



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 06:46 PM JST

PDB ID : 9WCY / pdb\_00009wcy  
EMDB ID : EMD-65879  
Title : Cryo-EM structure of the Mycobacterium abscessus cytochrome bcc:aa3 supercomplex in the presence of ND-011458  
Authors : Mathiyazakan, V.; Gruber, G.  
Deposited on : 2025-08-18  
Resolution : 2.26 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

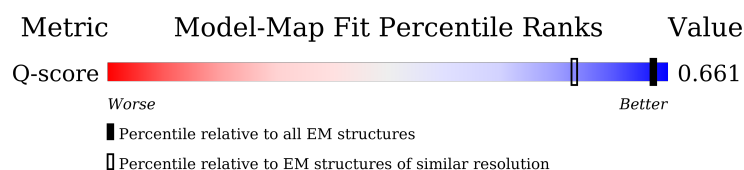
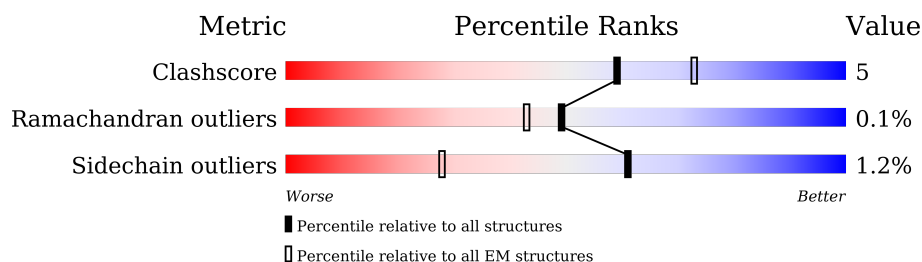
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.26 Å.

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







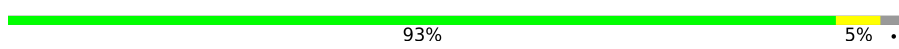
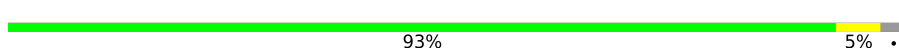


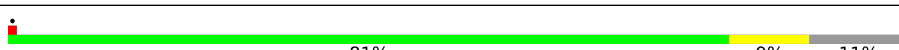

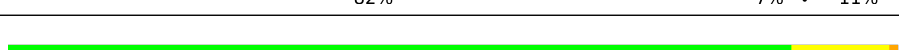
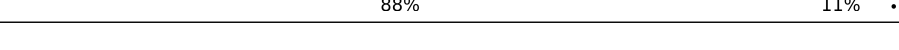

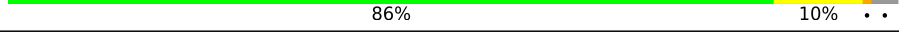


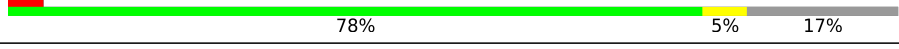
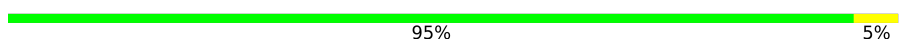


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3535 ( 1.76 - 2.76 )

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	G	99	
1	b	99	
2	I	564	
2	L	564	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	86	
3	h	86	
4	U	295	
4	o	295	
5	V	391	
5	p	391	
6	X	238	
6	a	238	
7	d	349	
7	e	349	
8	f	206	
8	g	206	
9	i	546	
9	j	546	
10	k	175	
10	l	175	
11	m	139	
11	n	139	
12	q	227	
12	r	227	

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 46789 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 Prokaryotic respiratory supercomplex associate factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	76	Total	C	N	O	S	0	0
			575	372	103	98	2		
1	b	76	Total	C	N	O	S	0	0
			575	372	103	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		
2	L	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	68	Total	C	N	O	S	0	0
			509	333	86	87	3		
3	h	68	Total	C	N	O	S	0	0
			509	333	86	87	3		

- Molecule 4 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		
4	o	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		

- Molecule 5 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		
5	p	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		

- Molecule 6 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	25	Total	C	N	O	S	0	0
			171	104	28	38	1		
6	a	25	Total	C	N	O	S	0	0
			171	104	28	38	1		

- Molecule 7 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		
7	e	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		

- Molecule 8 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		
8	g	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		
9	j	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		

- Molecule 10 is a protein called DUF5130 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	145	Total	C	N	O	S	0	0
			1068	672	185	210	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	145	Total	C	N	O	S	0	0
			1068	672	185	210	1		

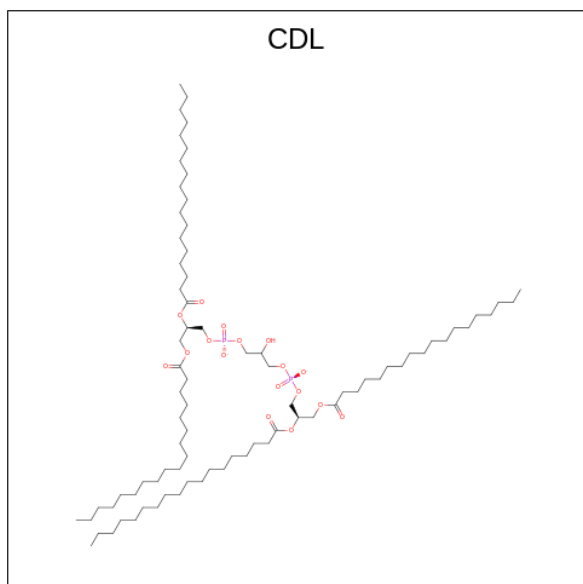
- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		
11	n	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		

- Molecule 12 is a protein called Lipoprotein lpqE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		
12	r	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



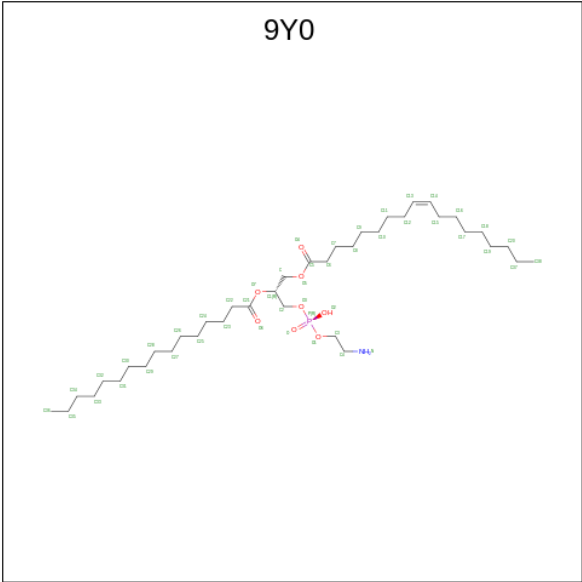
Mol	Chain	Residues	Atoms				AltConf
13	G	1	Total	C	O	P	0
			88	69	17	2	
13	I	1	Total	C	O	P	0
			76	57	17	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
13	I	1	Total	C	O	P	0
			81	62	17	2	
13	L	1	Total	C	O	P	0
			76	57	17	2	
13	L	1	Total	C	O	P	0
			81	62	17	2	
13	U	1	Total	C	O	P	0
			79	60	17	2	
13	V	1	Total	C	O	P	0
			95	76	17	2	
13	b	1	Total	C	O	P	0
			88	69	17	2	
13	i	1	Total	C	O	P	0
			66	47	17	2	
13	i	1	Total	C	O	P	0
			74	55	17	2	
13	i	1	Total	C	O	P	0
			77	58	17	2	
13	i	1	Total	C	O	P	0
			79	60	17	2	
13	i	1	Total	C	O	P	0
			74	55	17	2	
13	i	1	Total	C	O	P	0
			66	47	17	2	
13	j	1	Total	C	O	P	0
			77	58	17	2	
13	j	1	Total	C	O	P	0
			79	60	17	2	
13	j	1	Total	C	O	P	0
			79	60	17	2	
13	p	1	Total	C	O	P	0
			95	76	17	2	

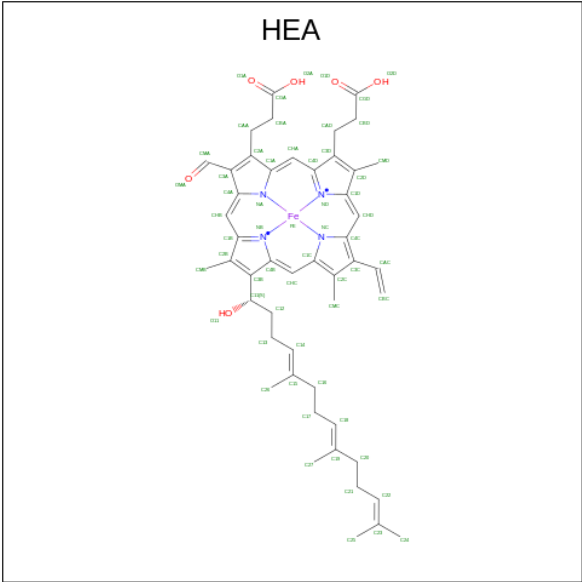
- Molecule 14 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	I	1	Total	C	N	O	P	0
			38	28	1	8	1	
14	I	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
14	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	f	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



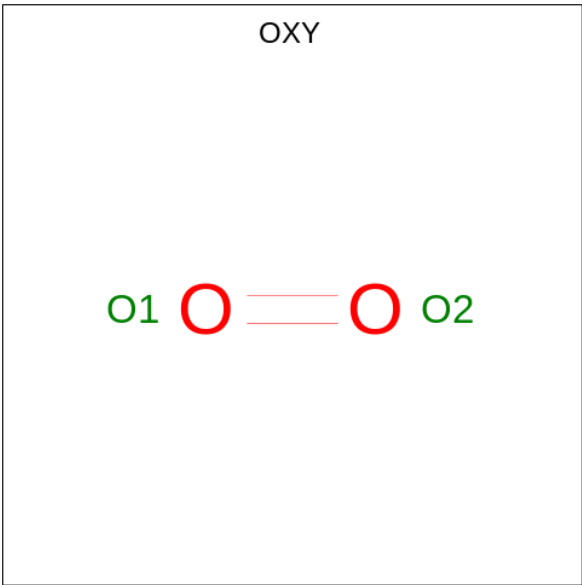


Mol	Chain	Residues	Atoms					AltConf
15	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
15	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
15	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
15	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

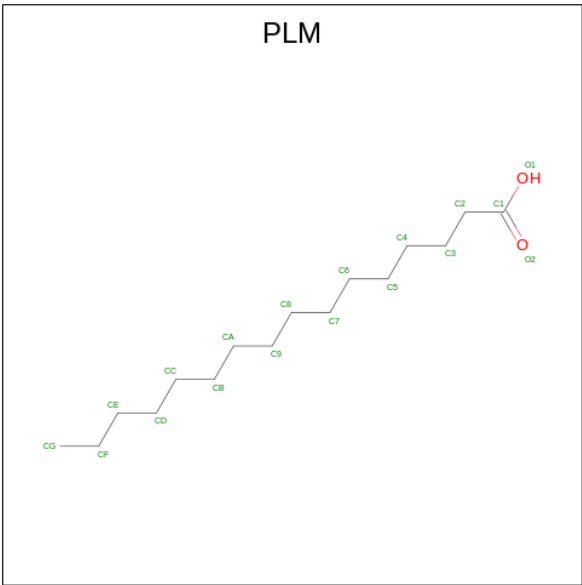
Mol	Chain	Residues	Atoms		AltConf
16	I	2	Total	Cu	0
			2	2	
16	L	2	Total	Cu	0
			2	2	
16	d	2	Total	Cu	0
			2	2	
16	e	2	Total	Cu	0
			2	2	

- Molecule 17 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
17	I	1	Total	O	0
			2	2	
17	L	1	Total	O	0
			2	2	

- Molecule 18 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



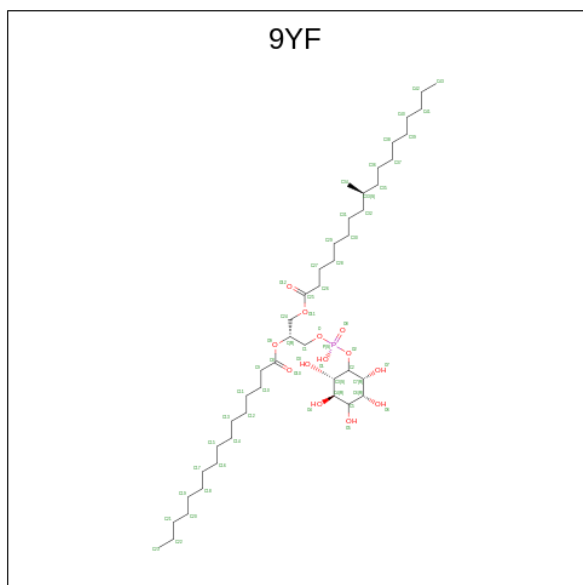
Mol	Chain	Residues	Atoms			AltConf
18	I	1	Total	C	O	0
			17	16	1	
18	j	1	Total	C	O	0
			11	10	1	

Continued on next page...

Continued from previous page...

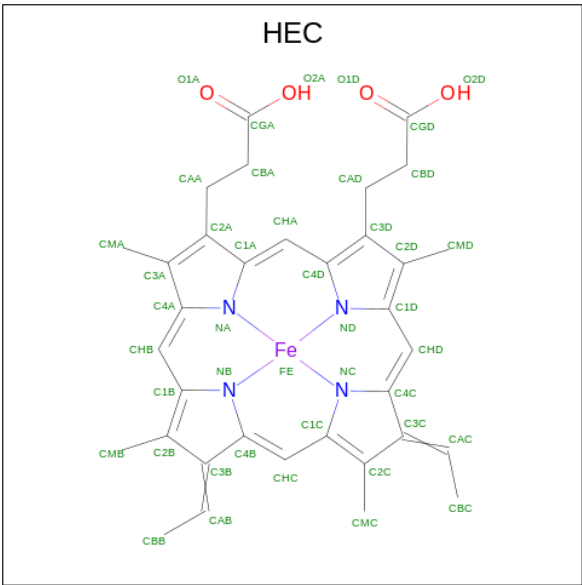
Mol	Chain	Residues	Atoms			AltConf
18	q	1	Total	C	O	0
			17	16	1	

- Molecule 19 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: C<sub>44</sub>H<sub>85</sub>O<sub>13</sub>P).



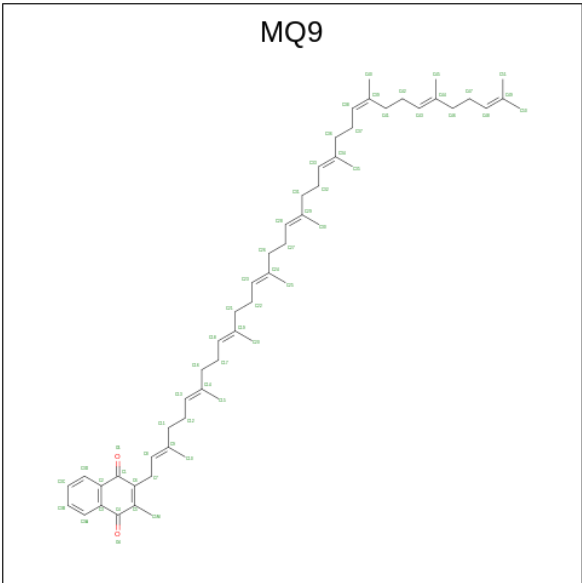
Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total	C	O	P	0
			58	44	13	1	
19	V	1	Total	C	O	P	0
			58	44	13	1	
19	i	1	Total	C	O	P	0
			58	44	13	1	
19	j	1	Total	C	O	P	0
			58	44	13	1	
19	o	1	Total	C	O	P	0
			58	44	13	1	
19	p	1	Total	C	O	P	0
			58	44	13	1	
19	p	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



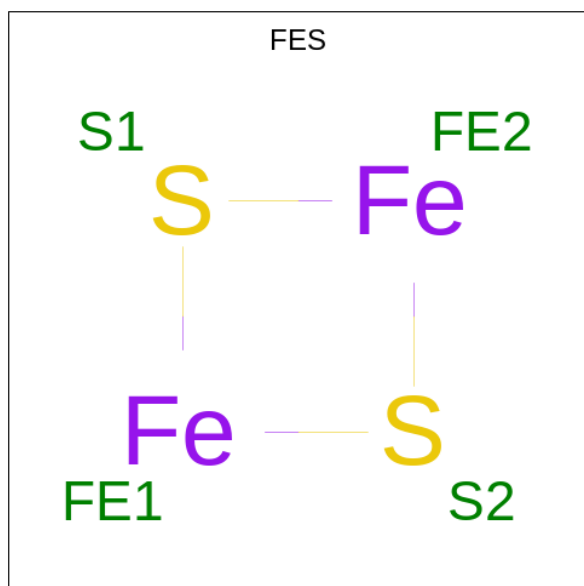
Mol	Chain	Residues	Atoms					AltConf
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C<sub>56</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	U	1	Total	C	O	0
			58	56	2	
21	i	1	Total	C	O	0
			43	41	2	
21	i	1	Total	C	O	0
			58	56	2	
21	j	1	Total	C	O	0
			43	41	2	
21	j	1	Total	C	O	0
			58	56	2	
21	m	1	Total	C	O	0
			48	46	2	
21	n	1	Total	C	O	0
			48	46	2	
21	o	1	Total	C	O	0
			58	56	2	

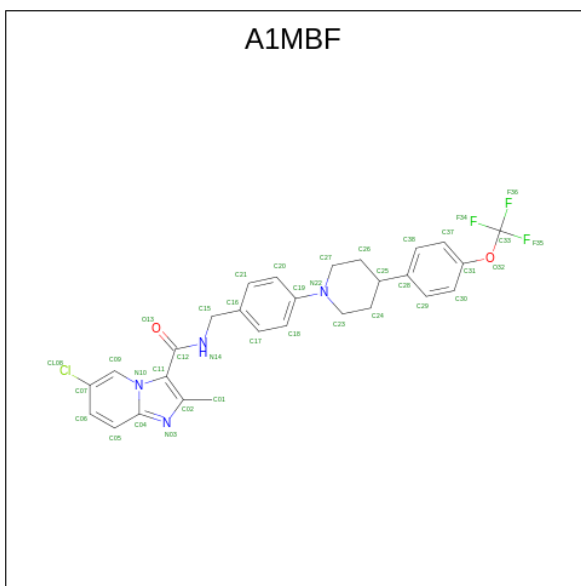
- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	V	1	Total	Fe	S	0
			4	2	2	
22	p	1	Total	Fe	S	0
			4	2	2	

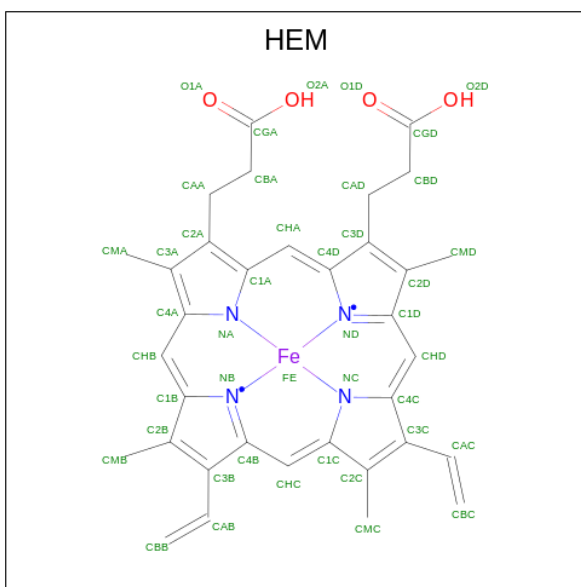
- Molecule 23 is 6-chloranyl-2-methyl- {N}-[[4-[4-(trifluoromethoxy)phenyl]piperidin-1-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (CCD ID: A1MBF) (formula:

C<sub>28</sub>H<sub>26</sub>ClF<sub>3</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



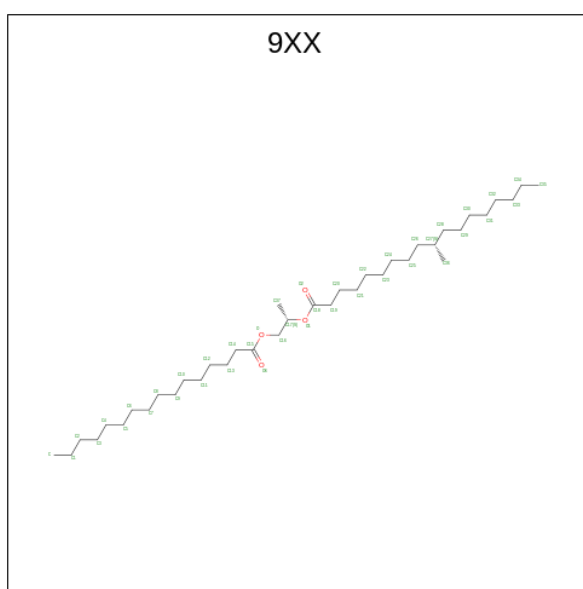
Mol	Chain	Residues	Atoms						AltConf
23	i	1	Total 38	C 28	Cl 1	F 3	N 4	O 2	0
23	j	1	Total 38	C 28	Cl 1	F 3	N 4	O 2	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	i	1	Total 42	C 33	Fe 1	N 4	O 4	0
24	i	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	j	1	Total 42	C 33	Fe 1	N 4	O 4	0
24	j	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 25 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C<sub>38</sub>H<sub>74</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
25	i	1	Total	C	O	0
			32	28	4	
25	j	1	Total	C	O	0
			32	28	4	
25	q	1	Total	C	O	0
			42	38	4	
25	r	1	Total	C	O	0
			42	38	4	

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	I	18	Total	O	0
			18	18	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
26	L	17	Total 17	O 17	0
26	U	5	Total 5	O 5	0
26	V	1	Total 1	O 1	0
26	d	2	Total 2	O 2	0
26	e	1	Total 1	O 1	0
26	i	8	Total 8	O 8	0
26	j	9	Total 9	O 9	0
26	m	2	Total 2	O 2	0
26	n	3	Total 3	O 3	0
26	o	6	Total 6	O 6	0
26	p	2	Total 2	O 2	0

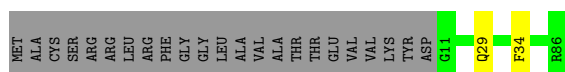


### 3 Residue-property plots [i](#)

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.

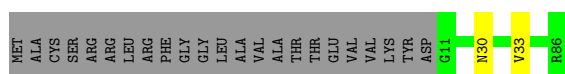
- Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

Chain G: 




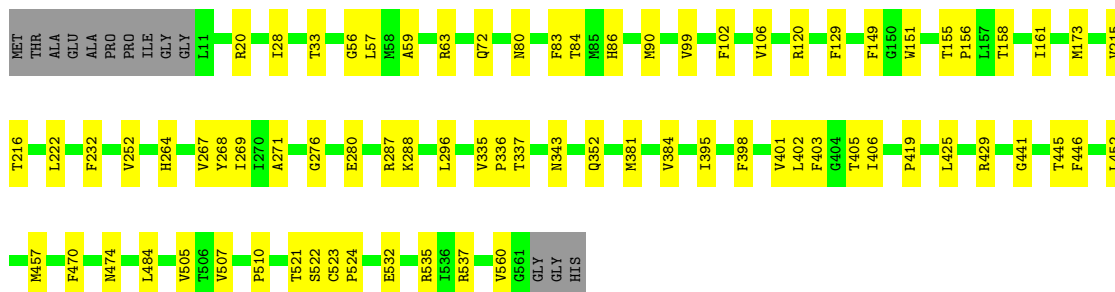
- Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

Chain b: 




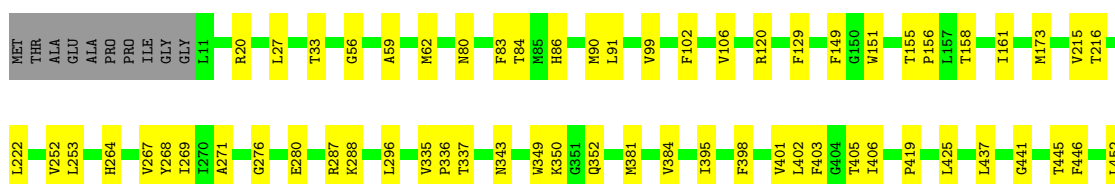
- Molecule 2: Cytochrome c oxidase subunit 1

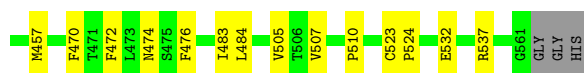
Chain I: 



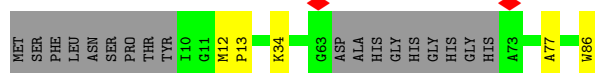
- Molecule 2: Cytochrome c oxidase subunit 1

Chain L: 

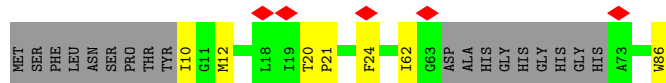




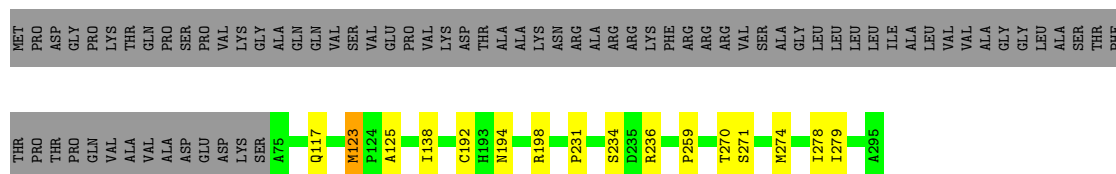
- Molecule 3: Cytochrome c oxidase subunit CtaJ



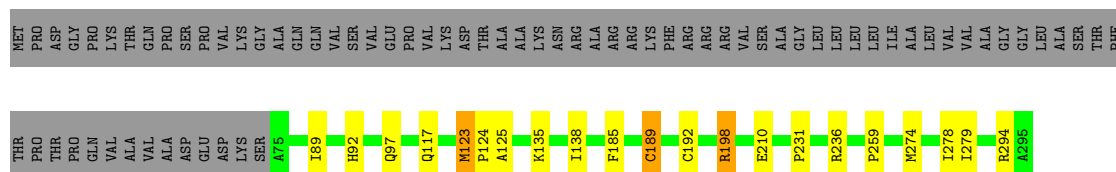
- Molecule 3: Cytochrome c oxidase subunit CtaJ



- Molecule 4: Cytochrome bc1 complex cytochrome c subunit



- Molecule 4: Cytochrome bc1 complex cytochrome c subunit



- Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit



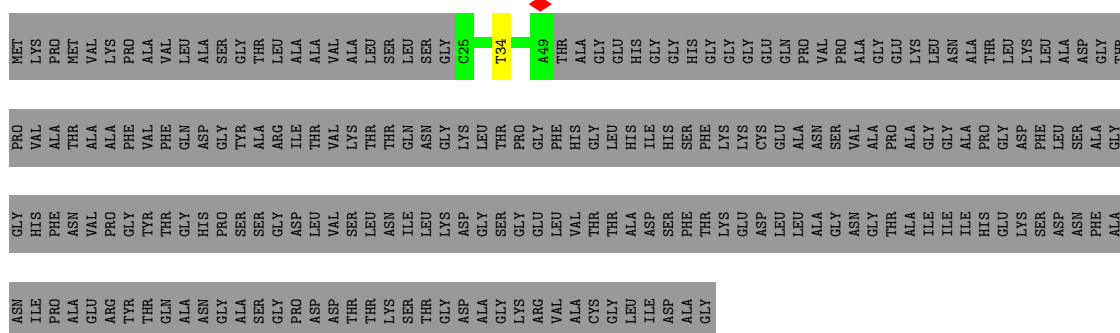
- Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit





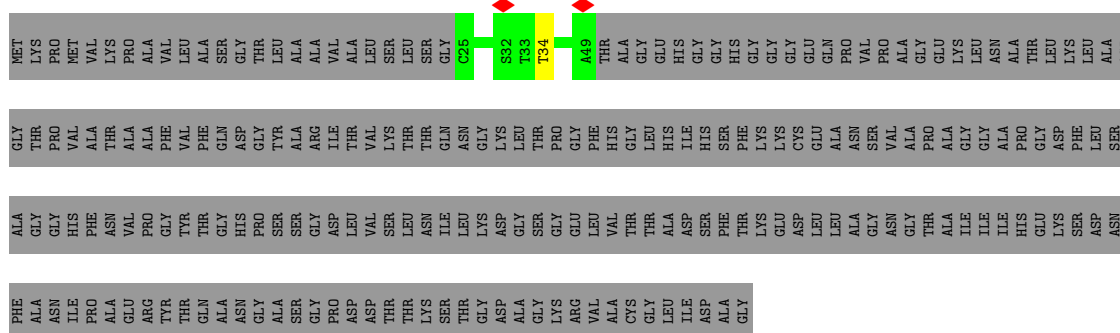
• Molecule 6: Superoxide dismutase [Cu-Zn]

Chain X: 10% 89%



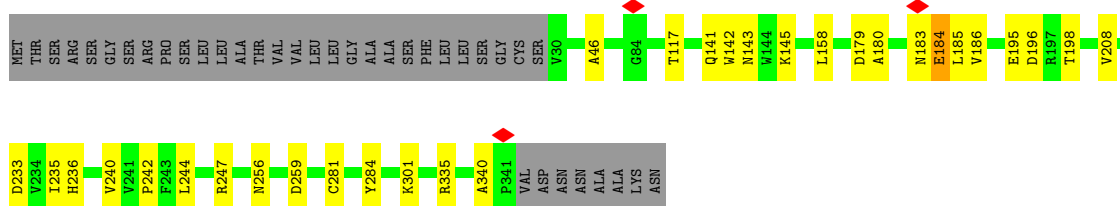
• Molecule 6: Superoxide dismutase [Cu-Zn]

Chain a: 10% 89%



• Molecule 7: cytochrome-c oxidase

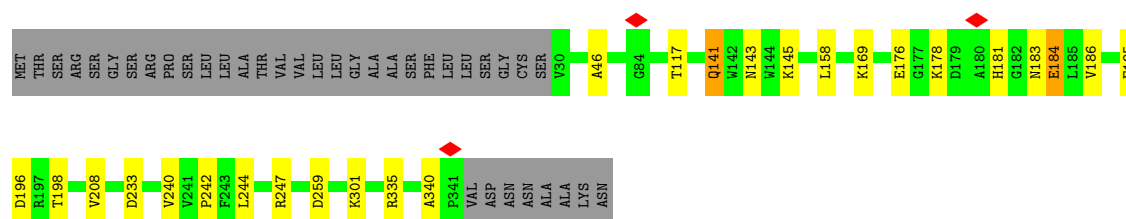
Chain d: 81% 9% 11%



• Molecule 7: cytochrome-c oxidase

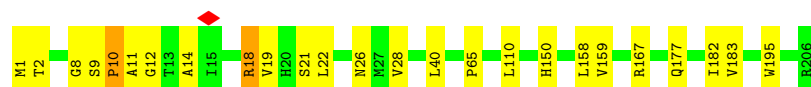
Chain e: 82% 7% 11%





- Molecule 8: Probable cytochrome c oxidase subunit 3

Chain f: 88% 11%



- Molecule 8: Probable cytochrome c oxidase subunit 3

Chain g: 90% 9%



- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain i: 86% 10%



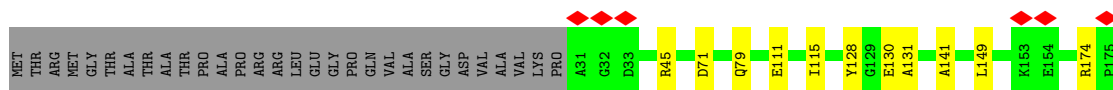
- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain j: 88% 8%

