



## wwPDB EM Validation Summary Report ⓘ

Apr 27, 2026 – 02:19 pm BST

PDB ID : 9TAJ / pdb\_00009taj  
EMDB ID : EMD-55748  
Title : E. coli Complex I WT purified in LMNG  
Authors : Kovalova, T.; Beghiah, A.; Kaila, V.R.I.  
Deposited on : 2025-11-18  
Resolution : 3.00 Å(reported)

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.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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)  
Validation Pipeline (wwPDB-VP) : 2.49

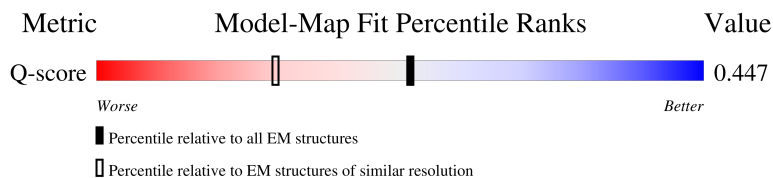
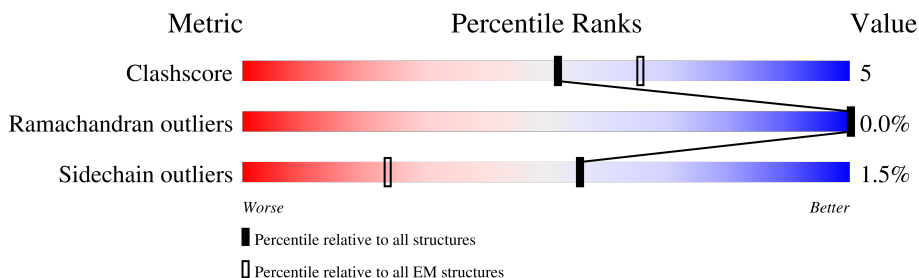
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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





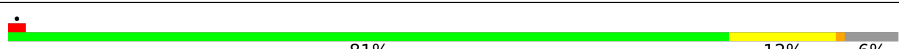
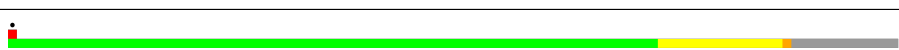

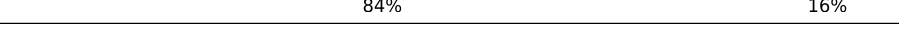
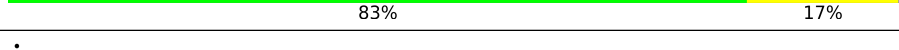

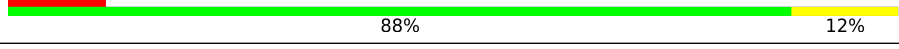
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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	E	166	
2	F	461	
3	G	910	
4	I	180	

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Mol	Chain	Length	Quality of chain
5	B	220	
6	C	600	
7	H	325	
8	J	184	
9	K	100	
10	M	509	
11	A	147	
12	L	613	
13	N	485	

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
17	SF4	B	301	-	-	X	-

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 38186 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 NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	156	Total	C	N	O	S	0	0
			1220	768	215	229	8		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	439	Total	C	N	O	S	0	0
			3407	2162	596	629	20		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	MET	-	initiating methionine	UNP P31979
F	-14	ARG	-	expression tag	UNP P31979
F	-13	GLY	-	expression tag	UNP P31979
F	-12	SER	-	expression tag	UNP P31979
F	-11	HIS	-	expression tag	UNP P31979
F	-10	HIS	-	expression tag	UNP P31979
F	-9	HIS	-	expression tag	UNP P31979
F	-8	HIS	-	expression tag	UNP P31979
F	-7	HIS	-	expression tag	UNP P31979
F	-6	HIS	-	expression tag	UNP P31979
F	-5	THR	-	expression tag	UNP P31979
F	-4	ASP	-	expression tag	UNP P31979
F	-3	PRO	-	expression tag	UNP P31979
F	-2	ALA	-	expression tag	UNP P31979
F	-1	LEU	-	expression tag	UNP P31979
F	0	ARG	-	expression tag	UNP P31979
F	1	ALA	-	expression tag	UNP P31979

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	905	Total	C	N	O	S	0	0
			7027	4392	1269	1329	37		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P33602
G	2	LEU	-	expression tag	UNP P33602

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	145	Total	C	N	O	S	0	0
			1149	728	192	217	12		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	195	Total	C	N	O	S	0	0
			1551	985	269	281	16		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	589	Total	C	N	O	S	0	0
			4760	3049	828	859	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P33599
C	2	VAL	-	expression tag	UNP P33599
C	3	ASN	-	expression tag	UNP P33599
C	4	ASN	-	expression tag	UNP P33599

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	307	Total	C	N	O	S	0	0
			2404	1614	373	399	18		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	504	Total	C	N	O	S	1	0
			3964	2671	618	646	29		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	98	Total	C	N	O	S	0	0
			788	543	120	121	4		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	613	Total	C	N	O	S	0	0
			4685	3113	753	787	32		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	485	Total	C	N	O	S	0	0
			3673	2448	582	623	20		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

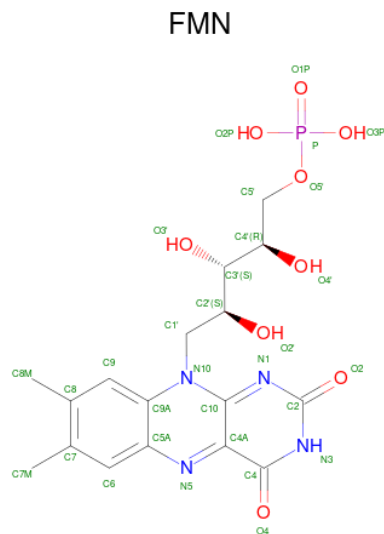


Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	Fe	S	0
			4	2	2	
14	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

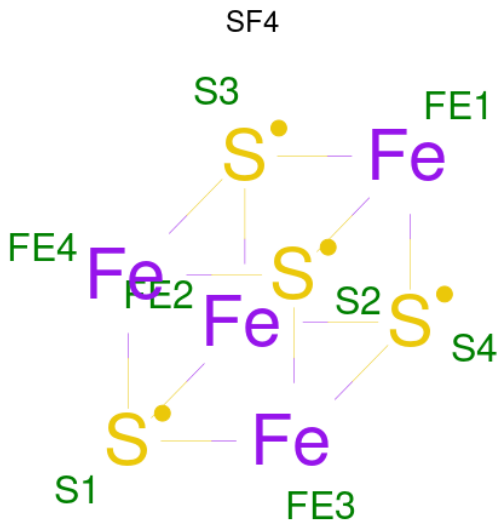
Mol	Chain	Residues	Atoms		AltConf
15	E	1	Total	Ca	0
			1	1	
15	G	3	Total	Ca	0
			3	3	
15	I	1	Total	Ca	0
			1	1	

- Molecule 16 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 17 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
17	F	1	Total 8	Fe 4	S 4	0
17	G	1	Total 8	Fe 4	S 4	0

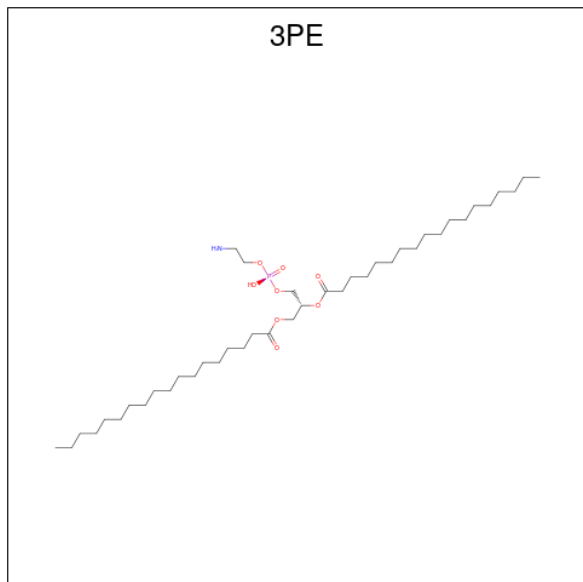
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Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	I	1	Total	Fe	S	0
			8	4	4	
17	I	1	Total	Fe	S	0
			8	4	4	
17	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



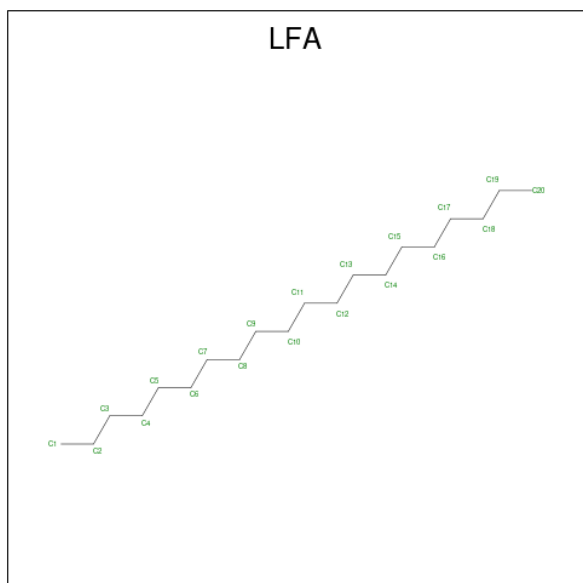
Mol	Chain	Residues	Atoms					AltConf
18	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	M	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	M	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 19 is EICOSANE (CCD ID: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



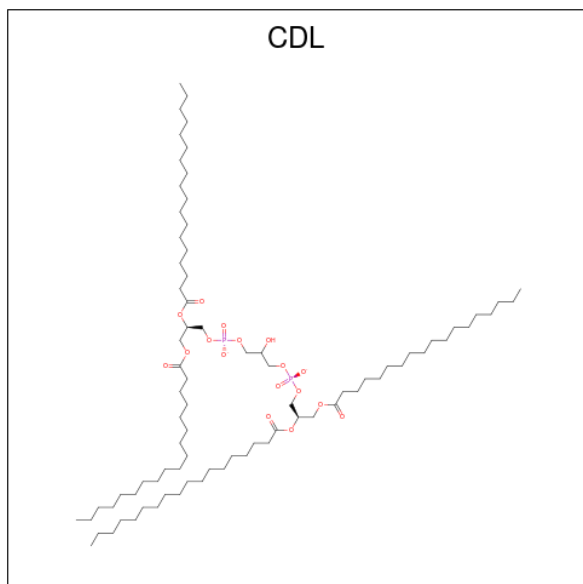
Mol	Chain	Residues	Atoms		AltConf
19	H	1	Total	C	0
			20	20	

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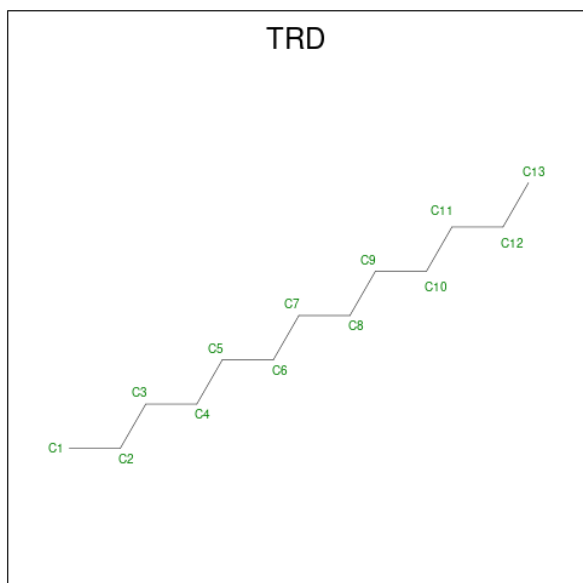
Mol	Chain	Residues	Atoms		AltConf
19	N	1	Total	C	0
			20	20	

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



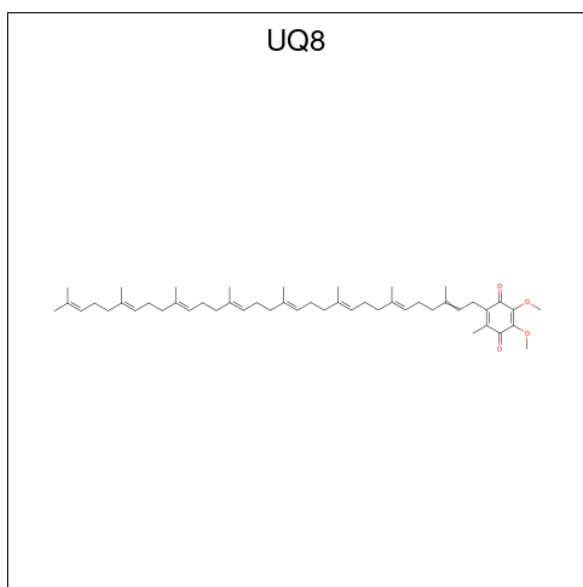
Mol	Chain	Residues	Atoms				AltConf
20	L	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 21 is TRIDECANE (CCD ID: TRD) (formula:  $C_{13}H_{28}$ ).



Mol	Chain	Residues	Atoms		AltConf
21	L	1	Total	C	0
			13	13	
21	L	1	Total	C	0
			13	13	
21	N	1	Total	C	0
			13	13	

- Molecule 22 is Ubiquinone-8 (CCD ID: UQ8) (formula:  $C_{49}H_{74}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	N	1	Total	C	O	0
			53	49	4	
22	N	1	Total	C	O	0
			53	49	4	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	E	5	Total	O	0
			5	5	
23	F	42	Total	O	0
			42	42	
23	G	138	Total	O	0
			138	138	
23	I	18	Total	O	0
			18	18	

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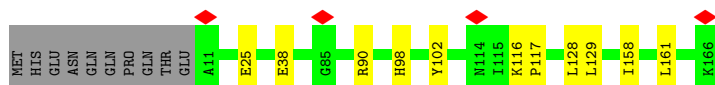
Mol	Chain	Residues	Atoms		AltConf
23	B	6	Total 6	O 6	0
23	C	53	Total 53	O 53	0
23	H	22	Total 22	O 22	0
23	J	8	Total 8	O 8	0
23	K	10	Total 10	O 10	0
23	M	40	Total 40	O 40	0
23	A	6	Total 6	O 6	0
23	L	44	Total 44	O 44	0
23	N	36	Total 36	O 36	0

### 3 Residue-property plots


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

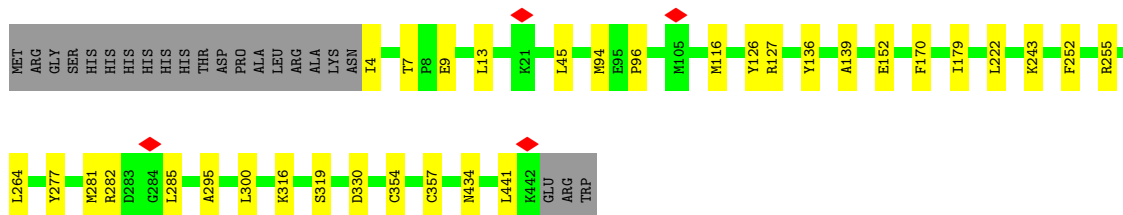
- Molecule 1: NADH-quinone oxidoreductase subunit E

Chain E: 




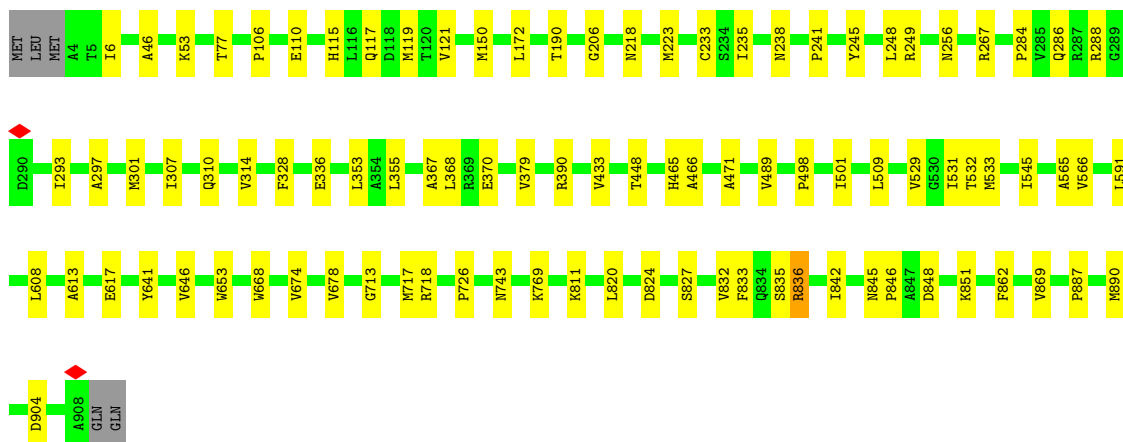
- Molecule 2: NADH-quinone oxidoreductase subunit F

Chain F: 



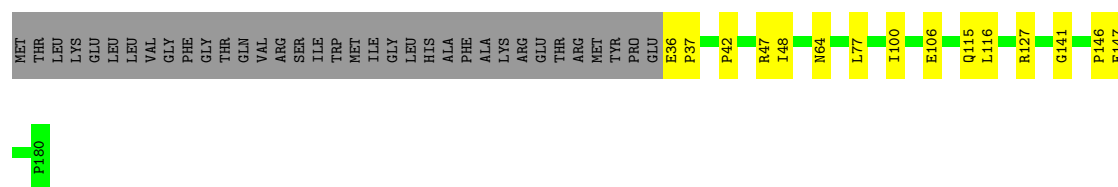
- Molecule 3: NADH-quinone oxidoreductase subunit G

Chain G: 



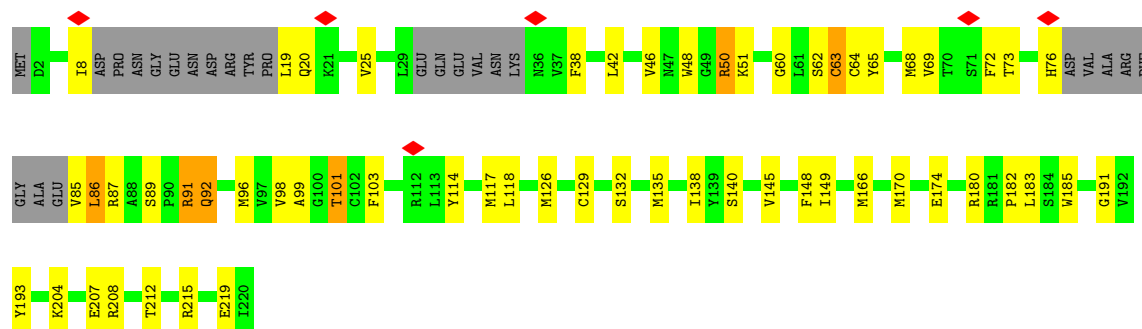
- Molecule 4: NADH-quinone oxidoreductase subunit I

Chain I:  72% 8% 19%




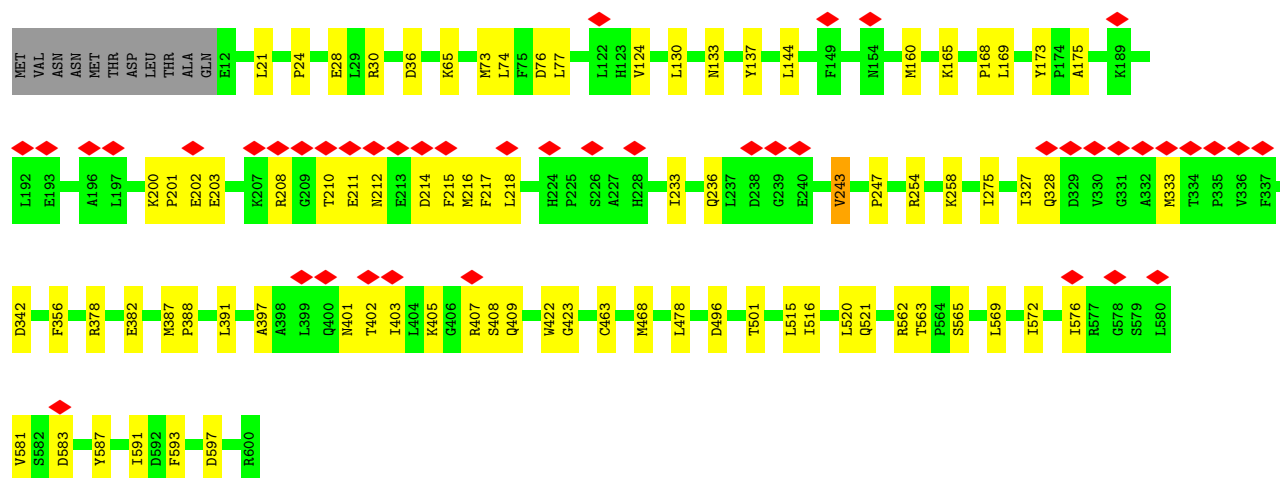
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:  62% 24% 11%




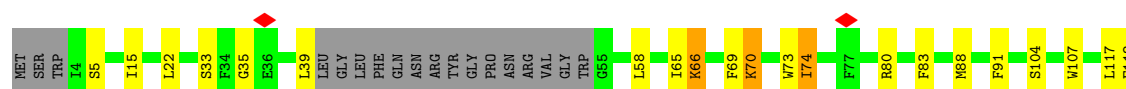
• Molecule 6: NADH-quinone oxidoreductase subunit C/D

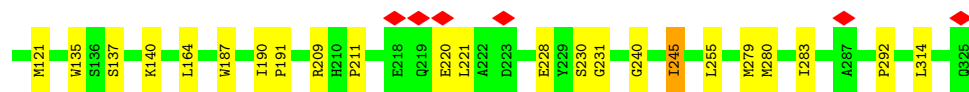
Chain C:  7% 84% 14%



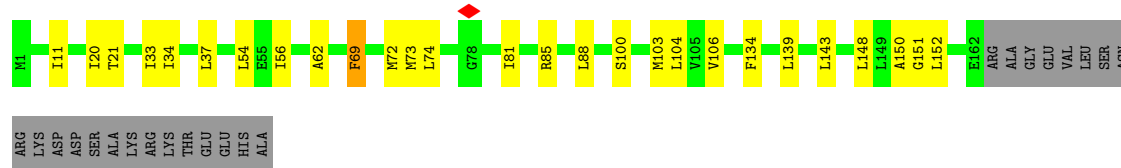
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:  81% 12% 6%

