



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 10:20 pm GMT

PDB ID : 8BEL  
EMDB ID : EMD-16007  
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (CIII membrane domain)  
Authors : Klusch, N.; Kuehlbrandt, W.  
Deposited on : 2022-10-21  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

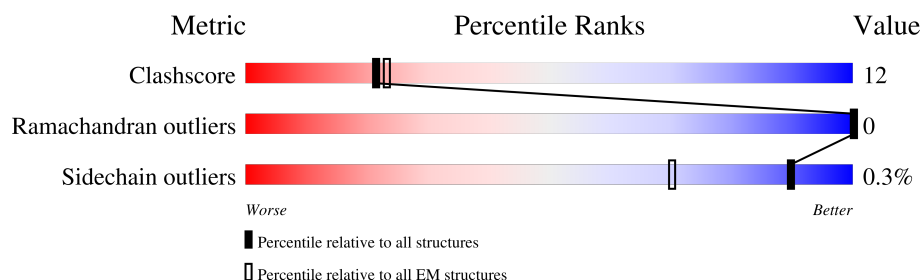
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.25 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	393	
1	M	393	
2	D	272	
2	N	272	
3	E	307	
3	O	307	
4	G	72	
4	Q	72	

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Mol	Chain	Length	Quality of chain
5	H	69	
5	R	69	
6	I	72	
6	S	72	
7	J	57	
7	T	57	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18929 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
1	M	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	SER	PRO	variant	UNP P42792
M	40	SER	PRO	variant	UNP P42792

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		
2	N	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		

- Molecule 3 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
3	O	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	69	Total	C	N	O	S	0	0
			581	387	95	98	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
5	R	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

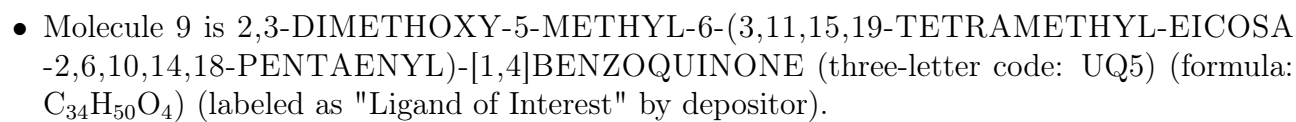
- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

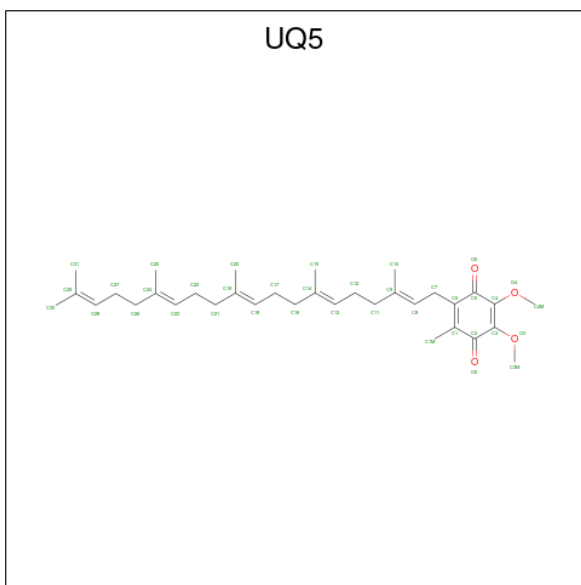
Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
6	S	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	28	Total	C	N	O	0	0
			203	137	33	33		
7	T	28	Total	C	N	O	0	0
			205	139	34	32		

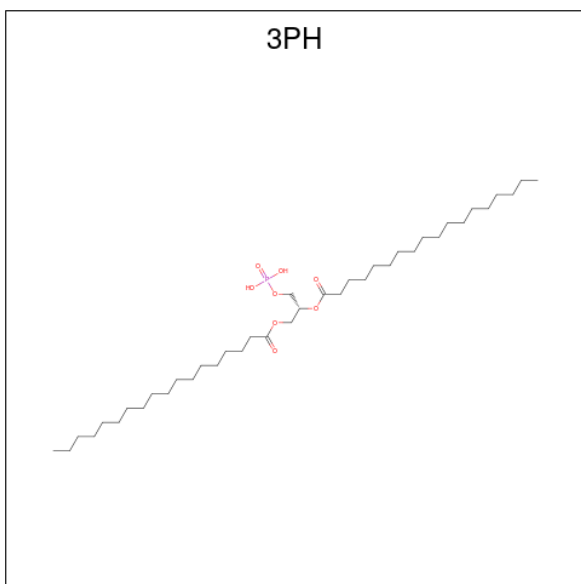
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).





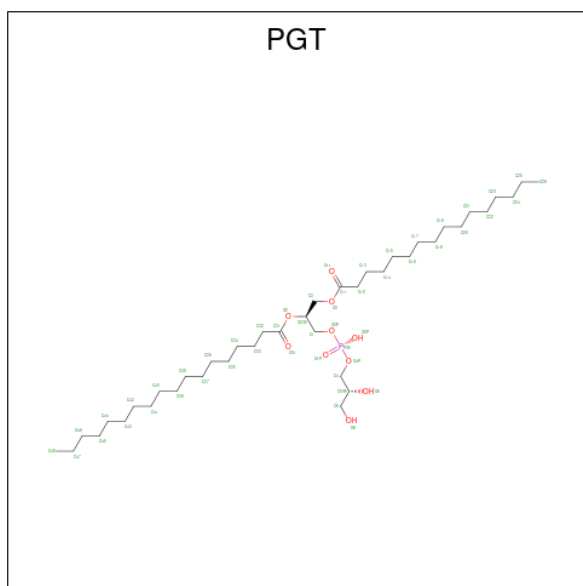
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			38	34	4	
9	C	1	Total	C	O	0
			38	34	4	
9	M	1	Total	C	O	0
			38	34	4	

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	O	P	0
			33	24	8	1	
10	G	1	Total	C	O	P	0
			33	24	8	1	
10	I	1	Total	C	O	P	0
			32	23	8	1	
10	M	1	Total	C	O	P	0
			44	35	8	1	
10	T	1	Total	C	O	P	0
			41	32	8	1	
10	T	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 11 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).

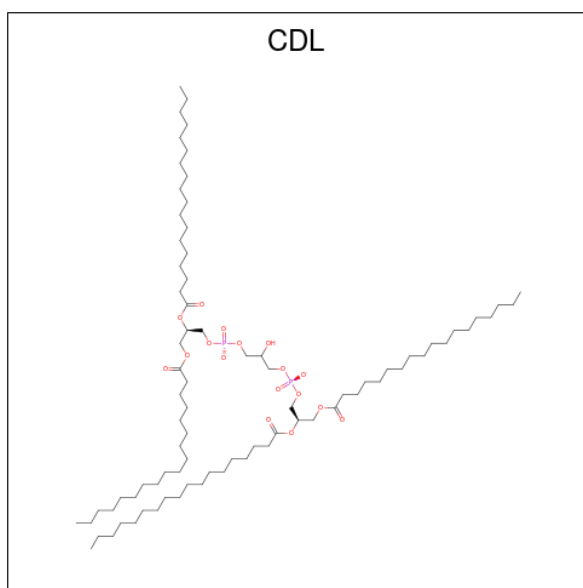


Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	P	0
			41	30	10	1	
11	C	1	Total	C	O	P	0
			51	40	10	1	
11	G	1	Total	C	O	P	0
			51	40	10	1	
11	M	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled

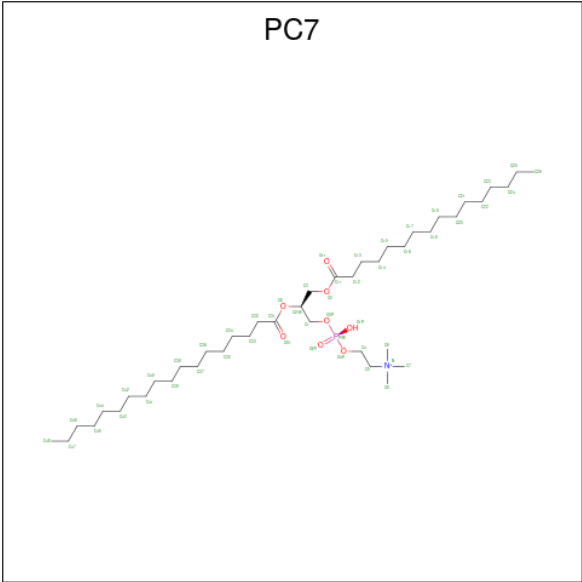


as "Ligand of Interest" by depositor).



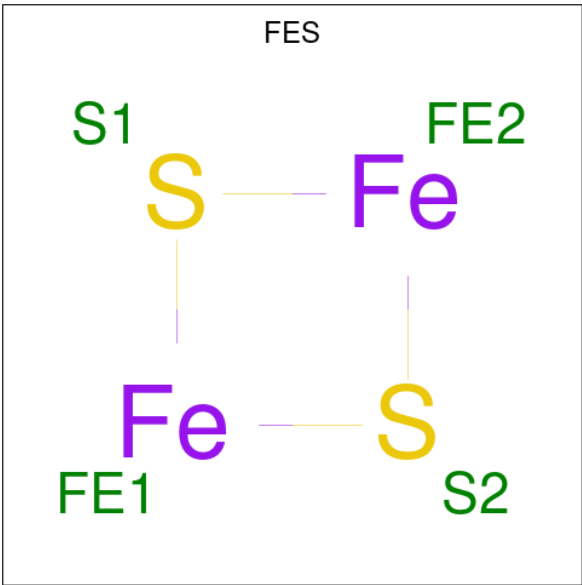
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			81	62	17	2	
12	C	1	Total	C	O	P	0
			85	66	17	2	
12	G	1	Total	C	O	P	0
			85	66	17	2	
12	M	1	Total	C	O	P	0
			77	58	17	2	
12	N	1	Total	C	O	P	0
			81	62	17	2	
12	O	1	Total	C	O	P	0
			88	69	17	2	
12	Q	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 13 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



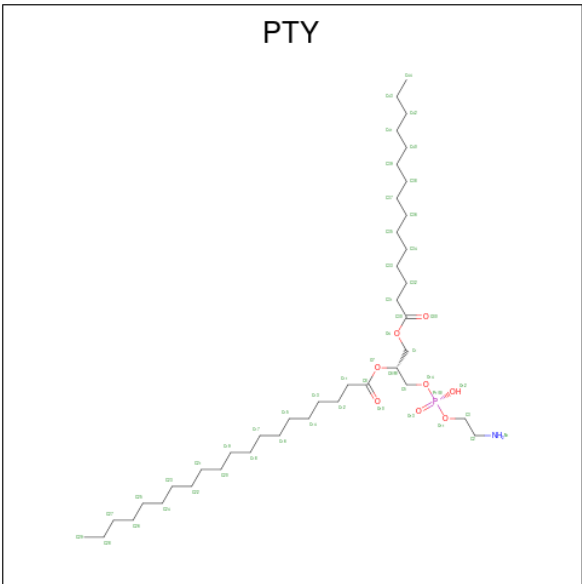
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
13	G	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	N	1	Total	C	N	O	P	0
			39	29	1	8	1	

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



Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	Fe	S	0
			4	2	2	
14	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



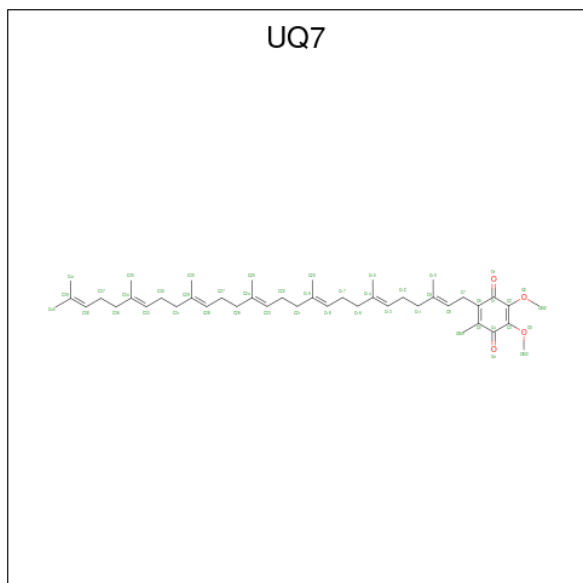
Mol	Chain	Residues	Atoms					AltConf
15	J	1	Total	C	N	O	P	0
			41	31	1	8	1	

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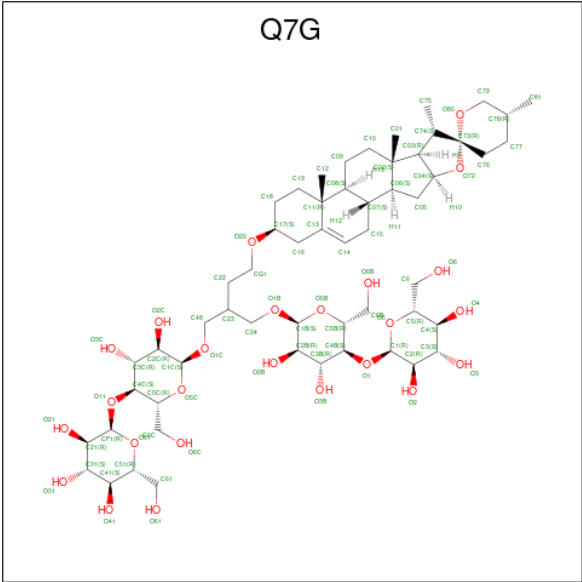
Mol	Chain	Residues	Atoms					AltConf
15	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	T	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 16 is UBIQUINONE-7 (three-letter code: UQ7) (formula:  $C_{44}H_{66}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			48	44	4	

- Molecule 17 is 2-([(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl)-4-([(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy)butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula:  $C_{56}H_{92}O_{25}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			39	34	5	
17	M	1	Total	C	O	0
			39	34	5	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	C	179	Total	O	0
			179	179	
18	D	32	Total	O	0
			32	32	
18	E	159	Total	O	0
			159	159	
18	G	30	Total	O	0
			30	30	
18	H	13	Total	O	0
			13	13	
18	I	20	Total	O	0
			20	20	
18	M	138	Total	O	0
			138	138	
18	N	33	Total	O	0
			33	33	
18	O	111	Total	O	0
			111	111	
18	Q	13	Total	O	0
			13	13	

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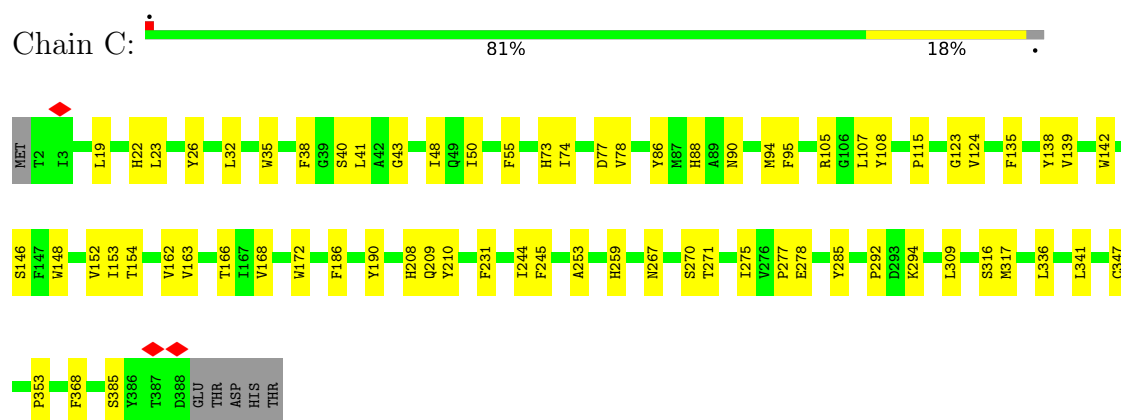
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Mol	Chain	Residues	Atoms		AltConf
18	R	2	Total 2	O 2	0
18	S	13	Total 13	O 13	0
18	T	1	Total 1	O 1	0

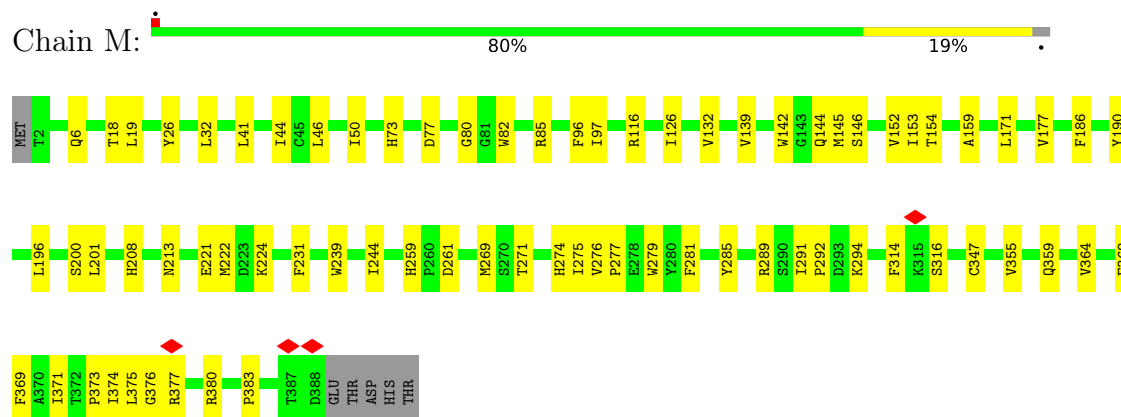
### 3 Residue-property plots [i](#)

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.

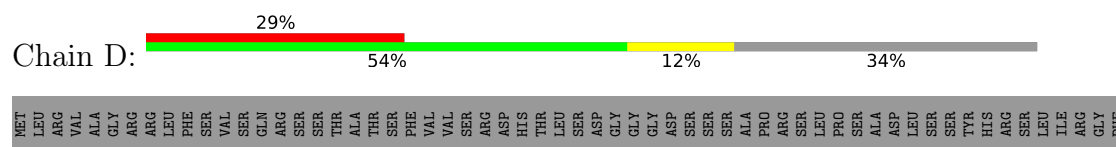
- Molecule 1: Cytochrome b

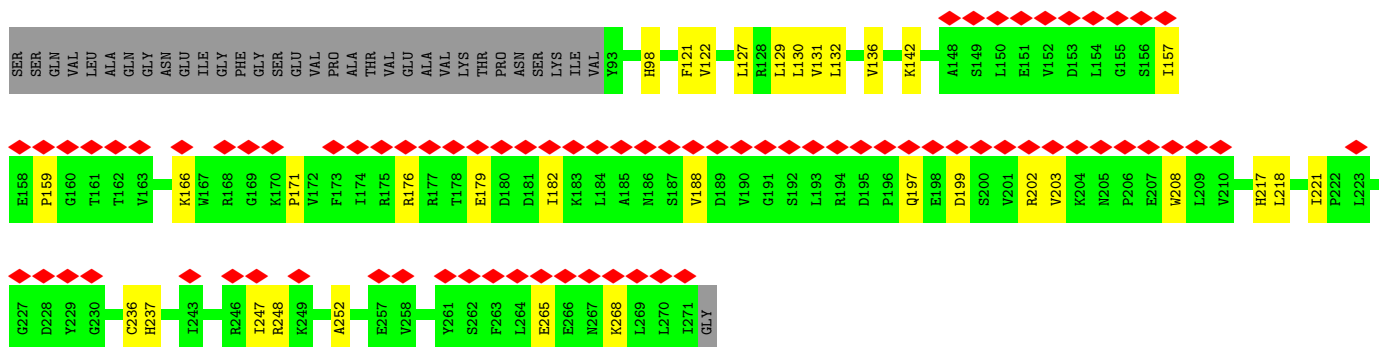


- Molecule 1: Cytochrome b

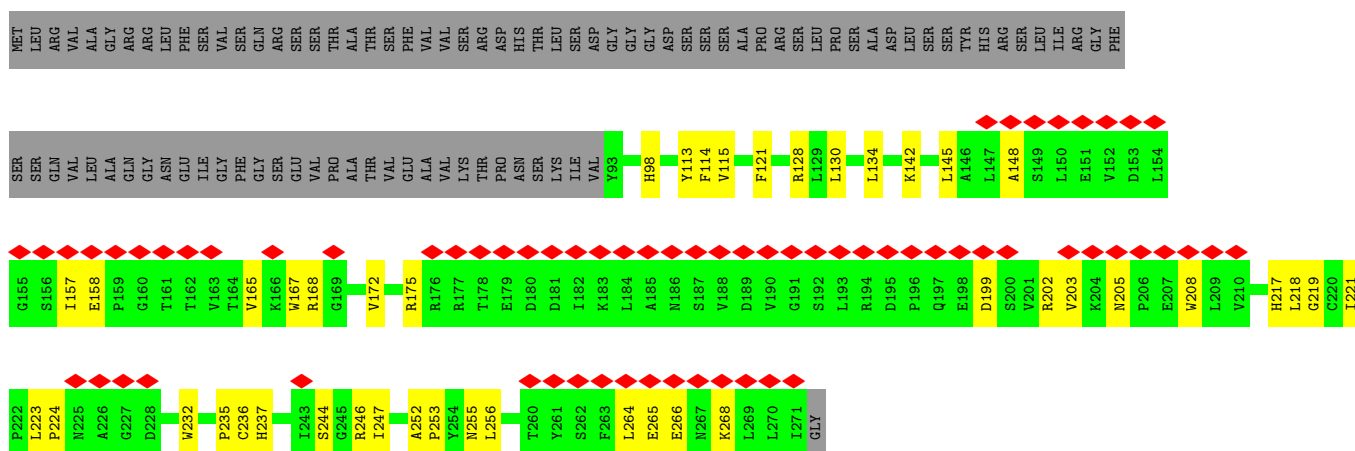


- Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

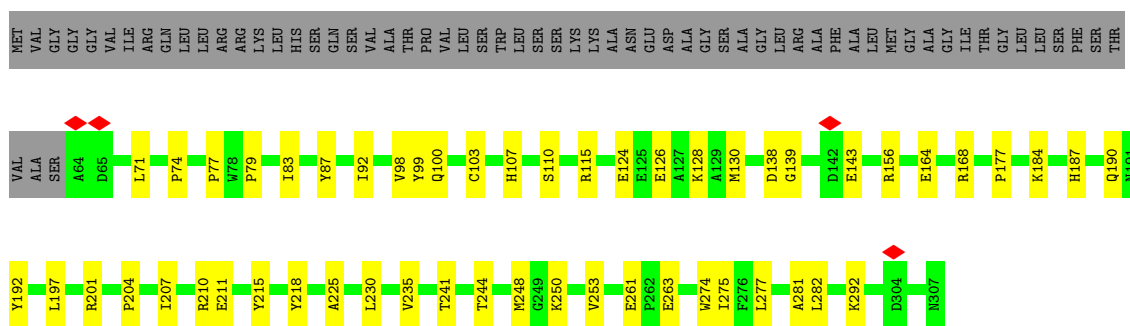




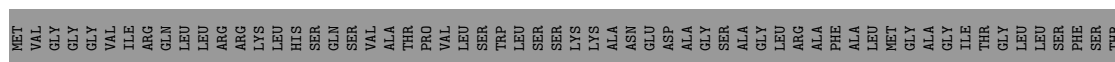
• Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



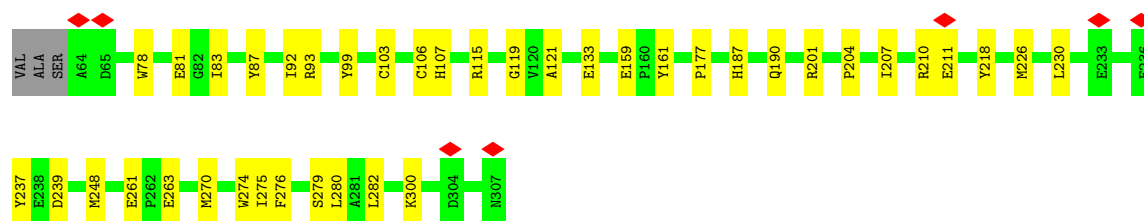
• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial



• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial



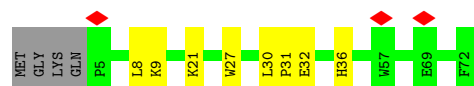
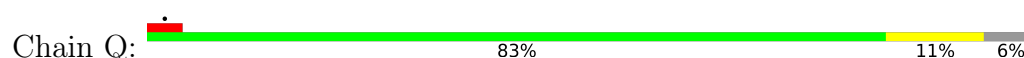




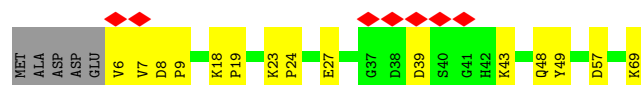
- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



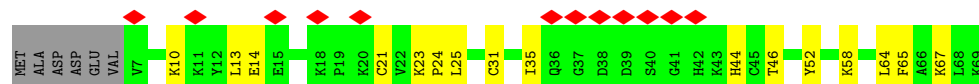
- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial

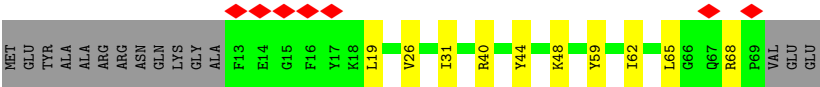


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

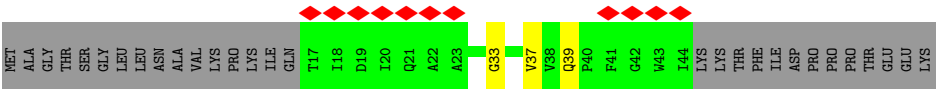
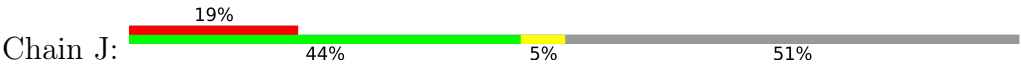


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

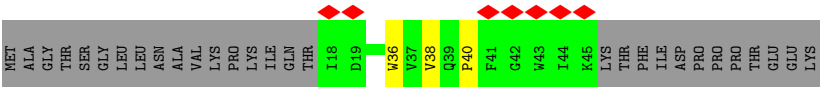
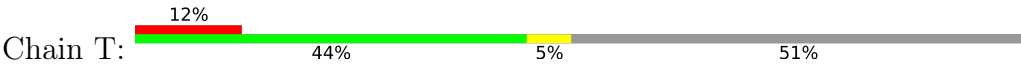




• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.977	Depositor
Minimum map value	-3.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.288	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	145.542, 163.30501, 142.677	wwPDB
Map dimensions	249, 285, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, PC7, HEM, CDL, UQ5, UQ7, PTY, Q7G, PGT, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.47	1/3208 (0.0%)	0.60	1/4395 (0.0%)
1	M	0.45	0/3208	0.64	2/4395 (0.0%)
2	D	0.31	0/1441	0.52	0/1961
2	N	0.38	0/1441	0.63	2/1961 (0.1%)
3	E	0.36	0/1968	0.56	0/2672
3	O	0.37	0/1968	0.55	0/2672
4	G	0.39	0/600	0.50	0/815
4	Q	0.34	0/591	0.60	0/802
5	H	0.29	0/531	0.47	0/713
5	R	0.43	0/524	0.69	1/703 (0.1%)
6	I	0.68	1/488 (0.2%)	0.77	0/655
6	S	0.39	0/488	0.69	0/655
7	J	0.44	0/210	0.78	1/290 (0.3%)
7	T	0.24	0/212	0.39	0/291
All	All	0.41	2/16878 (0.0%)	0.60	7/22980 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	63	SER	CA-CB	-6.47	1.43	1.52
1	C	88	HIS	C-O	-5.41	1.13	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	96	PHE	CB-CA-C	6.31	123.02	110.40
5	R	65	PHE	CB-CA-C	5.73	121.87	110.40
2	N	175	ARG	CB-CA-C	-5.73	98.94	110.40
2	N	114	PHE	CB-CA-C	5.38	121.16	110.40
1	C	86	TYR	CB-CA-C	5.36	121.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	39	GLN	CB-CA-C	5.03	120.47	110.40
1	M	383	PRO	N-CD-CG	-5.03	95.66	103.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3093	0	3074	75	0
1	M	3093	0	3074	94	0
2	D	1404	0	1395	31	0
2	N	1404	0	1395	38	0
3	E	1917	0	1844	47	0
3	O	1917	0	1844	36	0
4	G	581	0	589	17	0
4	Q	572	0	582	8	0
5	H	518	0	518	14	0
5	R	511	0	511	14	0
6	I	476	0	469	10	0
6	S	476	0	469	14	0
7	J	203	0	197	1	0
7	T	205	0	203	4	0
8	C	86	0	60	2	0
8	E	43	0	30	5	0
8	M	86	0	60	1	0
8	O	43	0	30	5	0
9	C	76	0	100	17	0
9	M	38	0	50	8	0
10	C	33	0	38	1	0
10	G	33	0	39	1	0
10	I	32	0	37	3	0
10	M	44	0	64	6	0
10	T	89	0	133	2	0
11	C	92	0	133	10	0
11	G	51	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	37	0	47	4	0
12	C	166	0	232	19	0
12	G	85	0	120	6	0
12	M	77	0	98	8	0
12	N	81	0	112	3	0
12	O	88	0	123	7	0
12	Q	70	0	87	6	0
13	C	51	0	79	9	0
13	D	34	0	42	1	0
13	G	52	0	84	5	0
13	M	45	0	60	2	0
13	N	39	0	52	6	0
14	D	4	0	0	0	0
14	N	4	0	0	1	0
15	J	41	0	58	0	0
15	M	40	0	56	2	0
15	T	29	0	31	1	0
16	M	48	0	66	12	0
17	M	78	0	0	0	0
18	C	179	0	0	17	0
18	D	32	0	0	1	0
18	E	159	0	0	14	0
18	G	30	0	0	3	0
18	H	13	0	0	1	0
18	I	20	0	0	1	0
18	M	138	0	0	21	0
18	N	33	0	0	4	0
18	O	111	0	0	8	0
18	Q	13	0	0	1	0
18	R	2	0	0	3	0
18	S	13	0	0	5	0
18	T	1	0	0	0	0
All	All	18929	0	18363	421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:316:SER:HB2	18:M:565:HOH:O	1.38	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:THR:HG22	1:M:171:LEU:HD21	1.18	1.13
1:M:154:THR:CG2	1:M:171:LEU:HD21	1.86	1.05
1:C:292:PRO:HA	18:N:425:HOH:O	1.57	1.01
1:M:154:THR:HG22	1:M:171:LEU:CD2	1.91	1.00
3:O:115:ARG:HD3	18:O:604:HOH:O	1.62	0.99
3:O:161:TYR:O	18:O:501:HOH:O	1.81	0.98
1:M:154:THR:CG2	1:M:171:LEU:CD2	2.44	0.94
1:C:107:LEU:HB3	18:C:615:HOH:O	1.68	0.93
4:G:28:LYS:HD2	18:G:223:HOH:O	1.72	0.90
5:H:6:VAL:HG12	5:H:7:VAL:H	1.35	0.90
1:M:274:HIS:CE1	1:M:276:VAL:CG1	2.57	0.88
3:E:77:PRO:O	18:E:501:HOH:O	1.92	0.87
5:H:6:VAL:HG12	5:H:7:VAL:N	1.87	0.87
1:M:6:GLN:HG2	18:M:625:HOH:O	1.73	0.87
1:M:369:PHE:CZ	18:M:626:HOH:O	2.29	0.84
5:H:6:VAL:HG12	5:H:7:VAL:HG22	1.60	0.84
1:C:294:LYS:HG2	2:N:217:HIS:HD2	1.42	0.83
1:M:316:SER:HA	18:M:565:HOH:O	1.79	0.81
1:M:316:SER:CA	18:M:565:HOH:O	2.26	0.81
1:M:18:THR:HG22	18:M:610:HOH:O	1.81	0.81
4:Q:32:GLU:O	4:Q:36:HIS:ND1	2.10	0.81
1:C:271:THR:OG1	18:C:501:HOH:O	1.98	0.80
1:M:213:ASN:HB2	18:M:609:HOH:O	1.81	0.80
1:M:154:THR:HB	1:M:171:LEU:HD22	1.62	0.80
1:M:274:HIS:CE1	1:M:276:VAL:HG13	2.16	0.80
1:M:274:HIS:CE1	1:M:276:VAL:HG11	2.18	0.79
3:E:74:PRO:HG3	5:H:57:ASP:HB3	1.63	0.79
1:C:26:TYR:HB3	9:C:403:UQ5:H3M1	1.66	0.78
3:E:138:ASP:OD1	3:E:139:GLY:N	2.17	0.78
1:C:259:HIS:CD2	18:E:540:HOH:O	2.36	0.78
1:C:186:PHE:HE2	1:M:186:PHE:HE2	1.31	0.77
1:M:77:ASP:OD1	18:M:501:HOH:O	2.02	0.77
2:D:265:GLU:HG2	2:D:268:LYS:HB2	1.66	0.77
11:M:406:PGT:H42	15:T:103:PTY:HC21	1.66	0.77
3:O:187:HIS:HB3	18:O:605:HOH:O	1.86	0.76
1:C:73:HIS:NE2	18:C:504:HOH:O	2.18	0.76
3:E:261:GLU:OE1	18:E:502:HOH:O	2.04	0.75
4:Q:9:LYS:O	18:Q:201:HOH:O	2.05	0.75
1:C:259:HIS:HD2	18:E:540:HOH:O	1.68	0.75
1:M:153:ILE:HG21	16:M:404:UQ7:H161	1.69	0.74
5:R:58:LYS:HG3	18:R:102:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:408:CDL:H871	2:D:130:LEU:HD22	1.69	0.74
1:M:44:ILE:HG13	11:M:406:PGT:H252	1.69	0.74
1:M:259:HIS:CE1	1:M:276:VAL:HG21	2.23	0.74
3:O:261:GLU:OE2	18:O:502:HOH:O	2.04	0.74
1:M:259:HIS:NE2	1:M:276:VAL:HG23	2.03	0.73
1:C:77:ASP:OD2	18:C:502:HOH:O	2.06	0.73
2:N:202:ARG:NH1	2:N:244:SER:O	2.21	0.73
3:O:210:ARG:NH1	3:O:211:GLU:O	2.21	0.73
1:C:142:TRP:HA	18:C:563:HOH:O	1.89	0.72
3:E:253:VAL:HG12	18:E:630:HOH:O	1.89	0.71
2:N:265:GLU:HG2	2:N:266:GLU:H	1.54	0.71
12:M:408:CDL:H131	13:M:409:PC7:H381	1.72	0.71
3:E:190:GLN:N	3:E:190:GLN:OE1	2.22	0.70
1:M:316:SER:CB	18:M:565:HOH:O	2.07	0.70
3:O:280:LEU:HB3	12:Q:101:CDL:H371	1.73	0.70
1:M:73:HIS:NE2	18:M:503:HOH:O	2.24	0.70
3:O:300:LYS:HD3	18:O:529:HOH:O	1.90	0.70
12:M:408:CDL:HB22	18:M:580:HOH:O	1.91	0.70
1:M:259:HIS:NE2	1:M:276:VAL:CG2	2.55	0.69
1:C:259:HIS:NE2	18:C:507:HOH:O	2.25	0.69
3:O:78:TRP:HB2	3:O:81:GLU:HG2	1.72	0.69
1:M:213:ASN:CB	18:M:609:HOH:O	2.38	0.69
3:O:204:PRO:HG2	3:O:207:ILE:HG13	1.73	0.69
2:D:98:HIS:NE2	18:D:401:HOH:O	2.26	0.69
4:G:27:TRP:HB3	12:G:103:CDL:H321	1.75	0.68
1:M:154:THR:CB	1:M:171:LEU:HD22	2.23	0.68
1:C:347:CYS:SG	18:C:507:HOH:O	2.52	0.68
1:M:26:TYR:HD2	9:M:403:UQ5:H3M1	1.59	0.68
1:M:269:MET:HE2	1:M:269:MET:HA	1.75	0.68
6:S:68:ARG:HD2	18:S:105:HOH:O	1.94	0.68
3:O:159:GLU:HB3	18:O:501:HOH:O	1.93	0.67
3:O:190:GLN:OE1	3:O:190:GLN:N	2.24	0.66
1:M:271:THR:CG2	1:M:275:ILE:HD11	2.25	0.66
3:E:210:ARG:NH1	3:E:211:GLU:O	2.29	0.66
1:C:208:HIS:NE2	9:C:403:UQ5:H4M3	2.11	0.65
1:C:294:LYS:HG2	2:N:217:HIS:CD2	2.30	0.65
3:O:230:LEU:HD22	3:O:248:MET:HE3	1.79	0.65
3:E:184:LYS:HG2	18:E:519:HOH:O	1.96	0.65
4:G:24:THR:O	18:G:201:HOH:O	2.15	0.65
1:C:163:VAL:HG12	10:T:101:3PH:H12	1.78	0.64
2:N:223:LEU:HD11	2:N:235:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:275:ILE:HB	18:M:534:HOH:O	1.97	0.63
12:C:408:CDL:H802	12:C:408:CDL:H201	1.79	0.63
2:D:218:LEU:HD13	1:M:152:VAL:HG13	1.81	0.62
1:C:253:ALA:HB2	11:C:407:PGT:H2	1.82	0.62
1:C:271:THR:HG21	2:N:221:ILE:O	1.99	0.62
2:N:202:ARG:NH2	2:N:256:LEU:O	2.32	0.62
1:M:144:GLN:NE2	18:M:506:HOH:O	2.32	0.62
3:E:282:LEU:HD23	12:G:103:CDL:H561	1.81	0.62
1:M:285:TYR:CZ	1:M:289:ARG:HD3	2.35	0.62
3:E:190:GLN:NE2	18:E:502:HOH:O	2.30	0.61
2:N:223:LEU:CD1	2:N:235:PRO:HG3	2.30	0.61
12:C:408:CDL:H751	2:D:127:LEU:HB2	1.82	0.61
10:M:405:3PH:H3D1	3:O:275:ILE:HG22	1.81	0.61
13:N:303:PC7:H182	7:T:36:TRP:HZ3	1.64	0.61
4:Q:27:TRP:HA	4:Q:30:LEU:HD13	1.81	0.61
3:E:225:ALA:HB3	8:E:400:HEM:HBD2	1.83	0.61
1:M:154:THR:CG2	1:M:171:LEU:HD22	2.30	0.61
2:N:113:TYR:CZ	13:N:303:PC7:H63	2.36	0.61
3:E:235:VAL:HG12	3:E:248:MET:SD	2.42	0.60
1:C:139:VAL:HA	1:C:146:SER:HB3	1.83	0.60
1:C:48:ILE:HG12	12:C:408:CDL:H822	1.83	0.60
2:D:237:HIS:HD2	1:M:289:ARG:HG2	1.66	0.60
1:M:153:ILE:HD11	16:M:404:UQ7:C5	2.31	0.59
1:C:77:ASP:HA	2:D:142:LYS:HD2	1.84	0.59
10:I:101:3PH:H241	10:I:101:3PH:H341	1.85	0.59
3:O:103:CYS:SG	8:O:401:HEM:CAB	2.91	0.59
1:M:139:VAL:HA	1:M:146:SER:HB3	1.83	0.59
2:N:115:VAL:HG11	12:Q:101:CDL:H312	1.84	0.59
3:O:133:GLU:OE2	6:S:68:ARG:NH2	2.21	0.59
1:C:138:TYR:CE1	1:C:278:GLU:OE2	2.56	0.59
3:O:99:TYR:HA	3:O:103:CYS:SG	2.43	0.59
1:M:376:GLY:HA3	18:M:565:HOH:O	2.02	0.58
4:G:26:LEU:HD21	12:G:103:CDL:HB32	1.86	0.58
4:G:38:VAL:HG11	10:G:101:3PH:H321	1.84	0.58
6:S:19:LEU:HD22	6:S:26:VAL:HG21	1.85	0.58
4:G:4:GLN:NE2	4:G:5:PRO:O	2.36	0.58
3:E:241:THR:HG23	5:H:69:LYS:HE3	1.85	0.58
10:M:405:3PH:H3B1	3:O:276:PHE:HB2	1.85	0.58
2:N:134:LEU:HD11	12:N:302:CDL:H861	1.85	0.58
1:C:152:VAL:HG21	9:C:404:UQ5:O3	2.04	0.57
3:E:277:LEU:HD21	6:I:42:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:13:LEU:HD11	5:R:67:LYS:HD3	1.86	0.57
12:C:409:CDL:H172	13:C:410:PC7:H422	1.86	0.57
8:E:400:HEM:HMC1	8:E:400:HEM:HBC2	1.85	0.57
1:M:285:TYR:HB2	16:M:404:UQ7:HM52	1.86	0.57
2:N:98:HIS:NE2	18:N:403:HOH:O	2.32	0.57
3:O:93:ARG:HB2	3:O:121:ALA:HB1	1.86	0.57
1:M:281:PHE:HB3	16:M:404:UQ7:H102	1.87	0.56
2:N:265:GLU:HG2	2:N:266:GLU:N	2.20	0.56
3:E:100:GLN:NE2	18:E:512:HOH:O	2.32	0.56
1:M:259:HIS:CE1	1:M:276:VAL:CG2	2.88	0.56
6:S:62:ILE:HB	6:S:65:LEU:HB2	1.88	0.56
3:E:99:TYR:CD1	3:E:103:CYS:HB2	2.41	0.56
1:M:153:ILE:CG2	16:M:404:UQ7:H161	2.35	0.56
1:C:209:GLN:NE2	18:C:517:HOH:O	2.35	0.56
8:E:400:HEM:HMB1	8:E:400:HEM:HBB2	1.87	0.56
2:N:246:ARG:HA	2:N:255:ASN:HB3	1.88	0.56
3:O:99:TYR:CD1	3:O:103:CYS:HB2	2.40	0.56
1:M:145:MET:CE	1:M:276:VAL:H	2.19	0.56
3:O:270:MET:HG2	3:O:274:TRP:HD1	1.71	0.55
5:H:57:ASP:OD1	18:H:101:HOH:O	2.18	0.55
3:E:126:GLU:HG2	6:I:68:ARG:HB3	1.87	0.55
1:M:271:THR:HG23	1:M:275:ILE:HD11	1.88	0.55
2:D:131:VAL:HG13	16:M:404:UQ7:H361	1.88	0.55
12:M:408:CDL:H552	12:O:402:CDL:H202	1.89	0.55
4:G:36:HIS:O	4:G:40:GLU:HG3	2.07	0.55
1:M:145:MET:HE1	1:M:276:VAL:H	1.71	0.55
1:C:26:TYR:CB	9:C:403:UQ5:H3M1	2.34	0.54
1:M:347:CYS:SG	18:M:632:HOH:O	2.57	0.54
1:C:154:THR:OG1	1:C:172:TRP:NE1	2.33	0.54
12:N:302:CDL:H752	12:N:302:CDL:H522	1.88	0.54
3:O:119:GLY:O	18:O:504:HOH:O	2.18	0.54
3:E:83:ILE:HD11	10:I:101:3PH:H332	1.90	0.54
3:O:270:MET:HG2	3:O:274:TRP:CD1	2.42	0.54
10:M:405:3PH:H3D2	3:O:276:PHE:HA	1.89	0.54
1:C:277:PRO:HB3	9:C:404:UQ5:C5	2.38	0.54
1:M:132:VAL:HG22	16:M:404:UQ7:H172	1.88	0.54
9:M:403:UQ5:H3M3	9:M:403:UQ5:H4M2	1.87	0.54
1:C:162:VAL:HG23	1:C:163:VAL:HG13	1.90	0.54
1:C:316:SER:HB2	18:C:631:HOH:O	2.07	0.53
1:C:277:PRO:HB3	9:C:404:UQ5:O5	2.07	0.53
2:N:115:VAL:CG1	12:Q:101:CDL:H312	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:247:ILE:HD13	2:N:252:ALA:HB3	1.89	0.53
5:R:10:LYS:HG3	5:R:64:LEU:HD22	1.90	0.53
6:S:44:TYR:CE1	6:S:48:LYS:HE2	2.44	0.53
2:D:121:PHE:HE1	6:I:31:ILE:HA	1.73	0.53
3:O:201:ARG:NH2	3:O:218:TYR:OH	2.41	0.53
1:C:368:PHE:HB2	11:G:102:PGT:H481	1.90	0.53
1:C:259:HIS:ND1	18:C:513:HOH:O	2.32	0.53
1:M:222:MET:CE	4:Q:8:LEU:HD23	2.38	0.53
3:E:184:LYS:CG	18:E:519:HOH:O	2.55	0.53
3:E:197:LEU:HB3	3:E:230:LEU:HD12	1.91	0.52
1:M:46:LEU:HD23	9:M:403:UQ5:H202	1.90	0.52
1:M:126:ILE:HD13	18:M:588:HOH:O	2.09	0.52
2:N:264:LEU:HB2	2:N:268:LYS:HB2	1.91	0.52
1:M:259:HIS:CD2	1:M:276:VAL:HG23	2.44	0.52
2:N:224:PRO:HA	2:N:232:TRP:CD1	2.45	0.52
1:C:50:ILE:HA	8:C:402:HEM:HAB	1.91	0.52
9:C:403:UQ5:H1M2	11:C:406:PGT:H392	1.91	0.52
1:M:239:TRP:HH2	11:M:406:PGT:H212	1.74	0.52
5:R:58:LYS:CG	18:R:102:HOH:O	2.51	0.52
1:M:244:ILE:HG21	12:O:402:CDL:H382	1.92	0.52
1:C:74:ILE:HA	1:C:78:VAL:HG13	1.92	0.52
12:C:409:CDL:H442	4:G:49:VAL:HG21	1.92	0.52
3:O:282:LEU:HD23	12:O:402:CDL:H342	1.92	0.51
12:M:408:CDL:H532	12:O:402:CDL:H181	1.91	0.51
2:D:157:ILE:H	2:D:208:TRP:HH2	1.58	0.51
7:J:33:GLY:O	7:J:37:VAL:HG23	2.10	0.51
1:C:385:SER:OG	18:C:505:HOH:O	2.18	0.51
1:C:275:ILE:HG21	2:N:236:CYS:SG	2.50	0.51
1:M:274:HIS:HE1	1:M:276:VAL:HG11	1.75	0.51
2:N:219:GLY:O	18:N:401:HOH:O	2.19	0.51
3:E:263:GLU:HA	18:E:588:HOH:O	2.11	0.51
4:G:72:PHE:C	18:G:206:HOH:O	2.49	0.51
1:C:267:ASN:OD1	1:C:270:SER:OG	2.29	0.51
4:G:56:TYR:O	4:G:60:GLN:HG2	2.11	0.51
12:C:409:CDL:O1	13:C:410:PC7:O31	2.29	0.51
3:E:192:TYR:OH	8:E:400:HEM:O1A	2.23	0.51
2:D:237:HIS:CD2	1:M:289:ARG:HG2	2.46	0.50
2:D:247:ILE:HD13	2:D:252:ALA:HB3	1.92	0.50
1:M:97:ILE:HG13	1:M:279:TRP:HH2	1.76	0.50
1:C:152:VAL:HG21	9:C:404:UQ5:C3	2.41	0.50
1:M:285:TYR:CE1	16:M:404:UQ7:HM32	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:403:UQ5:H18	11:C:406:PGT:C48	2.41	0.50
3:E:99:TYR:HA	3:E:103:CYS:SG	2.51	0.50
1:M:18:THR:HG23	1:M:19:LEU:HD22	1.92	0.50
4:G:30:LEU:O	4:G:34:ILE:HD12	2.11	0.50
5:H:6:VAL:CG1	5:H:7:VAL:H	2.06	0.50
3:E:244:THR:O	3:E:248:MET:HG3	2.11	0.50
1:C:245:PHE:HD1	11:C:407:PGT:H431	1.77	0.50
1:M:32:LEU:HB2	1:M:231:PHE:CE1	2.47	0.50
1:M:152:VAL:HG12	1:M:153:ILE:HD12	1.94	0.50
2:D:166:LYS:HG3	1:M:269:MET:SD	2.52	0.49
12:M:408:CDL:H712	12:M:408:CDL:H541	1.94	0.49
1:C:55:PHE:HZ	16:M:404:UQ7:H311	1.76	0.49
1:M:371:ILE:O	1:M:374:ILE:HG13	2.12	0.49
1:C:336:LEU:HD11	13:C:410:PC7:H411	1.94	0.49
1:C:277:PRO:O	18:C:506:HOH:O	2.20	0.49
5:R:25:LEU:HD23	5:R:52:TYR:CE1	2.48	0.49
1:M:97:ILE:HG13	1:M:279:TRP:CH2	2.48	0.49
2:N:148:ALA:HA	2:N:168:ARG:HD2	1.95	0.49
13:N:303:PC7:H182	7:T:36:TRP:CZ3	2.47	0.48
2:D:121:PHE:CE1	6:I:31:ILE:HA	2.49	0.48
1:M:377:ARG:HA	1:M:380:ARG:HD2	1.95	0.48
11:C:406:PGT:H351	12:C:408:CDL:H112	1.95	0.48
2:N:237:HIS:HB2	14:N:301:FES:S2	2.53	0.48
12:C:409:CDL:H432	4:G:49:VAL:HG11	1.96	0.48
12:C:408:CDL:H742	2:D:127:LEU:HD22	1.96	0.48
5:R:10:LYS:O	5:R:14:GLU:HG2	2.12	0.48
12:C:408:CDL:H711	13:D:302:PC7:H142	1.96	0.48
3:O:103:CYS:SG	8:O:401:HEM:HAB	2.54	0.48
1:M:314:PHE:CD2	1:M:373:PRO:HG3	2.48	0.48
6:I:62:ILE:HA	18:I:214:HOH:O	2.13	0.47
6:S:68:ARG:HG2	18:S:105:HOH:O	2.14	0.47
12:C:409:CDL:H422	12:C:409:CDL:H391	1.65	0.47
2:D:171:PRO:HG2	2:D:221:ILE:HD13	1.96	0.47
1:M:50:ILE:HA	8:M:402:HEM:HAB	1.96	0.47
1:M:159:ALA:HA	1:M:294:LYS:HD3	1.96	0.47
10:M:405:3PH:H2C1	12:O:402:CDL:H232	1.95	0.47
5:H:27:GLU:HG3	5:H:48:GLN:HG2	1.95	0.47
3:O:226:MET:HB2	8:O:401:HEM:C1D	2.49	0.47
6:I:58:ARG:HB2	6:I:61:ASP:OD1	2.15	0.47
1:M:142:TRP:HH2	1:M:177:VAL:HG12	1.78	0.47
1:M:126:ILE:HG23	1:M:196:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:ILE:HB	1:M:271:THR:OG1	2.15	0.47
2:D:236:CYS:SG	1:M:275:ILE:HD12	2.55	0.47
1:M:277:PRO:HB3	16:M:404:UQ7:H71	1.96	0.47
2:N:165:VAL:HG23	2:N:172:VAL:HB	1.97	0.47
12:C:409:CDL:H132	13:C:410:PC7:H152	1.97	0.47
1:M:116:ARG:HD2	18:M:609:HOH:O	2.14	0.47
2:D:188:VAL:HG11	2:D:248:ARG:NH2	2.30	0.46
16:M:404:UQ7:H322	16:M:404:UQ7:H28	1.60	0.46
2:D:159:PRO:HG3	2:D:176:ARG:HD3	1.98	0.46
2:D:179:GLU:HA	2:D:182:ILE:HD12	1.97	0.46
9:M:403:UQ5:H272	9:M:403:UQ5:H251	1.63	0.46
1:C:43:GLY:HA2	9:C:403:UQ5:H162	1.97	0.46
3:E:277:LEU:HD22	13:G:104:PC7:H242	1.98	0.46
1:M:26:TYR:CD2	9:M:403:UQ5:H3M1	2.47	0.46
1:M:154:THR:HG21	1:M:171:LEU:CD2	2.40	0.46
10:I:101:3PH:H321	10:I:101:3PH:H32	1.48	0.46
6:S:19:LEU:HB3	6:S:26:VAL:HG11	1.96	0.46
6:S:59:TYR:OH	18:S:101:HOH:O	2.20	0.46
1:M:239:TRP:CH2	11:M:406:PGT:H212	2.51	0.46
2:N:157:ILE:HG13	2:N:158:GLU:H	1.81	0.46
12:G:103:CDL:H572	12:G:103:CDL:H542	1.81	0.46
1:M:213:ASN:HB3	18:M:609:HOH:O	2.12	0.46
1:C:90:ASN:O	1:C:94:MET:HG2	2.16	0.46
1:C:317:MET:SD	18:C:589:HOH:O	2.61	0.46
3:O:237:TYR:HB3	3:O:239:ASP:OD1	2.15	0.46
1:C:35:TRP:HB3	1:C:105:ARG:HG3	1.98	0.45
2:N:121:PHE:HE1	6:S:31:ILE:HA	1.81	0.45
12:O:402:CDL:H621	4:Q:31:PRO:HG3	1.98	0.45
5:R:21:CYS:O	5:R:24:PRO:HD2	2.16	0.45
4:G:67:LYS:HB3	4:G:67:LYS:HE3	1.71	0.45
5:R:31:CYS:O	5:R:35:ILE:HG12	2.15	0.45
11:C:406:PGT:H431	11:C:406:PGT:H402	1.75	0.45
1:M:369:PHE:CE2	18:M:626:HOH:O	2.62	0.45
3:E:115:ARG:NH1	18:E:522:HOH:O	2.40	0.45
13:C:410:PC7:H41	13:C:410:PC7:H82	1.55	0.45
2:D:121:PHE:HE2	13:G:104:PC7:H442	1.82	0.45
1:M:375:LEU:HD23	1:M:375:LEU:HA	1.79	0.45
13:G:104:PC7:H362	13:G:104:PC7:H142	1.99	0.45
2:N:205:ASN:HD22	2:N:208:TRP:HD1	1.65	0.45
1:C:35:TRP:CH2	12:C:409:CDL:H712	2.52	0.45
11:C:407:PGT:H212	11:C:407:PGT:H181	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:113:TYR:CE2	13:N:303:PC7:H63	2.51	0.45
6:S:68:ARG:CG	18:S:105:HOH:O	2.63	0.45
1:C:123:GLY:O	8:C:401:HEM:HMC3	2.17	0.45
13:G:104:PC7:H41	13:G:104:PC7:H62	1.58	0.45
5:R:44:HIS:CE1	5:R:46:THR:HB	2.52	0.45
3:O:106:CYS:SG	8:O:401:HEM:CAC	3.05	0.44
12:O:402:CDL:H111	12:O:402:CDL:H141	1.62	0.44
9:C:403:UQ5:H222	9:C:403:UQ5:H262	1.87	0.44
3:E:87:TYR:HB3	3:E:92:ILE:HD11	1.99	0.44
3:E:201:ARG:NH2	3:E:218:TYR:OH	2.49	0.44
12:Q:101:CDL:H401	12:Q:101:CDL:H431	1.45	0.44
1:C:294:LYS:HD3	2:N:253:PRO:HG3	1.98	0.44
12:C:409:CDL:H271	12:C:409:CDL:H242	1.86	0.44
1:C:154:THR:O	1:C:168:VAL:HG22	2.17	0.44
3:E:204:PRO:HD3	3:E:215:TYR:CZ	2.53	0.44
1:M:82:TRP:CG	3:O:263:GLU:HG3	2.53	0.44
1:M:200:SER:HB3	9:M:403:UQ5:H161	1.98	0.44
2:N:128:ARG:HD2	7:T:36:TRP:CE2	2.52	0.44
5:H:39:ASP:HB2	5:H:43:LYS:HD2	1.98	0.44
1:C:115:PRO:HB2	1:C:210:TYR:CE2	2.53	0.44
4:G:23:MET:HG3	13:G:104:PC7:H32	2.00	0.44
1:C:108:TYR:CD1	13:C:410:PC7:H331	2.53	0.43
1:C:271:THR:CG2	2:N:221:ILE:O	2.66	0.43
11:C:407:PGT:H201	3:E:275:ILE:HG22	2.01	0.43
2:D:171:PRO:HG2	2:D:221:ILE:CD1	2.48	0.43
3:E:103:CYS:SG	8:E:400:HEM:CAB	3.06	0.43
3:E:207:ILE:HD13	3:E:207:ILE:HA	1.83	0.43
2:D:176:ARG:HB2	2:D:208:TRP:CZ3	2.53	0.43
3:O:107:HIS:HE1	3:O:177:PRO:HD2	1.83	0.43
4:Q:21:LYS:HB3	12:Q:101:CDL:HA21	2.01	0.43
1:C:32:LEU:HB2	1:C:231:PHE:CE1	2.54	0.43
1:C:40:SER:HB3	9:C:403:UQ5:H71	2.01	0.43
3:E:250:LYS:HE3	18:E:645:HOH:O	2.19	0.43
1:M:368:PHE:HB2	15:M:407:PTY:H441	2.00	0.43
3:E:98:VAL:HG22	3:E:235:VAL:HG11	2.00	0.43
1:C:163:VAL:O	1:C:166:THR:HG22	2.18	0.43
2:D:217:HIS:HD2	1:M:294:LYS:HB2	1.83	0.43
11:G:102:PGT:H242	11:G:102:PGT:H211	1.82	0.43
2:N:199:ASP:O	2:N:203:VAL:HG22	2.17	0.43
6:S:40:ARG:CZ	6:S:40:ARG:HA	2.48	0.43
1:C:19:LEU:HD13	1:C:23:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PHE:HA	1:C:41:LEU:HB2	2.01	0.43
3:E:187:HIS:HB3	18:E:654:HOH:O	2.17	0.43
1:M:80:GLY:C	18:M:551:HOH:O	2.57	0.43
12:M:408:CDL:H541	12:M:408:CDL:H511	1.61	0.43
3:E:130:MET:HG3	6:I:68:ARG:CZ	2.49	0.43
1:M:208:HIS:NE2	9:M:403:UQ5:O3	2.52	0.43
1:M:277:PRO:HG3	16:M:404:UQ7:C1	2.49	0.43
2:N:142:LYS:HA	2:N:145:LEU:HD12	2.00	0.43
3:O:226:MET:HG3	8:O:401:HEM:C4C	2.53	0.43
6:S:48:LYS:HA	6:S:48:LYS:HD3	1.79	0.43
10:M:405:3PH:H3G1	3:O:279:SER:HB2	2.00	0.42
12:M:408:CDL:H422	12:M:408:CDL:H391	1.81	0.42
6:S:68:ARG:CD	18:S:105:HOH:O	2.62	0.42
7:T:38:VAL:O	7:T:40:PRO:HD3	2.19	0.42
1:C:48:ILE:CG1	12:C:408:CDL:H822	2.46	0.42
1:C:148:TRP:CH2	2:N:221:ILE:HG12	2.55	0.42
1:M:364:VAL:HG13	15:M:407:PTY:H422	2.01	0.42
12:M:408:CDL:H1	13:M:409:PC7:H42	2.01	0.42
5:R:23:LYS:HB2	5:R:24:PRO:HD3	2.00	0.42
1:C:353:PRO:HG3	4:G:62:PHE:CG	2.54	0.42
1:M:355:VAL:O	1:M:359:GLN:HG3	2.19	0.42
1:C:26:TYR:CD2	9:C:403:UQ5:H3M1	2.55	0.42
5:R:10:LYS:HG3	5:R:64:LEU:CD2	2.49	0.42
2:D:132:LEU:O	2:D:136:VAL:HG23	2.19	0.42
3:E:204:PRO:HG3	5:H:49:TYR:CG	2.55	0.42
5:R:23:LYS:HB2	5:R:23:LYS:HE2	1.76	0.42
3:E:79:PRO:HG3	18:E:645:HOH:O	2.19	0.42
3:E:143:GLU:CD	3:E:143:GLU:H	2.23	0.42
1:C:142:TRP:CA	18:C:563:HOH:O	2.57	0.42
2:N:130:LEU:HB3	12:N:302:CDL:H862	2.02	0.42
13:N:303:PC7:H72	18:N:429:HOH:O	2.18	0.42
1:C:285:TYR:CZ	9:C:404:UQ5:H3M2	2.55	0.42
1:C:108:TYR:CG	13:C:410:PC7:H331	2.55	0.42
1:C:244:ILE:HG21	12:G:103:CDL:H602	2.02	0.42
13:C:410:PC7:H441	18:C:637:HOH:O	2.19	0.42
3:O:190:GLN:NE2	18:O:526:HOH:O	2.53	0.42
1:C:294:LYS:HB3	1:C:294:LYS:HE2	1.72	0.41
9:C:403:UQ5:H112	11:C:406:PGT:H462	2.02	0.41
3:E:124:GLU:HG2	3:E:128:LYS:HE3	2.01	0.41
12:G:103:CDL:H231	12:G:103:CDL:H262	1.80	0.41
1:M:291:ILE:HA	1:M:292:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:HIS:C	1:C:23:LEU:HD12	2.40	0.41
3:E:71:LEU:HD23	3:E:218:TYR:CE1	2.55	0.41
5:H:6:VAL:CG1	5:H:7:VAL:HG22	2.39	0.41
1:M:41:LEU:HD23	1:M:41:LEU:HA	1.89	0.41
5:R:10:LYS:NZ	18:R:101:HOH:O	2.42	0.41
1:C:124:VAL:HG11	1:C:309:LEU:HG	2.03	0.41
11:C:406:PGT:H471	11:C:406:PGT:H441	1.83	0.41
10:M:405:3PH:H322	10:M:405:3PH:H351	1.78	0.41
3:E:164:GLU:CD	3:E:168:ARG:HE	2.24	0.41
5:H:18:LYS:N	5:H:19:PRO:HD2	2.35	0.41
1:C:135:PHE:CZ	1:C:153:ILE:HB	2.56	0.41
9:C:403:UQ5:H1M1	9:C:403:UQ5:H72	1.66	0.41
12:C:409:CDL:H242	12:C:409:CDL:H211	1.78	0.41
3:E:107:HIS:HE1	3:E:177:PRO:HD2	1.86	0.41
4:G:61:TYR:O	4:G:65:GLN:HG2	2.21	0.41
5:H:23:LYS:HB3	5:H:24:PRO:HD3	2.02	0.41
9:C:404:UQ5:H151	9:C:404:UQ5:H171	1.82	0.41
12:C:409:CDL:H372	12:C:409:CDL:H341	1.93	0.41
2:D:197:GLN:HG2	2:D:202:ARG:HD2	2.03	0.41
2:D:199:ASP:O	2:D:203:VAL:HG12	2.21	0.41
5:H:8:ASP:HA	5:H:9:PRO:HD3	1.99	0.41
1:C:317:MET:HG2	18:C:572:HOH:O	2.20	0.41
1:C:341:LEU:HD21	4:G:52:VAL:HA	2.03	0.41
12:C:408:CDL:H851	2:D:130:LEU:HD13	2.03	0.41
1:M:221:GLU:HA	1:M:224:LYS:HZ3	1.86	0.41
13:N:303:PC7:H122	13:N:303:PC7:H32	1.65	0.41
10:T:101:3PH:H2A2	10:T:102:3PH:H371	2.03	0.41
1:M:145:MET:HG2	1:M:261:ASP:HB2	2.02	0.40
3:O:83:ILE:H	3:O:83:ILE:HG13	1.76	0.40
10:C:405:3PH:H221	10:C:405:3PH:H251	1.85	0.40
2:D:122:VAL:HG11	3:E:281:ALA:HB2	2.02	0.40
3:E:110:SER:O	3:E:156:ARG:HD2	2.21	0.40
5:R:35:ILE:O	5:R:35:ILE:HG22	2.21	0.40
6:I:23:ARG:HD3	6:I:23:ARG:HA	1.75	0.40
1:M:77:ASP:HA	2:N:142:LYS:HE3	2.02	0.40
4:Q:21:LYS:NZ	12:Q:101:CDL:OB4	2.53	0.40
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.91	0.40
1:C:152:VAL:HG23	1:C:153:ILE:HD12	2.02	0.40
3:E:143:GLU:CD	3:E:143:GLU:N	2.75	0.40
6:I:48:LYS:HD2	6:I:48:LYS:HA	1.57	0.40
1:M:201:LEU:HD23	9:M:403:UQ5:H152	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:167:TRP:CG	2:N:168:ARG:N	2.88	0.40
2:N:218:LEU:HD12	2:N:237:HIS:CE1	2.56	0.40
2:N:223:LEU:HA	2:N:224:PRO:HD3	1.96	0.40
4:Q:8:LEU:HD22	4:Q:9:LYS:N	2.36	0.40
6:S:59:TYR:O	6:S:65:LEU:HD22	2.21	0.40
1:C:316:SER:HB2	18:C:572:HOH:O	2.20	0.40
13:C:410:PC7:H322	13:C:410:PC7:H2	1.81	0.40
2:D:129:LEU:HD13	3:E:274:TRP:CZ2	2.56	0.40
6:I:58:ARG:HB2	6:I:58:ARG:HE	1.56	0.40
3:O:87:TYR:HB3	3:O:92:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	385/393 (98%)	376 (98%)	9 (2%)	0	100	100
1	M	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
2	D	177/272 (65%)	168 (95%)	9 (5%)	0	100	100
2	N	177/272 (65%)	166 (94%)	11 (6%)	0	100	100
3	E	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
3	O	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
4	G	67/72 (93%)	67 (100%)	0	0	100	100
4	Q	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
5	H	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
5	R	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
6	I	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
6	S	55/72 (76%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	J	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
7	T	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	2026/2484 (82%)	1966 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	330/336 (98%)	328 (99%)	2 (1%)	84	89
1	M	330/336 (98%)	328 (99%)	2 (1%)	84	89
2	D	155/232 (67%)	155 (100%)	0	100	100
2	N	155/232 (67%)	155 (100%)	0	100	100
3	E	200/247 (81%)	199 (100%)	1 (0%)	86	91
3	O	200/247 (81%)	200 (100%)	0	100	100
4	G	63/65 (97%)	63 (100%)	0	100	100
4	Q	62/65 (95%)	62 (100%)	0	100	100
5	H	58/62 (94%)	58 (100%)	0	100	100
5	R	57/62 (92%)	57 (100%)	0	100	100
6	I	48/59 (81%)	48 (100%)	0	100	100
6	S	48/59 (81%)	48 (100%)	0	100	100
7	J	16/41 (39%)	16 (100%)	0	100	100
7	T	16/41 (39%)	16 (100%)	0	100	100
All	All	1738/2084 (83%)	1733 (100%)	5 (0%)	90	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	PHE

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Mol	Chain	Res	Type
1	C	190	TYR
3	E	292	LYS
1	M	85	ARG
1	M	190	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	274	HIS
2	N	96	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

39 ligands are modelled in this entry.

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	$\# Z  > 2$
15	PTY	T	103	-	28,28,49	1.12	4 (14%)	31,33,54	1.18	2 (6%)
13	PC7	D	302	-	33,33,51	1.17	4 (12%)	39,41,59	1.07	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	HEM	C	402	1	41,50,50	1.60	8 (19%)	45,82,82	1.88	10 (22%)
8	HEM	M	402	1	41,50,50	1.78	8 (19%)	45,82,82	2.05	15 (33%)
11	PGT	M	406	-	36,36,50	1.20	3 (8%)	39,42,56	1.11	2 (5%)
12	CDL	Q	101	-	69,69,99	1.04	8 (11%)	75,81,111	1.16	5 (6%)
10	3PH	G	101	-	32,32,47	0.75	1 (3%)	36,37,52	0.67	1 (2%)
11	PGT	G	102	-	50,50,50	1.07	3 (6%)	53,56,56	1.06	2 (3%)
16	UQ7	M	404	-	48,48,48	0.66	2 (4%)	58,61,61	0.77	3 (5%)
8	HEM	E	400	3	41,50,50	1.44	3 (7%)	45,82,82	1.43	9 (20%)
11	PGT	C	407	-	50,50,50	1.09	3 (6%)	53,56,56	1.04	2 (3%)
10	3PH	T	101	-	40,40,47	0.68	1 (2%)	44,45,52	0.65	1 (2%)
14	FES	N	301	2	0,4,4	-	-	-	-	-
14	FES	D	301	2	0,4,4	-	-	-	-	-
13	PC7	M	409	-	43,43,51	1.03	4 (9%)	48,50,59	1.13	2 (4%)
15	PTY	J	101	-	40,40,49	0.33	0	43,45,54	0.38	0
9	UQ5	M	403	-	38,38,38	0.48	0	46,49,49	0.62	1 (2%)
10	3PH	I	101	-	31,31,47	0.76	1 (3%)	35,36,52	0.76	2 (5%)
13	PC7	C	410	-	50,50,51	0.97	4 (8%)	56,58,59	1.07	2 (3%)
15	PTY	M	407	-	39,39,49	0.97	4 (10%)	42,44,54	1.06	2 (4%)
12	CDL	C	408	-	80,80,99	0.37	0	86,92,111	0.56	2 (2%)
10	3PH	T	102	-	47,47,47	0.64	1 (2%)	51,52,52	0.59	1 (1%)
10	3PH	C	405	12	32,32,47	0.74	1 (3%)	36,37,52	0.77	1 (2%)
12	CDL	O	402	-	87,87,99	0.93	8 (9%)	93,99,111	1.11	4 (4%)
11	PGT	C	406	-	40,40,50	0.38	0	43,46,56	0.43	0
8	HEM	O	401	3	41,50,50	1.78	10 (24%)	45,82,82	2.41	14 (31%)
8	HEM	M	401	1	41,50,50	1.65	9 (21%)	45,82,82	1.92	14 (31%)
17	Q7G	M	411	-	44,44,90	0.76	1 (2%)	66,68,138	1.40	10 (15%)
12	CDL	C	409	10	84,84,99	0.94	7 (8%)	90,96,111	1.10	4 (4%)
17	Q7G	M	410	-	44,44,90	0.72	1 (2%)	66,68,138	1.36	11 (16%)
9	UQ5	C	403	-	38,38,38	0.94	2 (5%)	46,49,49	0.83	0
13	PC7	G	104	-	51,51,51	0.97	4 (7%)	57,59,59	1.02	2 (3%)
9	UQ5	C	404	-	38,38,38	0.46	0	46,49,49	0.82	1 (2%)
12	CDL	N	302	-	80,80,99	0.96	8 (10%)	86,92,111	1.16	4 (4%)
12	CDL	G	103	-	84,84,99	0.96	8 (9%)	90,96,111	1.11	4 (4%)
10	3PH	M	405	-	43,43,47	0.66	1 (2%)	47,48,52	0.62	1 (2%)
12	CDL	M	408	-	76,76,99	0.99	8 (10%)	82,88,111	1.11	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	PC7	N	303	-	38,38,51	0.39	0	44,46,59	0.64	1 (2%)
8	HEM	C	401	1	41,50,50	1.49	6 (14%)	45,82,82	1.45	6 (13%)

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
15	PTY	T	103	-	-	18/32/32/53	-
13	PC7	D	302	-	-	14/37/37/55	-
8	HEM	C	402	1	-	6/12/54/54	-
8	HEM	M	402	1	-	2/12/54/54	-
11	PGT	M	406	-	-	21/41/41/55	-
12	CDL	Q	101	-	-	38/80/80/110	-
10	3PH	G	101	-	-	16/34/34/49	-
11	PGT	G	102	-	-	37/55/55/55	-
16	UQ7	M	404	-	-	19/45/69/69	0/1/1/1
8	HEM	E	400	3	-	2/12/54/54	-
11	PGT	C	407	-	-	22/55/55/55	-
10	3PH	T	101	-	-	14/42/42/49	-
14	FES	N	301	2	-	-	0/1/1/1
14	FES	D	301	2	-	-	0/1/1/1
13	PC7	M	409	-	-	20/45/45/55	-
15	PTY	J	101	-	-	5/44/44/53	-
9	UQ5	M	403	-	-	9/33/57/57	0/1/1/1
10	3PH	I	101	-	-	15/33/33/49	-
13	PC7	C	410	-	-	19/54/54/55	-
15	PTY	M	407	-	-	18/43/43/53	-
12	CDL	C	408	-	-	48/91/91/110	-
10	3PH	T	102	-	-	13/49/49/49	-
10	3PH	C	405	12	-	17/34/34/49	-
12	CDL	O	402	-	-	35/98/98/110	-
11	PGT	C	406	-	-	14/45/45/55	-
8	HEM	O	401	3	-	4/12/54/54	-
8	HEM	M	401	1	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Q7G	M	411	-	-	0/12/100/200	0/6/6/10
12	CDL	C	409	10	-	43/95/95/110	-
17	Q7G	M	410	-	-	3/12/100/200	0/6/6/10
9	UQ5	C	403	-	-	10/33/57/57	0/1/1/1
13	PC7	G	104	-	-	20/55/55/55	-
9	UQ5	C	404	-	-	13/33/57/57	0/1/1/1
12	CDL	N	302	-	-	35/91/91/110	-
12	CDL	G	103	-	-	31/95/95/110	-
10	3PH	M	405	-	-	20/45/45/49	-
12	CDL	M	408	-	-	42/87/87/110	-
13	PC7	N	303	-	-	11/42/42/55	-
8	HEM	C	401	1	-	2/12/54/54	-

