



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 09:35 am BST

PDB ID : 4V4E
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici* complexed with inhibitor 1,2,4,5-tetrahydroxy-benzene
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

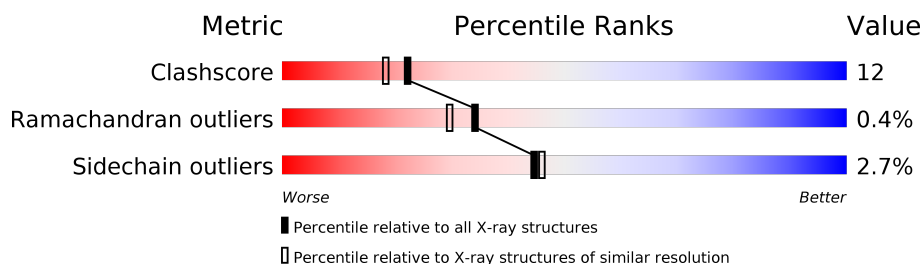
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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	80% 19% .
1	C	875	78% 21% .
1	E	875	81% 18% .
1	G	875	80% 19% .
1	I	875	80% 19% .
1	K	875	79% 20% .
1	M	875	79% 20% .
1	O	875	80% 19% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	Q	875		•
1	S	875		•
1	U	875		•
1	W	875		•
2	B	274		• •
2	D	274		• •
2	F	274		•
2	H	274		• •
2	J	274		• •
2	L	274		•
2	N	274		•
2	P	274		• •
2	R	274		•
2	T	274		• •
2	V	274		•
2	X	274		• •

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
6	BTT	E	905	-	X	-	-
6	BTT	S	905	-	X	-	-
7	SF4	B	303	-	-	X	-
7	SF4	D	303	-	-	X	-
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	J	303	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	303	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	R	303	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	V	303	-	-	X	-
7	SF4	X	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 121823 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	0	0
			6998	4464	1189	1297	48			
1	C	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	E	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	G	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	I	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	K	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	M	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	O	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	Q	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	S	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	U	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	W	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

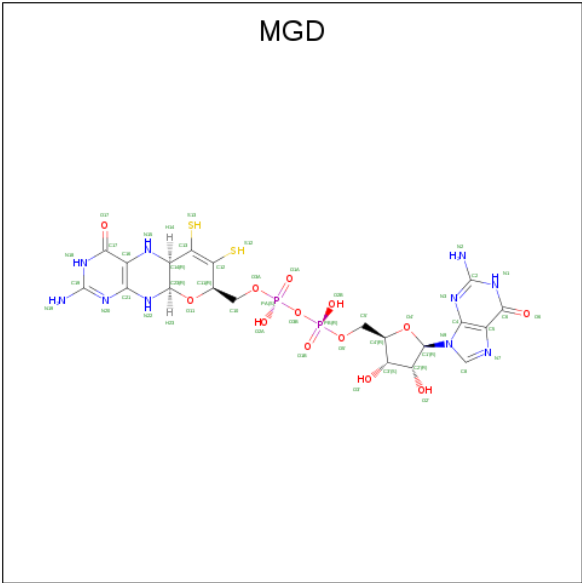
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	W	1	Total 1	Ca 1	0	0
3	N	1	Total 1	Ca 1	0	0
3	X	1	Total 1	Ca 1	0	0
3	S	1	Total 1	Ca 1	0	0
3	J	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	V	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	R	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0
3	D	1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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 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 (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



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

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

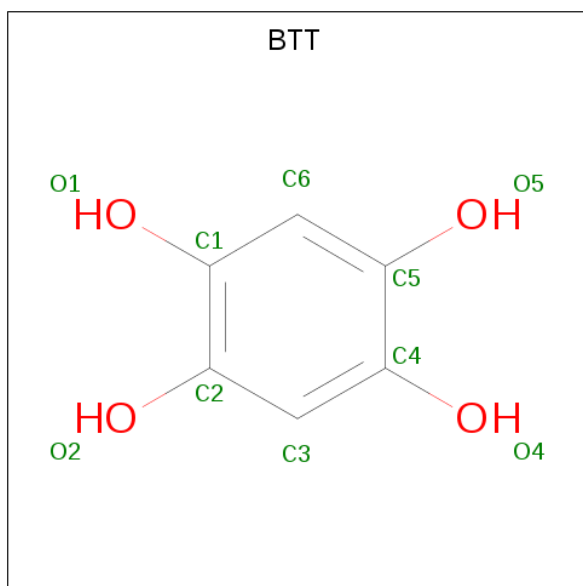
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mo	0	0
			1	1		
5	Q	1	Total	Mo	0	0
			1	1		
5	K	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	W	1	Total	Mo	0	0
			1	1		
5	A	1	Total	Mo	0	0
			1	1		
5	U	1	Total	Mo	0	0
			1	1		
5	O	1	Total	Mo	0	0
			1	1		
5	S	1	Total	Mo	0	0
			1	1		
5	M	1	Total	Mo	0	0
			1	1		

- Molecule 6 is BENZENE-1,2,4,5-TETROL (three-letter code: BTT) (formula: C₆H₆O₄).



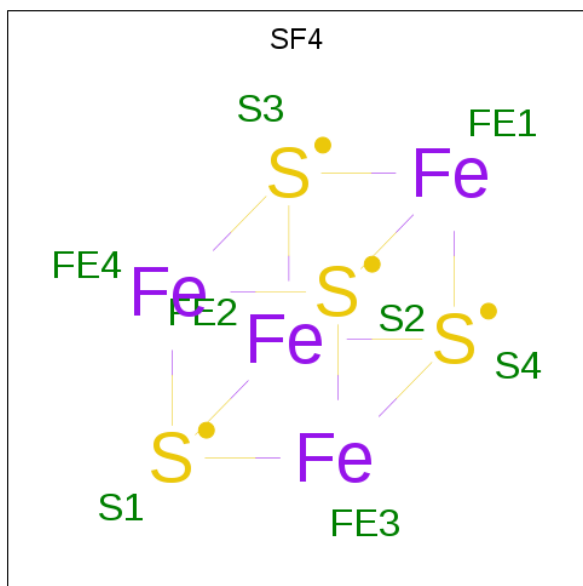
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		
6	K	1	Total	C	O	0	0
			10	6	4		
6	M	1	Total	C	O	0	0
			10	6	4		
6	O	1	Total	C	O	0	0
			10	6	4		
6	Q	1	Total	C	O	0	0
			10	6	4		
6	S	1	Total	C	O	0	0
			10	6	4		
6	U	1	Total	C	O	0	0
			10	6	4		
6	W	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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	681	Total 681	O 681	0	0
8	B	169	Total 169	O 169	0	0
8	C	684	Total 684	O 684	0	0
8	D	162	Total 162	O 162	0	0
8	E	688	Total 688	O 688	0	0
8	F	160	Total 160	O 160	0	0

Continued on next page...

Continued from previous page...

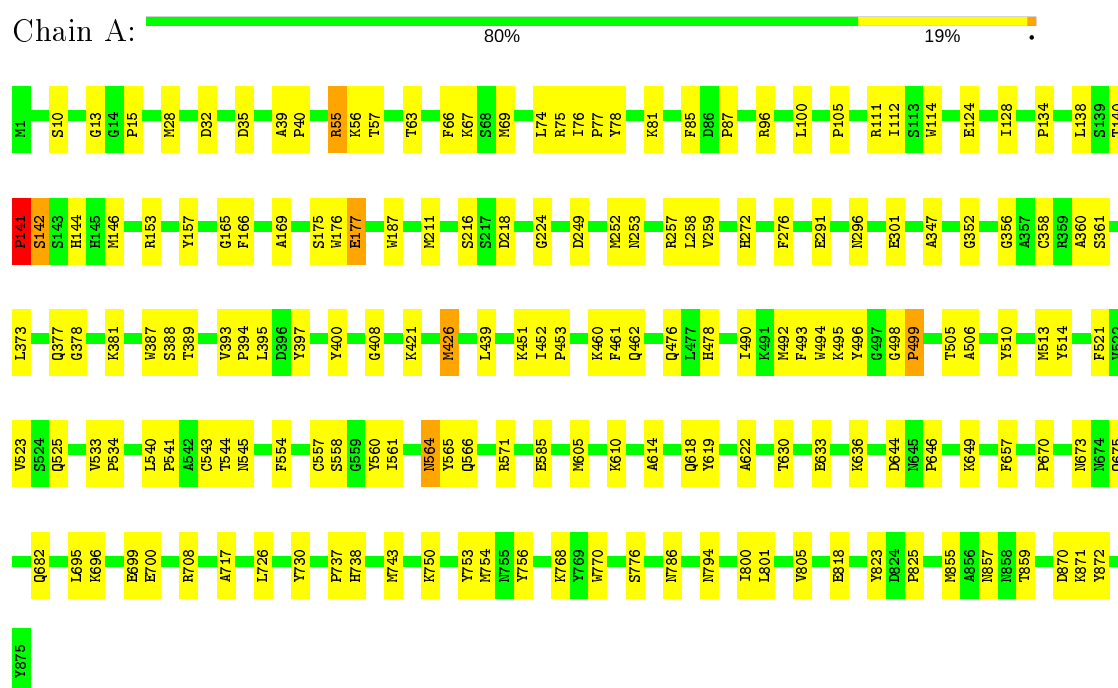
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	682	Total 682	O 682	0	0
8	H	161	Total 161	O 161	0	0
8	I	671	Total 671	O 671	0	0
8	J	168	Total 168	O 168	0	0
8	K	681	Total 681	O 681	0	0
8	L	165	Total 165	O 165	0	0
8	M	682	Total 682	O 682	0	0
8	N	160	Total 160	O 160	0	0
8	O	675	Total 675	O 675	0	0
8	P	160	Total 160	O 160	0	0
8	Q	693	Total 693	O 693	0	0
8	R	158	Total 158	O 158	0	0
8	S	665	Total 665	O 665	0	0
8	T	162	Total 162	O 162	0	0
8	U	670	Total 670	O 670	0	0
8	V	154	Total 154	O 154	0	0
8	W	675	Total 675	O 675	0	0
8	X	165	Total 165	O 165	0	0

3 Residue-property plots

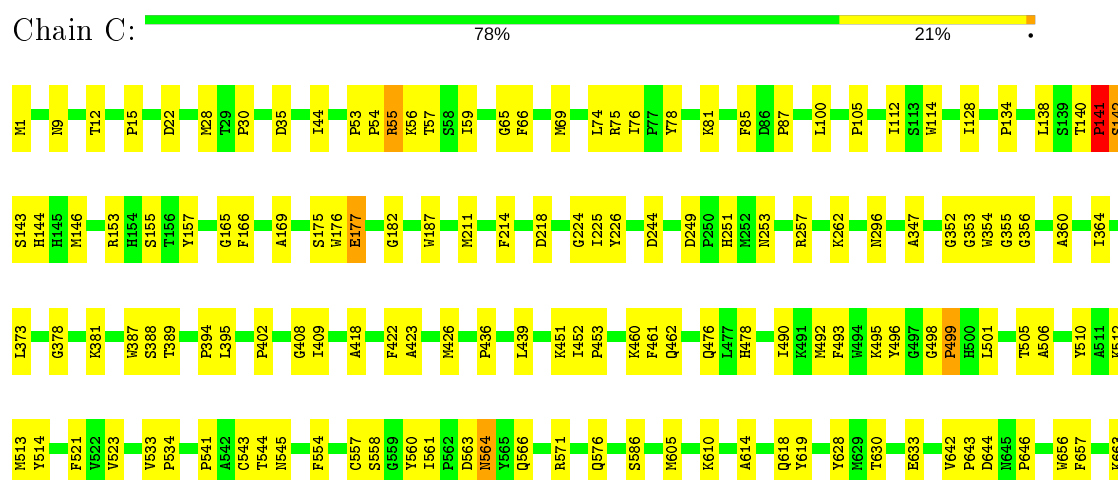
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

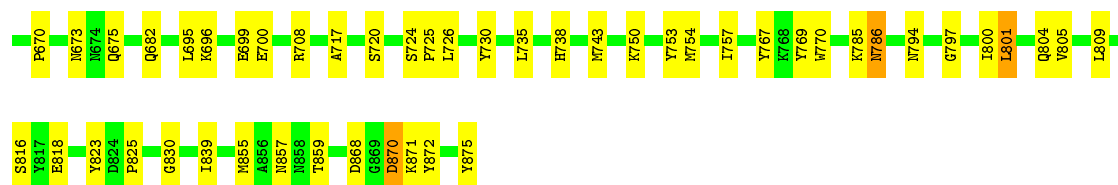
Note EDS was not executed.

- Molecule 1: Pyrogallol hydroxytransferase large subunit



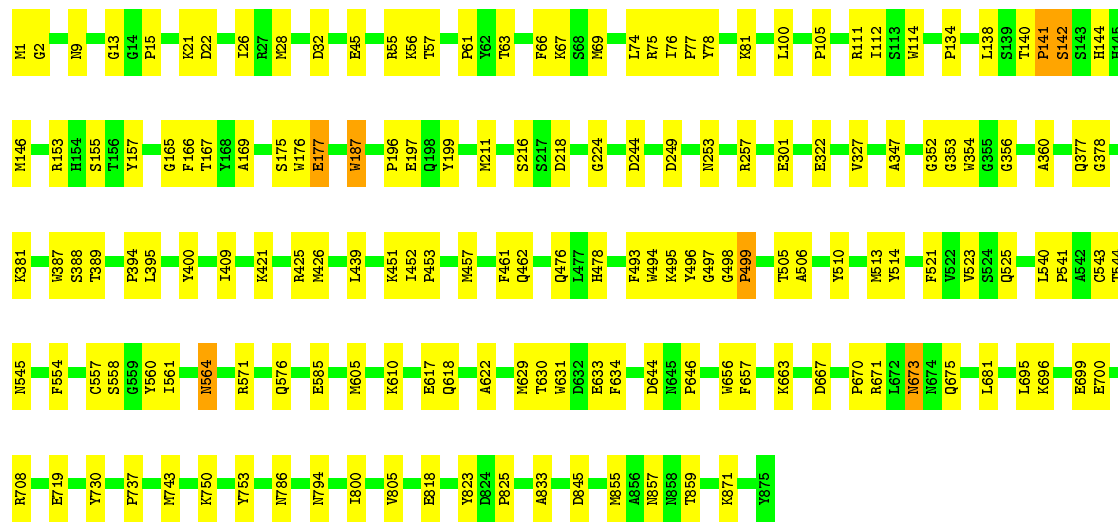
- Molecule 1: Pyrogallol hydroxytransferase large subunit





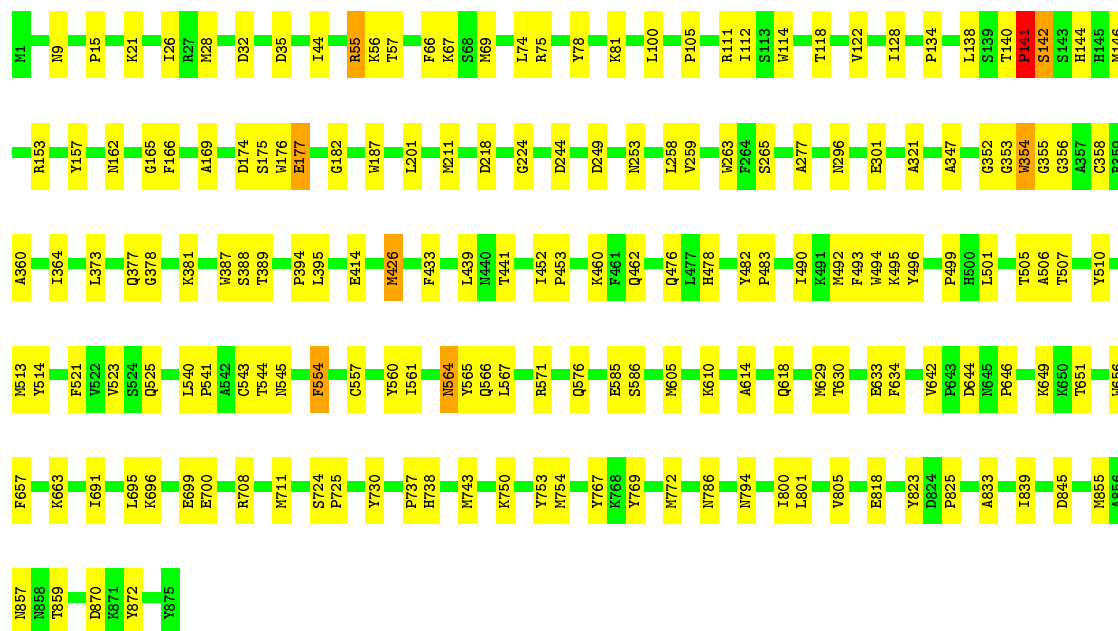
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain E: 81% 18%

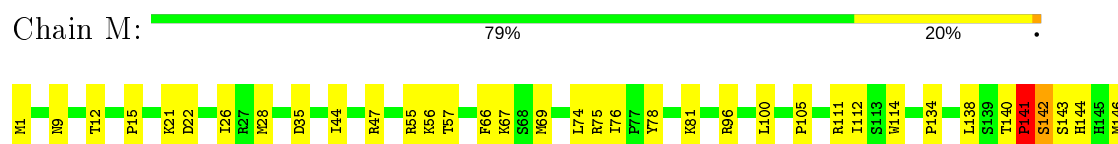
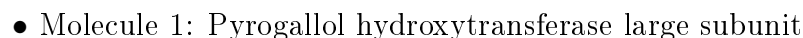
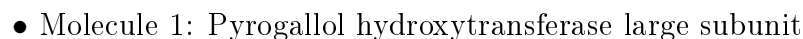


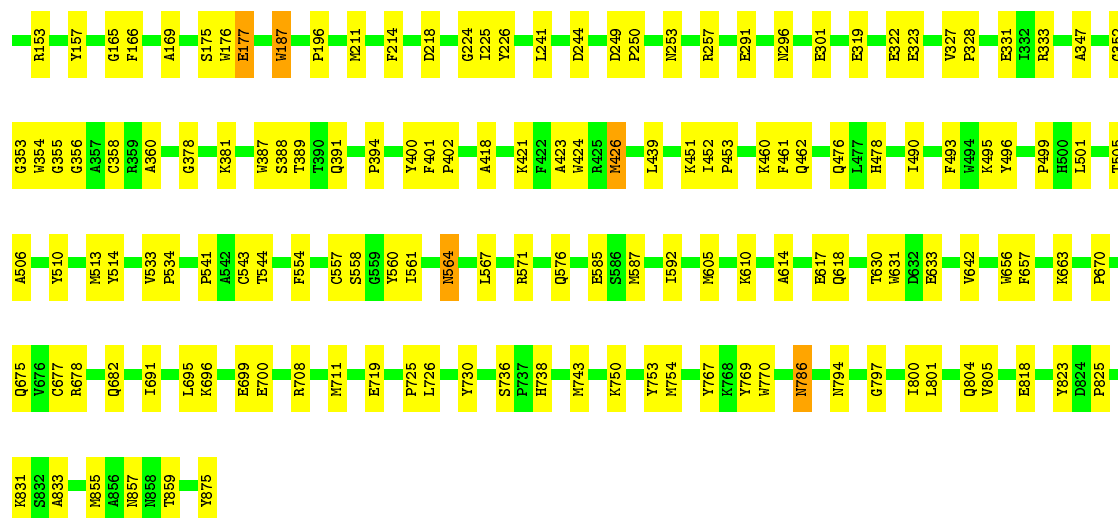
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain G: 80% 19%