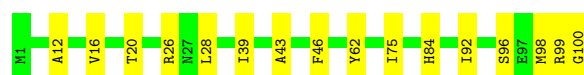
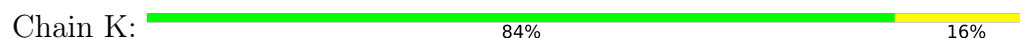




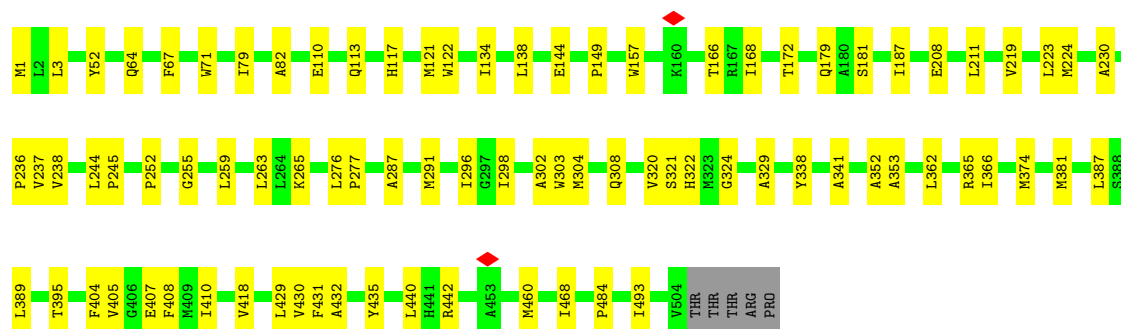
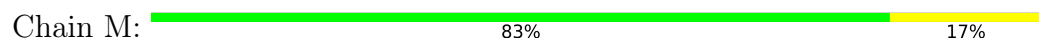
• Molecule 8: NADH-quinone oxidoreductase subunit J



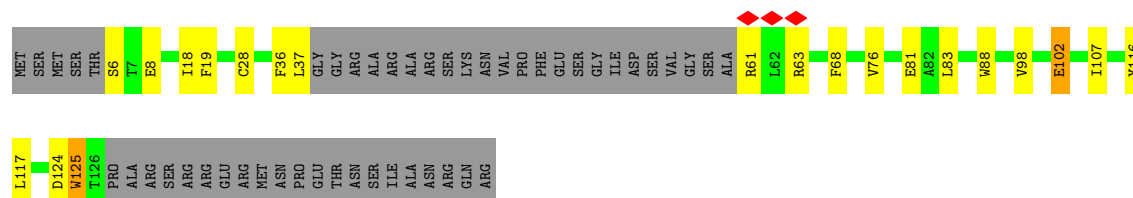
• Molecule 9: NADH-quinone oxidoreductase subunit K



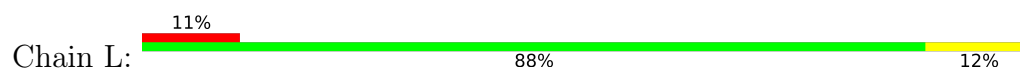
• Molecule 10: NADH-quinone oxidoreductase subunit M



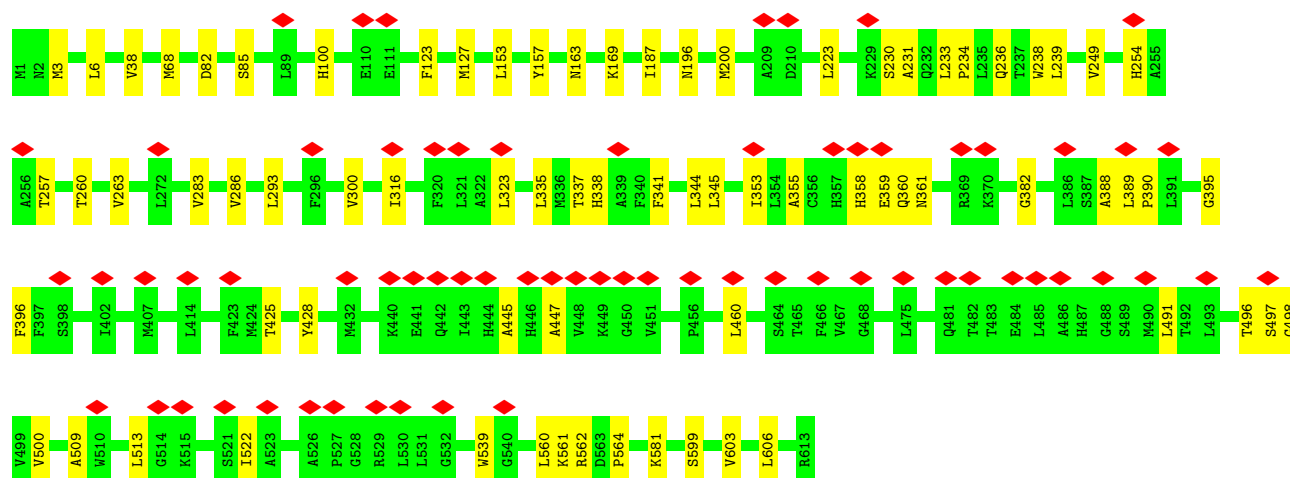
• Molecule 11: NADH-quinone oxidoreductase subunit A



• Molecule 12: NADH-quinone oxidoreductase subunit L

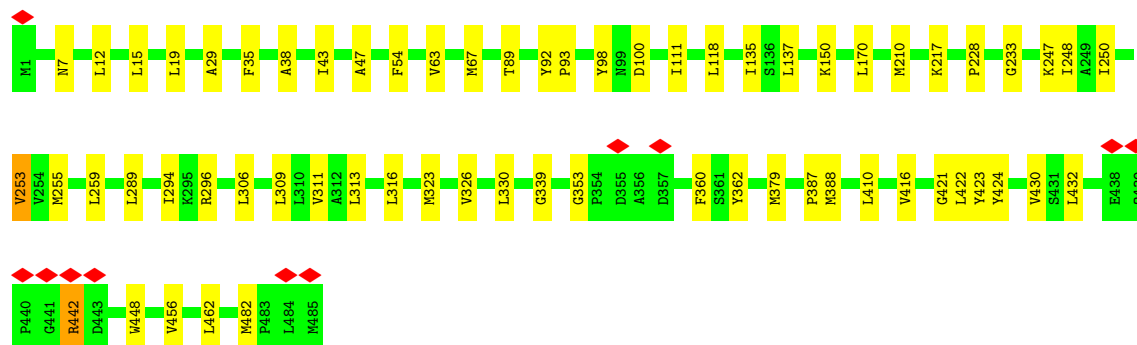






- Molecule 13: NADH-quinone oxidoreductase subunit N

Chain N: 87% 13%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.840	Depositor
Minimum map value	-0.721	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.234	Depositor
Map size (Å)	585.75, 585.75, 585.75	wwPDB
Map dimensions	710, 710, 710	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, FES, TRD, CA, UQ8, CDL, LFA, SF4, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	E	0.13	0/1248	0.25	0/1691
2	F	0.14	0/3486	0.24	0/4713
3	G	0.14	0/7178	0.25	0/9733
4	I	0.14	0/1176	0.27	0/1590
5	B	0.21	0/1582	0.36	0/2140
6	C	0.14	0/4891	0.29	0/6637
7	H	0.21	0/2472	0.36	0/3361
8	J	0.10	0/1252	0.24	0/1708
9	K	0.11	0/769	0.23	0/1040
10	M	0.11	0/4090	0.24	0/5569
11	A	0.17	0/812	0.35	0/1105
12	L	0.11	0/4806	0.29	0/6549
13	N	0.11	0/3764	0.26	0/5138
All	All	0.14	0/37526	0.28	0/50974

There are no bond length outliers.

There are no bond angle outliers.

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	E	1220	0	1187	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3407	0	3374	21	0
3	G	7027	0	6829	51	0
4	I	1149	0	1113	9	0
5	B	1551	0	1549	47	0
6	C	4760	0	4677	59	0
7	H	2404	0	2459	40	0
8	J	1226	0	1297	25	0
9	K	760	0	817	16	0
10	M	3964	0	4063	52	0
11	A	788	0	803	19	0
12	L	4685	0	4831	48	0
13	N	3673	0	3836	49	0
14	E	4	0	0	0	0
14	G	4	0	0	0	0
15	E	1	0	0	0	0
15	G	3	0	0	0	0
15	I	1	0	0	0	0
16	F	31	0	19	1	0
17	B	8	0	0	2	0
17	F	8	0	0	1	0
17	G	24	0	0	0	0
17	I	16	0	0	0	0
18	A	89	0	129	4	0
18	H	102	0	164	1	0
18	J	102	0	164	6	0
18	L	233	0	351	5	0
18	M	140	0	211	5	0
18	N	93	0	140	4	0
19	H	20	0	42	0	0
19	N	20	0	42	2	0
20	L	100	0	156	4	0
21	L	26	0	56	0	0
21	N	13	0	28	0	0
22	N	106	0	148	24	0
23	A	6	0	0	0	0
23	B	6	0	0	0	0
23	C	53	0	0	0	0
23	E	5	0	0	0	0
23	F	42	0	0	0	0
23	G	138	0	0	0	0
23	H	22	0	0	0	0
23	I	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J	8	0	0	0	0
23	K	10	0	0	0	0
23	L	44	0	0	0	0
23	M	40	0	0	0	0
23	N	36	0	0	0	0
All	All	38186	0	38485	410	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 5.

The worst 5 of 410 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)
6:C:581:VAL:HG11	7:H:220:GLU:HG3	1.52	0.91
6:C:563:THR:HG21	6:C:597:ASP:O	1.73	0.88
5:B:101:THR:HG21	6:C:254:ARG:HD3	1.60	0.83
12:L:522:ILE:HD11	18:L:704:3PE:H221	1.60	0.83
5:B:91:ARG:HG3	7:H:230:SER:HB3	1.66	0.77

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 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	E	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
2	F	437/461 (95%)	427 (98%)	10 (2%)	0	100	100
3	G	903/910 (99%)	874 (97%)	29 (3%)	0	100	100
4	I	143/180 (79%)	140 (98%)	3 (2%)	0	100	100
5	B	187/220 (85%)	177 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	587/600 (98%)	557 (95%)	30 (5%)	0	100	100
7	H	303/325 (93%)	289 (95%)	14 (5%)	0	100	100
8	J	160/184 (87%)	157 (98%)	3 (2%)	0	100	100
9	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
10	M	503/509 (99%)	486 (97%)	17 (3%)	0	100	100
11	A	94/147 (64%)	89 (95%)	5 (5%)	0	100	100
12	L	611/613 (100%)	574 (94%)	36 (6%)	1 (0%)	43	76
13	N	483/485 (100%)	467 (97%)	15 (3%)	1 (0%)	43	76
All	All	4663/4900 (95%)	4482 (96%)	179 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	N	353	GLY
12	L	361	ASN

### 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	E	129/139 (93%)	129 (100%)	0	100	100
2	F	353/372 (95%)	350 (99%)	3 (1%)	73	86
3	G	733/738 (99%)	722 (98%)	11 (2%)	57	80
4	I	124/154 (80%)	121 (98%)	3 (2%)	43	73
5	B	171/192 (89%)	156 (91%)	15 (9%)	9	35
6	C	509/519 (98%)	501 (98%)	8 (2%)	55	79
7	H	254/269 (94%)	247 (97%)	7 (3%)	38	70
8	J	128/146 (88%)	127 (99%)	1 (1%)	73	86
9	K	79/79 (100%)	77 (98%)	2 (2%)	42	72
10	M	414/418 (99%)	412 (100%)	2 (0%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	A	79/119 (66%)	76 (96%)	3 (4%)	29	63
12	L	485/485 (100%)	485 (100%)	0	100	100
13	N	385/385 (100%)	381 (99%)	4 (1%)	68	84
All	All	3843/4015 (96%)	3784 (98%)	59 (2%)	55	80

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	101	THR
13	N	135	ILE
6	C	243	VAL
11	A	125	TRP
9	K	46	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	20	GLN
6	C	236	GLN
12	L	254	HIS
3	G	598	GLN
3	G	286	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

Of 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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
17	SF4	G	1002	3	0,12,12	-	-	-		
17	SF4	I	203	4	0,12,12	-	-	-		
18	3PE	H	401	-	50,50,50	0.52	0	53,55,55	0.52	1 (1%)
14	FES	G	1003	3	0,4,4	-	-	-		
18	3PE	J	201	-	50,50,50	0.52	0	53,55,55	0.53	1 (1%)
17	SF4	B	301	5	0,12,12	-	-	-		
16	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.19	6 (12%)
18	3PE	L	705	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
19	LFA	H	402	-	19,19,19	0.24	0	18,18,18	0.23	0
17	SF4	F	502	2	0,12,12	-	-	-		
19	LFA	N	505	-	19,19,19	0.23	0	18,18,18	0.23	0
17	SF4	G	1001	3	0,12,12	-	-	-		
17	SF4	I	202	4	0,12,12	-	-	-		
14	FES	E	201	1	0,4,4	-	-	-		
18	3PE	J	202	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
18	3PE	L	704	-	41,41,50	0.56	0	44,46,55	0.55	1 (2%)
18	3PE	N	504	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
21	TRD	L	708	-	12,12,12	0.29	0	11,11,11	0.85	0
21	TRD	N	501	-	12,12,12	0.29	0	11,11,11	0.83	0
18	3PE	N	506	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
18	3PE	H	403	-	50,50,50	0.51	0	53,55,55	0.49	1 (1%)
22	UQ8	N	502	-	53,53,53	1.15	2 (3%)	64,67,67	1.74	17 (26%)
18	3PE	M	602	-	50,50,50	0.52	0	53,55,55	0.55	1 (1%)
18	3PE	A	502	-	46,46,50	0.53	0	49,51,55	0.53	1 (2%)
18	3PE	L	702	-	46,46,50	0.53	0	49,51,55	0.55	1 (2%)
21	TRD	L	707	-	12,12,12	0.29	0	11,11,11	0.83	0
18	3PE	A	501	-	41,41,50	0.56	0	44,46,55	0.57	1 (2%)
18	3PE	M	603	-	41,41,50	0.57	0	44,46,55	0.56	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	3PE	L	701	-	41,41,50	0.56	0	44,46,55	0.58	1 (2%)
17	SF4	G	1007	3	0,12,12	-	-	-		
20	CDL	L	703	-	99,99,99	0.91	7 (7%)	105,111,111	1.09	4 (3%)
18	3PE	L	706	-	50,50,50	0.51	0	53,55,55	0.51	1 (1%)
22	UQ8	N	503	-	53,53,53	1.14	2 (3%)	64,67,67	1.77	17 (26%)
18	3PE	M	601	-	46,46,50	0.53	0	49,51,55	0.57	1 (2%)

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
18	3PE	H	401	-	-	14/54/54/54	-
17	SF4	G	1002	3	-	-	0/6/5/5
17	SF4	I	203	4	-	-	0/6/5/5
14	FES	G	1003	3	-	-	0/1/1/1
18	3PE	J	201	-	-	22/54/54/54	-
17	SF4	B	301	5	-	-	0/6/5/5
16	FMN	F	501	-	-	5/18/18/18	0/3/3/3
18	3PE	L	705	-	-	33/54/54/54	-
19	LFA	H	402	-	-	1/17/17/17	-
17	SF4	F	502	2	-	-	0/6/5/5
19	LFA	N	505	-	-	7/17/17/17	-
17	SF4	G	1001	3	-	-	0/6/5/5
17	SF4	I	202	4	-	-	0/6/5/5
14	FES	E	201	1	-	-	0/1/1/1
18	3PE	J	202	-	-	19/54/54/54	-
18	3PE	L	704	-	-	12/45/45/54	-
18	3PE	N	504	-	-	16/45/45/54	-
21	TRD	L	708	-	-	3/10/10/10	-
21	TRD	N	501	-	-	1/10/10/10	-
18	3PE	N	506	-	-	30/54/54/54	-
18	3PE	H	403	-	-	18/54/54/54	-
22	UQ8	N	502	-	-	21/51/75/75	0/1/1/1
18	3PE	M	602	-	-	25/54/54/54	-
18	3PE	A	502	-	-	11/50/50/54	-
18	3PE	L	702	-	-	18/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TRD	L	707	-	-	2/10/10/10	-
18	3PE	A	501	-	-	16/45/45/54	-
18	3PE	M	603	-	-	13/45/45/54	-
18	3PE	L	701	-	-	7/45/45/54	-
17	SF4	G	1007	3	-	-	0/6/5/5
20	CDL	L	703	-	-	60/110/110/110	-
18	3PE	L	706	-	-	22/54/54/54	-
22	UQ8	N	503	-	-	15/51/75/75	0/1/1/1
18	3PE	M	601	-	-	18/50/50/54	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	502	UQ8	C6-C1	7.32	1.48	1.35
22	N	503	UQ8	C6-C1	7.21	1.48	1.35
16	F	501	FMN	C4A-N5	3.71	1.38	1.30
22	N	502	UQ8	C4-C3	2.97	1.48	1.36
22	N	503	UQ8	C4-C3	2.95	1.48	1.36

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	502	UQ8	C7-C8-C9	-5.10	118.30	126.79
22	N	503	UQ8	C7-C8-C9	-4.48	119.34	126.79
20	L	703	CDL	OA6-CA5-C11	3.89	119.89	111.50
20	L	703	CDL	OB6-CB5-C51	3.89	119.89	111.50
22	N	503	UQ8	C15-C14-C16	3.67	121.45	115.27

There are no chirality outliers.

5 of 409 torsion outliers are listed below:

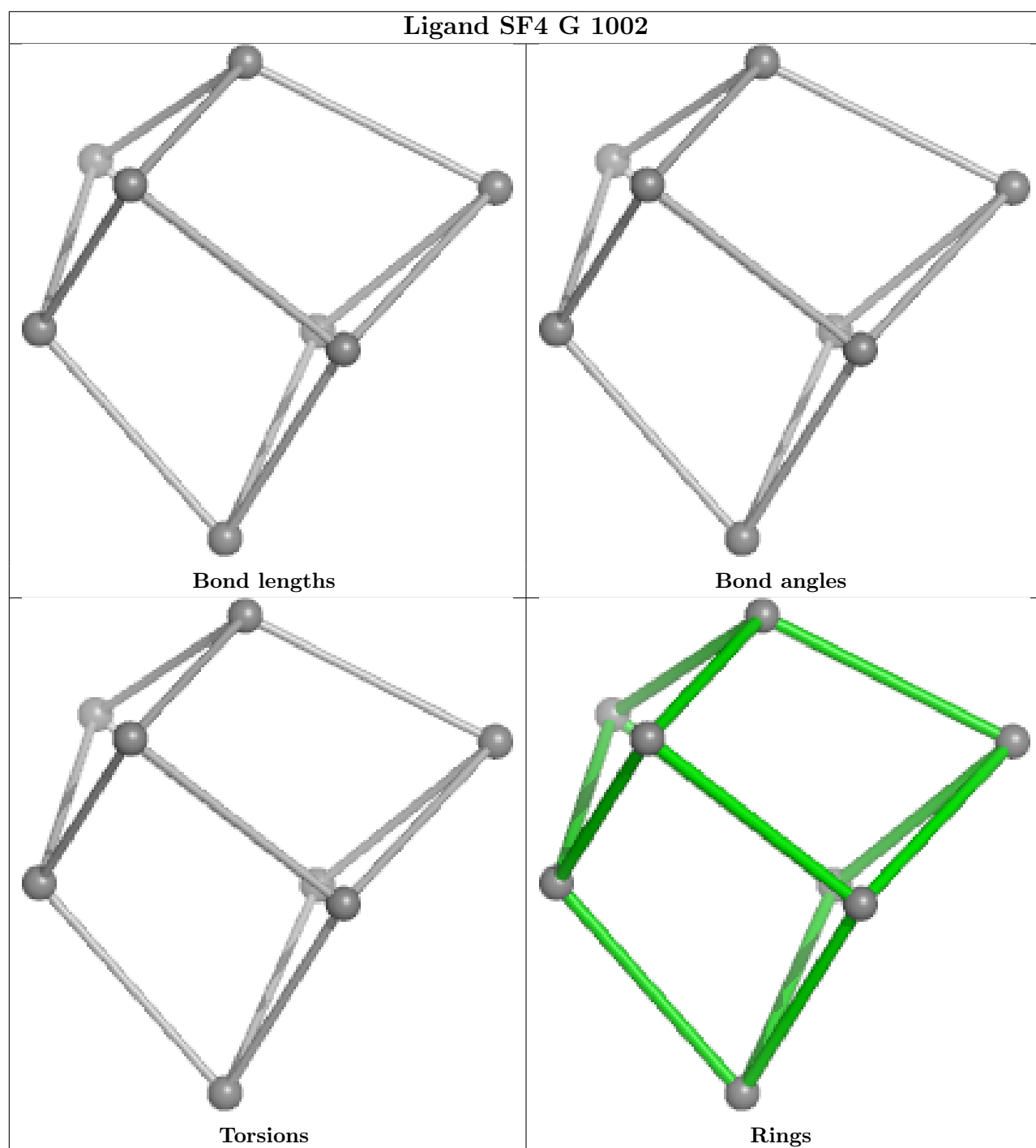
Mol	Chain	Res	Type	Atoms
16	F	501	FMN	C1'-C2'-C3'-O3'
16	F	501	FMN	C1'-C2'-C3'-C4'
18	H	401	3PE	C1-O11-P-O12
18	H	401	3PE	C2-C1-O11-P
18	H	401	3PE	C22-C21-O21-C2

There are no ring outliers.