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	HEM	C1B-NB	-6.39	1.29	1.40
8	O	401	HEM	C1B-NB	-5.57	1.30	1.40
8	M	401	HEM	C1B-NB	-4.83	1.32	1.40
8	C	402	HEM	C1B-NB	-4.13	1.33	1.40
8	M	402	HEM	FE-NB	4.07	2.17	1.96
8	M	401	HEM	C4D-ND	-4.01	1.33	1.40
8	M	402	HEM	C4D-ND	-3.99	1.33	1.40
8	E	400	HEM	C3C-C2C	-3.96	1.34	1.40
8	C	402	HEM	C4D-ND	-3.92	1.33	1.40
8	E	400	HEM	C3C-CAC	3.83	1.55	1.47
8	C	401	HEM	C3C-CAC	3.80	1.55	1.47
8	C	401	HEM	C3C-C2C	-3.79	1.35	1.40
8	O	401	HEM	C4B-NB	-3.70	1.31	1.38
8	O	401	HEM	C4D-ND	-3.67	1.34	1.40
8	M	402	HEM	C4B-NB	-3.63	1.31	1.38
8	C	402	HEM	FE-NB	3.42	2.13	1.96
8	C	402	HEM	C4B-NB	-3.41	1.31	1.38
8	M	401	HEM	O2A-CGA	-3.34	1.19	1.30
9	C	403	UQ5	C3-C2	-3.33	1.39	1.48
10	T	102	3PH	P-O11	3.30	1.70	1.60
10	M	405	3PH	P-O11	3.28	1.70	1.60
10	G	101	3PH	P-O11	3.28	1.70	1.60
10	T	101	3PH	P-O11	3.26	1.70	1.60
10	I	101	3PH	P-O11	3.26	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	405	3PH	P-O11	3.25	1.70	1.60
8	M	402	HEM	C1D-ND	-3.17	1.32	1.38
11	G	102	PGT	O3-C11	3.17	1.42	1.33
11	C	407	PGT	O3-C11	3.09	1.42	1.33
11	M	406	PGT	O3-C11	3.07	1.42	1.33
11	C	407	PGT	O2-C31	3.05	1.42	1.34
11	M	406	PGT	O2-C31	3.00	1.42	1.34
8	C	401	HEM	CAB-C3B	2.98	1.55	1.47
8	O	401	HEM	O2A-CGA	-2.98	1.20	1.30
8	C	402	HEM	O2D-CGD	-2.94	1.20	1.30
11	G	102	PGT	O2-C31	2.89	1.42	1.34
8	O	401	HEM	FE-NB	2.84	2.10	1.96
8	M	402	HEM	O2A-CGA	-2.83	1.21	1.30
8	E	400	HEM	CAB-C3B	2.82	1.55	1.47
8	O	401	HEM	C1D-ND	-2.82	1.33	1.38
12	M	408	CDL	OA6-CA4	-2.77	1.39	1.46
8	M	401	HEM	FE-NB	2.74	2.10	1.96
12	Q	101	CDL	OA6-CA4	-2.71	1.39	1.46
8	M	401	HEM	C1D-ND	-2.70	1.33	1.38
8	C	402	HEM	C1D-ND	-2.67	1.33	1.38
13	C	410	PC7	O2-C2	-2.67	1.39	1.46
8	C	402	HEM	O2A-CGA	-2.65	1.21	1.30
12	G	103	CDL	OB6-CB4	-2.63	1.40	1.46
13	G	104	PC7	O2-C2	-2.60	1.40	1.46
9	C	403	UQ5	C4-C5	-2.59	1.41	1.48
13	D	302	PC7	O2-C2	-2.59	1.40	1.46
12	G	103	CDL	OA6-CA4	-2.58	1.40	1.46
12	O	402	CDL	OB6-CB4	-2.57	1.40	1.46
12	Q	101	CDL	OB6-CB4	-2.57	1.40	1.46
12	C	409	CDL	OA6-CA4	-2.53	1.40	1.46
8	O	401	HEM	C3C-C2C	-2.52	1.36	1.40
15	M	407	PTY	O7-C6	-2.51	1.40	1.46
12	N	302	CDL	OA8-CA7	2.50	1.40	1.33
8	M	401	HEM	O2D-CGD	-2.49	1.22	1.30
12	Q	101	CDL	OA8-CA7	2.49	1.40	1.33
12	G	103	CDL	OA8-CA7	2.49	1.40	1.33
15	T	103	PTY	O7-C6	-2.49	1.40	1.46
12	M	408	CDL	OB8-CB7	2.49	1.40	1.33
8	O	401	HEM	O2D-CGD	-2.49	1.22	1.30
12	C	409	CDL	OA8-CA7	2.48	1.40	1.33
12	N	302	CDL	OB6-CB4	-2.48	1.40	1.46
13	M	409	PC7	O2-C2	-2.47	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	408	CDL	OA8-CA7	2.46	1.40	1.33
12	G	103	CDL	OB8-CB7	2.46	1.40	1.33
12	Q	101	CDL	OB8-CB7	2.46	1.40	1.33
17	M	411	Q7G	C11-C08	-2.46	1.51	1.56
16	M	404	UQ7	C3-C4	-2.45	1.41	1.48
12	O	402	CDL	OA8-CA7	2.43	1.40	1.33
12	N	302	CDL	OA6-CA4	-2.43	1.40	1.46
12	C	409	CDL	OB8-CB7	2.42	1.40	1.33
12	O	402	CDL	OB8-CB7	2.42	1.40	1.33
8	M	401	HEM	C3D-C2D	-2.40	1.31	1.36
12	N	302	CDL	OB8-CB7	2.38	1.40	1.33
13	G	104	PC7	O3-C11	2.38	1.40	1.33
8	M	401	HEM	C4B-NB	-2.38	1.33	1.38
13	D	302	PC7	O3-C11	2.37	1.40	1.33
8	M	402	HEM	O2D-CGD	-2.37	1.22	1.30
15	T	103	PTY	O4-C30	2.36	1.40	1.33
12	M	408	CDL	OB6-CB5	2.35	1.40	1.34
15	M	407	PTY	O4-C30	2.35	1.40	1.33
12	O	402	CDL	OA6-CA5	2.31	1.40	1.34
12	C	409	CDL	OB6-CB4	-2.31	1.40	1.46
8	M	401	HEM	C1B-C2B	-2.29	1.40	1.44
11	C	407	PGT	P-O3P	2.28	1.68	1.59
17	M	410	Q7G	C11-C08	-2.27	1.52	1.56
13	M	409	PC7	O3-C3	-2.26	1.40	1.45
13	M	409	PC7	O3-C11	2.25	1.39	1.33
11	M	406	PGT	P-O3P	2.25	1.68	1.59
13	C	410	PC7	O3-C11	2.25	1.39	1.33
13	D	302	PC7	O3-C3	-2.24	1.40	1.45
13	C	410	PC7	O3-C3	-2.24	1.40	1.45
8	O	401	HEM	C1B-C2B	-2.21	1.40	1.44
15	T	103	PTY	O4-C1	-2.21	1.40	1.45
12	C	409	CDL	OB6-CB5	2.20	1.40	1.34
11	G	102	PGT	P-O3P	2.19	1.68	1.59
12	N	302	CDL	OA6-CA5	2.19	1.40	1.34
13	M	409	PC7	O2-C31	2.18	1.40	1.34
13	G	104	PC7	O3-C3	-2.17	1.40	1.45
12	M	408	CDL	OB6-CB4	-2.17	1.41	1.46
12	O	402	CDL	OA8-CA6	-2.17	1.40	1.45
15	M	407	PTY	O7-C8	2.16	1.40	1.34
12	O	402	CDL	OA6-CA4	-2.16	1.41	1.46
15	T	103	PTY	O7-C8	2.16	1.40	1.34
16	M	404	UQ7	C2-C1	-2.16	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	408	CDL	OB8-CB6	-2.15	1.40	1.45
12	G	103	CDL	OA6-CA5	2.14	1.40	1.34
12	Q	101	CDL	OA8-CA6	-2.13	1.40	1.45
12	N	302	CDL	OB8-CB6	-2.13	1.40	1.45
15	M	407	PTY	O4-C1	-2.12	1.40	1.45
12	C	409	CDL	OA6-CA5	2.12	1.40	1.34
12	G	103	CDL	OA8-CA6	-2.12	1.40	1.45
12	O	402	CDL	OB8-CB6	-2.12	1.40	1.45
12	G	103	CDL	OB8-CB6	-2.12	1.40	1.45
12	Q	101	CDL	OA6-CA5	2.12	1.40	1.34
8	C	401	HEM	FE-ND	2.12	2.07	1.96
12	Q	101	CDL	OB8-CB6	-2.11	1.40	1.45
8	C	401	HEM	CMB-C2B	2.11	1.55	1.50
12	O	402	CDL	OB6-CB5	2.10	1.40	1.34
13	G	104	PC7	O2-C31	2.10	1.40	1.34
12	Q	101	CDL	OB6-CB5	2.10	1.40	1.34
12	G	103	CDL	OB6-CB5	2.09	1.40	1.34
12	N	302	CDL	OB6-CB5	2.09	1.40	1.34
13	C	410	PC7	O2-C31	2.08	1.40	1.34
12	C	409	CDL	OA8-CA6	-2.04	1.40	1.45
8	C	401	HEM	FE-NB	2.04	2.07	1.96
13	D	302	PC7	O2-C31	2.04	1.40	1.34
12	N	302	CDL	OA8-CA6	-2.03	1.40	1.45
8	C	402	HEM	C1B-C2B	-2.03	1.40	1.44
8	O	401	HEM	FE-ND	-2.02	1.86	1.96
12	M	408	CDL	OA6-CA5	2.02	1.40	1.34
8	M	402	HEM	C3B-C4B	2.02	1.48	1.44
12	M	408	CDL	OA8-CA6	-2.01	1.40	1.45

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	401	HEM	CHC-C4B-NB	7.94	133.06	124.43
8	M	402	HEM	C1B-NB-C4B	6.16	111.44	105.07
8	C	402	HEM	C1B-NB-C4B	6.11	111.38	105.07
8	O	401	HEM	C1B-NB-C4B	5.65	110.91	105.07
8	O	401	HEM	CHD-C1D-ND	5.16	130.04	124.43
8	O	401	HEM	O2A-CGA-O1A	-4.74	111.48	123.30
8	M	402	HEM	CHC-C4B-NB	4.65	129.49	124.43
8	C	402	HEM	CHC-C4B-NB	4.64	129.47	124.43
12	C	409	CDL	OB6-CB5-C51	4.54	121.29	111.50
8	M	401	HEM	C1B-NB-C4B	4.53	109.75	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	409	PC7	O2-C31-C32	4.48	121.16	111.50
17	M	411	Q7G	CG1-C22-C23	-4.46	108.24	113.88
13	C	410	PC7	O2-C31-C32	4.35	120.88	111.50
12	G	103	CDL	OA6-CA5-C11	4.31	120.78	111.50
12	O	402	CDL	OA6-CA5-C11	4.30	120.76	111.50
12	N	302	CDL	OB6-CB5-C51	4.29	120.75	111.50
12	N	302	CDL	OA6-CA5-C11	4.21	120.57	111.50
8	M	401	HEM	CHC-C4B-NB	4.14	128.93	124.43
12	M	408	CDL	OB6-CB5-C51	4.11	120.37	111.50
11	M	406	PGT	O2-C31-C32	4.04	120.22	111.50
15	T	103	PTY	O7-C8-C11	4.00	120.13	111.50
12	Q	101	CDL	OA6-CA5-C11	3.96	120.04	111.50
11	C	407	PGT	O2-C31-C32	3.92	119.95	111.50
12	C	409	CDL	OA6-CA5-C11	3.92	119.94	111.50
12	O	402	CDL	OB6-CB5-C51	3.90	119.90	111.50
12	G	103	CDL	OB6-CB5-C51	3.89	119.89	111.50
8	M	402	HEM	C4B-CHC-C1C	3.88	127.68	122.56
12	Q	101	CDL	OB6-CB5-C51	3.88	119.85	111.50
8	C	402	HEM	C4C-CHD-C1D	3.85	127.64	122.56
11	G	102	PGT	O2-C31-C32	3.84	119.78	111.50
13	G	104	PC7	O2-C31-C32	3.82	119.74	111.50
15	M	407	PTY	O7-C8-C11	3.82	119.74	111.50
13	D	302	PC7	O2-C31-C32	3.74	119.57	111.50
8	M	402	HEM	CHA-C4D-ND	3.70	128.96	124.38
17	M	410	Q7G	CG1-C22-C23	-3.63	109.29	113.88
8	M	402	HEM	C4D-ND-C1D	3.61	108.80	105.07
12	M	408	CDL	OA6-CA5-C11	3.60	119.26	111.50
8	M	401	HEM	O2A-CGA-O1A	-3.58	114.38	123.30
9	C	404	UQ5	C7-C6-C5	-3.57	114.18	118.48
17	M	410	Q7G	C02-C06-C07	-3.50	109.19	114.38
8	M	401	HEM	CMD-C2D-C1D	3.44	130.28	125.04
8	M	401	HEM	CHD-C1D-ND	3.40	128.13	124.43
8	C	401	HEM	C4D-ND-C1D	3.33	108.52	105.07
8	O	401	HEM	CBA-CAA-C2A	3.33	118.30	112.62
8	C	402	HEM	O2D-CGD-O1D	-3.29	115.11	123.30
8	C	401	HEM	C1B-NB-C4B	3.27	108.45	105.07
8	C	401	HEM	C4B-CHC-C1C	3.26	126.86	122.56
17	M	411	Q7G	C12-C11-C08	-3.25	107.81	111.68
8	O	401	HEM	CHD-C1D-C2D	-3.22	119.95	124.98
8	M	402	HEM	O2D-CGD-O1D	-3.20	115.31	123.30
8	O	401	HEM	O2A-CGA-CBA	3.09	123.96	114.03
8	M	402	HEM	CHD-C1D-ND	2.99	127.68	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	M	410	Q7G	C17-C16-C13	-2.97	106.90	111.52
8	O	401	HEM	CHA-C4D-ND	2.96	128.03	124.38
8	O	401	HEM	CHC-C4B-C3B	-2.93	120.08	124.57
8	M	401	HEM	CHA-C4D-ND	2.92	127.99	124.38
13	M	409	PC7	O3-C11-C12	2.91	121.03	111.91
8	C	402	HEM	CHA-C4D-ND	2.88	127.94	124.38
8	E	400	HEM	C1B-NB-C4B	2.88	108.04	105.07
8	O	401	HEM	O2D-CGD-O1D	-2.87	116.16	123.30
11	G	102	PGT	O3-C11-C12	2.86	120.90	111.91
17	M	410	Q7G	C12-C11-C08	-2.86	108.28	111.68
8	E	400	HEM	C4D-ND-C1D	2.76	107.92	105.07
17	M	410	Q7G	C02-C03-C74	-2.75	111.21	120.56
8	M	402	HEM	C4B-C3B-C2B	-2.75	104.94	107.11
8	C	402	HEM	CHD-C1D-ND	2.71	127.37	124.43
17	M	411	Q7G	C76-C73-C74	-2.68	110.19	115.69
8	M	402	HEM	O2D-CGD-CBD	2.67	122.60	114.03
8	M	402	HEM	O2A-CGA-O1A	-2.65	116.70	123.30
12	M	408	CDL	OA8-CA7-C31	2.64	120.20	111.91
8	M	401	HEM	O2D-CGD-CBD	2.63	122.48	114.03
12	N	302	CDL	OB8-CB7-C71	2.63	120.16	111.91
13	D	302	PC7	O3-C11-C12	2.63	120.15	111.91
12	G	103	CDL	OA8-CA7-C31	2.62	120.14	111.91
13	C	410	PC7	O3-C11-C12	2.61	120.11	111.91
12	G	103	CDL	OB8-CB7-C71	2.61	120.10	111.91
12	C	409	CDL	OA8-CA7-C31	2.61	120.10	111.91
8	M	401	HEM	CHB-C1B-NB	2.60	127.59	124.38
17	M	411	Q7G	C77-C76-C73	-2.59	107.45	111.93
8	M	401	HEM	CBD-CAD-C3D	-2.59	105.43	112.63
8	O	401	HEM	C4D-ND-C1D	2.57	107.73	105.07
8	C	401	HEM	C4C-CHD-C1D	2.57	125.95	122.56
12	O	402	CDL	OA8-CA7-C31	2.56	119.95	111.91
8	E	400	HEM	C4B-CHC-C1C	2.55	125.92	122.56
11	C	407	PGT	O3-C11-C12	2.54	119.89	111.91
12	Q	101	CDL	OB8-CB7-C71	2.53	119.85	111.91
15	M	407	PTY	O4-C30-C31	2.53	119.84	111.91
12	N	302	CDL	OA8-CA7-C31	2.51	119.79	111.91
12	Q	101	CDL	OA8-CA7-C31	2.51	119.79	111.91
13	G	104	PC7	O3-C11-C12	2.50	119.74	111.91
12	M	408	CDL	OB8-CB7-C71	2.49	119.73	111.91
17	M	410	Q7G	C76-C73-C74	-2.49	110.57	115.69
11	M	406	PGT	O3-C11-C12	2.48	119.69	111.91
8	M	402	HEM	CBD-CAD-C3D	-2.47	105.76	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	HEM	CHD-C1D-C2D	-2.47	121.13	124.98
15	T	103	PTY	O4-C30-C31	2.46	119.64	111.91
17	M	411	Q7G	C09-C10-C02	-2.46	108.56	112.78
12	O	402	CDL	OB8-CB7-C71	2.46	119.62	111.91
8	C	402	HEM	CBD-CAD-C3D	-2.44	105.84	112.63
8	E	400	HEM	CAA-CBA-CGA	-2.44	106.92	113.76
8	M	401	HEM	O2D-CGD-O1D	-2.43	117.23	123.30
16	M	404	UQ7	C17-C16-C14	2.37	120.78	112.98
12	C	409	CDL	OB8-CB7-C71	2.36	119.31	111.91
8	M	401	HEM	O2A-CGA-CBA	2.35	121.57	114.03
12	C	408	CDL	OB6-CB4-CB3	2.33	116.83	108.40
10	M	405	3PH	O13-P-O11	-2.32	100.56	106.73
12	C	408	CDL	OB6-CB5-C51	2.32	116.50	111.50
17	M	410	Q7G	C19-C11-C08	2.32	111.96	108.73
17	M	411	Q7G	C08-C07-C06	-2.31	105.99	109.09
10	C	405	3PH	O13-P-O11	-2.31	100.58	106.73
17	M	411	Q7G	C75-C74-C03	-2.31	109.38	114.50
8	E	400	HEM	C3B-C2B-C1B	2.30	108.19	106.49
8	M	401	HEM	C4B-C3B-C2B	-2.30	105.29	107.11
12	Q	101	CDL	CA4-OA6-CA5	-2.29	112.14	117.79
17	M	410	Q7G	C11-C08-C07	-2.29	109.30	112.73
17	M	410	Q7G	C09-C10-C02	-2.28	108.86	112.78
8	E	400	HEM	CMC-C2C-C3C	2.28	128.94	124.68
16	M	404	UQ7	C16-C17-C18	2.27	119.34	111.88
8	O	401	HEM	CHB-C1B-NB	2.23	127.14	124.38
8	E	400	HEM	C3D-C4D-ND	-2.22	107.69	110.17
8	C	401	HEM	CMC-C2C-C3C	2.20	128.79	124.68
8	C	402	HEM	CHB-C1B-NB	2.18	127.07	124.38
10	I	101	3PH	O13-P-O11	-2.18	100.94	106.73
17	M	411	Q7G	C02-C06-C07	-2.17	111.17	114.38
10	T	101	3PH	O13-P-O11	-2.17	100.96	106.73
8	C	401	HEM	C3D-C4D-ND	-2.17	107.75	110.17
8	O	401	HEM	CBD-CAD-C3D	-2.14	106.68	112.63
17	M	411	Q7G	C19-C11-C08	2.13	111.71	108.73
8	M	402	HEM	C4A-C3A-C2A	2.13	108.48	107.00
16	M	404	UQ7	C11-C12-C13	2.13	118.89	111.88
8	M	402	HEM	O2A-CGA-CBA	2.13	120.86	114.03
10	T	102	3PH	O13-P-O11	-2.12	101.08	106.73
10	G	101	3PH	O13-P-O11	-2.11	101.13	106.73
8	E	400	HEM	CBD-CAD-C3D	-2.10	106.79	112.63
13	N	303	PC7	O2-C2-C1	2.10	115.99	108.40
9	M	403	UQ5	C6-C1-C2	2.09	120.84	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	HEM	CAD-C3D-C4D	2.09	128.31	124.66
8	M	402	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
17	M	411	Q7G	C02-C03-C74	-2.09	113.47	120.56
8	C	402	HEM	CAD-CBD-CGD	2.06	118.04	113.60
17	M	410	Q7G	C75-C74-C03	-2.06	109.93	114.50
10	I	101	3PH	C3-C2-C1	2.05	116.62	111.79
8	E	400	HEM	CHC-C4B-NB	2.04	126.65	124.43
8	C	402	HEM	CMD-C2D-C1D	2.03	128.13	125.04
8	O	401	HEM	CMC-C2C-C3C	2.02	128.46	124.68
8	M	402	HEM	C4C-CHD-C1D	2.01	125.21	122.56
17	M	410	Q7G	C07-C15-C14	-2.00	109.86	112.73

There are no chirality outliers.

