



## wwPDB EM Validation Summary Report ⓘ

Nov 18, 2025 – 06:24 am GMT

PDB ID : 8RR0 / pdb\_00008rr0  
EMDB ID : EMD-19452  
Title : CryoEM structure of Molybdenum bispyranopterin guanine dinucleotide formate dehydrogenases ForCE1 from *Bacillus subtilis*  
Authors : Cherrier, M.V.; Arnoux, P.; Martin, L.; Nicolet, Y.; Schoehn, G.; Legrand, P.; Broc, M.; Seduk, F.; Brasseur, G.; Arias-Cartin, R.; Magalon, A.; Walburger, A.; Uzel, A.; Guigliarelli, B.; Grimaldi, S.; Pierrel, F.; Mate, M.  
Deposited on : 2024-01-22  
Resolution : 3.35 Å(reported)  
Based on initial model : 8RQZ

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

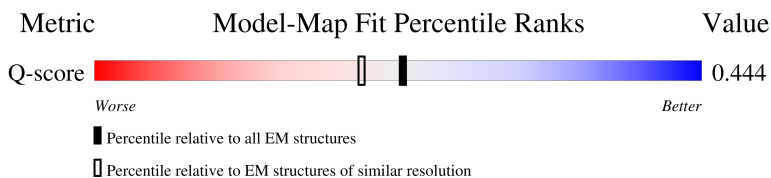
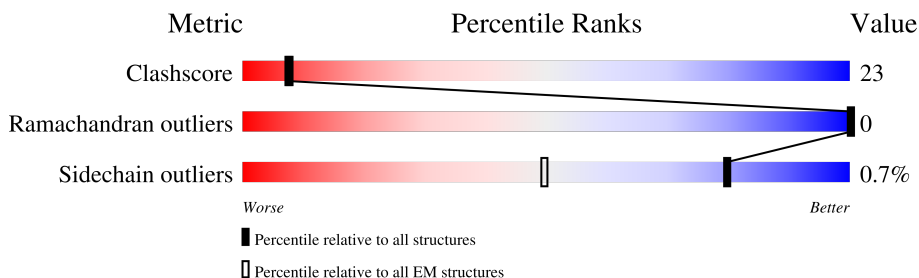
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14390 ( 2.85 - 3.85 )


The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	186	 52% 28% 20%
1	C	186	 52% 27% 20%
1	E	186	 53% 27% 20%

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Validation Pipeline (wwPDB-VP) : 2.46

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Mol	Chain	Length	Quality of chain
1	G	186	
2	B	985	
2	D	985	
2	F	985	
2	H	985	

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
9	SF4	B	1003	-	-	X	-
9	SF4	F	1003	-	-	X	-
9	SF4	H	1003	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 37080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

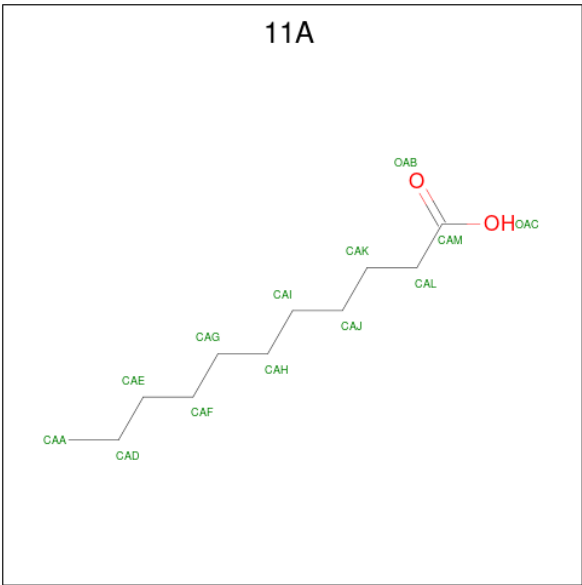
- Molecule 1 is a protein called Uncharacterized protein YjgD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	C	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	E	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		
1	G	148	Total	C	N	O	S	0	0
			1166	742	201	219	4		

- Molecule 2 is a protein called Probable oxidoreductase YjgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	D	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	F	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		
2	H	975	Total	C	N	O	S	0	0
			7636	4794	1307	1487	48		

- Molecule 3 is UNDECANOIC ACID (CCD ID: 11A) (formula: C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>).



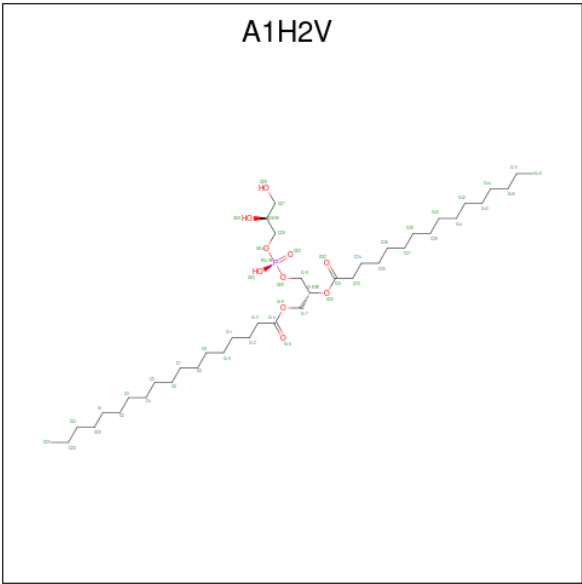
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			12	10	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	A	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			12	10	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	C	1	Total	C	O	0
			13	11	2	
3	E	1	Total	C	O	0
			12	10	2	
3	E	1	Total	C	O	0
			13	11	2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	E	1	13	11	2	0
3	E	1	13	11	2	0
3	E	1	13	11	2	0
3	E	1	13	11	2	0
3	G	1	12	10	2	0
3	G	1	13	11	2	0
3	G	1	13	11	2	0
3	G	1	13	11	2	0
3	G	1	13	11	2	0
3	G	1	13	11	2	0

- Molecule 4 is [(2 {R})-3-[[[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadecanoyloxy-propyl] octadecanoate (CCD ID: A1H2V) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



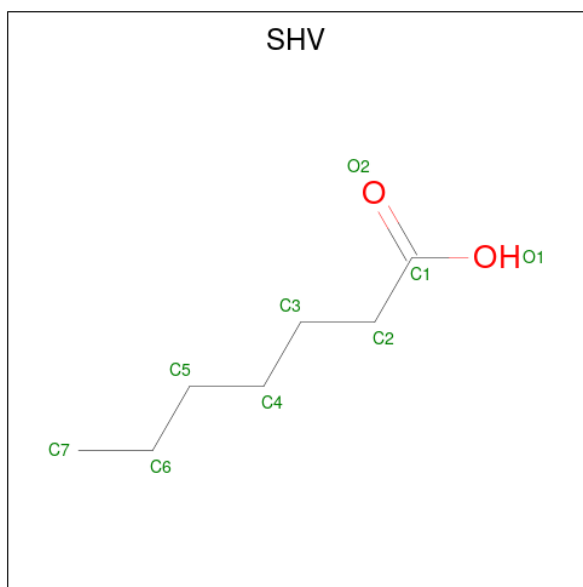
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	45	34	10	1	0

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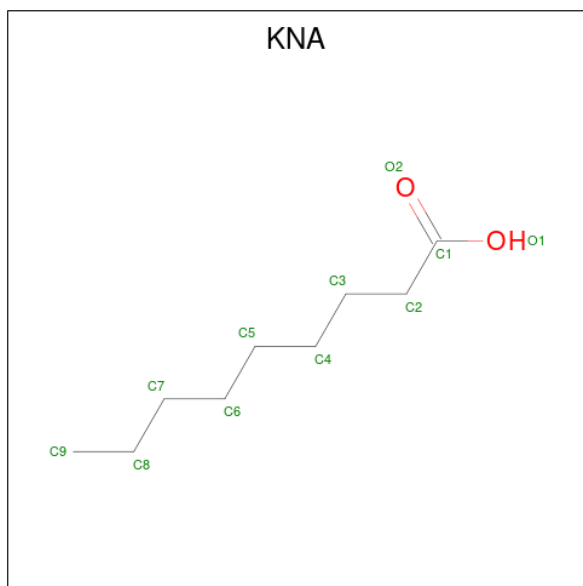
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			45	34	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	
4	E	1	Total	C	O	P	0
			51	40	10	1	
4	E	1	Total	C	O	P	0
			45	34	10	1	
4	E	1	Total	C	O	P	0
			51	40	10	1	
4	G	1	Total	C	O	P	0
			51	40	10	1	
4	G	1	Total	C	O	P	0
			45	34	10	1	
4	G	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 5 is HEPTANOIC ACID (CCD ID: SHV) (formula:  $C_7H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			9	7	2	
5	A	1	Total	C	O	0
			9	7	2	
5	C	1	Total	C	O	0
			9	7	2	
5	C	1	Total	C	O	0
			9	7	2	
5	E	1	Total	C	O	0
			9	7	2	
5	E	1	Total	C	O	0
			9	7	2	
5	G	1	Total	C	O	0
			9	7	2	
5	G	1	Total	C	O	0
			9	7	2	

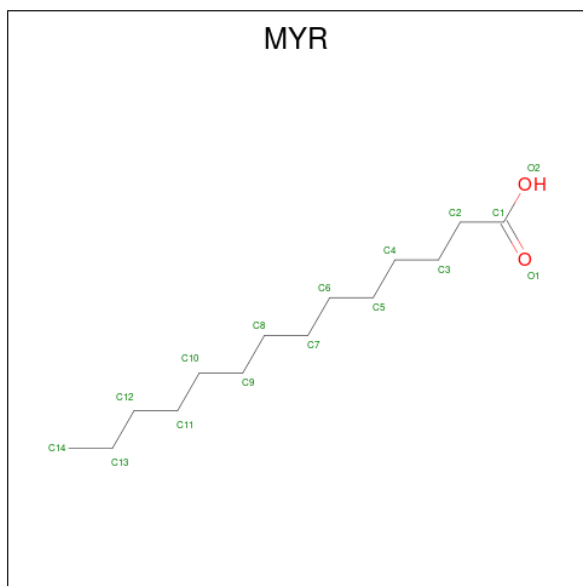
- Molecule 6 is nonanoic acid (CCD ID: KNA) (formula:  $C_9H_{18}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			11	9	2	
6	C	1	Total	C	O	0
			11	9	2	
6	E	1	Total	C	O	0
			11	9	2	
6	G	1	Total	C	O	0
			11	9	2	

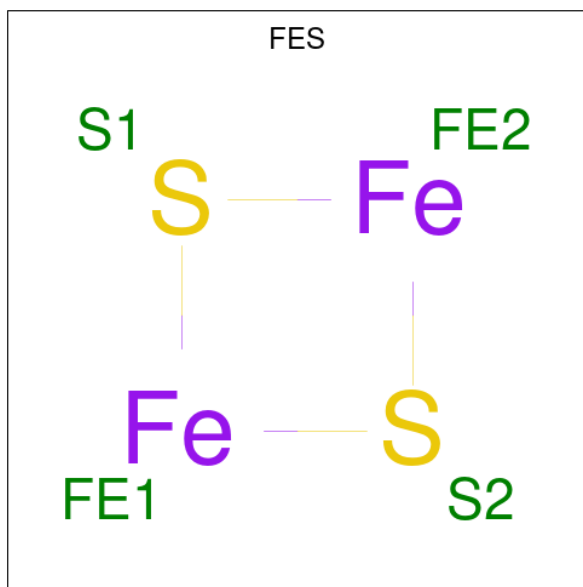


- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula:  $C_{14}H_{28}O_2$ ).



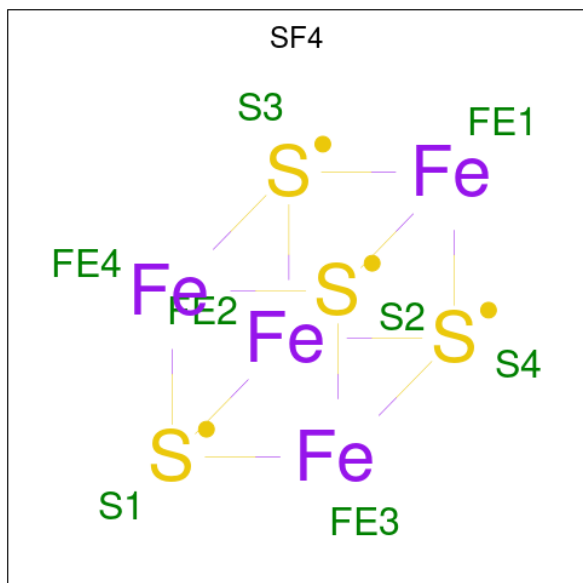
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			14	12	2	
7	C	1	Total	C	O	0
			14	12	2	
7	E	1	Total	C	O	0
			14	12	2	
7	G	1	Total	C	O	0
			14	12	2	

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ) (labeled as "Ligand of Interest" by depositor).



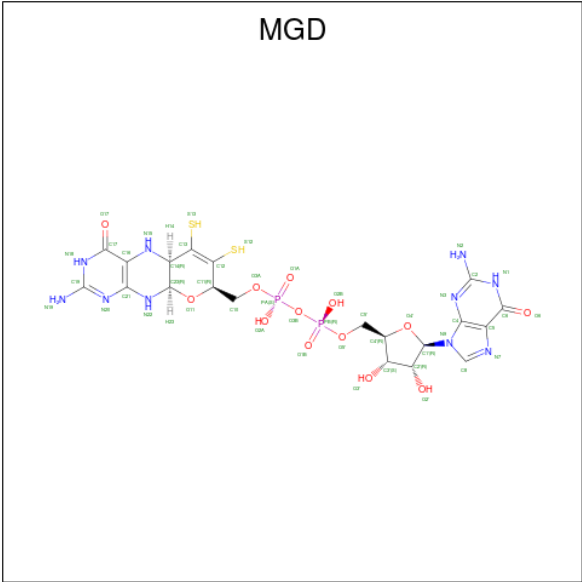
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			4	2	2	
8	D	1	Total	Fe	S	0
			4	2	2	
8	F	1	Total	Fe	S	0
			4	2	2	
8	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	D	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	F	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	
9	H	1	Total	Fe	S	0
			8	4	4	

- Molecule 10 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:  $C_{20}H_{26}N_{10}O_{13}P_2S_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	B	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	B	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	D	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	D	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	F	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	F	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	H	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
10	H	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	

- Molecule 11 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

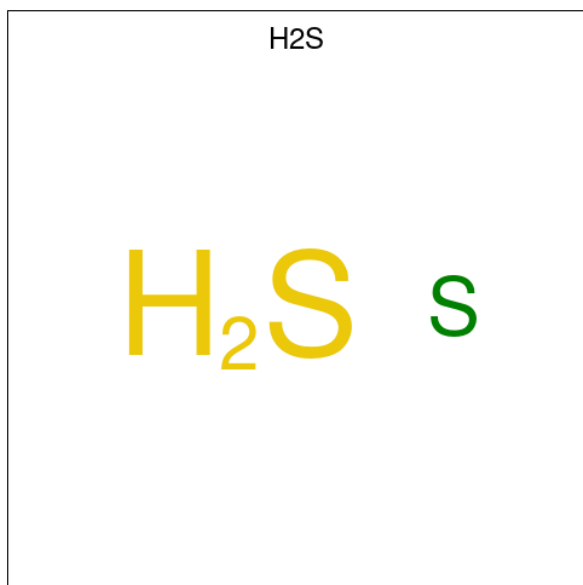
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Mo	0
			1	1	
11	D	1	Total	Mo	0
			1	1	
11	F	1	Total	Mo	0
			1	1	

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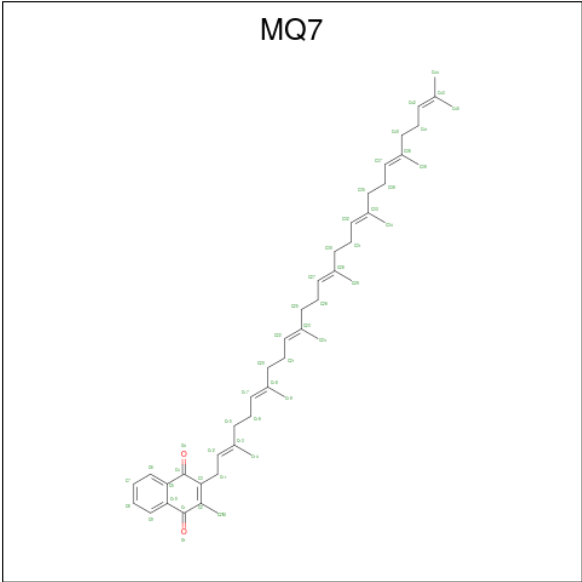
Mol	Chain	Residues	Atoms		AltConf
11	H	1	Total	Mo	0
			1	1	

- Molecule 12 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	S	0
			1	1	
12	D	1	Total	S	0
			1	1	
12	F	1	Total	S	0
			1	1	
12	H	1	Total	S	0
			1	1	

- Molecule 13 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	C	O	0
			48	46	2	
13	D	1	Total	C	O	0
			48	46	2	
13	F	1	Total	C	O	0
			48	46	2	
13	H	1	Total	C	O	0
			48	46	2	

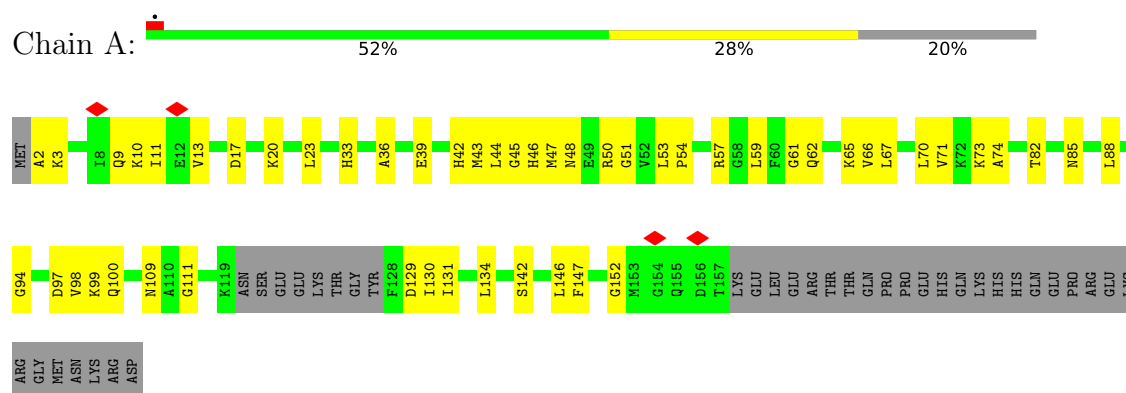
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	B	21	Total	O	0
			21	21	
14	D	21	Total	O	0
			21	21	
14	F	21	Total	O	0
			21	21	
14	H	21	Total	O	0
			21	21	

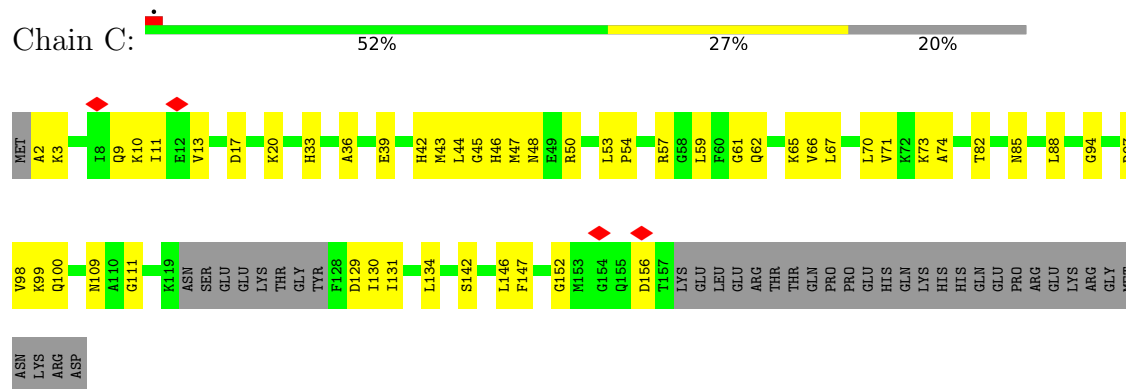
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

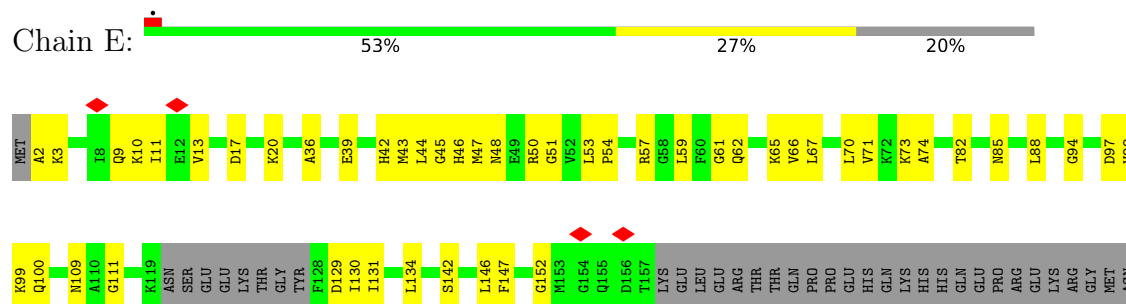
#### • Molecule 1: Uncharacterized protein YjgD



#### • Molecule 1: Uncharacterized protein YjgD



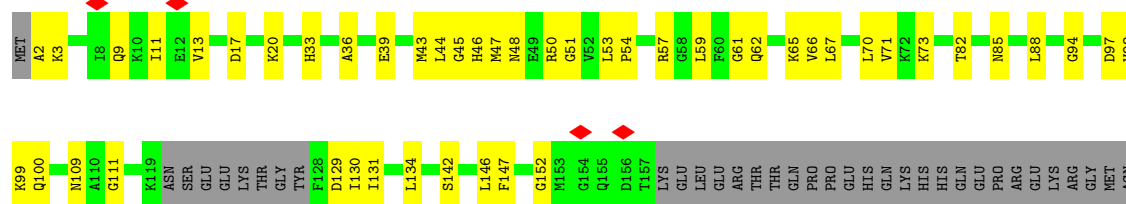
#### • Molecule 1: Uncharacterized protein YjgD



LYS  
ARG  
ASP

• Molecule 1: Uncharacterized protein YjgD

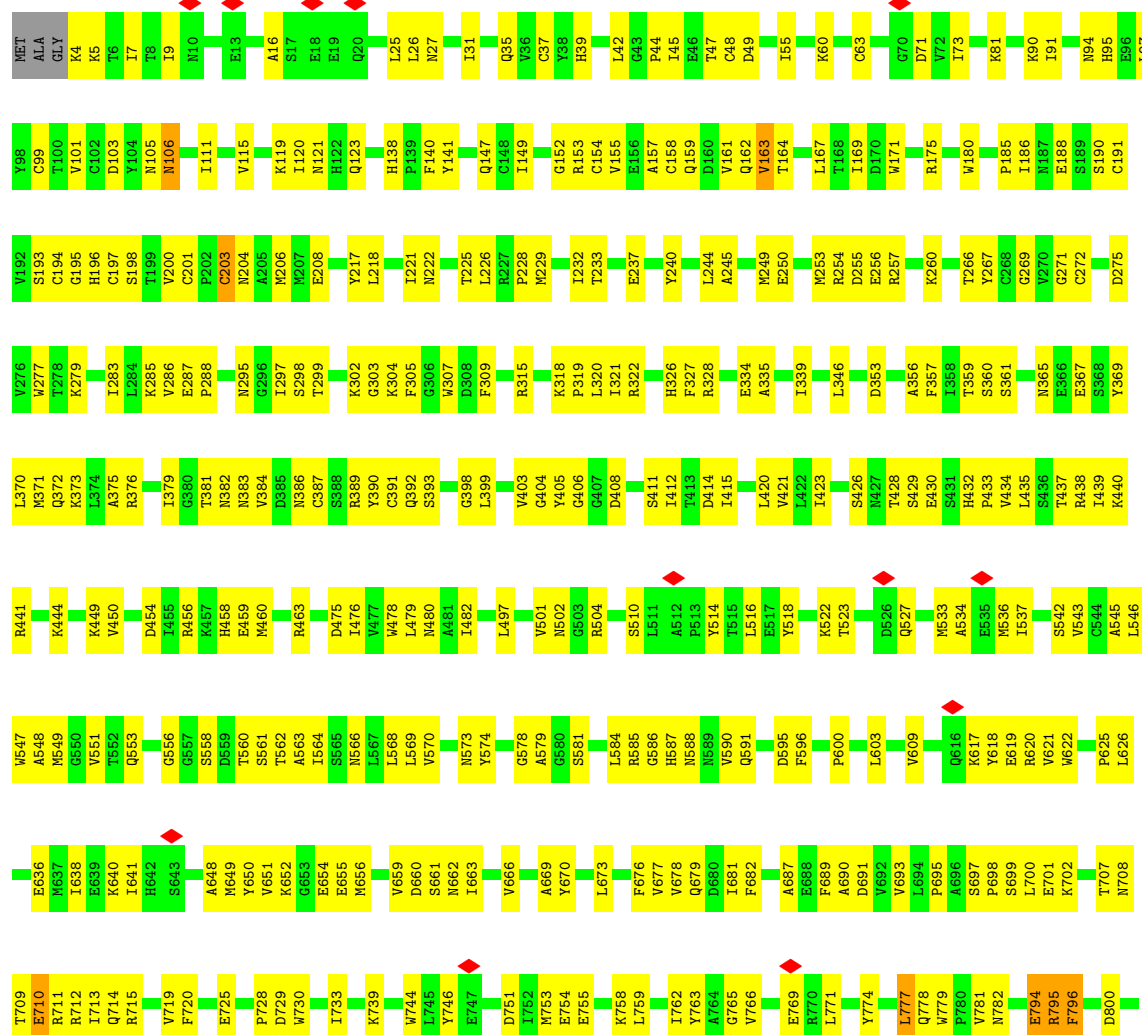
Chain G:  54% 26% 20%



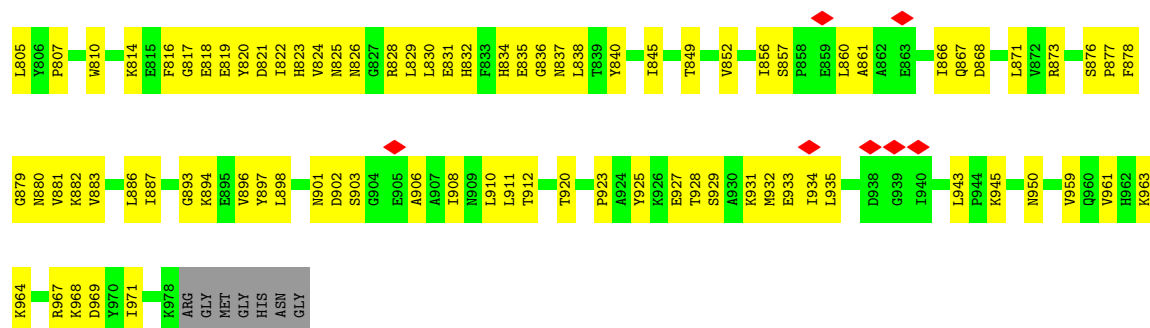
LYS  
ARG  
ASP

• Molecule 2: Probable oxidoreductase YjgC

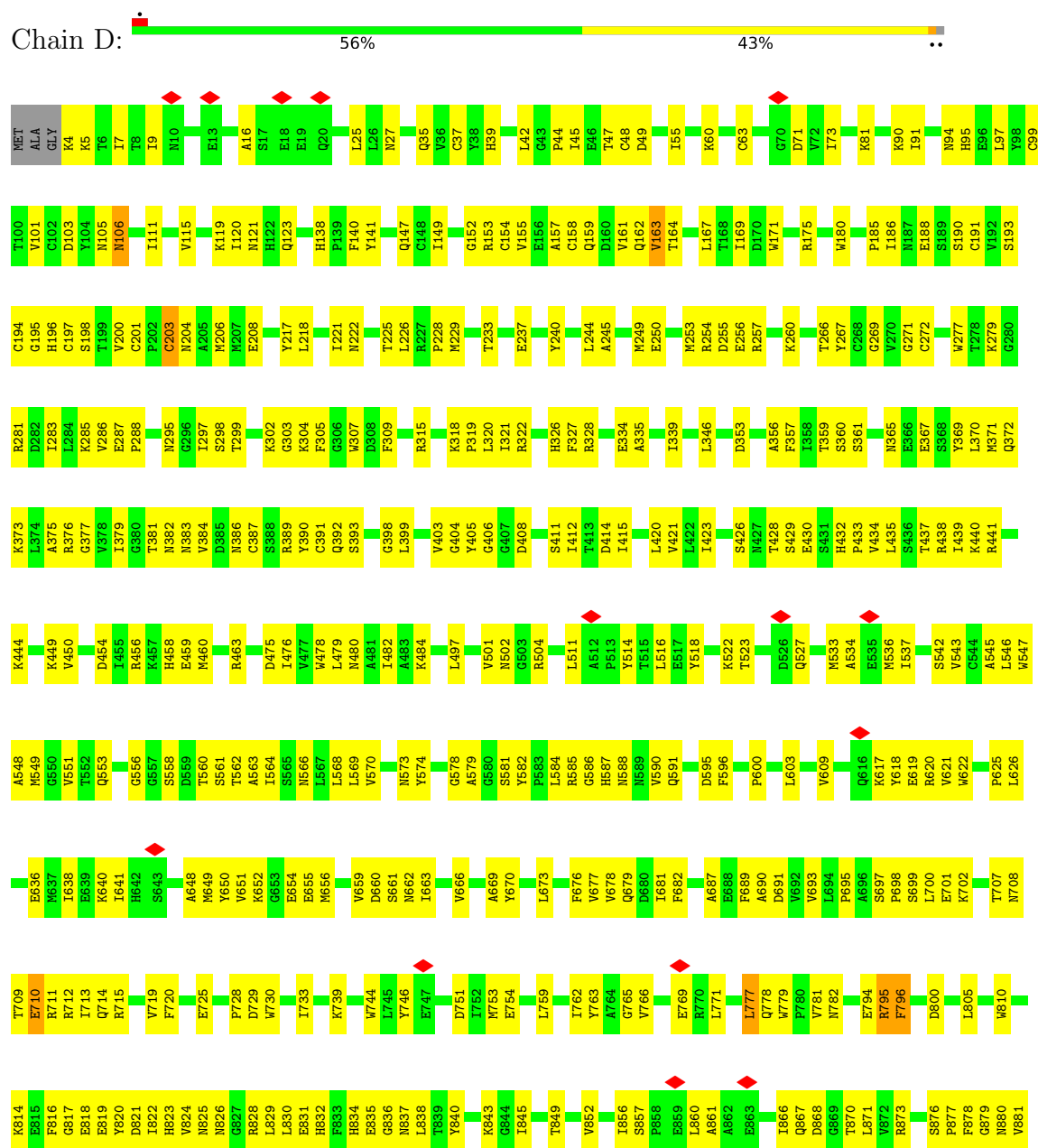
Chain B:  56% 43% ..