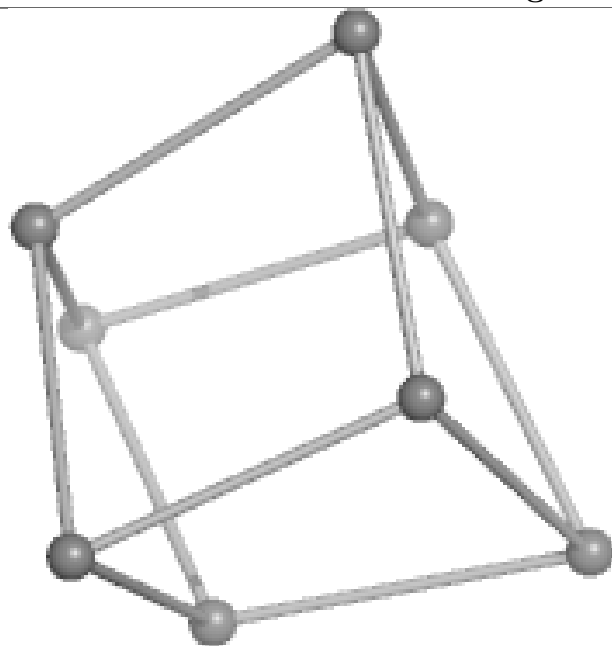
20 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	401	3PE	1	0
18	J	201	3PE	5	0
17	B	301	SF4	2	0
16	F	501	FMN	1	0
18	L	705	3PE	1	0
17	F	502	SF4	1	0
19	N	505	LFA	2	0
18	J	202	3PE	1	0
18	L	704	3PE	3	0
18	N	504	3PE	1	0
18	N	506	3PE	3	0
22	N	502	UQ8	10	0
18	M	602	3PE	1	0
18	A	502	3PE	2	0
18	A	501	3PE	2	0
18	M	603	3PE	3	0
18	L	701	3PE	1	0
20	L	703	CDL	4	0
22	N	503	UQ8	15	0
18	M	601	3PE	1	0

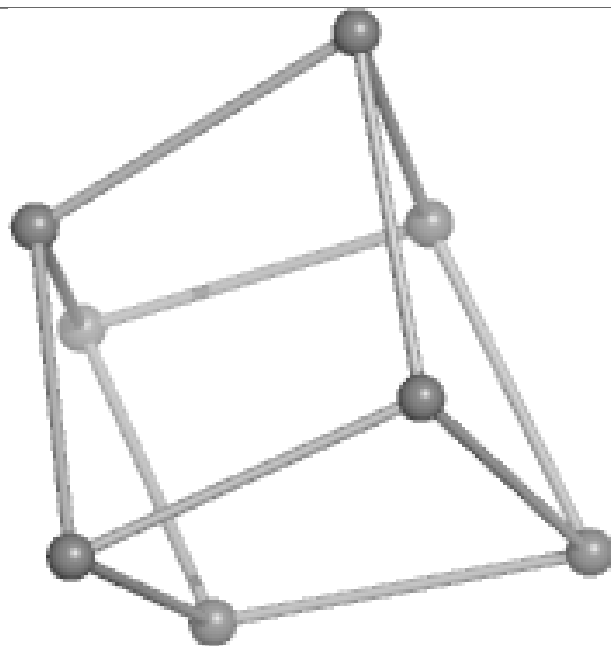
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



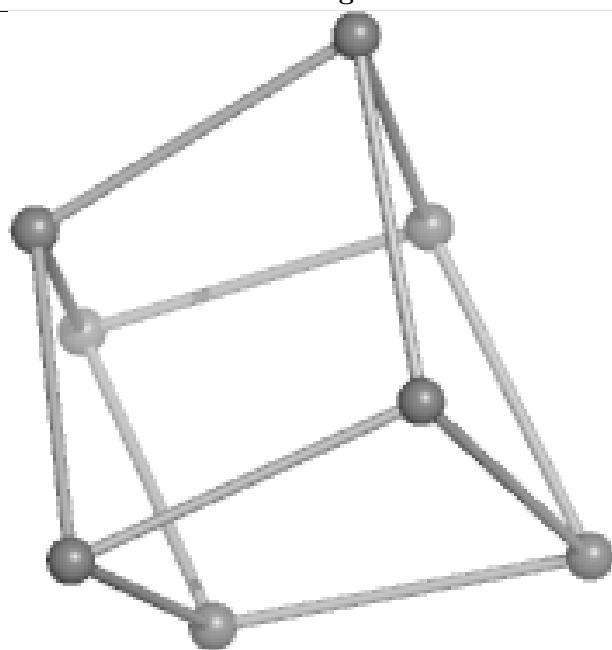
## Ligand SF4 I 203



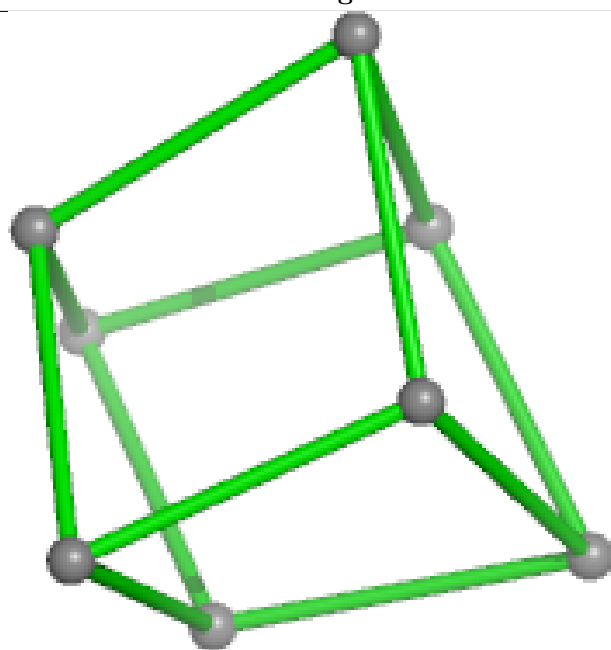
Bond lengths



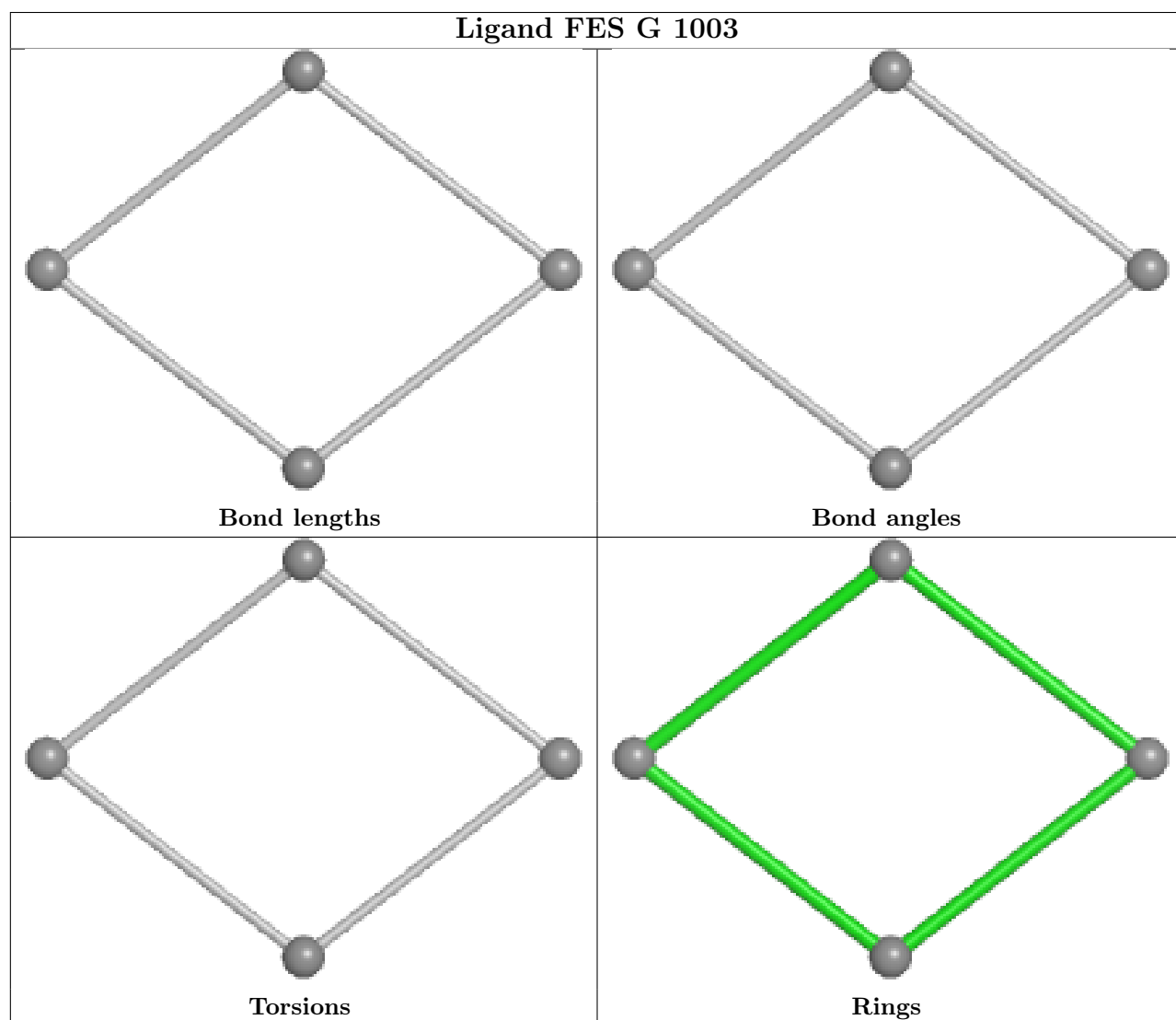
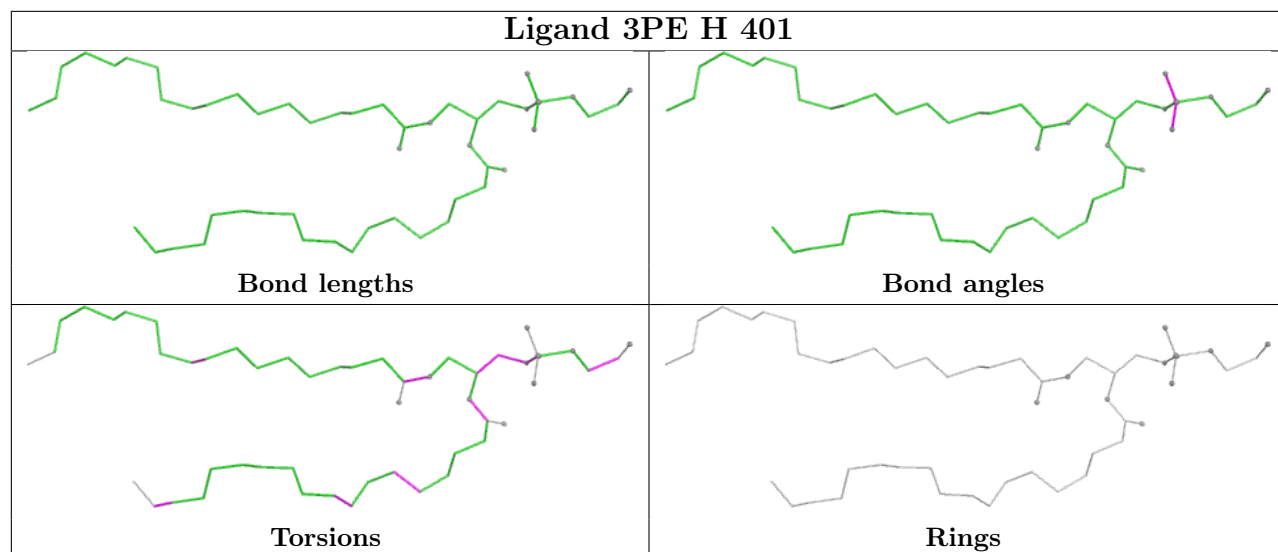
Bond angles

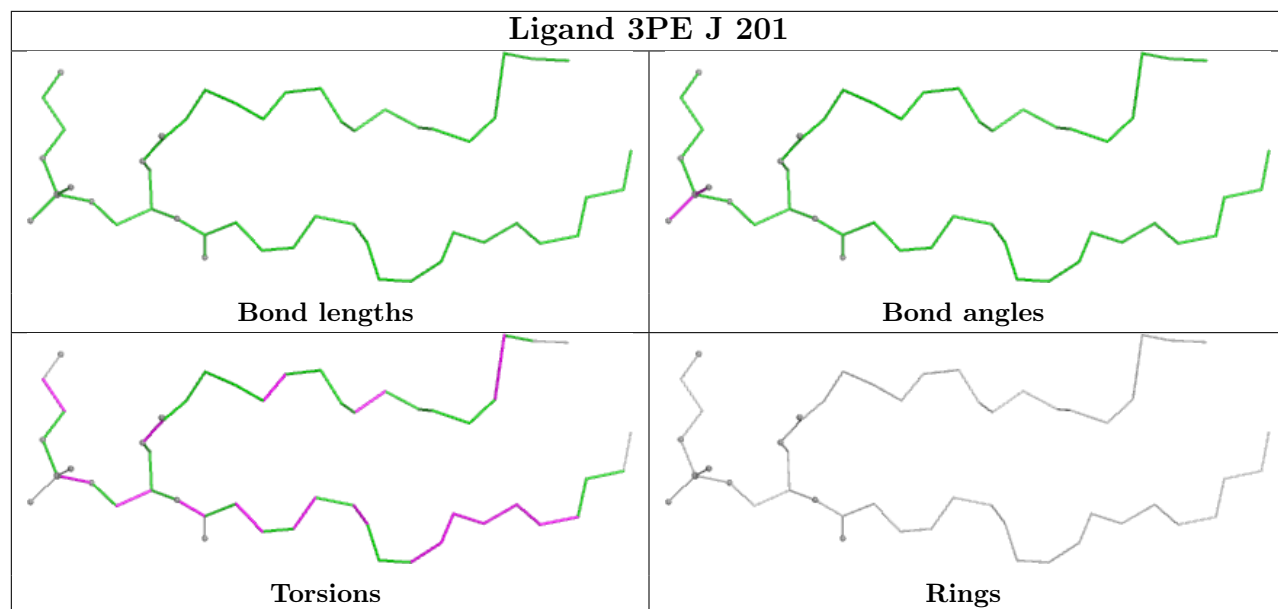


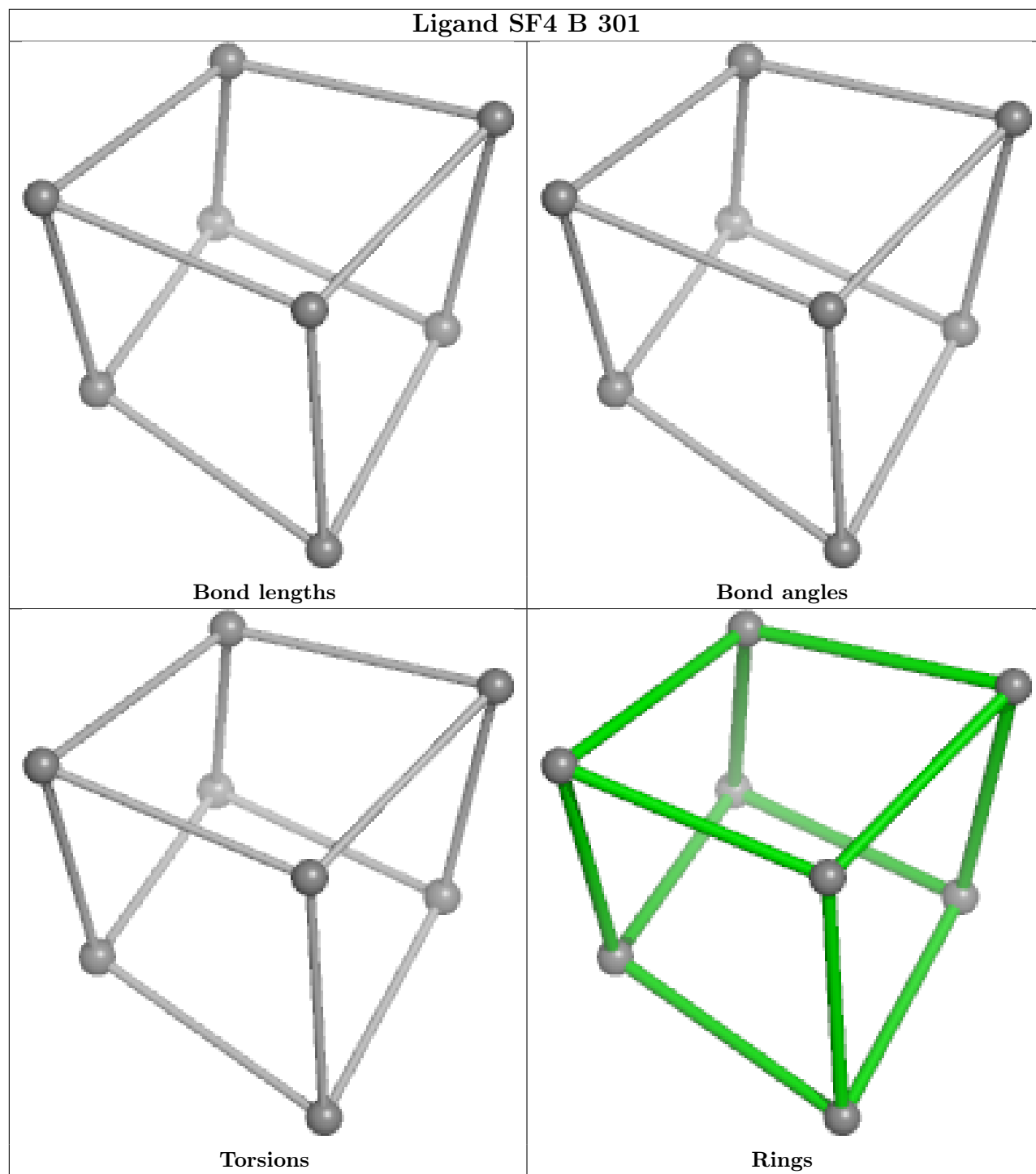
Torsions



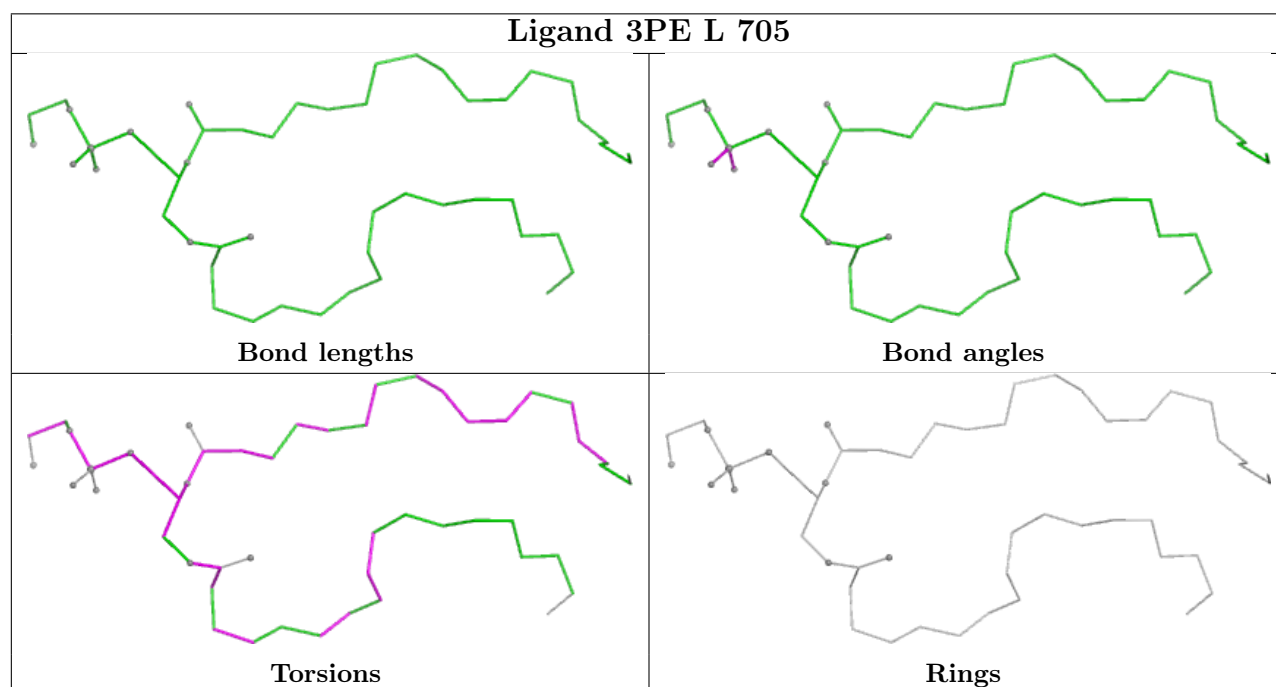
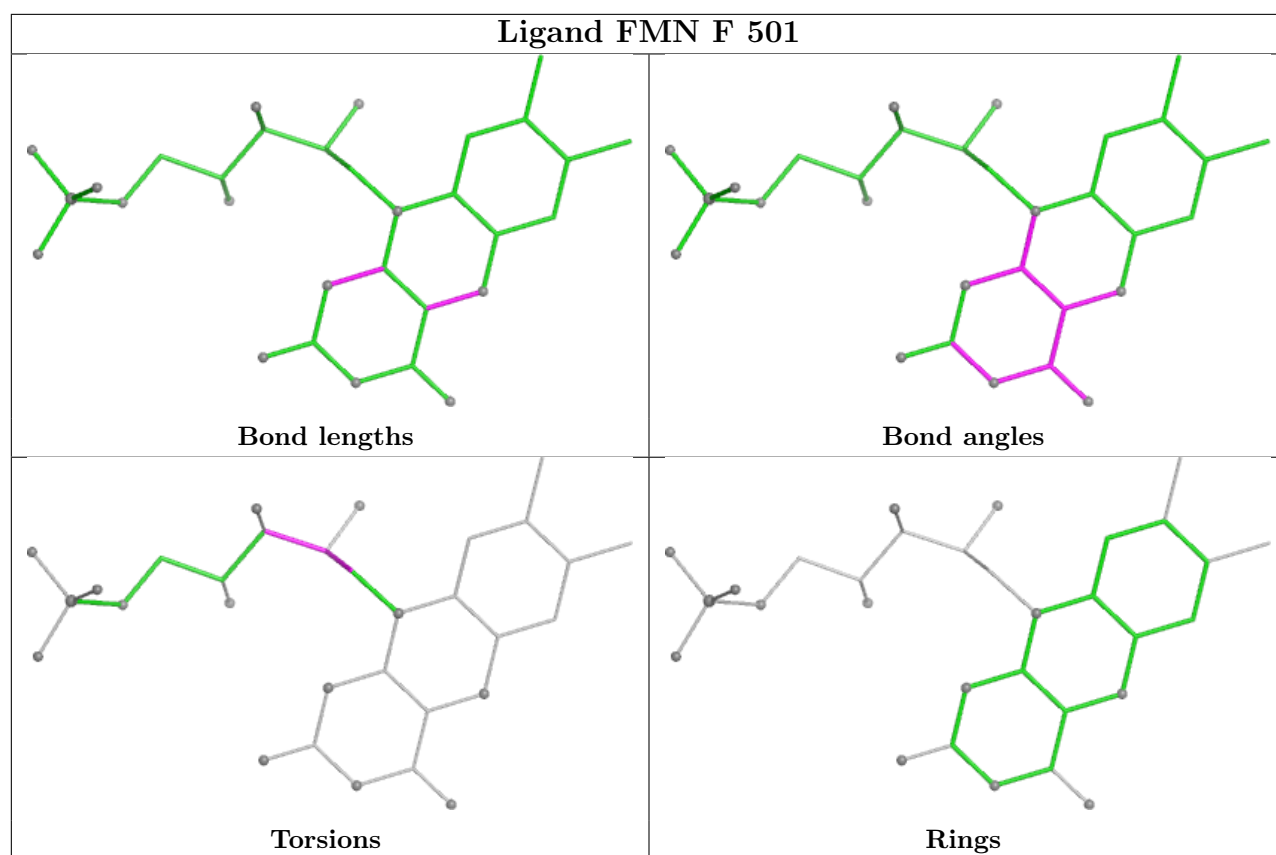
Rings

