



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:51 AM JST

PDB ID : 7E1W
EMDB ID : EMD-30944
Title : Cryo-EM structure of hybrid respiratory supercomplex consisting of Mycobacterium tuberculosis complexIII and Mycobacterium smegmatis complexIV in the presence of Q203
Authors : Zhou, S.; Wang, W.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on : 2021-02-03
Resolution : 2.67 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

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>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

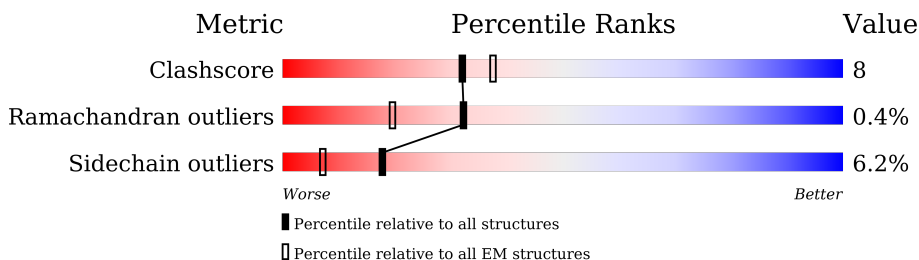
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 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.





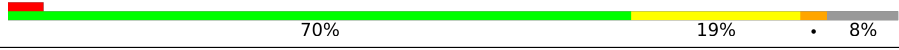



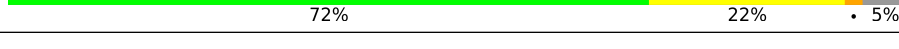
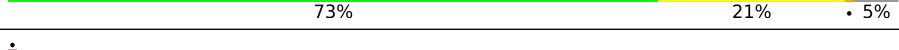
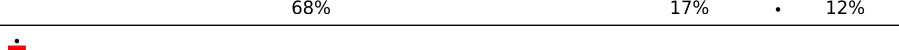
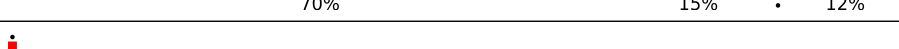

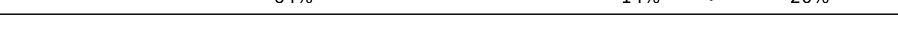
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	341	
1	Q	341	
2	F	575	
2	R	575	
3	G	203	
3	S	203	
4	H	139	
4	T	139	

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Mol	Chain	Length	Quality of chain
5	I	79	
5	U	79	
6	J	157	
6	V	157	
7	D	100	
7	P	100	
8	B	549	
8	N	549	
9	A	429	
9	M	429	
10	C	280	
10	O	280	

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
19	FES	A	501	-	-	X	-
19	FES	M	501	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 42695 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 Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	276	Total	C	N	O	S	0	0
			2191	1428	360	395	8		
1	Q	283	Total	C	N	O	S	0	0
			2242	1459	370	405	8		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		
2	R	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	186	Total	C	N	O	S	0	0
			1455	976	231	241	7		
3	S	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		

- Molecule 4 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
4	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 5 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	67	Total	C	N	O	S	0	0
			507	334	85	86	2		
5	U	67	Total	C	N	O	S	0	0
			507	334	85	86	2		

- Molecule 6 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		
6	V	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		

- Molecule 7 is a protein called Prokaryotic respiratory supercomplex associate factor 1 PRSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	76	Total	C	N	O	S	0	0
			607	397	112	94	4		
7	P	75	Total	C	N	O	S	0	0
			597	391	109	93	4		

- Molecule 8 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	524	Total	C	N	O	S	0	0
			4140	2734	707	682	17		
8	B	524	Total	C	N	O	S	0	0
			4140	2734	707	682	17		

- Molecule 9 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	378	Total	C	N	O	S	0	0
			2943	1900	501	531	11		
9	A	378	Total	C	N	O	S	0	0
			2943	1900	501	531	11		

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	223	Total	C	N	O	S	0	0
			1628	1018	293	306	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	218	Total	C	N	O	S	0	0
			1590	997	284	298	11		

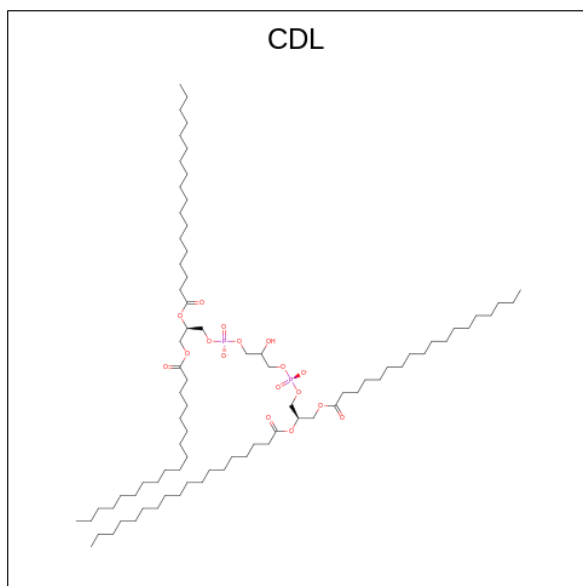
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	LEU	-	expression tag	UNP P9WP35
C	1	LEU	-	expression tag	UNP P9WP35

- Molecule 11 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
11	E	2	Total	Cu	0
			2	2	
11	F	2	Total	Cu	0
			2	2	
11	Q	2	Total	Cu	0
			2	2	
11	R	2	Total	Cu	0
			2	2	

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



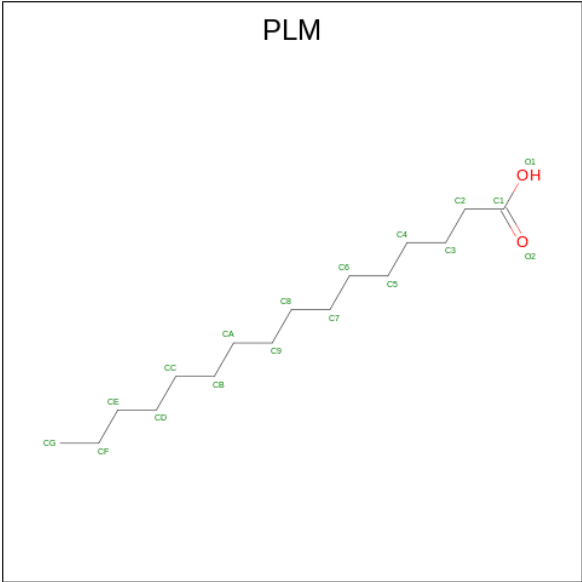
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total	C	O	P	0
			76	57	17	2	

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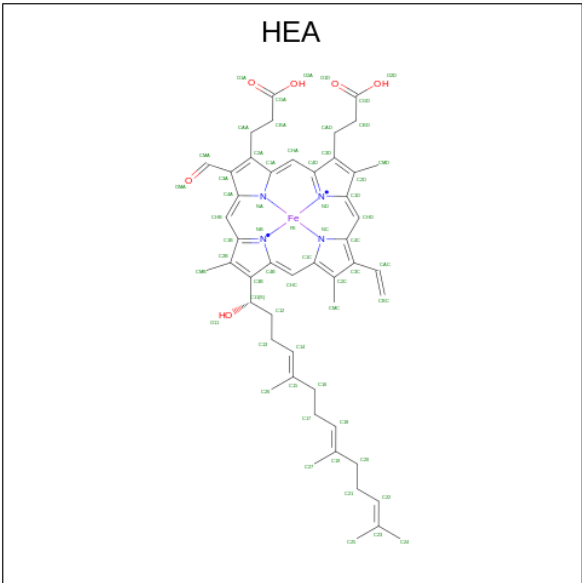
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total	C	O	P	0
			81	62	17	2	
12	D	1	Total	C	O	P	0
			88	69	17	2	
12	R	1	Total	C	O	P	0
			76	57	17	2	
12	R	1	Total	C	O	P	0
			81	62	17	2	
12	P	1	Total	C	O	P	0
			88	69	17	2	
12	N	1	Total	C	O	P	0
			74	55	17	2	
12	N	1	Total	C	O	P	0
			77	58	17	2	
12	N	1	Total	C	O	P	0
			79	60	17	2	
12	M	1	Total	C	O	P	0
			95	76	17	2	
12	O	1	Total	C	O	P	0
			79	60	17	2	
12	B	1	Total	C	O	P	0
			79	60	17	2	
12	B	1	Total	C	O	P	0
			66	47	17	2	
12	B	1	Total	C	O	P	0
			74	55	17	2	
12	B	1	Total	C	O	P	0
			77	58	17	2	
12	B	1	Total	C	O	P	0
			79	60	17	2	
12	A	1	Total	C	O	P	0
			95	76	17	2	

- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



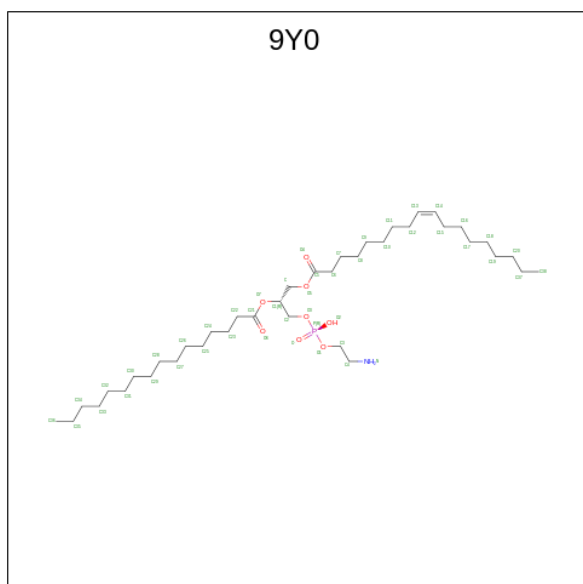
Mol	Chain	Residues	Atoms			AltConf
13	F	1	Total	C	O	0
			17	16	1	
13	R	1	Total	C	O	0
			17	16	1	
13	N	1	Total	C	O	0
			11	10	1	
13	B	1	Total	C	O	0
			11	10	1	

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



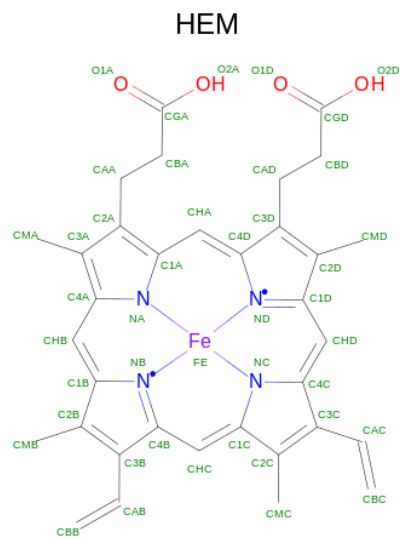
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 15 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (three-letter code: 9Y0) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



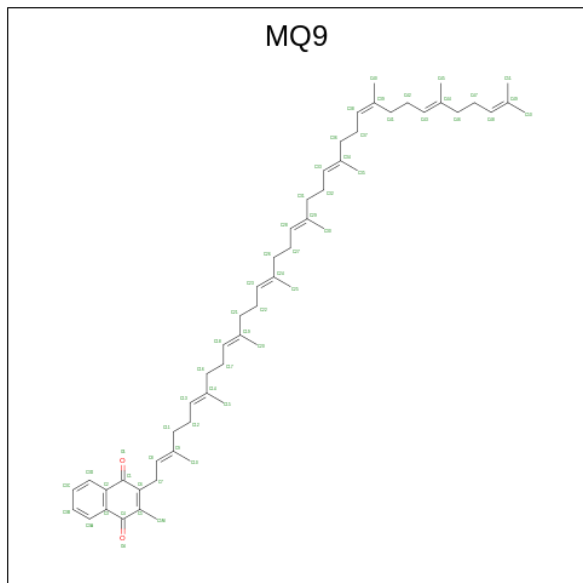
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



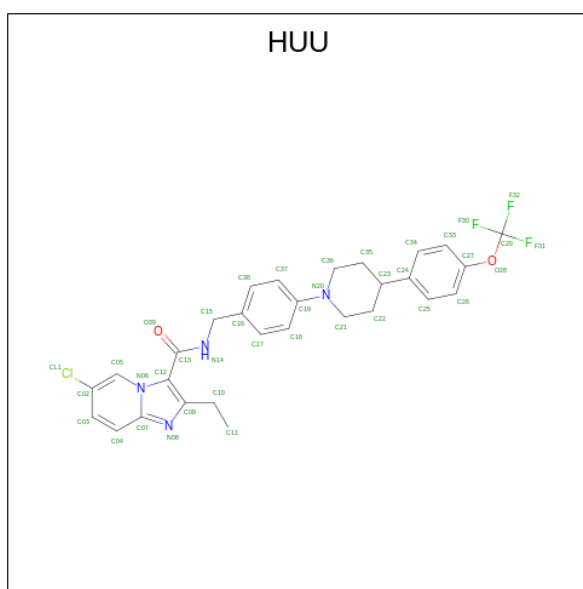
Mol	Chain	Residues	Atoms					AltConf
16	N	1	Total 42	C 33	Fe 1	N 4	O 4	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
16	B	1	Total 42	C 33	Fe 1	N 4	O 4	0
16	B	1	Total 43	C 34	Fe 1	N 4	O 4	0

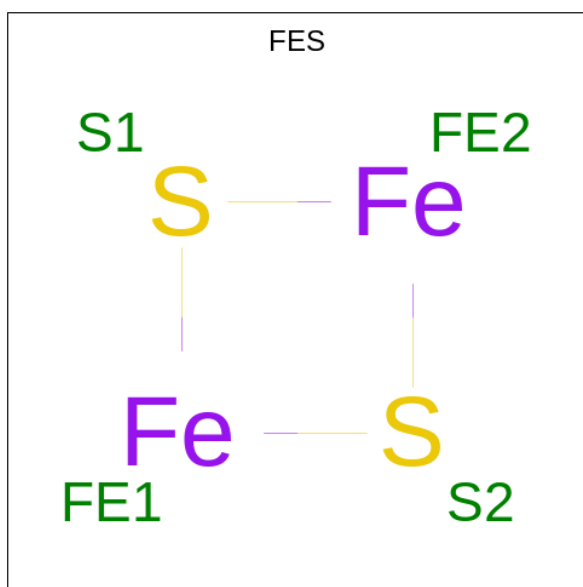
- Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $\text{C}_{56}\text{H}_{80}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	N	1	Total	C	O	0
			58	56	2	
17	N	1	Total	C	O	0
			58	56	2	
17	O	1	Total	C	O	0
			48	46	2	
17	O	1	Total	C	O	0
			58	56	2	
17	B	1	Total	C	O	0
			43	41	2	
17	B	1	Total	C	O	0
			58	56	2	
17	A	1	Total	C	O	0
			43	41	2	
17	C	1	Total	C	O	0
			48	46	2	

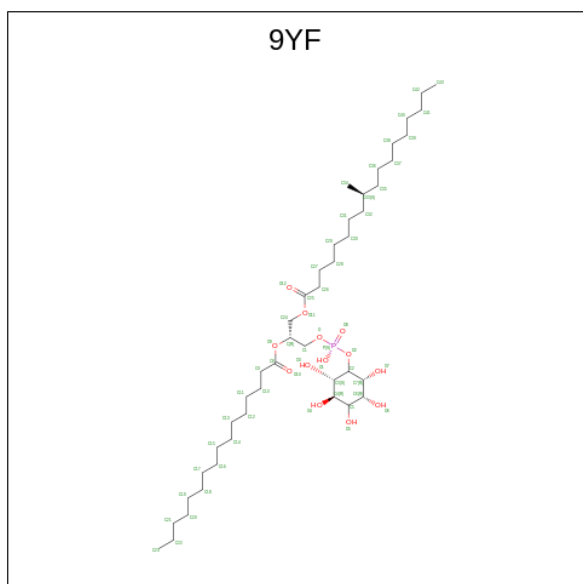
- Molecule 18 is 6-chloranyl-2-ethyl-N-[[4-[4-(trifluoromethoxy)phenyl]piperidin-1-yl]phenyl)methyl]imidazo[1,2-a]pyridine-3-carboxamide (three-letter code: HUU) (formula: C₂₉H₂₈ClF₃N₄O₂) (labeled as "Ligand of Interest" by depositor).





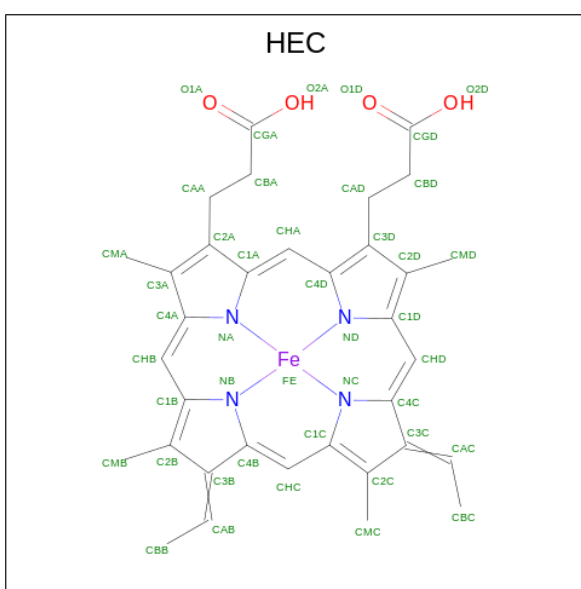
Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	Fe	S	0
			4	2	2	
19	A	1	Total	Fe	S	0
			4	2	2	

- Molecule 20 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: C₄₄H₈₅O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total 44	C 30	O 13	P 1	0
20	M	1	Total 40	C 26	O 13	P 1	0
20	A	1	Total 51	C 37	O 13	P 1	0
20	A	1	Total 42	C 28	O 13	P 1	0

- Molecule 21 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
21	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
21	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
21	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

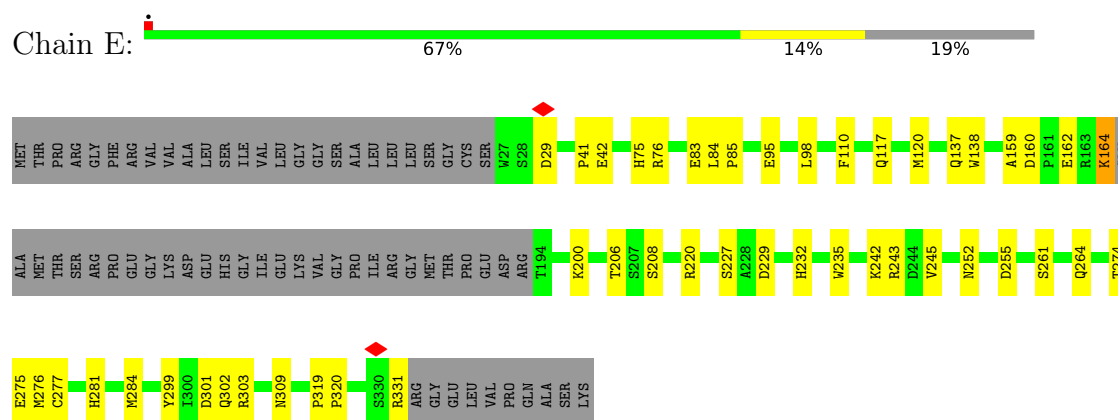
- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	N	1	Total O 1 1	0

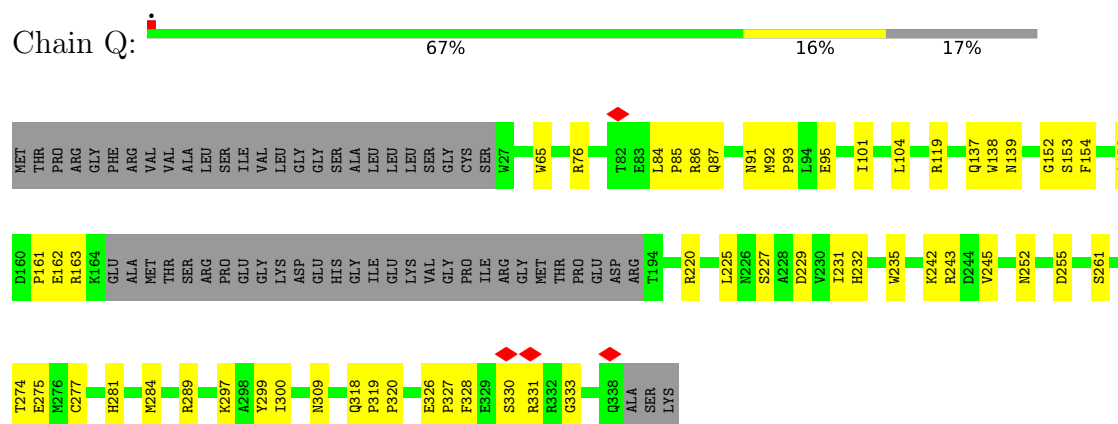
3 Residue-property plots

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.

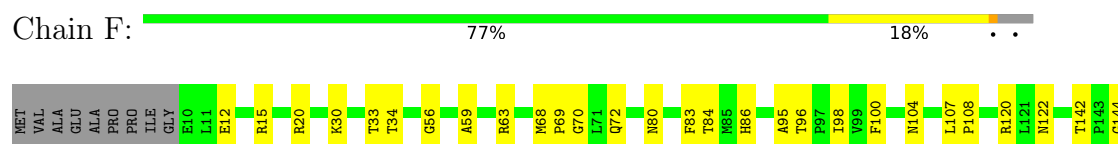
• Molecule 1: Cytochrome c oxidase subunit 2

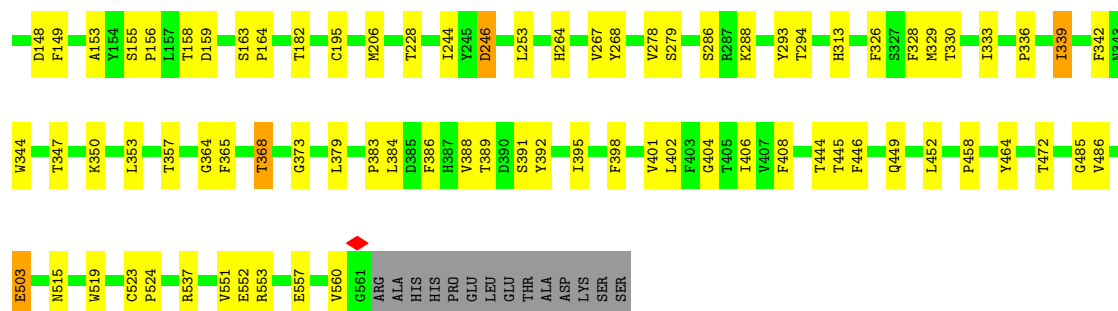


• Molecule 1: Cytochrome c oxidase subunit 2



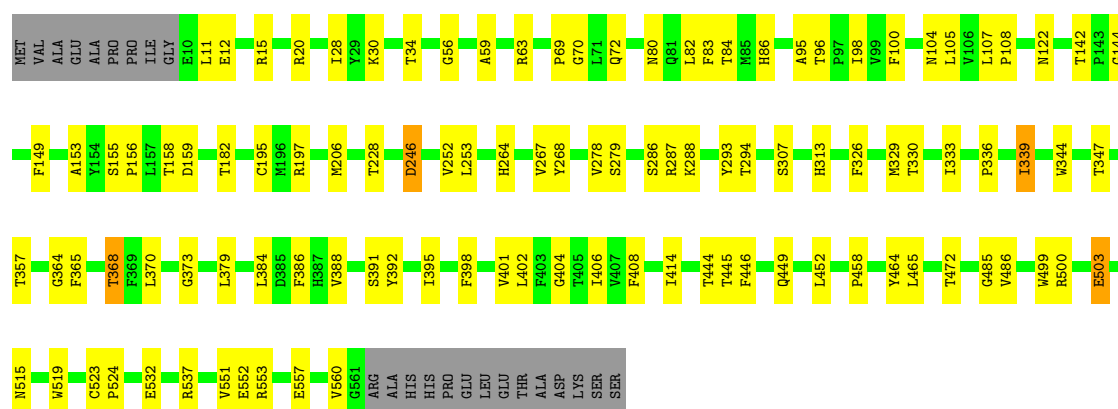
• Molecule 2: Cytochrome c oxidase subunit 1





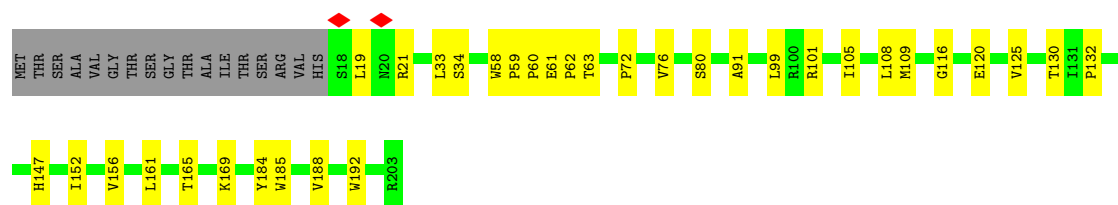
• Molecule 2: Cytochrome c oxidase subunit 1