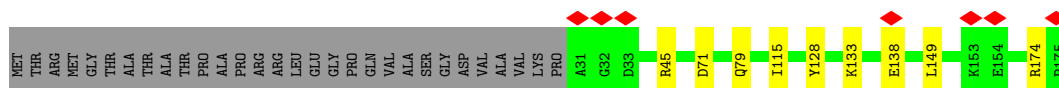
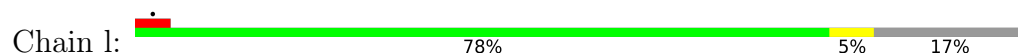


- Molecule 10: DUF5130 domain-containing protein

Chain k: 77% 6% 17%



- Molecule 10: DUF5130 domain-containing protein



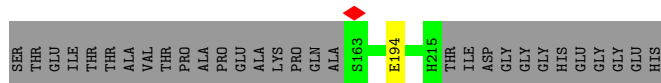
- Molecule 11: Cytochrome c oxidase polypeptide 4



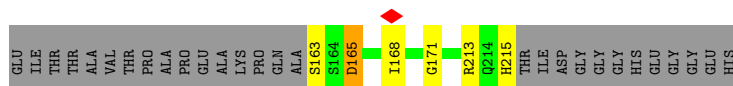
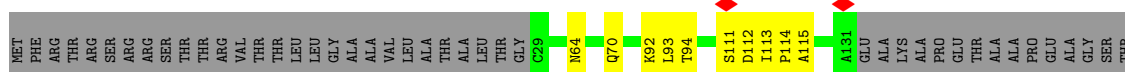
- Molecule 11: Cytochrome c oxidase polypeptide 4



- Molecule 12: Lipoprotein lpqE



- Molecule 12: Lipoprotein lpqE



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0332	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A1MBF, 9YF, 9XX, FES, HEC, 9Y0, CU, PLM, OXY, MQ9, CDL, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	G	0.12	0/585	0.23	0/789
1	b	0.13	0/585	0.29	0/789
2	I	0.16	0/4526	0.36	0/6181
2	L	0.16	0/4526	0.35	0/6181
3	J	0.11	0/526	0.25	0/718
3	h	0.11	0/526	0.29	0/718
4	U	0.13	0/1669	0.35	0/2257
4	o	0.19	0/1669	0.40	1/2257 (0.0%)
5	V	0.13	0/3033	0.30	0/4120
5	p	0.12	0/3033	0.29	0/4120
6	X	0.14	0/177	0.45	0/248
6	a	0.11	0/177	0.36	0/248
7	d	0.13	0/2547	0.31	0/3466
7	e	0.12	0/2547	0.30	0/3466
8	f	0.17	0/1644	0.32	0/2244
8	g	0.17	0/1644	0.35	0/2244
9	i	0.14	0/4252	0.33	0/5785
9	j	0.14	0/4252	0.33	0/5785
10	k	0.08	0/1088	0.23	0/1481
10	l	0.09	0/1088	0.26	0/1481
11	m	0.12	0/1097	0.28	0/1499
11	n	0.13	0/1097	0.28	0/1499
12	q	0.11	0/1144	0.31	0/1551
12	r	0.12	0/1144	0.33	0/1551
All	All	0.14	0/44576	0.32	1/60678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	o	89	ILE	N-CA-C	-6.67	107.37	113.71

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	575	0	591	1	0
1	b	575	0	591	1	0
2	I	4363	0	4322	70	0
2	L	4363	0	4322	64	0
3	J	509	0	500	5	0
3	h	509	0	500	6	0
4	U	1639	0	1598	14	0
4	o	1639	0	1600	17	0
5	V	2957	0	2964	14	0
5	p	2957	0	2964	15	0
6	X	171	0	156	0	0
6	a	171	0	156	0	0
7	d	2476	0	2445	19	0
7	e	2476	0	2445	13	0
8	f	1595	0	1581	19	0
8	g	1595	0	1581	15	0
9	i	4127	0	4157	41	0
9	j	4127	0	4158	32	0
10	k	1068	0	1054	7	0
10	l	1068	0	1054	6	0
11	m	1066	0	1052	7	0
11	n	1066	0	1052	13	0
12	q	1129	0	1126	10	0
12	r	1129	0	1126	10	0
13	G	88	0	126	8	0
13	I	157	0	208	8	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	157	0	208	4	0
13	U	79	0	105	2	0
13	V	95	0	143	14	0
13	b	88	0	126	6	0
13	i	436	0	539	14	0
13	j	235	0	308	2	0
13	p	95	0	143	4	0
14	G	41	0	0	0	0
14	I	81	0	0	11	0
14	L	38	0	0	1	0
14	b	41	0	0	0	0
14	f	43	0	0	0	0
15	I	120	0	108	9	0
15	L	120	0	108	8	0
16	I	2	0	0	0	0
16	L	2	0	0	0	0
16	d	2	0	0	0	0
16	e	2	0	0	0	0
17	I	2	0	0	0	0
17	L	2	0	0	0	0
18	I	17	0	31	1	0
18	j	11	0	16	0	0
18	q	17	0	31	5	0
19	L	58	0	0	0	0
19	V	58	0	0	0	0
19	i	58	0	0	0	0
19	j	58	0	0	0	0
19	o	58	0	0	0	0
19	p	116	0	0	0	0
20	U	86	0	62	4	0
20	o	86	0	64	4	0
21	U	58	0	80	1	0
21	i	101	0	133	17	0
21	j	101	0	130	11	0
21	m	48	0	61	2	0
21	n	48	0	61	5	0
21	o	58	0	80	3	0
22	V	4	0	0	0	0
22	p	4	0	0	0	0
23	i	38	0	0	0	0
23	j	38	0	0	0	0
24	i	85	0	57	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	j	85	0	57	3	0
25	i	32	0	0	0	0
25	j	32	0	0	0	0
25	q	42	0	0	3	0
25	r	42	0	0	0	0
26	I	18	0	0	0	0
26	L	17	0	0	0	0
26	U	5	0	0	0	0
26	V	1	0	0	0	0
26	d	2	0	0	0	0
26	e	1	0	0	0	0
26	i	8	0	0	0	0
26	j	9	0	0	0	0
26	m	2	0	0	0	0
26	n	3	0	0	0	0
26	o	6	0	0	0	0
26	p	2	0	0	0	0
All	All	46789	0	46080	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (426) 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)
13:i:607:CDL:C42	25:q:302:9XX:C35	1.78	1.57
2:I:232:PHE:CZ	14:I:610:9Y0:C15	1.85	1.56
2:I:155:THR:CG2	2:I:156:PRO:HD3	1.65	1.25
2:L:472:PHE:CZ	2:L:476:PHE:CE2	2.27	1.22
2:L:472:PHE:CE2	2:L:476:PHE:CE2	2.31	1.18
2:I:155:THR:HG22	2:I:156:PRO:HD3	1.27	1.13
2:I:155:THR:HG23	2:I:156:PRO:CD	1.80	1.11
2:L:472:PHE:CZ	2:L:476:PHE:CZ	2.41	1.08
2:I:232:PHE:CE2	8:g:149:PHE:HE1	1.75	1.05
2:I:232:PHE:CE2	8:g:149:PHE:CE1	2.47	1.02
2:I:232:PHE:CE1	14:I:610:9Y0:C15	2.42	1.01
2:L:472:PHE:CE2	2:L:476:PHE:HE2	1.71	0.99
2:I:155:THR:CG2	2:I:156:PRO:CD	2.39	0.98
2:I:155:THR:HG23	2:I:156:PRO:HD3	1.43	0.94
2:I:155:THR:HG21	2:I:252:VAL:HA	1.51	0.91
2:I:232:PHE:HZ	14:I:610:9Y0:C15	1.57	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:155:THR:CG2	2:L:156:PRO:HD3	2.06	0.85
5:p:283:MET:HG3	5:p:314:LYS:HG2	1.60	0.81
2:I:232:PHE:CZ	8:g:149:PHE:HE1	1.97	0.81
13:V:602:CDL:H632	13:V:602:CDL:H351	1.64	0.79
2:I:155:THR:HG23	2:I:156:PRO:N	1.98	0.79
2:I:521:THR:HG22	2:I:522:SER:N	1.98	0.78
2:L:155:THR:HG23	2:L:156:PRO:HD3	1.67	0.77
13:V:602:CDL:H222	13:V:602:CDL:H642	1.69	0.74
2:L:84:THR:OG1	2:L:149:PHE:O	2.06	0.73
2:L:59:ALA:HA	2:L:62:MET:HE2	1.72	0.71
9:i:137:ARG:HB3	9:i:138:PRO:HD3	1.73	0.71
9:i:501:THR:HG22	9:i:513:GLN:HG2	1.72	0.70
12:r:111:SER:HB3	12:r:171:GLY:HA3	1.71	0.70
4:U:259:PRO:O	9:i:282:GLN:NE2	2.24	0.70
9:j:137:ARG:HB3	9:j:138:PRO:HD3	1.74	0.70
2:I:84:THR:OG1	2:I:149:PHE:O	2.06	0.70
9:j:282:GLN:NE2	4:o:259:PRO:O	2.24	0.70
2:L:155:THR:HG22	2:L:156:PRO:HD3	1.73	0.69
21:j:608:MQ9:C8	21:j:608:MQ9:H5M3	2.23	0.69
2:I:232:PHE:CZ	8:g:149:PHE:CE1	2.79	0.69
12:r:165:ASP:OD1	12:r:165:ASP:N	2.25	0.69
9:j:501:THR:HG22	9:j:513:GLN:HG2	1.75	0.69
2:I:521:THR:HG22	2:I:522:SER:H	1.57	0.69
2:I:507:VAL:O	2:I:523:CYS:SG	2.50	0.68
2:I:232:PHE:CE1	14:I:610:9Y0:C16	2.77	0.68
4:U:231:PRO:HD3	20:U:602:HEC:HBC2	1.76	0.68
2:I:470:PHE:O	2:I:474:ASN:ND2	2.26	0.67
2:L:470:PHE:O	2:L:474:ASN:ND2	2.27	0.67
12:r:163:SER:HB2	12:r:168:ILE:HG21	1.77	0.66
2:L:155:THR:HG23	2:L:156:PRO:CD	2.26	0.66
4:U:117:GLN:HB3	4:U:123:MET:HG2	1.78	0.65
14:L:601:9Y0:O	14:L:601:9Y0:N	2.30	0.64
11:n:26:THR:HG21	11:n:35:GLU:HG2	1.78	0.64
3:J:86:TRP:HB3	10:k:149:LEU:HD22	1.80	0.63
2:I:72:GLN:HG2	3:J:12:MET:HG2	1.78	0.63
7:d:179:ASP:O	7:d:183:ASN:N	2.31	0.63
9:j:66:PHE:HA	9:j:93:THR:HG21	1.79	0.63
9:i:66:PHE:HA	9:i:93:THR:HG21	1.79	0.63
4:o:231:PRO:HD3	20:o:602:HEC:HBC2	1.81	0.62
13:L:606:CDL:HA62	13:L:606:CDL:HA22	1.81	0.62
13:V:602:CDL:H662	13:V:602:CDL:H251	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:454:ARG:HG3	9:j:459:GLU:HB3	1.82	0.62
21:n:201:MQ9:H101	21:n:201:MQ9:H5M3	1.81	0.62
9:i:72:GLU:OE2	9:i:86:GLN:NE2	2.34	0.61
12:r:92:LYS:HA	12:r:114:PRO:HD2	1.81	0.61
2:I:155:THR:HG23	2:I:156:PRO:CG	2.30	0.61
13:I:605:CDL:H171	13:I:605:CDL:H341	1.82	0.61
4:o:198:ARG:NH1	4:o:210:GLU:OE2	2.33	0.61
2:I:28:ILE:HD11	13:I:605:CDL:H652	1.83	0.60
2:L:337:THR:HG21	15:L:602:HEA:H263	1.82	0.60
7:d:186:VAL:HG21	8:f:65:PRO:HD3	1.82	0.60
9:i:449:THR:OG1	9:i:463:ILE:O	2.18	0.60
2:I:521:THR:CG2	2:I:522:SER:H	2.14	0.60
2:I:521:THR:CG2	2:I:522:SER:N	2.63	0.60
2:I:232:PHE:HZ	14:I:610:9Y0:C14	2.10	0.60
7:e:186:VAL:HG21	8:g:65:PRO:HD3	1.83	0.60
2:I:337:THR:HG21	15:I:601:HEA:H263	1.82	0.60
12:r:92:LYS:HG2	12:r:113:ILE:HG23	1.81	0.60
9:i:25:ALA:HA	9:i:28:MET:HB2	1.83	0.60
9:i:532:LYS:NZ	9:i:536:ASP:OD2	2.33	0.59
3:h:86:TRP:HB3	10:l:149:LEU:HD22	1.83	0.59
9:j:233:TRP:CE3	21:j:608:MQ9:H3C	2.36	0.59
12:q:29:CYS:N	18:q:301:PLM:O2	2.35	0.59
8:f:9:SER:N	8:f:10:PRO:HD3	2.18	0.59
12:r:213:ARG:HG2	12:r:215:HIS:H	1.67	0.59
8:f:18:ARG:H	8:f:18:ARG:HD3	1.68	0.59
2:L:155:THR:CG2	2:L:156:PRO:CD	2.79	0.58
2:L:33:THR:HG22	11:n:90:TRP:HB3	1.85	0.58
2:I:33:THR:HG22	11:m:90:TRP:HB3	1.85	0.58
9:i:212:MET:HG2	9:i:216:LEU:HD12	1.85	0.58
2:L:155:THR:HG21	2:L:252:VAL:HA	1.86	0.58
2:I:532:GLU:OE2	10:k:45:ARG:NH1	2.37	0.58
2:L:532:GLU:OE2	10:l:45:ARG:NH1	2.37	0.58
5:V:164:ARG:NH1	5:p:56:GLU:OE2	2.37	0.58
13:V:602:CDL:H222	13:V:602:CDL:H611	1.84	0.58
2:L:437:LEU:HD22	3:h:24:PHE:HE2	1.69	0.58
4:o:123:MET:O	4:o:125:ALA:N	2.37	0.58
9:i:243:PRO:O	9:i:535:GLN:NE2	2.37	0.57
9:j:243:PRO:O	9:j:535:GLN:NE2	2.37	0.57
5:V:242:GLU:O	4:o:236:ARG:NH1	2.37	0.57
12:q:100:ASP:OD1	12:q:101:GLU:N	2.37	0.57
9:j:396:ASP:OD1	9:j:396:ASP:N	2.36	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:236:HIS:ND1	7:d:281:CYS:SG	2.77	0.57
2:L:472:PHE:HZ	2:L:476:PHE:CZ	2.14	0.57
5:V:56:GLU:OE2	5:p:164:ARG:NH1	2.37	0.57
2:I:381:MET:SD	7:e:117:THR:OG1	2.63	0.57
12:r:93:LEU:HD23	12:r:112:ASP:HB3	1.86	0.57
2:L:507:VAL:O	2:L:523:CYS:SG	2.57	0.56
2:I:20:ARG:NH2	10:k:71:ASP:OD1	2.39	0.56
2:I:398:PHE:HA	2:I:401:VAL:HG22	1.87	0.56
13:V:602:CDL:H211	13:V:602:CDL:H162	1.87	0.56
2:I:161:ILE:HG21	4:o:138:ILE:HD11	1.87	0.56
2:L:398:PHE:HA	2:L:401:VAL:HG22	1.87	0.56
2:L:381:MET:SD	7:d:117:THR:OG1	2.63	0.56
2:L:20:ARG:NH2	10:l:71:ASP:OD1	2.39	0.56
4:o:123:MET:HE2	4:o:123:MET:HA	1.88	0.55
2:L:349:TRP:CD1	2:L:350:LYS:HG2	2.42	0.55
7:e:178:LYS:HD2	7:e:184:GLU:HG3	1.88	0.55
13:U:604:CDL:HA61	13:U:604:CDL:HA22	1.89	0.55
12:r:93:LEU:N	12:r:112:ASP:O	2.39	0.55
9:i:328:THR:OG1	5:p:386:PHE:O	2.24	0.55
4:U:236:ARG:NH1	5:p:242:GLU:O	2.38	0.55
2:I:232:PHE:CE2	14:I:610:9Y0:C15	2.74	0.55
7:e:335:ARG:NH2	7:e:340:ALA:O	2.35	0.55
9:j:67:ASP:H	9:j:93:THR:HG21	1.72	0.55
8:f:150:HIS:CE1	8:f:195:TRP:HB2	2.42	0.55
7:d:179:ASP:HA	7:d:184:GLU:HA	1.89	0.55
9:i:67:ASP:H	9:i:93:THR:HG21	1.72	0.55
7:d:196:ASP:OD1	7:d:198:THR:OG1	2.16	0.54
8:g:150:HIS:CE1	8:g:195:TRP:HB2	2.42	0.54
9:i:396:ASP:OD1	9:i:396:ASP:N	2.35	0.54
12:r:113:ILE:HG22	12:r:115:ALA:HB2	1.89	0.54
7:e:196:ASP:OD1	7:e:198:THR:OG1	2.16	0.54
2:I:271:ALA:HA	2:I:405:THR:HG21	1.90	0.53
2:L:287:ARG:HD2	2:L:352:GLN:HB2	1.90	0.53
8:g:19:VAL:HG13	8:g:20:HIS:H	1.72	0.53
2:I:287:ARG:HD2	2:I:352:GLN:HB2	1.91	0.53
2:L:271:ALA:HA	2:L:405:THR:HG21	1.90	0.53
12:q:92:LYS:HB2	12:q:113:ILE:HG23	1.91	0.53
2:L:155:THR:HG23	2:L:156:PRO:N	2.24	0.53
4:o:117:GLN:HB3	4:o:123:MET:HG2	1.90	0.53
9:j:532:LYS:NZ	9:j:536:ASP:OD2	2.33	0.53
2:I:429:ARG:NH1	3:J:34:LYS:O	2.40	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:354:PRO:HA	9:j:319:ALA:HB2	1.90	0.53
21:j:608:MQ9:H321	21:j:608:MQ9:H272	1.89	0.53
24:j:604:HEM:HBB2	24:j:604:HEM:HMB1	1.91	0.53
5:V:314:LYS:HE3	5:V:324:SER:HB3	1.90	0.52
8:f:150:HIS:NE2	8:f:195:TRP:HB2	2.24	0.52
13:i:613:CDL:H532	13:i:613:CDL:HB62	1.91	0.52
8:g:150:HIS:NE2	8:g:195:TRP:HB2	2.24	0.52
4:U:274:MET:HG2	21:n:201:MQ9:H5M1	1.92	0.52
2:L:483:ILE:HG23	3:h:24:PHE:CE2	2.44	0.52
7:e:46:ALA:HB1	7:e:244:LEU:HD12	1.92	0.52
2:I:264:HIS:NE2	2:I:268:TYR:HE2	2.09	0.51
13:I:604:CDL:HA62	13:I:604:CDL:HA22	1.92	0.51
7:e:183:ASN:ND2	8:g:130:GLU:O	2.43	0.51
13:i:606:CDL:OB7	21:i:610:MQ9:H3A	2.09	0.51
21:i:610:MQ9:H121	21:i:610:MQ9:H71	1.91	0.51
9:i:233:TRP:CE3	21:i:610:MQ9:H3C	2.46	0.51
2:I:80:ASN:HA	2:I:83:PHE:CE2	2.46	0.51
13:I:605:CDL:H162	13:b:101:CDL:H792	1.93	0.51
13:I:605:CDL:H873	13:b:101:CDL:H832	1.91	0.51
2:L:472:PHE:CE1	2:L:476:PHE:CZ	2.97	0.51
9:j:229:LEU:HD12	21:j:608:MQ9:C7	2.41	0.51
24:i:605:HEM:HBB2	24:i:605:HEM:HMB1	1.91	0.51
15:I:602:HEA:C24	14:I:608:9Y0:C20	2.89	0.51
2:L:264:HIS:NE2	2:L:268:TYR:HE2	2.09	0.51
2:L:437:LEU:HD22	3:h:24:PHE:CE2	2.46	0.51
7:d:46:ALA:HB1	7:d:244:LEU:HD12	1.92	0.51
9:i:214:ILE:HD11	9:j:214:ILE:HD11	1.93	0.51
4:o:125:ALA:HB3	20:o:601:HEC:HBC2	1.92	0.51
7:d:141:GLN:HG3	7:d:142:TRP:CD2	2.45	0.51
7:d:142:TRP:CG	7:d:284:TYR:HB2	2.46	0.51
13:i:608:CDL:H221	11:n:120:PHE:HB3	1.93	0.51
10:k:128:TYR:CE2	10:k:141:ALA:HB2	2.45	0.50
4:o:185:PHE:HA	4:o:189:CYS:SG	2.50	0.50
2:I:535:ARG:NH1	11:m:74:GLU:OE1	2.44	0.50
9:i:319:ALA:HB2	5:p:354:PRO:HA	1.92	0.50
8:f:19:VAL:O	8:f:21:SER:N	2.43	0.50
1:G:29:GLN:HG3	1:G:34:PHE:HE2	1.76	0.49
2:L:161:ILE:HG21	4:U:138:ILE:HD11	1.92	0.49
8:f:1:MET:HE3	9:i:490:MET:HB2	1.93	0.49
2:L:472:PHE:CZ	2:L:476:PHE:HZ	2.18	0.49
24:i:604:HEM:HMB1	24:i:604:HEM:HBB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:ASN:HA	2:L:83:PHE:CE2	2.46	0.49
13:V:602:CDL:H131	13:V:602:CDL:H312	1.94	0.49
12:q:93:LEU:HB3	12:q:194:GLU:HB2	1.94	0.49
3:h:10:ILE:HG21	3:h:12:MET:HE2	1.94	0.49
7:e:240:VAL:HG12	7:e:242:PRO:HD2	1.94	0.49
5:V:261:ASP:O	5:V:267:SER:OG	2.17	0.49
13:G:101:CDL:H272	25:q:302:9XX:C30	2.43	0.49
2:I:232:PHE:CZ	14:I:610:9Y0:C14	2.80	0.49
9:i:455:LEU:HB2	9:i:456:PRO:HD3	1.94	0.49
9:j:511:ASP:OD1	9:j:511:ASP:N	2.45	0.49
13:G:101:CDL:H832	15:L:603:HEA:H253	1.95	0.48
2:L:27:LEU:HD22	13:L:607:CDL:HB31	1.95	0.48
24:j:603:HEM:HMB1	24:j:603:HEM:HBB2	1.94	0.48
2:L:173:MET:HG3	11:n:107:ALA:HB2	1.95	0.48
9:i:511:ASP:OD1	9:i:511:ASP:N	2.45	0.48
9:j:455:LEU:HB3	9:j:456:PRO:HD3	1.95	0.48
7:d:141:GLN:HG3	7:d:142:TRP:CE2	2.48	0.48
7:e:145:LYS:HG3	7:e:208:VAL:HG22	1.95	0.48
21:i:610:MQ9:H121	21:i:610:MQ9:C7	2.42	0.48
5:p:231:SER:OG	5:p:233:SER:O	2.24	0.48
2:L:505:VAL:HG11	2:L:510:PRO:HG3	1.96	0.48
2:L:537:ARG:CZ	11:n:72:ASP:HA	2.44	0.48
13:j:611:CDL:H151	11:m:123:SER:HB3	1.95	0.48
12:q:29:CYS:N	18:q:301:PLM:H21	2.28	0.48
4:U:271:SER:HA	21:n:201:MQ9:H5M2	1.95	0.48
7:d:240:VAL:HG12	7:d:242:PRO:HD2	1.94	0.48
21:i:610:MQ9:H361	21:i:610:MQ9:H411	1.96	0.48
2:I:149:PHE:CD2	2:I:158:THR:HG22	2.49	0.48
5:V:325:LEU:HG	4:o:192:CYS:SG	2.54	0.47
9:i:28:MET:HE1	13:i:612:CDL:H342	1.95	0.47
4:o:92:HIS:O	4:o:97:GLN:O	2.32	0.47
7:d:145:LYS:HG3	7:d:208:VAL:HG22	1.96	0.47
2:I:505:VAL:HG11	2:I:510:PRO:HG3	1.96	0.47
4:U:123:MET:HG3	20:U:601:HEC:C4A	2.44	0.47
4:U:192:CYS:SG	5:p:325:LEU:HG	2.54	0.47
4:U:278:ILE:HG23	4:U:279:ILE:HG13	1.96	0.47
8:f:12:GLY:H	8:f:26:ASN:HB2	1.79	0.47
12:r:64:ASN:H	12:r:70:GLN:HE21	1.62	0.47
13:V:602:CDL:HB21	13:V:602:CDL:HB31	1.95	0.47
8:f:11:ALA:HB3	8:f:22:LEU:HD13	1.96	0.47
13:j:605:CDL:H572	13:j:605:CDL:H151	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:112:ASP:OD1	12:q:112:ASP:N	2.47	0.47
13:G:101:CDL:H411	9:i:427:ILE:HD11	1.96	0.47
2:I:173:MET:HG3	11:m:107:ALA:HB2	1.95	0.47
21:i:609:MQ9:H321	21:i:609:MQ9:H303	1.50	0.47
2:I:395:ILE:HA	2:I:398:PHE:CE2	2.49	0.47
2:I:537:ARG:CZ	11:m:72:ASP:HA	2.45	0.47
2:L:395:ILE:HA	2:L:398:PHE:CE2	2.49	0.47
5:V:145:ARG:NH1	9:i:19:ASP:OD2	2.47	0.47
13:b:101:CDL:H111	13:b:101:CDL:H141	1.61	0.47
9:i:501:THR:HG21	9:i:516:LEU:HD12	1.95	0.47
13:i:606:CDL:HA62	9:j:27:GLY:HA3	1.97	0.47
21:i:610:MQ9:H253	21:i:610:MQ9:H301	1.96	0.47
9:j:19:ASP:OD2	5:p:145:ARG:NH1	2.48	0.47
4:o:274:MET:SD	21:o:604:MQ9:H3D	2.54	0.47
9:j:61:TYR:CD1	9:j:107:VAL:HG11	2.49	0.47
2:L:472:PHE:CZ	2:L:476:PHE:HE2	1.91	0.47
4:U:125:ALA:HB3	20:U:601:HEC:HBC2	1.97	0.47
3:J:12:MET:HB2	3:J:13:PRO:HD3	1.96	0.46
2:L:56:GLY:C	15:L:603:HEA:H162	2.40	0.46
7:d:335:ARG:NH2	7:d:340:ALA:O	2.34	0.46
9:i:61:TYR:CD1	9:i:107:VAL:HG11	2.50	0.46
20:o:602:HEC:HMB3	20:o:602:HEC:HBB3	1.97	0.46
5:p:281:PRO:HB2	5:p:314:LYS:HD3	1.98	0.46
2:L:276:GLY:O	2:L:280:GLU:HG2	2.15	0.46
8:f:28:VAL:HG12	8:f:183:VAL:HG11	1.97	0.46
21:i:609:MQ9:H18	21:i:609:MQ9:H222	1.60	0.46
13:p:603:CDL:H112	13:p:603:CDL:HA4	1.62	0.46
2:L:149:PHE:CD2	2:L:158:THR:HG22	2.51	0.46
4:o:92:HIS:CD2	20:o:601:HEC:NC	2.84	0.46
2:L:288:LYS:HE2	2:L:288:LYS:HB3	1.73	0.46
13:L:607:CDL:H712	13:L:607:CDL:H742	1.72	0.46
2:I:56:GLY:C	15:I:602:HEA:H162	2.41	0.46
7:e:247:ARG:NH1	7:e:259:ASP:O	2.49	0.46
8:f:110:LEU:HD12	8:f:158:LEU:HD22	1.98	0.46
2:I:276:GLY:O	2:I:280:GLU:HG2	2.15	0.46
5:V:259:ASP:O	5:V:267:SER:OG	2.34	0.46
21:i:610:MQ9:H5M1	21:i:610:MQ9:H172	1.97	0.46
9:j:59:GLY:O	9:j:63:THR:OG1	2.33	0.46
9:j:66:PHE:HA	9:j:93:THR:CG2	2.45	0.46
7:e:181:HIS:O	7:e:181:HIS:ND1	2.49	0.46
13:i:603:CDL:H531	13:i:603:CDL:CB7	2.46	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:602:HEA:H261	15:I:602:HEA:H171	1.53	0.45
9:j:229:LEU:HD12	21:j:608:MQ9:H72	1.98	0.45
21:n:201:MQ9:H5M3	21:n:201:MQ9:C9	2.46	0.45
2:L:90:MET:HB3	15:L:603:HEA:CAC	2.46	0.45
9:j:156:GLU:HB2	9:j:217:ILE:HG21	1.98	0.45
21:i:610:MQ9:H253	21:i:610:MQ9:H271	1.57	0.45
9:j:256:LEU:HB3	9:j:257:PRO:HD3	1.99	0.45
9:j:501:THR:HG21	9:j:516:LEU:HD12	1.98	0.45
21:j:608:MQ9:H162	21:j:608:MQ9:H201	1.99	0.45
2:I:296:LEU:HG	2:I:343:ASN:HD22	1.81	0.45
10:l:133:LYS:NZ	10:l:138:GLU:OE2	2.45	0.45
13:V:602:CDL:H721	13:V:602:CDL:H551	1.99	0.45
13:i:607:CDL:H571	13:i:607:CDL:H151	1.98	0.45
2:L:445:THR:HG23	2:L:446:PHE:CD2	2.52	0.45
13:V:602:CDL:HB31	13:V:602:CDL:CB2	2.47	0.45
13:V:602:CDL:H381	13:V:602:CDL:H641	1.97	0.45
8:g:110:LEU:HD12	8:g:158:LEU:HD22	1.98	0.45
9:i:261:LEU:HD23	21:i:609:MQ9:H212	1.98	0.45
15:L:602:HEA:H261	15:L:602:HEA:H172	1.63	0.45
8:g:28:VAL:HG12	8:g:183:VAL:HG11	1.99	0.45
9:i:256:LEU:HB3	9:i:257:PRO:HD3	1.99	0.45
21:j:607:MQ9:H153	21:j:607:MQ9:H171	1.75	0.45
12:q:92:LYS:O	12:q:113:ILE:HG13	2.17	0.45
13:G:101:CDL:H131	9:i:422:ALA:HB1	1.98	0.45
13:L:607:CDL:H611	13:L:607:CDL:H641	1.64	0.44
5:V:322:PRO:HD2	9:j:297:ILE:HD12	1.99	0.44
9:i:279:GLY:HA3	5:p:103:GLY:HA3	1.98	0.44
9:i:455:LEU:HD23	11:n:79:ALA:HB1	1.99	0.44
2:I:445:THR:HG23	2:I:446:PHE:CD2	2.52	0.44
15:I:602:HEA:H241	14:I:608:9Y0:C20	2.48	0.44
2:L:222:LEU:HD23	11:n:48:LEU:HD13	1.99	0.44
13:b:101:CDL:HA4	9:j:426:TYR:HD1	1.82	0.44
7:d:158:LEU:HD22	7:d:301:LYS:HG2	1.99	0.44
21:U:603:MQ9:H172	21:U:603:MQ9:H153	1.51	0.44
9:i:156:GLU:HB2	9:i:217:ILE:HG21	2.00	0.44
13:i:603:CDL:H562	13:i:603:CDL:H711	1.98	0.44
2:L:296:LEU:HG	2:L:343:ASN:HD22	1.81	0.44
13:V:602:CDL:H532	13:V:602:CDL:OA7	2.18	0.44
2:I:523:CYS:HB2	2:I:524:PRO:HD3	2.00	0.44
7:d:247:ARG:NH1	7:d:259:ASP:O	2.49	0.44
4:o:124:PRO:O	4:o:135:LYS:NZ	2.49	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:602:HEA:H243	14:I:608:9Y0:C20	2.47	0.44
2:I:90:MET:HB3	15:I:602:HEA:CAC	2.47	0.44
13:V:602:CDL:H582	13:V:602:CDL:H552	1.35	0.44
13:i:608:CDL:H811	13:i:608:CDL:H782	1.88	0.44
9:j:233:TRP:CG	21:j:608:MQ9:H3B	2.53	0.44
7:d:142:TRP:CD1	7:d:284:TYR:HB2	2.53	0.44
7:e:158:LEU:HD22	7:e:301:LYS:HG2	2.00	0.44
8:f:10:PRO:HA	8:f:22:LEU:HD22	1.99	0.44
21:i:609:MQ9:H172	21:i:609:MQ9:H153	1.76	0.44
2:L:102:PHE:O	2:L:106:VAL:HG22	2.18	0.44
4:U:123:MET:HG3	20:U:601:HEC:CHB	2.48	0.44
2:I:57:LEU:HD21	18:I:609:PLM:HG2	2.00	0.43
2:I:288:LYS:HB3	2:I:288:LYS:HE2	1.72	0.43
13:I:605:CDL:H602	13:I:605:CDL:H571	1.64	0.43
9:i:314:LEU:HD23	9:i:335:VAL:HG21	2.00	0.43
2:I:59:ALA:HB2	2:I:86:HIS:CE1	2.53	0.43
3:J:77:ALA:O	10:k:130:GLU:N	2.52	0.43
21:j:608:MQ9:H5M3	21:j:608:MQ9:C9	2.48	0.43
13:V:602:CDL:H331	13:V:602:CDL:H362	1.69	0.43
11:n:40:THR:O	11:n:44:MET:HG2	2.18	0.43
13:p:603:CDL:H631	13:p:603:CDL:H601	1.43	0.43
5:V:283:MET:HE3	5:V:314:LYS:HG2	1.99	0.43
12:q:29:CYS:N	18:q:301:PLM:C1	2.81	0.43
13:G:101:CDL:H722	13:G:101:CDL:H751	1.54	0.43
2:I:335:VAL:HB	2:I:336:PRO:HD3	2.00	0.43
7:d:180:ALA:HB2	7:d:185:LEU:HD23	2.00	0.43
21:i:610:MQ9:H171	21:i:610:MQ9:H221	2.00	0.43
2:I:102:PHE:O	2:I:106:VAL:HG22	2.18	0.43
2:L:216:THR:HG23	2:L:269:ILE:HG23	2.00	0.43
8:f:159:VAL:HG22	13:p:603:CDL:H821	2.00	0.43
2:L:335:VAL:HB	2:L:336:PRO:HD3	2.00	0.43
4:o:294:ARG:HE	4:o:294:ARG:HB2	1.61	0.43
15:L:603:HEA:H171	15:L:603:HEA:H261	1.53	0.43
9:i:66:PHE:HA	9:i:93:THR:CG2	2.45	0.43
24:i:605:HEM:HBC2	24:i:605:HEM:HMC2	2.00	0.43
21:n:201:MQ9:H5M3	21:n:201:MQ9:C10	2.48	0.43
5:p:234:ASN:HB2	5:p:271:LEU:HB3	2.00	0.43
2:I:120:ARG:NH1	11:m:131:GLU:OE1	2.52	0.43
14:I:610:9Y0:O2	14:I:610:9Y0:N	2.52	0.43
3:h:20:THR:HB	3:h:21:PRO:HD3	2.01	0.43
8:f:18:ARG:HA	8:f:22:LEU:HD21	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:233:TRP:CD1	13:i:606:CDL:HB4	2.54	0.42
24:j:604:HEM:HMC2	24:j:604:HEM:HBC2	2.00	0.42
10:l:79:GLN:O	10:l:174:ARG:HD2	2.19	0.42
2:I:222:LEU:HD23	11:m:48:LEU:HD13	2.00	0.42
2:L:120:ARG:NH1	11:n:131:GLU:OE1	2.52	0.42
2:L:441:GLY:O	2:L:445:THR:HG22	2.19	0.42
13:U:604:CDL:H151	11:n:123:SER:HB3	2.00	0.42
5:V:103:GLY:HA3	9:j:279:GLY:HA3	2.01	0.42
2:I:264:HIS:O	2:I:267:VAL:HG22	2.19	0.42
2:L:151:TRP:CD1	15:L:603:HEA:HBD1	2.54	0.42
2:L:264:HIS:O	2:L:267:VAL:HG22	2.19	0.42
9:i:27:GLY:O	9:i:31:GLN:HG2	2.19	0.42
9:j:314:LEU:HD23	9:j:335:VAL:HG21	2.00	0.42
2:L:419:PRO:HG3	2:L:425:LEU:HD23	2.01	0.42
2:L:523:CYS:HB2	2:L:524:PRO:HD3	2.01	0.42
4:U:270:THR:HG23	9:i:394:MET:SD	2.59	0.42
1:b:30:ASN:O	1:b:33:VAL:HG22	2.20	0.42
21:m:201:MQ9:H303	21:m:201:MQ9:H322	1.72	0.42
2:L:59:ALA:HB2	2:L:86:HIS:CE1	2.55	0.42
2:I:151:TRP:CD1	15:I:602:HEA:HBD1	2.54	0.42
2:I:216:THR:HG23	2:I:269:ILE:HG23	2.00	0.42
13:i:603:CDL:H731	13:i:603:CDL:H582	2.00	0.42
2:I:419:PRO:HG3	2:I:425:LEU:HD23	2.01	0.42
13:b:101:CDL:H162	13:b:101:CDL:H132	1.66	0.42
8:f:14:ALA:HB1	8:f:182:ILE:HD13	2.00	0.42
8:g:167:ARG:HE	8:g:177:GLN:HE22	1.68	0.42
10:k:79:GLN:O	10:k:174:ARG:HD2	2.19	0.42
13:G:101:CDL:H401	13:G:101:CDL:H372	1.74	0.42
2:I:441:GLY:O	2:I:445:THR:HG22	2.19	0.42
13:G:101:CDL:H272	25:q:302:9XX:C31	2.50	0.42
21:o:604:MQ9:H271	21:o:604:MQ9:H253	1.84	0.42
2:L:91:LEU:HD23	2:L:91:LEU:HA	1.90	0.41
2:L:484:LEU:HD23	15:L:603:HEA:H11	2.01	0.41
9:j:317:ILE:HA	9:j:318:PRO:HD3	1.88	0.41
9:j:457:HIS:CD2	9:j:457:HIS:N	2.88	0.41
2:I:28:ILE:CD1	13:I:605:CDL:H652	2.50	0.41
2:L:381:MET:HE3	2:L:384:VAL:HG21	2.02	0.41
5:V:148:ILE:HG21	9:i:25:ALA:HB1	2.02	0.41
21:i:610:MQ9:H71	21:i:610:MQ9:H5M3	1.82	0.41
11:n:112:TRP:H	11:n:112:TRP:CD1	2.38	0.41
21:o:604:MQ9:H353	21:o:604:MQ9:H372	1.47	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:i:612:CDL:H152	13:i:612:CDL:H121	1.67	0.41
9:i:44:LEU:HD13	9:i:124:VAL:HG12	2.02	0.41
9:i:218:PRO:HB2	21:j:608:MQ9:C40	2.50	0.41
9:i:223:ALA:HA	21:i:610:MQ9:H221	2.02	0.41
2:I:452:LEU:HD13	2:I:457:MET:HE1	2.03	0.41
5:V:201:THR:OG1	5:V:204:GLY:O	2.33	0.41
7:e:141:GLN:HE21	7:e:141:GLN:HB2	1.66	0.41
21:j:608:MQ9:H203	21:j:608:MQ9:H221	1.37	0.41
5:p:314:LYS:HE2	5:p:314:LYS:HB3	1.95	0.41
8:f:2:THR:HG21	11:n:133:HIS:CE1	2.55	0.41
8:f:40:LEU:HG	11:n:44:MET:HE3	2.03	0.41
8:g:82:ALA:HB3	8:g:112:MET:HE1	2.02	0.41
2:I:155:THR:HG23	2:I:156:PRO:HG3	2.01	0.41
2:I:402:LEU:O	2:I:406:ILE:HG22	2.20	0.41
2:L:452:LEU:HD13	2:L:457:MET:HE1	2.03	0.41
9:i:233:TRP:HD1	13:i:606:CDL:HB4	1.85	0.41
10:k:111:GLU:HG2	10:k:131:ALA:HB3	2.03	0.41
21:i:610:MQ9:H28	21:i:610:MQ9:H322	1.83	0.41
9:j:22:TYR:O	9:j:24:LEU:HG	2.21	0.41
18:q:301:PLM:HF1	18:q:301:PLM:HC1	1.88	0.41
21:m:201:MQ9:H103	21:m:201:MQ9:H121	1.63	0.41
13:I:605:CDL:H362	13:b:101:CDL:H582	2.03	0.41
2:L:402:LEU:O	2:L:406:ILE:HG22	2.20	0.41
10:l:128:TYR:OH	10:l:138:GLU:OE1	2.37	0.41
13:G:101:CDL:H821	13:G:101:CDL:H851	1.94	0.40
2:I:484:LEU:HD23	15:I:602:HEA:H11	2.03	0.40
8:f:167:ARG:HE	8:f:177:GLN:HE22	1.68	0.40
8:g:74:ILE:HB	8:g:75:PRO:HD3	2.04	0.40
4:o:278:ILE:HG23	4:o:279:ILE:HG13	2.03	0.40
13:p:603:CDL:H811	13:p:603:CDL:H781	1.81	0.40
12:q:29:CYS:N	18:q:301:PLM:C2	2.84	0.40
4:U:234:SER:HB3	5:p:245:ASP:OD2	2.21	0.40
13:V:602:CDL:HB61	13:V:602:CDL:OB2	2.20	0.40
2:L:253:LEU:HD23	7:d:256:ASN:HB3	2.03	0.40
8:f:8:GLY:C	8:f:10:PRO:HD3	2.46	0.40
2:I:381:MET:HE3	2:I:384:VAL:HG21	2.02	0.40
2:L:252:VAL:HG13	7:d:235:ILE:HD11	2.04	0.40
8:g:16:THR:OG1	8:g:175:PRO:HB3	2.21	0.40
21:i:610:MQ9:H162	21:i:610:MQ9:H23	2.04	0.40
9:i:297:ILE:HD12	5:p:322:PRO:HD2	2.02	0.40
12:q:64:ASN:H	12:q:70:GLN:HE21	1.68	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	G	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
1	b	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
2	I	549/564 (97%)	530 (96%)	19 (4%)	0	100	100
2	L	549/564 (97%)	530 (96%)	19 (4%)	0	100	100
3	J	64/86 (74%)	62 (97%)	2 (3%)	0	100	100
3	h	64/86 (74%)	62 (97%)	2 (3%)	0	100	100
4	U	219/295 (74%)	208 (95%)	11 (5%)	0	100	100
4	o	219/295 (74%)	206 (94%)	13 (6%)	0	100	100
5	V	379/391 (97%)	372 (98%)	7 (2%)	0	100	100
5	p	379/391 (97%)	369 (97%)	10 (3%)	0	100	100
6	X	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
6	a	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
7	d	310/349 (89%)	290 (94%)	20 (6%)	0	100	100
7	e	310/349 (89%)	295 (95%)	14 (4%)	1 (0%)	36	40
8	f	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	24
8	g	204/206 (99%)	195 (96%)	7 (3%)	2 (1%)	12	10
9	i	525/546 (96%)	499 (95%)	25 (5%)	1 (0%)	43	50
9	j	525/546 (96%)	500 (95%)	24 (5%)	1 (0%)	43	50
10	k	143/175 (82%)	141 (99%)	2 (1%)	0	100	100
10	l	143/175 (82%)	141 (99%)	2 (1%)	0	100	100
11	m	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
11	n	137/139 (99%)	132 (96%)	5 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	q	152/227 (67%)	141 (93%)	11 (7%)	0	100	100
12	r	152/227 (67%)	140 (92%)	12 (8%)	0	100	100
All	All	5558/6630 (84%)	5320 (96%)	232 (4%)	6 (0%)	49	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	f	10	PRO
8	g	19	VAL
9	i	137	ARG
9	j	137	ARG
8	g	15	ILE
7	e	184	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	59/77 (77%)	59 (100%)	0	100	100
1	b	59/77 (77%)	59 (100%)	0	100	100
2	I	448/455 (98%)	442 (99%)	6 (1%)	61	72
2	L	448/455 (98%)	444 (99%)	4 (1%)	70	79
3	J	49/63 (78%)	49 (100%)	0	100	100
3	h	49/63 (78%)	48 (98%)	1 (2%)	48	59
4	U	164/223 (74%)	161 (98%)	3 (2%)	51	63
4	o	164/223 (74%)	161 (98%)	3 (2%)	51	63
5	V	312/321 (97%)	311 (100%)	1 (0%)	86	90
5	p	312/321 (97%)	311 (100%)	1 (0%)	86	90
6	X	20/173 (12%)	19 (95%)	1 (5%)	22	24
6	a	20/173 (12%)	19 (95%)	1 (5%)	22	24
7	d	269/298 (90%)	265 (98%)	4 (2%)	57	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	e	269/298 (90%)	263 (98%)	6 (2%)	45	56
8	f	163/163 (100%)	162 (99%)	1 (1%)	78	84
8	g	163/163 (100%)	161 (99%)	2 (1%)	63	74
9	i	421/437 (96%)	415 (99%)	6 (1%)	59	70
9	j	421/437 (96%)	412 (98%)	9 (2%)	47	58
10	k	108/130 (83%)	107 (99%)	1 (1%)	70	79
10	l	108/130 (83%)	107 (99%)	1 (1%)	70	79
11	m	103/103 (100%)	103 (100%)	0	100	100
11	n	103/103 (100%)	103 (100%)	0	100	100
12	q	121/171 (71%)	120 (99%)	1 (1%)	73	80
12	r	121/171 (71%)	119 (98%)	2 (2%)	53	65
All	All	4474/5228 (86%)	4420 (99%)	54 (1%)	61	74