All (658) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	403	UQ5	C17-C18-C19-C20
9	C	403	UQ5	C17-C18-C19-C21
9	M	403	UQ5	C9-C11-C12-C13
10	C	405	3PH	C1-O11-P-O13
10	C	405	3PH	C1-O11-P-O14
10	C	405	3PH	C22-C21-O21-C2
10	G	101	3PH	C1-O11-P-O13
10	G	101	3PH	C1-O11-P-O14
10	G	101	3PH	C2-C1-O11-P
10	I	101	3PH	C1-O11-P-O13
10	I	101	3PH	C1-O11-P-O14
10	I	101	3PH	C32-C31-O31-C3
10	T	101	3PH	C1-O11-P-O13
11	C	406	PGT	C1-O3P-P-O1P
11	C	407	PGT	C32-C31-O2-C2
11	C	407	PGT	C4-C5-C6-O6
11	G	102	PGT	C1-O3P-P-O2P
11	G	102	PGT	C1-O3P-P-O4P
11	G	102	PGT	C4-O4P-P-O2P
11	M	406	PGT	C32-C31-O2-C2
11	M	406	PGT	O2-C2-C3-O3
11	M	406	PGT	C2-C1-O3P-P
11	M	406	PGT	C1-O3P-P-O1P
11	M	406	PGT	C1-O3P-P-O2P
11	M	406	PGT	C1-O3P-P-O4P
12	C	408	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
12	C	408	CDL	CB2-OB2-PB2-OB4
12	C	408	CDL	C51-CB5-OB6-CB4
12	C	409	CDL	CA2-OA2-PA1-OA3
12	G	103	CDL	OA7-CA5-OA6-CA4
12	G	103	CDL	C11-CA5-OA6-CA4
12	G	103	CDL	CB3-OB5-PB2-OB4
12	M	408	CDL	C11-CA5-OA6-CA4
12	M	408	CDL	C51-CB5-OB6-CB4
12	N	302	CDL	OA7-CA5-OA6-CA4
12	N	302	CDL	C11-CA5-OA6-CA4
12	N	302	CDL	OB5-CB3-CB4-OB6
12	O	402	CDL	CA6-CA4-OA6-CA5
12	O	402	CDL	C11-CA5-OA6-CA4
12	O	402	CDL	CB3-OB5-PB2-OB2
12	O	402	CDL	CB3-OB5-PB2-OB3
12	O	402	CDL	CB3-OB5-PB2-OB4
12	Q	101	CDL	CA3-OA5-PA1-OA3
12	Q	101	CDL	CA3-OA5-PA1-OA4
12	Q	101	CDL	C11-CA5-OA6-CA4
12	Q	101	CDL	CB4-CB3-OB5-PB2
13	C	410	PC7	C32-C31-O2-C2
13	C	410	PC7	O31-C31-O2-C2
13	D	302	PC7	O31-C31-O2-C2
13	G	104	PC7	C32-C31-O2-C2
13	M	409	PC7	C32-C31-O2-C2
13	M	409	PC7	O2-C2-C3-O3
13	M	409	PC7	C21-C22-C23-C24
13	N	303	PC7	C32-C31-O2-C2
15	J	101	PTY	C11-C8-O7-C6
15	M	407	PTY	N1-C2-C3-O11
15	M	407	PTY	C3-O11-P1-O12
15	T	103	PTY	N1-C2-C3-O11
16	M	404	UQ7	C17-C18-C19-C20
16	M	404	UQ7	C17-C18-C19-C21
16	M	404	UQ7	C18-C19-C21-C22
16	M	404	UQ7	C20-C19-C21-C22
10	I	101	3PH	O32-C31-O31-C3
12	C	409	CDL	OB9-CB7-OB8-CB6
13	N	303	PC7	O11-C11-O3-C3
15	T	103	PTY	O30-C30-O4-C1
11	C	406	PGT	C12-C11-O3-C3
12	C	409	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
13	N	303	PC7	C12-C11-O3-C3
15	T	103	PTY	C31-C30-O4-C1
10	M	405	3PH	O32-C31-O31-C3
10	T	101	3PH	O32-C31-O31-C3
11	C	406	PGT	O11-C11-O3-C3
11	G	102	PGT	O11-C11-O3-C3
12	G	103	CDL	OA9-CA7-OA8-CA6
12	Q	101	CDL	OB9-CB7-OB8-CB6
10	C	405	3PH	O22-C21-O21-C2
11	C	407	PGT	O31-C31-O2-C2
12	C	408	CDL	OA7-CA5-OA6-CA4
12	C	408	CDL	OB7-CB5-OB6-CB4
12	M	408	CDL	OA7-CA5-OA6-CA4
12	M	408	CDL	OB7-CB5-OB6-CB4
12	Q	101	CDL	OA7-CA5-OA6-CA4
13	G	104	PC7	O31-C31-O2-C2
13	M	409	PC7	O31-C31-O2-C2
13	N	303	PC7	O31-C31-O2-C2
15	J	101	PTY	O10-C8-O7-C6
12	G	103	CDL	OB9-CB7-OB8-CB6
10	T	101	3PH	C32-C31-O31-C3
12	Q	101	CDL	C71-CB7-OB8-CB6
13	D	302	PC7	C32-C31-O2-C2
10	M	405	3PH	C32-C31-O31-C3
11	G	102	PGT	C12-C11-O3-C3
12	G	103	CDL	C31-CA7-OA8-CA6
12	G	103	CDL	C71-CB7-OB8-CB6
11	M	406	PGT	O31-C31-O2-C2
12	O	402	CDL	OA7-CA5-OA6-CA4
12	O	402	CDL	O1-C1-CA2-OA2
12	Q	101	CDL	O1-C1-CA2-OA2
12	C	408	CDL	C11-CA5-OA6-CA4
12	C	408	CDL	C1-CB2-OB2-PB2
9	C	403	UQ5	C12-C11-C9-C10
9	M	403	UQ5	C25-C24-C26-C27
16	M	404	UQ7	C15-C14-C16-C17
16	M	404	UQ7	C25-C24-C26-C27
9	C	403	UQ5	C12-C11-C9-C8
9	M	403	UQ5	C23-C24-C26-C27
16	M	404	UQ7	C13-C14-C16-C17
16	M	404	UQ7	C23-C24-C26-C27
9	C	404	UQ5	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	C	404	UQ5	C19-C21-C22-C23
9	C	404	UQ5	C24-C26-C27-C28
9	M	403	UQ5	C19-C21-C22-C23
12	C	409	CDL	C11-C12-C13-C14
12	Q	101	CDL	CB2-C1-CA2-OA2
12	C	408	CDL	C71-CB7-OB8-CB6
12	M	408	CDL	C31-CA7-OA8-CA6
11	C	406	PGT	C40-C41-C42-C43
12	M	408	CDL	C51-C52-C53-C54
12	M	408	CDL	OB6-CB4-CB6-OB8
15	T	103	PTY	C11-C8-O7-C6
12	Q	101	CDL	C40-C41-C42-C43
10	M	405	3PH	C21-C22-C23-C24
12	C	409	CDL	C31-CA7-OA8-CA6
12	M	408	CDL	CB5-C51-C52-C53
11	C	407	PGT	O5-C5-C6-O6
9	C	403	UQ5	C12-C13-C14-C15
10	C	405	3PH	C21-C22-C23-C24
10	T	101	3PH	C21-C22-C23-C24
10	T	102	3PH	C31-C32-C33-C34
12	C	408	CDL	CA5-C11-C12-C13
12	C	408	CDL	C31-CA7-OA8-CA6
12	C	408	CDL	C16-C17-C18-C19
13	N	303	PC7	C11-C12-C13-C14
9	M	403	UQ5	C24-C26-C27-C28
16	M	404	UQ7	C29-C31-C32-C33
12	Q	101	CDL	C31-CA7-OA8-CA6
12	C	408	CDL	OB9-CB7-OB8-CB6
12	M	408	CDL	OA9-CA7-OA8-CA6
11	C	406	PGT	C32-C31-O2-C2
12	N	302	CDL	C56-C57-C58-C59
11	G	102	PGT	C4-O4P-P-O3P
12	M	408	CDL	CB2-OB2-PB2-OB5
12	Q	101	CDL	CA3-OA5-PA1-OA2
12	Q	101	CDL	CB2-OB2-PB2-OB5
13	D	302	PC7	C4-O4P-P-O3P
13	M	409	PC7	C1-O3P-P-O4P
15	M	407	PTY	C3-O11-P1-O14
12	C	409	CDL	OA9-CA7-OA8-CA6
11	G	102	PGT	O4P-C4-C5-C6
12	O	402	CDL	CB2-C1-CA2-OA2
15	T	103	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
9	M	403	UQ5	C12-C11-C9-C10
13	M	409	PC7	C4-C5-N-C7
12	C	409	CDL	C37-C38-C39-C40
12	C	409	CDL	C11-CA5-OA6-CA4
11	C	407	PGT	C15-C16-C17-C18
12	C	409	CDL	C31-C32-C33-C34
12	N	302	CDL	C59-C60-C61-C62
12	O	402	CDL	C15-C16-C17-C18
13	C	410	PC7	C32-C33-C34-C35
15	M	407	PTY	C34-C35-C36-C37
11	G	102	PGT	C42-C43-C44-C45
11	M	406	PGT	C15-C16-C17-C18
12	M	408	CDL	C73-C74-C75-C76
10	C	405	3PH	C3-C2-O21-C21
12	M	408	CDL	CB3-CB4-OB6-CB5
11	C	406	PGT	O31-C31-O2-C2
12	C	409	CDL	OA7-CA5-OA6-CA4
10	I	101	3PH	C33-C34-C35-C36
11	C	407	PGT	C40-C41-C42-C43
11	C	407	PGT	C18-C19-C20-C21
12	O	402	CDL	C12-C13-C14-C15
13	G	104	PC7	C21-C22-C23-C24
13	G	104	PC7	C39-C40-C41-C42
11	C	407	PGT	O4P-C4-C5-O5
11	G	102	PGT	O4P-C4-C5-O5
12	C	409	CDL	C58-C59-C60-C61
12	Q	101	CDL	CB7-C71-C72-C73
10	G	101	3PH	C24-C25-C26-C27
10	I	101	3PH	C22-C23-C24-C25
12	C	408	CDL	C54-C55-C56-C57
12	M	408	CDL	C56-C57-C58-C59
12	Q	101	CDL	OA9-CA7-OA8-CA6
10	I	101	3PH	C38-C39-C3A-C3B
10	T	101	3PH	C22-C23-C24-C25
11	M	406	PGT	C17-C18-C19-C20
12	C	408	CDL	C83-C84-C85-C86
11	G	102	PGT	C2-C3-O3-C11
10	I	101	3PH	C36-C37-C38-C39
11	G	102	PGT	C40-C41-C42-C43
11	G	102	PGT	C37-C38-C39-C40
12	C	409	CDL	C39-C40-C41-C42
12	M	408	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	C	408	CDL	OA9-CA7-OA8-CA6
11	G	102	PGT	C4-C5-C6-O6
12	N	302	CDL	C51-CB5-OB6-CB4
12	C	409	CDL	C19-C20-C21-C22
16	M	404	UQ7	C12-C13-C14-C16
12	M	408	CDL	CA7-C31-C32-C33
12	O	402	CDL	CB7-C71-C72-C73
11	C	407	PGT	C19-C20-C21-C22
12	C	409	CDL	C36-C37-C38-C39
13	C	410	PC7	C16-C17-C18-C19
13	D	302	PC7	C13-C14-C15-C16
9	M	403	UQ5	C14-C16-C17-C18
12	C	408	CDL	C57-C58-C59-C60
12	C	408	CDL	C80-C81-C82-C83
12	N	302	CDL	C16-C17-C18-C19
12	N	302	CDL	C80-C81-C82-C83
12	O	402	CDL	C19-C20-C21-C22
12	G	103	CDL	C20-C21-C22-C23
13	C	410	PC7	C18-C19-C20-C21
12	C	409	CDL	CA7-C31-C32-C33
12	G	103	CDL	CB7-C71-C72-C73
13	M	409	PC7	C33-C34-C35-C36
11	G	102	PGT	C16-C17-C18-C19
12	C	408	CDL	C76-C77-C78-C79
10	M	405	3PH	C33-C34-C35-C36
11	C	407	PGT	C13-C14-C15-C16
12	N	302	CDL	C74-C75-C76-C77
13	M	409	PC7	C14-C15-C16-C17
11	C	407	PGT	C33-C34-C35-C36
12	C	408	CDL	C55-C56-C57-C58
13	N	303	PC7	C12-C13-C14-C15
16	M	404	UQ7	C37-C38-C39-C40
11	G	102	PGT	O5-C5-C6-O6
17	M	410	Q7G	CG1-C22-C23-C24
11	G	102	PGT	C36-C37-C38-C39
12	G	103	CDL	C32-C33-C34-C35
12	G	103	CDL	C36-C37-C38-C39
13	C	410	PC7	C15-C16-C17-C18
12	N	302	CDL	C71-CB7-OB8-CB6
12	C	408	CDL	C58-C59-C60-C61
12	C	409	CDL	C57-C58-C59-C60
13	C	410	PC7	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	C	408	CDL	CB7-C71-C72-C73
11	C	407	PGT	O4P-C4-C5-C6
12	C	408	CDL	C75-C76-C77-C78
12	O	402	CDL	C79-C80-C81-C82
15	M	407	PTY	C13-C14-C15-C16
12	N	302	CDL	OB7-CB5-OB6-CB4
15	J	101	PTY	C16-C17-C18-C19
15	M	407	PTY	C40-C41-C42-C43
11	C	407	PGT	C43-C44-C45-C46
13	C	410	PC7	C36-C37-C38-C39
10	T	102	3PH	C32-C33-C34-C35
13	C	410	PC7	C34-C35-C36-C37
12	N	302	CDL	CA5-C11-C12-C13
15	T	103	PTY	C30-C31-C32-C33
12	C	408	CDL	C12-C13-C14-C15
9	C	404	UQ5	C18-C19-C21-C22
10	G	101	3PH	O22-C21-O21-C2
10	M	405	3PH	C31-C32-C33-C34
12	G	103	CDL	CA5-C11-C12-C13
12	G	103	CDL	C35-C36-C37-C38
12	G	103	CDL	C11-C12-C13-C14
13	G	104	PC7	C20-C21-C22-C23
10	M	405	3PH	C34-C35-C36-C37
12	N	302	CDL	OB9-CB7-OB8-CB6
16	M	404	UQ7	C9-C11-C12-C13
12	M	408	CDL	C35-C36-C37-C38
12	N	302	CDL	C73-C74-C75-C76
12	G	103	CDL	CA7-C31-C32-C33
10	G	101	3PH	C22-C21-O21-C2
10	I	101	3PH	C22-C21-O21-C2
12	C	408	CDL	OB5-CB3-CB4-OB6
13	N	303	PC7	C33-C34-C35-C36
15	J	101	PTY	C31-C32-C33-C34
10	G	101	3PH	C29-C2A-C2B-C2C
10	I	101	3PH	O22-C21-O21-C2
12	G	103	CDL	C13-C14-C15-C16
12	C	408	CDL	OB6-CB4-CB6-OB8
13	D	302	PC7	C35-C36-C37-C38
13	M	409	PC7	C4-C5-N-C8
13	M	409	PC7	C4-C5-N-C6
9	M	403	UQ5	C12-C11-C9-C8
12	C	409	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	C	409	CDL	C53-C54-C55-C56
13	C	410	PC7	C19-C20-C21-C22
12	Q	101	CDL	C38-C39-C40-C41
13	M	409	PC7	C35-C36-C37-C38
12	C	408	CDL	CA3-OA5-PA1-OA2
10	G	101	3PH	C32-C33-C34-C35
9	C	403	UQ5	C27-C28-C29-C30
9	C	403	UQ5	C6-C7-C8-C9
11	C	406	PGT	C33-C34-C35-C36
13	M	409	PC7	C40-C41-C42-C43
12	C	409	CDL	C55-C56-C57-C58
11	C	407	PGT	C32-C33-C34-C35
12	M	408	CDL	C13-C14-C15-C16
11	G	102	PGT	C38-C39-C40-C41
9	C	404	UQ5	C20-C19-C21-C22
11	C	407	PGT	C31-C32-C33-C34
12	C	409	CDL	C16-C17-C18-C19
13	G	104	PC7	C14-C15-C16-C17
12	M	408	CDL	CB3-CB4-CB6-OB8
12	N	302	CDL	CA3-CA4-CA6-OA8
12	O	402	CDL	CA3-CA4-CA6-OA8
12	Q	101	CDL	CB3-CB4-CB6-OB8
13	D	302	PC7	C1-C2-C3-O3
13	M	409	PC7	C1-C2-C3-O3
16	M	404	UQ7	C37-C38-C39-C41
12	M	408	CDL	C40-C41-C42-C43
11	M	406	PGT	C20-C21-C22-C23
13	C	410	PC7	C44-C45-C46-C47
13	G	104	PC7	C15-C16-C17-C18
12	C	408	CDL	C32-C31-CA7-OA8
10	T	102	3PH	C23-C24-C25-C26
11	C	407	PGT	C42-C43-C44-C45
13	D	302	PC7	C31-C32-C33-C34
13	G	104	PC7	C32-C33-C34-C35
12	N	302	CDL	C81-C82-C83-C84
9	C	404	UQ5	C12-C11-C9-C10
12	C	409	CDL	C15-C16-C17-C18
9	C	404	UQ5	C12-C11-C9-C8
11	C	406	PGT	C45-C46-C47-C48
13	M	409	PC7	C32-C33-C34-C35
12	C	409	CDL	C74-C75-C76-C77
10	C	405	3PH	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
10	G	101	3PH	C1-O11-P-O12
10	I	101	3PH	C1-O11-P-O12
12	C	409	CDL	C18-C19-C20-C21
11	G	102	PGT	O3P-C1-C2-O2
10	T	101	3PH	C35-C36-C37-C38
11	G	102	PGT	C21-C22-C23-C24
12	M	408	CDL	C57-C58-C59-C60
13	M	409	PC7	C16-C17-C18-C19
15	T	103	PTY	O4-C1-C6-O7
10	T	102	3PH	C32-C31-O31-C3
10	T	102	3PH	C35-C36-C37-C38
11	C	406	PGT	C41-C42-C43-C44
13	M	409	PC7	C31-C32-C33-C34
12	M	408	CDL	C55-C56-C57-C58
12	O	402	CDL	C11-C12-C13-C14
10	G	101	3PH	C25-C26-C27-C28
10	G	101	3PH	O11-C1-C2-C3
12	C	408	CDL	OB5-CB3-CB4-CB6
12	C	409	CDL	OA5-CA3-CA4-CA6
12	N	302	CDL	C11-C12-C13-C14
15	M	407	PTY	C11-C12-C13-C14
15	J	101	PTY	C34-C35-C36-C37
16	M	404	UQ7	C11-C12-C13-C14
12	G	103	CDL	C53-C54-C55-C56
13	N	303	PC7	C17-C18-C19-C20
15	T	103	PTY	C11-C12-C13-C14
10	M	405	3PH	C2B-C2C-C2D-C2E
11	M	406	PGT	C12-C11-O3-C3
10	C	405	3PH	C1-C2-C3-O31
11	M	406	PGT	C1-C2-C3-O3
12	C	408	CDL	CA3-CA4-CA6-OA8
13	C	410	PC7	C1-C2-C3-O3
13	N	303	PC7	C1-C2-C3-O3
11	C	407	PGT	C34-C35-C36-C37
12	O	402	CDL	C52-C53-C54-C55
12	G	103	CDL	C41-C42-C43-C44
11	G	102	PGT	C32-C31-O2-C2
10	T	101	3PH	C36-C37-C38-C39
11	G	102	PGT	C41-C42-C43-C44
12	G	103	CDL	CB3-OB5-PB2-OB2
17	M	410	Q7G	CG1-C22-C23-C48
10	C	405	3PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
10	G	101	3PH	O11-C1-C2-O21
12	C	408	CDL	C72-C71-CB7-OB8
12	C	409	CDL	C17-C18-C19-C20
10	G	101	3PH	C33-C34-C35-C36
11	G	102	PGT	C34-C35-C36-C37
12	C	408	CDL	OA6-CA4-CA6-OA8
12	Q	101	CDL	OB6-CB4-CB6-OB8
13	C	410	PC7	O2-C2-C3-O3
13	D	302	PC7	O2-C2-C3-O3
13	C	410	PC7	C13-C14-C15-C16
12	M	408	CDL	C31-C32-C33-C34
10	C	405	3PH	C37-C38-C39-C3A
13	G	104	PC7	C17-C18-C19-C20
12	G	103	CDL	C74-C75-C76-C77
12	O	402	CDL	C18-C19-C20-C21
13	G	104	PC7	C16-C17-C18-C19
10	I	101	3PH	C2-C1-O11-P
11	G	102	PGT	C5-C4-O4P-P
10	T	102	3PH	O32-C31-O31-C3
12	N	302	CDL	C53-C54-C55-C56
11	G	102	PGT	O31-C31-O2-C2
12	M	408	CDL	OB5-CB3-CB4-CB6
12	N	302	CDL	OB5-CB3-CB4-CB6
12	Q	101	CDL	OA5-CA3-CA4-CA6
15	T	103	PTY	O14-C5-C6-C1
12	Q	101	CDL	C43-C44-C45-C46
12	C	409	CDL	C33-C34-C35-C36
9	C	403	UQ5	C27-C28-C29-C31
10	C	405	3PH	C25-C26-C27-C28
12	Q	101	CDL	C41-C42-C43-C44
12	Q	101	CDL	C51-C52-C53-C54
11	G	102	PGT	C17-C18-C19-C20
8	O	401	HEM	C2B-C3B-CAB-CBB
16	M	404	UQ7	C12-C13-C14-C15
11	G	102	PGT	C1-C2-C3-O3
12	C	409	CDL	CA3-CA4-CA6-OA8
12	M	408	CDL	CA3-CA4-CA6-OA8
10	T	102	3PH	O11-C1-C2-O21
12	C	409	CDL	OA5-CA3-CA4-OA6
12	G	103	CDL	C19-C20-C21-C22
11	M	406	PGT	O11-C11-O3-C3
10	C	405	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
11	G	102	PGT	O2-C2-C3-O3
12	M	408	CDL	OA6-CA4-CA6-OA8
12	O	402	CDL	OB6-CB4-CB6-OB8
10	C	405	3PH	C39-C3A-C3B-C3C
12	Q	101	CDL	CB4-CB6-OB8-CB7
10	C	405	3PH	C22-C23-C24-C25
10	M	405	3PH	C39-C3A-C3B-C3C
12	C	409	CDL	C59-C60-C61-C62
12	Q	101	CDL	C13-C14-C15-C16
17	M	410	Q7G	C22-CG1-O20-C17
12	C	408	CDL	O1-C1-CB2-OB2
12	Q	101	CDL	C31-C32-C33-C34
12	C	408	CDL	CB4-CB3-OB5-PB2
12	O	402	CDL	CB4-CB3-OB5-PB2
11	G	102	PGT	C1-O3P-P-O1P
11	G	102	PGT	C4-O4P-P-O1P
11	M	406	PGT	C4-O4P-P-O2P
12	C	408	CDL	CA2-OA2-PA1-OA4
12	C	408	CDL	CA3-OA5-PA1-OA3
12	C	408	CDL	CA3-OA5-PA1-OA4
12	G	103	CDL	CB3-OB5-PB2-OB3
12	M	408	CDL	CB2-OB2-PB2-OB4
12	N	302	CDL	CB2-OB2-PB2-OB3
12	Q	101	CDL	CB2-OB2-PB2-OB3
13	D	302	PC7	C4-O4P-P-O2P
13	G	104	PC7	C4-O4P-P-O2P
13	M	409	PC7	C1-O3P-P-O1P
15	M	407	PTY	C3-O11-P1-O13
11	M	406	PGT	C22-C23-C24-C25
10	C	405	3PH	O11-C1-C2-C3
10	T	102	3PH	O11-C1-C2-C3
11	G	102	PGT	O3P-C1-C2-C3
12	C	408	CDL	OA5-CA3-CA4-CA6
12	M	408	CDL	C74-C75-C76-C77
10	T	101	3PH	C33-C34-C35-C36
12	N	302	CDL	C77-C78-C79-C80
9	C	404	UQ5	C2-C3-O3-C3M
15	M	407	PTY	C2-C3-O11-P1
12	Q	101	CDL	CA2-C1-CB2-OB2
10	M	405	3PH	C36-C37-C38-C39
12	C	409	CDL	C56-C57-C58-C59
9	C	404	UQ5	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
11	G	102	PGT	C31-C32-C33-C34
12	C	408	CDL	OA5-CA3-CA4-OA6
12	M	408	CDL	OA5-CA3-CA4-OA6
12	M	408	CDL	OB5-CB3-CB4-OB6
12	Q	101	CDL	OA5-CA3-CA4-OA6
15	T	103	PTY	O14-C5-C6-O7
12	G	103	CDL	C22-C23-C24-C25
12	C	409	CDL	C44-C45-C46-C47
15	T	103	PTY	C8-C11-C12-C13
12	C	409	CDL	C20-C21-C22-C23
13	G	104	PC7	C13-C14-C15-C16
11	M	406	PGT	C23-C24-C25-C26
15	T	103	PTY	O4-C1-C6-C5
10	M	405	3PH	O21-C2-C3-O31
12	C	409	CDL	OA6-CA4-CA6-OA8
12	N	302	CDL	OA6-CA4-CA6-OA8
12	O	402	CDL	OA6-CA4-CA6-OA8
12	M	408	CDL	C16-C17-C18-C19
11	C	407	PGT	C35-C36-C37-C38
12	C	409	CDL	C23-C24-C25-C26
10	T	101	3PH	O22-C21-O21-C2
16	M	404	UQ7	C4-C3-O3-CM3
11	G	102	PGT	C19-C20-C21-C22
12	C	409	CDL	C72-C73-C74-C75
12	N	302	CDL	C78-C79-C80-C81
15	M	407	PTY	C41-C42-C43-C44
12	N	302	CDL	CA6-CA4-OA6-CA5
12	M	408	CDL	OA5-CA3-CA4-CA6
10	T	101	3PH	C1-O11-P-O12
12	G	103	CDL	C12-C13-C14-C15
12	O	402	CDL	C38-C39-C40-C41
9	C	404	UQ5	C15-C14-C16-C17
15	T	103	PTY	C33-C34-C35-C36
11	G	102	PGT	C11-C12-C13-C14
10	T	101	3PH	C22-C21-O21-C2
13	N	303	PC7	O2-C2-C3-O3
11	C	406	PGT	C1-O3P-P-O4P
12	C	408	CDL	CB2-OB2-PB2-OB5
12	C	409	CDL	CA2-OA2-PA1-OA5
12	N	302	CDL	CA2-OA2-PA1-OA5
12	N	302	CDL	CB2-OB2-PB2-OB5
12	O	402	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
12	Q	101	CDL	CA2-OA2-PA1-OA5
15	T	103	PTY	C3-O11-P1-O14
12	G	103	CDL	C17-C18-C19-C20
10	G	101	3PH	C28-C29-C2A-C2B
12	N	302	CDL	C63-C64-C65-C66
13	C	410	PC7	C4-C5-N-C8
12	C	408	CDL	C19-C20-C21-C22
12	C	409	CDL	C43-C44-C45-C46
12	N	302	CDL	C58-C59-C60-C61
12	M	408	CDL	CA2-C1-CB2-OB2
12	C	409	CDL	CB7-C71-C72-C73
11	G	102	PGT	C15-C16-C17-C18
12	M	408	CDL	C72-C73-C74-C75
10	C	405	3PH	C3A-C3B-C3C-C3D
10	C	405	3PH	C33-C34-C35-C36
12	C	409	CDL	OB5-CB3-CB4-OB6
8	O	401	HEM	C4B-C3B-CAB-CBB
10	T	102	3PH	C29-C2A-C2B-C2C
12	C	408	CDL	CA4-CA3-OA5-PA1
9	C	403	UQ5	C2-C3-O3-C3M
12	O	402	CDL	C78-C79-C80-C81
12	M	408	CDL	C52-C53-C54-C55
11	C	406	PGT	C44-C45-C46-C47
10	T	102	3PH	C26-C27-C28-C29
8	O	401	HEM	CAA-CBA-CGA-O1A
8	O	401	HEM	CAA-CBA-CGA-O2A
9	C	403	UQ5	C14-C16-C17-C18
8	E	400	HEM	CAA-CBA-CGA-O1A
8	M	402	HEM	CAD-CBD-CGD-O1D
12	G	103	CDL	C54-C55-C56-C57
10	M	405	3PH	O22-C21-O21-C2
10	T	102	3PH	O22-C21-O21-C2
15	M	407	PTY	O10-C8-O7-C6
12	C	408	CDL	C60-C61-C62-C63
13	C	410	PC7	C41-C42-C43-C44
11	M	406	PGT	C4-O4P-P-O3P
10	M	405	3PH	C32-C33-C34-C35
13	G	104	PC7	C12-C11-O3-C3
8	M	402	HEM	CAD-CBD-CGD-O2D
12	N	302	CDL	C83-C84-C85-C86
12	G	103	CDL	C16-C17-C18-C19
12	N	302	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	M	406	PGT	C21-C22-C23-C24
8	C	402	HEM	CAD-CBD-CGD-O2D
8	E	400	HEM	CAA-CBA-CGA-O2A
10	M	405	3PH	C37-C38-C39-C3A
10	T	102	3PH	C39-C3A-C3B-C3C
8	M	401	HEM	CAA-CBA-CGA-O1A
12	G	103	CDL	OB6-CB4-CB6-OB8
8	M	401	HEM	CAA-CBA-CGA-O2A
16	M	404	UQ7	C26-C27-C28-C29
12	N	302	CDL	CB2-C1-CA2-OA2
8	C	402	HEM	CAD-CBD-CGD-O1D
12	O	402	CDL	C34-C35-C36-C37
13	C	410	PC7	C35-C36-C37-C38
12	C	408	CDL	C32-C31-CA7-OA9
11	C	407	PGT	C36-C37-C38-C39
12	C	409	CDL	C38-C39-C40-C41
11	C	407	PGT	C41-C42-C43-C44
12	O	402	CDL	C37-C38-C39-C40
15	M	407	PTY	C39-C40-C41-C42
8	C	401	HEM	CAA-CBA-CGA-O2A
10	M	405	3PH	C3F-C3G-C3H-C3I
12	G	103	CDL	C71-C72-C73-C74
10	M	405	3PH	O11-C1-C2-O21
12	Q	101	CDL	OB5-CB3-CB4-OB6
10	M	405	3PH	C22-C23-C24-C25
12	C	408	CDL	C17-C18-C19-C20
12	Q	101	CDL	C11-C12-C13-C14
15	M	407	PTY	C16-C17-C18-C19
12	Q	101	CDL	OB5-CB3-CB4-CB6
13	G	104	PC7	O11-C11-O3-C3
15	M	407	PTY	C12-C13-C14-C15
12	O	402	CDL	C77-C78-C79-C80
9	C	404	UQ5	C4-C3-O3-C3M
12	C	408	CDL	C15-C16-C17-C18
10	T	102	3PH	C22-C21-O21-C2
10	T	101	3PH	C1-O11-P-O14
11	C	406	PGT	C4-O4P-P-O3P
9	C	404	UQ5	C23-C24-C26-C27
12	N	302	CDL	O1-C1-CA2-OA2
12	N	302	CDL	C51-C52-C53-C54
12	O	402	CDL	C76-C77-C78-C79
8	C	402	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	G	101	3PH	O21-C21-C22-C23
12	M	408	CDL	C12-C11-CA5-OA6
12	Q	101	CDL	C36-C37-C38-C39
12	C	408	CDL	C72-C71-CB7-OB9
12	O	402	CDL	C32-C31-CA7-OA8
13	D	302	PC7	O3-C11-C12-C13
15	T	103	PTY	C12-C11-C8-O7
16	M	404	UQ7	C14-C16-C17-C18
12	C	408	CDL	CB3-CB4-CB6-OB8
12	G	103	CDL	CB3-CB4-CB6-OB8
8	C	401	HEM	CAA-CBA-CGA-O1A
11	M	406	PGT	C18-C19-C20-C21
12	Q	101	CDL	C32-C31-CA7-OA8
12	Q	101	CDL	C72-C71-CB7-OB8
13	C	410	PC7	C4-C5-N-C7
13	D	302	PC7	C4-C5-N-C7
8	C	402	HEM	C4B-C3B-CAB-CBB
12	M	408	CDL	O1-C1-CB2-OB2
12	Q	101	CDL	O1-C1-CB2-OB2
10	M	405	3PH	C22-C21-O21-C2
10	M	405	3PH	O11-C1-C2-C3
10	I	101	3PH	O31-C31-C32-C33
13	G	104	PC7	O2-C31-C32-C33
15	M	407	PTY	O4-C30-C31-C32
13	C	410	PC7	C4-C5-N-C6
12	C	409	CDL	OB7-CB5-OB6-CB4
13	G	104	PC7	O3-C11-C12-C13
12	M	408	CDL	C58-C59-C60-C61
16	M	404	UQ7	C2-C3-O3-CM3
15	M	407	PTY	C11-C8-O7-C6
10	G	101	3PH	O22-C21-C22-C23
13	D	302	PC7	O11-C11-C12-C13
9	C	404	UQ5	C13-C14-C16-C17
12	M	408	CDL	C71-CB7-OB8-CB6
12	Q	101	CDL	C32-C31-CA7-OA9
12	Q	101	CDL	C72-C71-CB7-OB9
9	M	403	UQ5	C16-C17-C18-C19
10	T	101	3PH	C37-C38-C39-C3A
10	I	101	3PH	C1-C2-C3-O31
10	M	405	3PH	C1-C2-C3-O31
12	O	402	CDL	CB3-CB4-CB6-OB8
13	G	104	PC7	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
13	G	104	PC7	O11-C11-C12-C13
15	T	103	PTY	C12-C11-C8-O10
11	G	102	PGT	C44-C45-C46-C47
12	M	408	CDL	OB9-CB7-OB8-CB6
11	M	406	PGT	O2-C31-C32-C33
12	O	402	CDL	C72-C71-CB7-OB8
12	M	408	CDL	C15-C16-C17-C18
11	C	406	PGT	C4-O4P-P-O1P
12	C	408	CDL	CB2-OB2-PB2-OB3
12	C	409	CDL	CA3-OA5-PA1-OA3
12	G	103	CDL	CB2-OB2-PB2-OB3
12	N	302	CDL	CA2-OA2-PA1-OA3
13	D	302	PC7	C4-C5-N-C6
13	M	409	PC7	C1-O3P-P-O2P
15	T	103	PTY	C3-O11-P1-O13
15	T	103	PTY	C5-O14-P1-O13
11	C	407	PGT	C39-C40-C41-C42
15	M	407	PTY	C33-C34-C35-C36
12	M	408	CDL	C12-C11-CA5-OA7
11	C	407	PGT	C20-C21-C22-C23
13	G	104	PC7	C43-C44-C45-C46
13	G	104	PC7	C22-C23-C24-C25
12	O	402	CDL	C32-C31-CA7-OA9
15	M	407	PTY	O30-C30-C31-C32
13	M	409	PC7	C12-C11-O3-C3
13	N	303	PC7	C5-C4-O4P-P
13	M	409	PC7	O11-C11-O3-C3
10	I	101	3PH	O32-C31-C32-C33
12	O	402	CDL	C13-C14-C15-C16
12	O	402	CDL	CB5-C51-C52-C53
10	T	101	3PH	C39-C3A-C3B-C3C
8	C	402	HEM	C2A-CAA-CBA-CGA
12	O	402	CDL	C59-C60-C61-C62
11	G	102	PGT	C12-C13-C14-C15
10	M	405	3PH	O21-C21-C22-C23
12	C	409	CDL	C72-C71-CB7-OB8
13	D	302	PC7	O2-C31-C32-C33
11	C	406	PGT	C39-C40-C41-C42
11	M	406	PGT	O31-C31-C32-C33
11	G	102	PGT	C45-C46-C47-C48
12	N	302	CDL	C12-C13-C14-C15
12	O	402	CDL	C72-C71-CB7-OB9

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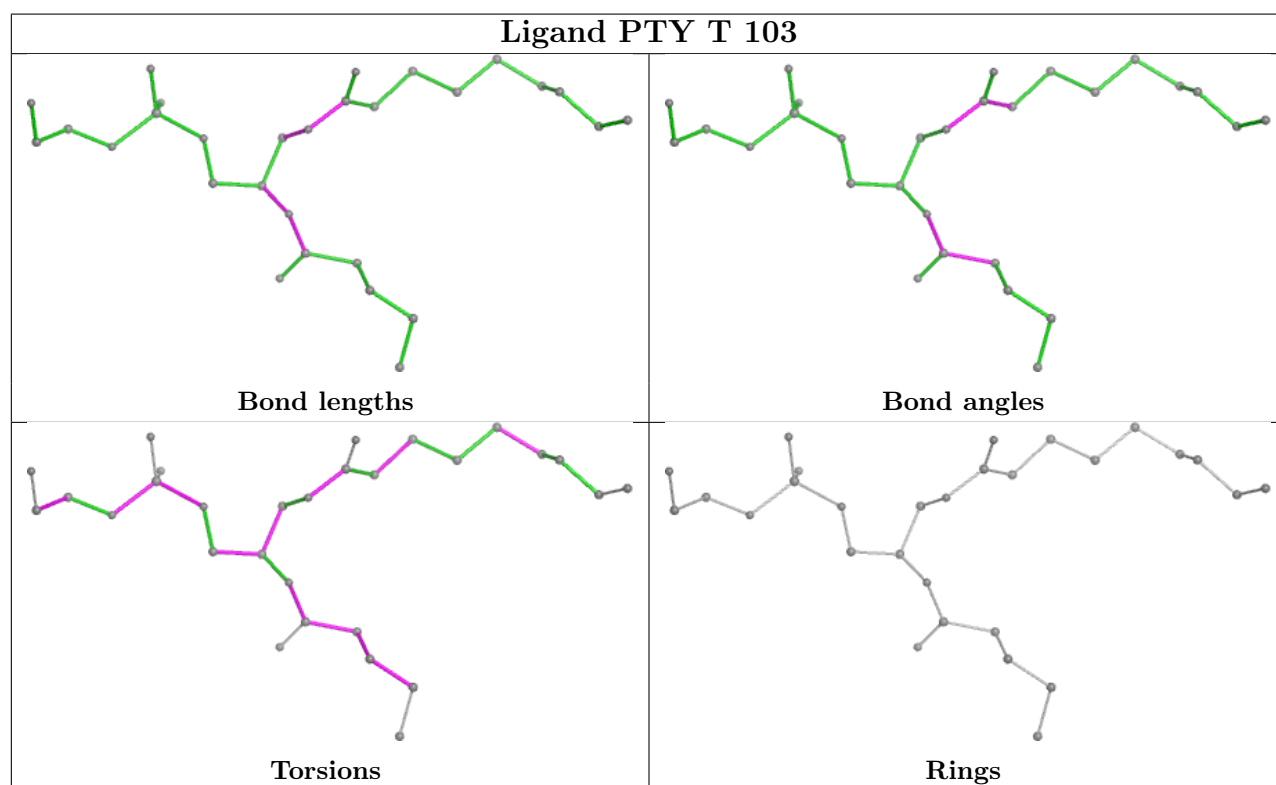
Mol	Chain	Res	Type	Atoms
12	M	408	CDL	C42-C43-C44-C45
8	C	402	HEM	CAA-CBA-CGA-O1A

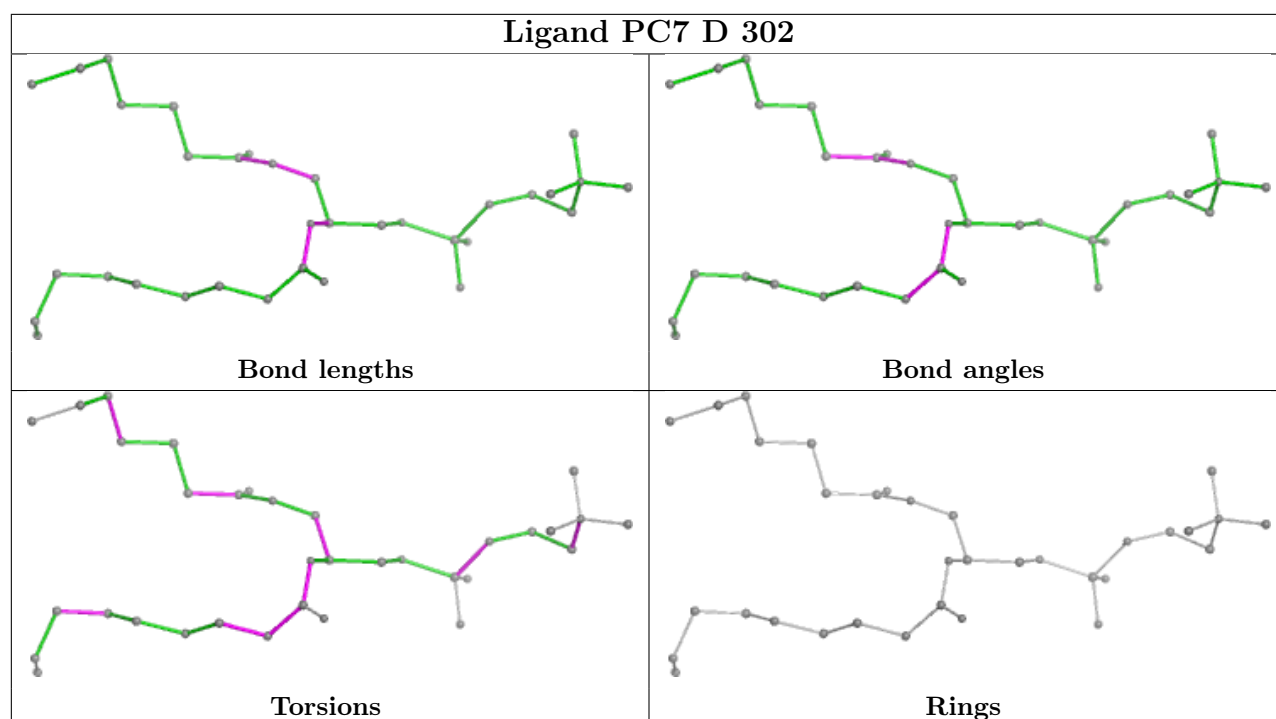
There are no ring outliers.

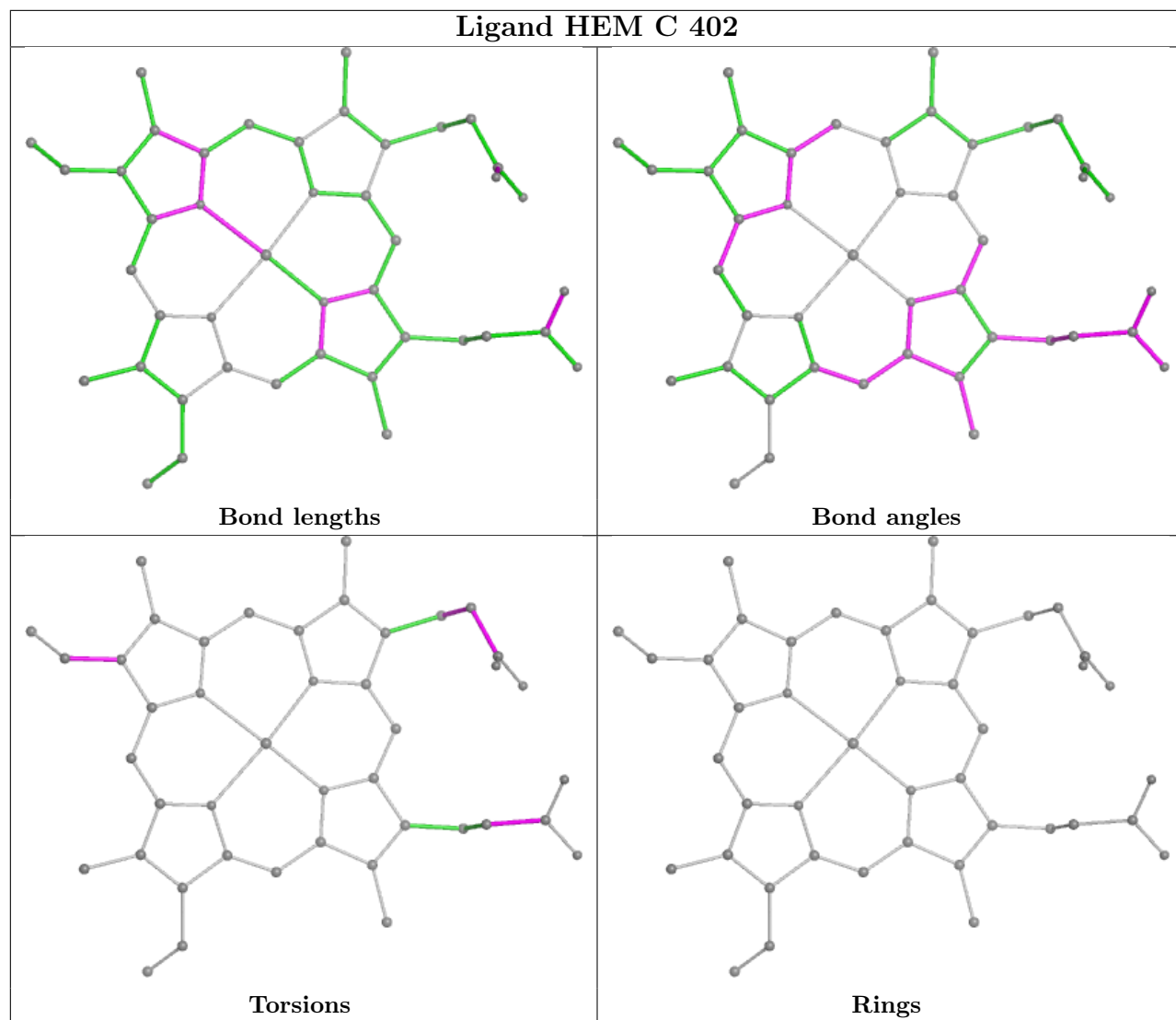
34 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	103	PTY	1	0
13	D	302	PC7	1	0
8	C	402	HEM	1	0
8	M	402	HEM	1	0
11	M	406	PGT	4	0
12	Q	101	CDL	6	0
10	G	101	3PH	1	0
11	G	102	PGT	2	0
16	M	404	UQ7	12	0
8	E	400	HEM	5	0
11	C	407	PGT	4	0
10	T	101	3PH	2	0
14	N	301	FES	1	0
13	M	409	PC7	2	0
9	M	403	UQ5	8	0
10	I	101	3PH	3	0
13	C	410	PC7	9	0
15	M	407	PTY	2	0
12	C	408	CDL	9	0
10	T	102	3PH	1	0
10	C	405	3PH	1	0
12	O	402	CDL	7	0
11	C	406	PGT	6	0
8	O	401	HEM	5	0
12	C	409	CDL	10	0
9	C	403	UQ5	11	0
13	G	104	PC7	5	0
9	C	404	UQ5	6	0
12	N	302	CDL	3	0
12	G	103	CDL	6	0
10	M	405	3PH	6	0
12	M	408	CDL	8	0
13	N	303	PC7	6	0
8	C	401	HEM	1	0