Chain R: 77% 18%



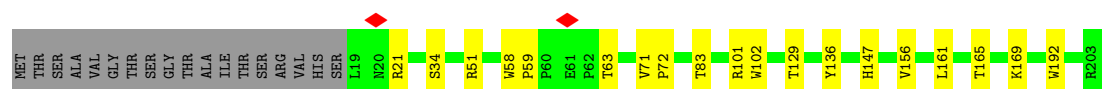
• Molecule 3: Cytochrome c oxidase subunit 3

Chain G: 74% 17% 8%



• Molecule 3: Cytochrome c oxidase subunit 3

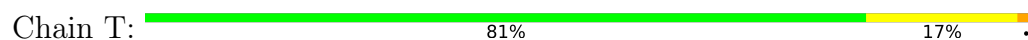
Chain S: 82% 9% 9%



• Molecule 4: Cytochrome c oxidase polypeptide 4

Chain H: 83% 15%

- Molecule 4: Cytochrome c oxidase polypeptide 4



- Molecule 5: Cytochrome c oxidase subunit CtaJ



- Molecule 5: Cytochrome c oxidase subunit CtaJ



- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

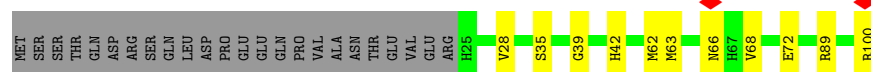


- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575



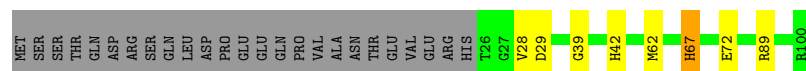
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain D:  65% 11% 24%



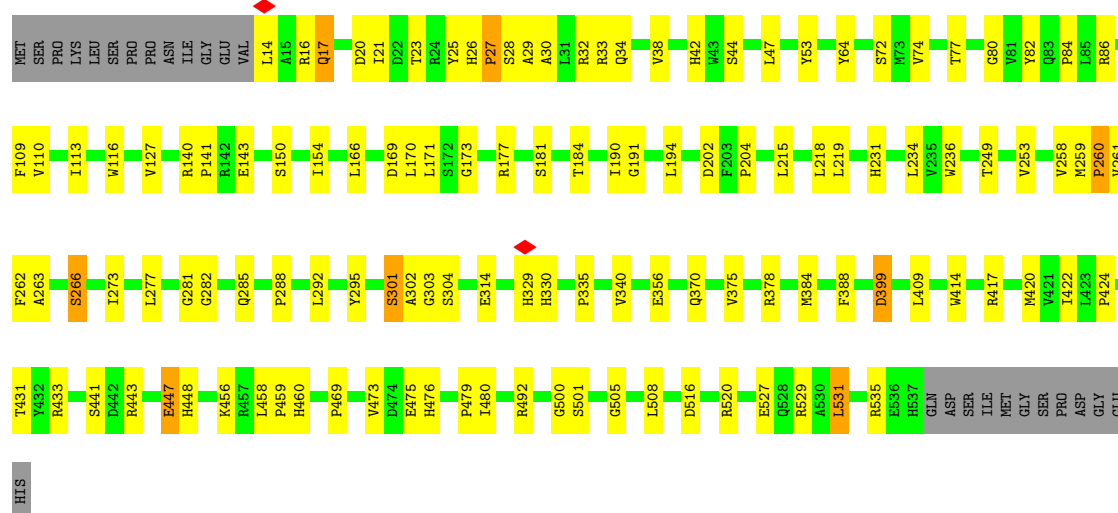
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain P:  67% 7% 25%



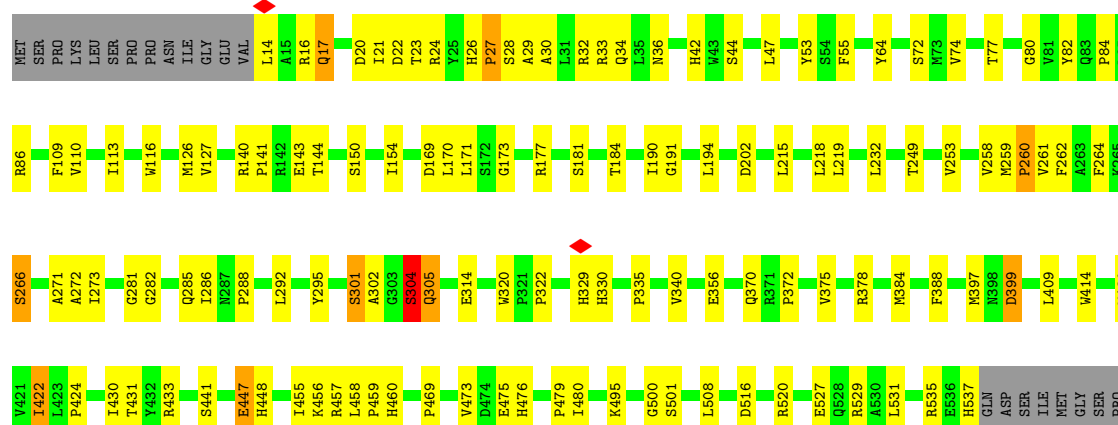
- Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain N:  73% 21% 5%



- Molecule 8: Cytochrome bc1 complex cytochrome b subunit

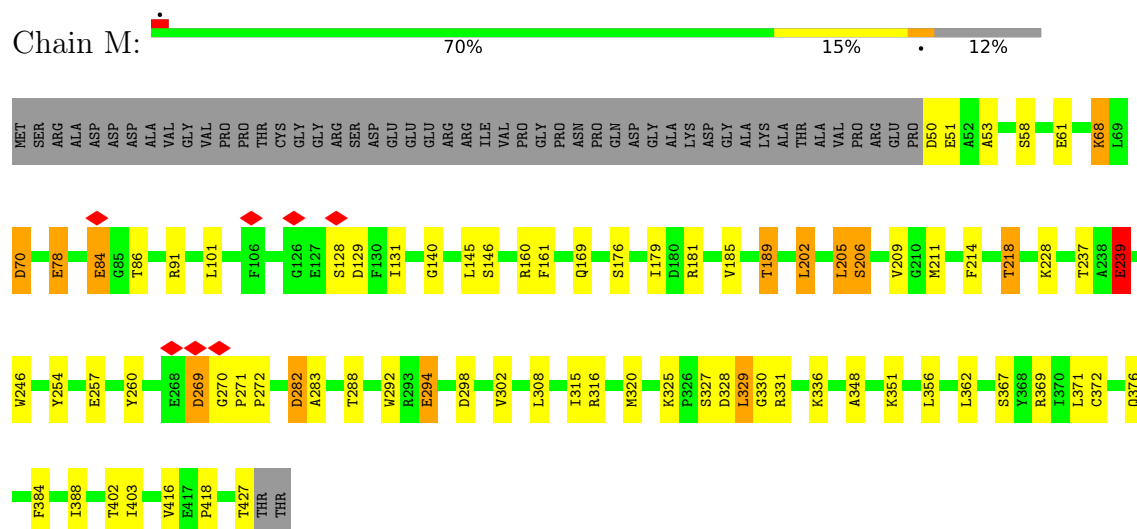
Chain B:  72% 22% 5%



ASP
GLY
GLU
HIS

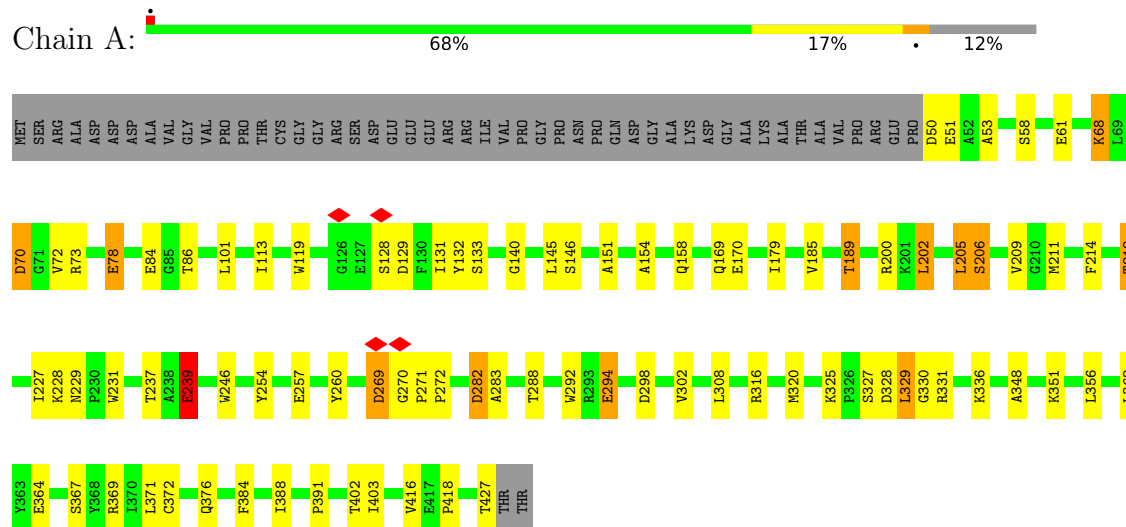
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M:



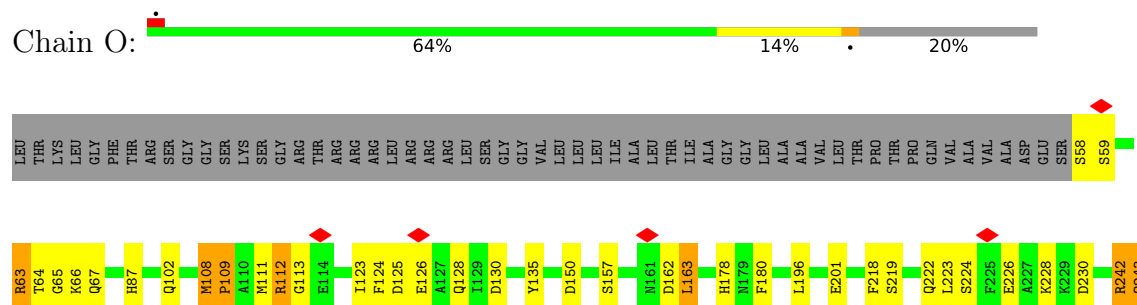
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A:



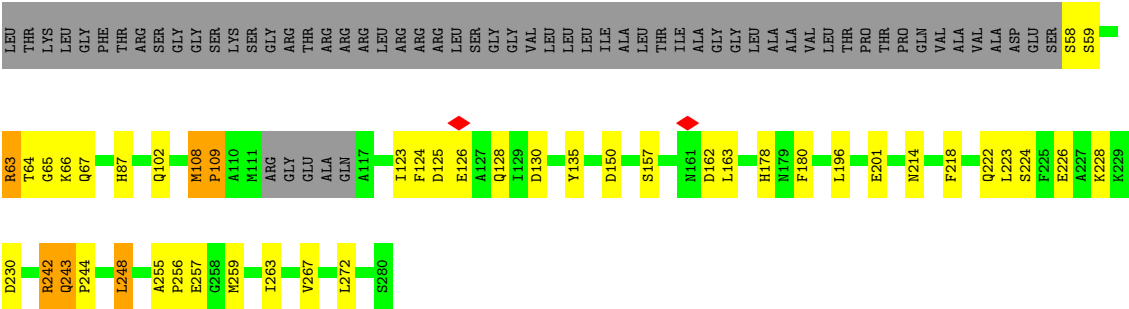
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain O:





• Molecule 10: Cytochrome bc1 complex cytochrome c subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106770	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.828	Depositor
Minimum map value	-1.206	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HUU, 9Y0, HEM, 9YF, CDL, MQ9, FES, PLM, HEC, HEA

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	0.30	0/2254	0.46	0/3072
1	Q	0.32	0/2306	0.47	0/3144
2	F	0.34	0/4533	0.48	0/6192
2	R	0.34	0/4533	0.48	0/6192
3	G	0.34	0/1502	0.49	0/2051
3	S	0.35	0/1496	0.48	0/2043
4	H	0.33	0/1112	0.47	0/1524
4	T	0.33	0/1112	0.47	0/1524
5	I	0.29	0/523	0.58	0/714
5	U	0.29	0/523	0.58	0/714
6	J	0.36	0/1059	0.56	0/1446
6	V	0.36	0/1059	0.56	0/1446
7	D	0.27	0/628	0.43	0/855
7	P	0.29	0/617	0.50	1/840 (0.1%)
8	B	0.34	0/4276	0.57	3/5833 (0.1%)
8	N	0.34	0/4276	0.50	2/5833 (0.0%)
9	A	0.33	0/3020	0.51	1/4094 (0.0%)
9	M	0.33	0/3020	0.51	1/4094 (0.0%)
10	C	0.31	0/1622	0.54	0/2195
10	O	0.31	0/1661	0.54	0/2248
All	All	0.33	0/41132	0.51	8/56054 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	C	0	1
10	O	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	304	SER	CB-CA-C	19.73	147.59	110.10
8	B	305	GLN	N-CA-CB	11.52	131.33	110.60
8	N	304	SER	N-CA-CB	-8.55	97.67	110.50
8	N	303	GLY	N-CA-C	-8.44	92.01	113.10
8	B	304	SER	N-CA-C	-6.64	93.07	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	C	108	MET	Peptide
10	O	108	MET	Peptide

5.2 Too-close contacts [i](#)

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	2191	0	2129	38	0
1	Q	2242	0	2175	41	0
2	F	4373	0	4347	66	0
2	R	4373	0	4347	83	0
3	G	1455	0	1455	23	0
3	S	1449	0	1450	15	0
4	H	1077	0	1058	11	0
4	T	1077	0	1058	15	0
5	I	507	0	516	8	0
5	U	507	0	516	11	0
6	J	1041	0	1052	19	0
6	V	1041	0	1052	22	0
7	D	607	0	594	9	0
7	P	597	0	586	7	0
8	B	4140	0	4163	87	0
8	N	4140	0	4165	75	0
9	A	2943	0	2931	80	0
9	M	2943	0	2931	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	1590	0	1572	36	0
10	O	1628	0	1608	34	0
11	E	2	0	0	0	0
11	F	2	0	0	0	0
11	Q	2	0	0	0	0
11	R	2	0	0	0	0
12	A	95	0	143	4	0
12	B	375	0	476	12	0
12	D	88	0	126	5	0
12	F	157	0	208	3	0
12	M	95	0	143	2	0
12	N	230	0	295	8	0
12	O	79	0	105	2	0
12	P	88	0	126	6	0
12	R	157	0	208	7	0
13	B	11	0	16	0	0
13	F	17	0	31	0	0
13	N	11	0	16	0	0
13	R	17	0	31	0	0
14	F	120	0	104	14	0
14	R	120	0	104	14	0
15	G	43	0	0	0	0
15	S	43	0	0	0	0
16	B	85	0	57	6	0
16	N	85	0	57	5	0
17	A	43	0	53	5	0
17	B	101	0	133	18	0
17	C	48	0	61	5	0
17	N	116	0	158	8	0
17	O	106	0	141	12	0
18	B	39	0	0	0	0
18	N	39	0	0	1	0
19	A	4	0	0	3	0
19	M	4	0	0	2	0
20	A	93	0	0	24	0
20	M	84	0	0	10	0
21	C	86	0	58	1	0
21	O	86	0	58	1	0
22	N	1	0	0	0	0
All	All	42695	0	42613	720	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 8.

The worst 5 of 720 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:R:268:TYR:OH	2:R:333:ILE:HD13	1.38	1.24
2:R:264:HIS:NE2	2:R:268:TYR:CE2	2.06	1.21
2:R:268:TYR:CD2	2:R:307:SER:HB2	1.82	1.13
20:M:504:9YF:O4	9:A:119:TRP:CZ2	2.04	1.10
9:A:228:LYS:NZ	20:A:503:9YF:O4	1.85	1.09

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	272/341 (80%)	243 (89%)	28 (10%)	1 (0%)	30	52
1	Q	279/341 (82%)	246 (88%)	33 (12%)	0	100	100
2	F	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
2	R	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
3	G	184/203 (91%)	177 (96%)	7 (4%)	0	100	100
3	S	183/203 (90%)	176 (96%)	7 (4%)	0	100	100
4	H	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
4	T	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
5	I	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
5	U	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
6	J	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
6	V	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
7	D	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
7	P	73/100 (73%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B	522/549 (95%)	475 (91%)	41 (8%)	6 (1%)	12	27
8	N	522/549 (95%)	477 (91%)	41 (8%)	4 (1%)	16	35
9	A	376/429 (88%)	334 (89%)	39 (10%)	3 (1%)	16	35
9	M	376/429 (88%)	336 (89%)	37 (10%)	3 (1%)	16	35
10	C	214/280 (76%)	187 (87%)	26 (12%)	1 (0%)	25	46
10	O	221/280 (79%)	190 (86%)	29 (13%)	2 (1%)	14	32
All	All	5082/5704 (89%)	4663 (92%)	399 (8%)	20 (0%)	32	52

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	28	SER
9	M	329	LEU
8	B	28	SER
9	A	329	LEU
8	B	304	SER

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	231/288 (80%)	230 (100%)	1 (0%)	89	96
1	Q	236/288 (82%)	235 (100%)	1 (0%)	89	96
2	F	453/471 (96%)	432 (95%)	21 (5%)	23	46
2	R	453/471 (96%)	432 (95%)	21 (5%)	23	46
3	G	148/161 (92%)	148 (100%)	0	100	100
3	S	147/161 (91%)	147 (100%)	0	100	100
4	H	106/106 (100%)	94 (89%)	12 (11%)	4	10
4	T	106/106 (100%)	94 (89%)	12 (11%)	4	10
5	I	52/59 (88%)	37 (71%)	15 (29%)	0	1
5	U	52/59 (88%)	37 (71%)	15 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	107/114 (94%)	90 (84%)	17 (16%)	2	4
6	V	107/114 (94%)	90 (84%)	17 (16%)	2	4
7	D	60/83 (72%)	59 (98%)	1 (2%)	56	79
7	P	59/83 (71%)	59 (100%)	0	100	100
8	B	424/446 (95%)	400 (94%)	24 (6%)	17	37
8	N	424/446 (95%)	401 (95%)	23 (5%)	18	39
9	A	304/343 (89%)	279 (92%)	25 (8%)	9	21
9	M	304/343 (89%)	280 (92%)	24 (8%)	10	23
10	C	161/207 (78%)	149 (92%)	12 (8%)	11	25
10	O	164/207 (79%)	152 (93%)	12 (7%)	11	26
All	All	4098/4556 (90%)	3845 (94%)	253 (6%)	18	33

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	U	78	LYS
9	A	86	THR
8	N	301	SER
9	A	78	GLU
9	A	282	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	104	ASN
10	C	87	HIS
3	S	186	HIS
10	C	67	GLN
8	B	36	ASN

5.3.3 RNA ⓘ

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 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 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$
16	HEM	N	602	8	41,50,50	1.48	4 (9%)	45,82,82	1.40	7 (15%)
12	CDL	A	505	-	94,94,99	1.05	7 (7%)	100,106,111	0.91	4 (4%)
17	MQ9	O	302	-	49,49,59	3.90	16 (32%)	60,63,75	3.25	25 (41%)
21	HEC	O	304	10	32,50,50	2.27	3 (9%)	24,82,82	1.31	1 (4%)
20	9YF	A	503	-	51,51,58	0.95	5 (9%)	62,64,71	1.01	4 (6%)
16	HEM	N	601	8	41,49,50	1.23	2 (4%)	46,81,82	1.26	4 (8%)
12	CDL	B	608	-	78,78,99	1.12	7 (8%)	84,90,111	1.03	4 (4%)
13	PLM	B	604	-	10,10,17	0.63	0	9,9,17	0.55	0
17	MQ9	O	303	-	59,59,59	3.87	18 (30%)	72,75,75	3.38	33 (45%)
18	HUU	B	611	-	40,43,43	2.02	9 (22%)	50,62,62	1.06	4 (8%)
12	CDL	F	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
12	CDL	O	301	-	78,78,99	1.12	7 (8%)	84,90,111	0.97	5 (5%)
13	PLM	F	603	-	16,16,17	0.56	0	15,15,17	0.42	0
12	CDL	N	606	-	78,78,99	1.12	8 (10%)	84,90,111	0.99	4 (4%)
21	HEC	O	305	10	32,50,50	2.23	3 (9%)	24,82,82	1.52	4 (16%)
14	HEA	R	607	2	57,67,67	2.57	30 (52%)	61,103,103	2.99	32 (52%)
12	CDL	P	201	-	87,87,99	1.07	6 (6%)	93,99,111	0.94	4 (4%)
17	MQ9	B	609	-	44,44,59	3.89	15 (34%)	54,57,75	3.16	22 (40%)
19	FES	M	501	9	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	HEC	C	301	10	32,50,50	2.30	3 (9%)	24,82,82	1.33	2 (8%)
12	CDL	B	603	-	78,78,99	1.14	8 (10%)	84,90,111	0.99	4 (4%)
17	MQ9	C	303	-	49,49,59	3.96	15 (30%)	60,63,75	3.16	26 (43%)
18	HUU	N	609	-	40,43,43	3.52	11 (27%)	50,62,62	1.52	7 (14%)
20	9YF	M	503	-	44,44,58	0.99	4 (9%)	55,57,71	1.10	5 (9%)
14	HEA	F	607	2	57,67,67	2.56	30 (52%)	61,103,103	3.00	32 (52%)
16	HEM	B	602	8	41,50,50	1.46	4 (9%)	45,82,82	1.40	7 (15%)
19	FES	A	501	9	0,4,4	-	-	-	-	-
14	HEA	F	606	2	57,67,67	2.54	30 (52%)	61,103,103	3.10	31 (50%)
17	MQ9	A	502	-	44,44,59	3.90	15 (34%)	54,57,75	3.21	23 (42%)
12	CDL	B	605	-	65,65,99	1.22	7 (10%)	71,77,111	0.98	4 (5%)
16	HEM	B	601	8	41,49,50	1.24	2 (4%)	46,81,82	1.26	5 (10%)
12	CDL	M	502	-	94,94,99	1.05	7 (7%)	100,106,111	0.85	4 (4%)
13	PLM	R	603	-	16,16,17	0.56	0	15,15,17	0.42	0
20	9YF	A	504	-	42,42,58	1.02	4 (9%)	52,54,71	1.27	6 (11%)
12	CDL	R	602	-	80,80,99	1.11	8 (10%)	86,92,111	0.97	4 (4%)
12	CDL	N	604	-	73,73,99	1.17	7 (9%)	79,85,111	1.03	4 (5%)
15	9Y0	S	301	-	42,42,48	0.95	4 (9%)	44,47,53	0.90	2 (4%)
17	MQ9	B	610	-	59,59,59	3.86	18 (30%)	72,75,75	3.40	33 (45%)
12	CDL	B	607	-	76,76,99	1.13	7 (9%)	82,88,111	1.03	4 (4%)
12	CDL	R	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
15	9Y0	G	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.91	2 (4%)
21	HEC	C	302	10	32,50,50	2.22	3 (9%)	24,82,82	1.51	4 (16%)
12	CDL	F	602	-	80,80,99	1.11	7 (8%)	86,92,111	0.97	4 (4%)
13	PLM	N	603	-	10,10,17	0.62	0	9,9,17	0.55	0
12	CDL	D	201	-	87,87,99	1.07	6 (6%)	93,99,111	0.96	4 (4%)
12	CDL	N	605	-	76,76,99	1.13	7 (9%)	82,88,111	0.98	4 (4%)
12	CDL	B	606	-	73,73,99	1.16	7 (9%)	79,85,111	1.01	4 (5%)
17	MQ9	N	607	-	59,59,59	3.94	18 (30%)	72,75,75	3.30	31 (43%)
20	9YF	M	504	-	40,40,58	1.01	3 (7%)	50,52,71	1.38	7 (14%)
14	HEA	R	606	2	57,67,67	2.53	30 (52%)	61,103,103	3.11	31 (50%)
17	MQ9	N	608	-	59,59,59	3.96	19 (32%)	72,75,75	3.33	33 (45%)

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
16	HEM	N	602	8	-	2/12/54/54	-
12	CDL	A	505	-	-	57/105/105/110	-
17	MQ9	O	302	-	-	26/41/61/73	0/2/2/2
21	HEC	O	304	10	-	7/10/54/54	-
20	9YF	A	503	-	-	30/47/71/78	0/1/1/1
16	HEM	N	601	8	-	1/12/52/54	-
12	CDL	B	608	-	-	45/89/89/110	-
13	PLM	B	604	-	-	1/7/8/15	-
17	MQ9	O	303	-	-	26/53/73/73	0/2/2/2
18	HUU	B	611	-	-	7/20/34/34	0/5/5/5
12	CDL	F	601	-	-	42/86/86/110	-
12	CDL	O	301	-	-	47/89/89/110	-
13	PLM	F	603	-	-	5/13/14/15	-
12	CDL	N	606	-	-	46/89/89/110	-
21	HEC	O	305	10	-	0/10/54/54	-
14	HEA	R	607	2	-	16/32/76/76	-
12	CDL	P	201	-	-	63/98/98/110	-
17	MQ9	B	609	-	-	20/35/55/73	0/2/2/2
19	FES	M	501	9	-	-	0/1/1/1
21	HEC	C	301	10	-	7/10/54/54	-
12	CDL	B	603	-	-	53/89/89/110	-
17	MQ9	C	303	-	-	24/41/61/73	0/2/2/2
18	HUU	N	609	-	-	5/20/34/34	0/5/5/5
20	9YF	M	503	-	-	19/39/63/78	0/1/1/1
14	HEA	F	607	2	-	16/32/76/76	-
16	HEM	B	602	8	-	2/12/54/54	-
19	FES	A	501	9	-	-	0/1/1/1
14	HEA	F	606	2	-	14/32/76/76	-
17	MQ9	A	502	-	-	21/35/55/73	0/2/2/2
12	CDL	B	605	-	-	48/76/76/110	-
16	HEM	B	601	8	-	2/12/52/54	-
12	CDL	M	502	-	-	65/105/105/110	-
13	PLM	R	603	-	-	4/13/14/15	-
20	9YF	A	504	-	-	15/37/61/78	0/1/1/1
12	CDL	R	602	-	-	58/91/91/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	N	604	-	-	51/84/84/110	-
15	9Y0	S	301	-	-	29/46/46/52	-
17	MQ9	B	610	-	-	24/53/73/73	0/2/2/2
12	CDL	B	607	-	-	38/87/87/110	-
12	CDL	R	601	-	-	42/86/86/110	-
15	9Y0	G	301	-	-	29/46/46/52	-
21	HEC	C	302	10	-	0/10/54/54	-
12	CDL	F	602	-	-	58/91/91/110	-
13	PLM	N	603	-	-	1/7/8/15	-
12	CDL	D	201	-	-	49/98/98/110	-
12	CDL	N	605	-	-	40/87/87/110	-
12	CDL	B	606	-	-	39/84/84/110	-
17	MQ9	N	607	-	-	30/53/73/73	0/2/2/2
20	9YF	M	504	-	-	18/35/59/78	0/1/1/1
14	HEA	R	606	2	-	14/32/76/76	-
17	MQ9	N	608	-	-	30/53/73/73	0/2/2/2

The worst 5 of 442 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	609	HUU	C07-N08	17.81	1.50	1.33
17	N	607	MQ9	C18-C19	9.33	1.55	1.33
17	C	303	MQ9	C23-C24	9.32	1.55	1.33
17	A	502	MQ9	C23-C24	9.32	1.55	1.33
17	N	608	MQ9	C18-C19	9.29	1.55	1.33

The worst 5 of 492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	608	MQ9	C7-C8-C9	-10.17	109.86	126.79
17	O	303	MQ9	C7-C8-C9	-9.88	110.35	126.79
17	B	610	MQ9	C7-C8-C9	-9.84	110.41	126.79
17	O	302	MQ9	C7-C8-C9	-9.83	110.43	126.79
17	N	607	MQ9	C7-C8-C9	-9.67	110.69	126.79

There are no chirality outliers.