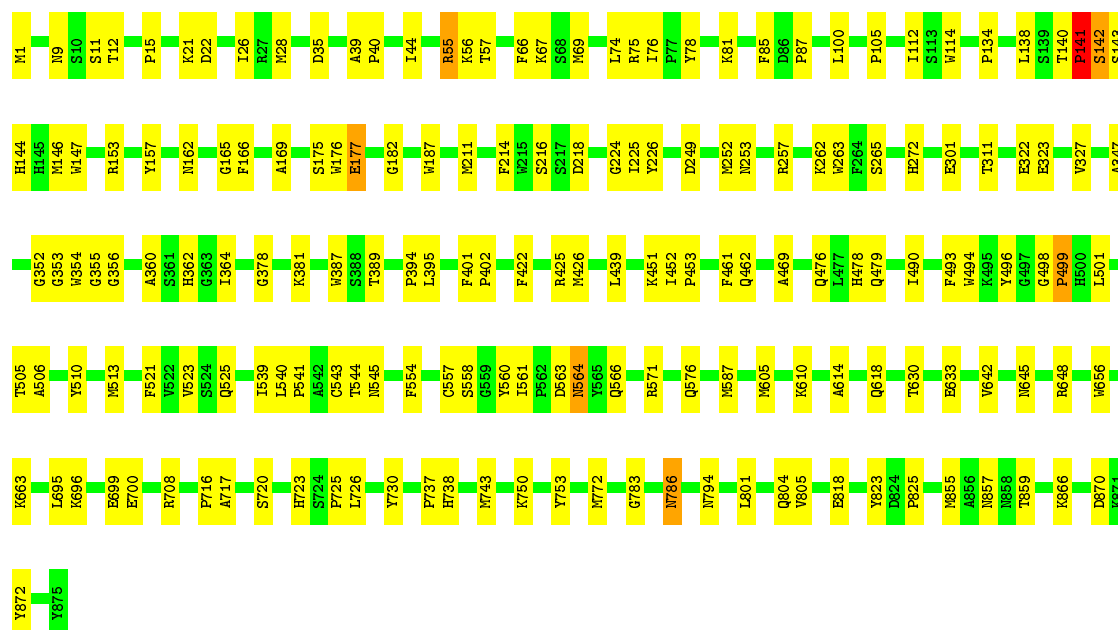
- Molecule 1: Pyrogallol hydroxytransferase large subunit





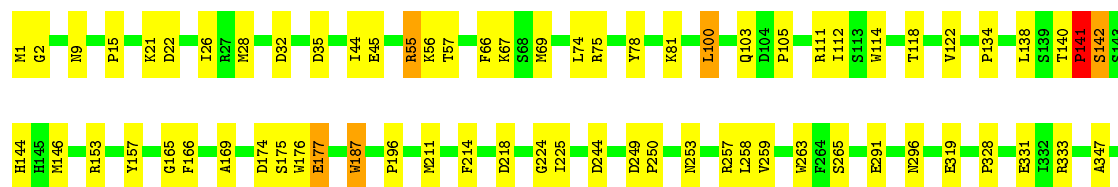
• Molecule 1: Pyrogallol hydroxytransferase large subunit

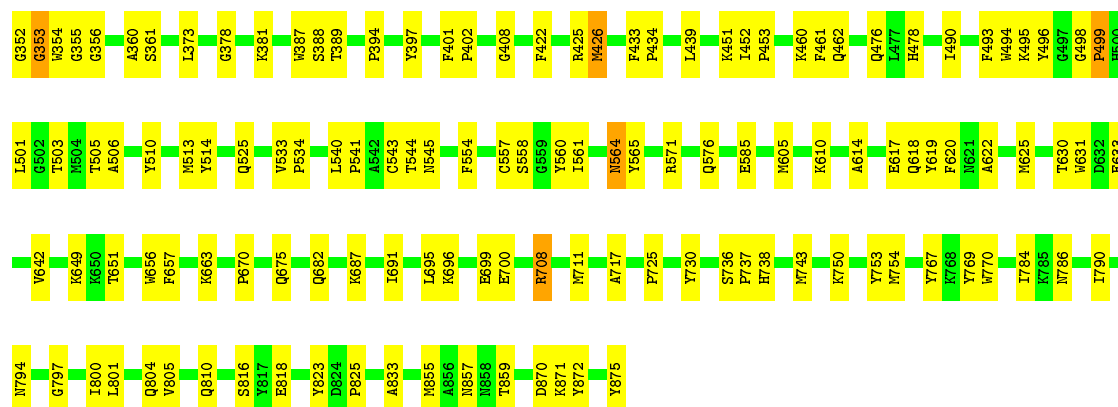
Chain O: 80% 19%



• Molecule 1: Pyrogallol hydroxytransferase large subunit

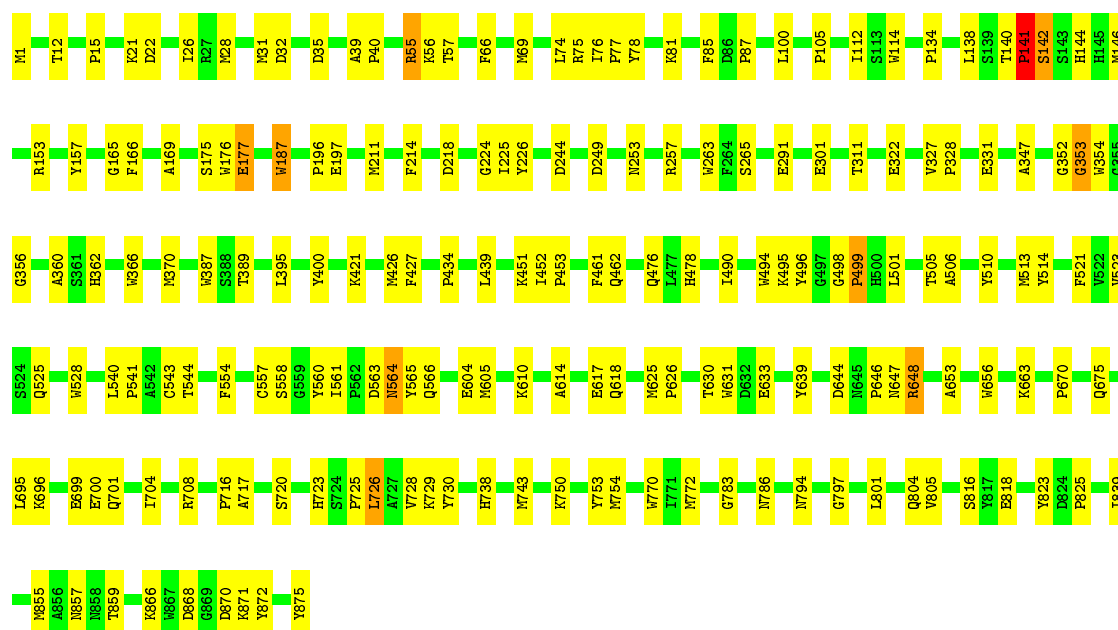
Chain Q: 77% 21%





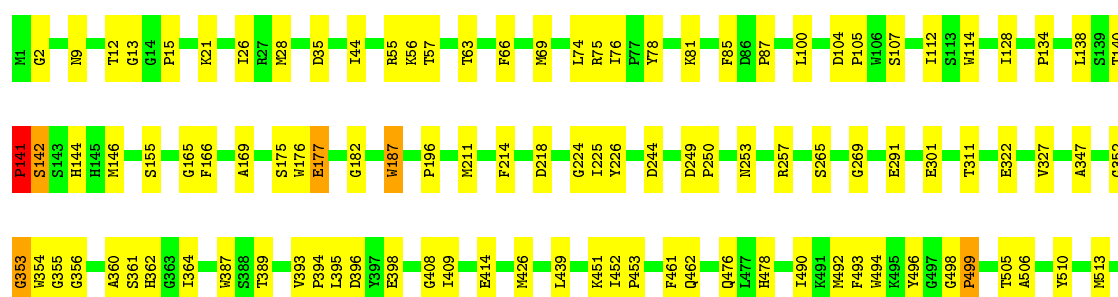
• Molecule 1: Pyrogallol hydroxytransferase large subunit

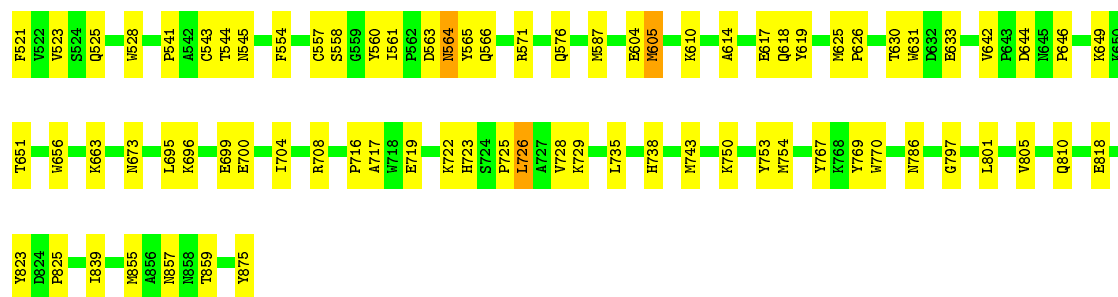
Chain S: 79% 20% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

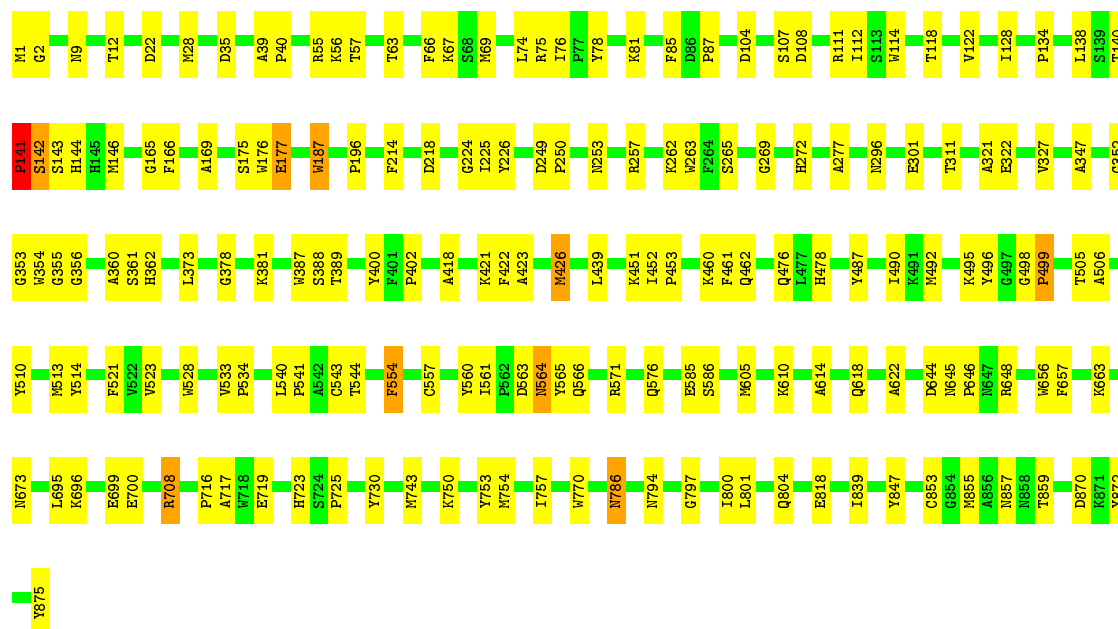
Chain U: 79% 20% .





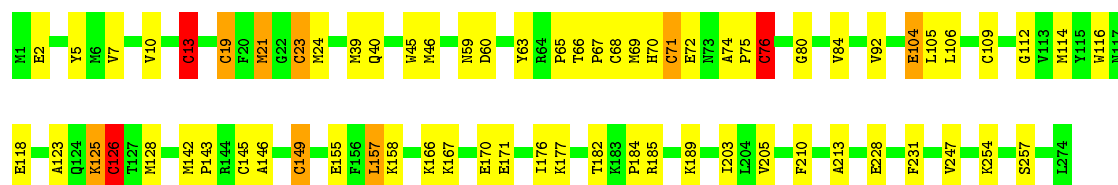
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain W: 80% 19%



• Molecule 2: Pyrogallol hydroxytransferase small subunit

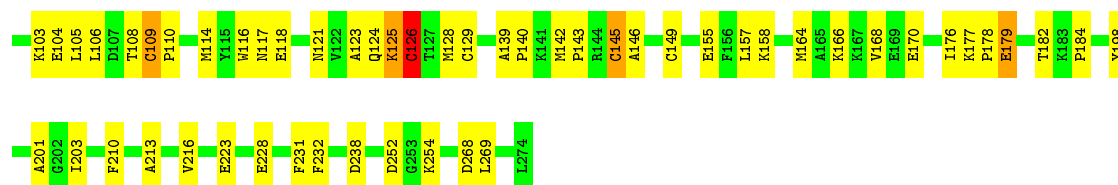
Chain B: 75% 21%



• Molecule 2: Pyrogallol hydroxytransferase small subunit

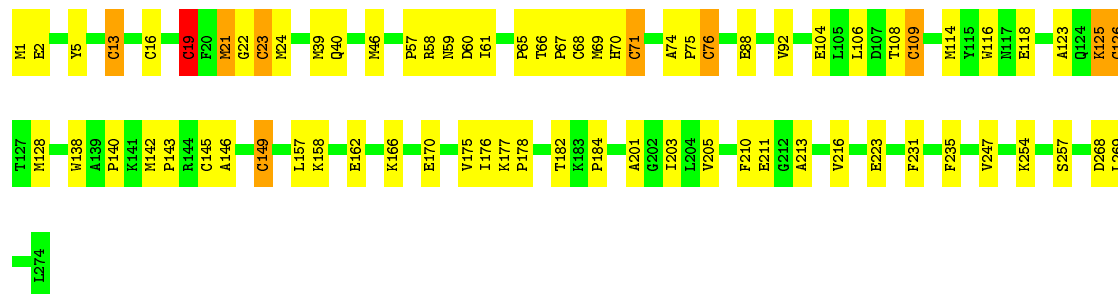
Chain D: 66% 30%





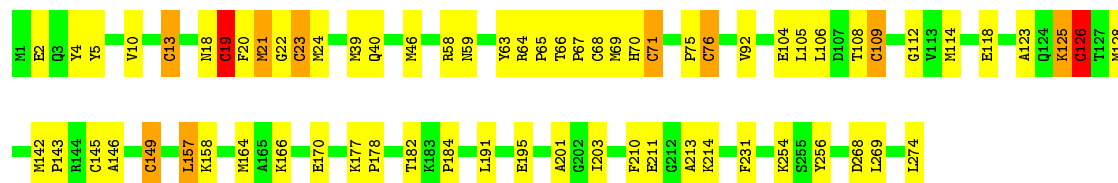
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain F: 73% 23% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H: 75% 21% . .



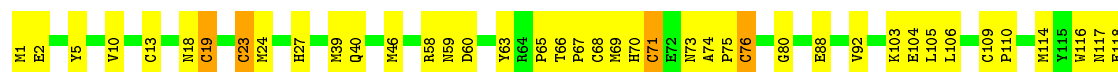
• Molecule 2: Pyrogallol hydroxytransferase small subunit

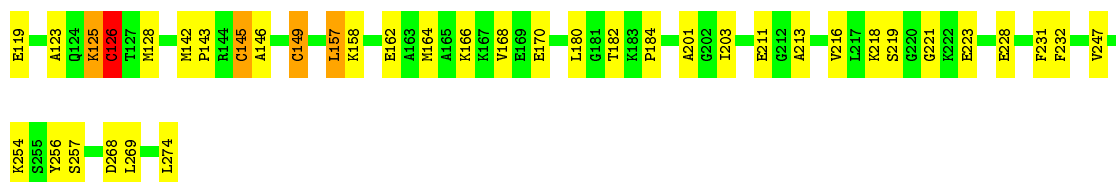
Chain J: 73% 23% . .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

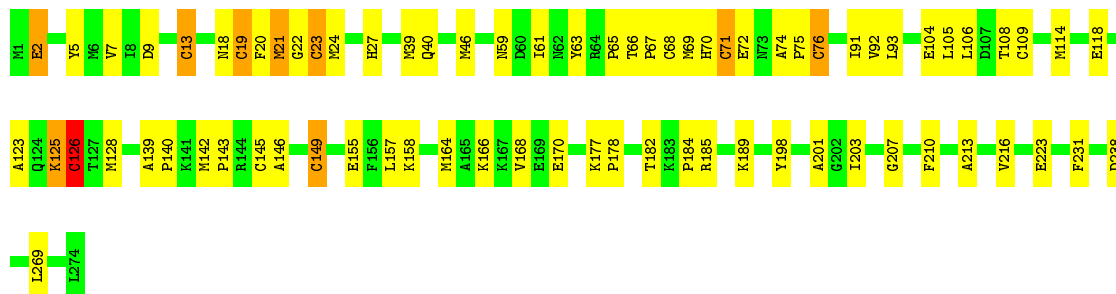
Chain L: 71% 26% .





