



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 09:54 pm GMT

PDB ID : 7Q21
EMDB ID : EMD-13777
Title : III2-IV2 respiratory supercomplex from *Corynebacterium glutamicum*
Authors : Kovalova, T.; Moe, A.; Krol, S.; Yanofsky, D.J.; Bott, M.; Sjostrand, D.;
Rubinstein, J.L.; Hogbom, M.; Brzezinski, P.
Deposited on : 2021-10-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation 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:

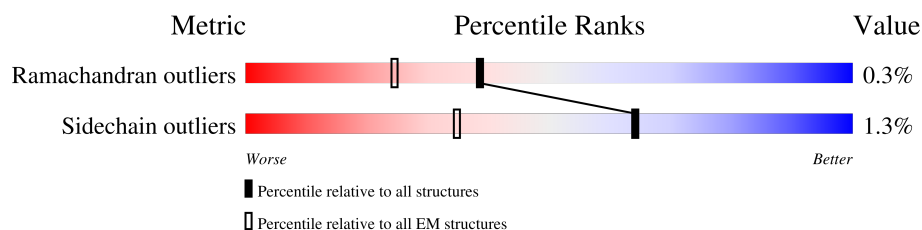
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.90 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.




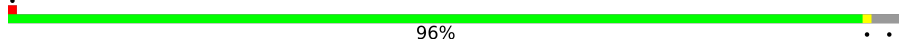
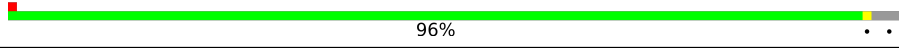
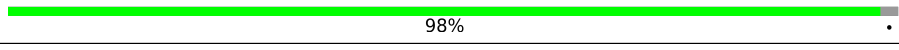
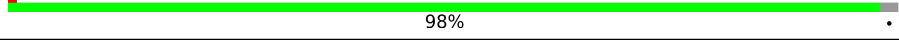

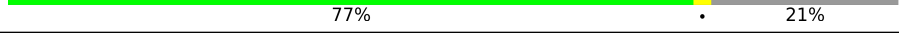
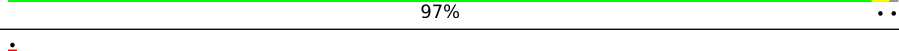
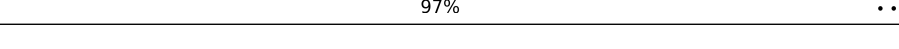
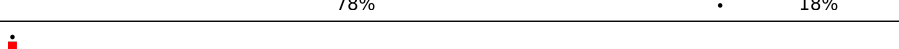
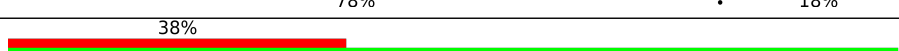
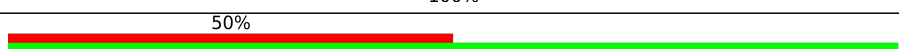


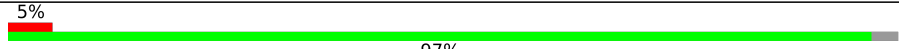
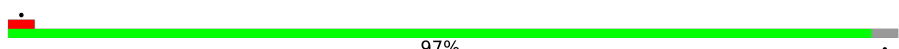

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	Y	96	100%
1	y	96	95% 5%
2	E	205	91% 8%
2	e	205	92% 8%
3	H	147	82% 15%
3	h	147	84% 14%
4	F	143	99% .
4	f	143	99% .
5	G	359	90% 9%

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Mol	Chain	Length	Quality of chain
5	g	359	
6	D	594	
6	d	594	
7	A	408	
7	a	408	
8	L	194	
8	l	194	
9	B	539	
9	b	539	
10	C	283	
10	c	283	
11	X	21	
12	x	22	
13	V	73	
13	v	73	
14	K	65	
14	k	65	

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
22	HAS	D	602	X	-	-	-
22	HAS	D	603	X	-	-	-
22	HAS	d	603	X	-	-	-
22	HAS	d	604	X	-	-	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 47749 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 Co-purified unknown transmembrane helices built as polyALA (AscD).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Y	96	Total	C	N	O	0	0
			480	288	96	96		
1	y	91	Total	C	N	O	0	0
			455	273	91	91		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	189	Total	C	N	O	S	0	0
			1478	987	235	249	7		
2	e	189	Total	C	N	O	S	0	0
			1478	987	235	249	7		

- Molecule 3 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total	C	N	O	S	0	0
			994	643	173	177	1		
3	h	126	Total	C	N	O	S	0	0
			1003	648	174	180	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	143	Total	C	N	O	S	0	0
			1094	728	167	190	9		
4	f	143	Total	C	N	O	S	0	0
			1094	728	167	190	9		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		
5	g	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		
6	d	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	-	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
d	585	ALA	-	expression tag	UNP Q79VD7
d	586	ALA	-	expression tag	UNP Q79VD7
d	587	TRP	-	expression tag	UNP Q79VD7
d	588	SER	-	expression tag	UNP Q79VD7
d	589	HIS	-	expression tag	UNP Q79VD7
d	590	PRO	-	expression tag	UNP Q79VD7
d	591	GLN	-	expression tag	UNP Q79VD7
d	592	PHE	-	expression tag	UNP Q79VD7
d	593	GLU	-	expression tag	UNP Q79VD7
d	594	LYS	-	expression tag	UNP Q79VD7

- Molecule 7 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		
8	l	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		

- Molecule 9 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		
9	b	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		
10	c	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		

- Molecule 11 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	21	Total	C	N	O	S	0	0
			106	63	21	21	1		

- Molecule 12 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	22	Total	C	N	O	S	0	0
			111	66	22	22	1		

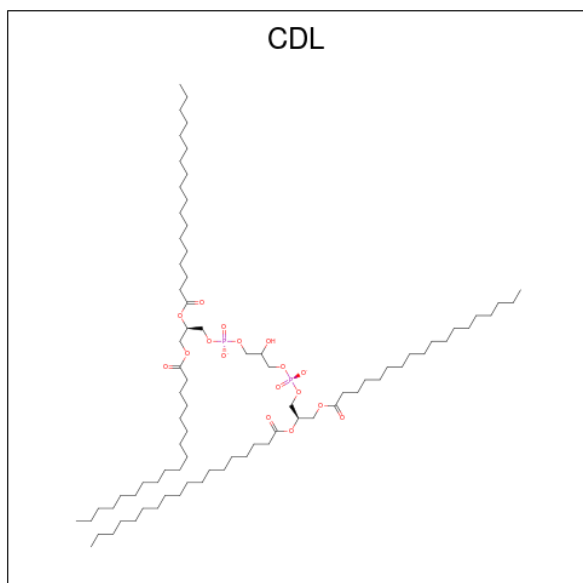
- Molecule 13 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	54	Total	C	N	O	0	0
			420	268	69	83		
13	v	54	Total	C	N	O	0	0
			420	268	69	83		

- Molecule 14 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	63	Total	C	N	O	S	0	0
			444	294	70	77	3		
14	k	63	Total	C	N	O	S	0	0
			444	294	70	77	3		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



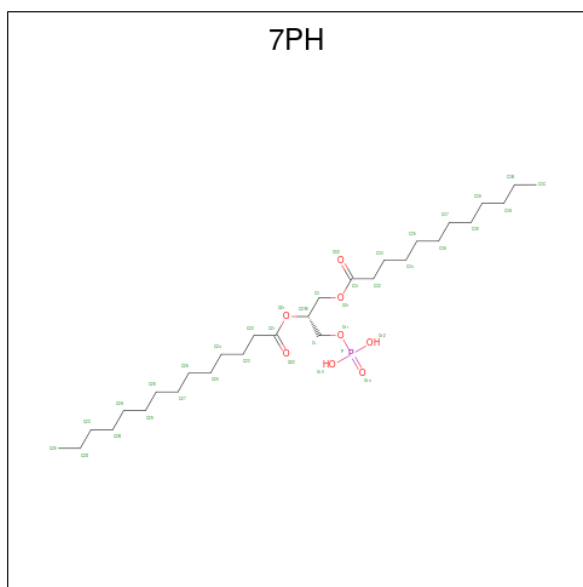
Mol	Chain	Residues	Atoms				AltConf
15	E	1	Total	C	O	P	0
			66	47	17	2	
15	F	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			74	55	17	2	
15	B	1	Total	C	O	P	0
			77	58	17	2	
15	B	1	Total	C	O	P	0
			74	55	17	2	

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Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			79	60	17	2	
15	e	1	Total	C	O	P	0
			66	47	17	2	
15	f	1	Total	C	O	P	0
			79	60	17	2	
15	d	1	Total	C	O	P	0
			79	60	17	2	
15	d	1	Total	C	O	P	0
			66	47	17	2	
15	b	1	Total	C	O	P	0
			74	55	17	2	
15	b	1	Total	C	O	P	0
			77	58	17	2	
15	c	1	Total	C	O	P	0
			79	60	17	2	

- Molecule 16 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



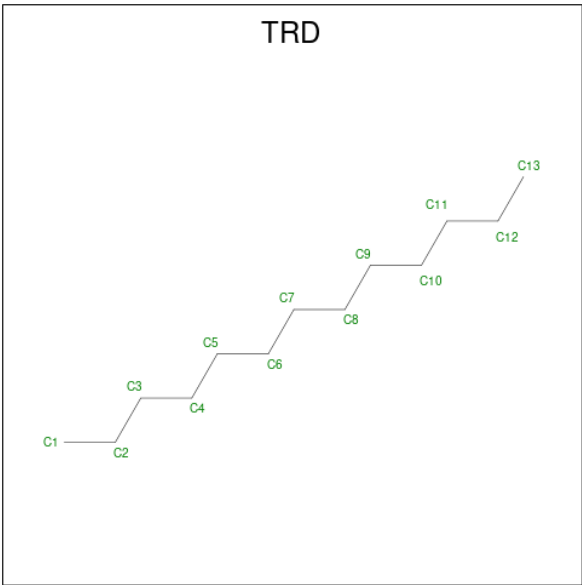
Mol	Chain	Residues	Atoms				AltConf
16	E	1	Total	C	O	P	0
			38	29	8	1	
16	H	1	Total	C	O	P	0
			38	29	8	1	
16	F	1	Total	C	O	P	0
			38	29	8	1	

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Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	e	1	Total	C	O	P	0
			38	29	8	1	
16	h	1	Total	C	O	P	0
			38	29	8	1	
16	f	1	Total	C	O	P	0
			38	29	8	1	
16	g	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	k	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 17 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



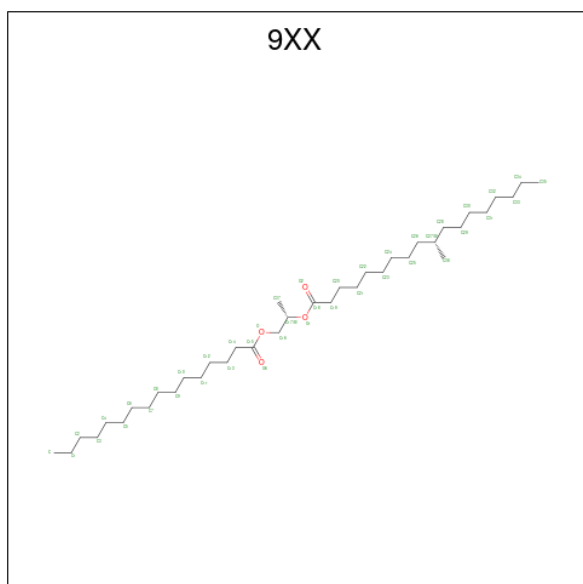
Mol	Chain	Residues	Atoms		AltConf
17	E	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	B	1	Total	C	0
			13	13	
17	e	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	

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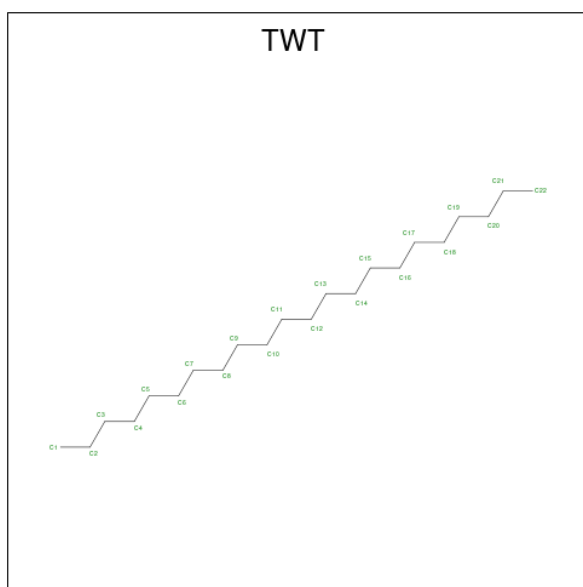
Mol	Chain	Residues	Atoms	AltConf
17	f	1	Total C 13 13	0
17	f	1	Total C 13 13	0
17	a	1	Total C 13 13	0
17	b	1	Total C 13 13	0

- Molecule 18 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C O 32 28 4	0
18	B	1	Total C O 32 28 4	0
18	h	1	Total C O 32 28 4	0
18	h	1	Total C O 32 28 4	0

- Molecule 19 is DOCOSANE (three-letter code: TWT) (formula: C₂₂H₄₆).



Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C 22 22	0
19	h	1	Total C 22 22	0

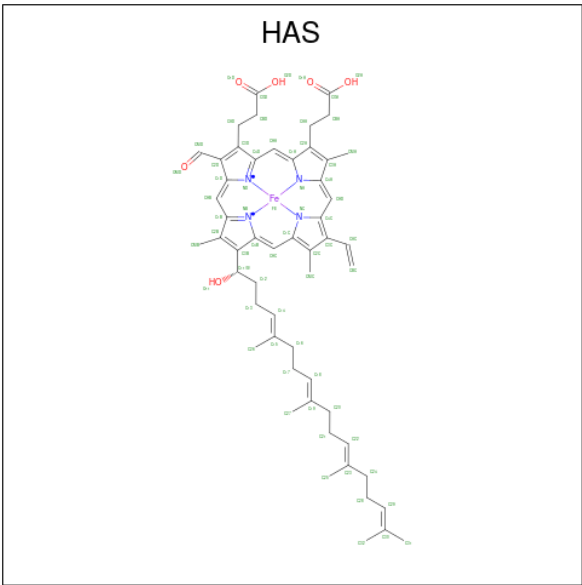
- Molecule 20 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
20	G	2	Total Cu 2 2	0
20	D	1	Total Cu 1 1	0
20	g	2	Total Cu 2 2	0
20	d	1	Total Cu 1 1	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total Mg 1 1	0
21	d	1	Total Mg 1 1	0

- Molecule 22 is HEME-AS (three-letter code: HAS) (formula: C₅₄H₆₄FeN₄O₆).

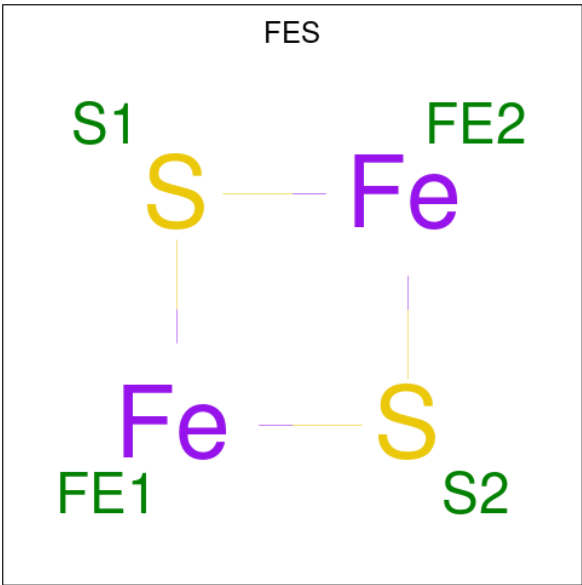


Mol	Chain	Residues	Atoms					AltConf
22	D	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	D	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	d	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	d	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

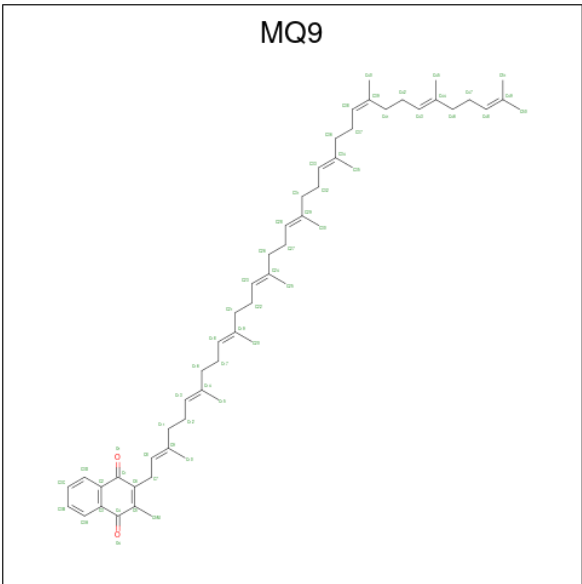
Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total	Ca	0
			1	1	
23	d	1	Total	Ca	0
			1	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	Fe	S	0
			4	2	2	
24	a	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



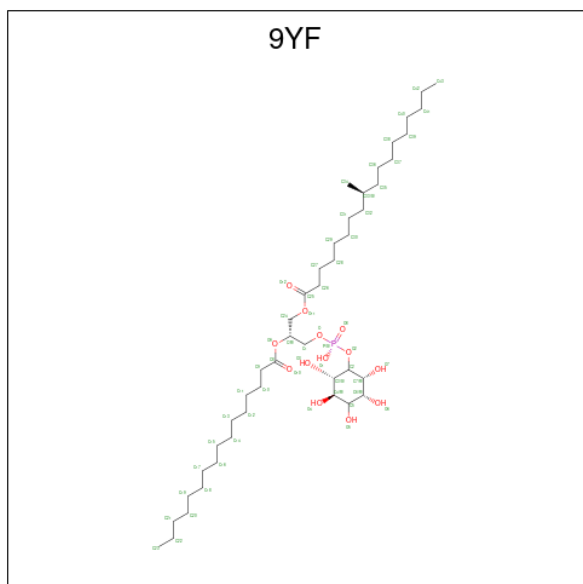
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			43	41	2	

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Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			43	41	2	
25	B	1	Total	C	O	0
			58	56	2	
25	a	1	Total	C	O	0
			43	41	2	
25	b	1	Total	C	O	0
			43	41	2	
25	b	1	Total	C	O	0
			58	56	2	

- Molecule 26 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).



Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			58	44	13	1	
26	a	1	Total	C	O	P	0
			58	44	13	1	
26	a	1	Total	C	O	P	0
			58	44	13	1	
26	l	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 27 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



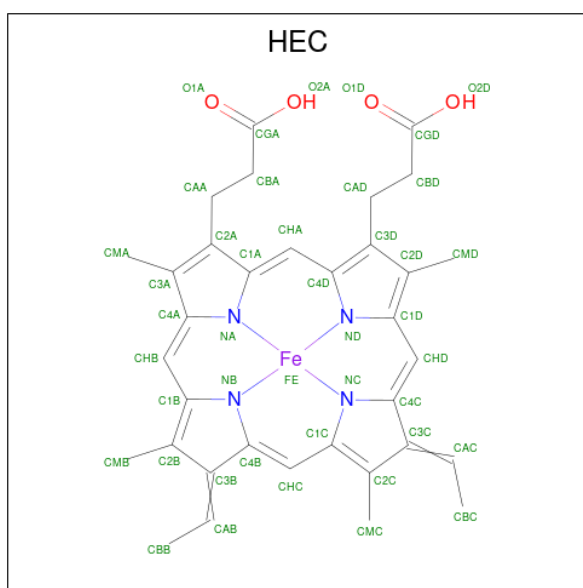
Mol	Chain	Residues	Atoms			AltConf
27	L	1	Total 11	C 10	O 1	0
27	d	1	Total 11	C 10	O 1	0
27	X	1	Total 11	C 10	O 1	0
27	x	1	Total 11	C 10	O 1	0

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	b	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	b	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 29 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).

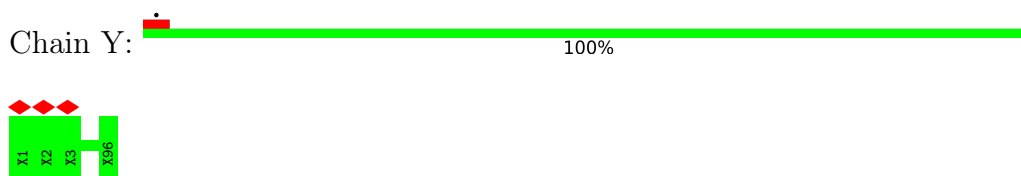


Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	c	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	c	1	Total 43	C 34	Fe 1	N 4	O 4	0

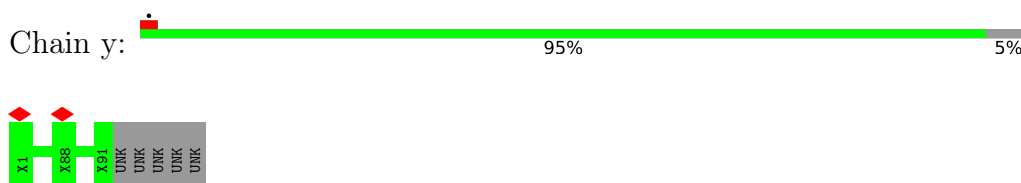
3 Residue-property plots [i](#)

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

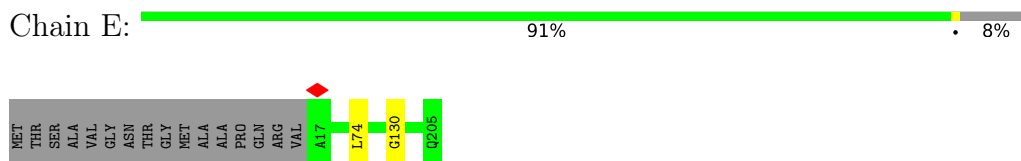
- Molecule 1: Co-purified unknown transmembrane helices built as polyALA (AscD)



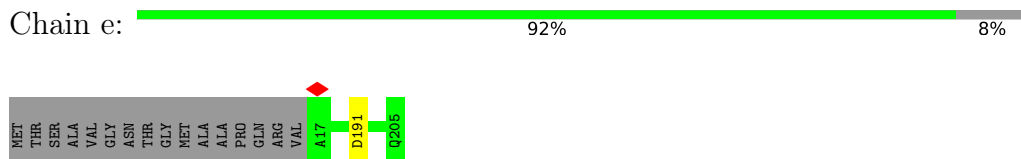
- Molecule 1: Co-purified unknown transmembrane helices built as polyALA (AscD)



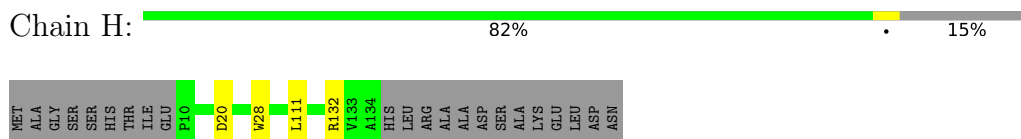
- Molecule 2: Cytochrome c oxidase subunit 3




- Molecule 2: Cytochrome c oxidase subunit 3



- Molecule 3: Uncharacterized membrane protein Cgl2017/cg2211



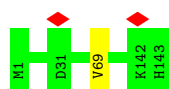
- Molecule 3: Uncharacterized membrane protein Cgl2017/cg2211

Chain h:  84% 14%



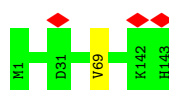
- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain F:  99%




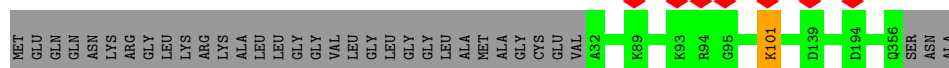
- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain f:  99%



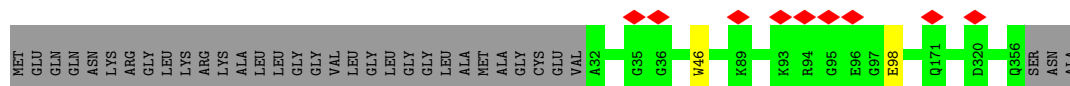
- Molecule 5: Cytochrome c oxidase subunit 2

Chain G:  90% 9%



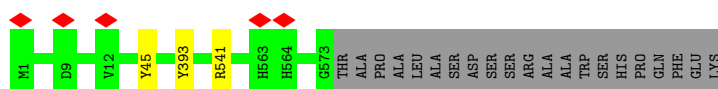
- Molecule 5: Cytochrome c oxidase subunit 2

Chain g:  90% 9%



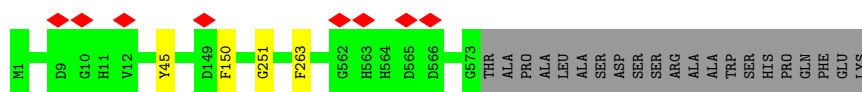
- Molecule 6: Cytochrome c oxidase subunit 1

Chain D:  96%



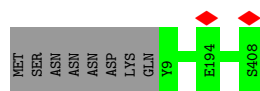
- Molecule 6: Cytochrome c oxidase subunit 1

Chain d:  96%



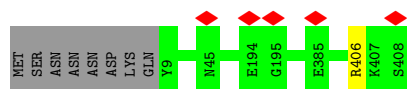
- Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A: 98%



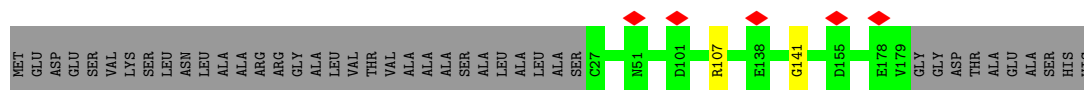
- Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain a: 98%



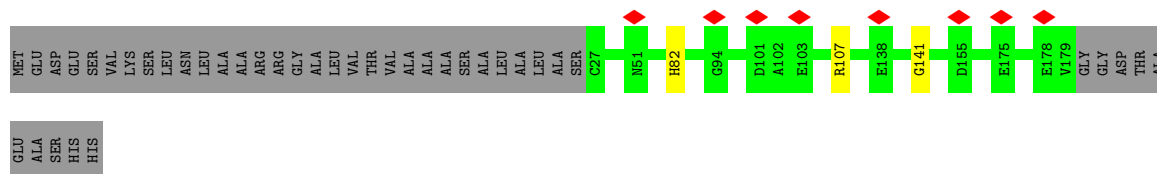
- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain L: 78% 21%



- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain l: 77% 21%



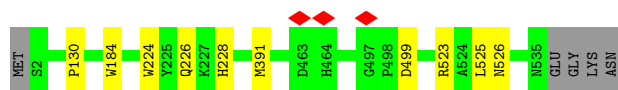
- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain B: 97%



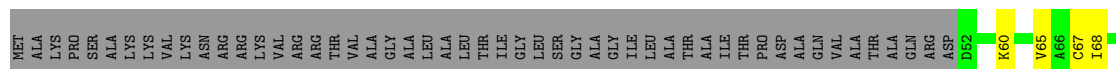
- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain b: 97%



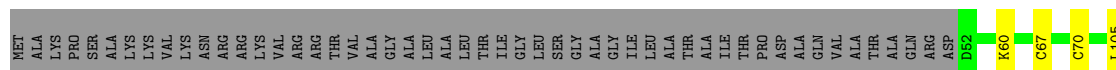
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain C: 78% 18%



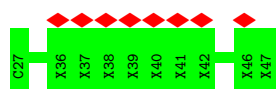
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain c: 78% 18%



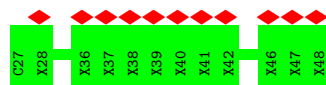
- Molecule 11: Co-purified unknown peptide built as polyALA (AscE)

Chain X: 38% 100%



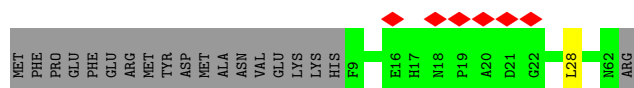
- Molecule 12: Co-purified unknown peptide built as polyALA (AscE)

Chain x: 50% 100%

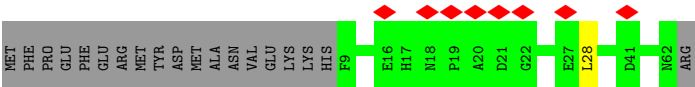


- Molecule 13: Actinobacterial supercomplex, subunit C (AscC)

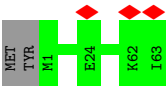
Chain V: 8% 73% 26%



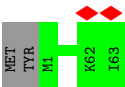
- Molecule 13: Actinobacterial supercomplex, subunit C (AscC)



• Molecule 14: Hypothetical membrane protein



• Molecule 14: Hypothetical membrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65391	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.331	Depositor
Minimum map value	-2.395	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.541	Depositor
Map size (Å)	328.59998, 328.59998, 328.59998	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRD, TWT, HEM, CU, HEC, HAS, MG, FES, 9XX, 7PH, PLM, 9YF, CA, CDL, MQ9

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
2	E	0.32	0/1520	0.58	0/2071
2	e	0.31	0/1520	0.58	0/2071
3	H	0.29	0/1022	0.61	0/1397
3	h	0.29	0/1031	0.59	0/1410
4	F	0.31	0/1125	0.60	0/1529
4	f	0.31	0/1125	0.57	0/1529
5	G	0.28	0/2629	0.55	0/3586
5	g	0.28	0/2629	0.54	0/3586
6	D	0.31	0/4701	0.59	0/6412
6	d	0.32	0/4701	0.58	0/6412
7	A	0.29	0/3197	0.59	0/4352
7	a	0.30	0/3197	0.60	0/4352
8	L	0.27	0/1134	0.58	0/1553
8	l	0.28	0/1134	0.57	0/1553
9	B	0.30	0/4301	0.58	0/5861
9	b	0.30	0/4301	0.58	0/5861
10	C	0.31	0/1761	0.58	0/2383
10	c	0.30	0/1761	0.58	0/2383
11	X	0.79	0/5	0.35	0/5
12	x	0.80	0/5	0.20	0/5
13	V	0.30	0/436	0.58	0/600
13	v	0.29	0/436	0.59	0/600
14	K	0.29	0/452	0.54	0/616
14	k	0.29	0/452	0.54	0/616
All	All	0.30	0/44575	0.58	0/60743

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	E	187/205 (91%)	182 (97%)	4 (2%)	1 (0%)	25	56
2	e	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
3	H	123/147 (84%)	109 (89%)	13 (11%)	1 (1%)	16	45
3	h	124/147 (84%)	114 (92%)	10 (8%)	0	100	100
4	F	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
4	f	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
5	G	323/359 (90%)	295 (91%)	27 (8%)	1 (0%)	37	66
5	g	323/359 (90%)	293 (91%)	30 (9%)	0	100	100
6	D	571/594 (96%)	543 (95%)	28 (5%)	0	100	100
6	d	571/594 (96%)	540 (95%)	30 (5%)	1 (0%)	44	73
7	A	398/408 (98%)	381 (96%)	17 (4%)	0	100	100
7	a	398/408 (98%)	372 (94%)	26 (6%)	0	100	100
8	L	151/194 (78%)	131 (87%)	19 (13%)	1 (1%)	19	49
8	l	151/194 (78%)	132 (87%)	18 (12%)	1 (1%)	19	49
9	B	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	30	60
9	b	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	30	60
10	C	230/283 (81%)	203 (88%)	24 (10%)	3 (1%)	10	33
10	c	230/283 (81%)	201 (87%)	28 (12%)	1 (0%)	30	60
13	V	52/73 (71%)	45 (86%)	7 (14%)	0	100	100
13	v	52/73 (71%)	45 (86%)	7 (14%)	0	100	100
14	K	61/65 (94%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	k	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
All	All	5539/6020 (92%)	5161 (93%)	364 (7%)	14 (0%)	38	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	141	GLY
8	l	141	GLY
2	E	130	GLY
5	G	101	LYS
3	H	111	LEU
9	b	499	ASP
10	c	143	GLU
9	B	227	LYS
9	B	462	ASP
6	d	251	GLY
10	C	68	ILE
10	C	65	VAL
10	C	215	PRO
9	b	130	PRO

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	
2	E	155/166 (93%)	154 (99%)	1 (1%)	84	95
2	e	155/166 (93%)	154 (99%)	1 (1%)	84	95
3	H	108/125 (86%)	105 (97%)	3 (3%)	38	73
3	h	109/125 (87%)	107 (98%)	2 (2%)	54	82
4	F	114/114 (100%)	113 (99%)	1 (1%)	75	92
4	f	114/114 (100%)	113 (99%)	1 (1%)	75	92
5	G	269/292 (92%)	268 (100%)	1 (0%)	89	97
5	g	269/292 (92%)	267 (99%)	2 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	472/488 (97%)	469 (99%)	3 (1%)	84	95
6	d	472/488 (97%)	469 (99%)	3 (1%)	84	95
7	A	324/332 (98%)	324 (100%)	0	100	100
7	a	324/332 (98%)	323 (100%)	1 (0%)	91	97
8	L	127/154 (82%)	126 (99%)	1 (1%)	79	93
8	l	127/154 (82%)	125 (98%)	2 (2%)	58	84
9	B	437/441 (99%)	428 (98%)	9 (2%)	48	78
9	b	437/441 (99%)	429 (98%)	8 (2%)	54	82
10	C	176/212 (83%)	169 (96%)	7 (4%)	27	61
10	c	176/212 (83%)	167 (95%)	9 (5%)	20	51
11	X	1/1 (100%)	1 (100%)	0	100	100
12	x	1/1 (100%)	1 (100%)	0	100	100
13	V	45/63 (71%)	44 (98%)	1 (2%)	47	78
13	v	45/63 (71%)	44 (98%)	1 (2%)	47	78
14	K	43/45 (96%)	43 (100%)	0	100	100
14	k	43/45 (96%)	43 (100%)	0	100	100
All	All	4543/4866 (93%)	4486 (99%)	57 (1%)	64	88

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	74	LEU
3	H	20	ASP
3	H	28	TRP
3	H	132	ARG
4	F	69	VAL
5	G	101	LYS
6	D	45	TYR
6	D	393	TYR
6	D	541	ARG
8	L	107	ARG
9	B	18	SER
9	B	168	MET
9	B	182	MET
9	B	280	LEU
9	B	515	HIS

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Mol	Chain	Res	Type
9	B	517	GLU
9	B	525	LEU
9	B	532	ARG
9	B	535	ASN
10	C	60	LYS
10	C	67	CYS
10	C	79	GLU
10	C	81	ARG
10	C	101	ARG
10	C	105	LEU
10	C	250	TYR
2	e	191	ASP
3	h	46	PHE
3	h	93	ARG
4	f	69	VAL
5	g	46	TRP
5	g	98	GLU
6	d	45	TYR
6	d	150	PHE
6	d	263	PHE
7	a	406	ARG
8	l	82	HIS
8	l	107	ARG
9	b	184	TRP
9	b	224	TRP
9	b	226	GLN
9	b	228	HIS
9	b	391	MET
9	b	523	ARG
9	b	525	LEU
9	b	526	ASN
10	c	60	LYS
10	c	67	CYS
10	c	70	CYS
10	c	105	LEU
10	c	147	LEU
10	c	153	ARG
10	c	186	ARG
10	c	216	GLN
10	c	250	TYR
13	V	28	LEU
13	v	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
6	D	105	ASN
6	D	314	HIS
8	l	85	HIS
9	b	287	GLN
9	b	445	GLN
10	c	182	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	$\# Z > 2$
22	HAS	d	604	6	69,72,72	2.10	17 (24%)	73,109,109	2.36	24 (32%)
16	7PH	D	609	-	37,37,37	0.87	2 (5%)	41,42,42	0.65	0
17	TRD	A	502	-	12,12,12	0.38	0	11,11,11	0.60	0
17	TRD	A	503	-	12,12,12	0.39	0	11,11,11	0.62	0
15	CDL	d	607	-	65,65,99	1.01	5 (7%)	71,77,111	0.73	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	MQ9	b	805	-	59,59,59	1.32	5 (8%)	72,75,75	1.22	9 (12%)
27	PLM	d	611	-	10,10,17	0.44	0	9,9,17	0.47	0
26	9YF	a	604	-	58,58,58	0.93	4 (6%)	69,71,71	1.00	3 (4%)
22	HAS	D	602	-	69,72,72	2.69	25 (36%)	73,109,109	2.43	31 (42%)
22	HAS	d	603	-	69,72,72	2.71	26 (37%)	73,109,109	2.34	30 (41%)
17	TRD	B	606	-	12,12,12	0.38	0	11,11,11	0.57	0
24	FES	a	603	7	0,4,4	-	-	-	-	-
17	TRD	f	205	-	12,12,12	0.37	0	11,11,11	0.71	0
17	TRD	F	201	-	12,12,12	0.39	0	11,11,11	0.67	0
18	9XX	B	608	-	31,31,41	1.12	4 (12%)	34,34,44	1.21	4 (11%)
15	CDL	B	605	-	76,76,99	0.95	5 (6%)	82,88,111	0.71	0
17	TRD	a	605	-	12,12,12	0.38	0	11,11,11	0.62	0
28	HEM	B	602	9	41,50,50	1.50	5 (12%)	45,82,82	2.20	17 (37%)
19	TWT	h	203	-	21,21,21	0.32	0	20,20,20	0.95	0
15	CDL	f	202	-	78,78,99	0.91	4 (5%)	84,90,111	0.82	2 (2%)
15	CDL	b	801	-	73,73,99	0.97	5 (6%)	79,85,111	0.81	2 (2%)
19	TWT	H	203	-	21,21,21	0.35	0	20,20,20	0.81	0
15	CDL	D	606	-	73,73,99	0.98	6 (8%)	79,85,111	0.76	2 (2%)
16	7PH	h	201	-	37,37,37	0.86	2 (5%)	41,42,42	0.71	0
29	HEC	C	302	10	32,50,50	1.44	6 (18%)	24,82,82	1.91	5 (20%)
17	TRD	A	505	-	12,12,12	0.38	0	11,11,11	0.62	0
16	7PH	G	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
16	7PH	H	201	-	37,37,37	0.90	2 (5%)	41,42,42	0.90	2 (4%)
16	7PH	e	302	-	37,37,37	0.95	3 (8%)	41,42,42	0.68	0
27	PLM	L	202	-	10,10,17	0.41	0	9,9,17	0.49	0
25	MQ9	b	804	-	44,44,59	1.51	6 (13%)	54,57,75	1.36	5 (9%)
17	TRD	f	204	-	12,12,12	0.38	0	11,11,11	0.66	0
24	FES	A	501	7	0,4,4	-	-	-	-	-
15	CDL	b	806	-	76,76,99	0.91	2 (2%)	82,88,111	0.80	1 (1%)
16	7PH	E	302	-	37,37,37	0.93	2 (5%)	41,42,42	0.92	1 (2%)
17	TRD	F	203	-	12,12,12	0.39	0	11,11,11	0.62	0
15	CDL	B	607	-	73,73,99	0.88	2 (2%)	79,85,111	0.87	4 (5%)
15	CDL	c	301	-	78,78,99	0.86	3 (3%)	84,90,111	0.75	1 (1%)
25	MQ9	B	604	-	59,59,59	1.25	5 (8%)	72,75,75	1.24	10 (13%)
26	9YF	l	201	-	58,58,58	0.90	4 (6%)	69,71,71	1.08	3 (4%)
17	TRD	b	807	-	12,12,12	0.37	0	11,11,11	0.65	0
25	MQ9	a	602	-	44,44,59	1.46	5 (11%)	54,57,75	1.33	9 (16%)
17	TRD	f	206	-	12,12,12	0.37	0	11,11,11	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	7PH	d	610	-	37,37,37	0.80	1 (2%)	41,42,42	0.72	0
25	MQ9	B	603	-	44,44,59	1.44	5 (11%)	54,57,75	1.36	9 (16%)
16	7PH	D	608	-	37,37,37	0.95	3 (8%)	41,42,42	0.89	1 (2%)
16	7PH	d	608	-	37,37,37	0.91	2 (5%)	41,42,42	0.72	1 (2%)
16	7PH	F	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
17	TRD	F	204	-	12,12,12	0.37	0	11,11,11	0.68	0
25	MQ9	A	504	-	44,44,59	1.46	5 (11%)	54,57,75	1.22	7 (12%)
28	HEM	b	803	9	41,50,50	1.47	5 (12%)	45,82,82	2.17	19 (42%)
17	TRD	f	201	-	12,12,12	0.38	0	11,11,11	0.69	0
16	7PH	d	609	-	37,37,37	0.84	0	41,42,42	0.88	1 (2%)
29	HEC	C	303	10	32,50,50	2.28	9 (28%)	24,82,82	4.06	11 (45%)
15	CDL	d	601	-	78,78,99	0.94	4 (5%)	84,90,111	0.69	0
22	HAS	D	603	6	69,72,72	2.50	21 (30%)	73,109,109	2.25	27 (36%)
17	TRD	f	203	-	12,12,12	0.38	0	11,11,11	0.60	0
18	9XX	h	204	-	31,31,41	1.10	3 (9%)	34,34,44	1.24	3 (8%)
15	CDL	e	301	-	65,65,99	1.01	4 (6%)	71,77,111	0.80	1 (1%)
26	9YF	L	201	-	58,58,58	0.91	5 (8%)	69,71,71	1.07	3 (4%)
16	7PH	f	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
16	7PH	k	101	-	37,37,37	0.83	1 (2%)	41,42,42	0.62	0
17	TRD	e	303	-	12,12,12	0.39	0	11,11,11	0.58	0
17	TRD	E	303	-	12,12,12	0.40	0	11,11,11	0.56	0
15	CDL	F	202	-	78,78,99	0.99	6 (7%)	84,90,111	0.81	1 (1%)
17	TRD	F	206	-	12,12,12	0.39	0	11,11,11	0.66	0
15	CDL	C	301	-	78,78,99	0.90	2 (2%)	84,90,111	0.85	2 (2%)
16	7PH	g	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
29	HEC	c	302	10	32,50,50	1.45	6 (18%)	24,82,82	1.86	5 (20%)
15	CDL	E	301	-	65,65,99	1.01	6 (9%)	71,77,111	0.75	0
16	7PH	D	610	-	37,37,37	0.89	2 (5%)	41,42,42	0.72	0
15	CDL	D	601	-	78,78,99	0.93	6 (7%)	84,90,111	0.64	0
29	HEC	c	303	10	32,50,50	2.23	11 (34%)	24,82,82	1.94	4 (16%)
27	PLM	x	101	-	10,10,17	0.42	0	9,9,17	0.45	0
28	HEM	b	802	9	41,50,50	1.35	4 (9%)	45,82,82	2.45	22 (48%)
28	HEM	B	601	9	41,50,50	1.43	4 (9%)	45,82,82	2.28	16 (35%)
18	9XX	h	202	-	31,31,41	1.10	3 (9%)	34,34,44	1.34	3 (8%)
17	TRD	F	205	-	12,12,12	0.37	0	11,11,11	0.64	0
16	7PH	D	607	-	37,37,37	0.89	2 (5%)	41,42,42	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	9XX	H	202	-	31,31,41	1.16	4 (12%)	34,34,44	1.30	3 (8%)
26	9YF	a	601	-	58,58,58	0.92	3 (5%)	69,71,71	1.22	6 (8%)
27	PLM	X	101	-	10,10,17	0.41	0	9,9,17	0.45	0

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
22	HAS	d	604	6	1/1/8/18	12/40/82/82	-
16	7PH	D	609	-	-	25/39/39/39	-
17	TRD	A	502	-	-	7/10/10/10	-
17	TRD	A	503	-	-	4/10/10/10	-
15	CDL	d	607	-	-	31/76/76/110	-
25	MQ9	b	805	-	-	11/53/73/73	0/2/2/2
27	PLM	d	611	-	-	3/7/8/15	-
26	9YF	a	604	-	-	29/54/78/78	0/1/1/1
22	HAS	D	602	-	1/1/8/18	16/40/82/82	-
22	HAS	d	603	-	1/1/8/18	11/40/82/82	-
17	TRD	B	606	-	-	7/10/10/10	-
24	FES	a	603	7	-	-	0/1/1/1
17	TRD	f	205	-	-	9/10/10/10	-
17	TRD	F	201	-	-	3/10/10/10	-
18	9XX	B	608	-	-	15/33/33/43	-
15	CDL	B	605	-	-	44/87/87/110	-
17	TRD	a	605	-	-	3/10/10/10	-
28	HEM	B	602	9	-	5/12/54/54	-
19	TWT	h	203	-	-	5/19/19/19	-
15	CDL	f	202	-	-	45/89/89/110	-
15	CDL	b	801	-	-	42/84/84/110	-
19	TWT	H	203	-	-	7/19/19/19	-
15	CDL	D	606	-	-	41/84/84/110	-
16	7PH	h	201	-	-	25/39/39/39	-
29	HEC	C	302	10	-	6/10/54/54	-
17	TRD	A	505	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	7PH	G	403	-	-	17/39/39/39	-
16	7PH	H	201	-	-	19/39/39/39	-
16	7PH	e	302	-	-	21/39/39/39	-
27	PLM	L	202	-	-	5/7/8/15	-
25	MQ9	b	804	-	-	8/35/55/73	0/2/2/2
17	TRD	f	204	-	-	4/10/10/10	-
24	FES	A	501	7	-	-	0/1/1/1
15	CDL	b	806	-	-	44/87/87/110	-
16	7PH	E	302	-	-	14/39/39/39	-
17	TRD	F	203	-	-	2/10/10/10	-
15	CDL	B	607	-	-	42/84/84/110	-
15	CDL	c	301	-	-	50/89/89/110	-
25	MQ9	B	604	-	-	21/53/73/73	0/2/2/2
26	9YF	l	201	-	-	23/54/78/78	0/1/1/1
17	TRD	b	807	-	-	2/10/10/10	-
25	MQ9	a	602	-	-	12/35/55/73	0/2/2/2
17	TRD	f	206	-	-	6/10/10/10	-
16	7PH	d	610	-	-	23/39/39/39	-
25	MQ9	B	603	-	-	7/35/55/73	0/2/2/2
16	7PH	D	608	-	-	18/39/39/39	-
16	7PH	d	608	-	-	16/39/39/39	-
16	7PH	F	207	-	-	19/39/39/39	-
17	TRD	F	204	-	-	4/10/10/10	-
25	MQ9	A	504	-	-	12/35/55/73	0/2/2/2
28	HEM	b	803	9	-	6/12/54/54	-
17	TRD	f	201	-	-	3/10/10/10	-
16	7PH	d	609	-	-	22/39/39/39	-
29	HEC	C	303	10	-	3/10/54/54	-
15	CDL	d	601	-	-	37/89/89/110	-
22	HAS	D	603	6	1/1/8/18	14/40/82/82	-
17	TRD	f	203	-	-	1/10/10/10	-
18	9XX	h	204	-	-	20/33/33/43	-
15	CDL	e	301	-	-	40/76/76/110	-
26	9YF	L	201	-	-	24/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	7PH	f	207	-	-	19/39/39/39	-
16	7PH	k	101	-	-	10/39/39/39	-
17	TRD	e	303	-	-	7/10/10/10	-
17	TRD	E	303	-	-	8/10/10/10	-
15	CDL	F	202	-	-	45/89/89/110	-
17	TRD	F	206	-	-	7/10/10/10	-
15	CDL	C	301	-	-	48/89/89/110	-
16	7PH	g	403	-	-	17/39/39/39	-
29	HEC	c	302	10	-	6/10/54/54	-
15	CDL	E	301	-	-	28/76/76/110	-
16	7PH	D	610	-	-	23/39/39/39	-
15	CDL	D	601	-	-	38/89/89/110	-
29	HEC	c	303	10	-	7/10/54/54	-
27	PLM	x	101	-	-	4/7/8/15	-
28	HEM	b	802	9	-	8/12/54/54	-
28	HEM	B	601	9	-	3/12/54/54	-
18	9XX	h	202	-	-	14/33/33/43	-
17	TRD	F	205	-	-	5/10/10/10	-
16	7PH	D	607	-	-	23/39/39/39	-
18	9XX	H	202	-	-	16/33/33/43	-
26	9YF	a	601	-	-	35/54/78/78	0/1/1/1
27	PLM	X	101	-	-	0/7/8/15	-