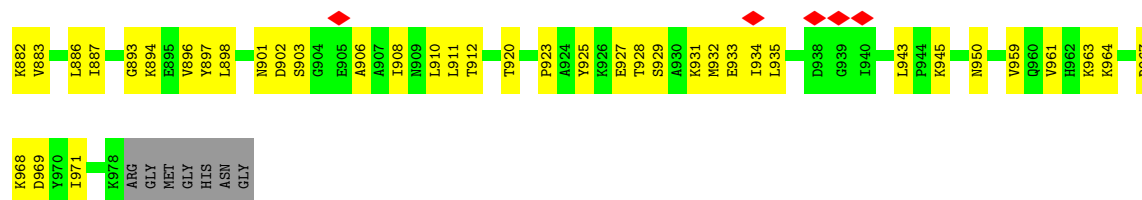




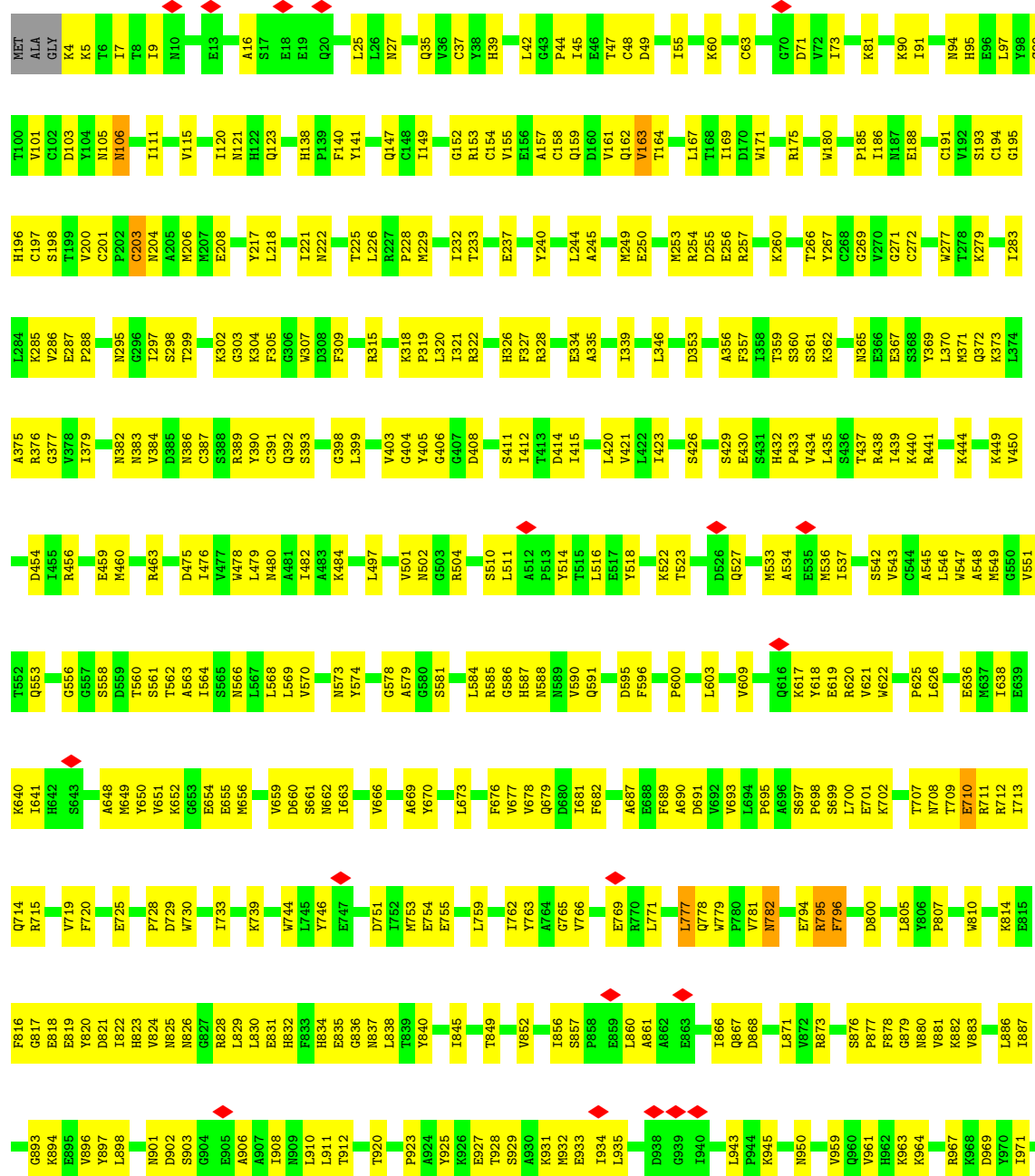


• Molecule 2: Probable oxidoreductase YjgC





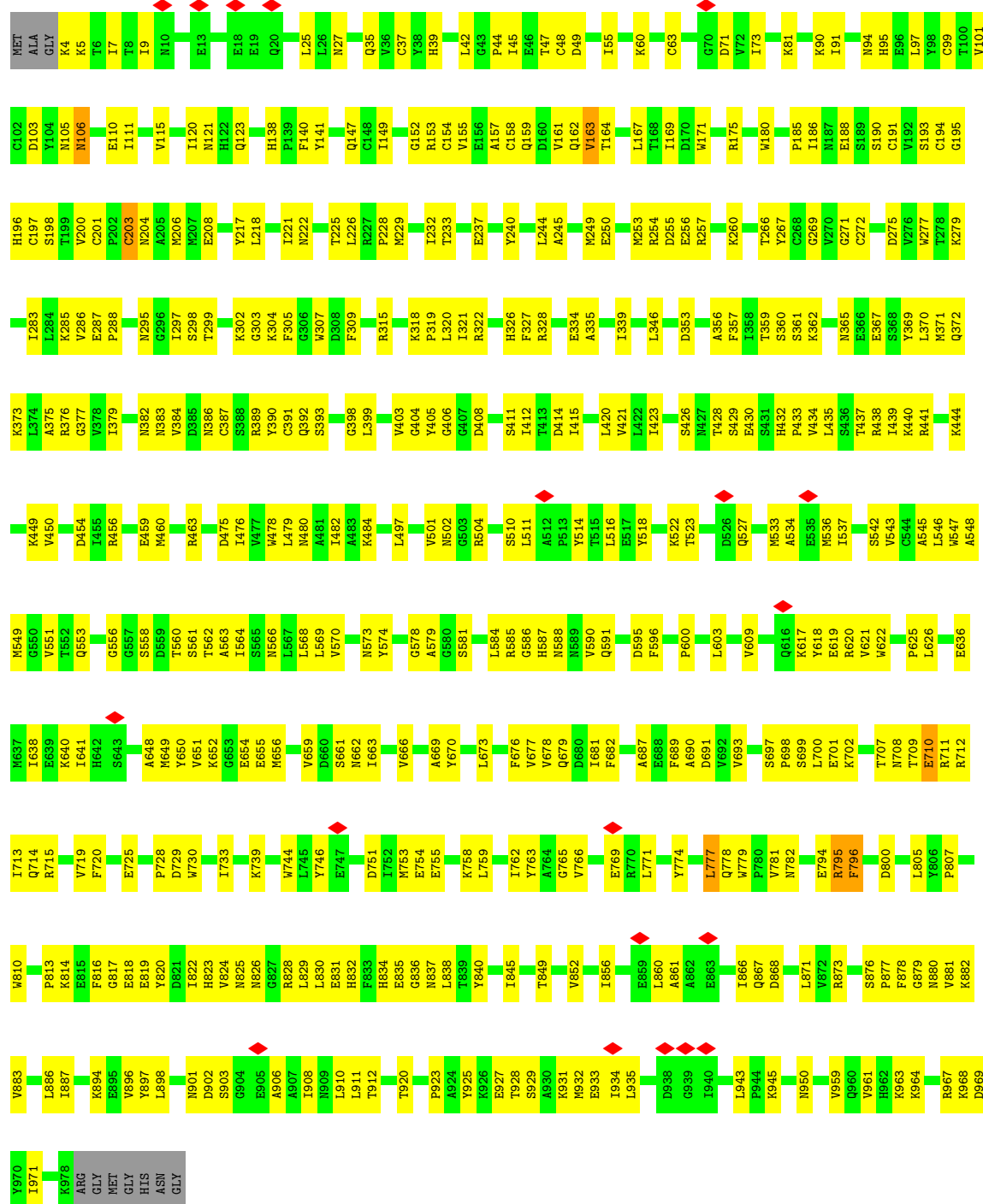
• Molecule 2: Probable oxidoreductase YjgC



K978  
ARG  
GLY  
MET  
GLY  
HIS  
ASN  
GLY

• Molecule 2: Probable oxidoreductase YjgC

Chain H:  56% 42% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	112095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.409	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, A1H2V, KNA, SHV, H2S, MQ7, MGD, MYR, 11A, 4MO, SF4

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	0.11	0/1175	0.29	0/1574
1	C	0.11	0/1175	0.29	0/1574
1	E	0.11	0/1175	0.29	0/1574
1	G	0.11	0/1175	0.29	0/1574
2	B	0.28	0/7797	0.54	8/10558 (0.1%)
2	D	0.28	0/7797	0.54	8/10558 (0.1%)
2	F	0.28	0/7797	0.54	8/10558 (0.1%)
2	H	0.28	0/7797	0.54	8/10558 (0.1%)
All	All	0.26	0/35888	0.51	32/48528 (0.1%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ASN	N-CA-C	-8.07	102.99	112.92
2	D	106	ASN	N-CA-C	-8.07	102.99	112.92
2	H	106	ASN	N-CA-C	-8.07	102.99	112.92
2	F	106	ASN	N-CA-C	-8.05	103.02	112.92
2	B	164	THR	N-CA-C	-6.53	104.01	112.23

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	1166	0	1237	59	0
1	C	1166	0	1237	60	0
1	E	1166	0	1237	55	0
1	G	1166	0	1237	55	0
2	B	7636	0	7467	380	0
2	D	7636	0	7467	379	0
2	F	7636	0	7467	370	0
2	H	7636	0	7467	370	0
3	A	77	0	121	4	0
3	C	77	0	121	3	0
3	E	77	0	121	3	0
3	G	77	0	121	3	0
4	A	147	0	0	6	0
4	C	147	0	0	6	0
4	E	147	0	0	6	0
4	G	147	0	0	6	0
5	A	18	0	26	0	0
5	C	18	0	26	0	0
5	E	18	0	26	0	0
5	G	18	0	26	0	0
6	A	11	0	17	0	0
6	C	11	0	17	0	0
6	E	11	0	17	0	0
6	G	11	0	17	0	0
7	A	14	0	20	2	0
7	C	14	0	20	2	0
7	E	14	0	20	2	0
7	G	14	0	20	2	0
8	B	4	0	0	1	0
8	D	4	0	0	1	0
8	F	4	0	0	1	0
8	H	4	0	0	1	0
9	B	32	0	0	5	0
9	D	32	0	0	4	0
9	F	32	0	0	5	0
9	H	32	0	0	5	0
10	B	94	0	44	20	0
10	D	94	0	44	22	0
10	F	94	0	44	22	0
10	H	94	0	44	22	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1	0	0	0	0
12	B	1	0	0	1	0
12	D	1	0	0	1	0
12	F	1	0	0	1	0
12	H	1	0	0	1	0
13	B	48	0	64	2	0
13	D	48	0	64	2	0
13	F	48	0	64	2	0
13	H	48	0	64	2	0
14	B	21	0	0	0	0
14	D	21	0	0	0	0
14	F	21	0	0	0	0
14	H	21	0	0	0	0
All	All	37080	0	35984	1647	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1647 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:387:CYS:SG	12:B:1009:H2S:S	2.30	1.30
2:H:387:CYS:SG	12:H:1009:H2S:S	2.30	1.30
2:D:387:CYS:SG	12:D:1009:H2S:S	2.30	1.29
2:F:387:CYS:SG	12:F:1009:H2S:S	2.30	1.27
2:B:387:CYS:SG	2:B:587:HIS:HD2	1.81	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	C	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	E	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
1	G	144/186 (77%)	141 (98%)	3 (2%)	0	100	100
2	B	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
2	D	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
2	F	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
2	H	973/985 (99%)	940 (97%)	33 (3%)	0	100	100
All	All	4468/4684 (95%)	4324 (97%)	144 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	129/165 (78%)	129 (100%)	0	100	100
1	C	129/165 (78%)	129 (100%)	0	100	100
1	E	129/165 (78%)	129 (100%)	0	100	100
1	G	129/165 (78%)	129 (100%)	0	100	100
2	B	840/845 (99%)	833 (99%)	7 (1%)	79	88
2	D	840/845 (99%)	833 (99%)	7 (1%)	79	88
2	F	840/845 (99%)	833 (99%)	7 (1%)	79	88
2	H	840/845 (99%)	833 (99%)	7 (1%)	79	88
All	All	3876/4040 (96%)	3848 (99%)	28 (1%)	80	89

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	47	THR
2	H	795	ARG

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Mol	Chain	Res	Type
2	F	203	CYS
2	H	203	CYS
2	F	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	182	ASN
2	H	502	ASN
2	H	642	HIS
2	D	502	ASN
2	D	417	GLN

### 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 92 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - leaving 84 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	11A	A	211	-	12,12,12	0.66	0	12,12,12	1.16	0
3	11A	A	206	-	12,12,12	0.66	0	12,12,12	1.17	1 (8%)
3	11A	G	213	-	12,12,12	0.66	0	12,12,12	1.16	0
3	11A	C	212	-	12,12,12	0.67	0	12,12,12	1.18	0
6	KNA	A	208	-	10,10,10	0.79	0	10,10,10	0.71	0
5	SHV	C	207	-	8,8,8	0.87	0	8,8,8	0.79	0
3	11A	E	203	-	11,11,12	0.68	0	11,11,12	1.19	0
5	SHV	C	206	-	8,8,8	0.87	0	8,8,8	0.73	0
5	SHV	G	206	-	8,8,8	0.87	0	8,8,8	0.73	0
4	A1H2V	C	202	-	50,50,50	0.30	0	53,56,56	0.27	0
5	SHV	E	206	-	8,8,8	0.87	0	8,8,8	0.73	0
5	SHV	A	205	-	8,8,8	0.87	0	8,8,8	0.79	0
9	SF4	D	1002	2	0,12,12	-	-	-		
9	SF4	B	1004	2	0,12,12	-	-	-		
8	FES	B	1001	2	0,4,4	-	-	-		
7	MYR	E	201	-	13,13,15	0.63	0	13,13,15	1.15	0
9	SF4	B	1005	2	0,12,12	-	-	-		
5	SHV	A	204	-	8,8,8	0.87	0	8,8,8	0.73	0
3	11A	C	211	-	12,12,12	0.67	0	12,12,12	1.17	0
9	SF4	F	1002	2	0,12,12	-	-	-		
6	KNA	C	210	-	10,10,10	0.79	0	10,10,10	0.71	0
9	SF4	F	1004	2	0,12,12	-	-	-		
4	A1H2V	G	205	-	50,50,50	0.29	0	53,56,56	0.40	0
10	MGD	D	1006	11	41,52,52	2.17	15 (36%)	40,81,81	1.68	8 (20%)
3	11A	G	211	-	12,12,12	0.67	0	12,12,12	1.17	0
9	SF4	H	1004	2	0,12,12	-	-	-		
10	MGD	F	1007	11,2	41,52,52	2.05	15 (36%)	40,81,81	1.82	9 (22%)
8	FES	H	1001	2	0,4,4	-	-	-		
3	11A	C	209	-	12,12,12	0.66	0	12,12,12	1.17	0
5	SHV	E	207	-	8,8,8	0.87	0	8,8,8	0.79	0
4	A1H2V	A	202	-	44,44,50	0.32	0	47,50,56	0.35	0
4	A1H2V	C	204	-	44,44,50	0.32	0	47,50,56	0.35	0
9	SF4	F	1005	2	0,12,12	-	-	-		
9	SF4	B	1003	2	0,12,12	-	-	-		
7	MYR	G	201	-	13,13,15	0.63	0	13,13,15	1.15	0
3	11A	E	208	-	12,12,12	0.66	0	12,12,12	1.18	1 (8%)
3	11A	E	212	-	12,12,12	0.67	0	12,12,12	1.18	0
9	SF4	H	1002	2	0,12,12	-	-	-		
4	A1H2V	A	213	-	50,50,50	0.30	0	53,56,56	0.27	0
13	MQ7	B	1010	-	49,49,49	0.22	0	60,63,63	0.36	1 (1%)
9	SF4	D	1004	2	0,12,12	-	-	-		
7	MYR	C	201	-	13,13,15	0.63	0	13,13,15	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	11A	C	208	-	12,12,12	0.66	0	12,12,12	1.17	1 (8%)
10	MGD	D	1007	11,2	41,52,52	2.05	15 (36%)	40,81,81	1.82	9 (22%)
13	MQ7	F	1010	-	49,49,49	0.22	0	60,63,63	0.36	1 (1%)
3	11A	A	209	-	12,12,12	0.67	0	12,12,12	1.17	0
10	MGD	F	1006	11	41,52,52	2.17	15 (36%)	40,81,81	1.68	8 (20%)
13	MQ7	H	1010	-	49,49,49	0.22	0	60,63,63	0.36	1 (1%)
4	A1H2V	C	205	-	50,50,50	0.29	0	53,56,56	0.40	0
4	A1H2V	E	204	-	44,44,50	0.32	0	47,50,56	0.35	0
9	SF4	D	1005	2	0,12,12	-	-	-	-	-
4	A1H2V	G	202	-	50,50,50	0.30	0	53,56,56	0.27	0
3	11A	C	203	-	11,11,12	0.68	0	11,11,12	1.18	0
3	11A	G	212	-	12,12,12	0.67	0	12,12,12	1.18	0
3	11A	C	213	-	12,12,12	0.66	0	12,12,12	1.16	0
10	MGD	B	1006	11	41,52,52	2.17	15 (36%)	40,81,81	1.68	8 (20%)
9	SF4	B	1002	2	0,12,12	-	-	-	-	-
3	11A	A	201	-	11,11,12	0.68	0	11,11,12	1.18	0
9	SF4	D	1003	2	0,12,12	-	-	-	-	-
3	11A	A	210	-	12,12,12	0.67	0	12,12,12	1.18	0
10	MGD	H	1006	11	41,52,52	2.17	15 (36%)	40,81,81	1.68	8 (20%)
3	11A	E	209	-	12,12,12	0.66	0	12,12,12	1.17	0
10	MGD	H	1007	11,2	41,52,52	2.05	15 (36%)	40,81,81	1.82	9 (22%)
4	A1H2V	A	203	-	50,50,50	0.29	0	53,56,56	0.40	0
7	MYR	A	212	-	13,13,15	0.63	0	13,13,15	1.15	0
6	KNA	G	210	-	10,10,10	0.79	0	10,10,10	0.71	0
3	11A	G	209	-	12,12,12	0.66	0	12,12,12	1.17	0
3	11A	E	211	-	12,12,12	0.67	0	12,12,12	1.17	0
8	FES	D	1001	2	0,4,4	-	-	-	-	-
4	A1H2V	E	202	-	50,50,50	0.30	0	53,56,56	0.27	0
9	SF4	F	1003	2	0,12,12	-	-	-	-	-
4	A1H2V	G	204	-	44,44,50	0.32	0	47,50,56	0.35	0
3	11A	E	213	-	12,12,12	0.67	0	12,12,12	1.17	0
13	MQ7	D	1010	-	49,49,49	0.22	0	60,63,63	0.36	1 (1%)
10	MGD	B	1007	11,2	41,52,52	2.05	15 (36%)	40,81,81	1.82	9 (22%)
9	SF4	H	1003	2	0,12,12	-	-	-	-	-
6	KNA	E	210	-	10,10,10	0.81	0	10,10,10	0.71	0
8	FES	F	1001	2	0,4,4	-	-	-	-	-
3	11A	G	208	-	12,12,12	0.66	0	12,12,12	1.17	1 (8%)
5	SHV	G	207	-	8,8,8	0.87	0	8,8,8	0.79	0
3	11A	G	203	-	11,11,12	0.68	0	11,11,12	1.18	0
3	11A	A	207	-	12,12,12	0.66	0	12,12,12	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	A1H2V	E	205	-	50,50,50	0.29	0	53,56,56	0.40	0
9	SF4	H	1005	2	0,12,12	-	-	-		

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
3	11A	A	211	-	-	4/10/10/10	-
3	11A	A	206	-	-	1/10/10/10	-
3	11A	G	213	-	-	4/10/10/10	-
3	11A	C	212	-	-	6/10/10/10	-
6	KNA	A	208	-	-	3/8/8/8	-
5	SHV	C	207	-	-	2/6/6/6	-
3	11A	E	203	-	-	1/9/9/10	-
5	SHV	C	206	-	-	3/6/6/6	-
5	SHV	G	206	-	-	3/6/6/6	-
4	A1H2V	C	202	-	-	4/55/55/55	-
5	SHV	E	206	-	-	3/6/6/6	-
5	SHV	A	205	-	-	2/6/6/6	-
9	SF4	D	1002	2	-	-	0/6/5/5
9	SF4	B	1004	2	-	-	0/6/5/5
8	FES	B	1001	2	-	-	0/1/1/1
7	MYR	E	201	-	-	5/11/11/13	-
9	SF4	B	1005	2	-	-	0/6/5/5
5	SHV	A	204	-	-	3/6/6/6	-
3	11A	C	211	-	-	2/10/10/10	-
9	SF4	F	1002	2	-	-	0/6/5/5
6	KNA	C	210	-	-	3/8/8/8	-
9	SF4	F	1004	2	-	-	0/6/5/5
4	A1H2V	G	205	-	-	22/55/55/55	-
10	MGD	D	1006	11	-	3/18/66/66	0/6/6/6
3	11A	G	211	-	-	2/10/10/10	-
10	MGD	F	1007	11,2	-	7/18/66/66	0/6/6/6
9	SF4	H	1004	2	-	-	0/6/5/5
8	FES	H	1001	2	-	-	0/1/1/1
3	11A	C	209	-	-	2/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SHV	E	207	-	-	2/6/6/6	-
4	A1H2V	A	202	-	-	11/49/49/55	-
4	A1H2V	C	204	-	-	11/49/49/55	-
9	SF4	F	1005	2	-	-	0/6/5/5
9	SF4	B	1003	2	-	-	0/6/5/5
7	MYR	G	201	-	-	5/11/11/13	-
3	11A	E	208	-	-	1/10/10/10	-
3	11A	E	212	-	-	6/10/10/10	-
9	SF4	H	1002	2	-	-	0/6/5/5
4	A1H2V	A	213	-	-	4/55/55/55	-
13	MQ7	B	1010	-	-	7/41/61/61	0/2/2/2
9	SF4	D	1004	2	-	-	0/6/5/5
7	MYR	C	201	-	-	5/11/11/13	-
3	11A	C	208	-	-	1/10/10/10	-
10	MGD	D	1007	11,2	-	7/18/66/66	0/6/6/6
13	MQ7	F	1010	-	-	7/41/61/61	0/2/2/2
3	11A	A	209	-	-	2/10/10/10	-
10	MGD	F	1006	11	-	3/18/66/66	0/6/6/6
13	MQ7	H	1010	-	-	7/41/61/61	0/2/2/2
4	A1H2V	C	205	-	-	22/55/55/55	-
4	A1H2V	E	204	-	-	11/49/49/55	-
9	SF4	D	1005	2	-	-	0/6/5/5
4	A1H2V	G	202	-	-	4/55/55/55	-
3	11A	C	203	-	-	1/9/9/10	-
3	11A	G	212	-	-	6/10/10/10	-
3	11A	C	213	-	-	4/10/10/10	-
10	MGD	B	1006	11	-	3/18/66/66	0/6/6/6
9	SF4	B	1002	2	-	-	0/6/5/5
3	11A	A	201	-	-	1/9/9/10	-
9	SF4	D	1003	2	-	-	0/6/5/5
3	11A	A	210	-	-	6/10/10/10	-
10	MGD	H	1006	11	-	3/18/66/66	0/6/6/6
3	11A	E	209	-	-	2/10/10/10	-
10	MGD	H	1007	11,2	-	7/18/66/66	0/6/6/6
4	A1H2V	A	203	-	-	22/55/55/55	-
7	MYR	A	212	-	-	5/11/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KNA	G	210	-	-	3/8/8/8	-
3	11A	G	209	-	-	2/10/10/10	-
3	11A	E	211	-	-	2/10/10/10	-
8	FES	D	1001	2	-	-	0/1/1/1
4	A1H2V	E	202	-	-	4/55/55/55	-
9	SF4	F	1003	2	-	-	0/6/5/5
4	A1H2V	G	204	-	-	11/49/49/55	-
3	11A	E	213	-	-	4/10/10/10	-
13	MQ7	D	1010	-	-	7/41/61/61	0/2/2/2
10	MGD	B	1007	11,2	-	7/18/66/66	0/6/6/6
9	SF4	H	1003	2	-	-	0/6/5/5
6	KNA	E	210	-	-	3/8/8/8	-
8	FES	F	1001	2	-	-	0/1/1/1
3	11A	G	208	-	-	1/10/10/10	-
5	SHV	G	207	-	-	2/6/6/6	-
3	11A	G	203	-	-	1/9/9/10	-
3	11A	A	207	-	-	2/10/10/10	-
4	A1H2V	E	205	-	-	22/55/55/55	-
9	SF4	H	1005	2	-	-	0/6/5/5

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1006	MGD	C23-C14	5.43	1.58	1.53
10	D	1006	MGD	C23-C14	5.43	1.58	1.53
10	F	1006	MGD	C23-C14	5.43	1.58	1.53
10	H	1006	MGD	C23-C14	5.43	1.58	1.53
10	B	1007	MGD	C21-N22	5.07	1.41	1.35

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1006	MGD	PA-O3B-PB	5.20	150.67	132.83
10	D	1006	MGD	PA-O3B-PB	5.20	150.67	132.83
10	F	1006	MGD	PA-O3B-PB	5.20	150.67	132.83
10	H	1006	MGD	PA-O3B-PB	5.20	150.67	132.83
10	B	1007	MGD	PA-O3B-PB	4.97	149.87	132.83

There are no chirality outliers.

5 of 332 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	A1H2V	C13-C14-O16-C17
4	A	202	A1H2V	O15-C14-O16-C17
4	C	204	A1H2V	C13-C14-O16-C17
4	C	204	A1H2V	O15-C14-O16-C17
4	E	204	A1H2V	C13-C14-O16-C17

There are no ring outliers.