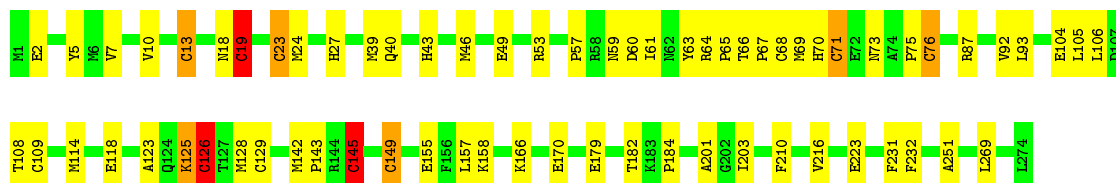
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N: 73% 24%



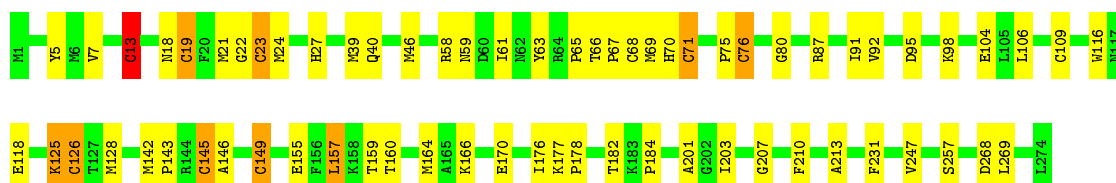
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P: 75% 22%



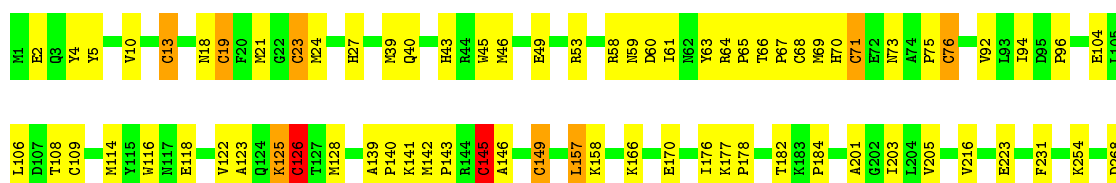
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R: 76% 21%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

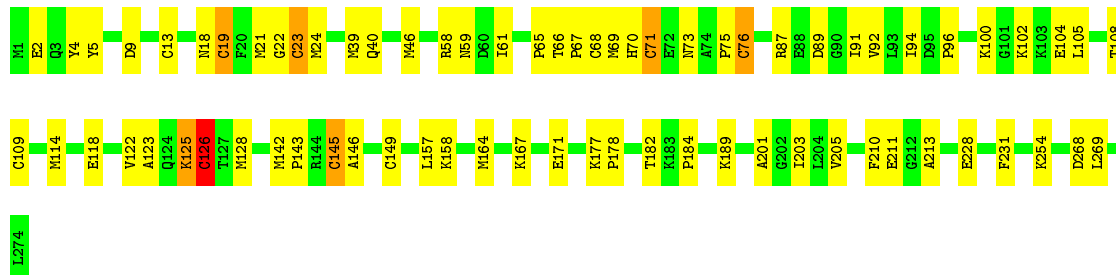
Chain T: 73% 24%





- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V: 74% 24%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X: 69% 27%



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	172.57Å 178.44Å 179.66Å 63.83° 64.40° 65.04°	Depositor
Resolution (Å)	24.99 – 2.00	Depositor
% Data completeness (in resolution range)	96.5 (24.99-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121823	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: BTT, SF4, 4MO, CA, MGD

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	0.33	0/7219	0.63	3/9786 (0.0%)
1	C	0.32	0/7219	0.61	3/9786 (0.0%)
1	E	0.33	0/7219	0.63	2/9786 (0.0%)
1	G	0.33	0/7219	0.63	3/9786 (0.0%)
1	I	0.32	0/7219	0.62	3/9786 (0.0%)
1	K	0.33	0/7219	0.63	4/9786 (0.0%)
1	M	0.33	0/7219	0.63	3/9786 (0.0%)
1	O	0.33	0/7219	0.62	3/9786 (0.0%)
1	Q	0.33	0/7219	0.63	4/9786 (0.0%)
1	S	0.32	0/7219	0.62	4/9786 (0.0%)
1	U	0.32	0/7219	0.62	4/9786 (0.0%)
1	W	0.32	0/7219	0.61	3/9786 (0.0%)
2	B	0.55	5/2231 (0.2%)	0.73	6/3009 (0.2%)
2	D	0.44	4/2231 (0.2%)	0.64	2/3009 (0.1%)
2	F	0.54	5/2231 (0.2%)	0.72	5/3009 (0.2%)
2	H	0.54	4/2231 (0.2%)	0.72	5/3009 (0.2%)
2	J	0.52	4/2231 (0.2%)	0.70	5/3009 (0.2%)
2	L	0.52	4/2231 (0.2%)	0.71	4/3009 (0.1%)
2	N	0.51	4/2231 (0.2%)	0.70	4/3009 (0.1%)
2	P	0.51	4/2231 (0.2%)	0.68	4/3009 (0.1%)
2	R	0.55	4/2231 (0.2%)	0.71	5/3009 (0.2%)
2	T	0.48	4/2231 (0.2%)	0.67	5/3009 (0.2%)
2	V	0.45	3/2231 (0.1%)	0.65	2/3009 (0.1%)
2	X	0.43	3/2231 (0.1%)	0.61	2/3009 (0.1%)
All	All	0.38	48/113400 (0.0%)	0.64	88/153540 (0.1%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	19	CYS	CB-SG	-9.78	1.65	1.82
2	P	23	CYS	CB-SG	-9.55	1.66	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	19	CYS	CB-SG	-9.47	1.66	1.82
2	J	23	CYS	CB-SG	-9.47	1.66	1.82
2	H	23	CYS	CB-SG	-9.46	1.66	1.82

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	352	GLY	N-CA-C	-9.07	90.42	113.10
1	I	352	GLY	N-CA-C	-8.62	91.55	113.10
1	Q	352	GLY	N-CA-C	-8.60	91.61	113.10
1	A	352	GLY	N-CA-C	-8.54	91.74	113.10
1	E	352	GLY	N-CA-C	-8.48	91.90	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6998	0	6632	150	0
1	C	6998	0	6632	157	0
1	E	6998	0	6632	140	0
1	G	6998	0	6632	141	0
1	I	6998	0	6632	141	0
1	K	6998	0	6632	149	0
1	M	6998	0	6632	152	0
1	O	6998	0	6632	140	1
1	Q	6998	0	6632	160	0
1	S	6998	0	6632	155	0
1	U	6998	0	6632	151	0
1	W	6998	0	6632	139	0
2	B	2182	0	2077	64	0
2	D	2182	0	2077	88	0
2	F	2182	0	2077	67	0
2	H	2182	0	2077	67	0
2	J	2182	0	2077	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2182	0	2077	75	0
2	N	2182	0	2077	73	0
2	P	2182	0	2077	61	0
2	R	2182	0	2077	64	0
2	T	2182	0	2077	61	0
2	V	2182	0	2077	66	0
2	X	2182	0	2077	74	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	94	0	44	11	0
4	C	94	0	44	15	0
4	E	94	0	44	13	0
4	G	94	0	44	15	0
4	I	94	0	44	10	0
4	K	94	0	44	14	0
4	M	94	0	44	16	0
4	O	94	0	44	17	0
4	Q	94	0	44	16	0
4	S	94	0	44	11	0
4	U	94	0	44	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	94	0	44	14	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
5	Q	1	0	0	0	0
5	S	1	0	0	0	0
5	U	1	0	0	0	0
5	W	1	0	0	0	0
6	A	10	0	2	1	0
6	C	10	0	2	1	0
6	E	10	0	2	1	0
6	G	10	0	2	1	0
6	I	10	0	2	1	0
6	K	10	0	2	1	0
6	M	10	0	2	1	0
6	O	10	0	2	1	0
6	Q	10	0	2	1	0
6	S	10	0	2	1	0
6	U	10	0	2	1	0
6	W	10	0	2	1	0
7	B	24	0	0	3	0
7	D	24	0	0	4	0
7	F	24	0	0	4	0
7	H	24	0	0	4	0
7	J	24	0	0	4	0
7	L	24	0	0	4	0
7	N	24	0	0	5	0
7	P	24	0	0	4	0
7	R	24	0	0	4	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	4	0
8	A	681	0	0	13	2
8	B	169	0	0	4	0
8	C	684	0	0	10	0
8	D	162	0	0	1	0
8	E	688	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	160	0	0	1	0
8	G	682	0	0	9	0
8	H	161	0	0	1	0
8	I	671	0	0	6	0
8	J	168	0	0	2	0
8	K	681	0	0	6	0
8	L	165	0	0	3	0
8	M	682	0	0	11	0
8	N	160	0	0	1	0
8	O	675	0	0	12	1
8	P	160	0	0	3	0
8	Q	693	0	0	13	0
8	R	158	0	0	2	0
8	S	665	0	0	13	0
8	T	162	0	0	1	0
8	U	670	0	0	9	0
8	V	154	0	0	0	0
8	W	675	0	0	8	0
8	X	165	0	0	2	0
All	All	121823	0	105060	2542	2

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 12.

The worst 5 of 2542 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:U:426:MET:HE1	1:U:618:GLN:HG2	1.31	1.10
1:I:356:GLY:N	4:I:903:MGD:O1B	1.86	1.09
1:C:356:GLY:N	4:C:903:MGD:O1B	1.86	1.09
1:C:557:CYS:H	1:C:564:ASN:HD21	1.08	1.00
2:D:19:CYS:HB3	2:D:145:CYS:HB3	1.44	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1584:HOH:O	8:O:1361:HOH:O[1_644]	2.06	0.14
1:O:162:ASN:O	8:A:1584:HOH:O[1_466]	2.19	0.01

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	873/875 (100%)	827 (95%)	44 (5%)	2 (0%)	47	44
1	C	873/875 (100%)	833 (95%)	37 (4%)	3 (0%)	41	37
1	E	873/875 (100%)	832 (95%)	39 (4%)	2 (0%)	47	44
1	G	873/875 (100%)	833 (95%)	37 (4%)	3 (0%)	41	37
1	I	873/875 (100%)	826 (95%)	44 (5%)	3 (0%)	41	37
1	K	873/875 (100%)	831 (95%)	39 (4%)	3 (0%)	41	37
1	M	873/875 (100%)	829 (95%)	41 (5%)	3 (0%)	41	37
1	O	873/875 (100%)	827 (95%)	43 (5%)	3 (0%)	41	37
1	Q	873/875 (100%)	835 (96%)	35 (4%)	3 (0%)	41	37
1	S	873/875 (100%)	826 (95%)	43 (5%)	4 (0%)	29	23
1	U	873/875 (100%)	829 (95%)	41 (5%)	3 (0%)	41	37
1	W	873/875 (100%)	826 (95%)	44 (5%)	3 (0%)	41	37
2	B	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	34	30
2	D	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	34	30
2	F	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	22	16
2	H	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	22	16
2	J	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	34	30
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	22	16
2	N	272/274 (99%)	262 (96%)	9 (3%)	1 (0%)	34	30
2	P	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	34	30
2	R	272/274 (99%)	260 (96%)	10 (4%)	2 (1%)	22	16
2	T	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	22	16
2	V	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	34	30
2	X	272/274 (99%)	252 (93%)	18 (7%)	2 (1%)	22	16
All	All	13740/13788 (100%)	13061 (95%)	626 (5%)	53 (0%)	34	30

5 of 53 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	K	177	GLU

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	729/729 (100%)	713 (98%)	16 (2%)	52	55	
1	C	729/729 (100%)	713 (98%)	16 (2%)	52	55	
1	E	729/729 (100%)	716 (98%)	13 (2%)	59	63	
1	G	729/729 (100%)	713 (98%)	16 (2%)	52	55	
1	I	729/729 (100%)	714 (98%)	15 (2%)	53	57	
1	K	729/729 (100%)	714 (98%)	15 (2%)	53	57	
1	M	729/729 (100%)	713 (98%)	16 (2%)	52	55	
1	O	729/729 (100%)	714 (98%)	15 (2%)	53	57	
1	Q	729/729 (100%)	713 (98%)	16 (2%)	52	55	
1	S	729/729 (100%)	717 (98%)	12 (2%)	62	67	
1	U	729/729 (100%)	715 (98%)	14 (2%)	57	61	
1	W	729/729 (100%)	713 (98%)	16 (2%)	52	55	
2	B	235/235 (100%)	223 (95%)	12 (5%)	24	19	
2	D	235/235 (100%)	221 (94%)	14 (6%)	19	14	
2	F	235/235 (100%)	227 (97%)	8 (3%)	37	36	
2	H	235/235 (100%)	226 (96%)	9 (4%)	33	31	
2	J	235/235 (100%)	223 (95%)	12 (5%)	24	19	
2	L	235/235 (100%)	225 (96%)	10 (4%)	29	26	
2	N	235/235 (100%)	226 (96%)	9 (4%)	33	31	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	235/235 (100%)	223 (95%)	12 (5%)	24	19
2	R	235/235 (100%)	227 (97%)	8 (3%)	37	36
2	T	235/235 (100%)	224 (95%)	11 (5%)	26	22
2	V	235/235 (100%)	225 (96%)	10 (4%)	29	26
2	X	235/235 (100%)	223 (95%)	12 (5%)	24	19
All	All	11568/11568 (100%)	11261 (97%)	307 (3%)	44	46

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	493	PHE
1	M	818	GLU
1	W	373	LEU
1	K	605	MET
2	L	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 229 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	564	ASN
2	N	27	HIS
1	W	171	HIS
1	K	697	ASN
1	M	162	ASN

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 carbohydrates 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
4	MGD	Q	903	5	41,52,52	2.48	12 (29%)	43,81,81	3.35	19 (44%)
7	SF4	T	302	2	0,12,12	0.00	-	-		
6	BTT	W	905	5	10,10,10	8.76	6 (60%)	14,14,14	2.20	3 (21%)
7	SF4	D	304	2	0,12,12	0.00	-	-		
4	MGD	M	903	5	41,52,52	2.48	12 (29%)	43,81,81	3.25	18 (41%)
6	BTT	O	905	5	10,10,10	8.77	6 (60%)	14,14,14	2.19	3 (21%)
7	SF4	V	303	2	0,12,12	0.00	-	-		
7	SF4	X	304	2	0,12,12	0.00	-	-		
4	MGD	A	903	5	41,52,52	2.55	13 (31%)	43,81,81	3.14	18 (41%)
7	SF4	V	304	2	0,12,12	0.00	-	-		
4	MGD	O	903	5	41,52,52	2.53	13 (31%)	43,81,81	3.25	21 (48%)
7	SF4	V	302	2	0,12,12	0.00	-	-		
4	MGD	K	903	5	41,52,52	2.50	14 (34%)	43,81,81	3.10	19 (44%)
4	MGD	E	903	5	41,52,52	2.48	12 (29%)	43,81,81	3.12	18 (41%)
6	BTT	K	905	5	10,10,10	8.76	6 (60%)	14,14,14	2.21	3 (21%)
4	MGD	S	903	5	41,52,52	2.48	14 (34%)	43,81,81	2.96	17 (39%)
7	SF4	L	303	2	0,12,12	0.00	-	-		
4	MGD	E	902	5	41,52,52	2.36	12 (29%)	43,81,81	2.46	17 (39%)
6	BTT	S	905	5	10,10,10	8.81	6 (60%)	14,14,14	2.19	4 (28%)
7	SF4	F	302	2	0,12,12	0.00	-	-		
7	SF4	J	302	2	0,12,12	0.00	-	-		
4	MGD	C	902	5	41,52,52	2.40	11 (26%)	43,81,81	2.49	18 (41%)
7	SF4	T	303	2	0,12,12	0.00	-	-		
4	MGD	M	902	5	41,52,52	2.34	11 (26%)	43,81,81	2.48	17 (39%)
7	SF4	R	304	2	0,12,12	0.00	-	-		
7	SF4	N	304	2	0,12,12	0.00	-	-		
7	SF4	B	302	2	0,12,12	0.00	-	-		
7	SF4	H	302	2	0,12,12	0.00	-	-		
4	MGD	W	902	5	41,52,52	2.37	10 (24%)	43,81,81	2.47	17 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	K	902	5	41,52,52	2.40	12 (29%)	43,81,81	2.38	14 (32%)
4	MGD	Q	902	5	41,52,52	2.42	12 (29%)	43,81,81	2.48	15 (34%)
6	BTT	I	905	5	10,10,10	8.74	6 (60%)	14,14,14	2.19	3 (21%)
7	SF4	P	302	2	0,12,12	0.00	-	-		
7	SF4	J	303	2	0,12,12	0.00	-	-		
7	SF4	B	304	2	0,12,12	0.00	-	-		
4	MGD	A	902	5	41,52,52	2.38	12 (29%)	43,81,81	2.46	16 (37%)
7	SF4	R	303	2	0,12,12	0.00	-	-		
4	MGD	G	902	5	41,52,52	2.36	11 (26%)	43,81,81	2.43	16 (37%)
7	SF4	P	303	2	0,12,12	0.00	-	-		
7	SF4	J	304	2	0,12,12	0.00	-	-		
6	BTT	C	905	5	10,10,10	8.79	6 (60%)	14,14,14	2.21	3 (21%)
4	MGD	U	903	5	41,52,52	2.39	10 (24%)	43,81,81	3.09	18 (41%)
4	MGD	G	903	5	41,52,52	2.53	16 (39%)	43,81,81	3.35	19 (44%)
4	MGD	O	902	5	41,52,52	2.36	12 (29%)	43,81,81	2.47	15 (34%)
7	SF4	X	303	2	0,12,12	0.00	-	-		
7	SF4	D	302	2	0,12,12	0.00	-	-		
6	BTT	G	905	5	10,10,10	8.77	6 (60%)	14,14,14	2.12	3 (21%)
4	MGD	U	902	5	41,52,52	2.43	11 (26%)	43,81,81	2.49	16 (37%)
4	MGD	I	902	5	41,52,52	2.30	12 (29%)	43,81,81	2.46	16 (37%)
7	SF4	B	303	2	0,12,12	0.00	-	-		
6	BTT	M	905	5	10,10,10	8.72	6 (60%)	14,14,14	2.15	3 (21%)
7	SF4	L	302	2	0,12,12	0.00	-	-		
7	SF4	F	303	2	0,12,12	0.00	-	-		
4	MGD	S	902	5	41,52,52	2.36	13 (31%)	43,81,81	2.47	16 (37%)
7	SF4	N	302	2	0,12,12	0.00	-	-		
6	BTT	Q	905	5	10,10,10	8.76	6 (60%)	14,14,14	2.14	3 (21%)
7	SF4	H	304	2	0,12,12	0.00	-	-		
6	BTT	U	905	5	10,10,10	8.77	6 (60%)	14,14,14	2.22	3 (21%)
7	SF4	N	303	2	0,12,12	0.00	-	-		
7	SF4	R	302	2	0,12,12	0.00	-	-		
7	SF4	X	302	2	0,12,12	0.00	-	-		
7	SF4	L	304	2	0,12,12	0.00	-	-		
6	BTT	A	905	5	10,10,10	8.76	6 (60%)	14,14,14	2.16	3 (21%)
7	SF4	P	304	2	0,12,12	0.00	-	-		
4	MGD	C	903	5	41,52,52	2.56	11 (26%)	43,81,81	2.96	17 (39%)
7	SF4	T	304	2	0,12,12	0.00	-	-		
7	SF4	F	304	2	0,12,12	0.00	-	-		
7	SF4	H	303	2	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	I	903	5	41,52,52	2.54	13 (31%)	43,81,81	3.00	17 (39%)
6	BTT	E	905	5	10,10,10	8.81	6 (60%)	14,14,14	2.13	4 (28%)
4	MGD	W	903	5	41,52,52	2.49	13 (31%)	43,81,81	3.17	18 (41%)
7	SF4	D	303	2	0,12,12	0.00	-	-		