All (290) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	603	HAS	CHD-C4A	10.37	1.49	1.35
22	D	602	HAS	CHD-C4A	10.12	1.49	1.35
22	D	603	HAS	CHD-C4A	8.74	1.47	1.35
29	C	303	HEC	C2B-C3B	7.23	1.48	1.40
22	d	604	HAS	CHD-C4A	6.92	1.45	1.35
22	D	602	HAS	C3B-C2B	6.70	1.49	1.34
22	d	603	HAS	C3C-C2C	6.29	1.49	1.40
22	d	603	HAS	C3B-C2B	6.14	1.48	1.34
22	D	603	HAS	C3B-C2B	6.13	1.48	1.34
25	b	804	MQ9	C6-C5	6.01	1.46	1.35
25	a	602	MQ9	C6-C5	5.94	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	602	HAS	C2A-C3A	5.90	1.49	1.36
25	B	603	MQ9	C6-C5	5.89	1.45	1.35
22	D	602	HAS	C3C-C2C	5.83	1.48	1.40
25	b	805	MQ9	C6-C5	5.74	1.45	1.35
22	d	603	HAS	C2D-C3D	5.69	1.48	1.36
25	A	504	MQ9	C6-C5	5.69	1.45	1.35
29	c	303	HEC	C2B-C3B	5.68	1.46	1.40
22	d	603	HAS	CHC-C4B	5.64	1.49	1.35
22	D	602	HAS	CHC-C4B	5.58	1.49	1.35
22	D	602	HAS	CHA-C1A	5.55	1.49	1.38
29	c	303	HEC	C3C-C2C	5.52	1.46	1.40
22	D	602	HAS	C2D-C3D	5.51	1.48	1.36
25	B	604	MQ9	C6-C5	5.38	1.45	1.35
22	D	603	HAS	C2A-C3A	5.37	1.48	1.36
22	D	603	HAS	C3C-C2C	5.37	1.47	1.40
22	d	603	HAS	CHA-C1A	5.36	1.48	1.38
29	C	303	HEC	C3C-C2C	5.28	1.46	1.40
22	d	603	HAS	C2A-C3A	5.27	1.47	1.36
22	d	604	HAS	C3B-C2B	5.20	1.46	1.34
22	d	604	HAS	C1D-ND	-5.13	1.31	1.40
22	D	603	HAS	CHC-C4B	5.03	1.47	1.35
22	D	602	HAS	CHB-C1D	4.98	1.48	1.38
22	d	603	HAS	CHB-C1D	4.95	1.48	1.38
22	D	603	HAS	C2D-C3D	4.77	1.47	1.36
22	d	604	HAS	C4B-NB	-4.74	1.32	1.40
22	D	603	HAS	CHA-C1A	4.69	1.47	1.38
22	d	603	HAS	CHB-C1B	4.53	1.49	1.39
22	D	603	HAS	CHB-C1D	4.53	1.47	1.38
22	d	604	HAS	C2A-C3A	4.36	1.46	1.36
22	D	602	HAS	CHB-C1B	4.34	1.49	1.39
22	D	603	HAS	C4B-NB	-4.32	1.32	1.40
28	B	602	HEM	C4D-ND	-4.27	1.33	1.40
18	H	202	9XX	O1-C17	-4.11	1.40	1.47
22	D	603	HAS	C1D-ND	-4.02	1.33	1.40
22	D	603	HAS	CHA-C4D	3.96	1.48	1.39
22	d	603	HAS	CHA-C4D	3.96	1.48	1.39
22	d	604	HAS	C3C-C2C	3.92	1.45	1.40
22	D	602	HAS	CHA-C4D	3.92	1.48	1.39
28	B	601	HEM	C1B-NB	-3.90	1.33	1.40
22	d	604	HAS	C2D-C3D	3.89	1.45	1.36
18	h	202	9XX	O1-C17	-3.89	1.40	1.47
29	c	303	HEC	C4B-C3B	3.80	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	608	9XX	O1-C17	-3.79	1.40	1.47
28	b	803	HEM	C4D-ND	-3.74	1.33	1.40
28	B	602	HEM	C1B-NB	-3.74	1.33	1.40
22	D	603	HAS	CHB-C1B	3.73	1.47	1.39
28	B	601	HEM	C4D-ND	-3.72	1.33	1.40
28	b	802	HEM	C4D-ND	-3.67	1.34	1.40
28	b	803	HEM	C1B-NB	-3.64	1.34	1.40
22	d	604	HAS	C4A-NA	-3.62	1.32	1.39
29	C	303	HEC	C4B-C3B	3.54	1.49	1.43
22	d	604	HAS	C4D-ND	-3.54	1.31	1.38
22	D	602	HAS	FE-NA	3.54	2.09	1.95
22	D	603	HAS	C1A-NA	-3.50	1.33	1.39
29	c	303	HEC	C3D-C2D	3.47	1.47	1.37
18	h	204	9XX	O1-C17	-3.43	1.41	1.47
29	c	303	HEC	C1C-CHC	3.43	1.50	1.41
22	d	603	HAS	C4B-NB	-3.41	1.34	1.40
28	b	802	HEM	FE-NB	3.37	2.13	1.96
22	d	604	HAS	C1A-NA	-3.35	1.33	1.39
29	C	303	HEC	C2A-C3A	3.35	1.47	1.37
29	C	303	HEC	C3D-C2D	3.32	1.47	1.37
22	D	602	HAS	C1D-ND	-3.28	1.34	1.40
22	d	603	HAS	C1D-ND	-3.25	1.34	1.40
29	c	303	HEC	C2A-C3A	3.24	1.47	1.37
22	d	604	HAS	CHC-C4B	3.22	1.43	1.35
22	d	604	HAS	C1B-NB	-3.22	1.32	1.38
22	d	603	HAS	FE-NA	3.18	2.08	1.95
29	c	302	HEC	C2A-C3A	3.17	1.47	1.37
22	D	602	HAS	C4B-NB	-3.16	1.34	1.40
22	D	602	HAS	C1C-CHC	3.15	1.49	1.41
22	D	603	HAS	C4A-NA	-3.13	1.33	1.39
15	F	202	CDL	OA6-CA4	-3.13	1.38	1.46
29	C	302	HEC	C2A-C3A	3.11	1.46	1.37
29	C	302	HEC	C3D-C2D	3.04	1.46	1.37
26	a	604	9YF	O11-C24	-3.02	1.38	1.45
28	b	802	HEM	C1B-NB	-2.98	1.35	1.40
29	c	302	HEC	C3D-C2D	2.97	1.46	1.37
25	b	804	MQ9	C2-C1	2.97	1.53	1.48
15	f	202	CDL	OA6-CA4	-2.93	1.39	1.46
22	d	603	HAS	C4D-C3D	2.92	1.50	1.45
22	d	603	HAS	C4B-C3B	2.91	1.49	1.44
28	b	802	HEM	C4B-NB	-2.91	1.32	1.38
22	d	603	HAS	C1B-C2B	2.91	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	603	HAS	C1B-NB	-2.89	1.32	1.38
15	D	601	CDL	OA6-CA4	-2.88	1.39	1.46
18	H	202	9XX	O-C15	2.87	1.41	1.33
22	d	603	HAS	C4C-CHD	2.86	1.48	1.41
28	B	602	HEM	C4B-NB	-2.85	1.32	1.38
28	B	602	HEM	FE-NB	2.85	2.10	1.96
28	B	601	HEM	FE-NB	2.85	2.10	1.96
22	d	603	HAS	C1A-NA	-2.84	1.34	1.39
25	a	602	MQ9	C2-C1	2.82	1.53	1.48
22	D	602	HAS	C4C-CHD	2.82	1.48	1.41
22	d	603	HAS	C1A-C2A	2.80	1.50	1.45
25	B	603	MQ9	C2-C1	2.80	1.53	1.48
22	d	603	HAS	C1C-CHC	2.79	1.48	1.41
22	D	603	HAS	C4C-CHD	2.79	1.48	1.41
28	b	803	HEM	FE-NB	2.77	2.10	1.96
22	D	602	HAS	C4B-C3B	2.76	1.49	1.44
25	B	603	MQ9	C3-C4	2.76	1.53	1.48
28	b	803	HEM	C4B-NB	-2.76	1.33	1.38
26	a	601	9YF	O11-C25	2.74	1.41	1.33
15	d	607	CDL	OB8-CB7	2.74	1.41	1.33
25	b	805	MQ9	C2-C1	2.74	1.53	1.48
22	D	602	HAS	C4A-NA	-2.73	1.34	1.39
22	D	603	HAS	FE-NA	2.72	2.06	1.95
18	h	204	9XX	O-C15	2.72	1.41	1.33
15	D	601	CDL	OB8-CB6	-2.71	1.39	1.45
25	a	602	MQ9	C3-C4	2.70	1.53	1.48
25	b	804	MQ9	C3-C4	2.69	1.53	1.48
26	L	201	9YF	O11-C25	2.69	1.41	1.33
26	l	201	9YF	O11-C25	2.69	1.41	1.33
25	a	602	MQ9	O1-C1	-2.66	1.17	1.23
25	A	504	MQ9	C3-C4	2.65	1.53	1.48
15	B	607	CDL	OB8-CB7	2.65	1.41	1.33
16	D	608	7PH	O21-C2	-2.65	1.40	1.46
22	D	602	HAS	C1A-NA	-2.64	1.34	1.39
15	B	605	CDL	OA6-CA4	-2.63	1.40	1.46
25	A	504	MQ9	C2-C1	2.63	1.53	1.48
18	B	608	9XX	O1-C18	2.62	1.41	1.34
29	c	302	HEC	C2A-C1A	2.62	1.48	1.42
16	F	207	7PH	O21-C2	-2.60	1.40	1.46
22	D	603	HAS	C4B-C3B	2.59	1.49	1.44
15	E	301	CDL	OA6-CA4	-2.59	1.40	1.46
16	f	207	7PH	O21-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	805	MQ9	O1-C1	-2.58	1.17	1.23
29	c	303	HEC	C4D-CHA	2.58	1.48	1.41
22	d	604	HAS	CHA-C1A	2.57	1.43	1.38
22	d	603	HAS	C4A-NA	-2.56	1.34	1.39
25	A	504	MQ9	O1-C1	-2.54	1.17	1.23
29	C	303	HEC	C2A-C1A	2.54	1.48	1.42
25	B	604	MQ9	C3-C4	2.53	1.53	1.48
18	B	608	9XX	O-C15	2.53	1.40	1.33
25	b	805	MQ9	C3-C4	2.52	1.53	1.48
15	d	607	CDL	OA8-CA6	-2.52	1.39	1.45
15	b	806	CDL	OA8-CA6	-2.51	1.39	1.45
26	L	201	9YF	O9-C	-2.51	1.40	1.46
22	D	602	HAS	C1B-C2B	2.51	1.49	1.44
18	h	204	9XX	O1-C18	2.51	1.41	1.34
18	H	202	9XX	O1-C18	2.49	1.41	1.34
15	F	202	CDL	OA8-CA7	2.49	1.40	1.33
22	d	604	HAS	FE-NA	2.49	2.05	1.95
15	B	605	CDL	OB6-CB5	2.49	1.41	1.34
26	l	201	9YF	O9-C	-2.48	1.40	1.46
22	d	604	HAS	C1C-NC	-2.48	1.31	1.36
25	B	604	MQ9	O1-C1	-2.48	1.18	1.23
15	d	607	CDL	OA8-CA7	2.47	1.40	1.33
22	d	603	HAS	C4A-C3A	2.47	1.50	1.45
16	k	101	7PH	O21-C2	-2.47	1.40	1.46
15	B	605	CDL	OB6-CB4	-2.46	1.40	1.46
15	E	301	CDL	OB6-CB5	2.46	1.41	1.34
15	E	301	CDL	OB6-CB4	-2.46	1.40	1.46
22	D	602	HAS	C4D-C3D	2.45	1.49	1.45
25	B	604	MQ9	O4-C4	-2.45	1.18	1.23
26	a	604	9YF	O9-C	-2.45	1.40	1.46
15	d	601	CDL	OA8-CA6	-2.45	1.39	1.45
16	g	403	7PH	O21-C2	-2.44	1.40	1.46
25	b	804	MQ9	O1-C1	-2.42	1.18	1.23
29	C	302	HEC	C2A-C1A	2.42	1.48	1.42
15	c	301	CDL	OA6-CA4	-2.41	1.40	1.46
16	e	302	7PH	O31-C3	-2.41	1.39	1.45
25	b	805	MQ9	O4-C4	-2.41	1.18	1.23
16	G	403	7PH	O21-C2	-2.41	1.40	1.46
16	E	302	7PH	O21-C21	2.40	1.41	1.34
29	c	302	HEC	C1D-CHD	2.39	1.47	1.41
15	e	301	CDL	OA6-CA4	-2.38	1.40	1.46
16	d	608	7PH	O21-C2	-2.38	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	201	7PH	O21-C21	2.38	1.41	1.34
16	D	610	7PH	O31-C3	-2.38	1.39	1.45
25	a	602	MQ9	O4-C4	-2.37	1.18	1.23
16	d	610	7PH	O21-C2	-2.36	1.40	1.46
15	D	601	CDL	OB6-CB5	2.36	1.41	1.34
15	d	607	CDL	OB6-CB4	-2.36	1.40	1.46
15	b	801	CDL	OB6-CB4	-2.35	1.40	1.46
25	B	603	MQ9	O1-C1	-2.34	1.18	1.23
25	B	604	MQ9	C2-C1	2.34	1.52	1.48
16	E	302	7PH	O21-C2	-2.34	1.40	1.46
29	C	302	HEC	C4D-CHA	2.34	1.47	1.41
29	C	303	HEC	C1C-CHC	2.34	1.47	1.41
29	c	303	HEC	C2A-C1A	2.33	1.47	1.42
16	D	607	7PH	O31-C3	-2.33	1.39	1.45
16	e	302	7PH	O21-C2	-2.32	1.40	1.46
15	d	601	CDL	OB8-CB7	2.32	1.40	1.33
16	D	609	7PH	O31-C3	-2.32	1.39	1.45
15	d	601	CDL	OA6-CA4	-2.31	1.40	1.46
22	D	602	HAS	FE-NB	2.31	2.09	1.97
15	D	606	CDL	OB6-CB4	-2.31	1.40	1.46
16	D	607	7PH	O31-C31	2.30	1.40	1.33
16	d	608	7PH	O31-C3	-2.30	1.39	1.45
15	f	202	CDL	OB8-CB7	2.30	1.40	1.33
26	a	604	9YF	O9-C8	2.30	1.40	1.34
28	B	601	HEM	C4B-NB	-2.29	1.34	1.38
22	D	602	HAS	C4A-C3A	2.29	1.49	1.45
29	C	302	HEC	C1D-CHD	2.29	1.47	1.41
15	b	801	CDL	OA8-CA7	2.29	1.40	1.33
16	H	201	7PH	O31-C31	2.28	1.40	1.33
29	C	303	HEC	CAA-C2A	-2.28	1.48	1.52
29	c	302	HEC	C4D-CHA	2.28	1.47	1.41
26	a	601	9YF	O9-C	-2.27	1.40	1.46
22	D	602	HAS	C1B-NB	-2.27	1.34	1.38
15	D	606	CDL	OB8-CB6	-2.27	1.40	1.45
18	h	202	9XX	O-C15	2.26	1.39	1.33
26	a	601	9YF	O9-C8	2.26	1.40	1.34
15	D	601	CDL	OB6-CB4	-2.25	1.41	1.46
22	D	603	HAS	C4D-ND	-2.25	1.34	1.38
26	l	201	9YF	O11-C24	-2.25	1.40	1.45
22	D	603	HAS	C1C-CHC	2.25	1.47	1.41
15	E	301	CDL	OA8-CA6	-2.25	1.40	1.45
29	c	303	HEC	C1B-CHB	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	605	CDL	OB8-CB6	-2.24	1.40	1.45
16	D	608	7PH	O21-C21	2.24	1.40	1.34
18	B	608	9XX	O-C16	-2.23	1.40	1.45
28	b	803	HEM	O2A-CGA	-2.23	1.23	1.30
15	f	202	CDL	OA6-CA5	2.23	1.40	1.34
15	B	605	CDL	OA8-CA7	2.22	1.39	1.33
15	D	606	CDL	OB6-CB5	2.22	1.40	1.34
15	b	801	CDL	OA6-CA5	2.21	1.40	1.34
16	D	610	7PH	O31-C31	2.21	1.39	1.33
25	A	504	MQ9	O4-C4	-2.21	1.18	1.23
15	E	301	CDL	OA6-CA5	2.21	1.40	1.34
15	d	607	CDL	OB6-CB5	2.21	1.40	1.34
16	h	201	7PH	O21-C2	-2.20	1.41	1.46
15	e	301	CDL	OB6-CB5	2.20	1.40	1.34
15	d	601	CDL	OB6-CB4	-2.19	1.41	1.46
22	d	604	HAS	CHB-C1B	2.19	1.44	1.39
16	D	609	7PH	O31-C31	2.17	1.39	1.33
26	a	604	9YF	O11-C25	2.17	1.39	1.33
15	D	606	CDL	OA6-CA5	2.16	1.40	1.34
15	D	606	CDL	OA6-CA4	-2.15	1.41	1.46
16	g	403	7PH	O31-C3	-2.15	1.40	1.45
22	d	603	HAS	C2D-C1D	2.15	1.49	1.44
26	L	201	9YF	O11-C24	-2.15	1.40	1.45
15	e	301	CDL	OB6-CB4	-2.15	1.41	1.46
15	F	202	CDL	OA6-CA5	2.15	1.40	1.34
28	B	602	HEM	O2D-CGD	-2.15	1.23	1.30
29	c	302	HEC	C1C-CHC	2.15	1.47	1.41
25	b	804	MQ9	O4-C4	-2.15	1.18	1.23
29	c	303	HEC	C3C-C4C	2.14	1.46	1.43
22	d	603	HAS	FE-ND	2.13	2.08	1.97
15	D	601	CDL	OB8-CB7	2.13	1.39	1.33
22	D	603	HAS	C4D-C3D	2.13	1.48	1.45
16	f	207	7PH	O31-C3	-2.13	1.40	1.45
15	B	607	CDL	OA8-CA7	2.13	1.39	1.33
29	C	302	HEC	C1C-CHC	2.13	1.46	1.41
15	b	806	CDL	OA6-CA5	2.11	1.40	1.34
15	F	202	CDL	OB6-CB4	-2.11	1.41	1.46
15	E	301	CDL	OB8-CB6	-2.11	1.40	1.45
15	b	801	CDL	OA6-CA4	-2.11	1.41	1.46
16	G	403	7PH	O31-C3	-2.10	1.40	1.45
18	H	202	9XX	O-C16	-2.10	1.40	1.45
15	c	301	CDL	OB8-CB7	2.10	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	301	CDL	OB6-CB5	2.10	1.40	1.34
22	D	602	HAS	C1A-C2A	2.09	1.48	1.45
26	L	201	9YF	O9-C8	2.09	1.40	1.34
16	F	207	7PH	O31-C3	-2.08	1.40	1.45
16	e	302	7PH	O31-C31	2.07	1.39	1.33
15	e	301	CDL	OA6-CA5	2.07	1.40	1.34
22	d	603	HAS	FE-NB	2.07	2.08	1.97
29	c	303	HEC	C3A-C4A	2.06	1.47	1.42
18	h	202	9XX	O1-C18	2.06	1.40	1.34
16	h	201	7PH	O31-C31	2.06	1.39	1.33
22	d	604	HAS	CHB-C1D	2.06	1.42	1.38
15	F	202	CDL	OA8-CA6	-2.05	1.40	1.45
25	B	603	MQ9	O4-C4	-2.05	1.18	1.23
29	C	303	HEC	C3A-C4A	2.05	1.47	1.42
26	L	201	9YF	P-O2	2.04	1.65	1.60
15	C	301	CDL	OB6-CB5	2.04	1.40	1.34
15	D	601	CDL	OA6-CA5	2.04	1.40	1.34
25	b	804	MQ9	C26-C24	2.04	1.55	1.51
22	d	603	HAS	C1B-NB	-2.03	1.34	1.38
15	F	202	CDL	OB8-CB7	2.03	1.39	1.33
15	b	801	CDL	OB8-CB7	2.02	1.39	1.33
15	D	606	CDL	OA8-CA6	-2.02	1.40	1.45
26	l	201	9YF	O9-C8	2.01	1.40	1.34
16	D	608	7PH	O31-C3	-2.01	1.40	1.45
15	f	202	CDL	OB8-CB6	-2.01	1.40	1.45
15	C	301	CDL	OB8-CB6	-2.01	1.40	1.45
22	D	602	HAS	FE-ND	2.01	2.08	1.97

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	303	HEC	CBA-CAA-C2A	-12.47	91.59	112.60
29	C	303	HEC	CMB-C2B-C3B	9.84	137.38	125.82
22	d	603	HAS	C2D-C3D-C4D	-7.98	100.80	106.49
29	C	303	HEC	C1D-C2D-C3D	-7.65	101.67	107.00
22	D	603	HAS	C2D-C3D-C4D	-7.55	101.10	106.49
22	D	602	HAS	C2D-C3D-C4D	-7.25	101.32	106.49
28	B	602	HEM	CAD-CBD-CGD	-7.20	98.11	113.60
28	b	803	HEM	CAD-CBD-CGD	-6.27	100.11	113.60
28	b	802	HEM	CAD-C3D-C4D	6.13	135.36	124.66
22	d	604	HAS	CAD-CBD-CGD	-6.04	100.61	113.60
28	b	802	HEM	CAD-C3D-C2D	-5.83	117.02	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	604	HAS	C1D-C2D-C3D	-5.58	102.69	107.11
29	c	303	HEC	C1D-C2D-C3D	-5.48	103.18	107.00
22	d	603	HAS	CHA-C4D-ND	-5.43	118.52	124.42
22	D	603	HAS	C25-C23-C24	5.41	124.38	115.27
29	C	302	HEC	C1D-C2D-C3D	-5.40	103.24	107.00
28	b	802	HEM	CAD-CBD-CGD	-5.34	102.11	113.60
22	D	602	HAS	CHD-C4A-NA	-5.20	118.80	124.43
22	d	604	HAS	C2D-C3D-C4D	-5.14	102.83	106.49
18	h	202	9XX	O1-C18-C19	5.08	122.45	111.50
29	c	303	HEC	CMB-C2B-C3B	5.07	131.79	125.82
22	d	604	HAS	CMA-C3A-C4A	4.95	133.44	124.71
22	d	603	HAS	CHD-C4A-NA	-4.92	119.10	124.43
22	D	602	HAS	CHA-C4D-ND	-4.90	119.09	124.42
22	d	604	HAS	C2A-C1A-NA	4.84	115.03	110.32
22	d	604	HAS	C3B-C4B-NB	4.83	115.56	109.84
29	c	302	HEC	C1D-C2D-C3D	-4.83	103.64	107.00
28	B	601	HEM	CBA-CAA-C2A	-4.83	104.38	112.62
25	b	804	MQ9	C10-C9-C11	4.78	123.31	115.27
22	d	604	HAS	C2B-C1B-NB	4.74	115.57	109.88
22	d	604	HAS	C3D-C4D-ND	4.73	114.94	110.36
28	B	601	HEM	CAD-C3D-C4D	4.69	132.85	124.66
29	C	303	HEC	CMB-C2B-C1B	-4.68	121.28	128.46
28	B	601	HEM	CAD-C3D-C2D	-4.64	119.24	127.88
28	B	601	HEM	CHD-C1D-ND	4.58	129.41	124.43
28	B	601	HEM	C2C-C3C-C4C	4.58	110.10	106.90
26	a	601	9YF	O9-C8-C9	4.49	121.17	111.50
22	d	603	HAS	CHB-C1B-NB	-4.47	119.56	124.42
22	D	602	HAS	CHB-C1B-NB	-4.40	119.64	124.42
22	D	602	HAS	CHA-C1A-NA	-4.32	119.77	124.44
22	D	602	HAS	CHC-C4B-NB	-4.28	119.09	124.38
28	b	802	HEM	CBA-CAA-C2A	-4.27	105.33	112.62
22	D	603	HAS	C3B-C4B-NB	4.23	114.85	109.84
22	D	603	HAS	C3D-C4D-ND	4.09	114.31	110.36
18	H	202	9XX	O1-C18-C19	4.02	120.16	111.50
28	b	802	HEM	CHD-C1D-ND	4.01	128.79	124.43
29	c	302	HEC	CBA-CAA-C2A	-4.00	105.87	112.60
29	C	302	HEC	CBA-CAA-C2A	-3.95	105.95	112.60
28	b	803	HEM	CHD-C1D-ND	3.93	128.70	124.43
22	D	603	HAS	CHC-C4B-NB	-3.92	119.54	124.38
28	B	601	HEM	CHC-C4B-NB	3.92	128.69	124.43
22	D	602	HAS	C26-C15-C16	3.91	121.86	115.27
22	D	603	HAS	CHA-C4D-ND	-3.87	120.21	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	604	HAS	OMD-CMD-C2D	-3.87	116.93	125.69
22	D	603	HAS	CHB-C1B-NB	-3.87	120.21	124.42
22	D	602	HAS	C25-C23-C24	3.86	121.77	115.27
18	h	204	9XX	O1-C18-C19	3.83	119.75	111.50
22	d	604	HAS	CMC-C2C-C3C	3.81	131.81	124.68
22	d	603	HAS	C3D-C4D-ND	3.79	114.03	110.36
22	d	603	HAS	CHA-C1A-NA	-3.74	120.39	124.44
22	D	602	HAS	CMB-C2B-C1B	3.74	130.74	125.04
22	D	602	HAS	C27-C19-C20	3.74	121.56	115.27
28	b	802	HEM	CHC-C4B-NB	3.66	128.41	124.43
22	d	603	HAS	CHC-C4B-NB	-3.65	119.87	124.38
28	b	803	HEM	CHC-C4B-NB	3.65	128.39	124.43
22	D	603	HAS	CHD-C4A-NA	-3.64	120.49	124.43
25	a	602	MQ9	C15-C14-C16	3.63	121.37	115.27
28	b	803	HEM	CMD-C2D-C1D	3.62	130.55	125.04
25	b	804	MQ9	C11-C9-C8	-3.62	113.80	121.12
25	B	604	MQ9	C7-C6-C1	3.57	122.33	118.50
22	D	603	HAS	C4B-C3B-C2B	-3.57	101.31	107.41
22	D	602	HAS	C3D-C4D-ND	3.57	113.81	110.36
29	C	303	HEC	C2B-C3B-C4B	-3.57	102.50	106.35
18	B	608	9XX	O1-C18-C19	3.52	119.09	111.50
28	B	602	HEM	CMD-C2D-C1D	3.50	130.38	125.04
22	d	603	HAS	CMB-C2B-C1B	3.50	130.37	125.04
22	d	603	HAS	C27-C19-C20	3.48	121.13	115.27
28	B	602	HEM	CHD-C1D-ND	3.48	128.21	124.43
28	B	601	HEM	CAD-CBD-CGD	-3.47	106.15	113.60
22	D	603	HAS	CAD-C3D-C4D	3.40	130.60	124.66
22	d	604	HAS	C1B-C2B-C3B	-3.40	102.74	106.80
25	B	603	MQ9	C25-C24-C26	3.38	120.96	115.27
28	B	602	HEM	CHC-C4B-NB	3.38	128.10	124.43
22	d	604	HAS	CHB-C1B-C2B	-3.37	119.72	124.98
15	b	806	CDL	OA6-CA5-C11	3.35	118.73	111.50
22	D	603	HAS	C2A-C1A-NA	3.33	113.56	110.32
22	D	602	HAS	CAD-C3D-C4D	3.33	130.47	124.66
28	B	601	HEM	CHD-C1D-C2D	-3.33	119.78	124.98
22	d	604	HAS	C4B-C3B-C2B	-3.32	101.74	107.41
22	D	602	HAS	CHB-C1D-ND	-3.32	120.29	124.37
26	L	201	9YF	O9-C8-C9	3.31	118.64	111.50
28	b	802	HEM	O2A-CGA-O1A	-3.29	115.11	123.30
28	b	803	HEM	C4C-CHD-C1D	-3.28	118.23	122.56
22	D	603	HAS	C2B-C1B-NB	3.27	113.80	109.88
28	B	602	HEM	CHA-C4D-ND	3.23	128.37	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	805	MQ9	C15-C14-C16	3.23	120.70	115.27
22	d	604	HAS	C26-C15-C16	3.22	120.69	115.27
22	d	604	HAS	C1A-C2A-C3A	-3.21	102.94	107.13
22	d	603	HAS	C1B-C2B-C3B	-3.20	102.98	106.80
25	B	604	MQ9	C20-C19-C21	3.19	120.64	115.27
22	d	604	HAS	CHA-C4D-C3D	-3.19	120.16	124.84
22	D	603	HAS	CMC-C2C-C3C	3.17	130.61	124.68
22	D	602	HAS	C1B-C2B-C3B	-3.13	103.05	106.80
22	D	603	HAS	C1A-C2A-C3A	-3.13	103.05	107.13
22	D	602	HAS	CMA-C3A-C4A	3.12	130.21	124.71
26	l	201	9YF	O9-C8-C9	3.11	118.21	111.50
26	a	601	9YF	C7-C6-C5	3.10	116.24	110.82
26	a	604	9YF	C7-C6-C5	3.10	116.23	110.82
28	b	803	HEM	CHA-C4D-ND	3.08	128.19	124.38
29	c	302	HEC	CMC-C2C-C1C	3.08	133.20	128.46
15	D	606	CDL	OA6-CA5-C11	3.07	118.13	111.50
29	C	302	HEC	CMC-C2C-C1C	3.07	133.18	128.46
26	a	601	9YF	O11-C25-C26	3.06	121.52	111.91
25	A	504	MQ9	C15-C14-C16	3.06	120.42	115.27
15	C	301	CDL	OB6-CB5-C51	3.06	118.08	111.50
25	B	603	MQ9	C30-C29-C31	3.05	120.40	115.27
28	B	601	HEM	C4C-CHD-C1D	-3.04	118.54	122.56
16	d	609	7PH	O21-C21-C22	3.04	118.06	111.50
22	D	603	HAS	C25-C23-C22	-3.02	115.92	123.68
22	D	602	HAS	CMC-C2C-C3C	3.00	130.30	124.68
22	D	602	HAS	C13-C14-C15	-2.99	120.47	127.66
28	b	803	HEM	C2C-C3C-C4C	2.99	108.98	106.90
22	D	602	HAS	C3B-C4B-NB	2.98	113.37	109.84
22	D	602	HAS	C4A-C3A-C2A	-2.97	102.60	106.94
29	C	302	HEC	CMA-C3A-C2A	2.97	130.55	124.94
22	d	604	HAS	C3C-C4C-NC	2.97	113.05	109.21
16	D	608	7PH	O21-C21-C22	2.96	117.88	111.50
28	B	601	HEM	CMA-C3A-C4A	-2.95	123.92	128.46
28	B	602	HEM	C4C-CHD-C1D	-2.95	118.66	122.56
28	b	802	HEM	C2C-C3C-C4C	2.95	108.96	106.90
25	a	602	MQ9	C15-C14-C13	-2.95	116.10	123.68
22	d	603	HAS	C1A-C2A-C3A	-2.94	103.30	107.13
16	H	201	7PH	O21-C21-C22	2.93	117.81	111.50
29	c	302	HEC	CMA-C3A-C2A	2.92	130.45	124.94
28	b	802	HEM	C4C-CHD-C1D	-2.92	118.71	122.56
29	C	303	HEC	C4C-C3C-C2C	-2.91	103.21	106.35
22	d	603	HAS	CMC-C2C-C3C	2.91	130.13	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	602	HAS	C2B-C1B-NB	2.90	113.35	109.88
28	B	602	HEM	C1B-NB-C4B	2.90	108.06	105.07
16	E	302	7PH	O21-C21-C22	2.90	117.74	111.50
28	B	601	HEM	CMD-C2D-C1D	2.89	129.44	125.04
22	d	604	HAS	CHA-C1A-C2A	-2.89	120.25	124.94
22	d	603	HAS	C1D-ND-C4D	2.87	108.04	105.07
15	B	607	CDL	CA6-CA4-CA3	-2.84	105.06	111.79
28	B	602	HEM	C2C-C3C-C4C	2.84	108.88	106.90
22	d	603	HAS	C26-C15-C16	2.83	120.04	115.27
22	d	603	HAS	C28-C29-C30	-2.82	118.12	127.75
22	d	603	HAS	CMA-C3A-C4A	2.80	129.66	124.71
22	d	603	HAS	C2A-C1A-NA	2.80	113.05	110.32
28	B	602	HEM	C4D-ND-C1D	2.80	107.96	105.07
28	b	803	HEM	CMA-C3A-C4A	-2.80	124.16	128.46
25	A	504	MQ9	C10-C9-C11	2.80	119.98	115.27
22	D	602	HAS	C2A-C1A-NA	2.79	113.04	110.32
22	d	604	HAS	C4A-C3A-C2A	-2.79	102.87	106.94
25	A	504	MQ9	C31-C29-C28	-2.78	115.50	121.12
18	h	204	9XX	O-C15-C14	2.77	120.61	111.91
22	D	603	HAS	C4A-C3A-C2A	-2.77	102.90	106.94
25	A	504	MQ9	C15-C14-C13	-2.76	116.61	123.68
25	B	603	MQ9	C10-C9-C11	2.76	119.91	115.27
28	b	803	HEM	C1B-NB-C4B	2.74	107.91	105.07
22	d	603	HAS	CAD-C3D-C4D	2.73	129.43	124.66
22	D	602	HAS	C1A-C2A-C3A	-2.73	103.57	107.13
22	D	603	HAS	O11-C11-C12	-2.73	101.80	109.42
26	l	201	9YF	O2-C2-C7	2.72	115.00	108.66
22	D	603	HAS	CHB-C1D-ND	-2.71	121.04	124.37
28	b	802	HEM	C1B-NB-C4B	2.71	107.87	105.07
22	d	603	HAS	C3B-C4B-NB	2.70	113.04	109.84
28	B	602	HEM	CHB-C1B-NB	2.70	127.71	124.38
22	d	603	HAS	CHB-C1D-ND	-2.69	121.06	124.37
25	b	805	MQ9	C16-C14-C13	-2.68	115.68	121.12
22	D	602	HAS	C4B-C3B-C2B	-2.68	102.83	107.41
28	b	802	HEM	CMD-C2D-C1D	2.68	129.12	125.04
15	f	202	CDL	OA6-CA5-C11	2.67	117.27	111.50
28	b	803	HEM	C3C-C4C-NC	-2.67	105.91	110.94
25	B	604	MQ9	C26-C24-C23	-2.66	115.73	121.12
18	H	202	9XX	O-C15-C14	2.66	120.26	111.91
22	d	603	HAS	C28-C24-C23	-2.66	104.24	112.98
25	B	603	MQ9	C20-C19-C21	2.65	119.73	115.27
26	L	201	9YF	O2-C2-C7	2.64	114.81	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	603	HAS	C17-C18-C19	-2.64	121.31	127.66
22	D	603	HAS	C1B-C2B-C3B	-2.63	103.66	106.80
25	a	602	MQ9	C25-C24-C26	2.63	119.70	115.27
25	a	602	MQ9	C30-C29-C31	2.62	119.68	115.27
28	B	602	HEM	C3C-C4C-NC	-2.61	106.01	110.94
28	b	802	HEM	O2A-CGA-CBA	2.60	122.39	114.03
26	l	201	9YF	O11-C25-C26	2.59	120.05	111.91
25	B	603	MQ9	C26-C24-C23	-2.59	115.87	121.12
15	B	607	CDL	OA6-CA5-C11	2.59	117.09	111.50
25	b	805	MQ9	C27-C28-C29	-2.59	121.43	127.66
22	D	602	HAS	C1D-ND-C4D	2.59	107.75	105.07
18	B	608	9XX	C37-C17-C16	-2.58	105.21	112.63
22	d	603	HAS	C13-C12-C11	-2.57	110.48	114.35
25	a	602	MQ9	C10-C9-C11	2.57	119.60	115.27
22	d	603	HAS	C2B-C1B-NB	2.56	112.95	109.88
28	b	803	HEM	CHD-C1D-C2D	-2.56	120.98	124.98
28	b	803	HEM	CHB-C1B-NB	2.55	127.53	124.38
25	B	604	MQ9	C25-C24-C26	2.55	119.55	115.27
22	D	603	HAS	CMA-C3A-C4A	2.54	129.19	124.71
25	B	603	MQ9	C11-C9-C8	-2.54	115.98	121.12
25	B	604	MQ9	C35-C34-C33	-2.54	117.17	123.68
22	d	603	HAS	C4A-C3A-C2A	-2.53	103.24	106.94
25	a	602	MQ9	C26-C24-C23	-2.53	115.99	121.12
25	B	604	MQ9	C30-C29-C31	2.53	119.53	115.27
28	b	802	HEM	CHD-C1D-C2D	-2.53	121.03	124.98
25	b	805	MQ9	C5M-C5-C6	-2.52	120.28	124.40
25	B	603	MQ9	C8-C7-C6	2.52	118.85	112.05
25	a	602	MQ9	C31-C29-C28	-2.52	116.02	121.12
22	D	602	HAS	C21-C22-C23	-2.48	121.70	127.66
18	h	202	9XX	O-C15-C14	2.48	119.68	111.91
18	h	202	9XX	O1-C18-O2	-2.46	117.75	123.70
15	e	301	CDL	OA6-CA5-C11	2.45	116.78	111.50
28	B	601	HEM	C3C-C4C-NC	-2.45	106.32	110.94
26	a	604	9YF	C6-C5-C4	2.44	115.08	110.82
25	B	604	MQ9	C35-C34-C36	2.44	119.38	115.27
26	a	604	9YF	O9-C8-C9	2.44	116.76	111.50
28	b	803	HEM	CMA-C3A-C2A	2.44	129.54	124.94
22	d	603	HAS	OMD-CMD-C2D	-2.44	120.18	125.69
28	b	802	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
26	L	201	9YF	O11-C25-C26	2.43	119.52	111.91
16	d	608	7PH	O21-C21-C22	2.42	116.72	111.50
28	b	802	HEM	C4B-CHC-C1C	2.42	125.76	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	603	HAS	CHA-C1A-NA	-2.42	121.82	124.44
22	d	603	HAS	C4B-NB-C1B	2.42	107.57	105.07
26	a	601	9YF	C6-C5-C4	2.41	115.03	110.82
28	b	803	HEM	C4D-ND-C1D	2.41	107.56	105.07
25	b	804	MQ9	C20-C19-C21	2.38	119.28	115.27
29	C	303	HEC	CMC-C2C-C1C	2.38	132.12	128.46
28	B	602	HEM	CHB-C1B-C2B	-2.38	120.15	126.72
25	b	805	MQ9	C45-C44-C46	2.37	119.26	115.27
18	B	608	9XX	O-C15-C14	2.37	119.34	111.91
25	b	804	MQ9	C25-C24-C23	-2.36	117.62	123.68
29	C	303	HEC	CMA-C3A-C2A	2.35	129.37	124.94
15	b	801	CDL	OA8-CA7-C31	2.33	119.21	111.91
28	B	601	HEM	CMA-C3A-C2A	2.33	129.33	124.94
25	B	604	MQ9	C21-C19-C18	-2.32	116.42	121.12
22	d	603	HAS	C4B-C3B-C2B	-2.32	103.45	107.41
28	b	802	HEM	CBD-CAD-C3D	2.32	119.07	112.63
28	b	803	HEM	CHB-C1B-C2B	-2.32	120.32	126.72
22	d	604	HAS	CAD-C3D-C4D	2.31	128.69	124.66
26	a	601	9YF	O11-C25-O12	-2.31	117.77	123.59
29	C	303	HEC	O1A-CGA-CBA	-2.31	115.67	123.08
15	f	202	CDL	OB8-CB7-C71	2.31	119.14	111.91
28	b	803	HEM	O2A-CGA-O1A	-2.30	117.57	123.30
15	d	607	CDL	OB8-CB7-C71	2.30	119.11	111.91
25	b	805	MQ9	C46-C44-C43	-2.29	116.49	121.12
28	b	802	HEM	O2D-CGD-CBD	2.28	121.37	114.03
28	B	602	HEM	CAD-C3D-C2D	-2.26	123.67	127.88
25	b	805	MQ9	C35-C34-C36	2.26	119.07	115.27
28	B	601	HEM	CHB-C1B-C2B	-2.26	120.47	126.72
22	D	603	HAS	C27-C19-C20	2.26	119.07	115.27
22	d	604	HAS	C3A-C4A-NA	2.25	113.84	109.69
28	B	601	HEM	CHB-C1B-NB	2.24	127.15	124.38
25	b	805	MQ9	C7-C6-C1	2.24	120.89	118.50
15	D	606	CDL	OB6-CB5-C51	2.24	116.32	111.50
28	B	602	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
22	D	602	HAS	C4B-NB-C1B	2.22	107.37	105.07
25	B	604	MQ9	C5M-C5-C6	-2.22	120.78	124.40
22	D	602	HAS	CAA-CBA-CGA	-2.22	108.82	113.60
15	F	202	CDL	OB8-CB7-C71	2.21	118.85	111.91
22	d	604	HAS	C27-C19-C20	2.21	118.99	115.27
29	C	303	HEC	CBD-CAD-C3D	-2.21	108.85	112.62
15	b	801	CDL	OA8-CA6-CA4	2.20	114.84	108.43
15	B	607	CDL	OA6-CA5-OA7	-2.19	118.40	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	603	HAS	C1D-C2D-C3D	-2.19	105.38	107.11
28	b	803	HEM	CAD-C3D-C2D	-2.18	123.81	127.88
22	d	603	HAS	C4A-NA-C1A	2.18	107.49	105.35
29	c	302	HEC	CMD-C2D-C3D	2.18	129.06	124.94
15	B	607	CDL	OA8-CA6-CA4	2.18	114.78	108.43
22	d	604	HAS	C25-C23-C24	2.18	118.93	115.27
18	B	608	9XX	O1-C17-C16	2.17	111.17	106.13
22	D	602	HAS	C4A-NA-C1A	2.17	107.47	105.35
22	D	602	HAS	CMB-C2B-C3B	-2.17	126.21	130.34
28	b	802	HEM	CHA-C4D-ND	2.16	127.05	124.38
29	c	303	HEC	CMD-C2D-C3D	2.15	129.00	124.94
25	B	603	MQ9	C36-C34-C35	2.14	119.33	114.60
28	B	601	HEM	C2B-C1B-NB	2.14	112.37	109.84
28	b	802	HEM	C3C-C4C-NC	-2.14	106.91	110.94
25	b	805	MQ9	C7-C8-C9	-2.14	123.24	126.79
25	b	804	MQ9	C8-C7-C6	2.13	117.79	112.05
28	b	803	HEM	C1D-C2D-C3D	-2.12	104.73	106.96
16	H	201	7PH	O31-C31-C32	2.11	118.53	111.91
15	c	301	CDL	OA5-PA1-OA3	2.11	117.30	109.07
28	b	803	HEM	CMC-C2C-C3C	2.10	128.60	124.68
25	a	602	MQ9	C20-C19-C21	2.09	118.80	115.27
22	D	602	HAS	OMD-CMD-C2D	-2.09	120.97	125.69
28	B	602	HEM	CMC-C2C-C3C	2.08	128.58	124.68
29	C	303	HEC	C3C-C4C-NC	2.08	114.86	110.94
15	d	607	CDL	OA6-CA5-C11	2.07	115.97	111.50
25	A	504	MQ9	C26-C24-C23	-2.07	116.92	121.12
29	C	302	HEC	CMD-C2D-C3D	2.07	128.85	124.94
28	B	602	HEM	C1D-C2D-C3D	-2.07	104.78	106.96
28	b	802	HEM	CMB-C2B-C1B	2.07	128.19	125.04
15	C	301	CDL	C52-C51-CB5	-2.06	106.13	113.62
26	a	601	9YF	O11-C24-C	2.06	114.42	108.43
25	A	504	MQ9	C30-C29-C31	2.06	118.73	115.27
28	b	802	HEM	O1D-CGD-CBD	-2.05	116.49	123.08
22	D	603	HAS	C13-C14-C15	-2.05	122.72	127.66
22	d	603	HAS	CAA-C2A-C1A	2.05	128.76	124.89
25	B	603	MQ9	C12-C13-C14	-2.05	122.72	127.66
18	H	202	9XX	C13-C14-C15	-2.05	106.17	113.62
29	c	303	HEC	CMA-C3A-C2A	2.05	128.80	124.94
22	D	602	HAS	C24-C23-C22	-2.04	116.98	121.12
22	d	604	HAS	C17-C18-C19	-2.04	122.75	127.66
28	B	602	HEM	CMA-C3A-C2A	2.04	128.78	124.94
25	B	604	MQ9	C40-C39-C41	2.03	118.69	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	602	MQ9	C5M-C5-C6	-2.03	121.08	124.40
18	h	204	9XX	O1-C17-C16	2.02	110.82	106.13
28	b	802	HEM	CMA-C3A-C2A	2.02	128.75	124.94
22	d	603	HAS	C25-C23-C24	2.02	118.66	115.27
22	D	603	HAS	CAA-C2A-C1A	2.01	128.69	124.89
25	A	504	MQ9	C36-C34-C35	2.01	119.04	114.60
22	D	603	HAS	C4A-NA-C1A	2.00	107.31	105.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	D	602	HAS	NA
22	D	603	HAS	NA
22	d	603	HAS	NA
22	d	604	HAS	NA