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	63	ARG
2	I	99	VAL
2	I	129	PHE
2	I	215	VAL
2	I	403	PHE
2	I	560	VAL
2	L	99	VAL
2	L	129	PHE
2	L	215	VAL
2	L	403	PHE
4	U	123	MET
4	U	194	ASN
4	U	198	ARG
5	V	323	THR
6	X	34	THR
6	a	34	THR
7	d	143	ASN
7	d	184	GLU
7	d	195	GLU
7	d	233	ASP
7	e	141	GLN
7	e	143	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	e	169	LYS
7	e	176	GLU
7	e	195	GLU
7	e	233	ASP
8	f	18	ARG
8	g	16	THR
8	g	145	LEU
3	h	62	ILE
9	i	93	THR
9	i	187	ILE
9	i	286	ILE
9	i	396	ASP
9	i	452	ILE
9	i	529	LEU
9	j	24	LEU
9	j	63	THR
9	j	93	THR
9	j	286	ILE
9	j	328	THR
9	j	396	ASP
9	j	452	ILE
9	j	457	HIS
9	j	529	LEU
10	k	115	ILE
10	l	115	ILE
4	o	123	MET
4	o	189	CYS
4	o	198	ARG
5	p	323	THR
12	q	94	THR
12	r	94	THR
12	r	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	239	HIS
2	I	343	ASN
2	I	434	HIS
2	I	449	GLN
2	L	72	GLN
2	L	76	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	L	239	HIS
2	L	343	ASN
2	L	387	HIS
2	L	434	HIS
2	L	449	GLN
4	U	128	ASN
4	U	228	GLN
5	V	31	ASN
5	V	206	GLN
5	V	273	HIS
6	X	30	GLN
7	d	31	GLN
7	d	141	GLN
7	d	193	ASN
7	d	263	GLN
7	e	141	GLN
7	e	193	ASN
8	f	177	GLN
8	g	56	GLN
8	g	129	HIS
8	g	177	GLN
9	i	80	GLN
9	i	86	GLN
9	i	109	GLN
9	i	445	HIS
9	i	524	HIS
9	i	535	GLN
9	j	31	GLN
9	j	80	GLN
9	j	109	GLN
9	j	445	HIS
9	j	457	HIS
9	j	524	HIS
9	j	535	GLN
11	m	133	HIS
11	n	133	HIS
4	o	128	ASN
4	o	228	GLN
5	p	31	ASN
5	p	135	HIS
5	p	206	GLN
5	p	234	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	p	268	HIS
12	q	70	GLN
12	q	174	GLN
12	r	70	GLN
12	r	170	HIS
12	r	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 72 ligands modelled in this entry, 8 are monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
18	PLM	q	301	-	16,16,17	0.40	0	15,15,17	0.39	0
21	MQ9	i	610	-	59,59,59	0.35	0	72,75,75	0.34	0
24	HEM	j	603	9	49,49,50	1.43	5 (10%)	66,81,82	1.14	5 (7%)
21	MQ9	n	201	-	49,49,59	0.32	0	60,63,75	0.47	0
14	9Y0	I	608	-	37,37,48	0.37	0	40,42,53	0.35	0
13	CDL	V	602	-	94,94,99	0.30	0	100,106,111	0.33	0
13	CDL	i	606	-	73,73,99	0.35	0	79,85,111	0.23	0
22	FES	V	601	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	9XX	r	301	-	41,41,41	0.38	0	44,44,44	0.35	0
14	9Y0	G	102	-	40,40,48	0.52	0	43,45,53	0.46	0
19	9YF	V	603	-	58,58,58	1.27	4 (6%)	69,71,71	1.14	3 (4%)
17	OXY	I	607	-	1,1,1	0.15	0	-		
23	A1MBF	j	602	-	42,42,42	2.68	14 (33%)	58,61,61	1.30	5 (8%)
13	CDL	G	101	-	87,87,99	0.33	0	93,99,111	0.21	0
15	HEA	I	602	2	66,67,67	1.18	6 (9%)	78,103,103	1.40	12 (15%)
14	9Y0	I	610	-	42,42,48	0.52	0	44,47,53	0.48	0
18	PLM	I	609	-	16,16,17	0.51	0	15,15,17	0.44	0
21	MQ9	i	609	-	44,44,59	0.34	0	54,57,75	0.65	2 (3%)
15	HEA	L	603	2	66,67,67	1.18	7 (10%)	78,103,103	1.40	11 (14%)
13	CDL	b	101	-	87,87,99	0.33	0	93,99,111	0.23	0
14	9Y0	b	102	-	40,40,48	0.51	0	43,45,53	0.59	1 (2%)
21	MQ9	j	608	-	59,59,59	0.41	0	72,75,75	0.32	0
25	9XX	q	302	-	41,41,41	0.31	0	44,44,44	0.39	0
15	HEA	L	602	2	66,67,67	1.19	7 (10%)	78,103,103	1.47	15 (19%)
13	CDL	j	611	-	78,78,99	0.35	0	84,90,111	0.22	0
14	9Y0	L	601	-	37,37,48	0.40	0	40,42,53	0.47	0
13	CDL	I	604	-	75,75,99	0.36	0	81,87,111	0.23	0
19	9YF	j	601	-	58,58,58	1.25	4 (6%)	69,71,71	1.19	5 (7%)
19	9YF	o	603	-	58,58,58	0.27	0	69,71,71	0.32	0
19	9YF	p	604	-	58,58,58	1.28	4 (6%)	69,71,71	1.12	3 (4%)
19	9YF	L	609	-	58,58,58	1.28	4 (6%)	69,71,71	1.19	5 (7%)
23	A1MBF	i	602	-	42,42,42	2.68	13 (30%)	58,61,61	1.32	5 (8%)
13	CDL	U	604	-	78,78,99	0.35	0	84,90,111	0.21	0
13	CDL	i	603	-	65,65,99	0.36	0	71,77,111	0.23	0
25	9XX	j	610	-	31,31,41	0.38	0	34,34,44	0.65	1 (2%)
21	MQ9	U	603	-	59,59,59	0.31	0	72,75,75	0.48	1 (1%)
17	OXY	L	608	-	1,1,1	0.15	0	-		
20	HEC	U	602	4	46,50,50	3.59	3 (6%)	60,82,82	2.04	7 (11%)
21	MQ9	o	604	-	59,59,59	0.31	0	72,75,75	0.50	1 (1%)
13	CDL	p	603	-	94,94,99	0.31	0	100,106,111	0.20	0
13	CDL	L	607	-	80,80,99	0.35	0	86,92,111	0.21	0
25	9XX	i	611	-	31,31,41	0.40	0	34,34,44	0.38	0
22	FES	p	602	5	0,4,4	-	-	-		
13	CDL	i	608	-	78,78,99	0.36	0	84,90,111	0.23	0
13	CDL	i	612	-	73,73,99	0.34	0	79,85,111	0.24	0
24	HEM	j	604	9	50,50,50	1.44	7 (14%)	66,82,82	1.16	6 (9%)
13	CDL	L	606	-	75,75,99	0.36	0	81,87,111	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CDL	I	605	-	80,80,99	0.34	0	86,92,111	0.36	0
21	MQ9	j	607	-	44,44,59	0.32	0	54,57,75	0.49	0
15	HEA	I	601	2	66,67,67	1.19	7 (10%)	78,103,103	1.47	15 (19%)
14	9Y0	f	601	-	42,42,48	0.52	0	44,47,53	0.47	0
20	HEC	U	601	4	46,50,50	3.58	4 (8%)	60,82,82	2.05	7 (11%)
19	9YF	i	601	-	58,58,58	0.34	0	69,71,71	0.52	0
13	CDL	j	605	-	76,76,99	0.36	0	82,88,111	0.21	0
20	HEC	o	601	4	46,50,50	3.58	4 (8%)	60,82,82	2.15	7 (11%)
13	CDL	j	606	-	78,78,99	0.36	0	84,90,111	0.23	0
20	HEC	o	602	4	46,50,50	3.58	3 (6%)	60,82,82	1.96	7 (11%)
24	HEM	i	604	9	49,49,50	1.45	5 (10%)	66,81,82	1.13	5 (7%)
24	HEM	i	605	9	50,50,50	1.44	8 (16%)	66,82,82	1.16	5 (7%)
19	9YF	p	601	-	58,58,58	1.27	4 (6%)	69,71,71	1.13	3 (4%)
21	MQ9	m	201	-	49,49,59	0.38	0	60,63,75	1.15	3 (5%)
13	CDL	i	607	-	76,76,99	0.36	0	82,88,111	0.21	0
18	PLM	j	609	-	10,10,17	0.65	0	9,9,17	0.53	0
13	CDL	i	613	-	65,65,99	0.36	0	71,77,111	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PLM	q	301	-	-	9/13/14/15	-
21	MQ9	i	610	-	-	31/53/73/73	0/2/2/2
24	HEM	j	603	9	-	2/12/52/54	-
21	MQ9	n	201	-	-	21/41/61/73	0/2/2/2
14	9Y0	I	608	-	-	18/41/41/52	-
13	CDL	V	602	-	-	52/105/105/110	-
13	CDL	i	606	-	-	44/84/84/110	-
22	FES	V	601	5	-	-	0/1/1/1
25	9XX	r	301	-	-	19/43/43/43	-
14	9Y0	G	102	-	-	18/44/44/52	-
19	9YF	V	603	-	-	22/54/78/78	0/1/1/1
23	A1MBF	j	602	-	-	2/22/32/32	0/5/5/5
13	CDL	G	101	-	-	64/98/98/110	-
15	HEA	I	602	2	-	17/36/76/76	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9Y0	I	610	-	-	18/46/46/52	-
18	PLM	I	609	-	-	4/13/14/15	-
21	MQ9	i	609	-	-	11/35/55/73	0/2/2/2
15	HEA	L	603	2	-	18/36/76/76	-
13	CDL	b	101	-	-	68/98/98/110	-
14	9Y0	b	102	-	-	13/44/44/52	-
21	MQ9	j	608	-	-	27/53/73/73	0/2/2/2
25	9XX	q	302	-	-	32/43/43/43	-
15	HEA	L	602	2	-	14/36/76/76	-
13	CDL	j	611	-	-	46/89/89/110	-
14	9Y0	L	601	-	-	23/41/41/52	-
13	CDL	I	604	-	-	46/86/86/110	-
19	9YF	j	601	-	-	26/54/78/78	0/1/1/1
19	9YF	o	603	-	-	24/54/78/78	0/1/1/1
19	9YF	p	604	-	-	34/54/78/78	0/1/1/1
19	9YF	L	609	-	-	25/54/78/78	0/1/1/1
23	A1MBF	i	602	-	-	3/22/32/32	0/5/5/5
13	CDL	U	604	-	-	43/89/89/110	-
13	CDL	i	603	-	-	42/76/76/110	-
25	9XX	j	610	-	-	12/33/33/43	-
21	MQ9	U	603	-	-	20/53/73/73	0/2/2/2
20	HEC	U	602	4	-	4/14/54/54	-
21	MQ9	o	604	-	-	19/53/73/73	0/2/2/2
13	CDL	p	603	-	-	62/105/105/110	-
13	CDL	L	607	-	-	58/91/91/110	-
25	9XX	i	611	-	-	5/33/33/43	-
22	FES	p	602	5	-	-	0/1/1/1
13	CDL	i	608	-	-	57/89/89/110	-
13	CDL	i	612	-	-	46/84/84/110	-
24	HEM	j	604	9	-	3/14/54/54	-
13	CDL	L	606	-	-	45/86/86/110	-
13	CDL	I	605	-	-	44/91/91/110	-
21	MQ9	j	607	-	-	9/35/55/73	0/2/2/2
15	HEA	I	601	2	-	14/36/76/76	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9Y0	f	601	-	-	21/46/46/52	-
20	HEC	U	601	4	-	6/14/54/54	-
19	9YF	i	601	-	-	22/54/78/78	0/1/1/1
13	CDL	j	605	-	-	36/87/87/110	-
20	HEC	o	601	4	-	4/14/54/54	-
13	CDL	j	606	-	-	55/89/89/110	-
20	HEC	o	602	4	-	4/14/54/54	-
24	HEM	i	604	9	-	3/12/52/54	-
24	HEM	i	605	9	-	3/14/54/54	-
19	9YF	p	601	-	-	26/54/78/78	0/1/1/1
21	MQ9	m	201	-	-	12/41/61/73	0/2/2/2
13	CDL	i	607	-	-	38/87/87/110	-
18	PLM	j	609	-	-	0/7/8/15	-
13	CDL	i	613	-	-	35/76/76/110	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	602	HEC	CAC-C3C	16.25	1.55	1.34
20	o	602	HEC	CAC-C3C	16.18	1.55	1.34
20	U	601	HEC	CAC-C3C	16.13	1.55	1.34
20	o	601	HEC	CAB-C3B	16.05	1.55	1.34
20	U	601	HEC	CAB-C3B	15.93	1.55	1.34
20	o	601	HEC	CAC-C3C	15.92	1.55	1.34
20	U	602	HEC	CAB-C3B	15.90	1.55	1.34
20	o	602	HEC	CAB-C3B	15.88	1.55	1.34
23	i	602	A1MBF	C12-N14	8.35	1.47	1.33
23	j	602	A1MBF	C12-N14	8.33	1.47	1.33
23	i	602	A1MBF	C04-N10	-6.22	1.31	1.39
23	j	602	A1MBF	C04-N10	-6.18	1.31	1.39
20	o	601	HEC	C3D-C2D	5.74	1.54	1.38
20	U	601	HEC	C3D-C2D	5.58	1.53	1.38
20	o	602	HEC	C3D-C2D	5.52	1.53	1.38
20	U	602	HEC	C3D-C2D	5.52	1.53	1.38
23	j	602	A1MBF	C09-C07	5.51	1.40	1.35
23	i	602	A1MBF	C27-N22	5.46	1.55	1.46
23	i	602	A1MBF	C09-C07	5.42	1.39	1.35
23	j	602	A1MBF	C27-N22	5.40	1.55	1.46
23	i	602	A1MBF	C28-C25	5.27	1.62	1.52