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
4	MGD	Q	903	5	-	6/18/66/66	0/6/6/6
7	SF4	T	302	2	-	-	0/6/5/5
6	BTT	W	905	5	-	-	0/1/1/1
7	SF4	D	304	2	-	-	0/6/5/5
4	MGD	M	903	5	-	5/18/66/66	0/6/6/6
7	SF4	R	304	2	-	-	0/6/5/5
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	X	304	2	-	-	0/6/5/5
4	MGD	A	903	5	-	9/18/66/66	0/6/6/6
7	SF4	V	304	2	-	-	0/6/5/5
4	MGD	O	903	5	-	8/18/66/66	0/6/6/6
7	SF4	V	302	2	-	-	0/6/5/5
4	MGD	K	903	5	-	8/18/66/66	0/6/6/6
4	MGD	E	903	5	-	8/18/66/66	0/6/6/6
6	BTT	K	905	5	-	-	0/1/1/1
4	MGD	S	903	5	-	4/18/66/66	0/6/6/6
7	SF4	L	303	2	-	-	0/6/5/5
4	MGD	E	902	5	-	8/18/66/66	0/6/6/6
6	BTT	S	905	5	-	-	0/1/1/1
7	SF4	F	302	2	-	-	0/6/5/5
7	SF4	J	302	2	-	-	0/6/5/5
4	MGD	C	902	5	-	8/18/66/66	0/6/6/6
7	SF4	T	303	2	-	-	0/6/5/5
4	MGD	M	902	5	-	8/18/66/66	0/6/6/6
6	BTT	O	905	5	-	-	0/1/1/1
4	MGD	I	902	5	-	8/18/66/66	0/6/6/6
7	SF4	N	304	2	-	-	0/6/5/5
4	MGD	K	902	5	-	10/18/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BTT	A	905	5	-	-	0/1/1/1
7	SF4	H	302	2	-	-	0/6/5/5
4	MGD	W	902	5	-	8/18/66/66	0/6/6/6
7	SF4	B	302	2	-	-	0/6/5/5
4	MGD	Q	902	5	-	8/18/66/66	0/6/6/6
7	SF4	J	304	2	-	-	0/6/5/5
7	SF4	P	302	2	-	-	0/6/5/5
4	MGD	W	903	5	-	5/18/66/66	0/6/6/6
7	SF4	B	304	2	-	-	0/6/5/5
7	SF4	R	303	2	-	-	0/6/5/5
4	MGD	G	902	5	-	8/18/66/66	0/6/6/6
7	SF4	P	303	2	-	-	0/6/5/5
4	MGD	A	902	5	-	8/18/66/66	0/6/6/6
4	MGD	U	903	5	-	4/18/66/66	0/6/6/6
4	MGD	G	903	5	-	7/18/66/66	0/6/6/6
4	MGD	O	902	5	-	8/18/66/66	0/6/6/6
7	SF4	X	303	2	-	-	0/6/5/5
7	SF4	D	302	2	-	-	0/6/5/5
6	BTT	G	905	5	-	-	0/1/1/1
4	MGD	U	902	5	-	8/18/66/66	0/6/6/6
7	SF4	H	303	2	-	-	0/6/5/5
7	SF4	B	303	2	-	-	0/6/5/5
6	BTT	M	905	5	-	-	0/1/1/1
7	SF4	L	302	2	-	-	0/6/5/5
7	SF4	F	303	2	-	-	0/6/5/5
4	MGD	S	902	5	-	8/18/66/66	0/6/6/6
7	SF4	N	302	2	-	-	0/6/5/5
6	BTT	Q	905	5	-	-	0/1/1/1
7	SF4	H	304	2	-	-	0/6/5/5
6	BTT	U	905	5	-	-	0/1/1/1
7	SF4	N	303	2	-	-	0/6/5/5
7	SF4	R	302	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
7	SF4	L	304	2	-	-	0/6/5/5
6	BTT	I	905	5	-	-	0/1/1/1
7	SF4	P	304	2	-	-	0/6/5/5
4	MGD	C	903	5	-	4/18/66/66	0/6/6/6
7	SF4	T	304	2	-	-	0/6/5/5
7	SF4	F	304	2	-	-	0/6/5/5
6	BTT	C	905	5	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	I	903	5	-	4/18/66/66	0/6/6/6
6	BTT	E	905	5	-	-	0/1/1/1
7	SF4	J	303	2	-	-	0/6/5/5
7	SF4	D	303	2	-	-	0/6/5/5

The worst 5 of 364 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	905	BTT	C3-C2	15.87	1.61	1.38
6	A	905	BTT	C3-C2	15.82	1.61	1.38
6	S	905	BTT	C3-C2	15.82	1.61	1.38
6	K	905	BTT	C3-C2	15.79	1.61	1.38
6	G	905	BTT	C3-C2	15.70	1.61	1.38

The worst 5 of 450 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	903	MGD	O11-C23-C14	-10.02	102.28	108.96
4	O	903	MGD	O11-C23-C14	-9.94	102.34	108.96
4	G	903	MGD	O11-C23-C14	-9.89	102.37	108.96
4	A	903	MGD	O11-C23-C14	-9.50	102.63	108.96
4	Q	903	MGD	O11-C23-C14	-9.49	102.63	108.96

There are no chirality outliers.

5 of 170 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	903	MGD	C5'-O5'-PB-O1B
4	M	903	MGD	C5'-O5'-PB-O2B
4	M	903	MGD	C5'-O5'-PB-O3B
4	E	903	MGD	C5'-O5'-PB-O1B
4	E	903	MGD	C5'-O5'-PB-O2B

There are no ring outliers.

70 monomers are involved in 227 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	903	MGD	11	0
7	T	302	SF4	1	0
6	W	905	BTT	1	0
7	D	304	SF4	1	0

Continued on next page...

Continued from previous page...

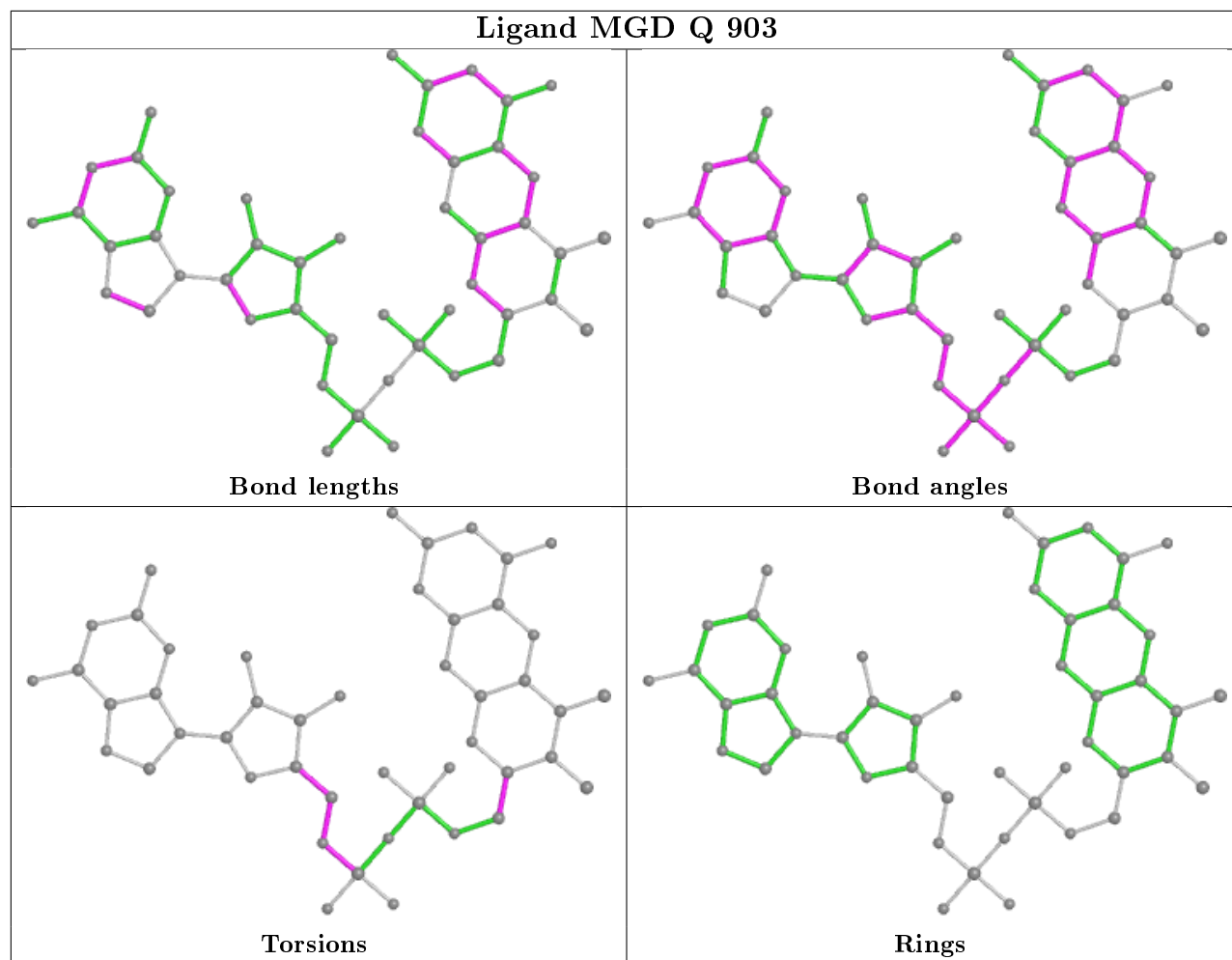
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	903	MGD	8	0
6	O	905	BTT	1	0
7	V	303	SF4	2	0
7	X	304	SF4	1	0
4	A	903	MGD	6	0
7	V	304	SF4	1	0
4	O	903	MGD	11	0
7	V	302	SF4	1	0
4	K	903	MGD	7	0
4	E	903	MGD	7	0
6	K	905	BTT	1	0
4	S	903	MGD	4	0
7	L	303	SF4	2	0
4	E	902	MGD	6	0
6	S	905	BTT	1	0
7	J	302	SF4	1	0
4	C	902	MGD	6	0
7	T	303	SF4	2	0
4	M	902	MGD	8	0
7	R	304	SF4	1	0
7	N	304	SF4	1	0
7	H	302	SF4	1	0
4	W	902	MGD	5	0
4	K	902	MGD	7	0
4	Q	902	MGD	5	0
6	I	905	BTT	1	0
7	P	302	SF4	1	0
7	J	303	SF4	2	0
7	B	304	SF4	1	0
4	A	902	MGD	5	0
7	R	303	SF4	2	0
4	G	902	MGD	6	0
7	P	303	SF4	2	0
7	J	304	SF4	1	0
6	C	905	BTT	1	0
4	U	903	MGD	9	0
4	G	903	MGD	9	0
4	O	902	MGD	6	0
7	X	303	SF4	2	0
7	D	302	SF4	1	0
6	G	905	BTT	1	0
4	U	902	MGD	6	0

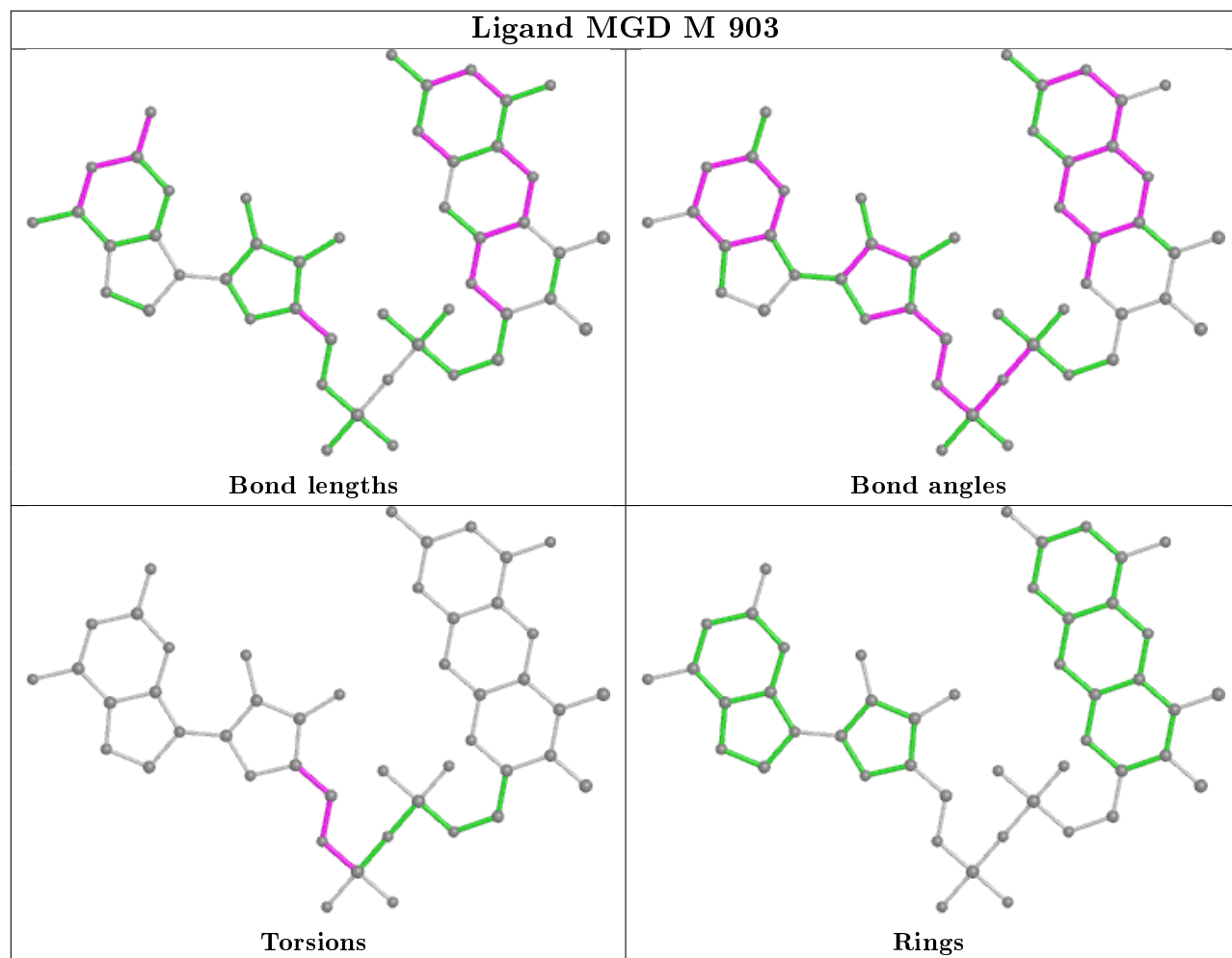
Continued on next page...

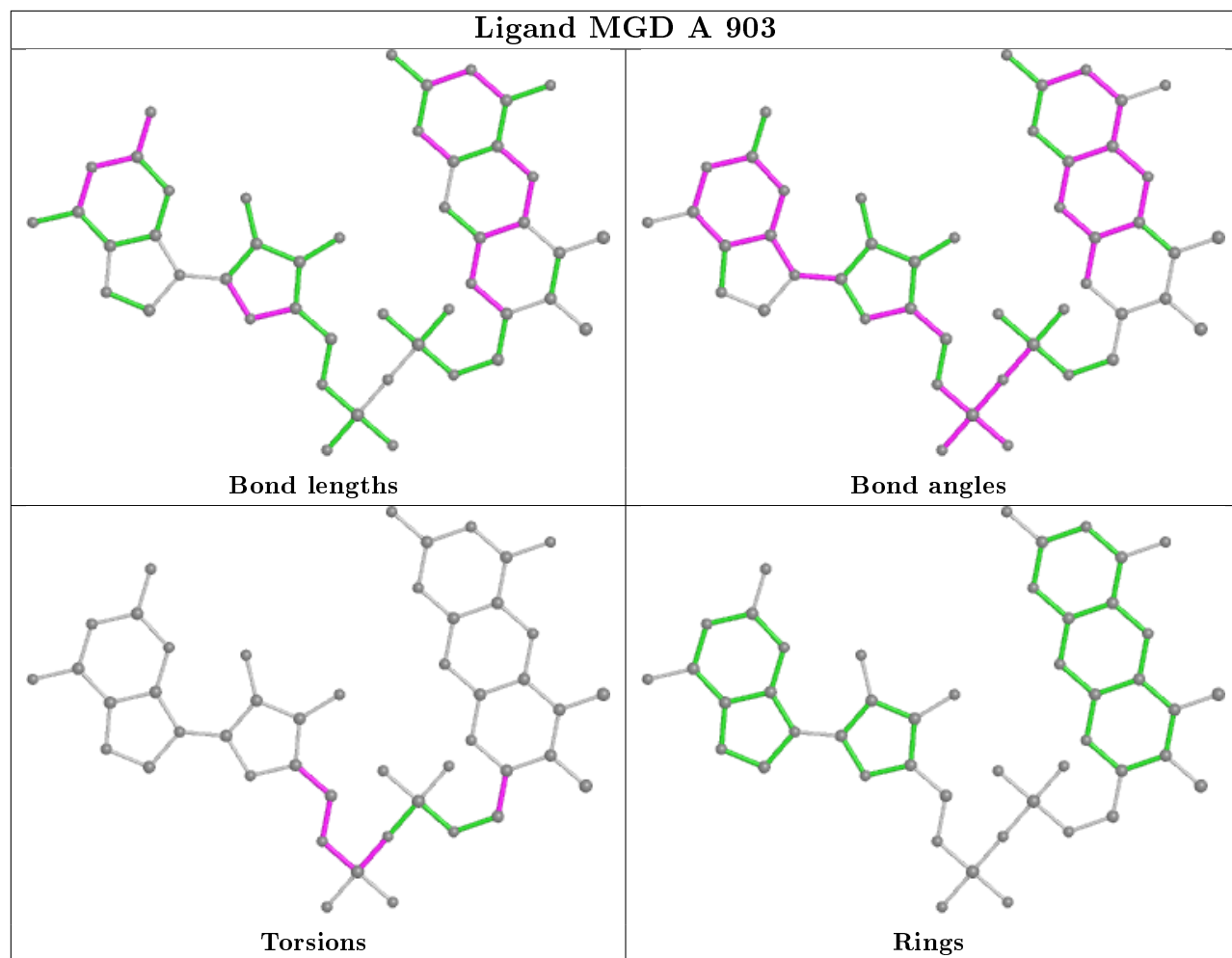
Continued from previous page...