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

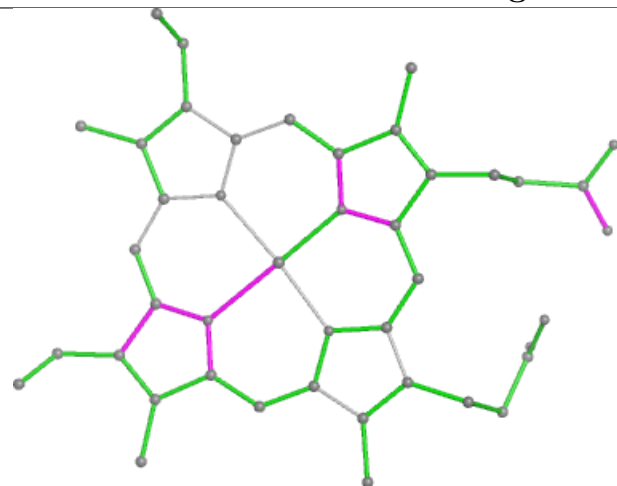




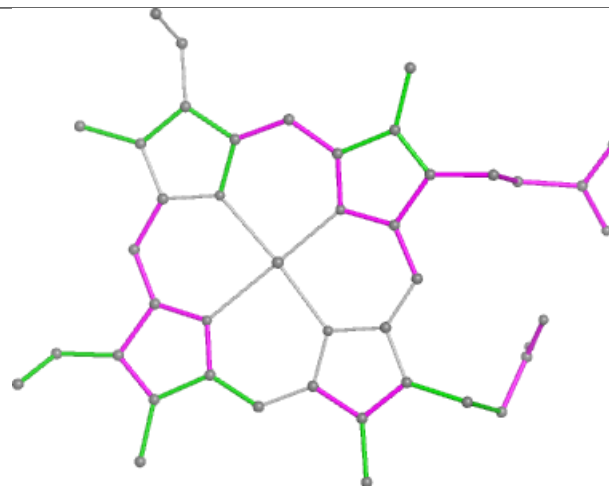




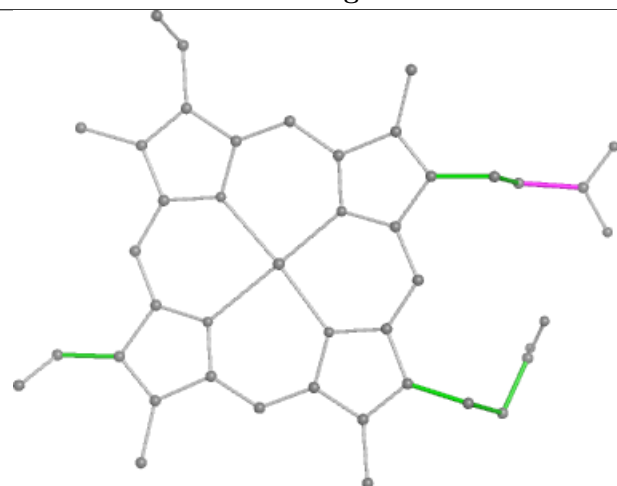
## Ligand HEM M 402



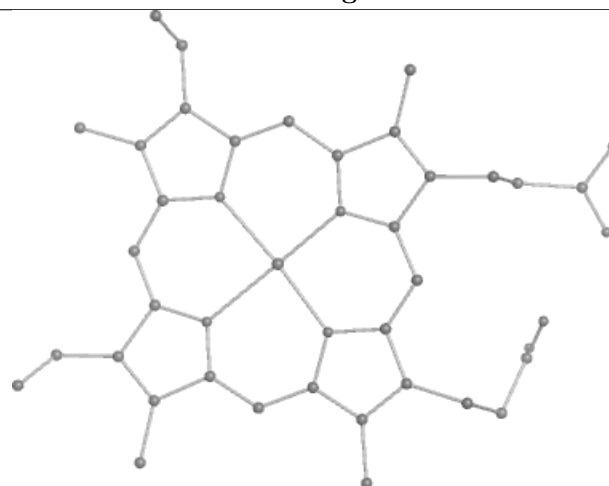
Bond lengths



Bond angles

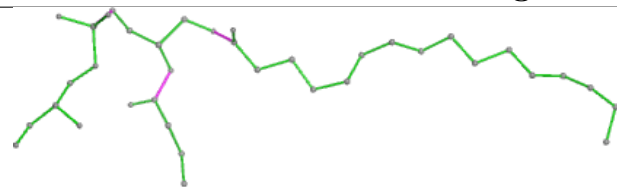


Torsions

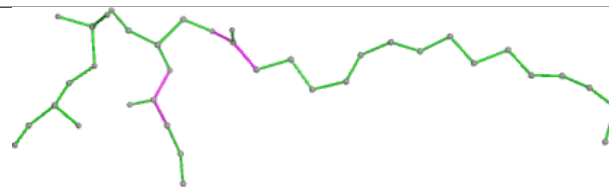


Rings

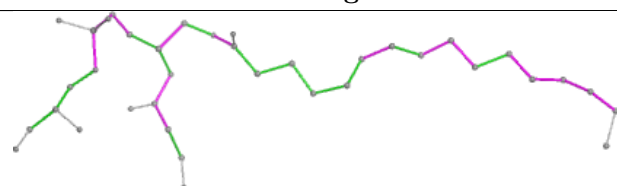
## Ligand PGT M 406



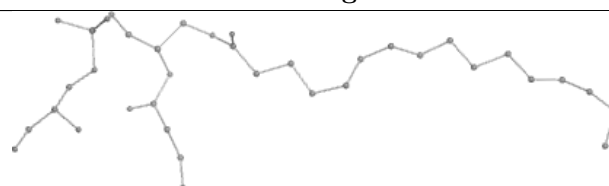
Bond lengths



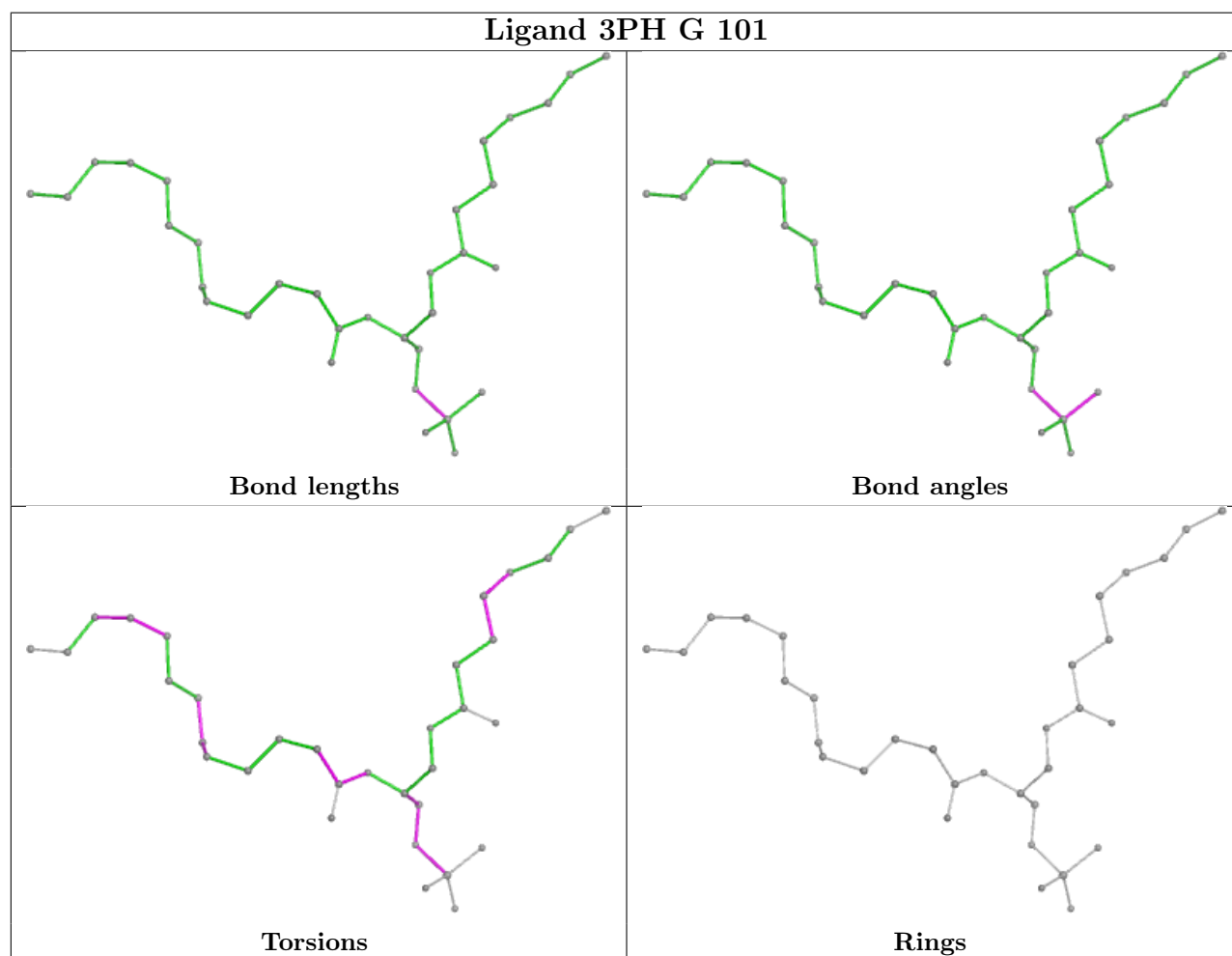
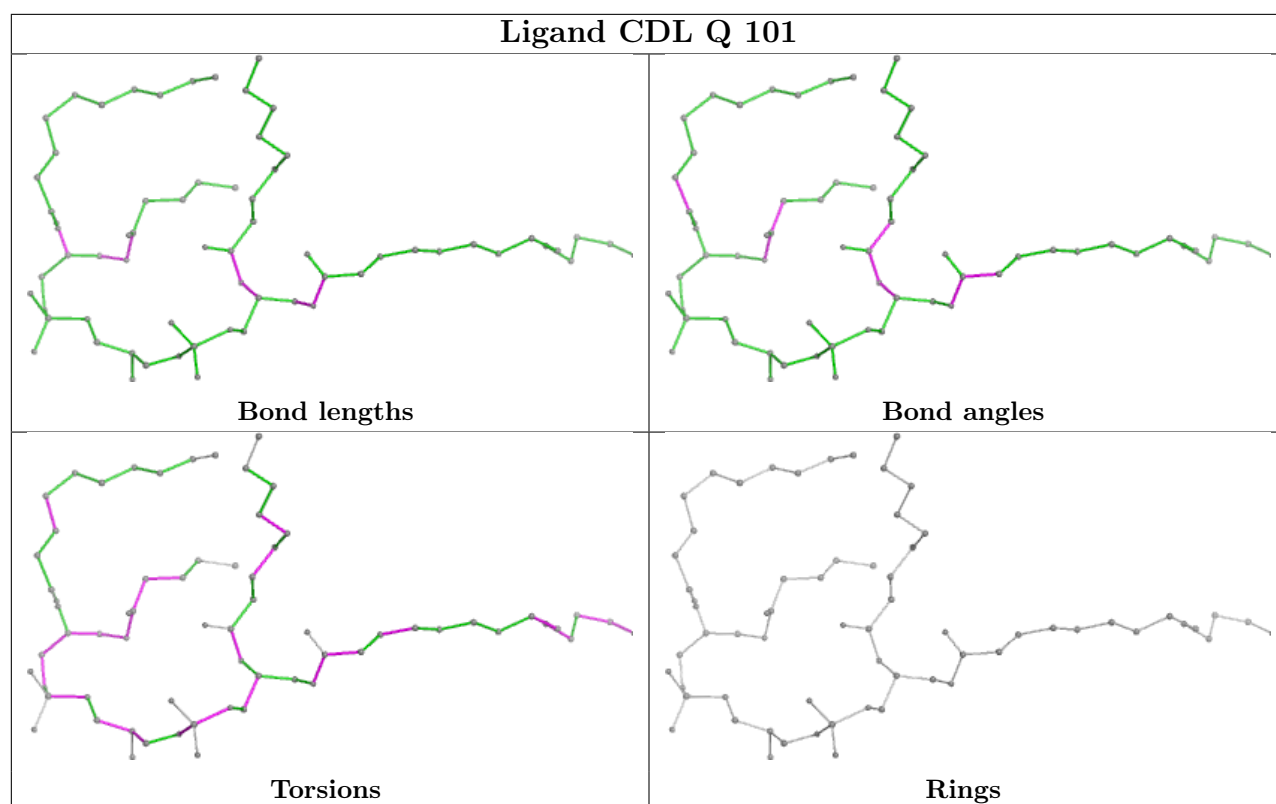
Bond angles

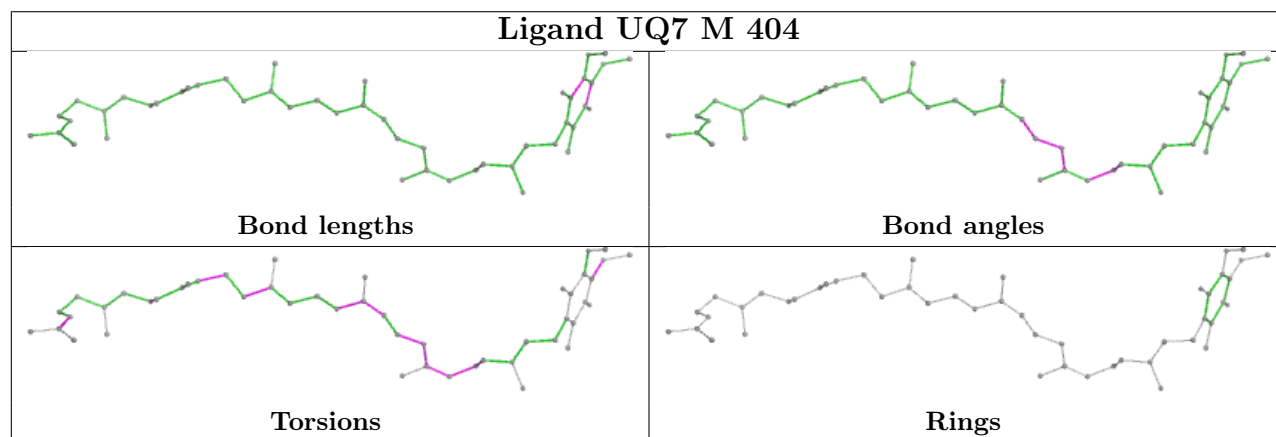
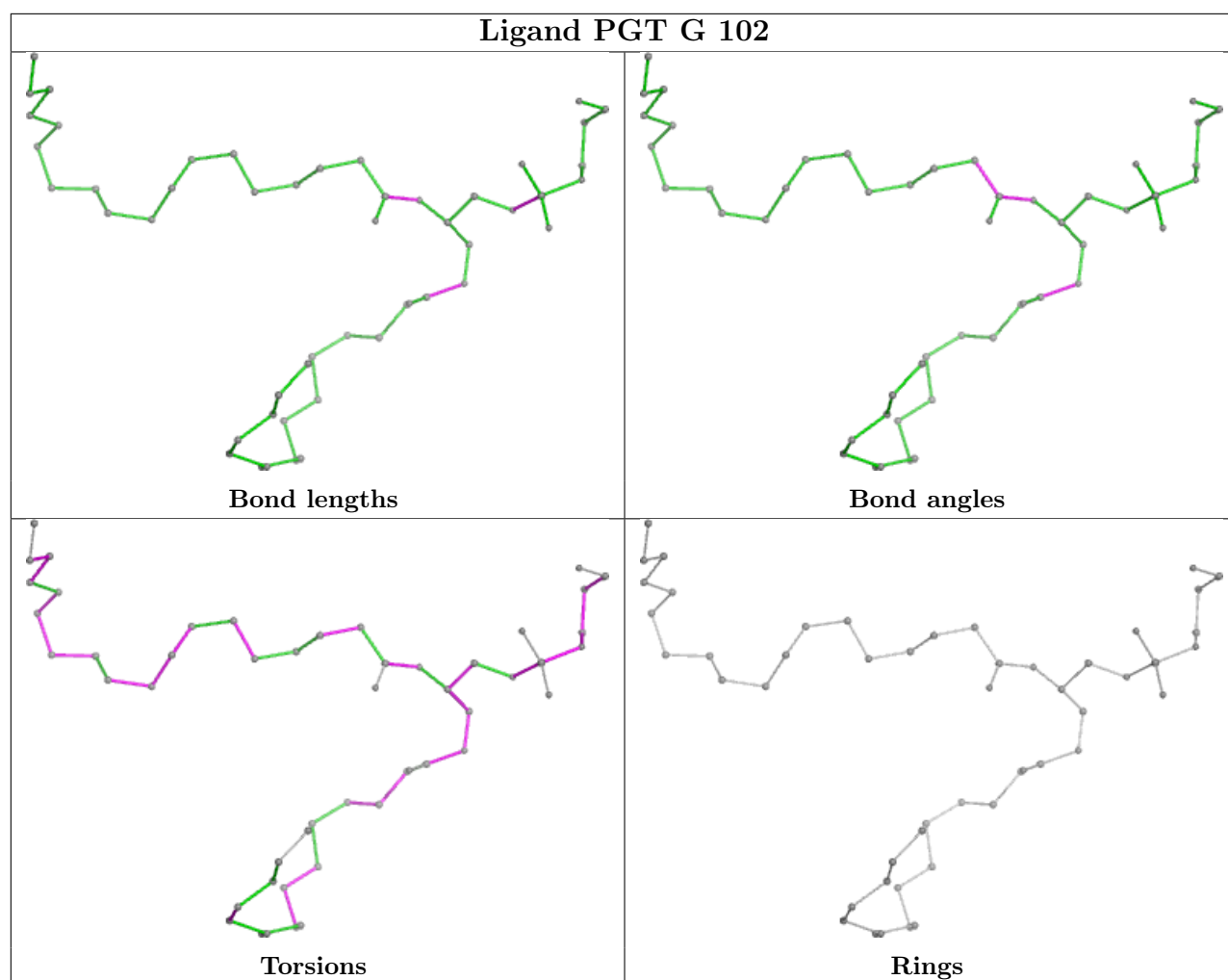


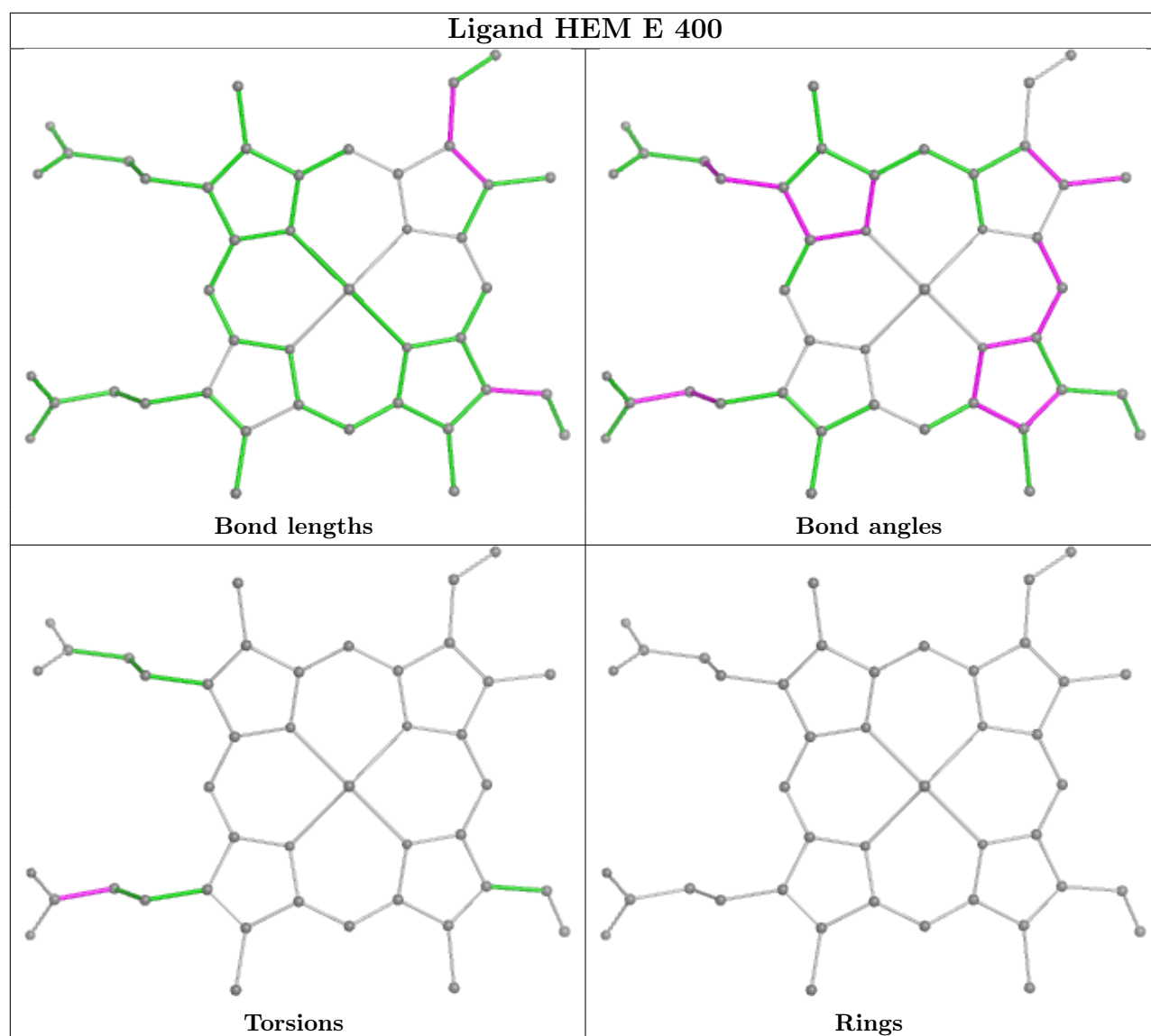
Torsions

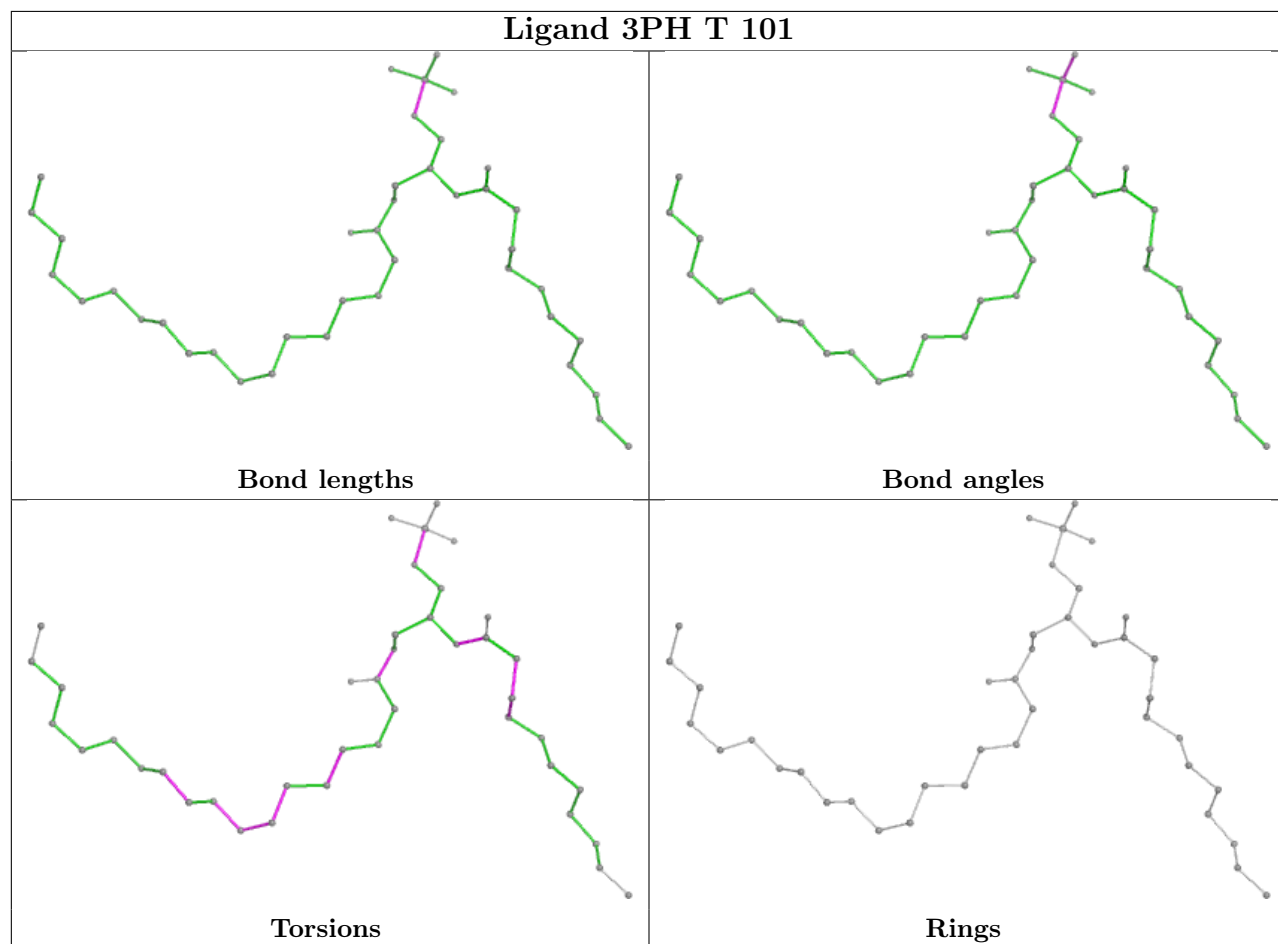
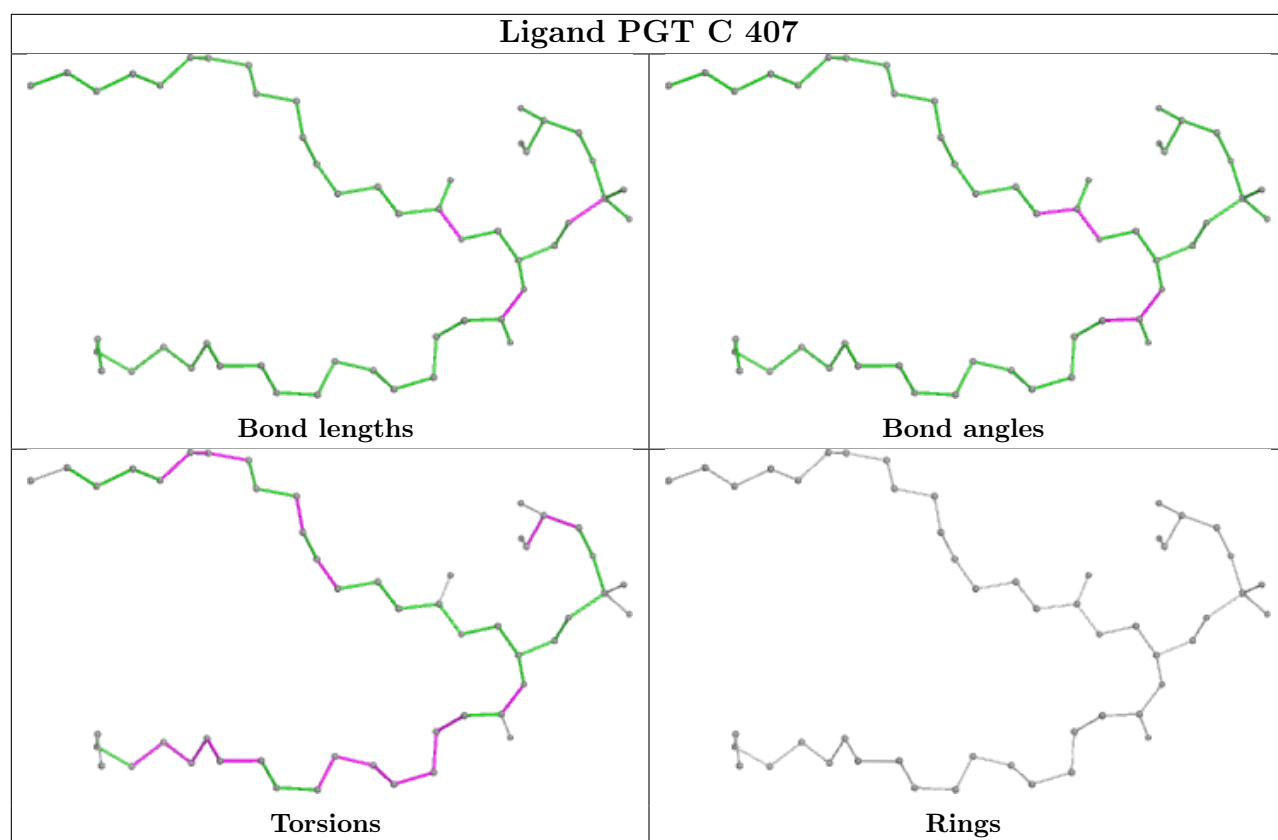


