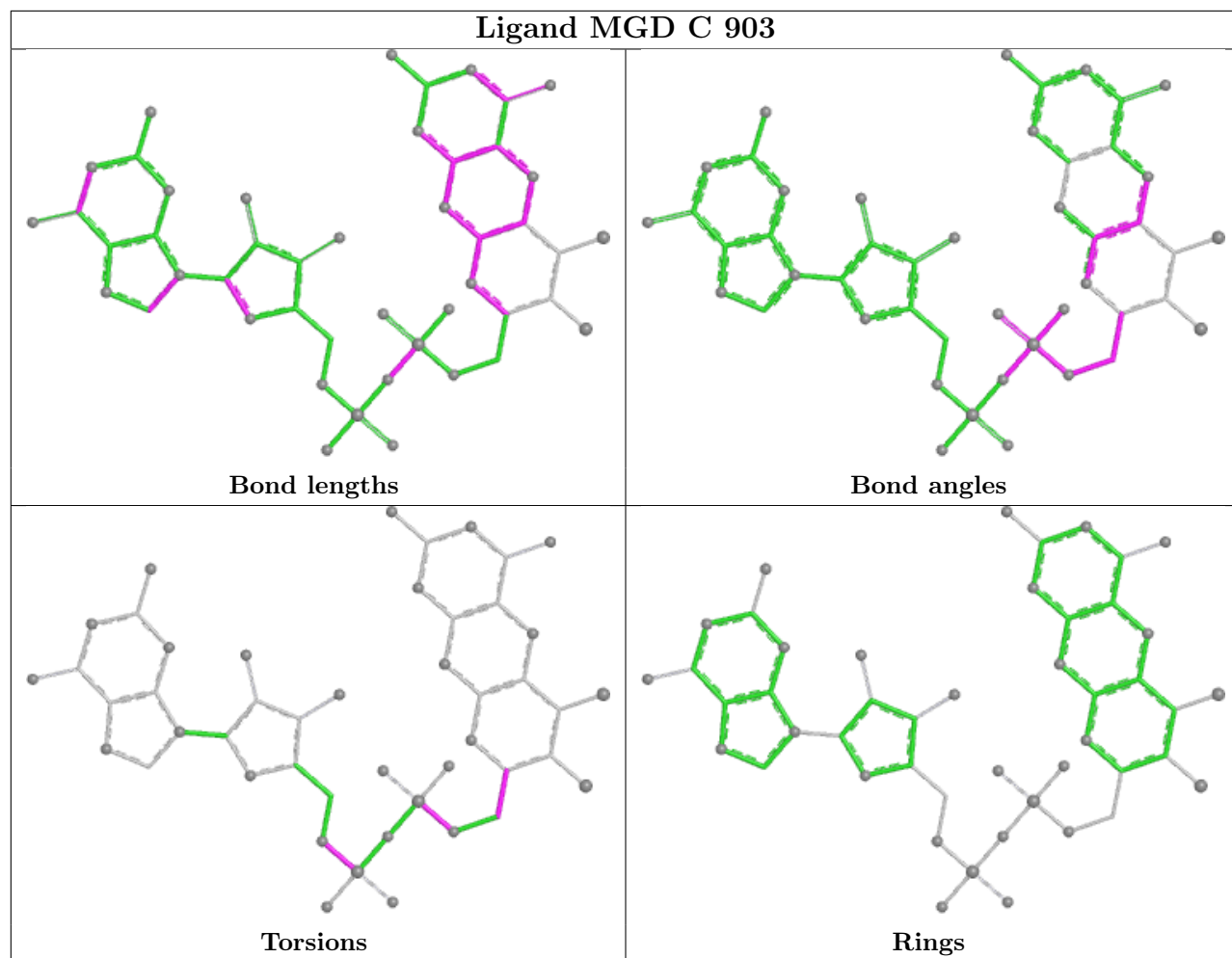


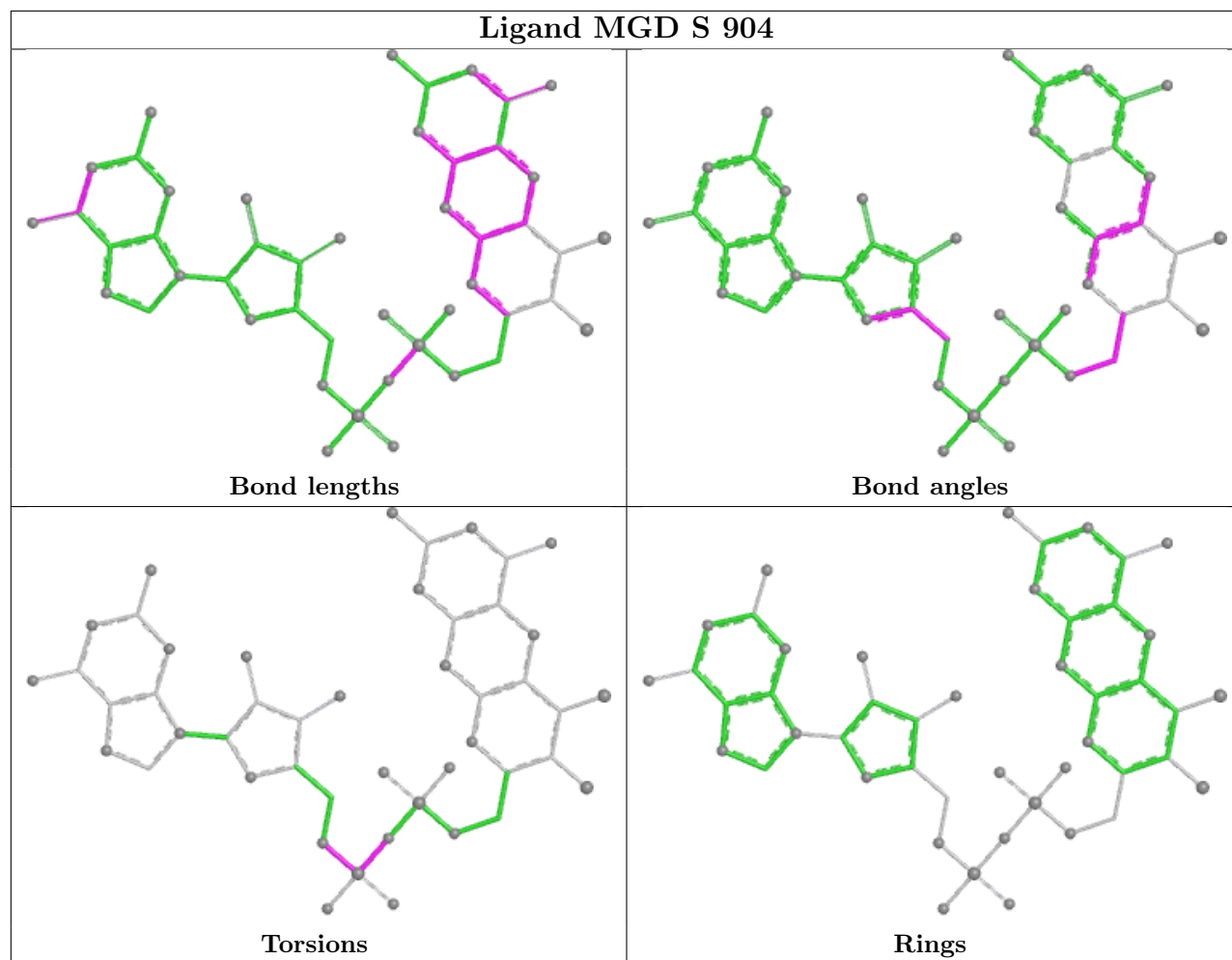


