



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:23 AM UTC

PDB ID : 4V4D / pdb_00004v4d
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici* complexed with pyrogallol
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.20 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

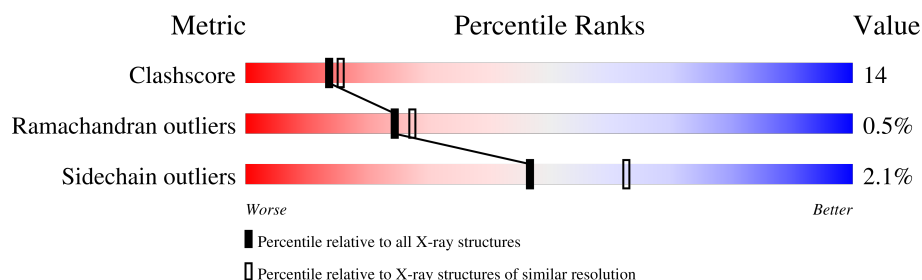
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

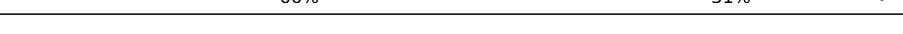
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	74% 24% .
1	C	875	71% 27% .
1	E	875	75% 23% .
1	G	875	76% 22% .
1	I	875	74% 23% .
1	K	875	74% 24% .
1	M	875	73% 25% .
1	O	875	72% 25% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	875	 72%25%.
1	S	875	 73%26%.
1	U	875	 72%26%.
1	W	875	 71%26%.
2	B	274	 67%29%..
2	D	274	 64%32%..
2	F	274	 68%30%.
2	H	274	 69%27%.
2	J	274	 69%26%5%.
2	L	274	 65%31%..
2	N	274	 67%28%..
2	P	274	 63%33%.
2	R	274	 69%27%.
2	T	274	 62%34%.
2	V	274	 66%31%.
2	X	274	 55%41%.

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	PYG	A	905	-	X	-	-
6	PYG	C	905	-	X	-	-
6	PYG	E	905	-	X	-	-
6	PYG	G	905	-	X	-	-
6	PYG	I	905	-	X	-	-
6	PYG	K	905	-	X	-	-
6	PYG	M	905	-	X	-	-
6	PYG	O	905	-	X	-	-
6	PYG	Q	905	-	X	-	-
6	PYG	S	905	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PYG	U	905	-	X	-	-
6	PYG	W	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	302	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	N	302	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	V	303	-	-	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 121808 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 (CCD ID: CA) (formula: Ca).

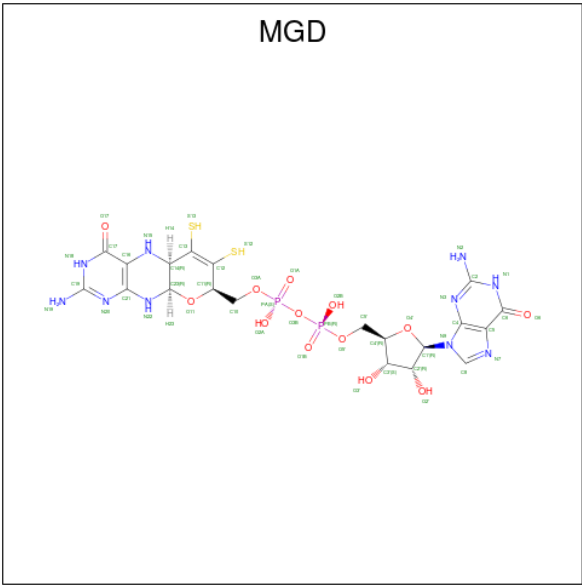
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- 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 (CCD ID: 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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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 (CCD ID: 4MO) (formula: Mo).

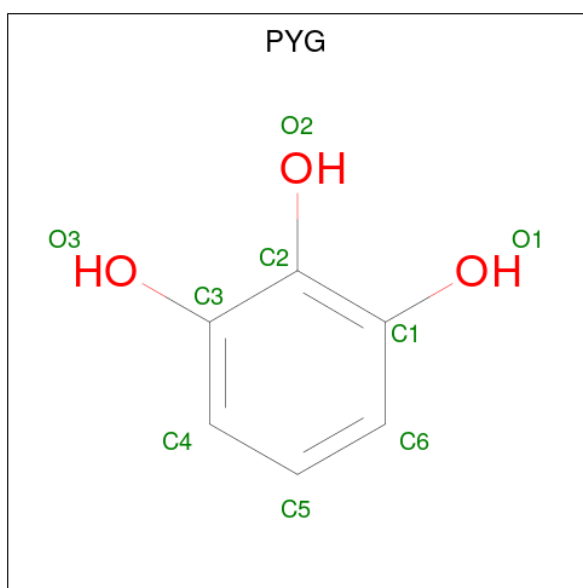
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	G	1	Total	Mo	0	0
			1	1		
5	I	1	Total	Mo	0	0
			1	1		
5	K	1	Total	Mo	0	0
			1	1		
5	M	1	Total	Mo	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	1	Total	Mo	0	0
			1	1		
5	Q	1	Total	Mo	0	0
			1	1		
5	S	1	Total	Mo	0	0
			1	1		
5	U	1	Total	Mo	0	0
			1	1		
5	W	1	Total	Mo	0	0
			1	1		

- Molecule 6 is BENZENE-1,2,3-TRIOL (CCD ID: PYG) (formula: $C_6H_6O_3$).



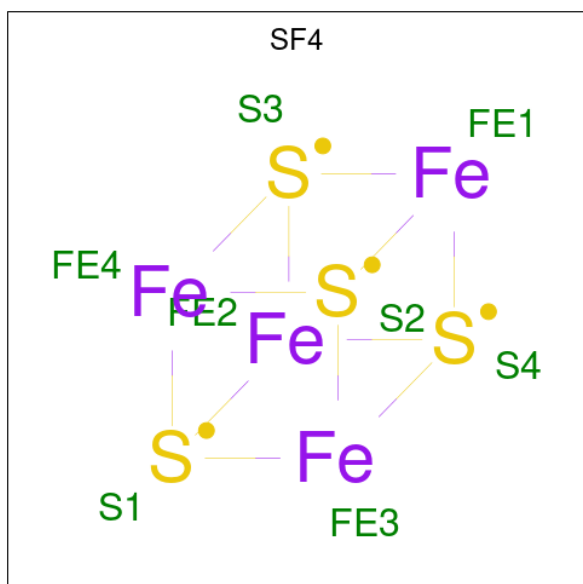
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			9	6	3		
6	E	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			9	6	3		
6	I	1	Total	C	O	0	0
			9	6	3		
6	K	1	Total	C	O	0	0
			9	6	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			9	6	3		
6	O	1	Total	C	O	0	0
			9	6	3		
6	Q	1	Total	C	O	0	0
			9	6	3		
6	S	1	Total	C	O	0	0
			9	6	3		
6	U	1	Total	C	O	0	0
			9	6	3		
6	W	1	Total	C	O	0	0
			9	6	3		

- 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		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	170	Total 170	O 170	0	0
8	C	681	Total 681	O 681	0	0
8	D	166	Total 166	O 166	0	0
8	E	684	Total 684	O 684	0	0
8	F	163	Total 163	O 163	0	0
8	G	683	Total 683	O 683	0	0
8	H	161	Total 161	O 161	0	0
8	I	671	Total 671	O 671	0	0

Continued on next page...

Continued from previous page...

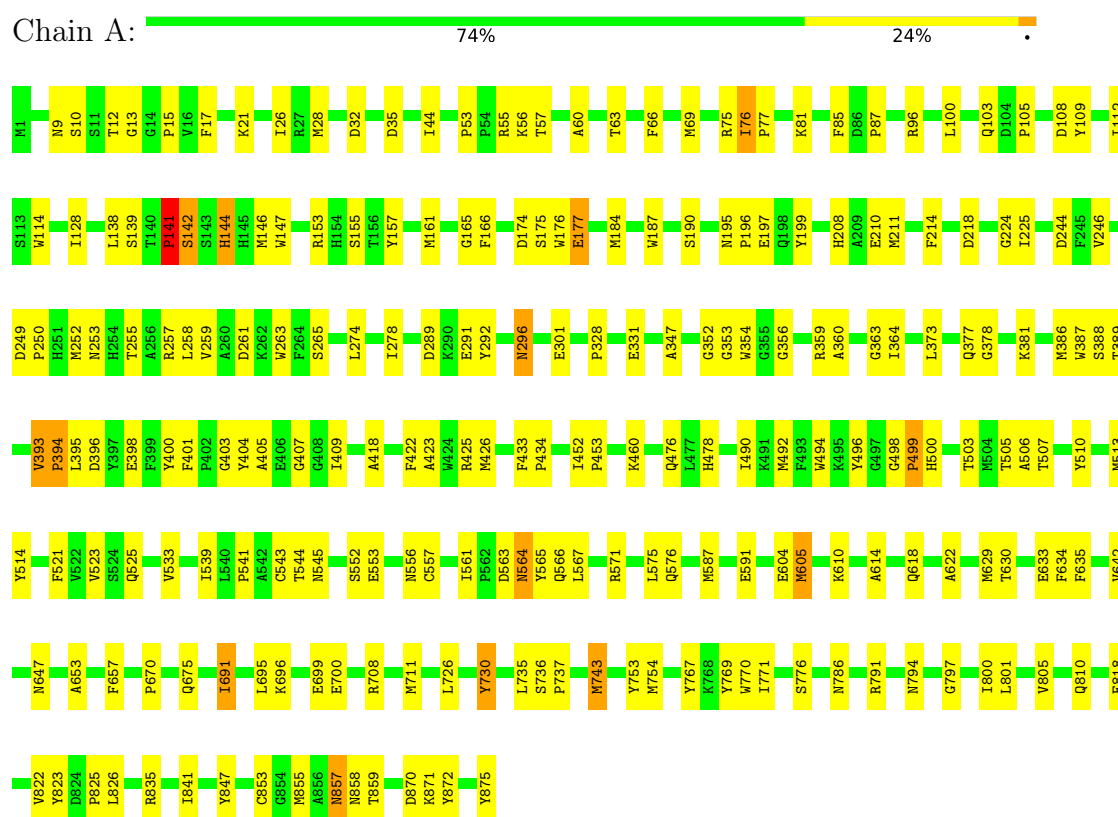
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	163	Total 163	O 163	0	0
8	K	681	Total 681	O 681	0	0
8	L	165	Total 165	O 165	0	0
8	M	684	Total 684	O 684	0	0
8	N	159	Total 159	O 159	0	0
8	O	672	Total 672	O 672	0	0
8	P	164	Total 164	O 164	0	0
8	Q	690	Total 690	O 690	0	0
8	R	161	Total 161	O 161	0	0
8	S	663	Total 663	O 663	0	0
8	T	163	Total 163	O 163	0	0
8	U	668	Total 668	O 668	0	0
8	V	157	Total 157	O 157	0	0
8	W	675	Total 675	O 675	0	0
8	X	164	Total 164	O 164	0	0

3 Residue-property plots [i](#)

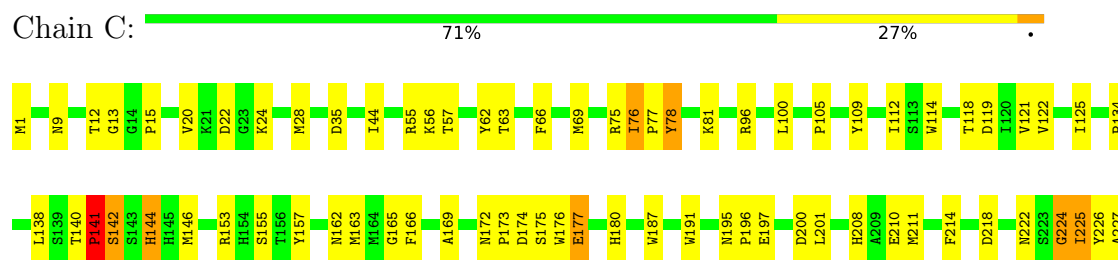
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

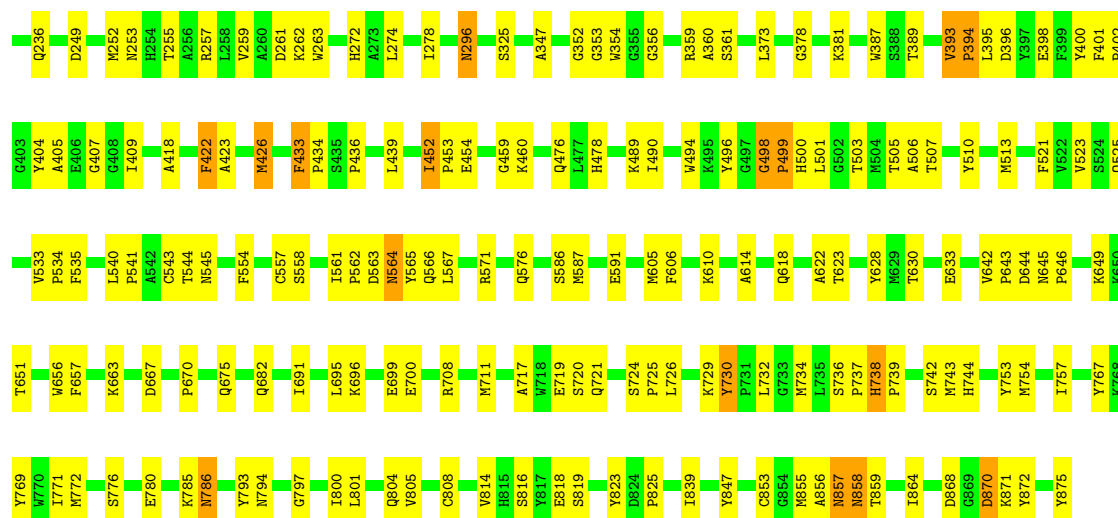
Note EDS was not executed.

- Molecule 1: Pyrogallol hydroxytransferase large subunit



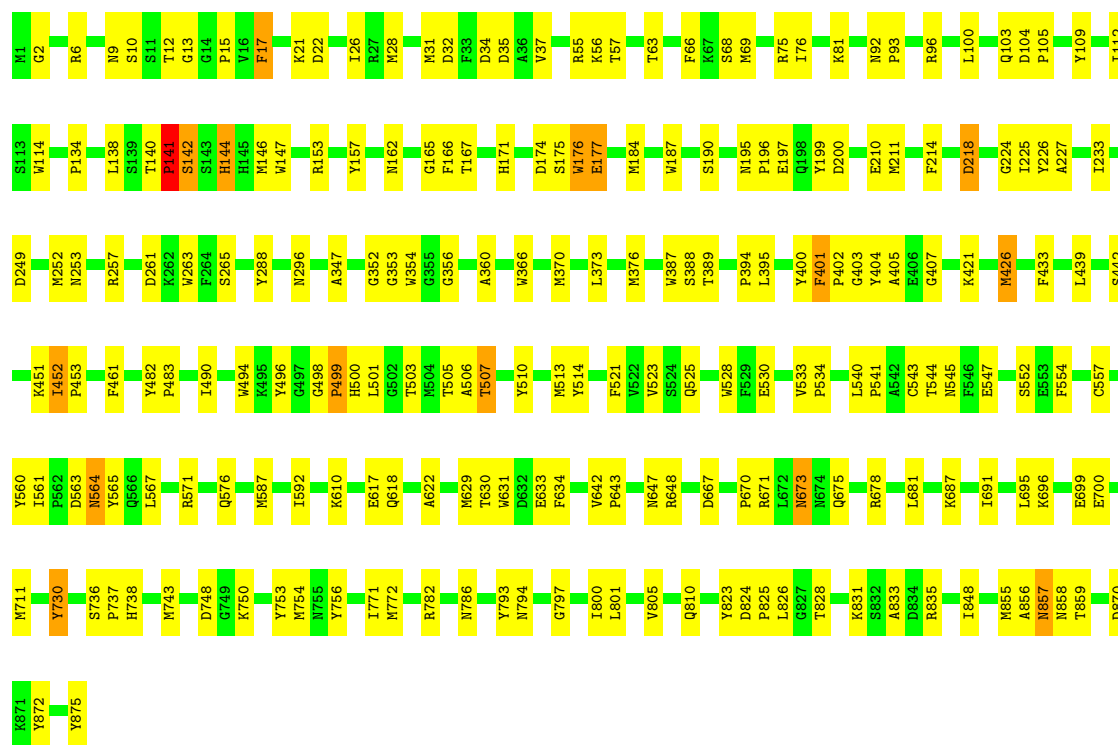
- Molecule 1: Pyrogallol hydroxytransferase large subunit





• Molecule 1: Pyrogallol hydroxytransferase large subunit

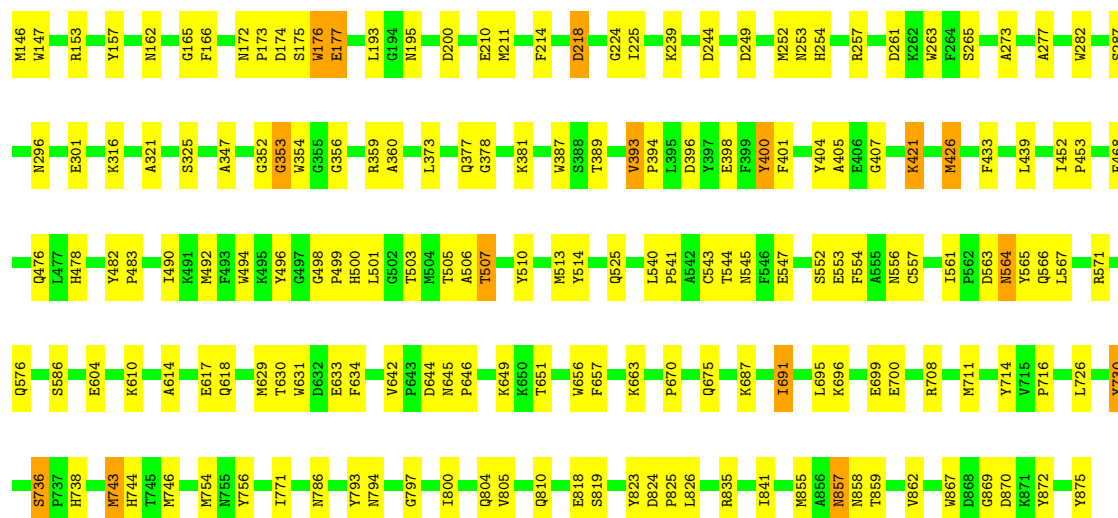
Chain E: 75% 23%



• Molecule 1: Pyrogallol hydroxytransferase large subunit

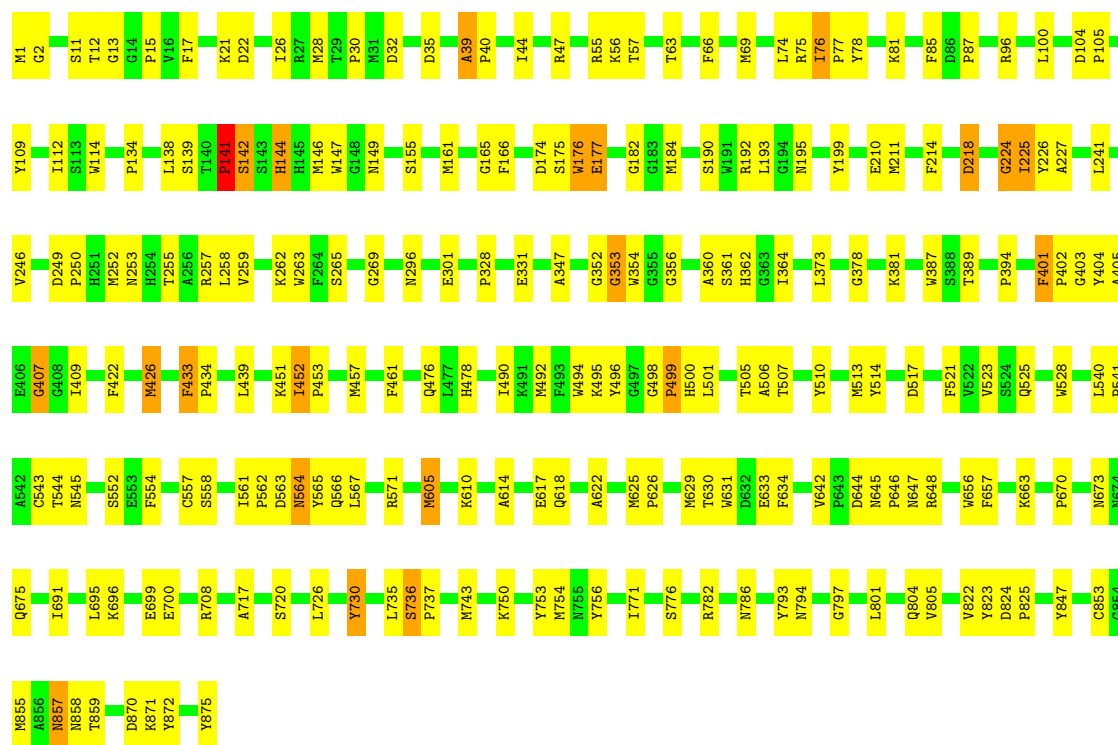
Chain G: 76% 22%





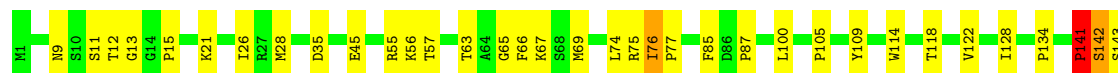
• Molecule 1: Pyrogallol hydroxytransferase large subunit