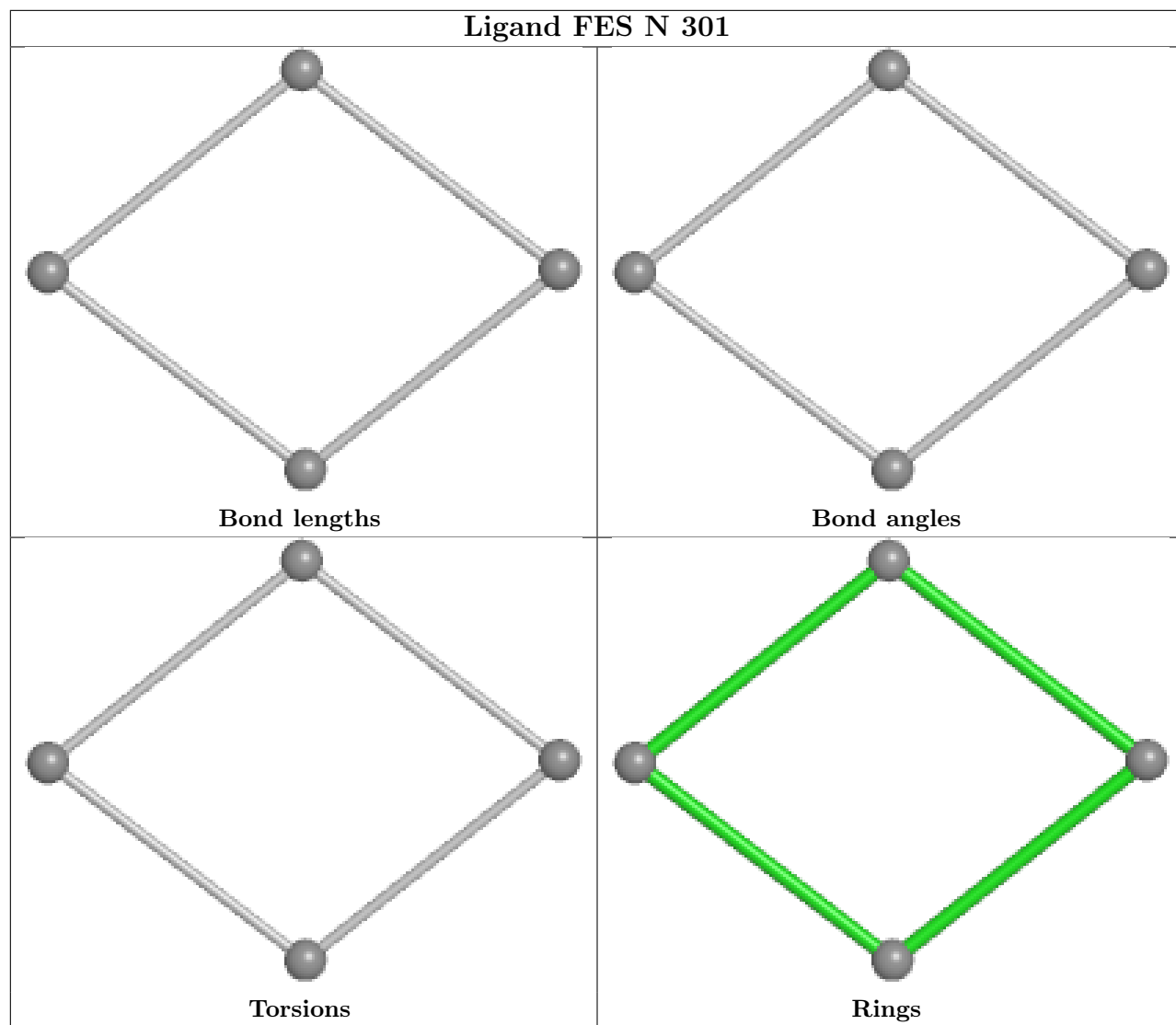
Rings

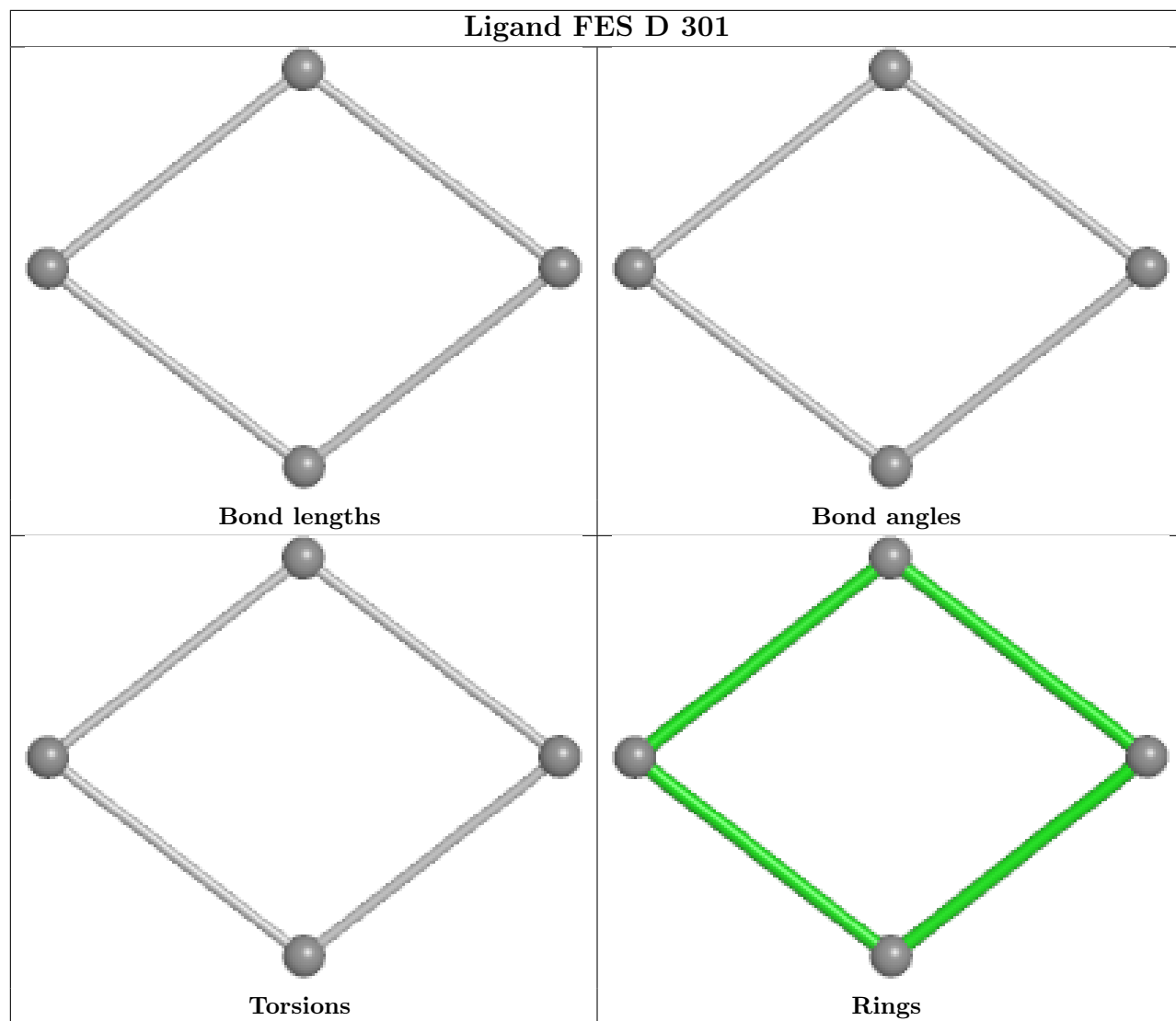


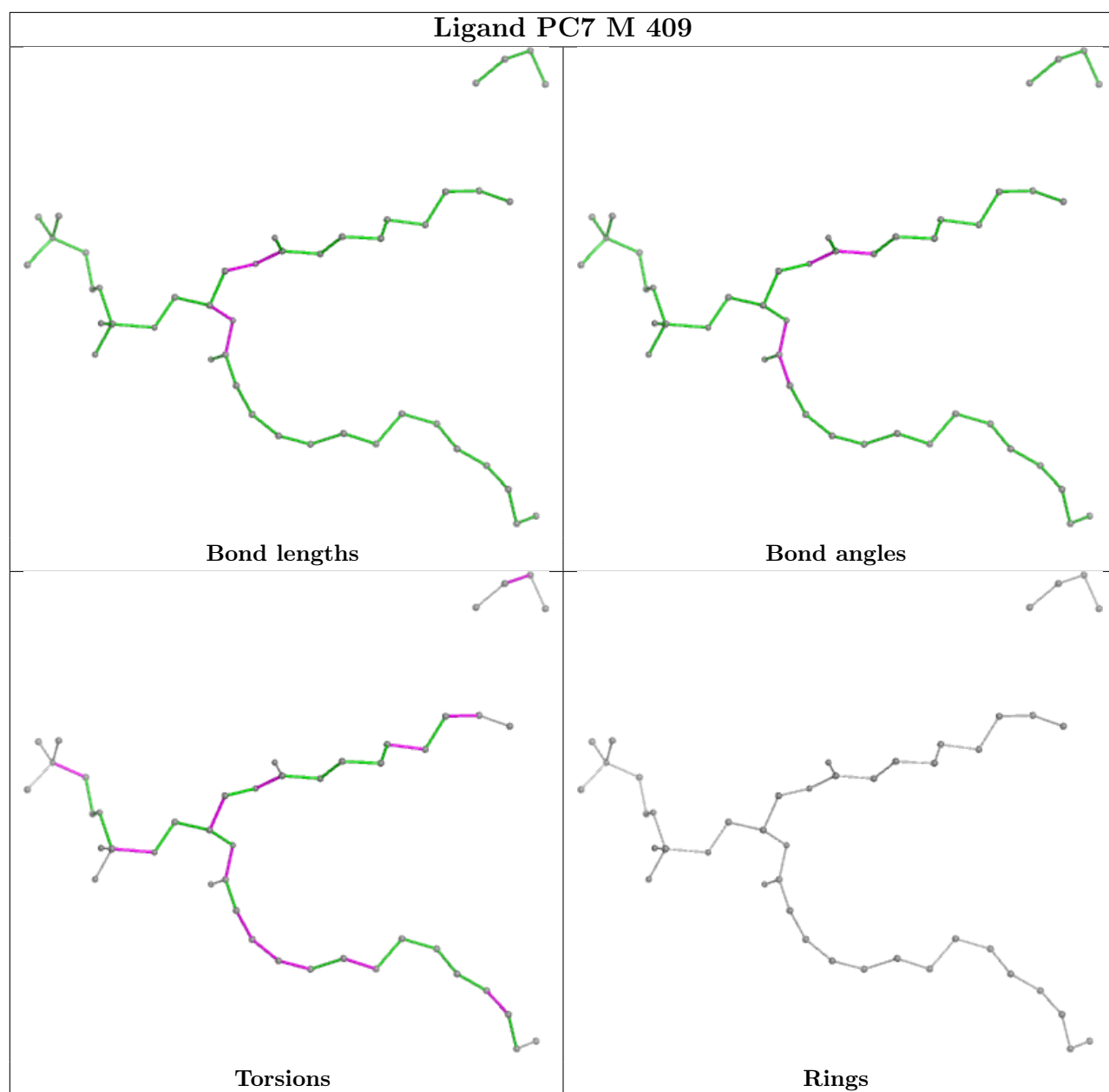




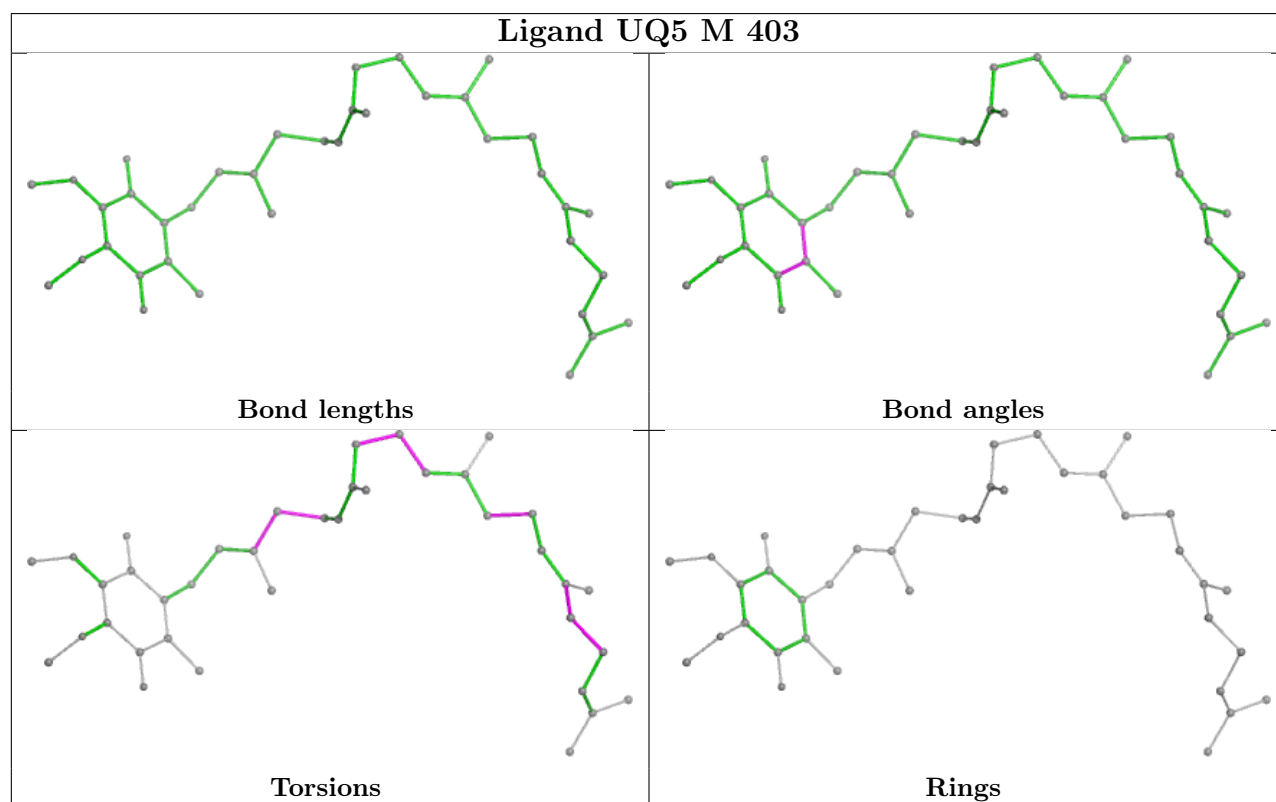
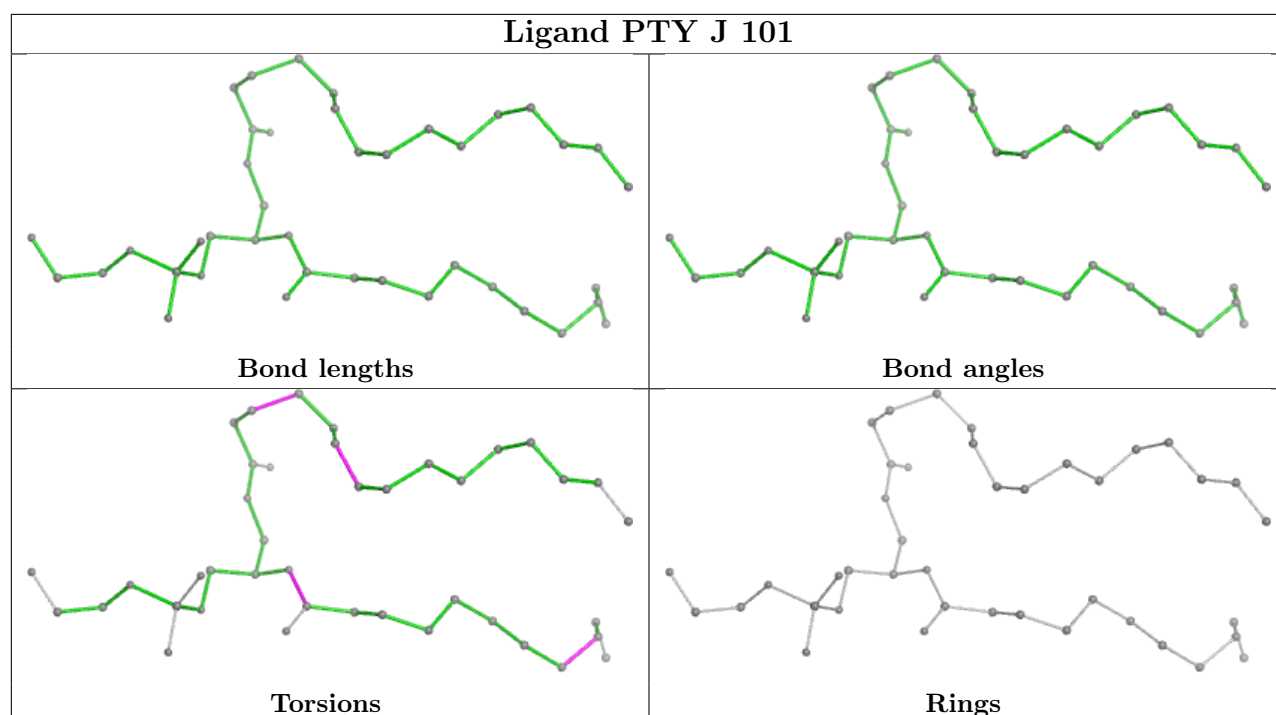


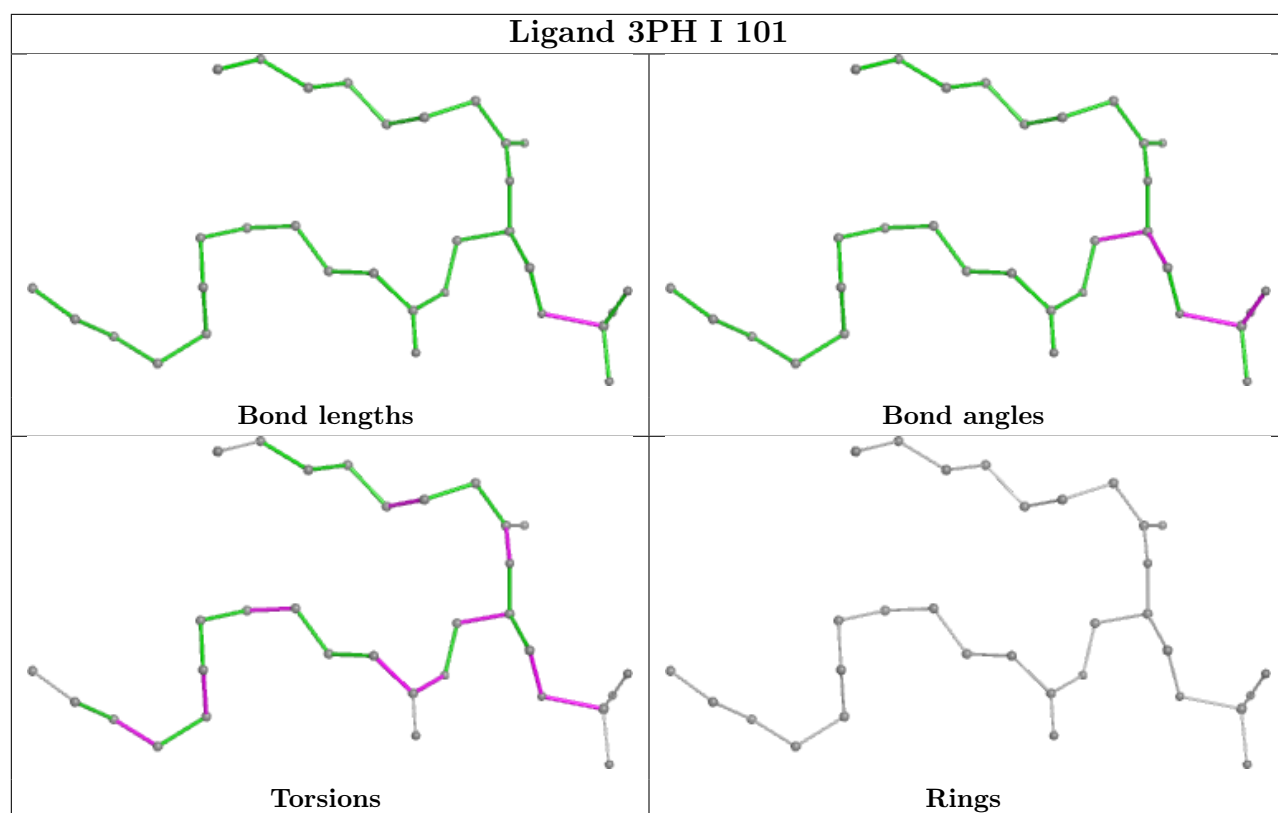


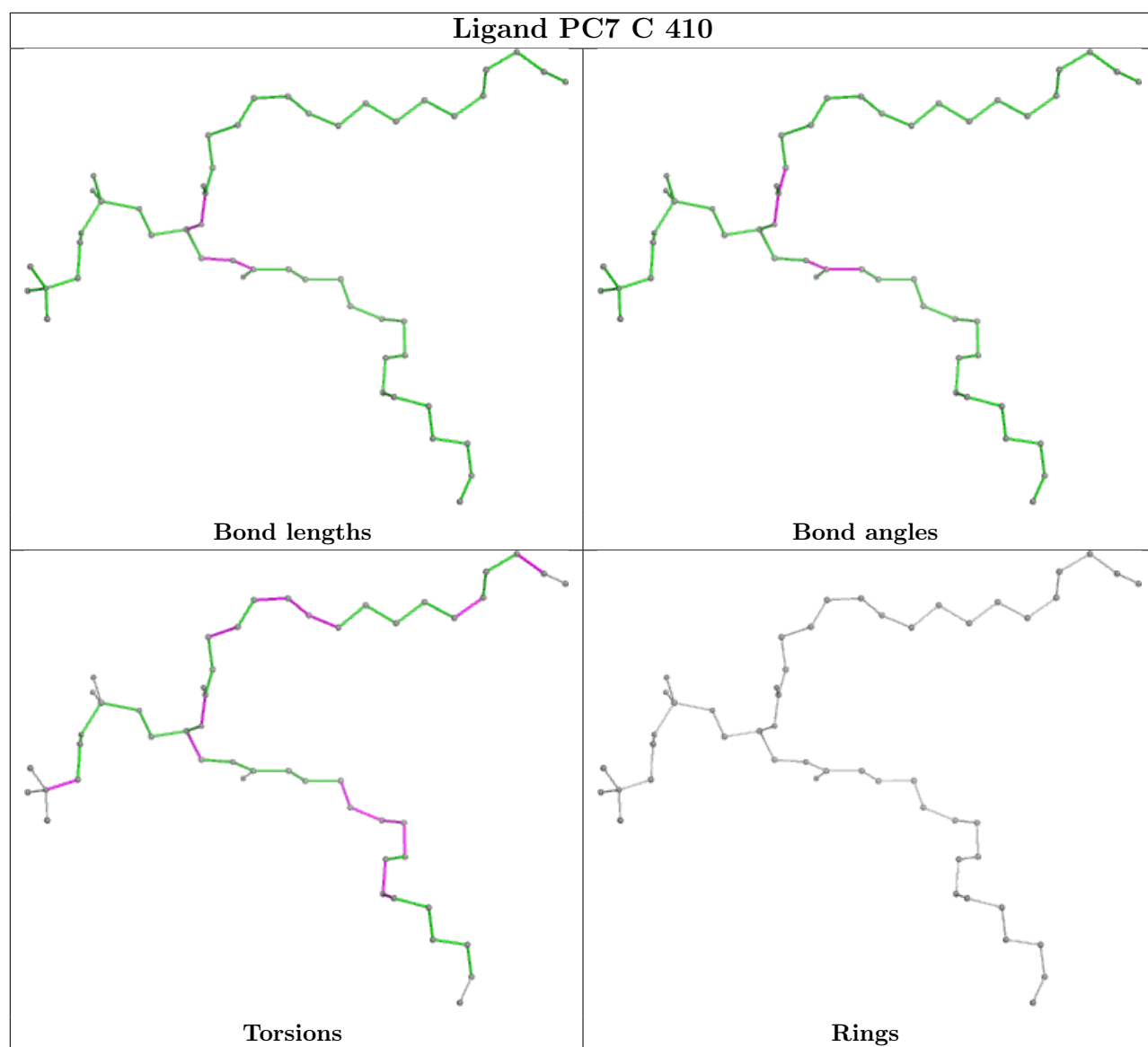


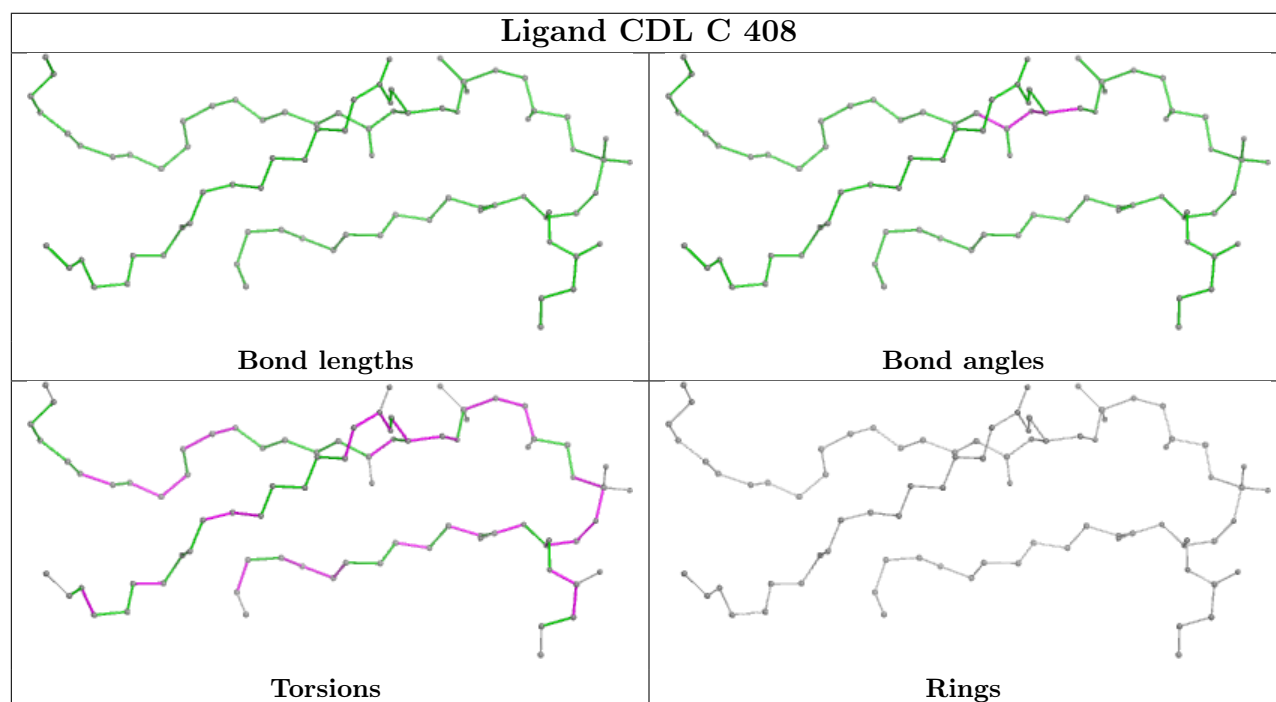
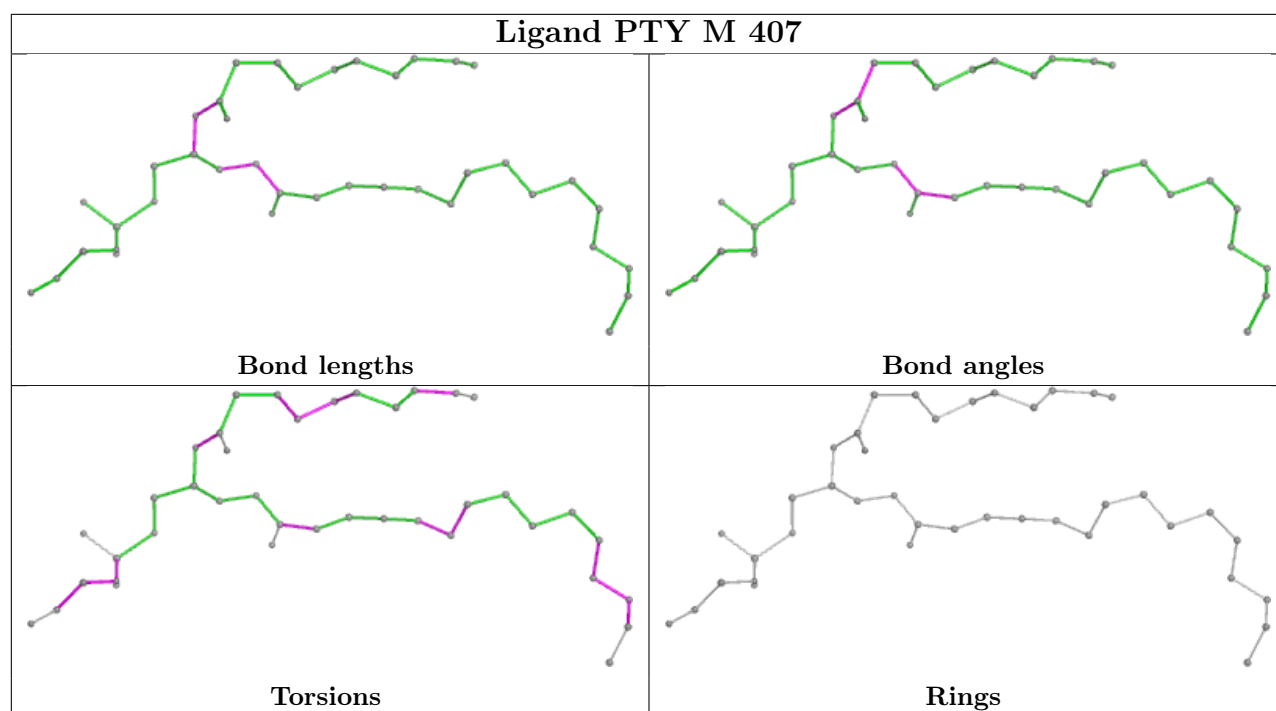


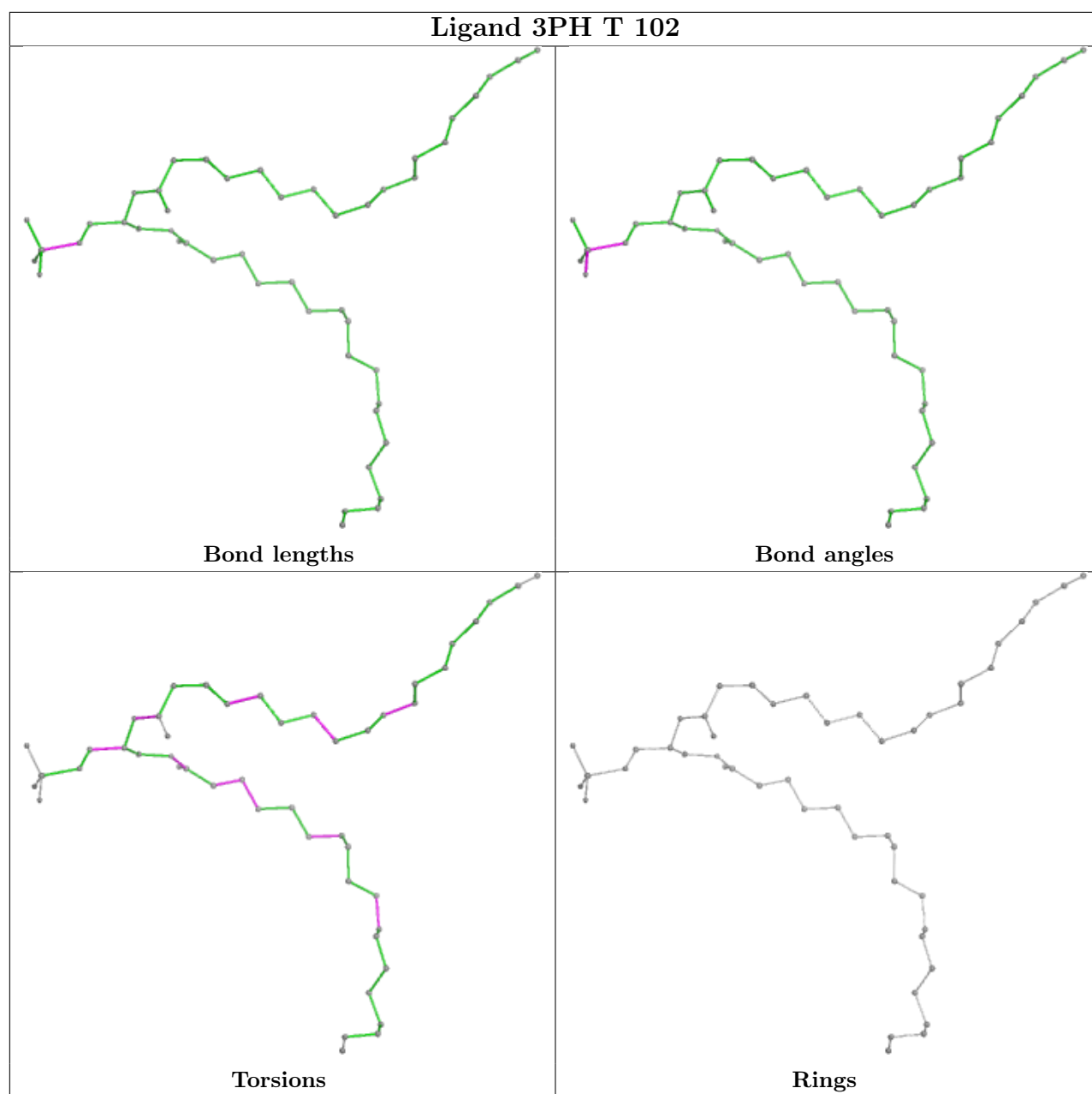


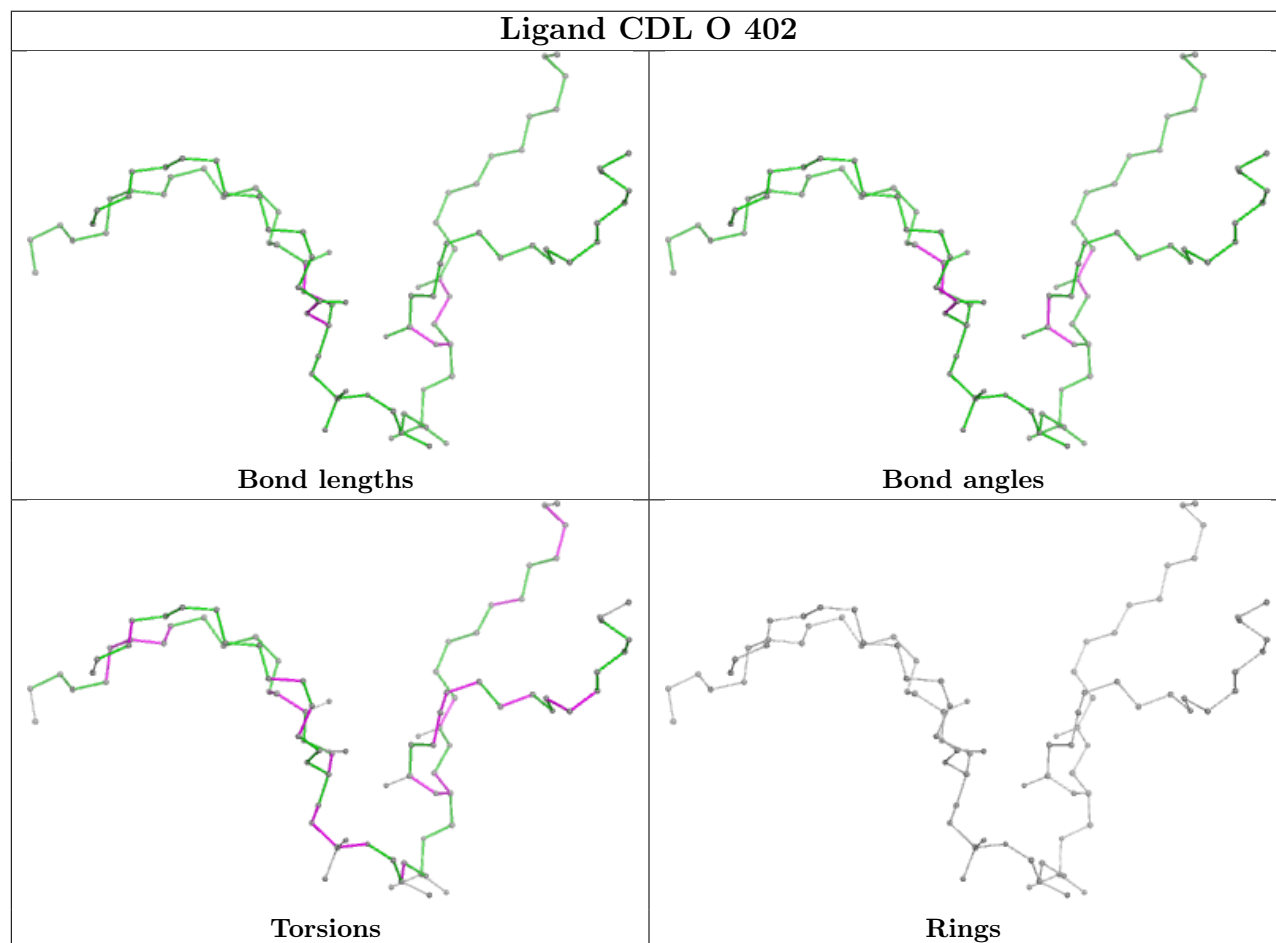
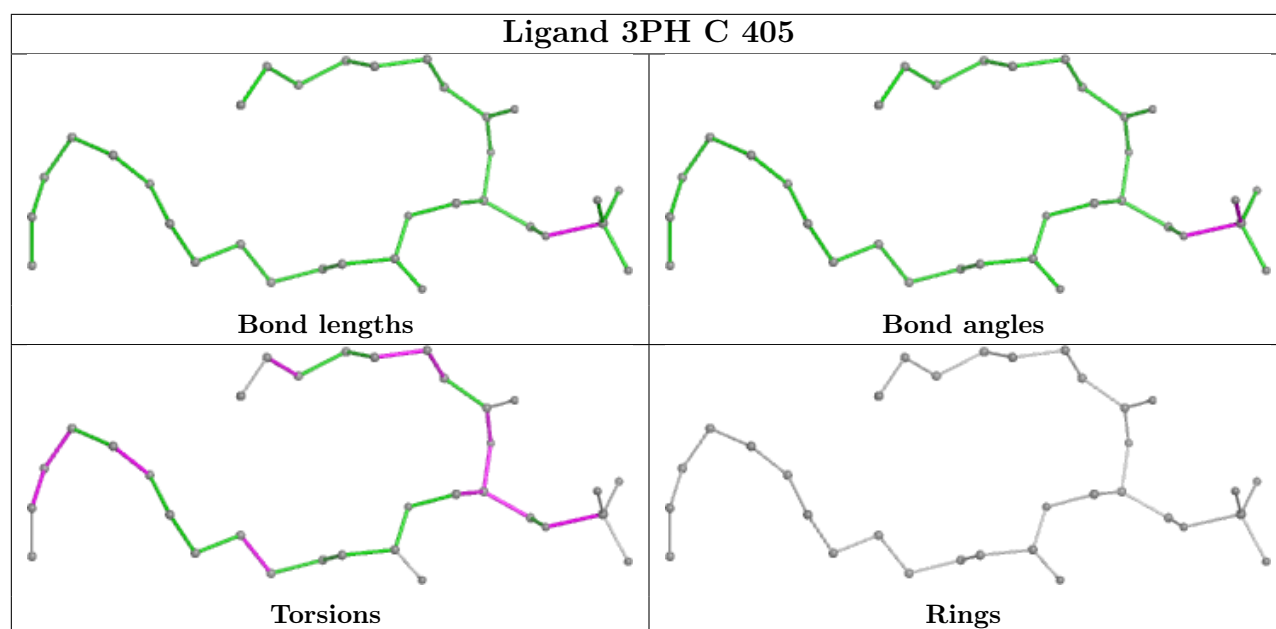