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	j	602	A1MBF	C28-C25	5.23	1.62	1.52
23	j	602	A1MBF	C23-N22	4.77	1.54	1.46
23	i	602	A1MBF	C23-N22	4.65	1.54	1.46
23	j	602	A1MBF	C11-C12	4.08	1.56	1.46
23	i	602	A1MBF	C11-C12	4.06	1.55	1.46
15	L	603	HEA	CMA-C3A	-3.93	1.36	1.45
15	I	601	HEA	CMA-C3A	-3.92	1.36	1.45
15	L	602	HEA	CMA-C3A	-3.92	1.36	1.45
19	p	601	9YF	O9-C	-3.90	1.36	1.46
15	I	602	HEA	CMA-C3A	-3.90	1.36	1.45
19	L	609	9YF	O11-C25	3.89	1.44	1.33
19	V	603	9YF	O9-C	-3.89	1.36	1.46
19	j	601	9YF	O9-C	-3.89	1.36	1.46
19	p	604	9YF	O11-C25	3.88	1.44	1.33
19	p	601	9YF	O11-C25	3.84	1.44	1.33
19	V	603	9YF	O11-C25	3.83	1.44	1.33
19	j	601	9YF	O11-C25	3.80	1.44	1.33
19	p	604	9YF	O9-C	-3.79	1.37	1.46
19	L	609	9YF	O9-C	-3.73	1.37	1.46
19	L	609	9YF	P-O2	3.69	1.70	1.60
24	i	605	HEM	FE-ND	3.64	2.06	1.94
24	j	604	HEM	FE-ND	3.64	2.06	1.94
24	i	604	HEM	FE-NC	3.60	2.07	1.95
24	i	604	HEM	FE-NA	3.60	2.07	1.95
19	p	601	9YF	P-O2	3.58	1.69	1.60
19	p	604	9YF	P-O2	3.58	1.69	1.60
19	V	603	9YF	P-O2	3.57	1.69	1.60
24	j	603	HEM	FE-NB	3.51	2.05	1.94
19	j	601	9YF	P-O2	3.42	1.69	1.60
24	j	603	HEM	FE-NA	3.41	2.06	1.95
24	j	603	HEM	FE-ND	3.41	2.05	1.94
24	i	605	HEM	FE-NB	3.41	2.05	1.94
24	i	604	HEM	FE-NB	3.39	2.05	1.94
24	j	604	HEM	FE-NB	3.38	2.05	1.94
24	i	604	HEM	FE-ND	3.30	2.05	1.94
23	j	602	A1MBF	C19-N22	3.26	1.47	1.38
23	i	602	A1MBF	C19-N22	3.26	1.47	1.38
24	j	603	HEM	FE-NC	3.25	2.06	1.95
24	i	605	HEM	FE-NA	3.19	2.05	1.95
24	j	604	HEM	FE-NA	3.18	2.05	1.95
24	j	604	HEM	FE-NC	3.00	2.05	1.95
24	i	605	HEM	FE-NC	2.99	2.05	1.95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	j	603	HEM	CAB-C3B	2.98	1.55	1.47
24	i	604	HEM	CAB-C3B	2.97	1.55	1.47
24	j	604	HEM	CAB-C3B	2.96	1.55	1.47
24	i	605	HEM	CAB-C3B	2.95	1.55	1.47
19	L	609	9YF	P-O	2.93	1.71	1.59
24	j	604	HEM	CAC-C3C	2.91	1.55	1.47
19	p	604	9YF	P-O	2.91	1.71	1.59
24	i	605	HEM	CAC-C3C	2.89	1.55	1.47
23	i	602	A1MBF	C07-CL08	2.84	1.79	1.73
19	j	601	9YF	P-O	2.82	1.70	1.59
19	V	603	9YF	P-O	2.81	1.70	1.59
19	p	601	9YF	P-O	2.81	1.70	1.59
23	j	602	A1MBF	C07-CL08	2.79	1.79	1.73
23	j	602	A1MBF	C26-C25	-2.77	1.45	1.53
23	i	602	A1MBF	C26-C25	-2.67	1.45	1.53
15	L	603	HEA	C4C-NC	-2.55	1.34	1.39
15	I	602	HEA	C4C-NC	-2.53	1.34	1.39
23	i	602	A1MBF	O13-C12	-2.49	1.18	1.23
15	I	601	HEA	C4C-NC	-2.48	1.34	1.39
23	j	602	A1MBF	O13-C12	-2.47	1.18	1.23
15	L	602	HEA	C4C-NC	-2.47	1.35	1.39
15	I	601	HEA	FE-NC	2.40	2.03	1.95
15	L	602	HEA	FE-NC	2.40	2.03	1.95
15	I	602	HEA	FE-NC	2.37	2.03	1.95
15	L	603	HEA	FE-NC	2.35	2.03	1.95
15	I	602	HEA	C4B-C3B	2.28	1.48	1.44
15	L	602	HEA	C4B-C3B	2.27	1.48	1.44
23	i	602	A1MBF	C06-C05	2.23	1.40	1.35
15	L	603	HEA	C4B-C3B	2.22	1.48	1.44
15	I	601	HEA	C4B-C3B	2.22	1.48	1.44
15	I	601	HEA	CMD-C2D	2.21	1.55	1.50
15	L	602	HEA	CMD-C2D	2.21	1.55	1.50
23	j	602	A1MBF	C06-C05	2.21	1.40	1.35
15	I	601	HEA	CHC-C1C	-2.17	1.34	1.39
15	L	603	HEA	CMD-C2D	2.17	1.55	1.50
15	I	602	HEA	CMD-C2D	2.15	1.55	1.50
15	I	602	HEA	CHC-C1C	-2.15	1.34	1.39
15	L	603	HEA	CHC-C1C	-2.15	1.34	1.39
15	I	601	HEA	C1D-C2D	2.14	1.48	1.44
15	L	602	HEA	C1D-C2D	2.14	1.48	1.44
15	L	602	HEA	CHC-C1C	-2.13	1.34	1.39
20	o	601	HEC	C3C-C2C	-2.09	1.34	1.41

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	j	602	A1MBF	C02-N03	-2.09	1.33	1.38
23	i	602	A1MBF	C02-N03	-2.05	1.33	1.38
23	j	602	A1MBF	C04-N03	2.04	1.37	1.33
24	i	605	HEM	CMB-C2B	2.03	1.55	1.50
24	i	605	HEM	CMC-C2C	2.03	1.55	1.50
24	j	604	HEM	CMB-C2B	2.03	1.55	1.50
20	U	601	HEC	C3B-C2B	-2.02	1.34	1.41
15	L	603	HEA	C1D-ND	-2.01	1.36	1.40

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	602	HEC	CBB-CAB-C3B	-9.00	111.31	127.86
20	U	601	HEC	CBB-CAB-C3B	-8.93	111.44	127.86
20	o	601	HEC	CBB-CAB-C3B	-8.54	112.16	127.86
20	o	601	HEC	C4D-ND-C1D	7.72	112.91	105.35
20	o	602	HEC	CBB-CAB-C3B	-7.61	113.88	127.86
20	o	601	HEC	CBC-CAC-C3C	-7.14	114.74	127.86
21	m	201	MQ9	C7-C6-C1	-6.94	111.07	118.50
20	U	601	HEC	CBC-CAC-C3C	-6.66	115.62	127.86
20	o	602	HEC	CBC-CAC-C3C	-6.63	115.68	127.86
20	o	602	HEC	C4D-ND-C1D	6.43	111.65	105.35
20	U	601	HEC	C4D-ND-C1D	6.34	111.55	105.35
20	U	602	HEC	CBC-CAC-C3C	-6.33	116.22	127.86
20	U	602	HEC	C4D-ND-C1D	6.32	111.54	105.35
19	V	603	9YF	C14-C13-C12	-5.88	84.59	114.42
19	p	604	9YF	C14-C13-C12	-5.86	84.66	114.42
19	p	601	9YF	C14-C13-C12	-5.86	84.66	114.42
19	L	609	9YF	C14-C13-C12	-5.83	84.83	114.42
19	j	601	9YF	C14-C13-C12	-5.77	85.14	114.42
23	i	602	A1MBF	C11-C02-N03	-4.53	107.49	111.01
23	j	602	A1MBF	C11-C02-N03	-4.41	107.58	111.01
15	I	602	HEA	C3C-C4C-NC	4.17	112.81	110.25
15	L	603	HEA	C3C-C4C-NC	4.16	112.81	110.25
19	L	609	9YF	O9-C8-C9	4.11	120.36	111.50
15	I	601	HEA	C3C-C4C-NC	4.06	112.75	110.25
15	L	602	HEA	C3C-C4C-NC	4.06	112.74	110.25
19	V	603	9YF	O9-C8-C9	4.02	120.16	111.50
19	p	604	9YF	O9-C8-C9	3.98	120.08	111.50
19	p	601	9YF	O9-C8-C9	3.98	120.08	111.50
19	j	601	9YF	O9-C8-C9	3.88	119.85	111.50
20	o	601	HEC	C4A-NA-C1A	3.60	108.87	105.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	o	601	HEC	C2A-C1A-NA	-3.28	107.13	110.32
23	i	602	A1MBF	C01-C02-N03	3.18	125.83	119.38
23	j	602	A1MBF	C01-C02-N03	3.14	125.75	119.38
15	I	602	HEA	CHB-C4A-NA	-3.01	121.18	124.44
15	L	603	HEA	CHB-C4A-NA	-2.99	121.20	124.44
24	i	605	HEM	C4A-NA-C1A	2.99	108.28	105.35
24	j	604	HEM	C4A-NA-C1A	2.98	108.27	105.35
24	i	604	HEM	C4D-ND-C1D	2.97	108.14	105.07
20	o	602	HEC	C4A-NA-C1A	2.97	108.25	105.35
15	L	602	HEA	CHB-C4A-NA	-2.94	121.26	124.44
24	j	603	HEM	C4D-ND-C1D	2.92	108.09	105.07
15	I	601	HEA	CHB-C4A-NA	-2.91	121.29	124.44
25	j	610	9XX	C17-O1-C18	2.87	121.57	117.88
20	U	601	HEC	C4A-NA-C1A	2.87	108.16	105.35
20	o	602	HEC	C2A-C1A-NA	-2.79	107.61	110.32
20	U	602	HEC	C4A-NA-C1A	2.78	108.08	105.35
21	m	201	MQ9	C5M-C5-C4	-2.78	111.66	116.27
24	i	605	HEM	C4D-ND-C1D	2.77	107.94	105.07
21	m	201	MQ9	C8-C7-C6	2.77	119.50	112.05
20	U	601	HEC	C4B-NB-C1B	2.75	108.04	105.35
24	j	604	HEM	C4D-ND-C1D	2.75	107.91	105.07
24	j	603	HEM	C4C-NC-C1C	2.74	108.03	105.35
21	i	609	MQ9	C7-C6-C1	-2.73	115.58	118.50
20	U	601	HEC	C2A-C1A-NA	-2.73	107.67	110.32
20	U	602	HEC	C4B-NB-C1B	2.73	108.02	105.35
20	U	602	HEC	C2A-C1A-NA	-2.72	107.68	110.32
20	o	601	HEC	C4B-NB-C1B	2.71	108.00	105.35
19	V	603	9YF	O11-C25-C26	2.70	120.39	111.91
19	L	609	9YF	O11-C25-C26	2.69	120.34	111.91
20	o	602	HEC	C4B-NB-C1B	2.66	107.95	105.35
19	p	604	9YF	O11-C25-C26	2.66	120.25	111.91
24	j	603	HEM	C4A-NA-C1A	2.65	107.94	105.35
19	p	601	9YF	O11-C25-C26	2.65	120.21	111.91
24	i	605	HEM	C1B-NB-C4B	2.64	107.80	105.07
24	i	604	HEM	C4C-NC-C1C	2.63	107.93	105.35
24	j	604	HEM	C1B-NB-C4B	2.62	107.78	105.07
24	i	604	HEM	C1B-NB-C4B	2.55	107.71	105.07
15	L	603	HEA	C20-C19-C18	-2.53	116.00	121.12
15	I	601	HEA	C1D-C2D-C3D	-2.53	104.30	106.96
15	I	602	HEA	C1D-C2D-C3D	-2.53	104.30	106.96
19	j	601	9YF	C7-C2-C3	2.52	114.49	110.85
24	i	604	HEM	C4A-NA-C1A	2.51	107.81	105.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	601	9YF	O11-C25-C26	2.51	119.77	111.91
15	L	603	HEA	C1D-C2D-C3D	-2.50	104.33	106.96
15	L	602	HEA	C1D-C2D-C3D	-2.49	104.34	106.96
15	L	602	HEA	C3D-C4D-ND	2.49	112.77	110.36
23	i	602	A1MBF	C02-C11-N10	2.48	106.33	104.69
23	j	602	A1MBF	C02-C11-N10	2.47	106.32	104.69
24	j	603	HEM	C1B-NB-C4B	2.47	107.62	105.07
20	U	601	HEC	C4C-NC-C1C	2.46	107.76	105.35
15	L	603	HEA	CMD-C2D-C1D	2.45	128.77	125.04
15	I	602	HEA	C20-C19-C18	-2.45	116.16	121.12
15	I	601	HEA	C3D-C4D-ND	2.44	112.72	110.36
15	L	602	HEA	CBA-CAA-C2A	2.44	119.39	112.63
15	I	601	HEA	CBA-CAA-C2A	2.44	119.39	112.63
19	j	601	9YF	C7-C6-C5	2.43	115.07	110.82
20	o	602	HEC	C4C-NC-C1C	2.43	107.72	105.35
15	I	602	HEA	CMD-C2D-C1D	2.42	128.73	125.04
23	j	602	A1MBF	C05-C04-N10	2.41	120.89	118.41
20	U	602	HEC	C4C-NC-C1C	2.39	107.69	105.35
23	i	602	A1MBF	C05-C04-N10	2.37	120.85	118.41
24	j	604	HEM	C4C-NC-C1C	2.37	107.67	105.35
15	I	601	HEA	CMD-C2D-C1D	2.35	128.62	125.04
15	L	602	HEA	CMD-C2D-C1D	2.35	128.62	125.04
15	I	602	HEA	CMB-C2B-C3B	-2.34	125.89	130.34
24	i	605	HEM	C4C-NC-C1C	2.33	107.63	105.35
15	I	601	HEA	C26-C15-C14	-2.29	117.80	123.68
15	L	602	HEA	C26-C15-C14	-2.29	117.80	123.68
21	o	604	MQ9	C7-C6-C1	-2.29	116.05	118.50
15	L	603	HEA	CMB-C2B-C3B	-2.29	125.98	130.34
15	I	601	HEA	C20-C19-C18	-2.28	116.50	121.12
15	L	602	HEA	C20-C19-C18	-2.28	116.50	121.12
21	U	603	MQ9	C7-C6-C1	-2.28	116.06	118.50
15	I	602	HEA	CBA-CAA-C2A	2.27	118.92	112.63
19	L	609	9YF	C7-C6-C5	2.26	114.76	110.82
24	j	604	HEM	C2A-C1A-NA	-2.25	107.63	110.15
15	L	603	HEA	CBA-CAA-C2A	2.23	118.84	112.63
15	L	602	HEA	C2B-C1B-NB	2.23	112.56	109.88
15	L	603	HEA	C3D-C4D-ND	2.23	112.52	110.36
15	L	602	HEA	C13-C14-C15	-2.23	122.30	127.66
15	I	601	HEA	CMB-C2B-C3B	-2.22	126.11	130.34
15	I	601	HEA	C13-C14-C15	-2.22	122.31	127.66
20	o	601	HEC	CHD-C4C-NC	2.22	126.84	124.44
24	i	605	HEM	C2A-C1A-NA	-2.22	107.66	110.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	601	HEA	C2B-C1B-NB	2.22	112.54	109.88
15	I	602	HEA	C3D-C4D-ND	2.19	112.48	110.36
15	L	602	HEA	CMB-C2B-C3B	-2.19	126.17	130.34
14	b	102	9Y0	C1-O7-C21	2.18	123.15	117.79
24	i	604	HEM	C3D-C4D-ND	-2.18	107.74	110.17
15	L	602	HEA	CBD-CAD-C3D	2.15	118.60	112.63
15	I	601	HEA	O1D-CGD-CBD	-2.14	116.20	123.08
15	L	602	HEA	O1D-CGD-CBD	-2.14	116.20	123.08
15	I	601	HEA	CBD-CAD-C3D	2.14	118.57	112.63
24	j	603	HEM	C3D-C4D-ND	-2.14	107.79	110.17
23	i	602	A1MBF	O13-C12-N14	-2.11	119.44	123.30
15	I	601	HEA	C2A-C1A-NA	2.11	112.37	110.32
15	L	602	HEA	C2A-C1A-NA	2.10	112.36	110.32
23	j	602	A1MBF	O13-C12-N14	-2.08	119.49	123.30
19	L	609	9YF	C6-C7-C2	2.07	114.42	109.68
15	I	601	HEA	CHA-C4D-C3D	-2.04	121.83	124.84
21	i	609	MQ9	C7-C8-C9	2.03	130.16	126.79
15	I	602	HEA	O11-C11-C12	-2.02	103.77	109.42
15	L	602	HEA	CHA-C4D-C3D	-2.02	121.87	124.84
15	L	603	HEA	C26-C15-C14	-2.02	118.50	123.68
15	I	602	HEA	C2B-C1B-NB	2.02	112.30	109.88
15	I	602	HEA	C26-C15-C14	-2.01	118.51	123.68
15	I	602	HEA	O1D-CGD-CBD	-2.01	116.62	123.08
15	L	603	HEA	O1D-CGD-CBD	-2.01	116.63	123.08
15	L	603	HEA	O11-C11-C12	-2.01	103.81	109.42
24	j	604	HEM	C3D-C4D-ND	-2.01	107.93	110.17

There are no chirality outliers.

All (1499) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	101	CDL	CA2-OA2-PA1-OA3
13	G	101	CDL	C11-CA5-OA6-CA4
13	G	101	CDL	CB2-OB2-PB2-OB3
13	I	604	CDL	CB2-OB2-PB2-OB3
13	I	604	CDL	CB2-OB2-PB2-OB4
13	I	604	CDL	CB3-OB5-PB2-OB3
13	I	604	CDL	CB3-OB5-PB2-OB4
13	I	605	CDL	CA2-OA2-PA1-OA3
13	I	605	CDL	CA2-OA2-PA1-OA4
13	I	605	CDL	CB2-OB2-PB2-OB4
13	L	606	CDL	CB2-OB2-PB2-OB3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	L	606	CDL	CB2-OB2-PB2-OB4
13	L	606	CDL	CB3-OB5-PB2-OB2
13	L	606	CDL	CB3-OB5-PB2-OB3
13	L	606	CDL	CB3-OB5-PB2-OB4
13	L	607	CDL	CA2-OA2-PA1-OA4
13	L	607	CDL	OA6-CA4-CA6-OA8
13	L	607	CDL	CB2-OB2-PB2-OB3
13	L	607	CDL	CB2-OB2-PB2-OB4
13	L	607	CDL	CB3-OB5-PB2-OB3
13	U	604	CDL	C11-CA5-OA6-CA4
13	U	604	CDL	CB2-OB2-PB2-OB3
13	U	604	CDL	CB2-OB2-PB2-OB4
13	U	604	CDL	CB2-OB2-PB2-OB5
13	U	604	CDL	CB3-OB5-PB2-OB3
13	V	602	CDL	O1-C1-CB2-OB2
13	V	602	CDL	CA2-OA2-PA1-OA3
13	V	602	CDL	CA2-OA2-PA1-OA4
13	V	602	CDL	CA2-OA2-PA1-OA5
13	V	602	CDL	CB2-OB2-PB2-OB3
13	V	602	CDL	CB3-OB5-PB2-OB2
13	V	602	CDL	CB3-OB5-PB2-OB4
13	V	602	CDL	C51-CB5-OB6-CB4
13	b	101	CDL	CA2-OA2-PA1-OA3
13	b	101	CDL	C11-CA5-OA6-CA4
13	b	101	CDL	CB2-OB2-PB2-OB3
13	b	101	CDL	CB2-OB2-PB2-OB4
13	b	101	CDL	CB2-OB2-PB2-OB5
13	b	101	CDL	C51-CB5-OB6-CB4
13	i	603	CDL	CA2-C1-CB2-OB2
13	i	603	CDL	CA2-OA2-PA1-OA3
13	i	603	CDL	CA2-OA2-PA1-OA4
13	i	603	CDL	CA3-OA5-PA1-OA4
13	i	603	CDL	C11-CA5-OA6-CA4
13	i	603	CDL	CB2-OB2-PB2-OB3
13	i	603	CDL	CB2-OB2-PB2-OB4
13	i	603	CDL	CB2-OB2-PB2-OB5
13	i	603	CDL	OB6-CB4-CB6-OB8
13	i	603	CDL	C51-CB5-OB6-CB4
13	i	606	CDL	CA2-OA2-PA1-OA3
13	i	606	CDL	CA2-OA2-PA1-OA4
13	i	606	CDL	OA6-CA4-CA6-OA8
13	i	606	CDL	CB2-OB2-PB2-OB3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	606	CDL	CB2-OB2-PB2-OB4
13	i	606	CDL	CB2-OB2-PB2-OB5
13	i	606	CDL	C51-CB5-OB6-CB4
13	i	607	CDL	O1-C1-CB2-OB2
13	i	607	CDL	CA2-OA2-PA1-OA3
13	i	607	CDL	CA3-OA5-PA1-OA3
13	i	607	CDL	CB3-OB5-PB2-OB2
13	i	608	CDL	CA2-OA2-PA1-OA3
13	i	608	CDL	CA3-OA5-PA1-OA2
13	i	608	CDL	CA3-OA5-PA1-OA3
13	i	608	CDL	CA3-OA5-PA1-OA4
13	i	608	CDL	CB2-OB2-PB2-OB3
13	i	608	CDL	CB2-OB2-PB2-OB4
13	i	608	CDL	CB2-OB2-PB2-OB5
13	i	608	CDL	CB3-OB5-PB2-OB3
13	i	608	CDL	CB3-OB5-PB2-OB4
13	i	608	CDL	OB5-CB3-CB4-OB6
13	i	608	CDL	C51-CB5-OB6-CB4
13	i	612	CDL	CB2-C1-CA2-OA2
13	i	612	CDL	CA2-OA2-PA1-OA3
13	i	612	CDL	CB2-OB2-PB2-OB3
13	i	612	CDL	CB2-OB2-PB2-OB4
13	i	613	CDL	CB2-OB2-PB2-OB3
13	i	613	CDL	CB2-OB2-PB2-OB4
13	j	605	CDL	O1-C1-CB2-OB2
13	j	605	CDL	CA2-OA2-PA1-OA3
13	j	605	CDL	CA3-OA5-PA1-OA3
13	j	605	CDL	CB3-OB5-PB2-OB2
13	j	606	CDL	CA2-OA2-PA1-OA3
13	j	606	CDL	CA2-OA2-PA1-OA4
13	j	606	CDL	CA2-OA2-PA1-OA5
13	j	606	CDL	CA3-OA5-PA1-OA3
13	j	606	CDL	C11-CA5-OA6-CA4
13	j	606	CDL	CB2-OB2-PB2-OB3
13	j	606	CDL	CB3-OB5-PB2-OB2
13	j	606	CDL	CB3-OB5-PB2-OB3
13	j	606	CDL	CB3-OB5-PB2-OB4
13	j	611	CDL	O1-C1-CA2-OA2
13	j	611	CDL	CA2-C1-CB2-OB2
13	j	611	CDL	CA2-OA2-PA1-OA3
13	j	611	CDL	C11-CA5-OA6-CA4
13	j	611	CDL	CB2-OB2-PB2-OB3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	j	611	CDL	CB2-OB2-PB2-OB4
13	j	611	CDL	CB3-OB5-PB2-OB3
13	j	611	CDL	CB3-OB5-PB2-OB4
13	p	603	CDL	O1-C1-CB2-OB2
13	p	603	CDL	CA2-OA2-PA1-OA3
13	p	603	CDL	CA2-OA2-PA1-OA4
13	p	603	CDL	CA2-OA2-PA1-OA5
13	p	603	CDL	OA5-CA3-CA4-OA6
13	p	603	CDL	OA7-CA5-OA6-CA4
13	p	603	CDL	C11-CA5-OA6-CA4
13	p	603	CDL	CB2-OB2-PB2-OB3
13	p	603	CDL	CB2-OB2-PB2-OB4
13	p	603	CDL	CB2-OB2-PB2-OB5
14	G	102	9Y0	C2-O3-P-O
14	G	102	9Y0	C2-O3-P-O2
14	I	608	9Y0	C12-C13-C14-C15
14	I	608	9Y0	O1-C3-C4-N
14	I	610	9Y0	C13-C14-C15-C16
14	I	610	9Y0	C22-C21-O7-C1
14	I	610	9Y0	C2-O3-P-O
14	I	610	9Y0	C2-O3-P-O2
14	L	601	9Y0	C2-O3-P-O
14	L	601	9Y0	C2-O3-P-O1
14	L	601	9Y0	C2-O3-P-O2
14	b	102	9Y0	C3-O1-P-O
14	b	102	9Y0	C2-O3-P-O
14	b	102	9Y0	C2-O3-P-O1
14	b	102	9Y0	C2-O3-P-O2
14	f	601	9Y0	C13-C14-C15-C16
14	f	601	9Y0	C2-O3-P-O
14	f	601	9Y0	C2-O3-P-O2
15	I	601	HEA	C2A-C3A-CMA-OMA
15	I	601	HEA	C4A-C3A-CMA-OMA
15	I	601	HEA	C2D-C3D-CAD-CBD
15	I	601	HEA	C4D-C3D-CAD-CBD
15	I	601	HEA	C26-C15-C16-C17
15	I	601	HEA	C15-C16-C17-C18
15	I	601	HEA	C17-C18-C19-C20
15	I	602	HEA	C2A-C3A-CMA-OMA
15	I	602	HEA	C4A-C3A-CMA-OMA
15	I	602	HEA	O11-C11-C3B-C4B
15	I	602	HEA	C3B-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	I	602	HEA	O11-C11-C12-C13
15	I	602	HEA	C13-C14-C15-C16
15	I	602	HEA	C26-C15-C16-C17
15	L	602	HEA	C2A-C3A-CMA-OMA
15	L	602	HEA	C4A-C3A-CMA-OMA
15	L	602	HEA	C2D-C3D-CAD-CBD
15	L	602	HEA	C4D-C3D-CAD-CBD
15	L	602	HEA	C26-C15-C16-C17
15	L	602	HEA	C15-C16-C17-C18
15	L	602	HEA	C17-C18-C19-C20
15	L	603	HEA	C2A-C3A-CMA-OMA
15	L	603	HEA	C4A-C3A-CMA-OMA
15	L	603	HEA	O11-C11-C3B-C4B
15	L	603	HEA	C3B-C11-C12-C13
15	L	603	HEA	O11-C11-C12-C13
15	L	603	HEA	C13-C14-C15-C16
15	L	603	HEA	C26-C15-C16-C17
15	L	603	HEA	C21-C22-C23-C25
19	L	609	9YF	C1-O-P-O1
19	L	609	9YF	C1-O-P-O8
19	i	601	9YF	O9-C-C24-O11
19	o	603	9YF	C1-O-P-O8
19	o	603	9YF	C9-C8-O9-C
19	o	603	9YF	O10-C8-O9-C
19	p	604	9YF	C1-O-P-O1
19	p	604	9YF	C1-O-P-O2
20	U	601	HEC	C2B-C3B-CAB-CBB
20	U	601	HEC	C4B-C3B-CAB-CBB
20	U	601	HEC	C2C-C3C-CAC-CBC
20	U	601	HEC	C4C-C3C-CAC-CBC
20	U	602	HEC	C2B-C3B-CAB-CBB
20	U	602	HEC	C4B-C3B-CAB-CBB
20	U	602	HEC	C2C-C3C-CAC-CBC
20	U	602	HEC	C4C-C3C-CAC-CBC
20	o	601	HEC	C2B-C3B-CAB-CBB
20	o	601	HEC	C4B-C3B-CAB-CBB
20	o	601	HEC	C2C-C3C-CAC-CBC
20	o	601	HEC	C4C-C3C-CAC-CBC
20	o	602	HEC	C2B-C3B-CAB-CBB
20	o	602	HEC	C4B-C3B-CAB-CBB
20	o	602	HEC	C2C-C3C-CAC-CBC
20	o	602	HEC	C4C-C3C-CAC-CBC