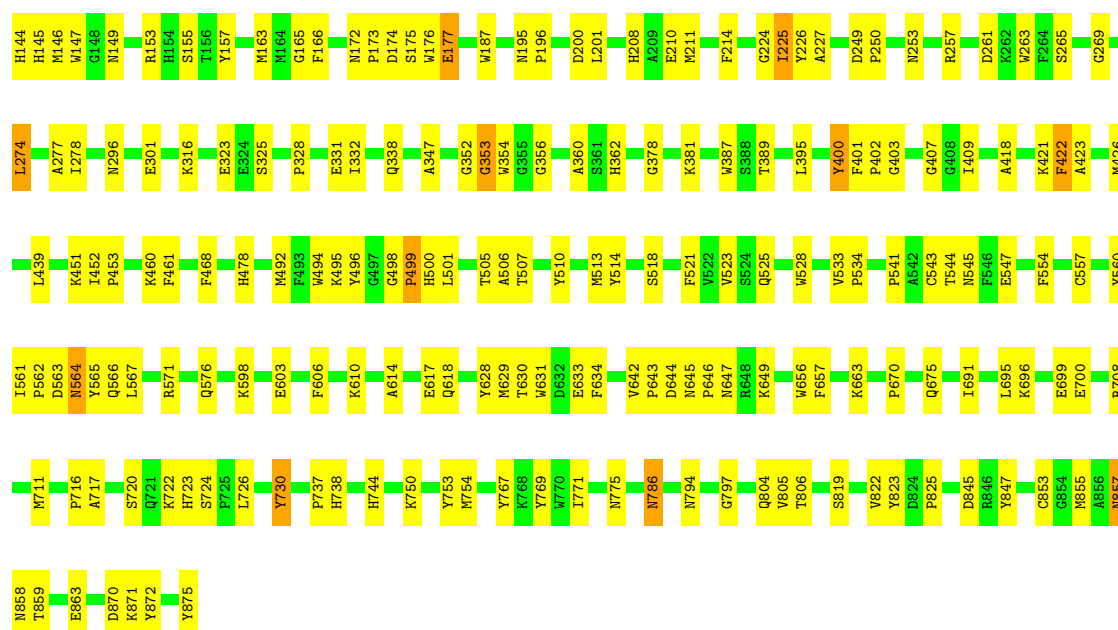
Chain I: 74% 23% •



• Molecule 1: Pyrogallol hydroxytransferase large subunit

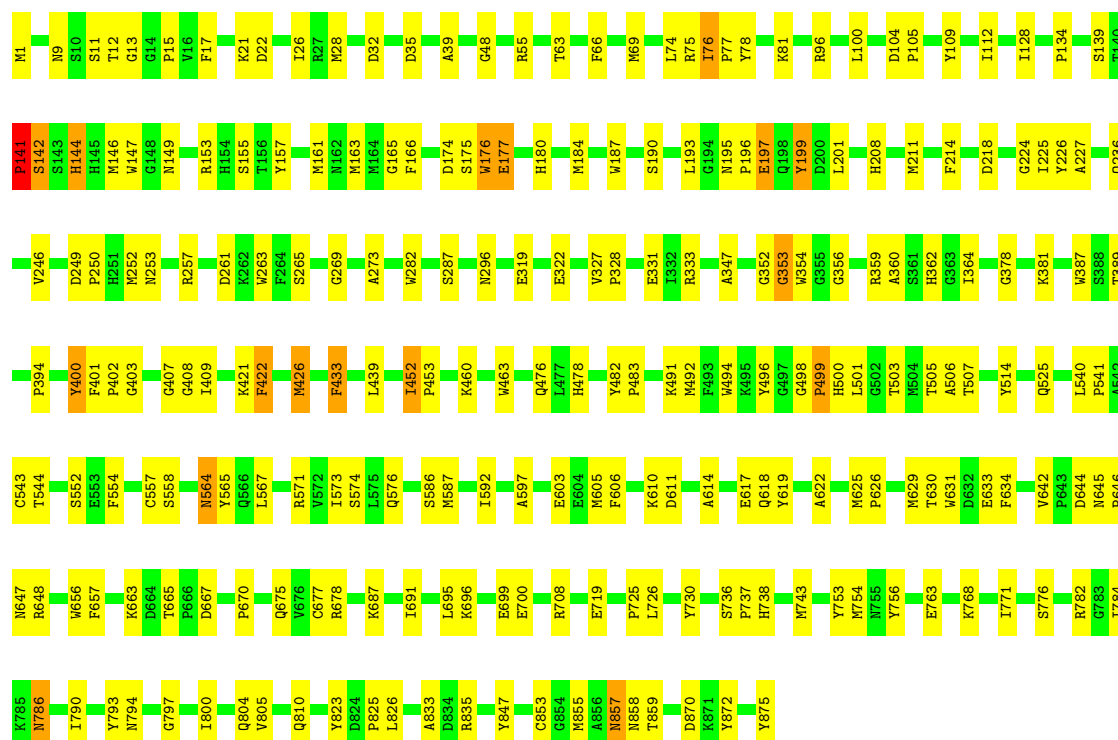
Chain K: 74% 24% •





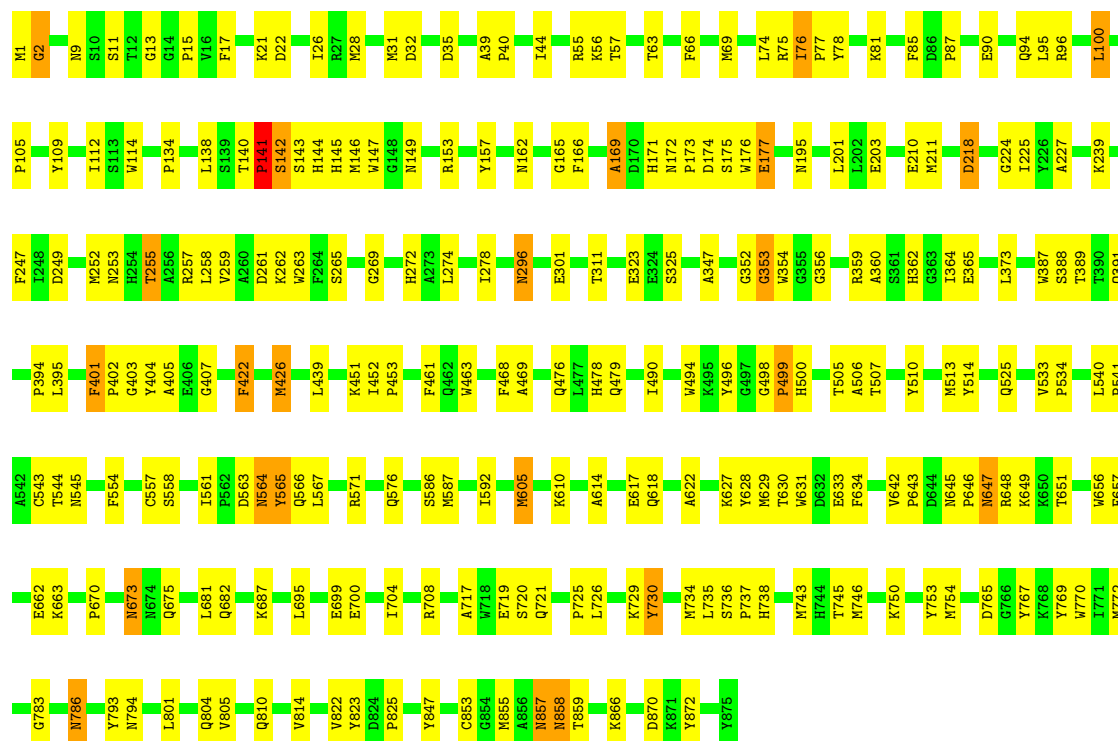
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain M: 73% 25% .



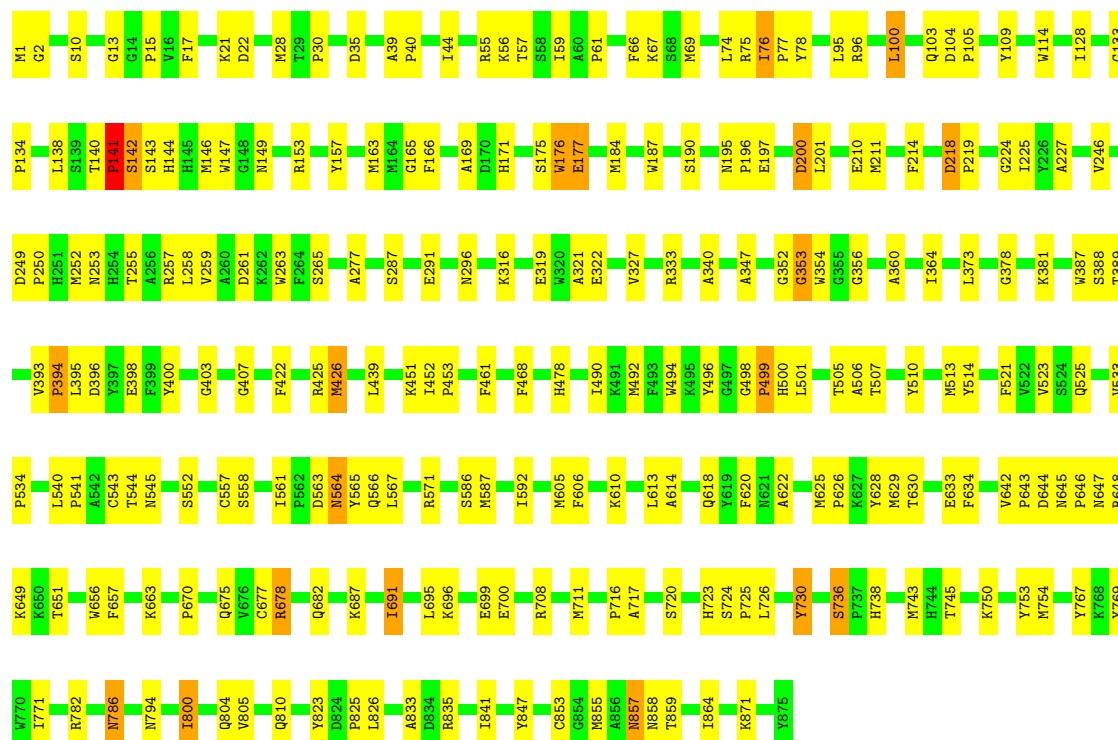
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O: 72% 25% .



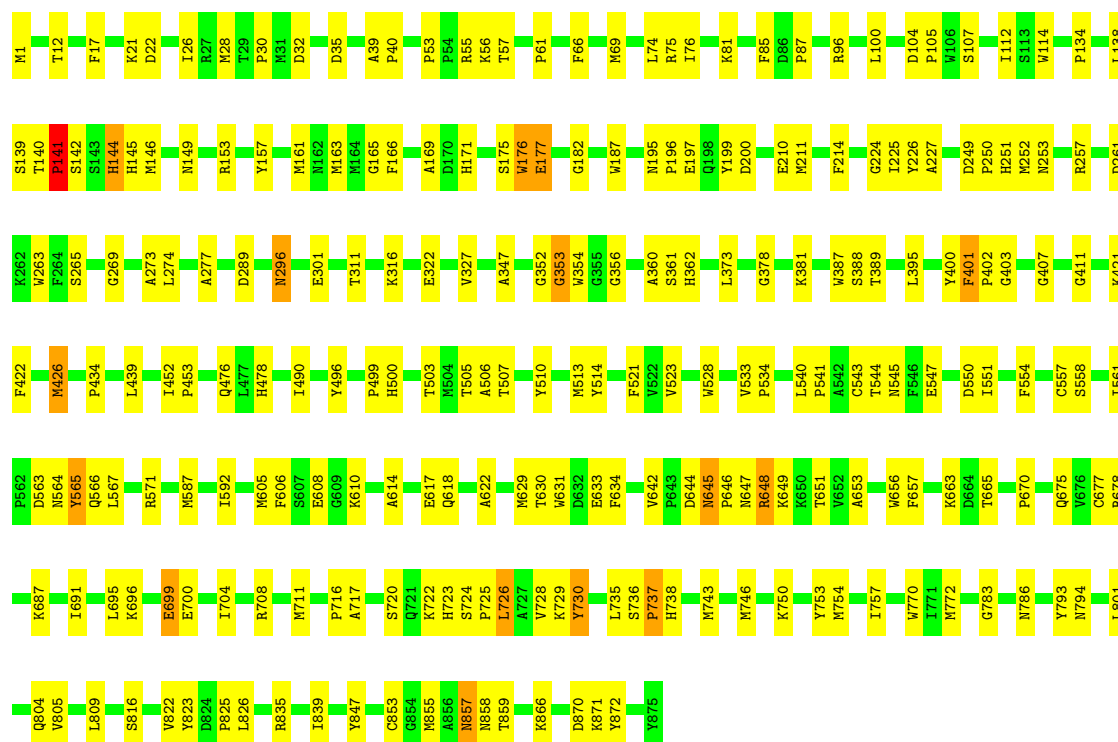
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain Q: 72% 25%



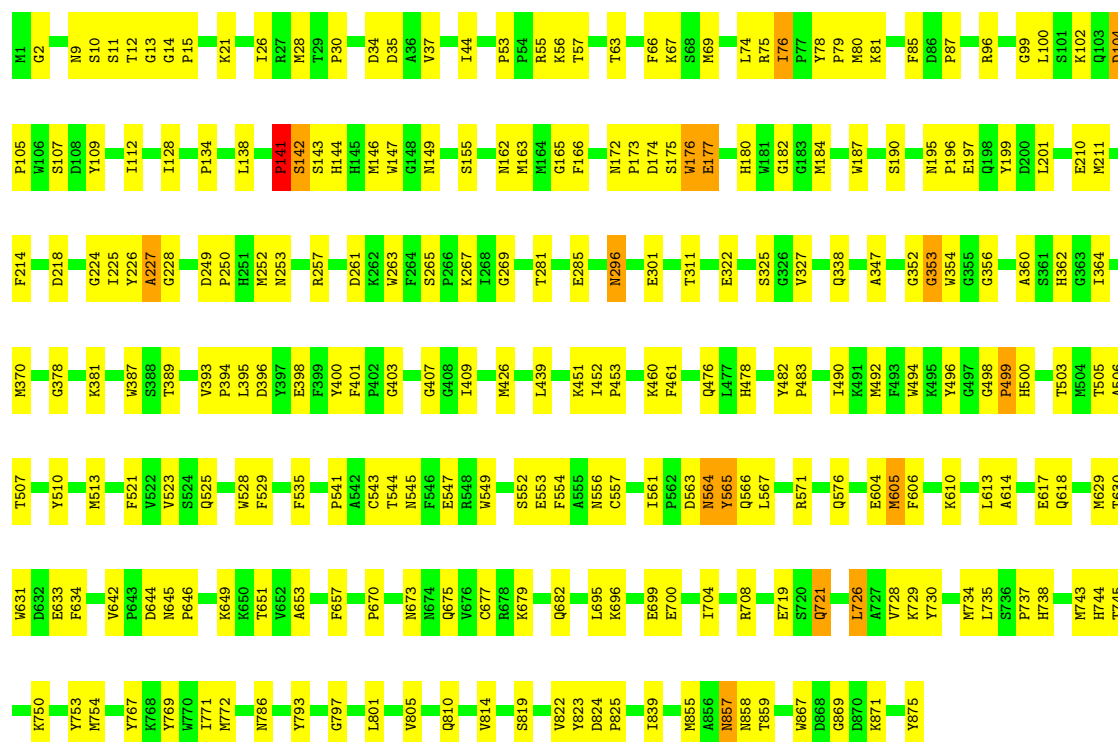
• Molecule 1: Pyrogallol hydroxytransferase large subunit

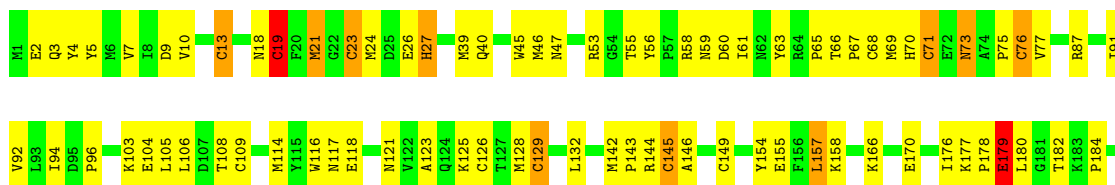
Chain S:  73% 26%

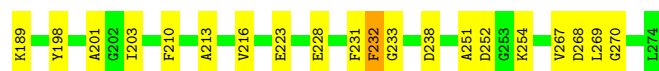


• Molecule 1: Pyrogallol hydroxytransferase large subunit

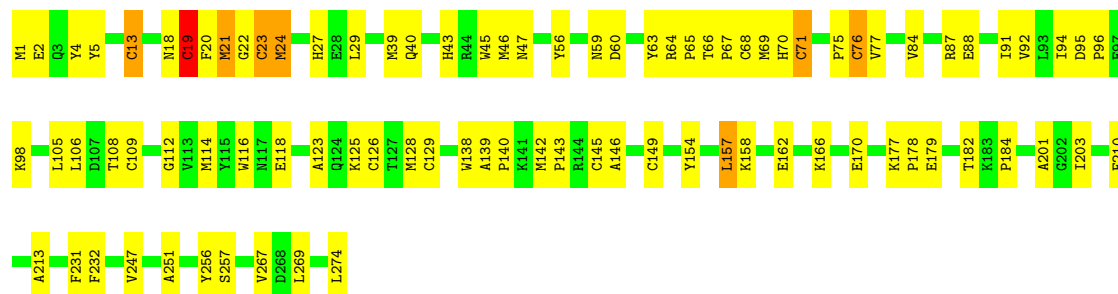
Chain U:  72% 26%







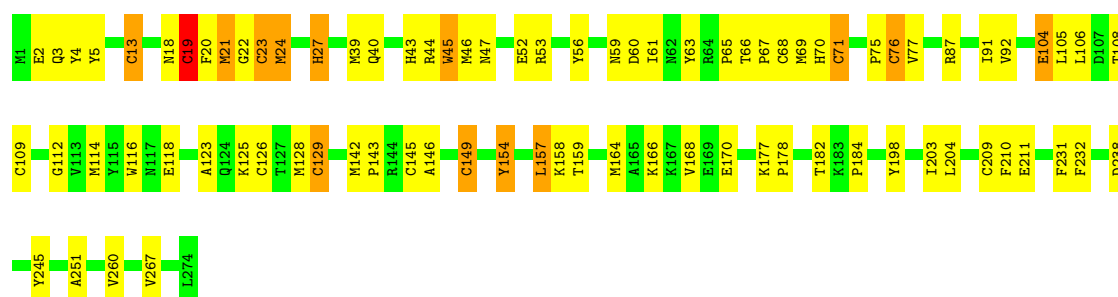
- Molecule 2: Pyrogallol hydroxytransferase small subunit