5 of 1286 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CB2-OB2-PB2-OB3
12	F	601	CDL	OB5-CB3-CB4-OB6
12	F	602	CDL	CA3-OA5-PA1-OA4
12	F	602	CDL	CB3-OB5-PB2-OB3
12	F	602	CDL	CB3-OB5-PB2-OB4

There are no ring outliers.

42 monomers are involved in 173 short contacts:

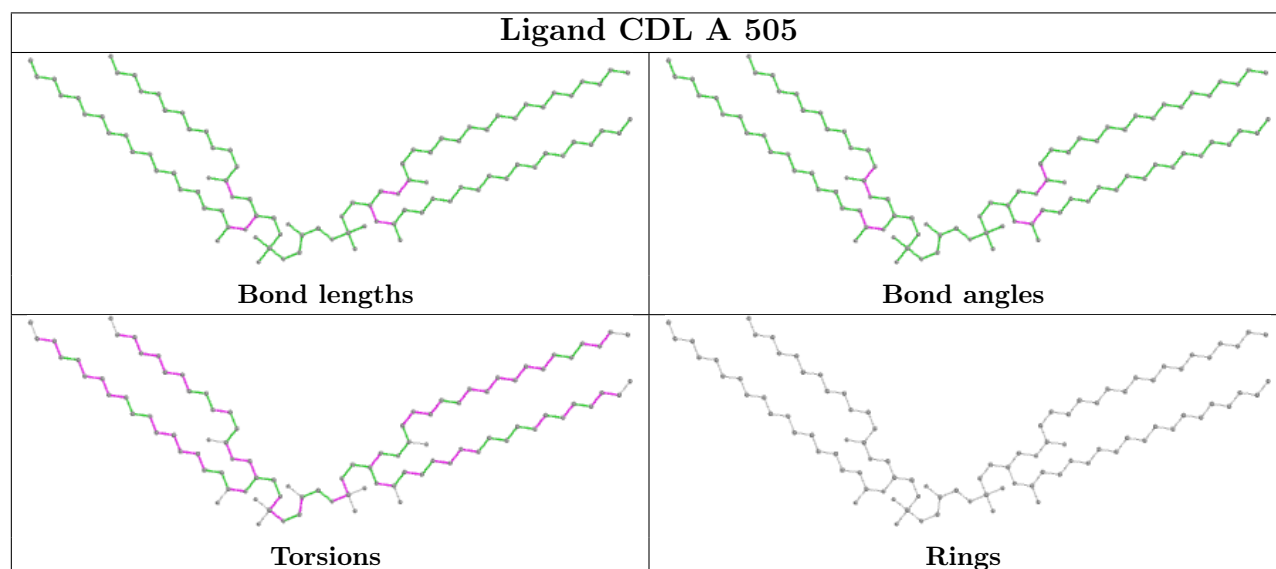
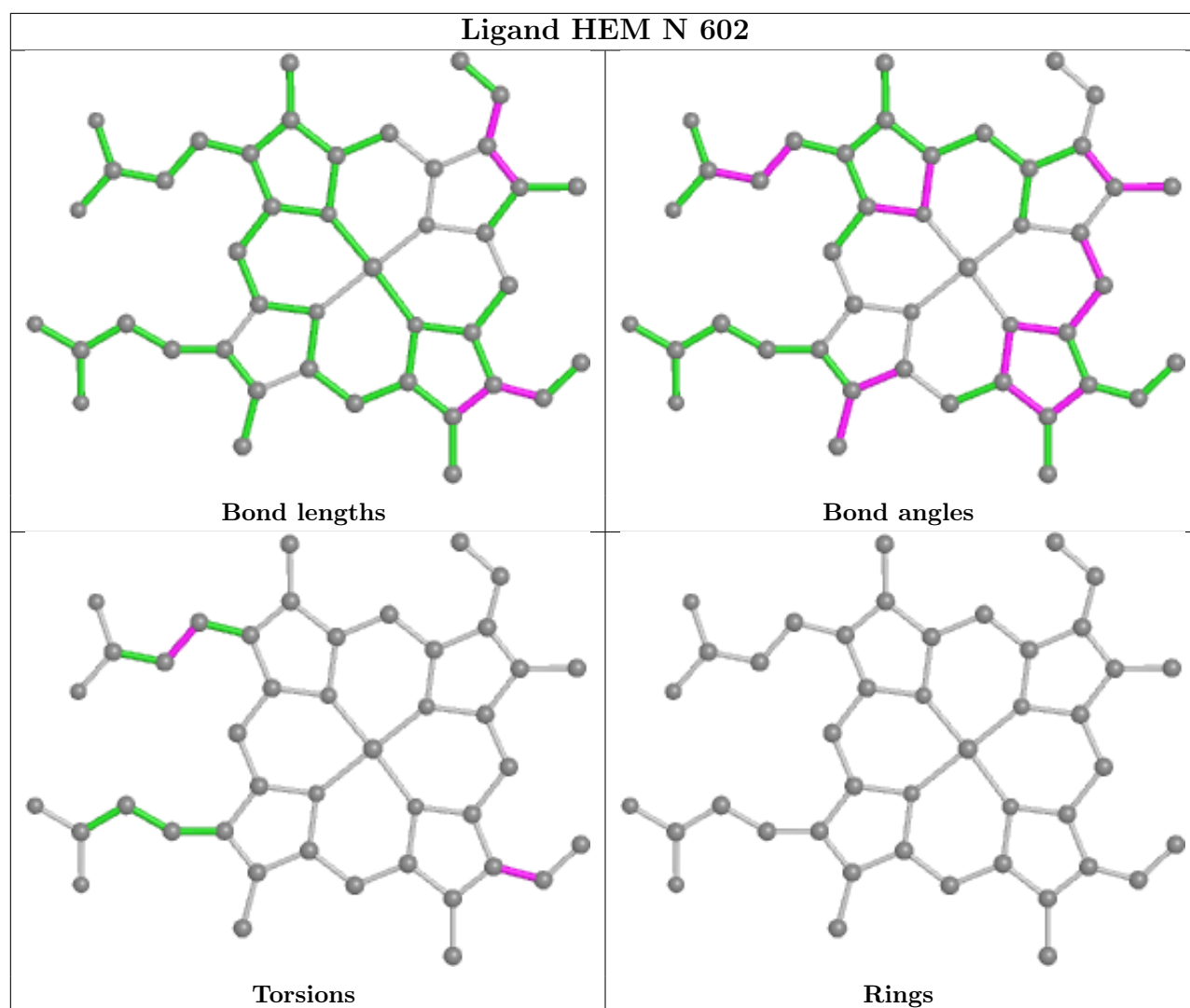
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	602	HEM	3	0
12	A	505	CDL	4	0
17	O	302	MQ9	8	0
21	O	304	HEC	1	0
20	A	503	9YF	6	0
16	N	601	HEM	2	0
12	B	608	CDL	3	0
17	O	303	MQ9	4	0
12	F	601	CDL	1	0
12	O	301	CDL	2	0
12	N	606	CDL	3	0
14	R	607	HEA	8	0
12	P	201	CDL	6	0
17	B	609	MQ9	4	0
19	M	501	FES	2	0
21	C	301	HEC	1	0
12	B	603	CDL	3	0
17	C	303	MQ9	5	0
18	N	609	HUU	1	0
20	M	503	9YF	6	0
14	F	607	HEA	9	0
16	B	602	HEM	5	0
19	A	501	FES	3	0
14	F	606	HEA	5	0
17	A	502	MQ9	5	0
12	B	605	CDL	3	0
16	B	601	HEM	1	0
12	M	502	CDL	2	0
20	A	504	9YF	18	0
12	R	602	CDL	6	0
12	N	604	CDL	2	0
17	B	610	MQ9	14	0
12	B	607	CDL	2	0

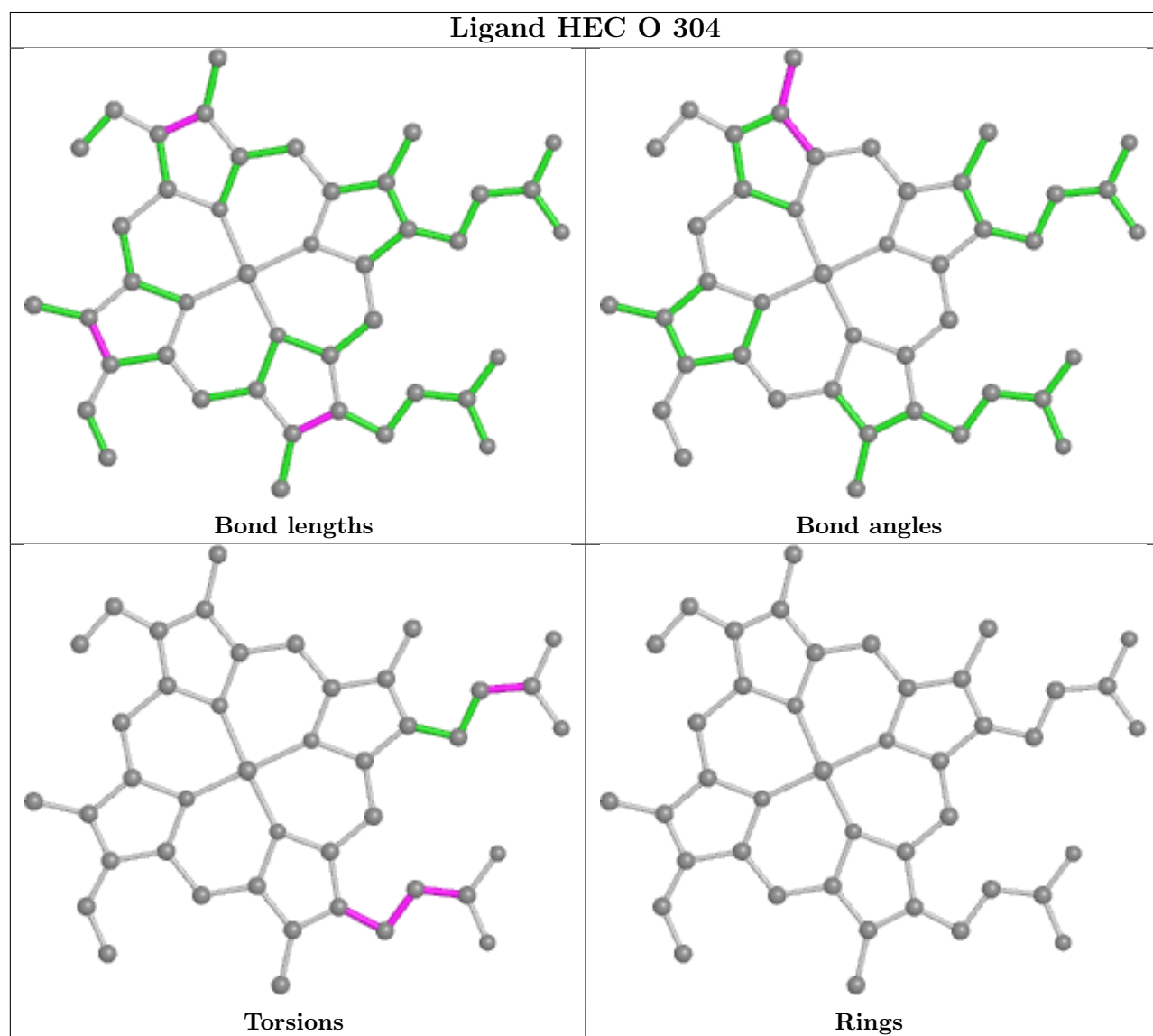
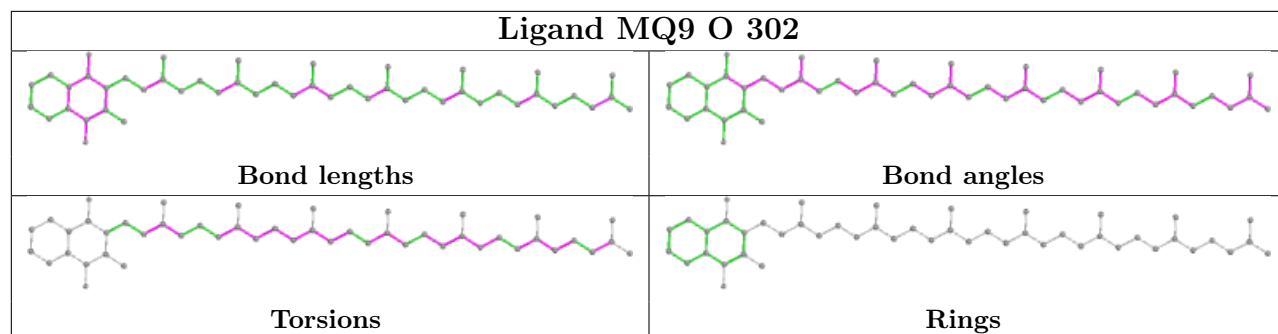
Continued on next page...

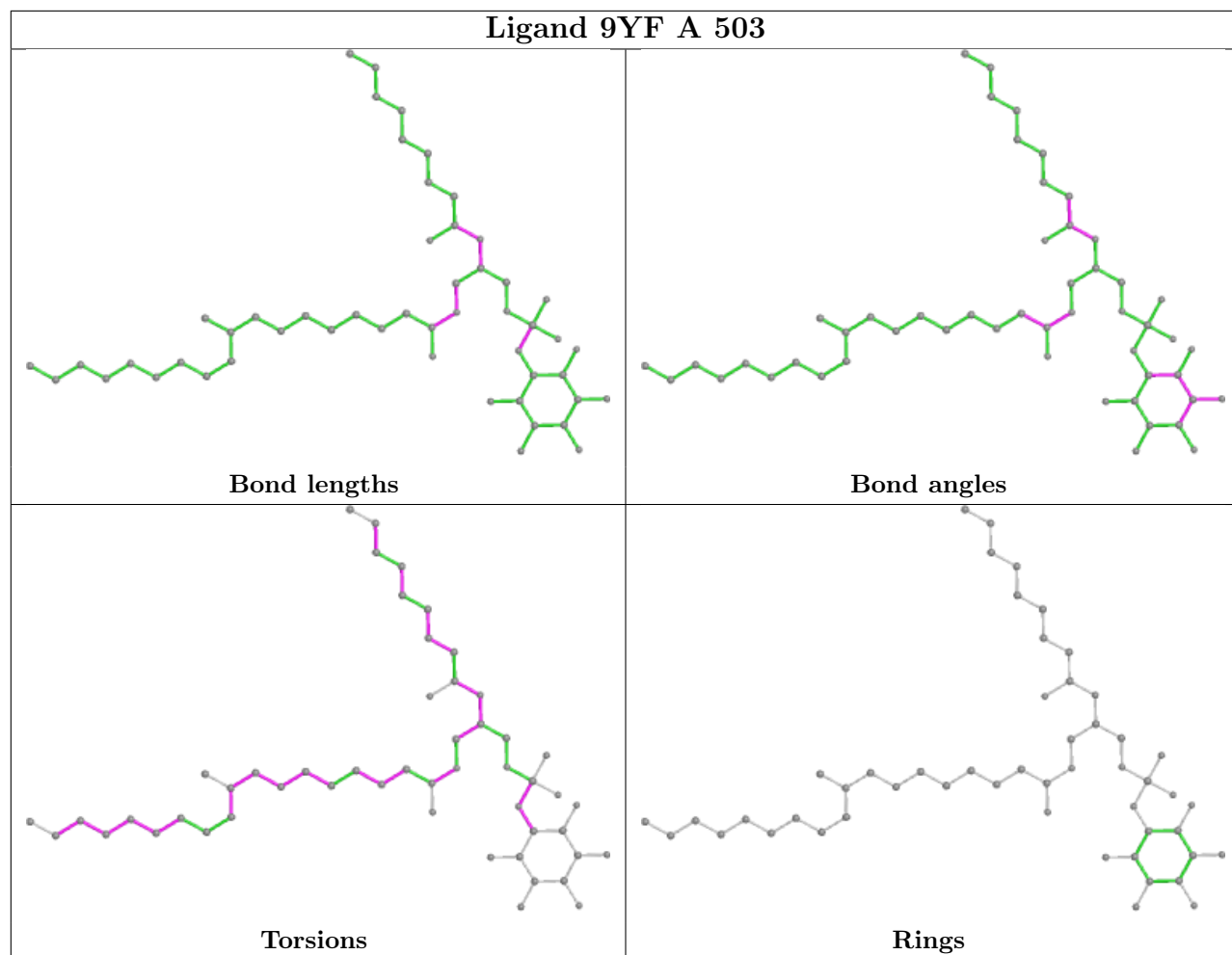
Continued from previous page...

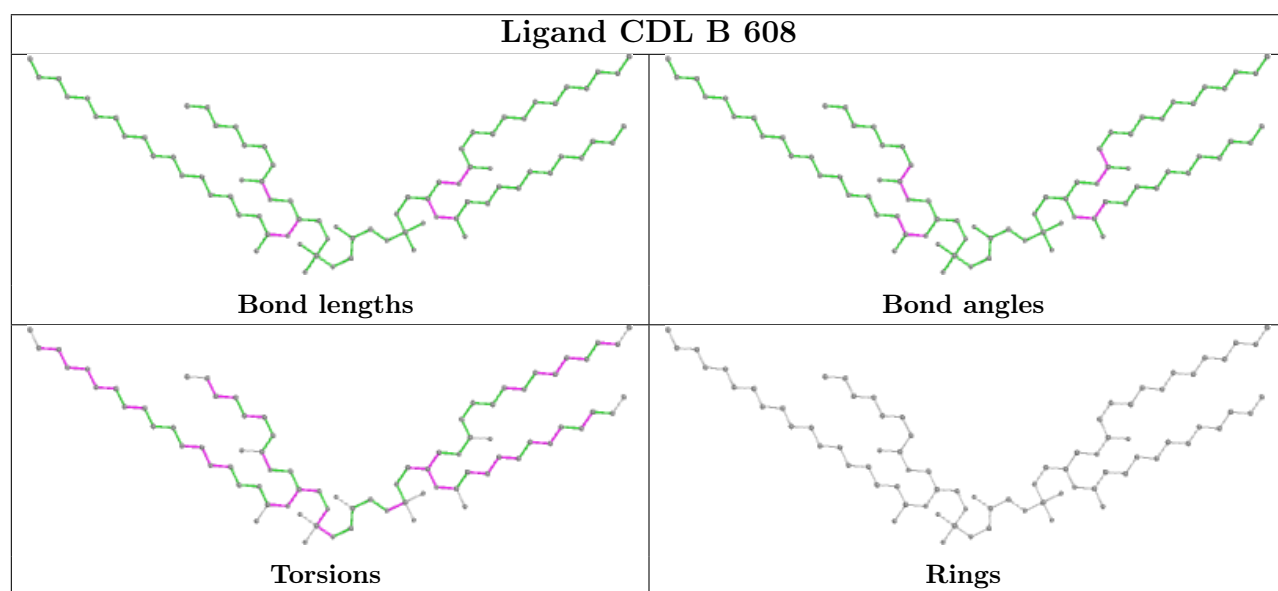
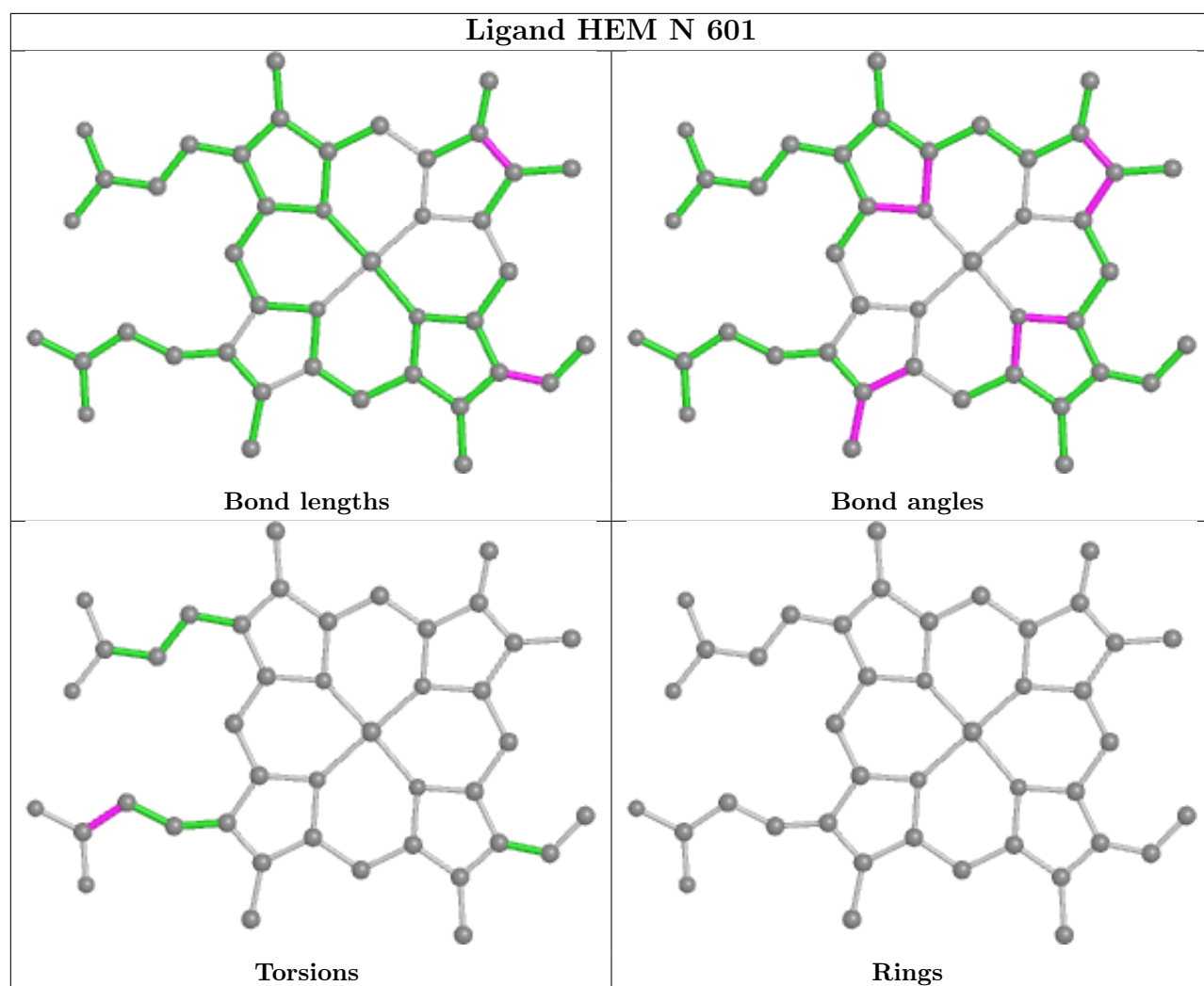
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	601	CDL	1	0
12	F	602	CDL	2	0
12	D	201	CDL	5	0
12	N	605	CDL	5	0
12	B	606	CDL	3	0
17	N	607	MQ9	3	0
20	M	504	9YF	4	0
14	R	606	HEA	6	0
17	N	608	MQ9	5	0