All (1340) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	301	CDL	CA2-OA2-PA1-OA3
15	E	301	CDL	CB2-OB2-PB2-OB3
15	E	301	CDL	CB2-OB2-PB2-OB4
15	E	301	CDL	CB3-OB5-PB2-OB2
15	F	202	CDL	CA2-OA2-PA1-OA4
15	F	202	CDL	CA3-OA5-PA1-OA3
15	F	202	CDL	C51-CB5-OB6-CB4
15	D	601	CDL	CA2-OA2-PA1-OA3
15	D	601	CDL	CA2-OA2-PA1-OA5
15	D	601	CDL	CB2-OB2-PB2-OB4
15	D	606	CDL	CA2-OA2-PA1-OA3
15	D	606	CDL	CA2-OA2-PA1-OA5
15	D	606	CDL	OA7-CA5-OA6-CA4
15	B	605	CDL	CA2-OA2-PA1-OA4
15	B	605	CDL	CA3-OA5-PA1-OA3
15	B	605	CDL	CA3-OA5-PA1-OA4
15	B	605	CDL	C51-CB5-OB6-CB4
15	B	607	CDL	CA2-OA2-PA1-OA3
15	B	607	CDL	CA2-OA2-PA1-OA4
15	B	607	CDL	CA2-OA2-PA1-OA5
15	B	607	CDL	C11-CA5-OA6-CA4
15	B	607	CDL	CB2-OB2-PB2-OB3
15	B	607	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	B	607	CDL	CB2-OB2-PB2-OB5
15	C	301	CDL	CA2-OA2-PA1-OA3
15	C	301	CDL	C31-CA7-OA8-CA6
15	C	301	CDL	CB6-CB4-OB6-CB5
15	C	301	CDL	C51-CB5-OB6-CB4
15	e	301	CDL	CA3-OA5-PA1-OA3
15	e	301	CDL	CB2-OB2-PB2-OB3
15	e	301	CDL	CB2-OB2-PB2-OB4
15	e	301	CDL	CB2-OB2-PB2-OB5
15	f	202	CDL	CA2-OA2-PA1-OA4
15	f	202	CDL	CB2-OB2-PB2-OB3
15	f	202	CDL	CB2-OB2-PB2-OB4
15	f	202	CDL	CB3-OB5-PB2-OB3
15	f	202	CDL	CB3-OB5-PB2-OB4
15	f	202	CDL	OB7-CB5-OB6-CB4
15	f	202	CDL	C51-CB5-OB6-CB4
15	d	601	CDL	CA2-OA2-PA1-OA4
15	d	607	CDL	CA3-OA5-PA1-OA3
15	d	607	CDL	CA3-OA5-PA1-OA4
15	d	607	CDL	CB2-OB2-PB2-OB3
15	d	607	CDL	CB2-OB2-PB2-OB4
15	b	801	CDL	CA2-C1-CB2-OB2
15	b	801	CDL	CA2-OA2-PA1-OA3
15	b	801	CDL	CA2-OA2-PA1-OA4
15	b	806	CDL	CA2-OA2-PA1-OA4
15	b	806	CDL	CA2-OA2-PA1-OA5
15	b	806	CDL	CA6-CA4-OA6-CA5
15	b	806	CDL	C11-CA5-OA6-CA4
15	b	806	CDL	C51-CB5-OB6-CB4
15	c	301	CDL	CB2-C1-CA2-OA2
15	c	301	CDL	CA3-OA5-PA1-OA3
15	c	301	CDL	CA3-OA5-PA1-OA4
15	c	301	CDL	OA9-CA7-OA8-CA6
15	c	301	CDL	CB3-OB5-PB2-OB3
15	c	301	CDL	CB3-OB5-PB2-OB4
16	E	302	7PH	C22-C21-O21-C2
16	H	201	7PH	O22-C21-O21-C2
16	F	207	7PH	C1-O11-P-O14
16	D	607	7PH	C3-C2-O21-C21
16	D	607	7PH	C22-C21-O21-C2
16	D	609	7PH	C1-O11-P-O13
16	D	609	7PH	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
16	D	610	7PH	C1-O11-P-O12
16	D	610	7PH	C1-O11-P-O13
16	h	201	7PH	C1-O11-P-O12
16	h	201	7PH	C1-O11-P-O13
16	h	201	7PH	C1-O11-P-O14
16	f	207	7PH	C1-O11-P-O13
16	f	207	7PH	C1-O11-P-O14
16	d	609	7PH	C22-C21-O21-C2
16	d	610	7PH	C1-O11-P-O12
16	d	610	7PH	C1-O11-P-O13
18	h	202	9XX	C19-C18-O1-C17
18	h	202	9XX	O2-C18-O1-C17
18	h	204	9XX	O-C16-C17-C37
18	h	204	9XX	O-C16-C17-O1
18	h	204	9XX	C19-C18-O1-C17
22	D	602	HAS	C12-C11-C3B-C2B
22	D	602	HAS	C12-C11-C3B-C4B
22	D	603	HAS	C12-C11-C3B-C2B
22	D	603	HAS	C2D-C3D-CAD-CBD
22	D	603	HAS	C4D-C3D-CAD-CBD
22	D	603	HAS	C23-C24-C28-C29
22	d	603	HAS	O11-C11-C3B-C4B
22	d	603	HAS	C1D-C2D-CMD-OMD
22	d	603	HAS	C3D-C2D-CMD-OMD
22	d	604	HAS	C3D-C2D-CMD-OMD
22	d	604	HAS	C3B-C11-C12-C13
25	A	504	MQ9	C9-C11-C12-C13
25	A	504	MQ9	C23-C24-C26-C27
25	A	504	MQ9	C25-C24-C26-C27
25	A	504	MQ9	C24-C26-C27-C28
25	A	504	MQ9	C28-C29-C31-C32
25	A	504	MQ9	C30-C29-C31-C32
25	A	504	MQ9	C29-C31-C32-C33
25	B	604	MQ9	C5-C6-C7-C8
25	B	604	MQ9	C1-C6-C7-C8
25	B	604	MQ9	C20-C19-C21-C22
25	B	604	MQ9	C29-C31-C32-C33
25	a	602	MQ9	C13-C14-C16-C17
25	a	602	MQ9	C15-C14-C16-C17
25	a	602	MQ9	C30-C29-C31-C32
25	a	602	MQ9	C29-C31-C32-C33
25	b	804	MQ9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
25	b	804	MQ9	C29-C31-C32-C33
25	b	805	MQ9	C39-C41-C42-C43
26	L	201	9YF	C7-C2-O2-P
26	a	601	9YF	C2-O2-P-O1
26	a	604	9YF	O9-C-C24-O11
26	l	201	9YF	C7-C2-O2-P
28	B	602	HEM	C2B-C3B-CAB-CBB
28	B	602	HEM	C4B-C3B-CAB-CBB
28	b	802	HEM	C2D-C3D-CAD-CBD
28	b	802	HEM	C4D-C3D-CAD-CBD
28	b	803	HEM	C1A-C2A-CAA-CBA
28	b	803	HEM	C3A-C2A-CAA-CBA
28	b	803	HEM	C2B-C3B-CAB-CBB
28	b	803	HEM	C4B-C3B-CAB-CBB
29	C	302	HEC	C2D-C3D-CAD-CBD
29	C	302	HEC	C4D-C3D-CAD-CBD
29	c	302	HEC	C2D-C3D-CAD-CBD
29	c	302	HEC	C4D-C3D-CAD-CBD
29	c	303	HEC	C2D-C3D-CAD-CBD
29	c	303	HEC	C4D-C3D-CAD-CBD
15	C	301	CDL	OA9-CA7-OA8-CA6
15	C	301	CDL	OB9-CB7-OB8-CB6
15	c	301	CDL	OB9-CB7-OB8-CB6
16	F	207	7PH	C2-C3-O31-C31
16	f	207	7PH	C2-C3-O31-C31
15	F	202	CDL	C71-CB7-OB8-CB6
15	C	301	CDL	C71-CB7-OB8-CB6
15	f	202	CDL	C71-CB7-OB8-CB6
15	c	301	CDL	C31-CA7-OA8-CA6
15	c	301	CDL	C71-CB7-OB8-CB6
15	F	202	CDL	OB9-CB7-OB8-CB6
15	f	202	CDL	OB9-CB7-OB8-CB6
15	d	607	CDL	OB9-CB7-OB8-CB6
15	b	806	CDL	OA9-CA7-OA8-CA6
16	H	201	7PH	O32-C31-O31-C3
16	d	609	7PH	O32-C31-O31-C3
15	F	202	CDL	OB7-CB5-OB6-CB4
15	B	605	CDL	OB7-CB5-OB6-CB4
15	e	301	CDL	OB7-CB5-OB6-CB4
15	b	806	CDL	OA7-CA5-OA6-CA4
15	b	806	CDL	OB7-CB5-OB6-CB4
15	c	301	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
16	E	302	7PH	O22-C21-O21-C2
16	D	609	7PH	O22-C21-O21-C2
18	h	204	9XX	O2-C18-O1-C17
26	L	201	9YF	O10-C8-O9-C
26	l	201	9YF	O10-C8-O9-C
15	B	605	CDL	OA9-CA7-OA8-CA6
15	d	607	CDL	C71-CB7-OB8-CB6
15	D	606	CDL	C11-CA5-OA6-CA4
15	e	301	CDL	C51-CB5-OB6-CB4
16	H	201	7PH	C22-C21-O21-C2
26	L	201	9YF	C9-C8-O9-C
22	d	603	HAS	C3A-C2A-CAA-CBA
22	d	604	HAS	C26-C15-C16-C17
25	A	504	MQ9	C15-C14-C16-C17
25	A	504	MQ9	C20-C19-C21-C22
25	A	504	MQ9	C18-C19-C21-C22
25	B	604	MQ9	C18-C19-C21-C22
25	a	602	MQ9	C28-C29-C31-C32
25	b	804	MQ9	C12-C11-C9-C8
15	B	605	CDL	C31-CA7-OA8-CA6
15	b	801	CDL	C31-CA7-OA8-CA6
15	b	801	CDL	C71-CB7-OB8-CB6
15	b	806	CDL	C31-CA7-OA8-CA6
16	H	201	7PH	C32-C31-O31-C3
16	h	201	7PH	C32-C31-O31-C3
16	d	609	7PH	C32-C31-O31-C3
18	h	204	9XX	C14-C15-O-C16
22	d	603	HAS	C1A-C2A-CAA-CBA
15	B	607	CDL	OA7-CA5-OA6-CA4
15	C	301	CDL	OB7-CB5-OB6-CB4
15	d	607	CDL	OA7-CA5-OA6-CA4
16	D	607	7PH	O22-C21-O21-C2
16	d	609	7PH	O22-C21-O21-C2
15	b	801	CDL	OB9-CB7-OB8-CB6
15	D	606	CDL	O1-C1-CA2-OA2
15	D	606	CDL	O1-C1-CB2-OB2
15	f	202	CDL	O1-C1-CA2-OA2
15	b	801	CDL	O1-C1-CB2-OB2
15	c	301	CDL	O1-C1-CA2-OA2
18	h	204	9XX	O6-C15-O-C16
15	d	607	CDL	C11-CA5-OA6-CA4
15	c	301	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
26	l	201	9YF	C9-C8-O9-C
26	a	601	9YF	C9-C10-C11-C12
15	d	601	CDL	CA5-C11-C12-C13
15	B	607	CDL	C75-C76-C77-C78
15	f	202	CDL	C19-C20-C21-C22
16	h	201	7PH	O32-C31-O31-C3
22	D	602	HAS	C26-C15-C16-C17
22	D	602	HAS	C25-C23-C24-C28
25	B	604	MQ9	C30-C29-C31-C32
25	a	602	MQ9	C25-C24-C26-C27
22	D	602	HAS	C14-C15-C16-C17
22	D	602	HAS	C22-C23-C24-C28
25	B	604	MQ9	C28-C29-C31-C32
25	a	602	MQ9	C23-C24-C26-C27
15	b	801	CDL	OA9-CA7-OA8-CA6
16	G	403	7PH	O32-C31-O31-C3
16	g	403	7PH	O32-C31-O31-C3
22	d	603	HAS	C23-C24-C28-C29
22	d	604	HAS	C23-C24-C28-C29
25	A	504	MQ9	C19-C21-C22-C23
25	B	604	MQ9	C14-C16-C17-C18
25	B	604	MQ9	C39-C41-C42-C43
25	a	602	MQ9	C9-C11-C12-C13
25	b	804	MQ9	C14-C16-C17-C18
25	b	805	MQ9	C29-C31-C32-C33
16	G	403	7PH	C32-C31-O31-C3
16	g	403	7PH	C32-C31-O31-C3
16	d	610	7PH	C32-C31-O31-C3
18	h	202	9XX	C14-C15-O-C16
26	a	601	9YF	C26-C25-O11-C24
15	D	601	CDL	CA5-C11-C12-C13
15	F	202	CDL	C19-C20-C21-C22
15	F	202	CDL	CA2-C1-CB2-OB2
15	D	606	CDL	CB2-C1-CA2-OA2
15	D	606	CDL	CA2-C1-CB2-OB2
15	B	605	CDL	CB2-C1-CA2-OA2
16	D	607	7PH	C37-C38-C39-C3A
15	B	607	CDL	C31-CA7-OA8-CA6
15	B	607	CDL	C71-CB7-OB8-CB6
15	D	606	CDL	CA7-C31-C32-C33
15	b	806	CDL	O1-C1-CB2-OB2
16	d	608	7PH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	B	607	CDL	OA9-CA7-OA8-CA6
16	d	610	7PH	O32-C31-O31-C3
18	h	202	9XX	O6-C15-O-C16
22	d	604	HAS	C14-C15-C16-C17
25	A	504	MQ9	C13-C14-C16-C17
18	h	204	9XX	C25-C26-C27-C36
15	C	301	CDL	C11-CA5-OA6-CA4
15	D	601	CDL	CA7-C31-C32-C33
15	D	601	CDL	CB7-C71-C72-C73
15	B	607	CDL	CB5-C51-C52-C53
15	C	301	CDL	CB5-C51-C52-C53
15	b	806	CDL	CA7-C31-C32-C33
16	D	610	7PH	C21-C22-C23-C24
15	B	607	CDL	OB9-CB7-OB8-CB6
29	c	303	HEC	C2A-CAA-CBA-CGA
26	a	604	9YF	C33-C35-C36-C37
15	E	301	CDL	CB7-C71-C72-C73
15	e	301	CDL	CA5-C11-C12-C13
15	d	601	CDL	CB5-C51-C52-C53
16	D	609	7PH	C21-C22-C23-C24
26	L	201	9YF	C25-C26-C27-C28
15	B	607	CDL	CA5-C11-C12-C13
15	f	202	CDL	CB5-C51-C52-C53
15	d	607	CDL	CB5-C51-C52-C53
15	b	801	CDL	CB5-C51-C52-C53
15	b	806	CDL	CA5-C11-C12-C13
16	E	302	7PH	C21-C22-C23-C24
16	D	607	7PH	C21-C22-C23-C24
16	k	101	7PH	C31-C32-C33-C34
18	h	202	9XX	C12-C13-C14-C15
18	h	204	9XX	C18-C19-C20-C21
26	l	201	9YF	C25-C26-C27-C28
26	a	604	9YF	C30-C31-C32-C33
15	D	601	CDL	C17-C18-C19-C20
15	b	806	CDL	CB5-C51-C52-C53
16	D	608	7PH	C31-C32-C33-C34
22	D	602	HAS	C3D-CAD-CBD-CGD
28	B	601	HEM	C3D-CAD-CBD-CGD
28	b	802	HEM	C3D-CAD-CBD-CGD
26	a	601	9YF	C30-C31-C32-C33
26	l	201	9YF	C32-C33-C35-C36
26	a	601	9YF	O12-C25-O11-C24

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Mol	Chain	Res	Type	Atoms
22	D	602	HAS	C15-C16-C17-C18
25	B	603	MQ9	C9-C11-C12-C13
25	B	603	MQ9	C14-C16-C17-C18
25	B	603	MQ9	C29-C31-C32-C33
25	a	602	MQ9	C19-C21-C22-C23
25	a	602	MQ9	C24-C26-C27-C28
25	b	805	MQ9	C14-C16-C17-C18
25	b	805	MQ9	C24-C26-C27-C28
16	d	609	7PH	C21-C22-C23-C24
15	F	202	CDL	O1-C1-CB2-OB2
15	B	605	CDL	O1-C1-CA2-OA2
15	B	605	CDL	C11-CA5-OA6-CA4
16	D	610	7PH	C22-C21-O21-C2
16	h	201	7PH	C22-C21-O21-C2
15	E	301	CDL	CA2-OA2-PA1-OA5
15	E	301	CDL	CB2-OB2-PB2-OB5
15	F	202	CDL	CA2-OA2-PA1-OA5
15	D	601	CDL	CA3-OA5-PA1-OA2
15	D	601	CDL	CB2-OB2-PB2-OB5
15	B	605	CDL	CA2-OA2-PA1-OA5
15	B	605	CDL	CA3-OA5-PA1-OA2
15	B	605	CDL	CB3-OB5-PB2-OB2
15	C	301	CDL	CB3-OB5-PB2-OB2
15	e	301	CDL	CA3-OA5-PA1-OA2
15	f	202	CDL	CA3-OA5-PA1-OA2
15	f	202	CDL	CB2-OB2-PB2-OB5
15	d	601	CDL	CA2-OA2-PA1-OA5
15	d	601	CDL	CA3-OA5-PA1-OA2
15	d	607	CDL	CA3-OA5-PA1-OA2
15	d	607	CDL	CB2-OB2-PB2-OB5
15	b	801	CDL	CA2-OA2-PA1-OA5
15	b	801	CDL	CB2-OB2-PB2-OB5
15	c	301	CDL	CA3-OA5-PA1-OA2
15	c	301	CDL	CB3-OB5-PB2-OB2
15	D	601	CDL	CB5-C51-C52-C53
16	F	207	7PH	C32-C31-O31-C3
16	f	207	7PH	C32-C31-O31-C3
15	d	607	CDL	CA5-C11-C12-C13
15	f	202	CDL	CB2-C1-CA2-OA2
15	B	605	CDL	OA7-CA5-OA6-CA4
15	C	301	CDL	OA7-CA5-OA6-CA4
16	D	610	7PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
16	h	201	7PH	O22-C21-O21-C2
25	b	804	MQ9	C30-C29-C31-C32
16	D	610	7PH	C33-C34-C35-C36
26	a	601	9YF	C2-O2-P-O
15	C	301	CDL	C16-C17-C18-C19
15	c	301	CDL	C16-C17-C18-C19
17	F	206	TRD	C2-C3-C4-C5
16	D	608	7PH	C22-C21-O21-C2
15	D	606	CDL	C17-C18-C19-C20
15	D	606	CDL	C77-C78-C79-C80
16	h	201	7PH	C26-C27-C28-C29
16	d	610	7PH	C27-C28-C29-C2A
18	H	202	9XX	C9-C10-C11-C12
18	h	202	9XX	C20-C21-C22-C23
26	a	601	9YF	C17-C18-C19-C20
26	l	201	9YF	C16-C17-C18-C19
15	F	202	CDL	C21-C22-C23-C24
15	D	601	CDL	C75-C76-C77-C78
15	D	606	CDL	C72-C73-C74-C75
15	B	605	CDL	C55-C56-C57-C58
16	D	608	7PH	C34-C35-C36-C37
17	F	203	TRD	C11-C10-C9-C8
26	L	201	9YF	C16-C17-C18-C19
26	a	601	9YF	C27-C28-C29-C30
26	a	601	9YF	C36-C37-C38-C39
27	x	101	PLM	C4-C5-C6-C7
15	B	607	CDL	CA3-CA4-OA6-CA5
16	D	608	7PH	O22-C21-O21-C2
15	C	301	CDL	CA7-C31-C32-C33
15	D	606	CDL	C75-C76-C77-C78
15	f	202	CDL	C21-C22-C23-C24
15	d	607	CDL	C34-C35-C36-C37
15	b	801	CDL	C18-C19-C20-C21
16	D	610	7PH	C27-C28-C29-C2A
16	h	201	7PH	C28-C29-C2A-C2B
17	F	205	TRD	C11-C10-C9-C8
15	b	806	CDL	C17-C18-C19-C20
15	b	806	CDL	C59-C60-C61-C62
16	D	609	7PH	C26-C27-C28-C29
18	h	204	9XX	C11-C12-C13-C14
26	a	601	9YF	C35-C36-C37-C38
27	x	101	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	f	202	CDL	C78-C79-C80-C81
15	b	806	CDL	C54-C55-C56-C57
15	c	301	CDL	C22-C23-C24-C25
15	c	301	CDL	C77-C78-C79-C80
16	H	201	7PH	C28-C29-C2A-C2B
17	f	205	TRD	C11-C10-C9-C8
26	a	604	9YF	C11-C12-C13-C14
15	F	202	CDL	C78-C79-C80-C81
15	f	202	CDL	C55-C56-C57-C58
16	E	302	7PH	C33-C34-C35-C36
16	D	610	7PH	C38-C39-C3A-C3B
16	d	610	7PH	C38-C39-C3A-C3B
17	f	205	TRD	C2-C3-C4-C5
26	L	201	9YF	C26-C27-C28-C29
15	B	607	CDL	C18-C19-C20-C21
15	d	607	CDL	C31-C32-C33-C34
15	b	801	CDL	C13-C14-C15-C16
16	e	302	7PH	C33-C34-C35-C36
17	A	502	TRD	C5-C6-C7-C8
26	l	201	9YF	C34-C33-C35-C36
15	E	301	CDL	C73-C74-C75-C76
15	D	601	CDL	C22-C23-C24-C25
15	D	606	CDL	C51-C52-C53-C54
15	C	301	CDL	C55-C56-C57-C58
15	C	301	CDL	C75-C76-C77-C78
15	f	202	CDL	C17-C18-C19-C20
16	D	609	7PH	C33-C34-C35-C36
16	g	403	7PH	C34-C35-C36-C37
17	E	303	TRD	C11-C10-C9-C8
18	H	202	9XX	C19-C20-C21-C22
26	a	604	9YF	C37-C38-C39-C40
15	C	301	CDL	C15-C16-C17-C18
26	L	201	9YF	C9-C10-C11-C12
26	l	201	9YF	C9-C10-C11-C12
16	d	610	7PH	C22-C21-O21-C2
15	d	607	CDL	C56-C57-C58-C59
15	b	806	CDL	C51-C52-C53-C54
15	c	301	CDL	C72-C73-C74-C75
16	D	607	7PH	C32-C33-C34-C35
17	E	303	TRD	C7-C8-C9-C10
18	B	608	9XX	C7-C8-C9-C10
26	a	601	9YF	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
26	l	201	9YF	C39-C40-C41-C42
27	d	611	PLM	C2-C3-C4-C5
15	e	301	CDL	CA7-C31-C32-C33
15	e	301	CDL	CB5-C51-C52-C53
15	D	606	CDL	C14-C15-C16-C17
15	D	606	CDL	C71-C72-C73-C74
15	D	606	CDL	C78-C79-C80-C81
15	B	605	CDL	C16-C17-C18-C19
15	B	605	CDL	C74-C75-C76-C77
15	B	607	CDL	C77-C78-C79-C80
15	C	301	CDL	C20-C21-C22-C23
15	e	301	CDL	C12-C13-C14-C15
15	d	601	CDL	C32-C33-C34-C35
15	d	601	CDL	C75-C76-C77-C78
15	d	607	CDL	C72-C73-C74-C75
15	b	806	CDL	C33-C34-C35-C36
16	E	302	7PH	C28-C29-C2A-C2B
16	D	609	7PH	C22-C23-C24-C25
16	D	610	7PH	C22-C23-C24-C25
16	D	610	7PH	C2A-C2B-C2C-C2D
16	e	302	7PH	C32-C33-C34-C35
16	e	302	7PH	C38-C39-C3A-C3B
16	d	608	7PH	C26-C27-C28-C29
18	H	202	9XX	C20-C21-C22-C23
26	a	604	9YF	C12-C13-C14-C15
15	D	601	CDL	OA5-CA3-CA4-CA6
15	F	202	CDL	C33-C34-C35-C36
15	D	601	CDL	C71-C72-C73-C74
15	D	606	CDL	C57-C58-C59-C60
15	B	607	CDL	C16-C17-C18-C19
16	G	403	7PH	C34-C35-C36-C37
17	e	303	TRD	C3-C4-C5-C6
17	e	303	TRD	C11-C10-C9-C8
26	L	201	9YF	C39-C40-C41-C42
26	a	604	9YF	C17-C18-C19-C20
15	B	607	CDL	C17-C18-C19-C20
15	d	601	CDL	C71-C72-C73-C74
15	d	607	CDL	C52-C53-C54-C55
15	c	301	CDL	C17-C18-C19-C20
16	D	610	7PH	C28-C29-C2A-C2B
16	e	302	7PH	C23-C24-C25-C26
16	f	207	7PH	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
16	d	608	7PH	C32-C33-C34-C35
17	B	606	TRD	C6-C7-C8-C9
26	a	604	9YF	C18-C19-C20-C21
15	E	301	CDL	CB5-C51-C52-C53
15	d	607	CDL	CA7-C31-C32-C33
15	F	202	CDL	C17-C18-C19-C20
15	B	607	CDL	C74-C75-C76-C77
15	B	607	CDL	C79-C80-C81-C82
15	f	202	CDL	C71-C72-C73-C74
15	b	806	CDL	C56-C57-C58-C59
16	d	610	7PH	C24-C25-C26-C27
17	E	303	TRD	C2-C3-C4-C5
17	F	204	TRD	C2-C3-C4-C5
15	D	606	CDL	C73-C74-C75-C76
16	D	608	7PH	C38-C39-C3A-C3B
16	f	207	7PH	C26-C27-C28-C29
18	h	202	9XX	C10-C11-C12-C13
27	d	611	PLM	C3-C4-C5-C6
16	E	302	7PH	C32-C33-C34-C35
16	F	207	7PH	C2A-C2B-C2C-C2D
16	G	403	7PH	C38-C39-C3A-C3B
16	e	302	7PH	C35-C36-C37-C38
17	A	505	TRD	C6-C7-C8-C9
18	h	204	9XX	C7-C8-C9-C10
16	F	207	7PH	O32-C31-O31-C3
16	f	207	7PH	O32-C31-O31-C3
15	D	601	CDL	C32-C33-C34-C35
15	D	606	CDL	C15-C16-C17-C18
15	D	606	CDL	C31-C32-C33-C34
15	B	607	CDL	C78-C79-C80-C81
15	C	301	CDL	C22-C23-C24-C25
16	F	207	7PH	C26-C27-C28-C29
16	g	403	7PH	C38-C39-C3A-C3B
16	d	608	7PH	C36-C37-C38-C39
17	f	206	TRD	C9-C10-C11-C12
18	h	204	9XX	C19-C20-C21-C22
26	a	604	9YF	C27-C28-C29-C30
26	l	201	9YF	C26-C27-C28-C29
26	a	601	9YF	C1-C-C24-O11
15	c	301	CDL	OA7-CA5-OA6-CA4
15	E	301	CDL	C32-C33-C34-C35
16	D	607	7PH	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
16	k	101	7PH	C28-C29-C2A-C2B
15	E	301	CDL	CA5-C11-C12-C13
15	B	605	CDL	CB5-C51-C52-C53
15	B	607	CDL	C76-C77-C78-C79
17	f	201	TRD	C5-C6-C7-C8
17	f	205	TRD	C4-C5-C6-C7
22	d	604	HAS	C27-C19-C20-C21
25	B	604	MQ9	C12-C11-C9-C10
22	d	604	HAS	C18-C19-C20-C21
25	B	604	MQ9	C12-C11-C9-C8
25	b	804	MQ9	C28-C29-C31-C32
15	c	301	CDL	C11-CA5-OA6-CA4
16	F	207	7PH	C22-C21-O21-C2
16	f	207	7PH	C22-C21-O21-C2
26	a	601	9YF	C9-C8-O9-C
15	C	301	CDL	C74-C75-C76-C77
15	b	806	CDL	C53-C54-C55-C56
15	F	202	CDL	C23-C24-C25-C26
15	F	202	CDL	C53-C54-C55-C56
15	f	202	CDL	C23-C24-C25-C26
15	f	202	CDL	C33-C34-C35-C36
15	c	301	CDL	C11-C12-C13-C14
16	d	609	7PH	C28-C29-C2A-C2B
16	d	610	7PH	C26-C27-C28-C29
18	B	608	9XX	C19-C20-C21-C22
19	H	203	TWT	C11-C12-C13-C14
26	a	601	9YF	C29-C30-C31-C32
26	a	601	9YF	C39-C40-C41-C42
15	c	301	CDL	CA5-C11-C12-C13
16	F	207	7PH	C37-C38-C39-C3A
16	f	207	7PH	C37-C38-C39-C3A
16	d	609	7PH	C23-C24-C25-C26
15	D	601	CDL	C14-C15-C16-C17
15	d	601	CDL	C18-C19-C20-C21
17	f	205	TRD	C9-C10-C11-C12
18	H	202	9XX	C22-C23-C24-C25
26	a	601	9YF	C18-C19-C20-C21
15	B	607	CDL	CA7-C31-C32-C33
18	h	202	9XX	C18-C19-C20-C21
15	f	202	CDL	C53-C54-C55-C56
16	D	609	7PH	C23-C24-C25-C26
16	e	302	7PH	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
15	b	801	CDL	OA7-CA5-OA6-CA4
16	F	207	7PH	O22-C21-O21-C2
16	f	207	7PH	O22-C21-O21-C2
16	d	610	7PH	O22-C21-O21-C2
26	a	601	9YF	O10-C8-O9-C
15	D	606	CDL	C56-C57-C58-C59
15	f	202	CDL	C16-C17-C18-C19
16	h	201	7PH	C25-C26-C27-C28
17	f	204	TRD	C9-C10-C11-C12
15	F	202	CDL	C16-C17-C18-C19
15	B	607	CDL	C54-C55-C56-C57
16	d	609	7PH	C33-C34-C35-C36
17	e	303	TRD	C2-C3-C4-C5
15	b	806	CDL	CB7-C71-C72-C73
16	e	302	7PH	C31-C32-C33-C34
18	H	202	9XX	C18-C19-C20-C21
15	b	806	CDL	C32-C33-C34-C35
15	c	301	CDL	C76-C77-C78-C79
16	E	302	7PH	C32-C31-O31-C3
16	D	609	7PH	C32-C31-O31-C3
15	C	301	CDL	C21-C22-C23-C24
15	e	301	CDL	C32-C33-C34-C35
16	H	201	7PH	C37-C38-C39-C3A
17	b	807	TRD	C3-C4-C5-C6
16	D	610	7PH	C31-C32-C33-C34
18	H	202	9XX	C12-C13-C14-C15
15	d	601	CDL	C22-C23-C24-C25
15	b	806	CDL	C37-C38-C39-C40
16	E	302	7PH	C22-C23-C24-C25
15	C	301	CDL	C72-C73-C74-C75
15	b	801	CDL	C75-C76-C77-C78
26	L	201	9YF	C32-C33-C35-C36
15	D	606	CDL	C53-C54-C55-C56
22	D	602	HAS	C1A-C2A-CAA-CBA
15	E	301	CDL	OB7-CB5-OB6-CB4
26	a	604	9YF	C11-C10-C9-C8
15	F	202	CDL	C31-CA7-OA8-CA6
15	C	301	CDL	C18-C19-C20-C21
18	h	202	9XX	C24-C25-C26-C27
15	b	801	CDL	C51-C52-C53-C54
16	H	201	7PH	C36-C37-C38-C39
16	d	608	7PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	k	101	7PH	C22-C23-C24-C25
15	c	301	CDL	C75-C76-C77-C78
16	h	201	7PH	C38-C39-C3A-C3B
15	B	605	CDL	CA5-C11-C12-C13
15	d	601	CDL	CB7-C71-C72-C73
15	c	301	CDL	CA7-C31-C32-C33
15	c	301	CDL	CB5-C51-C52-C53
22	D	602	HAS	C3A-C2A-CAA-CBA
15	b	806	CDL	C15-C16-C17-C18
16	D	609	7PH	C34-C35-C36-C37
17	A	502	TRD	C4-C5-C6-C7
17	A	503	TRD	C7-C8-C9-C10
28	b	802	HEM	C2B-C3B-CAB-CBB
16	D	608	7PH	C33-C34-C35-C36
16	e	302	7PH	C37-C38-C39-C3A
15	F	202	CDL	C51-C52-C53-C54
15	C	301	CDL	C76-C77-C78-C79
15	e	301	CDL	C56-C57-C58-C59
15	d	601	CDL	C33-C34-C35-C36
16	D	610	7PH	C25-C26-C27-C28
16	d	610	7PH	C28-C29-C2A-C2B
17	E	303	TRD	C3-C4-C5-C6
17	e	303	TRD	C7-C8-C9-C10
19	H	203	TWT	C18-C19-C20-C21
15	c	301	CDL	CB7-C71-C72-C73
15	E	301	CDL	C51-CB5-OB6-CB4
15	d	601	CDL	C11-CA5-OA6-CA4
15	b	801	CDL	C11-CA5-OA6-CA4
16	G	403	7PH	C22-C21-O21-C2
16	g	403	7PH	C22-C21-O21-C2
16	G	403	7PH	C26-C27-C28-C29
17	F	204	TRD	C4-C5-C6-C7
18	h	202	9XX	C11-C12-C13-C14
15	B	605	CDL	O1-C1-CB2-OB2
15	d	601	CDL	OA7-CA5-OA6-CA4
15	b	806	CDL	C55-C56-C57-C58
16	g	403	7PH	C24-C25-C26-C27
17	f	206	TRD	C5-C6-C7-C8
15	C	301	CDL	C11-C12-C13-C14
15	d	607	CDL	C71-C72-C73-C74
16	d	610	7PH	C22-C23-C24-C25
16	e	302	7PH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	B	603	MQ9	C12-C11-C9-C8
15	F	202	CDL	C71-C72-C73-C74
16	H	201	7PH	C38-C39-C3A-C3B
26	a	604	9YF	C28-C29-C30-C31
26	L	201	9YF	C34-C33-C35-C36
15	C	301	CDL	C71-C72-C73-C74
18	h	204	9XX	C11-C10-C9-C8
15	E	301	CDL	C51-C52-C53-C54
15	e	301	CDL	C76-C77-C78-C79
15	b	801	CDL	C57-C58-C59-C60
15	b	806	CDL	C74-C75-C76-C77
16	G	403	7PH	C24-C25-C26-C27
16	d	608	7PH	C22-C23-C24-C25
22	d	603	HAS	C4D-C3D-CAD-CBD
16	E	302	7PH	O32-C31-O31-C3
16	D	609	7PH	O32-C31-O31-C3
16	G	403	7PH	O22-C21-O21-C2
16	g	403	7PH	O22-C21-O21-C2
15	B	605	CDL	C12-C13-C14-C15
15	B	605	CDL	C58-C59-C60-C61
15	f	202	CDL	C51-C52-C53-C54
16	G	403	7PH	C35-C36-C37-C38
17	a	605	TRD	C7-C8-C9-C10
26	L	201	9YF	C15-C16-C17-C18
15	B	605	CDL	CB2-OB2-PB2-OB5
15	e	301	CDL	C53-C54-C55-C56
17	E	303	TRD	C4-C5-C6-C7
17	f	204	TRD	C11-C10-C9-C8
15	d	601	CDL	C31-C32-C33-C34
15	b	801	CDL	C78-C79-C80-C81
16	D	610	7PH	C32-C33-C34-C35
16	d	610	7PH	C29-C2A-C2B-C2C
15	F	202	CDL	OB5-CB3-CB4-CB6
15	e	301	CDL	OA5-CA3-CA4-CA6
16	H	201	7PH	O11-C1-C2-C3
16	D	608	7PH	O11-C1-C2-C3
16	D	609	7PH	C32-C33-C34-C35
16	d	610	7PH	C25-C26-C27-C28
22	d	604	HAS	O11-C11-C12-C13
27	L	202	PLM	C2-C3-C4-C5
27	L	202	PLM	C3-C4-C5-C6
15	B	605	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
15	d	607	CDL	C73-C74-C75-C76
17	e	303	TRD	C4-C5-C6-C7
15	B	605	CDL	C37-C38-C39-C40
16	H	201	7PH	C33-C34-C35-C36
17	F	205	TRD	C7-C8-C9-C10
19	h	203	TWT	C18-C19-C20-C21
15	b	801	CDL	C72-C73-C74-C75
15	c	301	CDL	C71-C72-C73-C74
16	H	201	7PH	C27-C28-C29-C2A
16	g	403	7PH	C26-C27-C28-C29
16	D	610	7PH	C37-C38-C39-C3A
17	B	606	TRD	C11-C10-C9-C8
15	B	605	CDL	C15-C16-C17-C18
26	l	201	9YF	C15-C16-C17-C18
15	F	202	CDL	C55-C56-C57-C58
15	F	202	CDL	C56-C57-C58-C59
15	f	202	CDL	C75-C76-C77-C78
16	f	207	7PH	C27-C28-C29-C2A
16	g	403	7PH	C35-C36-C37-C38
15	E	301	CDL	C74-C75-C76-C77
15	D	606	CDL	CB3-CB4-CB6-OB8
15	B	605	CDL	CA3-CA4-CA6-OA8
15	B	607	CDL	CB3-CB4-CB6-OB8
15	e	301	CDL	CA3-CA4-CA6-OA8
15	b	801	CDL	CB3-CB4-CB6-OB8
15	b	806	CDL	CA3-CA4-CA6-OA8
15	b	806	CDL	CB3-CB4-CB6-OB8
15	c	301	CDL	C31-C32-C33-C34
15	c	301	CDL	CB3-CB4-CB6-OB8
15	c	301	CDL	C73-C74-C75-C76
16	D	607	7PH	C1-C2-C3-O31
16	h	201	7PH	C1-C2-C3-O31
17	a	605	TRD	C10-C11-C12-C13
17	F	206	TRD	C5-C6-C7-C8
17	A	503	TRD	C2-C3-C4-C5
15	B	605	CDL	C72-C73-C74-C75
26	a	601	9YF	C33-C35-C36-C37
15	e	301	CDL	C75-C76-C77-C78
25	B	604	MQ9	C24-C26-C27-C28
25	b	805	MQ9	C9-C11-C12-C13
15	f	202	CDL	C18-C19-C20-C21
15	b	806	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
18	h	204	9XX	C6-C7-C8-C9
15	C	301	CDL	C53-C54-C55-C56
15	e	301	CDL	C31-C32-C33-C34
16	F	207	7PH	C27-C28-C29-C2A
18	h	202	9XX	C9-C10-C11-C12
26	l	201	9YF	C27-C28-C29-C30
16	e	302	7PH	C34-C35-C36-C37
16	d	608	7PH	C27-C28-C29-C2A
26	a	601	9YF	C10-C11-C12-C13
15	D	601	CDL	C24-C25-C26-C27
25	B	604	MQ9	C15-C14-C16-C17
15	b	806	CDL	C13-C14-C15-C16
16	H	201	7PH	C2A-C2B-C2C-C2D
16	d	610	7PH	C39-C3A-C3B-C3C
16	D	607	7PH	C32-C31-O31-C3
16	g	403	7PH	C39-C3A-C3B-C3C
17	f	205	TRD	C10-C11-C12-C13
15	b	801	CDL	CA3-CA4-OA6-CA5
15	c	301	CDL	CB6-CB4-OB6-CB5
16	F	207	7PH	C3-C2-O21-C21
16	D	610	7PH	C1-C2-O21-C21
16	f	207	7PH	C3-C2-O21-C21
15	b	806	CDL	C57-C58-C59-C60
16	G	403	7PH	C39-C3A-C3B-C3C
15	b	806	CDL	C75-C76-C77-C78
16	D	610	7PH	C1-O11-P-O14
16	d	610	7PH	C1-O11-P-O14
15	E	301	CDL	C35-C36-C37-C38
15	B	607	CDL	C56-C57-C58-C59
15	e	301	CDL	C35-C36-C37-C38
16	d	608	7PH	C25-C26-C27-C28
17	b	807	TRD	C7-C8-C9-C10
15	e	301	CDL	C31-CA7-OA8-CA6
16	k	101	7PH	C32-C31-O31-C3
26	a	604	9YF	O9-C-C1-O
16	H	201	7PH	C35-C36-C37-C38
15	d	601	CDL	C24-C25-C26-C27
16	k	101	7PH	C26-C27-C28-C29
18	h	202	9XX	C22-C23-C24-C25
26	l	201	9YF	C38-C39-C40-C41
18	B	608	9XX	C24-C25-C26-C27
15	B	607	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
15	C	301	CDL	OB6-CB4-CB6-OB8
15	c	301	CDL	C58-C59-C60-C61
15	F	202	CDL	OA9-CA7-OA8-CA6
16	D	607	7PH	O32-C31-O31-C3
16	k	101	7PH	O32-C31-O31-C3
15	f	202	CDL	C14-C15-C16-C17
15	b	806	CDL	C60-C61-C62-C63
17	A	502	TRD	C1-C2-C3-C4
17	B	606	TRD	C2-C3-C4-C5
18	h	204	9XX	C26-C27-C28-C29
25	B	604	MQ9	C13-C14-C16-C17
26	a	604	9YF	C32-C33-C35-C36
16	h	201	7PH	C32-C33-C34-C35
26	a	601	9YF	C34-C33-C35-C36
15	d	601	CDL	C11-C12-C13-C14
15	c	301	CDL	C14-C15-C16-C17
15	D	601	CDL	C31-CA7-OA8-CA6
15	e	301	CDL	C71-CB7-OB8-CB6
16	D	608	7PH	C32-C31-O31-C3
26	a	601	9YF	C40-C41-C42-C43
26	a	604	9YF	C35-C36-C37-C38
15	C	301	CDL	CA2-C1-CB2-OB2
15	b	806	CDL	CA2-C1-CB2-OB2
15	D	601	CDL	C54-C55-C56-C57
15	D	606	CDL	C74-C75-C76-C77
15	C	301	CDL	C58-C59-C60-C61
15	d	607	CDL	C53-C54-C55-C56
15	F	202	CDL	C75-C76-C77-C78
15	d	607	CDL	C51-C52-C53-C54
15	C	301	CDL	CA5-C11-C12-C13
16	F	207	7PH	C29-C2A-C2B-C2C
16	d	610	7PH	C33-C34-C35-C36
26	a	601	9YF	C15-C16-C17-C18
15	F	202	CDL	C14-C15-C16-C17
16	D	609	7PH	C25-C26-C27-C28
16	f	207	7PH	C29-C2A-C2B-C2C
15	E	301	CDL	OB5-CB3-CB4-CB6
15	d	601	CDL	OA5-CA3-CA4-CA6
15	d	601	CDL	OB5-CB3-CB4-CB6
16	d	609	7PH	O11-C1-C2-C3
26	a	601	9YF	C24-C-C1-O
25	B	604	MQ9	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
15	D	606	CDL	C79-C80-C81-C82
16	F	207	7PH	C28-C29-C2A-C2B
17	f	204	TRD	C6-C7-C8-C9
16	k	101	7PH	C21-C22-C23-C24
26	a	604	9YF	C15-C16-C17-C18
18	h	204	9XX	C24-C25-C26-C27
22	d	603	HAS	C2D-C3D-CAD-CBD
16	E	302	7PH	C37-C38-C39-C3A
17	F	204	TRD	C6-C7-C8-C9
22	D	603	HAS	C25-C23-C24-C28
25	B	604	MQ9	C40-C39-C41-C42
15	b	801	CDL	O1-C1-CA2-OA2
15	b	806	CDL	O1-C1-CA2-OA2
16	d	609	7PH	C24-C25-C26-C27
18	h	204	9XX	C27-C28-C29-C30
17	A	502	TRD	C3-C4-C5-C6
16	h	201	7PH	C31-C32-C33-C34
16	G	403	7PH	C33-C34-C35-C36
16	e	302	7PH	C25-C26-C27-C28
18	B	608	9XX	C23-C24-C25-C26
16	F	207	7PH	C2-C1-O11-P
16	f	207	7PH	C2-C1-O11-P
15	C	301	CDL	C14-C15-C16-C17
15	D	601	CDL	C18-C19-C20-C21
16	d	609	7PH	C27-C28-C29-C2A
17	B	606	TRD	C10-C11-C12-C13
26	a	601	9YF	C38-C39-C40-C41
17	F	205	TRD	C9-C10-C11-C12
15	d	601	CDL	C71-CB7-OB8-CB6
16	d	610	7PH	C23-C24-C25-C26
16	H	201	7PH	C1-C2-C3-O31
18	H	202	9XX	O-C16-C17-C37
26	a	604	9YF	C1-C-C24-O11
15	c	301	CDL	C54-C55-C56-C57
15	e	301	CDL	C51-C52-C53-C54
16	g	403	7PH	C33-C34-C35-C36
26	a	601	9YF	C2-O2-P-O8
26	a	604	9YF	C2-O2-P-O8
15	C	301	CDL	C32-C33-C34-C35
16	e	302	7PH	C36-C37-C38-C39
17	F	206	TRD	C9-C10-C11-C12
15	F	202	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
15	e	301	CDL	OA9-CA7-OA8-CA6
15	e	301	CDL	OB9-CB7-OB8-CB6
17	A	505	TRD	C11-C10-C9-C8
15	b	806	CDL	C36-C37-C38-C39
17	f	206	TRD	C7-C8-C9-C10
15	F	202	CDL	OB5-CB3-CB4-OB6
15	D	601	CDL	OA5-CA3-CA4-OA6
15	d	601	CDL	OB5-CB3-CB4-OB6
16	d	609	7PH	O11-C1-C2-O21
15	e	301	CDL	CB7-C71-C72-C73
15	b	801	CDL	C14-C15-C16-C17
15	f	202	CDL	C79-C80-C81-C82
16	d	609	7PH	C26-C27-C28-C29
18	H	202	9XX	O-C16-C17-O1
15	b	801	CDL	OB6-CB4-CB6-OB8
16	D	607	7PH	O21-C2-C3-O31
26	a	601	9YF	O9-C-C24-O11
15	C	301	CDL	C73-C74-C75-C76
25	b	805	MQ9	C34-C36-C37-C38
17	f	205	TRD	C6-C7-C8-C9
15	F	202	CDL	C18-C19-C20-C21
15	D	601	CDL	C73-C74-C75-C76
18	h	204	9XX	C36-C27-C28-C29
26	a	604	9YF	C34-C33-C35-C36
15	d	601	CDL	C13-C14-C15-C16
16	D	608	7PH	C22-C23-C24-C25
15	f	202	CDL	C1-CA2-OA2-PA1
15	d	607	CDL	C1-CA2-OA2-PA1
15	c	301	CDL	CB4-CB3-OB5-PB2
16	D	610	7PH	C2-C1-O11-P
15	D	601	CDL	C33-C34-C35-C36
16	D	609	7PH	C27-C28-C29-C2A
18	H	202	9XX	C21-C22-C23-C24
15	F	202	CDL	C79-C80-C81-C82
17	B	606	TRD	C7-C8-C9-C10
15	b	801	CDL	C55-C56-C57-C58
26	L	201	9YF	C40-C41-C42-C43
26	l	201	9YF	C30-C31-C32-C33
15	b	801	CDL	CB7-C71-C72-C73
16	h	201	7PH	C36-C37-C38-C39
16	f	207	7PH	C28-C29-C2A-C2B
15	B	605	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
15	B	607	CDL	C19-C20-C21-C22
15	B	605	CDL	CB7-C71-C72-C73
15	b	806	CDL	C11-C12-C13-C14
17	F	206	TRD	C1-C2-C3-C4
15	d	607	CDL	OB5-CB3-CB4-CB6
16	D	609	7PH	O11-C1-C2-C3
15	F	202	CDL	C34-C35-C36-C37
18	h	204	9XX	C25-C26-C27-C28
26	L	201	9YF	C31-C32-C33-C35
26	a	601	9YF	C32-C33-C35-C36
26	l	201	9YF	C31-C32-C33-C35
16	d	608	7PH	C39-C3A-C3B-C3C
15	F	202	CDL	C72-C73-C74-C75
16	e	302	7PH	C2B-C2C-C2D-C2E
15	b	801	CDL	C56-C57-C58-C59
16	F	207	7PH	C1-O11-P-O13
16	G	403	7PH	C1-O11-P-O13
16	D	609	7PH	C1-O11-P-O12
16	g	403	7PH	C1-O11-P-O13
26	L	201	9YF	C30-C31-C32-C33
16	d	608	7PH	C32-C31-O31-C3
15	D	606	CDL	C19-C20-C21-C22
17	f	206	TRD	C11-C10-C9-C8
19	H	203	TWT	C13-C14-C15-C16
16	d	610	7PH	C31-C32-C33-C34
15	B	607	CDL	C51-C52-C53-C54
16	D	608	7PH	C28-C29-C2A-C2B
17	A	502	TRD	C6-C7-C8-C9
17	A	503	TRD	C5-C6-C7-C8
18	H	202	9XX	C6-C7-C8-C9
18	H	202	9XX	C24-C25-C26-C27
16	d	609	7PH	C22-C23-C24-C25
17	F	206	TRD	C7-C8-C9-C10
16	h	201	7PH	C3-C2-O21-C21
16	D	608	7PH	C32-C33-C34-C35
17	B	606	TRD	C4-C5-C6-C7
26	L	201	9YF	C17-C18-C19-C20
26	l	201	9YF	C40-C41-C42-C43
25	B	603	MQ9	C12-C11-C9-C10
17	E	303	TRD	C5-C6-C7-C8
18	B	608	9XX	C12-C13-C14-C15
15	B	605	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
15	d	607	CDL	C1-CB2-OB2-PB2
16	D	609	7PH	C1-C2-C3-O31
15	D	601	CDL	OA9-CA7-OA8-CA6
15	D	601	CDL	OB5-CB3-CB4-OB6
15	e	301	CDL	OA5-CA3-CA4-OA6
16	D	607	7PH	O11-C1-C2-O21
16	D	608	7PH	O11-C1-C2-O21
26	a	601	9YF	O9-C-C1-O
26	L	201	9YF	C33-C35-C36-C37
15	B	607	CDL	C72-C73-C74-C75
16	F	207	7PH	C34-C35-C36-C37
28	b	802	HEM	C4B-C3B-CAB-CBB
15	C	301	CDL	C17-C18-C19-C20
16	f	207	7PH	C34-C35-C36-C37
17	f	201	TRD	C9-C10-C11-C12
26	l	201	9YF	C17-C18-C19-C20
16	D	608	7PH	O32-C31-O31-C3
15	D	606	CDL	OB6-CB4-CB6-OB8
15	B	605	CDL	OB6-CB4-CB6-OB8
15	B	607	CDL	OB6-CB4-CB6-OB8
15	e	301	CDL	OA6-CA4-CA6-OA8
16	H	201	7PH	O21-C2-C3-O31
15	E	301	CDL	C55-C56-C57-C58
17	f	206	TRD	C4-C5-C6-C7
27	x	101	PLM	C5-C6-C7-C8
26	a	601	9YF	C7-C2-O2-P
17	A	505	TRD	C7-C8-C9-C10
19	H	203	TWT	C14-C15-C16-C17
16	e	302	7PH	C26-C27-C28-C29
15	d	601	CDL	OB9-CB7-OB8-CB6
26	L	201	9YF	C31-C32-C33-C34
26	l	201	9YF	C31-C32-C33-C34
15	b	801	CDL	C54-C55-C56-C57
17	F	206	TRD	C3-C4-C5-C6
26	a	604	9YF	O12-C25-O11-C24
15	f	202	CDL	CB3-OB5-PB2-OB2
15	E	301	CDL	C75-C76-C77-C78
15	d	601	CDL	C21-C22-C23-C24
18	H	202	9XX	C5-C6-C7-C8
15	E	301	CDL	C1-CA2-OA2-PA1
15	F	202	CDL	C1-CA2-OA2-PA1
15	F	202	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
15	D	606	CDL	C1-CB2-OB2-PB2
15	e	301	CDL	C1-CB2-OB2-PB2
15	b	801	CDL	C1-CB2-OB2-PB2
16	d	610	7PH	C2-C1-O11-P
16	D	610	7PH	O32-C31-O31-C3
16	d	608	7PH	O32-C31-O31-C3
15	E	301	CDL	CA2-OA2-PA1-OA4
15	D	601	CDL	CA3-OA5-PA1-OA3
15	D	601	CDL	CA3-OA5-PA1-OA4
15	D	601	CDL	CB2-OB2-PB2-OB3
15	D	601	CDL	CB3-OB5-PB2-OB3
15	B	605	CDL	CB3-OB5-PB2-OB3
15	C	301	CDL	CB3-OB5-PB2-OB4
15	f	202	CDL	CA3-OA5-PA1-OA3
15	f	202	CDL	CA3-OA5-PA1-OA4
15	d	601	CDL	CA3-OA5-PA1-OA3
15	d	601	CDL	CB2-OB2-PB2-OB3
15	d	601	CDL	CB3-OB5-PB2-OB3
15	b	801	CDL	CB2-OB2-PB2-OB3
15	b	806	CDL	CA2-OA2-PA1-OA3
25	B	604	MQ9	C6-C7-C8-C9
16	G	403	7PH	C31-C32-C33-C34
26	a	604	9YF	C26-C25-O11-C24
15	D	601	CDL	OB5-CB3-CB4-CB6
16	D	607	7PH	O11-C1-C2-C3
15	c	301	CDL	C21-C22-C23-C24
15	d	601	CDL	C12-C13-C14-C15
22	D	602	HAS	O11-C11-C12-C13
16	g	403	7PH	C22-C23-C24-C25
15	E	301	CDL	C33-C34-C35-C36
16	D	609	7PH	C29-C2A-C2B-C2C
16	h	201	7PH	C27-C28-C29-C2A
16	G	403	7PH	C22-C23-C24-C25
17	e	303	TRD	C6-C7-C8-C9
26	l	201	9YF	C28-C29-C30-C31
16	D	607	7PH	C36-C37-C38-C39
16	E	302	7PH	C39-C3A-C3B-C3C
15	B	605	CDL	CA2-C1-CB2-OB2
16	D	608	7PH	C37-C38-C39-C3A
25	b	805	MQ9	C30-C29-C31-C32
15	E	301	CDL	OB5-CB3-CB4-OB6
15	f	202	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
15	d	601	CDL	OA5-CA3-CA4-OA6
16	H	201	7PH	O11-C1-C2-O21
16	D	609	7PH	O11-C1-C2-O21
16	d	610	7PH	O11-C1-C2-O21
22	D	603	HAS	C22-C23-C24-C28
22	d	603	HAS	O11-C11-C3B-C2B
29	C	303	HEC	C2A-CAA-CBA-CGA
15	d	601	CDL	C23-C24-C25-C26
16	D	607	7PH	C38-C39-C3A-C3B
26	a	604	9YF	C39-C40-C41-C42
17	f	205	TRD	C7-C8-C9-C10
15	f	202	CDL	C12-C11-CA5-OA6
17	f	201	TRD	C3-C4-C5-C6
18	h	204	9XX	C9-C10-C11-C12
18	H	202	9XX	C23-C24-C25-C26
26	l	201	9YF	C33-C35-C36-C37
15	B	605	CDL	C71-C72-C73-C74
15	e	301	CDL	C71-C72-C73-C74
16	e	302	7PH	C39-C3A-C3B-C3C
16	h	201	7PH	C2B-C2C-C2D-C2E
15	B	607	CDL	CA3-CA4-CA6-OA8
16	d	609	7PH	C29-C2A-C2B-C2C
22	D	602	HAS	O11-C11-C3B-C4B
22	D	603	HAS	O11-C11-C3B-C4B
22	d	604	HAS	C1D-C2D-CMD-OMD
27	L	202	PLM	C1-C2-C3-C4
15	B	605	CDL	OA6-CA4-CA6-OA8
15	C	301	CDL	OA6-CA4-CA6-OA8
15	b	806	CDL	OB6-CB4-CB6-OB8
15	c	301	CDL	OA6-CA4-CA6-OA8
15	F	202	CDL	C57-C58-C59-C60
15	B	605	CDL	C14-C15-C16-C17
15	B	607	CDL	C12-C13-C14-C15
26	a	601	9YF	C16-C17-C18-C19
15	D	606	CDL	C59-C60-C61-C62
15	B	607	CDL	C71-C72-C73-C74
15	c	301	CDL	C52-C53-C54-C55
16	D	609	7PH	C24-C25-C26-C27
17	B	606	TRD	C5-C6-C7-C8
16	d	609	7PH	C25-C26-C27-C28
16	h	201	7PH	C2A-C2B-C2C-C2D
15	f	202	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	D	607	7PH	C23-C24-C25-C26
16	D	608	7PH	C25-C26-C27-C28
16	E	302	7PH	C2B-C2C-C2D-C2E
16	h	201	7PH	C24-C25-C26-C27
17	f	205	TRD	C5-C6-C7-C8
17	A	502	TRD	C2-C3-C4-C5
16	g	403	7PH	C31-C32-C33-C34
16	D	608	7PH	C27-C28-C29-C2A
25	B	604	MQ9	C38-C39-C41-C42
16	E	302	7PH	C29-C2A-C2B-C2C
25	B	603	MQ9	C1-C6-C7-C8
25	b	804	MQ9	C1-C6-C7-C8
16	d	608	7PH	C38-C39-C3A-C3B
15	E	301	CDL	C52-C51-CB5-OB6
16	D	607	7PH	O31-C31-C32-C33
17	f	206	TRD	C1-C2-C3-C4
19	H	203	TWT	C6-C7-C8-C9
19	H	203	TWT	C10-C11-C12-C13
19	h	203	TWT	C16-C17-C18-C19
16	H	201	7PH	C1-C2-O21-C21
16	D	609	7PH	C3-C2-O21-C21
16	e	302	7PH	C3-C2-O21-C21
15	f	202	CDL	OB5-CB3-CB4-CB6
16	d	610	7PH	O11-C1-C2-C3
26	a	604	9YF	C24-C-C1-O
16	D	610	7PH	C32-C31-O31-C3
22	D	603	HAS	C11-C12-C13-C14
15	b	806	CDL	C35-C36-C37-C38
15	e	301	CDL	C77-C78-C79-C80
16	D	609	7PH	C1-O11-P-O14
16	h	201	7PH	C22-C23-C24-C25
15	f	202	CDL	C31-CA7-OA8-CA6
15	b	801	CDL	C53-C54-C55-C56
16	d	608	7PH	C37-C38-C39-C3A
15	b	806	CDL	OA6-CA4-CA6-OA8
15	c	301	CDL	OB6-CB4-CB6-OB8
16	h	201	7PH	O21-C2-C3-O31
15	e	301	CDL	C54-C55-C56-C57
15	F	202	CDL	CB2-OB2-PB2-OB5
15	C	301	CDL	CA2-OA2-PA1-OA5
15	C	301	CDL	CA3-OA5-PA1-OA2
15	e	301	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
15	d	607	CDL	CA2-OA2-PA1-OA5
26	L	201	9YF	C1-O-P-O2
26	l	201	9YF	C1-O-P-O2
16	d	610	7PH	C21-C22-C23-C24
27	L	202	PLM	C5-C6-C7-C8
15	f	202	CDL	C57-C58-C59-C60
15	C	301	CDL	CA3-CA4-CA6-OA8
27	d	611	PLM	C5-C6-C7-C8
26	a	604	9YF	C2-O2-P-O
16	D	608	7PH	C23-C24-C25-C26
17	E	303	TRD	C9-C10-C11-C12
15	c	301	CDL	C15-C16-C17-C18
15	c	301	CDL	C1-CA2-OA2-PA1
16	d	609	7PH	O21-C21-C22-C23
15	f	202	CDL	C72-C73-C74-C75
22	D	602	HAS	C16-C17-C18-C19
17	F	206	TRD	C4-C5-C6-C7
15	B	605	CDL	C56-C57-C58-C59
17	F	201	TRD	C11-C10-C9-C8
16	d	609	7PH	C2-C3-O31-C31
15	d	601	CDL	C54-C55-C56-C57
15	e	301	CDL	OB5-CB3-CB4-CB6
17	e	303	TRD	C9-C10-C11-C12
16	D	610	7PH	C34-C35-C36-C37
15	b	806	CDL	C58-C59-C60-C61
15	F	202	CDL	C12-C11-CA5-OA6
26	L	201	9YF	C27-C28-C29-C30
27	x	101	PLM	C2-C3-C4-C5
29	c	303	HEC	CAD-CBD-CGD-O2D
16	H	201	7PH	C29-C2A-C2B-C2C
18	h	204	9XX	C12-C13-C14-C15
28	b	802	HEM	CAA-CBA-CGA-O1A
15	B	607	CDL	C53-C54-C55-C56
16	D	607	7PH	C26-C27-C28-C29
17	F	205	TRD	C5-C6-C7-C8
15	F	202	CDL	CB5-C51-C52-C53
17	f	203	TRD	C6-C7-C8-C9
26	L	201	9YF	C11-C12-C13-C14
15	D	601	CDL	C11-C12-C13-C14
16	D	607	7PH	C34-C35-C36-C37
19	h	203	TWT	C15-C16-C17-C18
26	L	201	9YF	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
15	F	202	CDL	O1-C1-CA2-OA2
17	a	605	TRD	C3-C4-C5-C6
22	d	604	HAS	CAD-CBD-CGD-O1D
29	c	303	HEC	CAD-CBD-CGD-O1D
15	F	202	CDL	C31-C32-C33-C34
15	c	301	CDL	C78-C79-C80-C81
15	C	301	CDL	CA6-CA4-OA6-CA5
15	d	607	CDL	C77-C78-C79-C80
26	a	604	9YF	C19-C20-C21-C22
15	d	607	CDL	CA4-CA3-OA5-PA1
15	c	301	CDL	C1-CB2-OB2-PB2
18	B	608	9XX	C18-C19-C20-C21
15	D	606	CDL	OA5-CA3-CA4-OA6
15	d	607	CDL	OB5-CB3-CB4-OB6
22	D	602	HAS	CAD-CBD-CGD-O1D
16	F	207	7PH	O11-C1-C2-C3
16	f	207	7PH	O11-C1-C2-C3
28	b	802	HEM	CAA-CBA-CGA-O2A
15	D	606	CDL	C80-C81-C82-C83
18	B	608	9XX	C11-C10-C9-C8
22	d	604	HAS	CAD-CBD-CGD-O2D
27	L	202	PLM	C6-C7-C8-C9
15	f	202	CDL	OB6-CB4-CB6-OB8
15	d	607	CDL	OA6-CA4-CA6-OA8
15	f	202	CDL	C31-C32-C33-C34
15	d	601	CDL	C19-C20-C21-C22
26	a	604	9YF	C36-C37-C38-C39
25	B	604	MQ9	C21-C22-C23-C24
16	k	101	7PH	C36-C37-C38-C39
26	a	601	9YF	C11-C12-C13-C14
18	B	608	9XX	O6-C15-O-C16
25	b	804	MQ9	C9-C11-C12-C13
15	f	202	CDL	C54-C55-C56-C57
28	b	803	HEM	C2A-CAA-CBA-CGA
16	D	607	7PH	C33-C34-C35-C36
15	C	301	CDL	C23-C24-C25-C26
15	C	301	CDL	C31-C32-C33-C34
18	B	608	9XX	C22-C23-C24-C25
15	b	801	CDL	CA7-C31-C32-C33
28	B	602	HEM	CAA-CBA-CGA-O2A
15	B	607	CDL	C14-C15-C16-C17
25	a	602	MQ9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
16	k	101	7PH	C33-C34-C35-C36
16	k	101	7PH	C24-C25-C26-C27
17	F	204	TRD	C11-C10-C9-C8
22	D	602	HAS	CAD-CBD-CGD-O2D
22	d	603	HAS	CAD-CBD-CGD-O2D
16	G	403	7PH	C2A-C2B-C2C-C2D
16	g	403	7PH	C25-C26-C27-C28
15	c	301	CDL	OA5-CA3-CA4-OA6
22	d	603	HAS	CAD-CBD-CGD-O1D
18	h	202	9XX	C5-C6-C7-C8
18	B	608	9XX	C14-C15-O-C16
15	D	606	CDL	C52-C51-CB5-OB6
15	b	801	CDL	C74-C75-C76-C77
18	H	202	9XX	C25-C26-C27-C28
16	D	607	7PH	C35-C36-C37-C38
15	F	202	CDL	OB6-CB4-CB6-OB8
15	D	601	CDL	OA6-CA4-CA6-OA8
15	D	601	CDL	C79-C80-C81-C82
16	h	201	7PH	C29-C2A-C2B-C2C
17	E	303	TRD	C6-C7-C8-C9
16	D	610	7PH	C24-C25-C26-C27
18	h	202	9XX	C23-C24-C25-C26
17	F	201	TRD	C5-C6-C7-C8
29	C	302	HEC	CAD-CBD-CGD-O1D
15	b	806	CDL	C34-C35-C36-C37
16	H	201	7PH	C1-O11-P-O12
16	F	207	7PH	C1-O11-P-O12
16	f	207	7PH	C1-O11-P-O12
16	d	609	7PH	C1-O11-P-O13
17	F	205	TRD	C4-C5-C6-C7
22	D	603	HAS	C26-C15-C16-C17
29	c	302	HEC	CAD-CBD-CGD-O1D
29	c	303	HEC	CAA-CBA-CGA-O1A
15	c	301	CDL	C18-C19-C20-C21
15	E	301	CDL	C12-C11-CA5-OA6
15	E	301	CDL	C54-C55-C56-C57
15	b	801	CDL	C80-C81-C82-C83
16	d	608	7PH	O21-C21-C22-C23
15	B	605	CDL	C32-C33-C34-C35
15	e	301	CDL	C73-C74-C75-C76
16	D	610	7PH	C36-C37-C38-C39
15	D	601	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
16	F	207	7PH	C39-C3A-C3B-C3C
15	E	301	CDL	C57-C58-C59-C60
15	b	801	CDL	C19-C20-C21-C22
16	E	302	7PH	C31-C32-C33-C34
15	B	605	CDL	C72-C71-CB7-OB8
25	b	805	MQ9	C12-C11-C9-C10
22	D	603	HAS	CAD-CBD-CGD-O2D
15	D	606	CDL	C12-C11-CA5-OA6
15	d	601	CDL	C12-C11-CA5-OA6
16	e	302	7PH	O21-C21-C22-C23
17	A	505	TRD	C2-C3-C4-C5
15	C	301	CDL	CB3-CB4-CB6-OB8
15	c	301	CDL	CA3-CA4-CA6-OA8
22	D	603	HAS	CAD-CBD-CGD-O1D
15	B	607	CDL	C55-C56-C57-C58
15	e	301	CDL	C34-C35-C36-C37
15	D	606	CDL	OB5-CB3-CB4-OB6
15	B	607	CDL	OA5-CA3-CA4-OA6
15	C	301	CDL	OA5-CA3-CA4-OA6
16	D	609	7PH	O31-C31-C32-C33
17	f	204	TRD	C5-C6-C7-C8
29	C	302	HEC	CAD-CBD-CGD-O2D
16	D	608	7PH	C2A-C2B-C2C-C2D
17	F	203	TRD	C4-C5-C6-C7
16	d	609	7PH	C32-C33-C34-C35
28	B	602	HEM	CAA-CBA-CGA-O1A
29	C	302	HEC	CAA-CBA-CGA-O1A
29	C	302	HEC	CAA-CBA-CGA-O2A
29	c	302	HEC	CAA-CBA-CGA-O2A
29	c	302	HEC	CAD-CBD-CGD-O2D
18	B	608	9XX	C6-C7-C8-C9
15	C	301	CDL	O1-C1-CB2-OB2
19	h	203	TWT	C14-C15-C16-C17
15	B	607	CDL	OA5-CA3-CA4-CA6
22	D	603	HAS	CAA-CBA-CGA-O2A
29	c	302	HEC	CAA-CBA-CGA-O1A
16	e	302	7PH	C2-C3-O31-C31
26	a	601	9YF	O9-C8-C9-C10
15	D	606	CDL	OA6-CA4-CA6-OA8
15	d	601	CDL	OA6-CA4-CA6-OA8
16	d	608	7PH	O21-C2-C3-O31
15	B	605	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
26	L	201	9YF	C18-C19-C20-C21
15	b	801	CDL	C72-C71-CB7-OB8
29	c	303	HEC	CAA-CBA-CGA-O2A
15	D	606	CDL	C51-CB5-OB6-CB4
15	e	301	CDL	C12-C11-CA5-OA6
17	F	201	TRD	C3-C4-C5-C6
26	a	601	9YF	C12-C13-C14-C15
18	B	608	9XX	C26-C27-C28-C29
25	a	602	MQ9	C18-C19-C21-C22
25	b	805	MQ9	C12-C11-C9-C8
16	D	607	7PH	C2-C1-O11-P
26	a	604	9YF	O11-C25-C26-C27
25	B	603	MQ9	C24-C26-C27-C28
25	B	604	MQ9	C19-C21-C22-C23
17	A	502	TRD	C7-C8-C9-C10
15	B	607	CDL	C72-C71-CB7-OB8
15	e	301	CDL	C55-C56-C57-C58
22	D	603	HAS	CAA-CBA-CGA-O1A
25	b	805	MQ9	C25-C24-C26-C27
19	h	203	TWT	C2-C3-C4-C5
15	E	301	CDL	C12-C11-CA5-OA7
16	e	302	7PH	O22-C21-C22-C23
15	F	202	CDL	CB2-C1-CA2-OA2
26	a	604	9YF	C16-C17-C18-C19
15	f	202	CDL	CB3-CB4-CB6-OB8
16	h	201	7PH	C39-C3A-C3B-C3C
16	d	609	7PH	C2A-C2B-C2C-C2D
17	A	503	TRD	C9-C10-C11-C12
15	D	606	CDL	C12-C11-CA5-OA7
15	B	605	CDL	C72-C71-CB7-OB9
16	G	403	7PH	O21-C21-C22-C23
16	g	403	7PH	O21-C21-C22-C23
16	D	609	7PH	C2-C1-O11-P
19	H	203	TWT	C15-C16-C17-C18
15	F	202	CDL	CB2-OB2-PB2-OB3
15	F	202	CDL	CB3-OB5-PB2-OB3
15	D	601	CDL	CB3-OB5-PB2-OB4
15	D	606	CDL	CA3-OA5-PA1-OA3
15	D	606	CDL	CB3-OB5-PB2-OB3
15	C	301	CDL	CA3-OA5-PA1-OA3
15	f	202	CDL	CA2-OA2-PA1-OA3
15	d	601	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
15	b	806	CDL	CB2-OB2-PB2-OB3
15	c	301	CDL	CA2-OA2-PA1-OA3
26	a	604	9YF	C1-O-P-O8
22	D	603	HAS	C20-C21-C22-C23
16	d	608	7PH	O22-C21-C22-C23
15	D	606	CDL	OA5-CA3-CA4-CA6
15	c	301	CDL	OA5-CA3-CA4-CA6
28	B	602	HEM	CAD-CBD-CGD-O2D
15	d	607	CDL	C52-C51-CB5-OB6
16	e	302	7PH	O31-C31-C32-C33
15	d	601	CDL	C12-C11-CA5-OA7
28	B	601	HEM	CAA-CBA-CGA-O1A
28	B	601	HEM	CAA-CBA-CGA-O2A
18	H	202	9XX	C13-C14-C15-O
26	a	601	9YF	C25-C26-C27-C28
25	B	604	MQ9	C31-C32-C33-C34
22	D	602	HAS	C3B-C11-C12-C13
15	b	801	CDL	C76-C77-C78-C79
18	H	202	9XX	C25-C26-C27-C36
18	B	608	9XX	C36-C27-C28-C29
29	C	303	HEC	CAA-CBA-CGA-O1A
26	a	601	9YF	O10-C8-C9-C10
16	d	609	7PH	C38-C39-C3A-C3B
28	b	802	HEM	CAD-CBD-CGD-O1D
16	e	302	7PH	C29-C2A-C2B-C2C
17	f	205	TRD	C1-C2-C3-C4
15	e	301	CDL	C52-C51-CB5-OB6
18	B	608	9XX	C13-C14-C15-O
18	B	608	9XX	O1-C18-C19-C20
15	D	601	CDL	C31-C32-C33-C34
15	B	605	CDL	C73-C74-C75-C76
15	b	801	CDL	C72-C71-CB7-OB9
16	D	607	7PH	C39-C3A-C3B-C3C
16	h	201	7PH	O11-C1-C2-O21
15	e	301	CDL	C12-C11-CA5-OA7
16	G	403	7PH	O22-C21-C22-C23
16	g	403	7PH	O22-C21-C22-C23
26	l	201	9YF	O12-C25-C26-C27
29	C	303	HEC	CAA-CBA-CGA-O2A
26	L	201	9YF	O11-C25-C26-C27
26	a	604	9YF	O9-C8-C9-C10
15	b	801	CDL	C52-C51-CB5-OB7