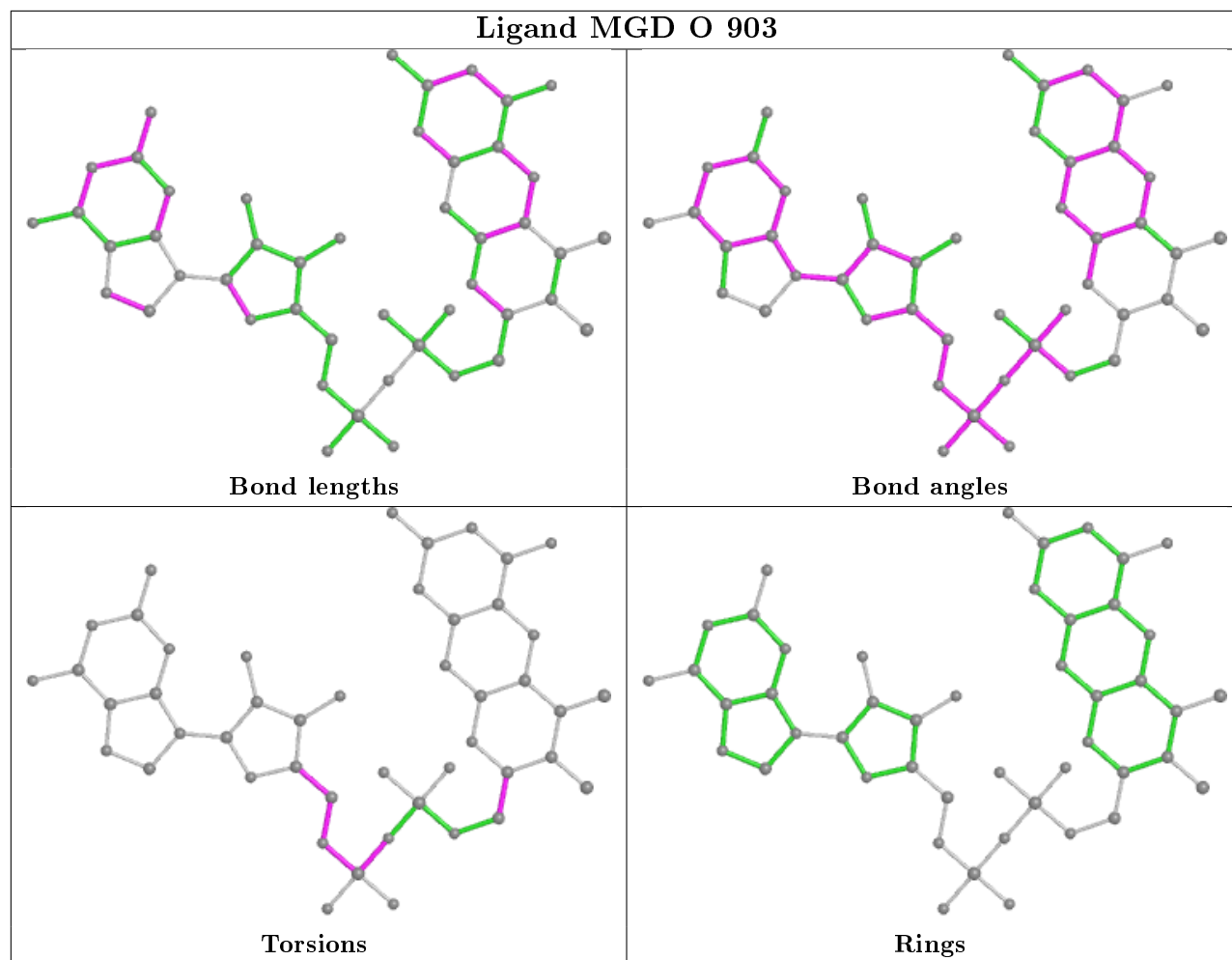
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	902	MGD	5	0
7	B	303	SF4	2	0
6	M	905	BTT	1	0
7	L	302	SF4	1	0
7	F	303	SF4	3	0
4	S	902	MGD	7	0
7	N	302	SF4	1	0
6	Q	905	BTT	1	0
7	H	304	SF4	1	0
6	U	905	BTT	1	0
7	N	303	SF4	3	0
7	R	302	SF4	1	0
7	X	302	SF4	1	0
7	L	304	SF4	1	0
6	A	905	BTT	1	0
7	P	304	SF4	1	0
4	C	903	MGD	9	0
7	T	304	SF4	1	0
7	F	304	SF4	1	0
7	H	303	SF4	2	0
4	I	903	MGD	5	0
6	E	905	BTT	1	0
4	W	903	MGD	9	0
7	D	303	SF4	2	0

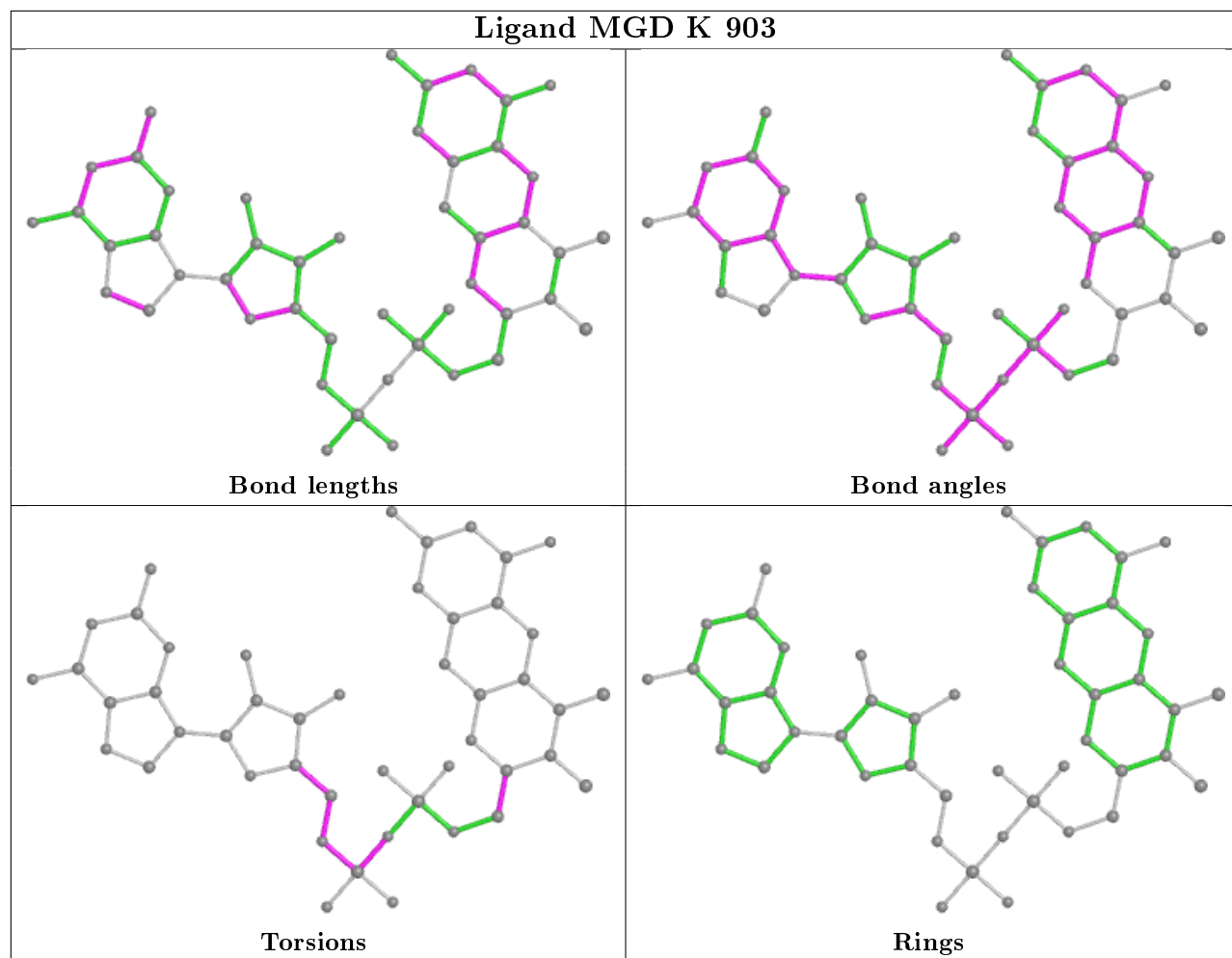
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