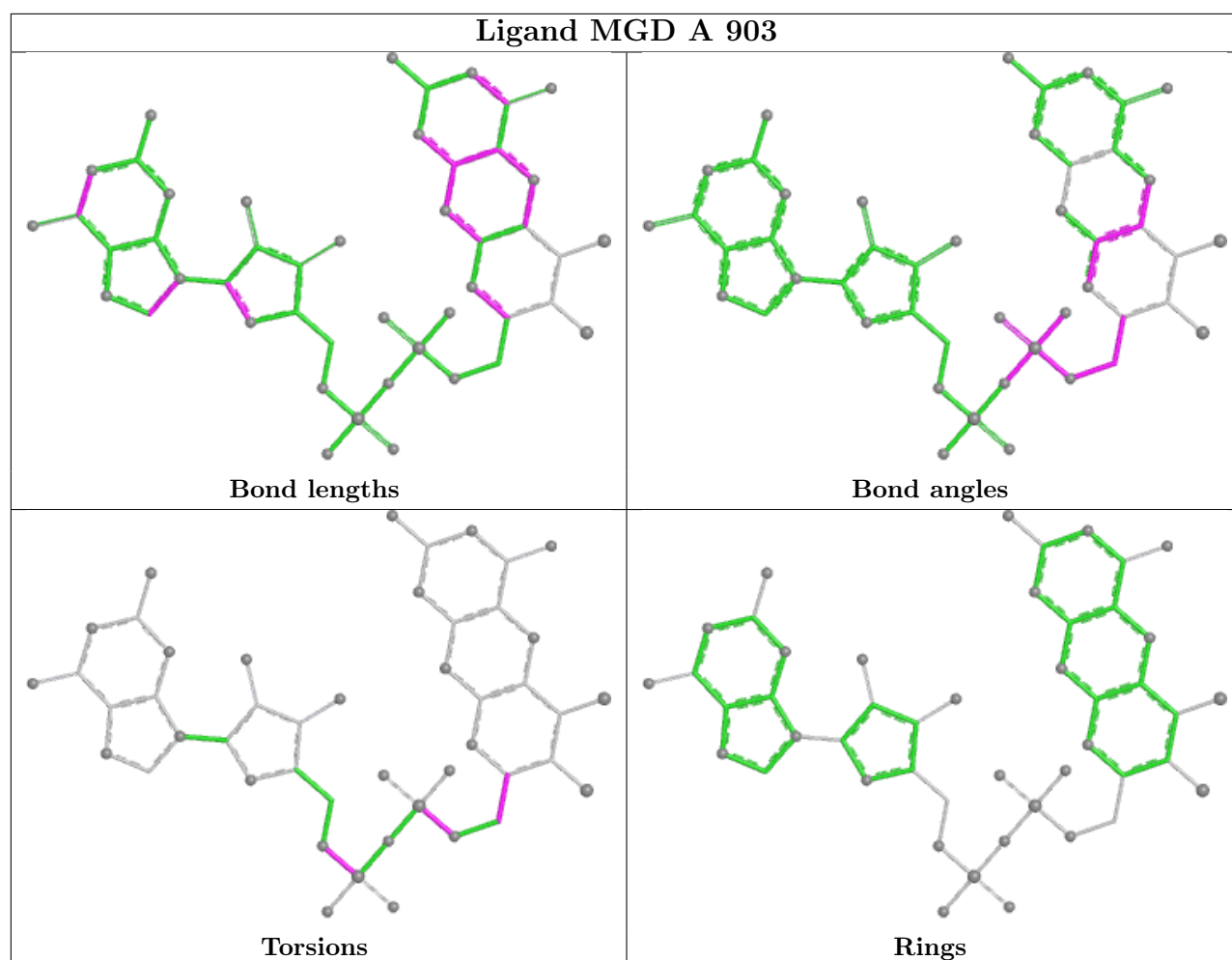












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.