- Molecule 2: Pyrogallol hydroxytransferase small subunit

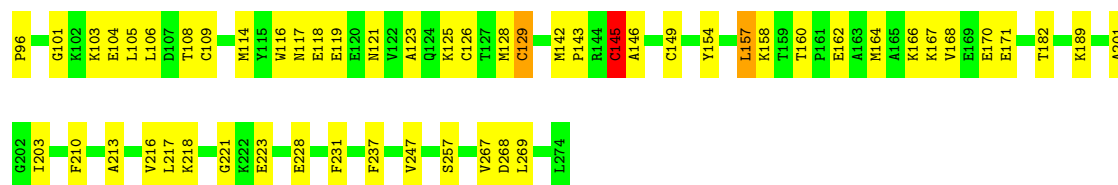


- Molecule 2: Pyrogallol hydroxytransferase small subunit



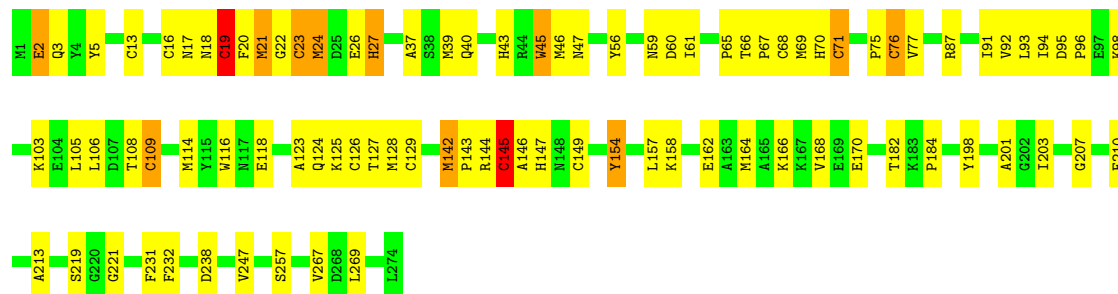
- Molecule 2: Pyrogallol hydroxytransferase small subunit





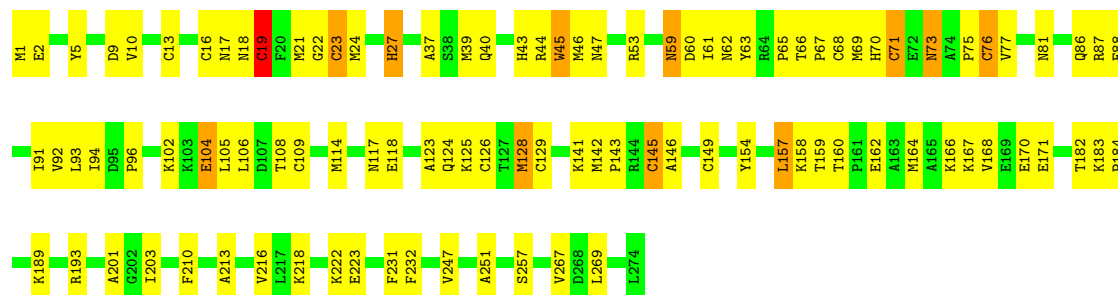
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N: 67% 28% . .



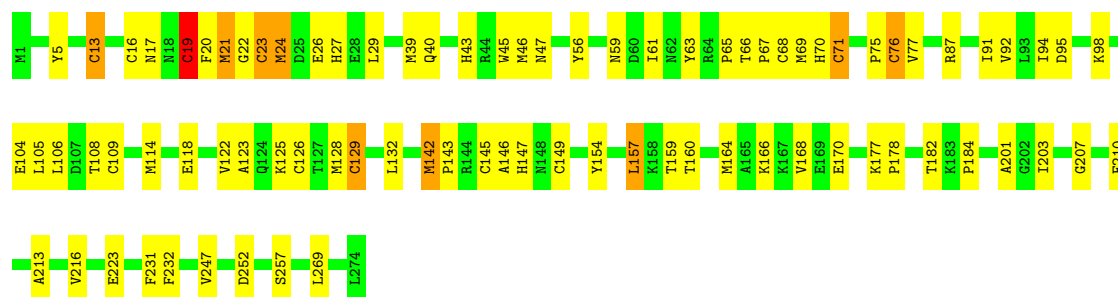
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P: 63% 33% .



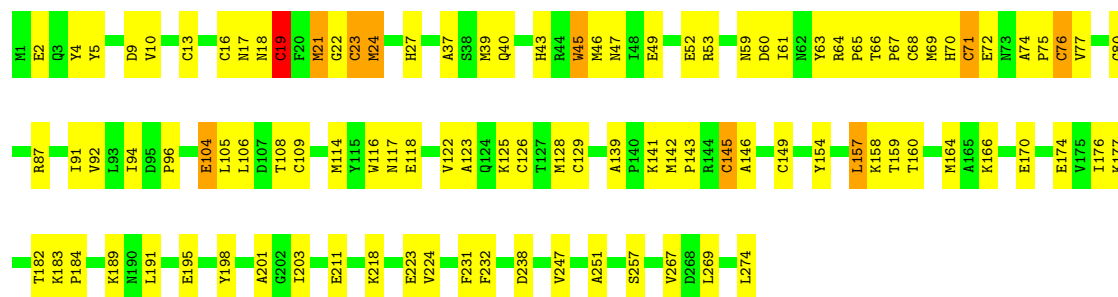
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R: 69% 27% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T: 62% 34% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V: 66% 31% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X: 55% 41% .



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	172.47Å 178.14Å 179.05Å 64.11° 64.45° 65.11°	Depositor
Resolution (Å)	24.99 – 2.20	Depositor
% Data completeness (in resolution range)	96.7 (24.99-2.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121808	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: PYG, SF4, MGD, CA, 4MO

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	0.38	0/7219	0.98	41/9786 (0.4%)
1	C	0.37	0/7219	0.97	45/9786 (0.5%)
1	E	0.38	0/7219	0.97	36/9786 (0.4%)
1	G	0.38	0/7219	0.98	45/9786 (0.5%)
1	I	0.37	0/7219	0.97	45/9786 (0.5%)
1	K	0.39	0/7219	0.97	37/9786 (0.4%)
1	M	0.38	0/7219	0.97	43/9786 (0.4%)
1	O	0.38	0/7219	0.96	42/9786 (0.4%)
1	Q	0.38	0/7219	0.97	44/9786 (0.4%)
1	S	0.37	0/7219	0.97	39/9786 (0.4%)
1	U	0.37	0/7219	0.97	42/9786 (0.4%)
1	W	0.37	0/7219	0.97	41/9786 (0.4%)
2	B	0.47	1/2231 (0.0%)	0.97	10/3009 (0.3%)
2	D	0.39	0/2231	0.92	8/3009 (0.3%)
2	F	0.45	0/2231	0.96	6/3009 (0.2%)
2	H	0.44	0/2231	0.97	9/3009 (0.3%)
2	J	0.43	0/2231	0.95	8/3009 (0.3%)
2	L	0.43	0/2231	0.97	8/3009 (0.3%)
2	N	0.47	1/2231 (0.0%)	0.96	11/3009 (0.4%)
2	P	0.43	0/2231	0.95	9/3009 (0.3%)
2	R	0.45	1/2231 (0.0%)	0.98	6/3009 (0.2%)
2	T	0.41	0/2231	0.95	11/3009 (0.4%)
2	V	0.40	0/2231	0.94	7/3009 (0.2%)
2	X	0.38	0/2231	0.93	13/3009 (0.4%)
All	All	0.39	3/113400 (0.0%)	0.97	606/153540 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	MET	SD-CE	-6.04	1.64	1.79
2	R	142	MET	SD-CE	-5.89	1.64	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	142	MET	SD-CE	-5.21	1.66	1.79

The worst 5 of 606 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	77	VAL	N-CA-C	-9.71	101.29	111.58
1	Q	76	ILE	CA-C-N	9.41	128.75	118.97
1	Q	76	ILE	C-N-CA	9.41	128.75	118.97
1	G	76	ILE	CA-C-N	9.19	128.52	118.97
1	G	76	ILE	C-N-CA	9.19	128.52	118.97

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	169	0
1	C	6998	0	6632	193	0
1	E	6998	0	6632	176	0
1	G	6998	0	6632	161	0
1	I	6998	0	6632	178	0
1	K	6998	0	6632	164	0
1	M	6998	0	6632	188	0
1	O	6998	0	6632	199	0
1	Q	6998	0	6632	194	0
1	S	6998	0	6632	182	0
1	U	6998	0	6632	197	0
1	W	6998	0	6632	195	0
2	B	2182	0	2077	79	0
2	D	2182	0	2077	92	0
2	F	2182	0	2077	85	0
2	H	2182	0	2077	75	0
2	J	2182	0	2077	81	0
2	L	2182	0	2077	84	0
2	N	2182	0	2077	92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	2182	0	2077	93	0
2	R	2182	0	2077	78	0
2	T	2182	0	2077	84	0
2	V	2182	0	2077	68	0
2	X	2182	0	2077	105	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	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	13	0
4	C	94	0	44	13	0
4	E	94	0	44	14	0
4	G	94	0	44	11	0
4	I	94	0	44	12	0
4	K	94	0	44	13	0
4	M	94	0	44	15	0
4	O	94	0	44	12	0
4	Q	94	0	44	10	0
4	S	94	0	44	11	0
4	U	94	0	44	13	0
4	W	94	0	44	12	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0	5	1	0
6	C	9	0	5	0	0
6	E	9	0	5	1	0
6	G	9	0	5	0	0
6	I	9	0	5	1	0
6	K	9	0	5	0	0
6	M	9	0	5	1	0
6	O	9	0	5	1	0
6	Q	9	0	5	1	0
6	S	9	0	5	1	0
6	U	9	0	5	1	0
6	W	9	0	5	0	0
7	B	24	0	0	4	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	3	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	5	0
8	A	681	0	0	10	0
8	B	170	0	0	1	0
8	C	681	0	0	15	0
8	D	166	0	0	2	0
8	E	684	0	0	9	0
8	F	163	0	0	4	0
8	G	683	0	0	9	0
8	H	161	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	671	0	0	11	0
8	J	163	0	0	2	0
8	K	681	0	0	10	0
8	L	165	0	0	2	0
8	M	684	0	0	11	0
8	N	159	0	0	5	0
8	O	672	0	0	21	0
8	P	164	0	0	4	0
8	Q	690	0	0	14	0
8	R	161	0	0	0	0
8	S	663	0	0	16	0
8	T	163	0	0	1	0
8	U	668	0	0	12	0
8	V	157	0	0	0	0
8	W	675	0	0	20	0
8	X	164	0	0	7	0
All	All	121808	0	105096	3135	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 14.

The worst 5 of 3135 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:B:68:CYS:HB2	2:B:126:CYS:HB3	1.36	1.05
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.40	1.04
1:E:66:PHE:HZ	1:E:146:MET:HE1	1.23	1.03
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.38	1.03
2:L:68:CYS:HB2	2:L:126:CYS:HB3	1.38	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	873/875 (100%)	815 (93%)	54 (6%)	4 (0%)	24	27
1	C	873/875 (100%)	822 (94%)	46 (5%)	5 (1%)	21	23
1	E	873/875 (100%)	820 (94%)	50 (6%)	3 (0%)	36	42
1	G	873/875 (100%)	823 (94%)	46 (5%)	4 (0%)	24	27
1	I	873/875 (100%)	821 (94%)	49 (6%)	3 (0%)	36	42
1	K	873/875 (100%)	822 (94%)	48 (6%)	3 (0%)	36	42
1	M	873/875 (100%)	825 (94%)	45 (5%)	3 (0%)	36	42
1	O	873/875 (100%)	816 (94%)	51 (6%)	6 (1%)	18	19
1	Q	873/875 (100%)	821 (94%)	48 (6%)	4 (0%)	24	27
1	S	873/875 (100%)	814 (93%)	52 (6%)	7 (1%)	16	16
1	U	873/875 (100%)	820 (94%)	49 (6%)	4 (0%)	24	27
1	W	873/875 (100%)	815 (93%)	55 (6%)	3 (0%)	36	42
2	B	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	30	34
2	D	272/274 (99%)	256 (94%)	14 (5%)	2 (1%)	18	19
2	F	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	30	34
2	H	272/274 (99%)	258 (95%)	11 (4%)	3 (1%)	11	10
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	18	19
2	N	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	P	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	30	34
2	R	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	34
2	T	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	30	34
2	V	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	18	19
2	X	272/274 (99%)	245 (90%)	25 (9%)	2 (1%)	18	19
All	All	13740/13788 (100%)	12921 (94%)	752 (6%)	67 (0%)	24	27

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	177	GLU
1	I	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%)	720 (99%)	9 (1%)	63	78
1	C	729/729 (100%)	717 (98%)	12 (2%)	55	71
1	E	729/729 (100%)	722 (99%)	7 (1%)	68	81
1	G	729/729 (100%)	722 (99%)	7 (1%)	68	81
1	I	729/729 (100%)	719 (99%)	10 (1%)	59	75
1	K	729/729 (100%)	723 (99%)	6 (1%)	73	85
1	M	729/729 (100%)	721 (99%)	8 (1%)	65	79
1	O	729/729 (100%)	718 (98%)	11 (2%)	57	73
1	Q	729/729 (100%)	718 (98%)	11 (2%)	57	73
1	S	729/729 (100%)	720 (99%)	9 (1%)	63	78
1	U	729/729 (100%)	723 (99%)	6 (1%)	73	85
1	W	729/729 (100%)	719 (99%)	10 (1%)	59	75
2	B	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	D	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	F	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	H	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	J	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	L	235/235 (100%)	224 (95%)	11 (5%)	23	31
2	N	235/235 (100%)	224 (95%)	11 (5%)	23	31
2	P	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	R	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	T	235/235 (100%)	223 (95%)	12 (5%)	21	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	V	235/235 (100%)	223 (95%)	12 (5%)	21 27
2	X	235/235 (100%)	226 (96%)	9 (4%)	29 40
All	All	11568/11568 (100%)	11323 (98%)	245 (2%)	47 63

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	71	CYS
2	V	104	GLU
1	O	373	LEU
2	V	73	ASN
2	X	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 267 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	674	ASN
2	V	73	ASN
1	W	810	GLN
1	I	462	GLN
1	I	171	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 35 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	W	903	5	47,52,52	2.66	13 (27%)	58,81,81	1.20	3 (5%)
4	MGD	A	902	5	47,52,52	2.21	13 (27%)	58,81,81	2.24	9 (15%)
4	MGD	K	902	5	47,52,52	2.08	12 (25%)	58,81,81	1.98	8 (13%)
4	MGD	Q	903	5	47,52,52	2.23	12 (25%)	58,81,81	1.47	3 (5%)
6	PYG	Q	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.11	4 (33%)
7	SF4	R	302	2	0,12,12	-	-	-	-	-
6	PYG	O	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.17	5 (41%)
7	SF4	X	304	2	0,12,12	-	-	-	-	-
4	MGD	U	902	5	47,52,52	2.17	16 (34%)	58,81,81	2.10	8 (13%)
7	SF4	J	303	2	0,12,12	-	-	-	-	-
4	MGD	G	902	5	47,52,52	2.25	12 (25%)	58,81,81	2.18	7 (12%)
4	MGD	M	902	5	47,52,52	2.03	14 (29%)	58,81,81	2.04	9 (15%)
7	SF4	F	303	2	0,12,12	-	-	-	-	-
7	SF4	L	302	2	0,12,12	-	-	-	-	-
4	MGD	Q	902	5	47,52,52	2.06	13 (27%)	58,81,81	2.02	7 (12%)
6	PYG	I	905	5	9,9,9	4.67	9 (100%)	12,12,12	3.13	5 (41%)
4	MGD	C	903	5	47,52,52	2.60	18 (38%)	58,81,81	1.30	3 (5%)
4	MGD	W	902	5	47,52,52	2.12	13 (27%)	58,81,81	2.01	8 (13%)
6	PYG	E	905	5	9,9,9	4.69	9 (100%)	12,12,12	3.12	4 (33%)
4	MGD	I	903	5	47,52,52	2.31	14 (29%)	58,81,81	1.55	4 (6%)
7	SF4	P	304	2	0,12,12	-	-	-	-	-
7	SF4	D	304	2	0,12,12	-	-	-	-	-
6	PYG	K	905	5	9,9,9	4.71	9 (100%)	12,12,12	3.16	4 (33%)
6	PYG	A	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.09	4 (33%)
7	SF4	T	302	2	0,12,12	-	-	-	-	-
4	MGD	K	903	5	47,52,52	2.35	15 (31%)	58,81,81	2.16	9 (15%)
7	SF4	L	303	2	0,12,12	-	-	-	-	-
7	SF4	X	302	2	0,12,12	-	-	-	-	-
7	SF4	R	304	2	0,12,12	-	-	-	-	-
4	MGD	G	903	5	47,52,52	2.29	17 (36%)	58,81,81	1.52	2 (3%)
4	MGD	C	902	5	47,52,52	2.22	13 (27%)	58,81,81	2.05	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	X	303	2	0,12,12	-	-	-		
4	MGD	I	902	5	47,52,52	2.03	12 (25%)	58,81,81	1.99	8 (13%)
4	MGD	E	902	5	47,52,52	2.12	13 (27%)	58,81,81	2.08	8 (13%)
7	SF4	N	302	2	0,12,12	-	-	-		
4	MGD	S	902	5	47,52,52	2.12	14 (29%)	58,81,81	2.13	8 (13%)
7	SF4	B	304	2	0,12,12	-	-	-		
7	SF4	F	304	2	0,12,12	-	-	-		
7	SF4	H	303	2	0,12,12	-	-	-		
7	SF4	T	303	2	0,12,12	-	-	-		
7	SF4	J	302	2	0,12,12	-	-	-		
7	SF4	F	302	2	0,12,12	-	-	-		
6	PYG	W	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.21	5 (41%)
7	SF4	B	303	2	0,12,12	-	-	-		
4	MGD	U	903	5	47,52,52	2.46	12 (25%)	58,81,81	1.32	4 (6%)
7	SF4	V	304	2	0,12,12	-	-	-		
7	SF4	V	302	2	0,12,12	-	-	-		
7	SF4	L	304	2	0,12,12	-	-	-		
6	PYG	C	905	5	9,9,9	4.63	9 (100%)	12,12,12	3.15	5 (41%)
7	SF4	R	303	2	0,12,12	-	-	-		
6	PYG	S	905	5	9,9,9	4.72	9 (100%)	12,12,12	3.10	4 (33%)
4	MGD	S	903	5	47,52,52	2.34	14 (29%)	58,81,81	1.38	3 (5%)
6	PYG	G	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.12	4 (33%)
6	PYG	M	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.12	5 (41%)
7	SF4	P	302	2	0,12,12	-	-	-		
7	SF4	V	303	2	0,12,12	-	-	-		
7	SF4	D	302	2	0,12,12	-	-	-		
4	MGD	E	903	5	47,52,52	2.37	15 (31%)	58,81,81	1.40	4 (6%)
7	SF4	N	303	2	0,12,12	-	-	-		
7	SF4	B	302	2	0,12,12	-	-	-		
4	MGD	O	903	5	47,52,52	2.46	16 (34%)	58,81,81	1.32	4 (6%)
4	MGD	A	903	5	47,52,52	2.31	14 (29%)	58,81,81	2.26	10 (17%)
7	SF4	H	304	2	0,12,12	-	-	-		
7	SF4	H	302	2	0,12,12	-	-	-		
7	SF4	J	301	2	0,12,12	-	-	-		
4	MGD	M	903	5	47,52,52	2.42	16 (34%)	58,81,81	1.43	5 (8%)
7	SF4	D	303	2	0,12,12	-	-	-		
7	SF4	P	303	2	0,12,12	-	-	-		
7	SF4	T	304	2	0,12,12	-	-	-		
6	PYG	U	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.13	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	N	304	2	0,12,12	-	-	-		
4	MGD	O	902	5	47,52,52	2.11	12 (25%)	58,81,81	2.03	9 (15%)