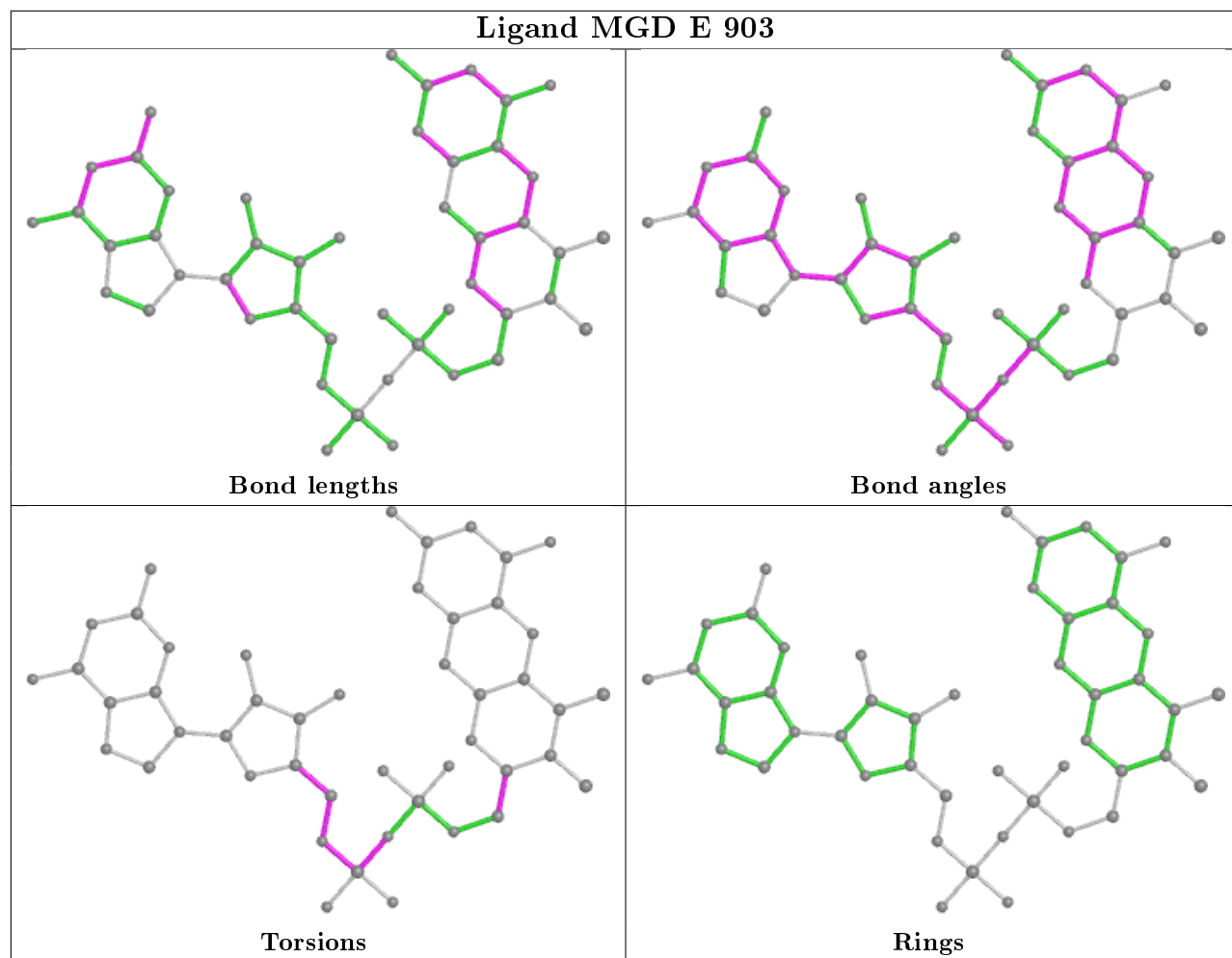


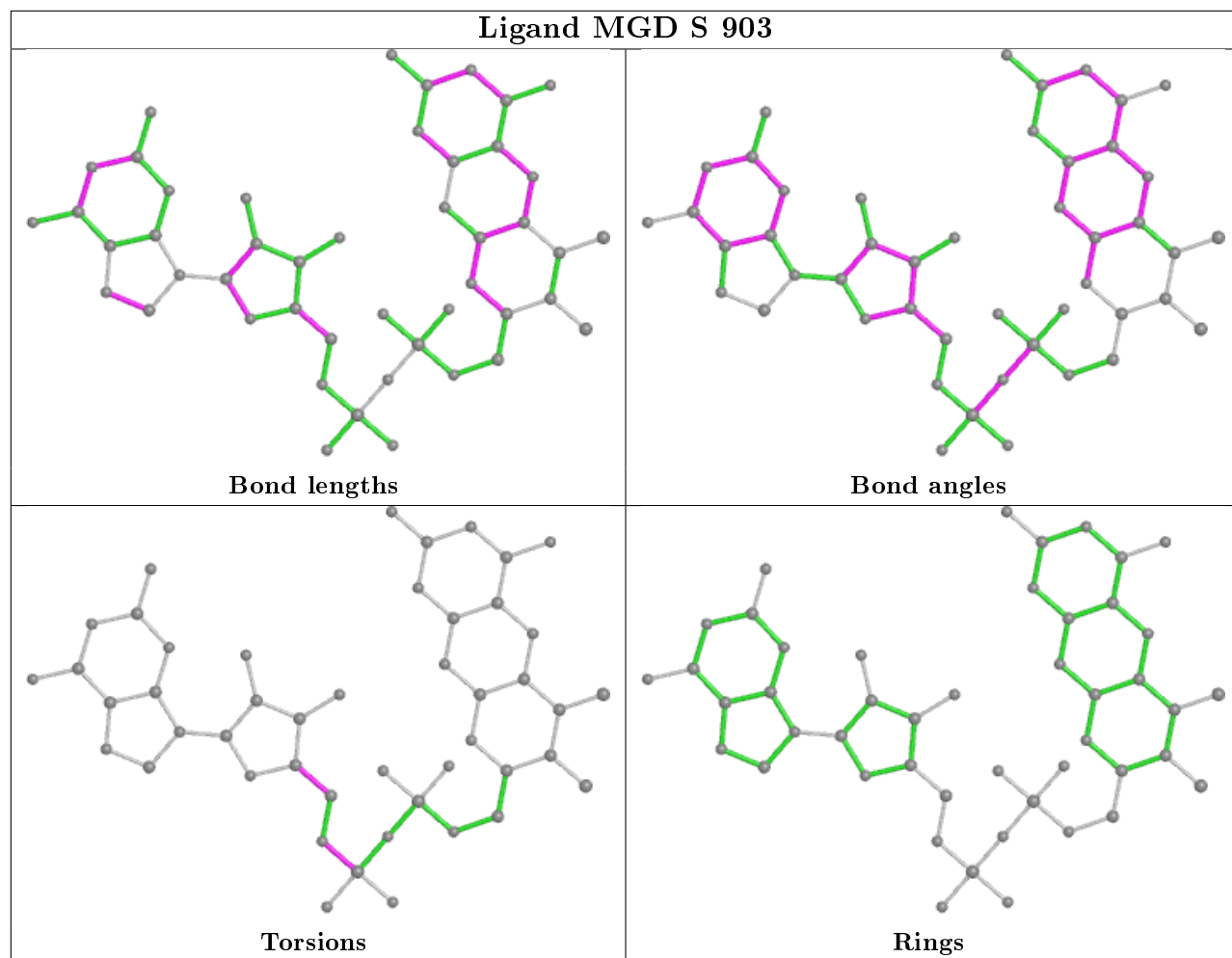


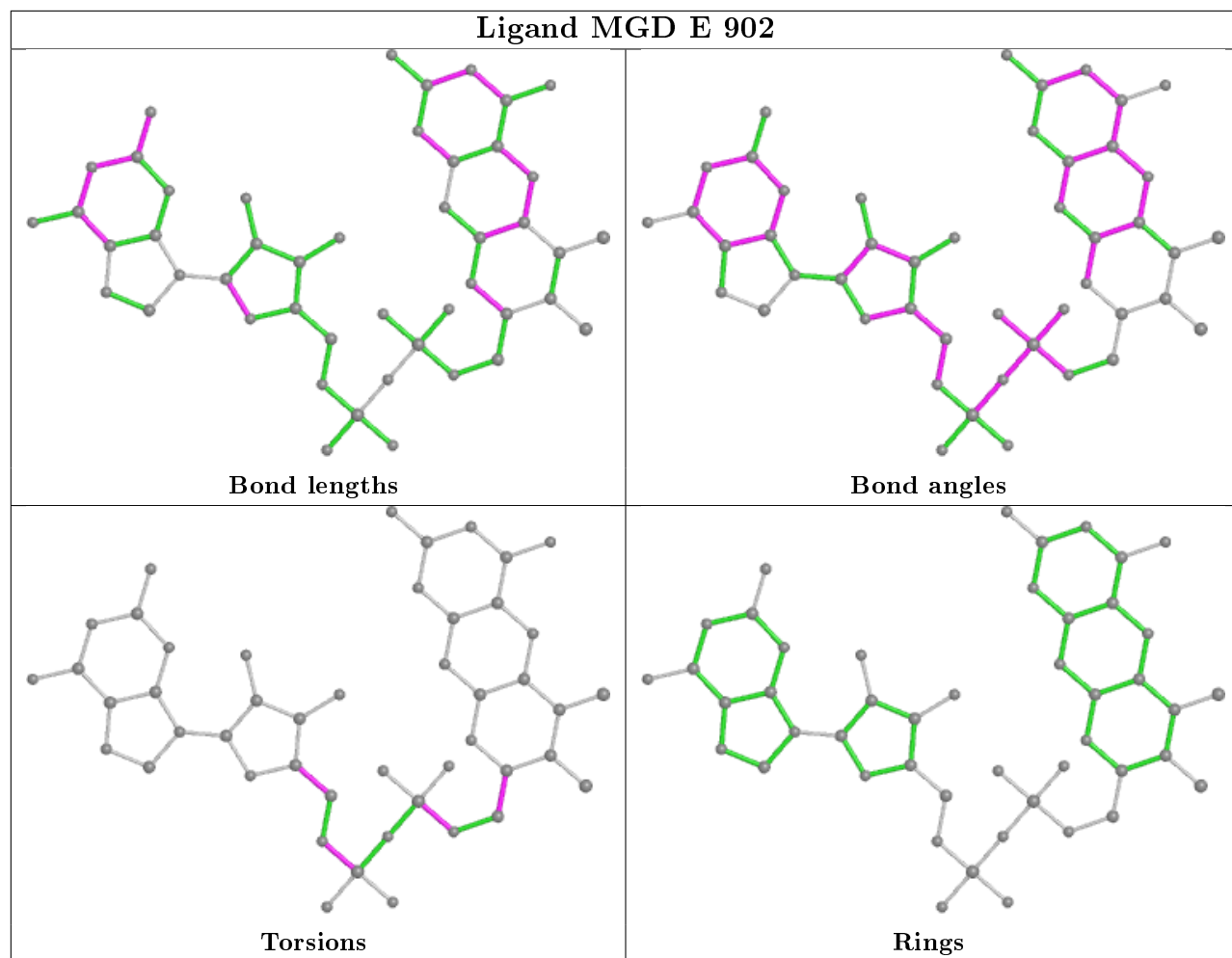


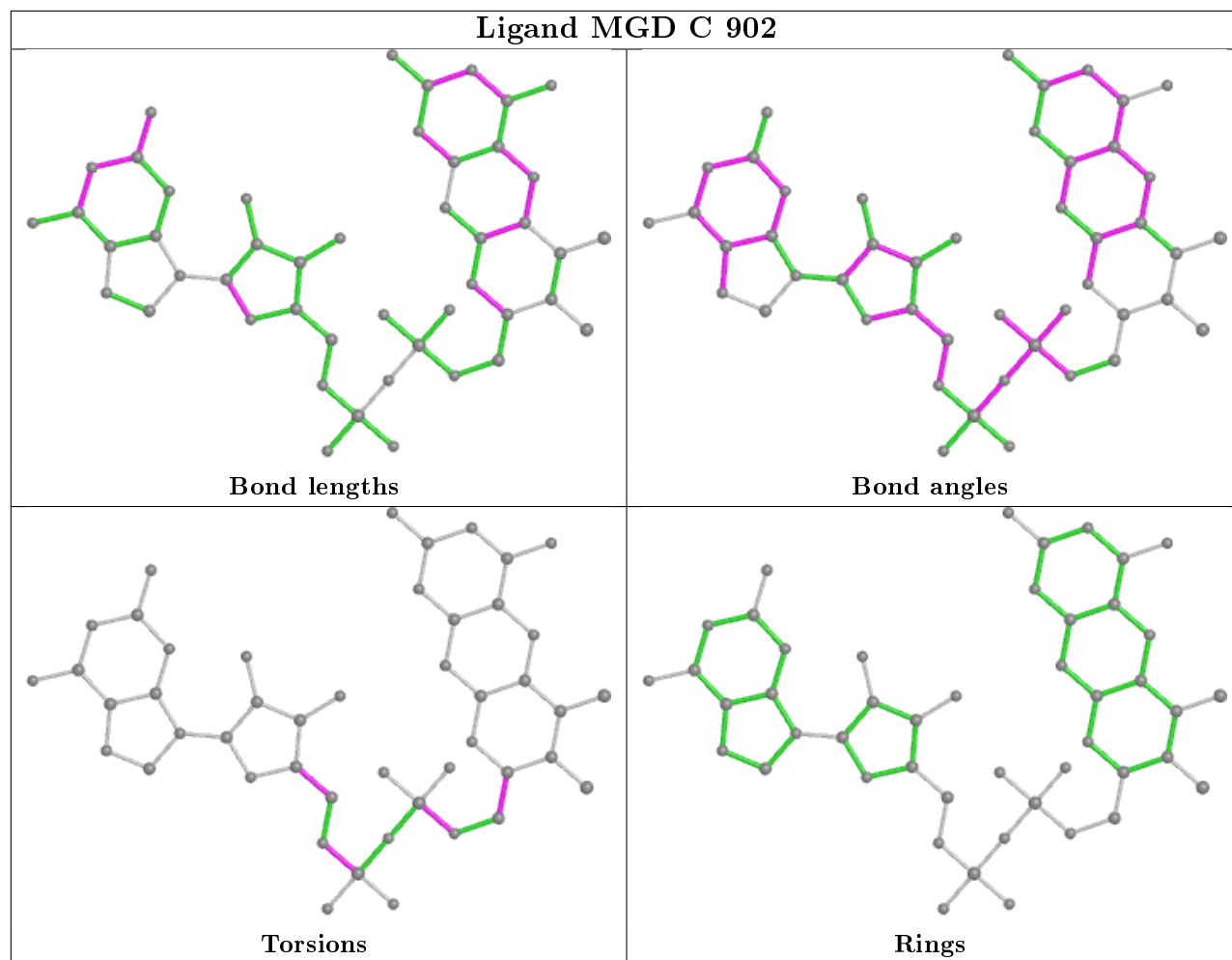


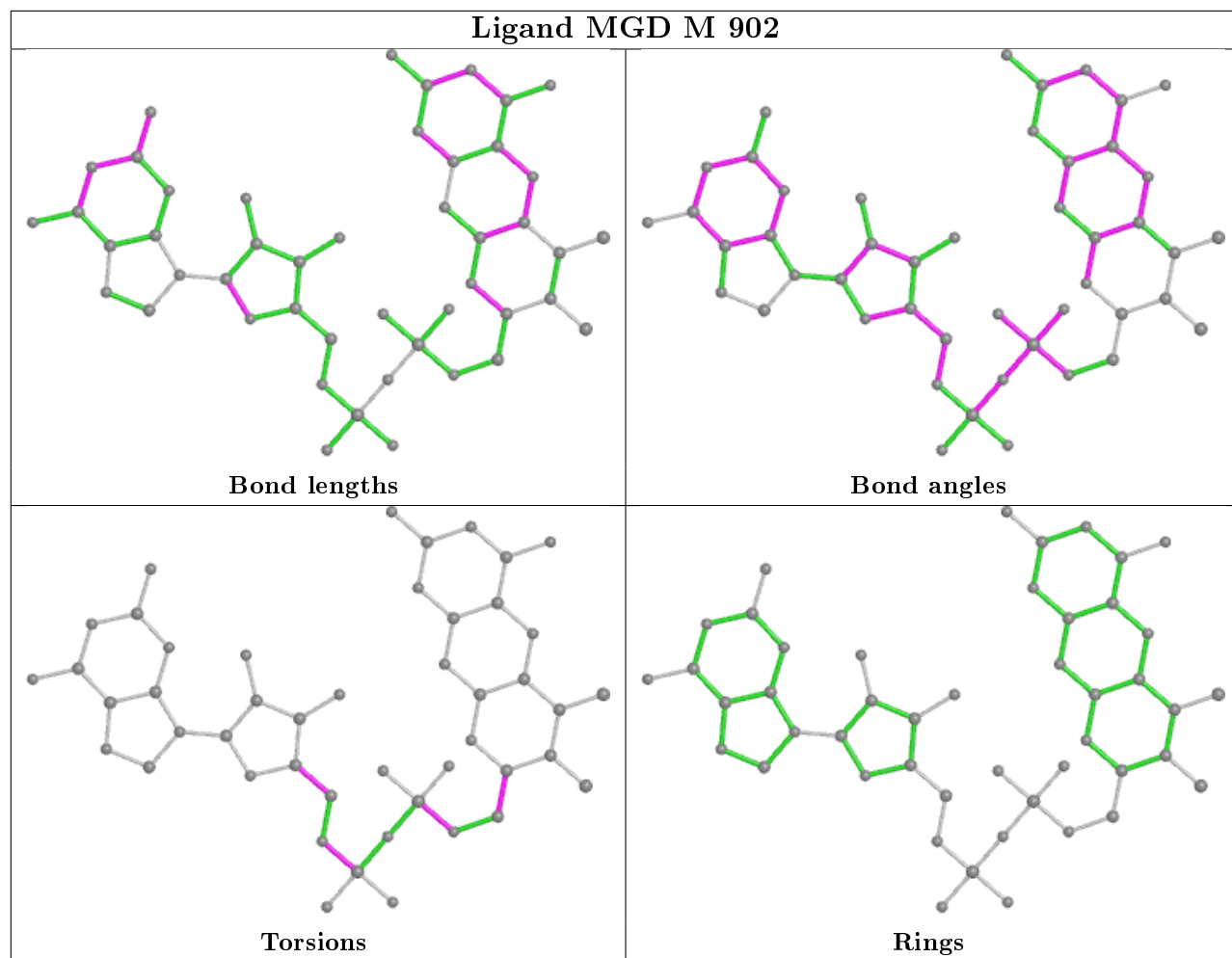


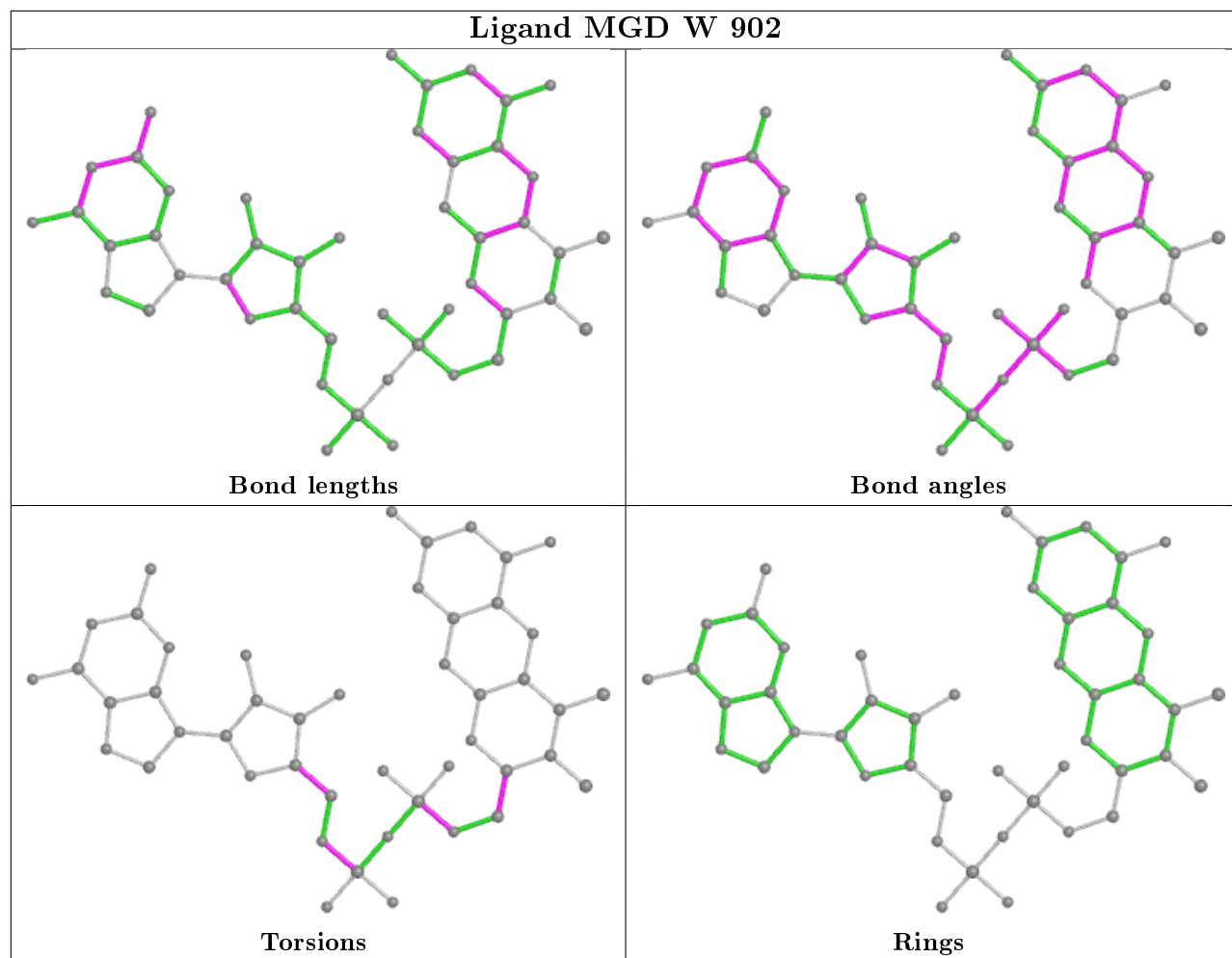


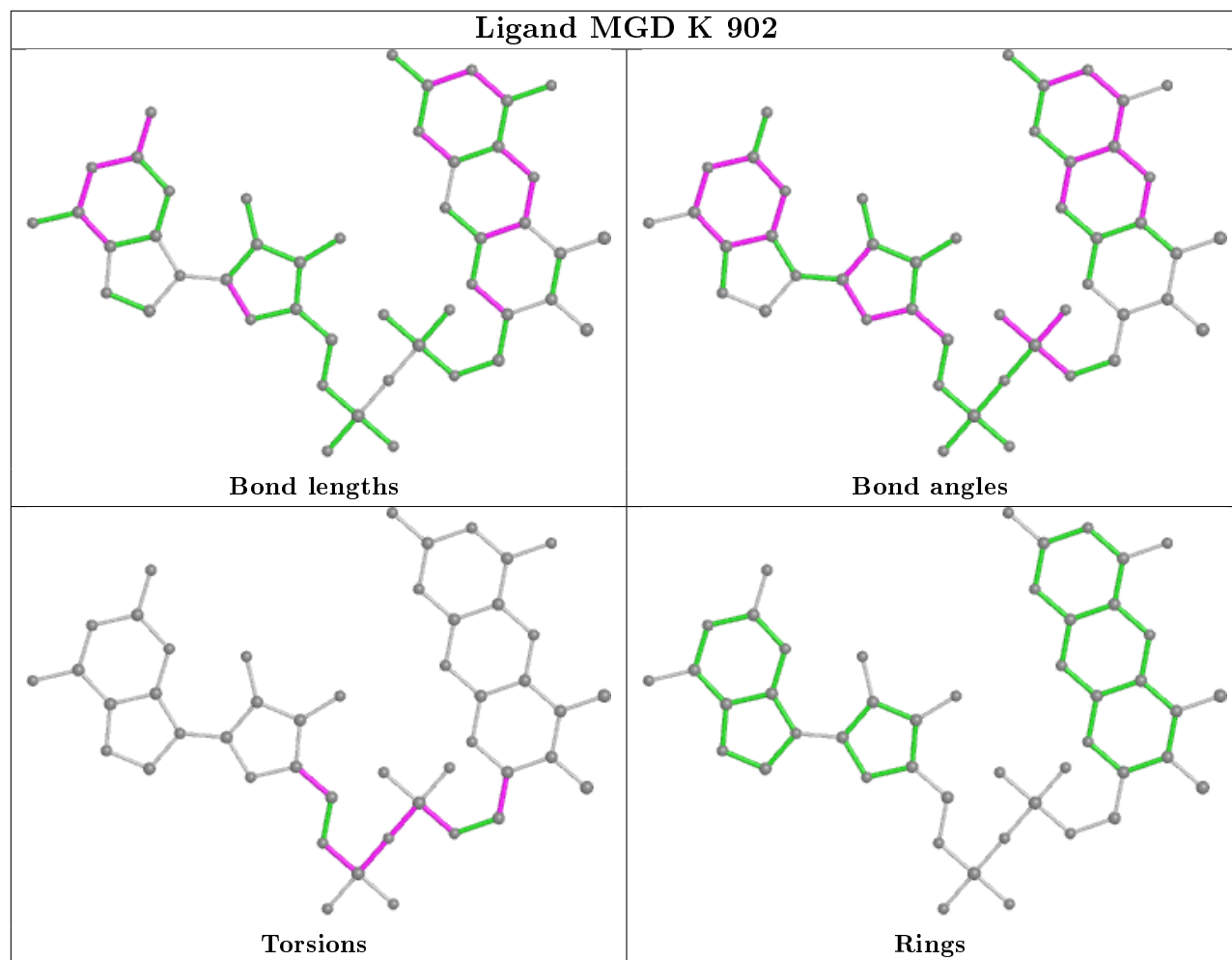