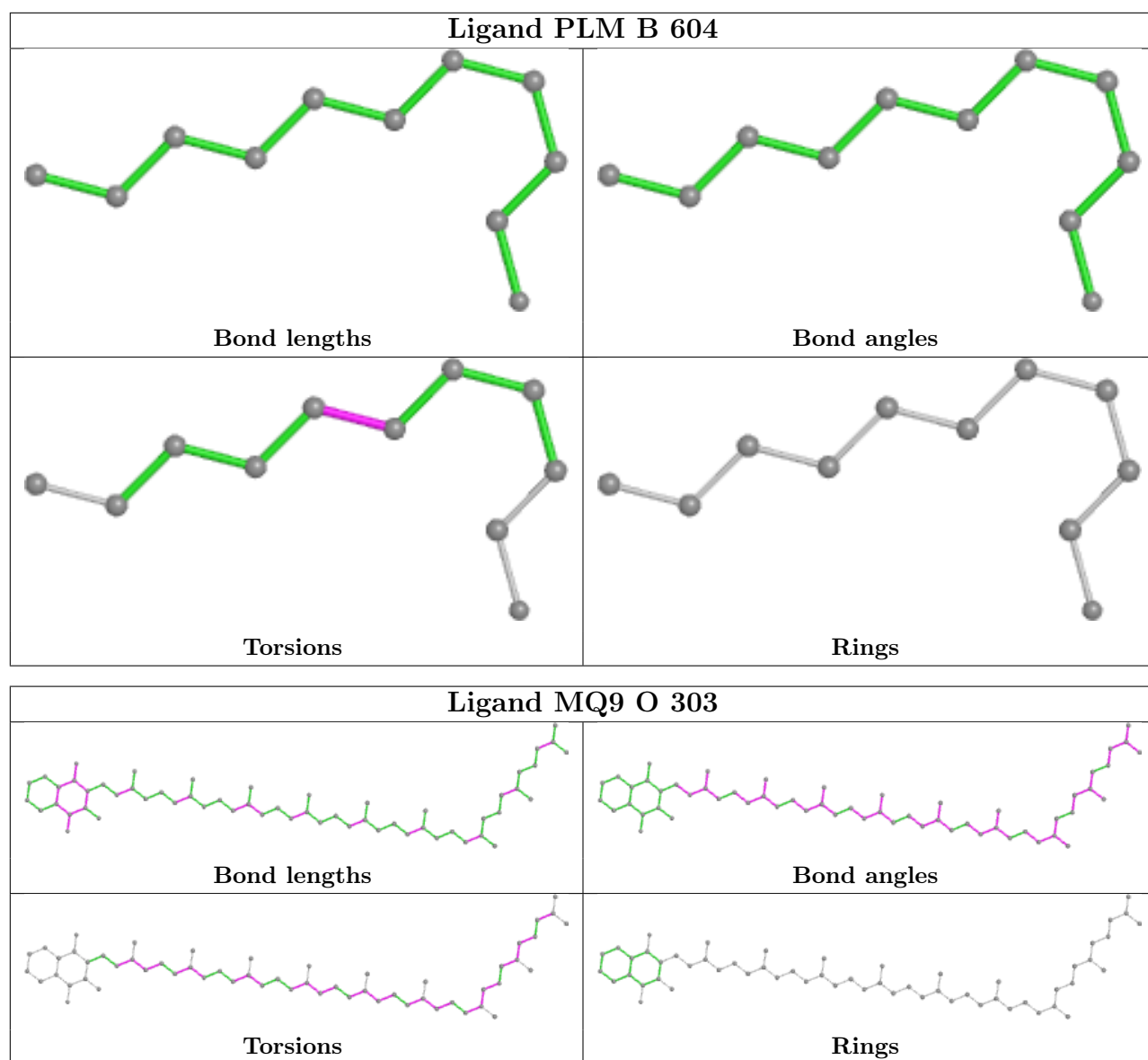
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

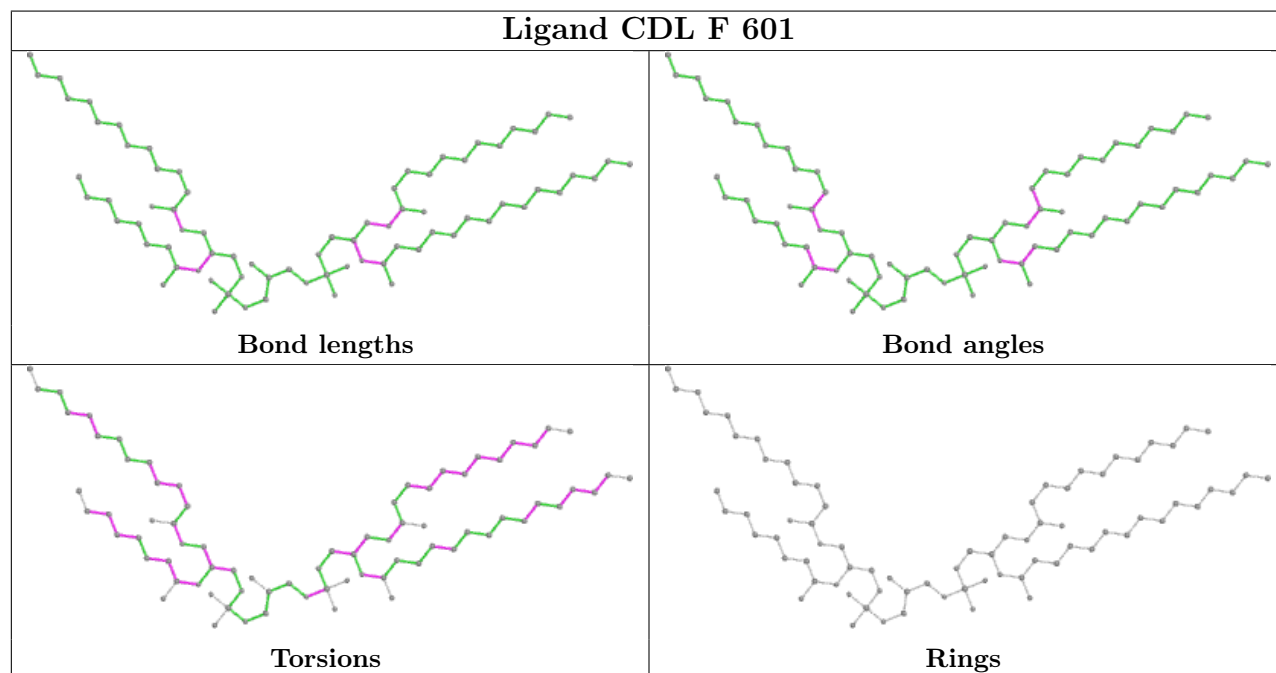
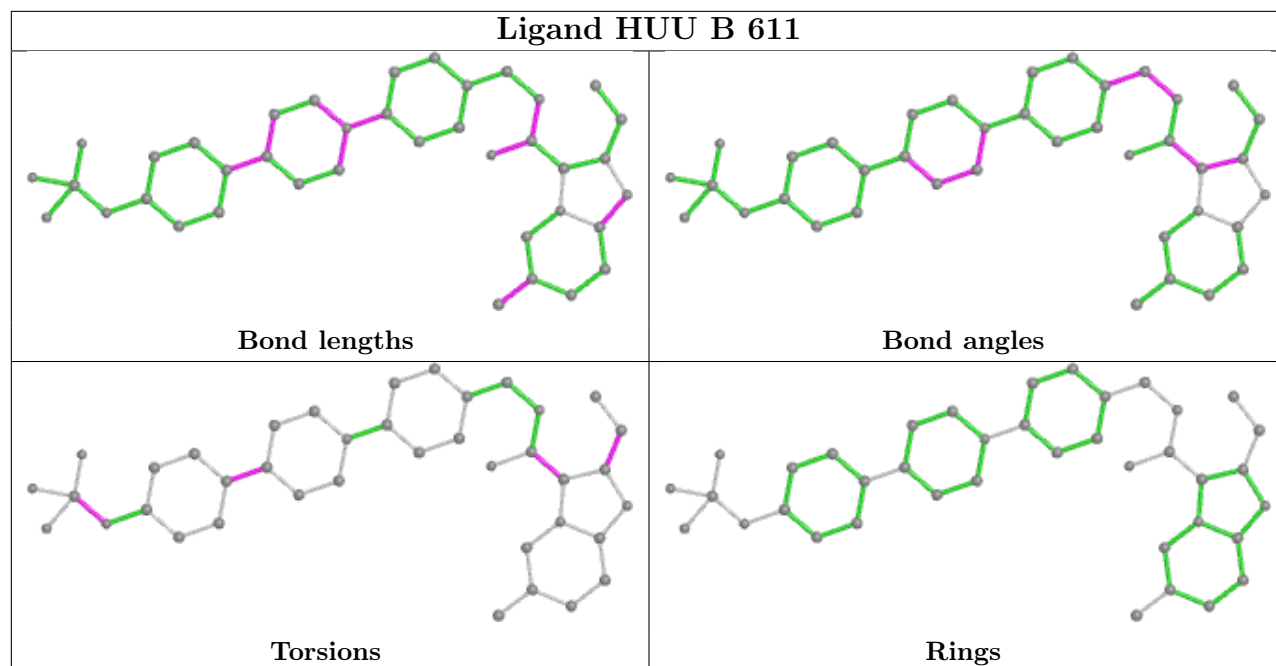


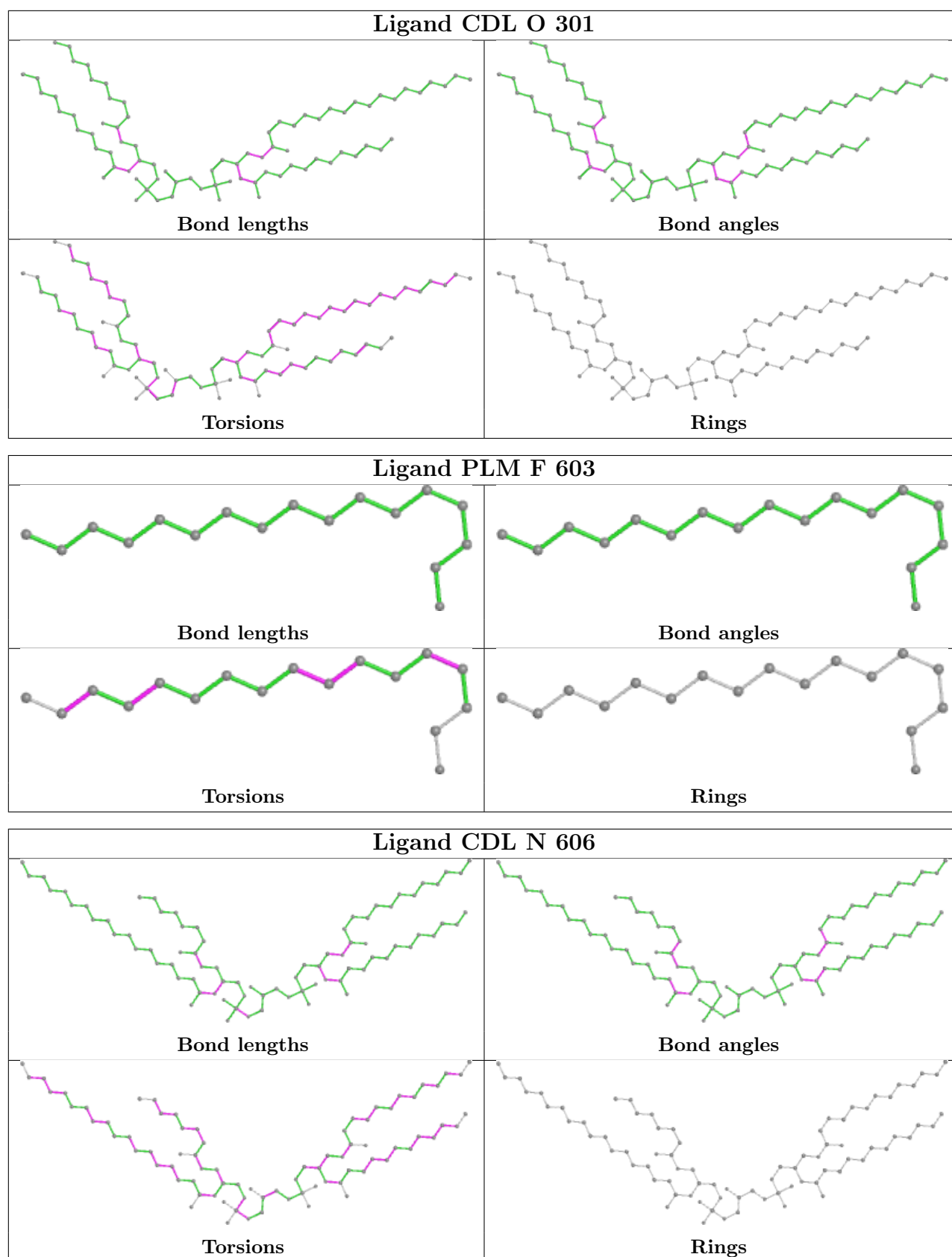


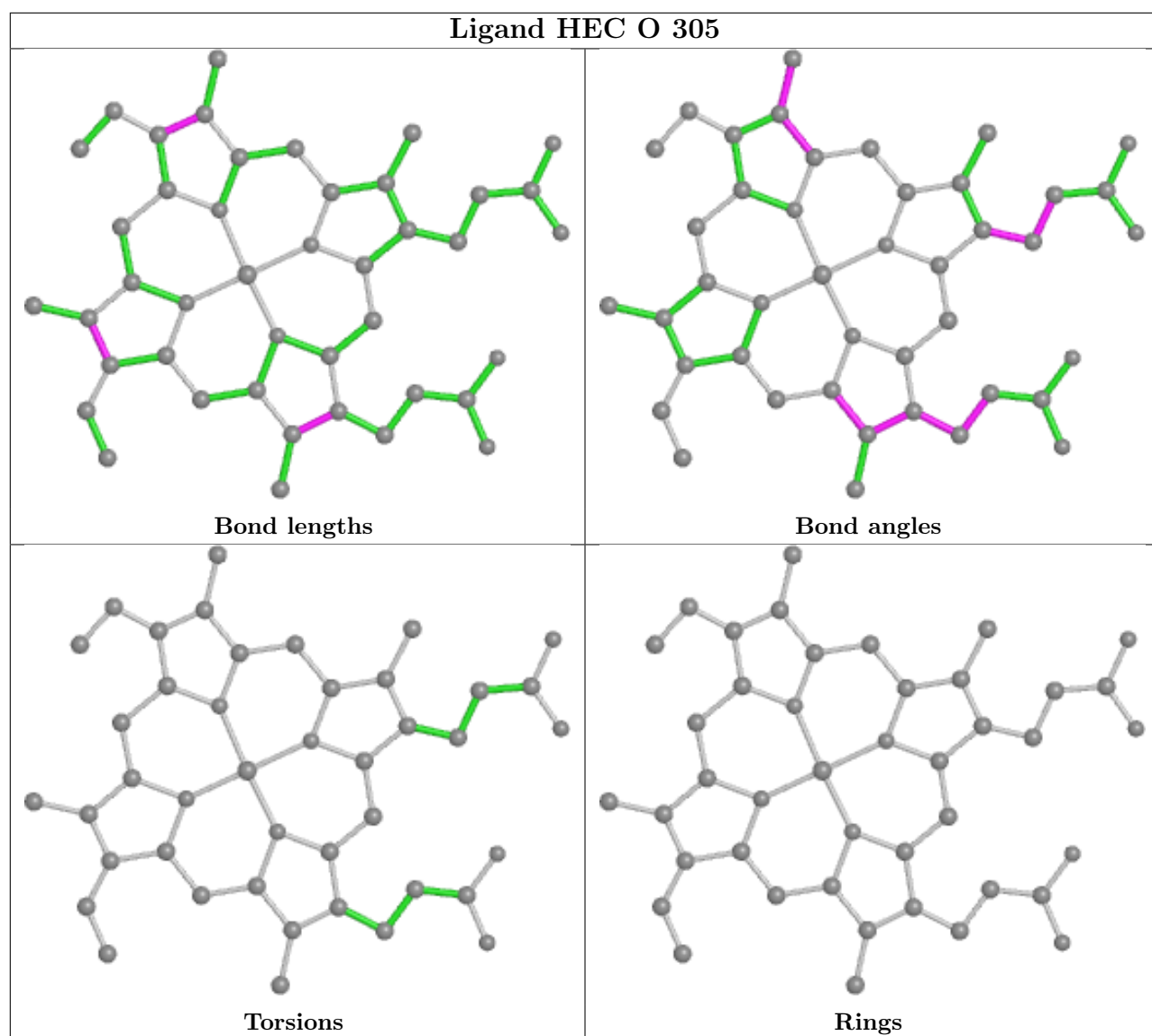


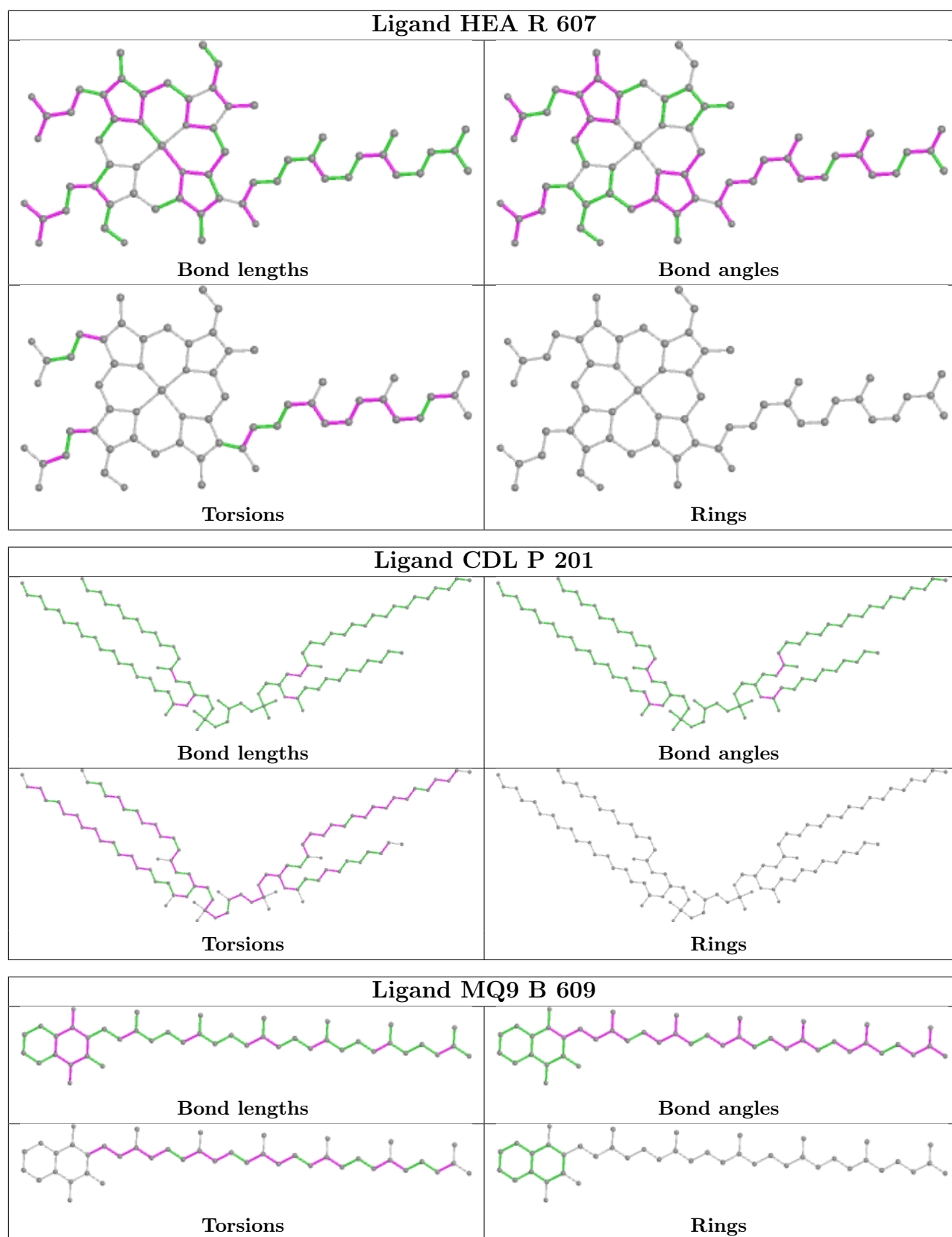


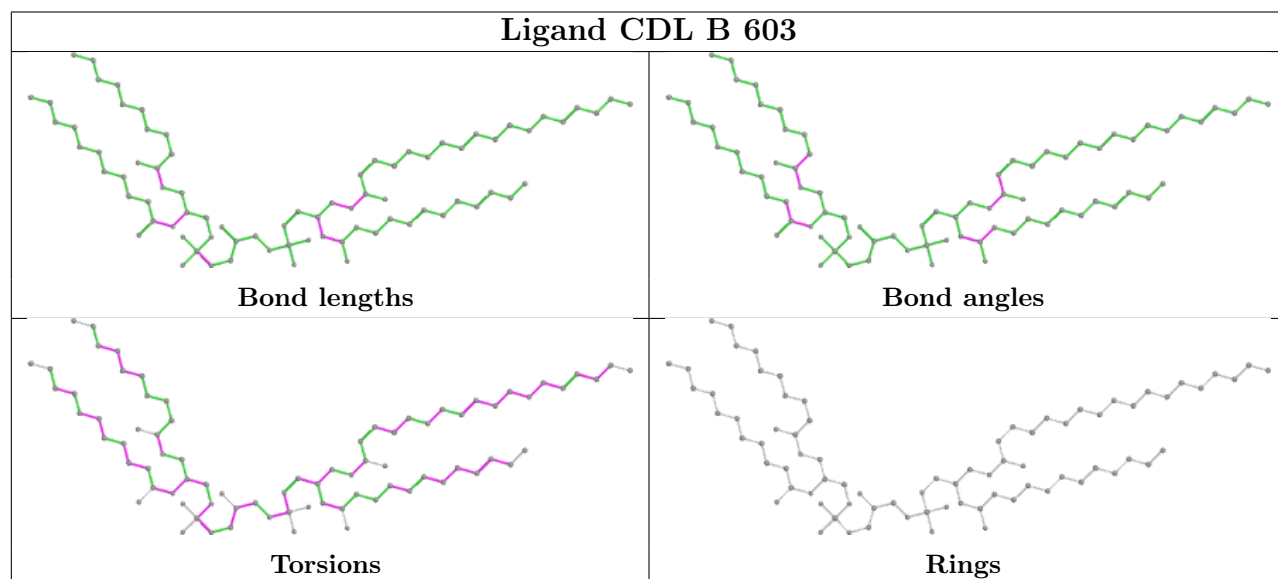
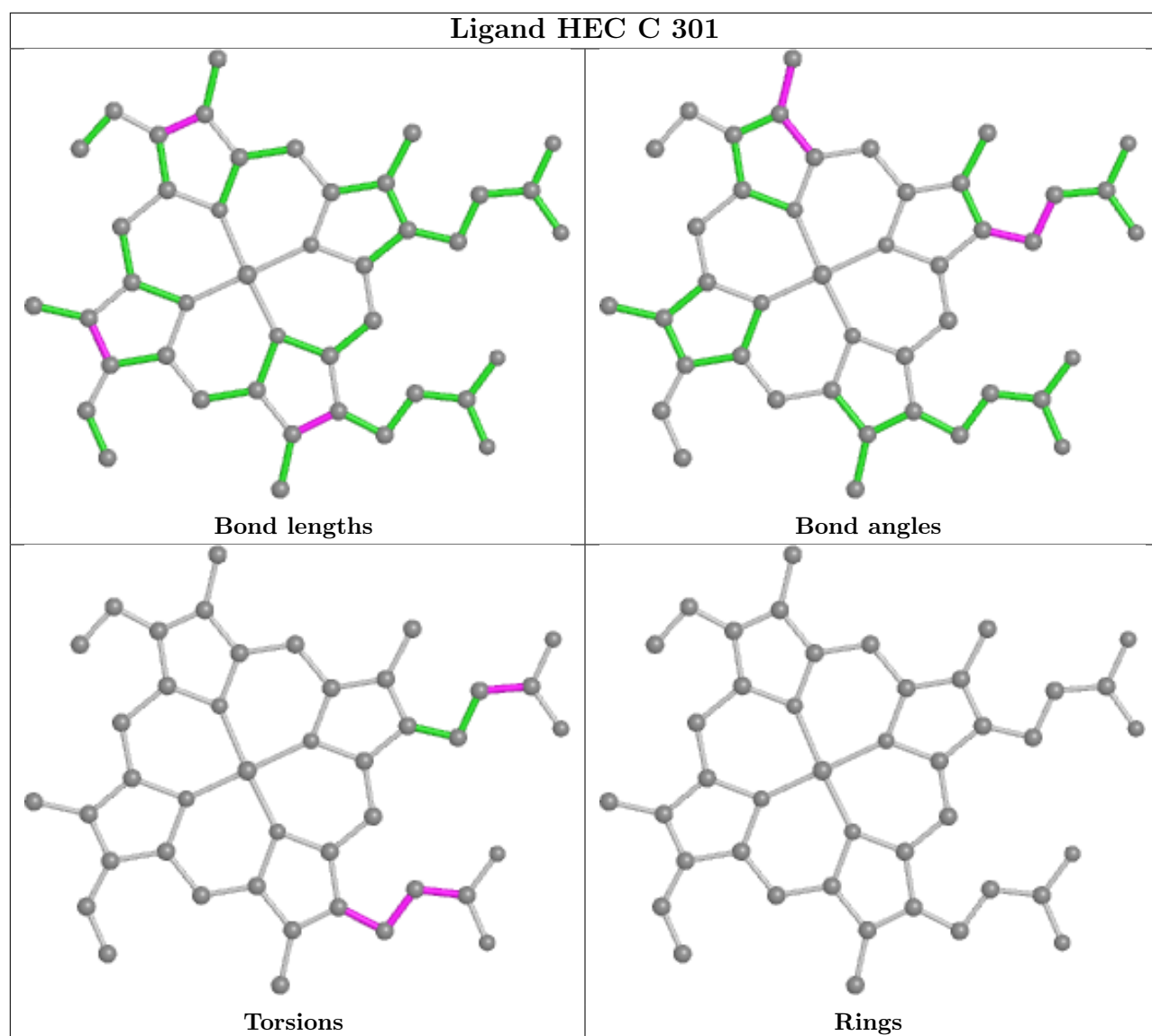