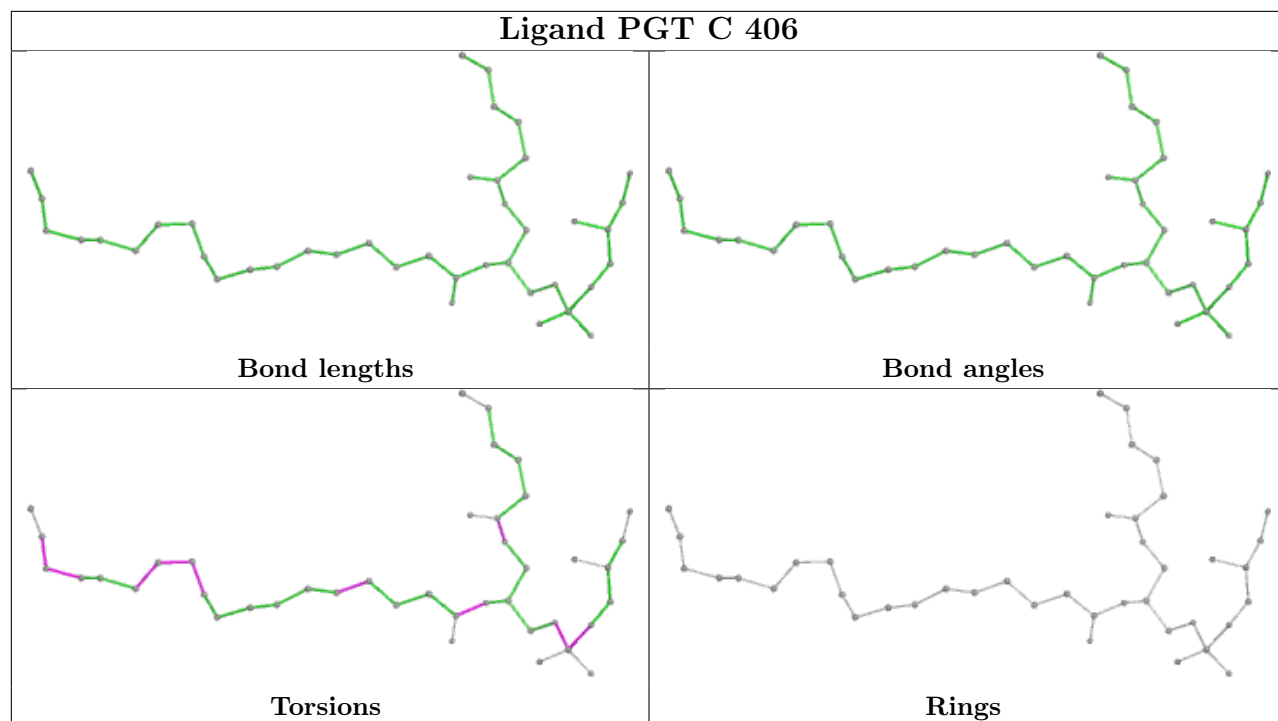


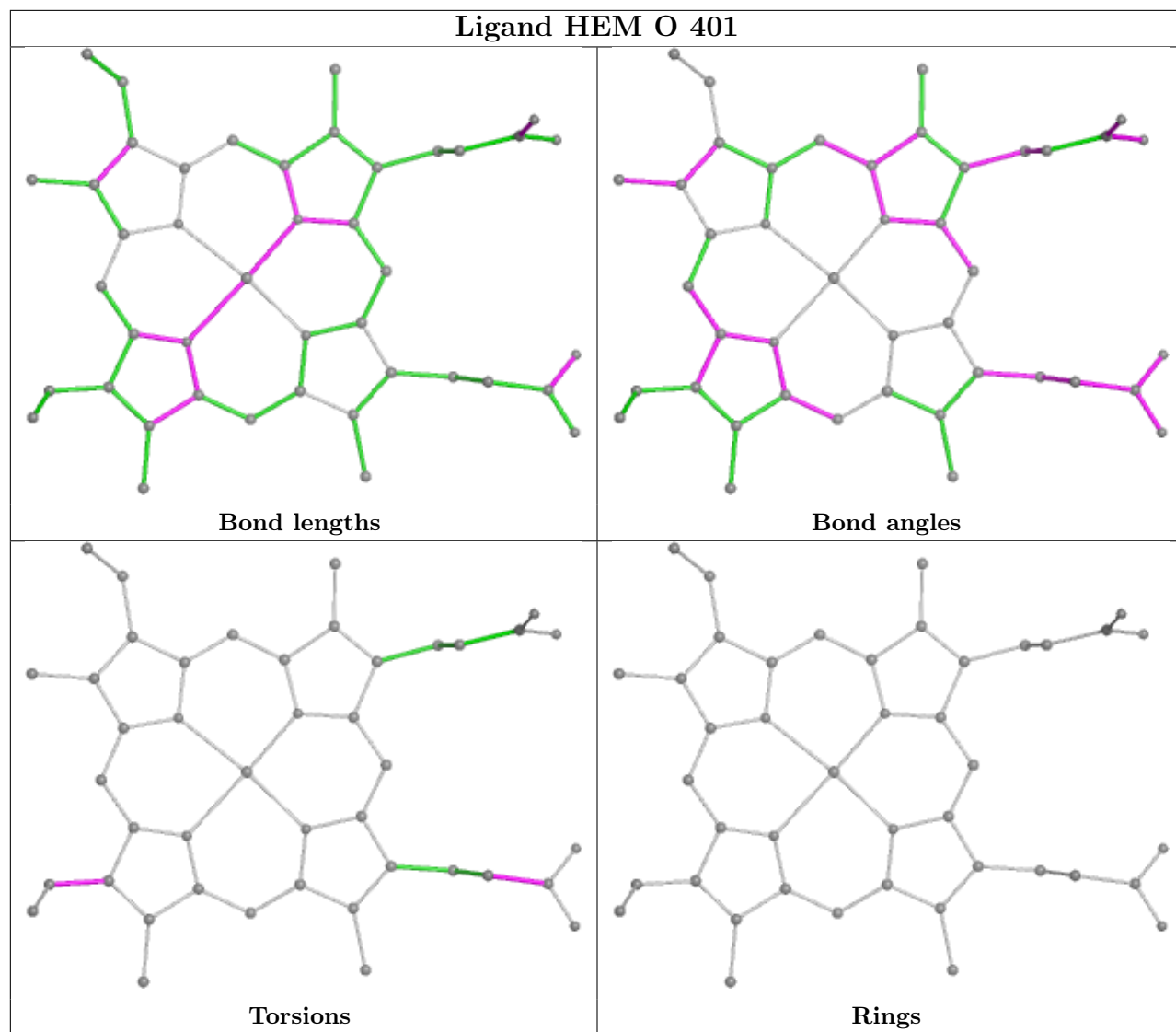






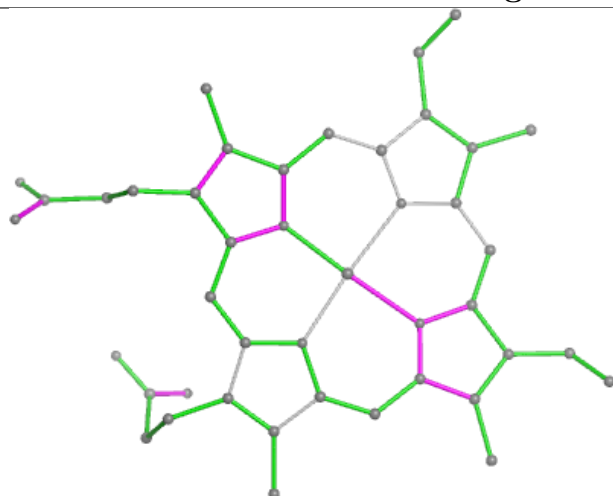




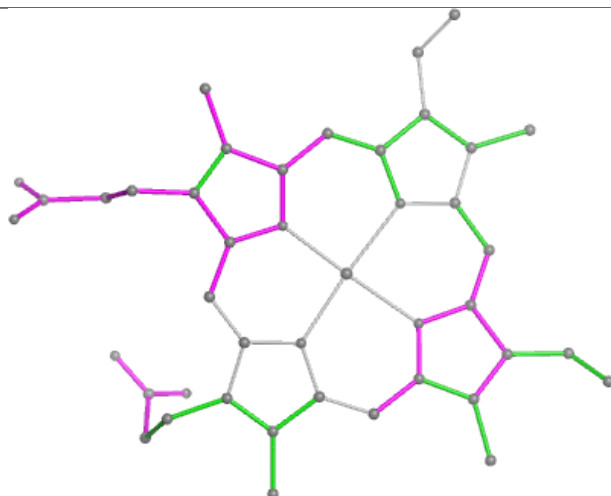




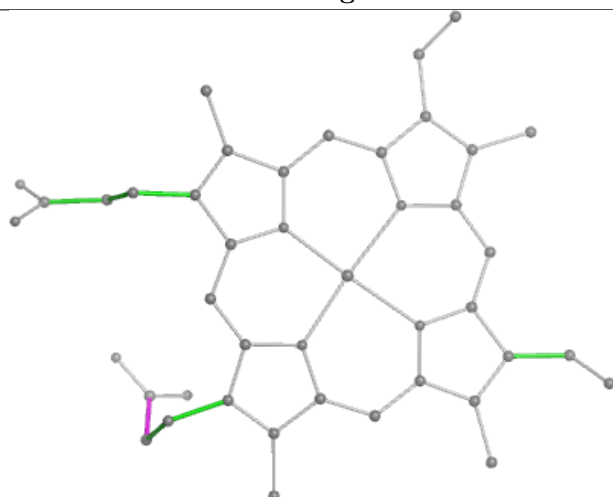
## Ligand HEM M 401



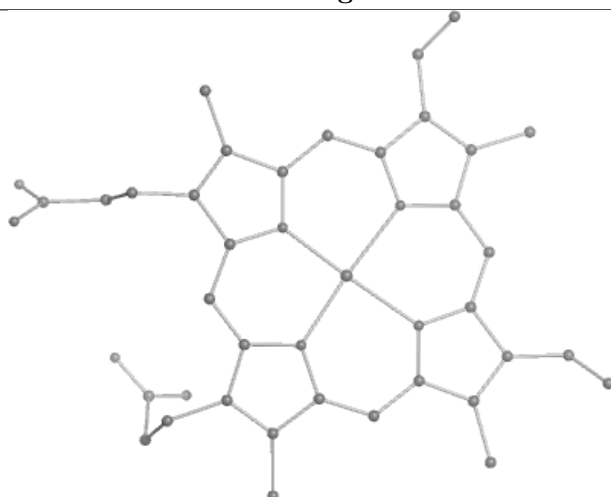
Bond lengths



Bond angles

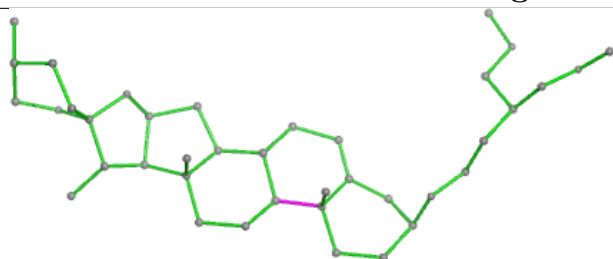


Torsions

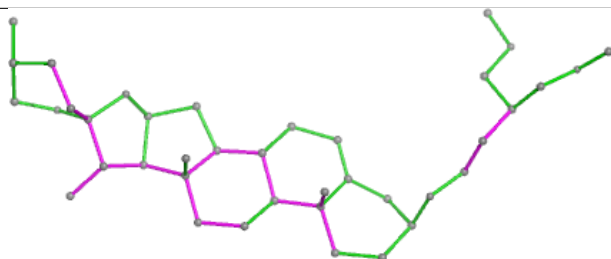


Rings

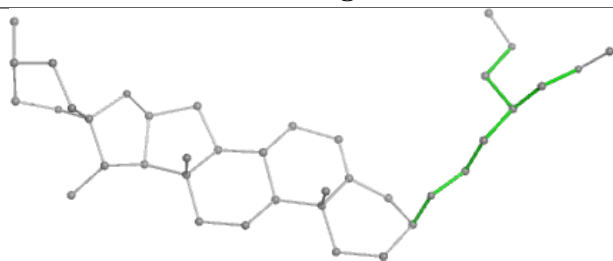
## Ligand Q7G M 411



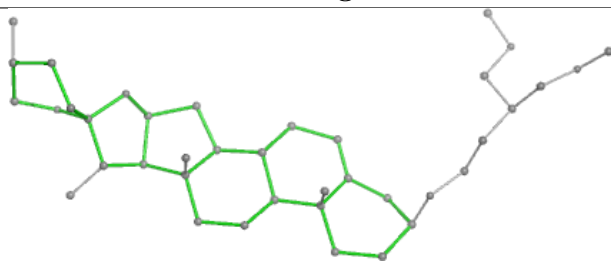
Bond lengths



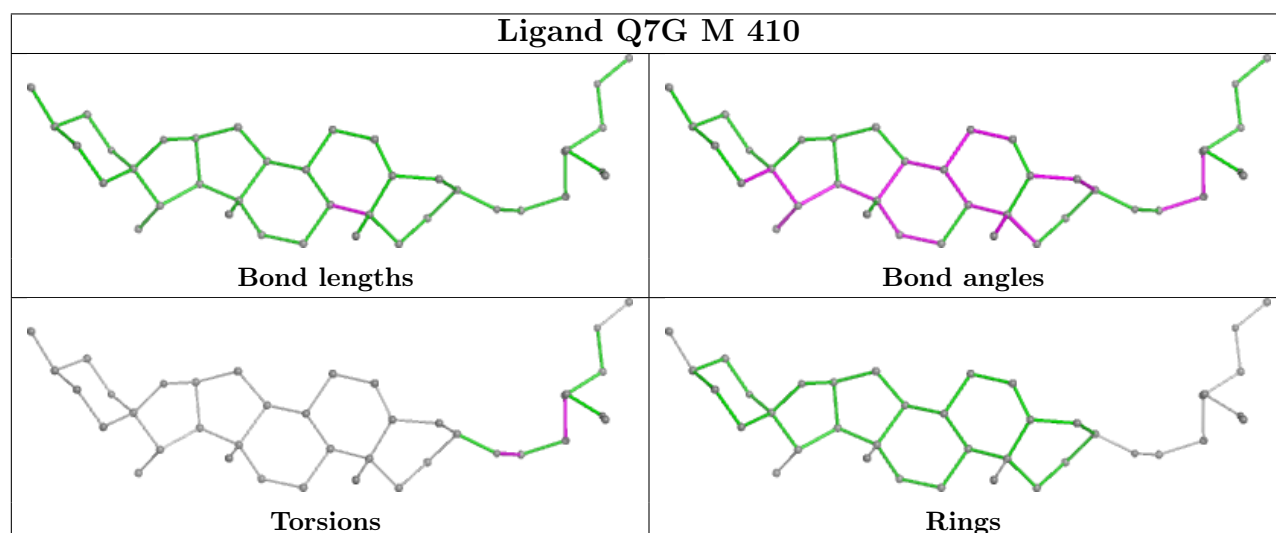
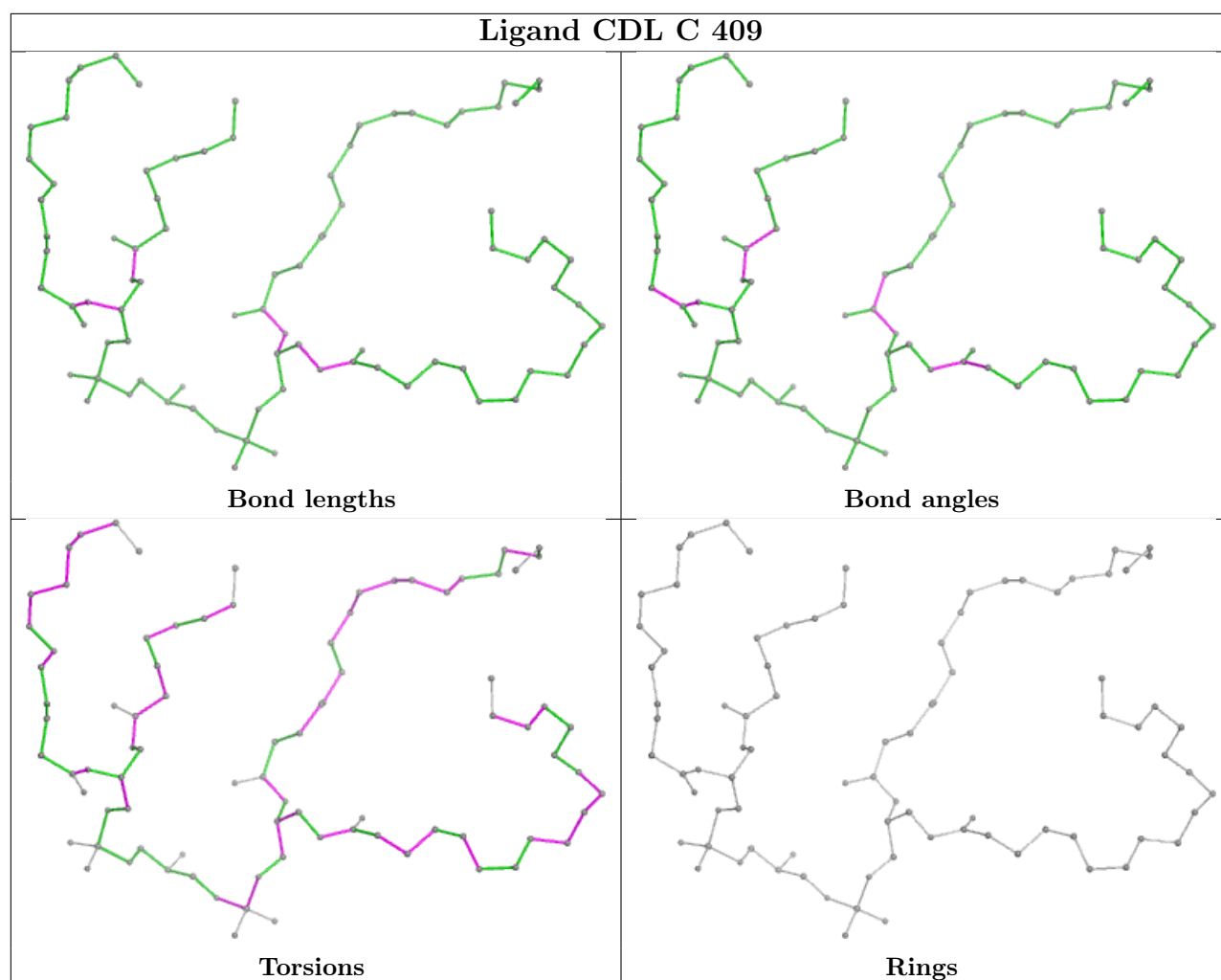
Bond angles

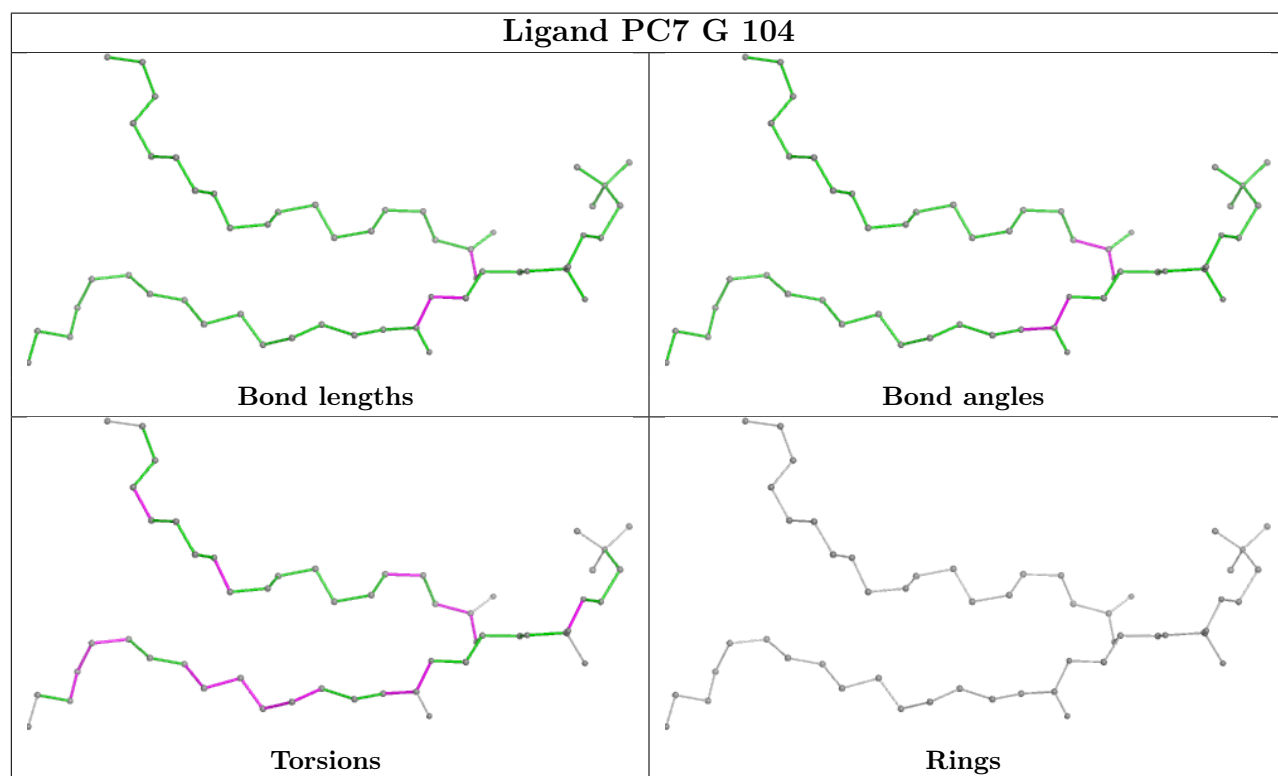
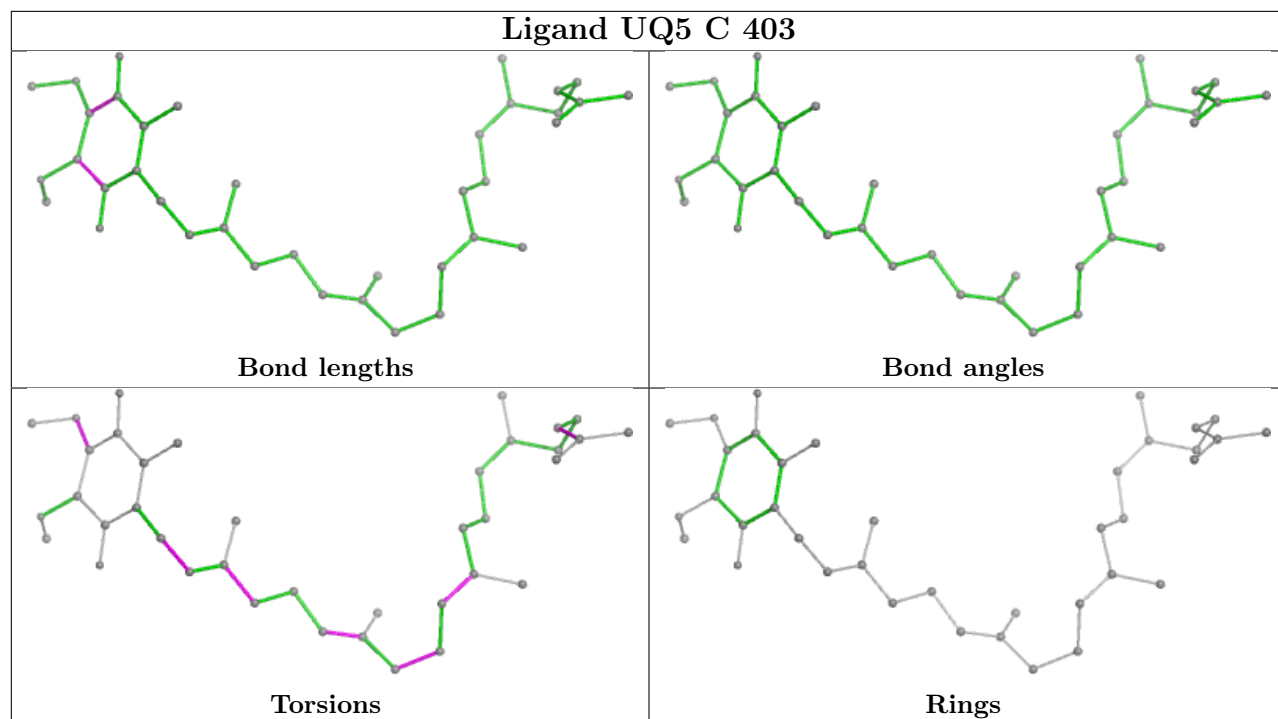


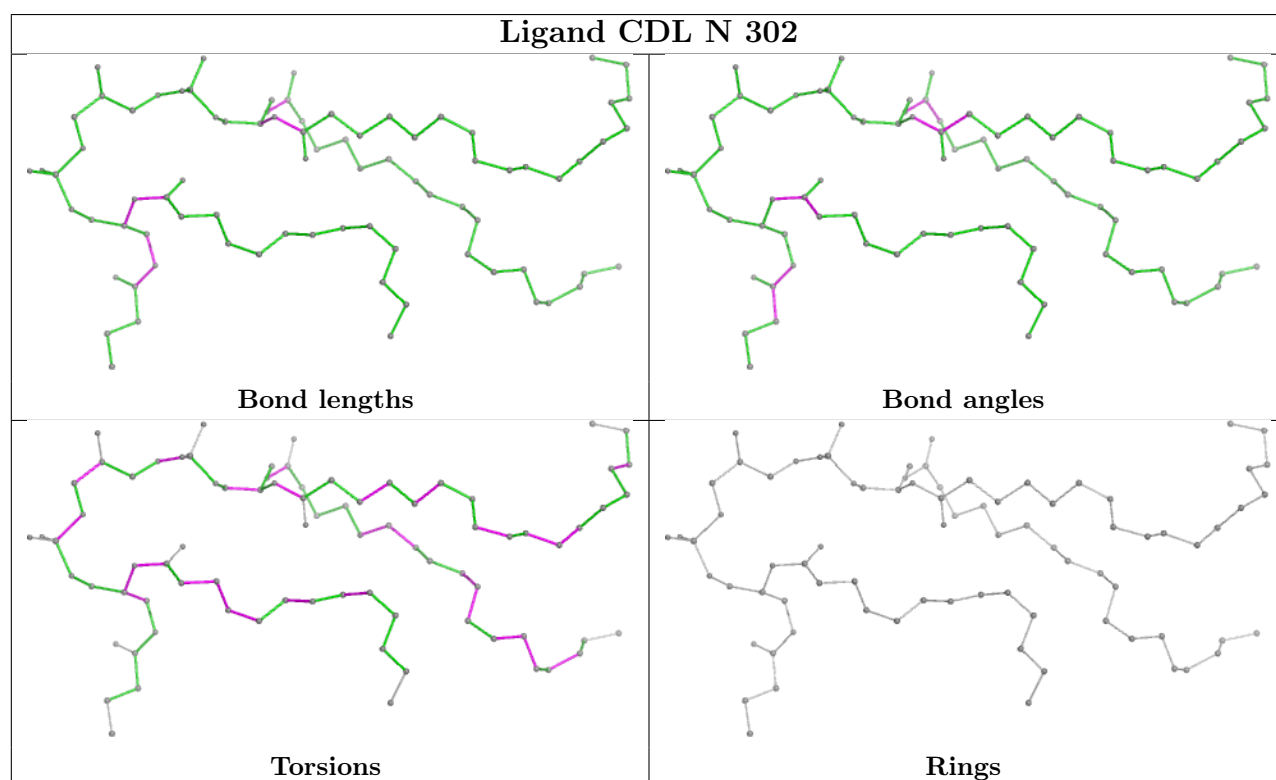
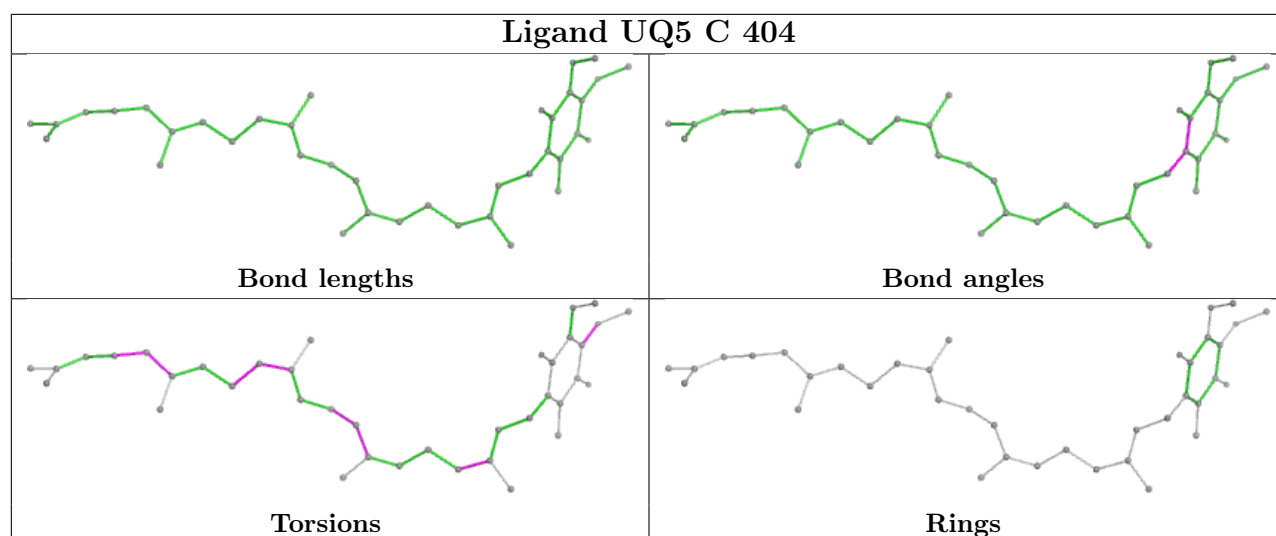
Torsions