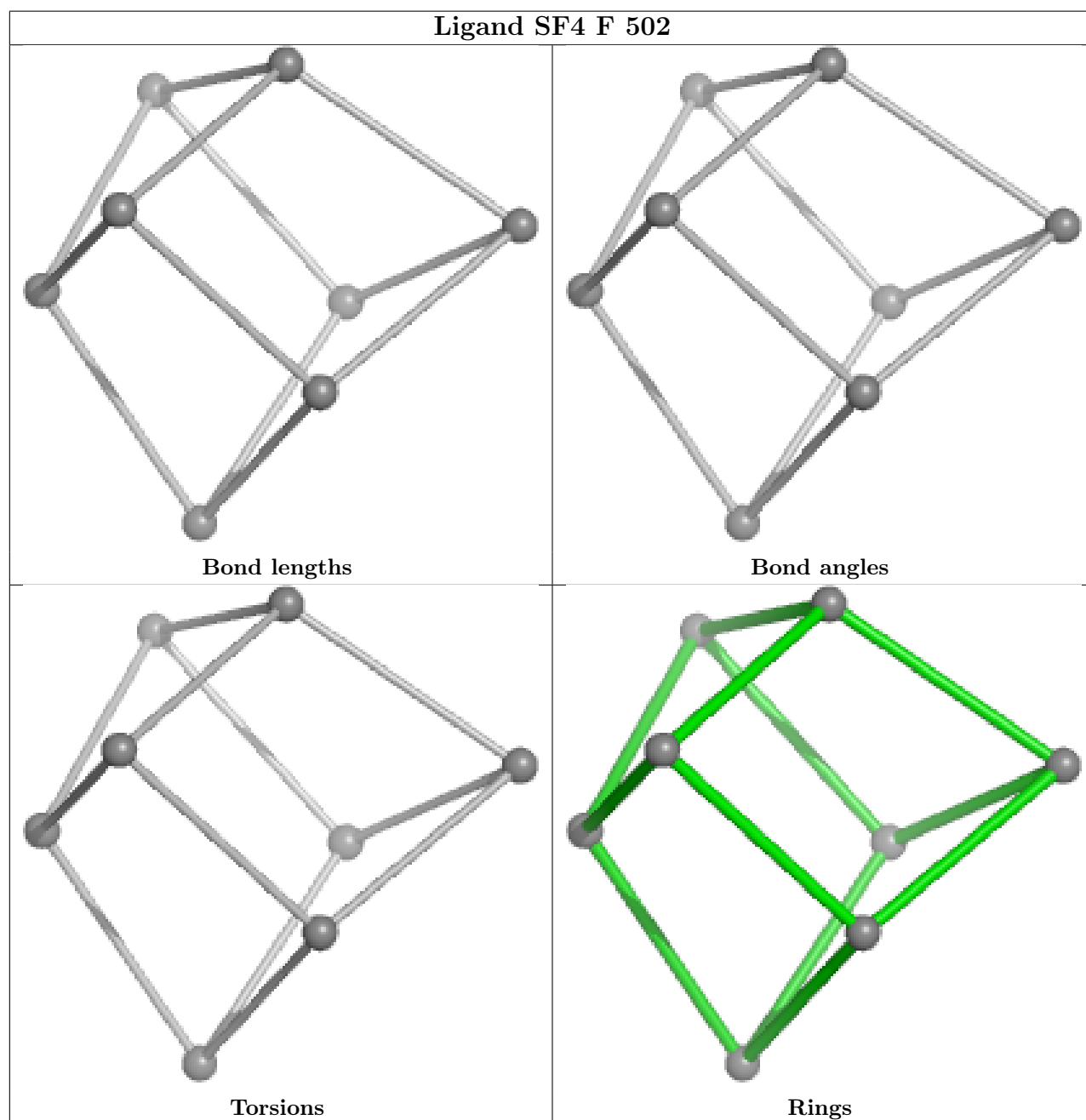
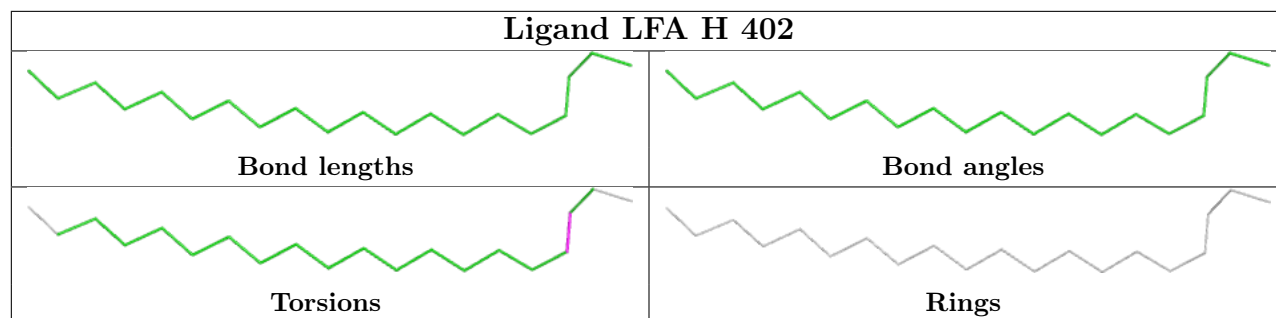


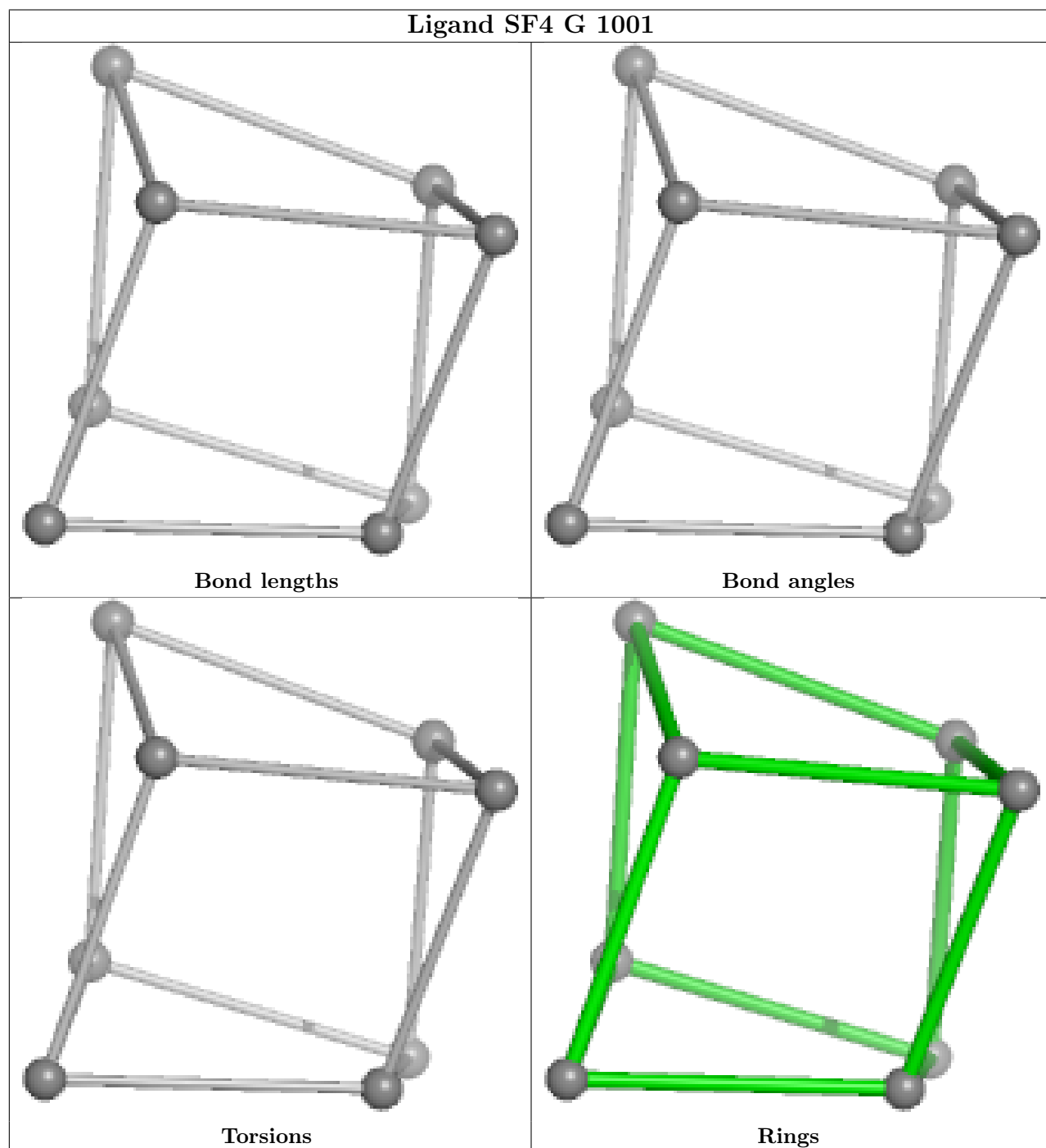
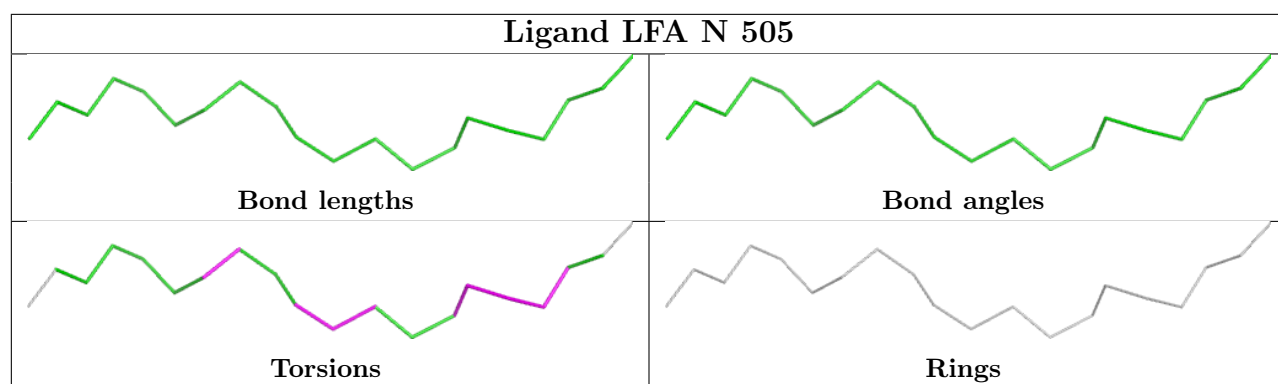