49 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	211	11A	1	0
3	G	213	11A	1	0
3	E	203	11A	2	0
9	D	1002	SF4	1	0
9	B	1004	SF4	1	0
8	B	1001	FES	1	0
7	E	201	MYR	2	0
9	B	1005	SF4	1	0
9	F	1002	SF4	1	0
9	F	1004	SF4	1	0
4	G	205	A1H2V	6	0
10	D	1006	MGD	10	0
9	H	1004	SF4	1	0
10	F	1007	MGD	11	0
8	H	1001	FES	1	0
9	F	1005	SF4	1	0
9	B	1003	SF4	2	0
7	G	201	MYR	2	0
9	H	1002	SF4	1	0
13	B	1010	MQ7	2	0
9	D	1004	SF4	1	0
7	C	201	MYR	2	0
10	D	1007	MGD	12	0
13	F	1010	MQ7	2	0
3	A	209	11A	1	0
10	F	1006	MGD	11	0
13	H	1010	MQ7	2	0
4	C	205	A1H2V	6	0
9	D	1005	SF4	1	0
3	C	203	11A	2	0
3	C	213	11A	1	0

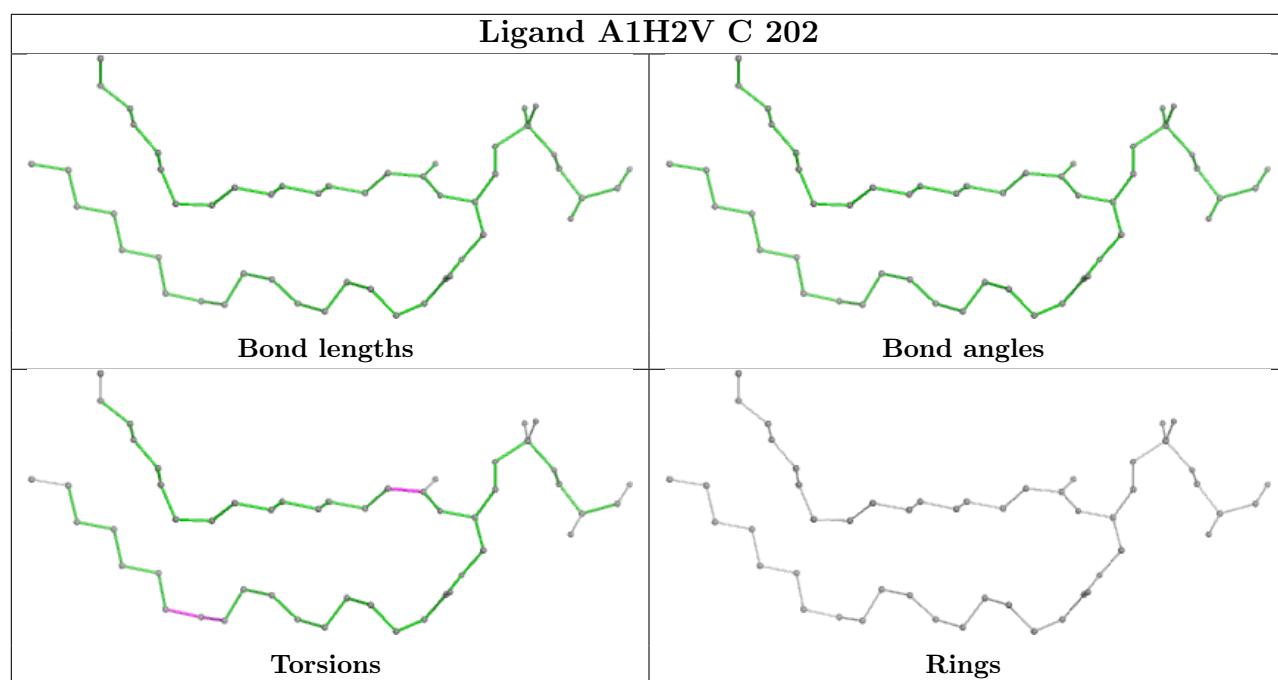
*Continued on next page...*

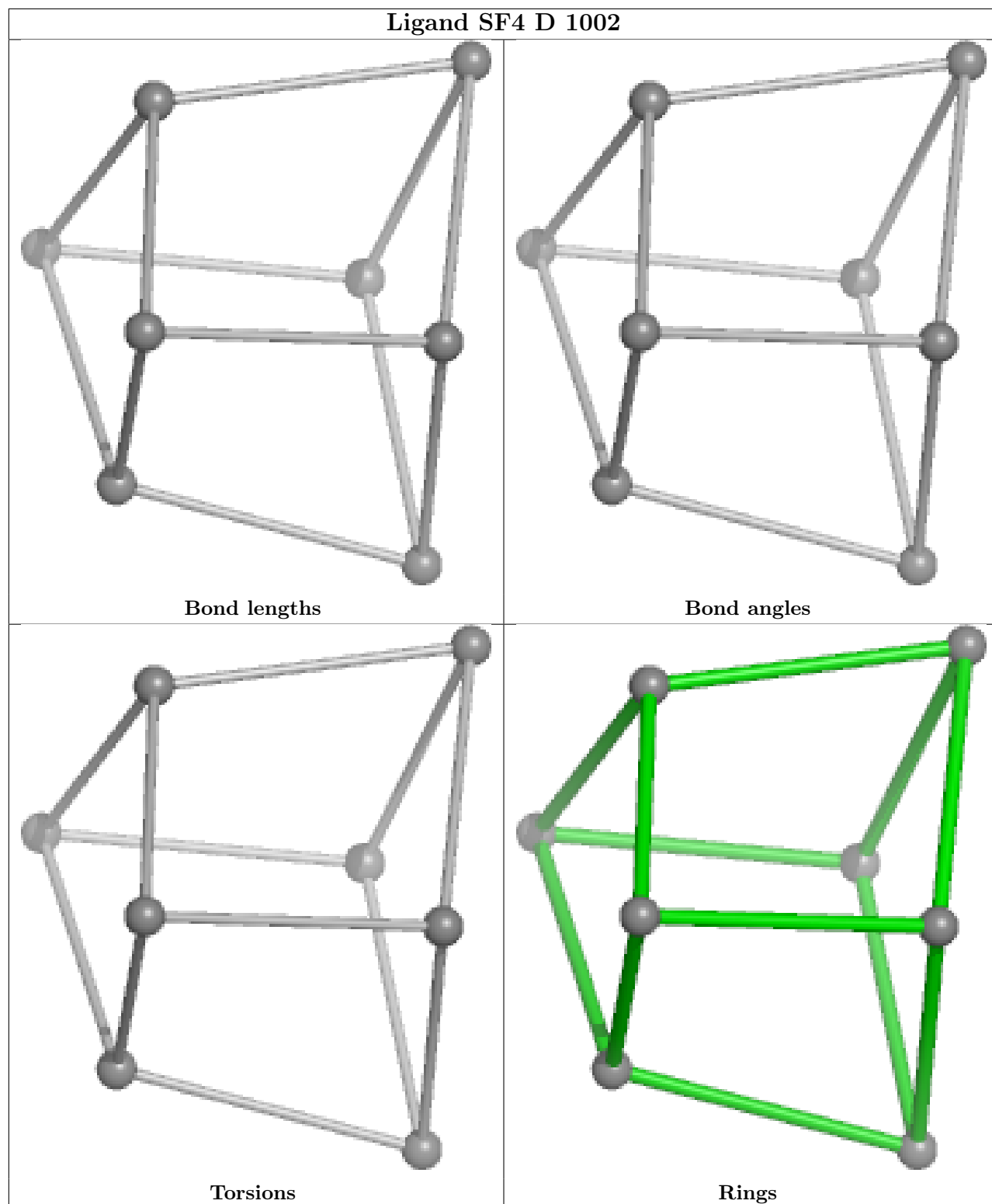
*Continued from previous page...*

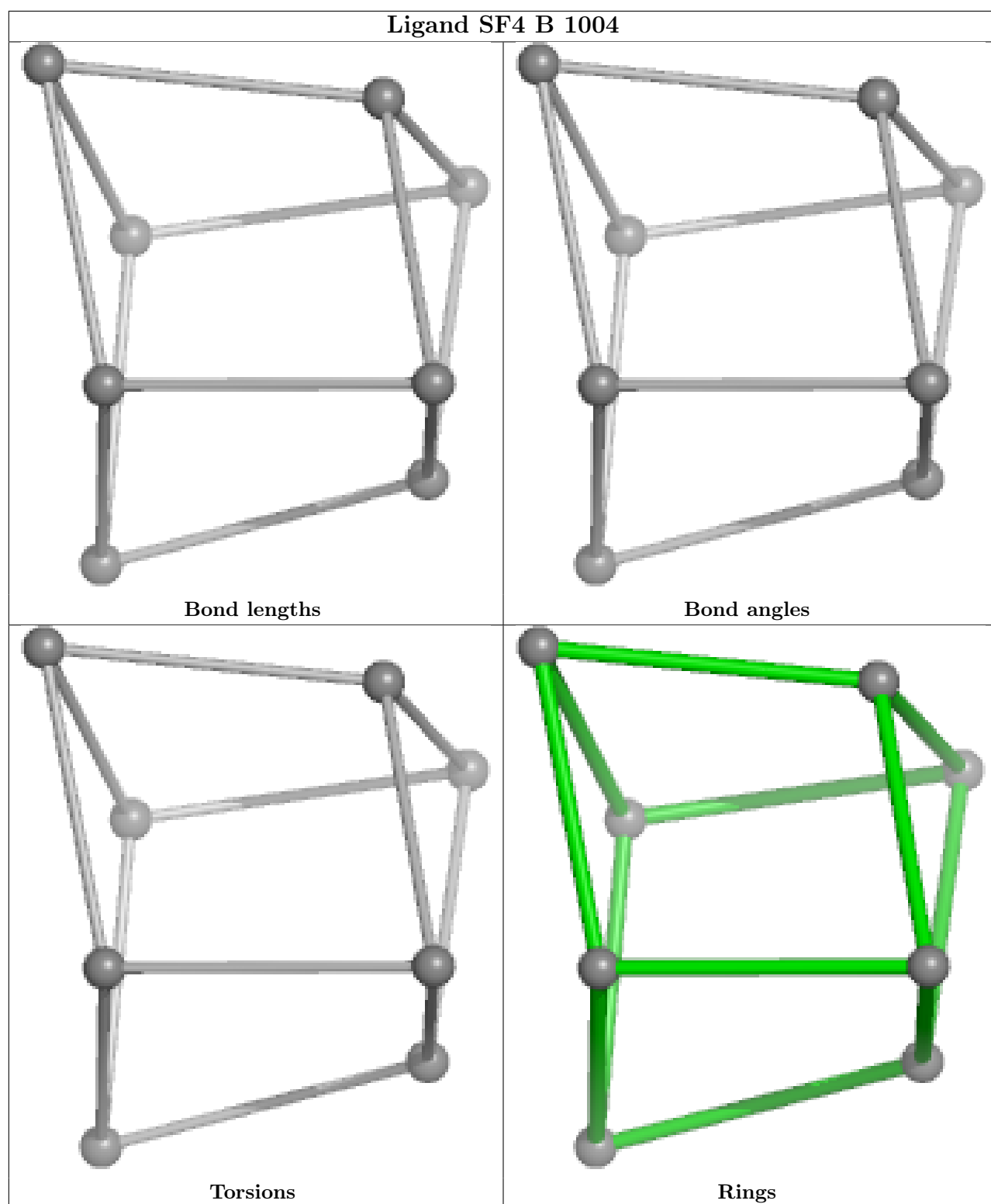
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1006	MGD	10	0
9	B	1002	SF4	1	0
3	A	201	11A	2	0
9	D	1003	SF4	1	0
10	H	1006	MGD	11	0
10	H	1007	MGD	11	0
4	A	203	A1H2V	6	0
7	A	212	MYR	2	0
8	D	1001	FES	1	0
9	F	1003	SF4	2	0
3	E	213	11A	1	0
13	D	1010	MQ7	2	0
10	B	1007	MGD	10	0
9	H	1003	SF4	2	0
8	F	1001	FES	1	0
3	G	203	11A	2	0
4	E	205	A1H2V	6	0
9	H	1005	SF4	1	0

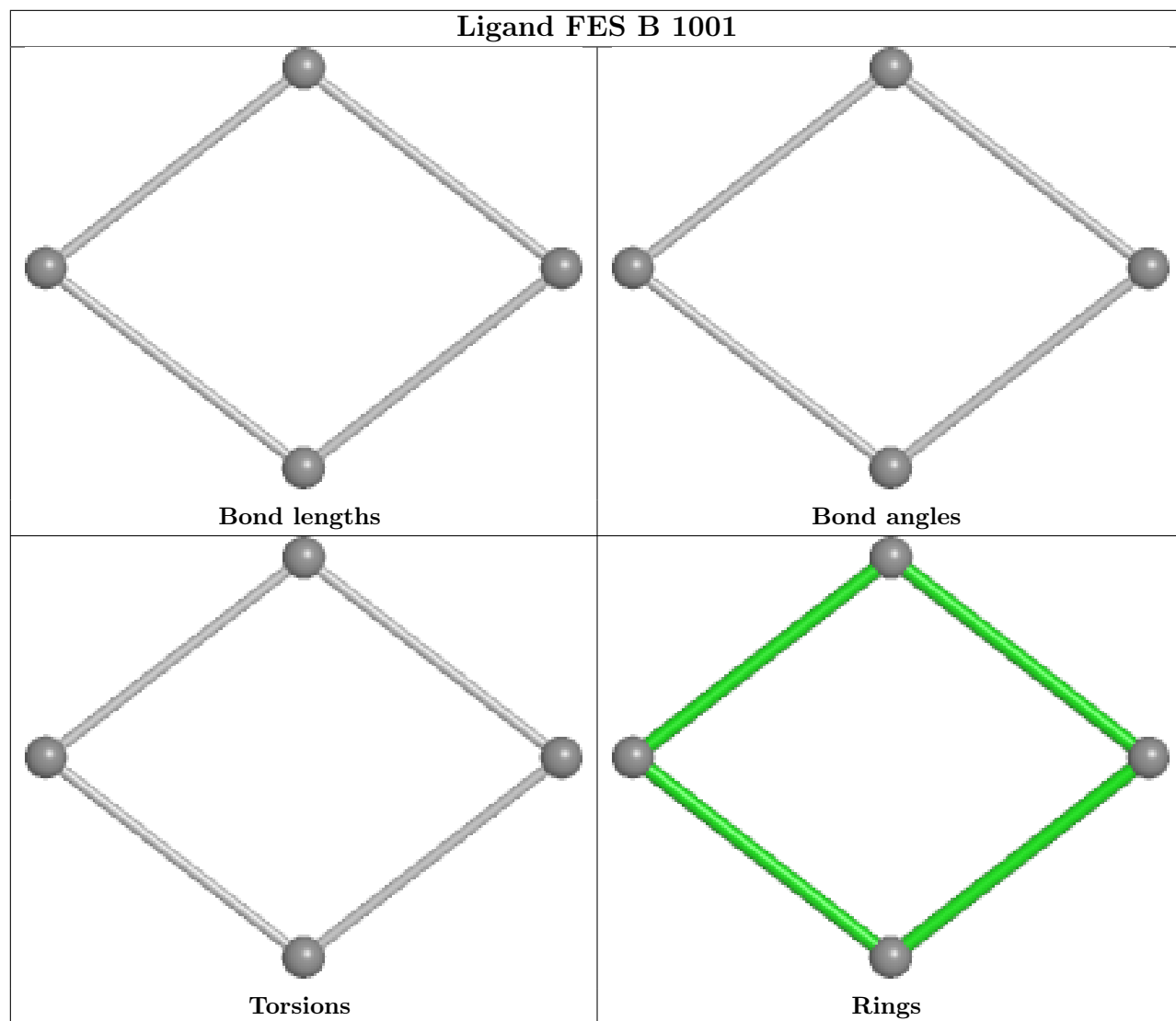
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

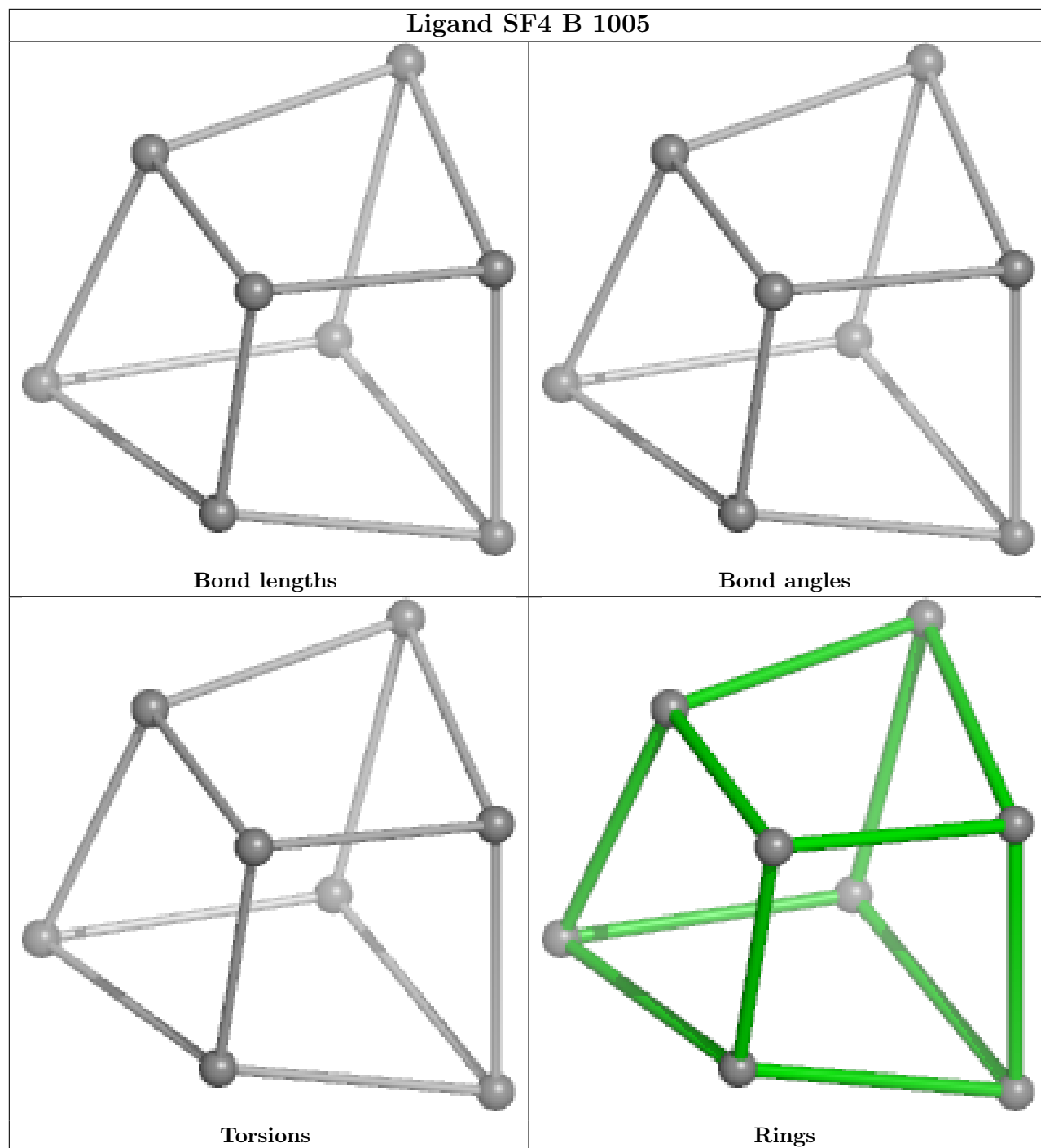


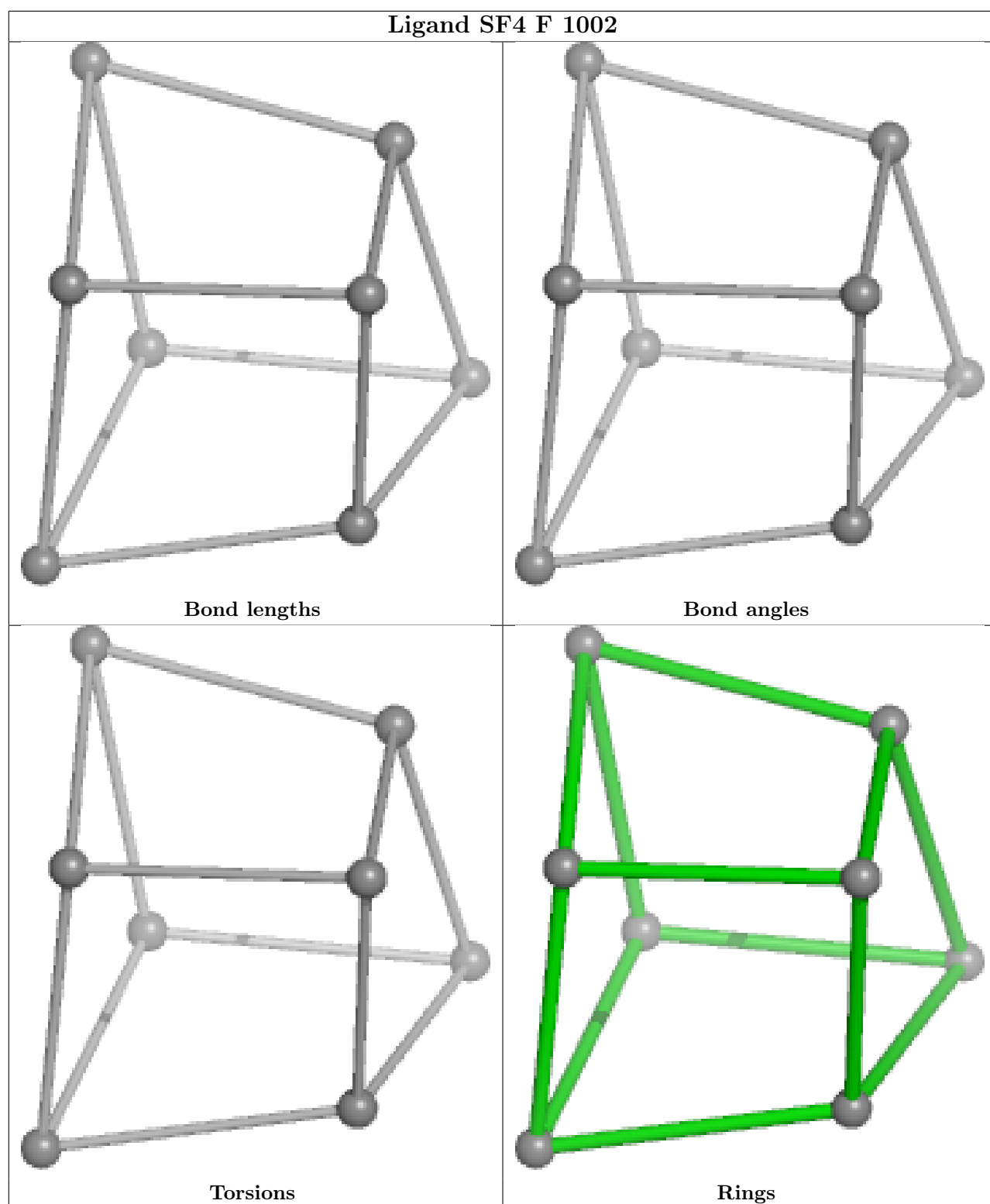


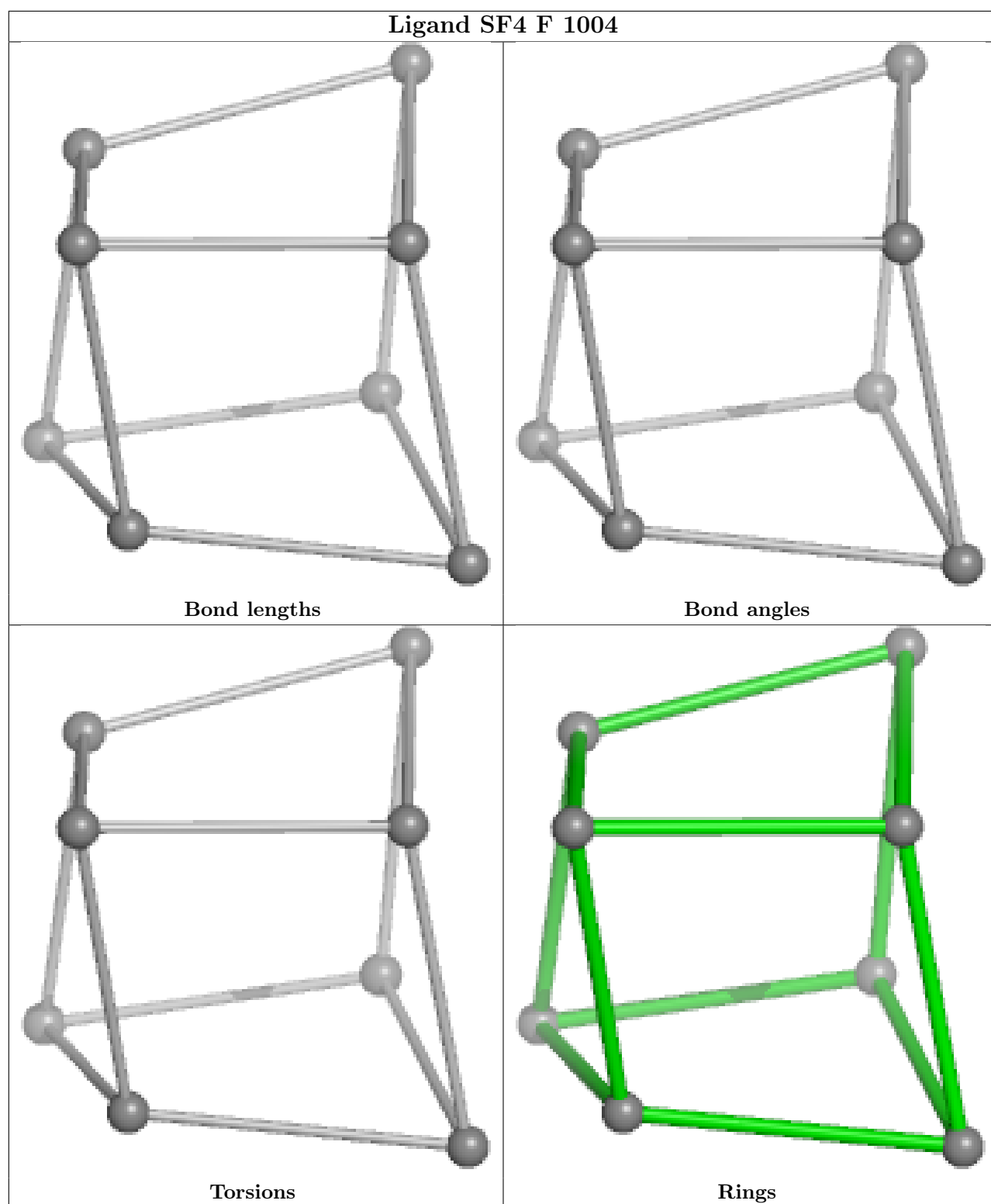


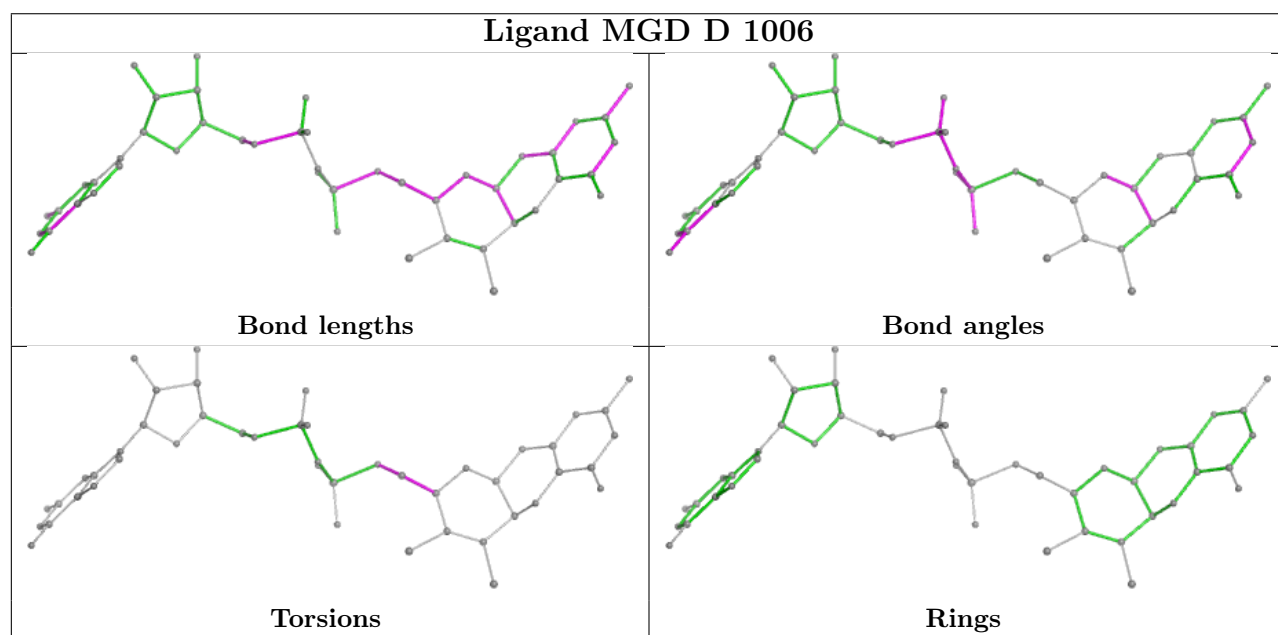
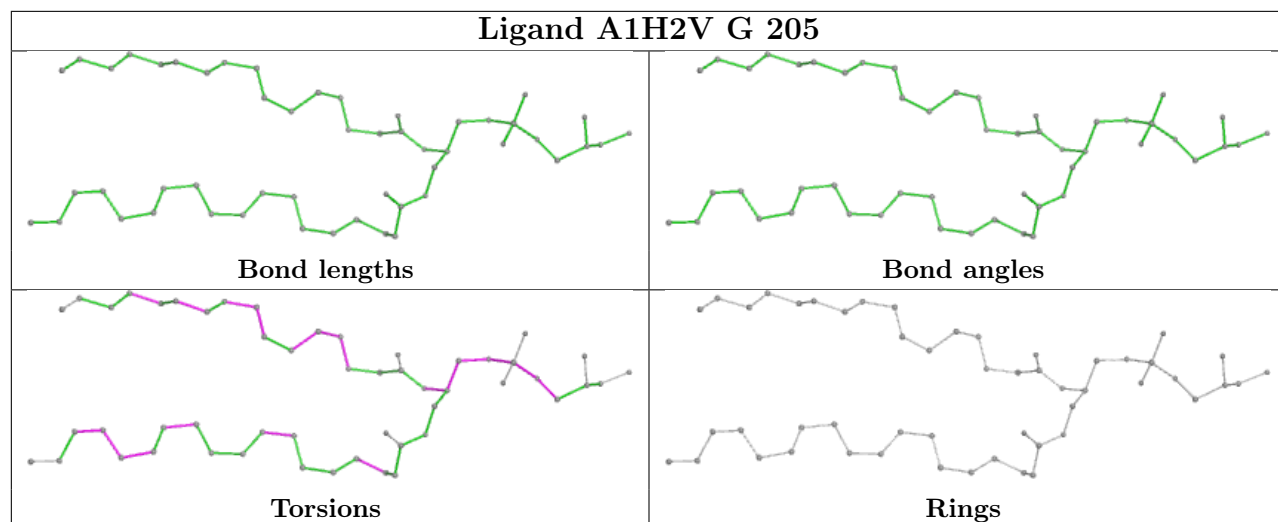