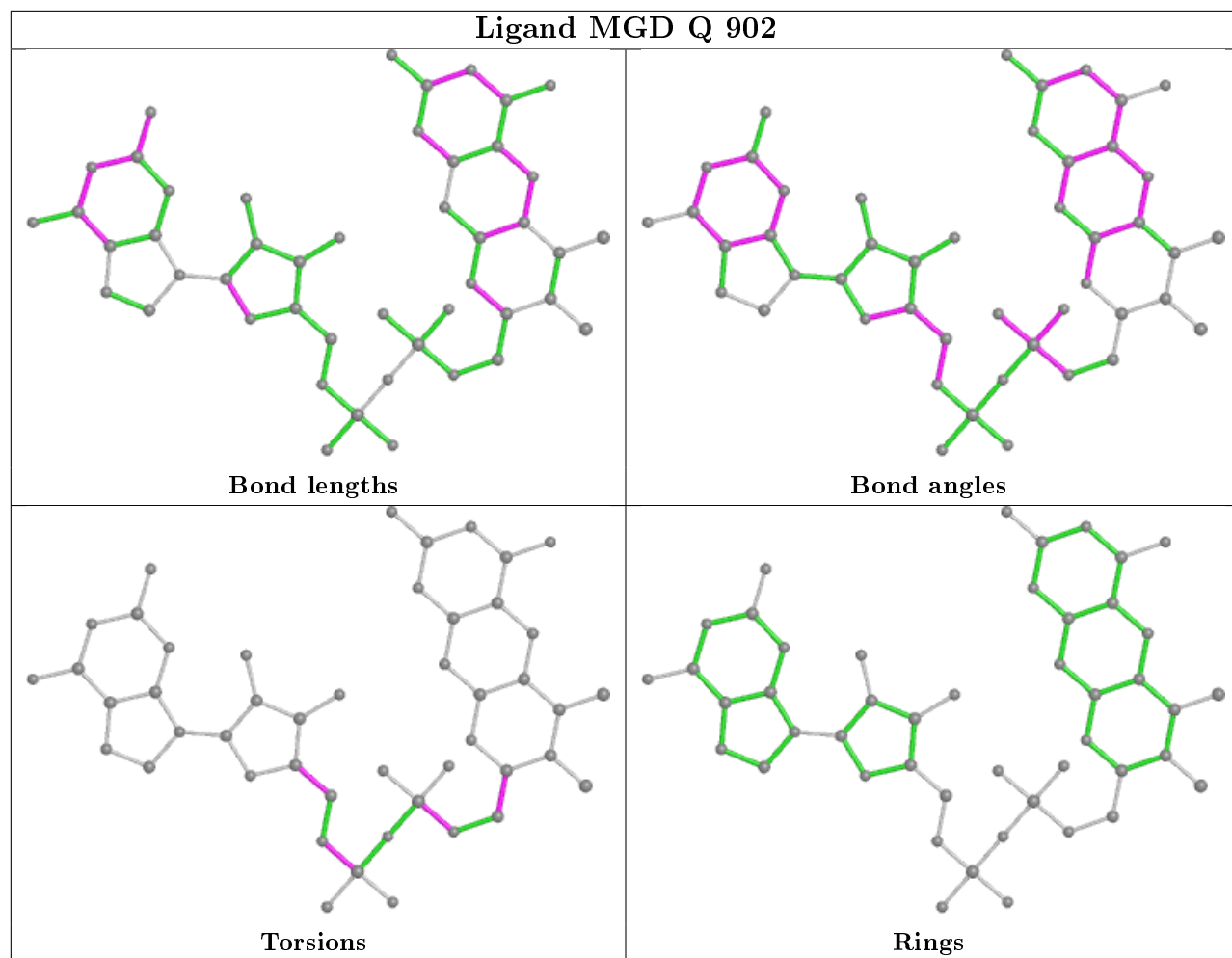


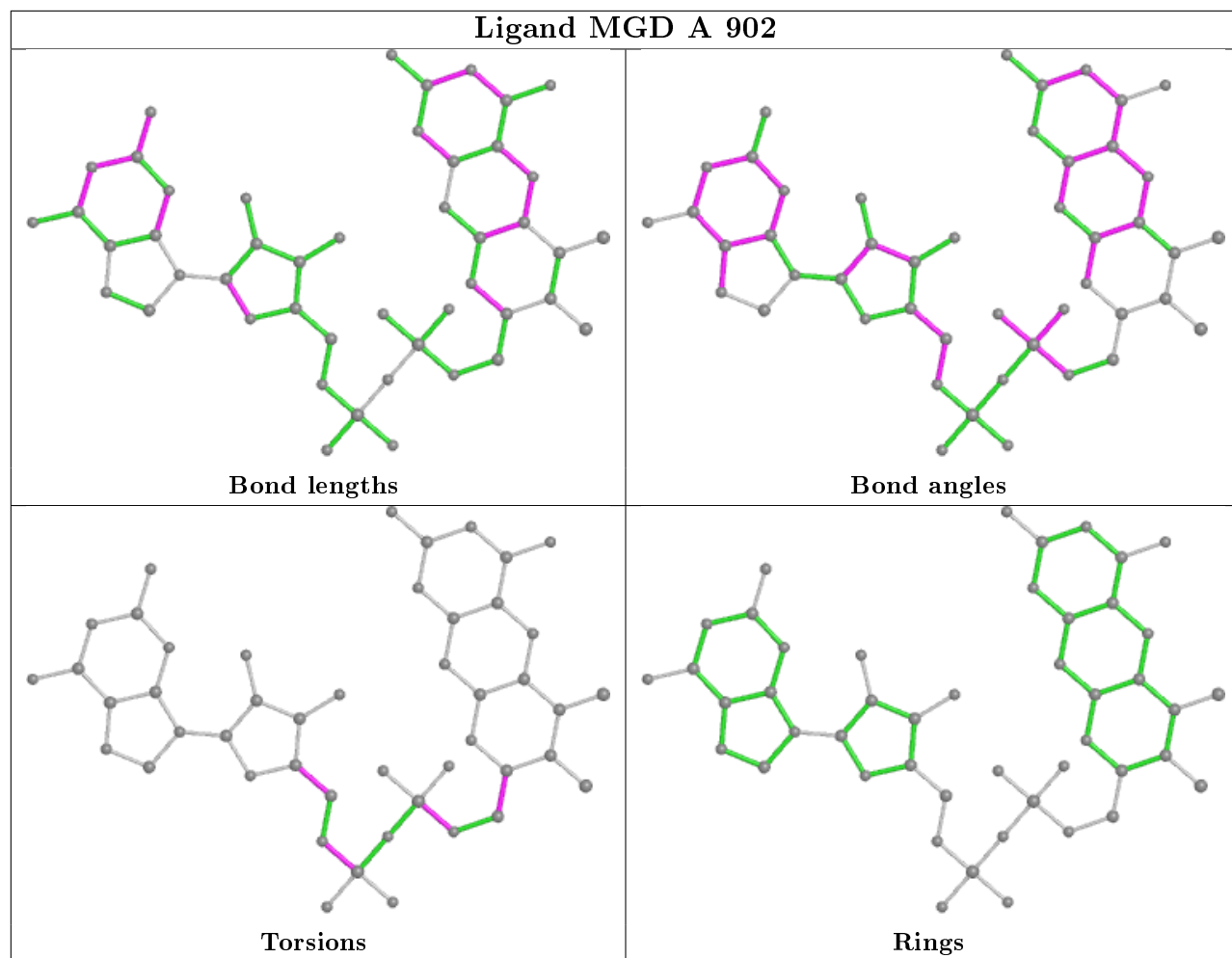


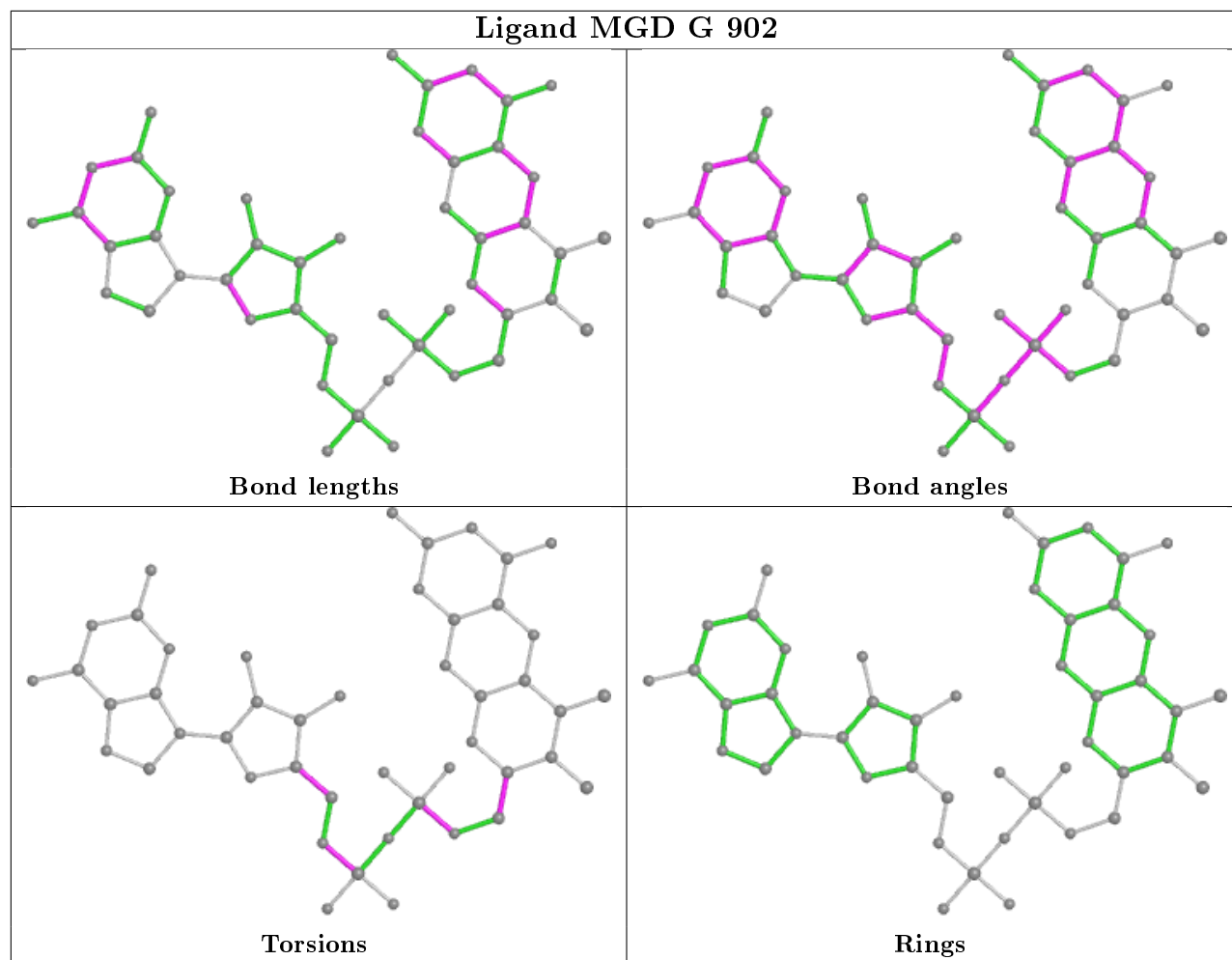


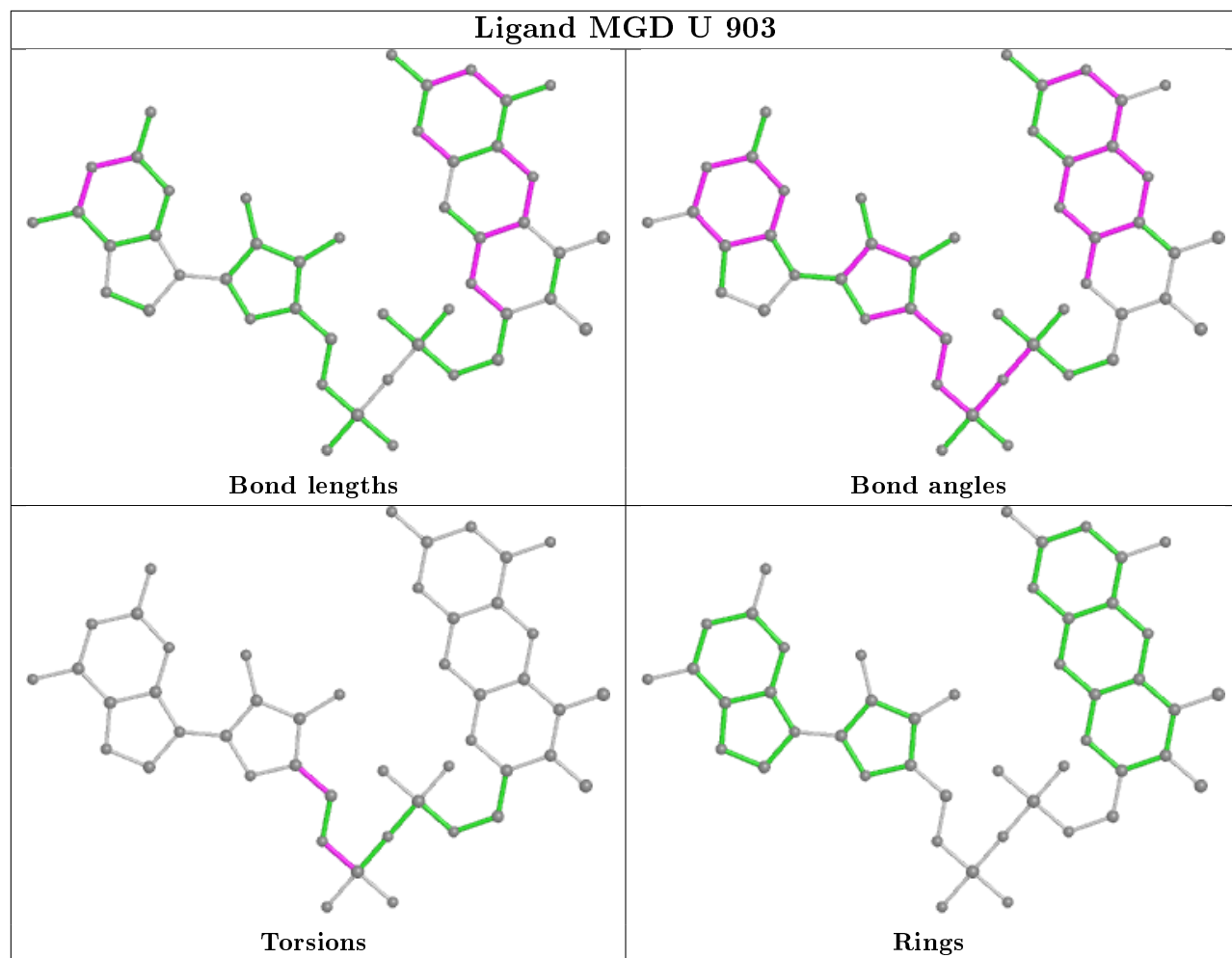


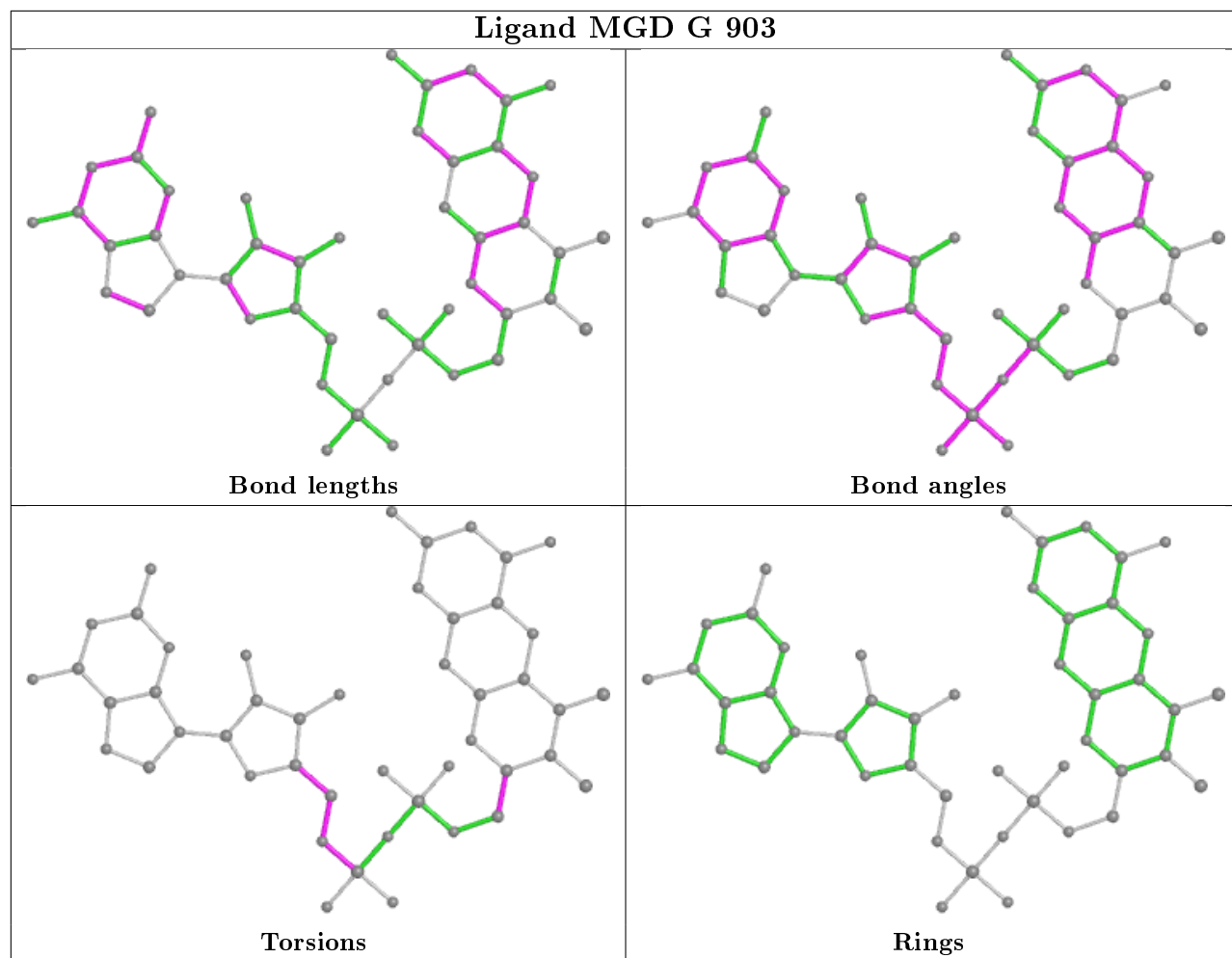


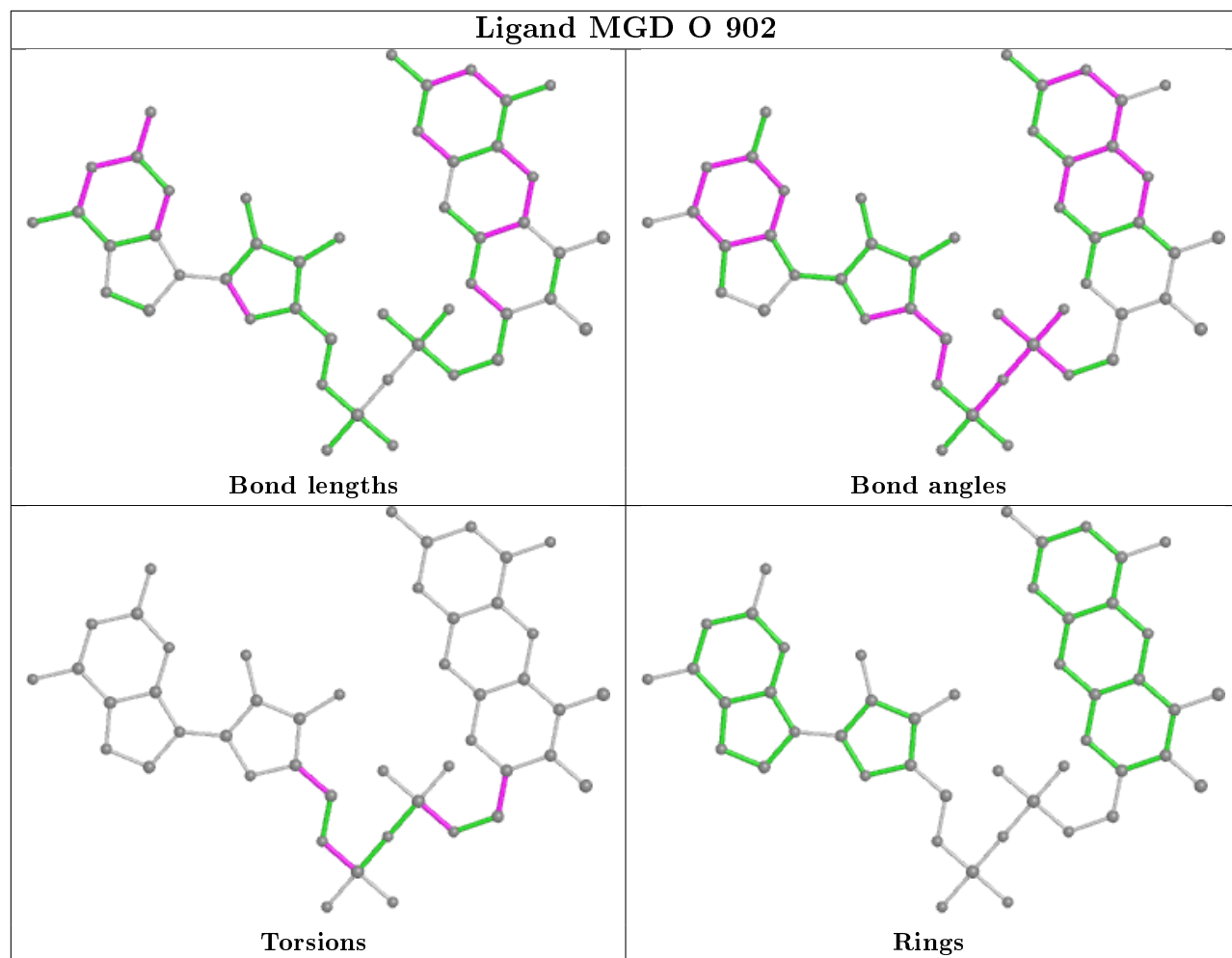


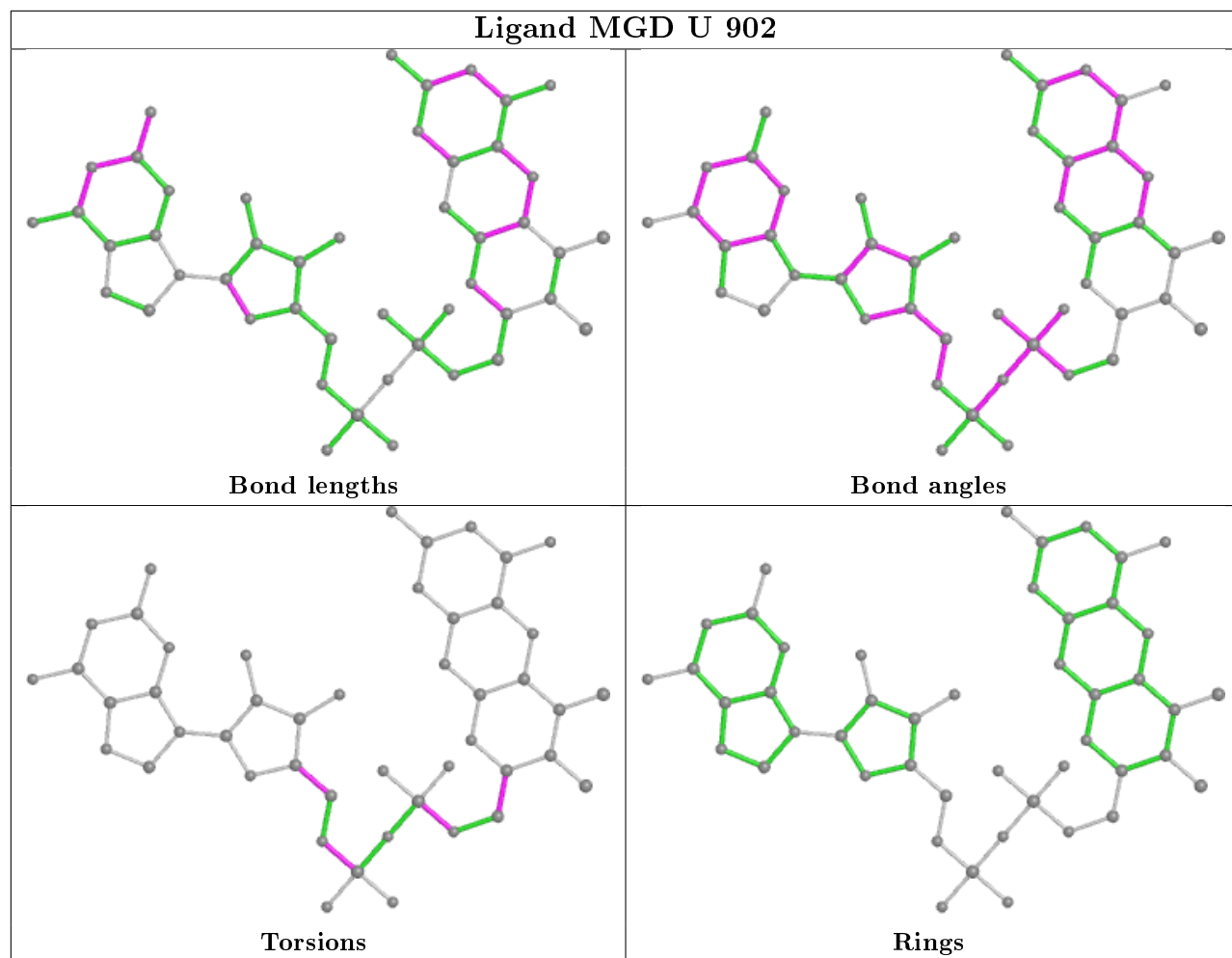