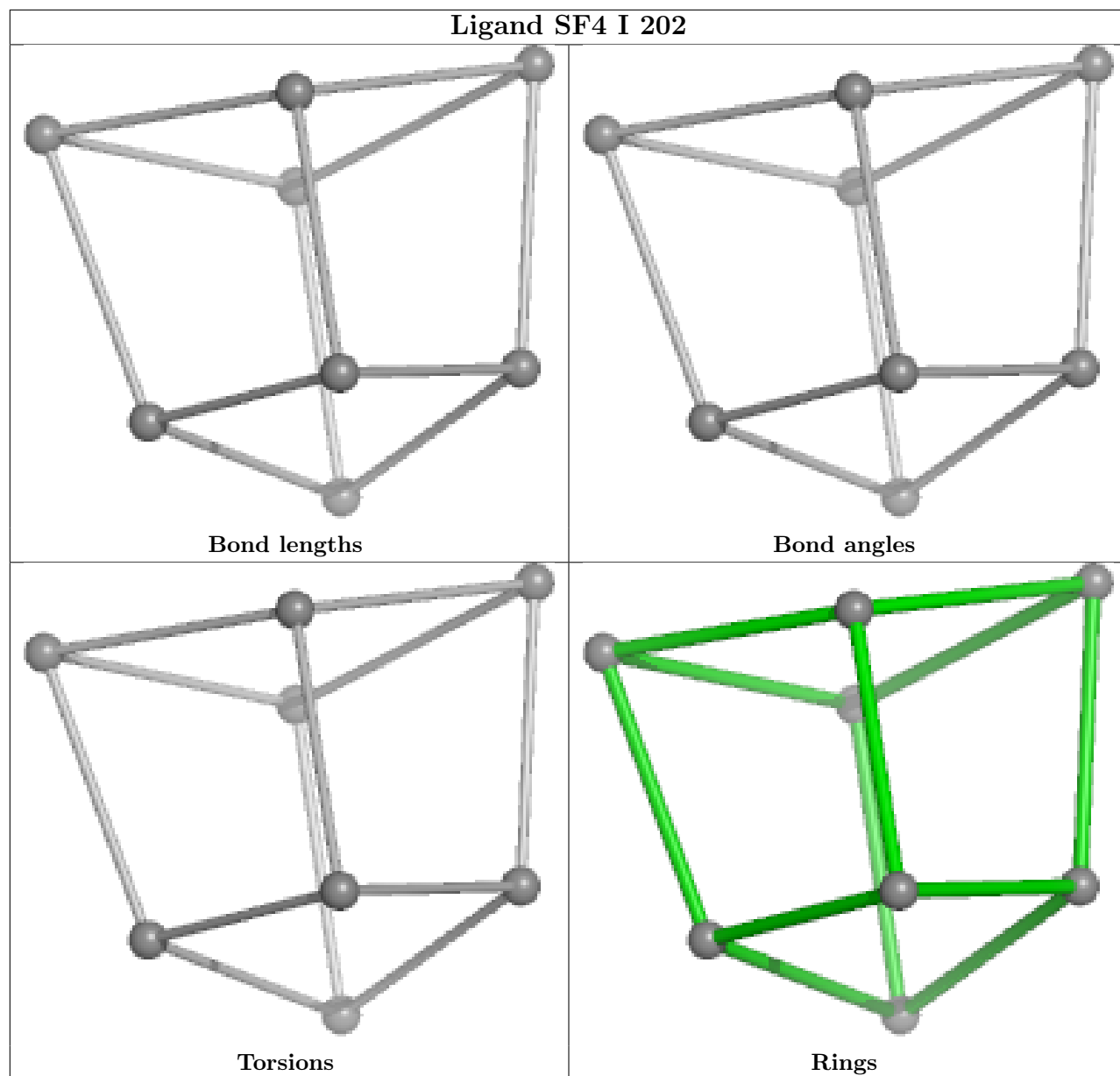


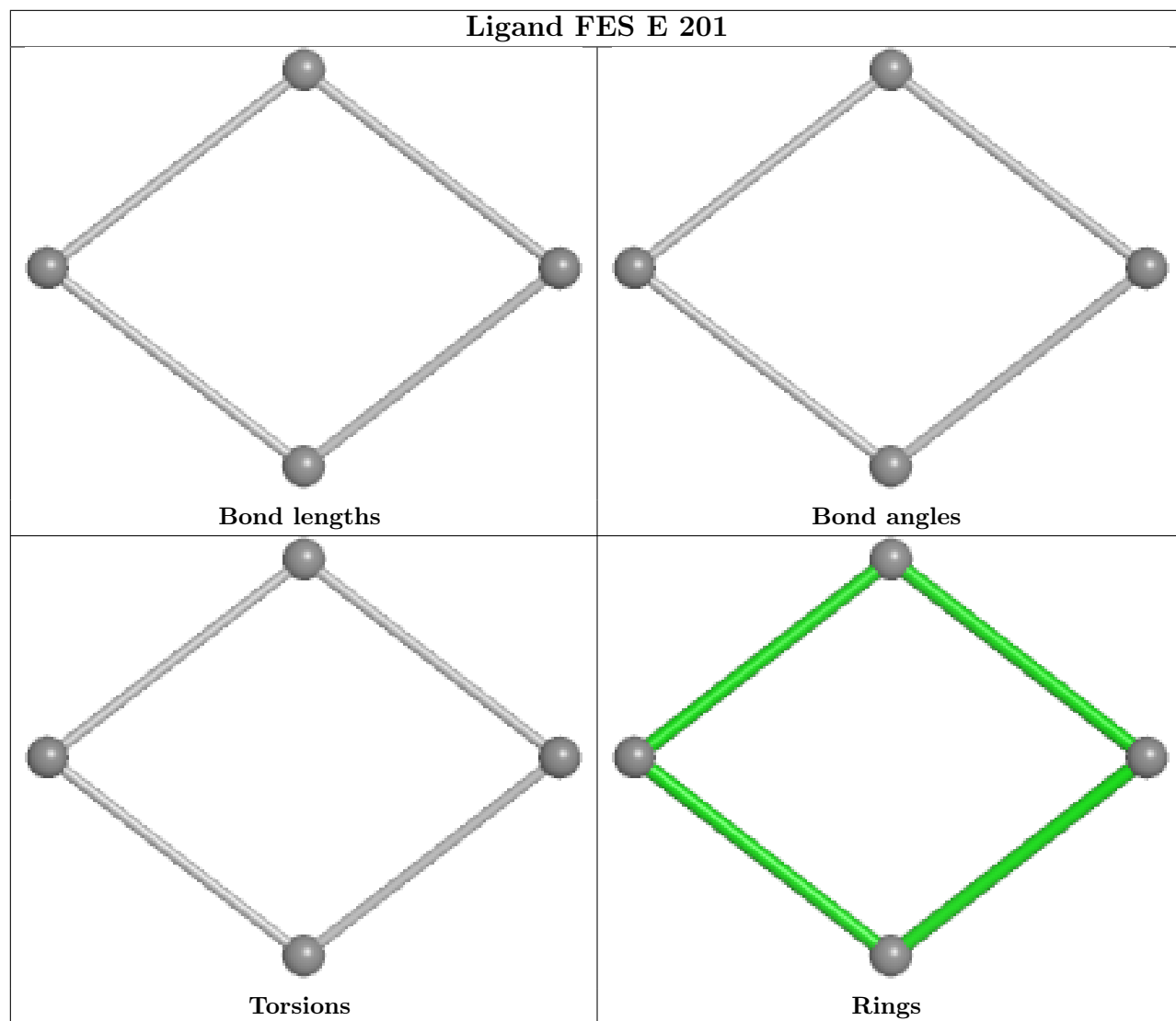


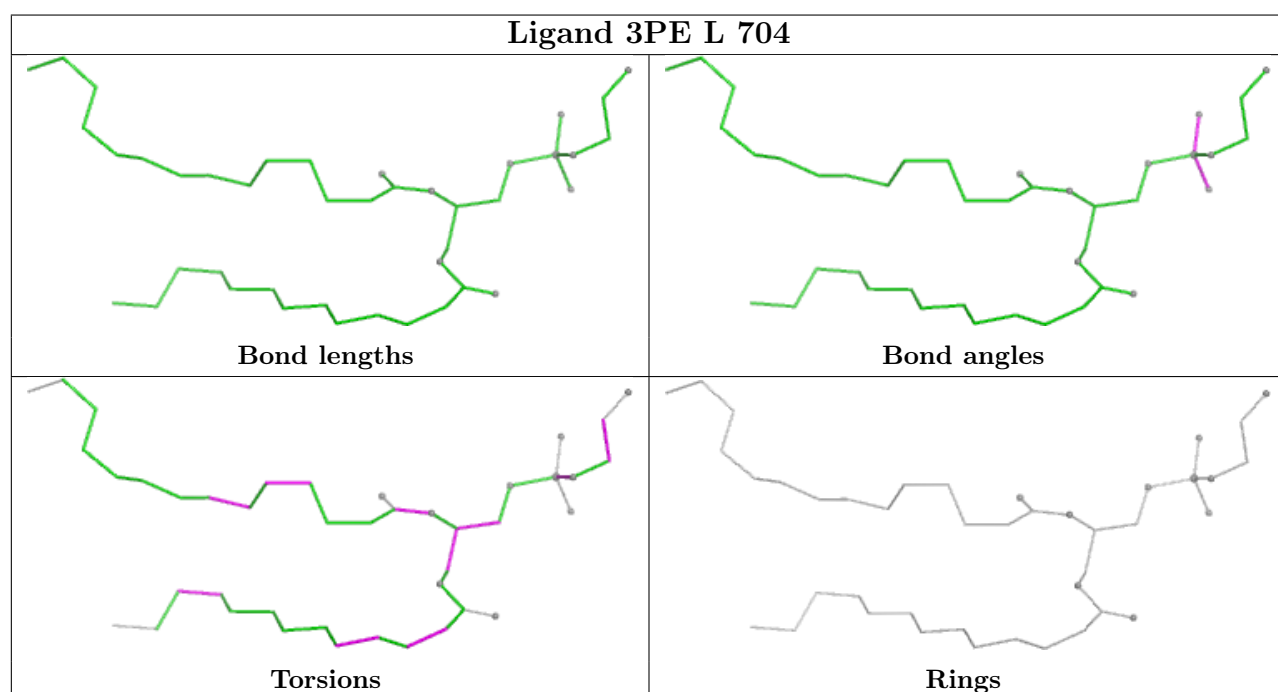
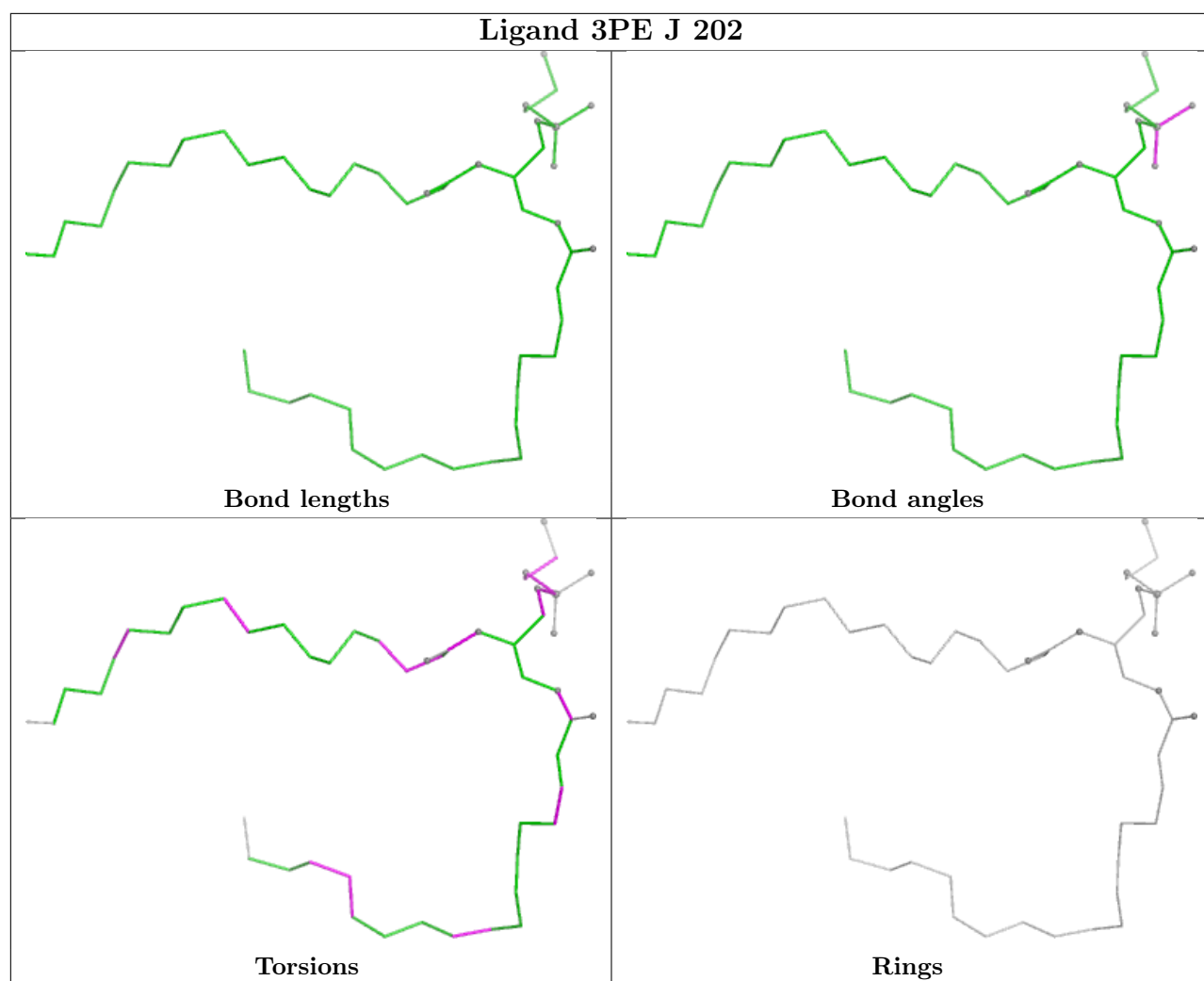


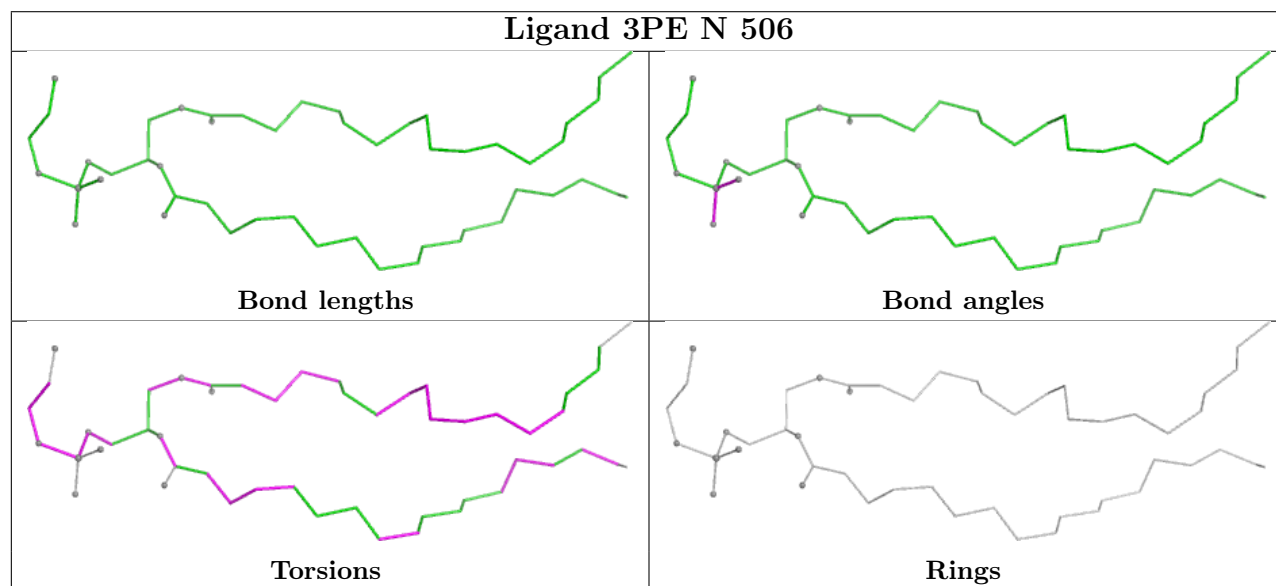
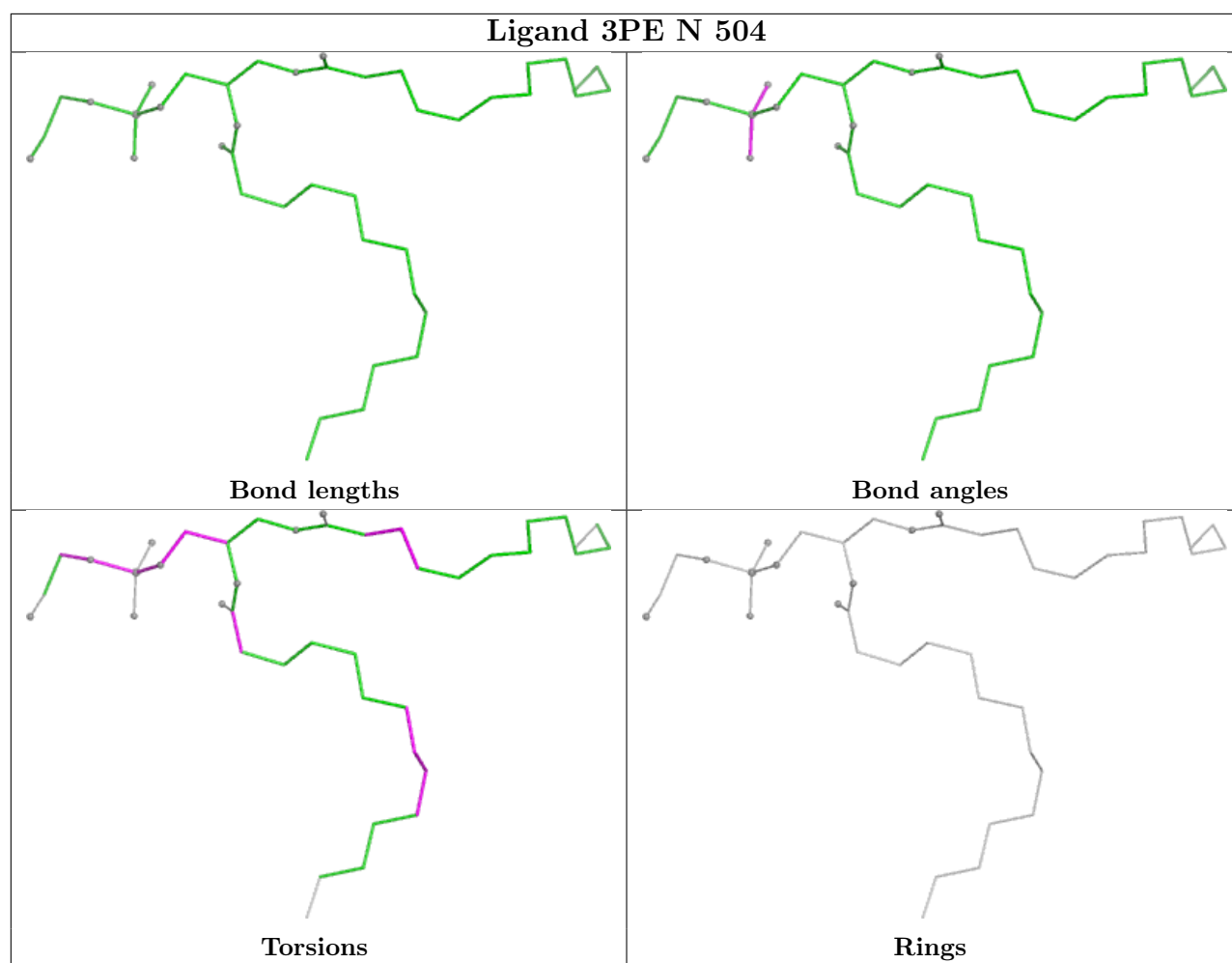


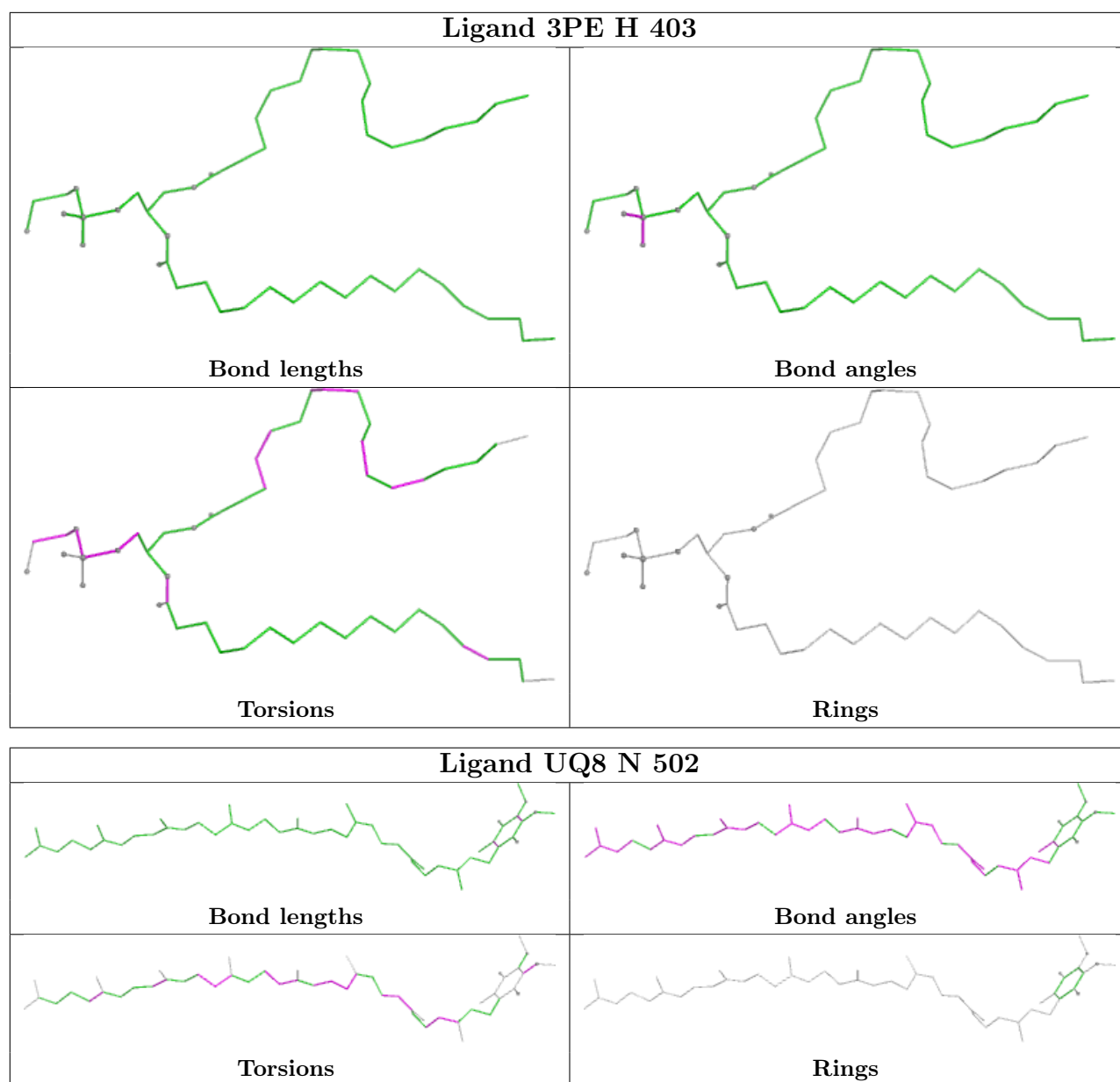




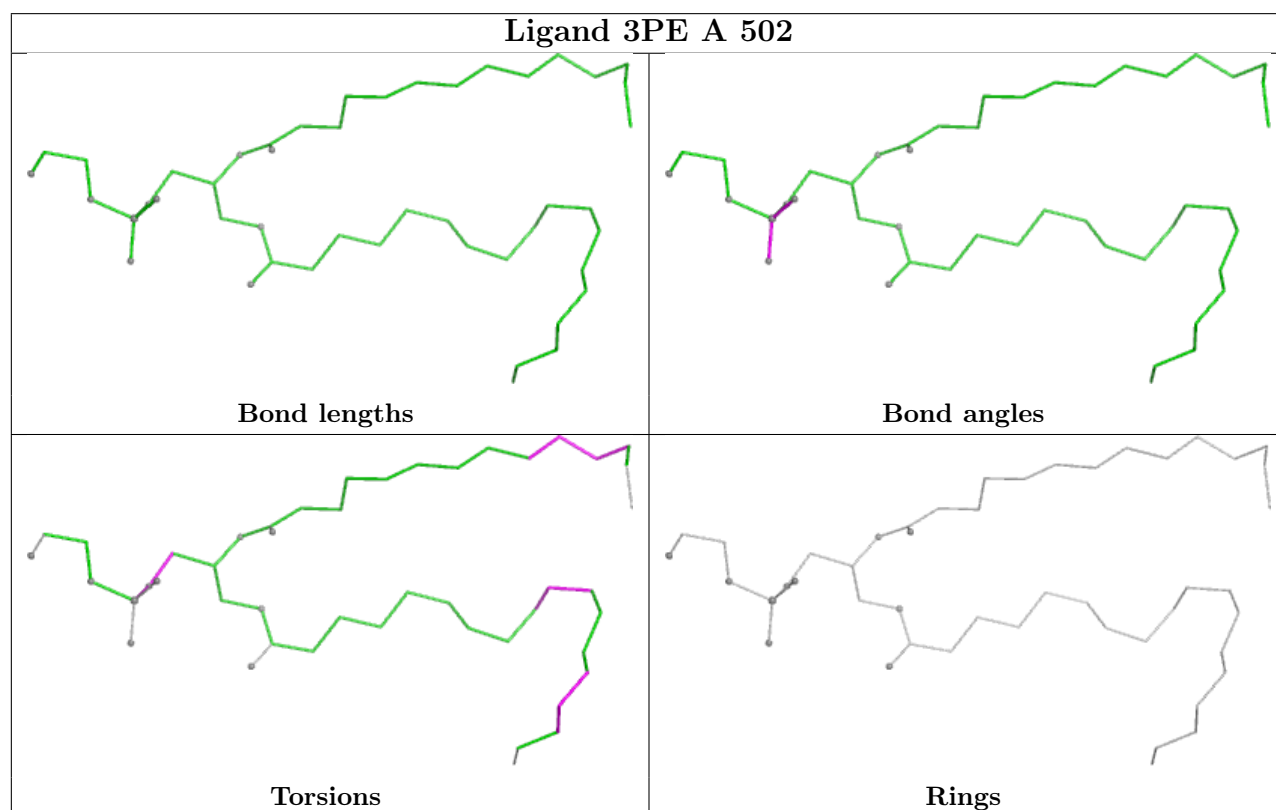
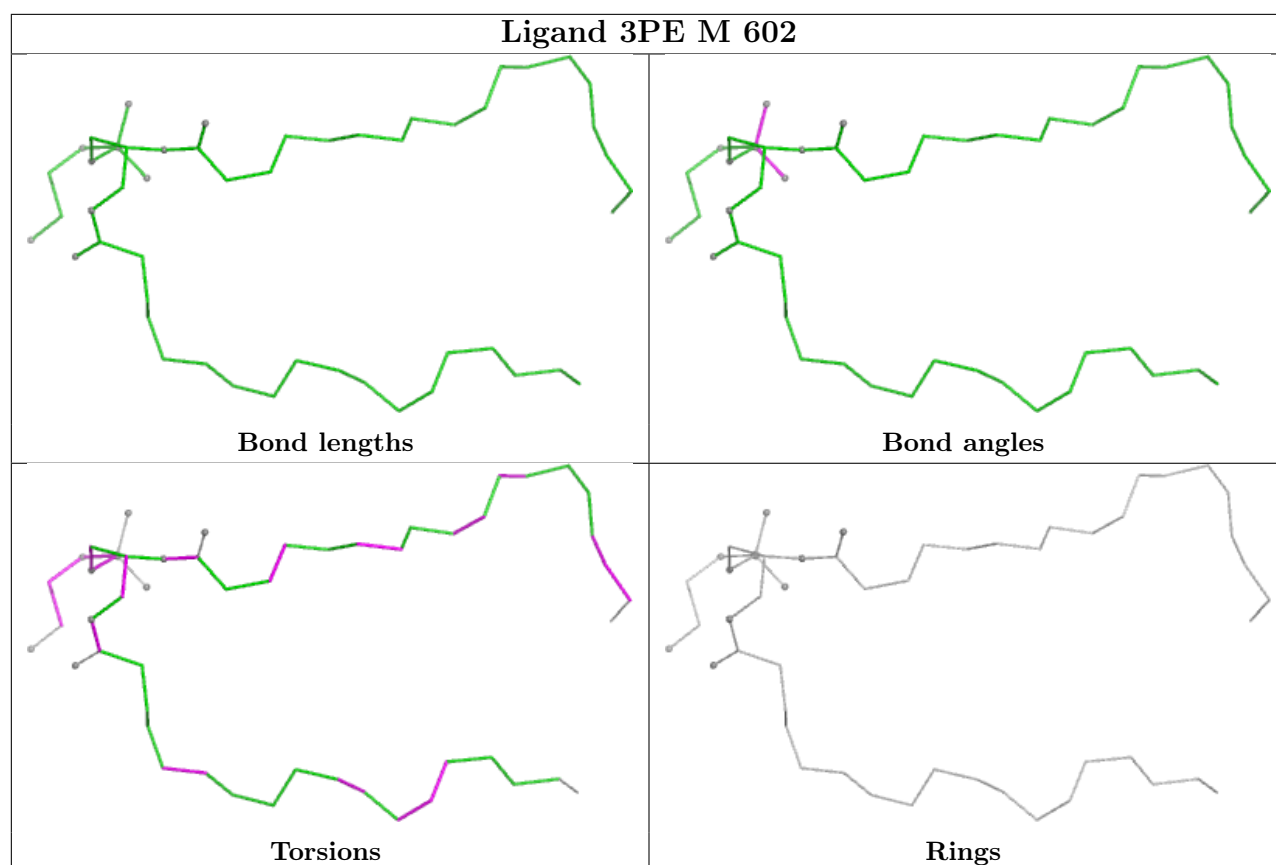