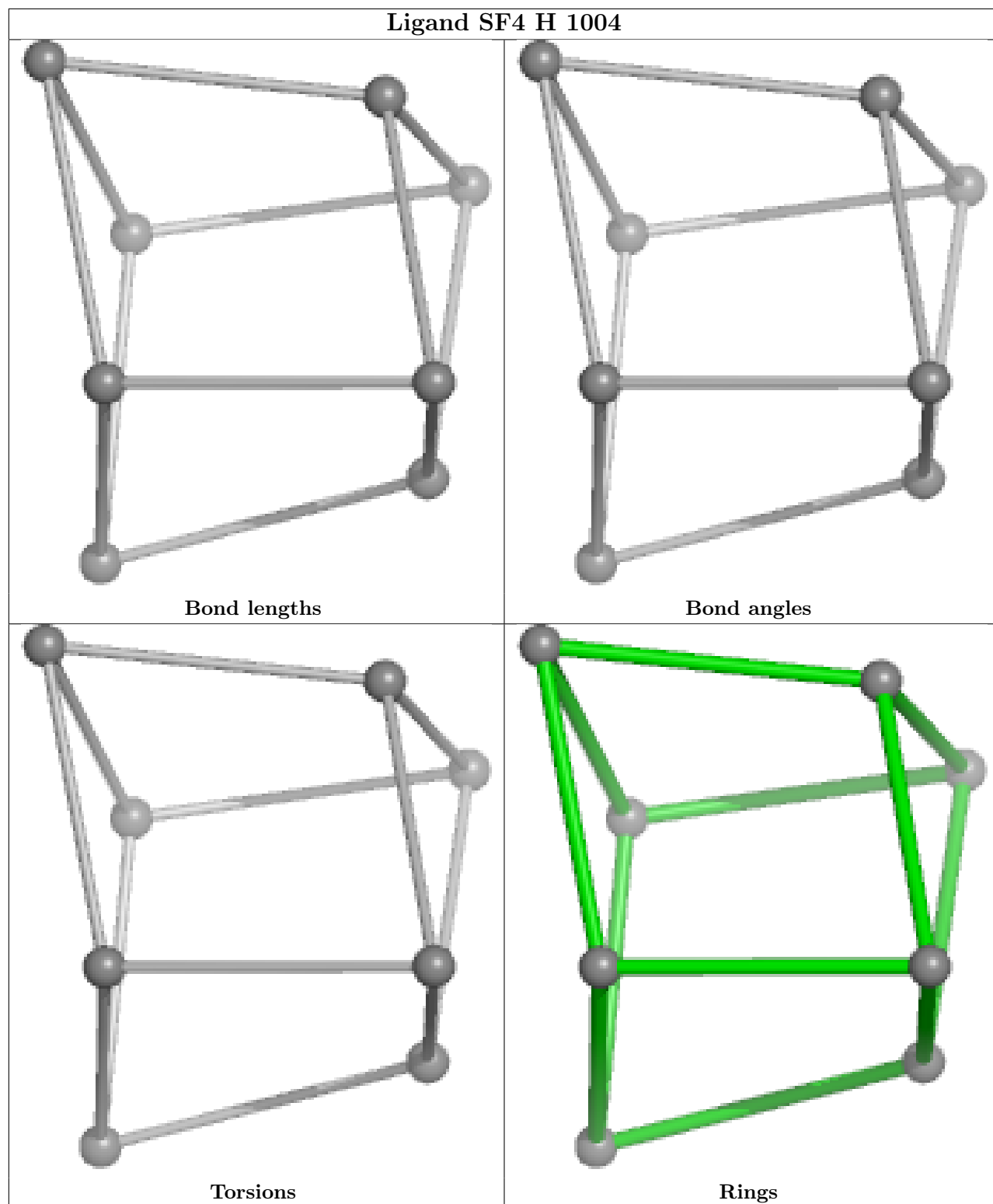


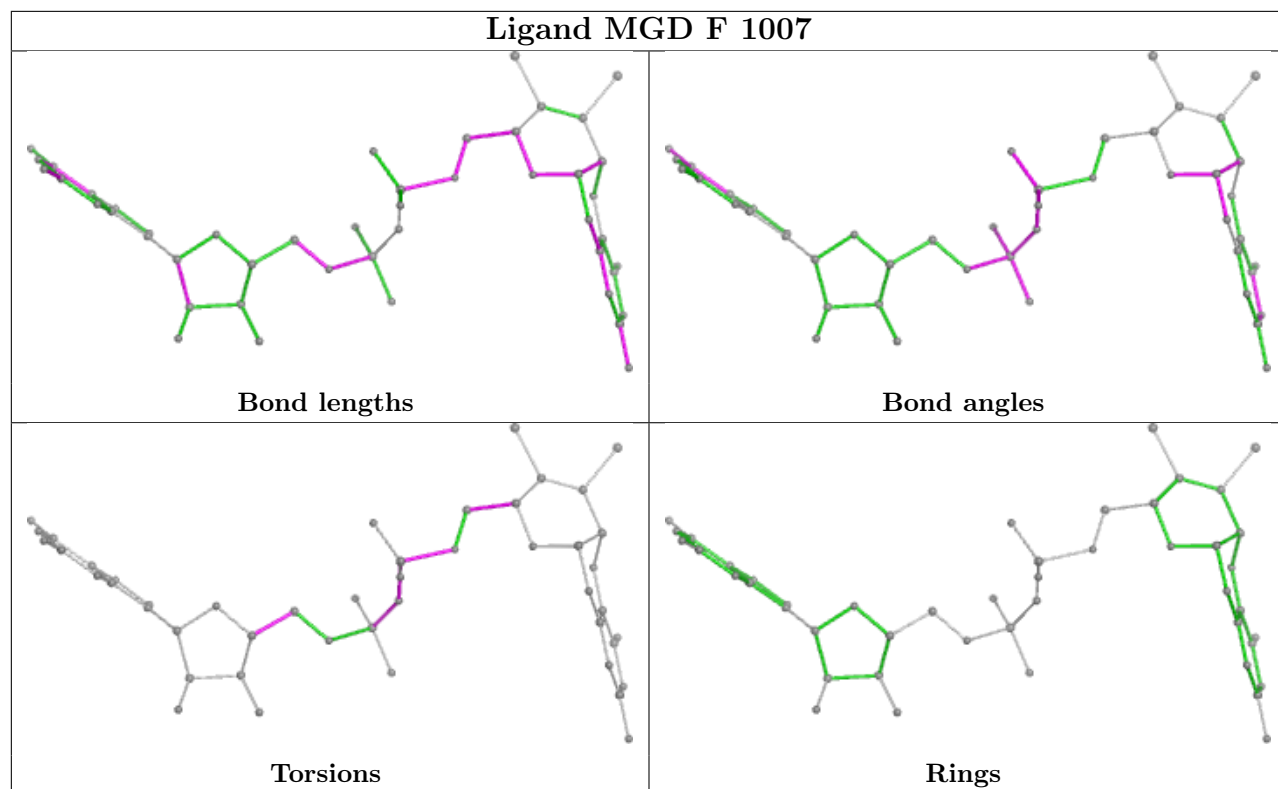


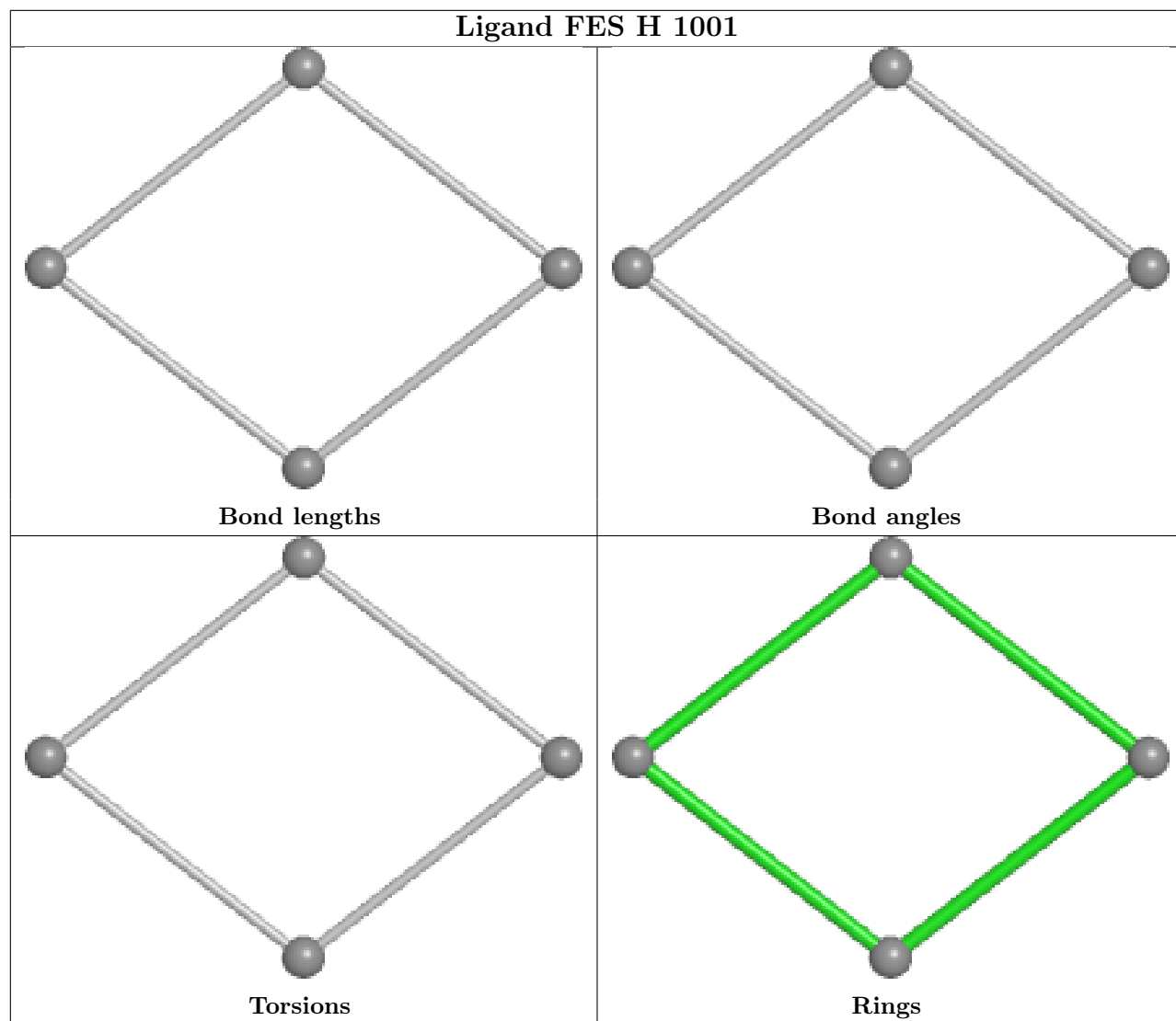


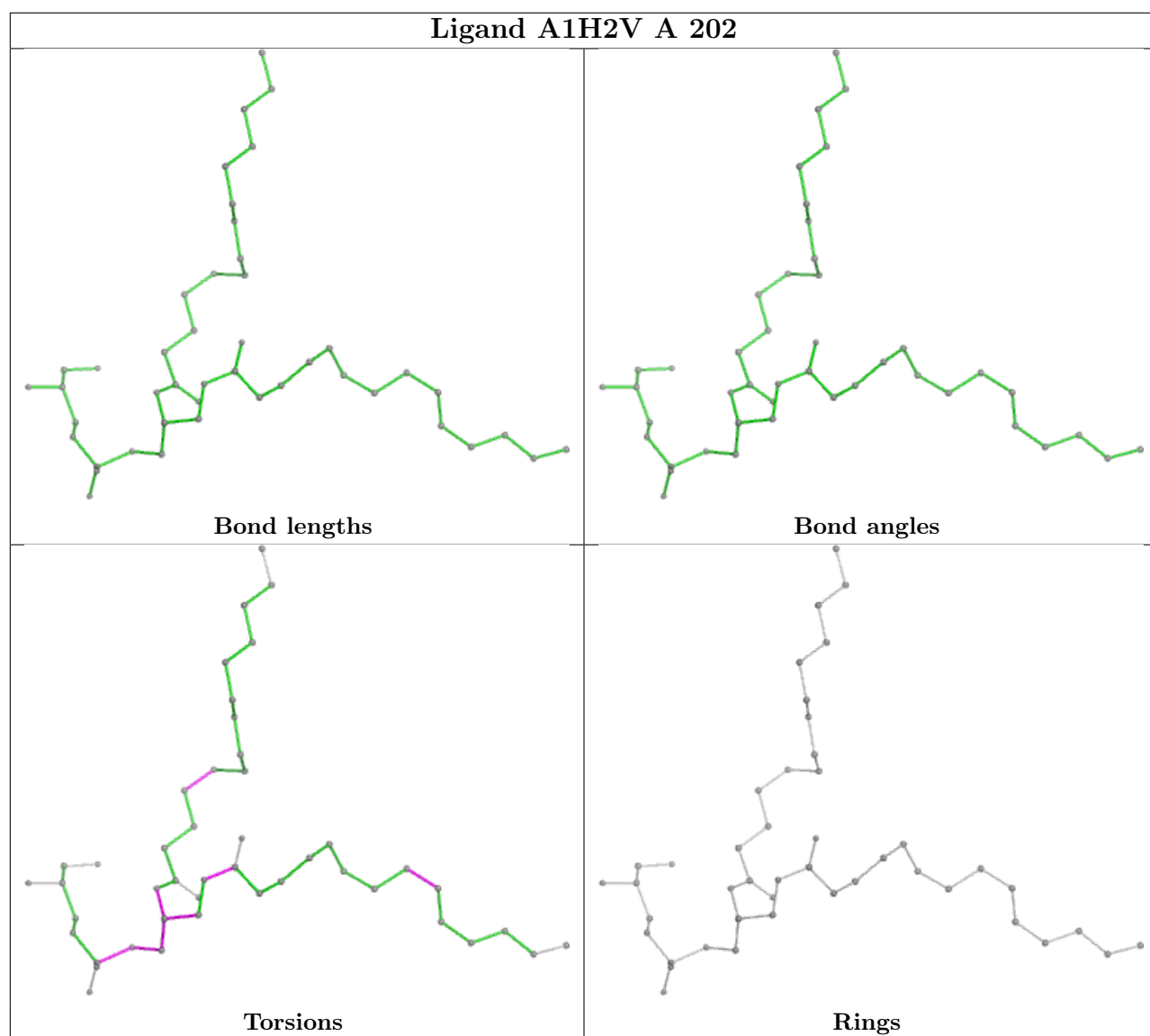


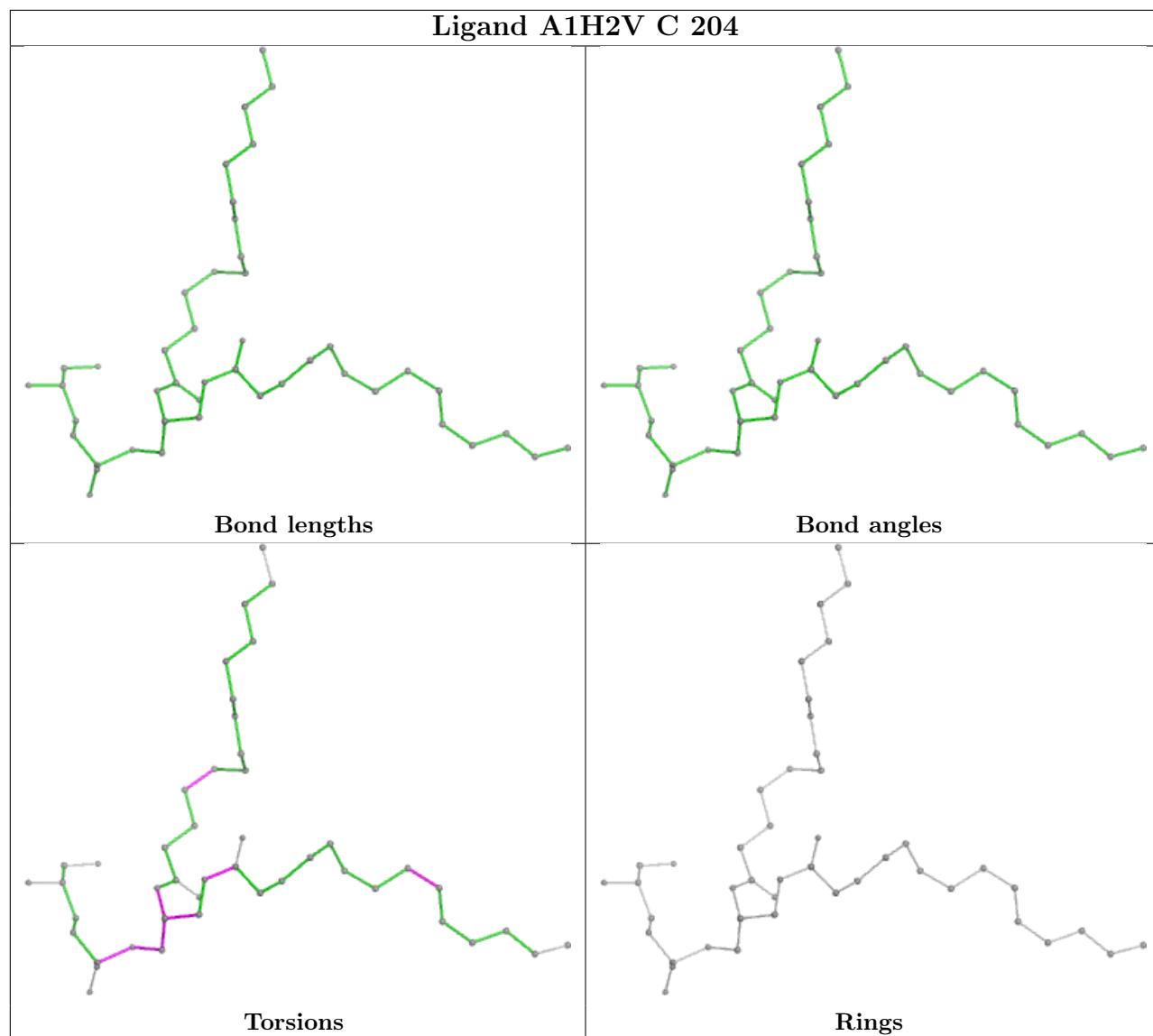


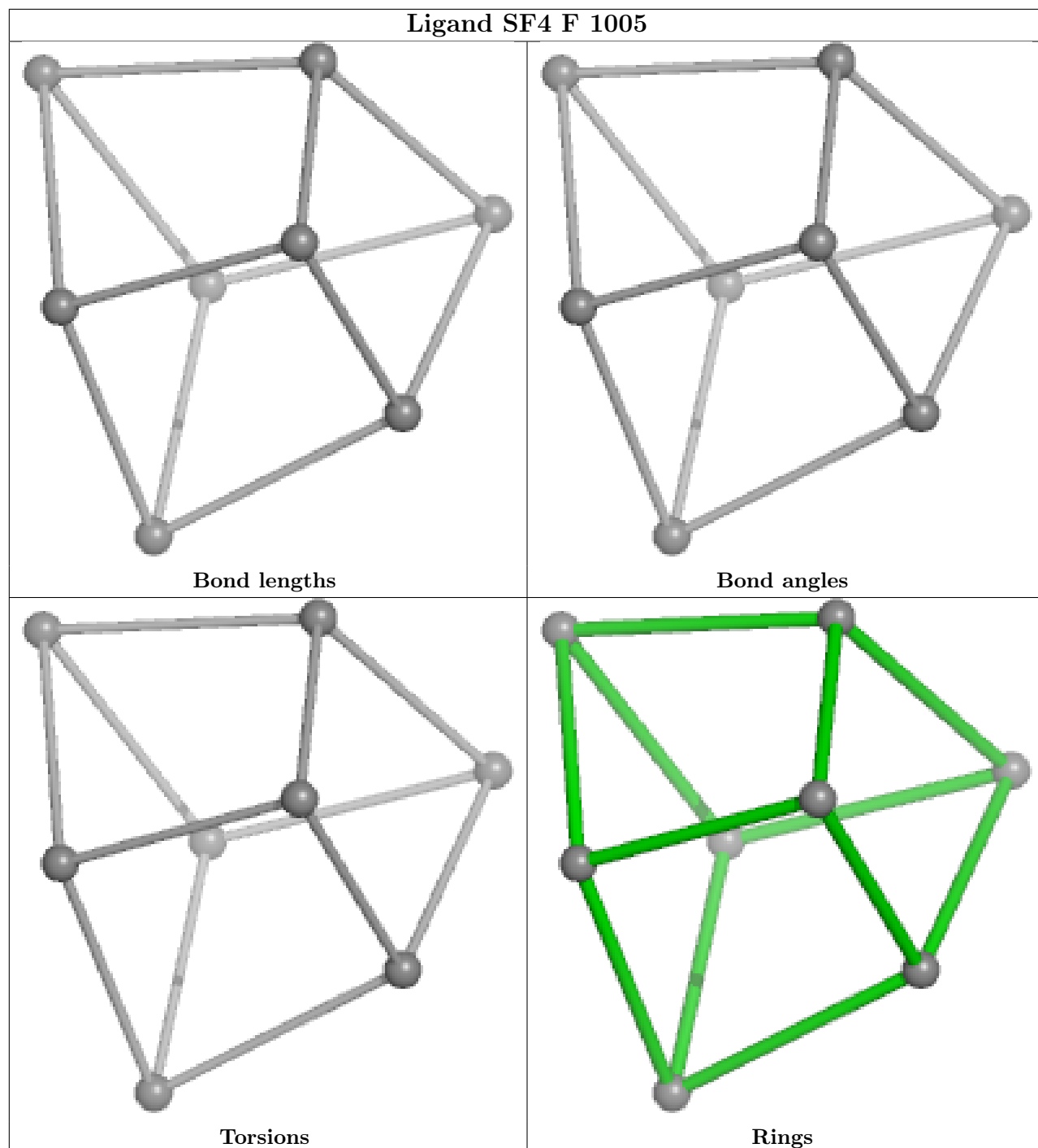


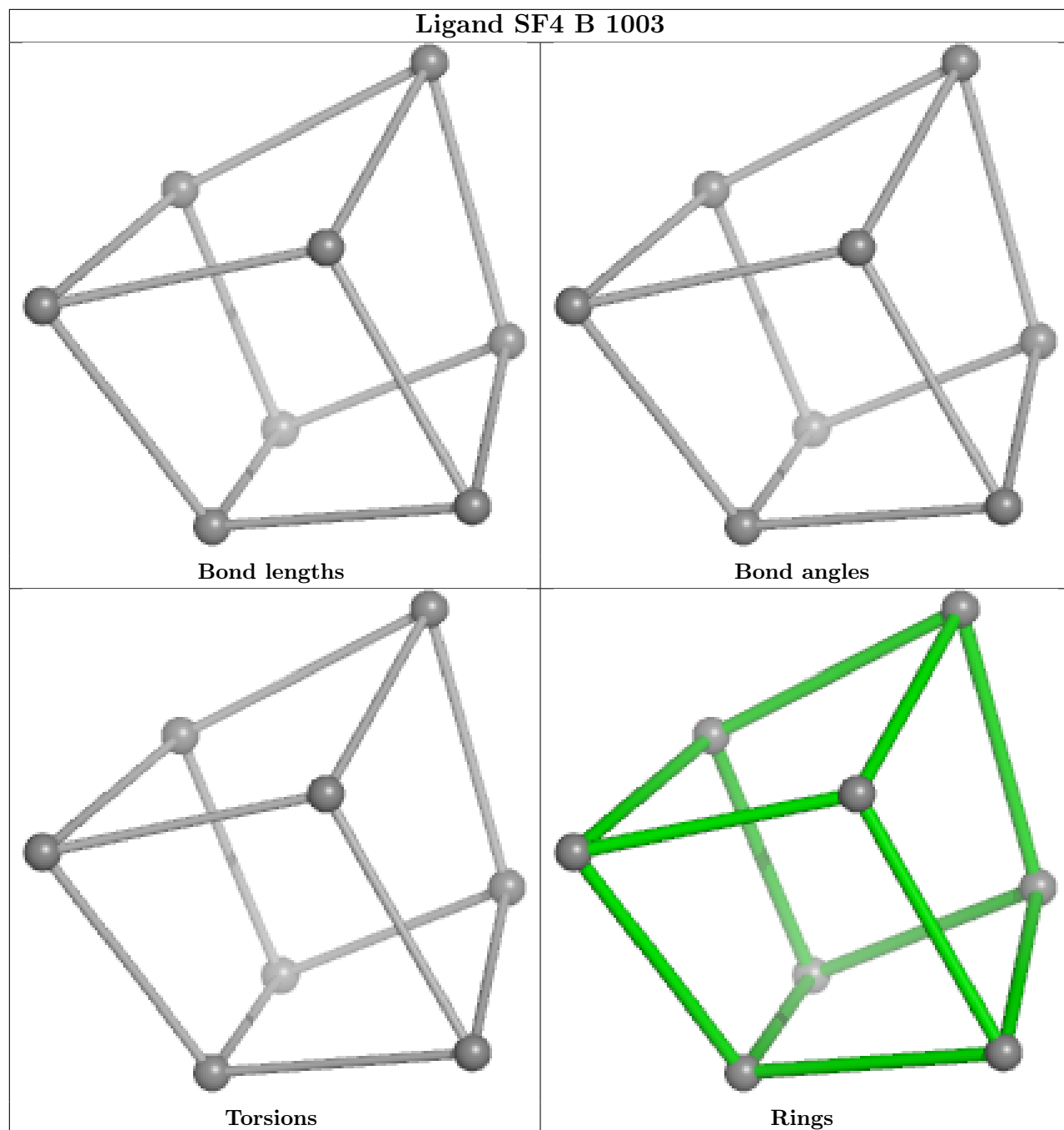


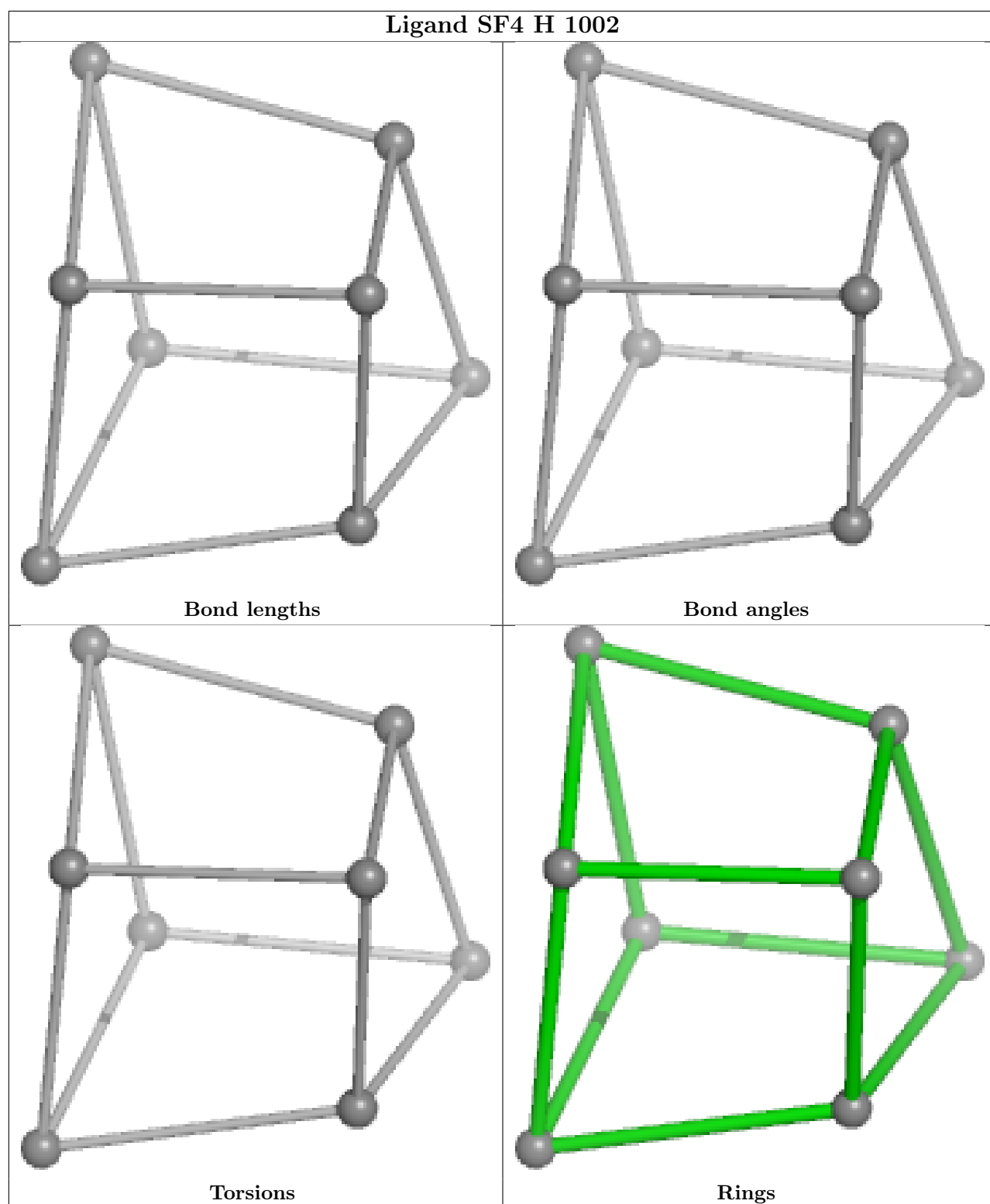




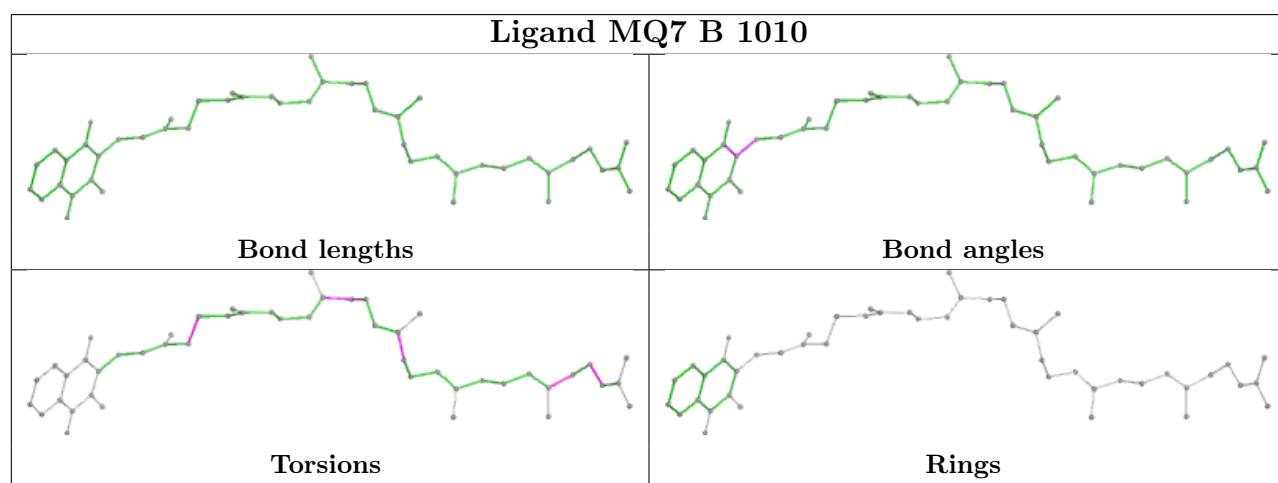
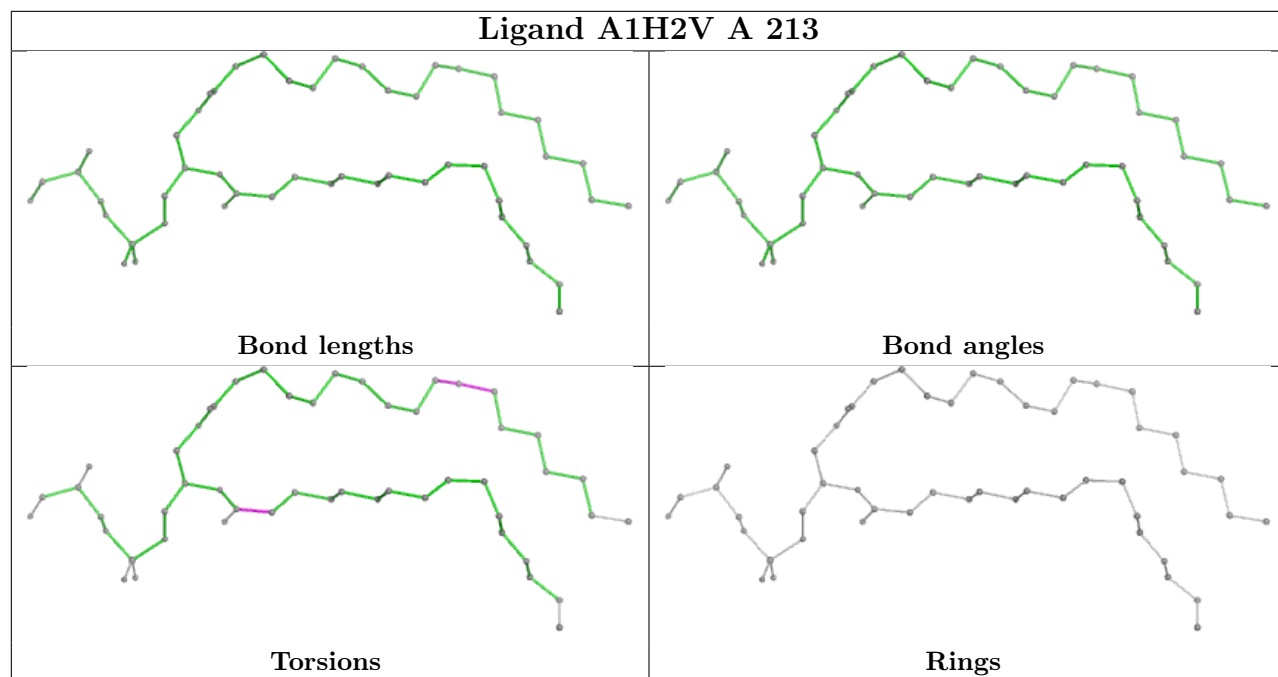