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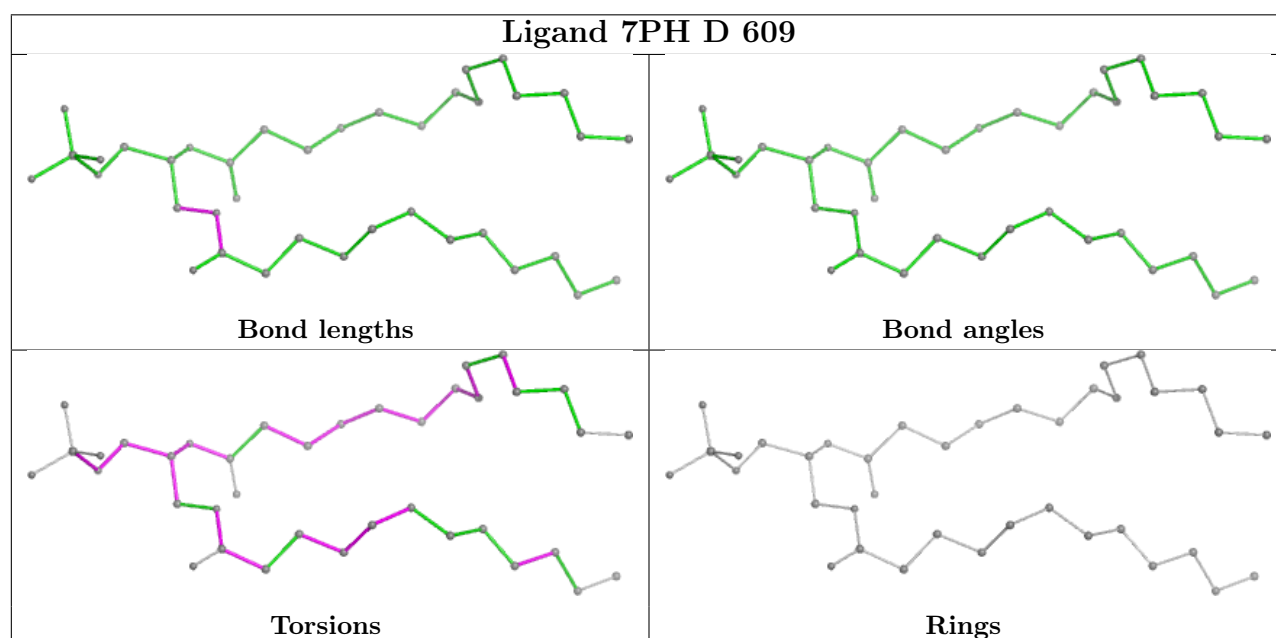
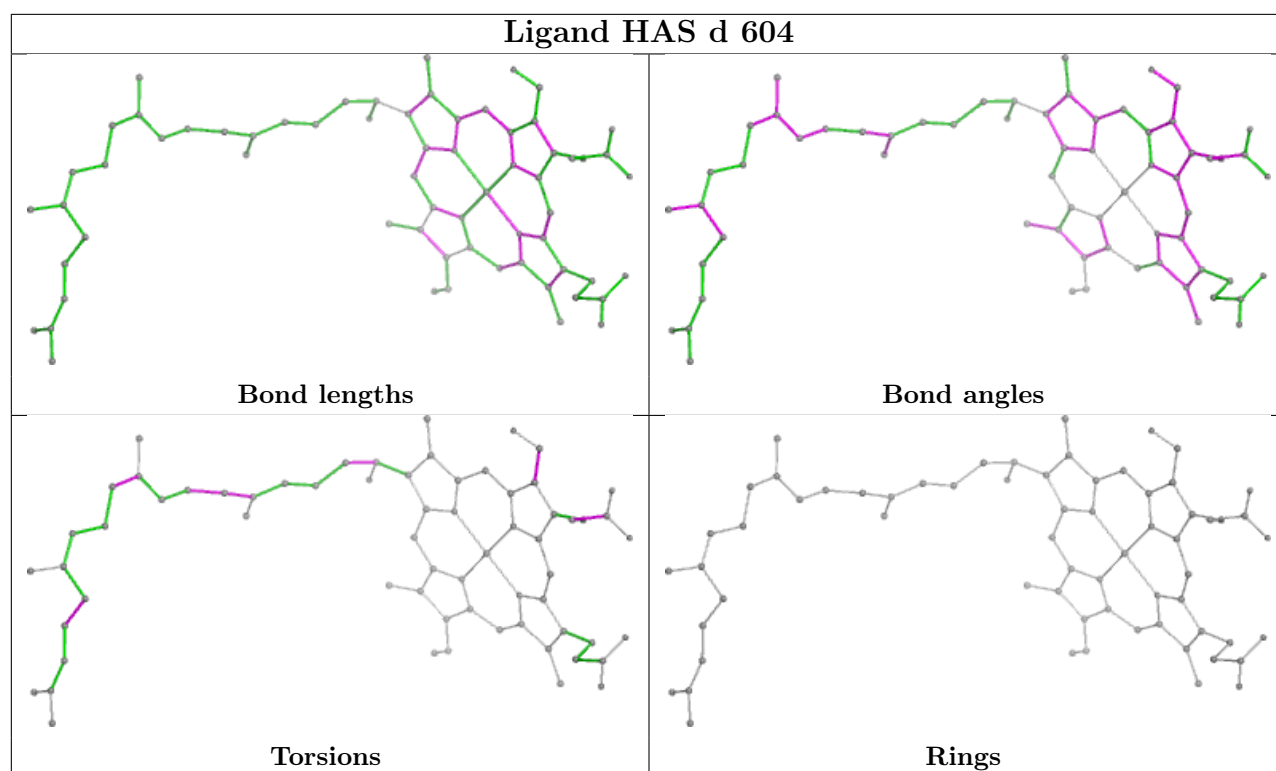
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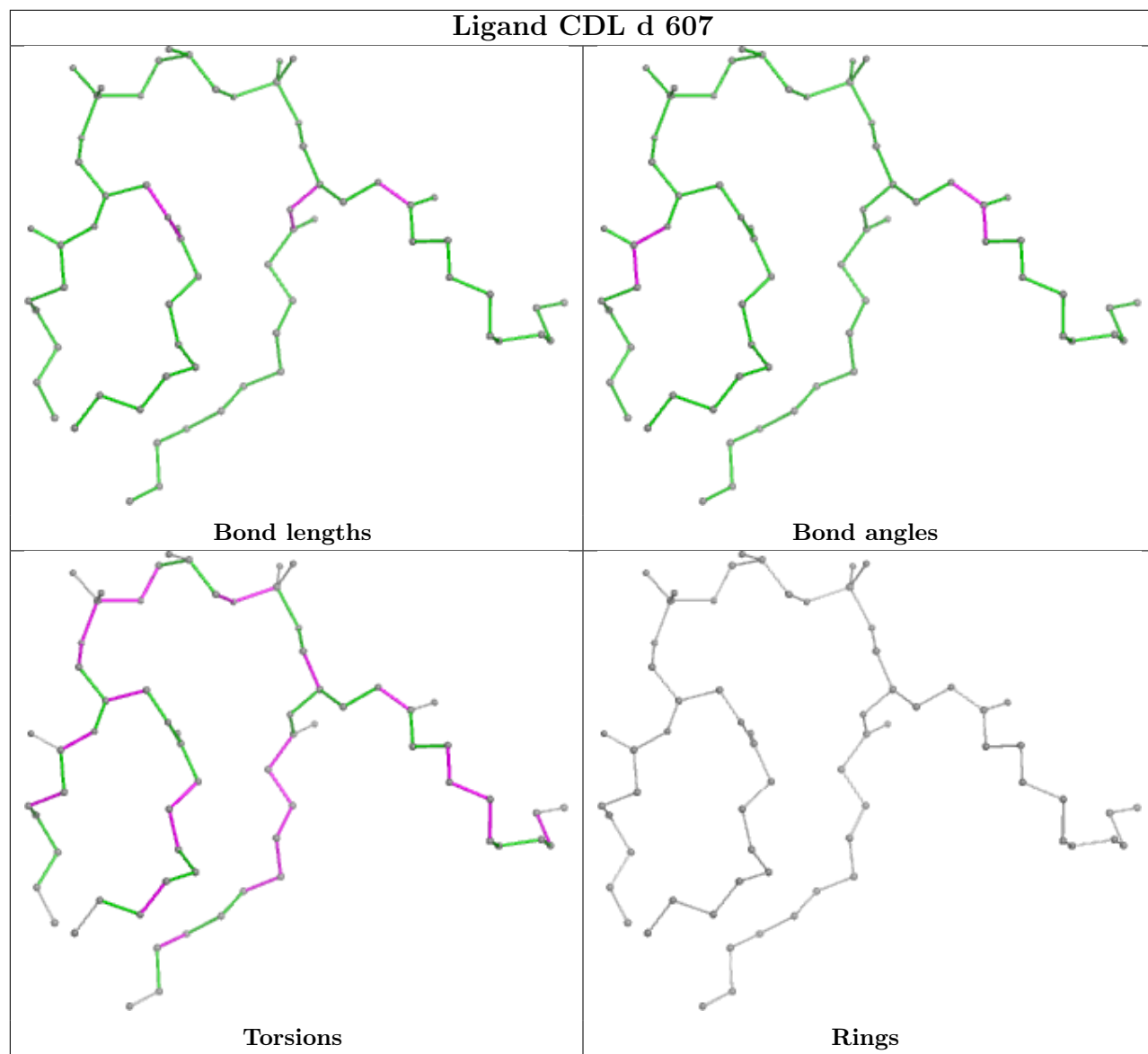
Mol	Chain	Res	Type	Atoms
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15	d	601	CDL	C52-C51-CB5-OB6
15	b	801	CDL	C52-C51-CB5-OB6
26	l	201	9YF	O11-C25-C26-C27
22	d	604	HAS	C15-C16-C17-C18
25	b	805	MQ9	C19-C21-C22-C23
15	B	605	CDL	C33-C34-C35-C36
15	C	301	CDL	C77-C78-C79-C80
15	F	202	CDL	C12-C13-C14-C15
15	D	601	CDL	C12-C11-CA5-OA6
15	b	801	CDL	C32-C31-CA7-OA8
28	b	803	HEM	CAA-CBA-CGA-O1A
15	D	601	CDL	C12-C13-C14-C15
16	f	207	7PH	C39-C3A-C3B-C3C
26	L	201	9YF	O12-C25-C26-C27

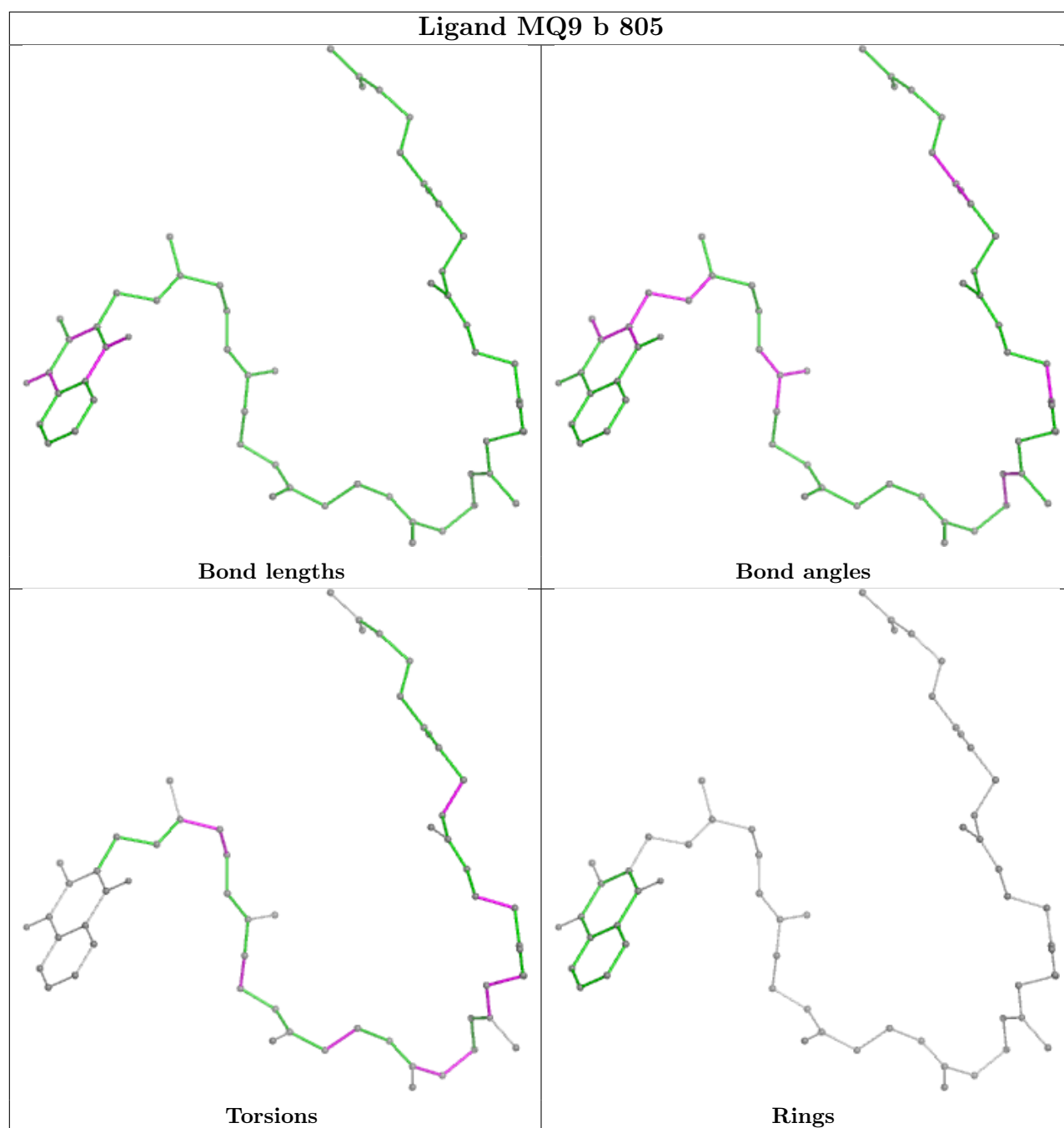
There are no ring outliers.

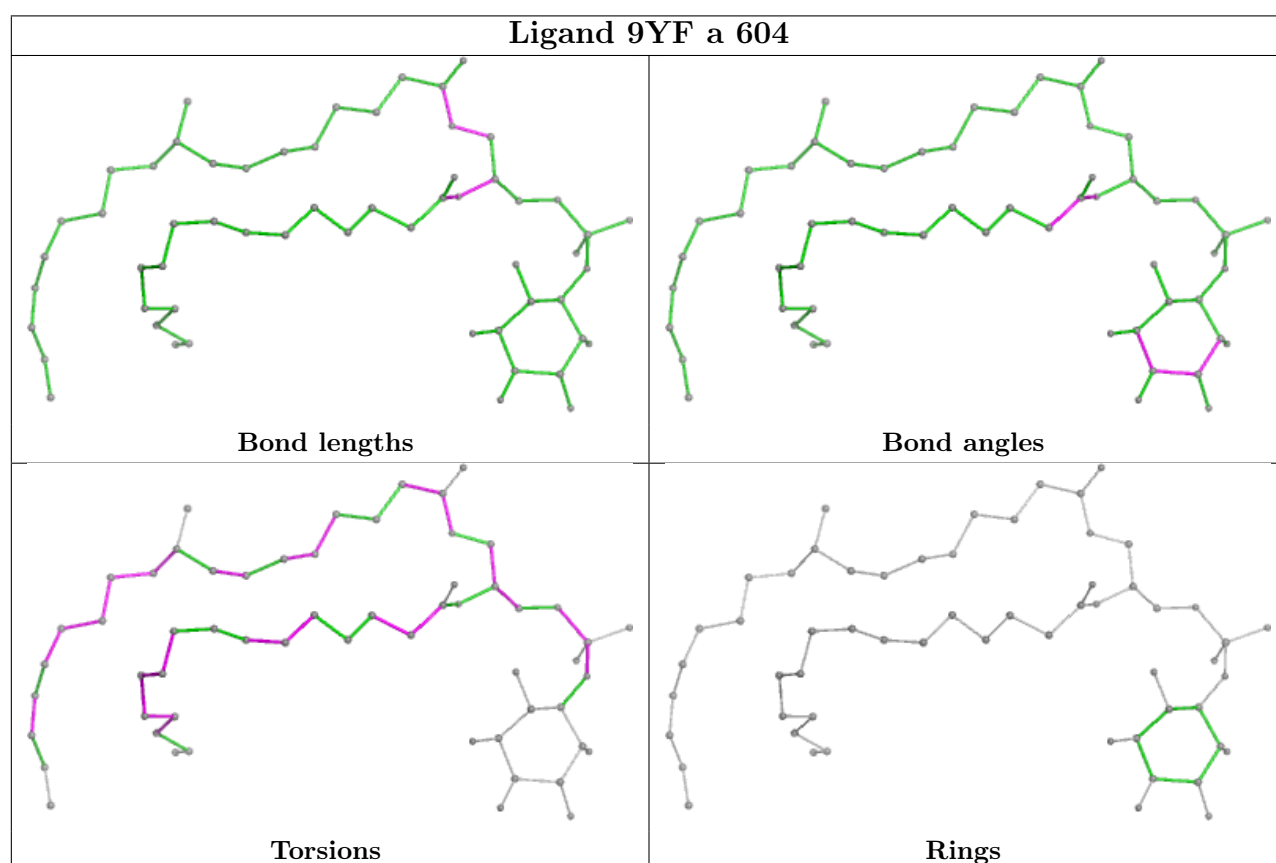
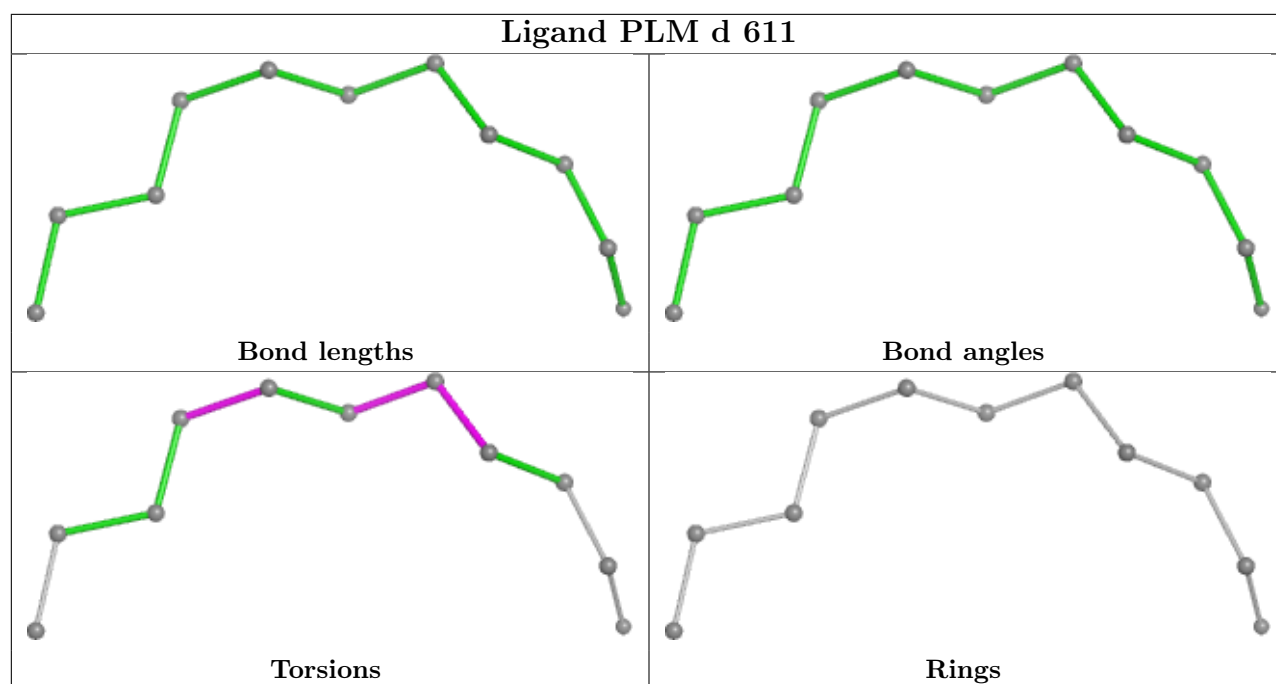
No monomer is involved in short contacts.