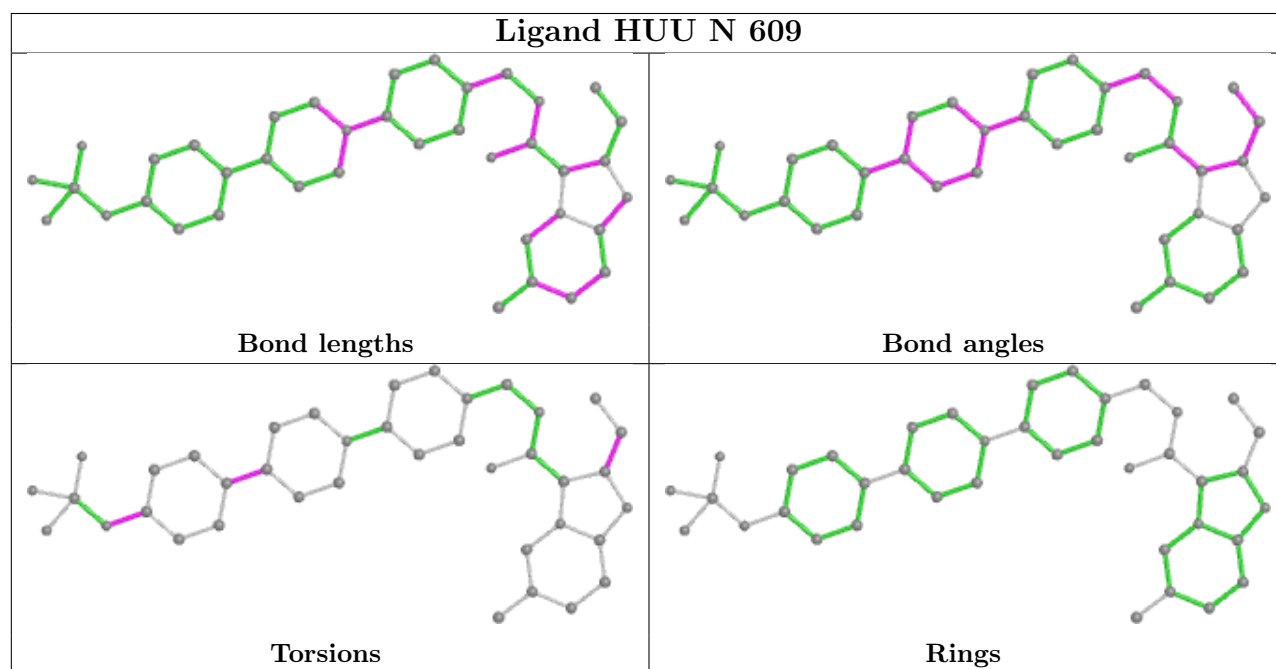
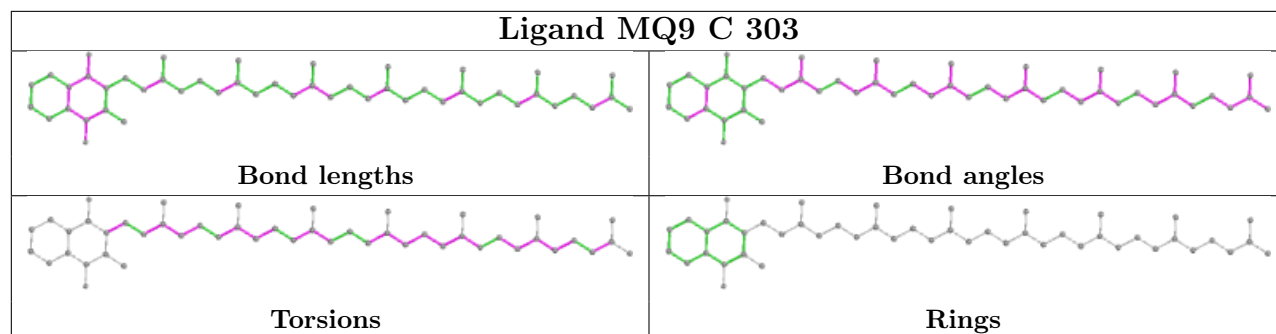


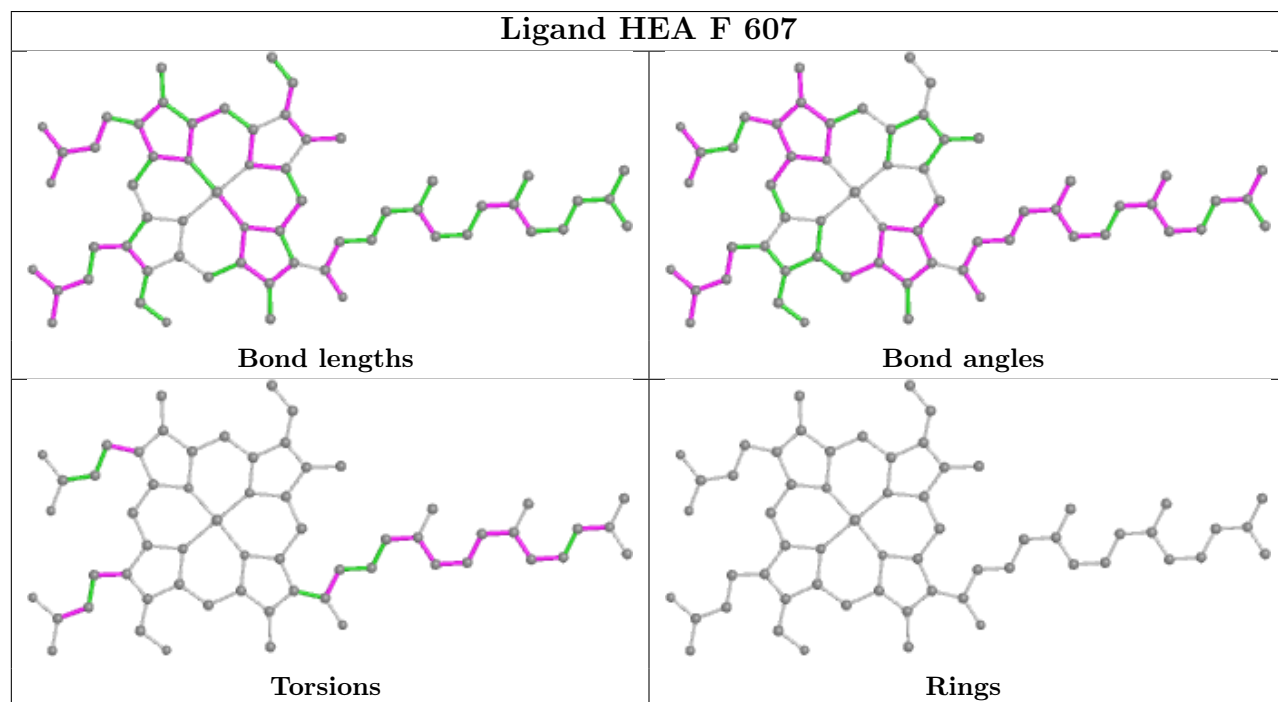
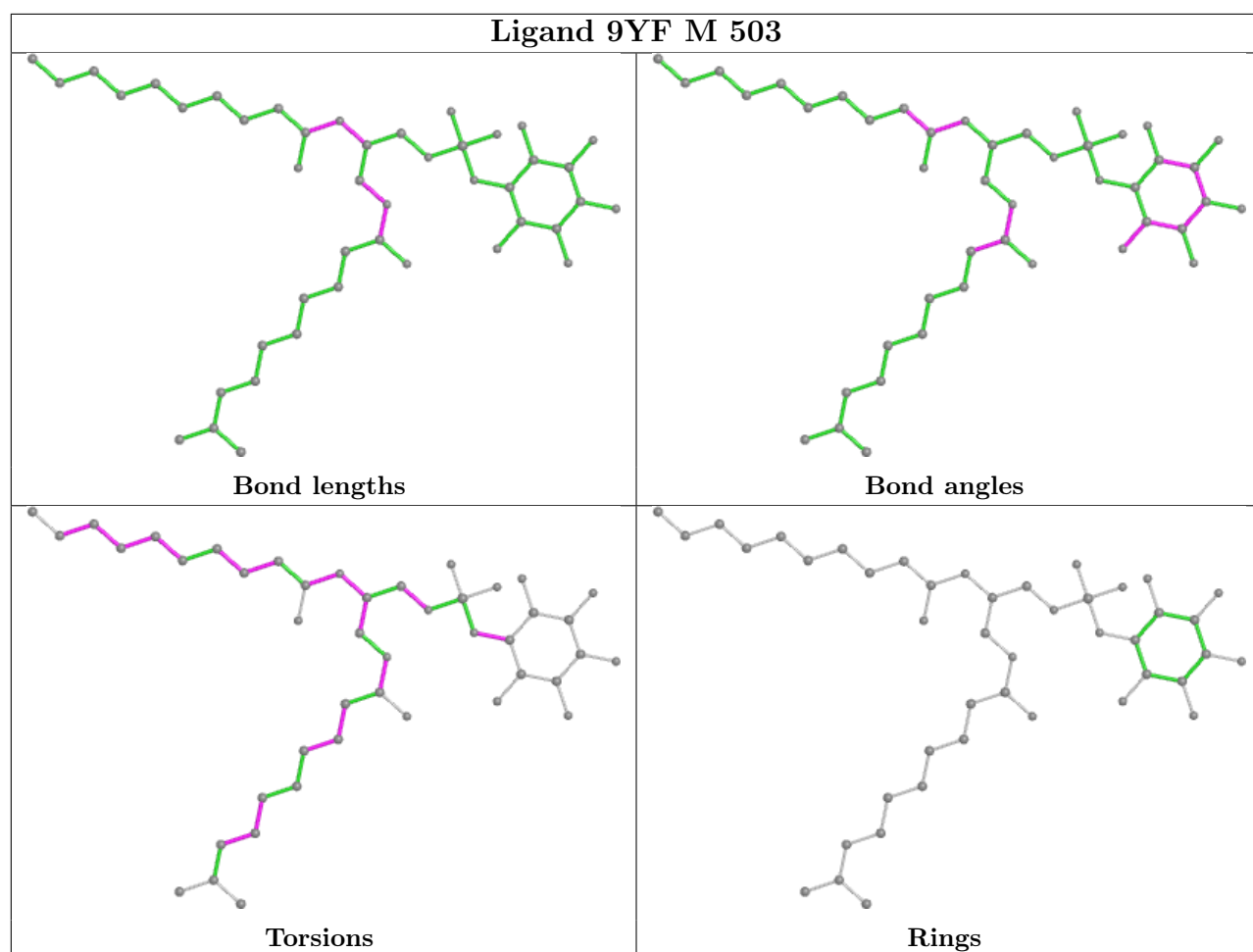


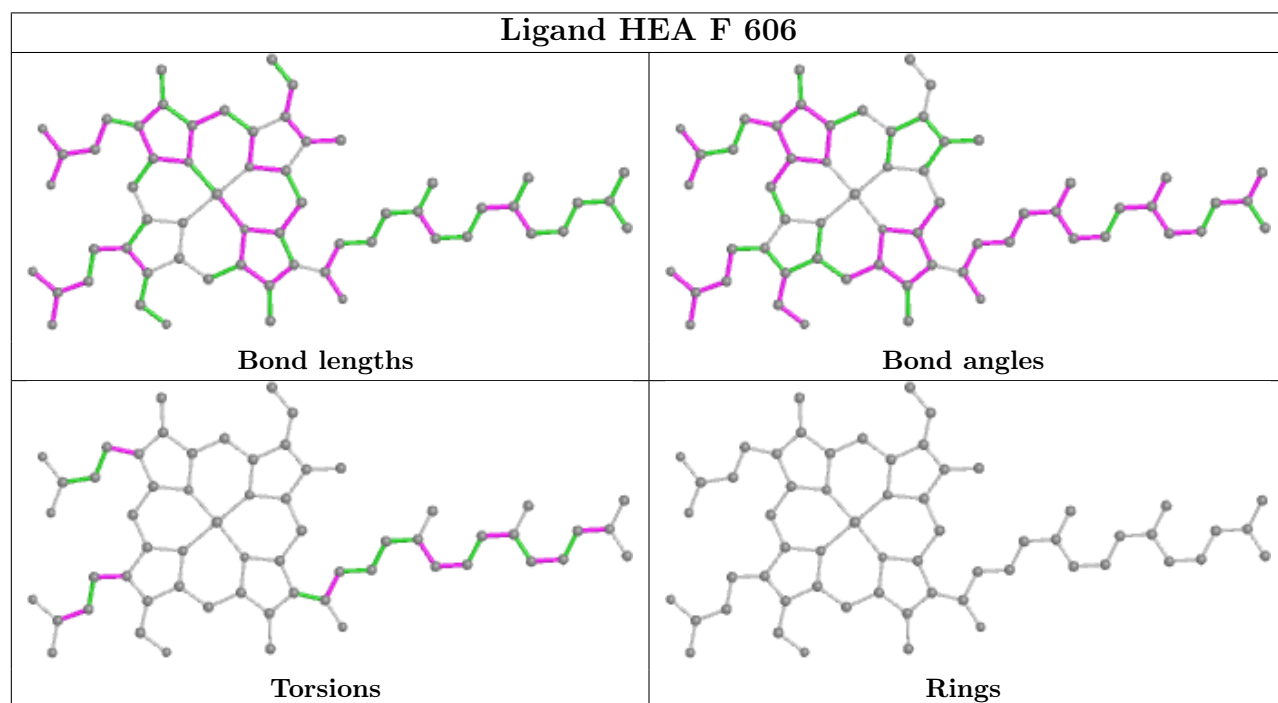
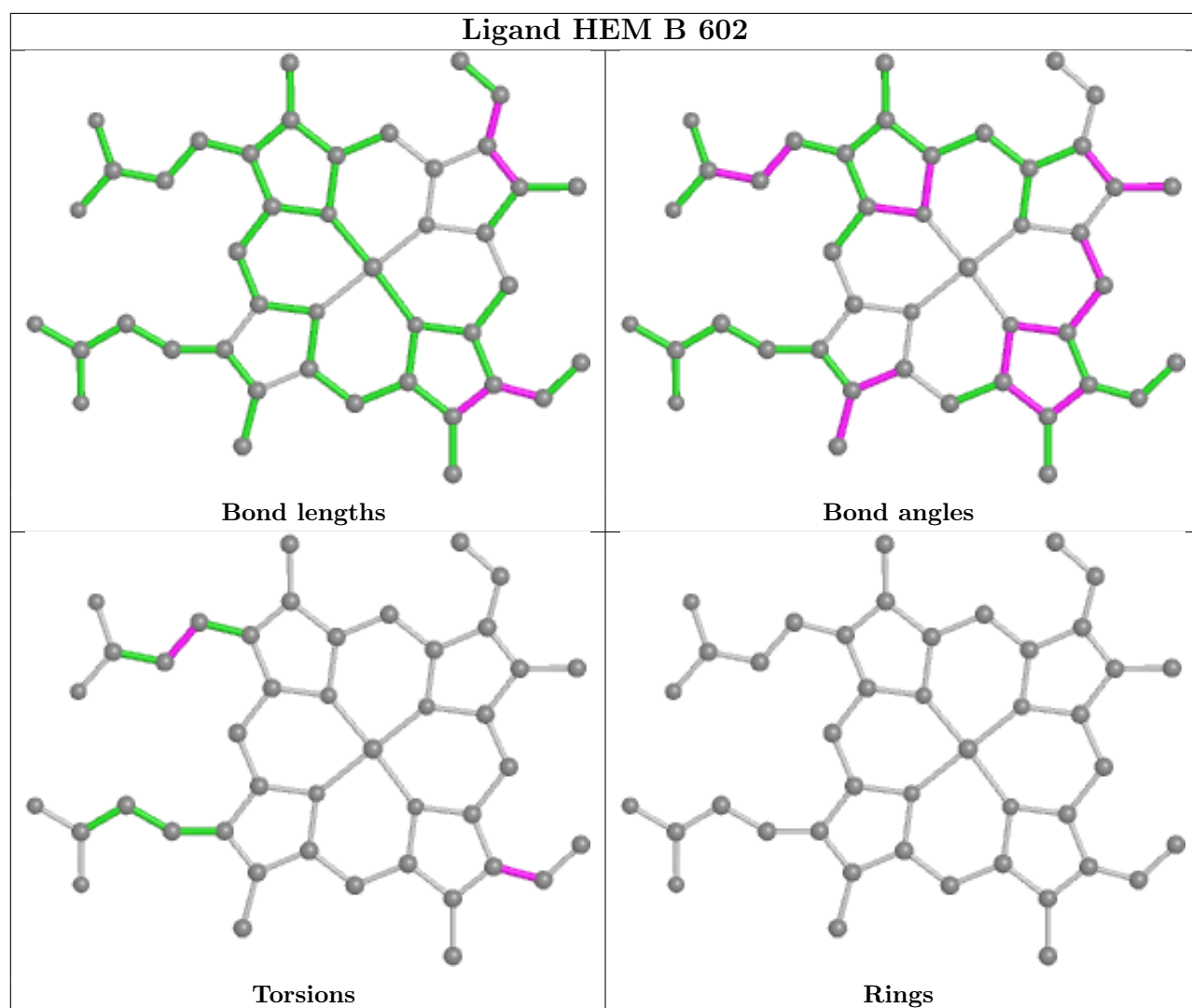


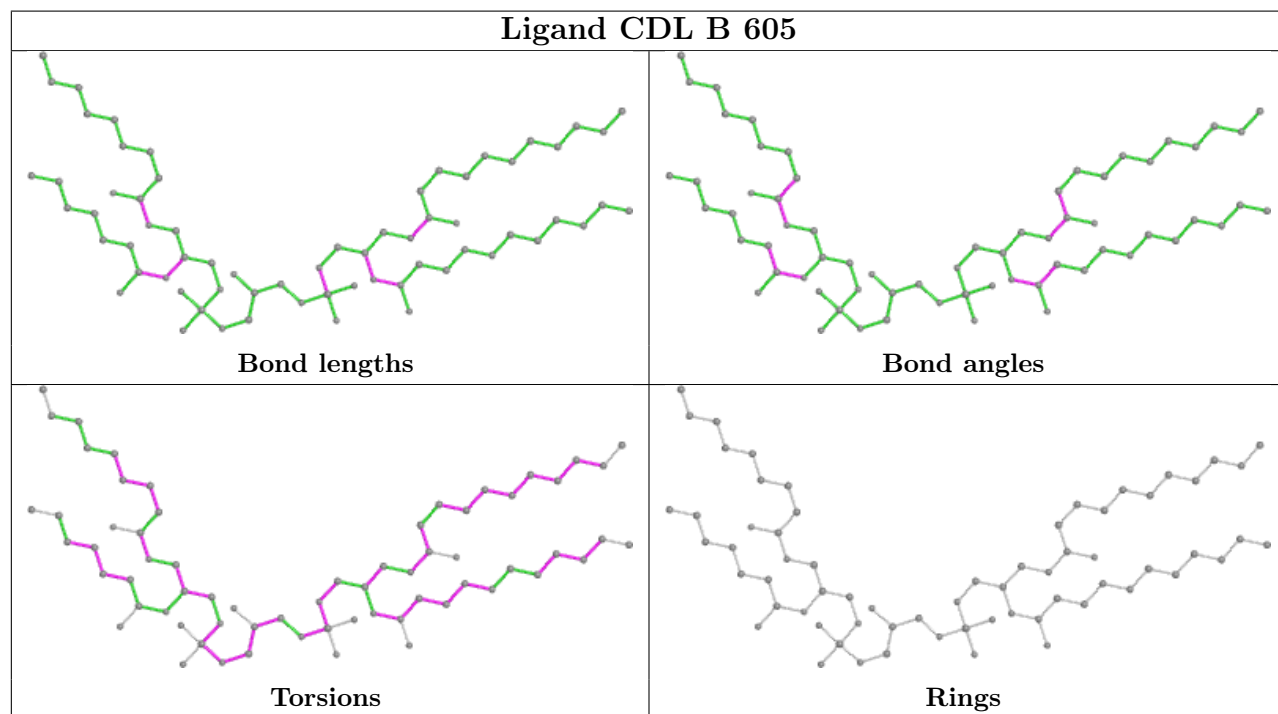
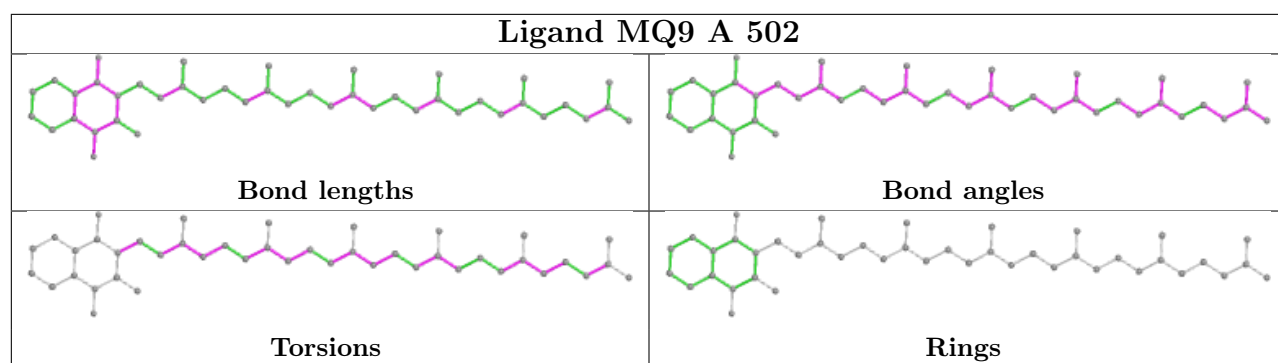