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	W	903	5	-	5/22/66/66	0/6/6/6
4	MGD	A	902	5	-	9/22/66/66	0/6/6/6
4	MGD	K	902	5	-	8/22/66/66	0/6/6/6
4	MGD	Q	903	5	-	4/22/66/66	0/6/6/6
6	PYG	Q	905	5	-	-	0/1/1/1
7	SF4	R	302	2	-	-	0/6/5/5
6	PYG	O	905	5	-	-	0/1/1/1
7	SF4	X	304	2	-	-	0/6/5/5
4	MGD	U	902	5	-	7/22/66/66	0/6/6/6
7	SF4	J	303	2	-	-	0/6/5/5
4	MGD	G	902	5	-	10/22/66/66	0/6/6/6
4	MGD	M	902	5	-	7/22/66/66	0/6/6/6
7	SF4	F	303	2	-	-	0/6/5/5
7	SF4	L	302	2	-	-	0/6/5/5
4	MGD	Q	902	5	-	7/22/66/66	0/6/6/6
6	PYG	I	905	5	-	-	0/1/1/1
4	MGD	C	903	5	-	4/22/66/66	0/6/6/6
4	MGD	W	902	5	-	8/22/66/66	0/6/6/6
6	PYG	E	905	5	-	-	0/1/1/1
4	MGD	I	903	5	-	6/22/66/66	0/6/6/6
7	SF4	P	304	2	-	-	0/6/5/5
7	SF4	D	304	2	-	-	0/6/5/5
6	PYG	K	905	5	-	-	0/1/1/1
6	PYG	A	905	5	-	-	0/1/1/1
7	SF4	T	302	2	-	-	0/6/5/5
4	MGD	K	903	5	-	4/22/66/66	0/6/6/6
7	SF4	L	303	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
7	SF4	R	304	2	-	-	0/6/5/5
4	MGD	G	903	5	-	3/22/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	C	902	5	-	7/22/66/66	0/6/6/6
7	SF4	X	303	2	-	-	0/6/5/5
4	MGD	I	902	5	-	8/22/66/66	0/6/6/6
4	MGD	E	902	5	-	8/22/66/66	0/6/6/6
7	SF4	N	302	2	-	-	0/6/5/5
4	MGD	S	902	5	-	9/22/66/66	0/6/6/6
7	SF4	B	304	2	-	-	0/6/5/5
7	SF4	F	304	2	-	-	0/6/5/5
7	SF4	H	303	2	-	-	0/6/5/5
7	SF4	T	303	2	-	-	0/6/5/5
7	SF4	J	302	2	-	-	0/6/5/5
7	SF4	F	302	2	-	-	0/6/5/5
6	PYG	W	905	5	-	-	0/1/1/1
7	SF4	B	303	2	-	-	0/6/5/5
4	MGD	U	903	5	-	4/22/66/66	0/6/6/6
7	SF4	V	304	2	-	-	0/6/5/5
7	SF4	V	302	2	-	-	0/6/5/5
7	SF4	L	304	2	-	-	0/6/5/5
6	PYG	C	905	5	-	-	0/1/1/1
7	SF4	R	303	2	-	-	0/6/5/5
6	PYG	S	905	5	-	-	0/1/1/1
4	MGD	S	903	5	-	4/22/66/66	0/6/6/6
6	PYG	G	905	5	-	-	0/1/1/1
6	PYG	M	905	5	-	-	0/1/1/1
7	SF4	P	302	2	-	-	0/6/5/5
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	D	302	2	-	-	0/6/5/5
4	MGD	E	903	5	-	4/22/66/66	0/6/6/6
7	SF4	N	303	2	-	-	0/6/5/5
7	SF4	B	302	2	-	-	0/6/5/5
4	MGD	O	903	5	-	4/22/66/66	0/6/6/6
4	MGD	A	903	5	-	5/22/66/66	0/6/6/6
7	SF4	H	304	2	-	-	0/6/5/5
7	SF4	H	302	2	-	-	0/6/5/5
7	SF4	J	301	2	-	-	0/6/5/5
4	MGD	M	903	5	-	4/22/66/66	0/6/6/6
7	SF4	D	303	2	-	-	0/6/5/5
7	SF4	P	303	2	-	-	0/6/5/5
7	SF4	T	304	2	-	-	0/6/5/5
6	PYG	U	905	5	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	N	304	2	-	-	0/6/5/5
4	MGD	O	902	5	-	8/22/66/66	0/6/6/6

The worst 5 of 441 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	905	PYG	C1-C2	8.07	1.49	1.40
6	I	905	PYG	C1-C2	8.04	1.49	1.40
6	E	905	PYG	C1-C2	8.01	1.49	1.40
6	U	905	PYG	C1-C2	7.99	1.49	1.40
6	C	905	PYG	C1-C2	7.98	1.49	1.40

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	MGD	O2A-PA-O3B	-11.71	75.62	107.27
4	G	902	MGD	O2A-PA-O3B	-11.59	75.95	107.27
4	S	902	MGD	O2A-PA-O3B	-11.18	77.06	107.27
4	Q	902	MGD	O2A-PA-O3B	-10.63	78.54	107.27
4	W	902	MGD	O2A-PA-O3B	-10.63	78.55	107.27

There are no chirality outliers.

5 of 147 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	MGD	C5'-O5'-PB-O1B
4	A	902	MGD	C5'-O5'-PB-O2B
4	A	902	MGD	C5'-O5'-PB-O3B
4	A	902	MGD	C10-O3A-PA-O2A
4	A	902	MGD	O3A-C10-C11-O11

There are no ring outliers.

67 monomers are involved in 206 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	903	MGD	4	0
4	A	902	MGD	5	0
4	K	902	MGD	5	0
4	Q	903	MGD	4	0
6	Q	905	PYG	1	0
6	O	905	PYG	1	0

Continued on next page...

Continued from previous page...

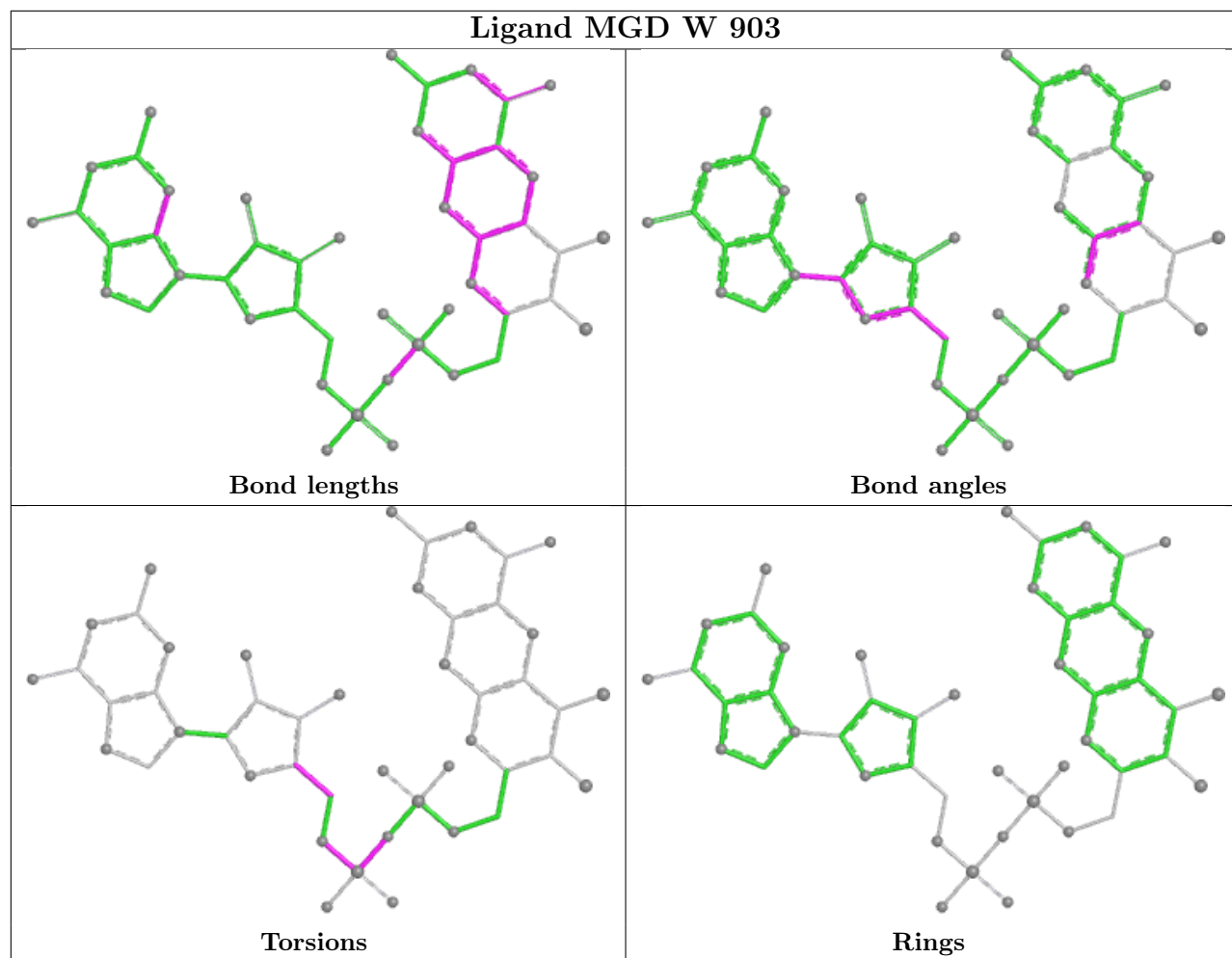
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	304	SF4	2	0
4	U	902	MGD	8	0
7	J	303	SF4	1	0
4	G	902	MGD	7	0
4	M	902	MGD	8	0
7	F	303	SF4	2	0
7	L	302	SF4	1	0
4	Q	902	MGD	6	0
6	I	905	PYG	1	0
4	C	903	MGD	5	0
4	W	902	MGD	8	0
6	E	905	PYG	1	0
4	I	903	MGD	6	0
7	P	304	SF4	1	0
7	D	304	SF4	1	0
6	A	905	PYG	1	0
7	T	302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

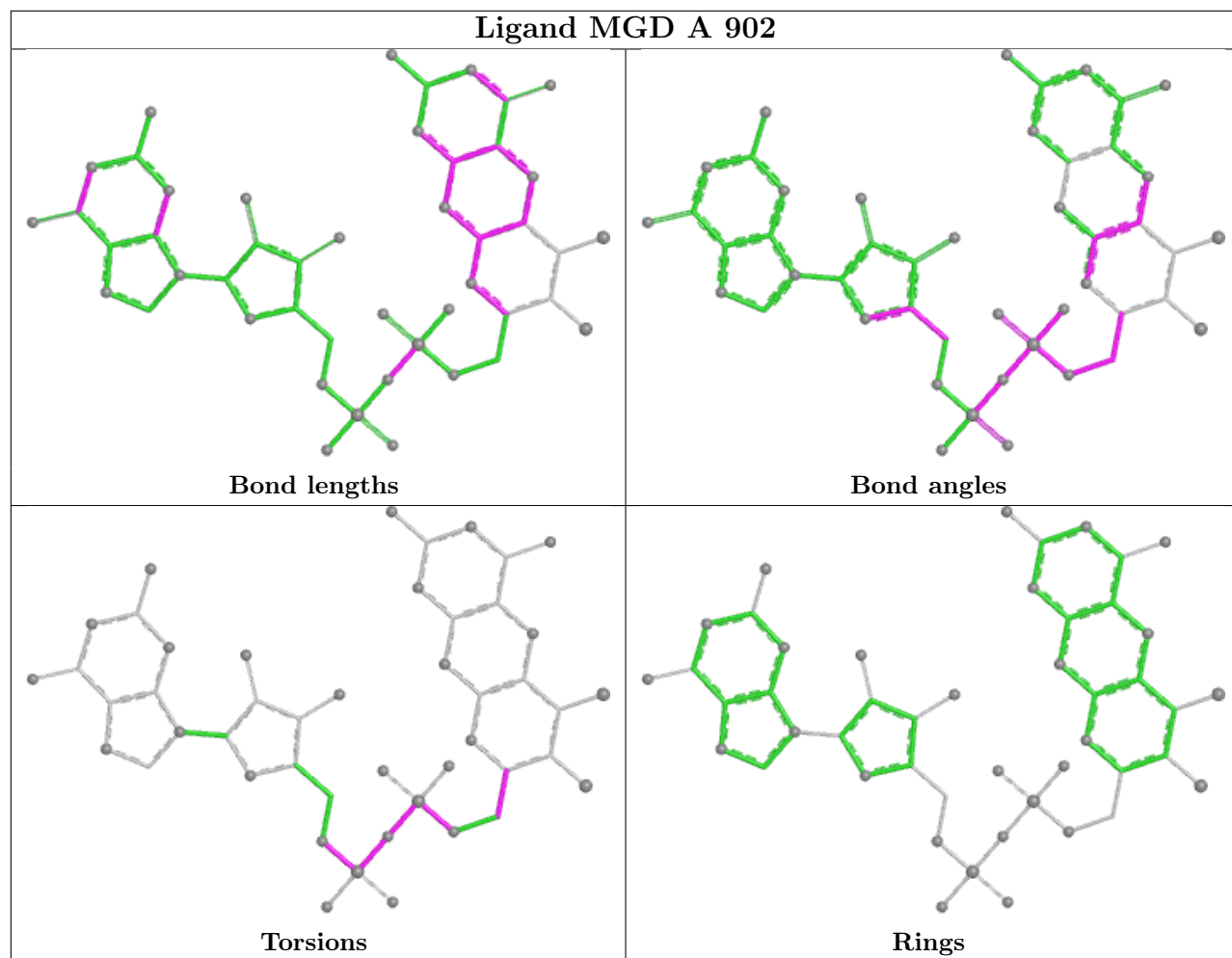
Continued on next page...

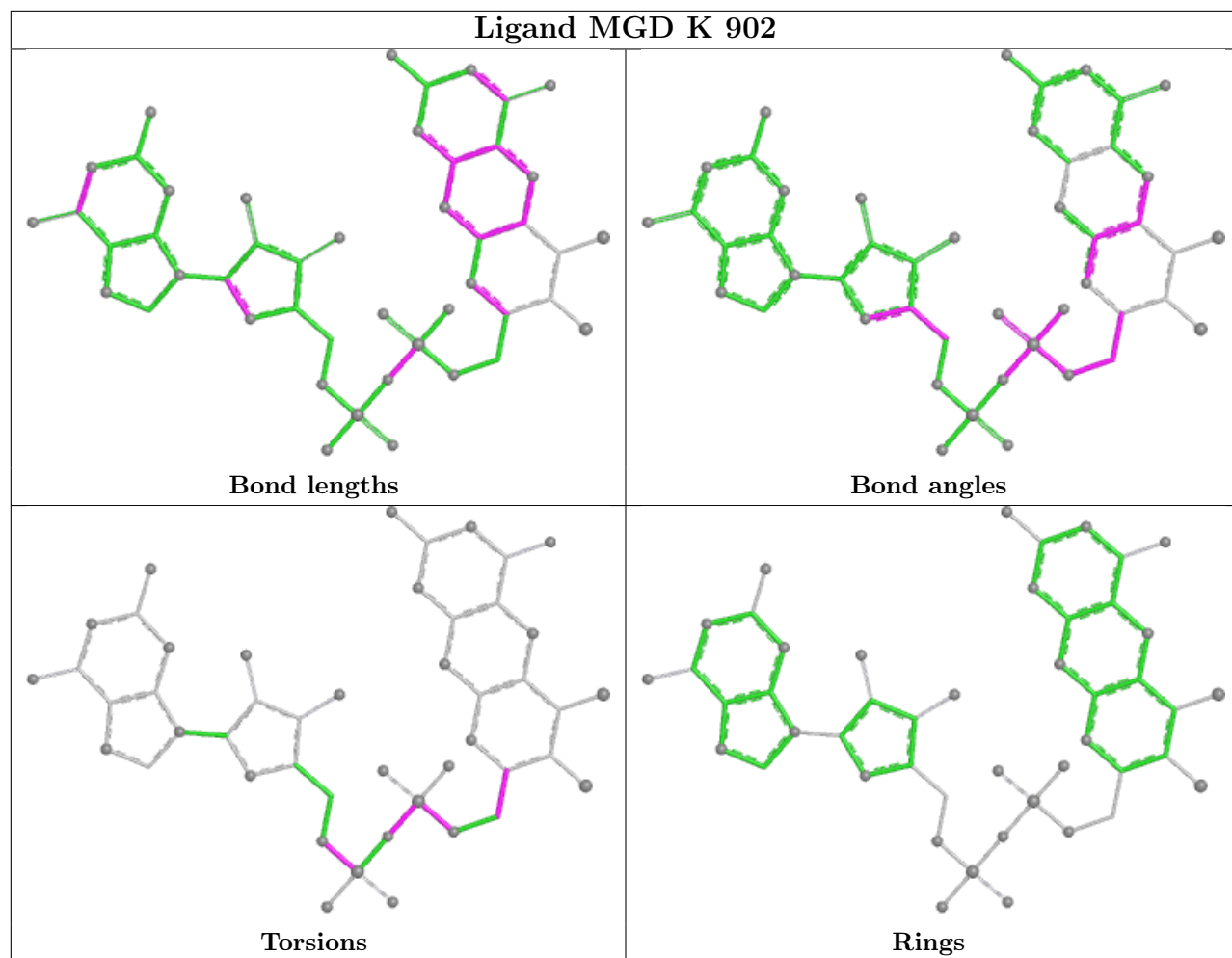
Continued from previous page...