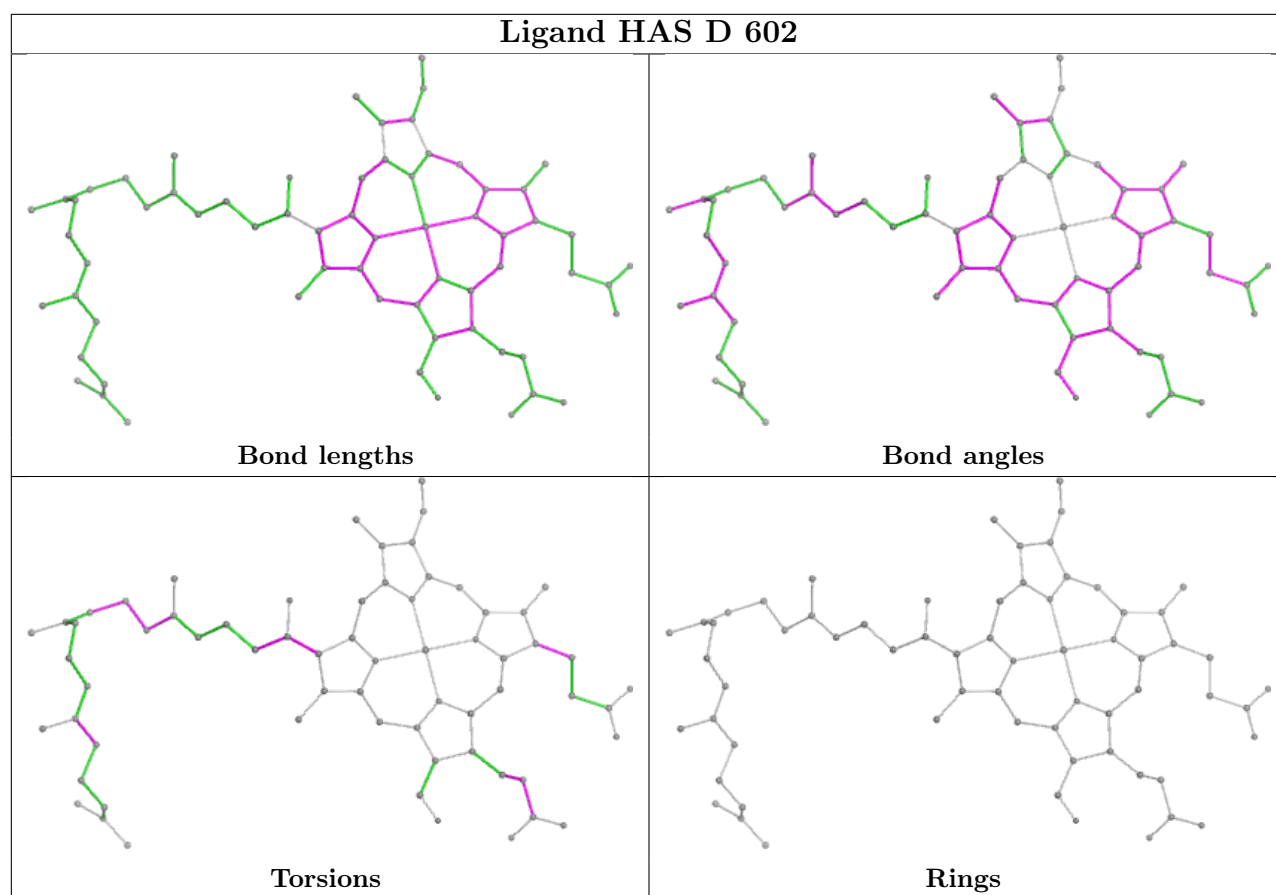
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



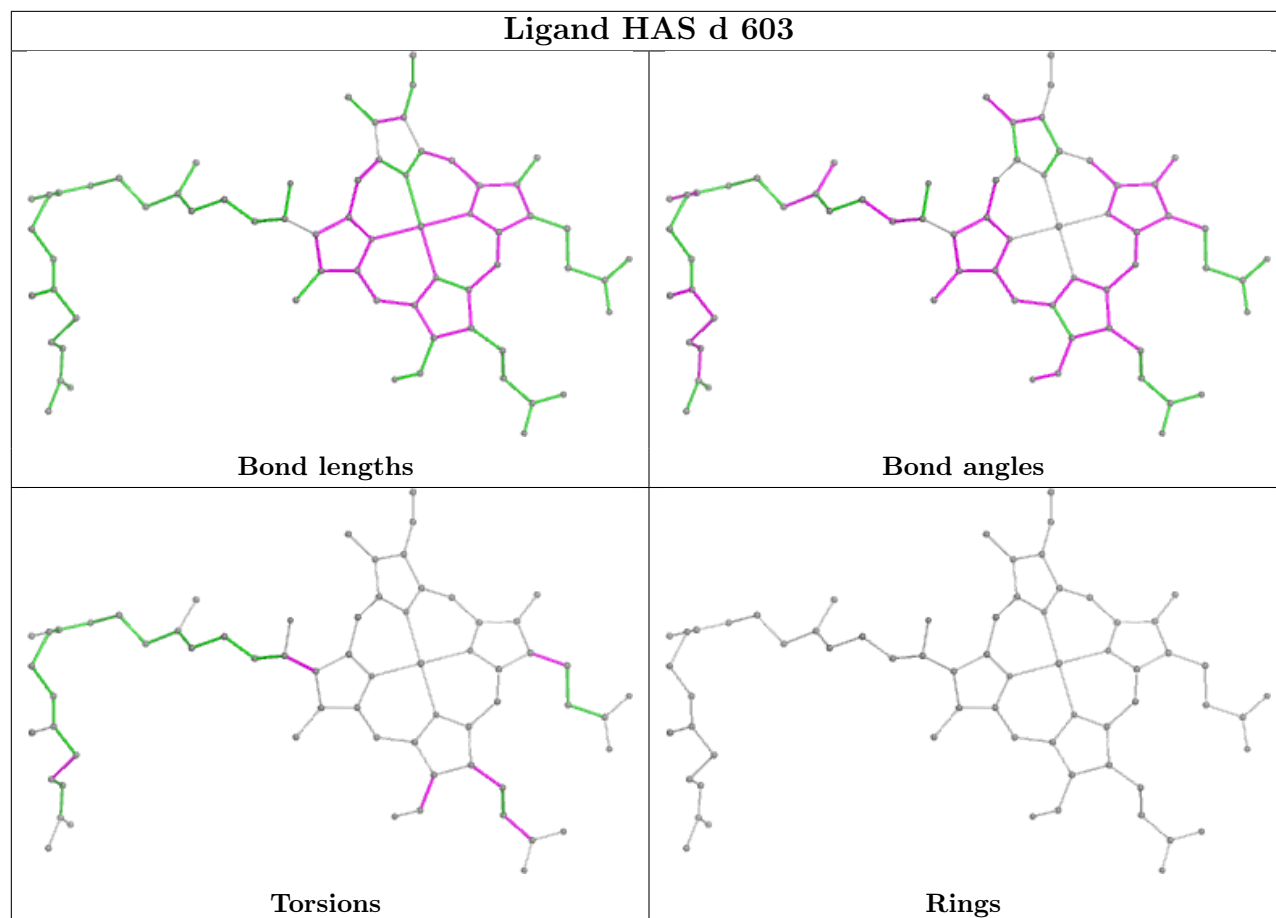




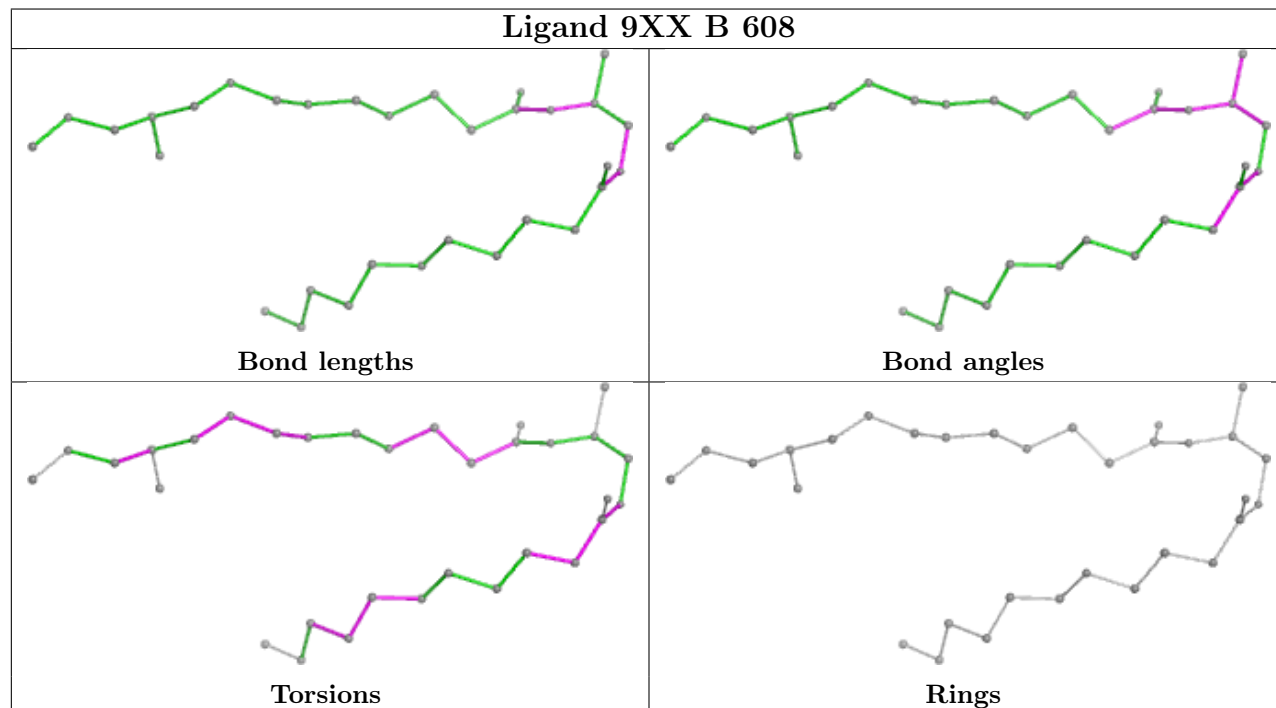


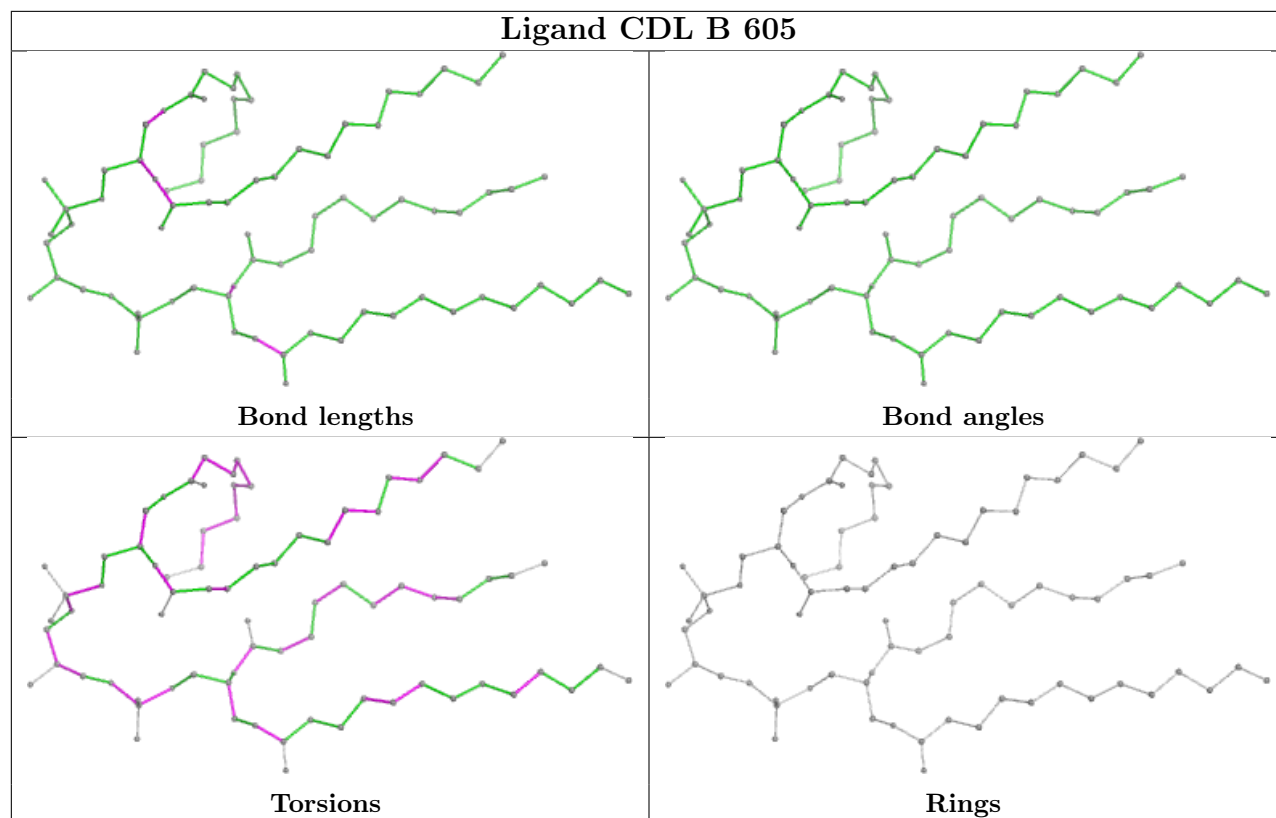


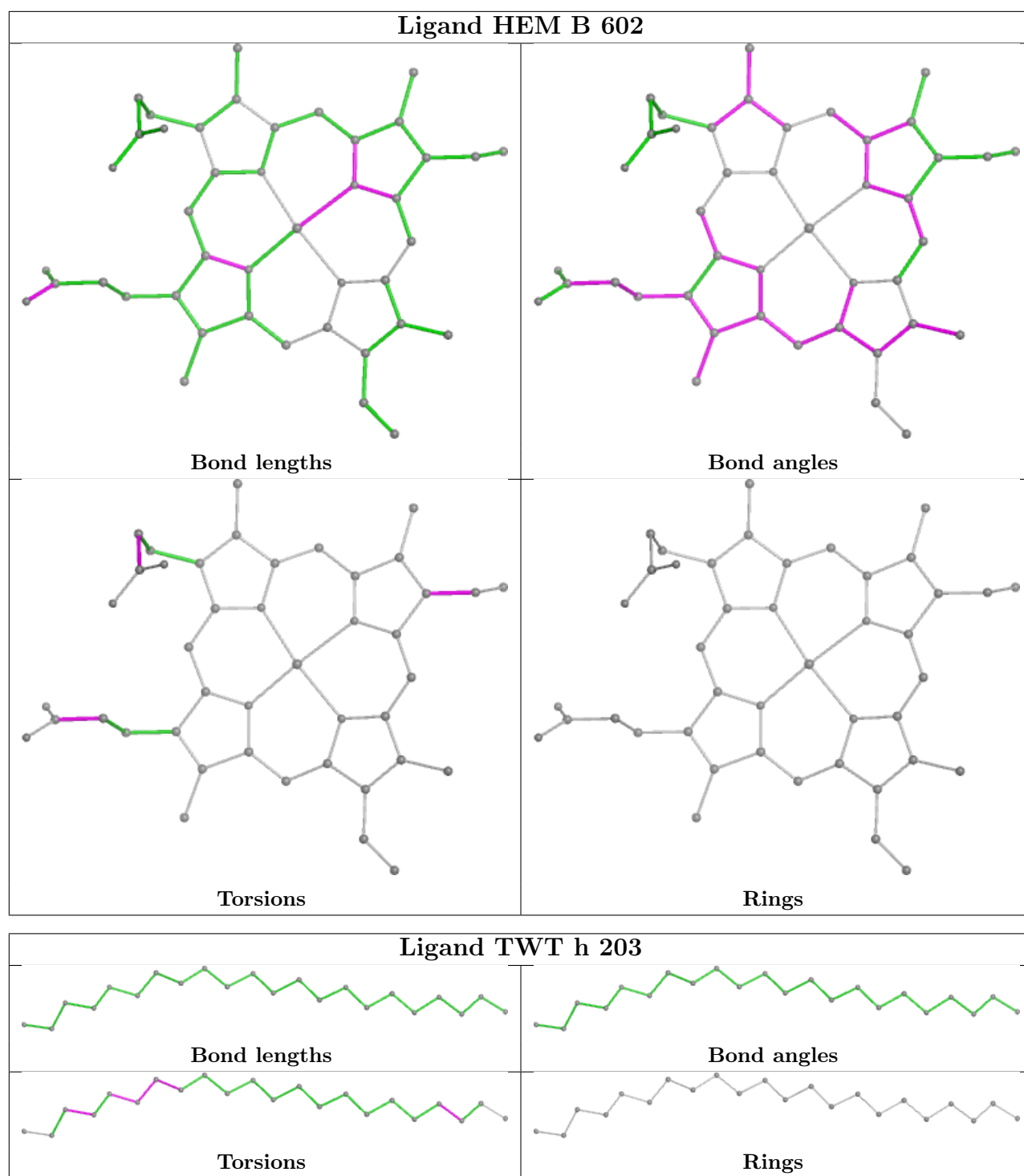
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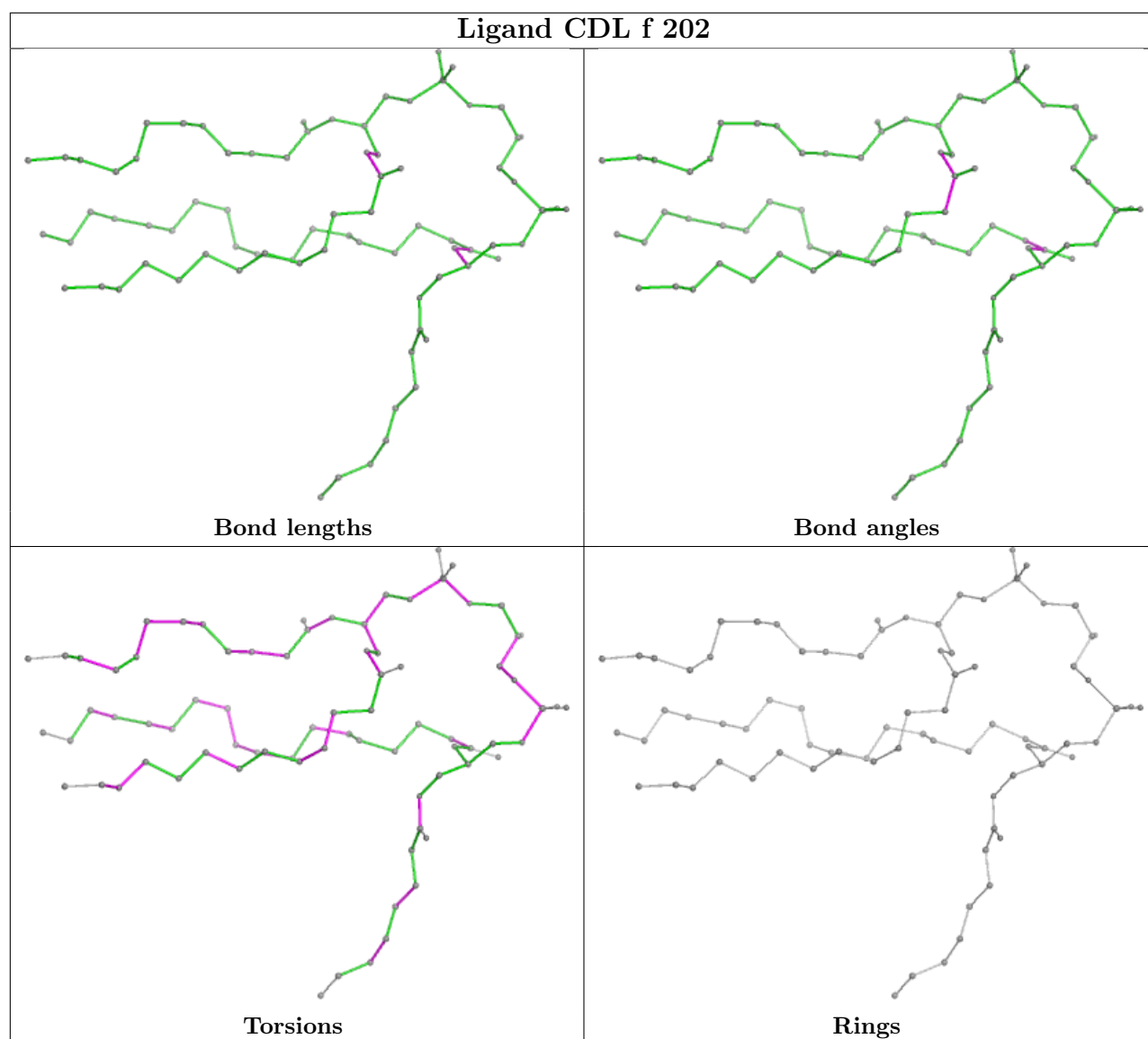


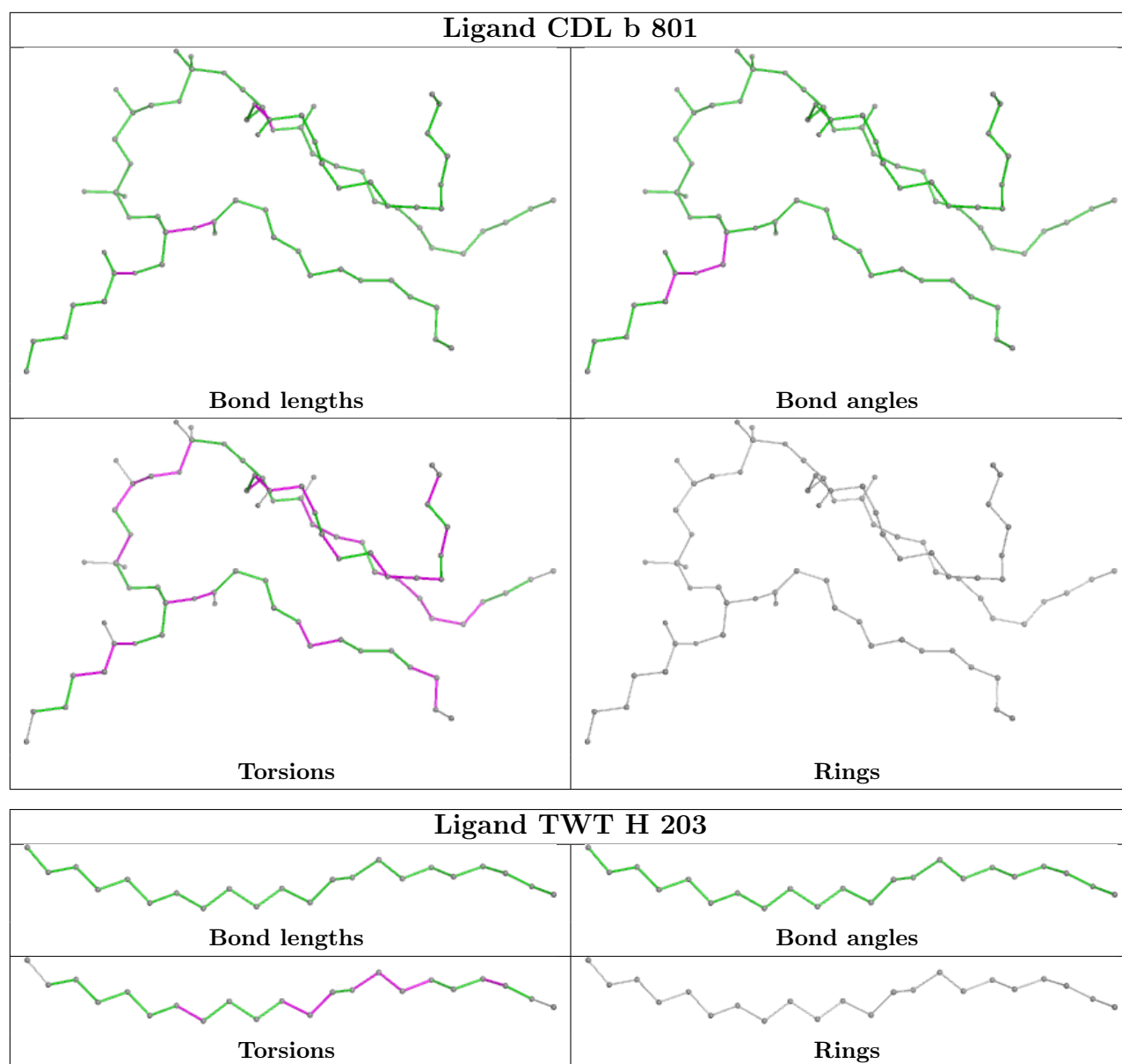
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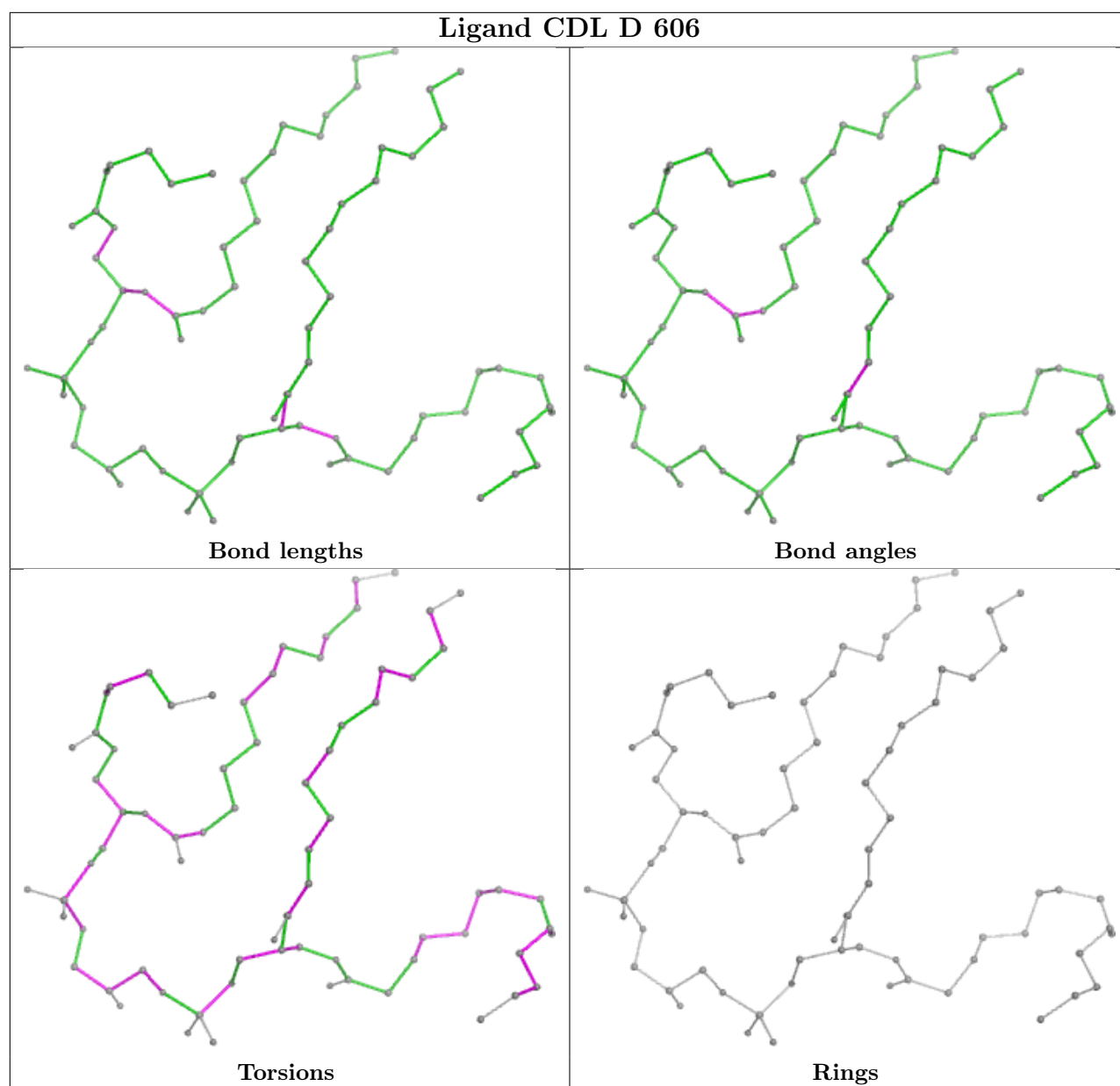


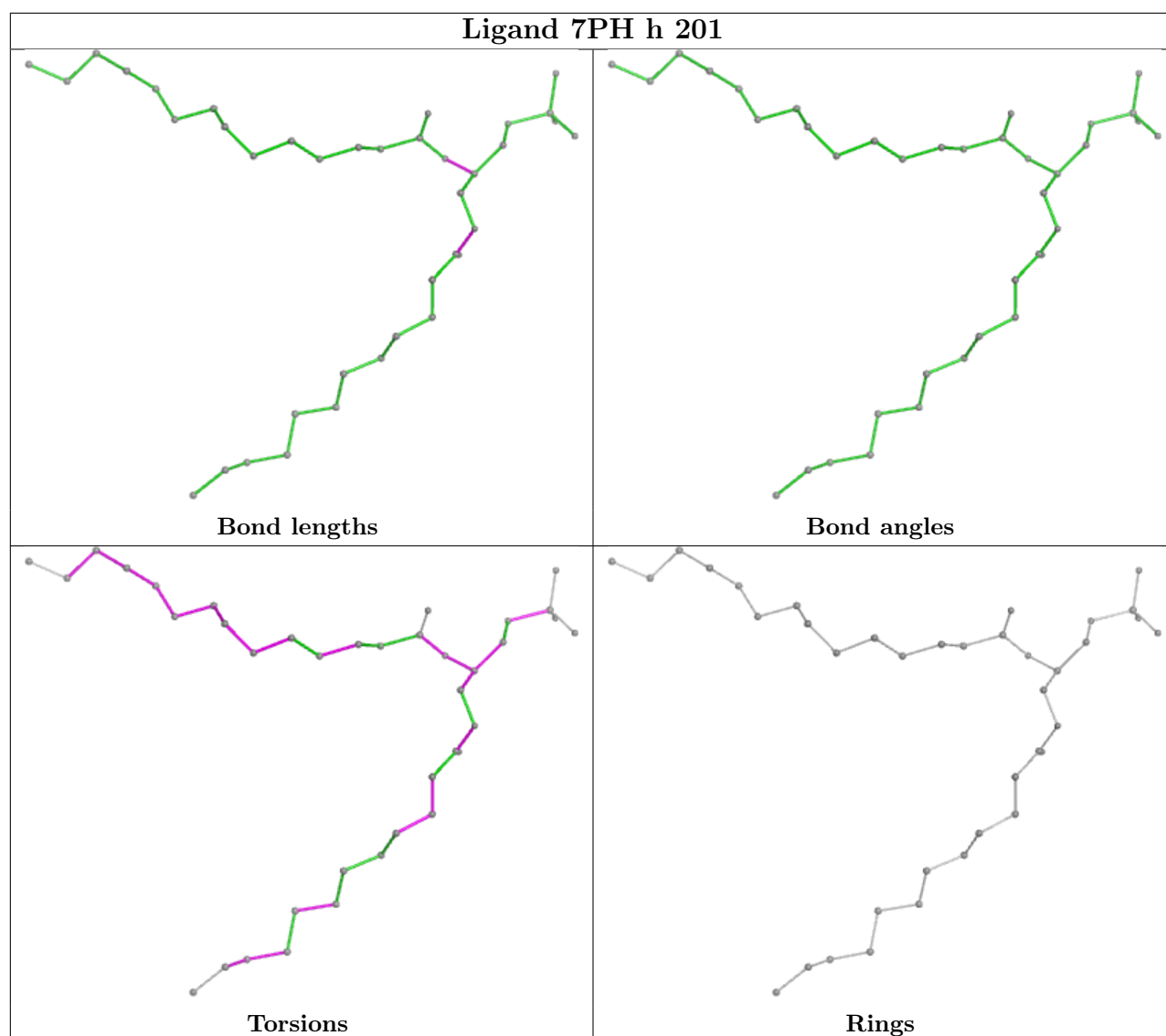


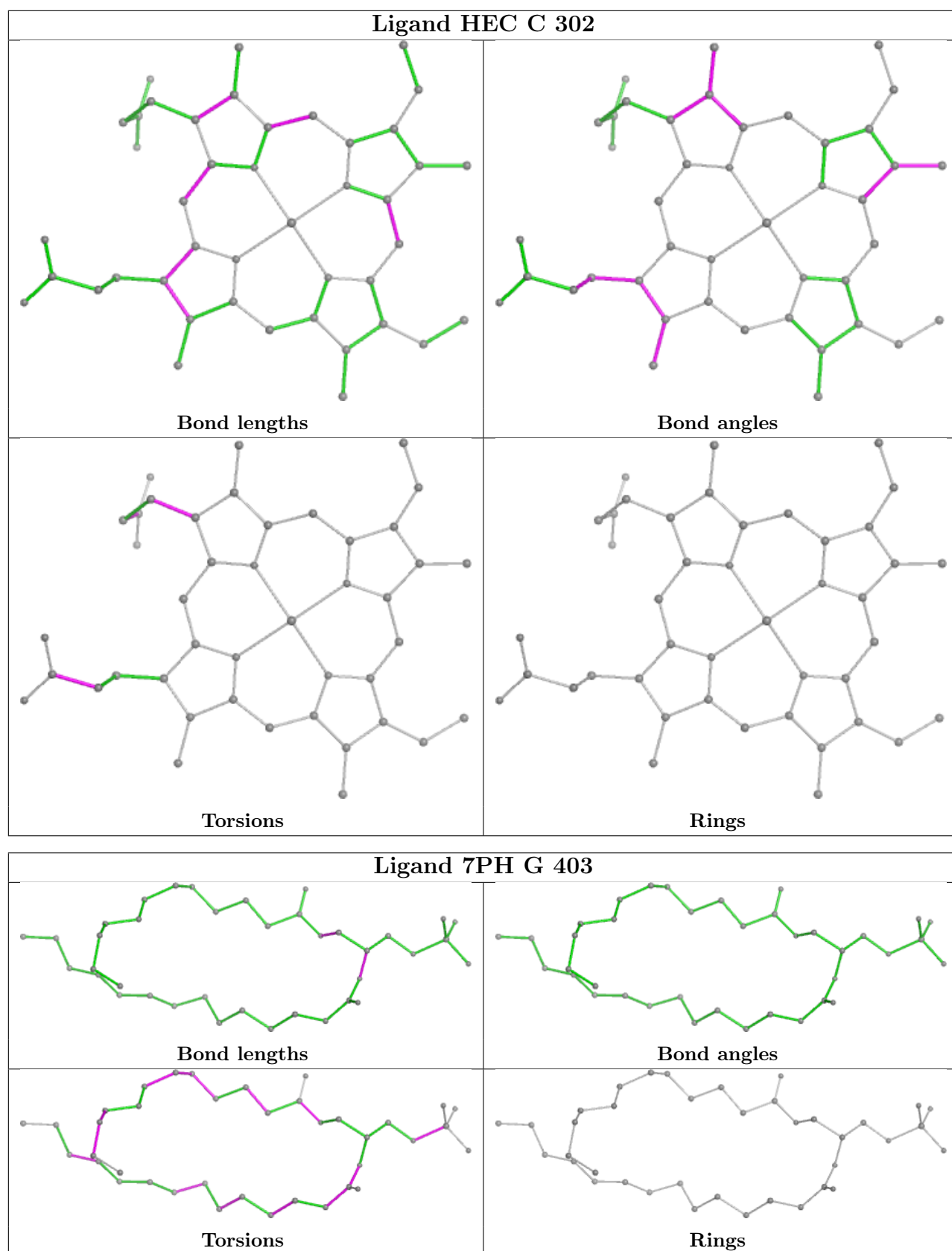


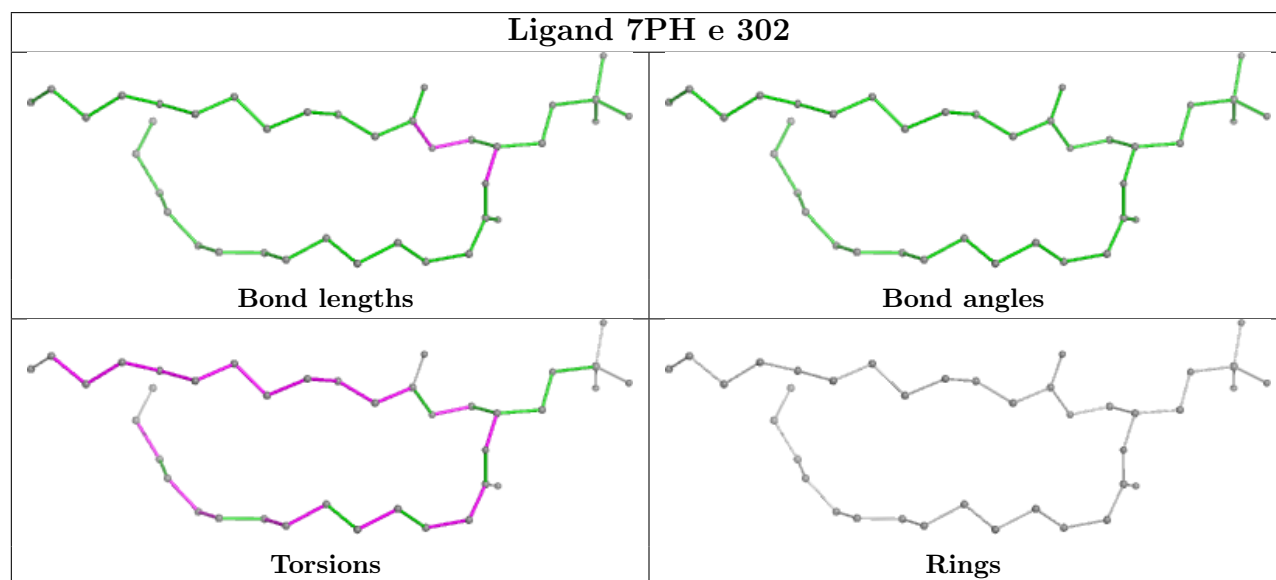
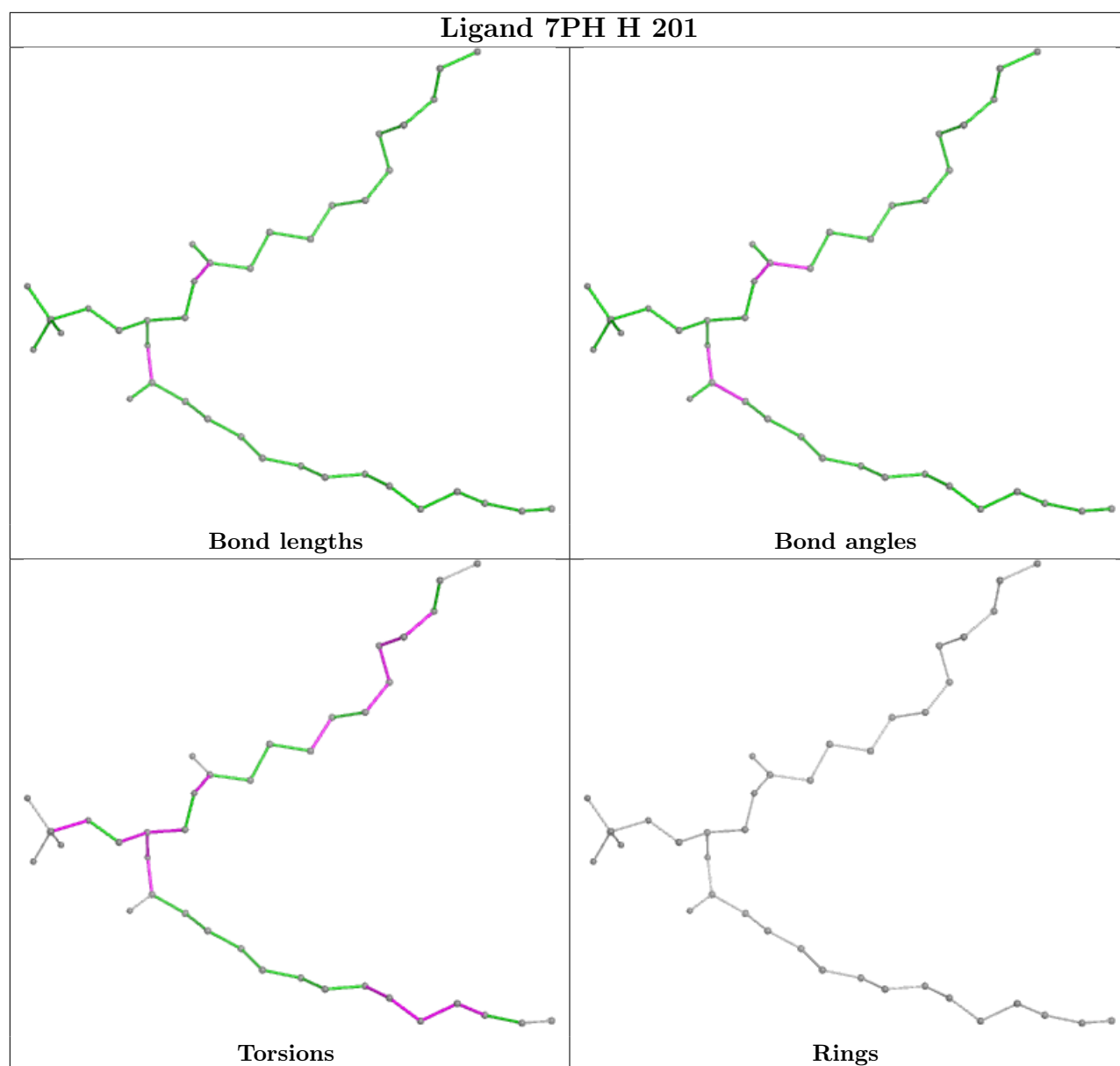


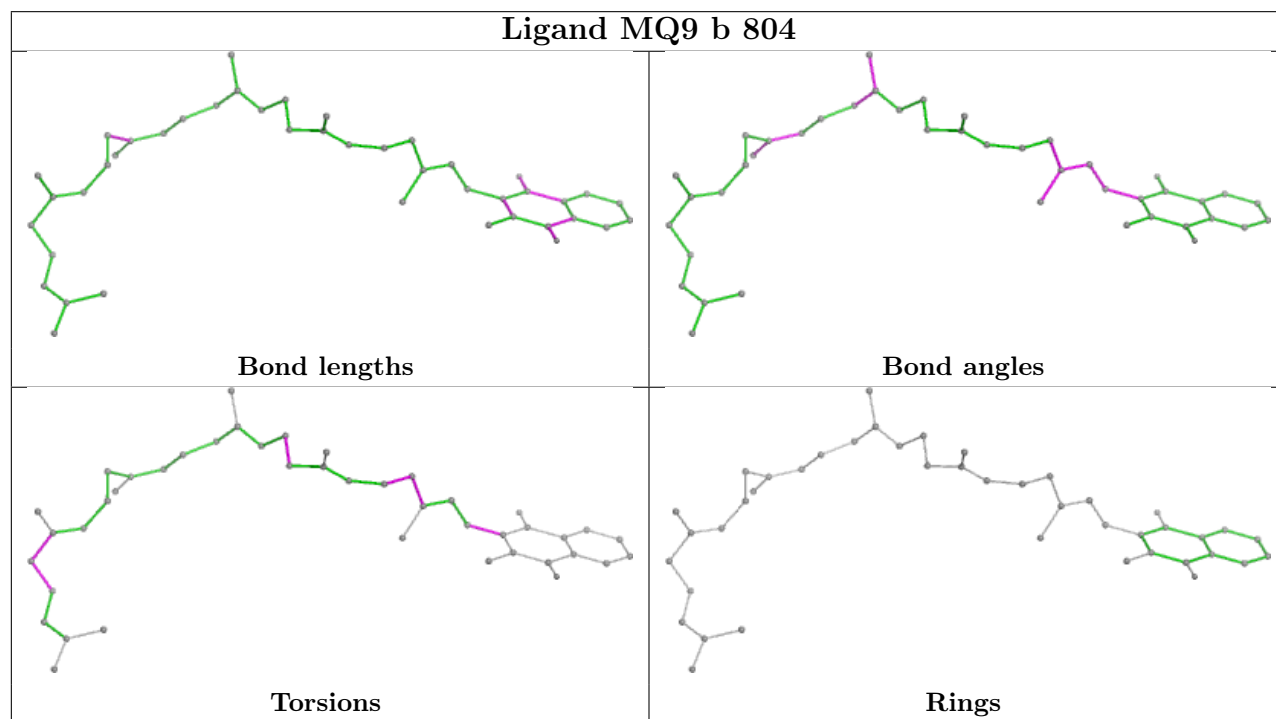
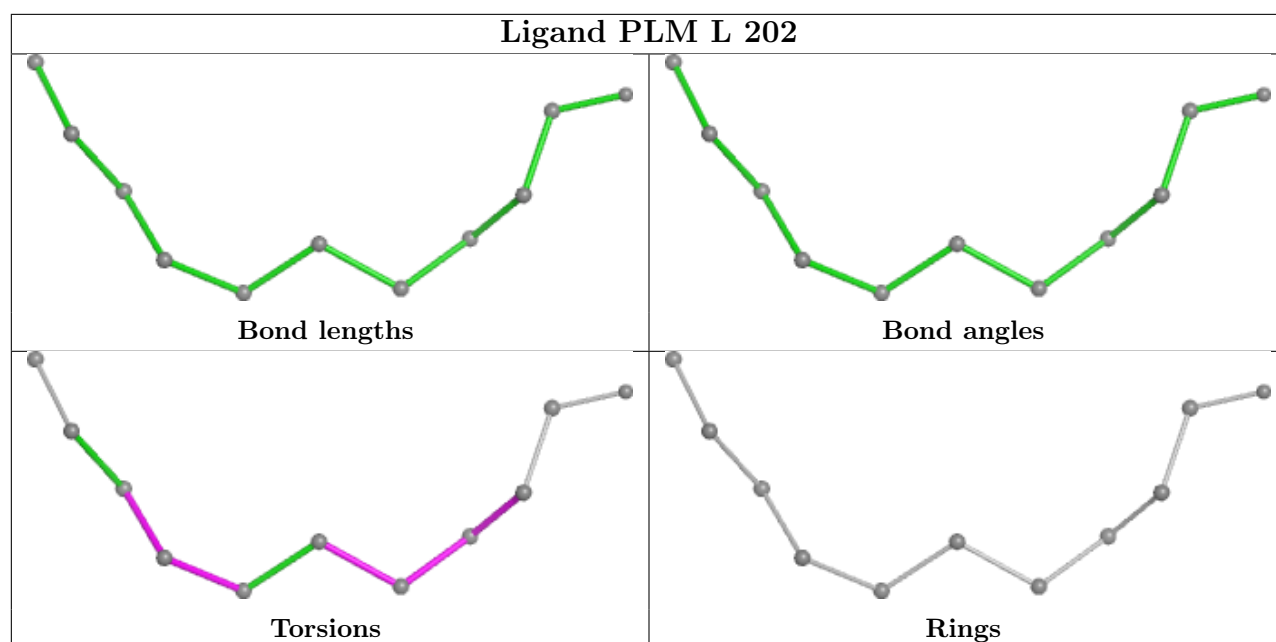