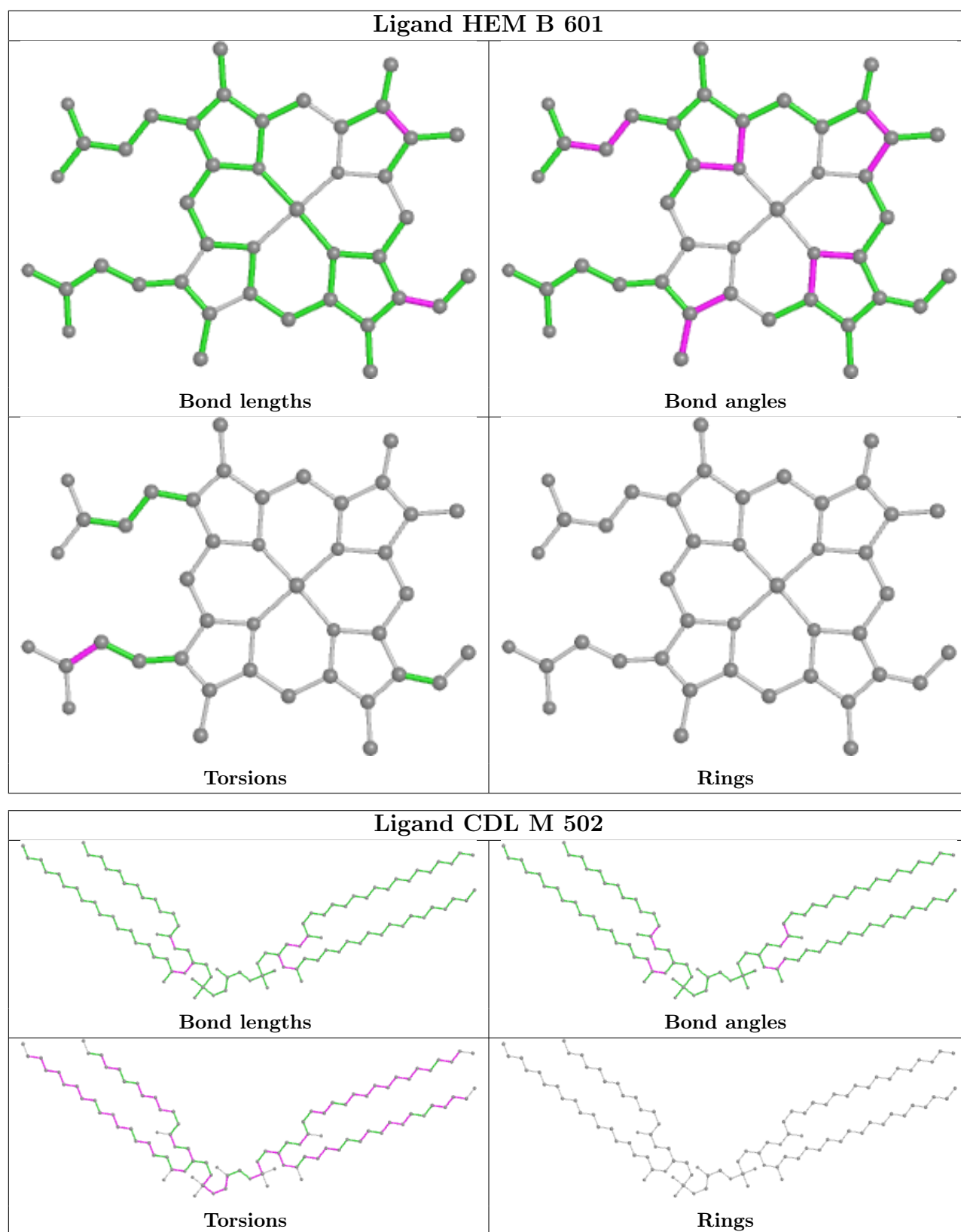


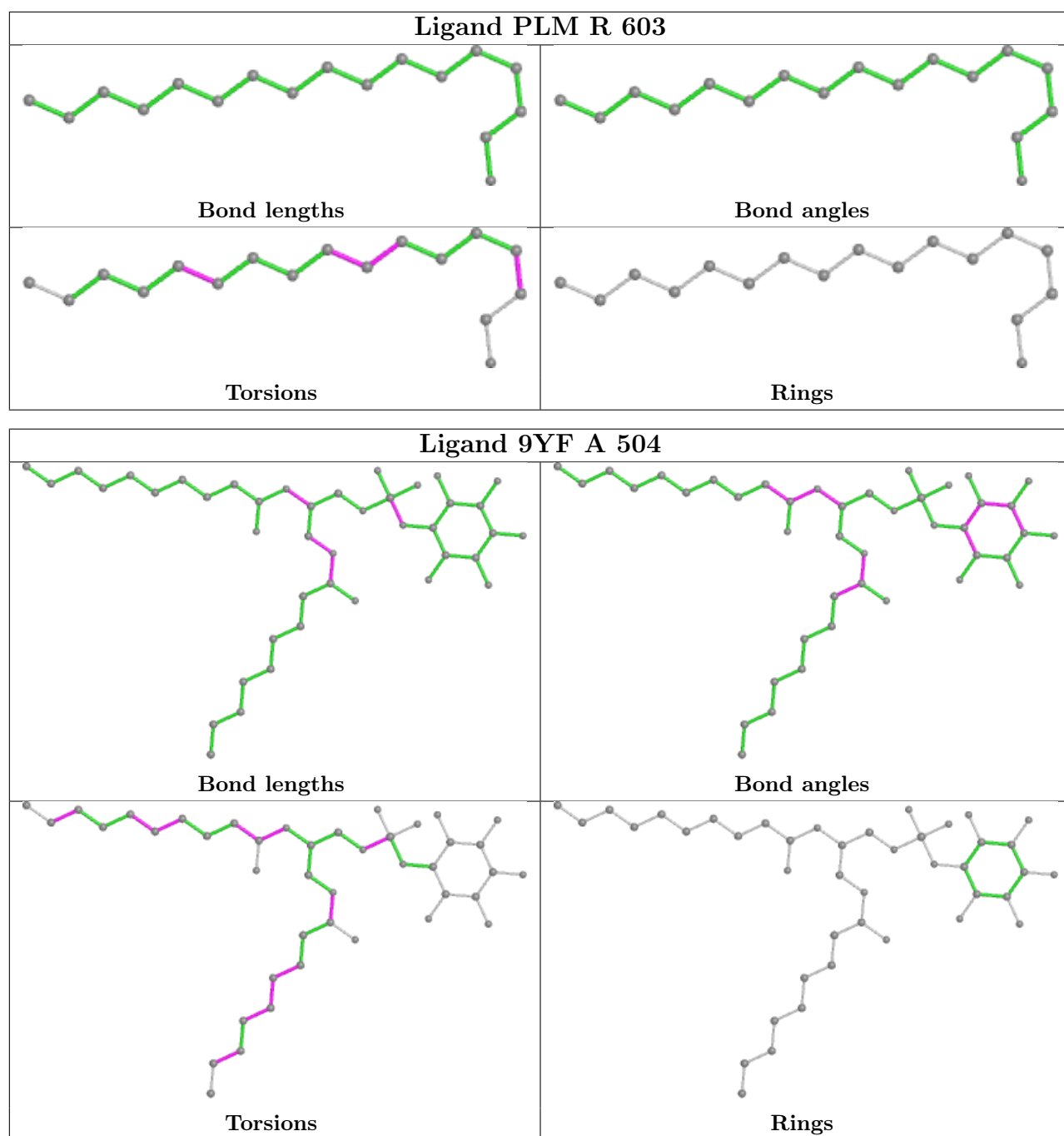


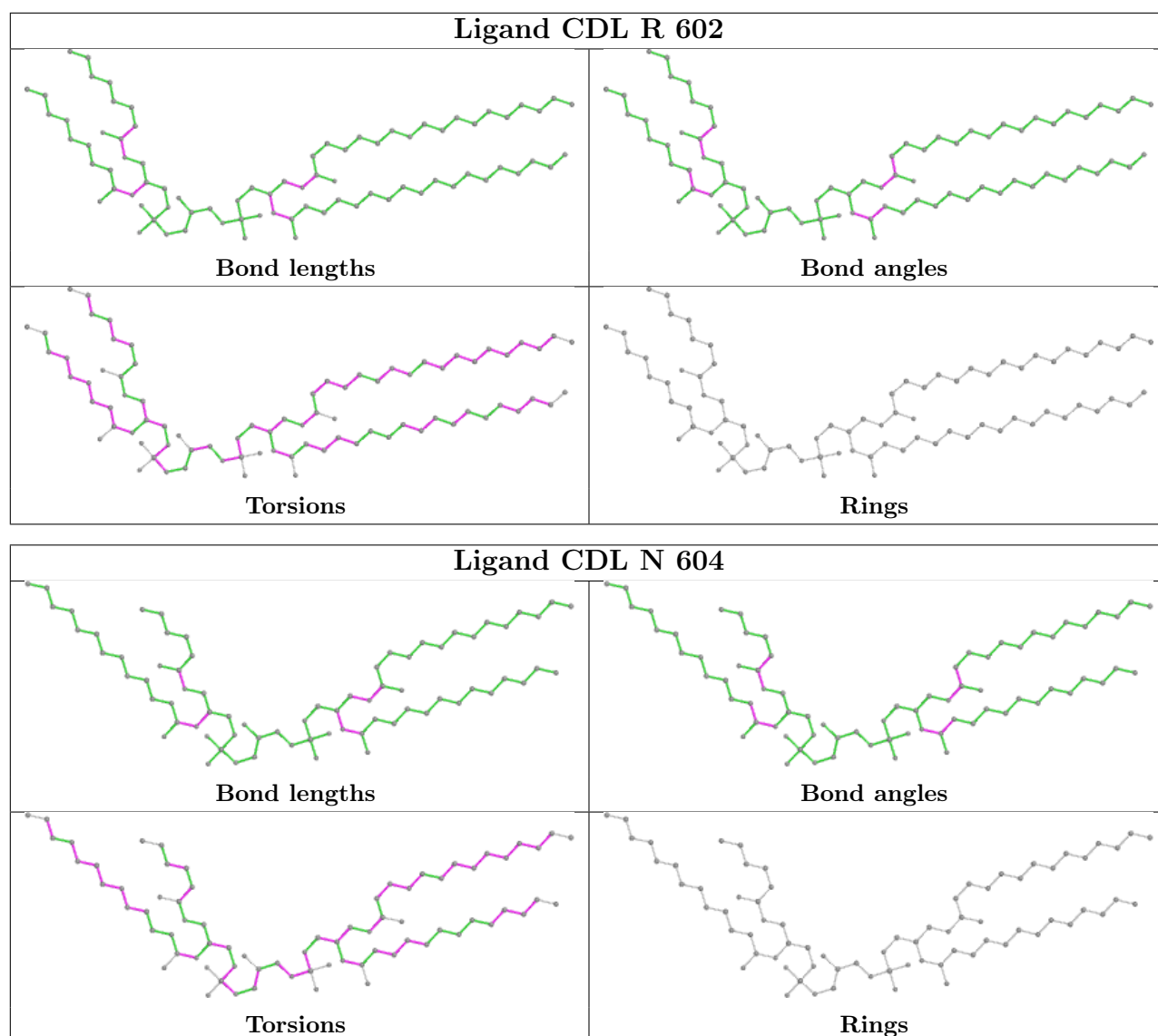


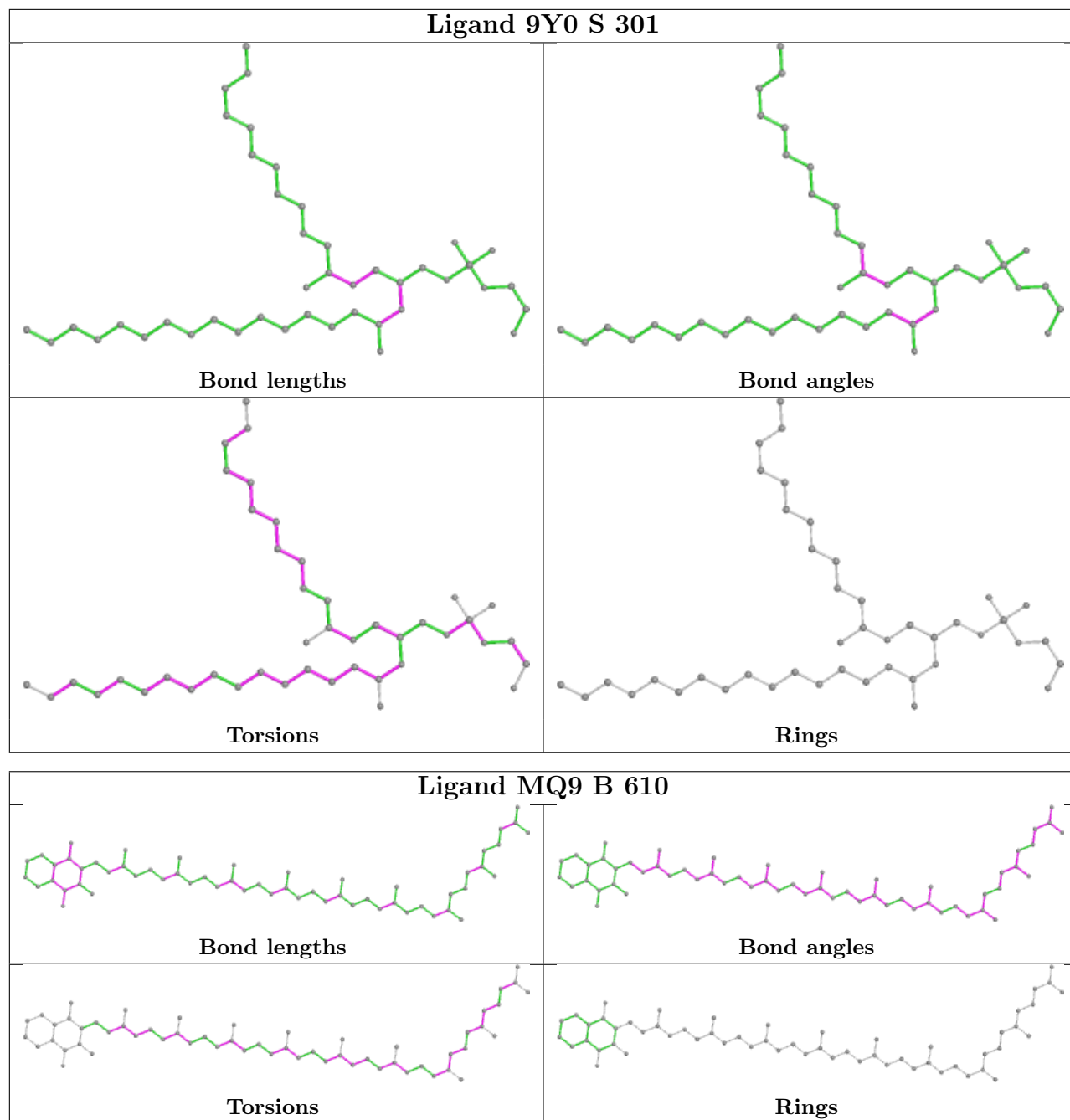


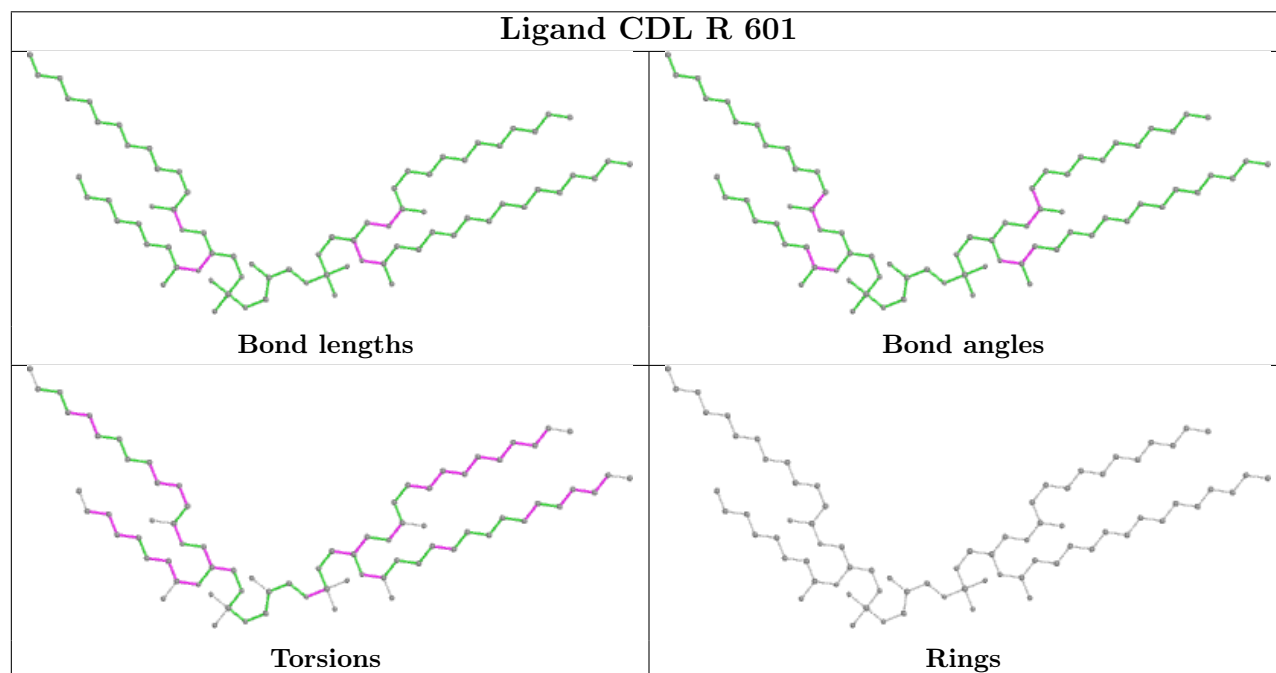
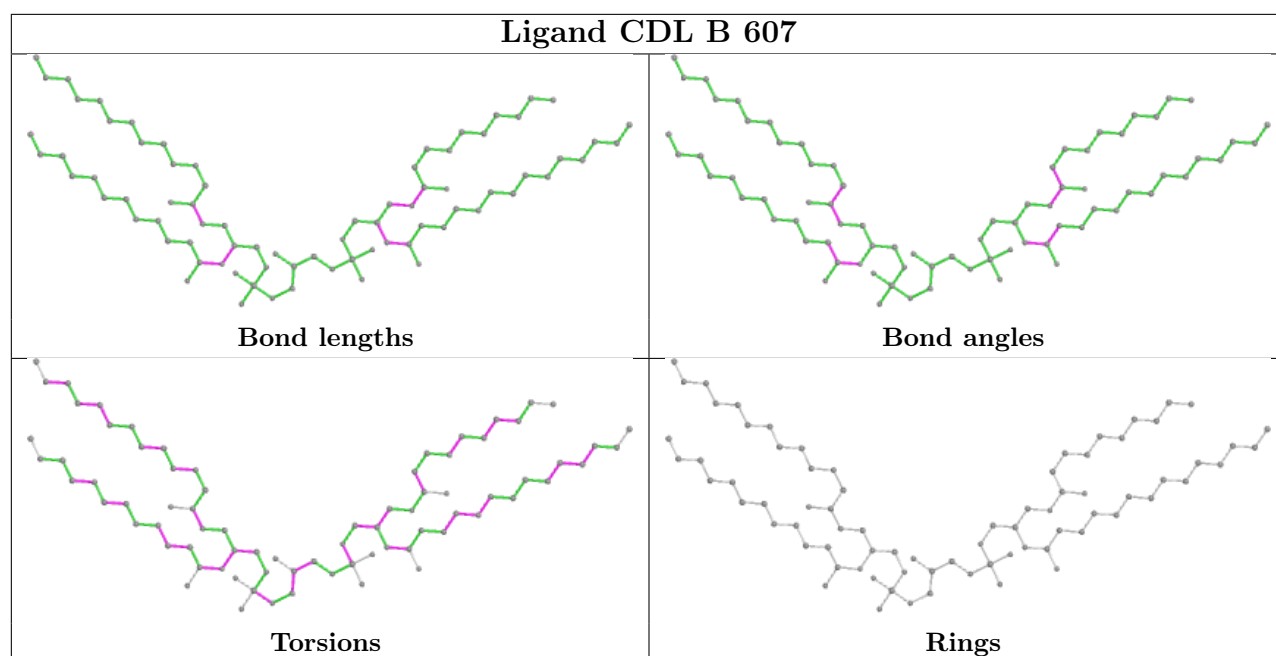