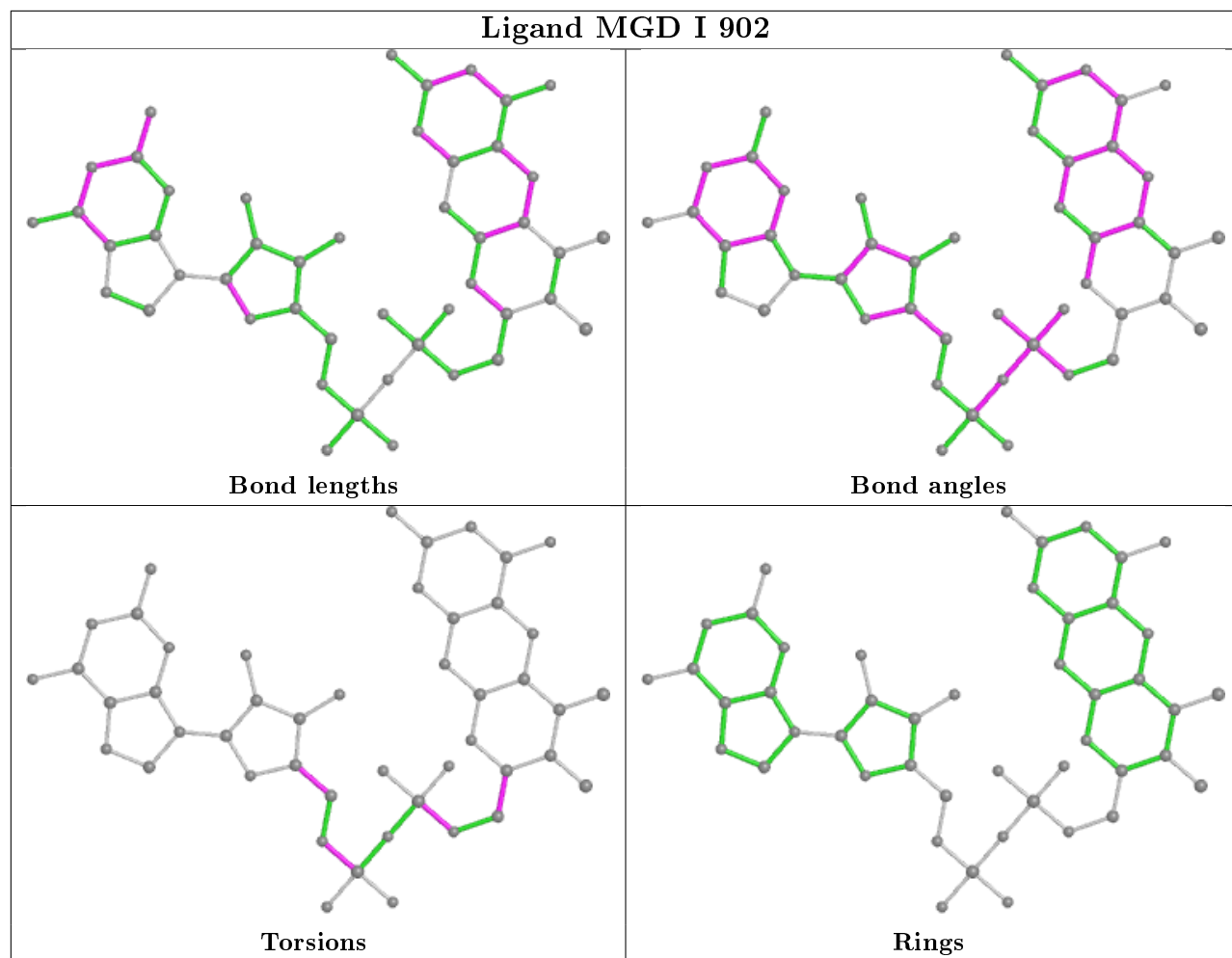


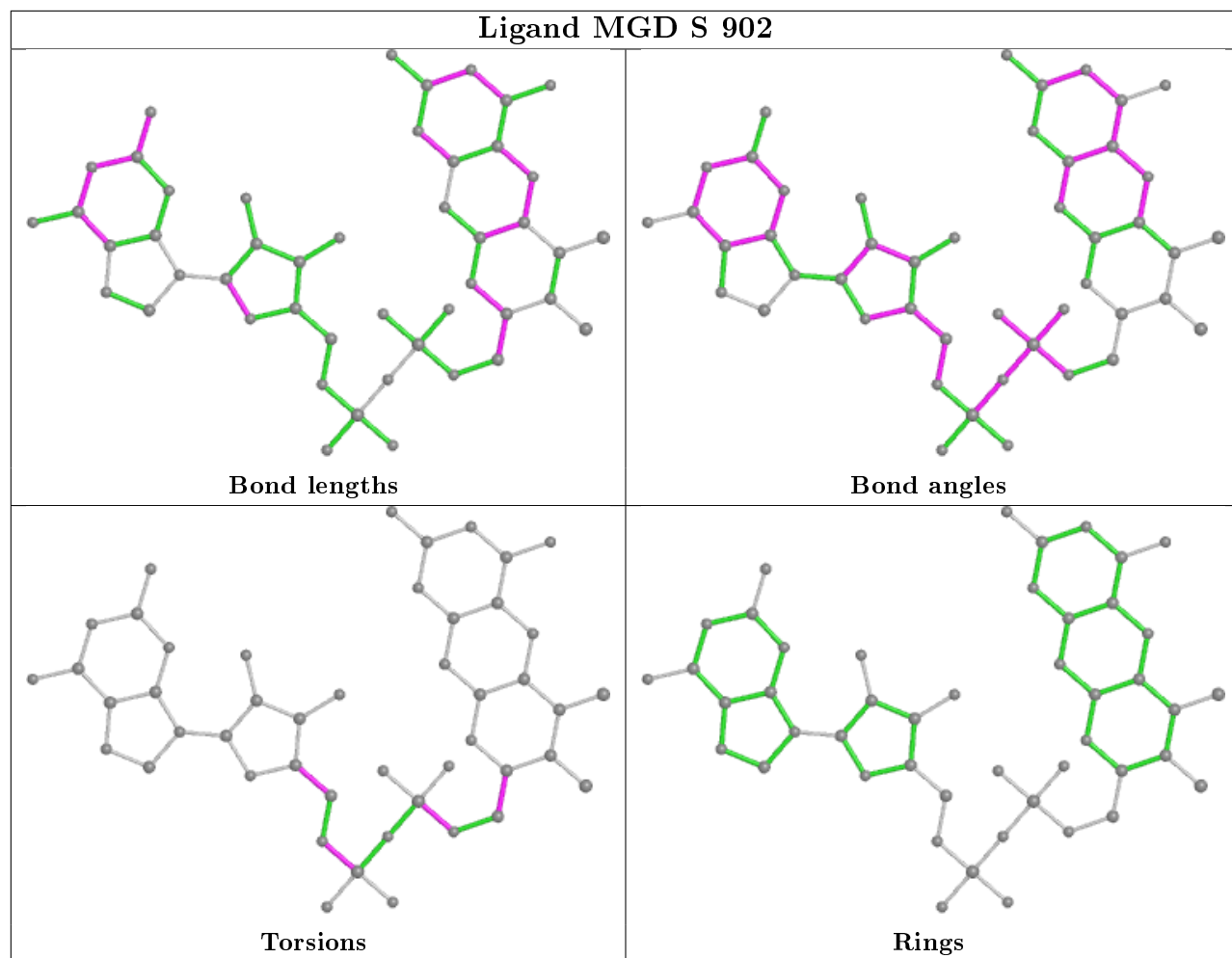


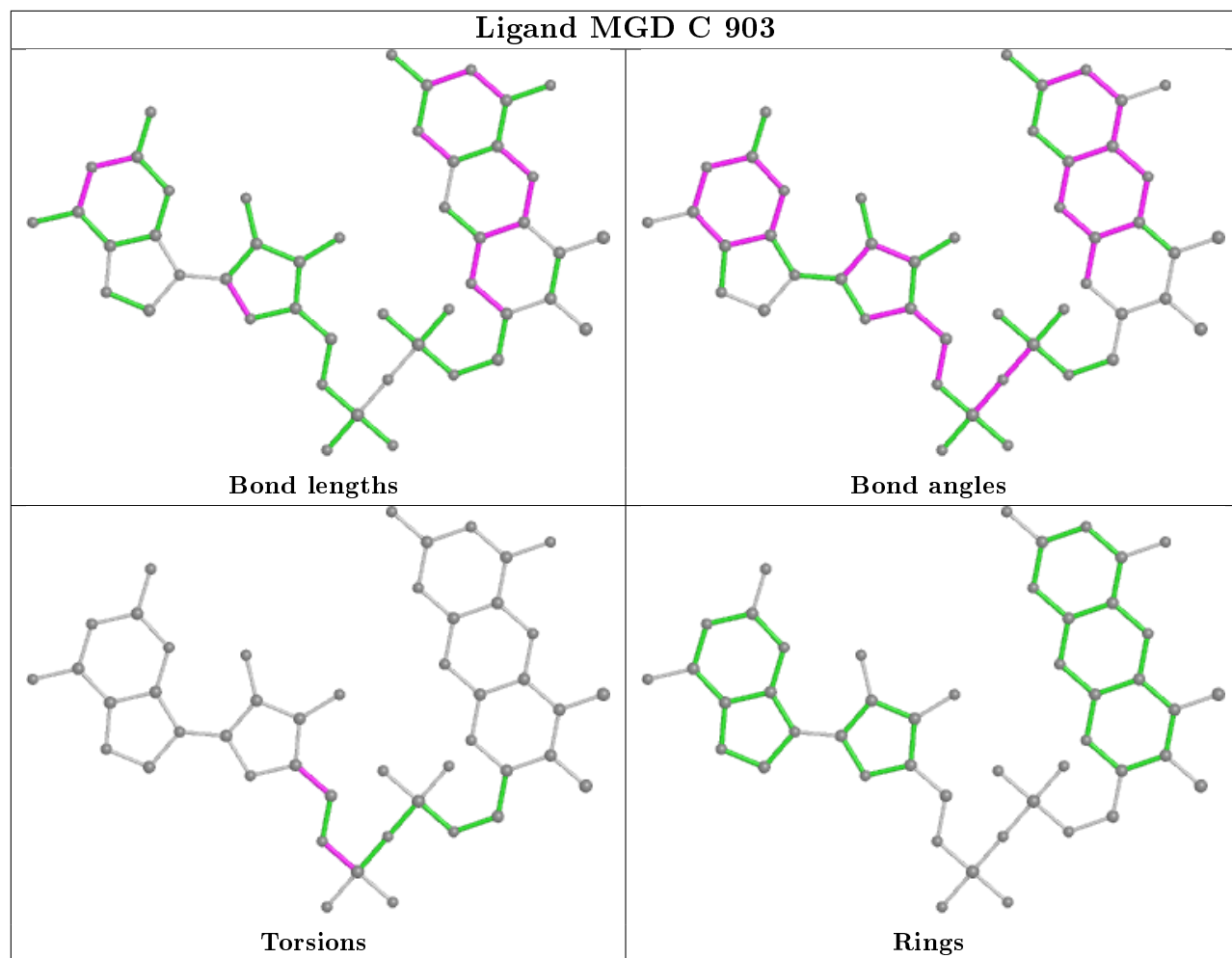


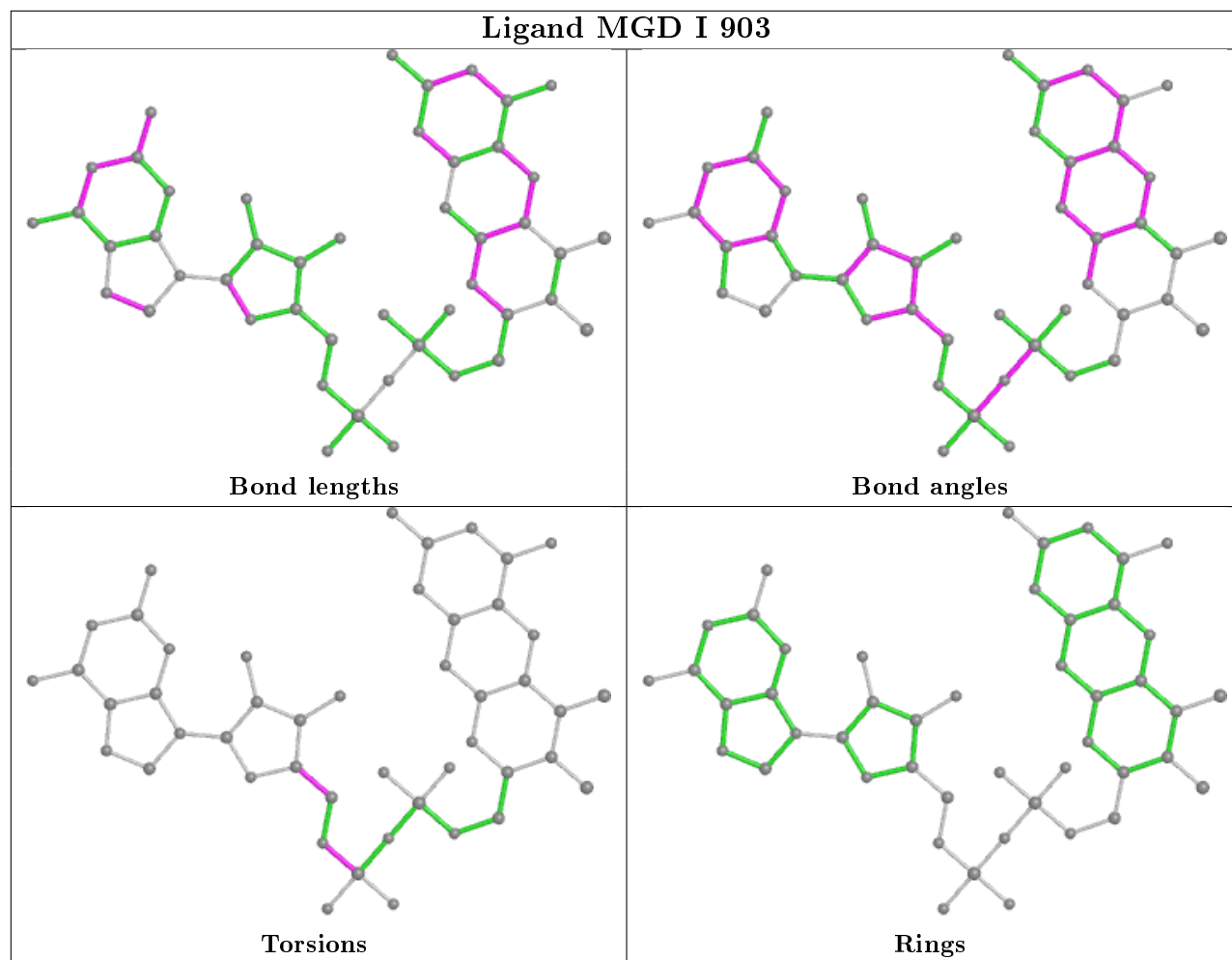


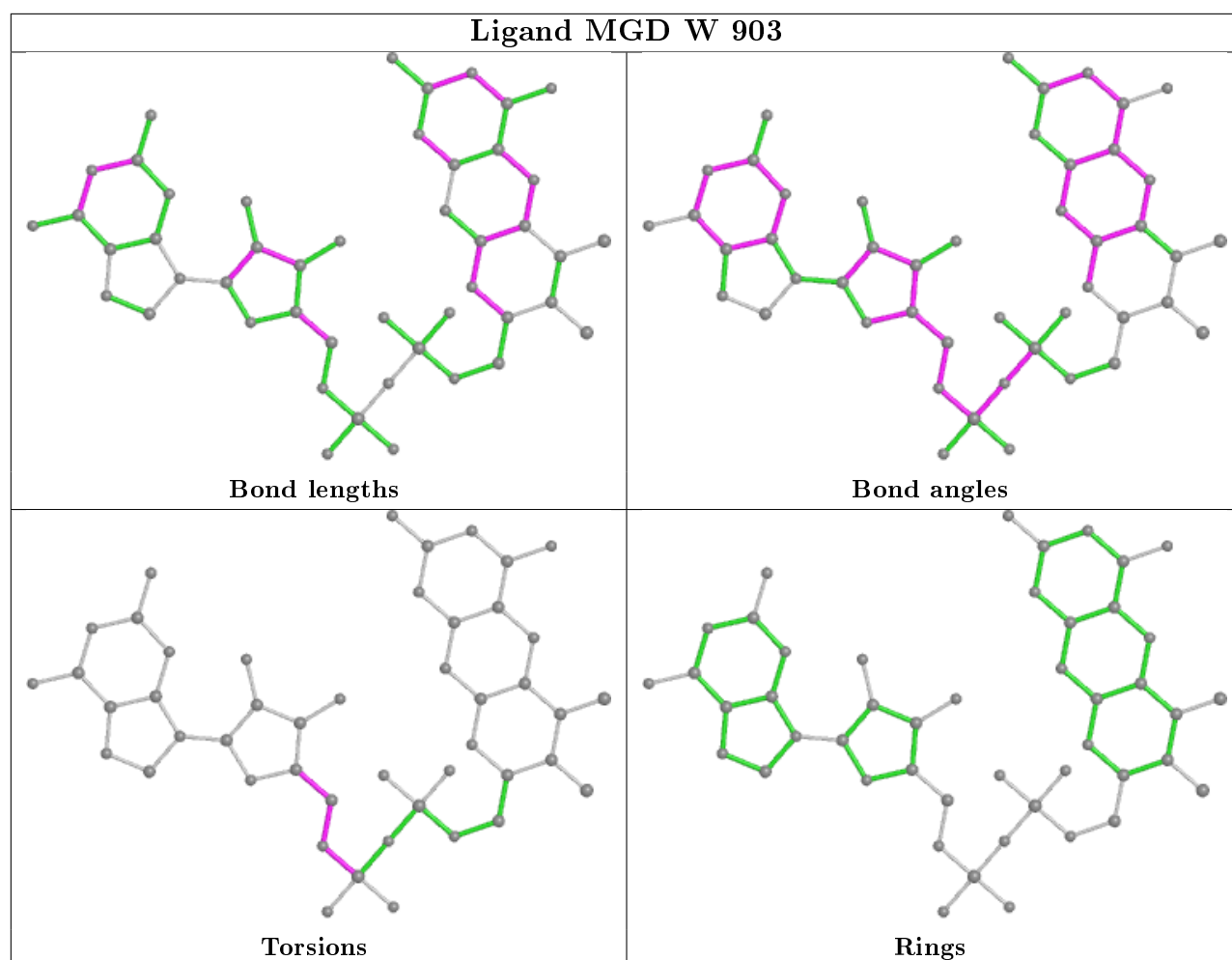












5.7 Other polymers [i](#)

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.