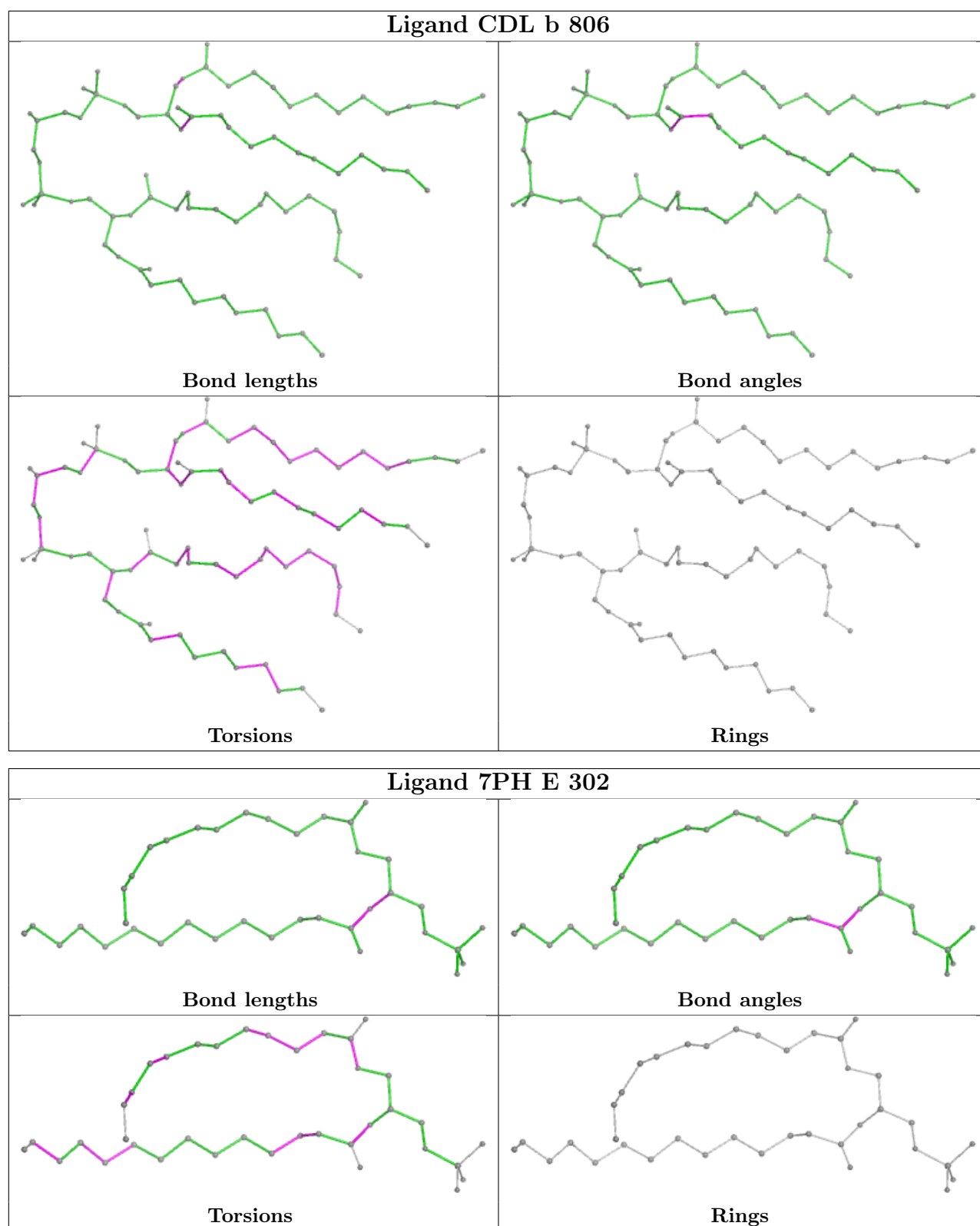


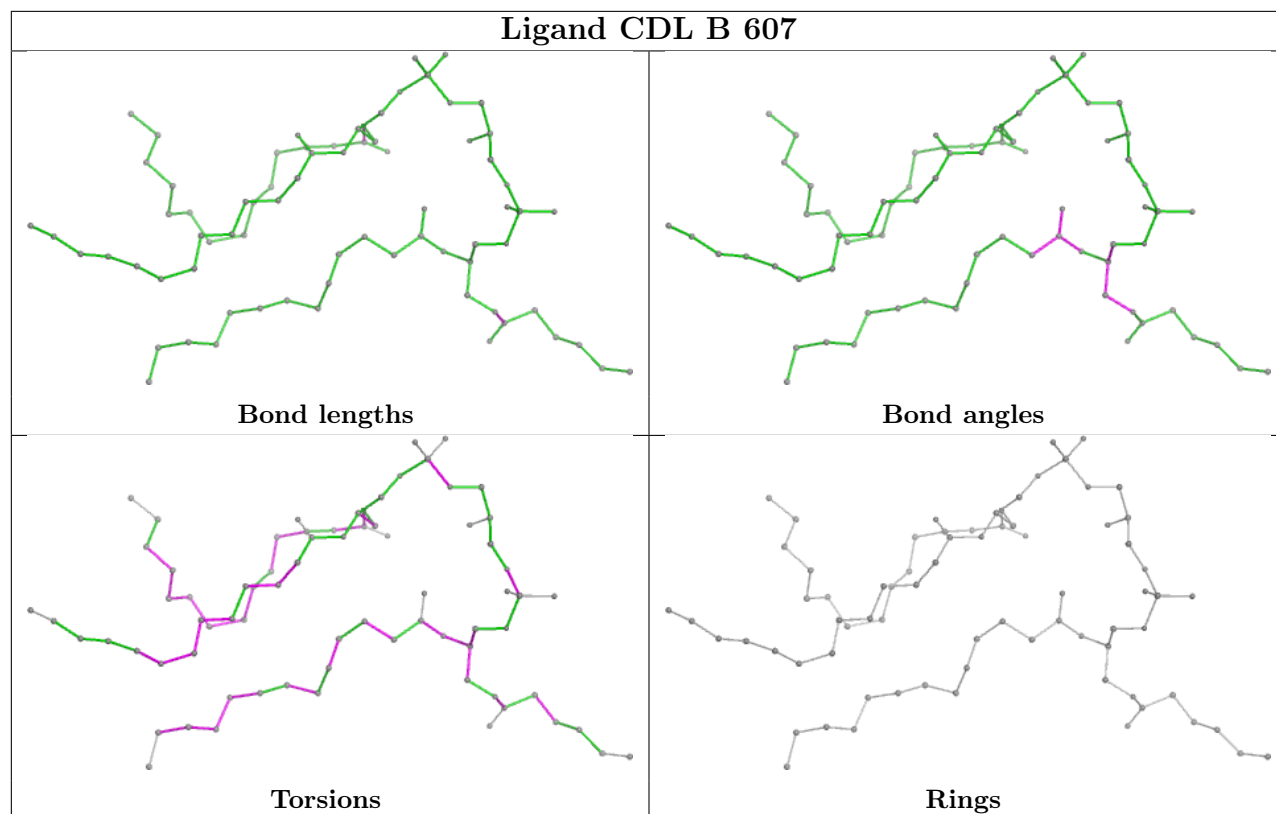


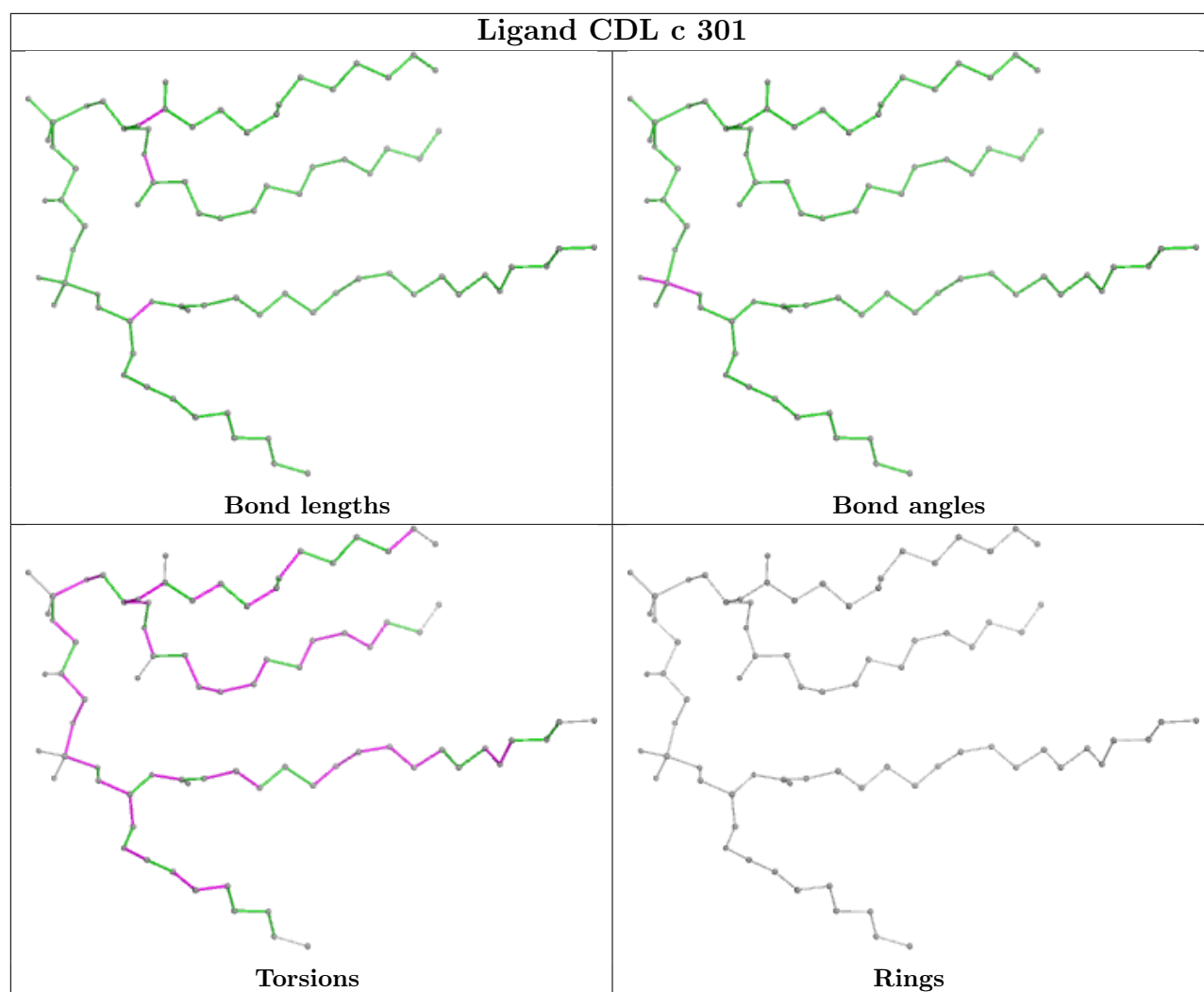


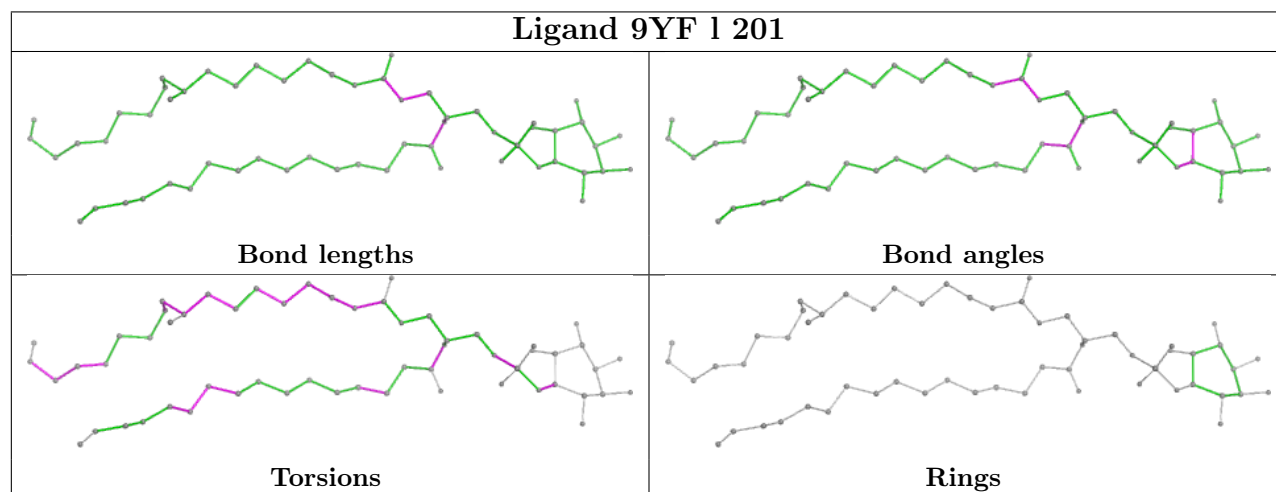
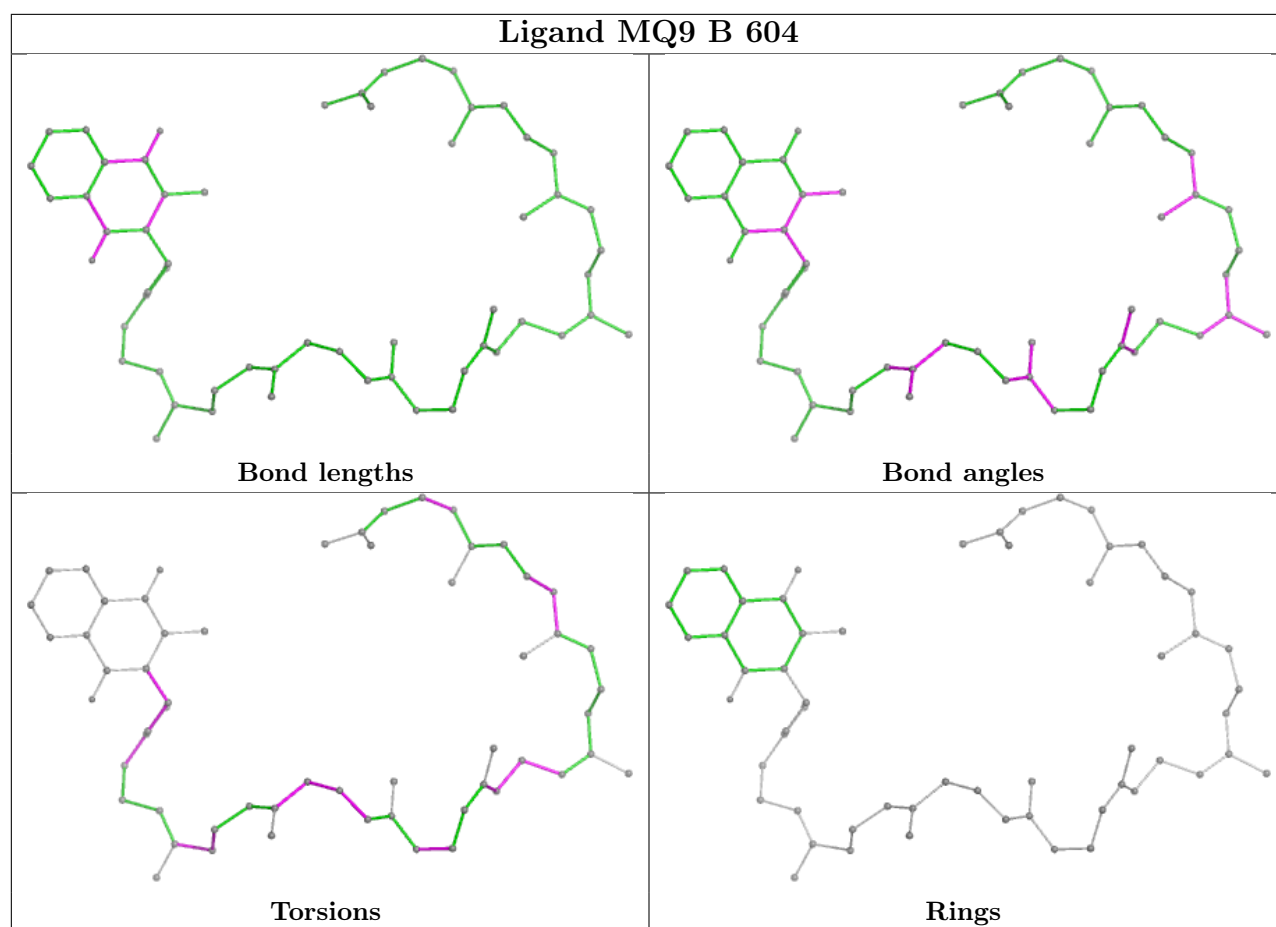


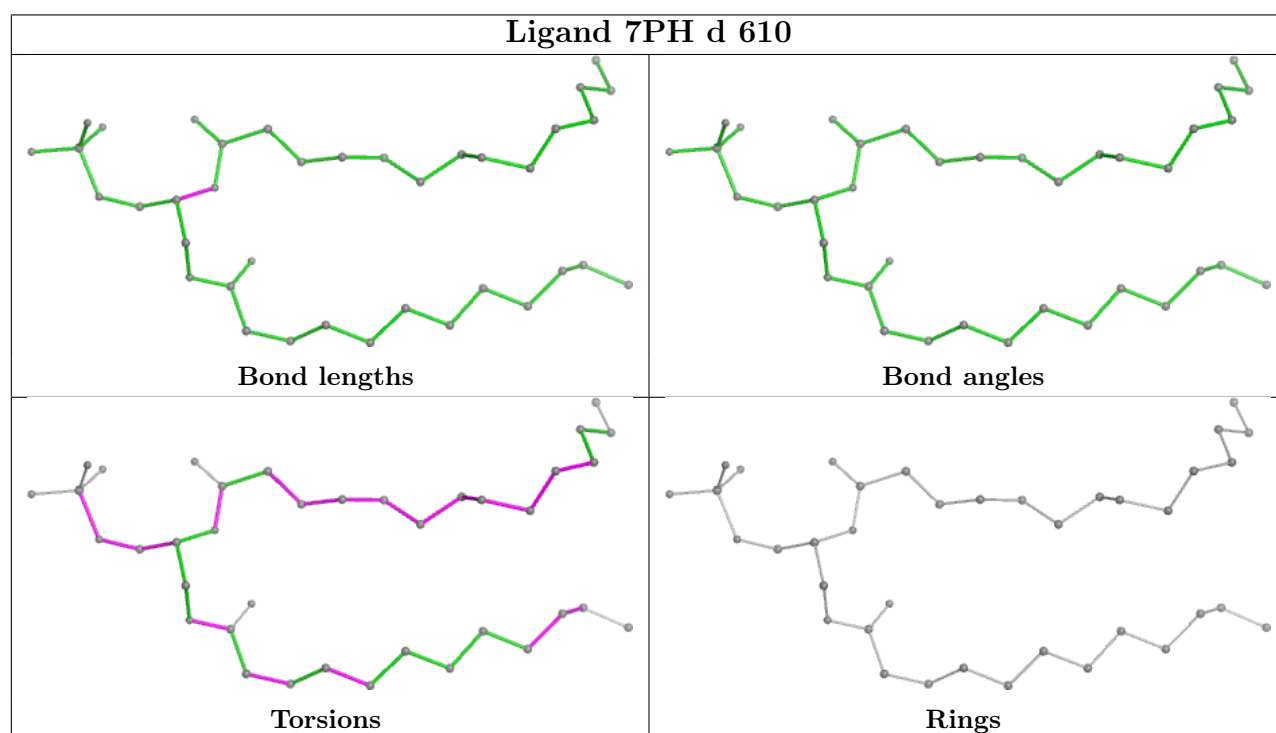
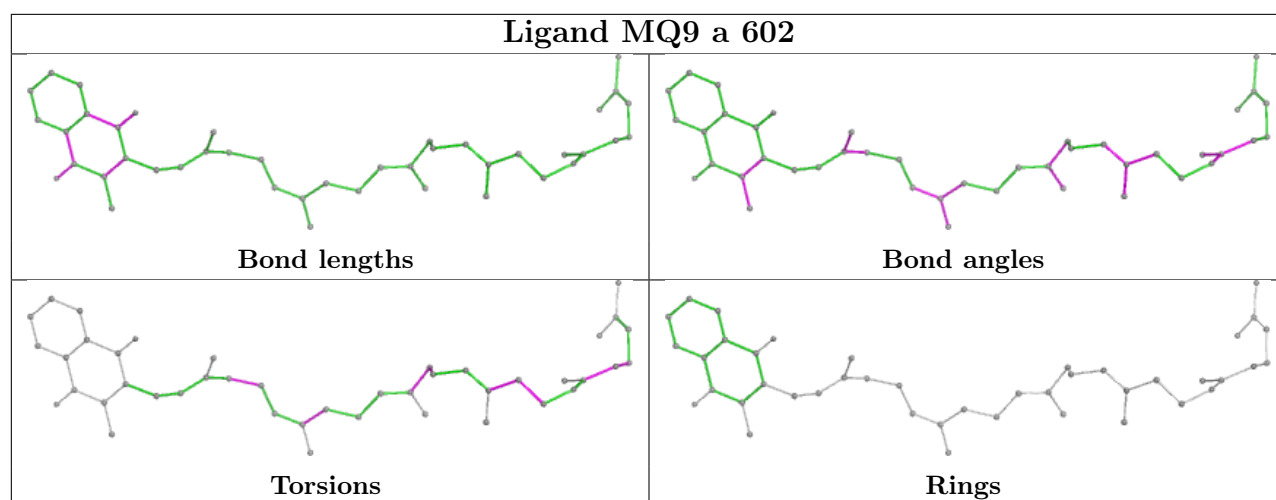


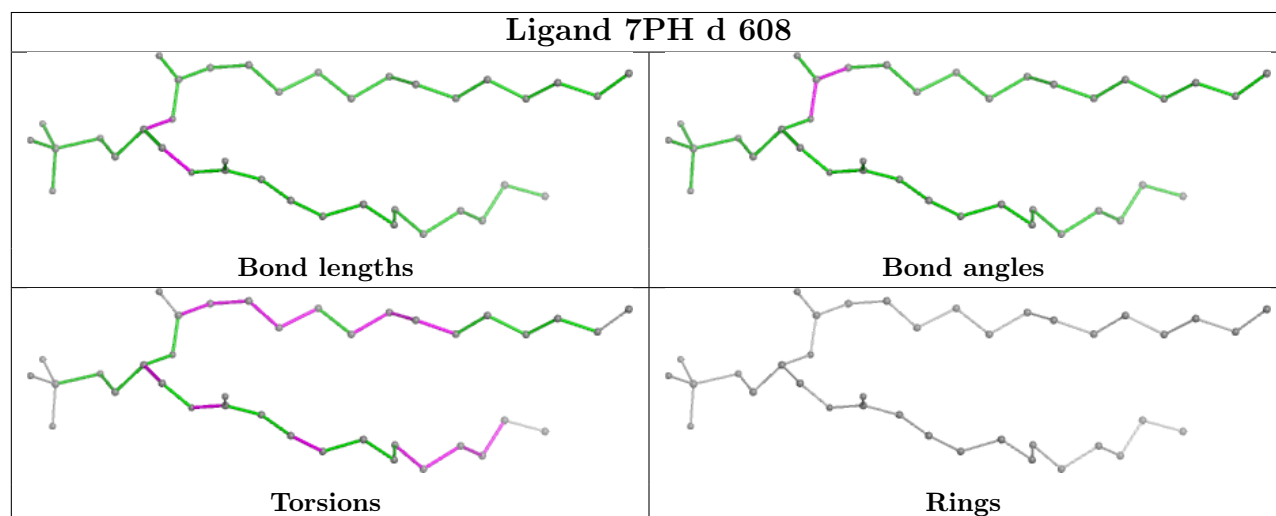
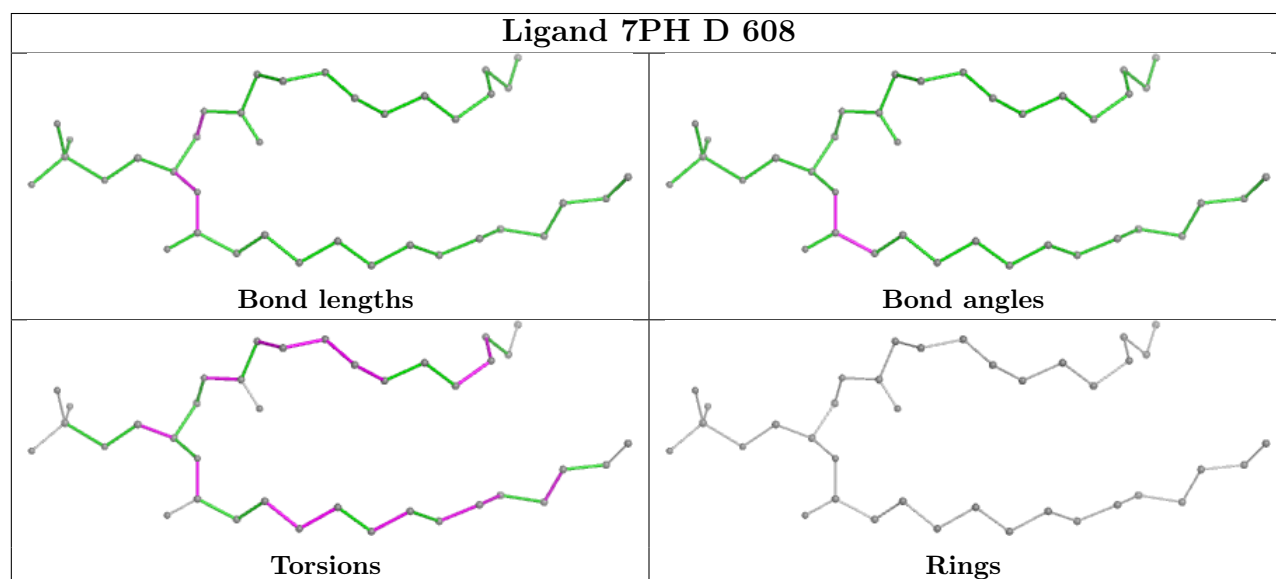
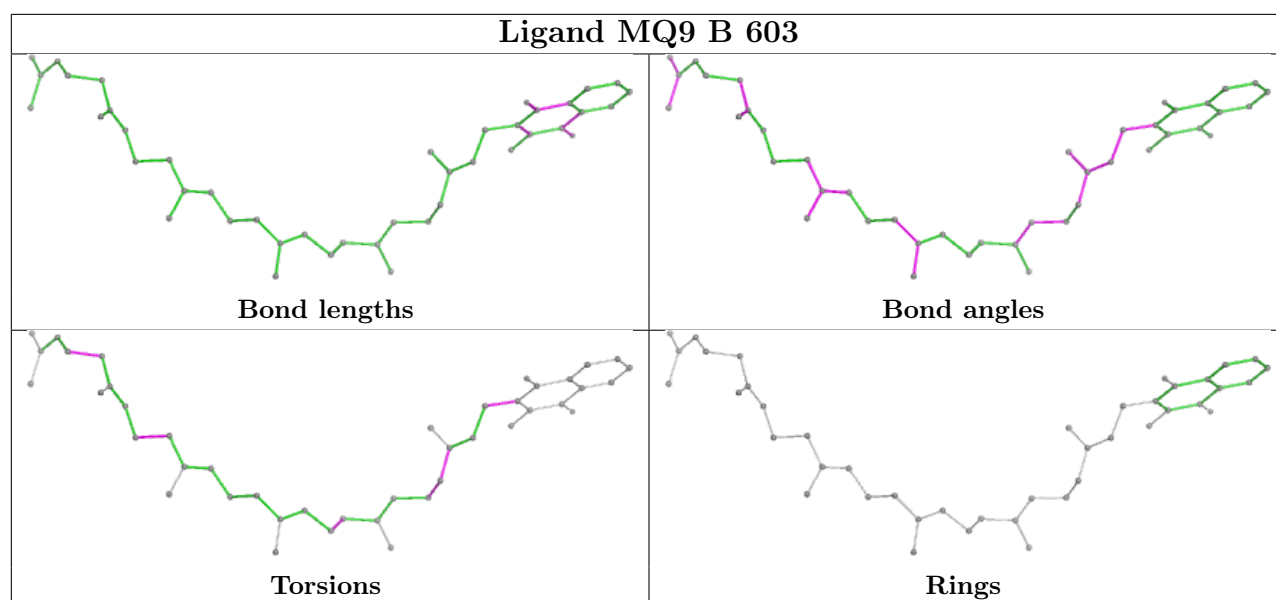


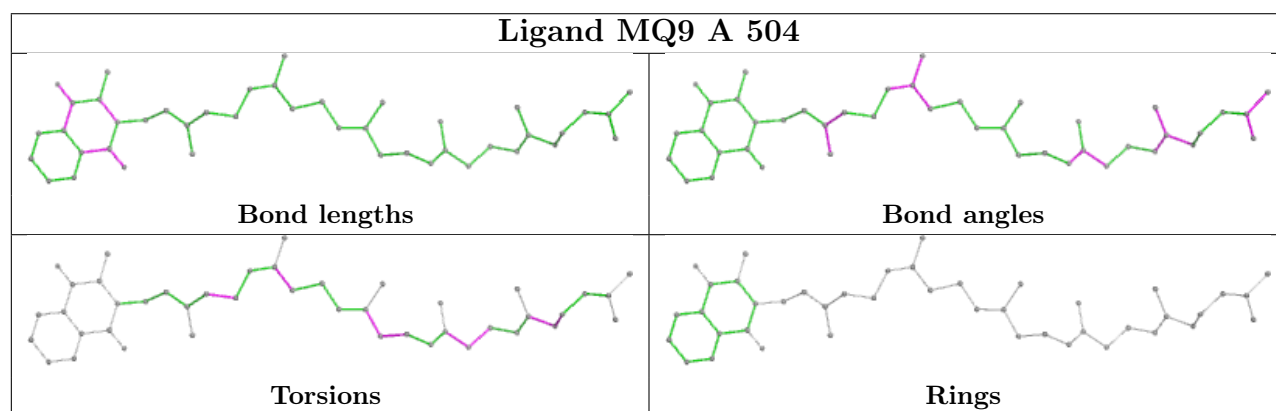
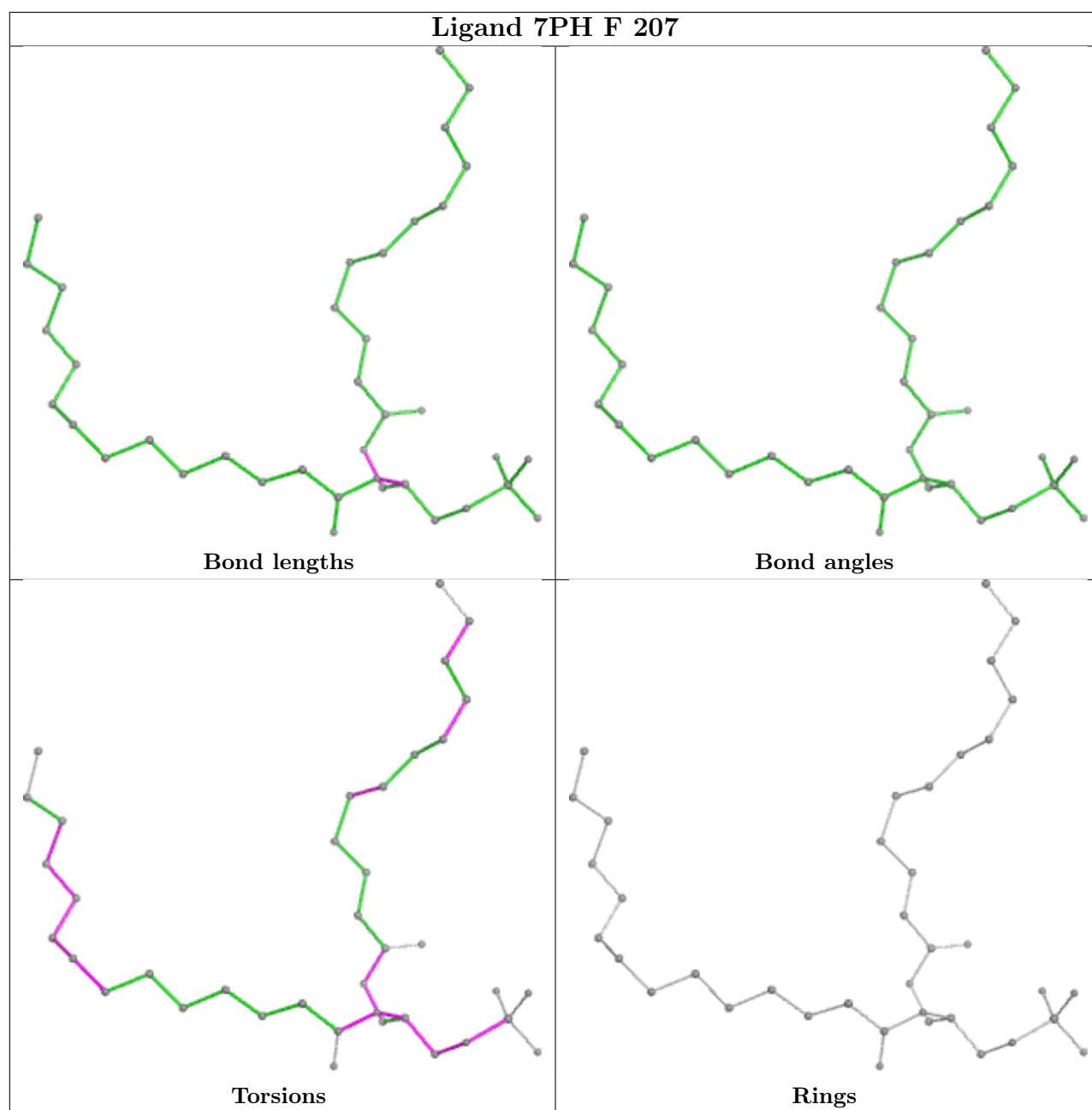


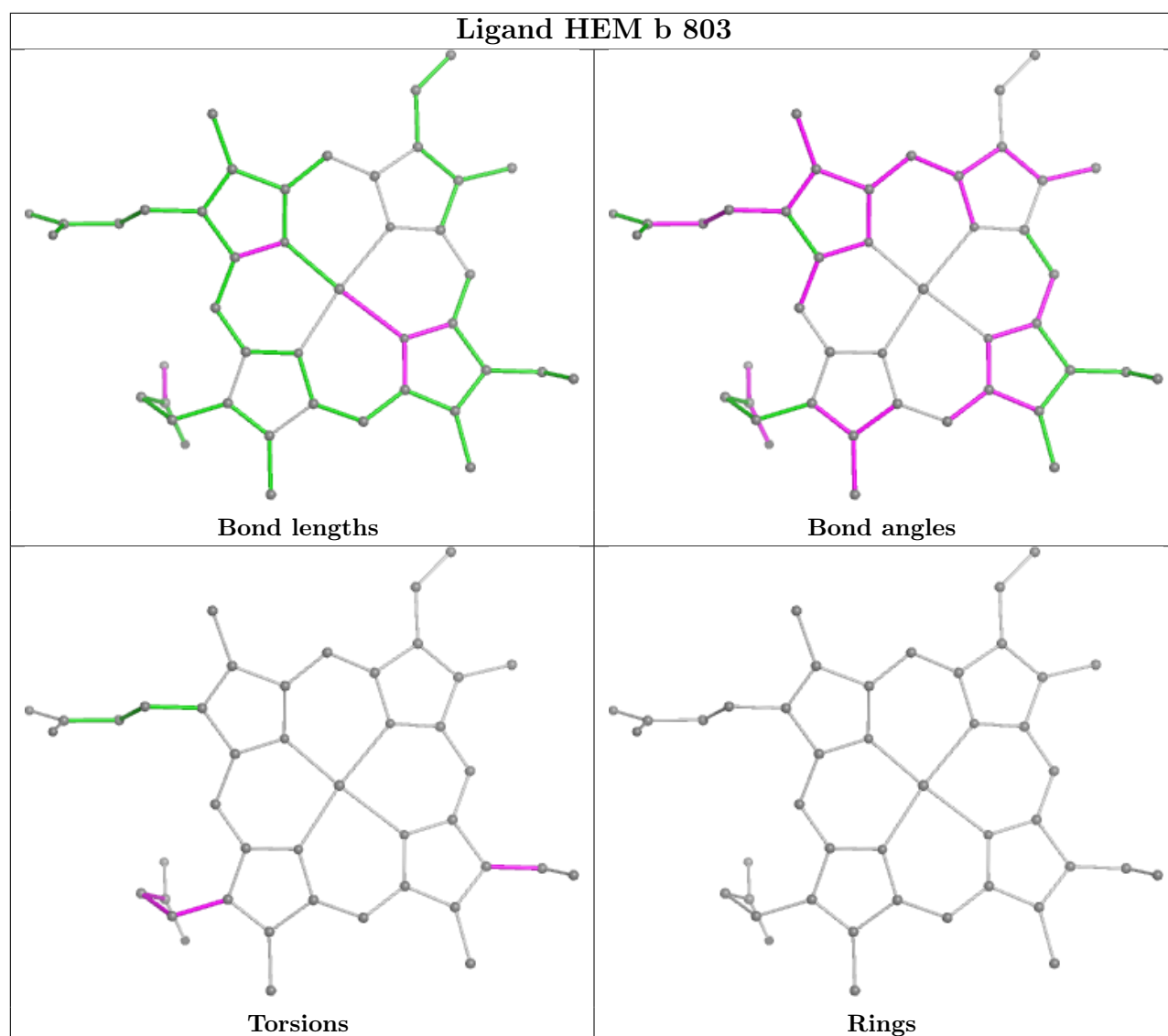


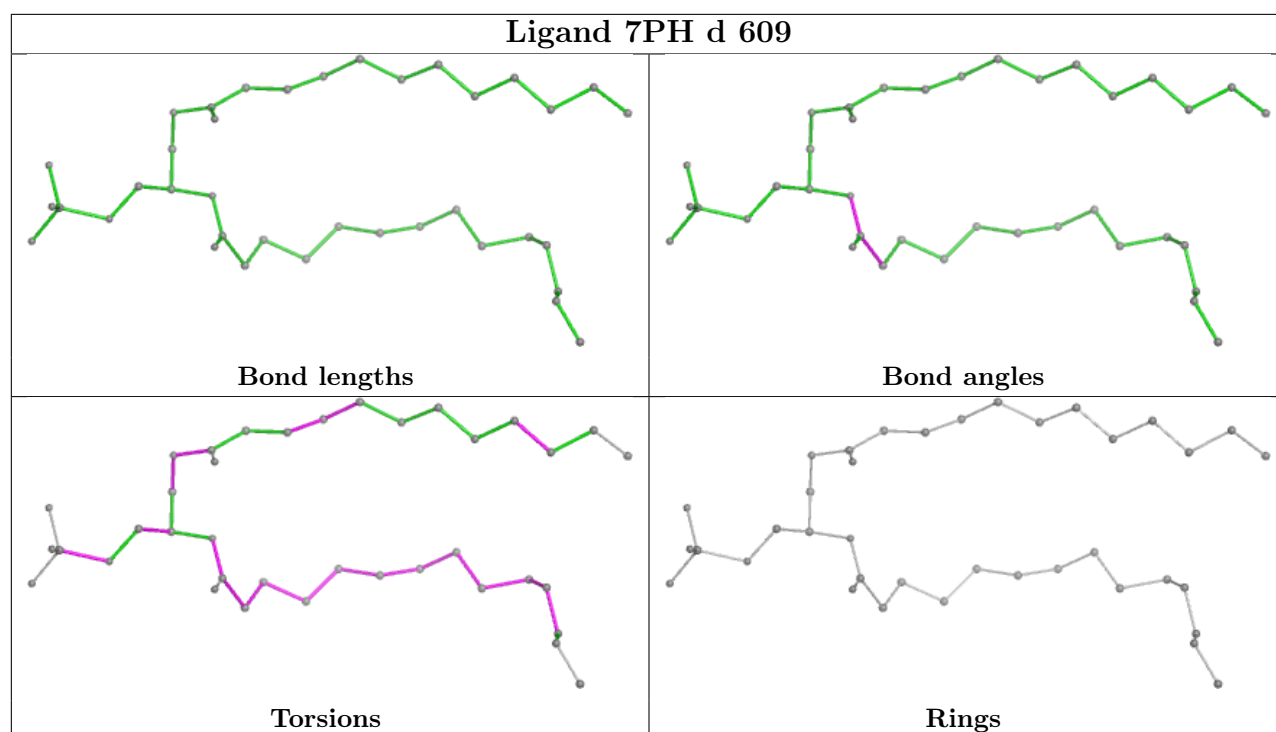


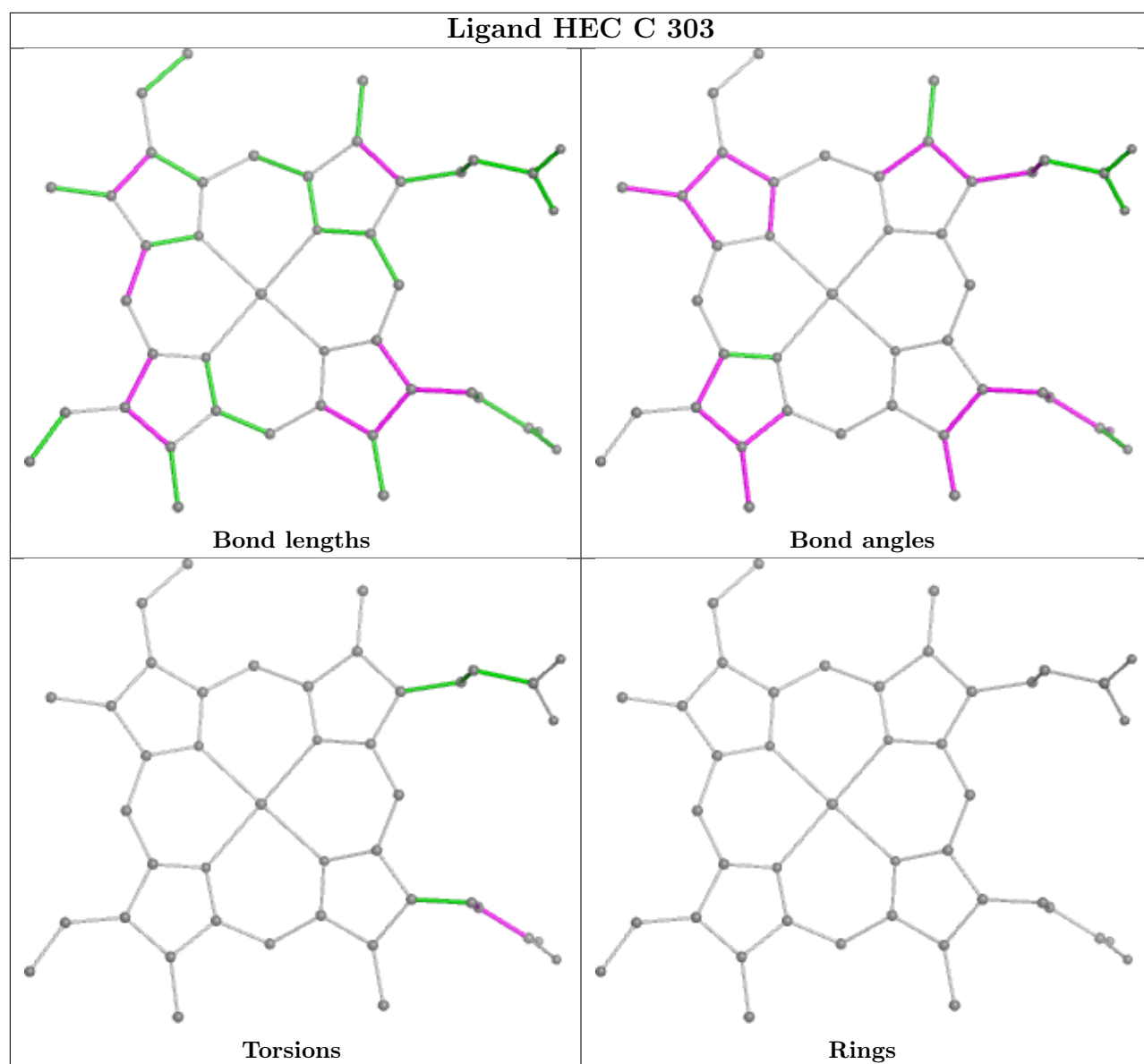


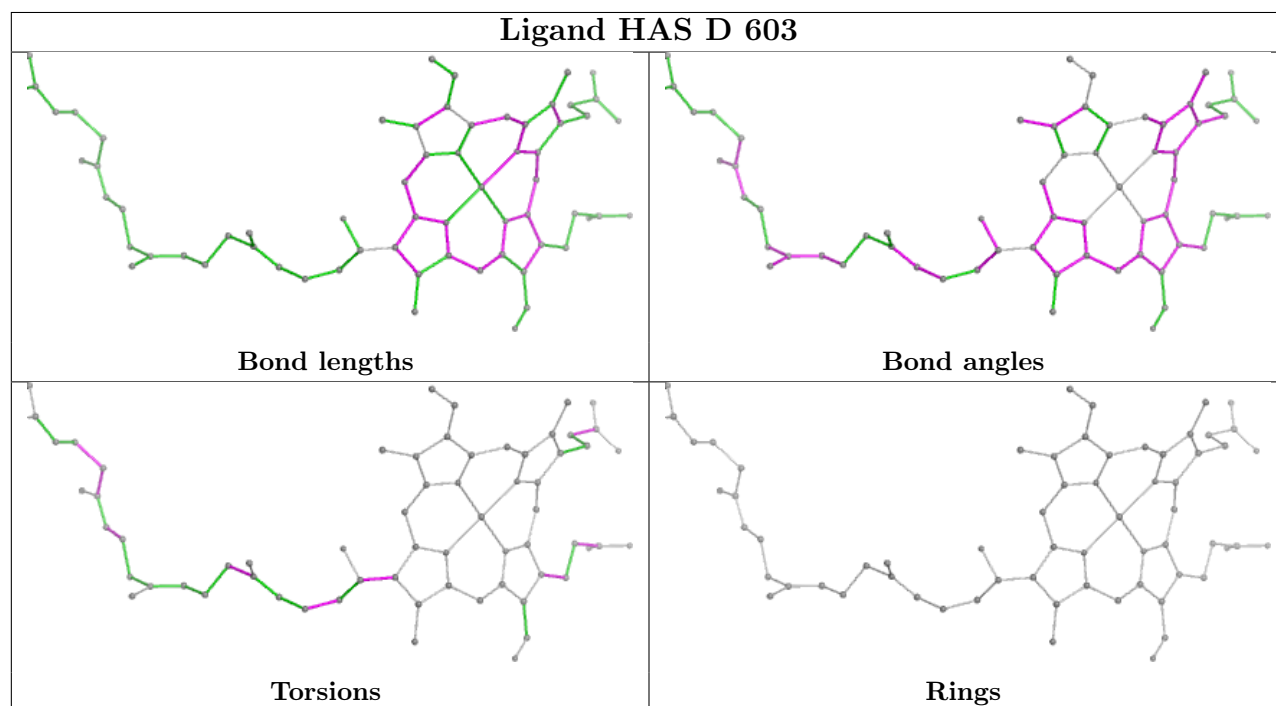
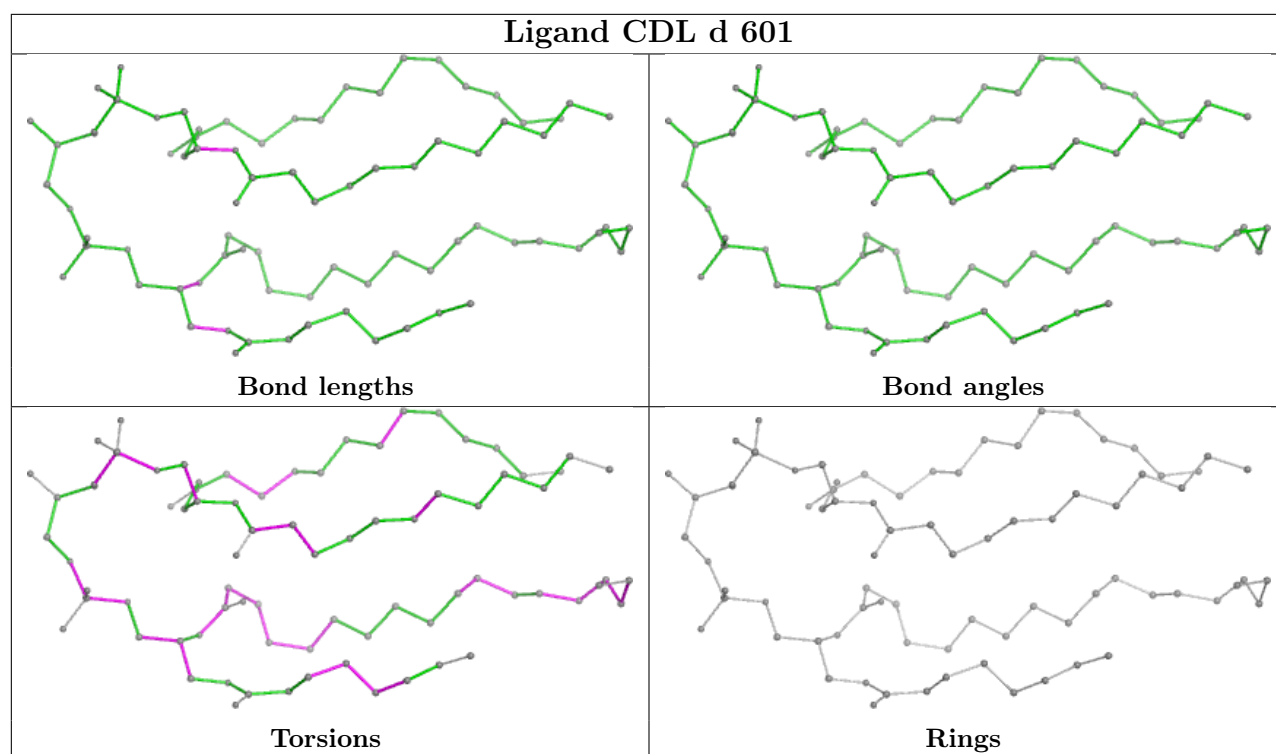