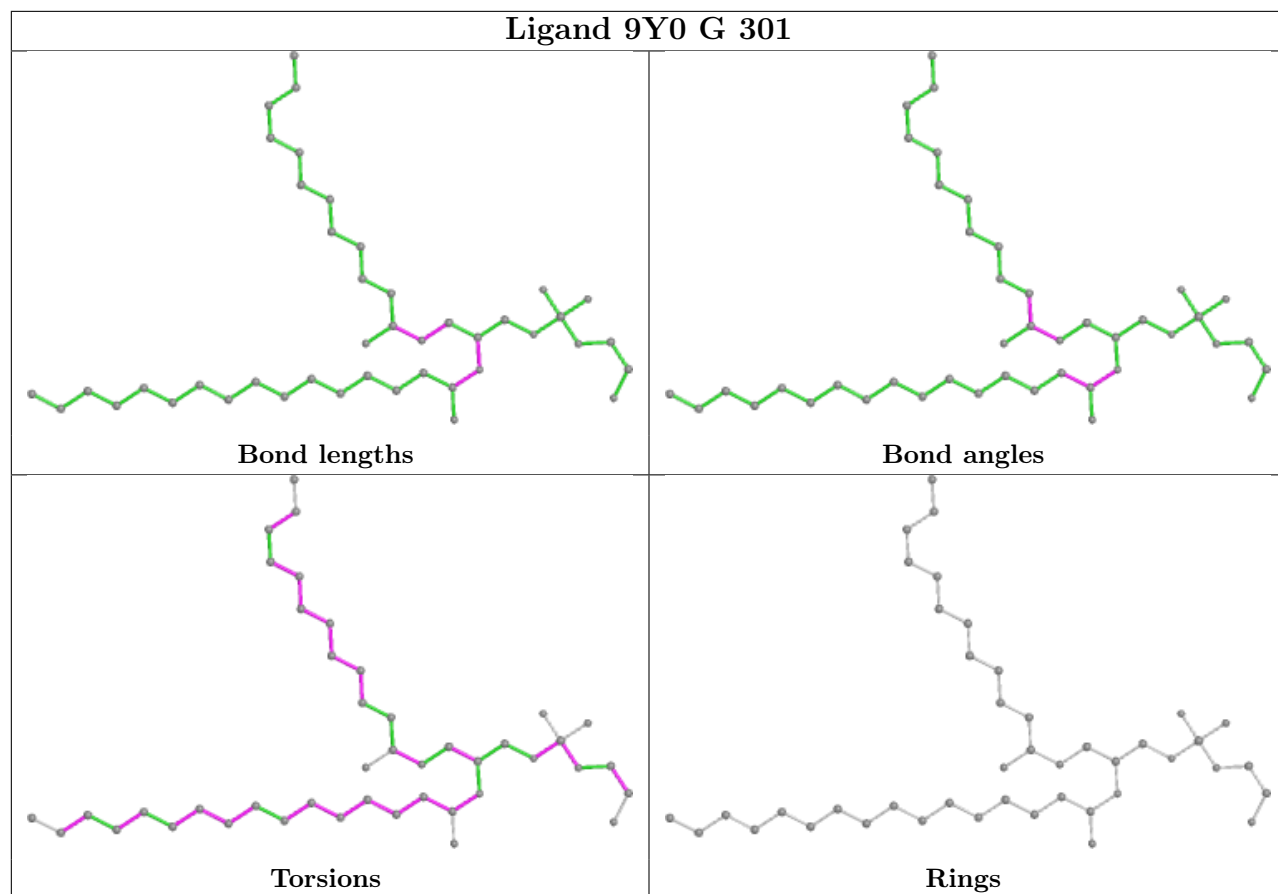


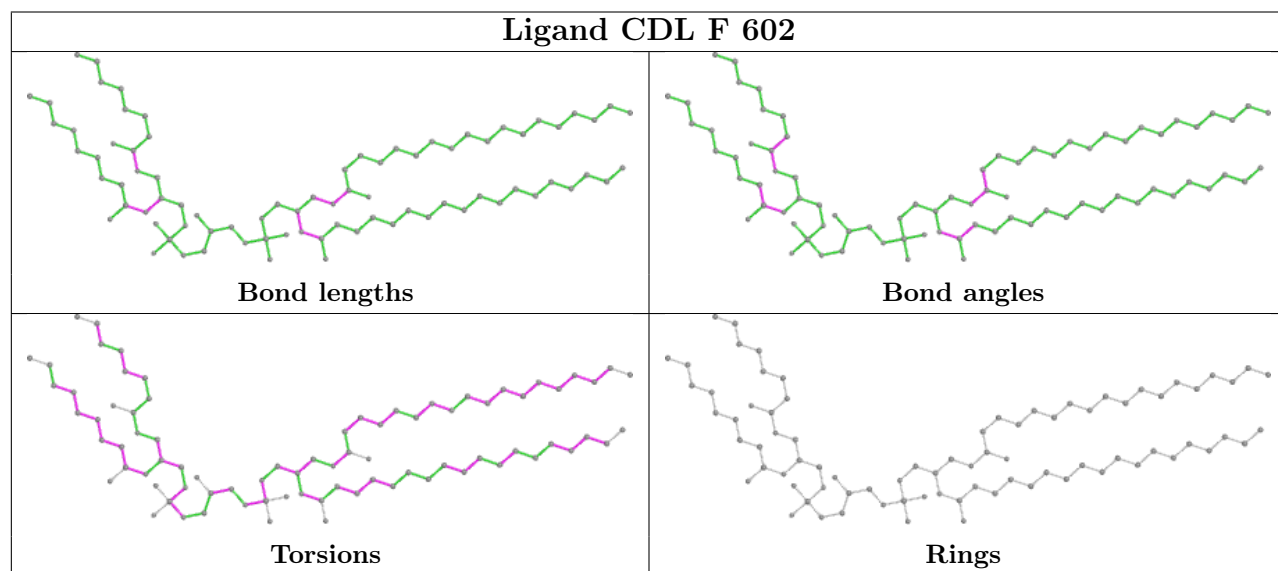
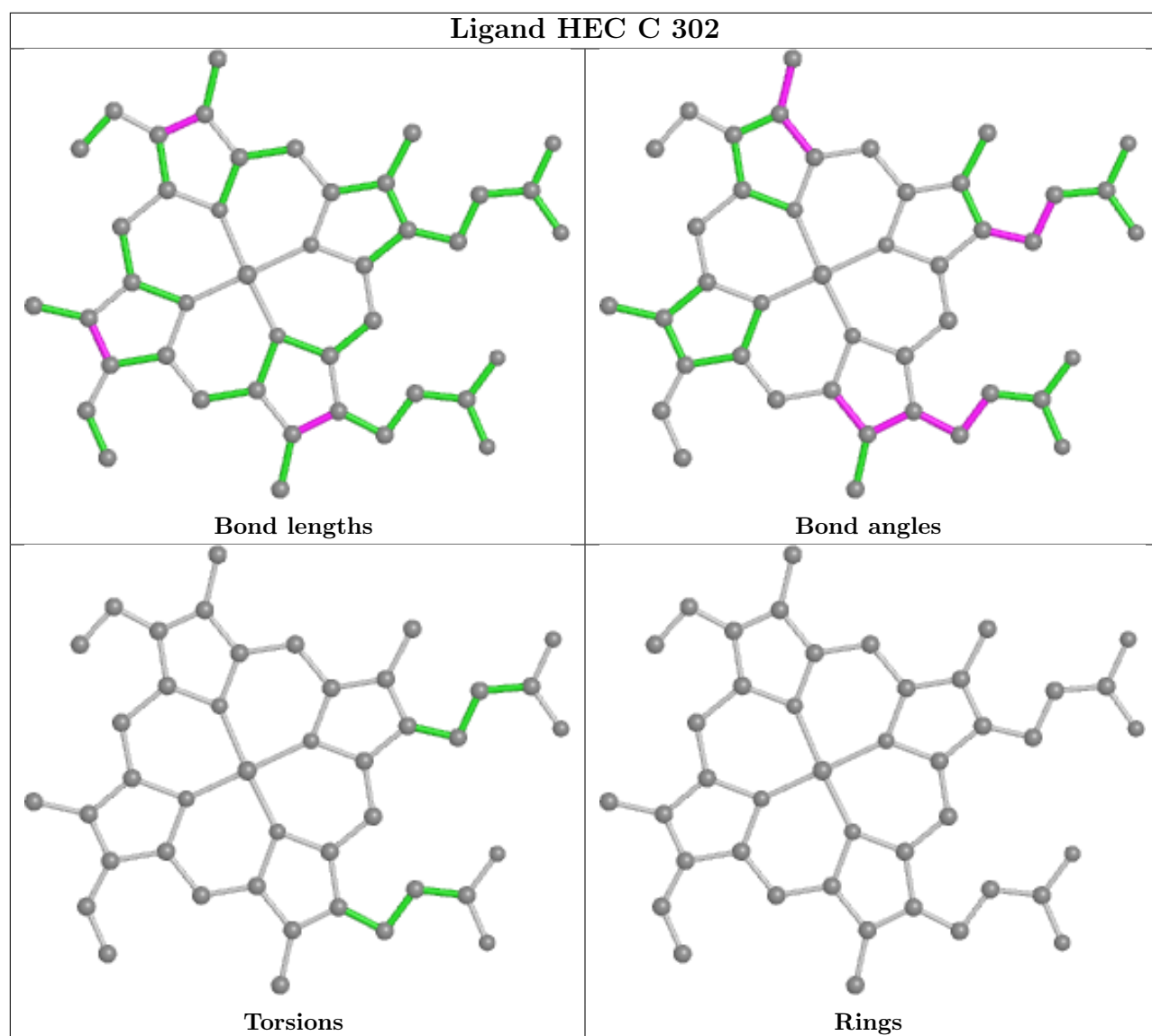


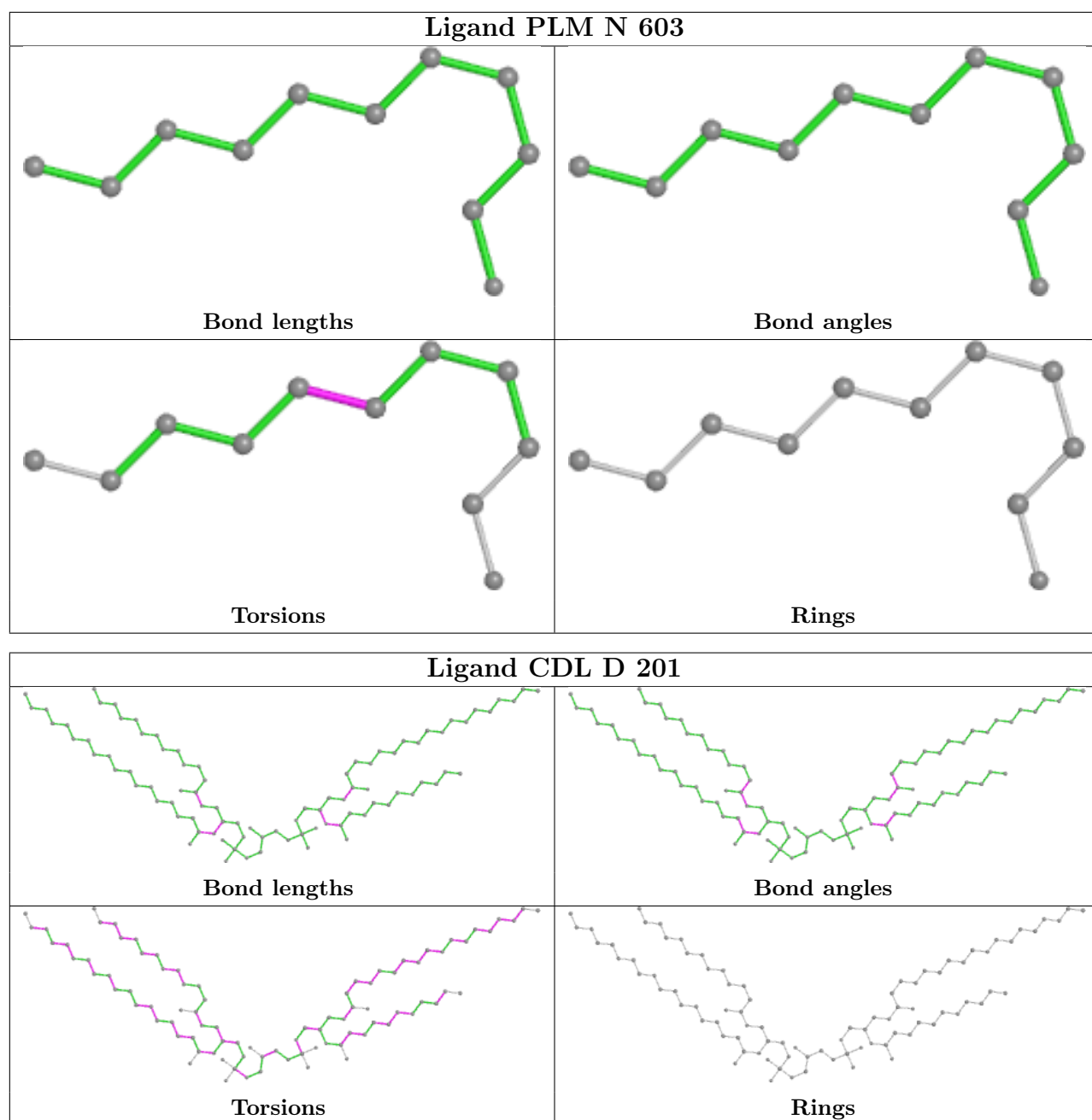


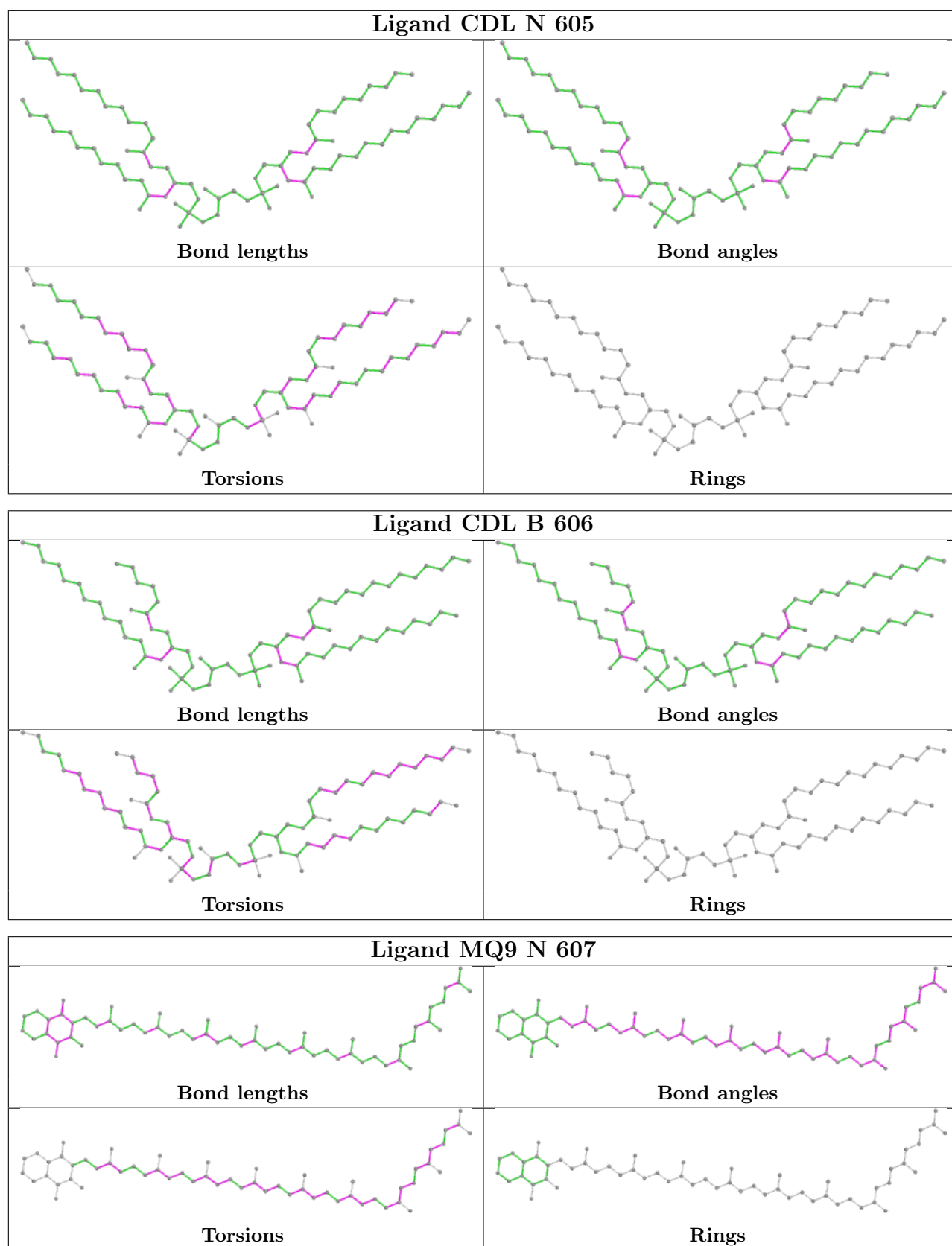


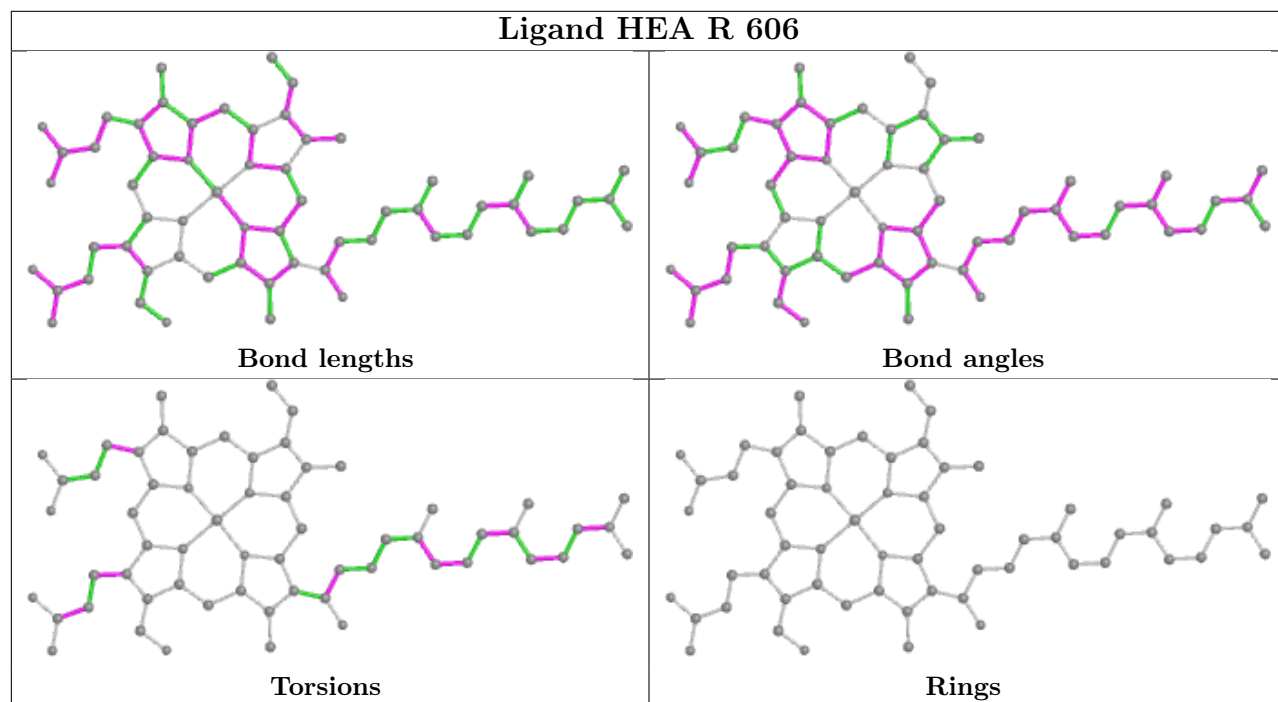
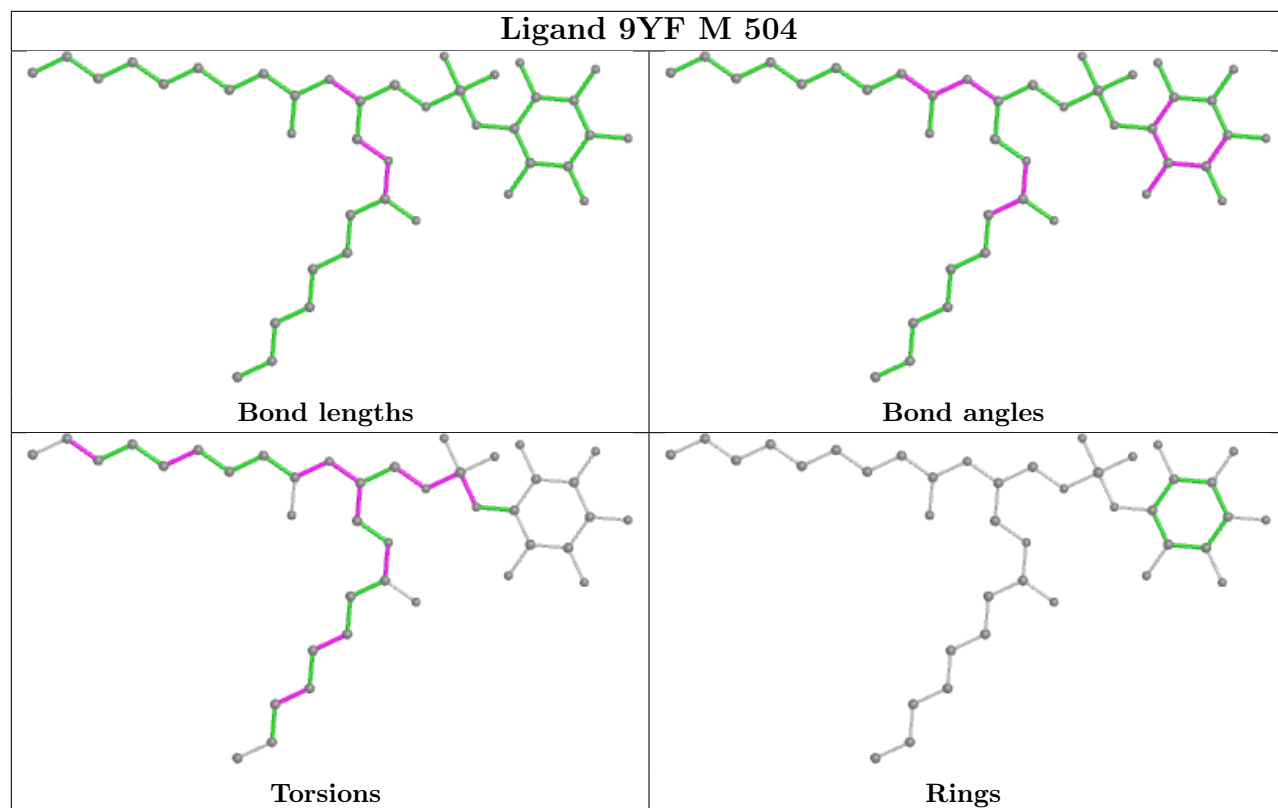


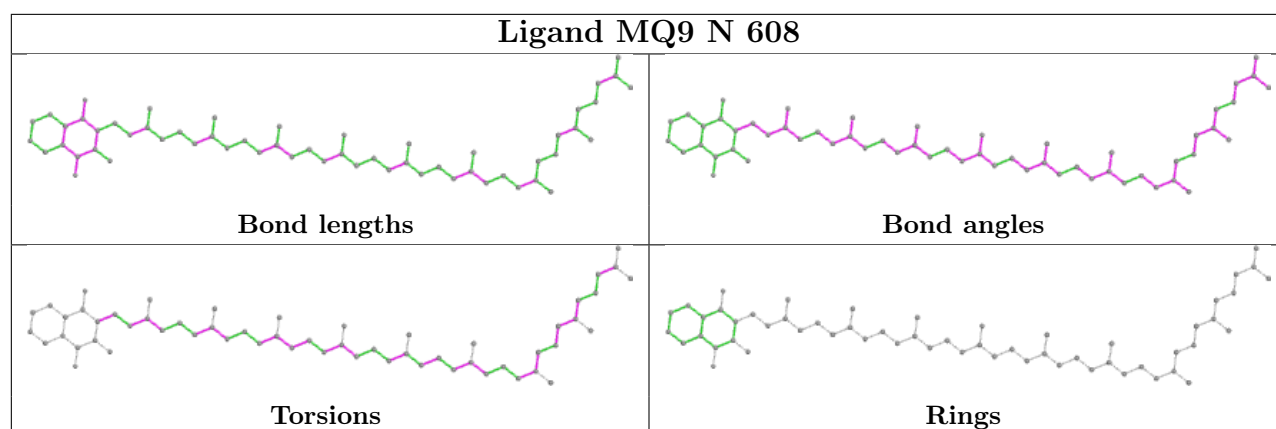












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

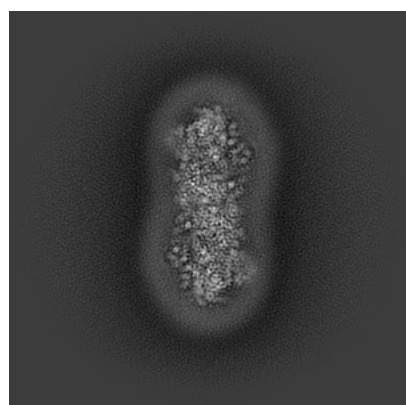
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30944. These allow visual inspection of the internal detail of the map and identification of artifacts.