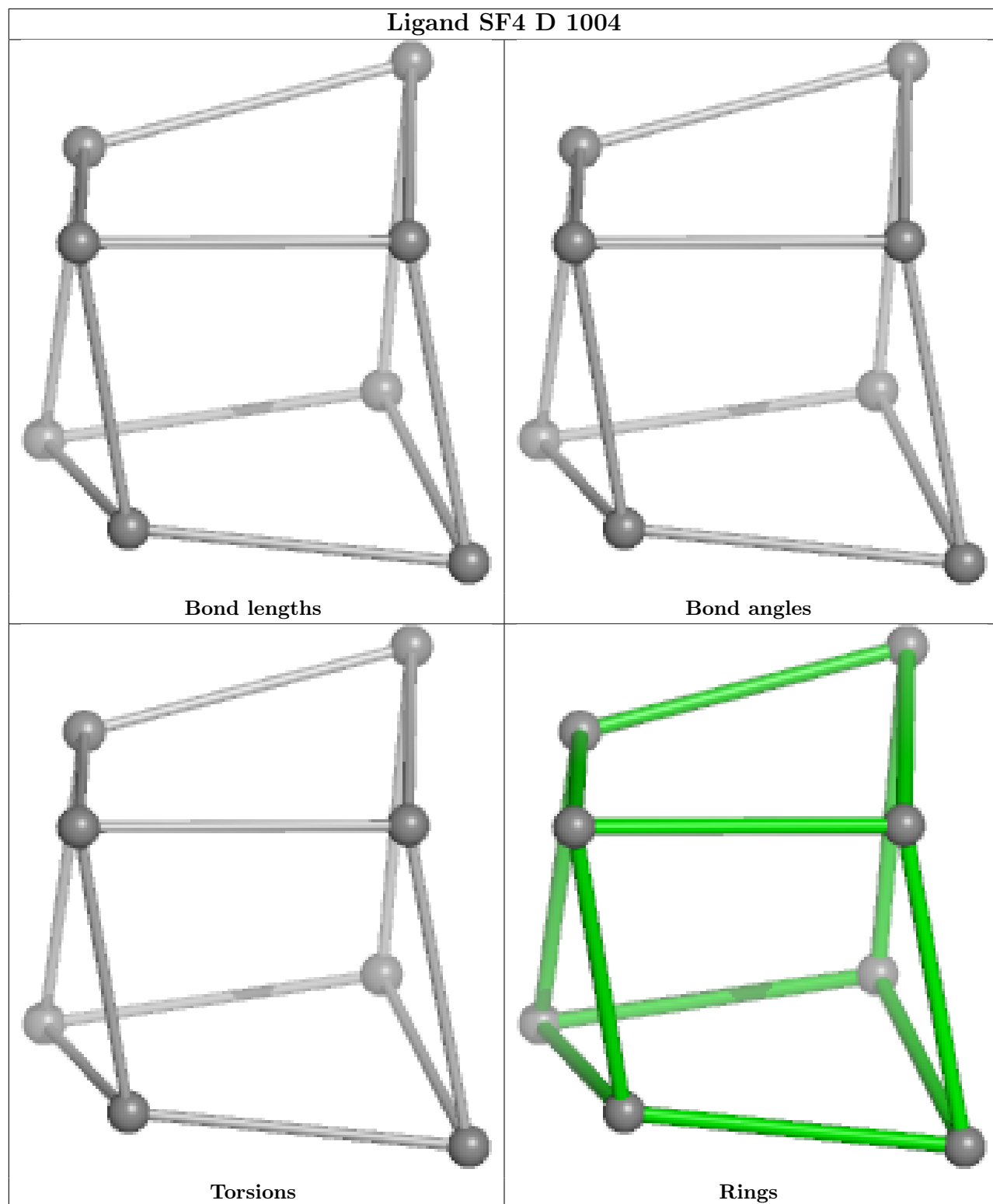




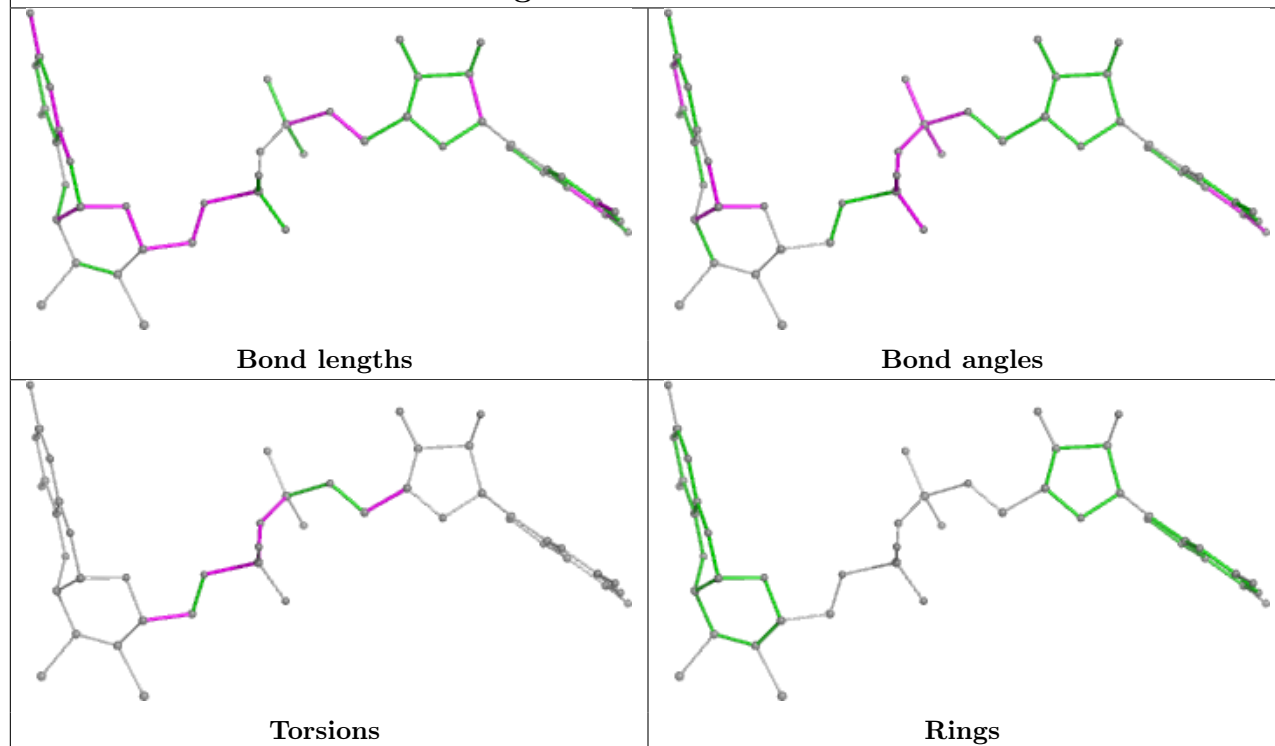




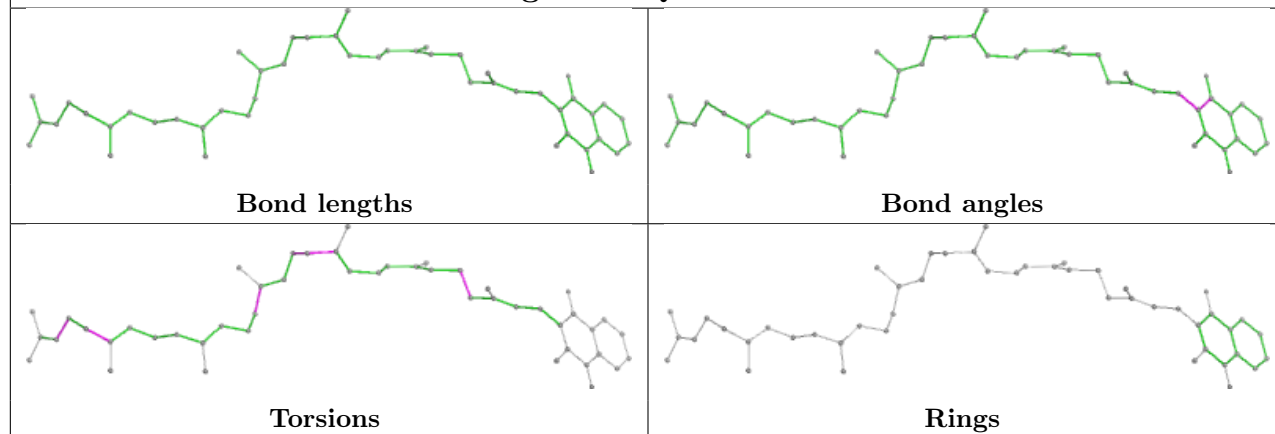


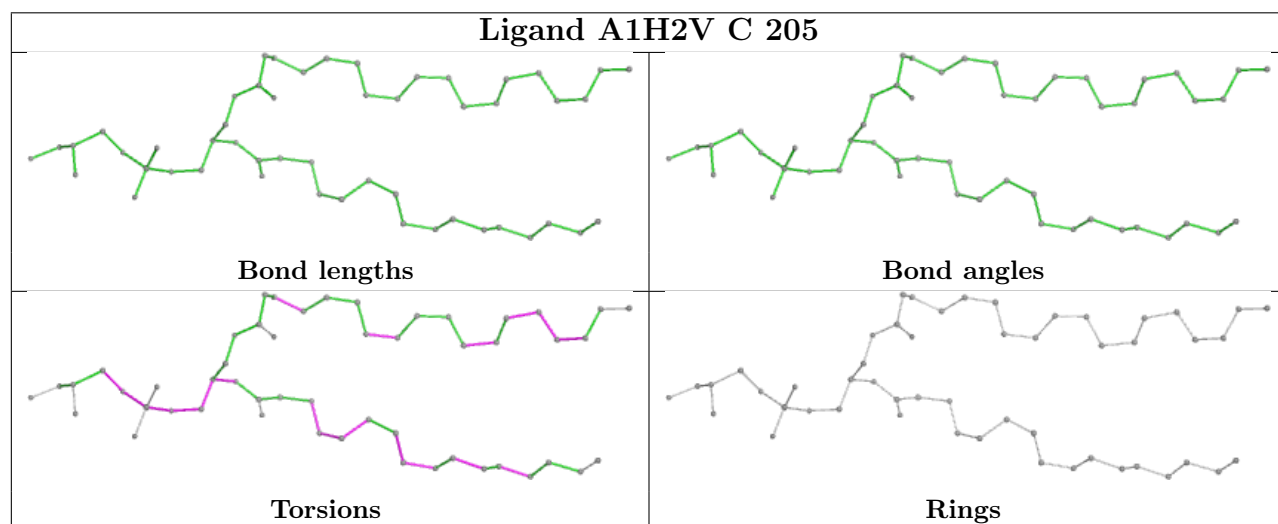
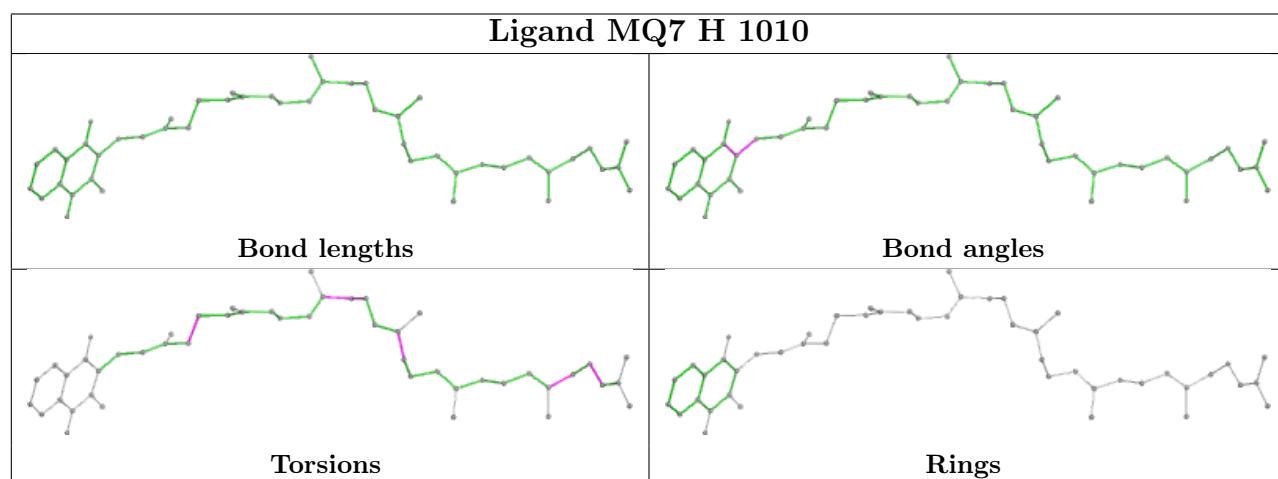
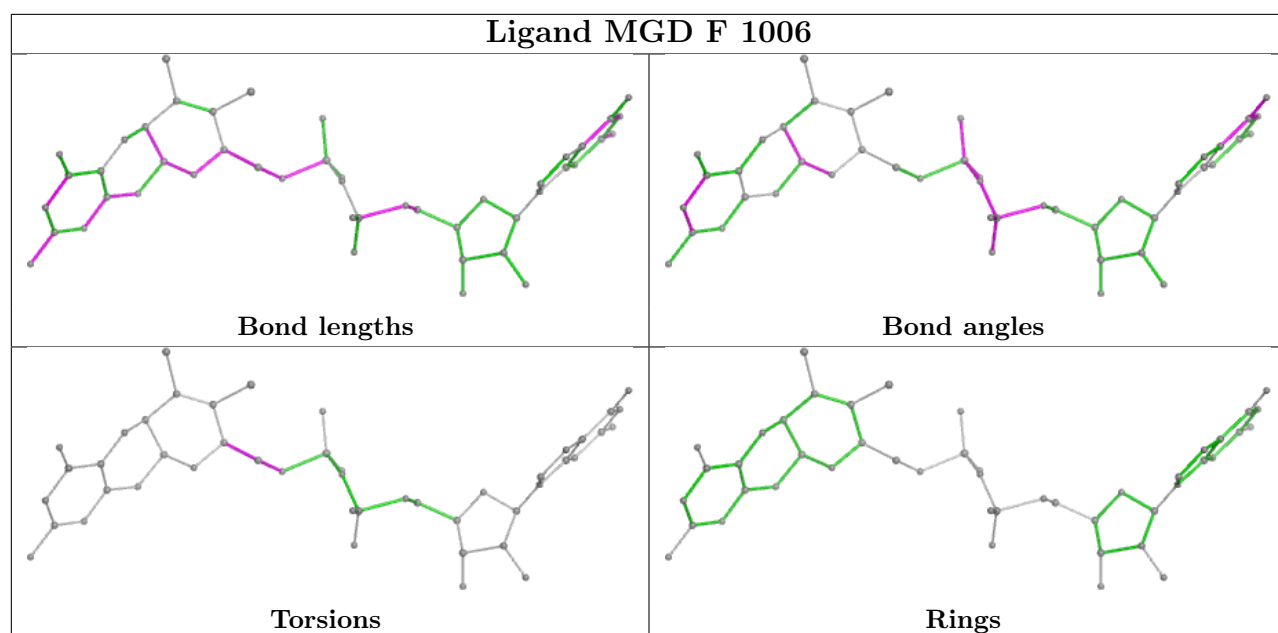


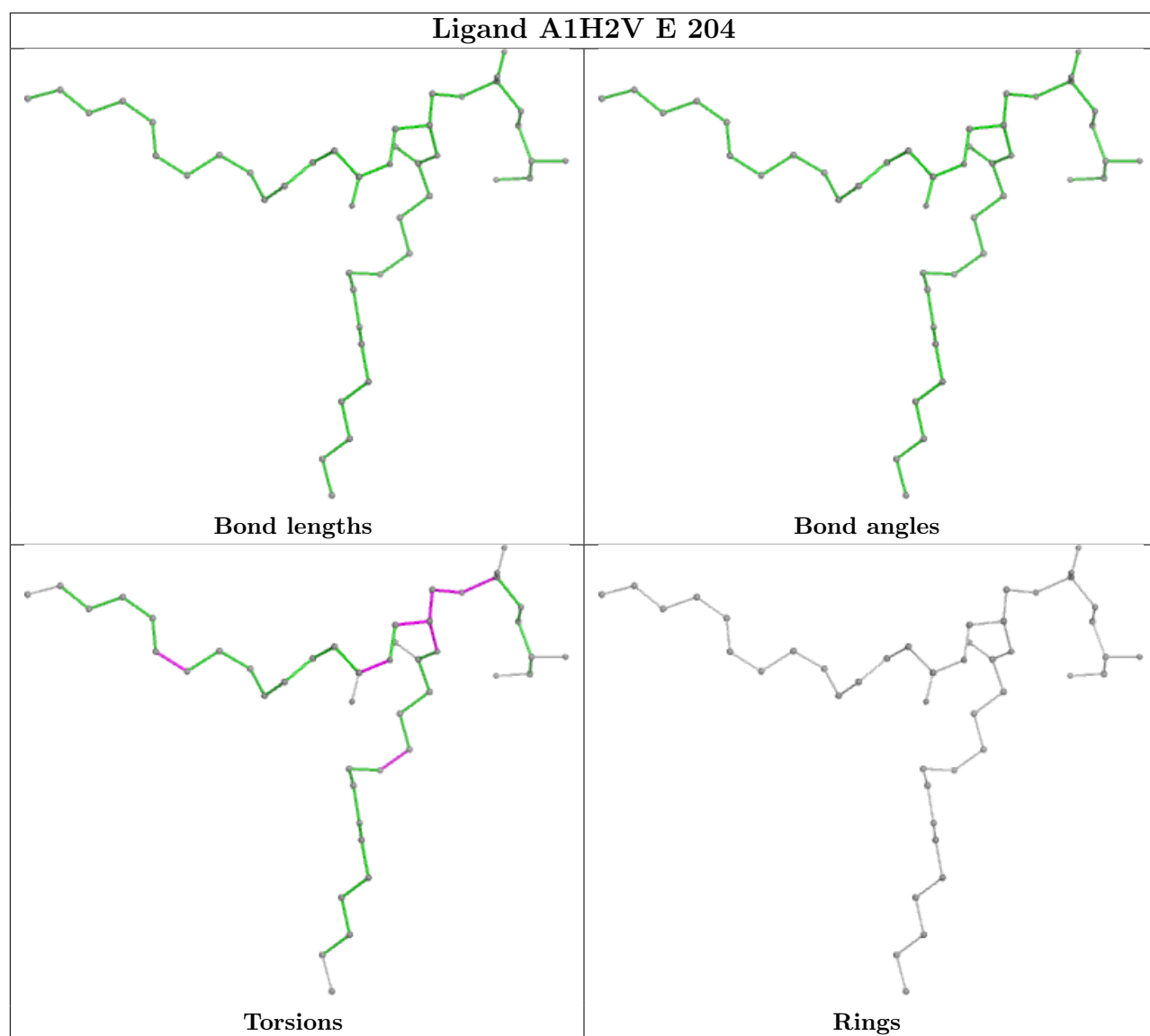
## Ligand MGD D 1007

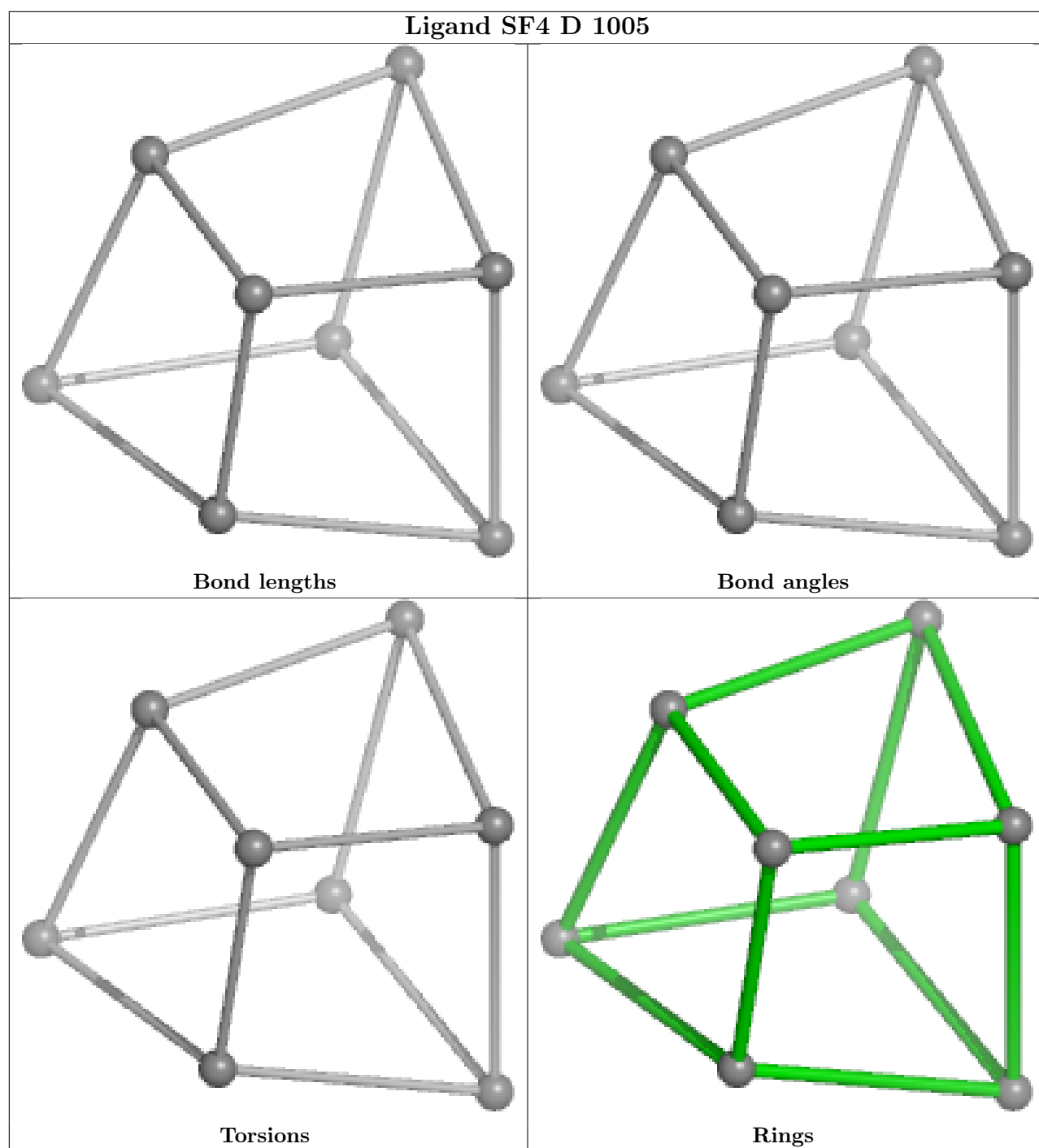


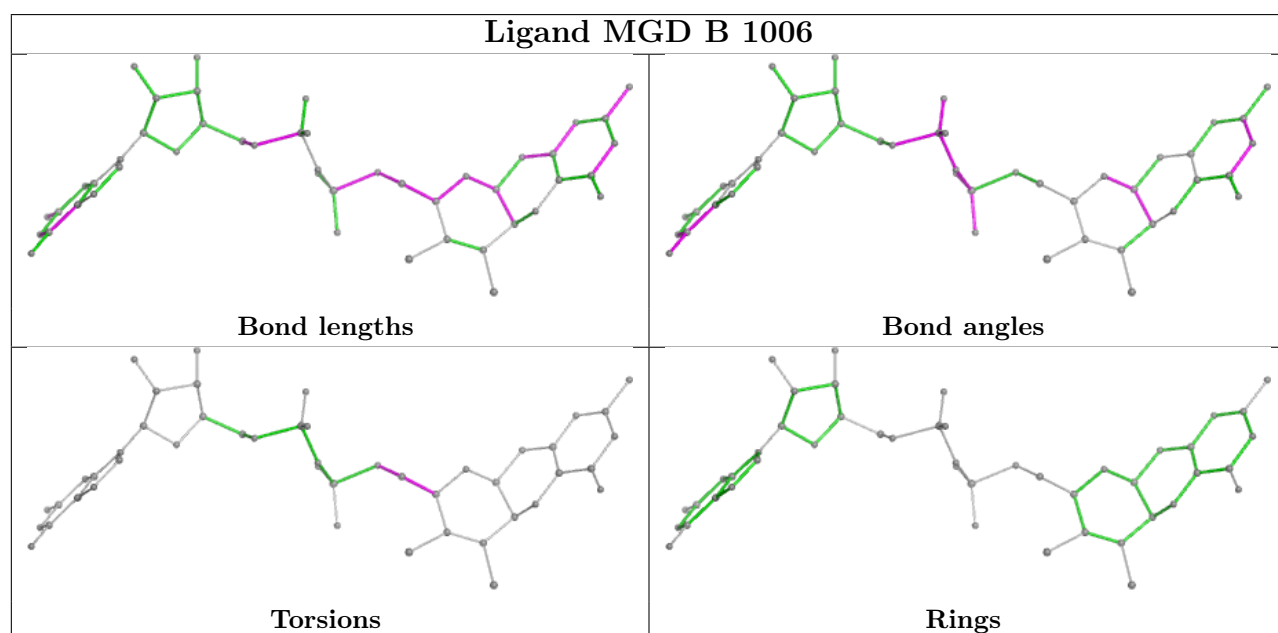
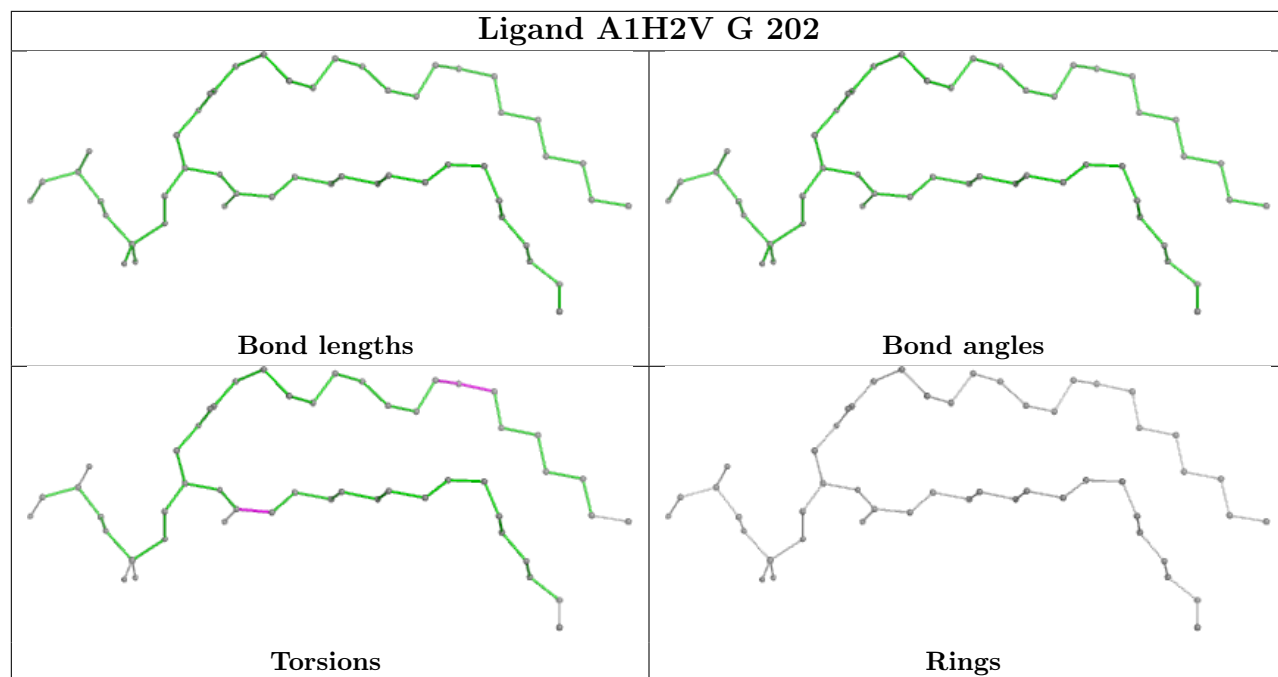
## Ligand MQ7 F 1010