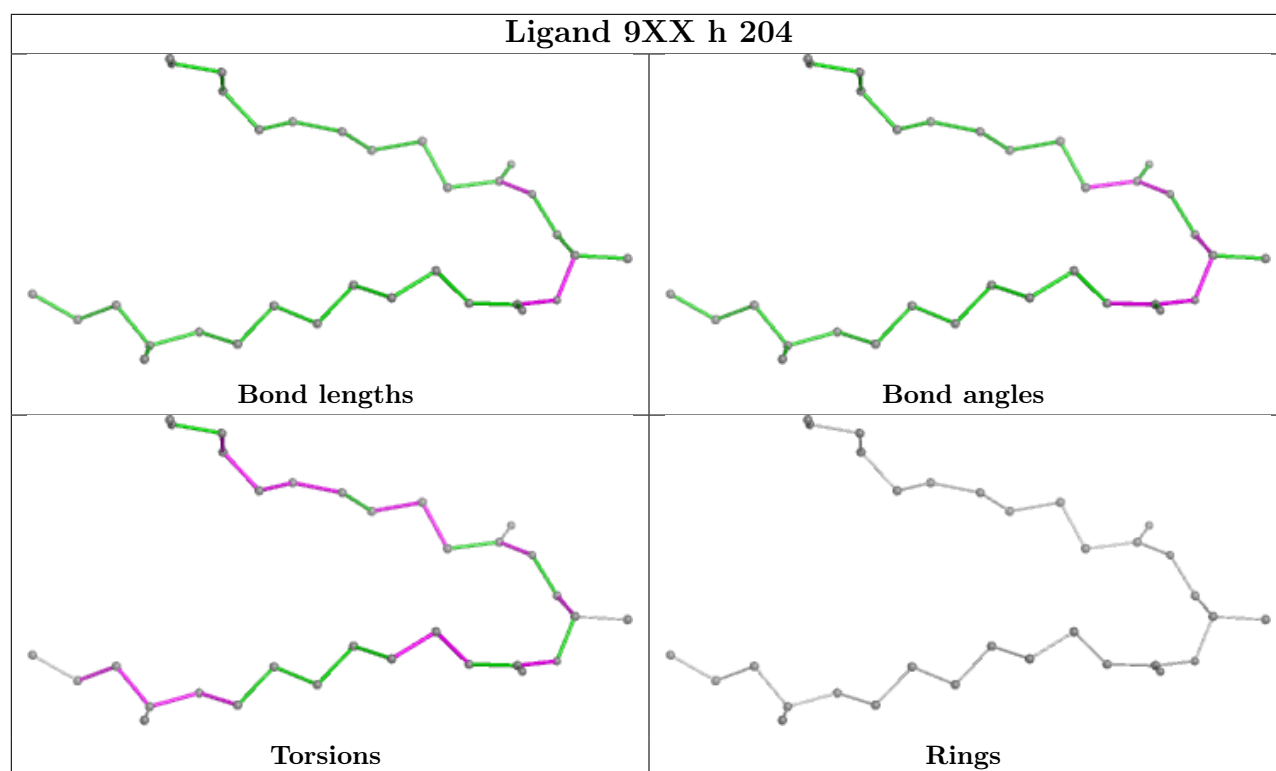


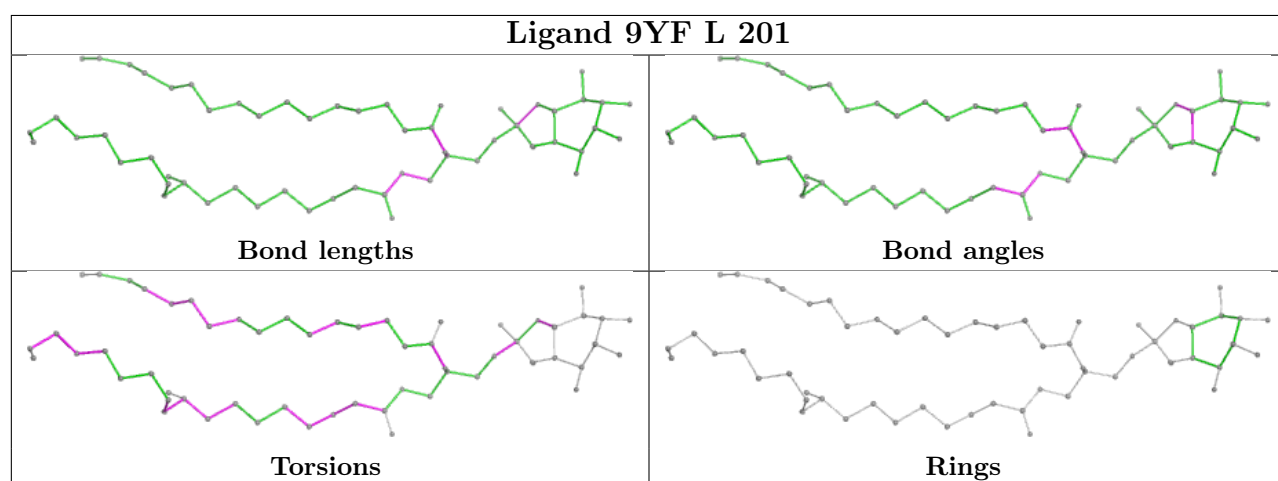
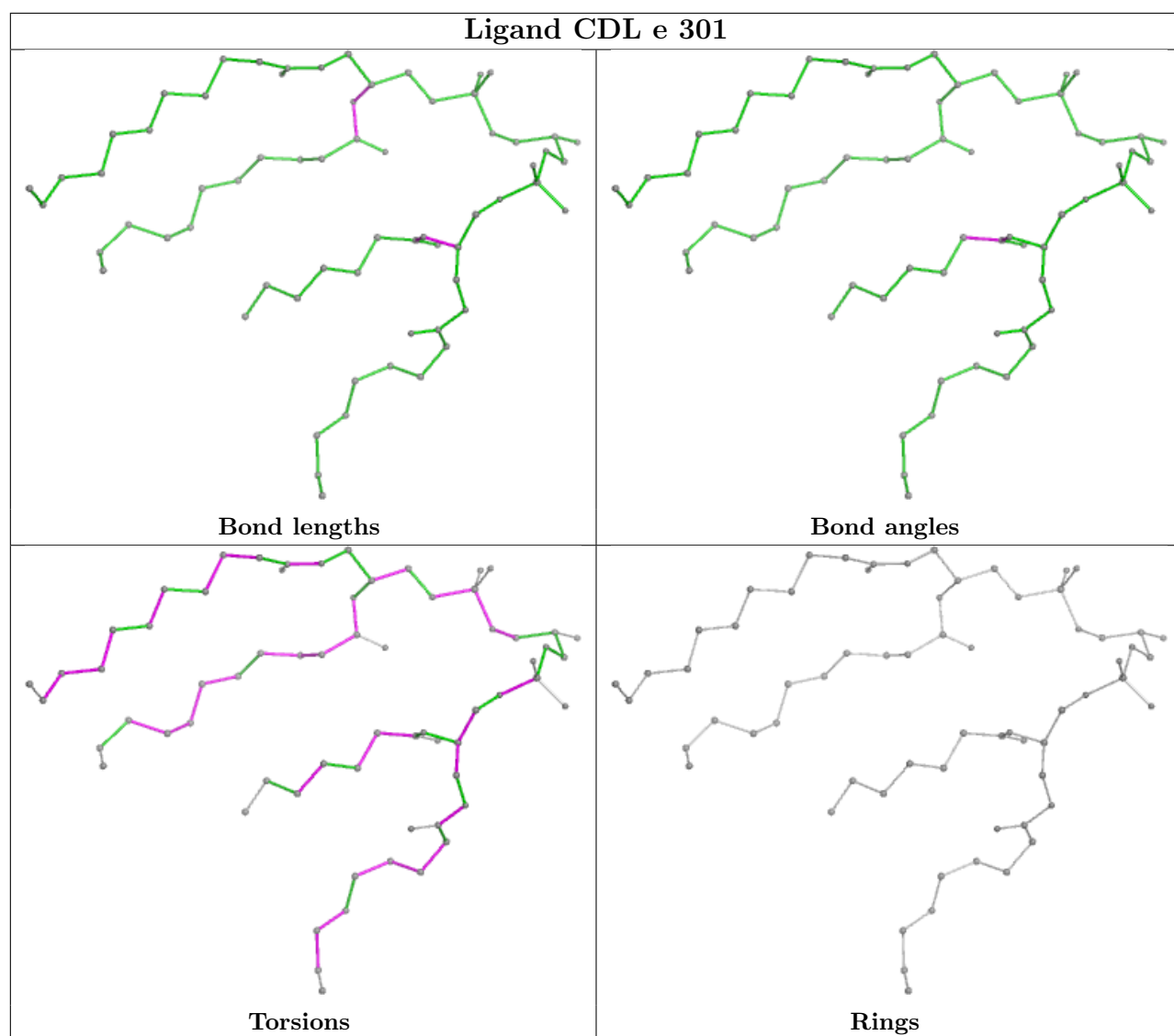