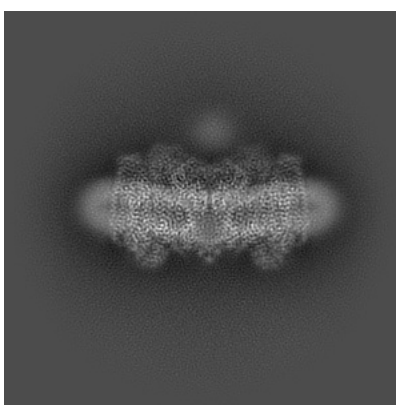
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

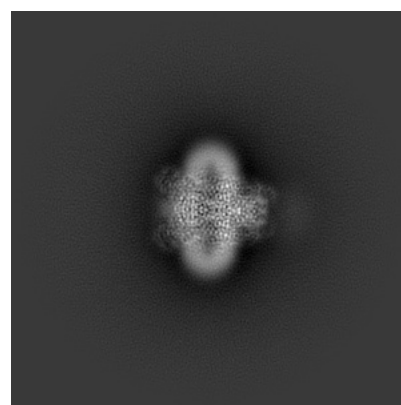
6.1.1 Primary map



X



Y

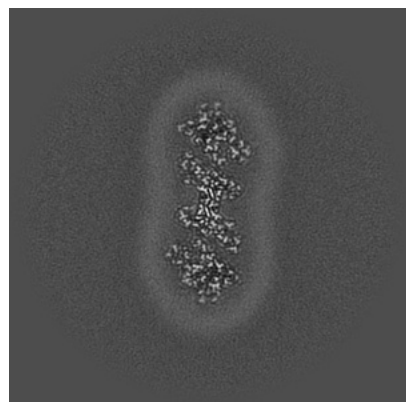


Z

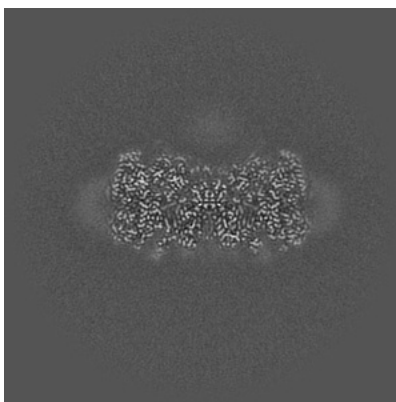
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

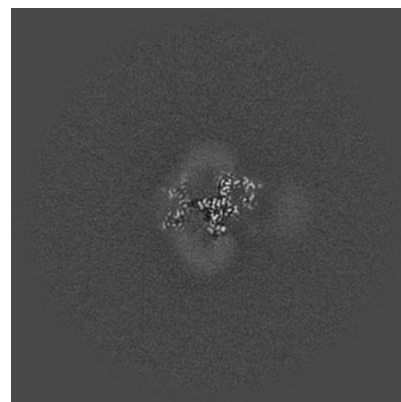
6.2.1 Primary map



X Index: 256



Y Index: 256

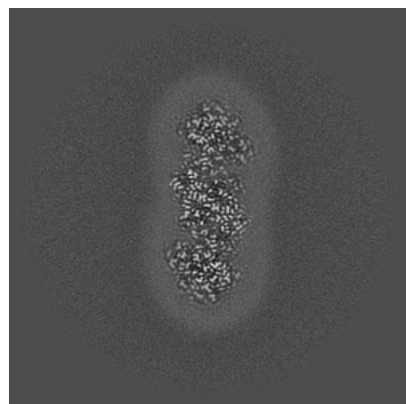


Z Index: 256

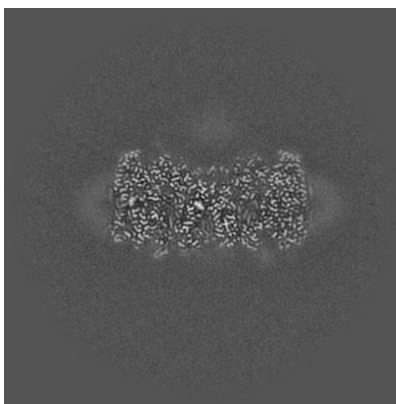
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

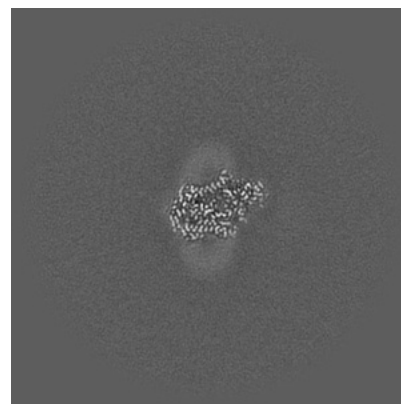
6.3.1 Primary map



X Index: 272



Y Index: 253

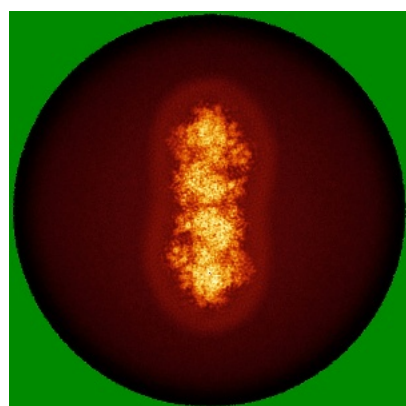


Z Index: 236

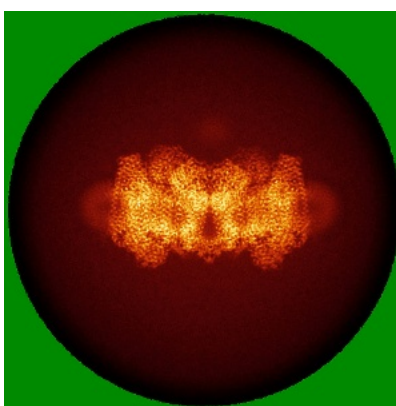
The images above show the largest variance slices of the map in three orthogonal directions.

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

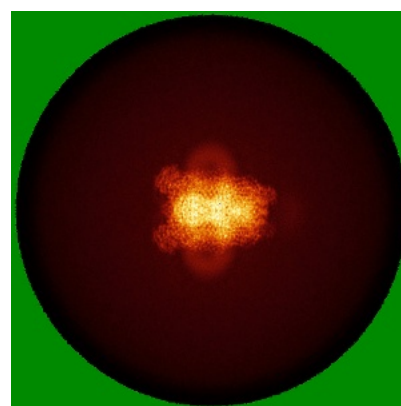
6.4.1 Primary map



X



Y



Z

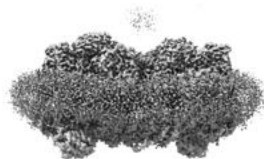
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

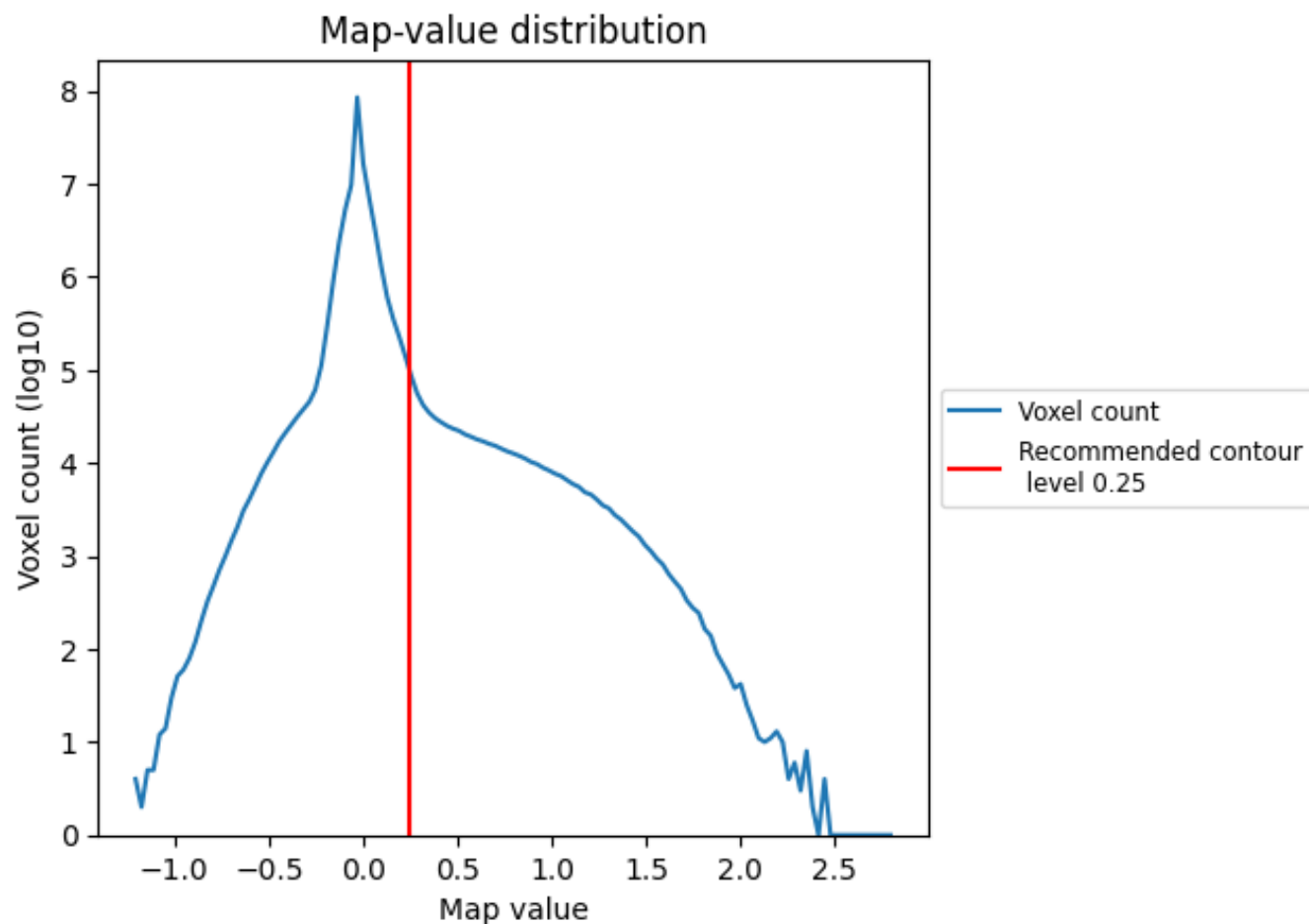
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

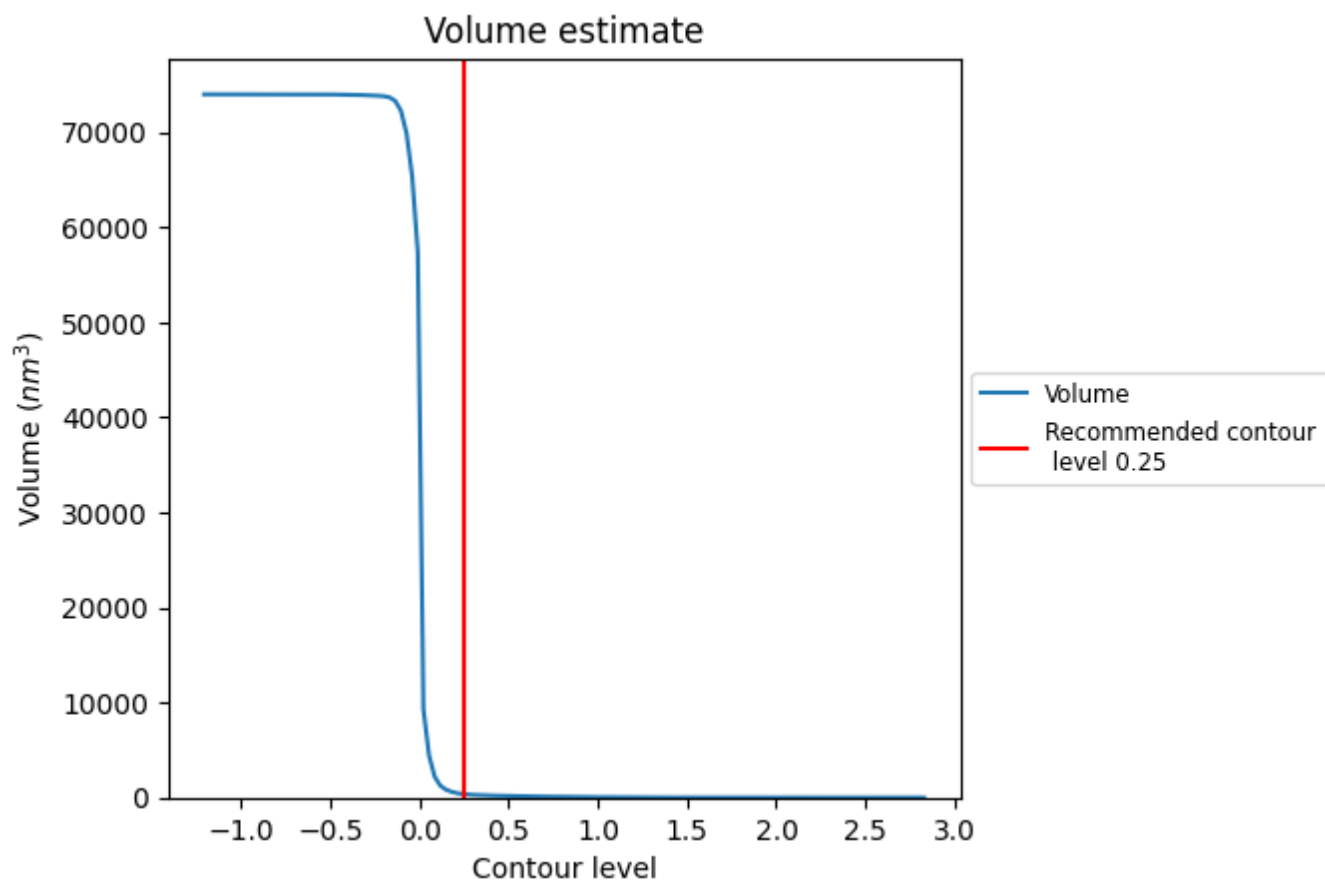
This section contains the results of statistical analysis of the map.

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.

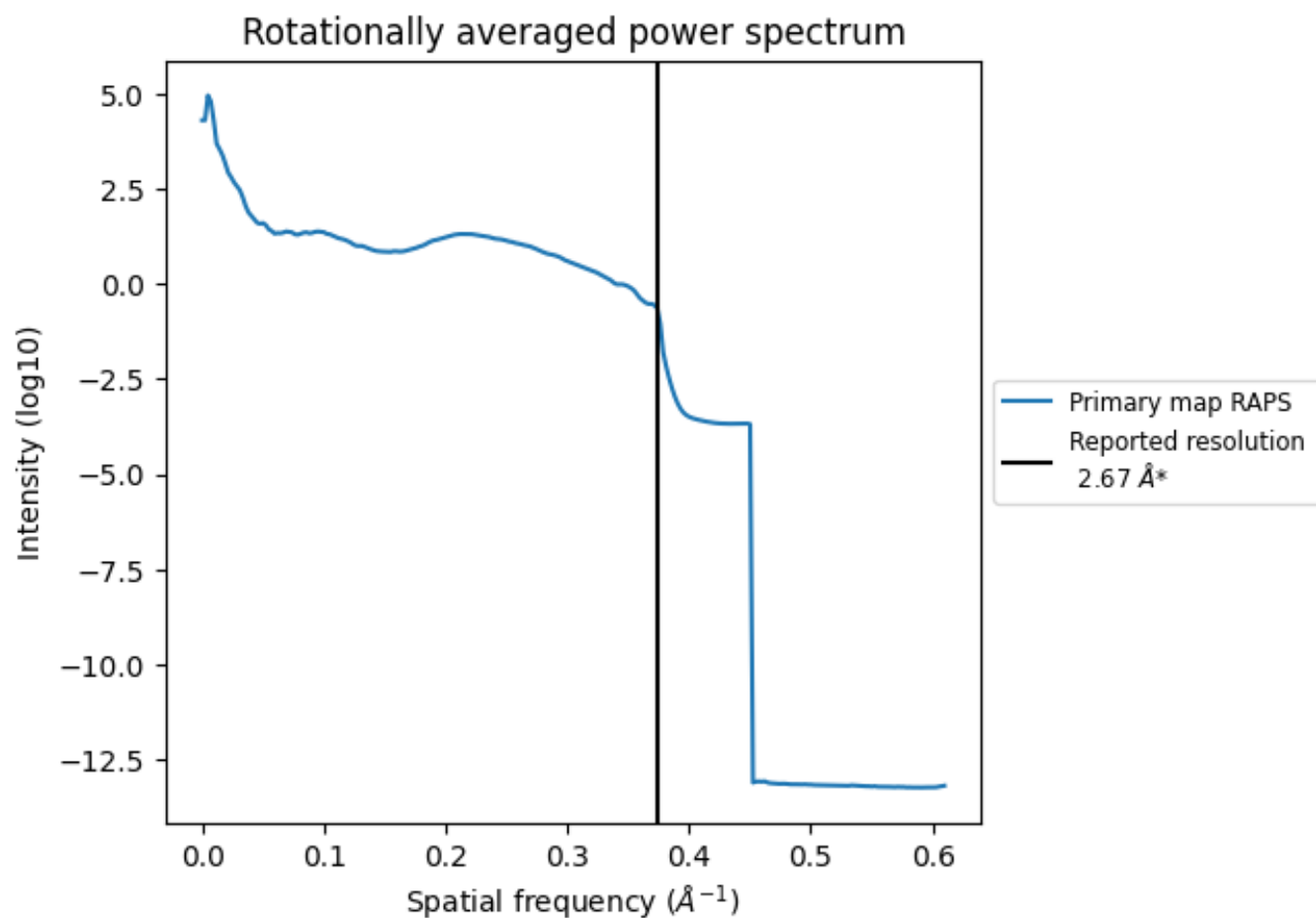
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm³; this corresponds to an approximate mass of 323 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 0.375 Å⁻¹

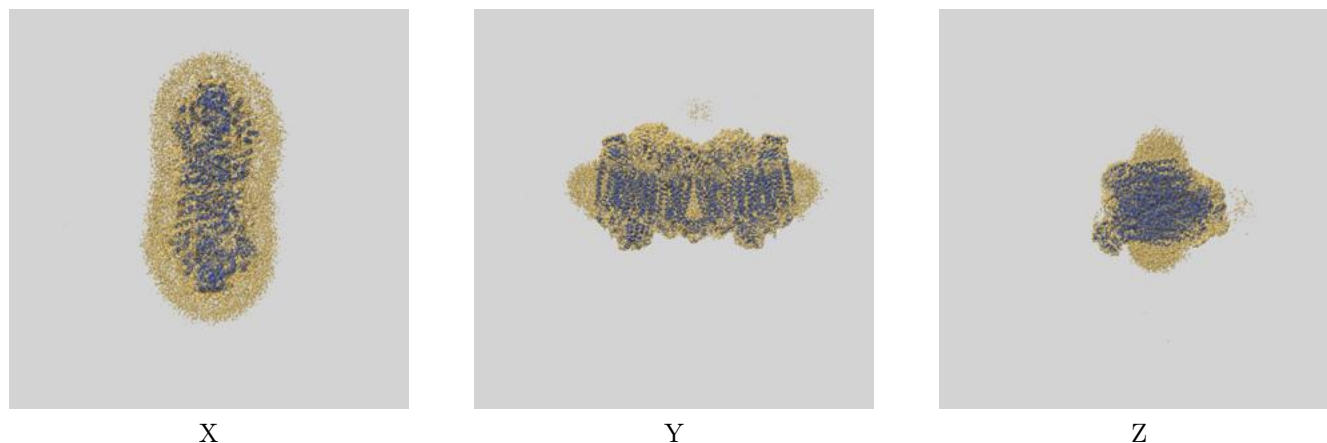
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

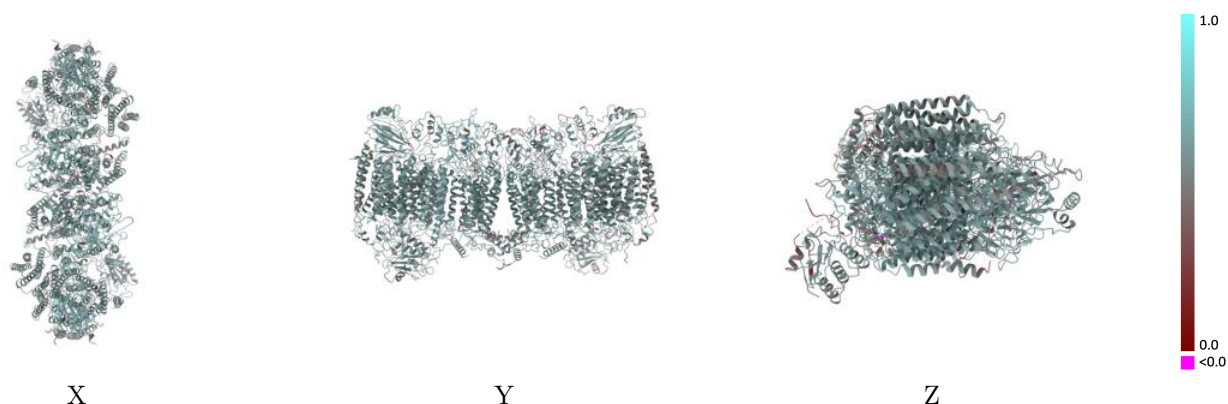
This section contains information regarding the fit between EMDB map EMD-30944 and PDB model 7E1W. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



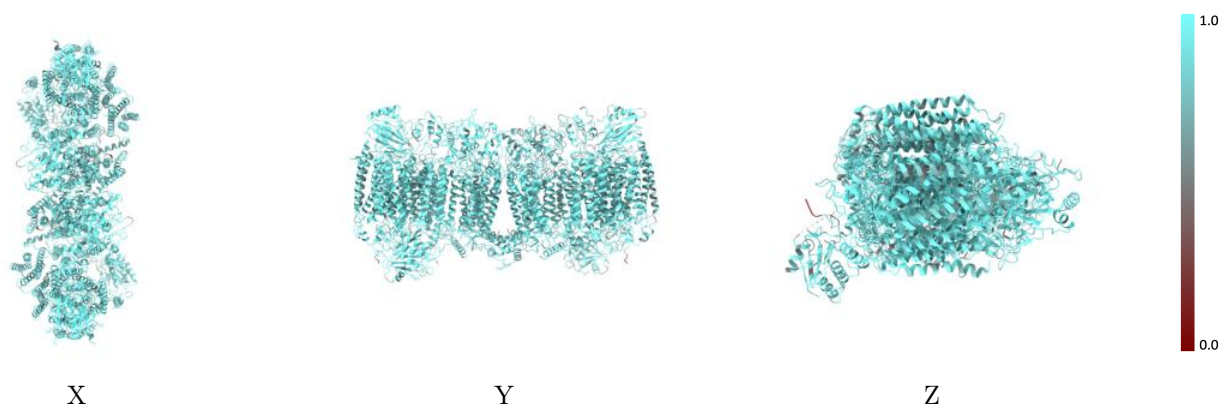
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



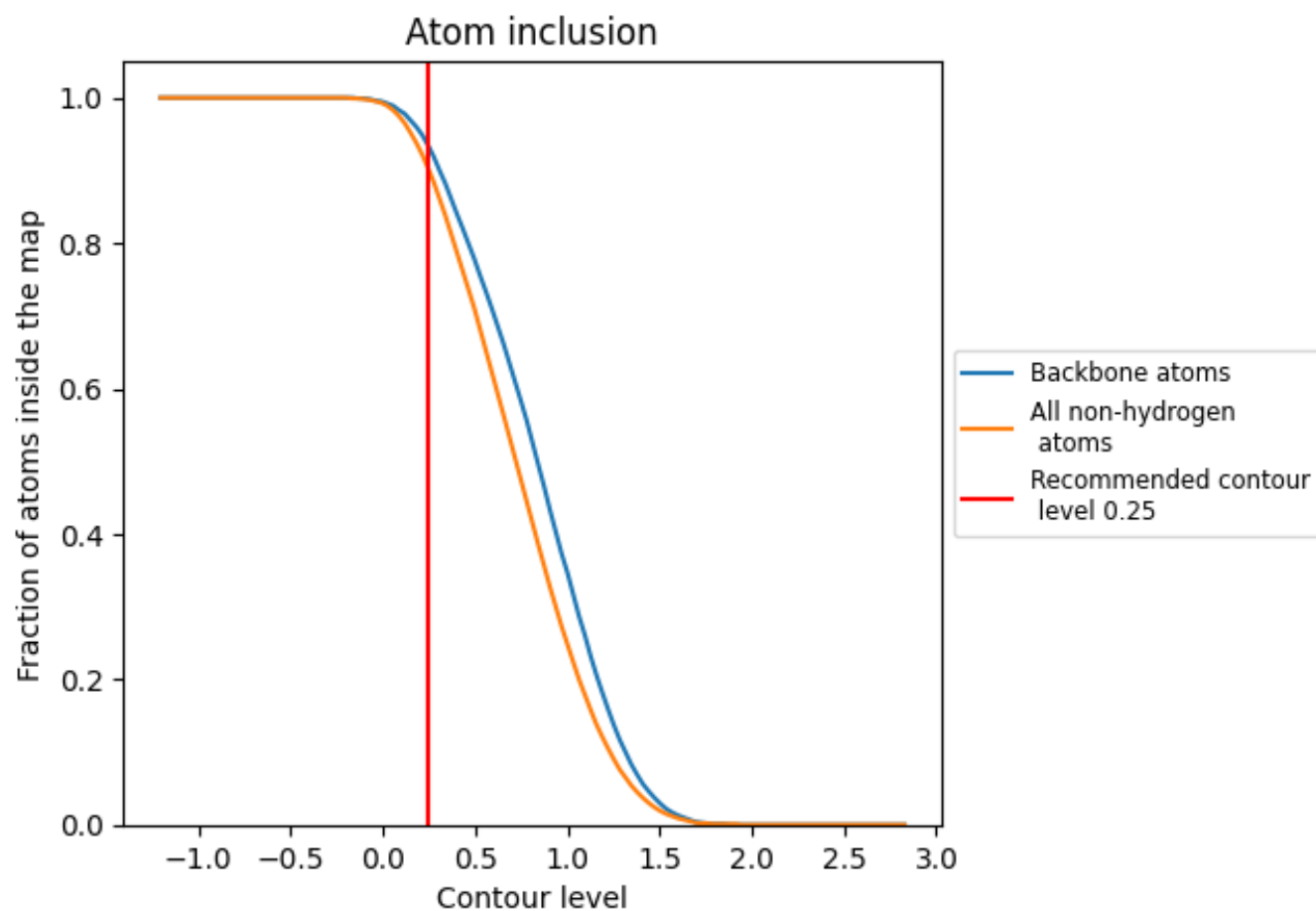
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.5690
A	 0.8900	 0.5640
B	 0.9160	 0.5880
C	 0.8940	 0.5670
D	 0.8610	 0.5590
E	 0.8820	 0.5460
F	 0.9250	 0.5870
G	 0.8730	 0.5480
H	 0.8870	 0.5590
I	 0.8280	 0.5070
J	 0.8390	 0.5020
M	 0.8850	 0.5600
N	 0.9110	 0.5880
O	 0.8480	 0.5560
P	 0.9040	 0.5820
Q	 0.9020	 0.5540
R	 0.9440	 0.5940
S	 0.9020	 0.5600
T	 0.9150	 0.5720
U	 0.8560	 0.5290
V	 0.8830	 0.5270