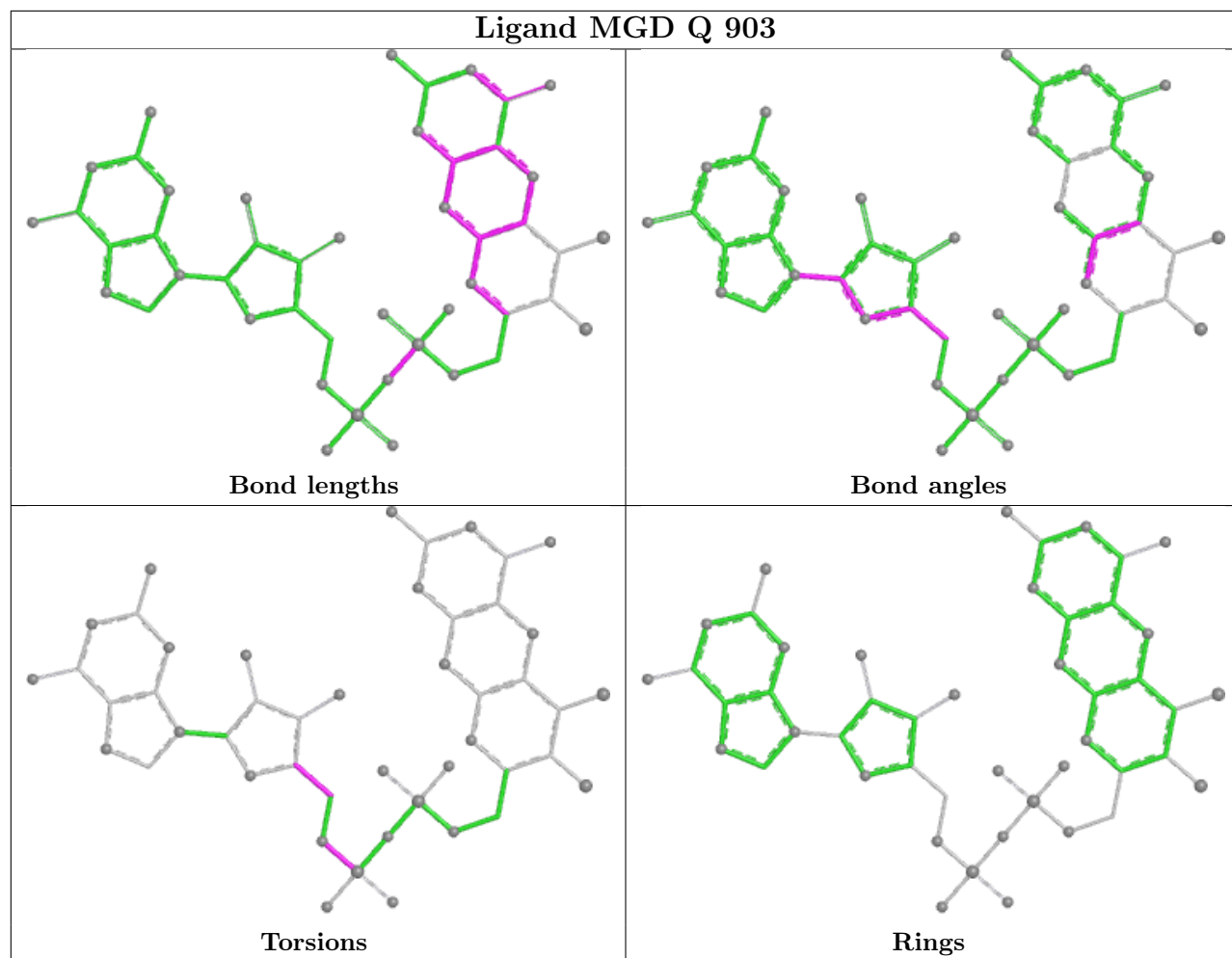
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	905	PYG	1	0
7	P	302	SF4	1	0
7	V	303	SF4	2	0
7	D	302	SF4	1	0
4	E	903	MGD	5	0
7	N	303	SF4	2	0
7	B	302	SF4	1	0
4	O	903	MGD	4	0
4	A	903	MGD	8	0
7	H	304	SF4	1	0
7	H	302	SF4	1	0
7	J	301	SF4	1	0
4	M	903	MGD	7	0
7	D	303	SF4	2	0
7	P	303	SF4	2	0
7	T	304	SF4	1	0
6	U	905	PYG	1	0
7	N	304	SF4	1	0
4	O	902	MGD	8	0

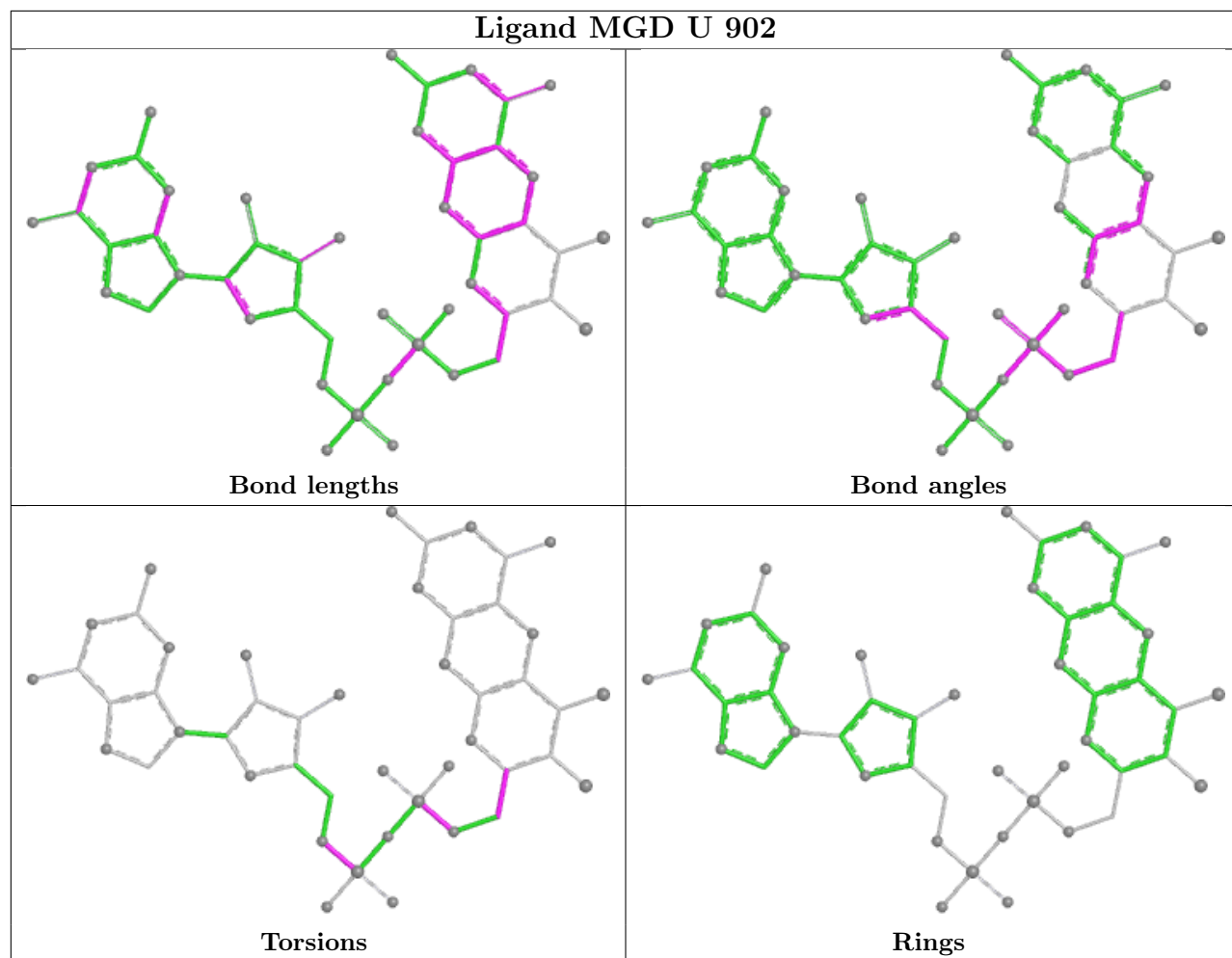
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