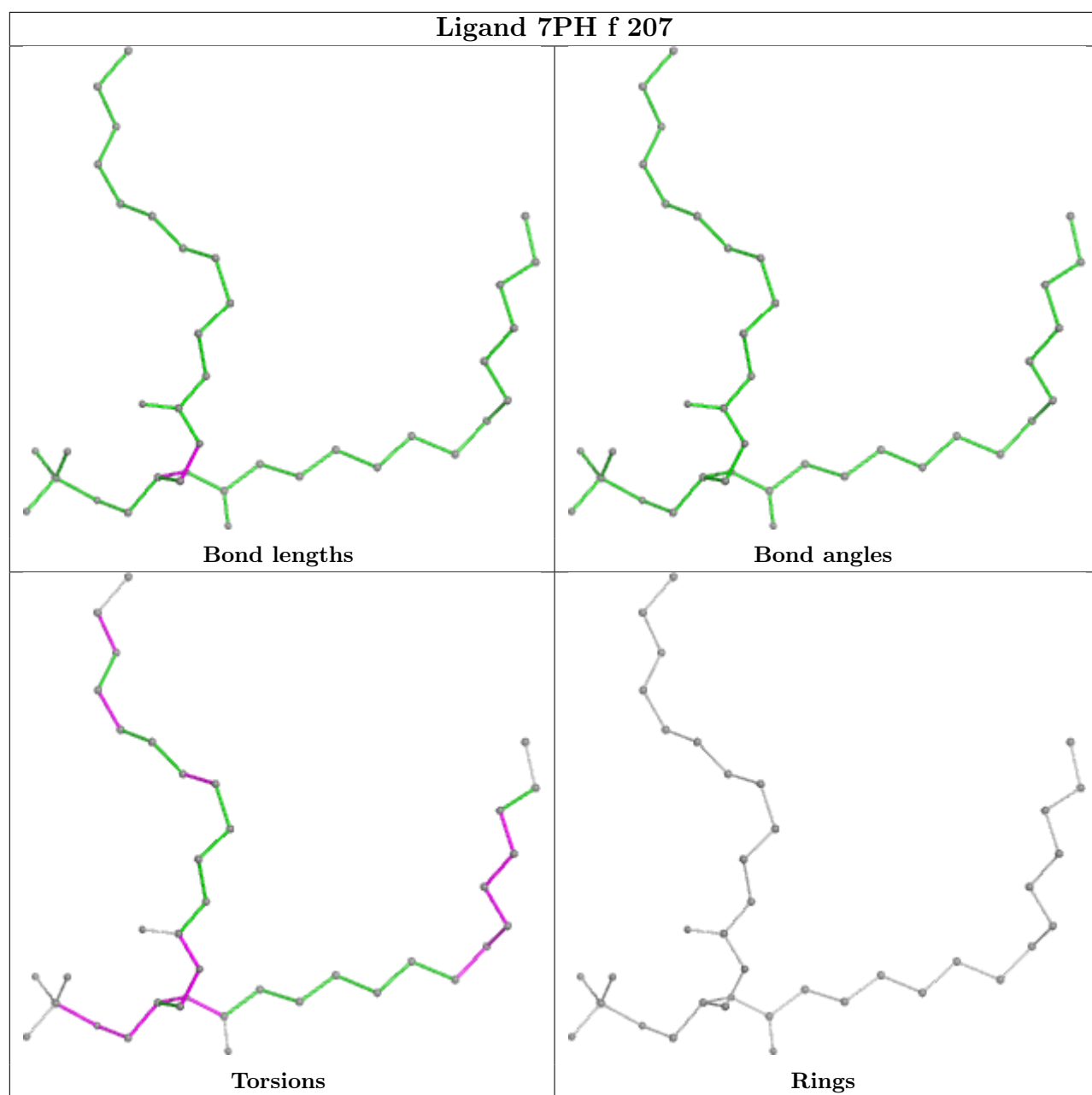


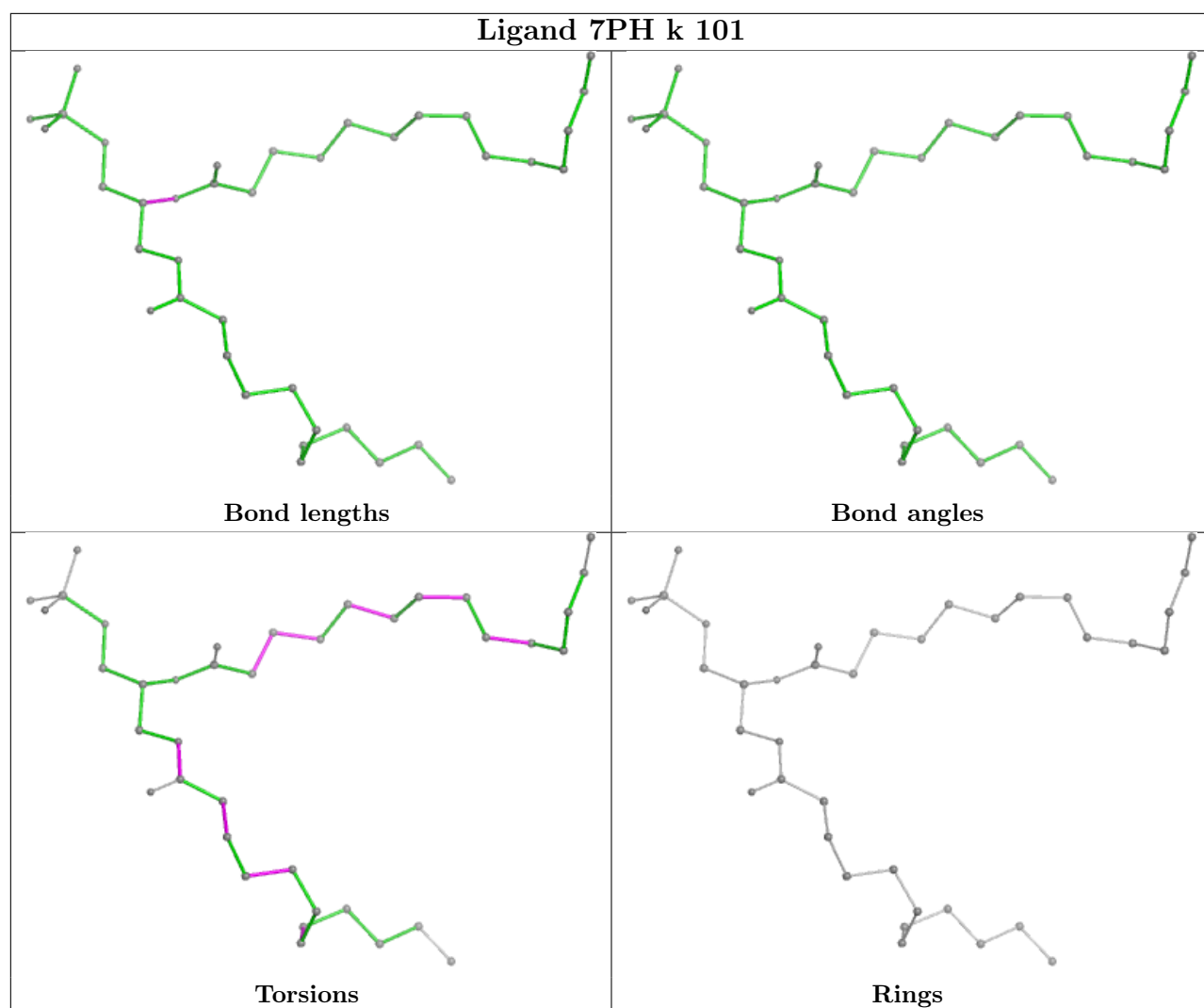


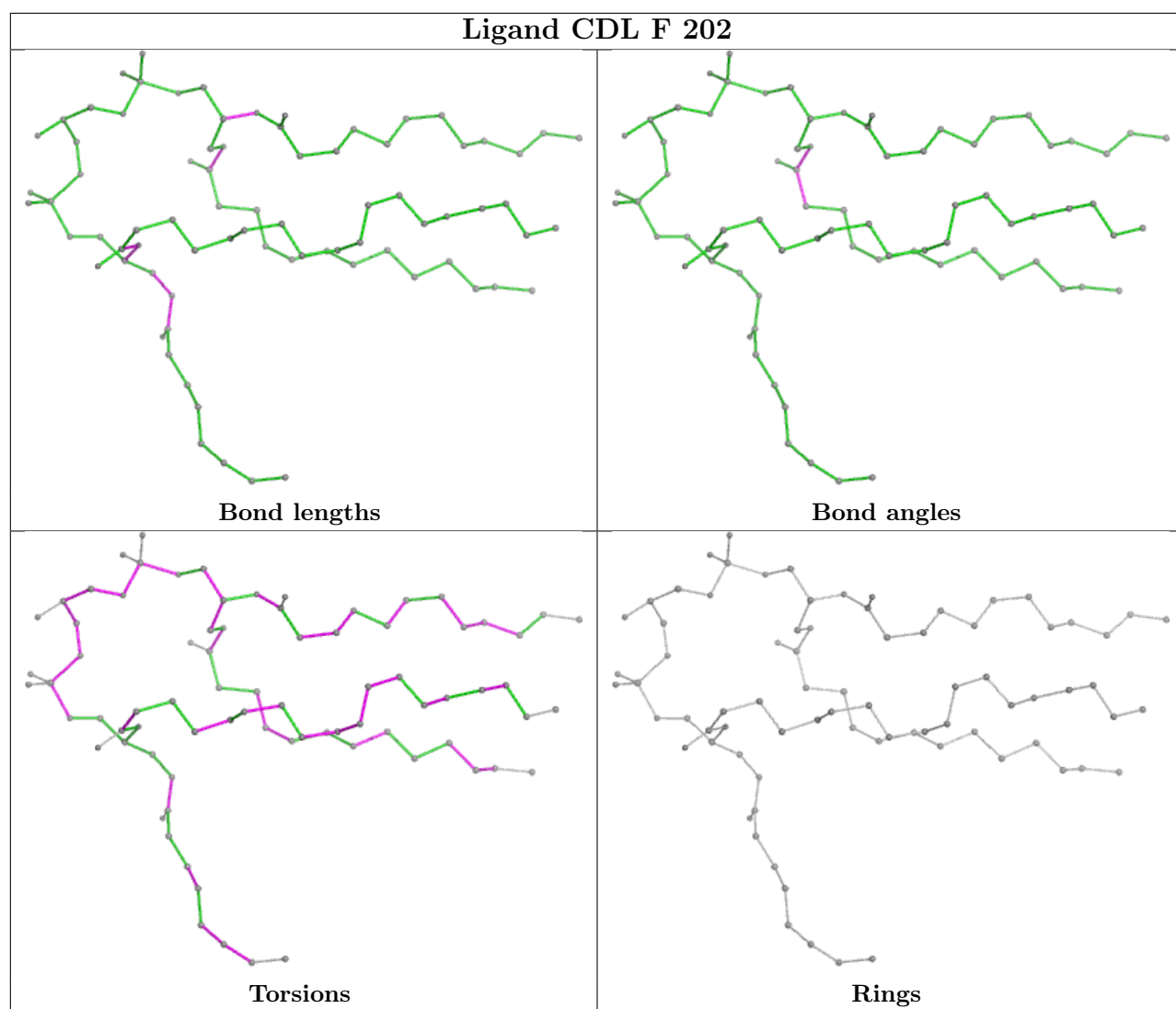




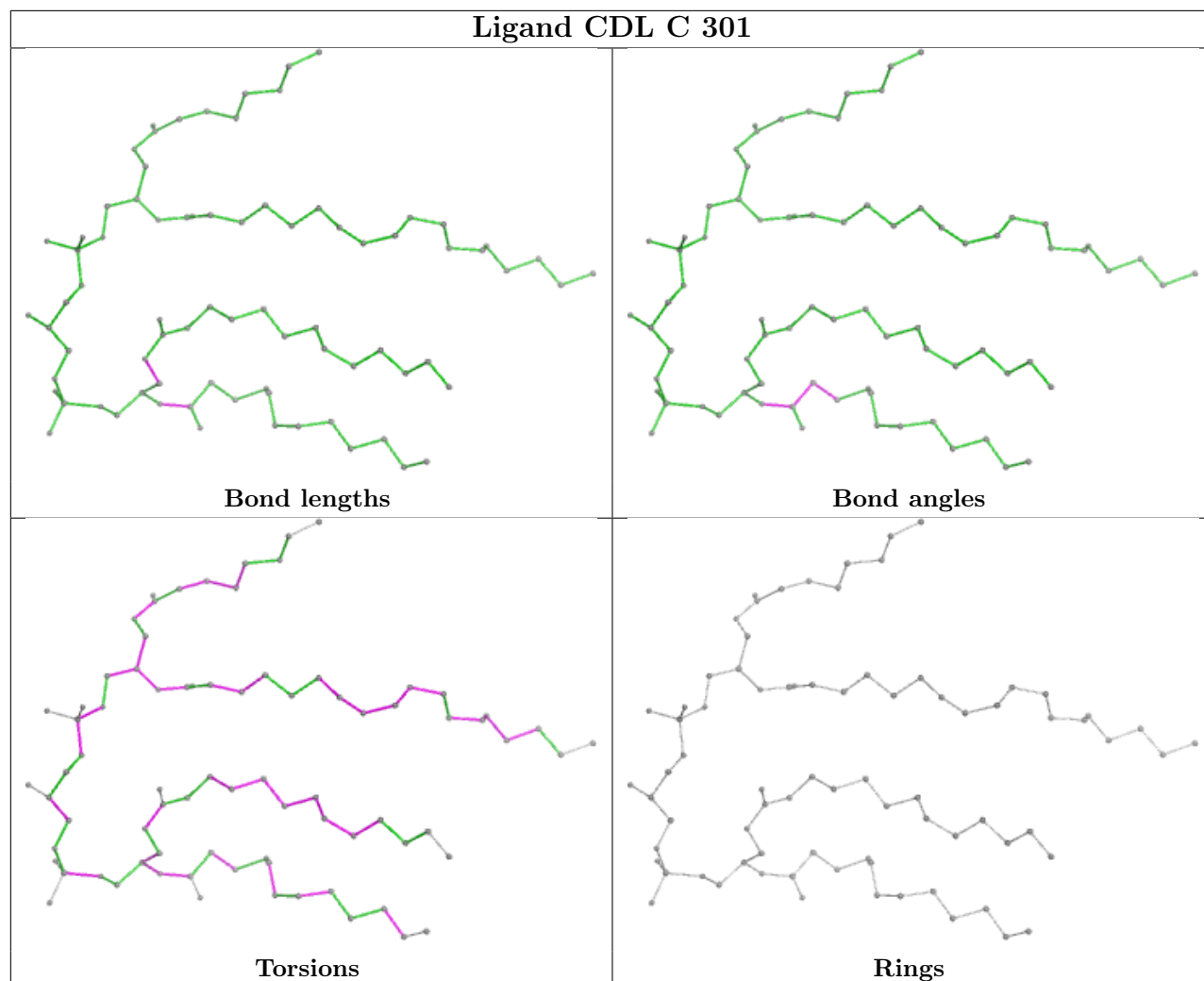




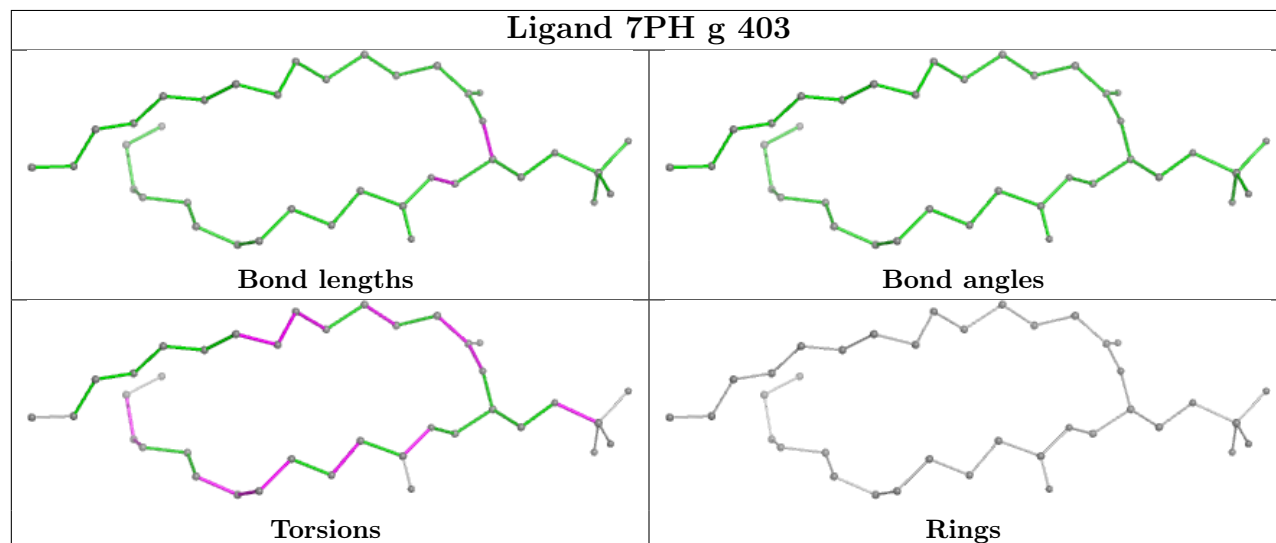




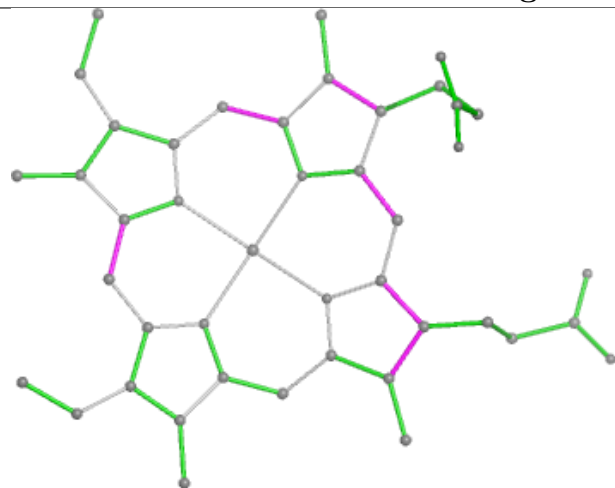
Ligand CDL C 301



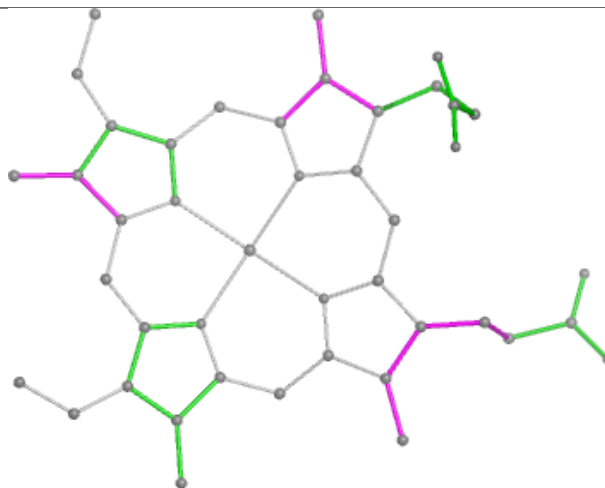
Ligand 7PH g 403



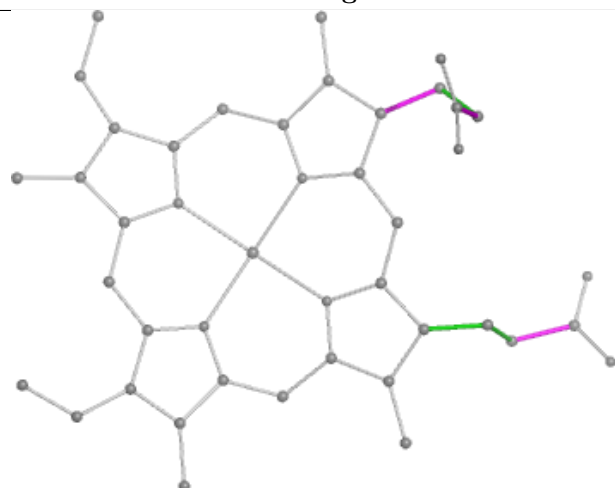
Ligand HEC c 302



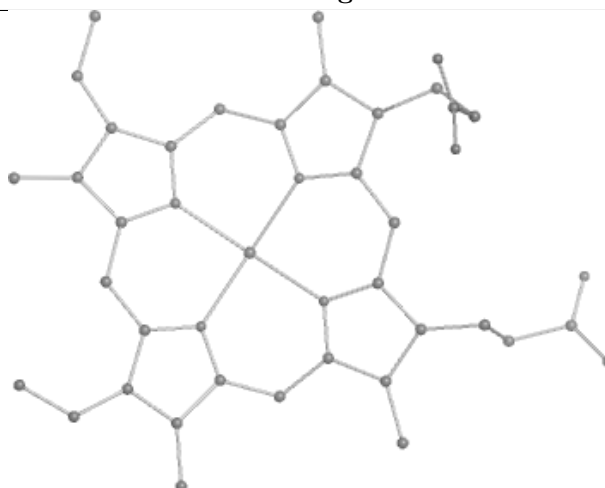
Bond lengths



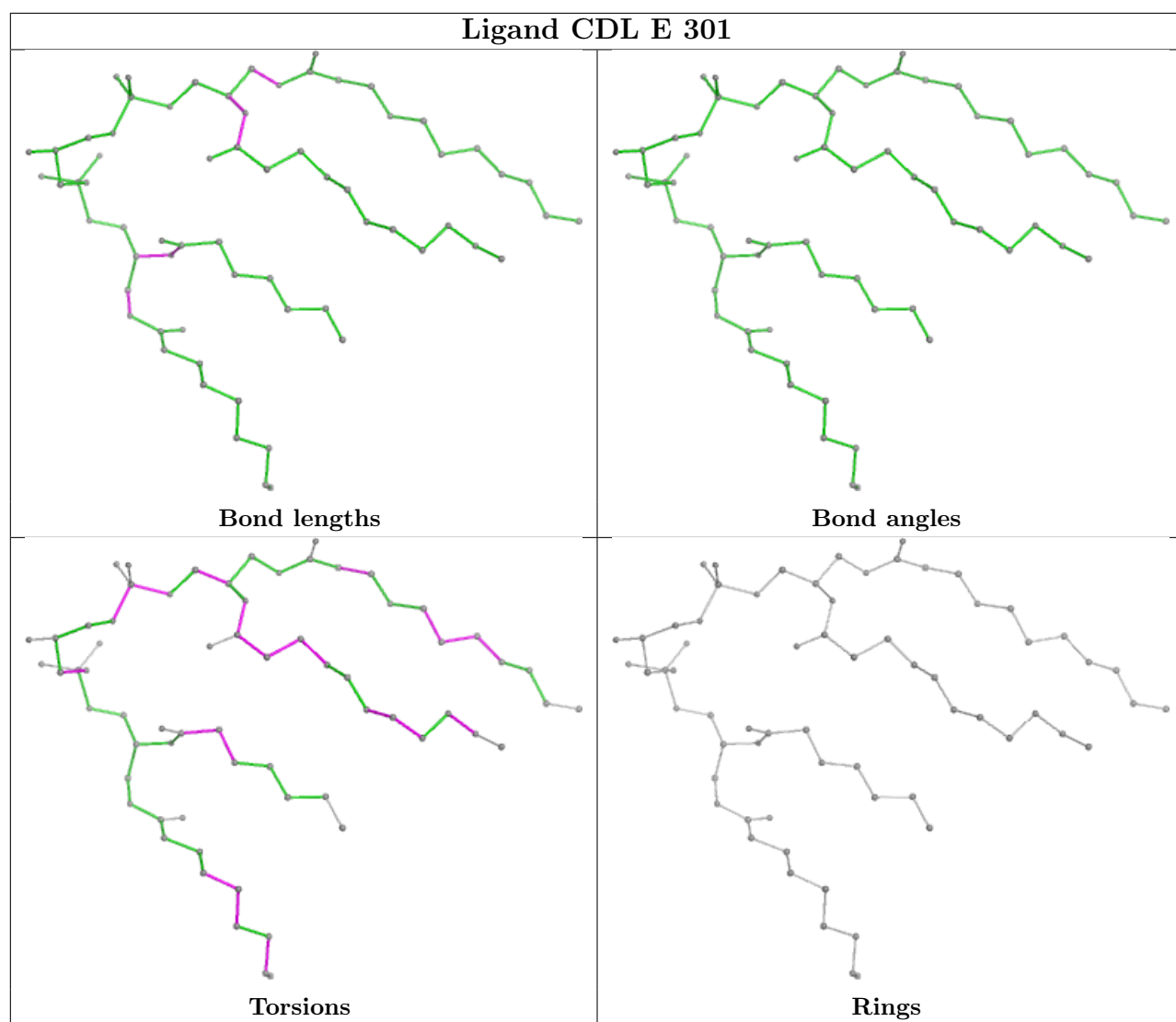
Bond angles

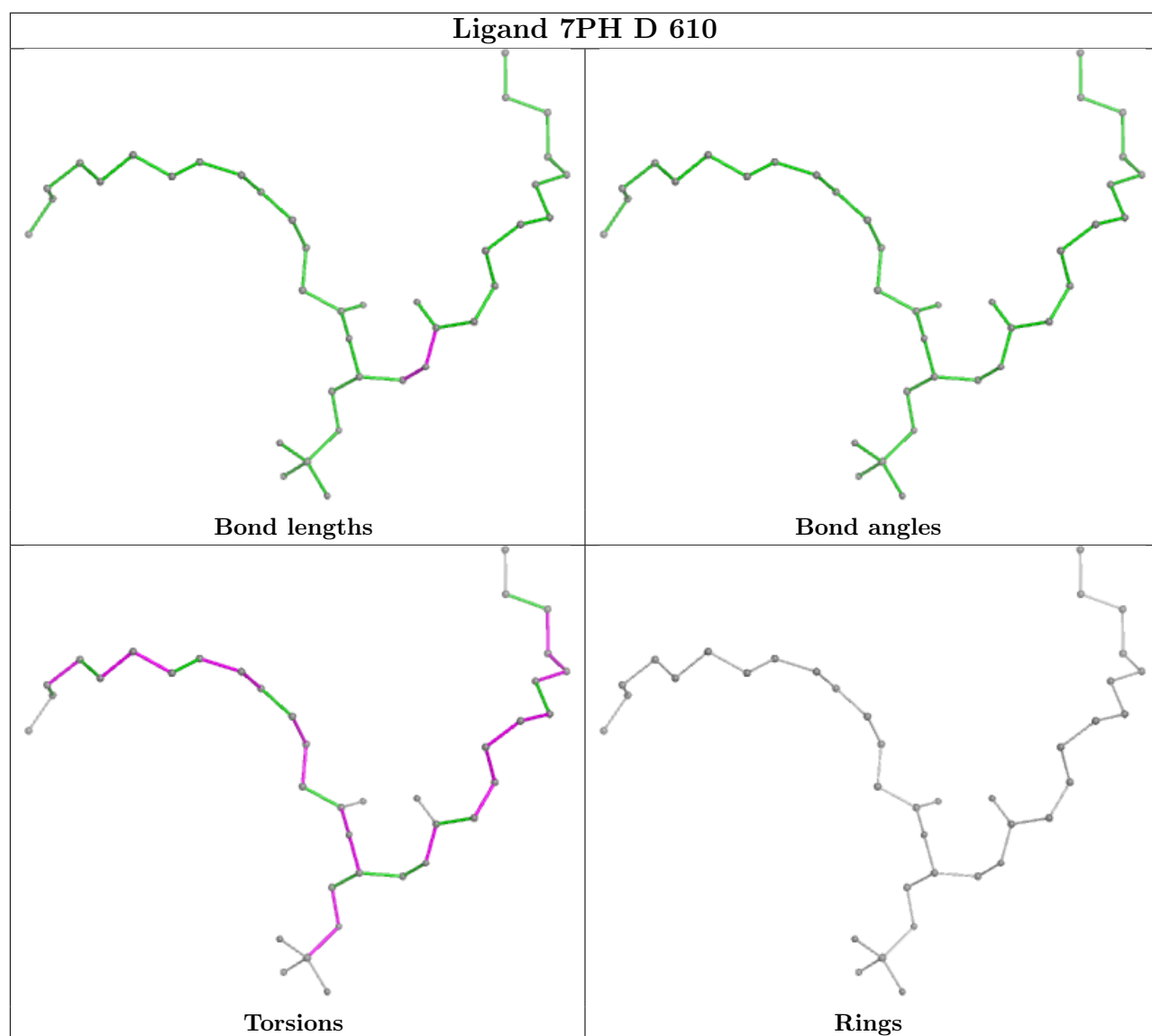


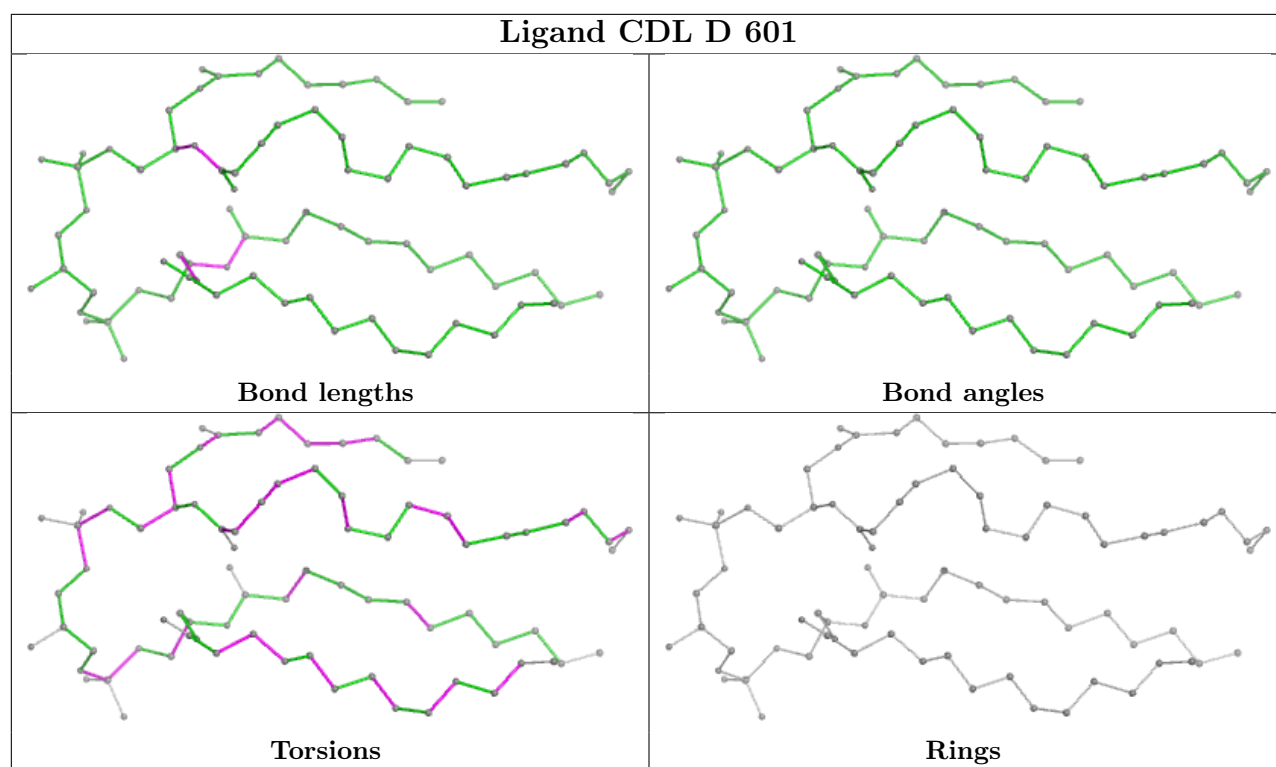
Torsions

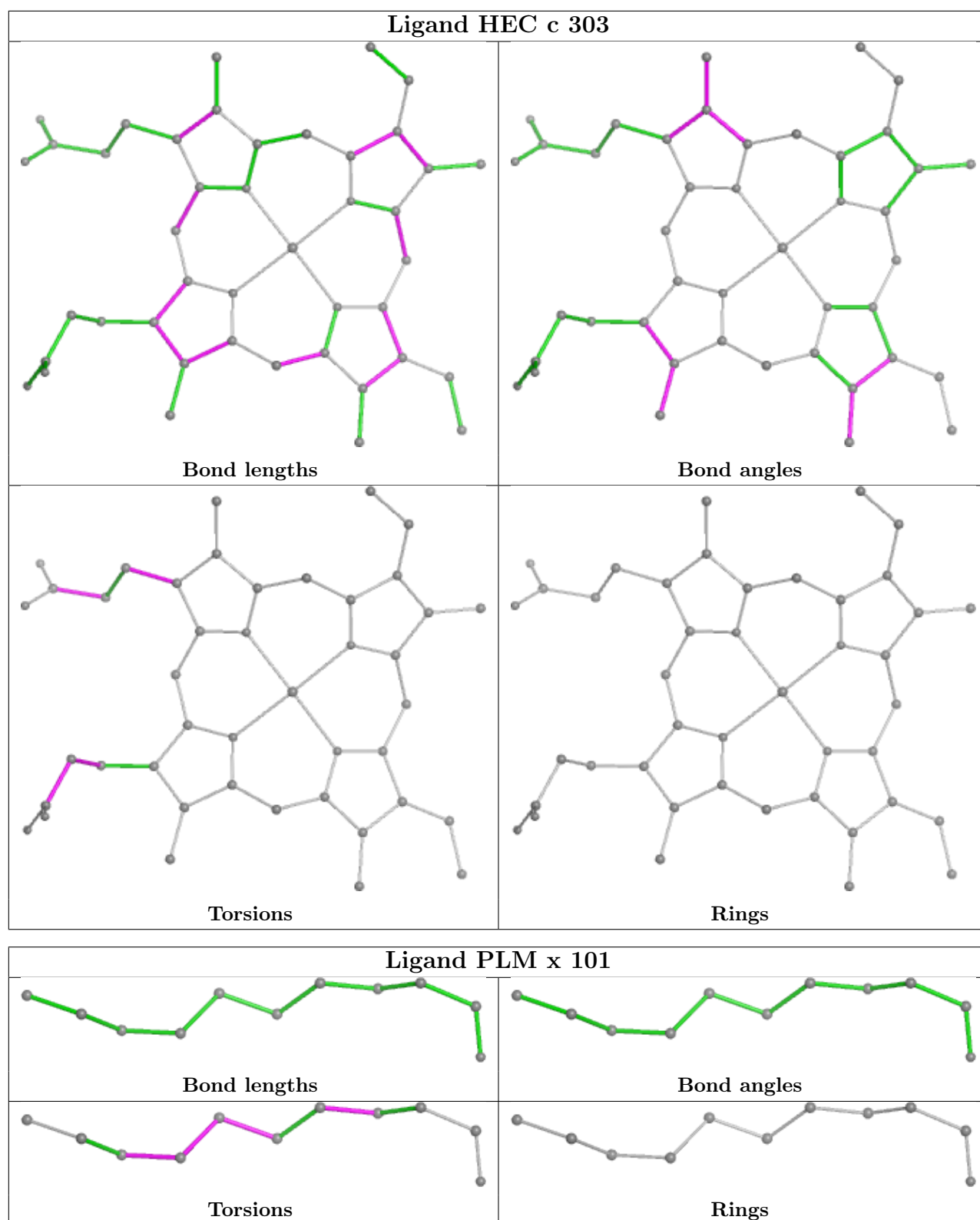


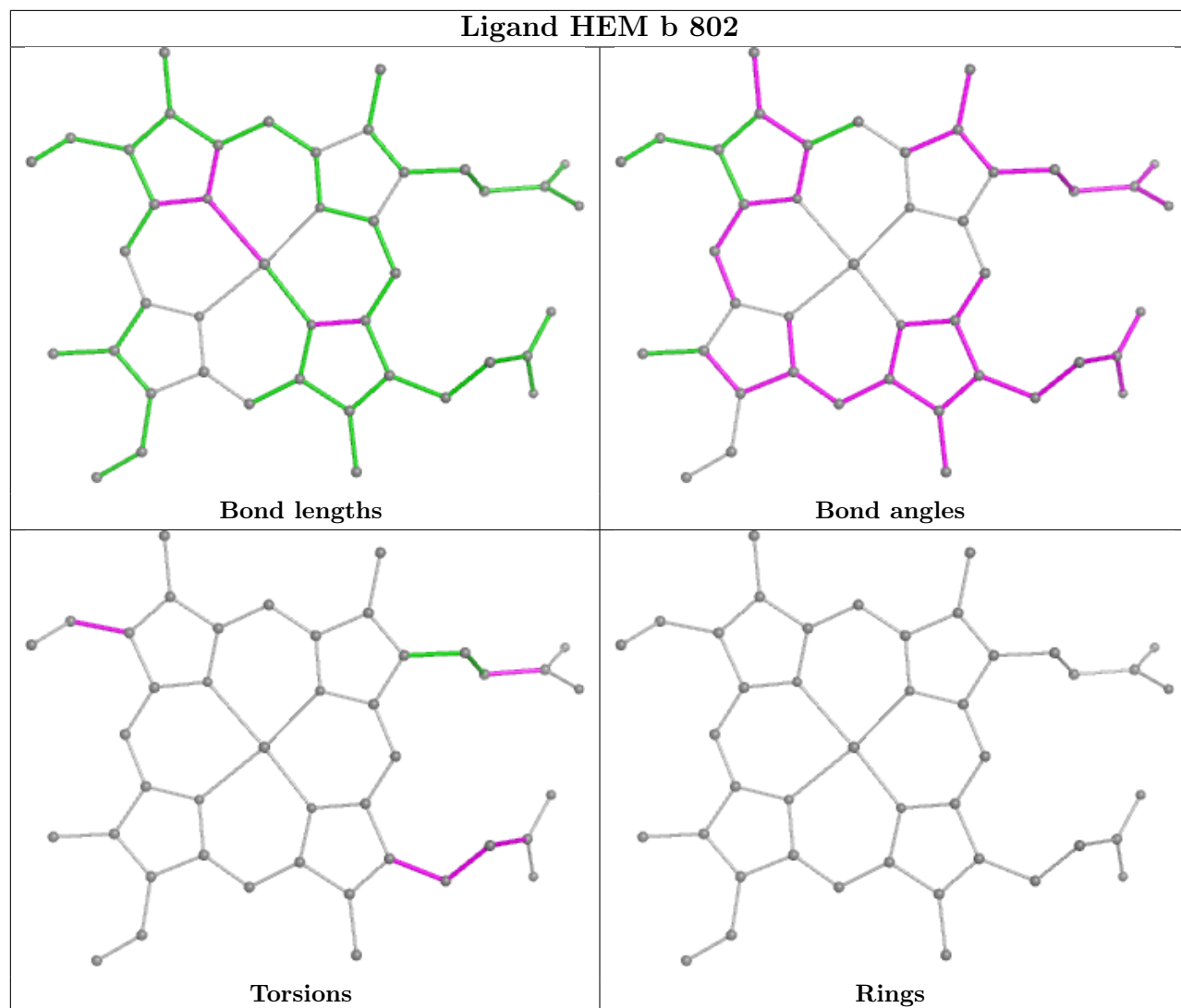
Rings

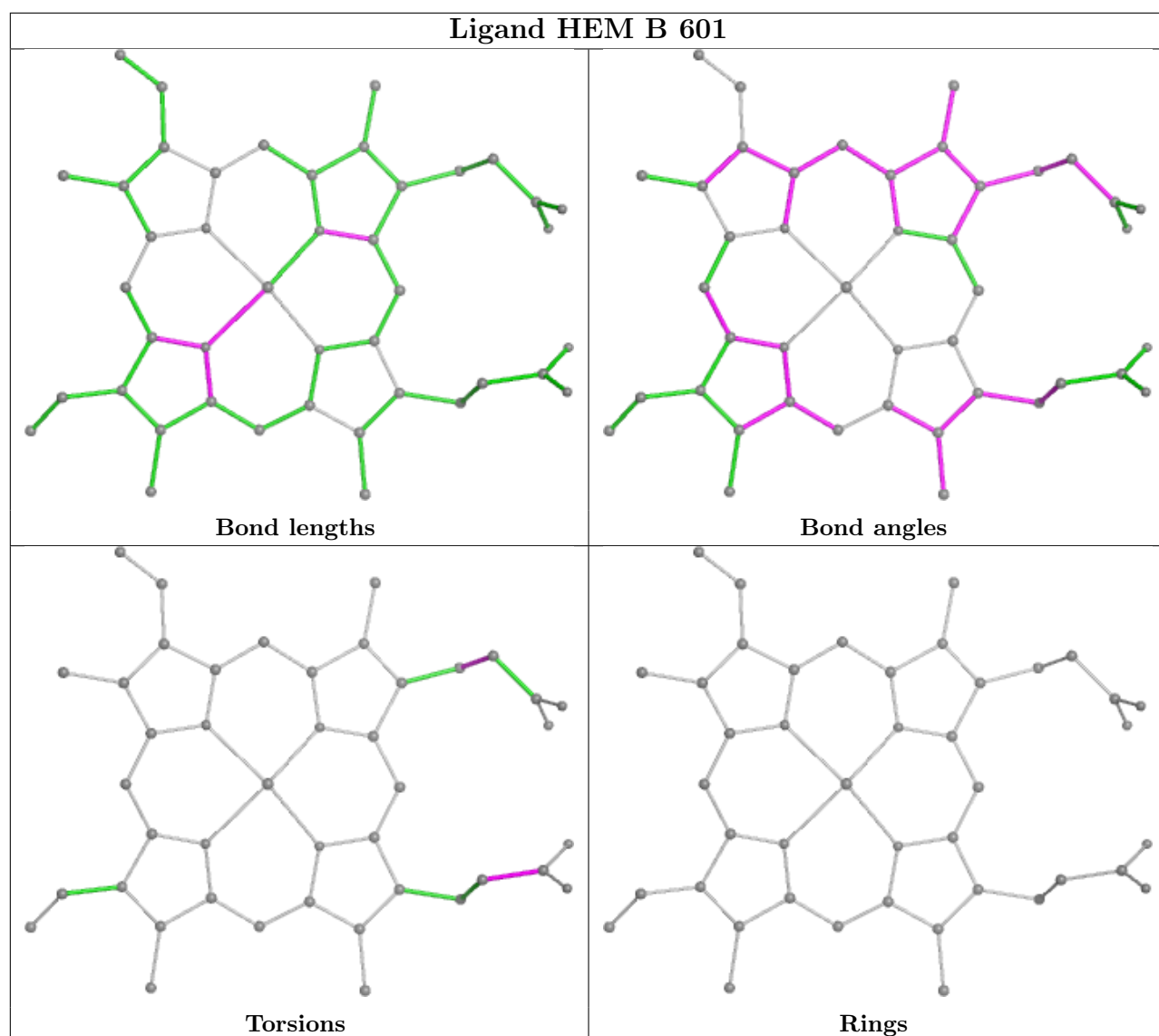


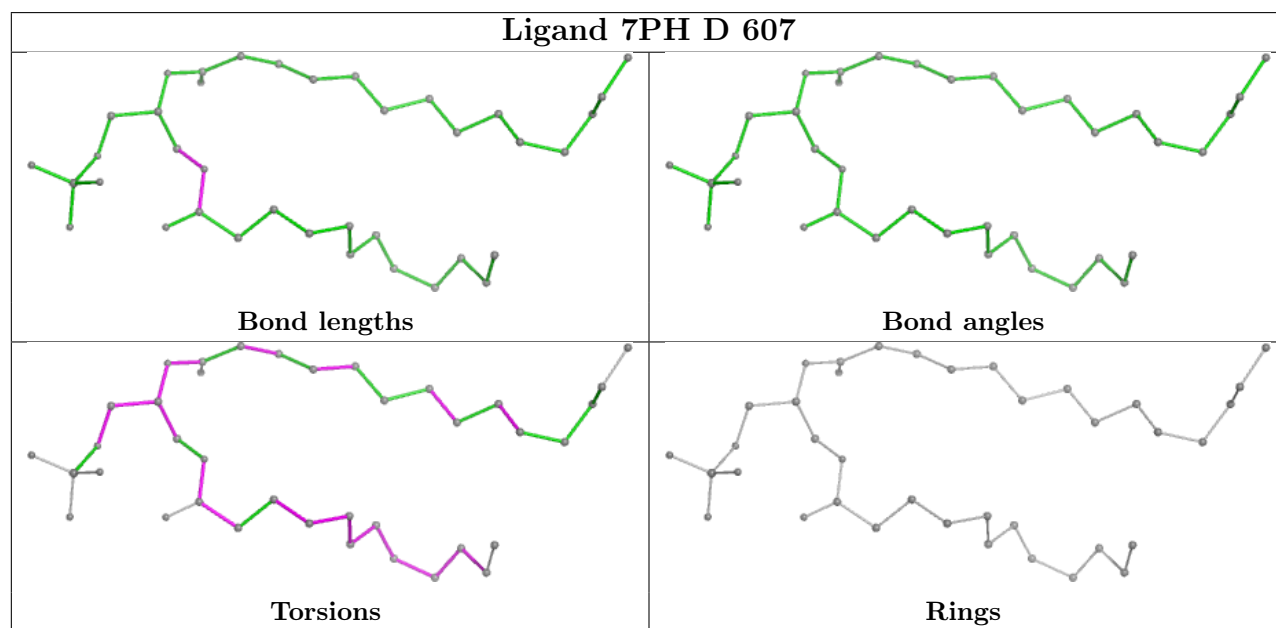
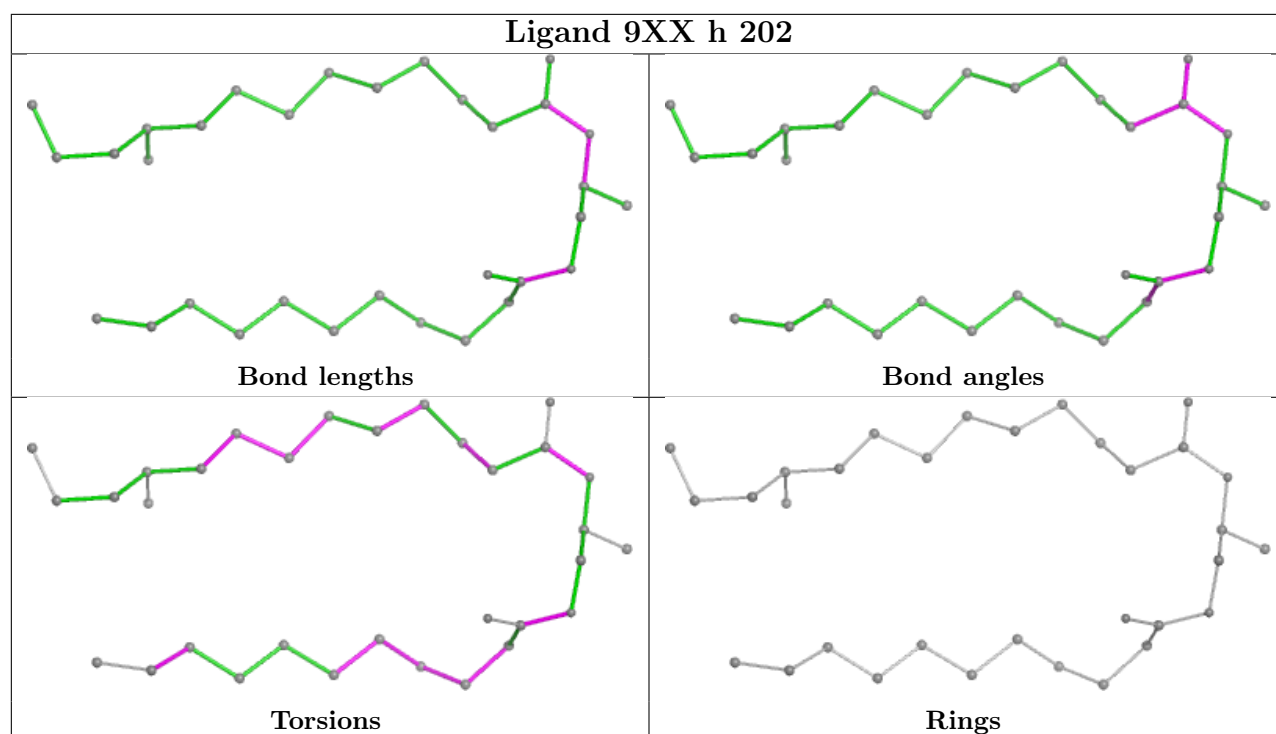


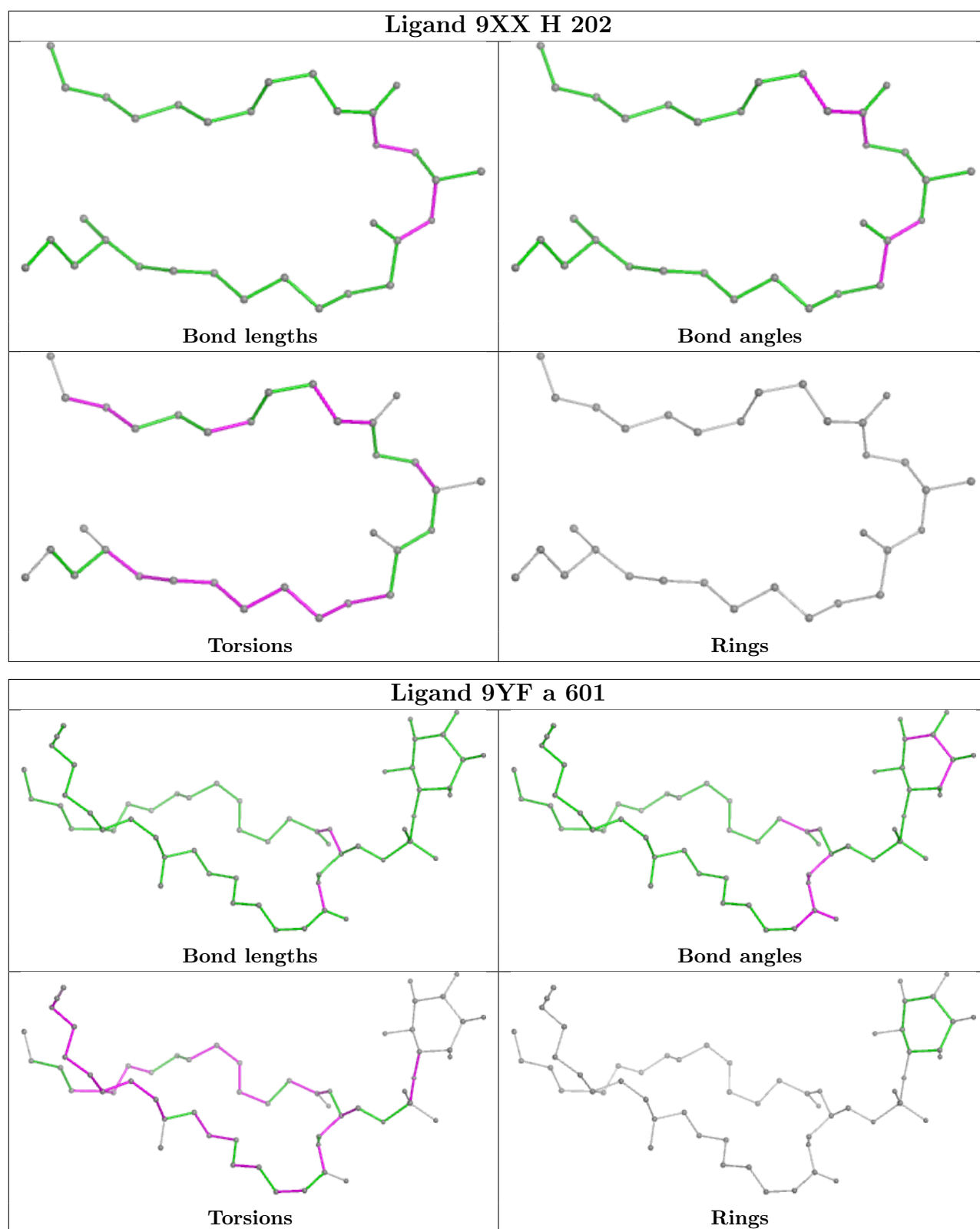












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13777. These allow visual inspection of the internal detail of the map and identification of artifacts.

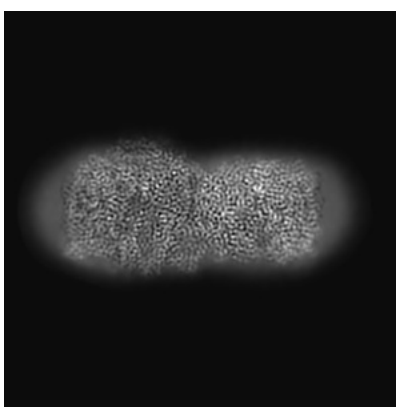
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

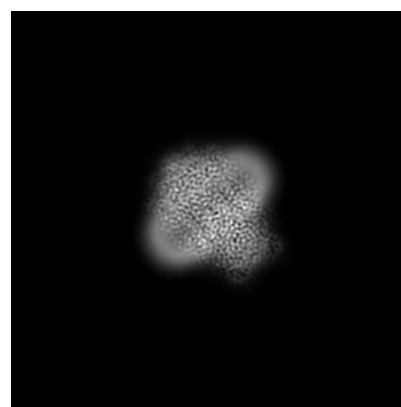
6.1.1 Primary map



X



Y

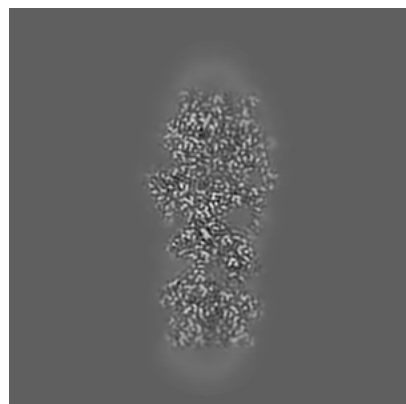


Z

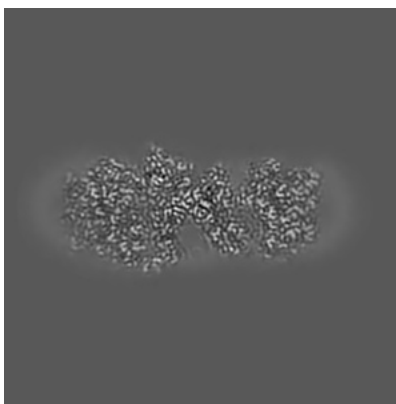
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

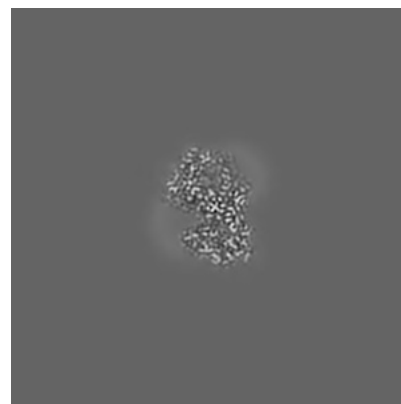
6.2.1 Primary map



X Index: 155



Y Index: 155

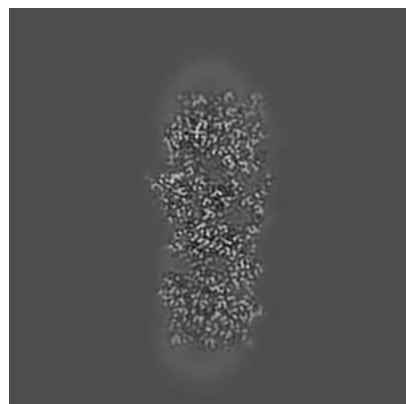


Z Index: 155

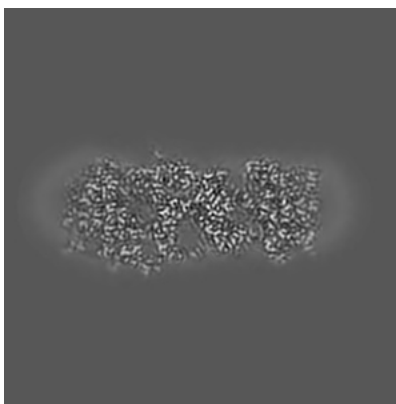
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

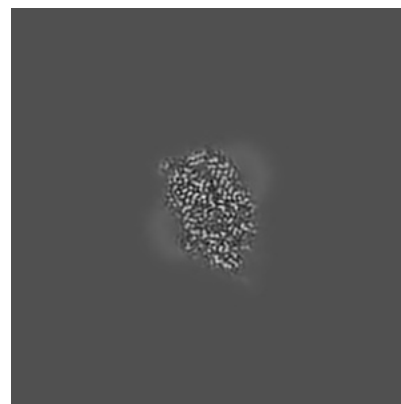
6.3.1 Primary map



X Index: 149



Y Index: 160

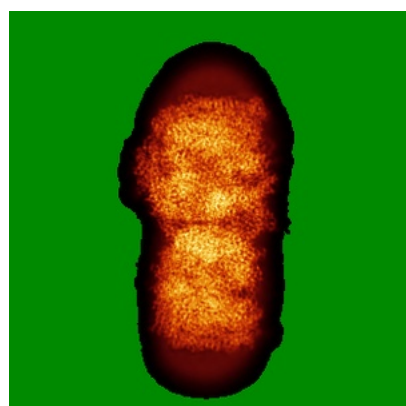


Z Index: 166

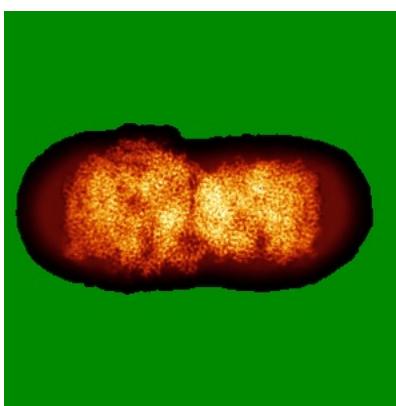
The images above show the largest variance slices of the map in three orthogonal directions.

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

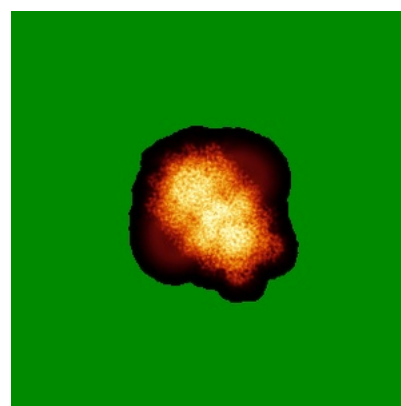
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.541. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

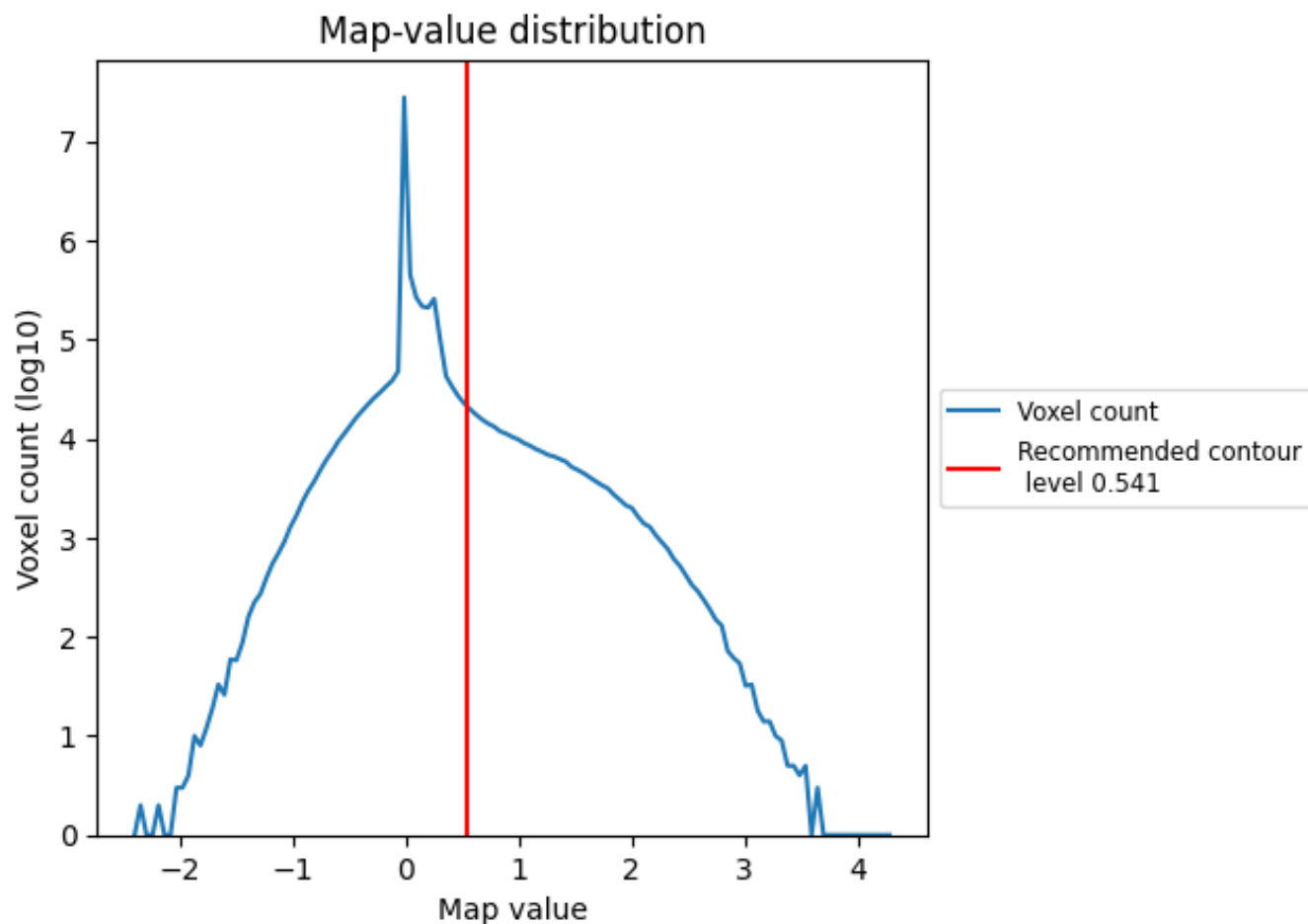
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

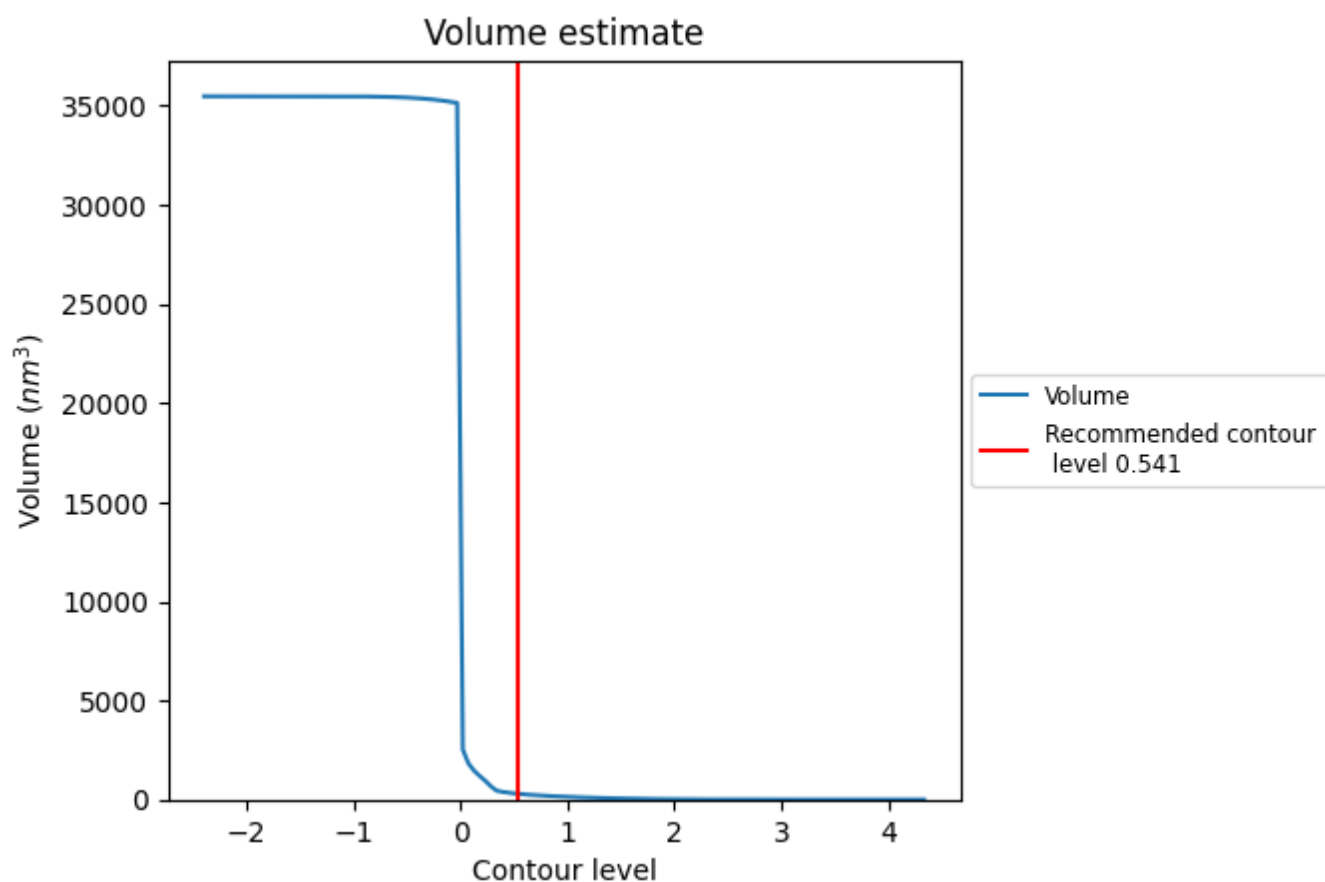
This section contains the results of statistical analysis of the map.

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.

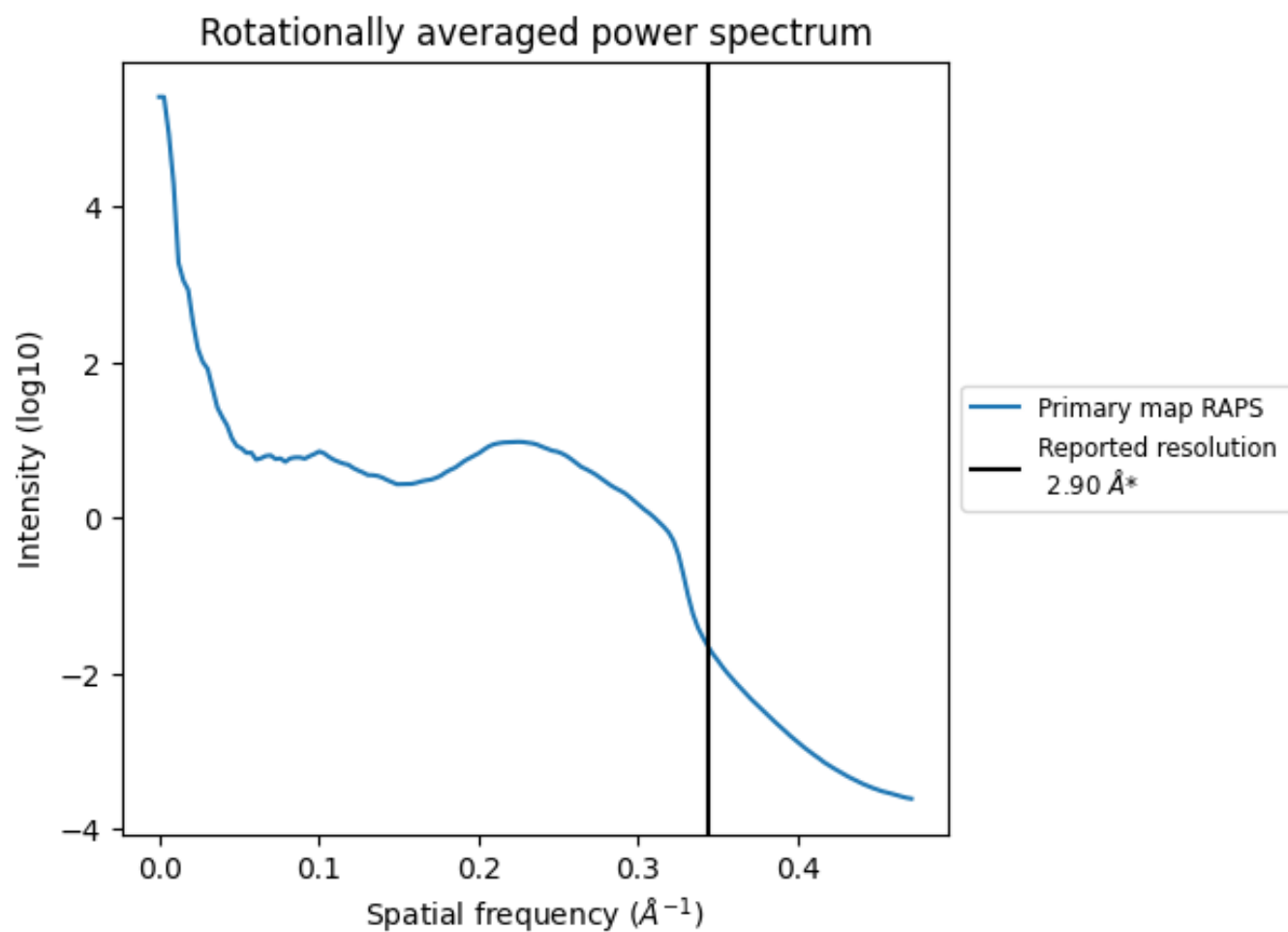
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm^3 ; this corresponds to an approximate mass of 261 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 0.345 Å⁻¹

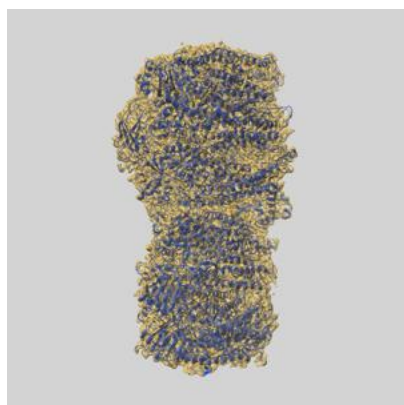
8 Fourier-Shell correlation ⓘ

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

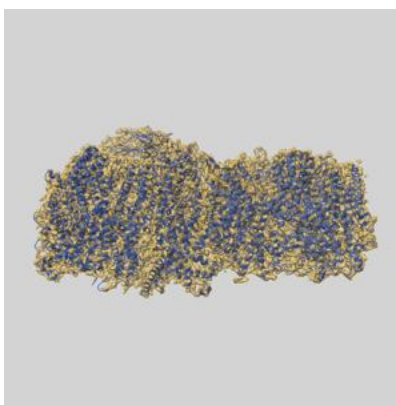
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13777 and PDB model 7Q21. Per-residue inclusion information can be found in section [3](#) on page [18](#).

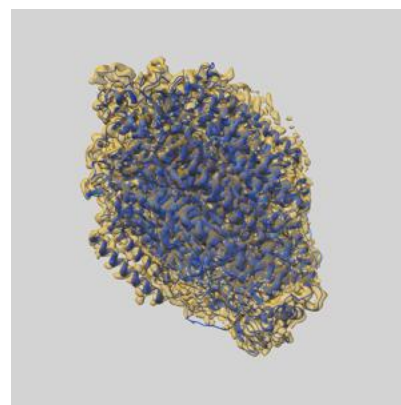
9.1 Map-model overlay [i](#)



X



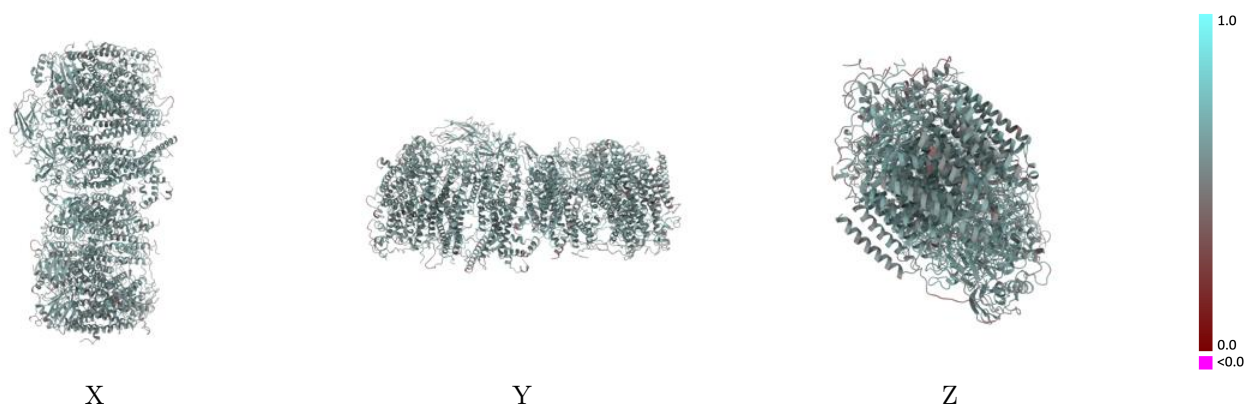
Y



Z

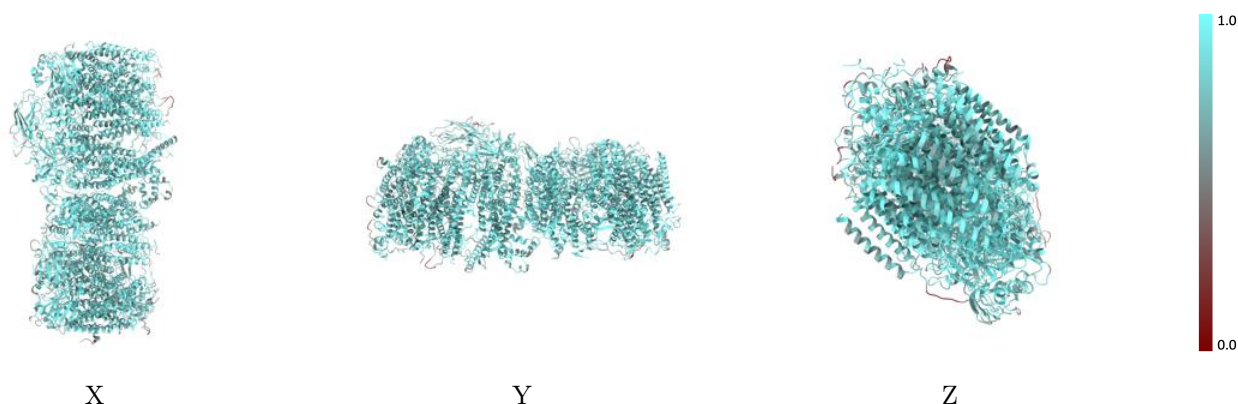
The images above show the 3D surface view of the map at the recommended contour level 0.541 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



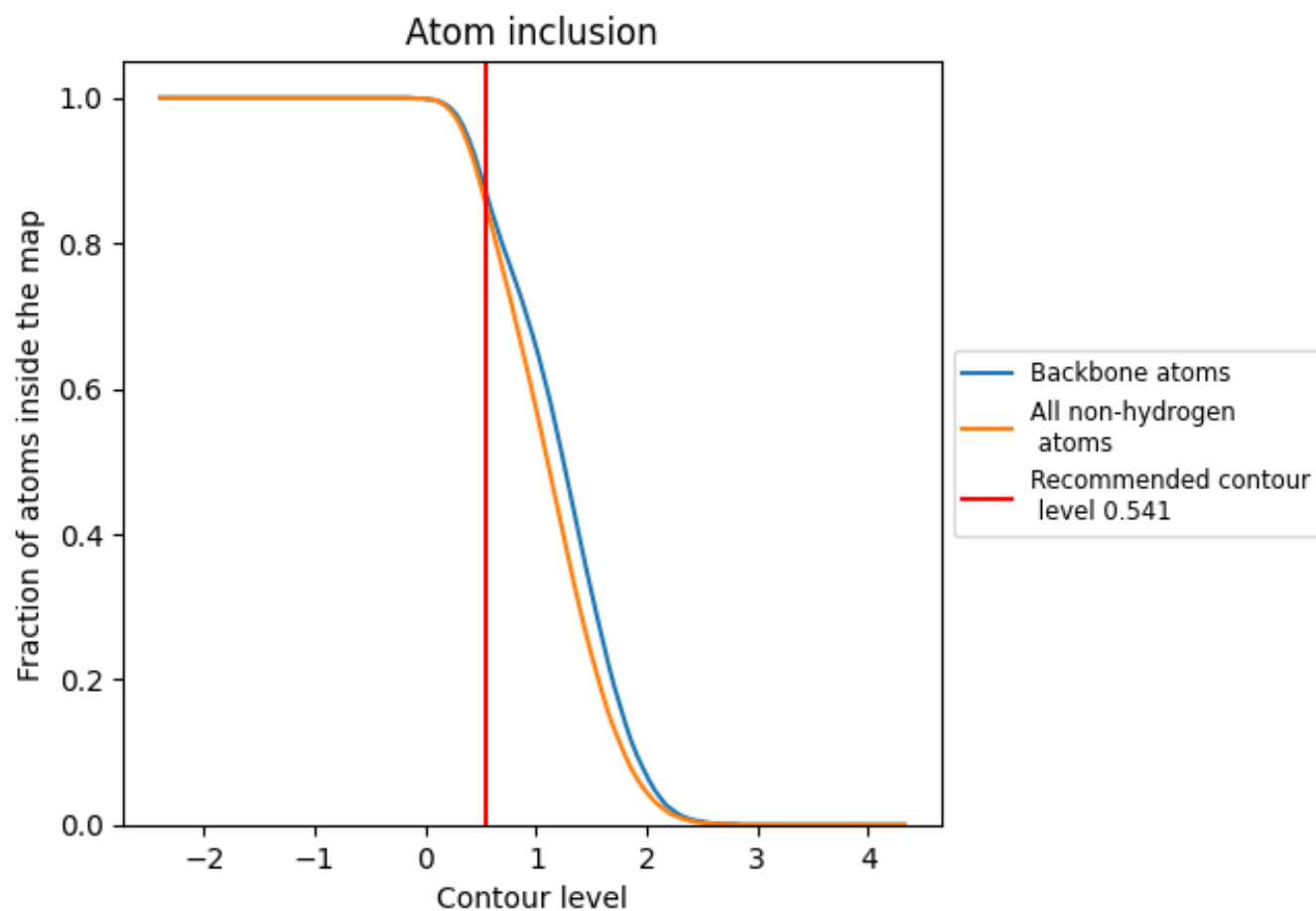
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.541).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.541) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.5710
A	 0.8860	 0.5850
B	 0.8970	 0.5910
C	 0.9010	 0.5860
D	 0.8940	 0.5860
E	 0.8820	 0.5770
F	 0.8460	 0.5750
G	 0.8390	 0.5550
H	 0.8570	 0.5590
K	 0.7210	 0.5210
L	 0.8040	 0.5490
V	 0.7660	 0.5320
X	 0.5210	 0.4590
Y	 0.8440	 0.5190
a	 0.8600	 0.5800
b	 0.8910	 0.5860
c	 0.8740	 0.5730
d	 0.8610	 0.5740
e	 0.8610	 0.5720
f	 0.8100	 0.5670
g	 0.8000	 0.5480
h	 0.8160	 0.5510
k	 0.6880	 0.5210
l	 0.7530	 0.5290
v	 0.7440	 0.5280
x	 0.4590	 0.4420
y	 0.8220	 0.5120