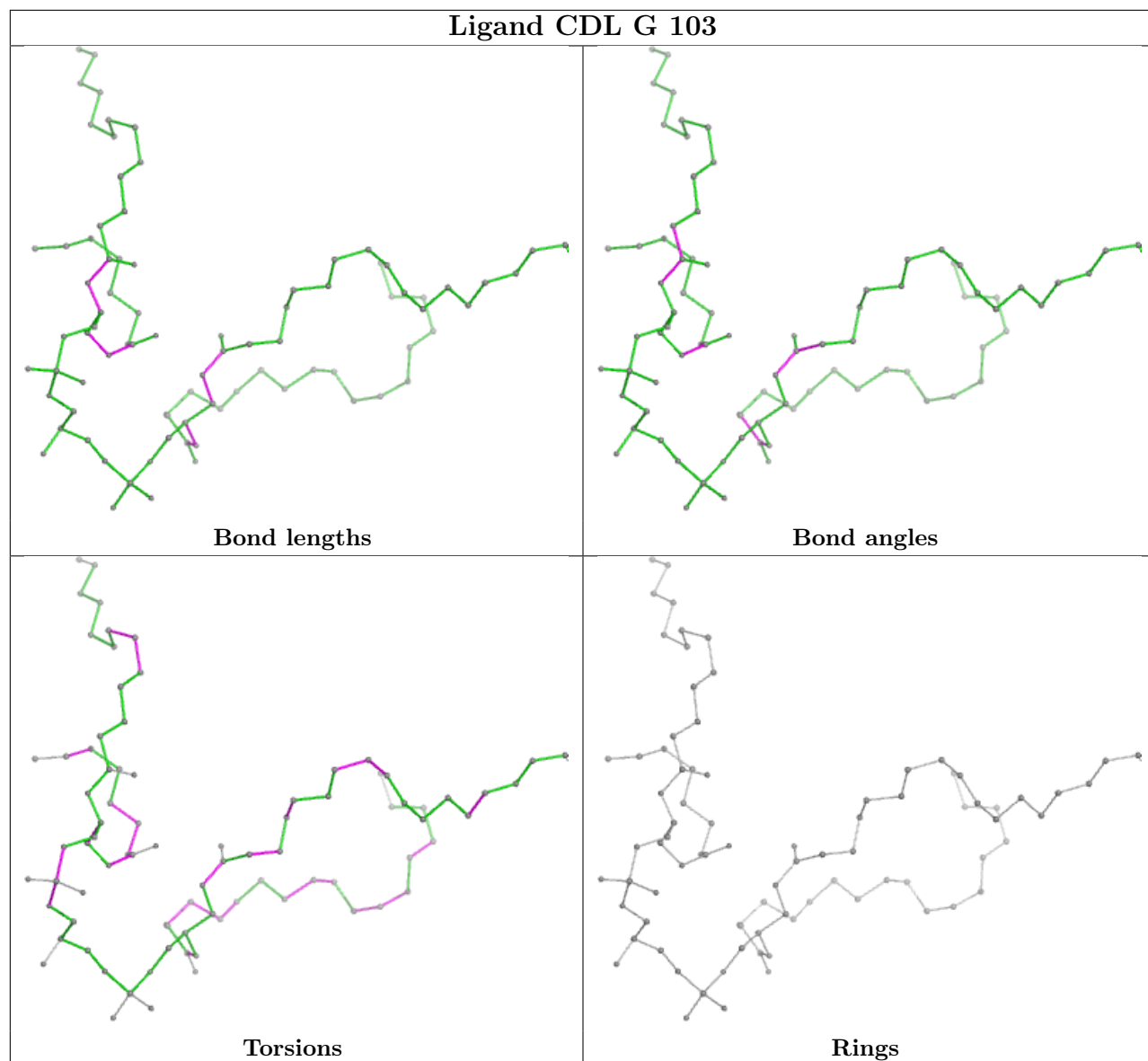


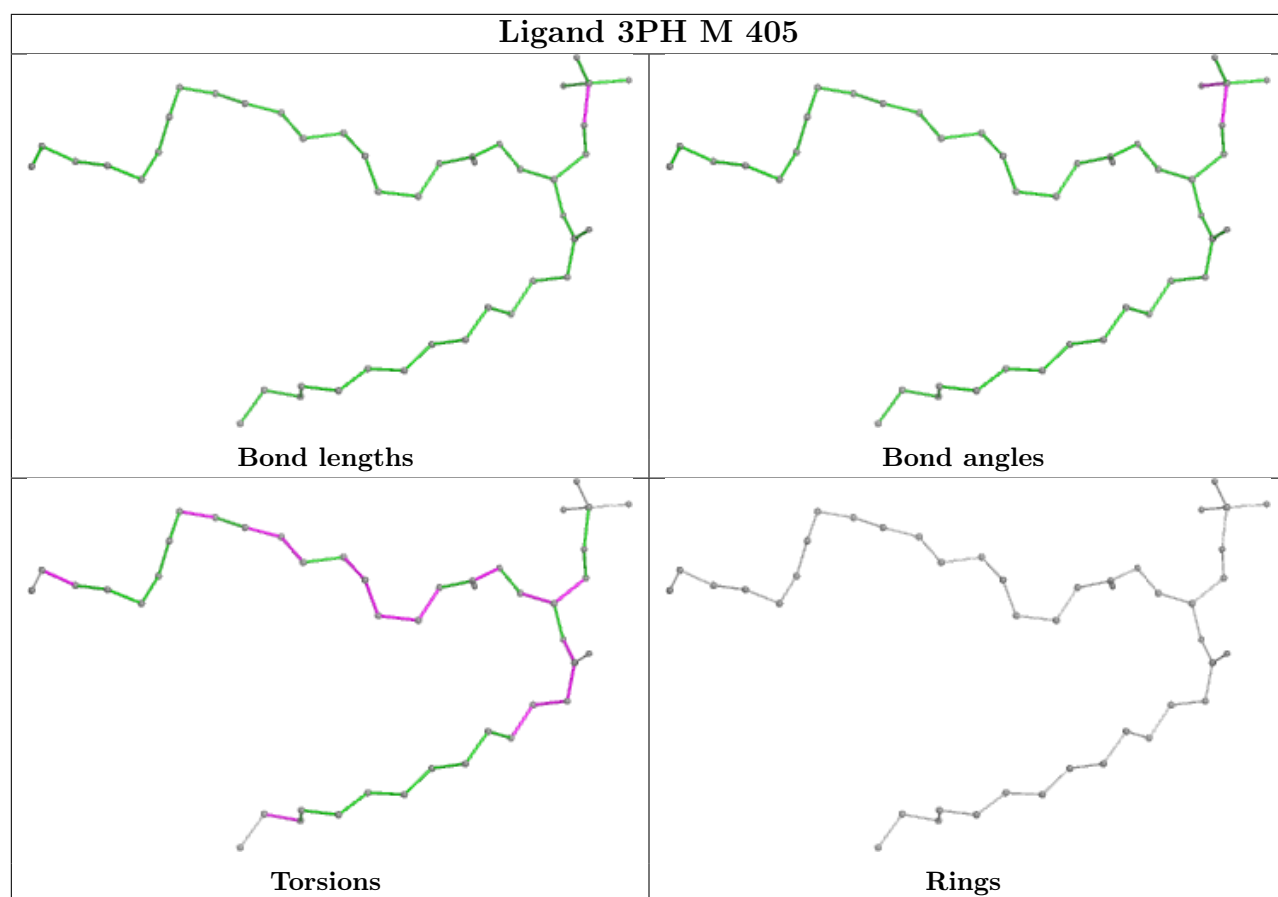
Rings

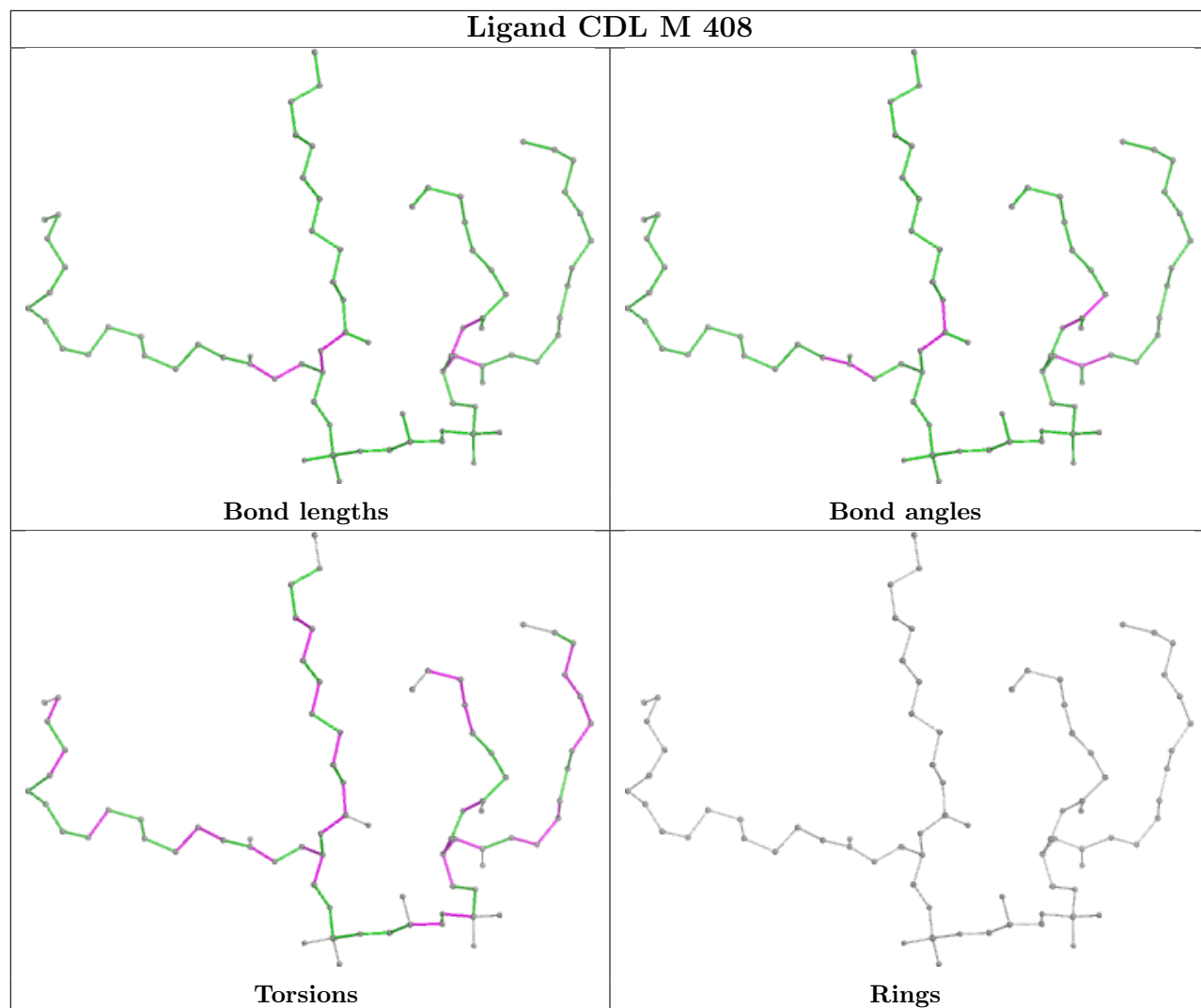


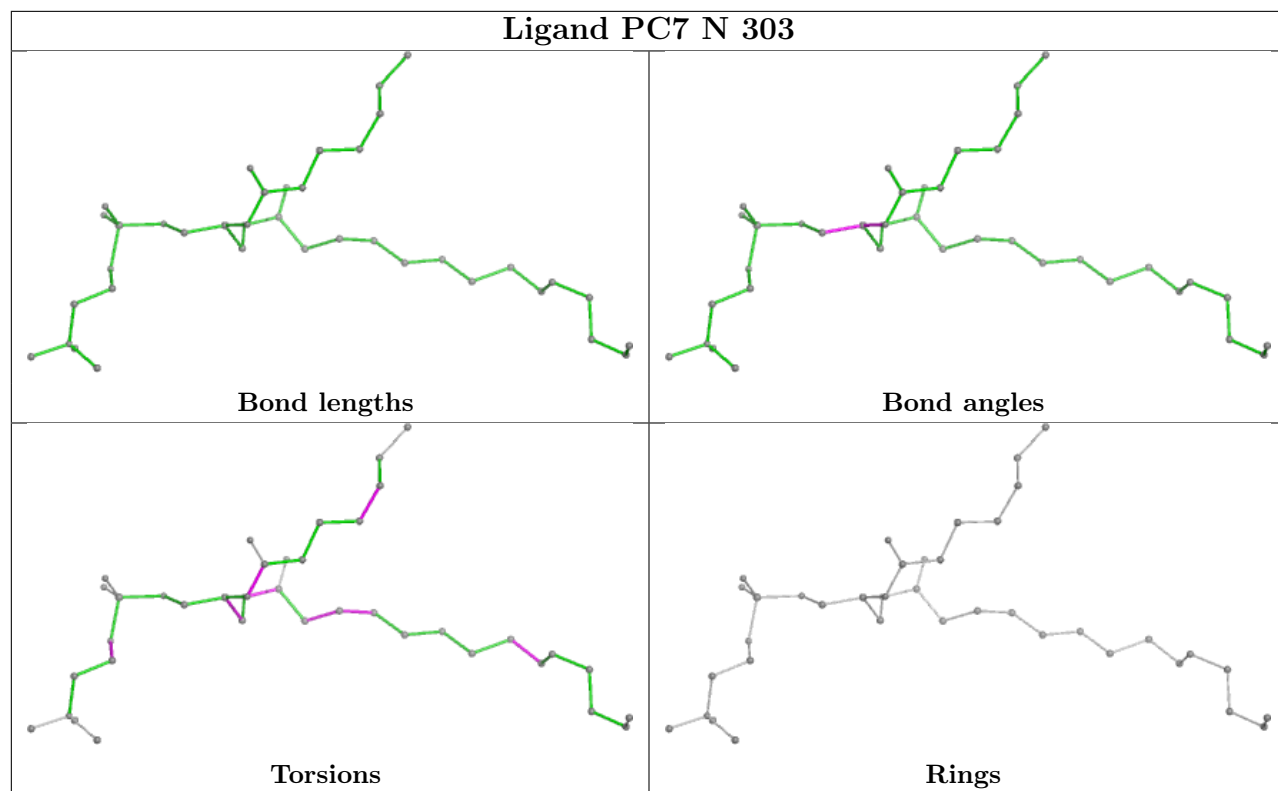




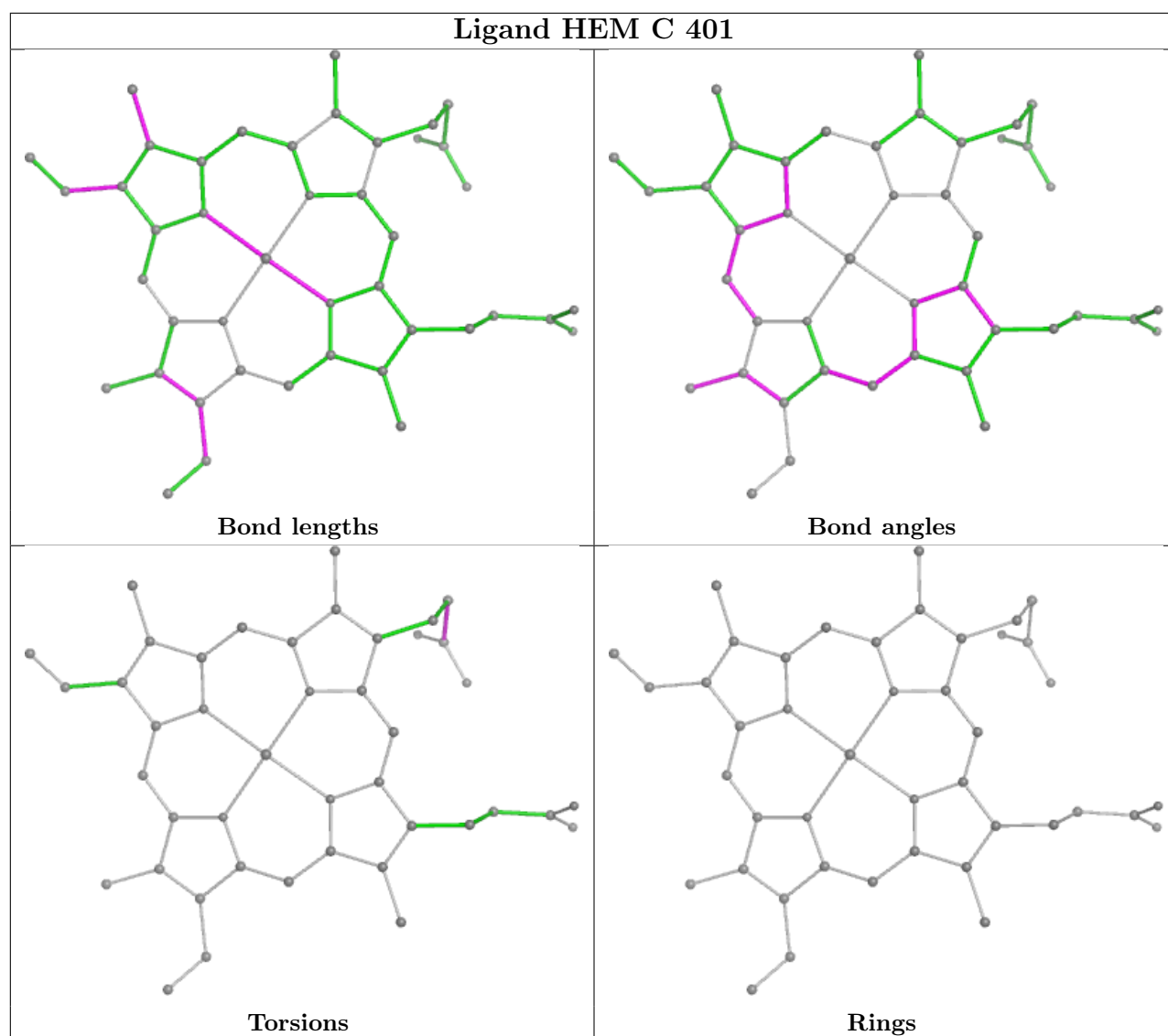












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

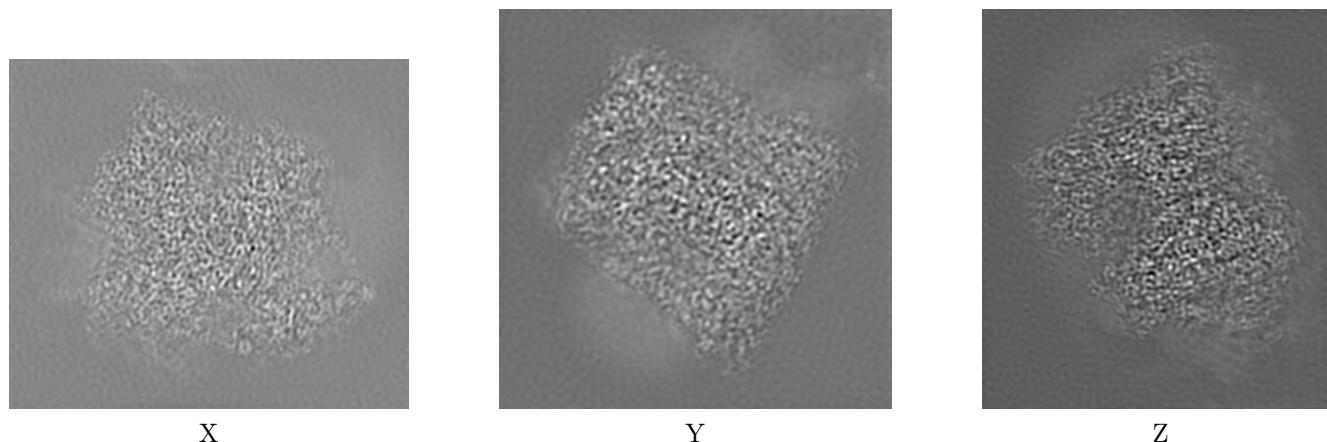
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16007. These allow visual inspection of the internal detail of the map and identification of artifacts.

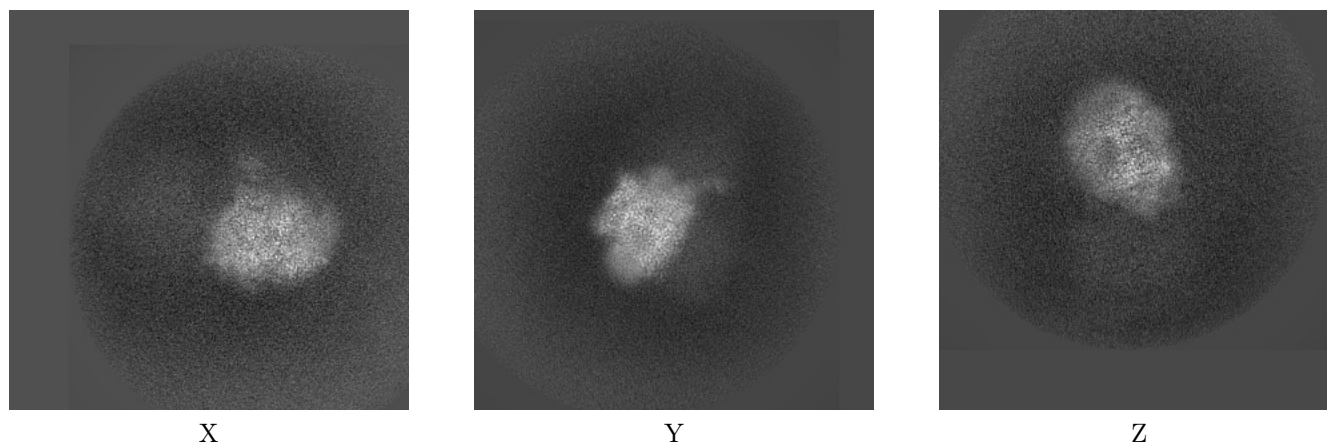
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



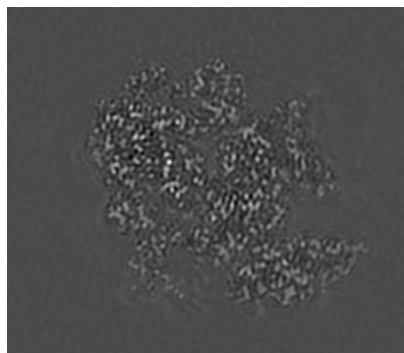
#### 6.1.2 Raw map



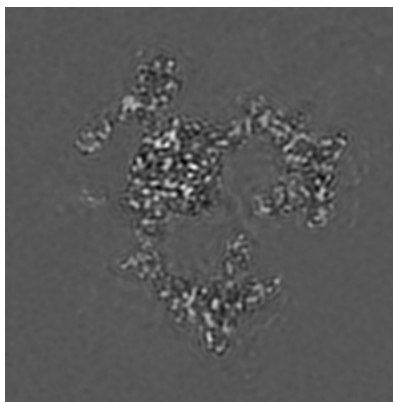
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

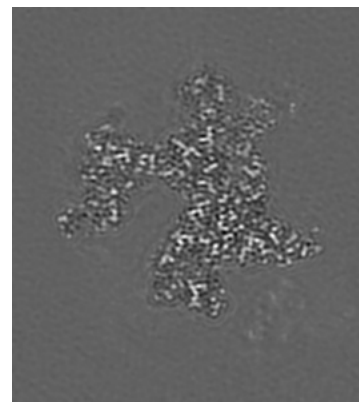
### 6.2.1 Primary map



X Index: 127

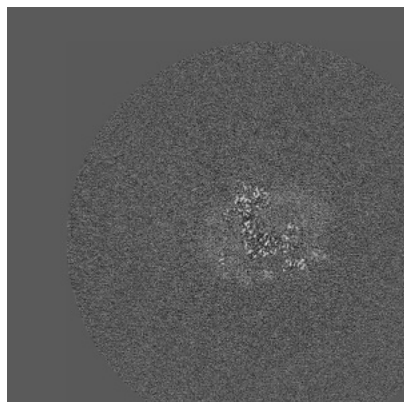


Y Index: 142

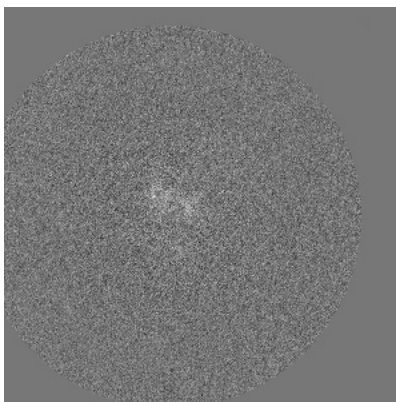


Z Index: 124

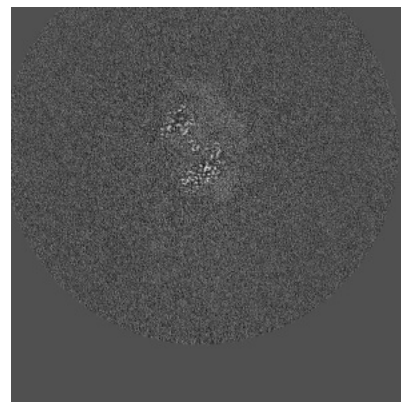
### 6.2.2 Raw map



X Index: 375



Y Index: 375

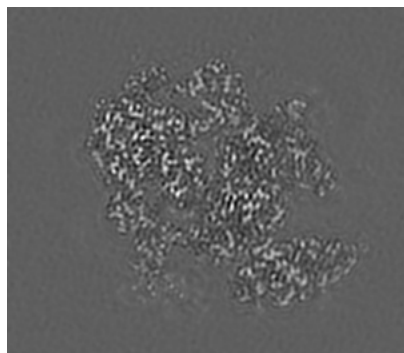


Z Index: 375

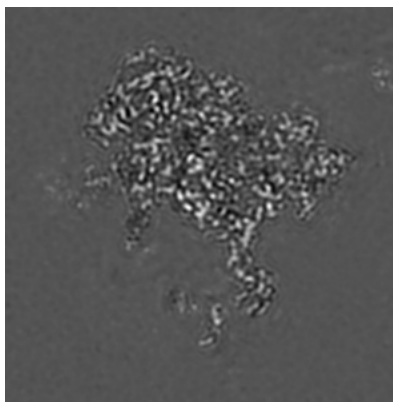
The images above show central slices of the map in three orthogonal directions.

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

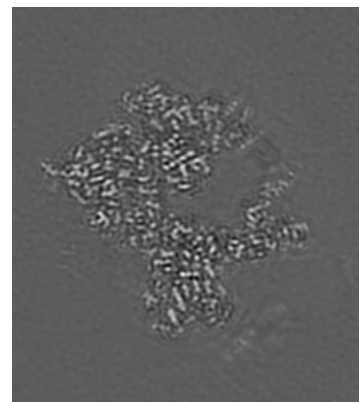
### 6.3.1 Primary map



X Index: 126

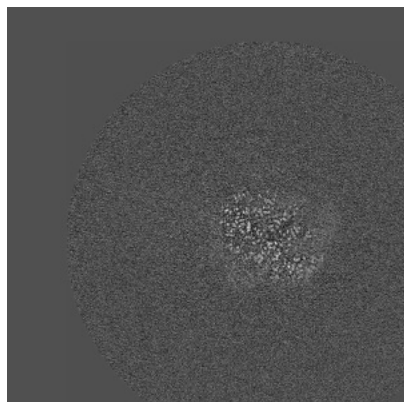


Y Index: 121

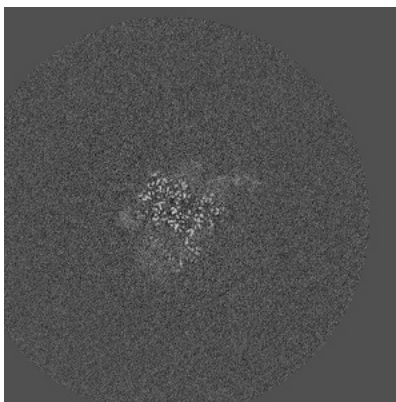


Z Index: 146

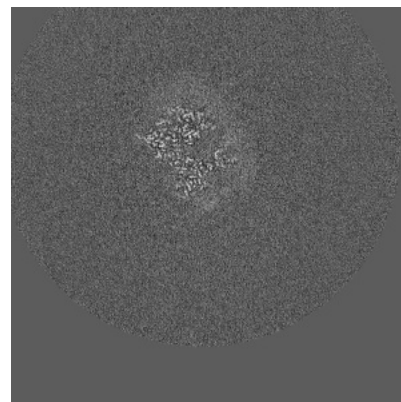
### 6.3.2 Raw map



X Index: 343



Y Index: 458

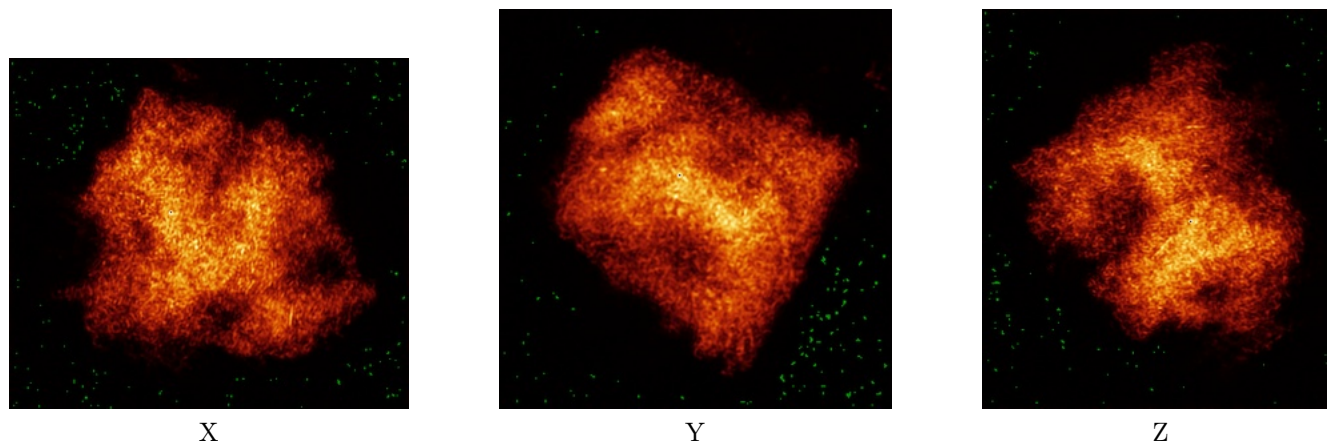


Z Index: 344

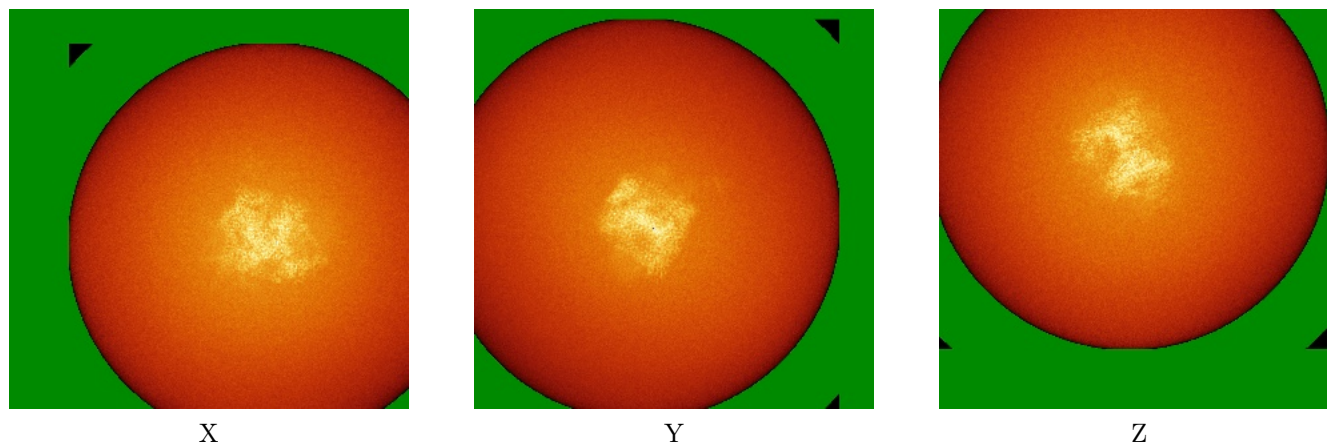
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

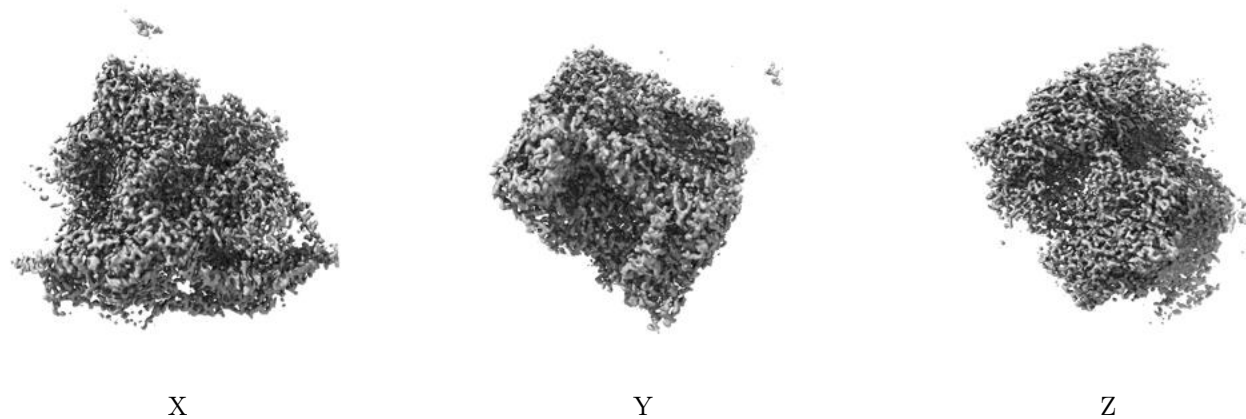


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



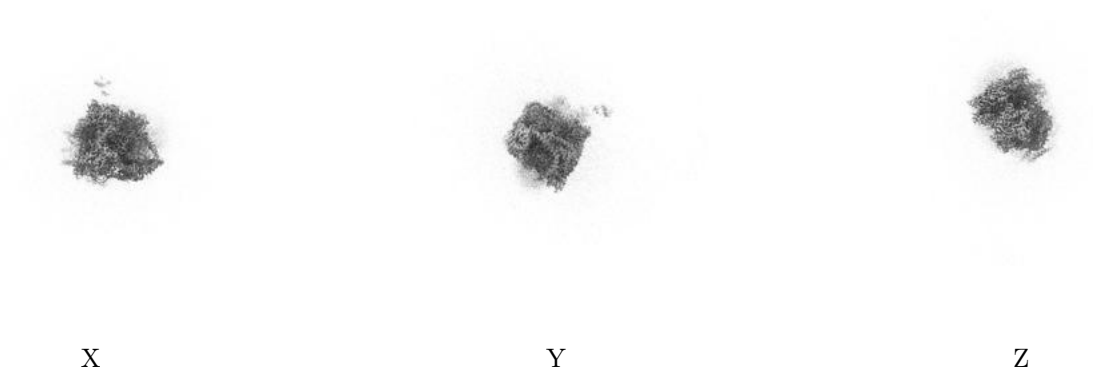
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

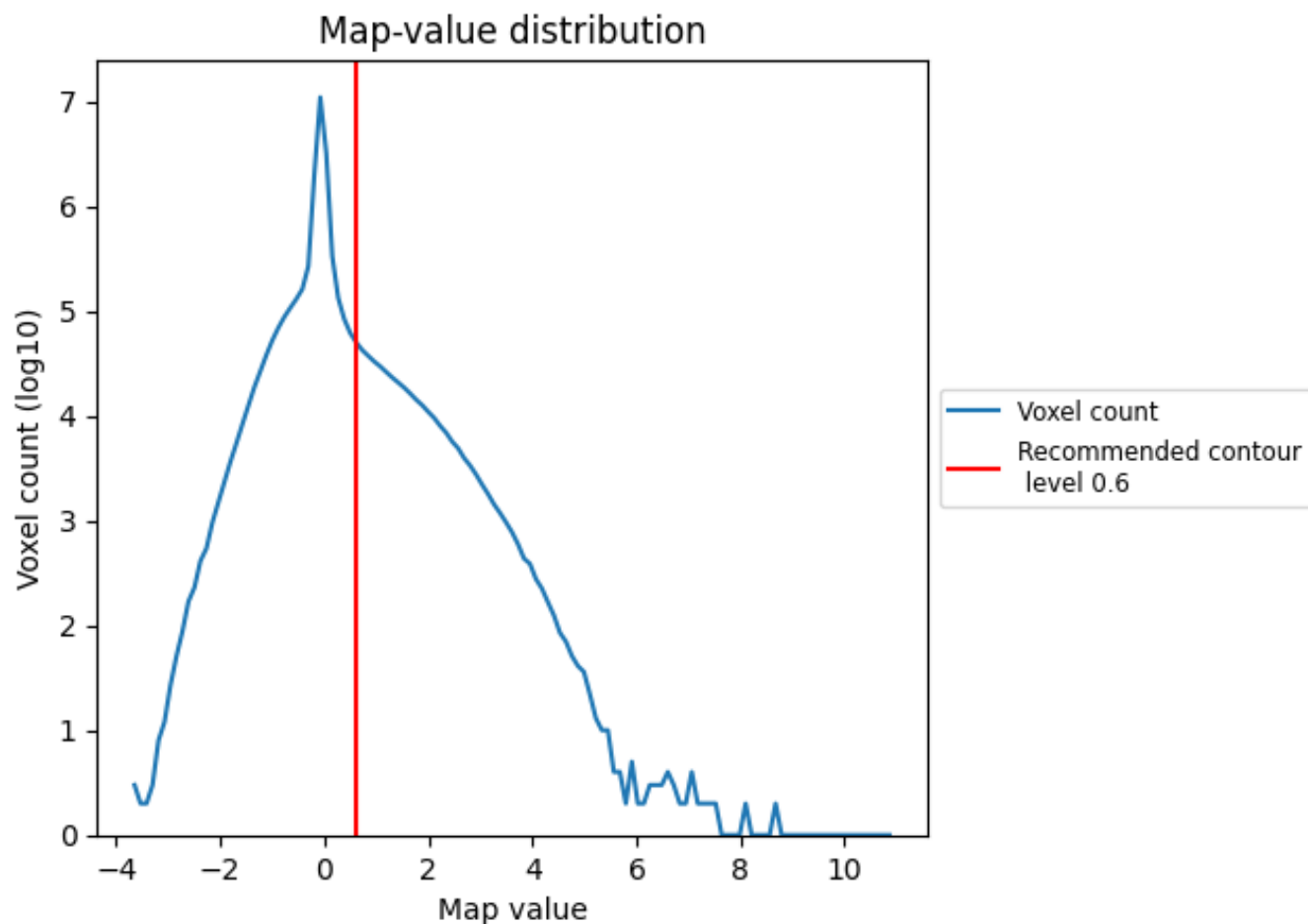
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

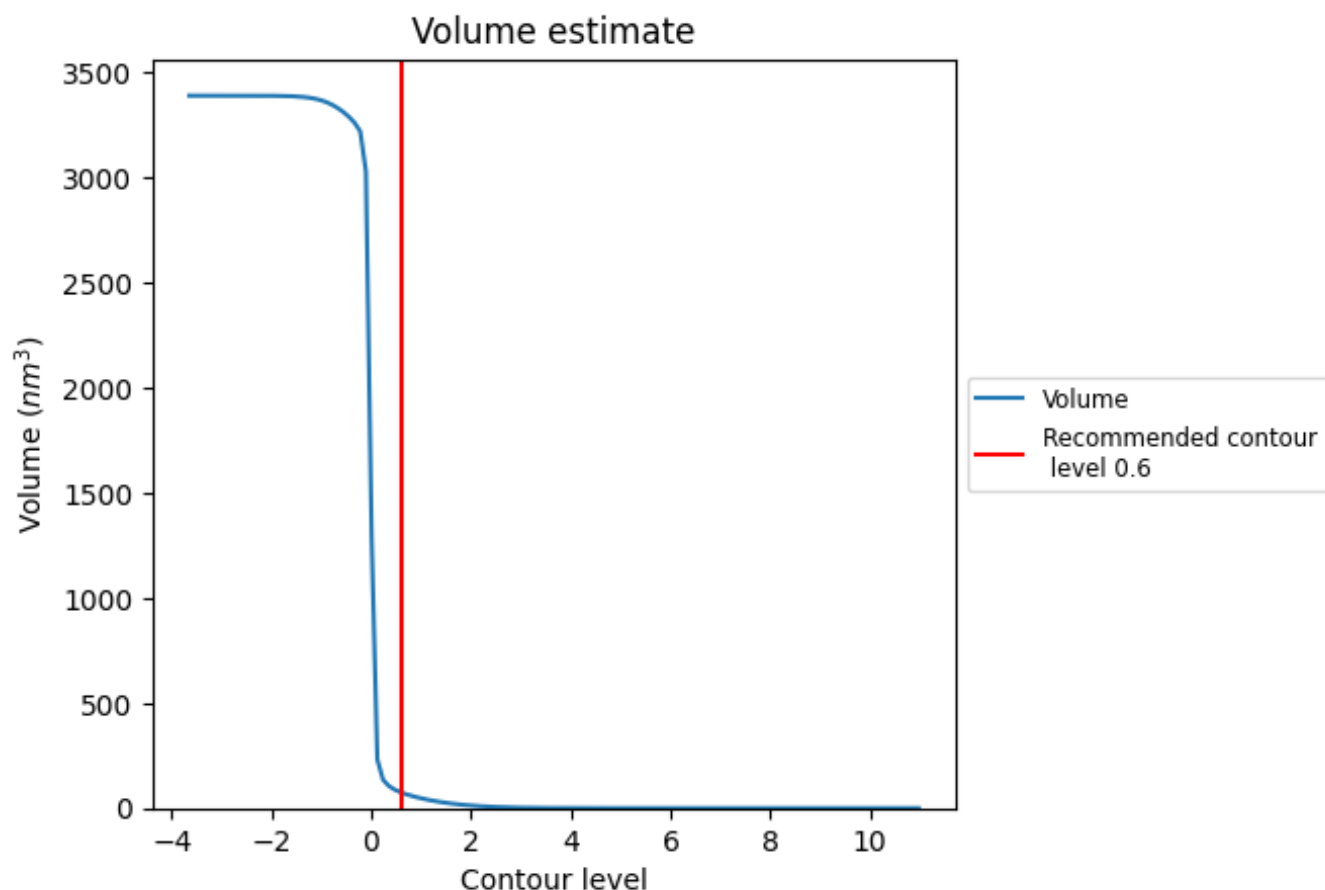
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm<sup>3</sup>; this corresponds to an approximate mass of 68 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



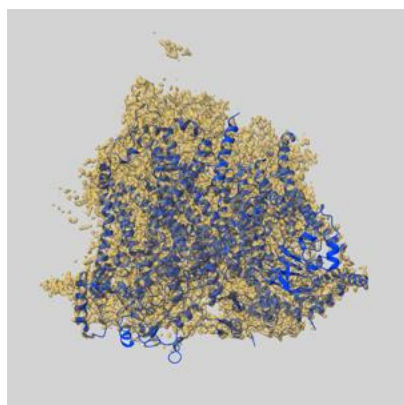
## 8 Fourier-Shell correlation

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

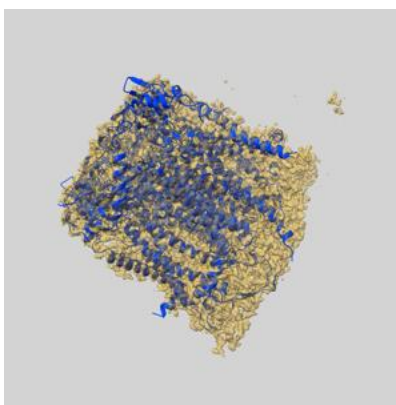
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16007 and PDB model 8BEL. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

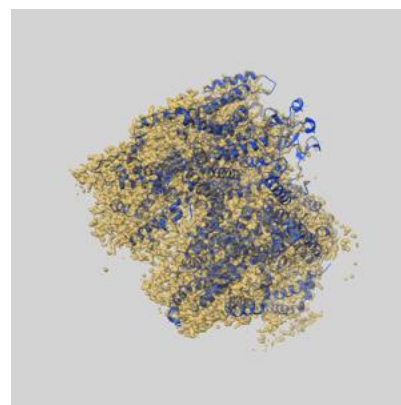
### 9.1 Map-model overlay [i](#)



X



Y



Z

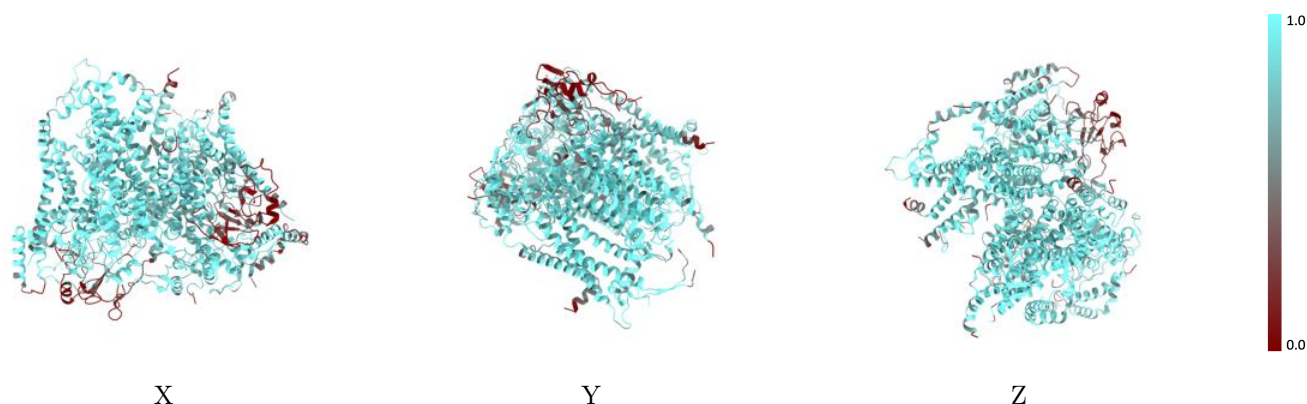
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



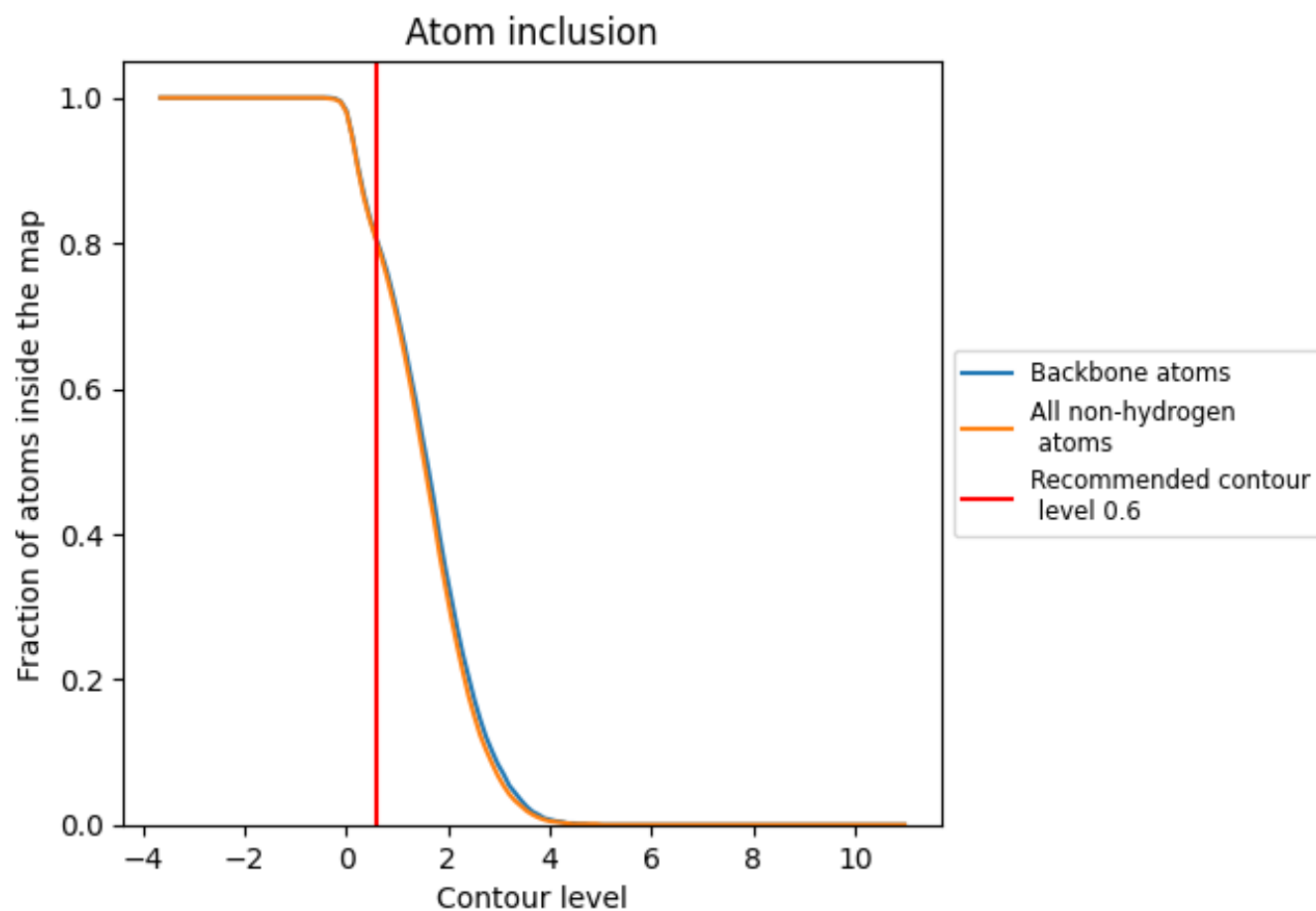
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).































## 9.4 Atom inclusion [i](#)



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

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.6820
C	 0.9050	 0.7310
D	 0.5210	 0.5940
E	 0.9330	 0.7410
G	 0.7630	 0.6610
H	 0.7980	 0.6640
I	 0.8270	 0.7040
J	 0.4560	 0.5700
M	 0.8830	 0.7050
N	 0.5570	 0.5950
O	 0.8840	 0.7010
Q	 0.7650	 0.6440
R	 0.6490	 0.5850
S	 0.7690	 0.6440
T	 0.5490	 0.6090