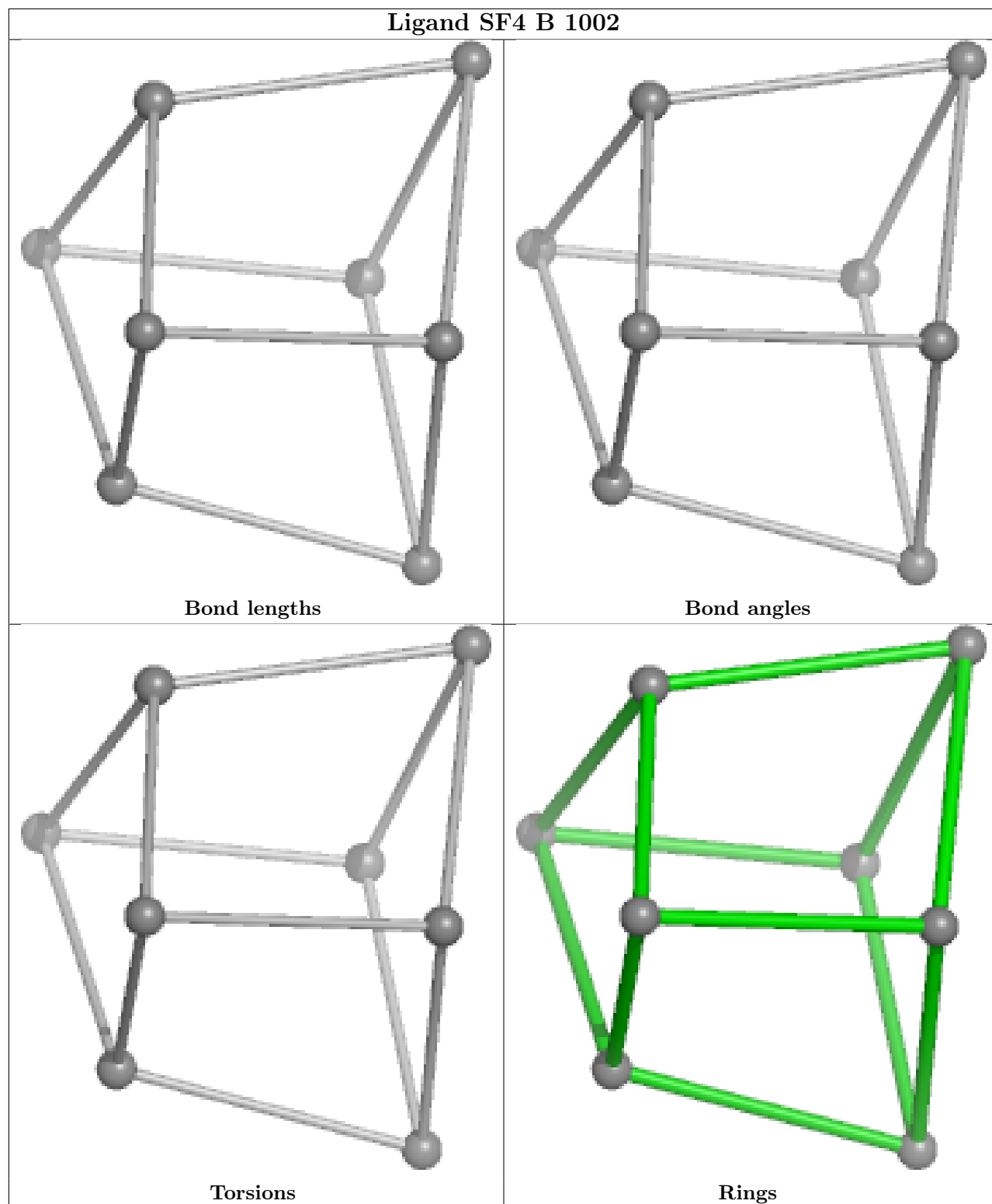




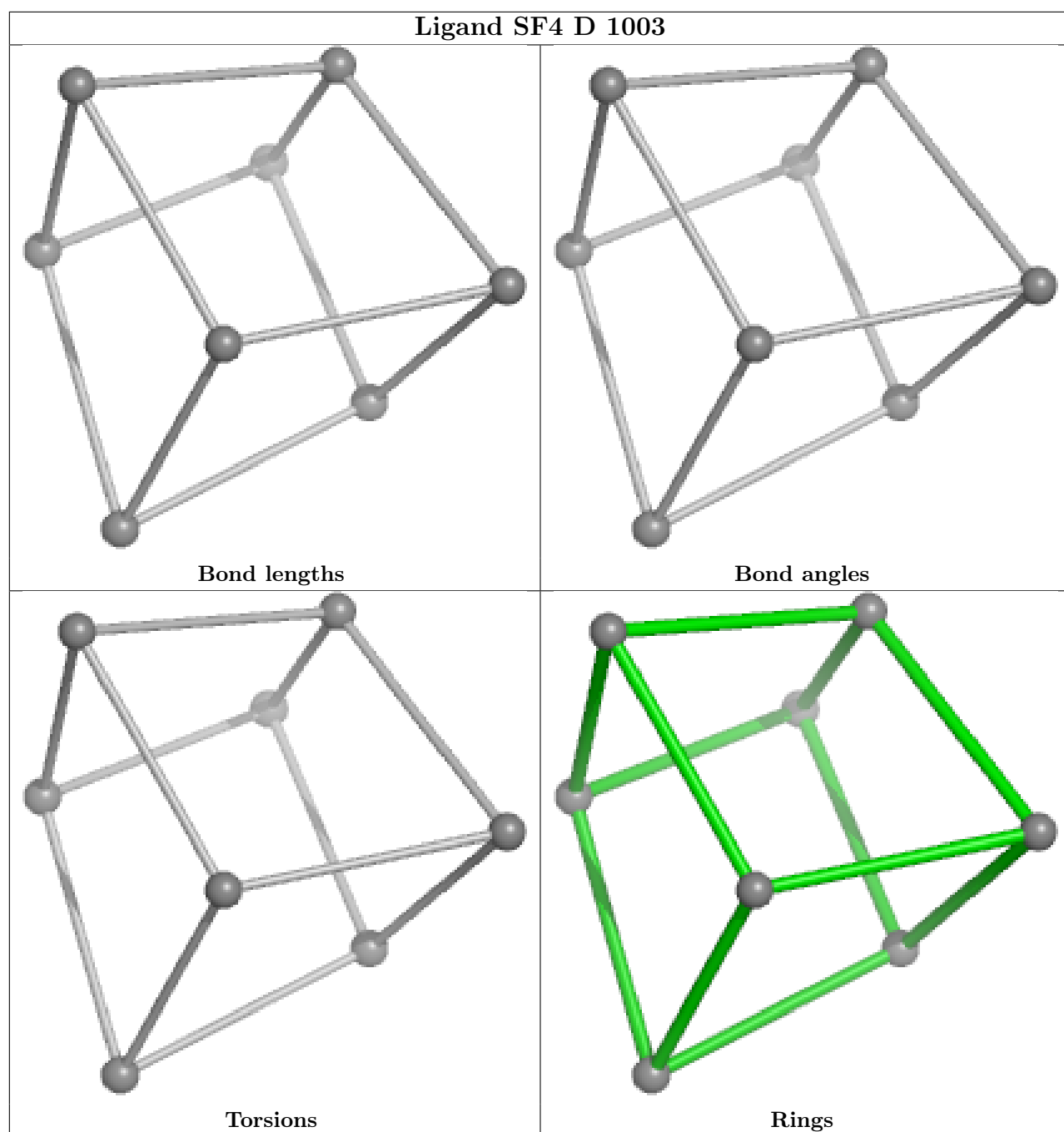


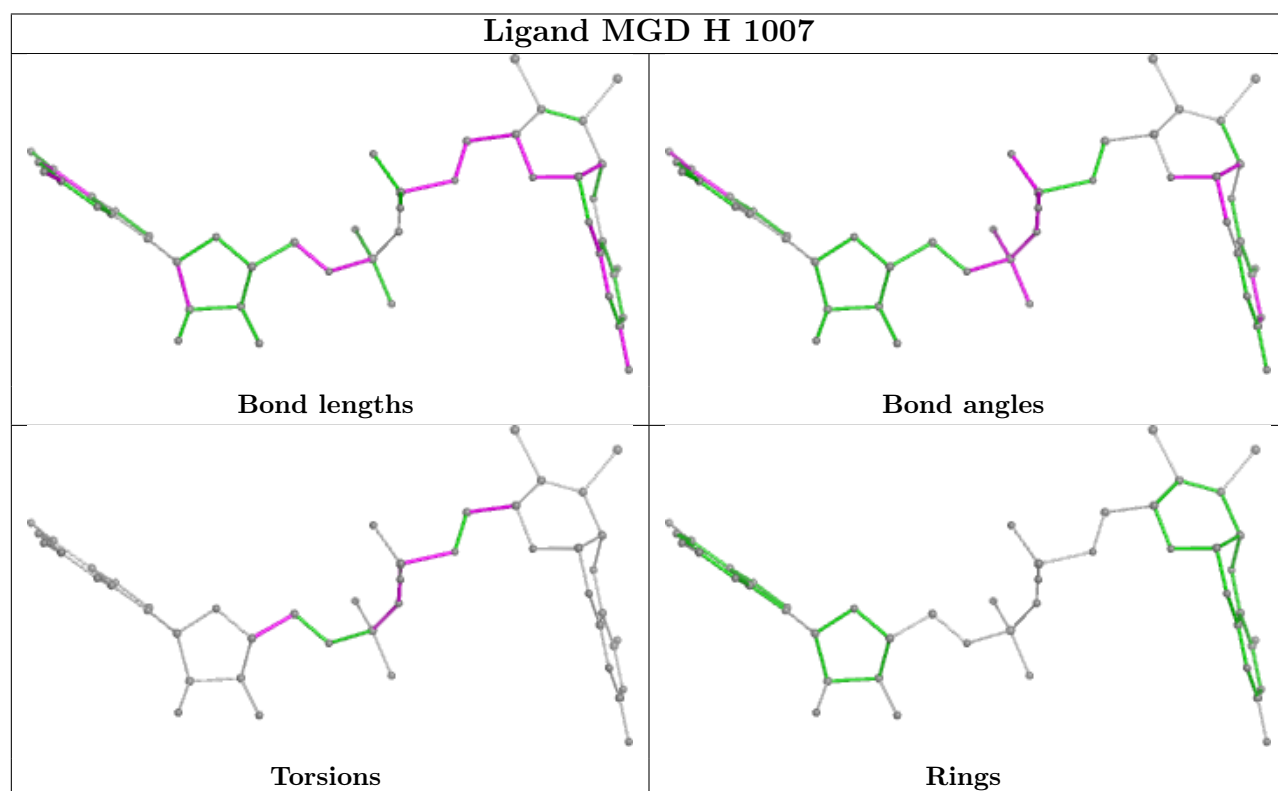
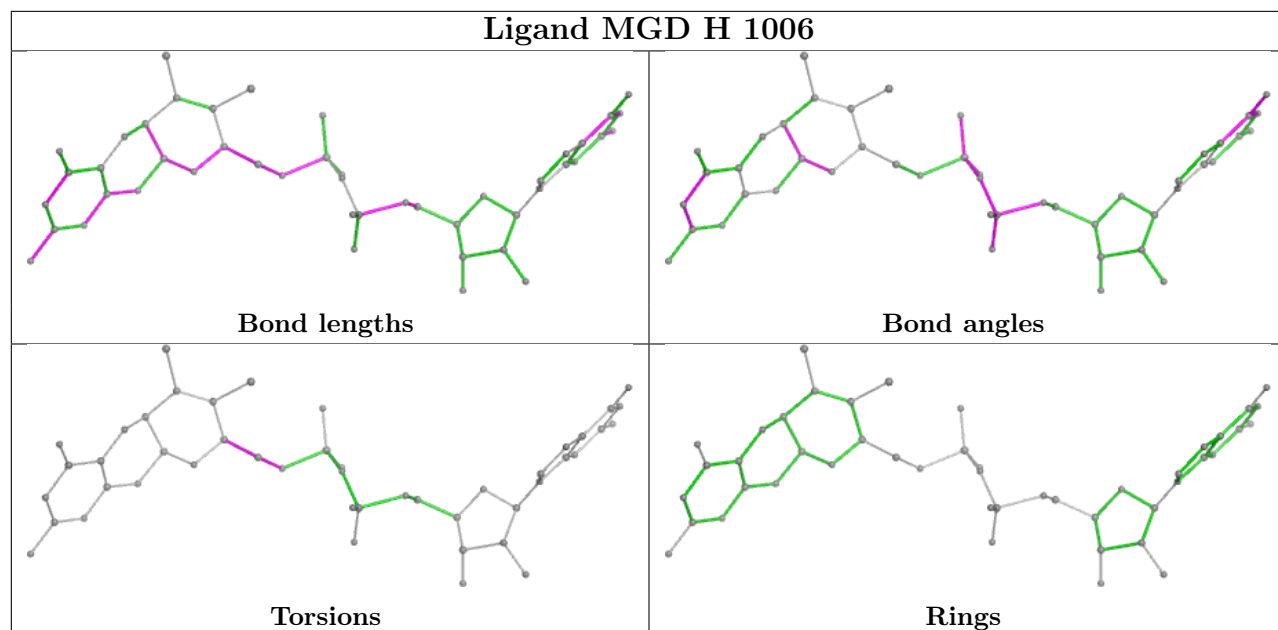


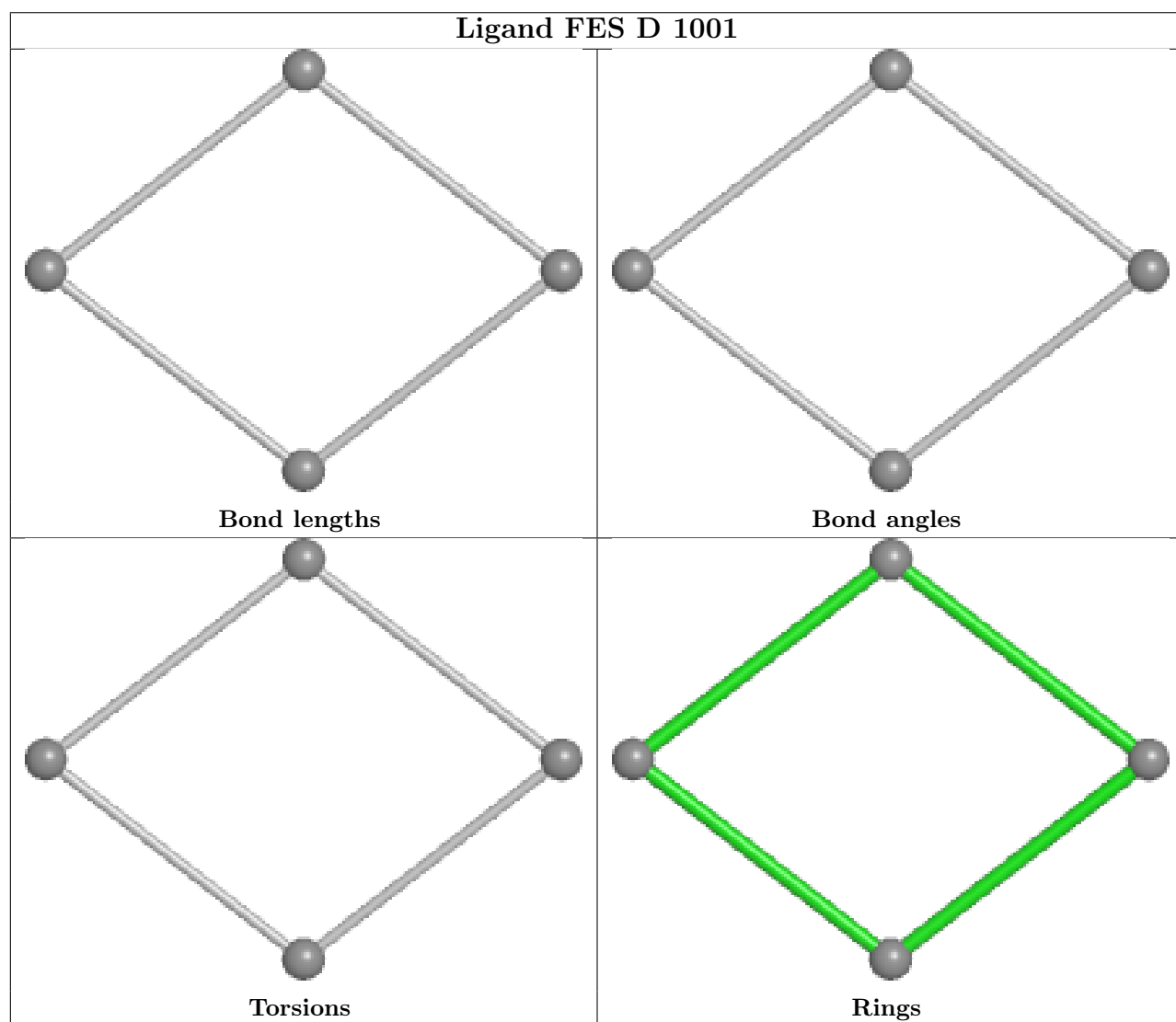
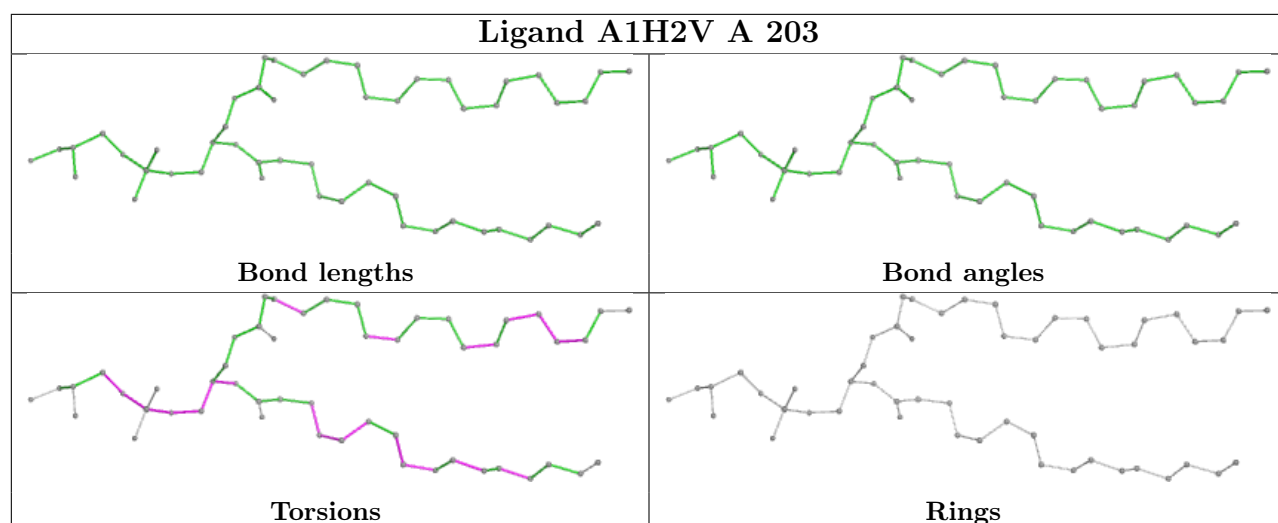


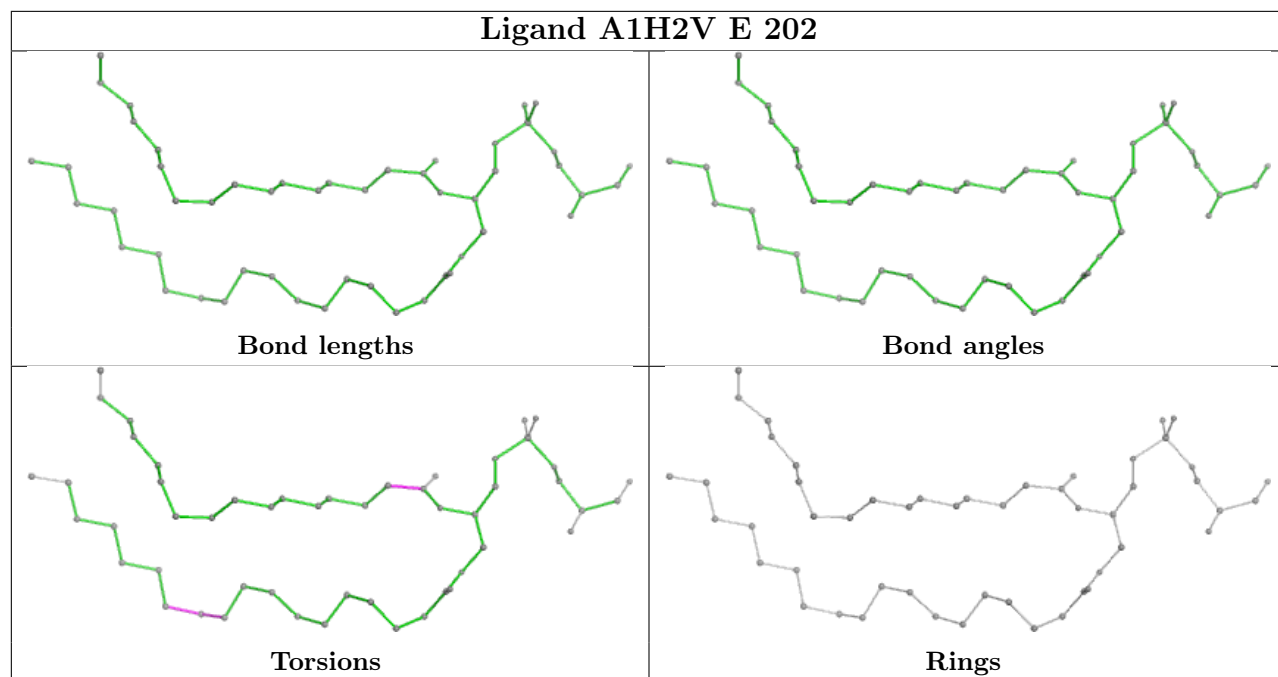


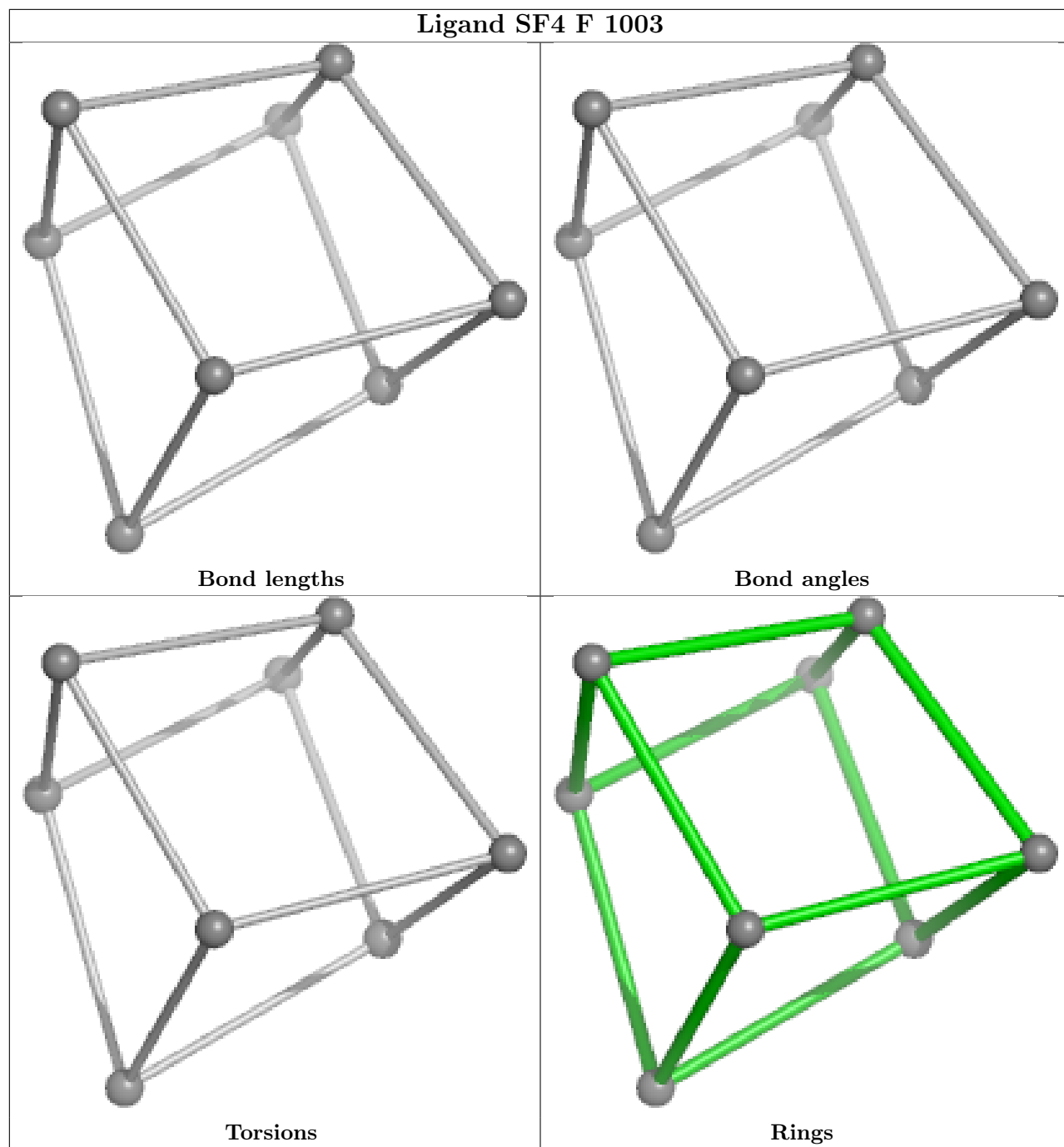


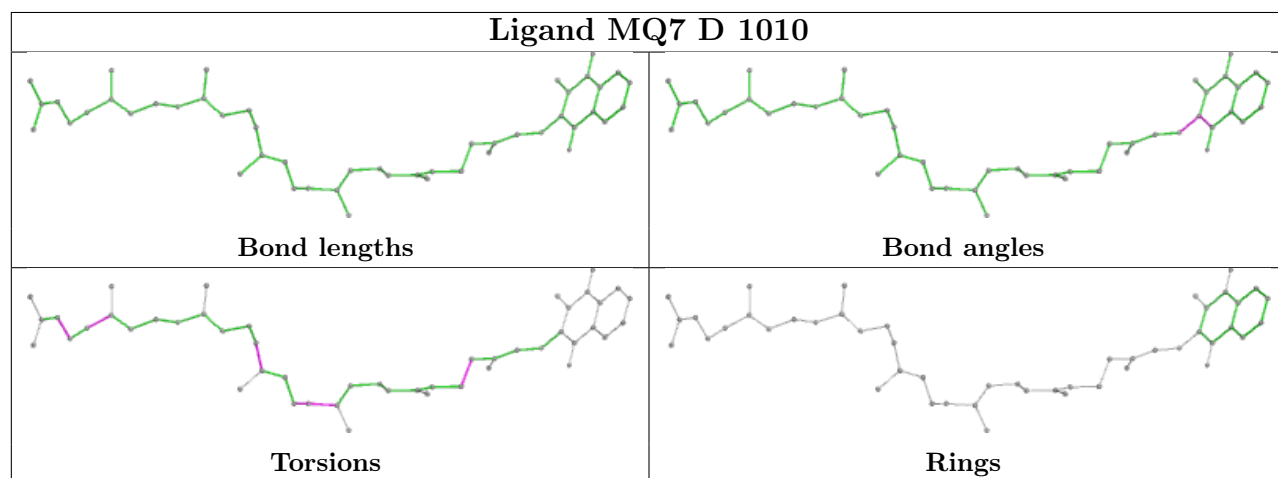
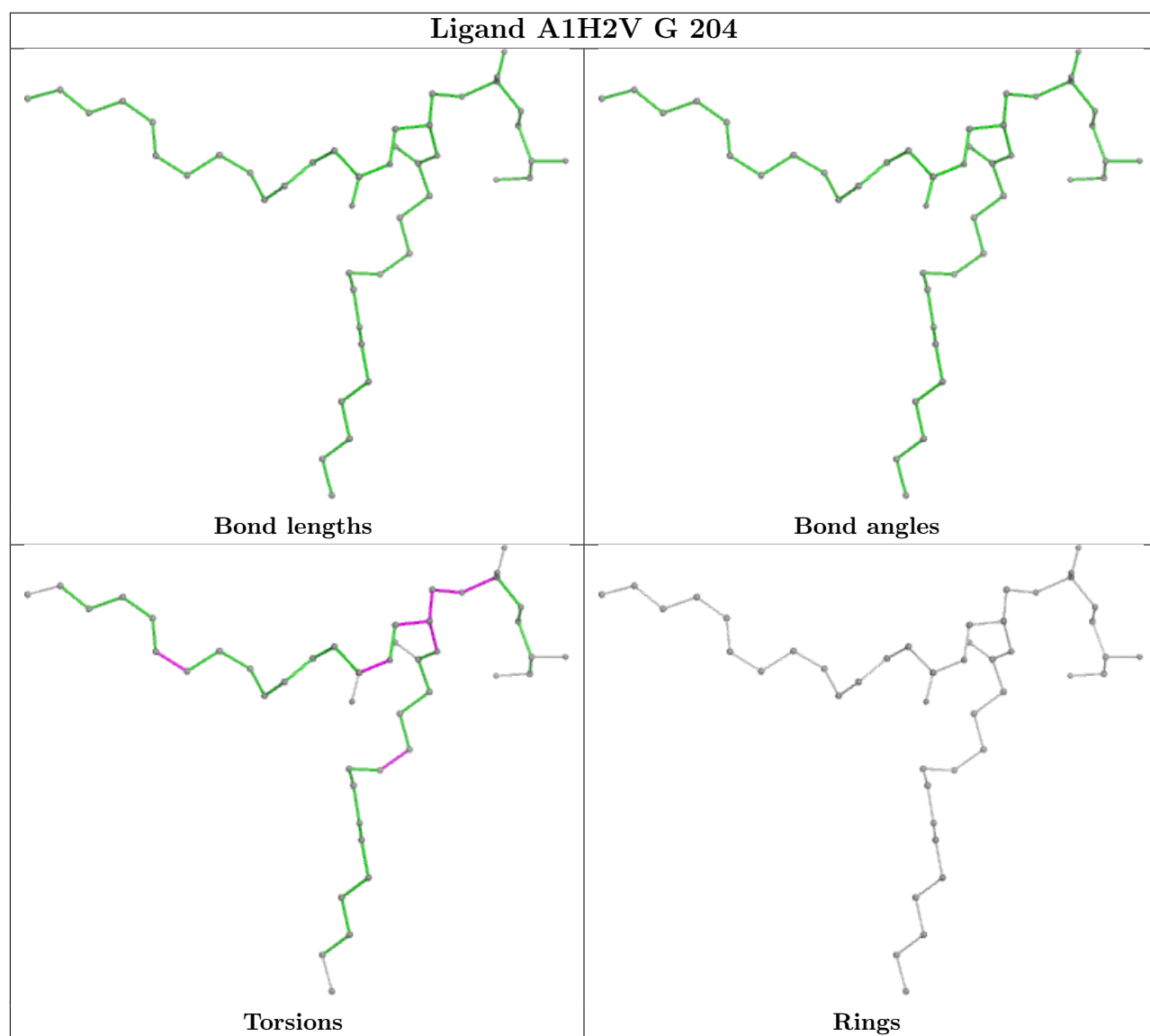