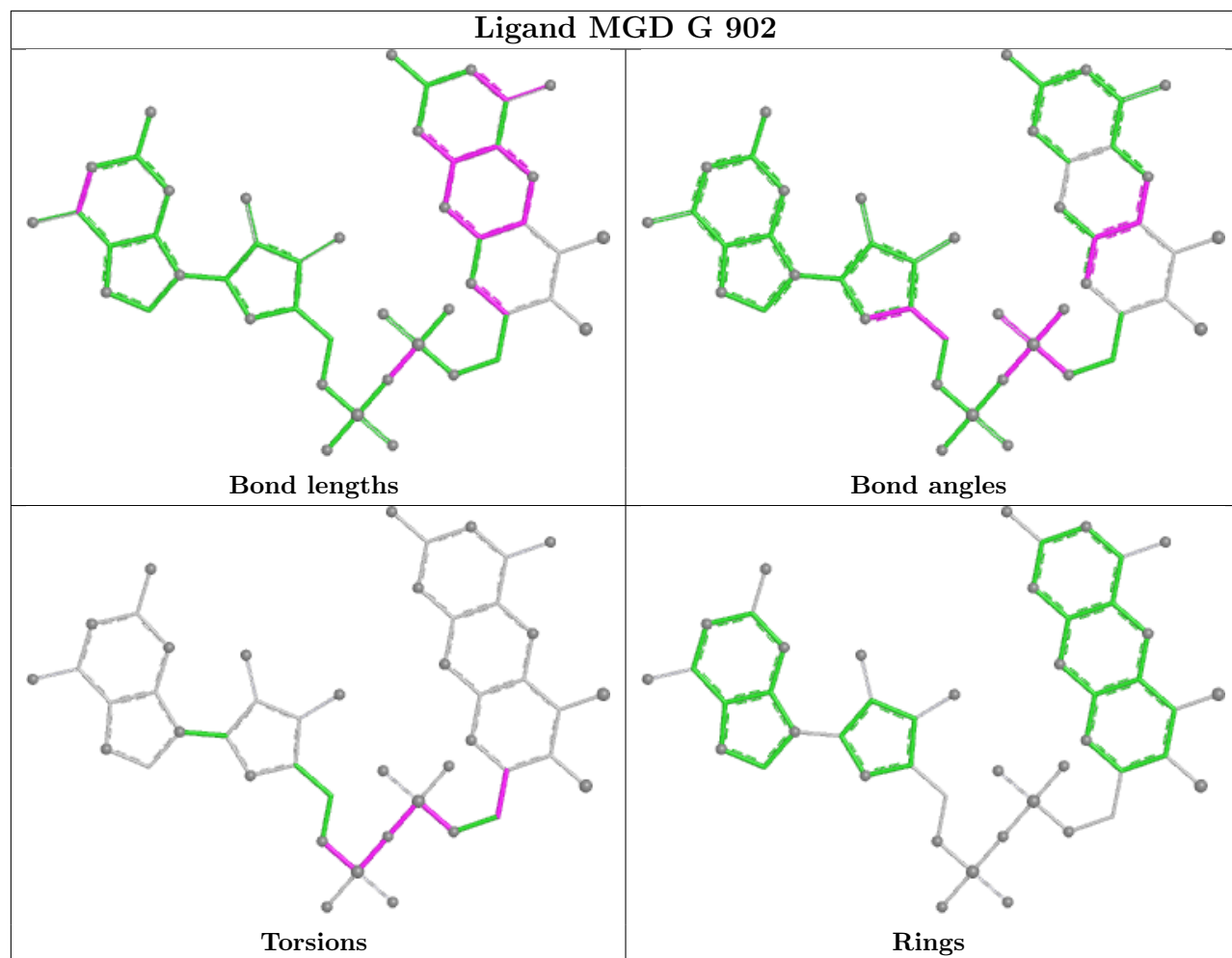


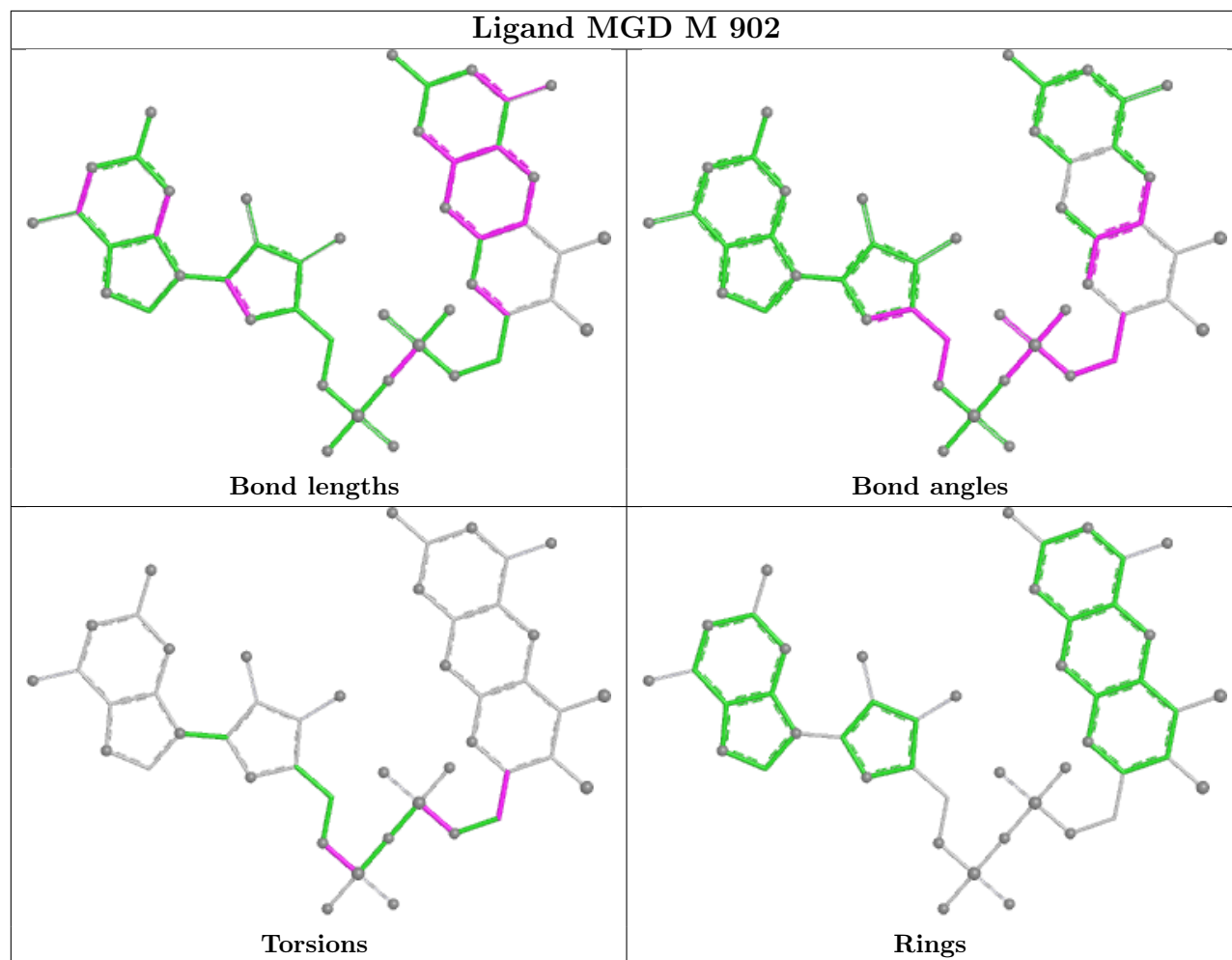


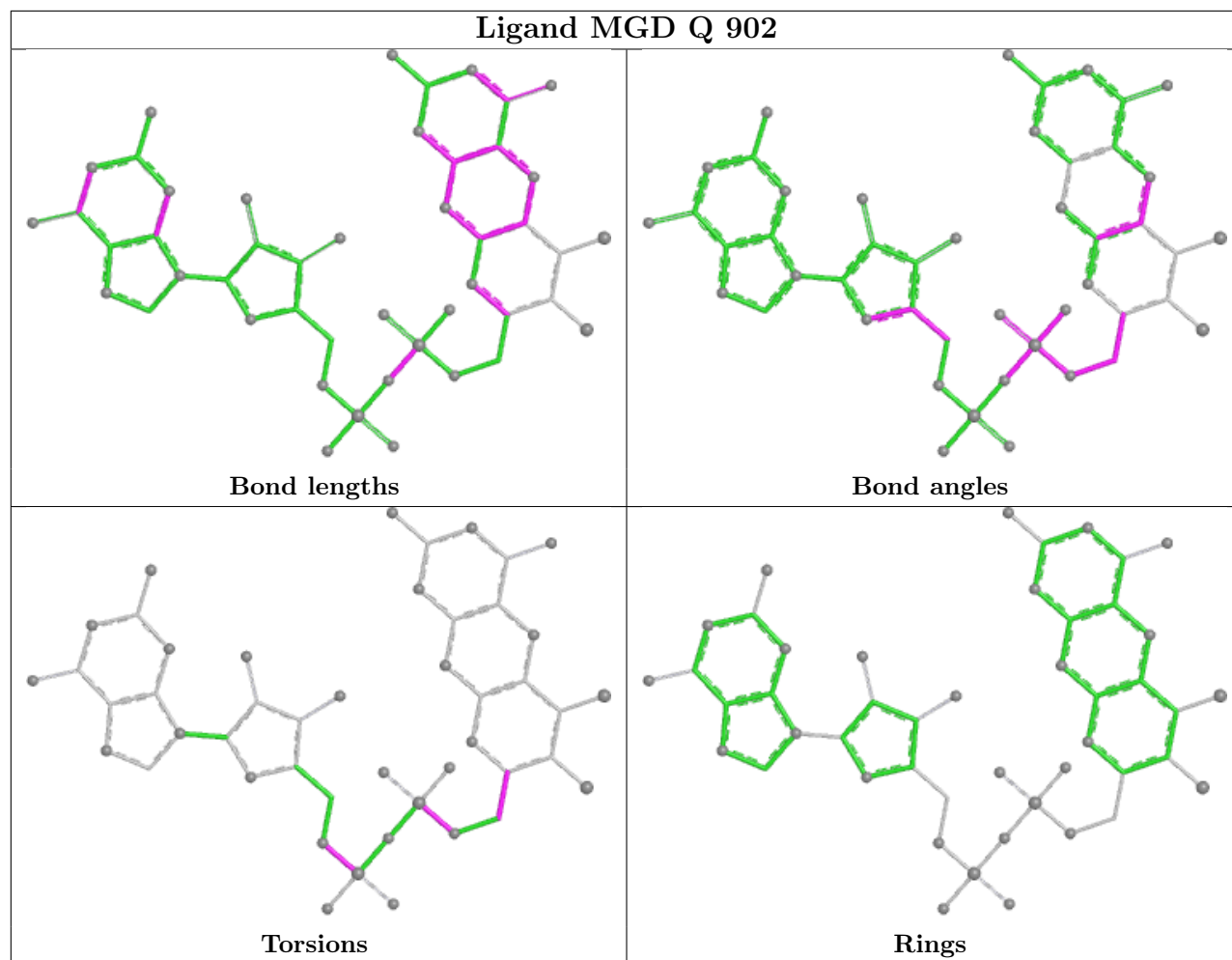


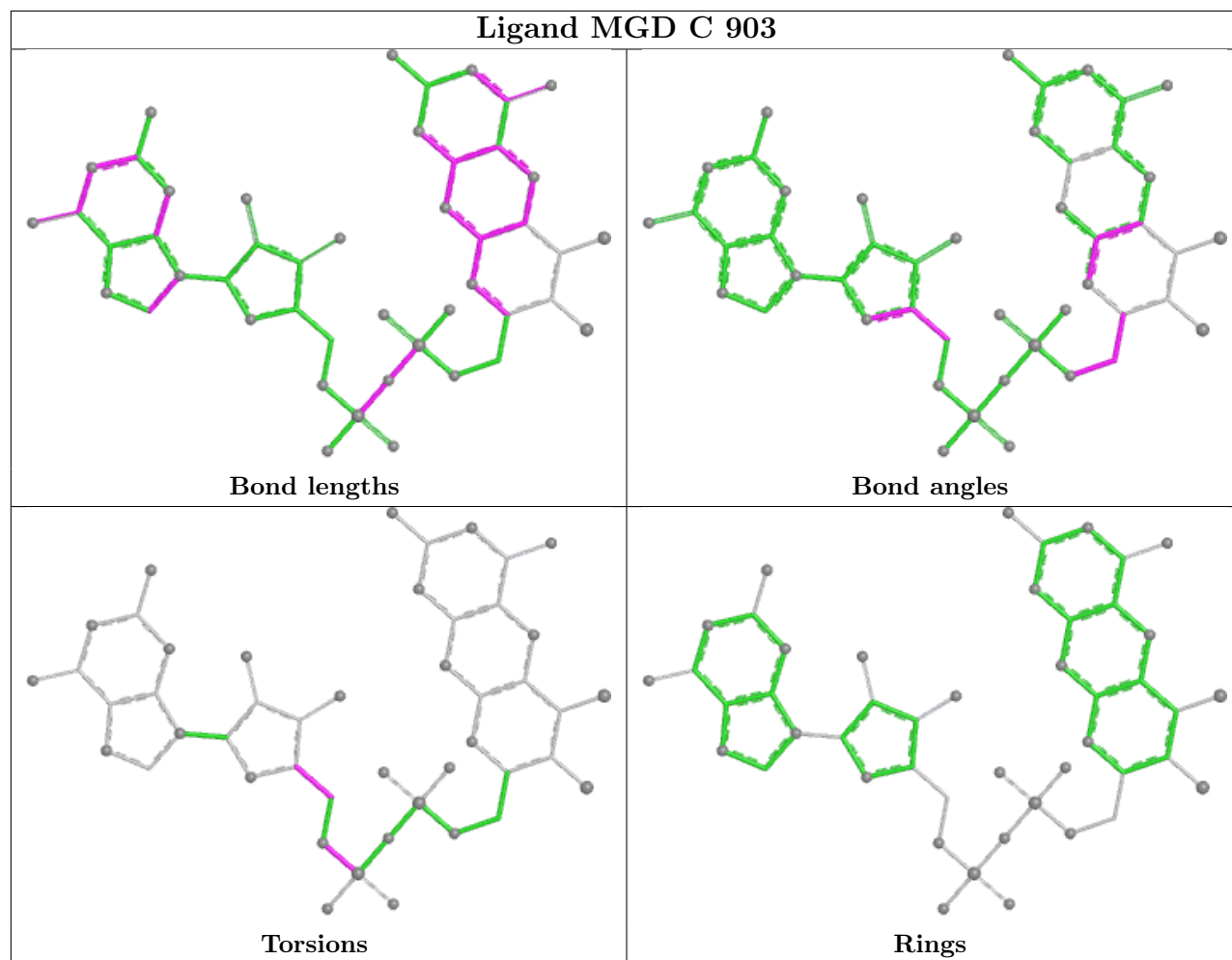


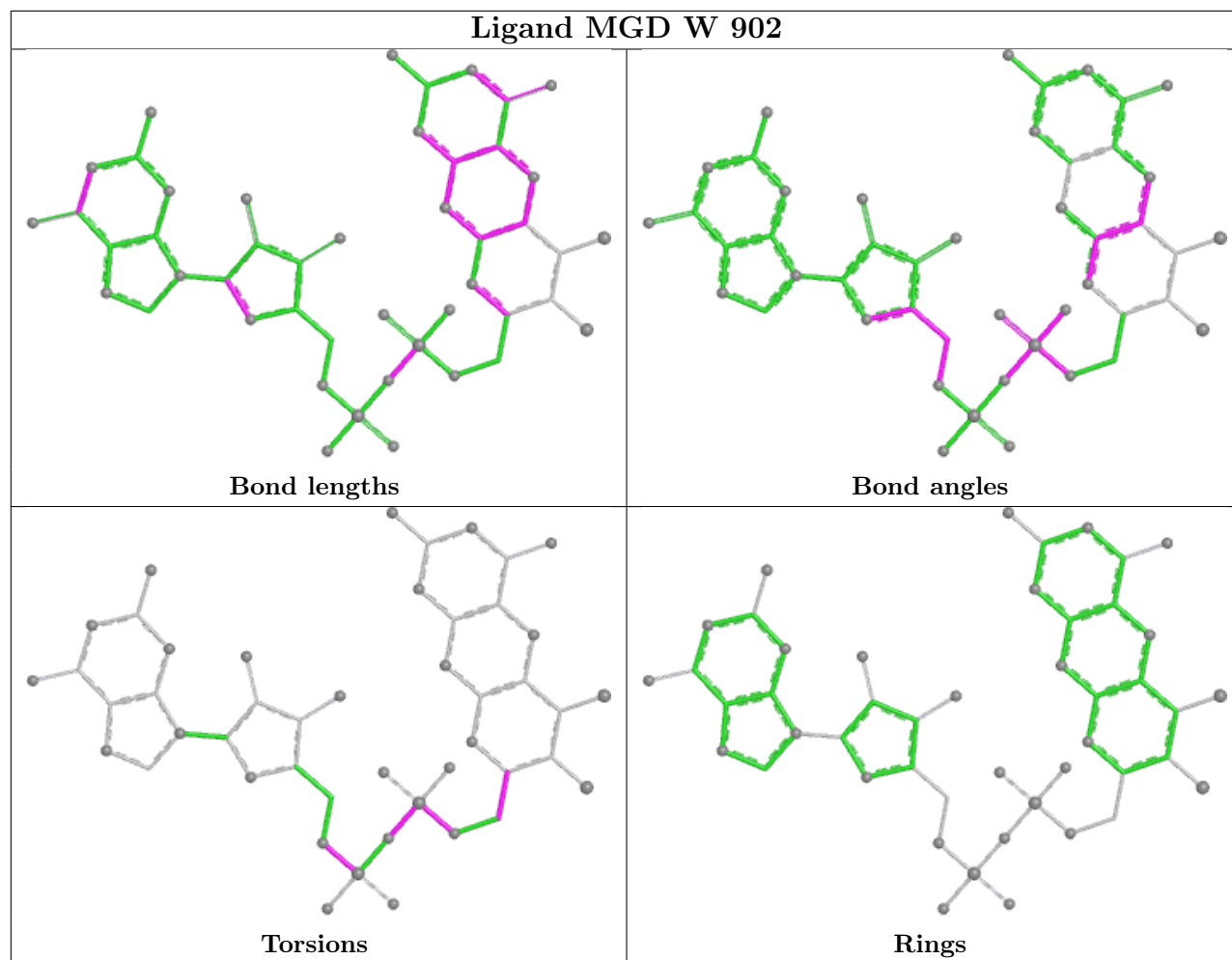


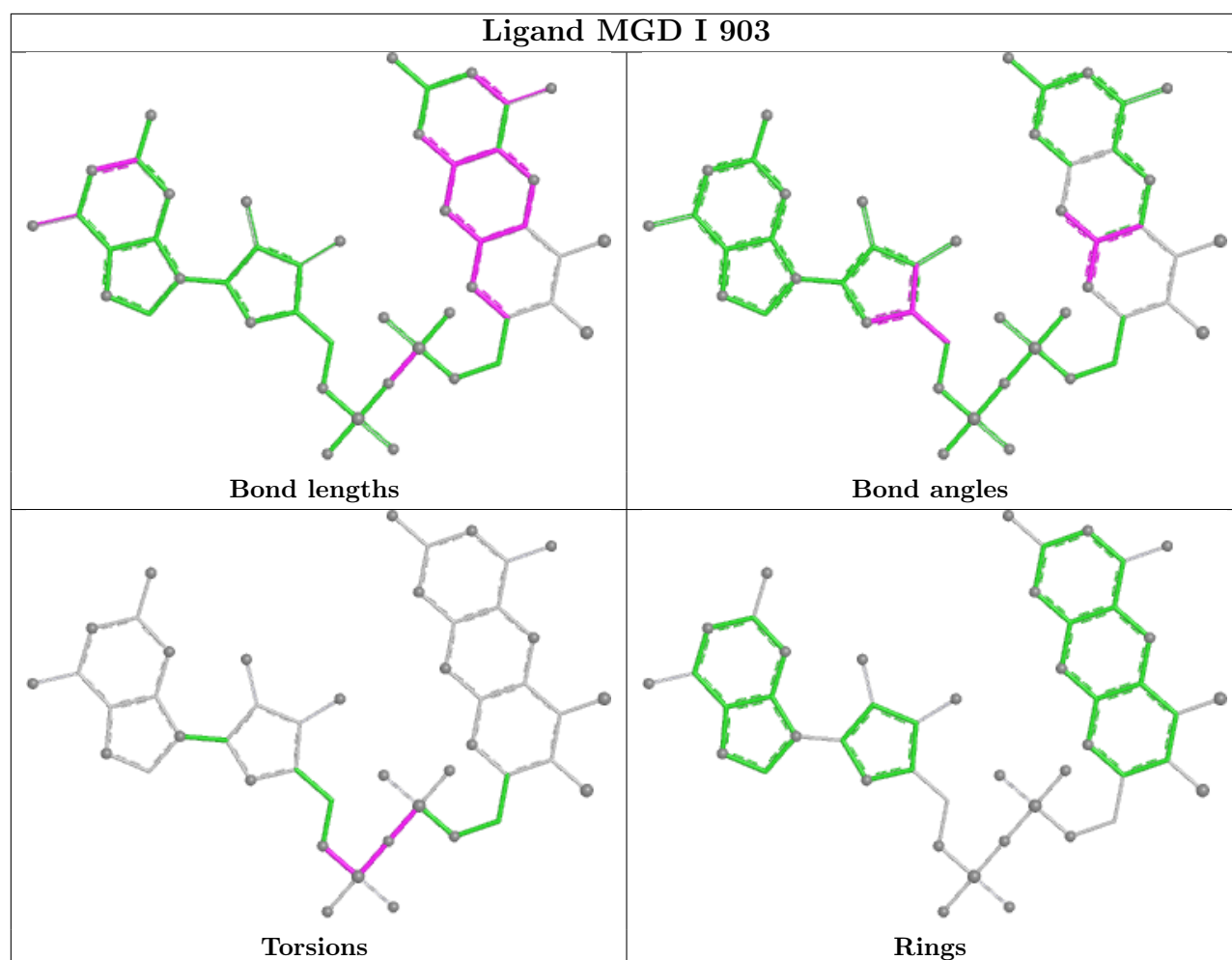


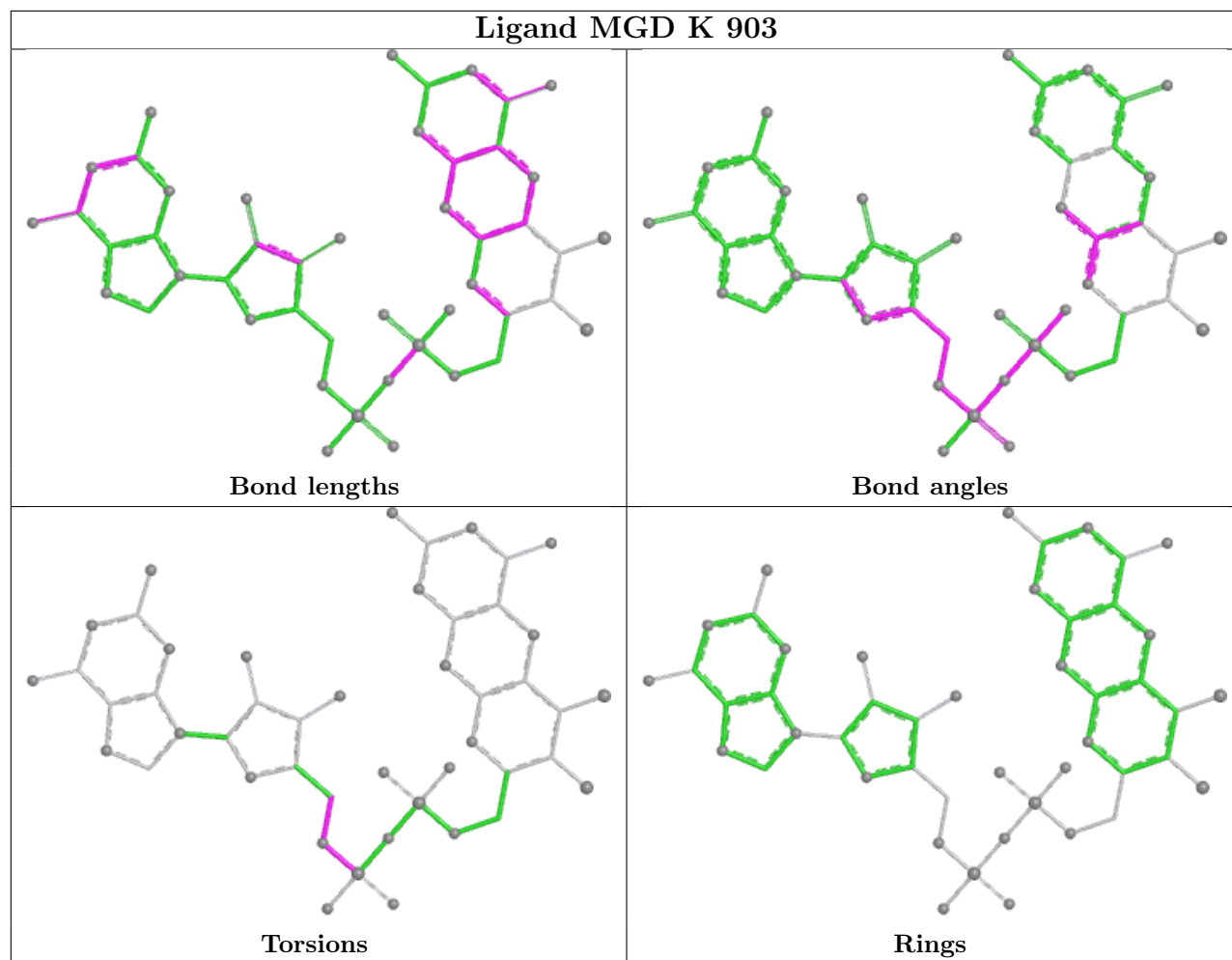