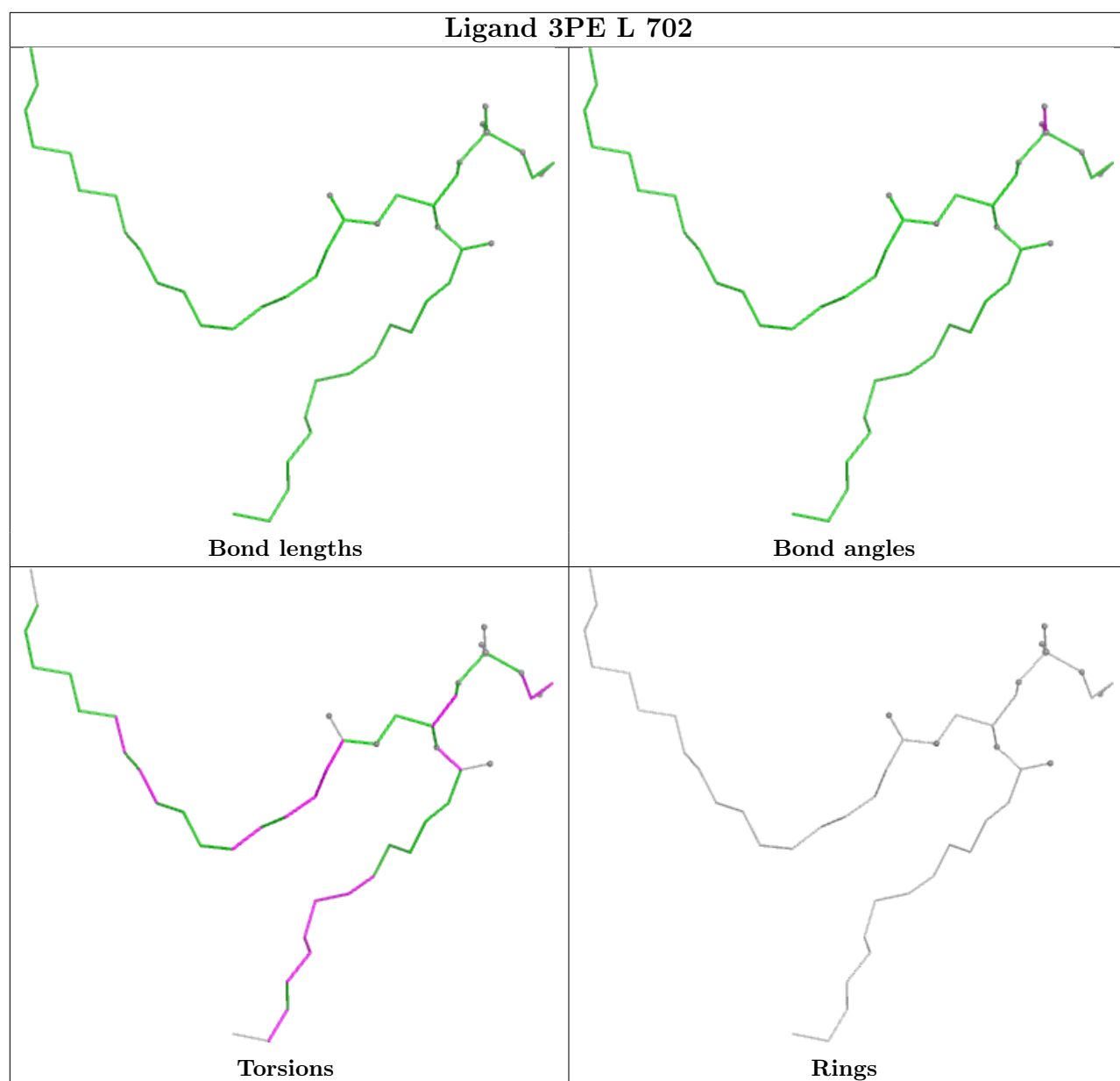


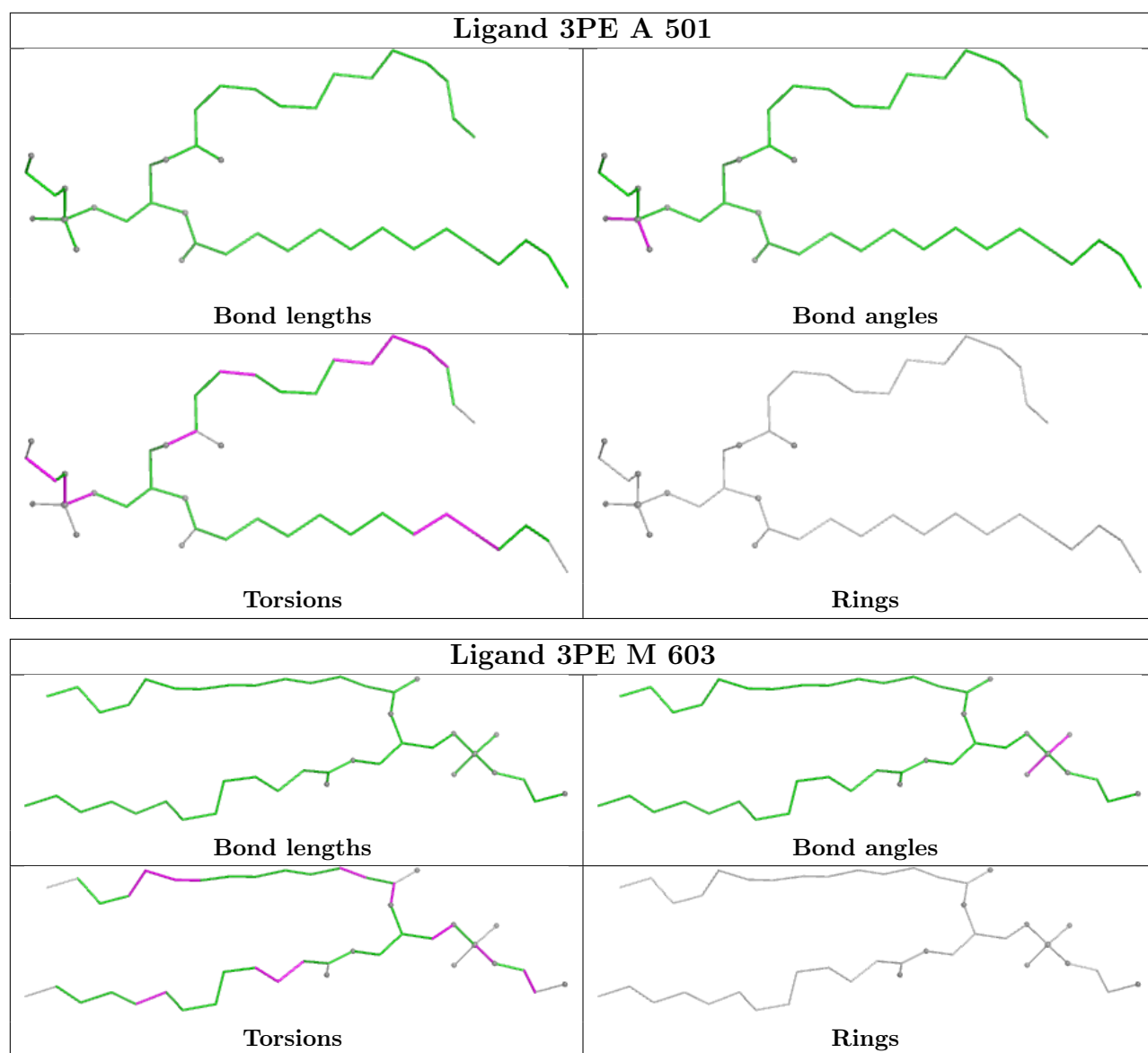


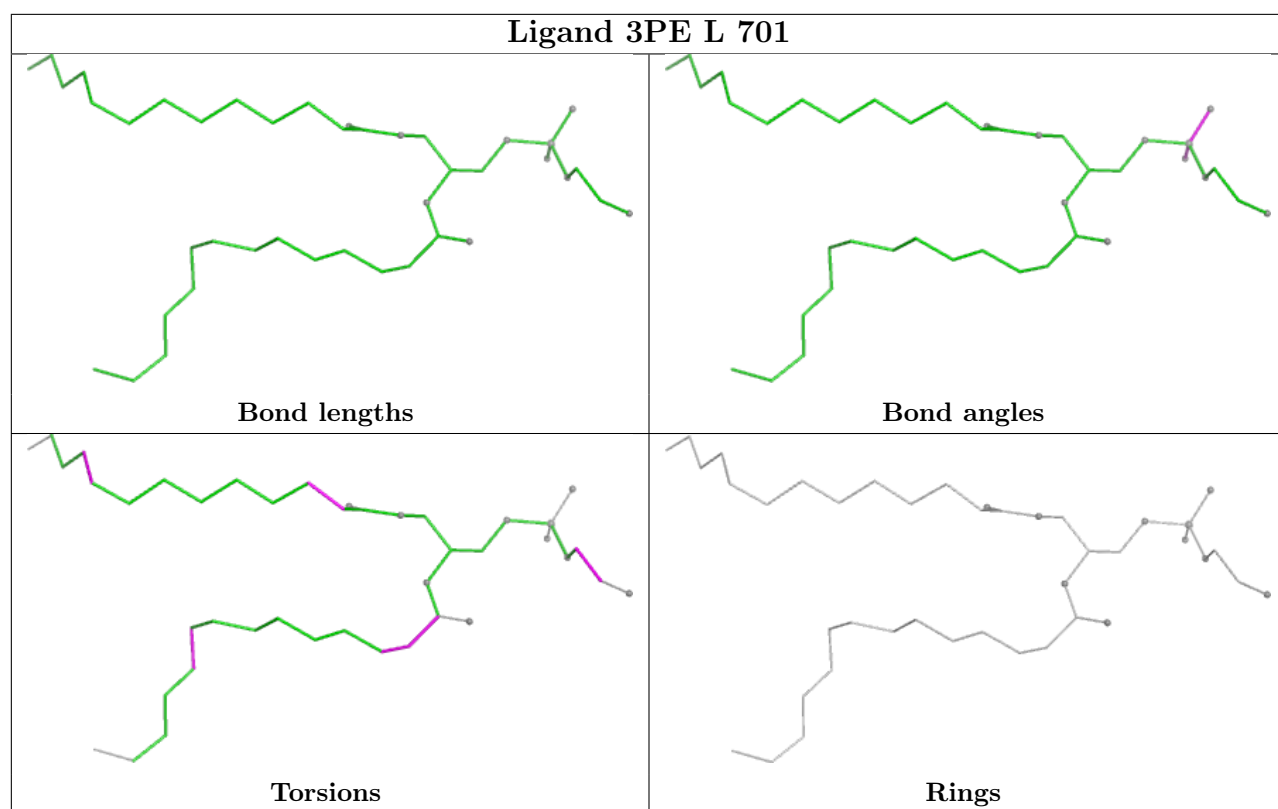


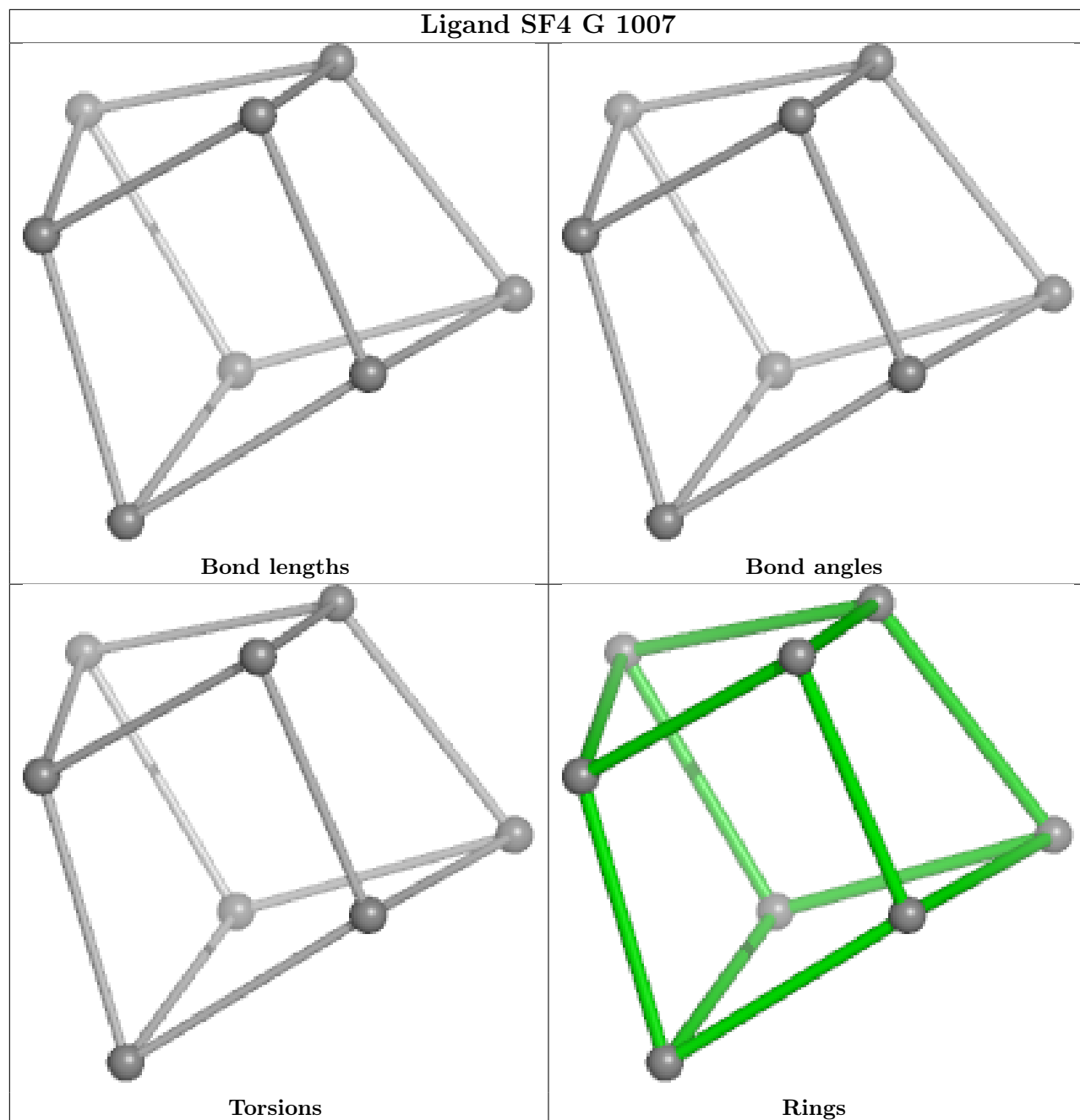


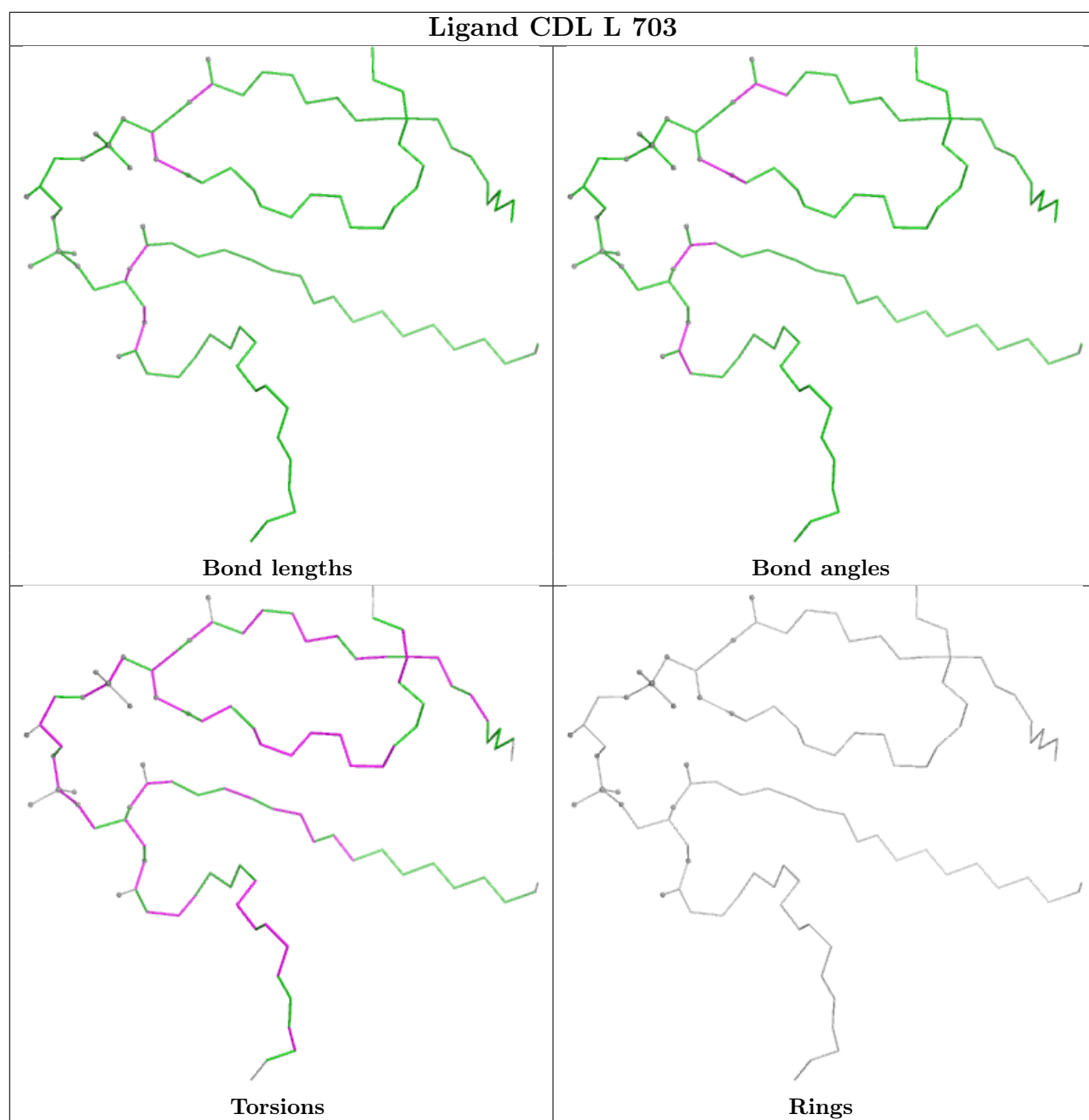


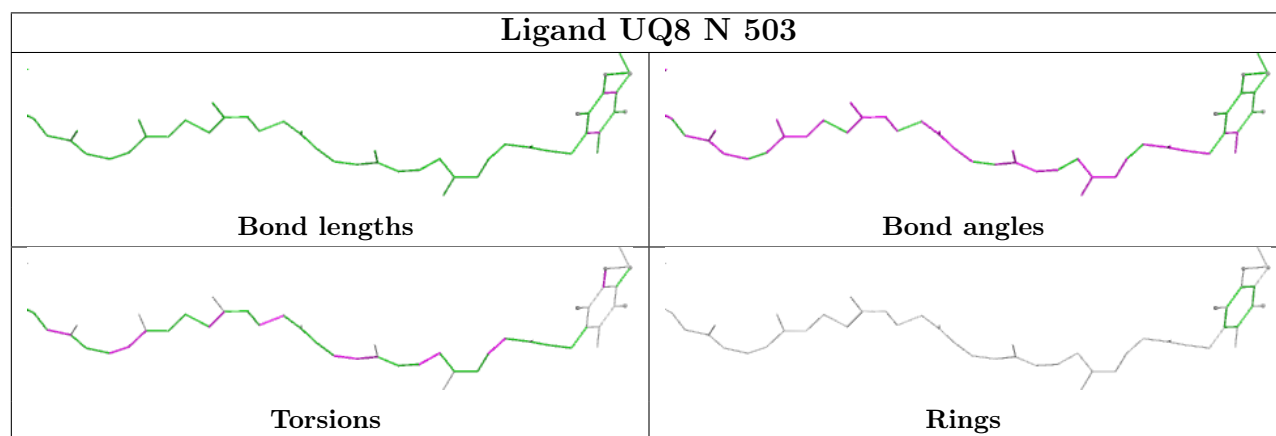
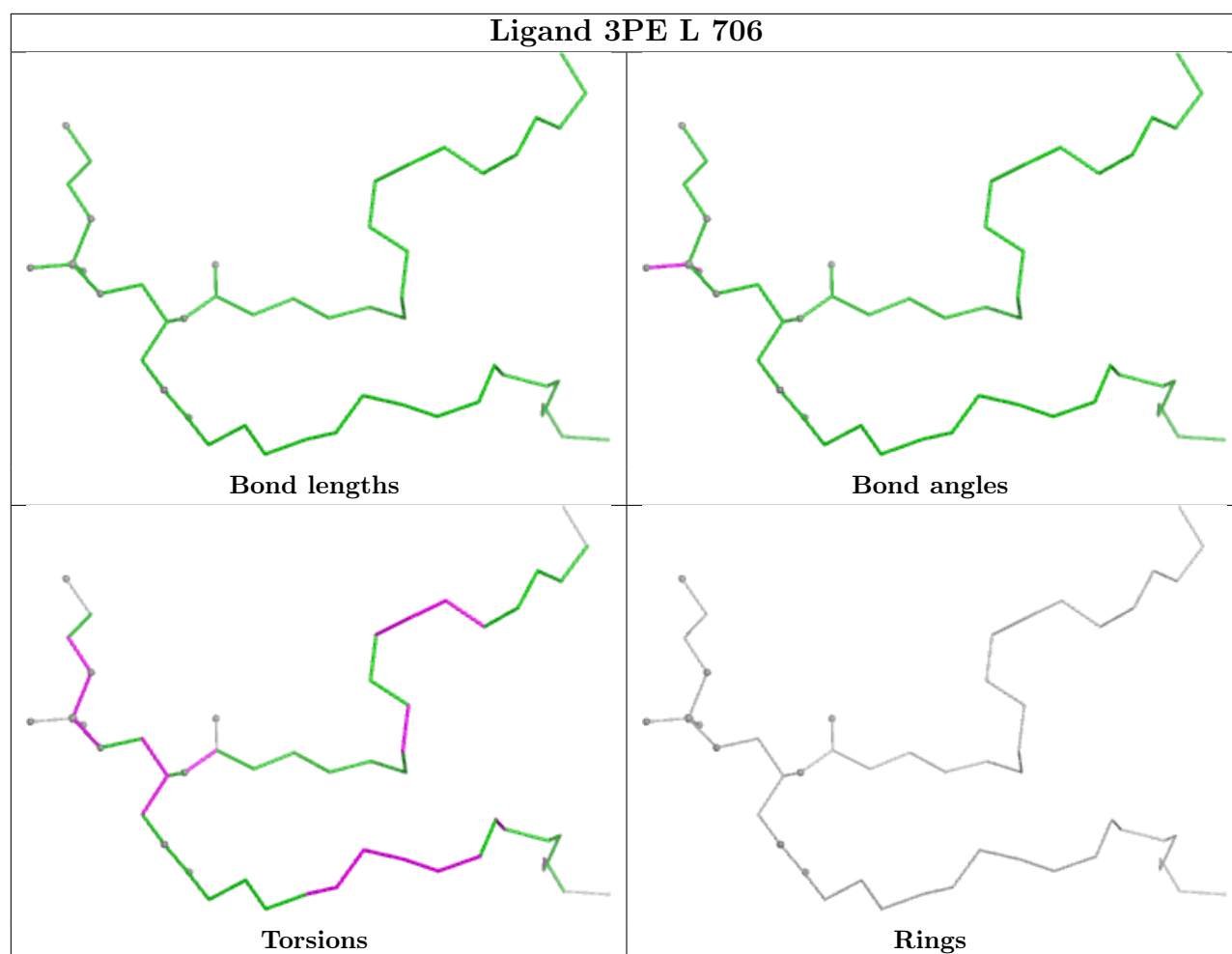