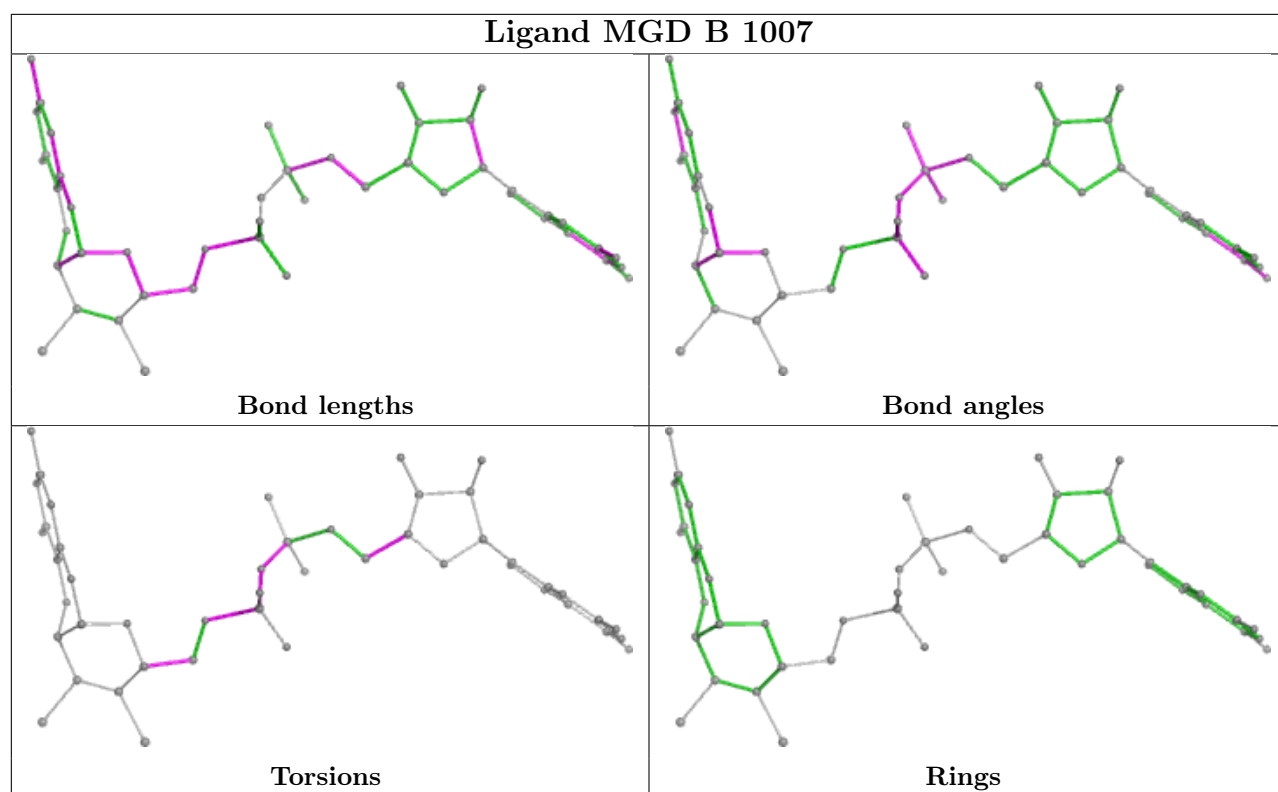


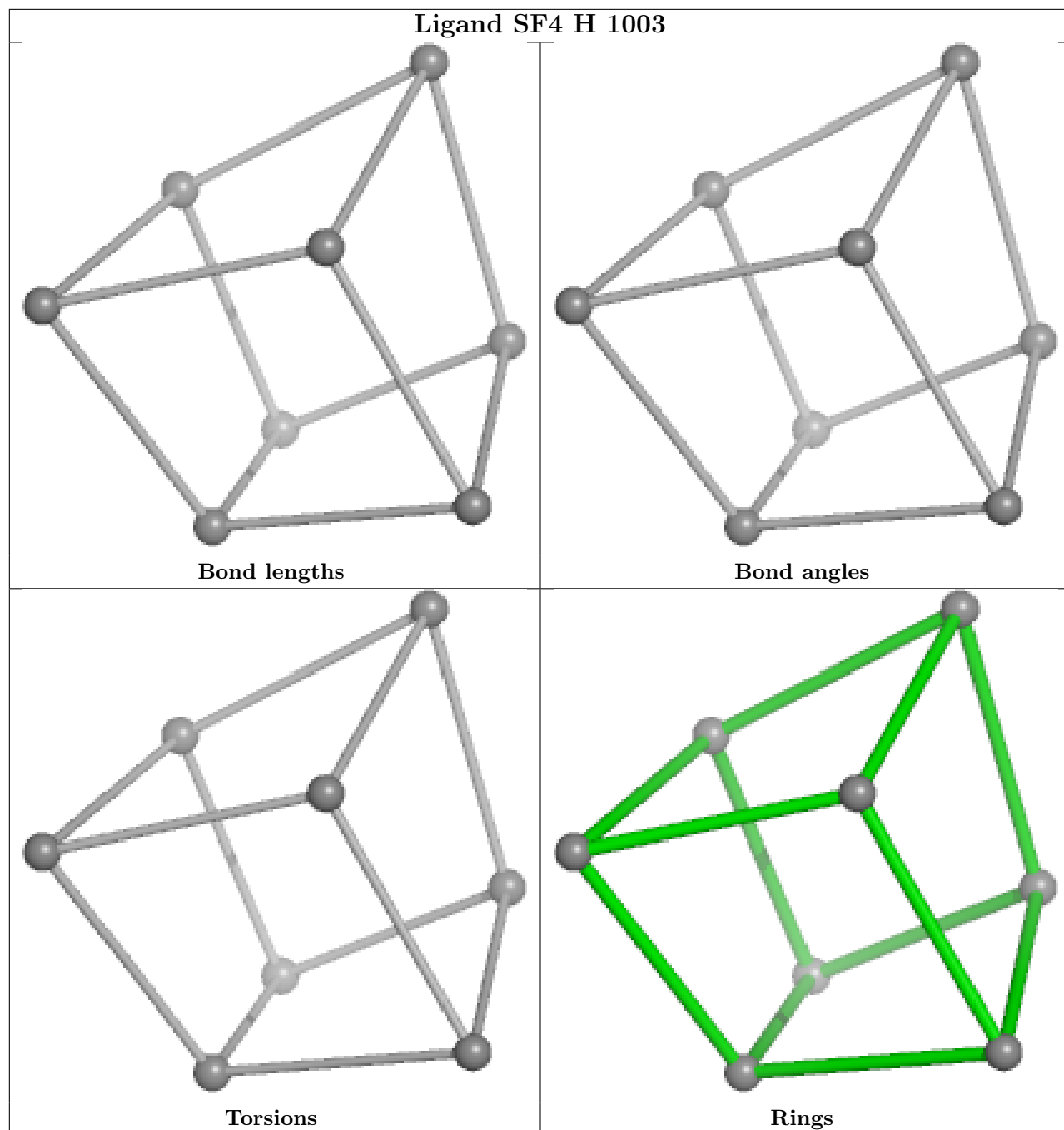




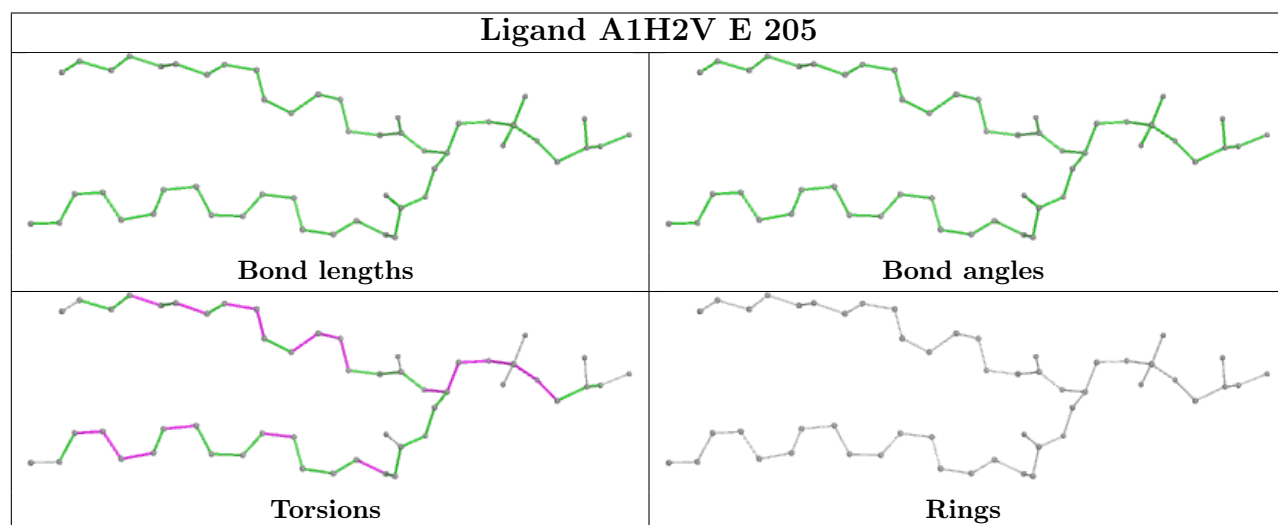
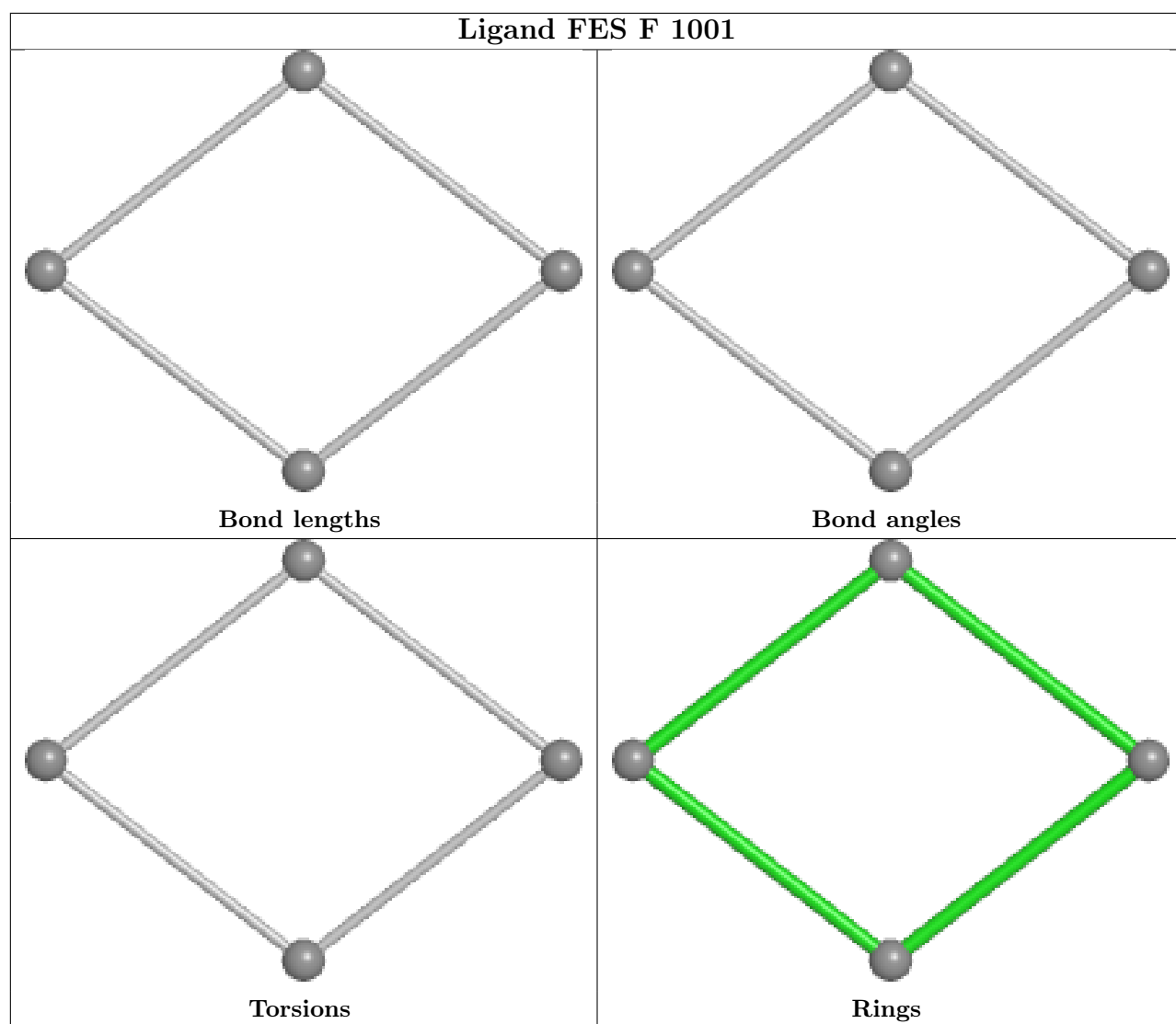


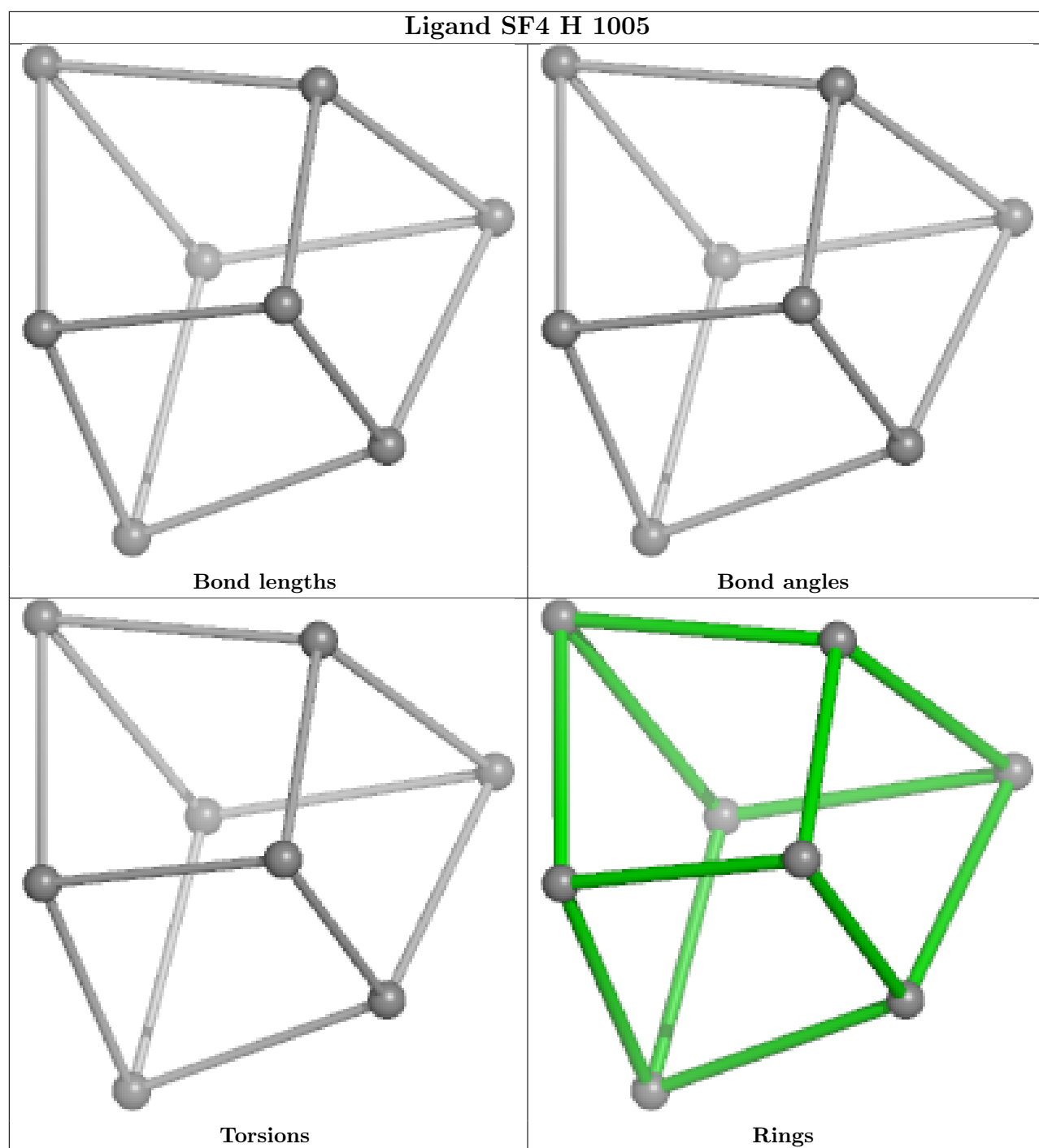












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

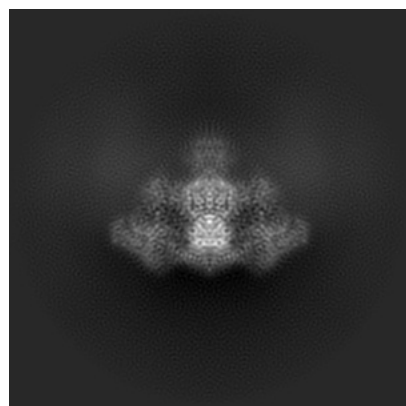
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19452. These allow visual inspection of the internal detail of the map and identification of artifacts.

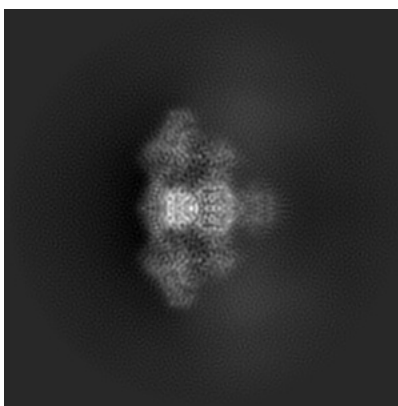
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

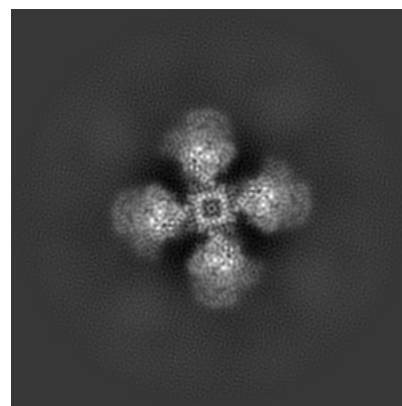
#### 6.1.1 Primary map



X

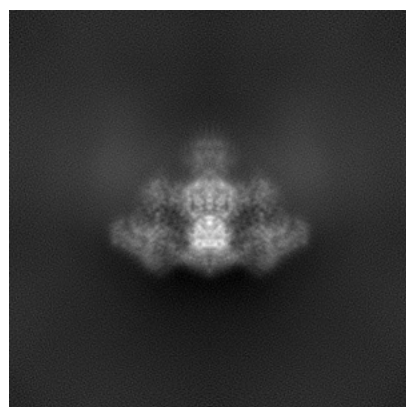


Y

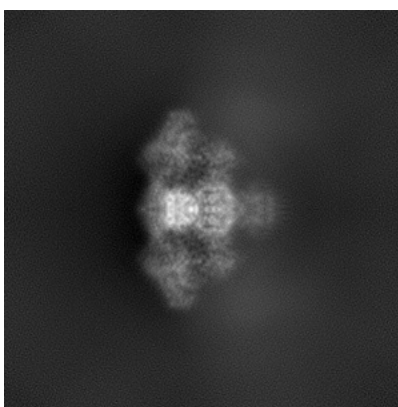


Z

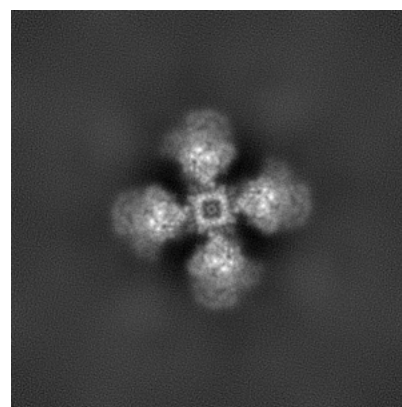
#### 6.1.2 Raw map



X



Y

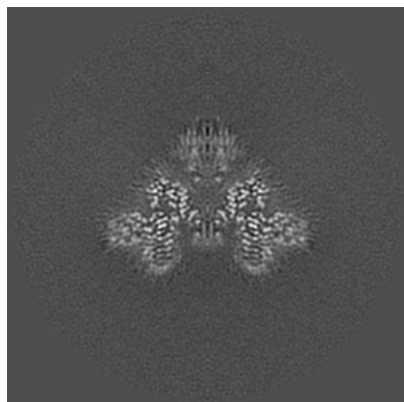


Z

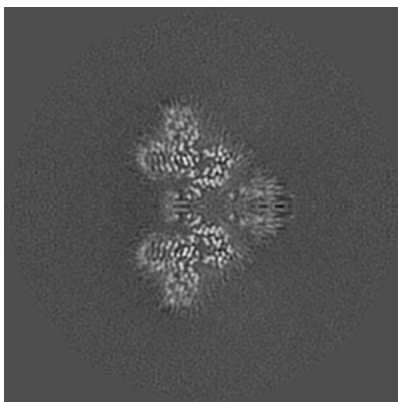
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

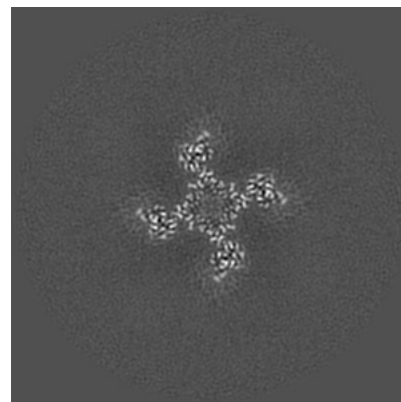
### 6.2.1 Primary map



X Index: 160

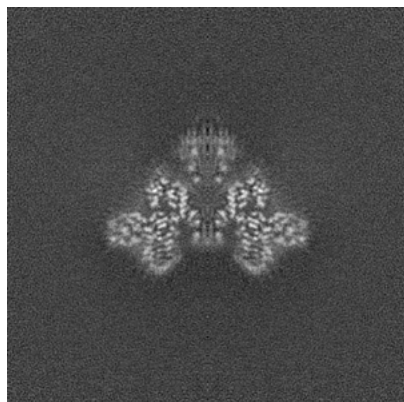


Y Index: 160

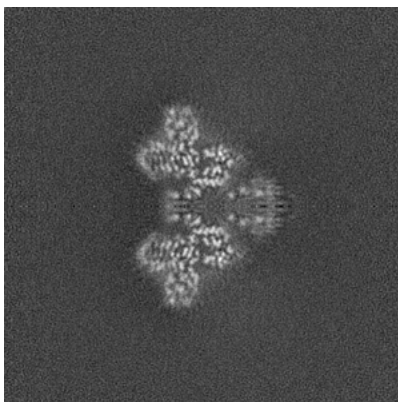


Z Index: 160

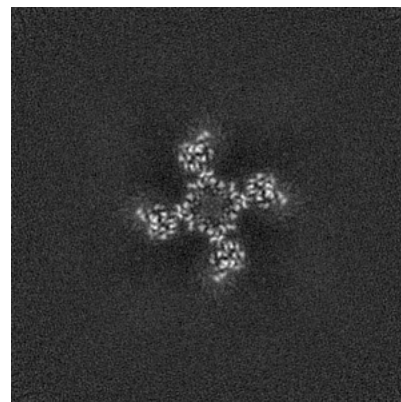
### 6.2.2 Raw map



X Index: 160



Y Index: 160

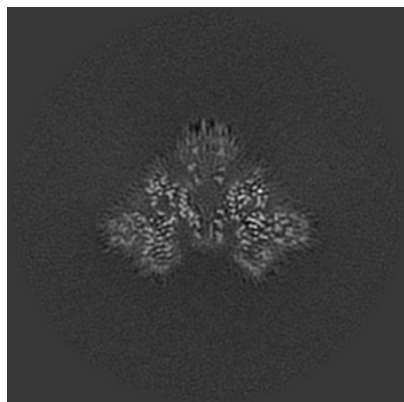


Z Index: 160

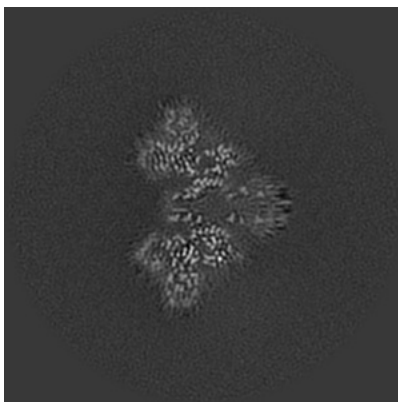
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

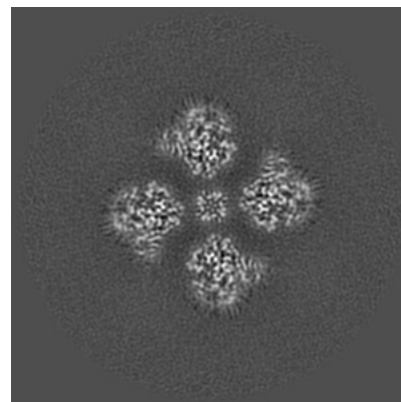
### 6.3.1 Primary map



X Index: 159

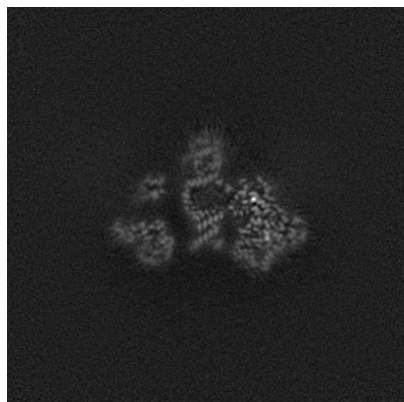


Y Index: 159

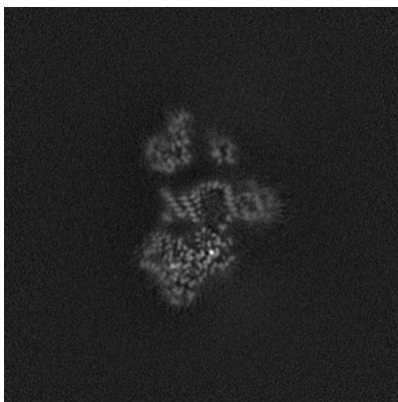


Z Index: 139

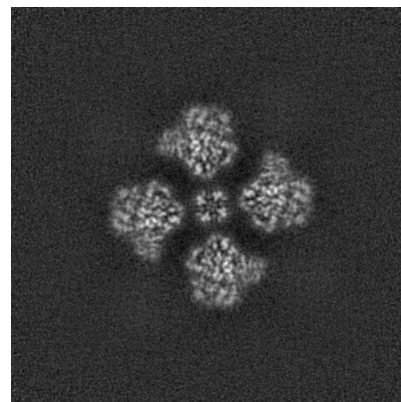
### 6.3.2 Raw map



X Index: 150



Y Index: 150

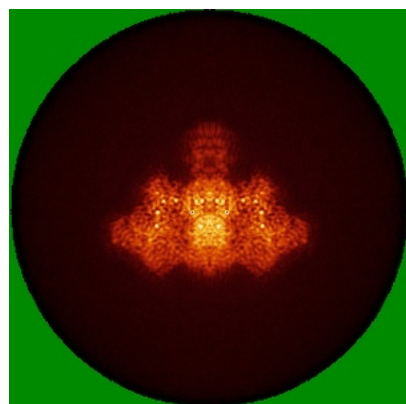


Z Index: 140

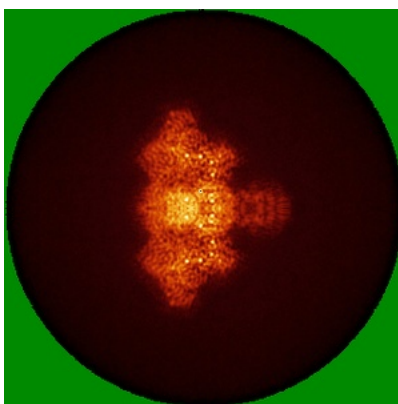
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