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	U	603	MQ9	C23-C24-C26-C27
21	U	603	MQ9	C25-C24-C26-C27
21	U	603	MQ9	C24-C26-C27-C28
21	U	603	MQ9	C33-C34-C36-C37
21	U	603	MQ9	C35-C34-C36-C37
21	U	603	MQ9	C40-C39-C41-C42
21	i	609	MQ9	C28-C29-C31-C32
21	i	609	MQ9	C30-C29-C31-C32
21	i	610	MQ9	C7-C8-C9-C10
21	i	610	MQ9	C7-C8-C9-C11
21	i	610	MQ9	C12-C13-C14-C15
21	i	610	MQ9	C12-C13-C14-C16
21	i	610	MQ9	C17-C18-C19-C20
21	i	610	MQ9	C17-C18-C19-C21
21	i	610	MQ9	C22-C23-C24-C25
21	i	610	MQ9	C22-C23-C24-C26
21	j	607	MQ9	C24-C26-C27-C28
21	j	608	MQ9	C7-C8-C9-C10
21	j	608	MQ9	C7-C8-C9-C11
21	j	608	MQ9	C22-C23-C24-C25
21	j	608	MQ9	C22-C23-C24-C26
21	j	608	MQ9	C31-C32-C33-C34
21	j	608	MQ9	C32-C33-C34-C35
21	j	608	MQ9	C32-C33-C34-C36
21	m	201	MQ9	C5-C6-C7-C8
21	m	201	MQ9	C1-C6-C7-C8
21	m	201	MQ9	C24-C26-C27-C28
21	n	201	MQ9	C12-C13-C14-C15
21	n	201	MQ9	C12-C13-C14-C16
21	n	201	MQ9	C17-C18-C19-C20
21	n	201	MQ9	C22-C23-C24-C25
21	n	201	MQ9	C22-C23-C24-C26
21	n	201	MQ9	C24-C26-C27-C28
21	n	201	MQ9	C32-C33-C34-C35
21	n	201	MQ9	C32-C33-C34-C36
21	n	201	MQ9	C34-C36-C37-C38
21	o	604	MQ9	C23-C24-C26-C27
21	o	604	MQ9	C25-C24-C26-C27
21	o	604	MQ9	C24-C26-C27-C28
21	o	604	MQ9	C33-C34-C36-C37
21	o	604	MQ9	C35-C34-C36-C37
21	o	604	MQ9	C34-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	i	611	9XX	O-C16-C17-O1
25	q	302	9XX	O-C16-C17-C37
25	q	302	9XX	O-C16-C17-O1
25	q	302	9XX	C19-C18-O1-C17
25	q	302	9XX	O2-C18-O1-C17
25	r	301	9XX	C37-C17-O1-C18
19	p	604	9YF	C30-C31-C32-C33
19	L	609	9YF	O12-C25-O11-C24
19	p	604	9YF	O12-C25-O11-C24
25	q	302	9XX	O6-C15-O-C16
19	L	609	9YF	C26-C25-O11-C24
19	p	604	9YF	C26-C25-O11-C24
13	b	101	CDL	OA9-CA7-OA8-CA6
13	i	606	CDL	OB9-CB7-OB8-CB6
13	p	603	CDL	OB9-CB7-OB8-CB6
13	U	604	CDL	OA7-CA5-OA6-CA4
13	V	602	CDL	OB7-CB5-OB6-CB4
13	b	101	CDL	OA7-CA5-OA6-CA4
13	b	101	CDL	OB7-CB5-OB6-CB4
13	i	603	CDL	OB7-CB5-OB6-CB4
13	i	606	CDL	OB7-CB5-OB6-CB4
13	i	608	CDL	OB7-CB5-OB6-CB4
13	i	613	CDL	OB7-CB5-OB6-CB4
13	j	606	CDL	OA7-CA5-OA6-CA4
13	j	611	CDL	OA7-CA5-OA6-CA4
14	I	610	9Y0	O6-C21-O7-C1
13	G	101	CDL	C31-CA7-OA8-CA6
13	b	101	CDL	C31-CA7-OA8-CA6
13	i	606	CDL	C71-CB7-OB8-CB6
13	j	606	CDL	C31-CA7-OA8-CA6
13	p	603	CDL	C71-CB7-OB8-CB6
25	q	302	9XX	C14-C15-O-C16
13	i	613	CDL	C51-CB5-OB6-CB4
15	I	601	HEA	C21-C22-C23-C24
15	I	601	HEA	C21-C22-C23-C25
15	I	602	HEA	C21-C22-C23-C24
15	I	602	HEA	C21-C22-C23-C25
15	L	602	HEA	C21-C22-C23-C24
15	L	602	HEA	C21-C22-C23-C25
15	L	603	HEA	C21-C22-C23-C24
21	o	604	MQ9	C40-C39-C41-C42
15	L	603	HEA	C14-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	U	603	MQ9	C38-C39-C41-C42
13	V	602	CDL	C14-C15-C16-C17
13	p	603	CDL	C60-C61-C62-C63
13	U	604	CDL	C71-CB7-OB8-CB6
13	i	603	CDL	C71-CB7-OB8-CB6
14	L	601	9Y0	C12-C13-C14-C15
13	G	101	CDL	C37-C38-C39-C40
13	p	603	CDL	C11-C12-C13-C14
25	q	302	9XX	C29-C30-C31-C32
15	I	601	HEA	C17-C18-C19-C27
15	I	602	HEA	C13-C14-C15-C26
15	L	602	HEA	C17-C18-C19-C27
15	L	603	HEA	C13-C14-C15-C26
21	i	610	MQ9	C42-C43-C44-C45
18	q	301	PLM	C7-C8-C9-CA
13	G	101	CDL	OA7-CA5-OA6-CA4
13	i	603	CDL	OA7-CA5-OA6-CA4
13	p	603	CDL	OB7-CB5-OB6-CB4
21	i	610	MQ9	C42-C43-C44-C46
21	n	201	MQ9	C17-C18-C19-C21
13	i	603	CDL	OB9-CB7-OB8-CB6
13	G	101	CDL	C72-C73-C74-C75
25	j	610	9XX	C16-C17-O1-C18
13	U	604	CDL	O1-C1-CB2-OB2
13	V	602	CDL	O1-C1-CA2-OA2
13	b	101	CDL	O1-C1-CB2-OB2
13	i	603	CDL	O1-C1-CB2-OB2
13	i	608	CDL	O1-C1-CB2-OB2
13	i	612	CDL	O1-C1-CA2-OA2
13	i	612	CDL	O1-C1-CB2-OB2
13	i	613	CDL	O1-C1-CB2-OB2
13	j	611	CDL	O1-C1-CB2-OB2
14	I	608	9Y0	C6-C5-O5-C
19	o	603	9YF	C26-C25-O11-C24
13	L	607	CDL	C61-C62-C63-C64
13	G	101	CDL	OA9-CA7-OA8-CA6
13	U	604	CDL	OB9-CB7-OB8-CB6
13	j	606	CDL	OA9-CA7-OA8-CA6
13	i	612	CDL	C11-CA5-OA6-CA4
13	j	606	CDL	C51-CB5-OB6-CB4
13	p	603	CDL	C51-CB5-OB6-CB4
13	j	611	CDL	C77-C78-C79-C80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	V	602	CDL	C55-C56-C57-C58
13	b	101	CDL	C11-C12-C13-C14
13	i	612	CDL	C17-C18-C19-C20
13	p	603	CDL	C17-C18-C19-C20
13	p	603	CDL	C20-C21-C22-C23
13	p	603	CDL	C51-C52-C53-C54
18	q	301	PLM	CC-CD-CE-CF
19	o	603	9YF	C11-C12-C13-C14
19	o	603	9YF	C13-C14-C15-C16
25	q	302	9XX	C6-C7-C8-C9
25	q	302	9XX	C3-C4-C5-C6
13	i	612	CDL	C12-C13-C14-C15
13	j	606	CDL	OB7-CB5-OB6-CB4
13	V	602	CDL	C33-C34-C35-C36
14	f	601	9Y0	C23-C24-C25-C26
14	I	608	9Y0	O4-C5-O5-C
19	o	603	9YF	O12-C25-O11-C24
13	j	611	CDL	C34-C35-C36-C37
14	f	601	9Y0	C25-C26-C27-C28
21	i	610	MQ9	C47-C48-C49-C50
21	U	603	MQ9	C15-C14-C16-C17
21	i	610	MQ9	C25-C24-C26-C27
21	j	608	MQ9	C20-C19-C21-C22
21	m	201	MQ9	C12-C11-C9-C10
21	n	201	MQ9	C30-C29-C31-C32
21	o	604	MQ9	C15-C14-C16-C17
21	U	603	MQ9	C13-C14-C16-C17
21	i	610	MQ9	C23-C24-C26-C27
21	j	608	MQ9	C18-C19-C21-C22
21	m	201	MQ9	C12-C11-C9-C8
21	n	201	MQ9	C28-C29-C31-C32
21	o	604	MQ9	C13-C14-C16-C17
14	I	610	9Y0	C21-C22-C23-C24
13	I	605	CDL	C74-C75-C76-C77
21	U	603	MQ9	C14-C16-C17-C18
21	i	610	MQ9	C14-C16-C17-C18
21	i	610	MQ9	C44-C46-C47-C48
21	j	607	MQ9	C14-C16-C17-C18
21	j	608	MQ9	C19-C21-C22-C23
21	m	201	MQ9	C14-C16-C17-C18
21	m	201	MQ9	C29-C31-C32-C33
13	i	612	CDL	C72-C73-C74-C75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	q	302	9XX	C21-C22-C23-C24
13	I	605	CDL	CA7-C31-C32-C33
13	I	604	CDL	C51-CB5-OB6-CB4
13	L	606	CDL	C51-CB5-OB6-CB4
13	b	101	CDL	C13-C14-C15-C16
21	j	608	MQ9	C12-C13-C14-C15
21	j	608	MQ9	C27-C28-C29-C30
13	G	101	CDL	CA2-C1-CB2-OB2
13	I	604	CDL	CA2-C1-CB2-OB2
13	L	606	CDL	CA2-C1-CB2-OB2
13	L	607	CDL	CA2-C1-CB2-OB2
13	V	602	CDL	CB2-C1-CA2-OA2
13	V	602	CDL	CA2-C1-CB2-OB2
13	i	606	CDL	CB2-C1-CA2-OA2
13	i	606	CDL	CA2-C1-CB2-OB2
13	i	607	CDL	CA2-C1-CB2-OB2
13	i	608	CDL	CA2-C1-CB2-OB2
13	i	612	CDL	CA2-C1-CB2-OB2
13	j	605	CDL	CA2-C1-CB2-OB2
13	j	606	CDL	CA2-C1-CB2-OB2
13	j	611	CDL	CB2-C1-CA2-OA2
13	p	603	CDL	CA2-C1-CB2-OB2
13	i	612	CDL	OA7-CA5-OA6-CA4
21	j	608	MQ9	C12-C13-C14-C16
21	j	608	MQ9	C27-C28-C29-C31
13	L	607	CDL	C71-C72-C73-C74
13	V	602	CDL	C20-C21-C22-C23
13	L	607	CDL	C71-CB7-OB8-CB6
25	i	611	9XX	C14-C15-O-C16
13	I	605	CDL	C57-C58-C59-C60
13	i	613	CDL	CB7-C71-C72-C73
13	L	607	CDL	C12-C13-C14-C15
13	j	611	CDL	C82-C83-C84-C85
14	I	610	9Y0	C23-C24-C25-C26
13	V	602	CDL	C18-C19-C20-C21
13	i	612	CDL	OB5-CB3-CB4-OB6
13	G	101	CDL	O1-C1-CB2-OB2
13	I	605	CDL	O1-C1-CB2-OB2
13	L	607	CDL	O1-C1-CB2-OB2
13	i	606	CDL	O1-C1-CB2-OB2
13	j	606	CDL	O1-C1-CB2-OB2
13	p	603	CDL	C78-C79-C80-C81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	I	602	HEA	C14-C15-C16-C17
21	o	604	MQ9	C38-C39-C41-C42
19	p	601	9YF	C31-C32-C33-C34
25	r	301	9XX	C36-C27-C28-C29
13	i	606	CDL	C51-C52-C53-C54
19	p	604	9YF	C38-C39-C40-C41
13	I	604	CDL	CA7-C31-C32-C33
19	j	601	9YF	C25-C26-C27-C28
13	L	607	CDL	OB9-CB7-OB8-CB6
19	p	604	9YF	C33-C35-C36-C37
13	i	606	CDL	C18-C19-C20-C21
13	j	606	CDL	C78-C79-C80-C81
13	G	101	CDL	CB7-C71-C72-C73
14	I	608	9Y0	C21-C22-C23-C24
14	f	601	9Y0	C21-C22-C23-C24
13	p	603	CDL	C71-C72-C73-C74
13	i	613	CDL	C12-C13-C14-C15
13	L	606	CDL	CA7-C31-C32-C33
13	L	607	CDL	CB5-C51-C52-C53
13	L	607	CDL	CB7-C71-C72-C73
13	V	602	CDL	CB7-C71-C72-C73
13	i	606	CDL	CB7-C71-C72-C73
13	i	608	CDL	CB7-C71-C72-C73
13	j	606	CDL	CB7-C71-C72-C73
19	L	609	9YF	C11-C10-C9-C8
19	L	609	9YF	C25-C26-C27-C28
19	o	603	9YF	C11-C10-C9-C8
19	p	601	9YF	C25-C26-C27-C28
13	V	602	CDL	C61-C62-C63-C64
19	j	601	9YF	C30-C31-C32-C33
13	I	604	CDL	CB7-C71-C72-C73
13	L	606	CDL	CB7-C71-C72-C73
13	b	101	CDL	CB7-C71-C72-C73
13	i	603	CDL	CB5-C51-C52-C53
19	i	601	9YF	C25-C26-C27-C28
21	i	610	MQ9	C47-C48-C49-C51
25	i	611	9XX	O6-C15-O-C16
13	L	607	CDL	C78-C79-C80-C81
13	i	608	CDL	C78-C79-C80-C81
15	L	603	HEA	C19-C20-C21-C22
21	U	603	MQ9	C9-C11-C12-C13
21	U	603	MQ9	C19-C21-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	i	609	MQ9	C19-C21-C22-C23
21	i	609	MQ9	C29-C31-C32-C33
21	i	610	MQ9	C9-C11-C12-C13
21	i	610	MQ9	C29-C31-C32-C33
21	j	607	MQ9	C19-C21-C22-C23
21	j	608	MQ9	C9-C11-C12-C13
21	m	201	MQ9	C9-C11-C12-C13
21	o	604	MQ9	C9-C11-C12-C13
21	o	604	MQ9	C14-C16-C17-C18
21	o	604	MQ9	C19-C21-C22-C23
21	o	604	MQ9	C29-C31-C32-C33
13	i	603	CDL	CA5-C11-C12-C13
14	b	102	9Y0	C21-C22-C23-C24
21	n	201	MQ9	C37-C38-C39-C41
13	I	604	CDL	O1-C1-CB2-OB2
13	L	606	CDL	O1-C1-CB2-OB2
13	I	604	CDL	OB7-CB5-OB6-CB4
13	L	606	CDL	OB7-CB5-OB6-CB4
19	L	609	9YF	C30-C31-C32-C33
19	p	601	9YF	C26-C25-O11-C24
13	G	101	CDL	C35-C36-C37-C38
19	p	601	9YF	C30-C31-C32-C33
19	i	601	9YF	C35-C36-C37-C38
13	L	606	CDL	C59-C60-C61-C62
13	I	604	CDL	CA2-OA2-PA1-OA5
13	I	604	CDL	CA3-OA5-PA1-OA2
13	I	604	CDL	CB2-OB2-PB2-OB5
13	I	604	CDL	CB3-OB5-PB2-OB2
13	I	605	CDL	CA2-OA2-PA1-OA5
13	I	605	CDL	CB2-OB2-PB2-OB5
13	L	606	CDL	CA3-OA5-PA1-OA2
13	L	606	CDL	CB2-OB2-PB2-OB5
13	L	607	CDL	CA2-OA2-PA1-OA5
13	L	607	CDL	CB2-OB2-PB2-OB5
13	L	607	CDL	CB3-OB5-PB2-OB2
13	U	604	CDL	CB3-OB5-PB2-OB2
13	b	101	CDL	CA2-OA2-PA1-OA5
13	b	101	CDL	CA3-OA5-PA1-OA2
13	i	603	CDL	CA2-OA2-PA1-OA5
13	i	603	CDL	CA3-OA5-PA1-OA2
13	i	606	CDL	CA2-OA2-PA1-OA5
13	i	606	CDL	CB3-OB5-PB2-OB2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	607	CDL	CA3-OA5-PA1-OA2
13	i	607	CDL	CB2-OB2-PB2-OB5
13	i	608	CDL	CA2-OA2-PA1-OA5
13	i	608	CDL	CB3-OB5-PB2-OB2
13	i	612	CDL	CA3-OA5-PA1-OA2
13	i	612	CDL	CB2-OB2-PB2-OB5
13	i	613	CDL	CB2-OB2-PB2-OB5
13	j	605	CDL	CA3-OA5-PA1-OA2
13	j	606	CDL	CA3-OA5-PA1-OA2
13	j	606	CDL	CB2-OB2-PB2-OB5
13	j	611	CDL	CA2-OA2-PA1-OA5
13	j	611	CDL	CB2-OB2-PB2-OB5
13	j	611	CDL	CB3-OB5-PB2-OB2
14	G	102	9Y0	C3-O1-P-O3
14	G	102	9Y0	C2-O3-P-O1
14	I	610	9Y0	C2-O3-P-O1
14	L	601	9Y0	C3-O1-P-O3
14	f	601	9Y0	C2-O3-P-O1
19	L	609	9YF	C1-O-P-O2
13	b	101	CDL	CB5-C51-C52-C53
13	I	605	CDL	C31-CA7-OA8-CA6
13	L	607	CDL	C31-CA7-OA8-CA6
13	i	603	CDL	C57-C58-C59-C60
25	j	610	9XX	C12-C13-C14-C15
13	U	604	CDL	CA2-C1-CB2-OB2
13	b	101	CDL	CA2-C1-CB2-OB2
13	i	613	CDL	CA2-C1-CB2-OB2
13	j	611	CDL	C16-C17-C18-C19
13	L	607	CDL	C57-C58-C59-C60
19	L	609	9YF	C2-O2-P-O
19	o	603	9YF	C2-O2-P-O
13	b	101	CDL	C18-C19-C20-C21
13	i	606	CDL	C12-C13-C14-C15
13	i	607	CDL	C35-C36-C37-C38
13	i	607	CDL	C36-C37-C38-C39
13	L	607	CDL	C51-CB5-OB6-CB4
13	i	606	CDL	C11-CA5-OA6-CA4
14	G	102	9Y0	C22-C21-O7-C1
14	f	601	9Y0	C22-C21-O7-C1
13	G	101	CDL	C14-C15-C16-C17
13	G	101	CDL	C18-C19-C20-C21
13	L	607	CDL	C77-C78-C79-C80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	603	CDL	C11-C12-C13-C14
13	i	603	CDL	C34-C35-C36-C37
13	i	606	CDL	C74-C75-C76-C77
13	i	608	CDL	C11-C12-C13-C14
13	i	608	CDL	C54-C55-C56-C57
13	i	612	CDL	C13-C14-C15-C16
13	i	612	CDL	C71-C72-C73-C74
13	i	612	CDL	C74-C75-C76-C77
13	j	605	CDL	C36-C37-C38-C39
13	j	605	CDL	C38-C39-C40-C41
13	j	611	CDL	C32-C33-C34-C35
14	L	601	9Y0	C16-C17-C18-C19
18	q	301	PLM	C3-C4-C5-C6
19	j	601	9YF	C14-C15-C16-C17
19	j	601	9YF	C37-C38-C39-C40
19	p	604	9YF	C18-C19-C20-C21
19	V	603	9YF	C26-C25-O11-C24
13	G	101	CDL	C51-C52-C53-C54
13	G	101	CDL	C77-C78-C79-C80
13	I	605	CDL	C51-C52-C53-C54
13	b	101	CDL	C32-C33-C34-C35
13	i	606	CDL	C75-C76-C77-C78
13	i	607	CDL	C13-C14-C15-C16
13	i	608	CDL	C23-C24-C25-C26
13	j	606	CDL	C20-C21-C22-C23
13	j	606	CDL	C75-C76-C77-C78
13	p	603	CDL	C38-C39-C40-C41
13	p	603	CDL	C59-C60-C61-C62
14	G	102	9Y0	C27-C28-C29-C30
19	L	609	9YF	C18-C19-C20-C21
19	p	604	9YF	C29-C30-C31-C32
13	V	602	CDL	CB6-CB4-OB6-CB5
13	b	101	CDL	CA6-CA4-OA6-CA5
13	i	608	CDL	CB6-CB4-OB6-CB5
13	i	606	CDL	OA7-CA5-OA6-CA4
14	f	601	9Y0	O6-C21-O7-C1
25	r	301	9XX	C16-C17-O1-C18
13	L	607	CDL	CA5-C11-C12-C13
13	U	604	CDL	C55-C56-C57-C58
13	i	613	CDL	C52-C53-C54-C55
13	i	613	CDL	C74-C75-C76-C77
13	j	611	CDL	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	p	603	CDL	C13-C14-C15-C16
14	L	601	9Y0	C11-C10-C9-C8
19	j	601	9YF	C18-C19-C20-C21
13	G	101	CDL	C20-C21-C22-C23
13	G	101	CDL	C73-C74-C75-C76
13	G	101	CDL	C80-C81-C82-C83
13	I	604	CDL	C56-C57-C58-C59
13	L	607	CDL	C63-C64-C65-C66
13	U	604	CDL	C11-C12-C13-C14
13	U	604	CDL	C71-C72-C73-C74
13	b	101	CDL	C80-C81-C82-C83
13	i	607	CDL	C38-C39-C40-C41
13	i	608	CDL	C73-C74-C75-C76
13	j	611	CDL	C11-C12-C13-C14
19	V	603	9YF	C29-C30-C31-C32
19	i	601	9YF	C12-C13-C14-C15
19	i	601	9YF	C27-C28-C29-C30
19	i	601	9YF	C28-C29-C30-C31
19	o	603	9YF	C36-C37-C38-C39
24	i	605	HEM	C3D-CAD-CBD-CGD
24	j	604	HEM	C3D-CAD-CBD-CGD
13	i	606	CDL	C72-C73-C74-C75
13	j	606	CDL	C13-C14-C15-C16
13	j	606	CDL	C73-C74-C75-C76
13	p	603	CDL	C12-C13-C14-C15
19	o	603	9YF	C17-C18-C19-C20
19	p	604	9YF	C25-C26-C27-C28
13	G	101	CDL	OB6-CB4-CB6-OB8
13	I	605	CDL	C58-C59-C60-C61
13	L	606	CDL	C57-C58-C59-C60
13	b	101	CDL	C19-C20-C21-C22
13	b	101	CDL	C75-C76-C77-C78
13	i	612	CDL	C11-C12-C13-C14
13	j	606	CDL	C74-C75-C76-C77
13	p	603	CDL	C61-C62-C63-C64
13	I	604	CDL	C55-C56-C57-C58
13	I	605	CDL	C33-C34-C35-C36
13	I	605	CDL	C79-C80-C81-C82
13	L	606	CDL	C55-C56-C57-C58
13	L	607	CDL	C75-C76-C77-C78
13	U	604	CDL	C57-C58-C59-C60
13	V	602	CDL	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	V	602	CDL	C54-C55-C56-C57
13	V	602	CDL	C60-C61-C62-C63
13	i	603	CDL	C73-C74-C75-C76
13	i	612	CDL	C77-C78-C79-C80
13	j	606	CDL	C16-C17-C18-C19
13	j	611	CDL	C78-C79-C80-C81
19	i	601	9YF	C29-C30-C31-C32
19	p	601	9YF	C39-C40-C41-C42
25	q	302	9XX	C2-C3-C4-C5
13	G	101	CDL	C11-C12-C13-C14
13	I	604	CDL	C11-C12-C13-C14
13	I	605	CDL	C52-C53-C54-C55
13	L	606	CDL	C11-C12-C13-C14
13	U	604	CDL	C12-C13-C14-C15
13	b	101	CDL	C76-C77-C78-C79
13	i	607	CDL	C14-C15-C16-C17
13	i	608	CDL	C55-C56-C57-C58
13	j	606	CDL	C55-C56-C57-C58
18	q	301	PLM	C6-C7-C8-C9
19	i	601	9YF	C14-C15-C16-C17
19	p	601	9YF	C14-C15-C16-C17
19	p	601	9YF	C16-C17-C18-C19
25	q	302	9XX	C20-C21-C22-C23
13	I	605	CDL	OA9-CA7-OA8-CA6
19	p	601	9YF	O12-C25-O11-C24
13	I	604	CDL	C51-C52-C53-C54
13	I	605	CDL	C53-C54-C55-C56
13	I	605	CDL	C76-C77-C78-C79
13	L	606	CDL	C56-C57-C58-C59
13	V	602	CDL	C58-C59-C60-C61
13	i	607	CDL	C37-C38-C39-C40
13	j	611	CDL	C80-C81-C82-C83
13	p	603	CDL	C74-C75-C76-C77
19	j	601	9YF	C29-C30-C31-C32
13	L	607	CDL	OB7-CB5-OB6-CB4
14	G	102	9Y0	O6-C21-O7-C1
13	i	608	CDL	C11-CA5-OA6-CA4
14	L	601	9Y0	C22-C21-O7-C1
13	U	604	CDL	C32-C33-C34-C35
13	i	608	CDL	C77-C78-C79-C80
13	p	603	CDL	C15-C16-C17-C18
14	I	608	9Y0	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	L	609	9YF	C29-C30-C31-C32
19	V	603	9YF	C10-C11-C12-C13
19	V	603	9YF	C14-C15-C16-C17
19	p	601	9YF	C10-C11-C12-C13
19	p	604	9YF	C37-C38-C39-C40
25	q	302	9XX	C30-C31-C32-C33
13	i	613	CDL	CA5-C11-C12-C13
19	V	603	9YF	C25-C26-C27-C28
13	G	101	CDL	C13-C14-C15-C16
13	G	101	CDL	C16-C17-C18-C19
13	L	606	CDL	C51-C52-C53-C54
13	L	607	CDL	C59-C60-C61-C62
13	L	607	CDL	C60-C61-C62-C63
13	U	604	CDL	C75-C76-C77-C78
13	V	602	CDL	C71-C72-C73-C74
13	V	602	CDL	C78-C79-C80-C81
13	b	101	CDL	C16-C17-C18-C19
13	b	101	CDL	C37-C38-C39-C40
13	b	101	CDL	C55-C56-C57-C58
13	b	101	CDL	C72-C73-C74-C75
13	i	606	CDL	C78-C79-C80-C81
13	i	607	CDL	C59-C60-C61-C62
13	i	608	CDL	C20-C21-C22-C23
13	i	612	CDL	C52-C53-C54-C55
13	j	605	CDL	C17-C18-C19-C20
13	j	605	CDL	C57-C58-C59-C60
13	j	611	CDL	C51-C52-C53-C54
13	p	603	CDL	C63-C64-C65-C66
18	q	301	PLM	C5-C6-C7-C8
19	V	603	9YF	C16-C17-C18-C19
19	V	603	9YF	C39-C40-C41-C42
19	i	601	9YF	C39-C40-C41-C42
19	o	603	9YF	C35-C36-C37-C38
25	q	302	9XX	C22-C23-C24-C25
21	m	201	MQ9	C19-C21-C22-C23
13	G	101	CDL	C75-C76-C77-C78
13	I	604	CDL	C57-C58-C59-C60
13	L	606	CDL	C37-C38-C39-C40
13	V	602	CDL	C51-C52-C53-C54
13	b	101	CDL	C74-C75-C76-C77
13	i	608	CDL	C12-C13-C14-C15
13	j	605	CDL	C55-C56-C57-C58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	j	611	CDL	C52-C53-C54-C55
13	p	603	CDL	C77-C78-C79-C80
25	j	610	9XX	C11-C12-C13-C14
13	I	604	CDL	C60-C61-C62-C63
13	L	606	CDL	C60-C61-C62-C63
13	U	604	CDL	C80-C81-C82-C83
13	p	603	CDL	C57-C58-C59-C60
13	L	607	CDL	C33-C34-C35-C36
19	p	604	9YF	C35-C36-C37-C38
25	q	302	9XX	C23-C24-C25-C26
13	I	604	CDL	C37-C38-C39-C40
13	U	604	CDL	C52-C53-C54-C55
13	b	101	CDL	C20-C21-C22-C23
13	i	606	CDL	C77-C78-C79-C80
13	j	606	CDL	C12-C13-C14-C15
13	j	606	CDL	C54-C55-C56-C57
19	i	601	9YF	C33-C35-C36-C37
13	I	605	CDL	C62-C63-C64-C65
13	V	602	CDL	C15-C16-C17-C18
13	i	603	CDL	C54-C55-C56-C57
13	i	607	CDL	C57-C58-C59-C60
13	i	608	CDL	C57-C58-C59-C60
13	j	611	CDL	C75-C76-C77-C78
13	p	603	CDL	C19-C20-C21-C22
13	p	603	CDL	C36-C37-C38-C39
14	I	608	9Y0	C6-C7-C8-C9
18	q	301	PLM	C2-C3-C4-C5
18	q	301	PLM	C4-C5-C6-C7
19	p	604	9YF	C14-C15-C16-C17
13	j	605	CDL	C59-C60-C61-C62
19	L	609	9YF	C12-C13-C14-C15
19	i	601	9YF	C18-C19-C20-C21
14	f	601	9Y0	O5-C-C1-C2
13	i	608	CDL	OA7-CA5-OA6-CA4
14	L	601	9Y0	O6-C21-O7-C1
13	V	602	CDL	C12-C13-C14-C15
13	V	602	CDL	C52-C53-C54-C55
13	i	603	CDL	C75-C76-C77-C78
13	i	607	CDL	C12-C13-C14-C15
13	i	608	CDL	C75-C76-C77-C78
19	p	601	9YF	C37-C38-C39-C40
13	U	604	CDL	CB7-C71-C72-C73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	j	611	CDL	C15-C16-C17-C18
14	I	608	9Y0	C15-C16-C17-C18
25	q	302	9XX	C10-C11-C12-C13
21	i	610	MQ9	C45-C44-C46-C47
25	r	301	9XX	C14-C15-O-C16
21	U	603	MQ9	C18-C19-C21-C22
21	i	610	MQ9	C43-C44-C46-C47
21	j	608	MQ9	C38-C39-C41-C42
13	i	607	CDL	C51-CB5-OB6-CB4
25	q	302	9XX	C16-C17-O1-C18
13	I	604	CDL	C73-C74-C75-C76
13	L	607	CDL	C80-C81-C82-C83
19	j	601	9YF	C12-C13-C14-C15
13	G	101	CDL	C12-C13-C14-C15
13	I	605	CDL	C59-C60-C61-C62
13	i	606	CDL	C71-C72-C73-C74
13	i	608	CDL	C32-C33-C34-C35
13	j	611	CDL	C14-C15-C16-C17
13	j	611	CDL	C73-C74-C75-C76
13	L	607	CDL	OA9-CA7-OA8-CA6
13	V	602	CDL	C82-C83-C84-C85
13	b	101	CDL	C12-C13-C14-C15
13	j	606	CDL	C18-C19-C20-C21
19	i	601	9YF	C37-C38-C39-C40
25	r	301	9XX	C2-C3-C4-C5
13	L	606	CDL	C73-C74-C75-C76
13	V	602	CDL	C56-C57-C58-C59
13	j	605	CDL	C37-C38-C39-C40
13	j	606	CDL	C32-C33-C34-C35
13	j	606	CDL	C71-C72-C73-C74
13	j	611	CDL	C57-C58-C59-C60
25	r	301	9XX	C5-C6-C7-C8
13	G	101	CDL	C31-C32-C33-C34
13	I	605	CDL	C56-C57-C58-C59
13	U	604	CDL	C78-C79-C80-C81
19	L	609	9YF	C38-C39-C40-C41
19	V	603	9YF	O12-C25-O11-C24
13	i	612	CDL	C55-C56-C57-C58
19	V	603	9YF	C37-C38-C39-C40
13	U	604	CDL	C74-C75-C76-C77
13	j	605	CDL	C74-C75-C76-C77
13	I	605	CDL	C11-CA5-OA6-CA4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	U	604	CDL	C51-CB5-OB6-CB4
13	V	602	CDL	C57-C58-C59-C60
13	i	603	CDL	C52-C53-C54-C55
13	i	612	CDL	C76-C77-C78-C79
13	i	613	CDL	C32-C33-C34-C35
25	q	302	9XX	C19-C20-C21-C22
14	L	601	9Y0	C5-C6-C7-C8
13	U	604	CDL	C54-C55-C56-C57
13	i	608	CDL	C76-C77-C78-C79
21	n	201	MQ9	C37-C38-C39-C40
13	b	101	CDL	C54-C55-C56-C57
13	i	608	CDL	C71-C72-C73-C74
19	o	603	9YF	C19-C20-C21-C22
25	q	302	9XX	C9-C10-C11-C12
21	U	603	MQ9	C20-C19-C21-C22
21	j	608	MQ9	C40-C39-C41-C42
25	r	301	9XX	C25-C26-C27-C28
13	i	613	CDL	C55-C56-C57-C58
14	I	608	9Y0	C17-C18-C19-C20
14	G	102	9Y0	C10-C11-C12-C13
13	i	607	CDL	OB7-CB5-OB6-CB4
25	j	610	9XX	O2-C18-O1-C17
13	I	604	CDL	CA5-C11-C12-C13
13	I	605	CDL	CB7-C71-C72-C73
13	L	606	CDL	CA5-C11-C12-C13
13	b	101	CDL	CA5-C11-C12-C13
13	i	613	CDL	CA7-C31-C32-C33
19	j	601	9YF	C26-C25-O11-C24
13	b	101	CDL	C84-C85-C86-C87
13	p	603	CDL	C34-C35-C36-C37
13	i	612	CDL	C54-C55-C56-C57
13	i	612	CDL	C59-C60-C61-C62
19	V	603	9YF	C35-C36-C37-C38
25	q	302	9XX	C37-C17-O1-C18
13	G	101	CDL	C39-C40-C41-C42
13	i	608	CDL	C14-C15-C16-C17
25	q	302	9XX	C11-C12-C13-C14
25	r	301	9XX	O6-C15-O-C16
15	I	602	HEA	C15-C16-C17-C18
13	L	607	CDL	C51-C52-C53-C54
19	j	601	9YF	C39-C40-C41-C42
19	p	601	9YF	C36-C37-C38-C39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	101	CDL	C51-CB5-OB6-CB4
13	j	605	CDL	C51-CB5-OB6-CB4
25	j	610	9XX	C19-C18-O1-C17
25	r	301	9XX	C19-C18-O1-C17
13	i	603	CDL	OB5-CB3-CB4-OB6
13	L	607	CDL	C73-C74-C75-C76
13	V	602	CDL	C79-C80-C81-C82
13	i	613	CDL	C51-C52-C53-C54
13	j	605	CDL	C35-C36-C37-C38
13	V	602	CDL	C53-C54-C55-C56
19	i	601	9YF	C15-C16-C17-C18
13	i	606	CDL	O1-C1-CA2-OA2
13	G	101	CDL	OB7-CB5-OB6-CB4
13	U	604	CDL	OB7-CB5-OB6-CB4
13	j	605	CDL	OB7-CB5-OB6-CB4
25	r	301	9XX	O2-C18-O1-C17
19	o	603	9YF	C25-C26-C27-C28
13	i	607	CDL	C71-C72-C73-C74
13	p	603	CDL	C75-C76-C77-C78
13	L	607	CDL	OB6-CB4-CB6-OB8
14	f	601	9Y0	O5-C-C1-O7
19	L	609	9YF	C37-C38-C39-C40
13	i	612	CDL	C75-C76-C77-C78
21	j	607	MQ9	C25-C24-C26-C27
21	j	607	MQ9	C30-C29-C31-C32
21	m	201	MQ9	C30-C29-C31-C32
21	o	604	MQ9	C20-C19-C21-C22
21	i	610	MQ9	C28-C29-C31-C32
13	L	606	CDL	C72-C73-C74-C75