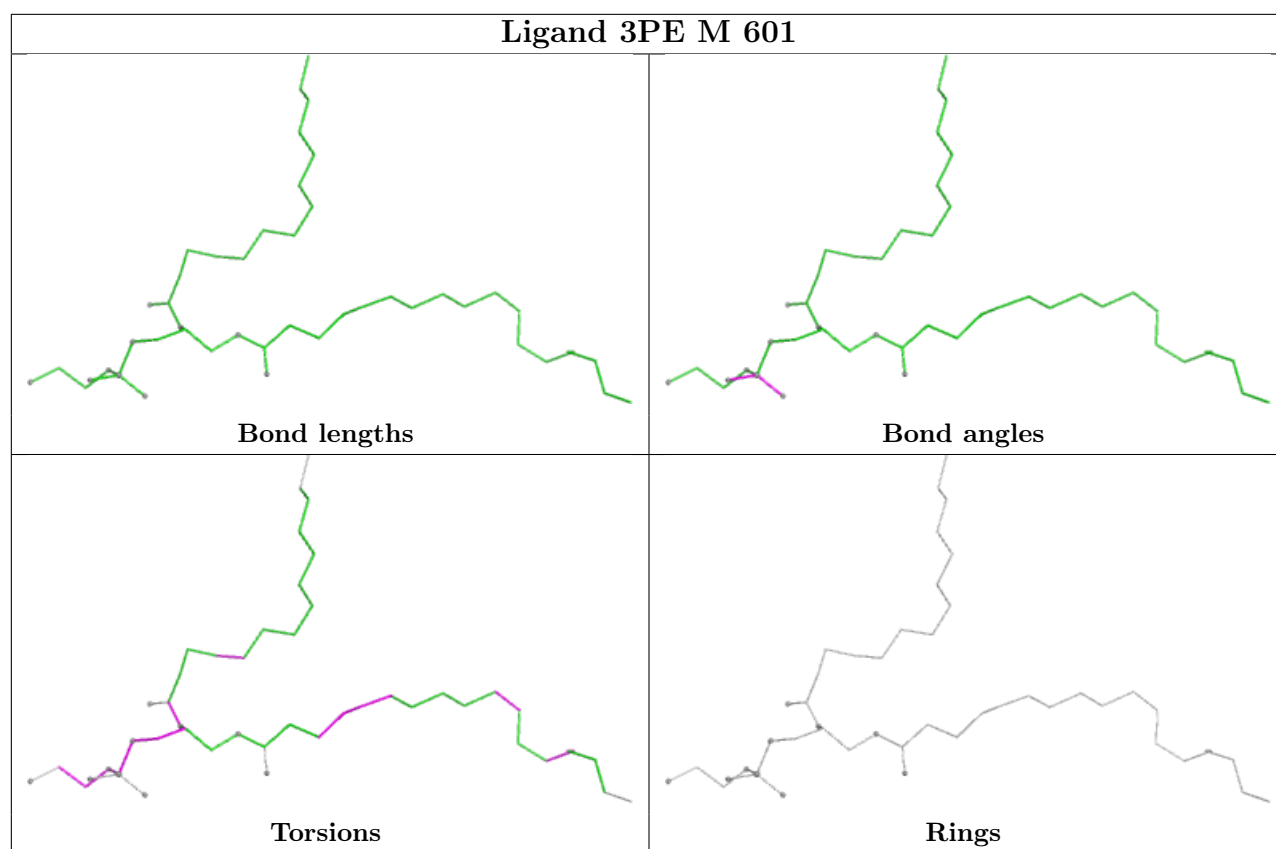












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



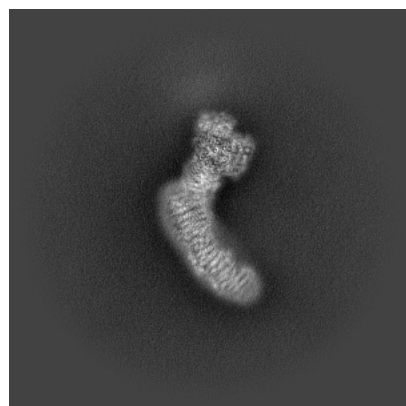
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55748. These allow visual inspection of the internal detail of the map and identification of artifacts.

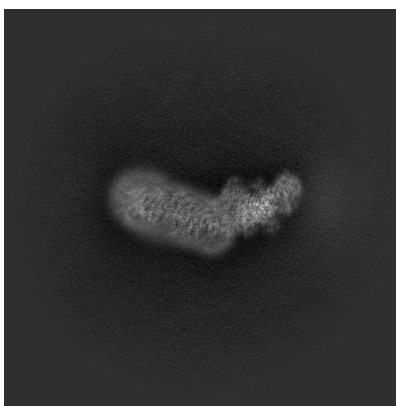
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

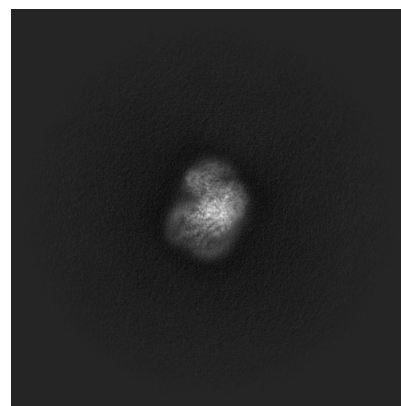
#### 6.1.1 Primary map



X

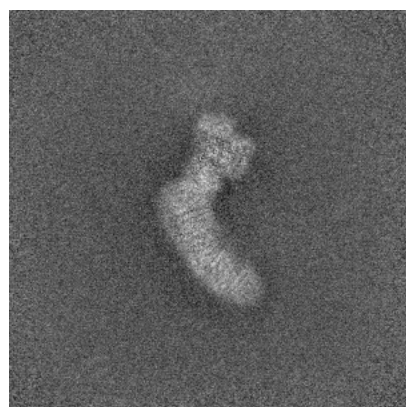


Y

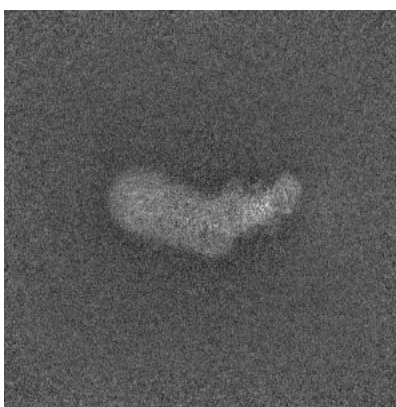


Z

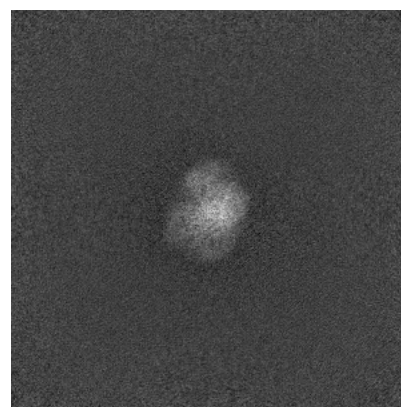
#### 6.1.2 Raw map



X



Y

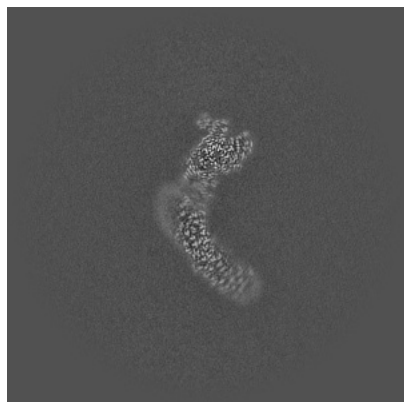


Z

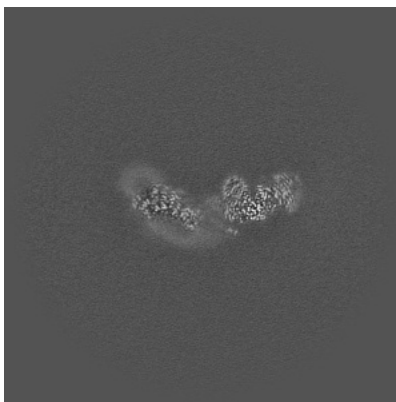
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

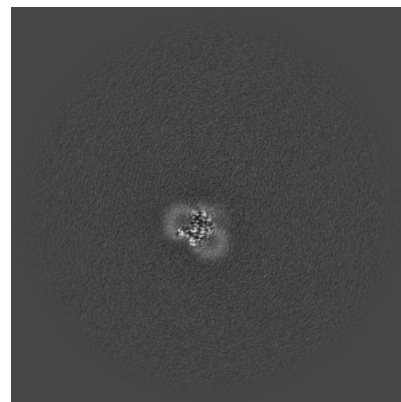
### 6.2.1 Primary map



X Index: 355

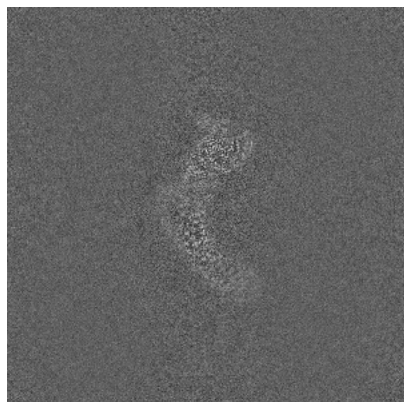


Y Index: 355

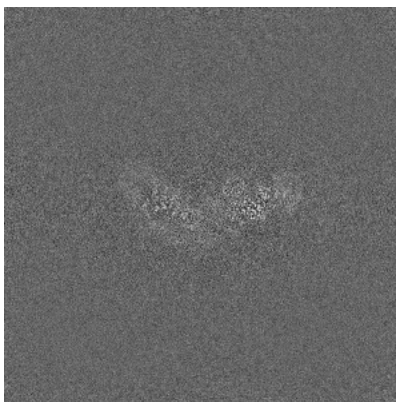


Z Index: 355

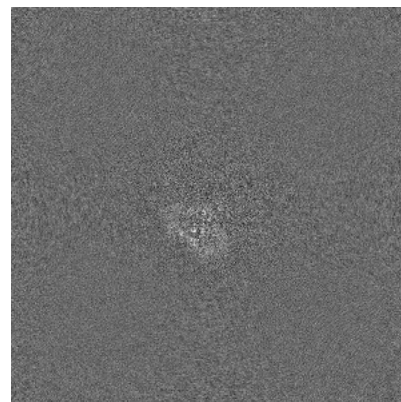
### 6.2.2 Raw map



X Index: 355



Y Index: 355



Z Index: 355

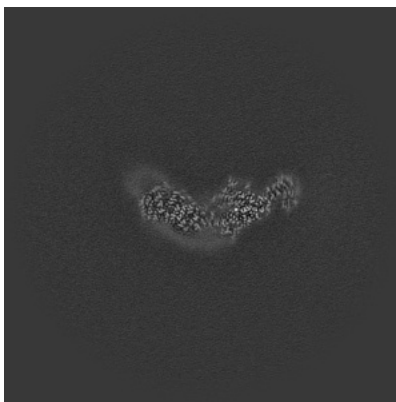
The images above show central slices of the map in three orthogonal directions.

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

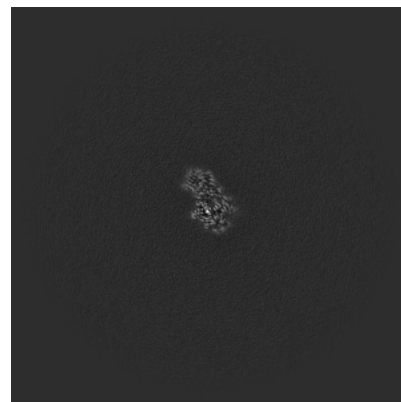
### 6.3.1 Primary map



X Index: 349

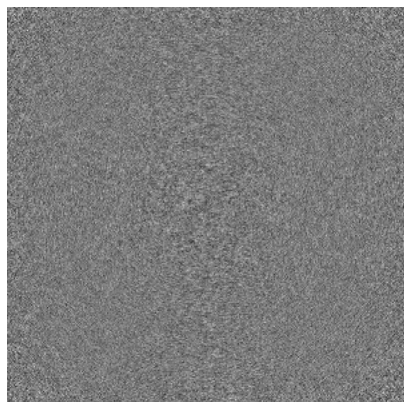


Y Index: 344

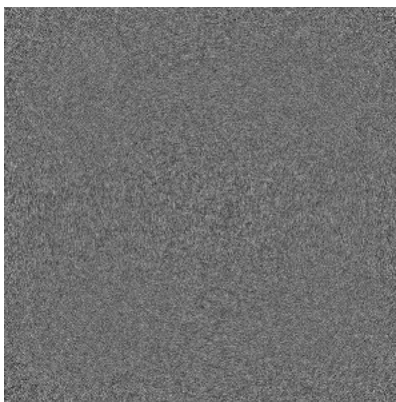


Z Index: 427

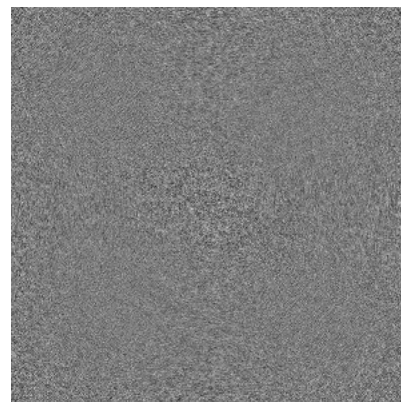
### 6.3.2 Raw map



X Index: 0



Y Index: 0



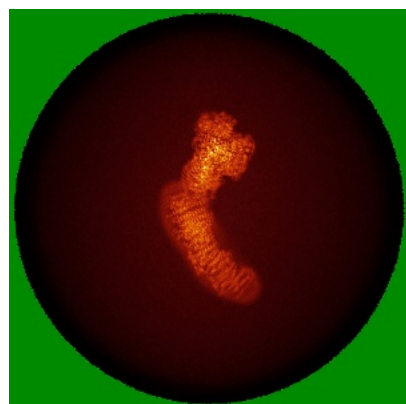
Z Index: 0

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

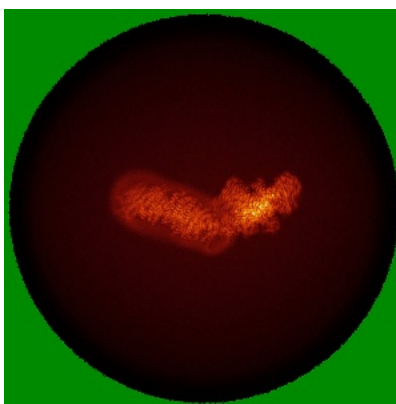


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

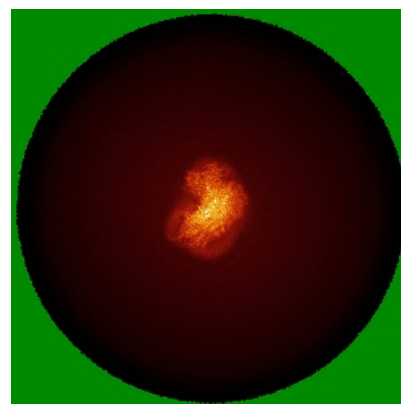
### 6.4.1 Primary map



X

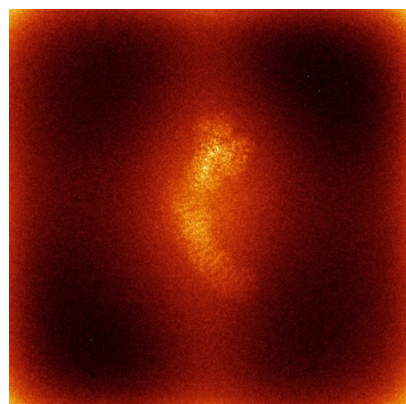


Y

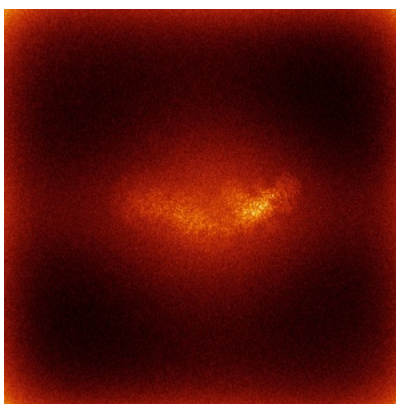


Z

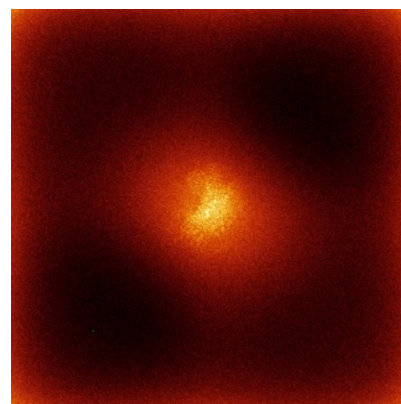
### 6.4.2 Raw map



X



Y

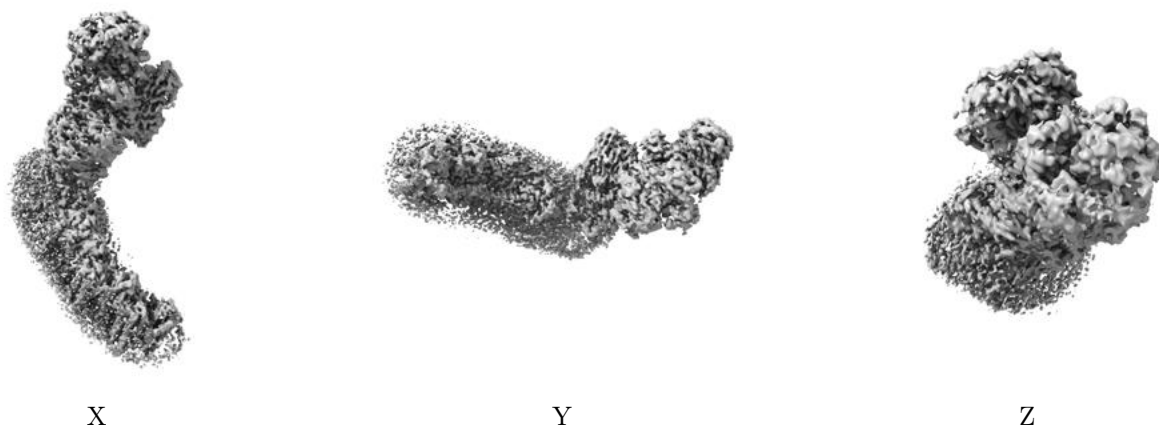


Z

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.

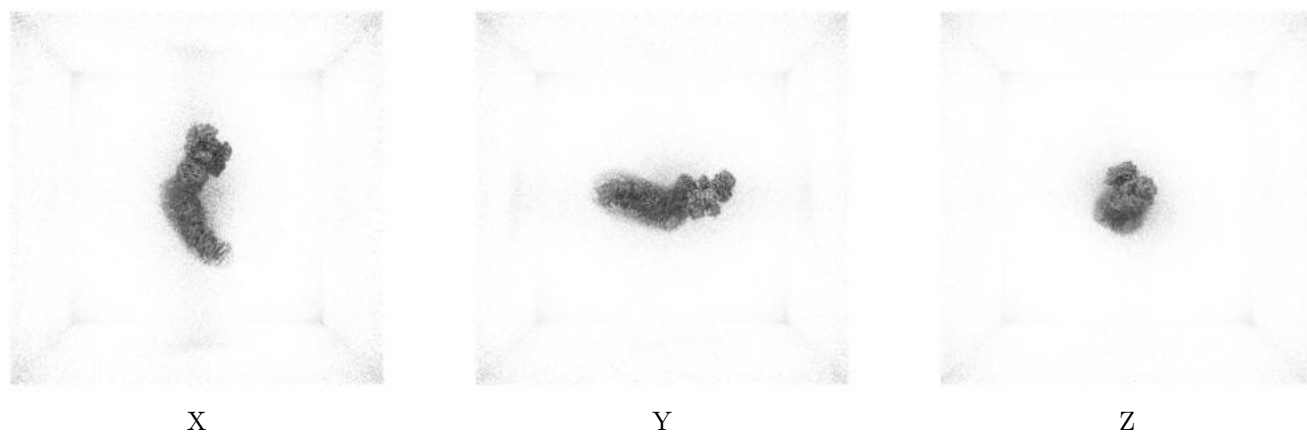
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.234. 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.