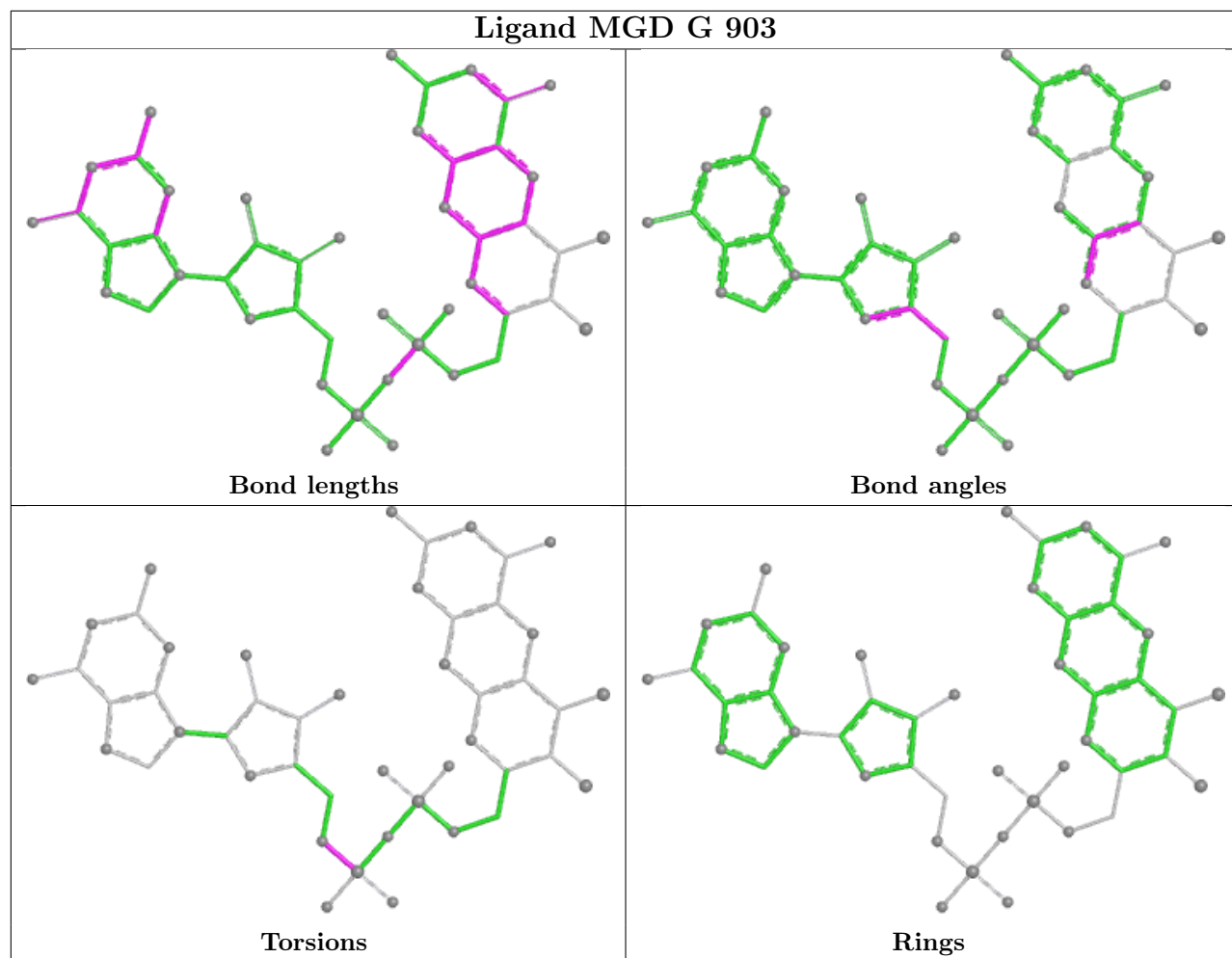


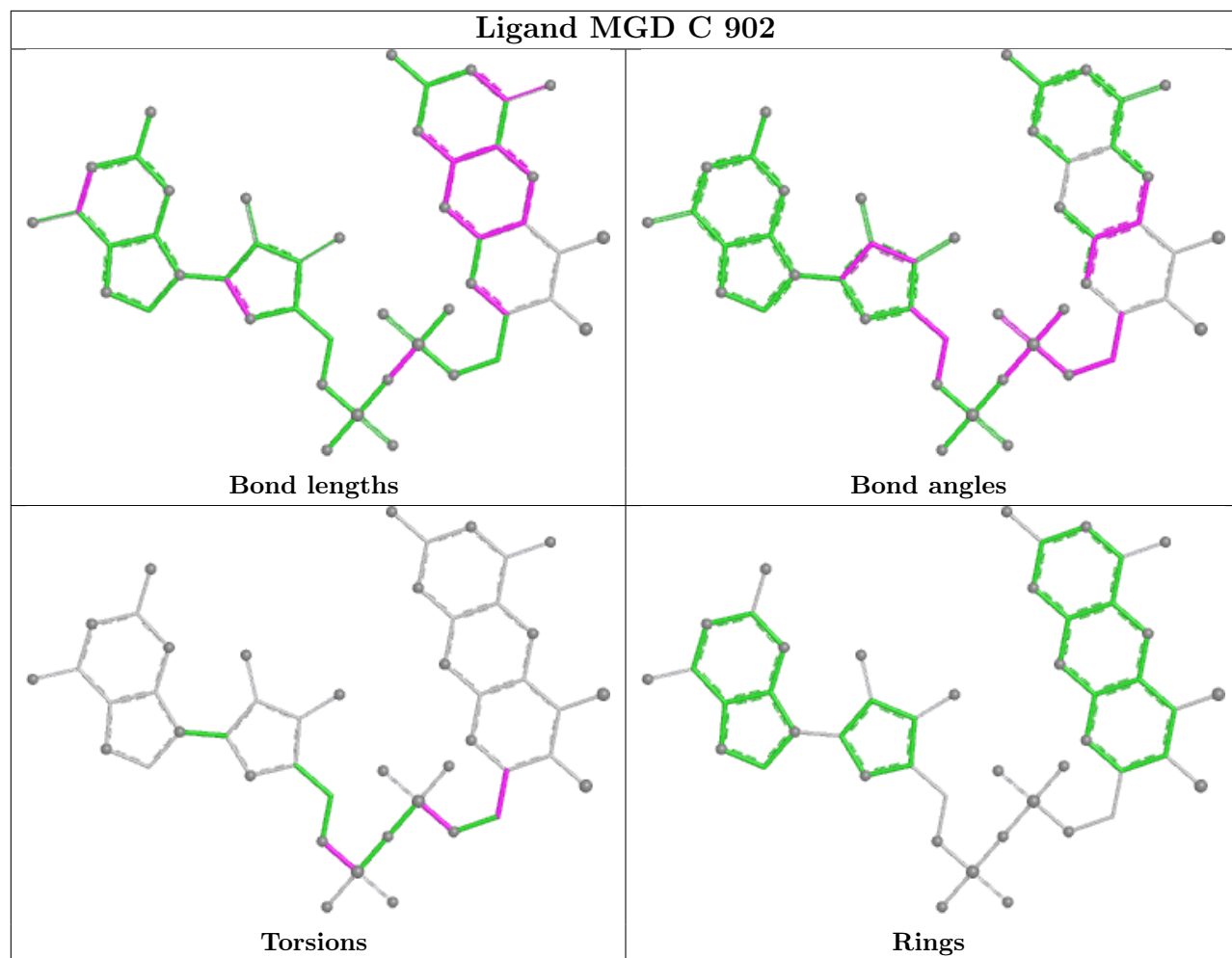


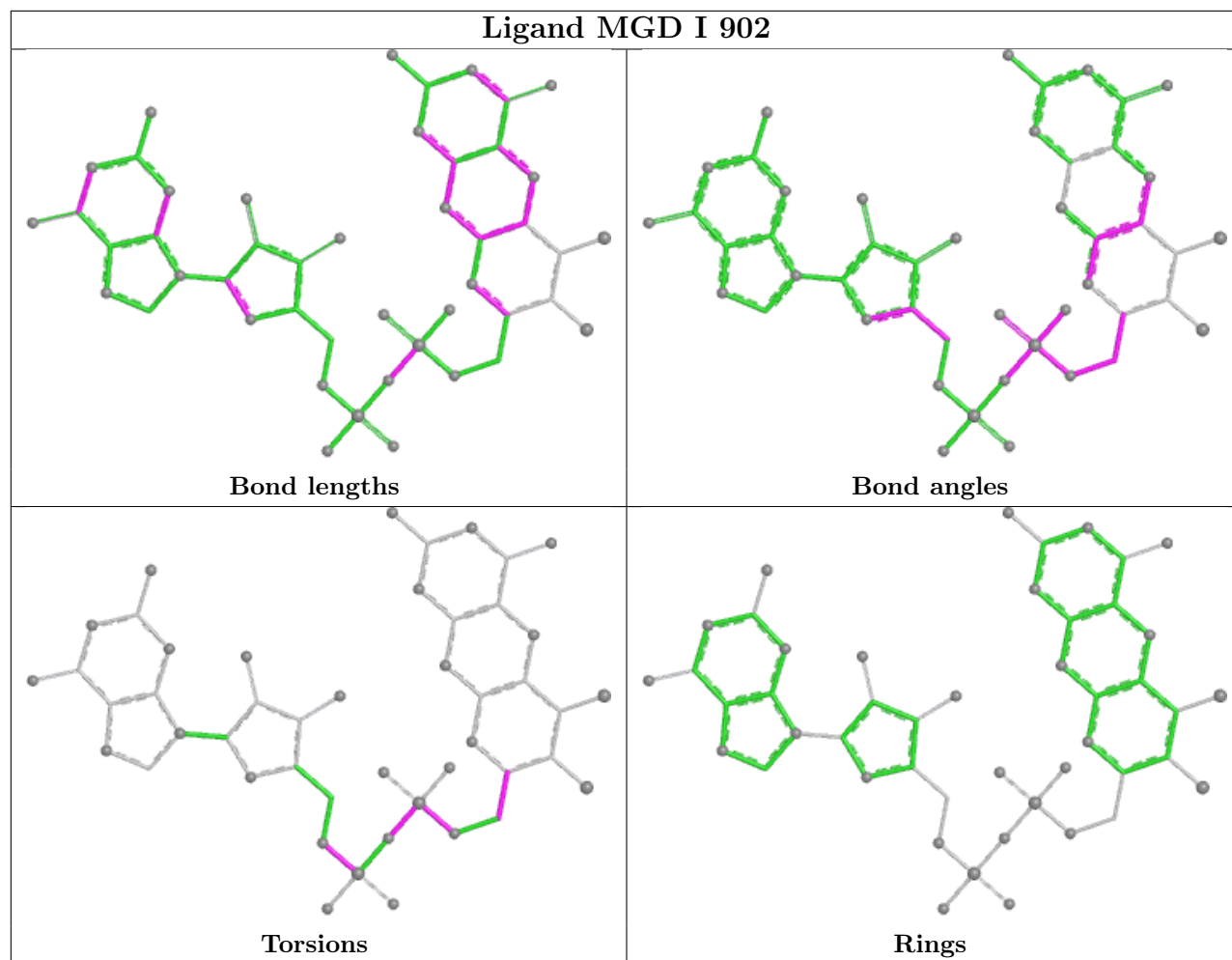


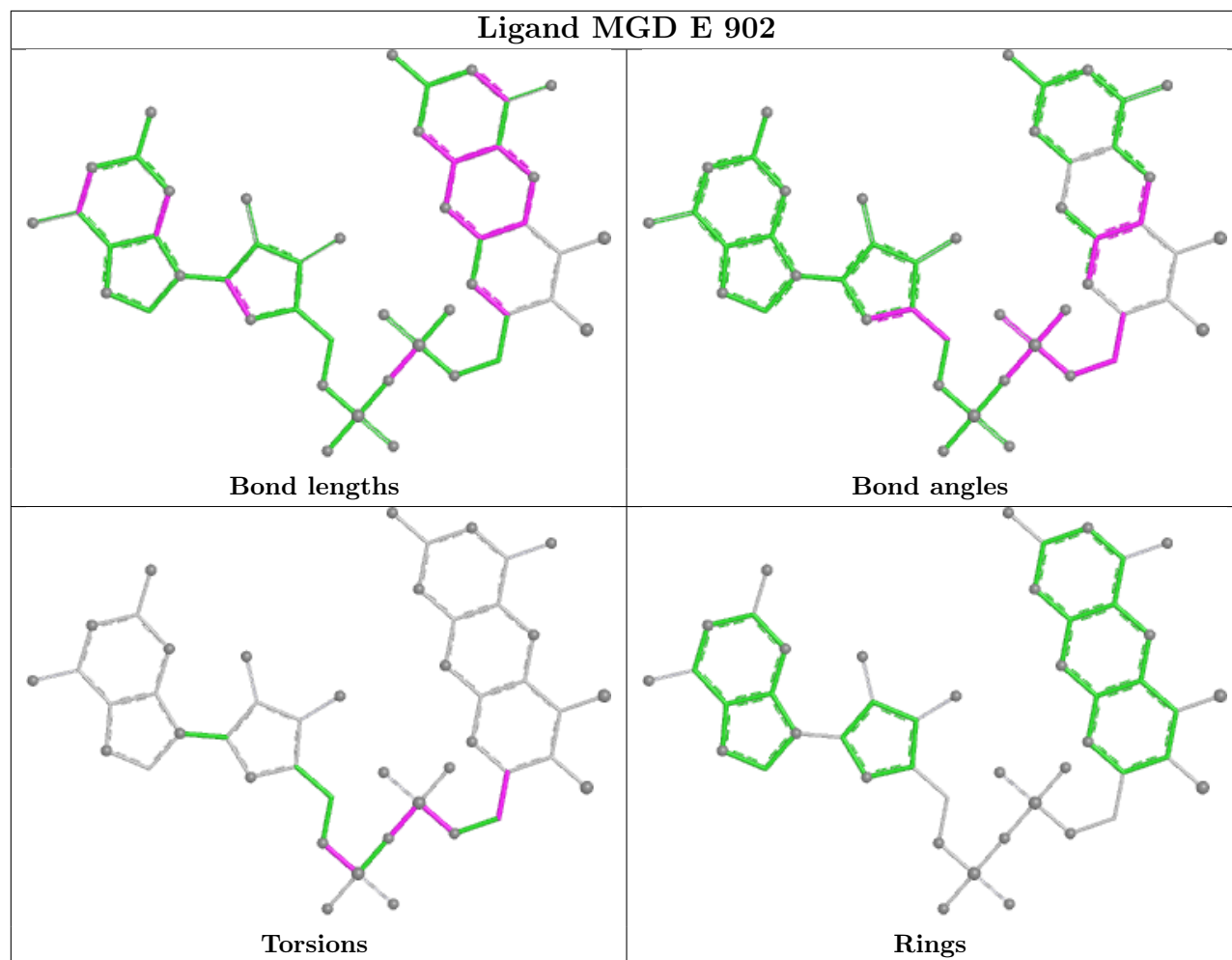


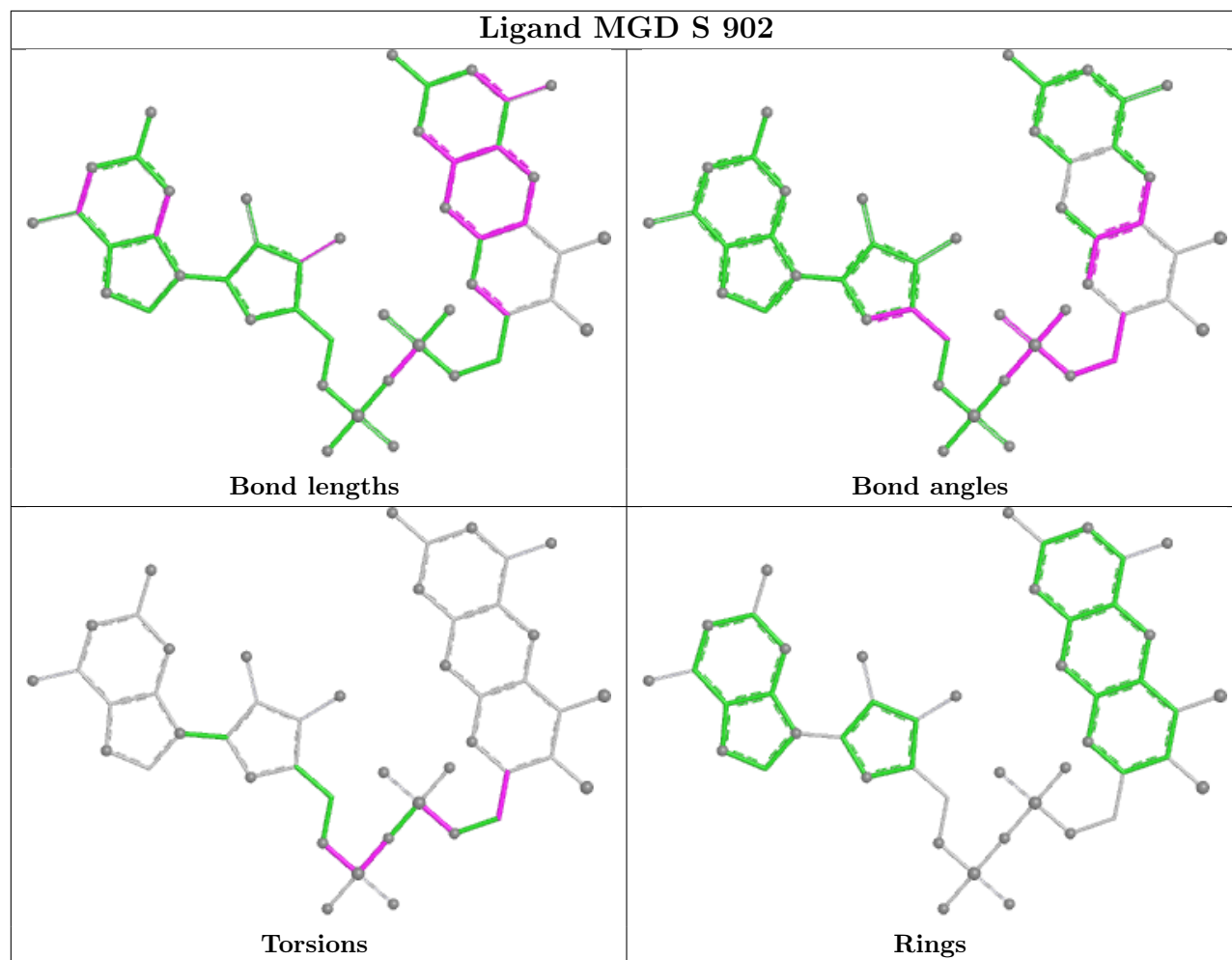


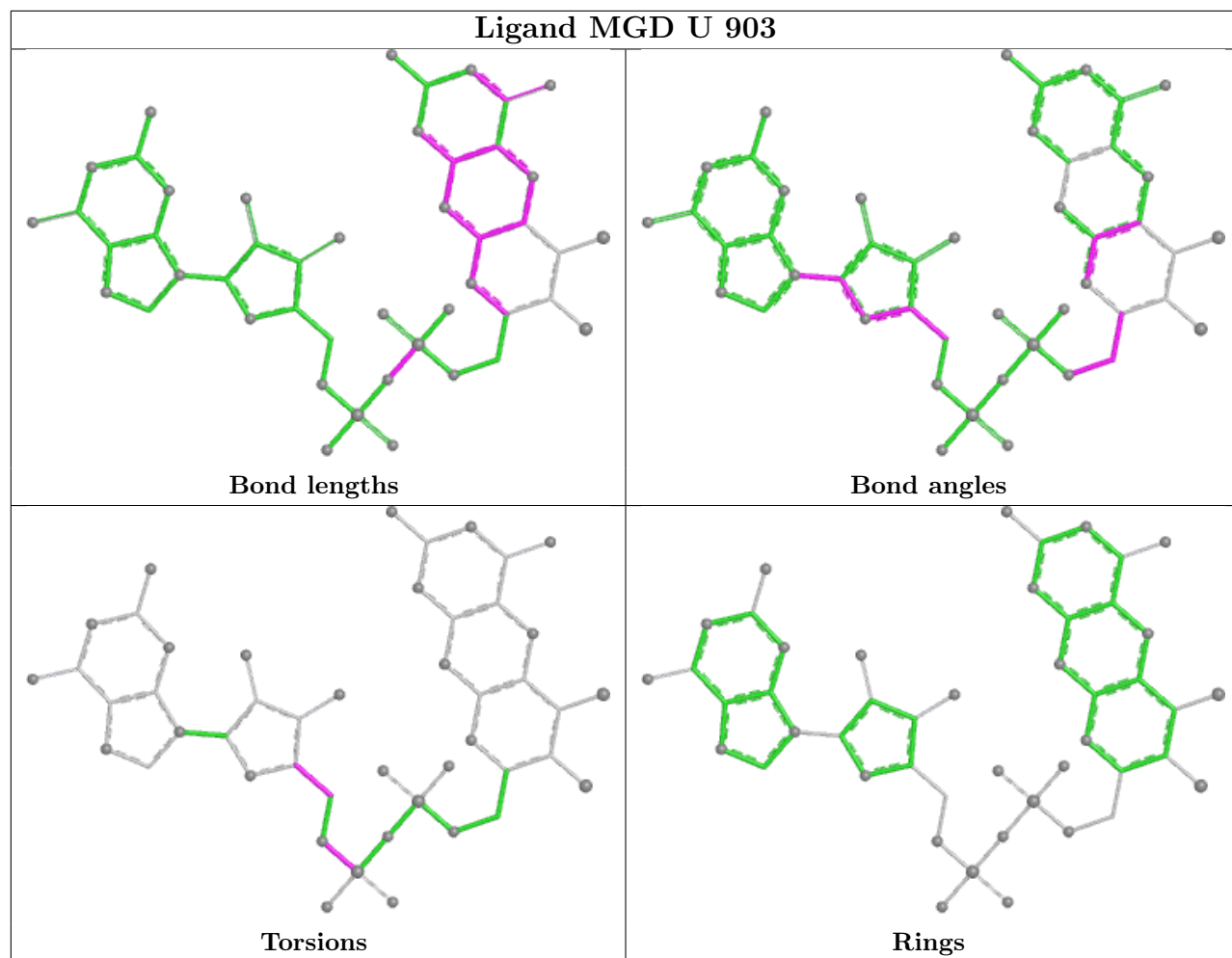


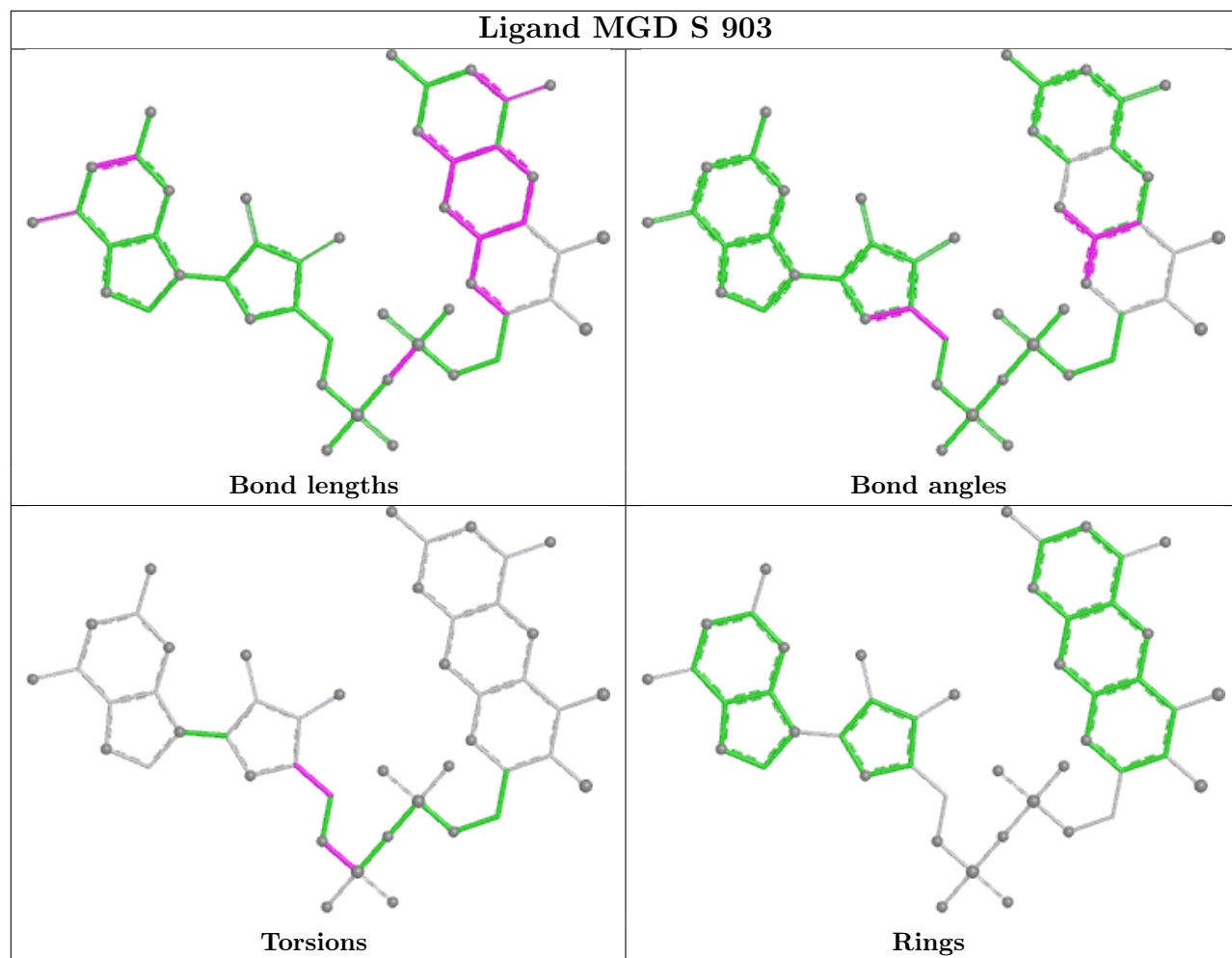