13	b	101	CDL	C15-C16-C17-C18
25	r	301	9XX	C25-C26-C27-C36
13	j	605	CDL	C71-C72-C73-C74
13	I	604	CDL	C32-C33-C34-C35
13	L	606	CDL	C32-C33-C34-C35
13	i	606	CDL	C76-C77-C78-C79
13	p	603	CDL	C18-C19-C20-C21
19	o	603	9YF	C20-C21-C22-C23
19	p	601	9YF	C18-C19-C20-C21
13	I	605	CDL	OA7-CA5-OA6-CA4
13	G	101	CDL	CB2-OB2-PB2-OB5
13	L	606	CDL	CA2-OA2-PA1-OA5
13	V	602	CDL	CA3-OA5-PA1-OA2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	j	605	CDL	CA2-OA2-PA1-OA5
13	j	605	CDL	CB2-OB2-PB2-OB5
13	p	603	CDL	CA3-OA5-PA1-OA2
19	o	603	9YF	C1-O-P-O2
13	V	602	CDL	C59-C60-C61-C62
13	b	101	CDL	C53-C54-C55-C56
13	b	101	CDL	C56-C57-C58-C59
13	i	612	CDL	C57-C58-C59-C60
13	i	603	CDL	OA5-CA3-CA4-CA6
13	i	603	CDL	OB5-CB3-CB4-CB6
13	i	612	CDL	OB5-CB3-CB4-CB6
13	j	606	CDL	OB5-CB3-CB4-CB6
13	p	603	CDL	OA5-CA3-CA4-CA6
13	L	607	CDL	C32-C33-C34-C35
13	j	606	CDL	C51-C52-C53-C54
13	V	602	CDL	C21-C22-C23-C24
13	i	603	CDL	C55-C56-C57-C58
19	V	603	9YF	C28-C29-C30-C31
13	L	606	CDL	C31-C32-C33-C34
13	i	613	CDL	C11-C12-C13-C14
13	i	613	CDL	C71-C72-C73-C74
13	j	606	CDL	C14-C15-C16-C17
19	p	601	9YF	C27-C28-C29-C30
19	p	601	9YF	C11-C10-C9-C8
13	i	607	CDL	CB2-C1-CA2-OA2
13	j	605	CDL	CB2-C1-CA2-OA2
21	i	610	MQ9	C30-C29-C31-C32
13	G	101	CDL	C36-C37-C38-C39
13	I	604	CDL	C72-C73-C74-C75
13	b	101	CDL	C36-C37-C38-C39
25	q	302	9XX	C24-C25-C26-C27
13	L	607	CDL	C74-C75-C76-C77
19	j	601	9YF	O12-C25-O11-C24
13	G	101	CDL	C78-C79-C80-C81
13	p	603	CDL	C37-C38-C39-C40
13	G	101	CDL	CA3-CA4-CA6-OA8
13	G	101	CDL	CB3-CB4-CB6-OB8
13	L	607	CDL	CA3-CA4-CA6-OA8
13	L	607	CDL	CB3-CB4-CB6-OB8
13	i	606	CDL	C80-C81-C82-C83
13	i	608	CDL	CB3-CB4-CB6-OB8
14	I	608	9Y0	O5-C-C1-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	I	608	9Y0	C23-C24-C25-C26
19	p	601	9YF	C29-C30-C31-C32
13	i	612	CDL	C53-C54-C55-C56
13	j	611	CDL	C54-C55-C56-C57
19	L	609	9YF	C20-C21-C22-C23
21	n	201	MQ9	C5-C6-C7-C8
13	G	101	CDL	C84-C85-C86-C87
13	i	612	CDL	C19-C20-C21-C22
13	G	101	CDL	C83-C84-C85-C86
13	b	101	CDL	C82-C83-C84-C85
13	b	101	CDL	C72-C71-CB7-OB8
13	G	101	CDL	CA5-C11-C12-C13
19	V	603	9YF	C11-C10-C9-C8
13	G	101	CDL	C57-C58-C59-C60
13	i	606	CDL	C59-C60-C61-C62
19	V	603	9YF	C36-C37-C38-C39
19	p	604	9YF	C9-C10-C11-C12
15	I	602	HEA	C19-C20-C21-C22
21	i	610	MQ9	C34-C36-C37-C38
21	n	201	MQ9	C9-C11-C12-C13
13	V	602	CDL	C39-C40-C41-C42
13	V	602	CDL	C75-C76-C77-C78
13	i	613	CDL	C13-C14-C15-C16
25	r	301	9XX	C32-C33-C34-C35
13	G	101	CDL	C32-C33-C34-C35
13	V	602	CDL	C24-C25-C26-C27
13	i	607	CDL	C52-C53-C54-C55
14	L	601	9Y0	C14-C15-C16-C17
13	G	101	CDL	C17-C18-C19-C20
14	L	601	9Y0	C17-C18-C19-C20
21	i	610	MQ9	C15-C14-C16-C17
21	i	610	MQ9	C20-C19-C21-C22
21	n	201	MQ9	C35-C34-C36-C37
13	I	605	CDL	C84-C85-C86-C87
25	j	610	9XX	C14-C15-O-C16
13	p	603	CDL	C80-C81-C82-C83
21	j	608	MQ9	C1-C6-C7-C8
21	n	201	MQ9	C1-C6-C7-C8
13	I	604	CDL	C61-C62-C63-C64
13	i	603	CDL	C77-C78-C79-C80
13	j	606	CDL	C24-C25-C26-C27
19	o	603	9YF	C39-C40-C41-C42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	I	604	CDL	CB3-CB4-OB6-CB5
13	L	606	CDL	CB3-CB4-OB6-CB5
13	i	608	CDL	CA6-CA4-OA6-CA5
13	j	606	CDL	CA6-CA4-OA6-CA5
13	L	606	CDL	C61-C62-C63-C64
13	G	101	CDL	C74-C75-C76-C77
13	I	605	CDL	C71-C72-C73-C74
13	L	607	CDL	C84-C85-C86-C87
13	i	607	CDL	C74-C75-C76-C77
13	j	611	CDL	C84-C85-C86-C87
19	p	604	9YF	C36-C37-C38-C39
14	I	610	9Y0	C6-C5-O5-C
14	L	601	9Y0	C6-C5-O5-C
13	p	603	CDL	C35-C36-C37-C38
25	q	302	9XX	C4-C5-C6-C7
25	r	301	9XX	C4-C5-C6-C7
13	I	605	CDL	C83-C84-C85-C86
13	U	604	CDL	C17-C18-C19-C20
13	i	607	CDL	C60-C61-C62-C63
19	j	601	9YF	C20-C21-C22-C23
13	j	605	CDL	O1-C1-CA2-OA2
13	i	606	CDL	C16-C17-C18-C19
13	i	613	CDL	C73-C74-C75-C76
13	p	603	CDL	C84-C85-C86-C87
13	j	611	CDL	C17-C18-C19-C20
13	p	603	CDL	OB6-CB4-CB6-OB8
13	I	605	CDL	C60-C61-C62-C63
13	U	604	CDL	C84-C85-C86-C87
13	j	606	CDL	C57-C58-C59-C60
14	G	102	9Y0	C26-C27-C28-C29
19	L	609	9YF	C13-C14-C15-C16
19	V	603	9YF	C18-C19-C20-C21
21	i	610	MQ9	C12-C11-C9-C10
21	j	608	MQ9	C45-C44-C46-C47
13	I	604	CDL	C31-C32-C33-C34
13	I	605	CDL	C54-C55-C56-C57
13	i	612	CDL	C58-C59-C60-C61
19	j	601	9YF	C31-C32-C33-C35
21	i	610	MQ9	C12-C11-C9-C8
21	n	201	MQ9	C33-C34-C36-C37
13	i	612	CDL	C18-C19-C20-C21
13	j	611	CDL	C36-C37-C38-C39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	j	601	9YF	C31-C32-C33-C34
13	j	606	CDL	C22-C23-C24-C25
13	G	101	CDL	C23-C24-C25-C26
13	G	101	CDL	C52-C53-C54-C55
13	V	602	CDL	C38-C39-C40-C41
13	G	101	CDL	CB2-C1-CA2-OA2
13	L	607	CDL	C83-C84-C85-C86
13	b	101	CDL	C73-C74-C75-C76
19	j	601	9YF	C15-C16-C17-C18
13	b	101	CDL	C71-CB7-OB8-CB6
13	i	608	CDL	C31-CA7-OA8-CA6
13	i	613	CDL	C57-C58-C59-C60
14	I	608	9Y0	C24-C25-C26-C27
25	q	302	9XX	C-C1-C2-C3
13	I	604	CDL	OB5-CB3-CB4-CB6
13	L	607	CDL	OA5-CA3-CA4-CA6
13	i	606	CDL	OB5-CB3-CB4-CB6
13	i	608	CDL	OA5-CA3-CA4-CA6
13	i	608	CDL	OB5-CB3-CB4-CB6
13	i	613	CDL	OB5-CB3-CB4-CB6
14	f	601	9Y0	C-C1-C2-O3
19	o	603	9YF	C24-C-C1-O
21	U	603	MQ9	C29-C31-C32-C33
21	U	603	MQ9	C34-C36-C37-C38
13	I	605	CDL	C34-C35-C36-C37
19	i	601	9YF	C38-C39-C40-C41
25	i	611	9XX	C11-C12-C13-C14
21	i	610	MQ9	C13-C14-C16-C17
21	i	610	MQ9	C18-C19-C21-C22
21	j	607	MQ9	C23-C24-C26-C27
21	j	608	MQ9	C43-C44-C46-C47
21	o	604	MQ9	C18-C19-C21-C22
13	j	611	CDL	CB7-C71-C72-C73
25	j	610	9XX	O6-C15-O-C16
13	I	604	CDL	C71-C72-C73-C74
13	L	607	CDL	C55-C56-C57-C58
13	b	101	CDL	C34-C35-C36-C37
19	p	601	9YF	C20-C21-C22-C23
13	j	611	CDL	C71-CB7-OB8-CB6
13	b	101	CDL	C17-C18-C19-C20
13	p	603	CDL	C54-C55-C56-C57
19	p	604	9YF	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	L	609	9YF	C-C1-O-P
19	p	604	9YF	C2-O2-P-O
14	L	601	9Y0	O4-C5-O5-C
13	I	605	CDL	C61-C62-C63-C64
19	L	609	9YF	C14-C15-C16-C17
19	L	609	9YF	C9-C10-C11-C12
19	V	603	9YF	C20-C21-C22-C23
13	i	603	CDL	CB3-CB4-CB6-OB8
13	j	606	CDL	CA3-CA4-CA6-OA8
13	p	603	CDL	CA3-CA4-CA6-OA8
19	p	604	9YF	C1-C-C24-O11
25	i	611	9XX	O-C16-C17-C37
25	j	610	9XX	O-C16-C17-C37
13	I	605	CDL	C75-C76-C77-C78
13	i	608	CDL	C17-C18-C19-C20
13	i	603	CDL	C13-C14-C15-C16
13	i	612	CDL	C73-C74-C75-C76
13	L	606	CDL	C77-C78-C79-C80
19	p	601	9YF	C13-C14-C15-C16
19	p	604	9YF	C20-C21-C22-C23
14	I	610	9Y0	O4-C5-O5-C
13	I	604	CDL	C77-C78-C79-C80
13	b	101	CDL	C51-C52-C53-C54
13	G	101	CDL	CA2-OA2-PA1-OA5
14	I	608	9Y0	C3-O1-P-O3
14	b	102	9Y0	C3-O1-P-O3
25	q	302	9XX	C18-C19-C20-C21
13	b	101	CDL	C57-C58-C59-C60
13	i	608	CDL	C56-C57-C58-C59
18	I	609	PLM	C8-C9-CA-CB
13	I	604	CDL	OA5-CA3-CA4-OA6
13	L	606	CDL	OA5-CA3-CA4-OA6
13	b	101	CDL	OB5-CB3-CB4-OB6
13	i	603	CDL	OA5-CA3-CA4-OA6
13	i	606	CDL	OB5-CB3-CB4-OB6
13	i	608	CDL	OA5-CA3-CA4-OA6
13	i	613	CDL	OB5-CB3-CB4-OB6
13	i	607	CDL	C53-C54-C55-C56
13	j	606	CDL	C11-C12-C13-C14
13	i	612	CDL	CB7-C71-C72-C73
13	j	606	CDL	C72-C73-C74-C75
25	j	610	9XX	O-C16-C17-O1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	101	CDL	OB6-CB4-CB6-OB8
14	I	610	9Y0	O5-C-C1-O7
19	p	604	9YF	O9-C-C24-O11
13	i	603	CDL	C51-C52-C53-C54
15	L	603	HEA	C15-C16-C17-C18
21	n	201	MQ9	C14-C16-C17-C18
13	i	608	CDL	C31-C32-C33-C34
13	i	613	CDL	C77-C78-C79-C80
13	p	603	CDL	C32-C33-C34-C35
25	r	301	9XX	C27-C28-C29-C30
13	V	602	CDL	C1-CA2-OA2-PA1
13	L	607	CDL	C11-C12-C13-C14
13	b	101	CDL	C52-C53-C54-C55
13	j	605	CDL	C39-C40-C41-C42
18	I	609	PLM	C2-C3-C4-C5
13	I	605	CDL	OA5-CA3-CA4-CA6
13	i	607	CDL	O1-C1-CA2-OA2
13	G	101	CDL	C21-C22-C23-C24
13	L	606	CDL	C71-C72-C73-C74
19	p	601	9YF	C31-C32-C33-C35
13	b	101	CDL	OB9-CB7-OB8-CB6
13	U	604	CDL	C33-C34-C35-C36
14	I	610	9Y0	C25-C26-C27-C28
19	V	603	9YF	C26-C27-C28-C29
13	i	608	CDL	OA9-CA7-OA8-CA6
14	f	601	9Y0	C22-C23-C24-C25
13	p	603	CDL	C31-C32-C33-C34
13	L	606	CDL	C76-C77-C78-C79
13	U	604	CDL	C73-C74-C75-C76
14	L	601	9Y0	C7-C8-C9-C10
13	i	613	CDL	CB6-CB4-OB6-CB5
13	p	603	CDL	CB6-CB4-OB6-CB5
13	p	603	CDL	C14-C15-C16-C17
19	V	603	9YF	C13-C14-C15-C16
13	j	605	CDL	C60-C61-C62-C63
14	b	102	9Y0	C14-C15-C16-C17
13	U	604	CDL	CA3-CA4-CA6-OA8
13	V	602	CDL	CB4-CB3-OB5-PB2
13	i	606	CDL	CA3-CA4-CA6-OA8
13	i	608	CDL	CA3-CA4-CA6-OA8
23	j	602	A1MBF	C24-C25-C28-C29
23	j	602	A1MBF	C24-C25-C28-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	608	CDL	C72-C73-C74-C75
13	j	606	CDL	C23-C24-C25-C26
13	G	101	CDL	OB5-CB3-CB4-OB6
13	I	604	CDL	OB5-CB3-CB4-OB6
13	I	605	CDL	OA5-CA3-CA4-OA6
13	L	607	CDL	OA5-CA3-CA4-OA6
14	b	102	9Y0	O7-C1-C2-O3
13	G	101	CDL	OA6-CA4-CA6-OA8
13	j	606	CDL	OA6-CA4-CA6-OA8
14	I	608	9Y0	O5-C-C1-O7
13	j	611	CDL	OB9-CB7-OB8-CB6
13	I	605	CDL	C12-C13-C14-C15
19	L	609	9YF	C3-C2-O2-P
13	I	604	CDL	C76-C77-C78-C79
14	G	102	9Y0	C14-C15-C16-C17
13	G	101	CDL	C76-C77-C78-C79
13	j	606	CDL	C56-C57-C58-C59
13	I	605	CDL	C52-C51-CB5-OB6
13	b	101	CDL	C79-C80-C81-C82
13	i	603	CDL	C12-C13-C14-C15
13	p	603	CDL	C73-C74-C75-C76
25	r	301	9XX	C6-C7-C8-C9
13	i	607	CDL	CA2-OA2-PA1-OA5
13	i	613	CDL	CA2-OA2-PA1-OA5
19	j	601	9YF	C36-C37-C38-C39
19	p	601	9YF	C17-C18-C19-C20
21	o	604	MQ9	C45-C44-C46-C47
21	j	607	MQ9	C28-C29-C31-C32
21	m	201	MQ9	C28-C29-C31-C32
13	G	101	CDL	CB2-OB2-PB2-OB4
13	I	604	CDL	CA2-OA2-PA1-OA3
13	I	604	CDL	CA2-OA2-PA1-OA4
13	I	604	CDL	CA3-OA5-PA1-OA3
13	L	606	CDL	CA2-OA2-PA1-OA4
13	L	606	CDL	CA3-OA5-PA1-OA3
13	L	607	CDL	CB3-OB5-PB2-OB4
13	U	604	CDL	CB3-OB5-PB2-OB4
13	V	602	CDL	CB3-OB5-PB2-OB3
13	b	101	CDL	CA2-OA2-PA1-OA4
13	b	101	CDL	CA3-OA5-PA1-OA3
13	i	606	CDL	CB3-OB5-PB2-OB3
13	i	606	CDL	CB3-OB5-PB2-OB4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	607	CDL	CA2-OA2-PA1-OA4
13	i	607	CDL	CA3-OA5-PA1-OA4
13	i	607	CDL	CB2-OB2-PB2-OB3
13	i	607	CDL	CB2-OB2-PB2-OB4
13	i	607	CDL	CB3-OB5-PB2-OB4
13	i	608	CDL	CA2-OA2-PA1-OA4
13	i	612	CDL	CA2-OA2-PA1-OA4
13	i	612	CDL	CA3-OA5-PA1-OA3
13	i	612	CDL	CA3-OA5-PA1-OA4
13	j	605	CDL	CA2-OA2-PA1-OA4
13	j	605	CDL	CA3-OA5-PA1-OA4
13	j	605	CDL	CB2-OB2-PB2-OB4
13	j	605	CDL	CB3-OB5-PB2-OB4
13	j	606	CDL	CA3-OA5-PA1-OA4
13	j	606	CDL	CB2-OB2-PB2-OB4
13	j	611	CDL	CA2-OA2-PA1-OA4
14	G	102	9Y0	C3-O1-P-O
14	G	102	9Y0	C3-O1-P-O2
14	L	601	9Y0	C3-O1-P-O2
19	j	601	9YF	C1-O-P-O8
19	p	604	9YF	C1-O-P-O8
13	U	604	CDL	C81-C82-C83-C84
13	i	608	CDL	C13-C14-C15-C16
13	G	101	CDL	OB5-CB3-CB4-CB6
13	I	604	CDL	OA5-CA3-CA4-CA6
13	L	606	CDL	OA5-CA3-CA4-CA6
13	b	101	CDL	OB5-CB3-CB4-CB6
14	I	610	9Y0	C-C1-C2-O3
21	U	603	MQ9	C39-C41-C42-C43
23	i	602	A1MBF	C26-C25-C28-C29
19	j	601	9YF	C28-C29-C30-C31
14	L	601	9Y0	C4-C3-O1-P
13	I	604	CDL	C52-C53-C54-C55
23	i	602	A1MBF	C26-C25-C28-C38
13	L	607	CDL	C72-C73-C74-C75
19	j	601	9YF	C35-C36-C37-C38
13	L	607	CDL	CA7-C31-C32-C33
13	L	607	CDL	OB5-CB3-CB4-OB6
13	j	606	CDL	OB5-CB3-CB4-OB6
15	I	602	HEA	O11-C11-C3B-C2B
15	L	603	HEA	O11-C11-C3B-C2B
19	i	601	9YF	C31-C32-C33-C35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	o	603	9YF	O9-C-C1-O
19	p	604	9YF	C31-C32-C33-C35
25	j	610	9XX	C25-C26-C27-C28
25	q	302	9XX	C26-C27-C28-C29
19	V	603	9YF	C9-C10-C11-C12
14	L	601	9Y0	C6-C7-C8-C9
13	j	606	CDL	C15-C16-C17-C18
19	j	601	9YF	C38-C39-C40-C41
13	i	603	CDL	CA7-C31-C32-C33
14	L	601	9Y0	C21-C22-C23-C24
13	i	613	CDL	C32-C31-CA7-OA8
13	p	603	CDL	CB3-CB4-CB6-OB8
14	b	102	9Y0	C27-C28-C29-C30
18	q	301	PLM	C1-C2-C3-C4
19	i	601	9YF	C1-C-C24-O11
13	i	608	CDL	OB6-CB4-CB6-OB8
13	p	603	CDL	OA6-CA4-CA6-OA8
19	L	609	9YF	C26-C27-C28-C29
19	p	601	9YF	C9-C10-C11-C12
21	j	608	MQ9	C5-C6-C7-C8
13	j	605	CDL	C32-C33-C34-C35
19	p	601	9YF	C28-C29-C30-C31
13	i	608	CDL	C51-C52-C53-C54
13	i	612	CDL	C80-C81-C82-C83
21	i	609	MQ9	C9-C11-C12-C13
21	j	608	MQ9	C29-C31-C32-C33
13	L	606	CDL	C54-C55-C56-C57
19	L	609	9YF	C17-C18-C19-C20
19	p	604	9YF	C39-C40-C41-C42
13	L	606	CDL	C75-C76-C77-C78
13	j	605	CDL	C12-C13-C14-C15
19	p	604	9YF	C10-C11-C12-C13
13	i	608	CDL	C33-C34-C35-C36
13	i	608	CDL	C18-C19-C20-C21
13	L	607	CDL	CB6-CB4-OB6-CB5
13	j	606	CDL	CB6-CB4-OB6-CB5
19	o	603	9YF	C1-C-O9-C8
13	I	605	CDL	CA2-C1-CB2-OB2
13	i	608	CDL	C15-C16-C17-C18
15	I	602	HEA	C11-C12-C13-C14
15	L	603	HEA	C11-C12-C13-C14
13	i	607	CDL	C39-C40-C41-C42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	V	603	9YF	C17-C18-C19-C20
13	U	604	CDL	C13-C14-C15-C16
13	b	101	CDL	CA4-CA3-OA5-PA1
13	i	603	CDL	CB4-CB3-OB5-PB2
19	L	609	9YF	O9-C-C1-O
13	I	604	CDL	C75-C76-C77-C78
13	b	101	CDL	C22-C23-C24-C25
21	o	604	MQ9	C43-C44-C46-C47
13	p	603	CDL	C76-C77-C78-C79
13	p	603	CDL	C56-C57-C58-C59
13	G	101	CDL	CA3-OA5-PA1-OA2
13	V	602	CDL	CB5-C51-C52-C53
14	I	610	9Y0	O5-C-C1-C2
25	r	301	9XX	C26-C27-C28-C29
13	G	101	CDL	C55-C56-C57-C58
13	p	603	CDL	C52-C53-C54-C55
25	r	301	9XX	C20-C21-C22-C23
19	p	604	9YF	C31-C32-C33-C34
13	j	611	CDL	C53-C54-C55-C56
13	i	612	CDL	C78-C79-C80-C81
13	b	101	CDL	C72-C71-CB7-OB9
19	j	601	9YF	C19-C20-C21-C22
13	V	602	CDL	CA4-CA3-OA5-PA1
18	I	609	PLM	C9-CA-CB-CC
13	i	612	CDL	OB7-CB5-OB6-CB4
21	j	608	MQ9	C16-C17-C18-C19
19	o	603	9YF	C29-C30-C31-C32
14	I	610	9Y0	C10-C11-C12-C13
15	I	602	HEA	C3D-CAD-CBD-CGD
15	L	603	HEA	C3D-CAD-CBD-CGD
13	G	101	CDL	C34-C35-C36-C37
21	m	201	MQ9	C34-C36-C37-C38
14	I	610	9Y0	C6-C7-C8-C9
14	L	601	9Y0	C9-C10-C11-C12
13	j	611	CDL	OB5-CB3-CB4-OB6
13	j	605	CDL	C33-C34-C35-C36
21	i	609	MQ9	C15-C14-C16-C17
21	j	607	MQ9	C15-C14-C16-C17
13	I	605	CDL	C82-C83-C84-C85
14	f	601	9Y0	C10-C11-C12-C13
13	j	606	CDL	C52-C53-C54-C55
13	p	603	CDL	O1-C1-CA2-OA2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	q	302	9XX	C27-C28-C29-C30
13	j	606	CDL	C77-C78-C79-C80
13	i	603	CDL	C33-C34-C35-C36
24	i	604	HEM	CAA-CBA-CGA-O1A
15	I	601	HEA	CAD-CBD-CGD-O2D
15	L	602	HEA	CAD-CBD-CGD-O2D
24	j	603	HEM	CAA-CBA-CGA-O1A
13	G	101	CDL	C71-C72-C73-C74
21	U	603	MQ9	C45-C44-C46-C47
19	o	603	9YF	C34-C33-C35-C36
25	q	302	9XX	C36-C27-C28-C29
13	U	604	CDL	C82-C83-C84-C85
13	V	602	CDL	C64-C65-C66-C67
14	b	102	9Y0	C24-C25-C26-C27
13	i	607	CDL	CB3-CB4-CB6-OB8
13	U	604	CDL	C15-C16-C17-C18
13	j	611	CDL	C56-C57-C58-C59
13	b	101	CDL	O1-C1-CA2-OA2
13	i	613	CDL	O1-C1-CA2-OA2
13	i	613	CDL	C34-C35-C36-C37
19	p	604	9YF	C2-O2-P-O1
13	I	604	CDL	C38-C39-C40-C41
13	U	604	CDL	C77-C78-C79-C80
15	I	601	HEA	CAD-CBD-CGD-O1D
15	L	602	HEA	CAD-CBD-CGD-O1D
13	L	607	CDL	CB3-CB4-OB6-CB5
14	b	102	9Y0	C-C1-O7-C21
21	i	609	MQ9	C12-C11-C9-C10
13	V	602	CDL	C34-C35-C36-C37
13	j	606	CDL	C19-C20-C21-C22
19	o	603	9YF	C14-C15-C16-C17
25	r	301	9XX	C31-C32-C33-C34
13	U	604	CDL	CA3-OA5-PA1-OA2
13	i	606	CDL	C58-C59-C60-C61
13	I	605	CDL	CB5-C51-C52-C53
13	L	606	CDL	C52-C53-C54-C55
13	j	605	CDL	C51-C52-C53-C54
25	q	302	9XX	C31-C32-C33-C34
13	L	606	CDL	C53-C54-C55-C56
14	f	601	9Y0	O7-C1-C2-O3
13	i	612	CDL	OA5-CA3-CA4-CA6
13	j	605	CDL	OB5-CB3-CB4-CB6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	612	CDL	C51-CB5-OB6-CB4
18	I	609	PLM	CB-CC-CD-CE
14	I	610	9Y0	C24-C25-C26-C27
24	i	604	HEM	CAA-CBA-CGA-O2A
19	L	609	9YF	C10-C11-C12-C13
19	j	601	9YF	C26-C27-C28-C29
13	b	101	CDL	CB2-C1-CA2-OA2
13	i	608	CDL	CB2-C1-CA2-OA2
21	i	610	MQ9	C19-C21-C22-C23
13	L	607	CDL	C34-C35-C36-C37
21	U	603	MQ9	C43-C44-C46-C47
13	I	604	CDL	C59-C60-C61-C62
13	I	605	CDL	C72-C71-CB7-OB8
13	V	602	CDL	C72-C73-C74-C75
14	f	601	9Y0	C6-C7-C8-C9
13	i	613	CDL	C1-CA2-OA2-PA1
14	L	601	9Y0	C15-C16-C17-C18
13	G	101	CDL	C38-C39-C40-C41
13	L	607	CDL	C13-C14-C15-C16
14	G	102	9Y0	C11-C12-C13-C14
13	i	608	CDL	C52-C53-C54-C55
13	j	606	CDL	C33-C34-C35-C36
24	j	603	HEM	CAA-CBA-CGA-O2A
19	j	601	9YF	C10-C11-C12-C13
13	p	603	CDL	OB5-CB3-CB4-OB6
19	p	604	9YF	O9-C-C1-O
19	j	601	9YF	C11-C10-C9-C8
25	r	301	9XX	C-C1-C2-C3
15	I	601	HEA	CAA-CBA-CGA-O2A
13	L	606	CDL	C38-C39-C40-C41
13	j	611	CDL	OB5-CB3-CB4-CB6
13	i	607	CDL	C72-C71-CB7-OB8
21	i	609	MQ9	C25-C24-C26-C27
21	U	603	MQ9	C44-C46-C47-C48
21	o	604	MQ9	C44-C46-C47-C48
21	i	609	MQ9	C12-C11-C9-C8
13	L	606	CDL	C13-C14-C15-C16
13	i	612	CDL	C32-C33-C34-C35
14	b	102	9Y0	O7-C21-C22-C23
14	f	601	9Y0	C28-C29-C30-C31
13	U	604	CDL	OA6-CA4-CA6-OA8
24	j	604	HEM	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	101	CDL	C72-C71-CB7-OB8
14	L	601	9Y0	O7-C21-C22-C23
19	j	601	9YF	O9-C8-C9-C10
13	I	604	CDL	C13-C14-C15-C16
13	i	607	CDL	C32-C33-C34-C35
15	L	602	HEA	CAA-CBA-CGA-O2A
24	i	605	HEM	CAA-CBA-CGA-O2A
13	i	606	CDL	C19-C20-C21-C22
13	L	607	CDL	C52-C51-CB5-OB6
19	p	604	9YF	O9-C8-C9-C10
21	j	608	MQ9	C15-C14-C16-C17
20	U	601	HEC	CAD-CBD-CGD-O1D
19	p	604	9YF	C27-C28-C29-C30
13	j	605	CDL	C72-C71-CB7-OB8
19	i	601	9YF	C31-C32-C33-C34
19	p	601	9YF	C34-C33-C35-C36
25	j	610	9XX	C25-C26-C27-C36
19	p	604	9YF	C26-C27-C28-C29
15	L	602	HEA	CAA-CBA-CGA-O1A
13	G	101	CDL	C52-C51-CB5-OB6
19	V	603	9YF	O9-C8-C9-C10
19	p	601	9YF	O9-C8-C9-C10
14	I	608	9Y0	C13-C14-C15-C16
13	b	101	CDL	C31-C32-C33-C34
15	I	601	HEA	CAA-CBA-CGA-O1A
13	j	611	CDL	C52-C51-CB5-OB6
25	q	302	9XX	C1-C2-C3-C4
14	f	601	9Y0	C27-C28-C29-C30
13	i	606	CDL	C73-C74-C75-C76
13	p	603	CDL	C39-C40-C41-C42
14	I	608	9Y0	O7-C21-C22-C23
13	U	604	CDL	C51-C52-C53-C54
13	i	613	CDL	C75-C76-C77-C78
13	G	101	CDL	C33-C34-C35-C36
13	i	608	CDL	C34-C35-C36-C37
13	j	605	CDL	C54-C55-C56-C57
19	i	601	9YF	O9-C8-C9-C10
14	f	601	9Y0	O4-C5-O5-C
15	L	603	HEA	CAA-CBA-CGA-O1A
13	i	607	CDL	C15-C16-C17-C18
13	G	101	CDL	O1-C1-CA2-OA2
21	j	608	MQ9	C30-C29-C31-C32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	603	CDL	C12-C11-CA5-OA6
14	f	601	9Y0	C6-C5-O5-C
21	j	608	MQ9	C13-C14-C16-C17
13	L	607	CDL	OB5-CB3-CB4-CB6
13	p	603	CDL	OB5-CB3-CB4-CB6
19	p	604	9YF	C24-C-C1-O
13	G	101	CDL	C32-C31-CA7-OA8
13	U	604	CDL	C12-C11-CA5-OA6
13	b	101	CDL	C32-C31-CA7-OA8
19	i	601	9YF	C20-C21-C22-C23
20	U	601	HEC	CAD-CBD-CGD-O2D
15	I	602	HEA	CAA-CBA-CGA-O1A
24	j	604	HEM	CAA-CBA-CGA-O1A
25	q	302	9XX	C32-C33-C34-C35
19	o	603	9YF	C31-C32-C33-C35
21	i	609	MQ9	C23-C24-C26-C27
13	I	604	CDL	C12-C11-CA5-OA6
13	L	607	CDL	C12-C11-CA5-OA6
13	j	611	CDL	C12-C11-CA5-OA6
13	V	602	CDL	C31-C32-C33-C34
13	L	606	CDL	C12-C11-CA5-OA6
13	I	605	CDL	OB9-CB7-OB8-CB6
24	i	605	HEM	CAA-CBA-CGA-O1A
13	i	607	CDL	CB7-C71-C72-C73
21	i	610	MQ9	C46-C47-C48-C49
13	j	611	CDL	C52-C51-CB5-OB7
13	b	101	CDL	C33-C34-C35-C36
14	I	610	9Y0	C30-C31-C32-C33
13	G	101	CDL	C52-C51-CB5-OB7
19	V	603	9YF	O10-C8-C9-C10
19	p	601	9YF	O10-C8-C9-C10
21	n	201	MQ9	C20-C19-C21-C22
13	b	101	CDL	C21-C22-C23-C24
14	L	601	9Y0	O6-C21-C22-C23
13	I	605	CDL	C71-CB7-OB8-CB6
13	i	612	CDL	C14-C15-C16-C17
13	i	607	CDL	C33-C34-C35-C36
14	f	601	9Y0	C30-C31-C32-C33
13	G	101	CDL	C72-C71-CB7-OB9
13	L	607	CDL	C52-C51-CB5-OB7
14	I	608	9Y0	O6-C21-C22-C23
13	j	606	CDL	C34-C35-C36-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	101	CDL	CB3-CB4-CB6-OB8
13	j	611	CDL	C12-C11-CA5-OA7
19	j	601	9YF	O10-C8-C9-C10
23	i	602	A1MBF	F36-C33-O32-C31
19	L	609	9YF	C39-C40-C41-C42
13	i	613	CDL	C12-C11-CA5-OA6
19	i	601	9YF	C-C1-O-P
19	p	604	9YF	O10-C8-C9-C10
13	I	605	CDL	CA3-OA5-PA1-OA3
13	L	606	CDL	CA2-OA2-PA1-OA3
13	U	604	CDL	CA3-OA5-PA1-OA3
13	V	602	CDL	CA3-OA5-PA1-OA3
13	i	612	CDL	CB3-OB5-PB2-OB3
13	j	605	CDL	CB2-OB2-PB2-OB3
13	p	603	CDL	CA3-OA5-PA1-OA3
14	I	608	9Y0	C3-O1-P-O
13	L	607	CDL	C12-C11-CA5-OA7
13	i	603	CDL	C12-C11-CA5-OA7
14	G	102	9Y0	C-C1-C2-O3
19	p	601	9YF	C26-C27-C28-C29
14	G	102	9Y0	C23-C24-C25-C26
13	I	604	CDL	C12-C11-CA5-OA7
13	p	603	CDL	C23-C24-C25-C26
19	p	601	9YF	C35-C36-C37-C38
14	b	102	9Y0	C22-C23-C24-C25
13	L	606	CDL	C12-C11-CA5-OA7
19	i	601	9YF	C10-C11-C12-C13
13	b	101	CDL	C77-C78-C79-C80
14	G	102	9Y0	C25-C26-C27-C28
19	i	601	9YF	O10-C8-C9-C10
19	j	601	9YF	C27-C28-C29-C30
25	j	610	9XX	C19-C20-C21-C22
13	G	101	CDL	C12-C11-CA5-OA6
13	I	605	CDL	C32-C31-CA7-OA8
25	q	302	9XX	C25-C26-C27-C36
13	i	606	CDL	C72-C71-CB7-OB8
13	i	613	CDL	C72-C71-CB7-OB8
19	V	603	9YF	C38-C39-C40-C41
19	p	604	9YF	O11-C25-C26-C27
18	q	301	PLM	CA-CB-CC-CD
13	U	604	CDL	C12-C11-CA5-OA7
13	i	606	CDL	C32-C31-CA7-OA9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	j	608	MQ9	C12-C11-C9-C10
13	i	606	CDL	OA5-CA3-CA4-OA6
14	G	102	9Y0	O7-C1-C2-O3
21	i	609	MQ9	C13-C14-C16-C17
21	j	607	MQ9	C13-C14-C16-C17
13	i	613	CDL	C72-C71-CB7-OB9
15	L	603	HEA	CAA-CBA-CGA-O2A
24	i	604	HEM	CAD-CBD-CGD-O2D
13	i	603	CDL	C52-C51-CB5-OB6
13	I	604	CDL	C12-C13-C14-C15
13	L	607	CDL	C15-C16-C17-C18
14	G	102	9Y0	C7-C8-C9-C10
13	b	101	CDL	C35-C36-C37-C38
13	b	101	CDL	C32-C31-CA7-OA9
13	i	613	CDL	C12-C11-CA5-OA7
13	i	606	CDL	C32-C31-CA7-OA8
19	p	604	9YF	O12-C25-C26-C27
13	i	612	CDL	C72-C71-CB7-OB8