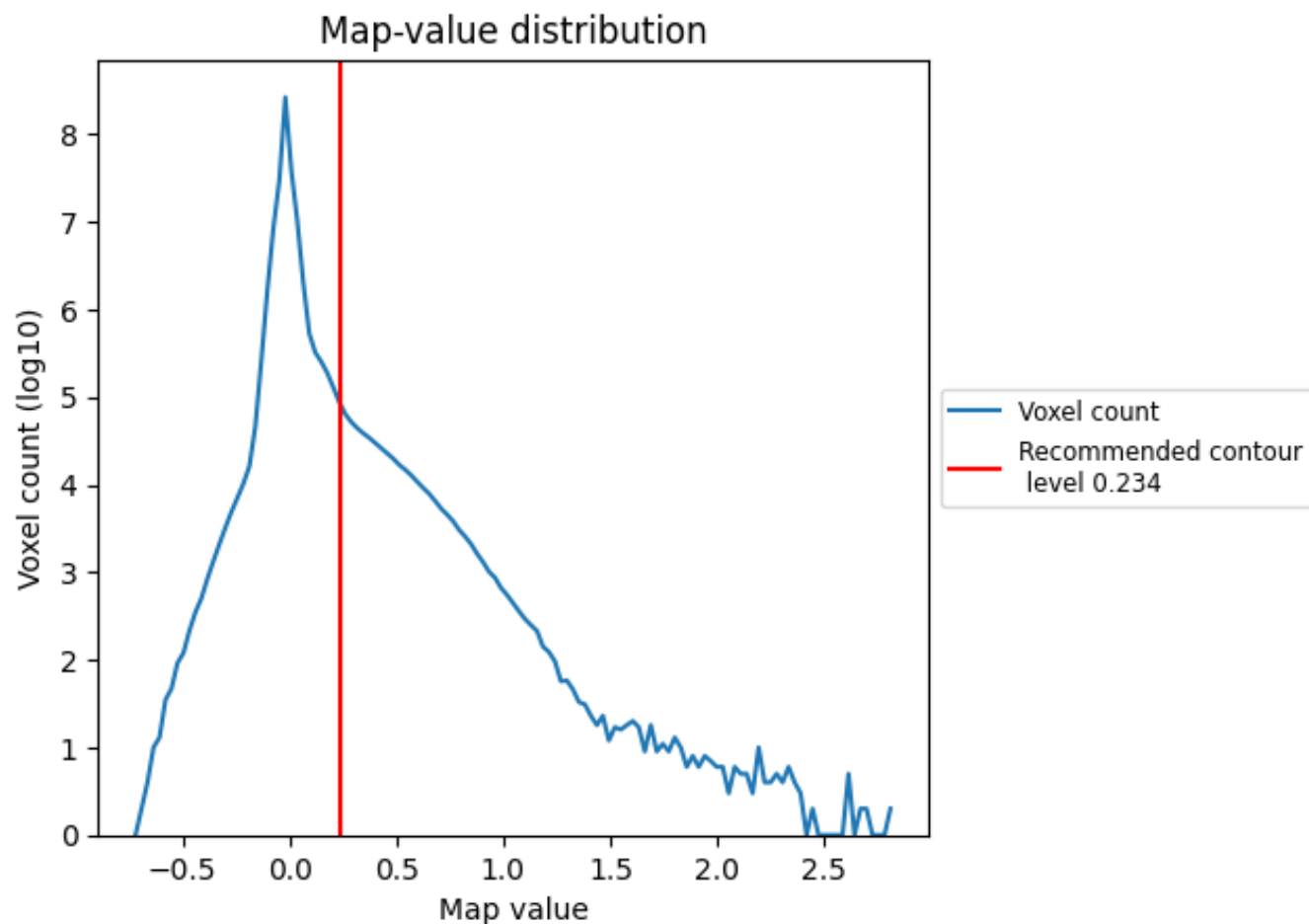
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

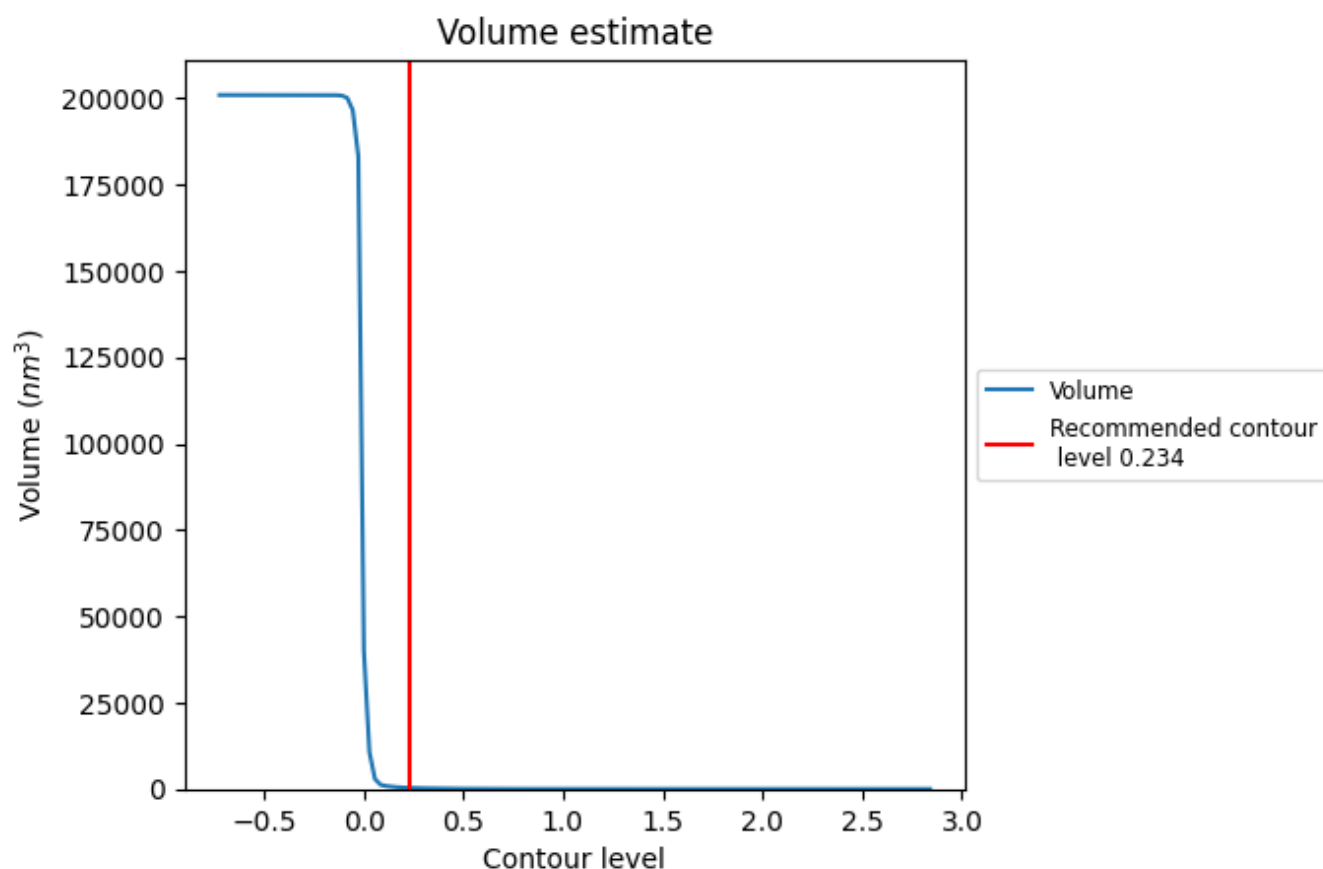
This section contains the results of statistical analysis of the map.

### 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.

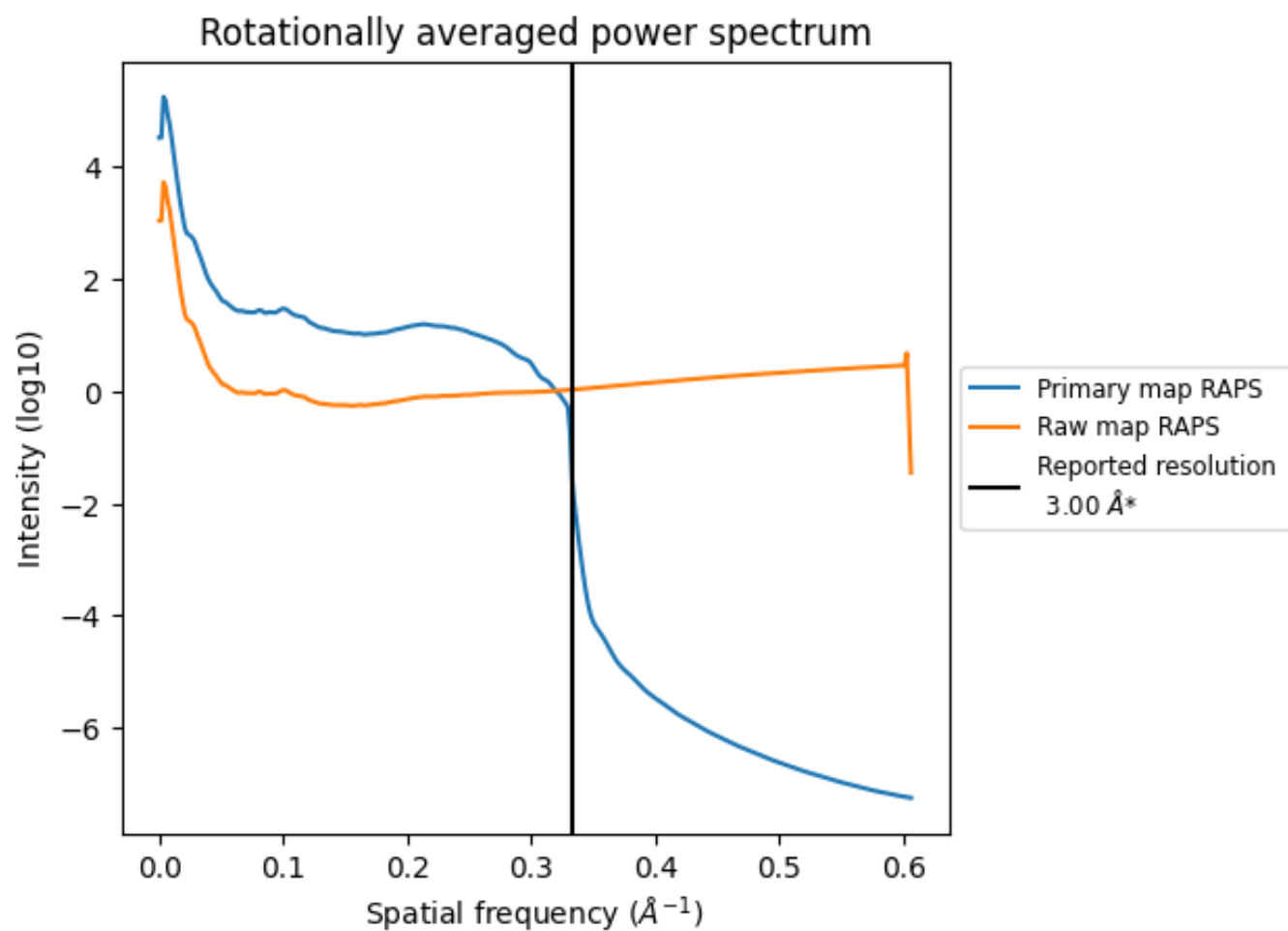
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296  $\text{nm}^3$ ; this corresponds to an approximate mass of 267 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 ⓘ



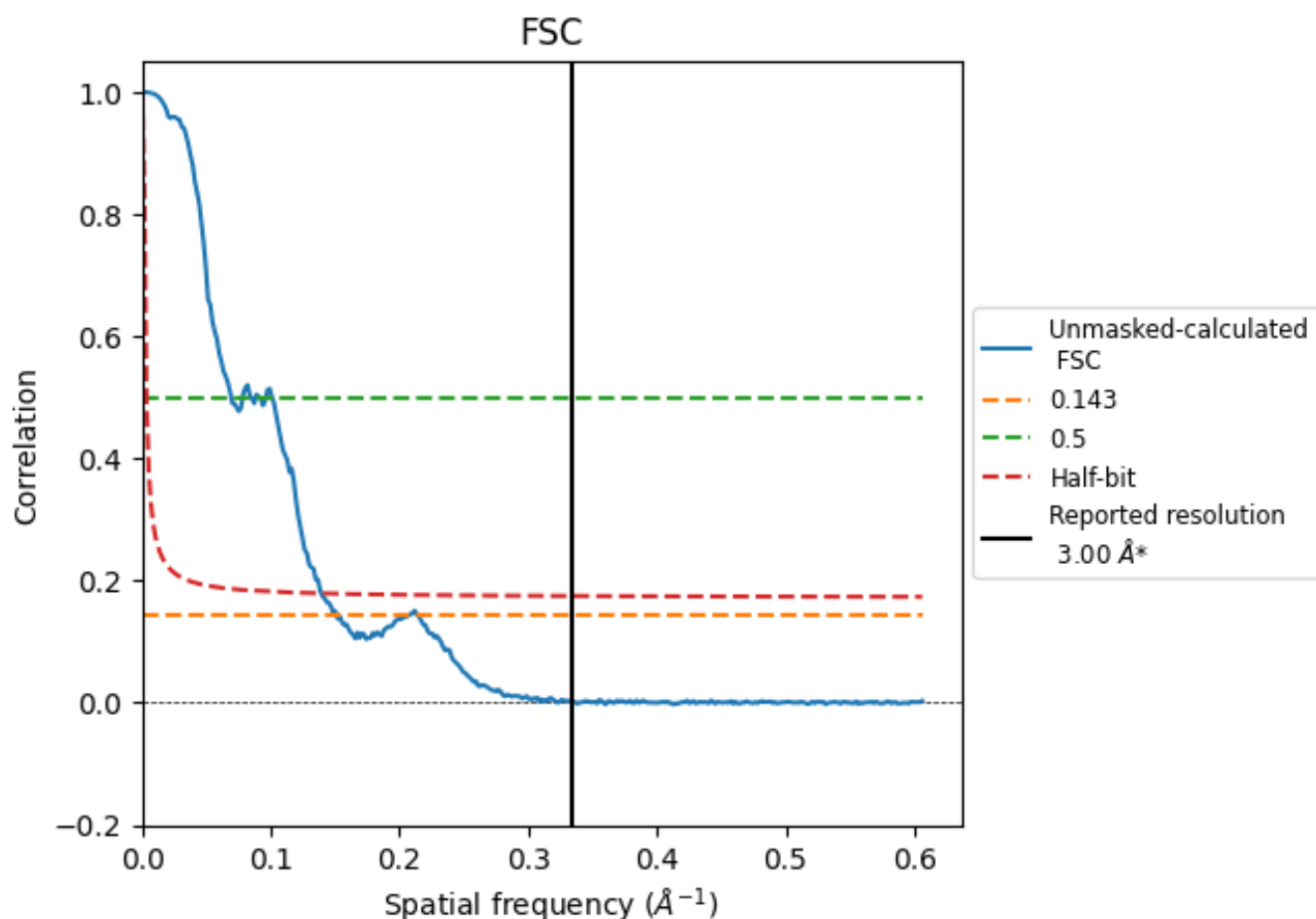
\*Reported resolution corresponds to spatial frequency of 0.333  $\text{\AA}^{-1}$



## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

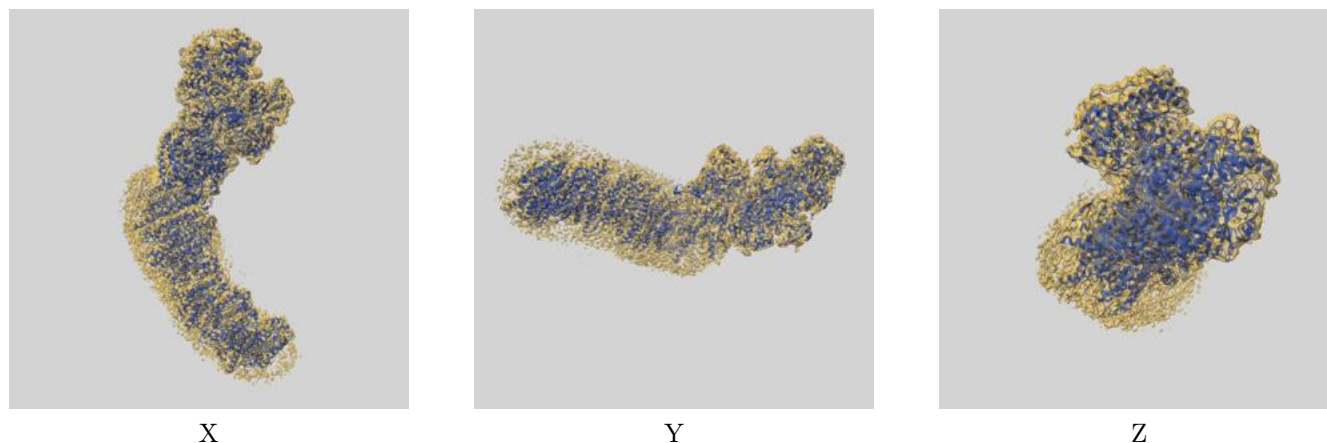
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.62	14.47	7.19

\*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 6.62 differs from the reported value 3.0 by more than 10 %

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

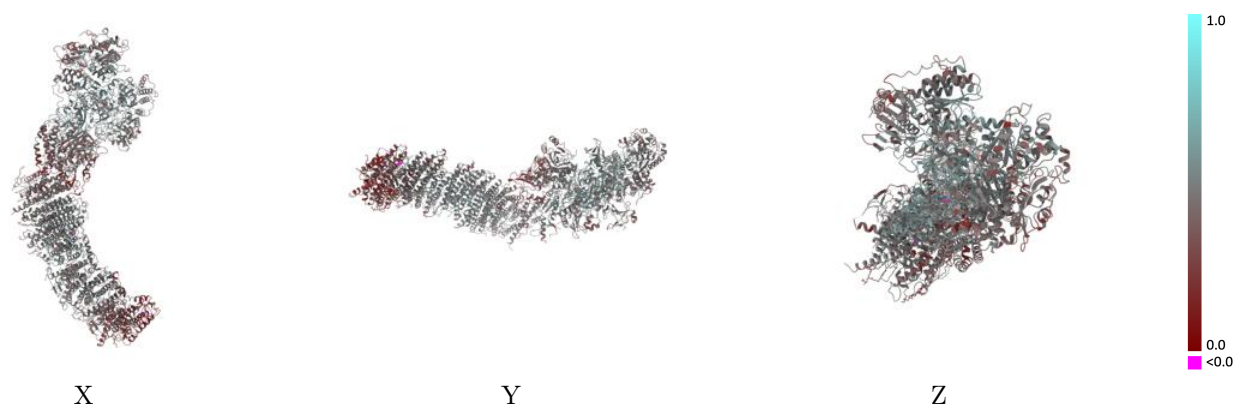
This section contains information regarding the fit between EMDB map EMD-55748 and PDB model 9TAJ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



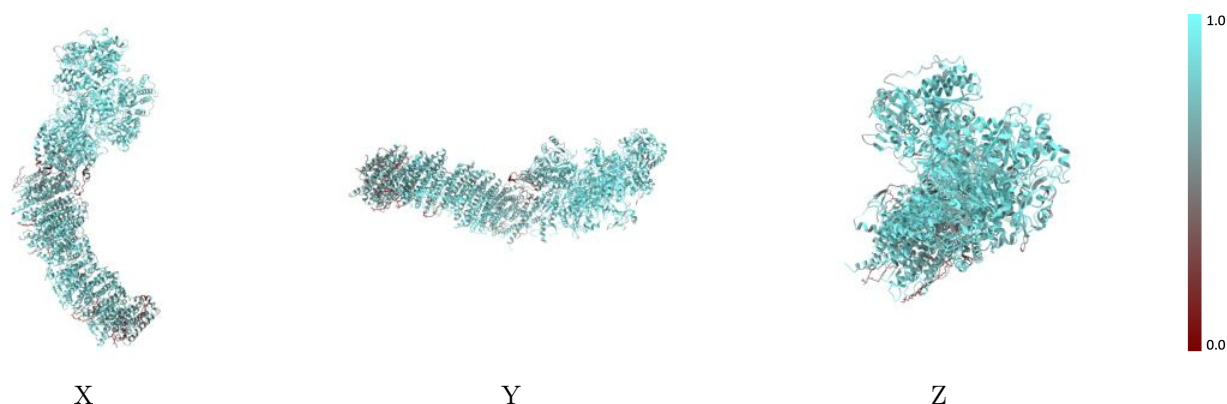
The images above show the 3D surface view of the map at the recommended contour level 0.234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



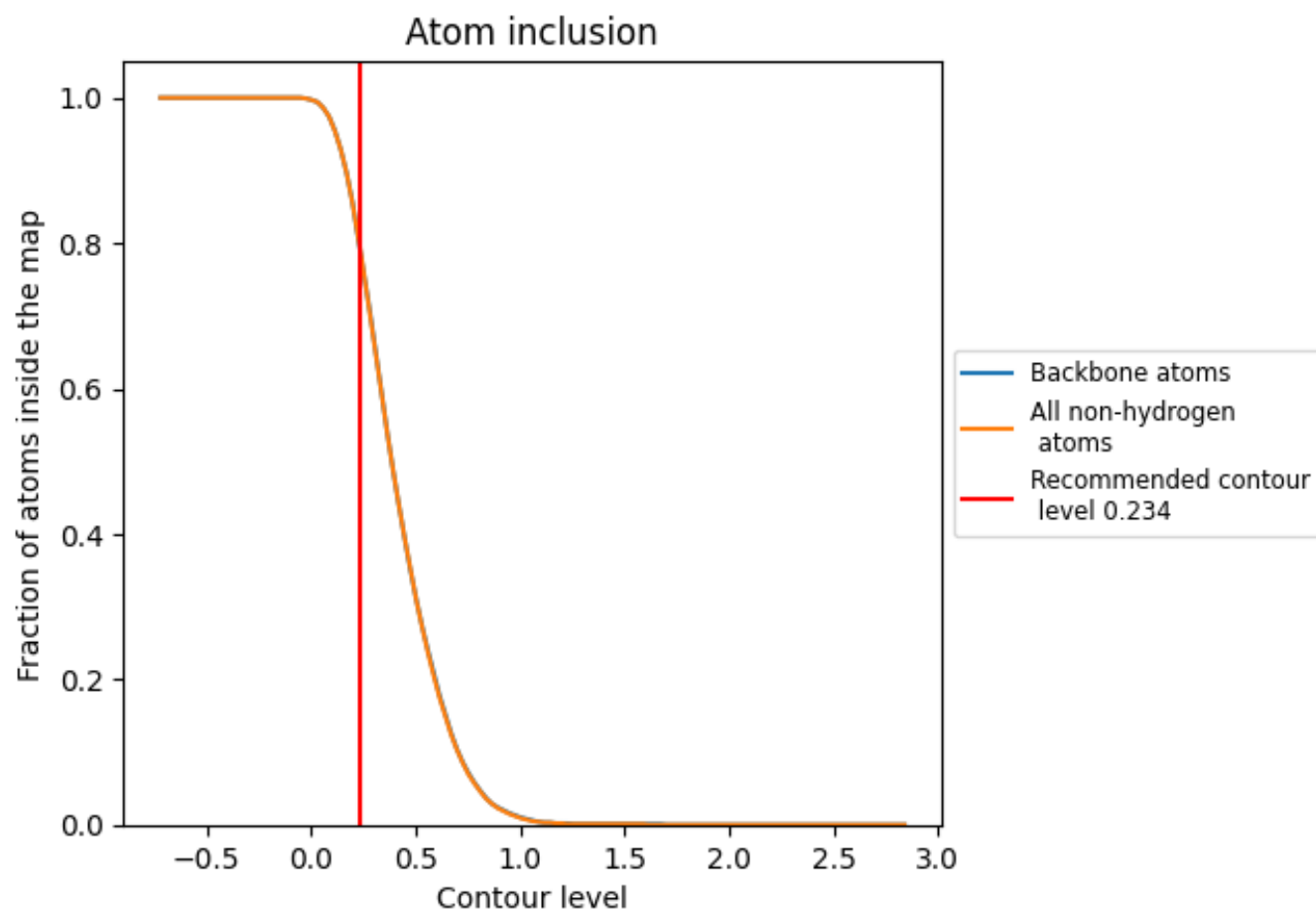
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.234).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.4470
A	 0.7450	 0.4380
B	 0.8300	 0.4730
C	 0.7700	 0.4010
E	 0.8200	 0.4330
F	 0.8310	 0.4550
G	 0.8850	 0.4990
H	 0.7460	 0.4060
I	 0.9300	 0.5450
J	 0.7900	 0.4710
K	 0.8540	 0.5000
L	 0.6450	 0.3470
M	 0.8000	 0.4670
N	 0.8270	 0.4850