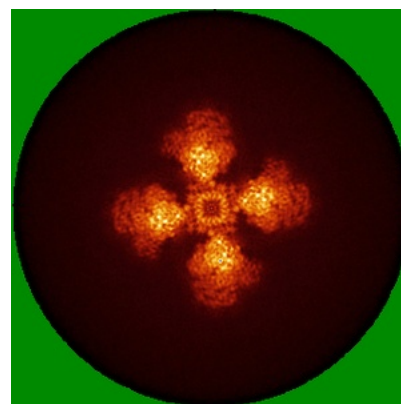
### 6.4.1 Primary map



X

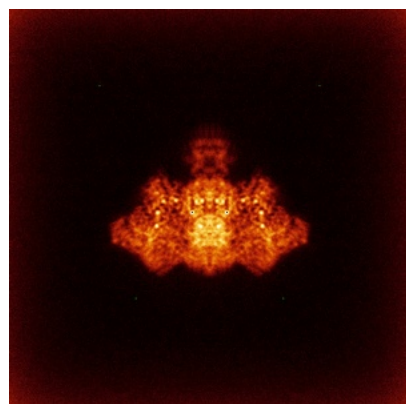


Y

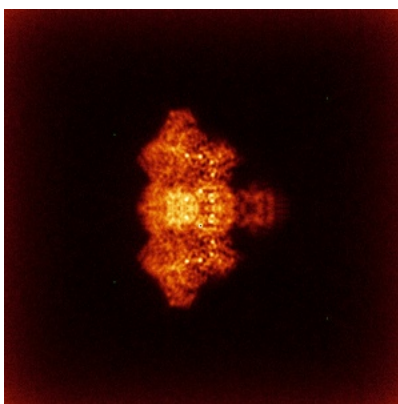


Z

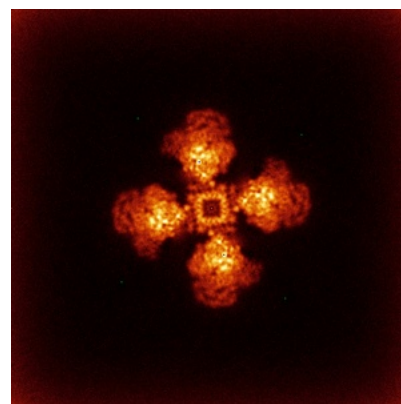
### 6.4.2 Raw map



X



Y



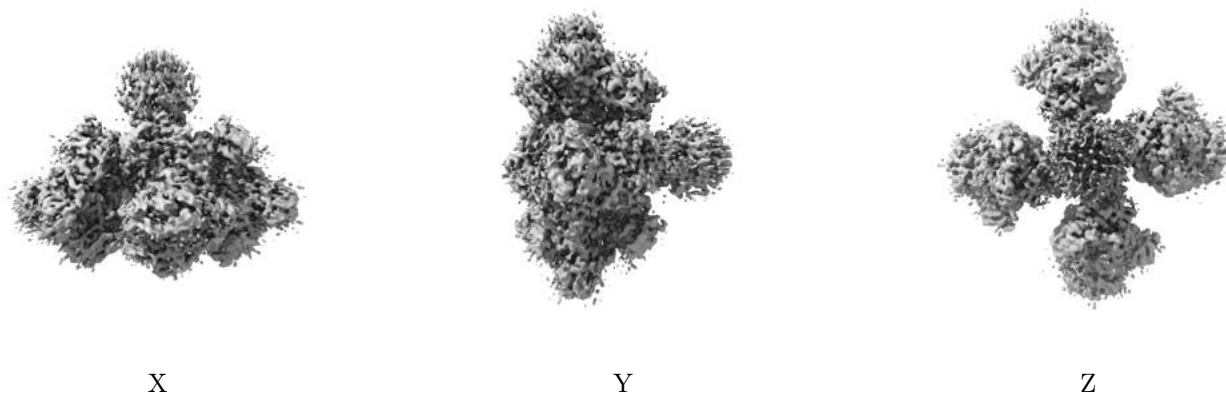
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



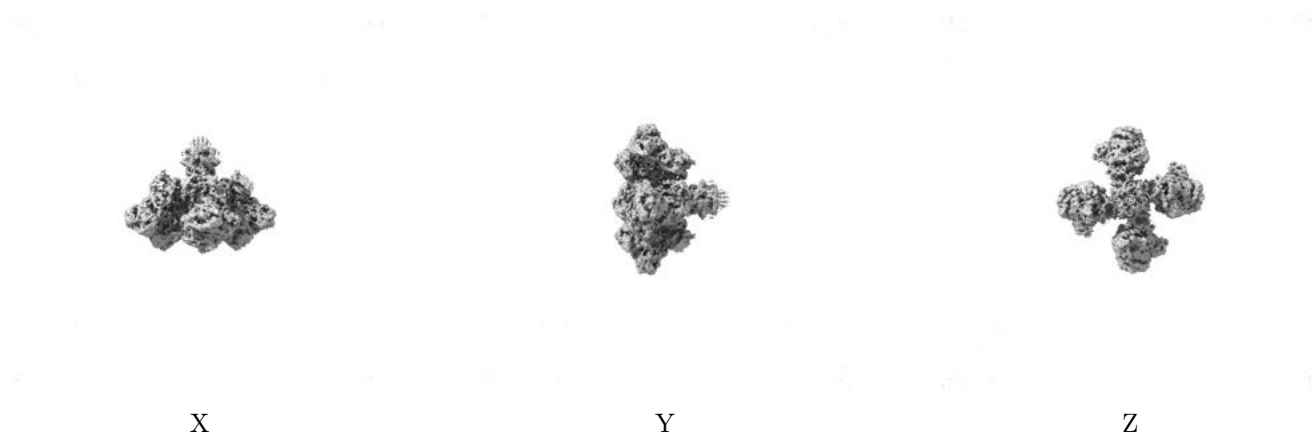
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

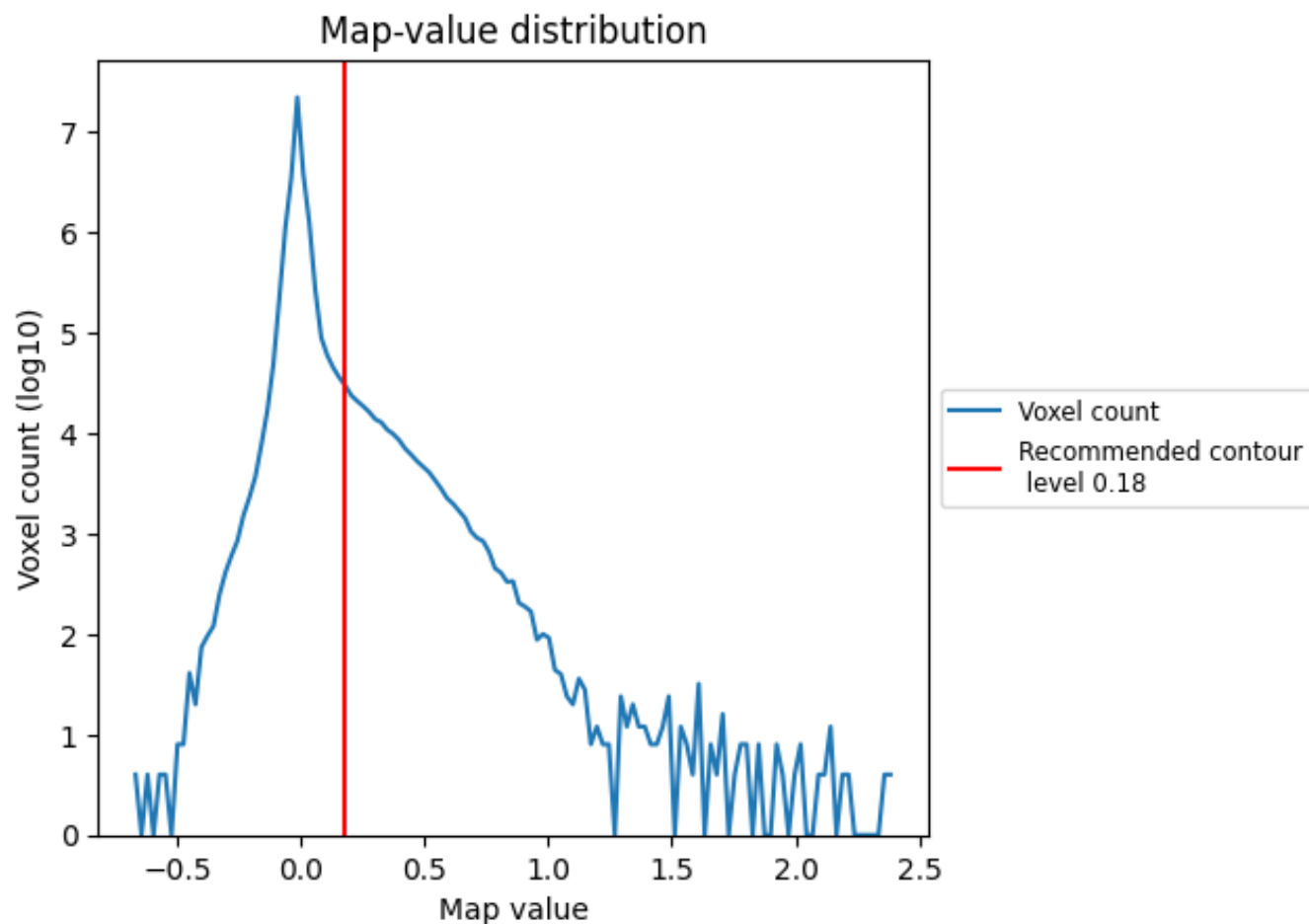
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

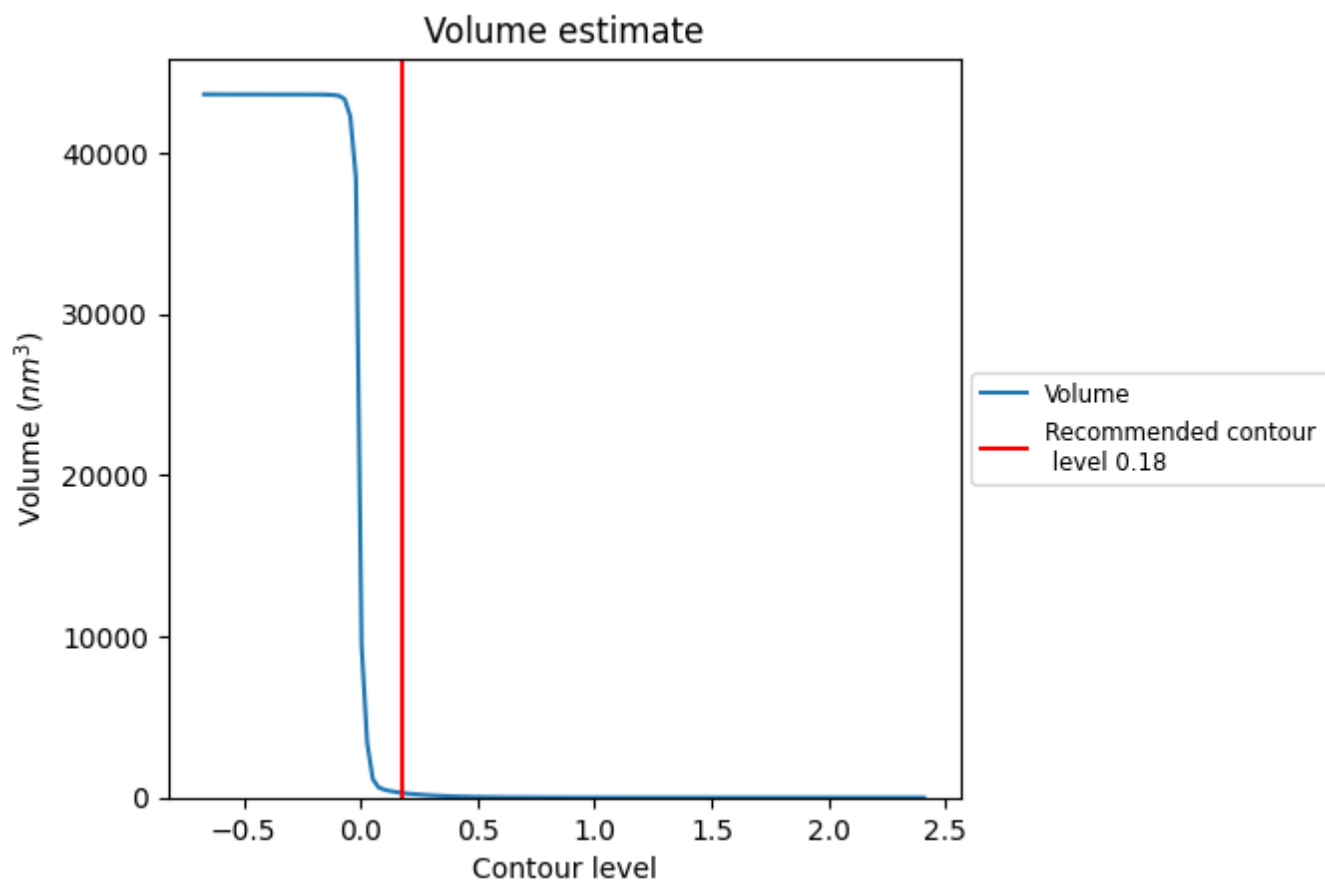
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



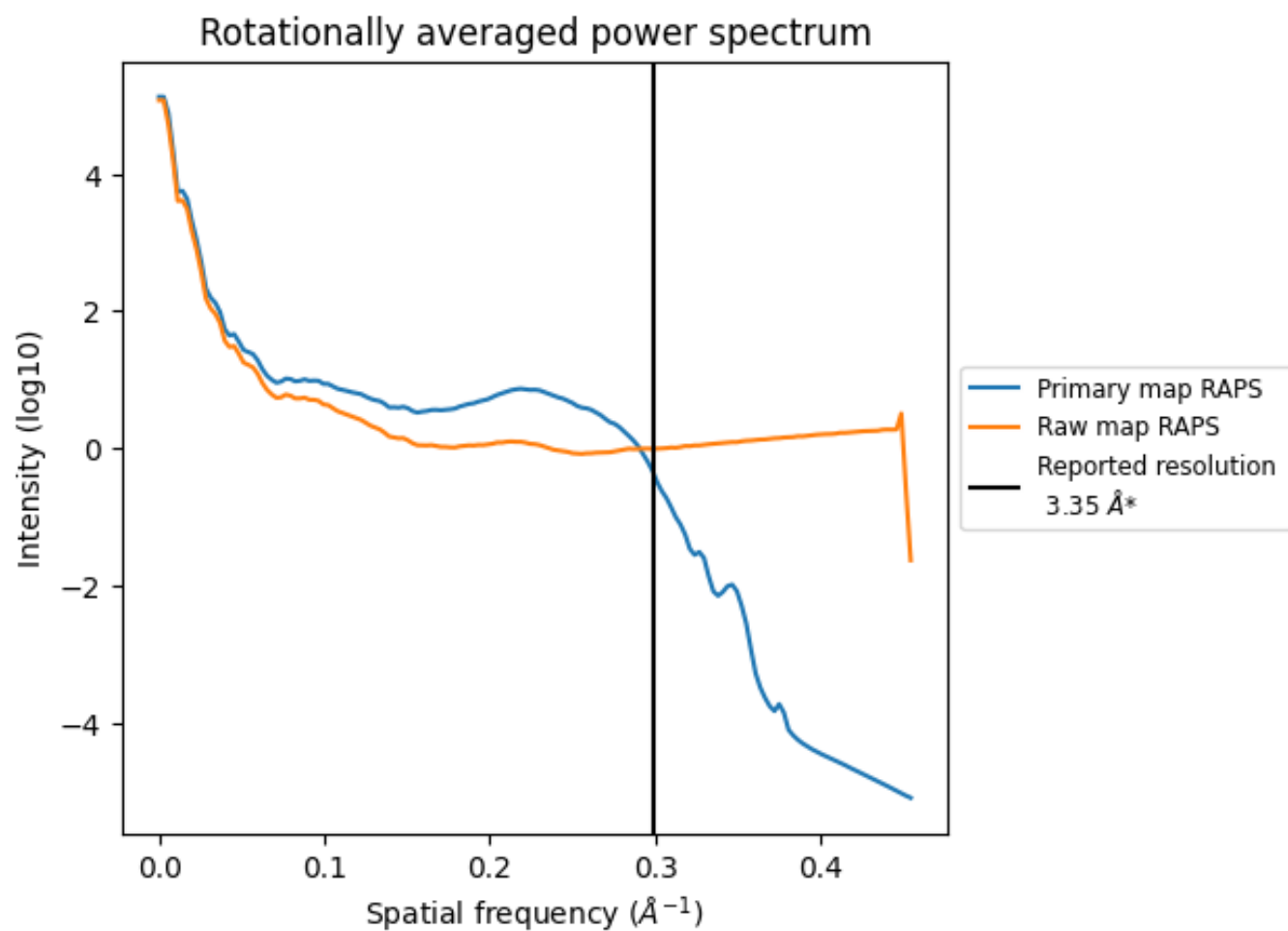
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282  $\text{nm}^3$ ; this corresponds to an approximate mass of 254 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

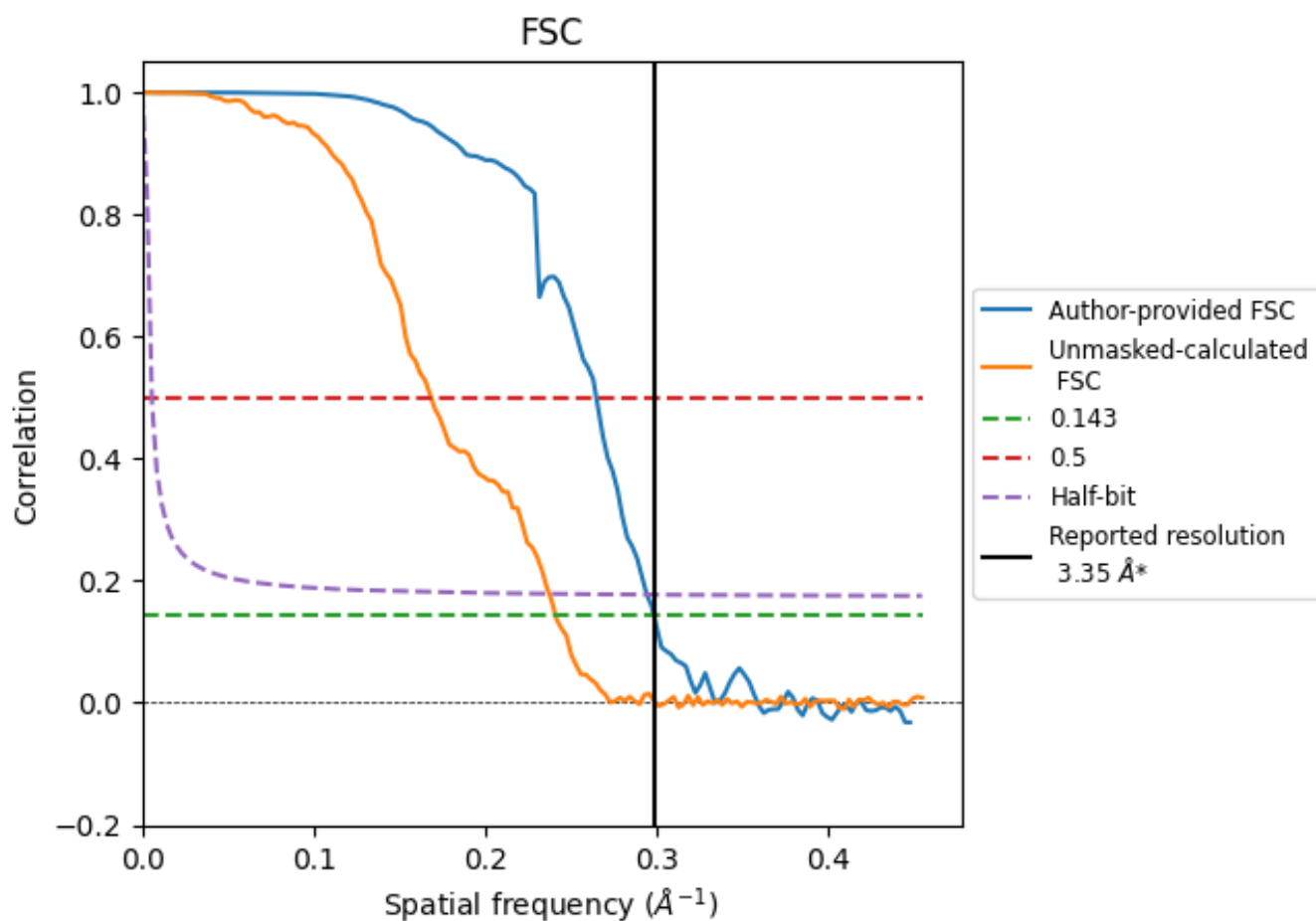


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.299  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

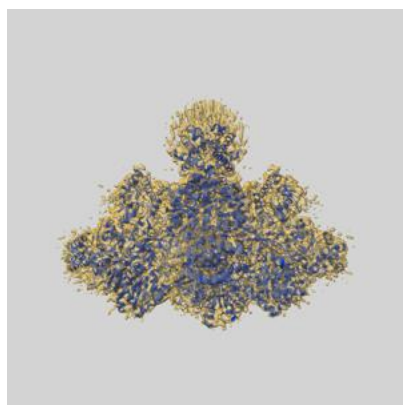
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.40
Unmasked-calculated*	4.15	5.94	4.22

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.35 by more than 10 %

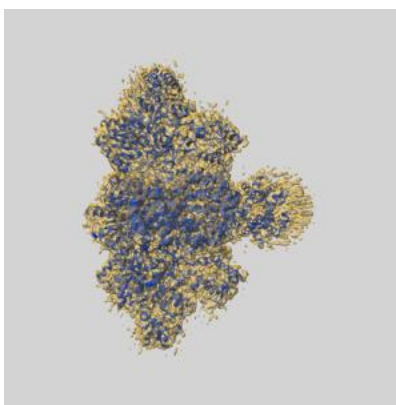
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19452 and PDB model 8RR0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

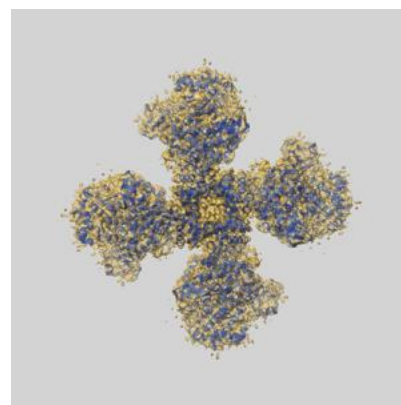
### 9.1 Map-model overlay [i](#)



X



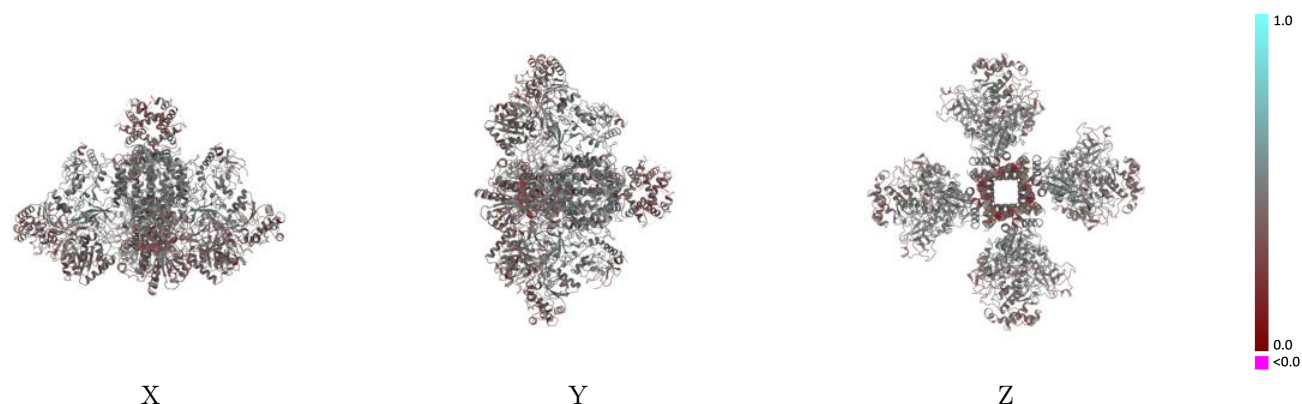
Y



Z

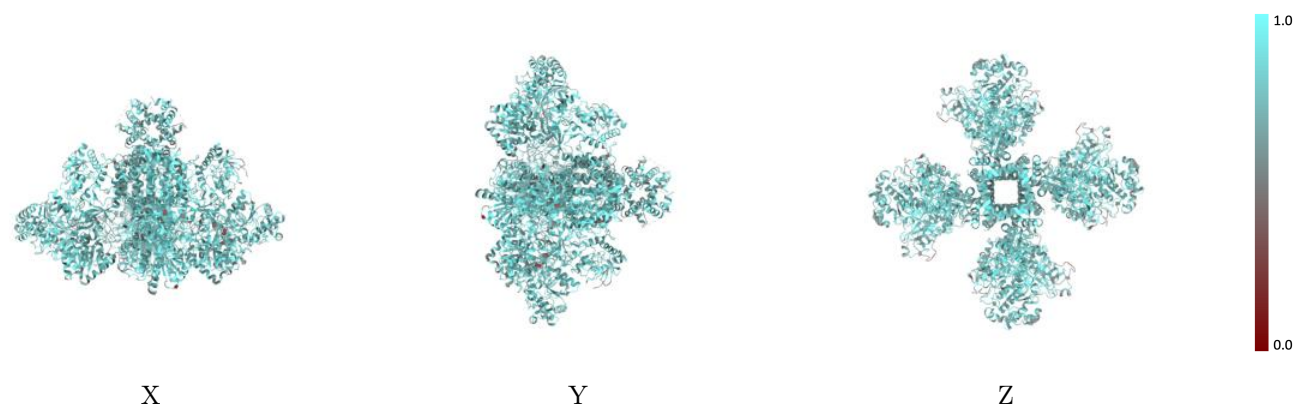
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



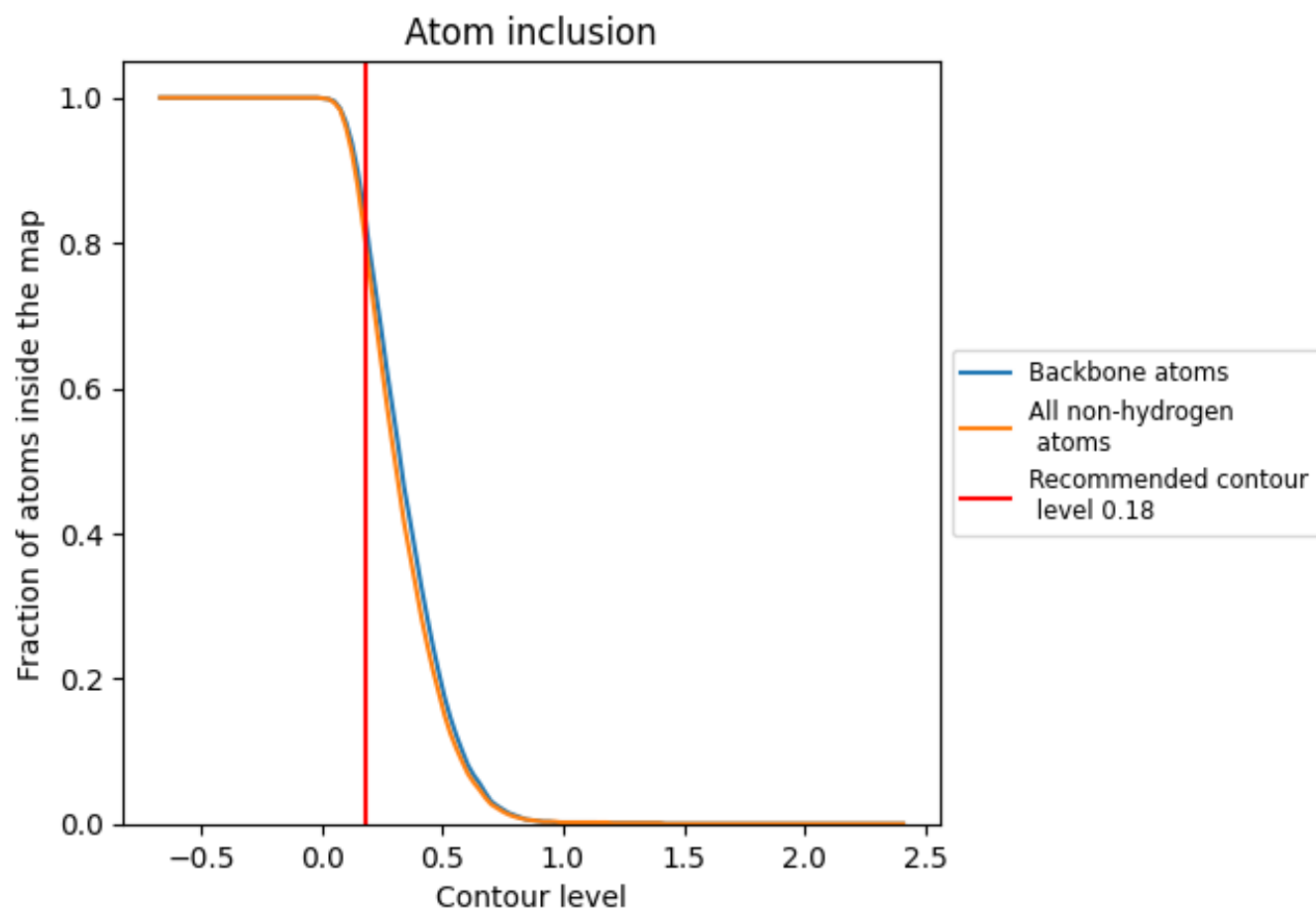
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8040	<div><div></div></div> 0.4440
A	<div><div></div></div> 0.7150	<div><div></div></div> 0.4420
B	<div><div></div></div> 0.8240	<div><div></div></div> 0.4440
C	<div><div></div></div> 0.7150	<div><div></div></div> 0.4450
D	<div><div></div></div> 0.8240	<div><div></div></div> 0.4450
E	<div><div></div></div> 0.7150	<div><div></div></div> 0.4440
F	<div><div></div></div> 0.8240	<div><div></div></div> 0.4440
G	<div><div></div></div> 0.7140	<div><div></div></div> 0.4420
H	<div><div></div></div> 0.8240	<div><div></div></div> 0.4430

1.0

0.0

<0.0