There are no ring outliers.

43 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	q	301	PLM	5	0
21	i	610	MQ9	13	0
24	j	603	HEM	1	0
21	n	201	MQ9	5	0
14	I	608	9Y0	3	0
13	V	602	CDL	14	0
13	i	606	CDL	4	0
13	G	101	CDL	8	0
15	I	602	HEA	8	0
14	I	610	9Y0	8	0
18	I	609	PLM	1	0
21	i	609	MQ9	4	0
15	L	603	HEA	6	0
13	b	101	CDL	6	0
21	j	608	MQ9	10	0
25	q	302	9XX	3	0
15	L	602	HEA	2	0
13	j	611	CDL	1	0
14	L	601	9Y0	1	0

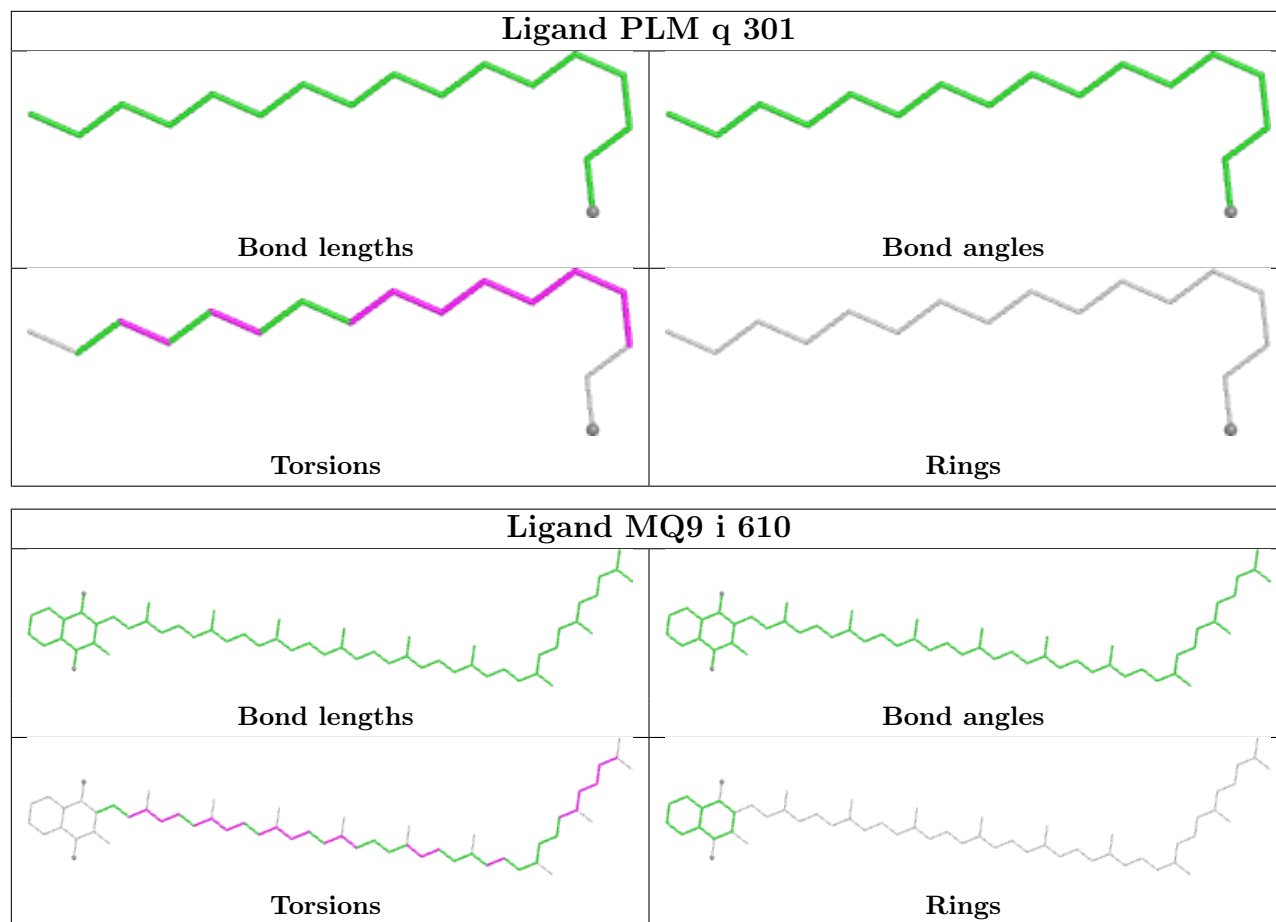
*Continued on next page...*

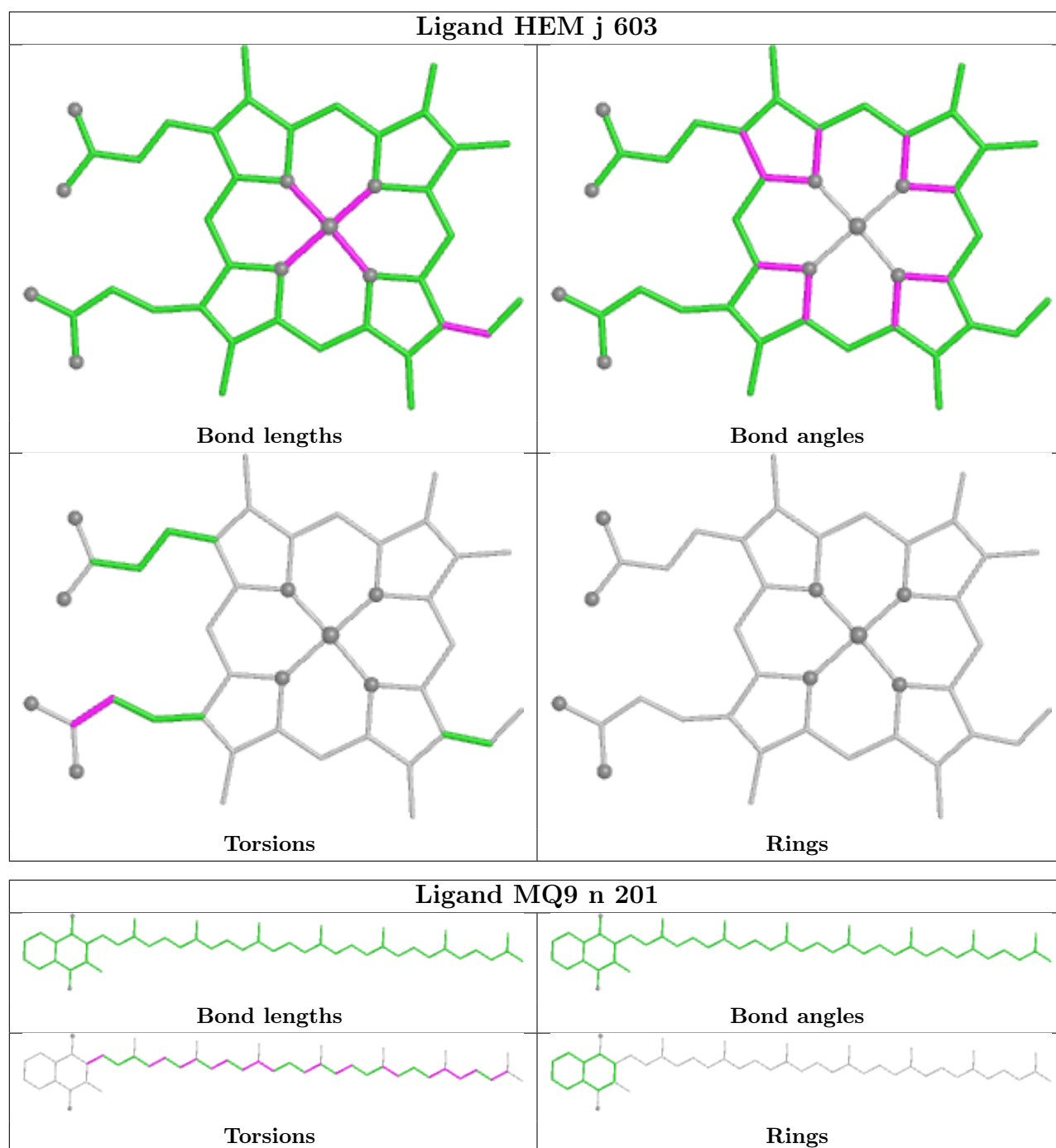


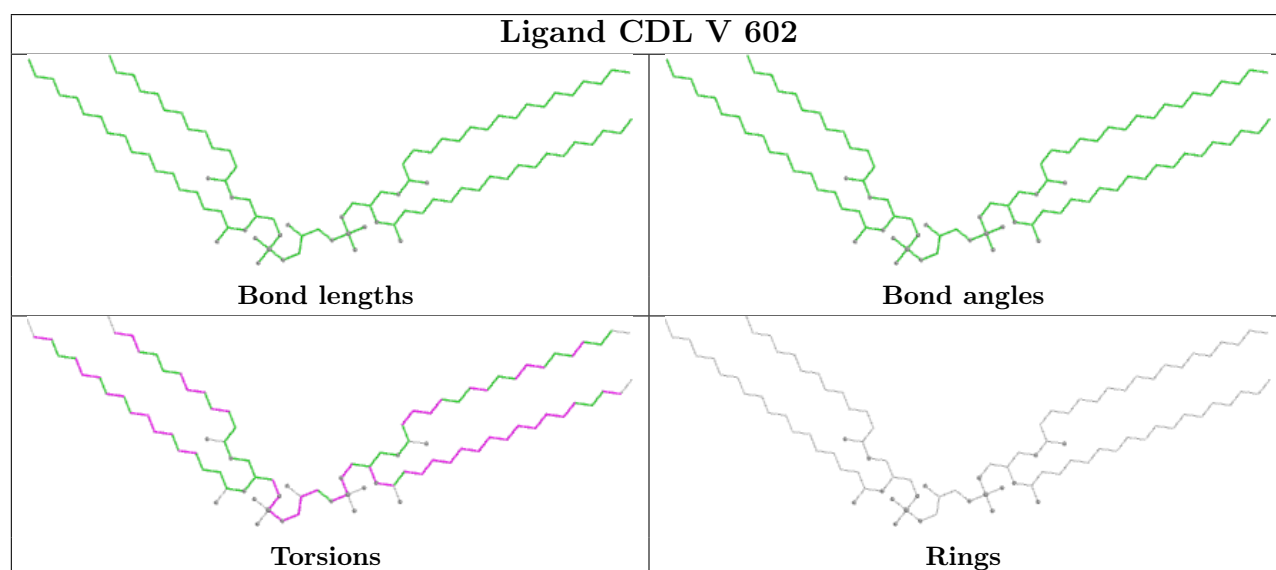
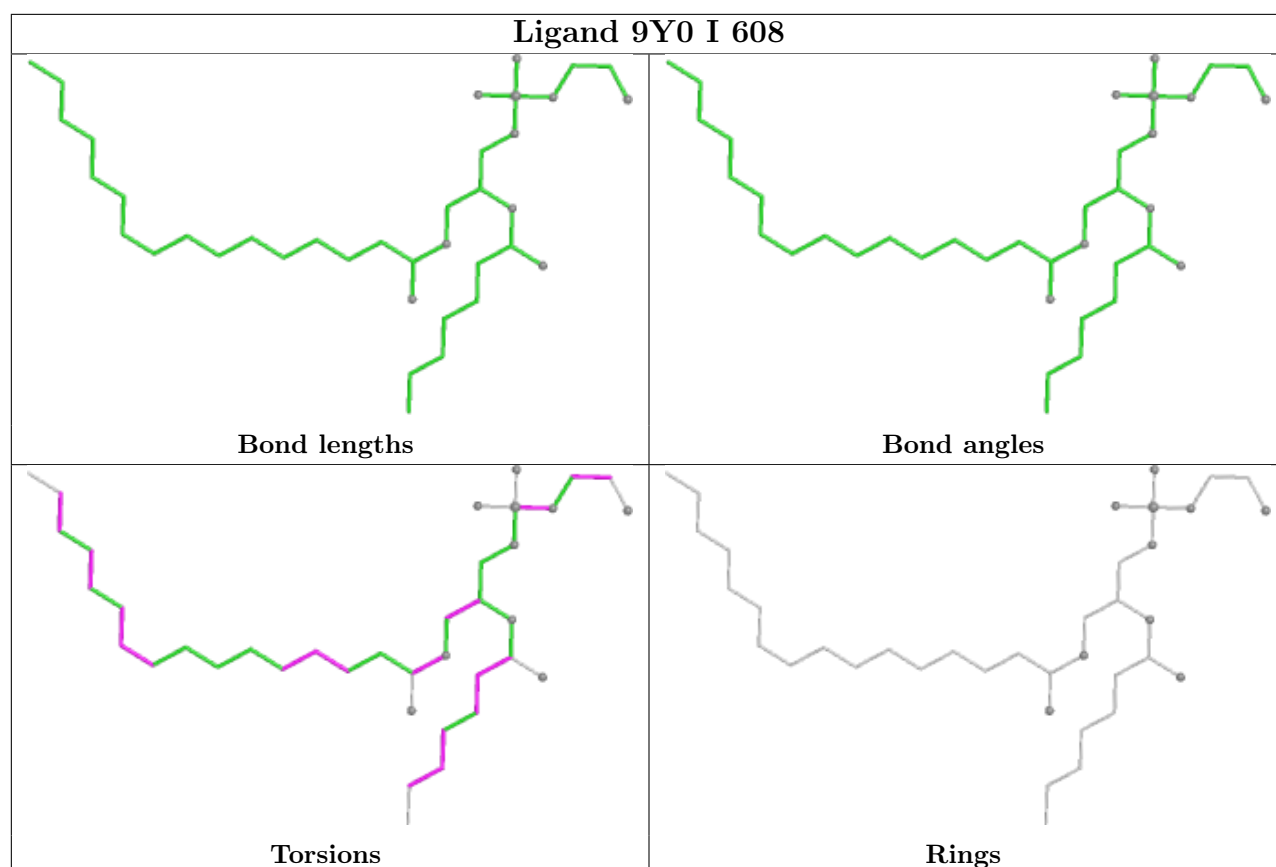
*Continued from previous page...*

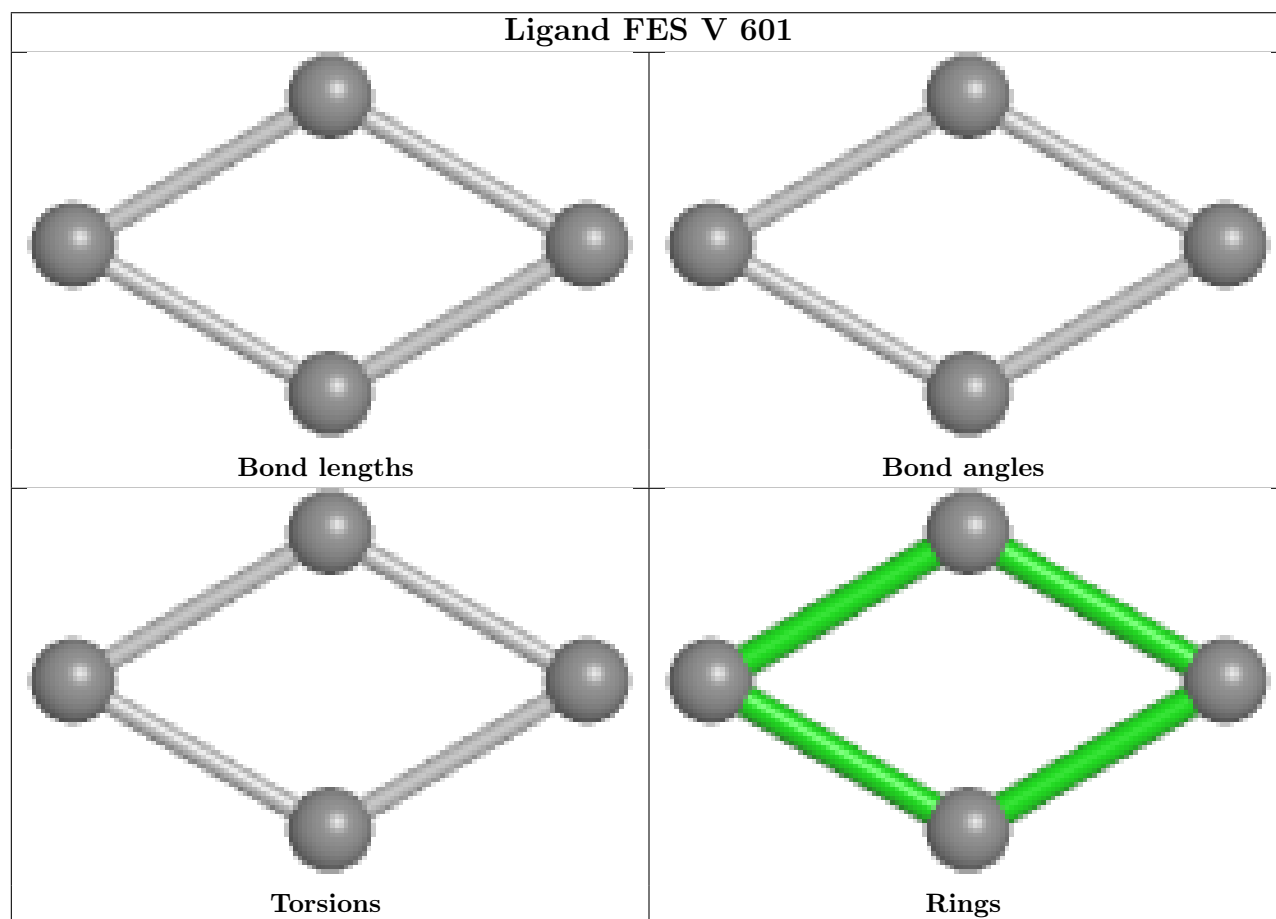
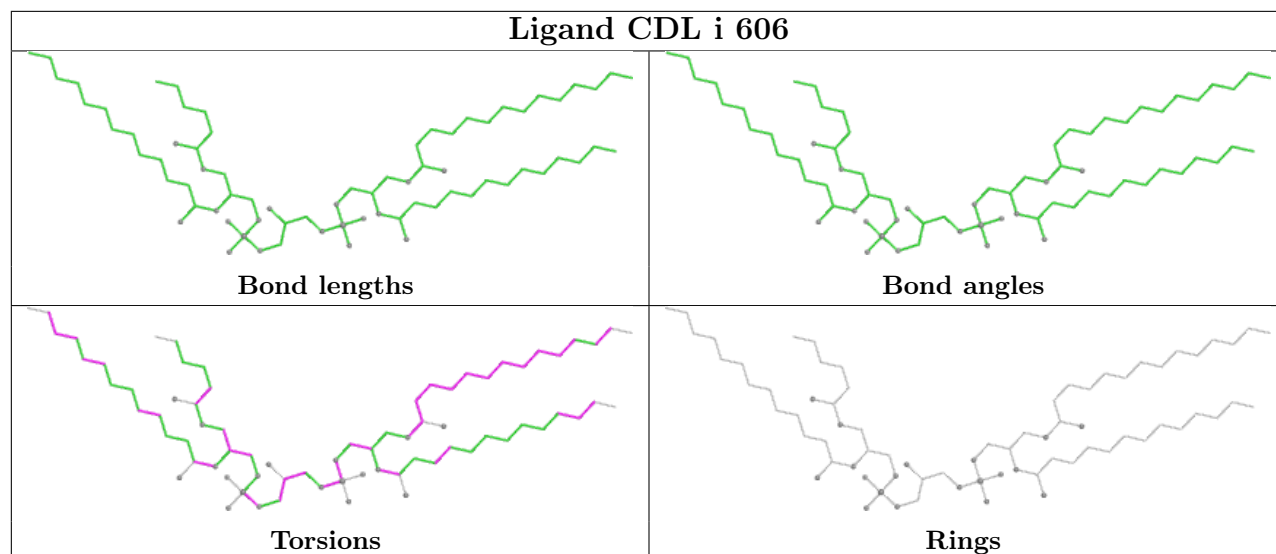
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	604	CDL	1	0
13	U	604	CDL	2	0
13	i	603	CDL	3	0
21	U	603	MQ9	1	0
20	U	602	HEC	1	0
21	o	604	MQ9	3	0
13	p	603	CDL	4	0
13	L	607	CDL	3	0
13	i	608	CDL	2	0
13	i	612	CDL	2	0
24	j	604	HEM	2	0
13	L	606	CDL	1	0
13	I	605	CDL	7	0
21	j	607	MQ9	1	0
15	I	601	HEA	1	0
20	U	601	HEC	3	0
13	j	605	CDL	1	0
20	o	601	HEC	2	0
20	o	602	HEC	2	0
24	i	604	HEM	1	0
24	i	605	HEM	2	0
21	m	201	MQ9	2	0
13	i	607	CDL	2	0
13	i	613	CDL	1	0

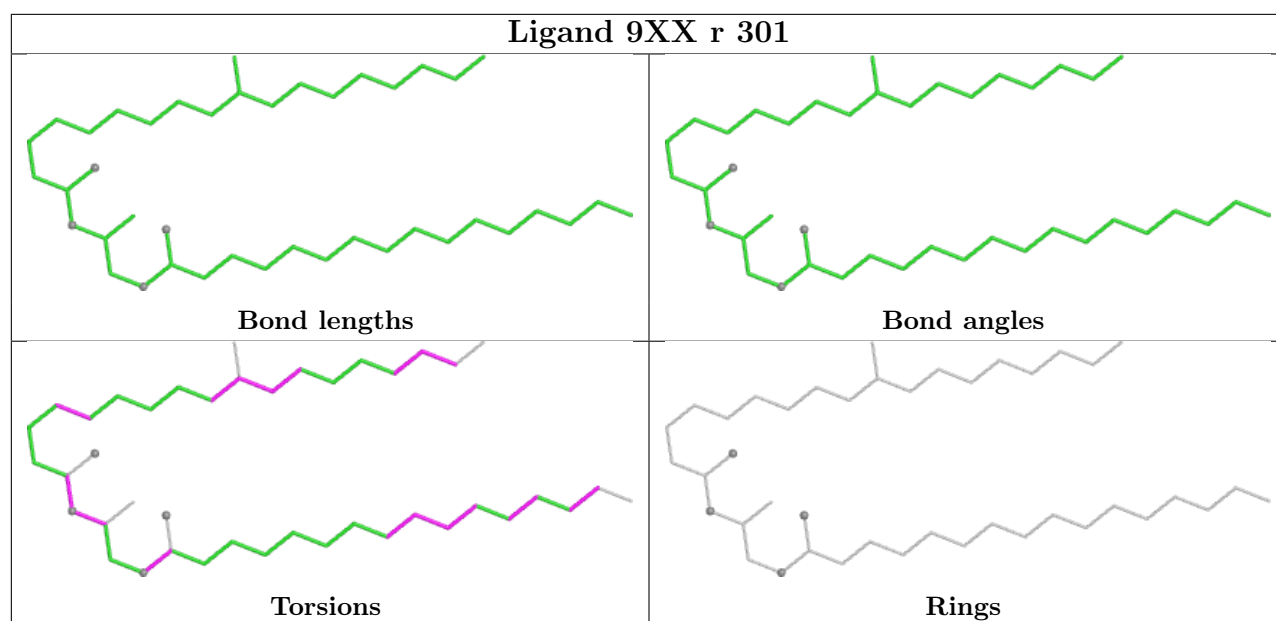
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