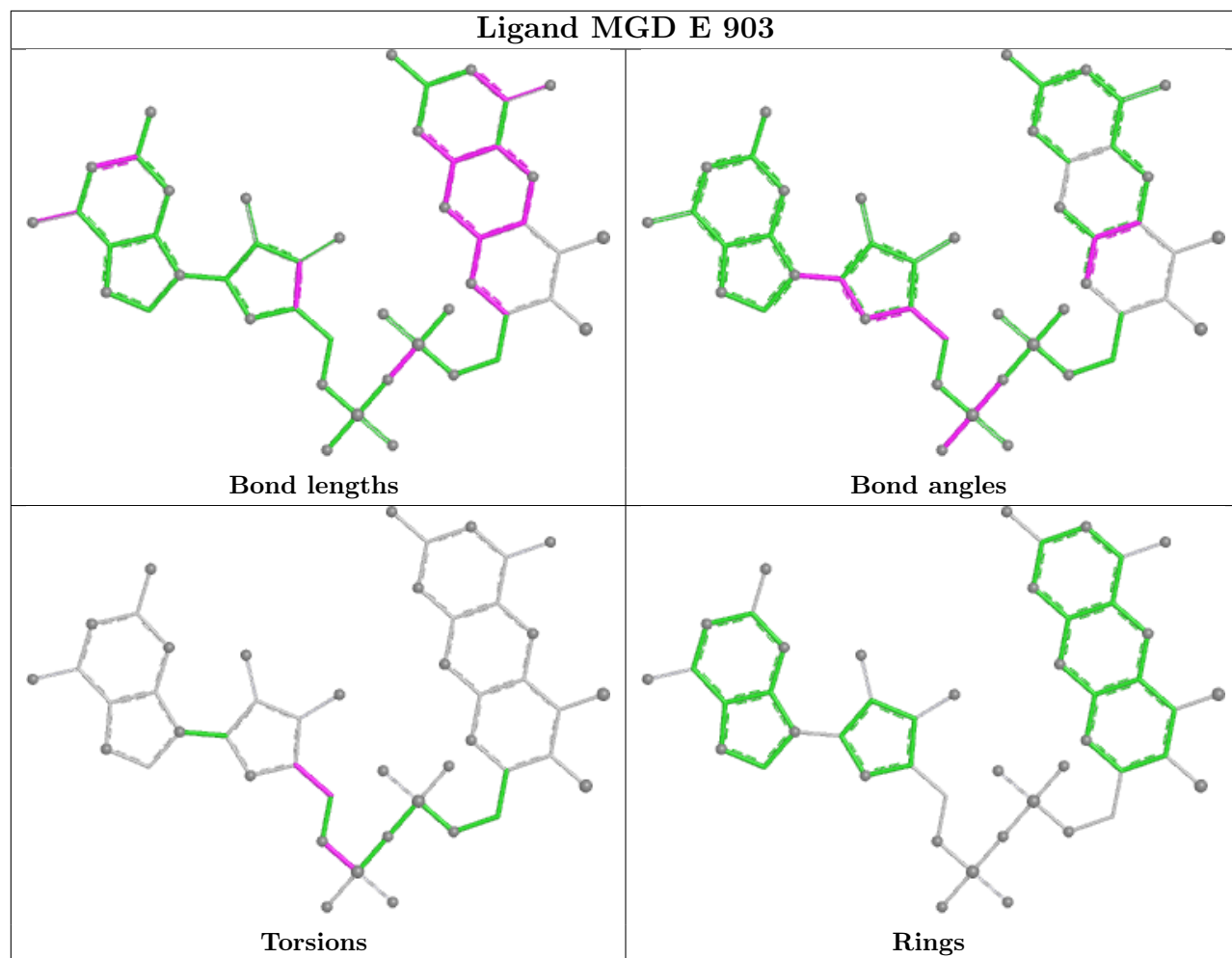


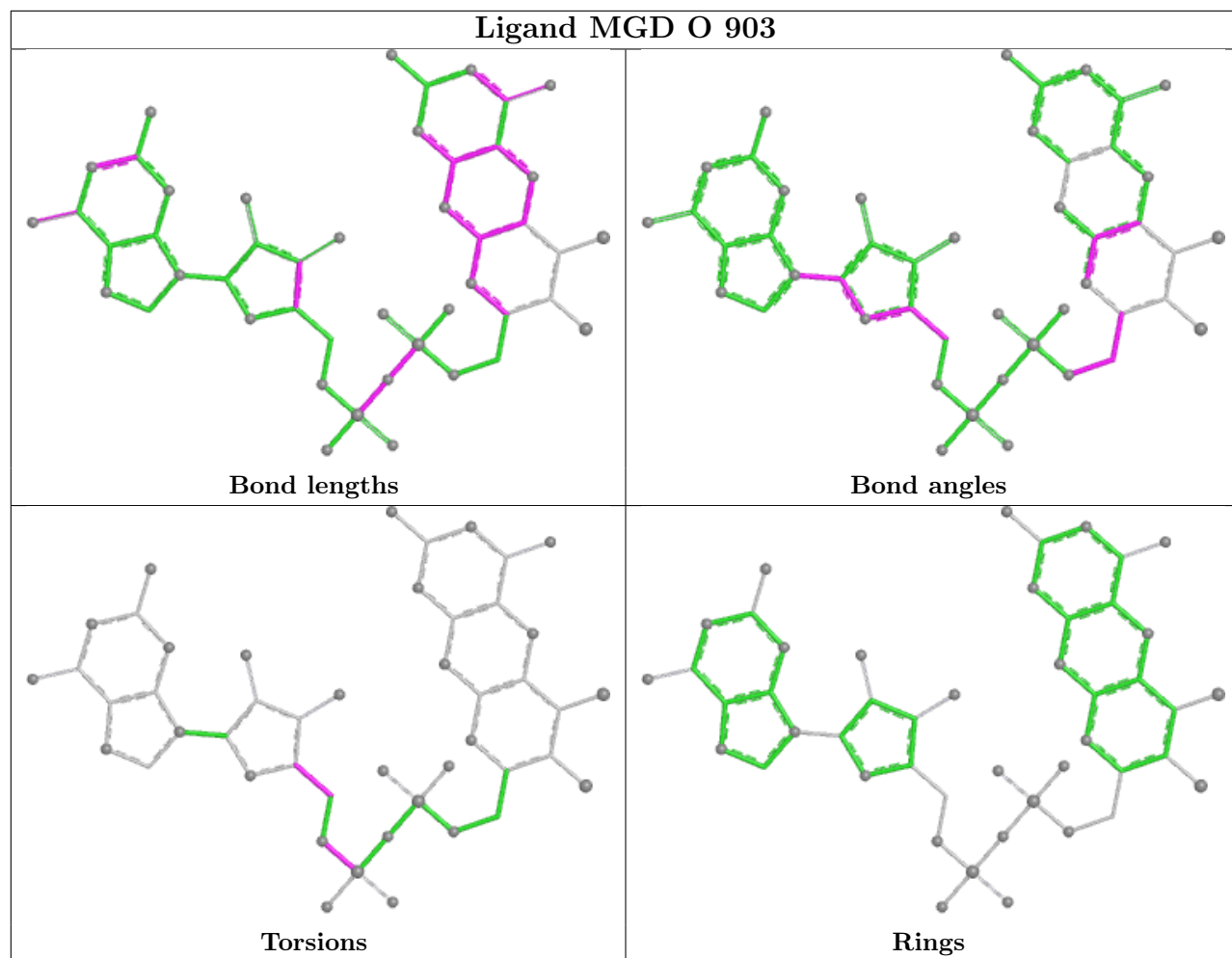


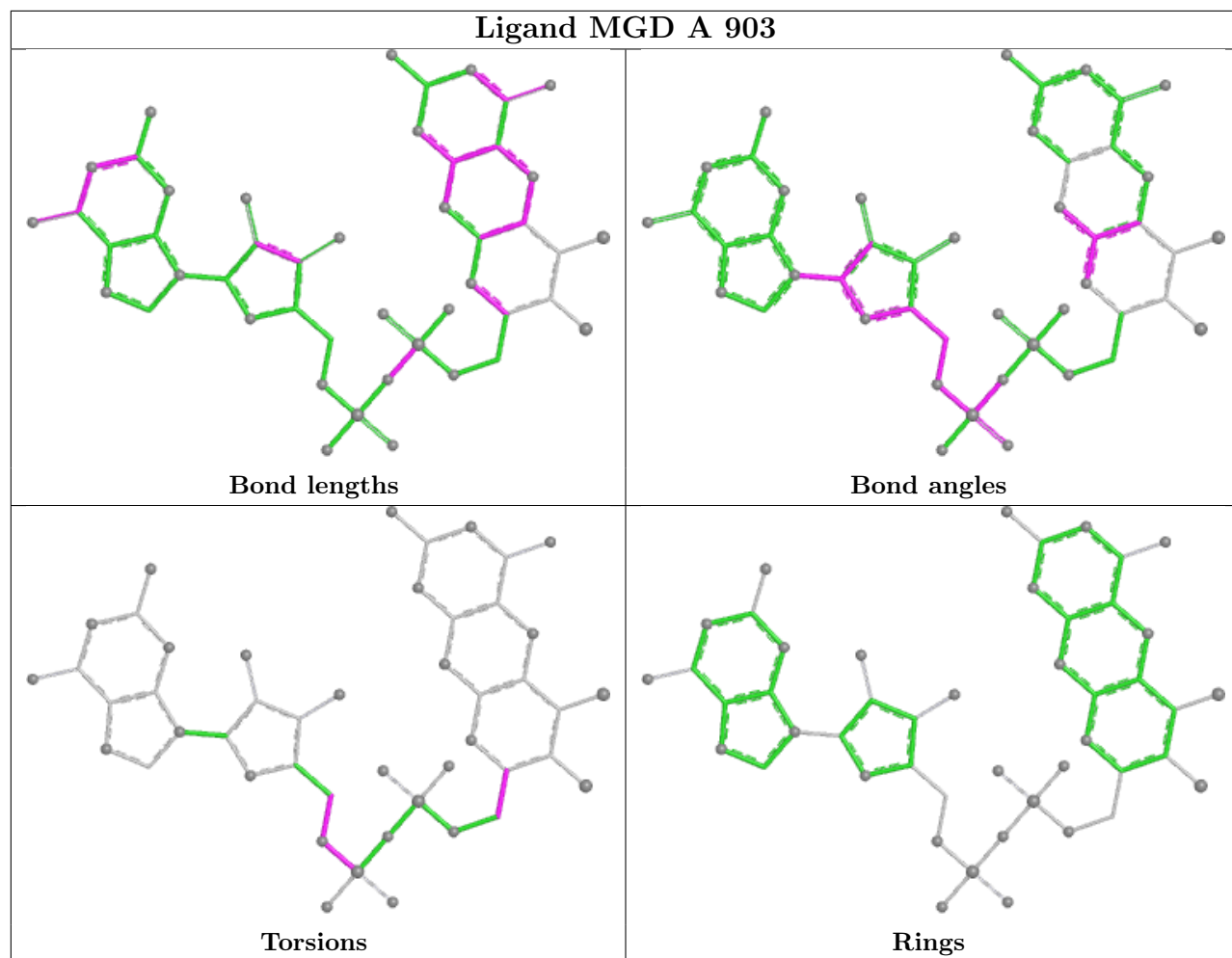


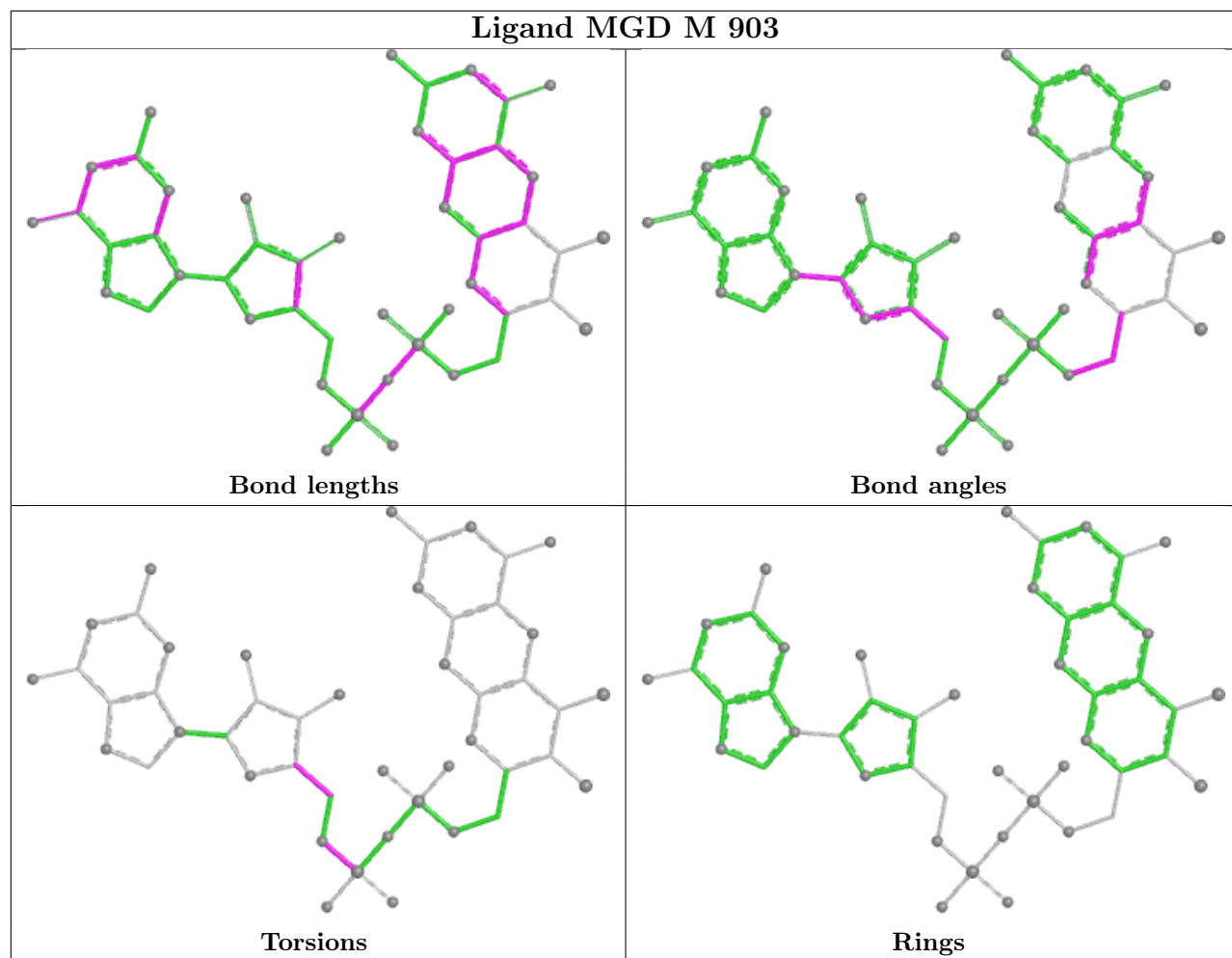


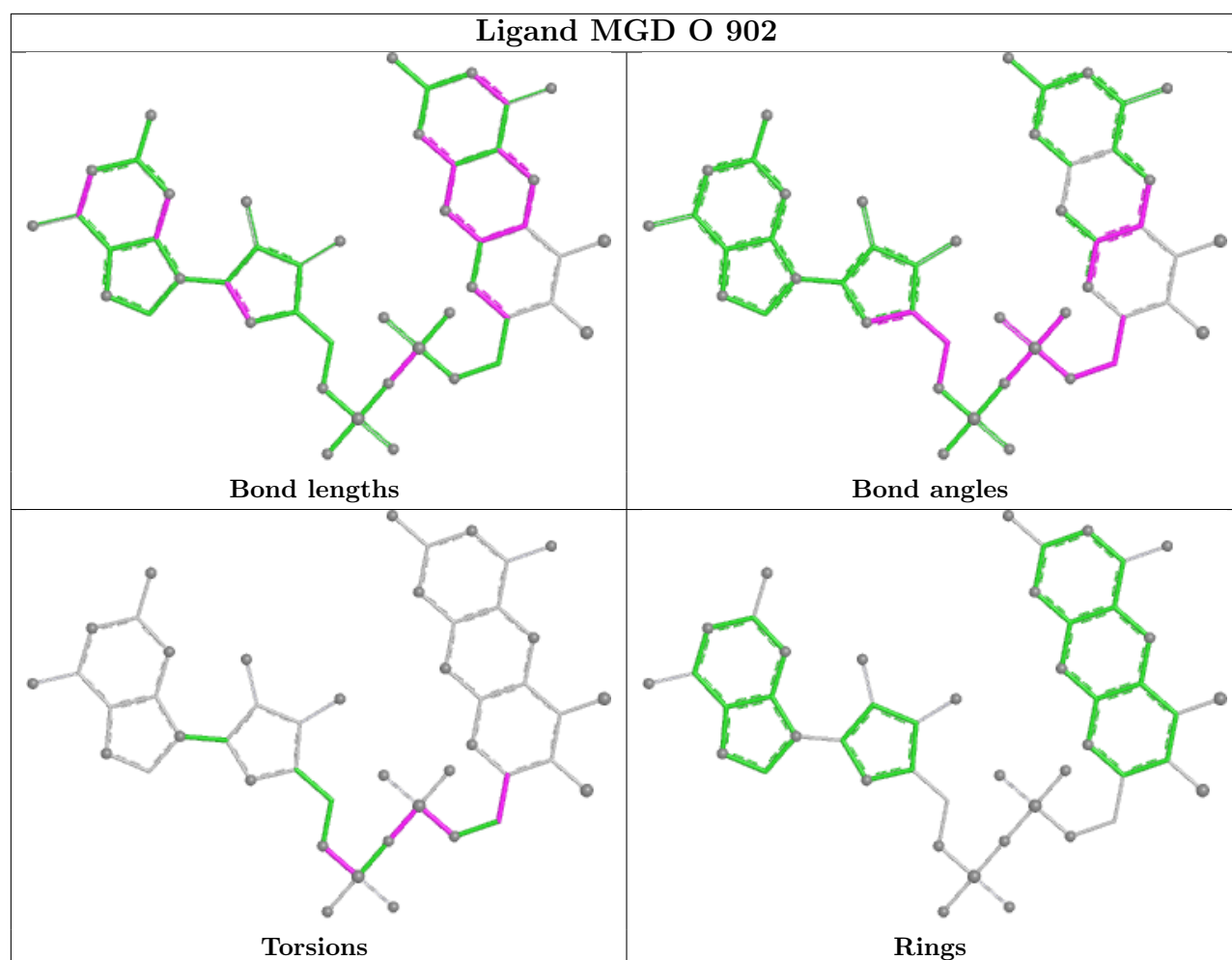












5.7 Other polymers [i](#)

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.