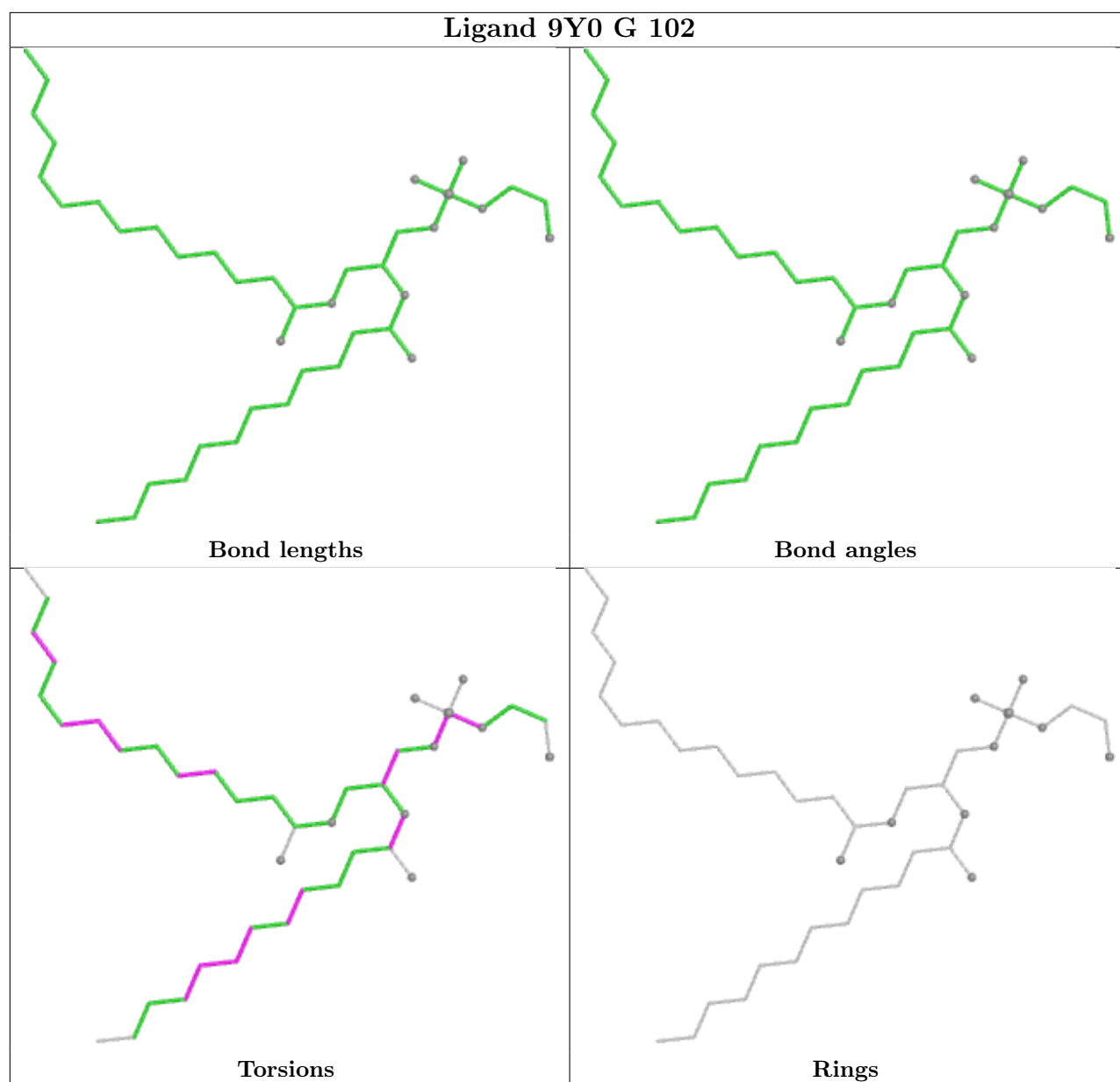


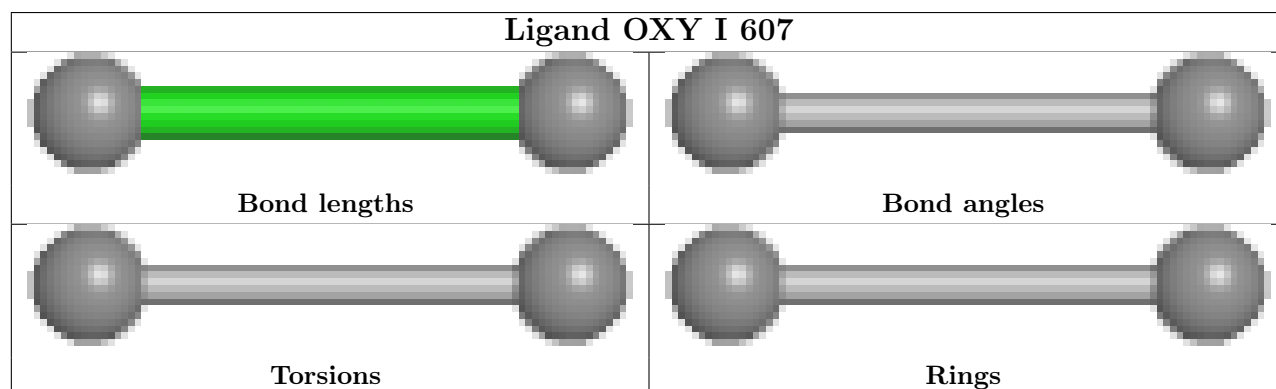
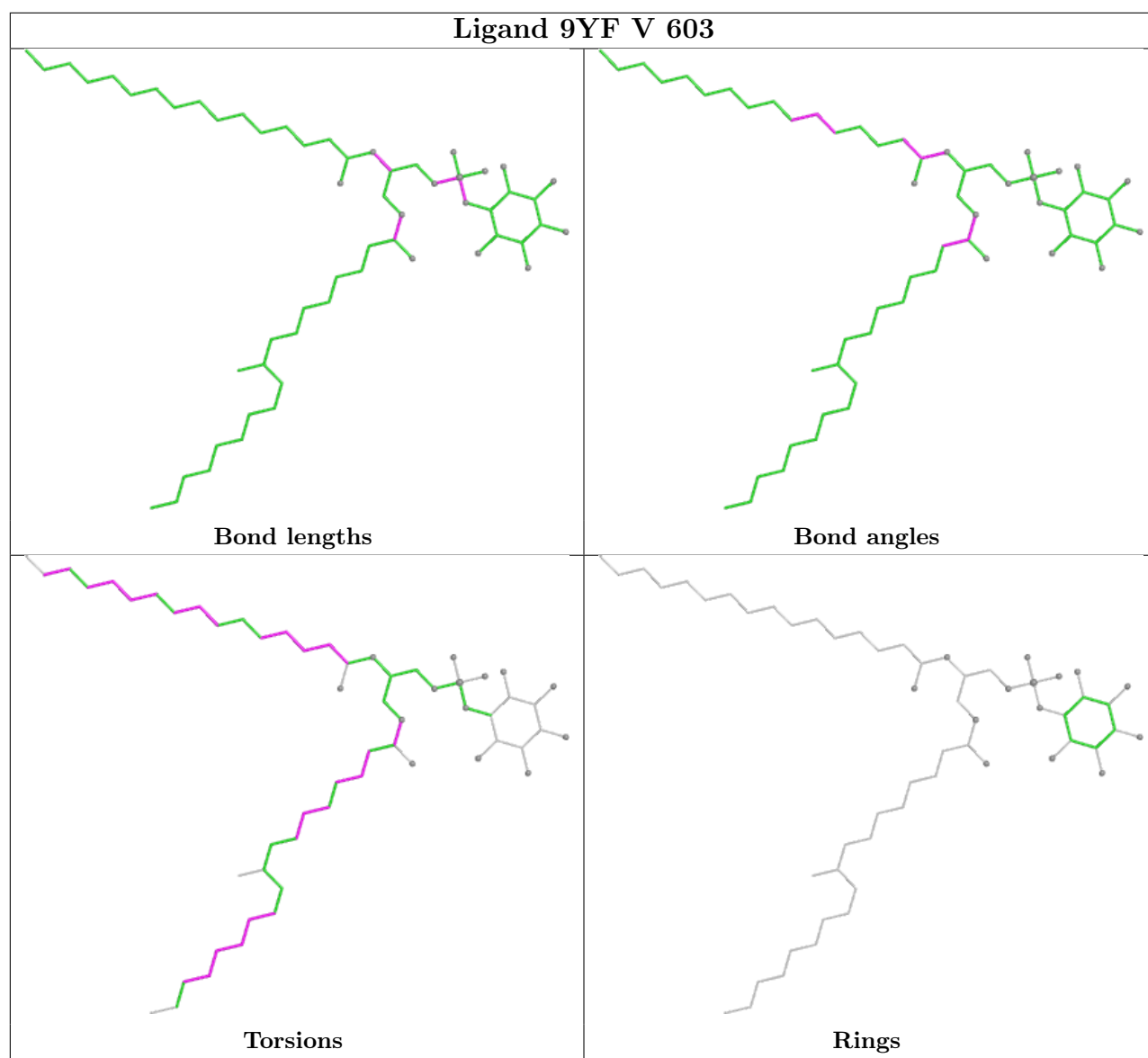




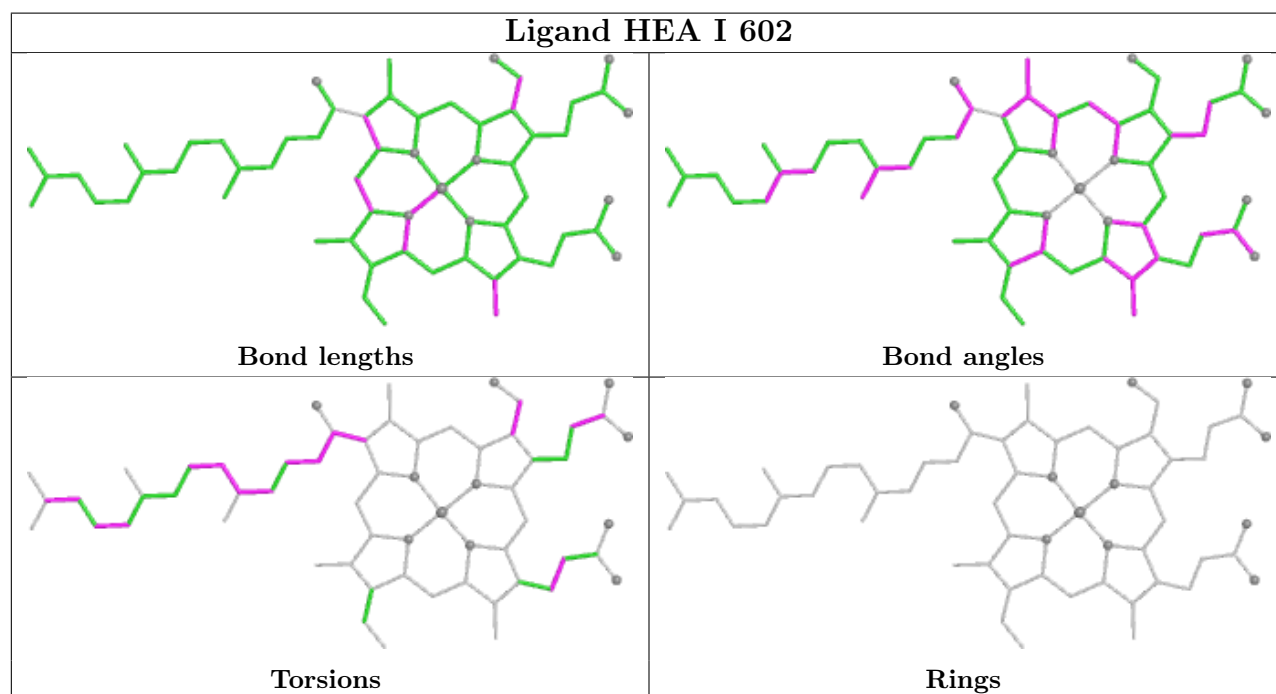
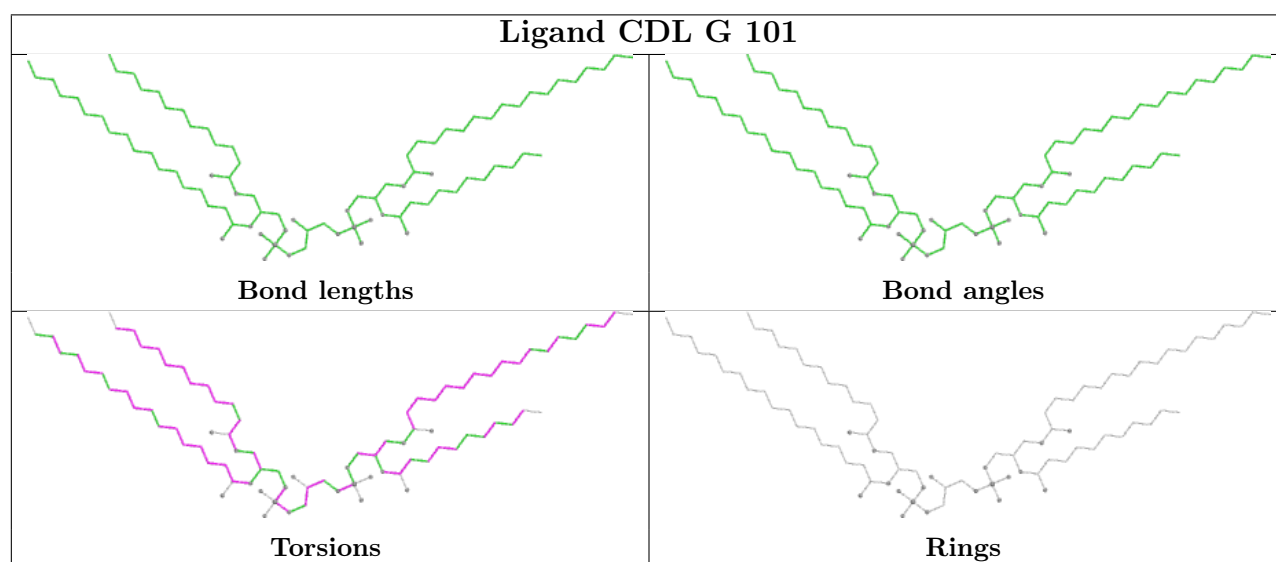
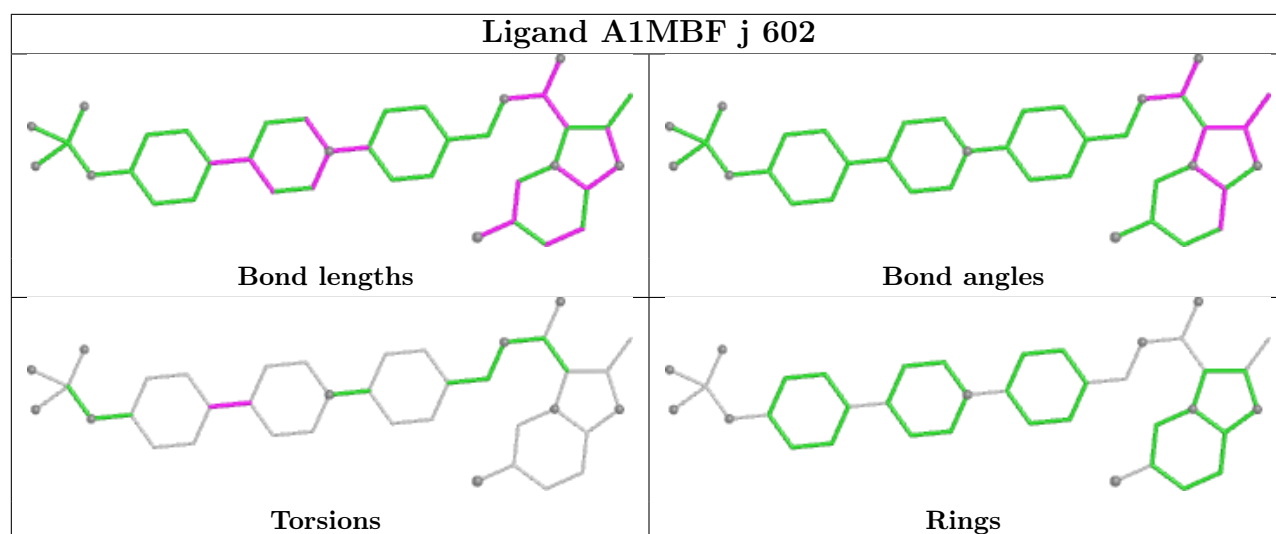


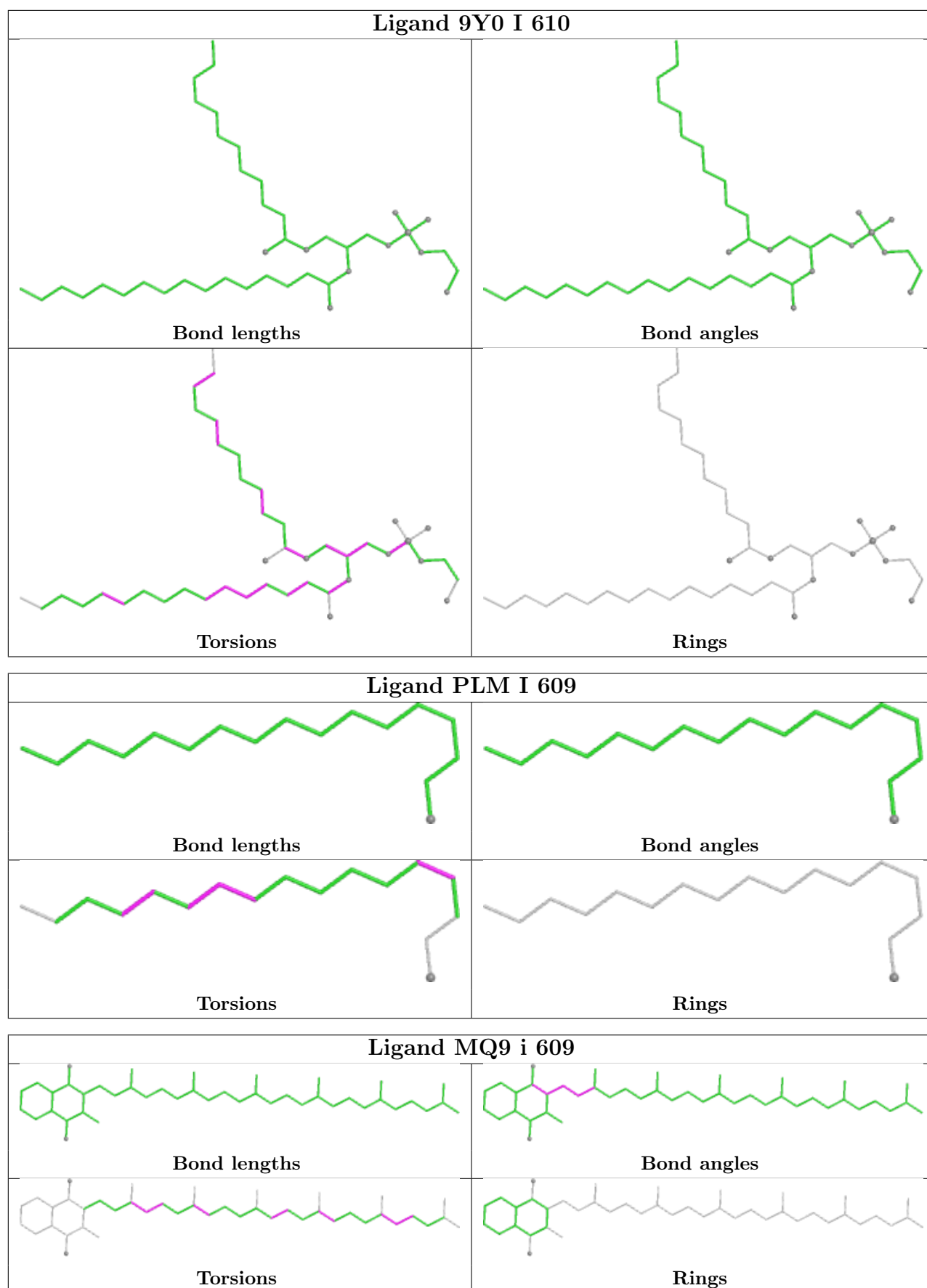


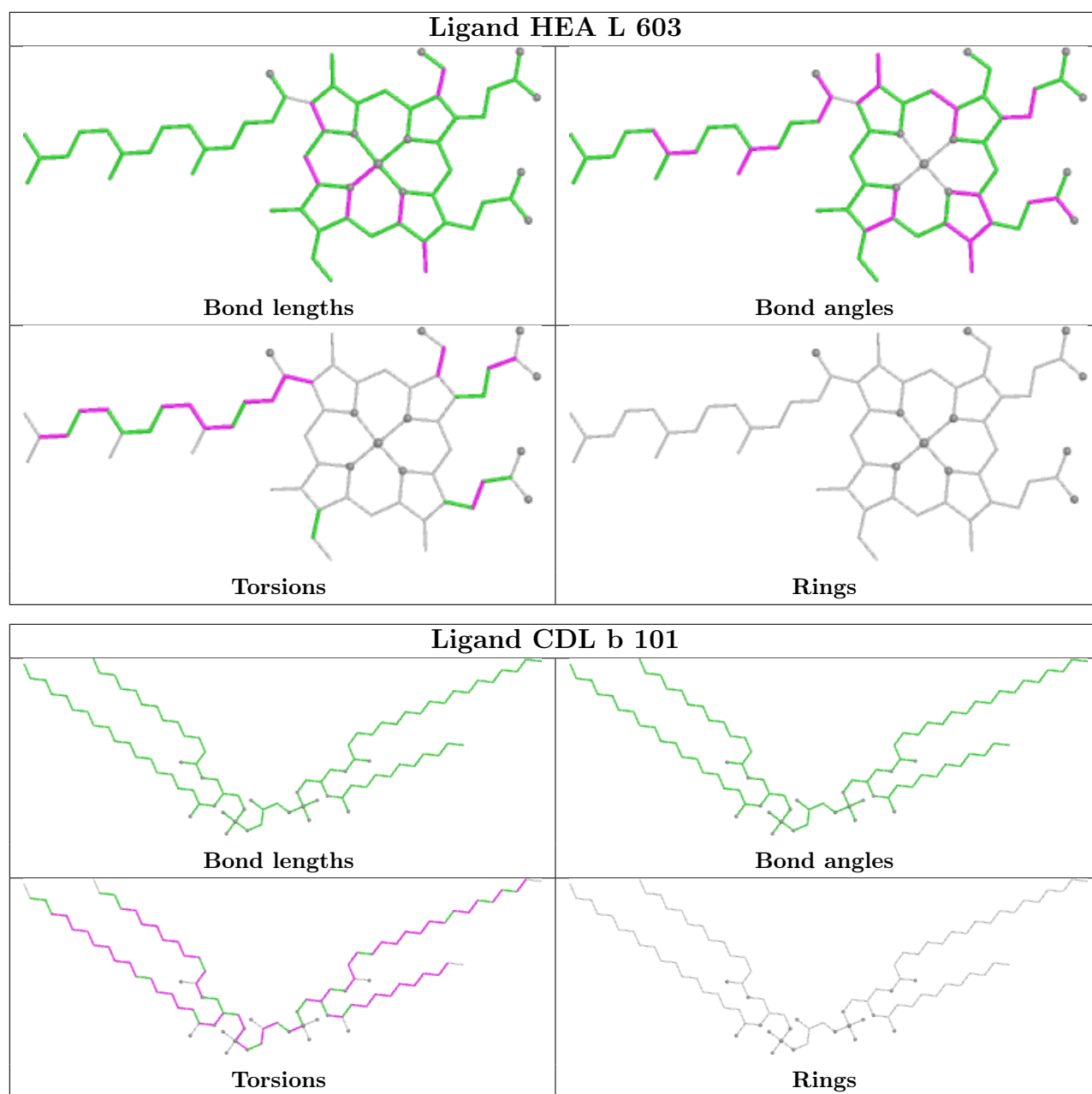


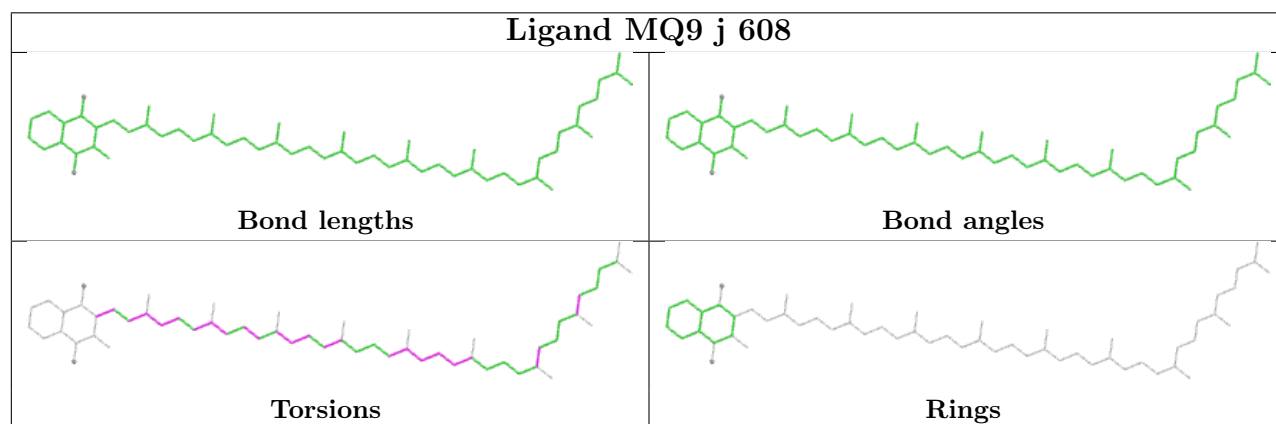
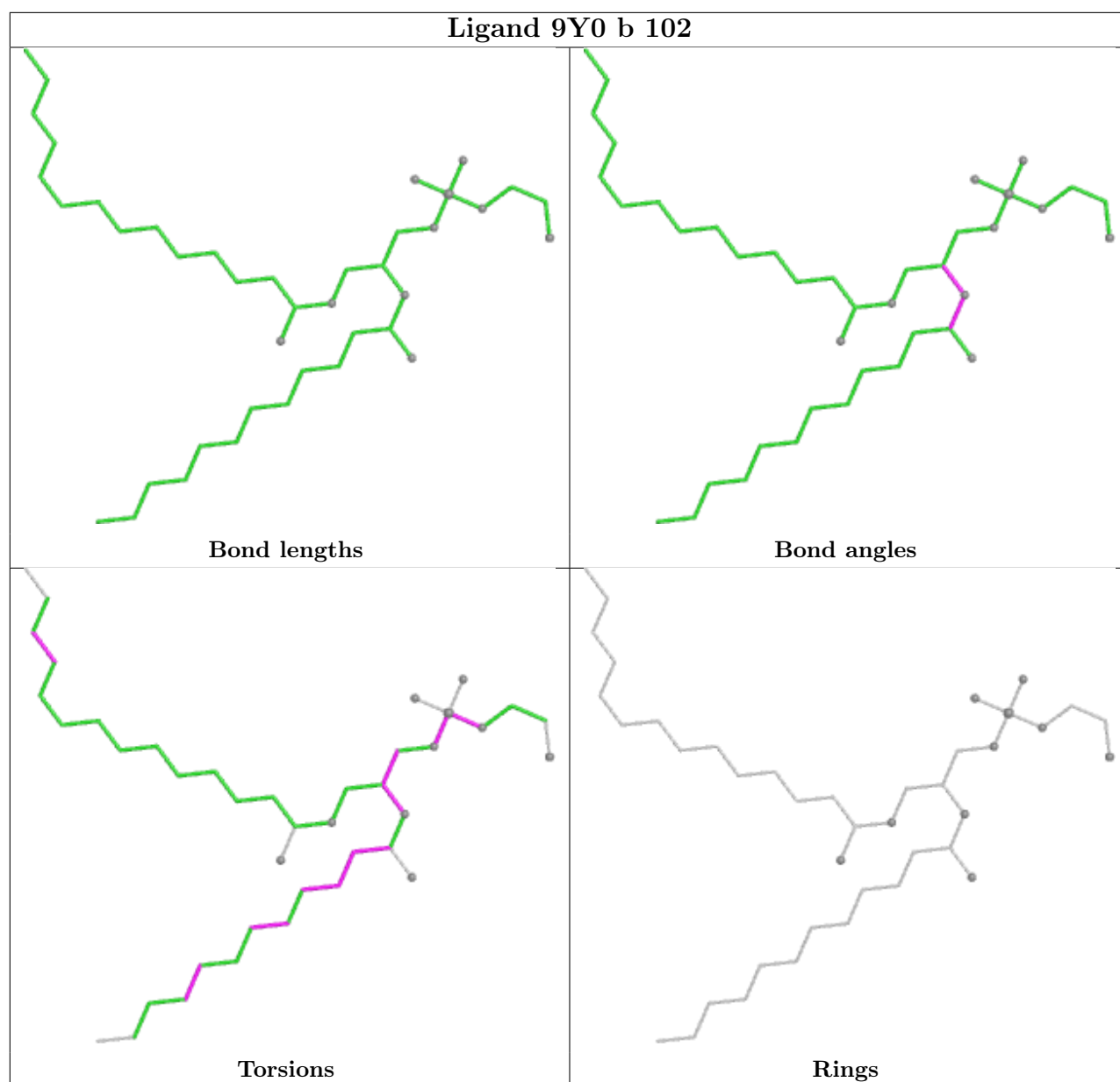


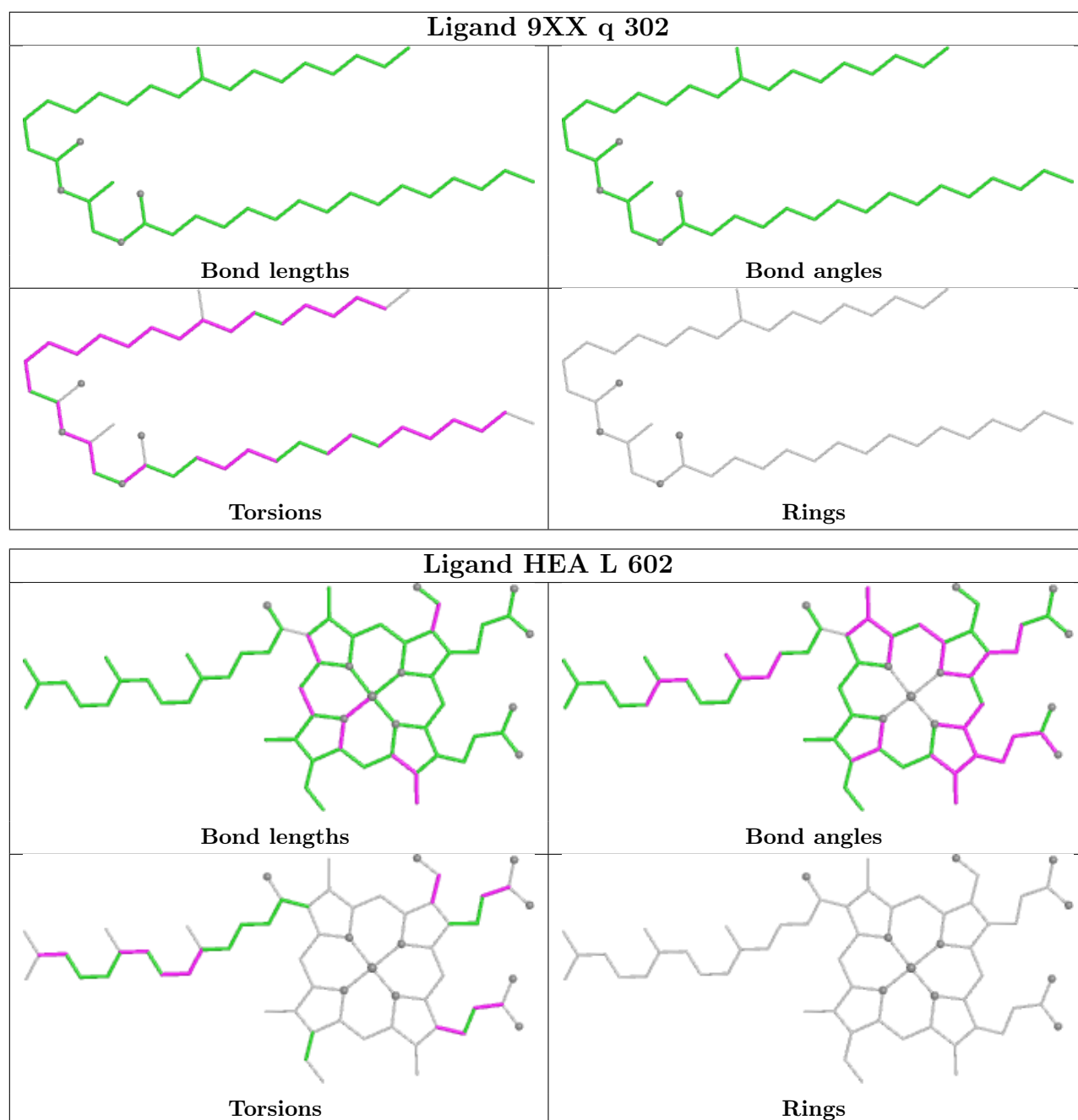


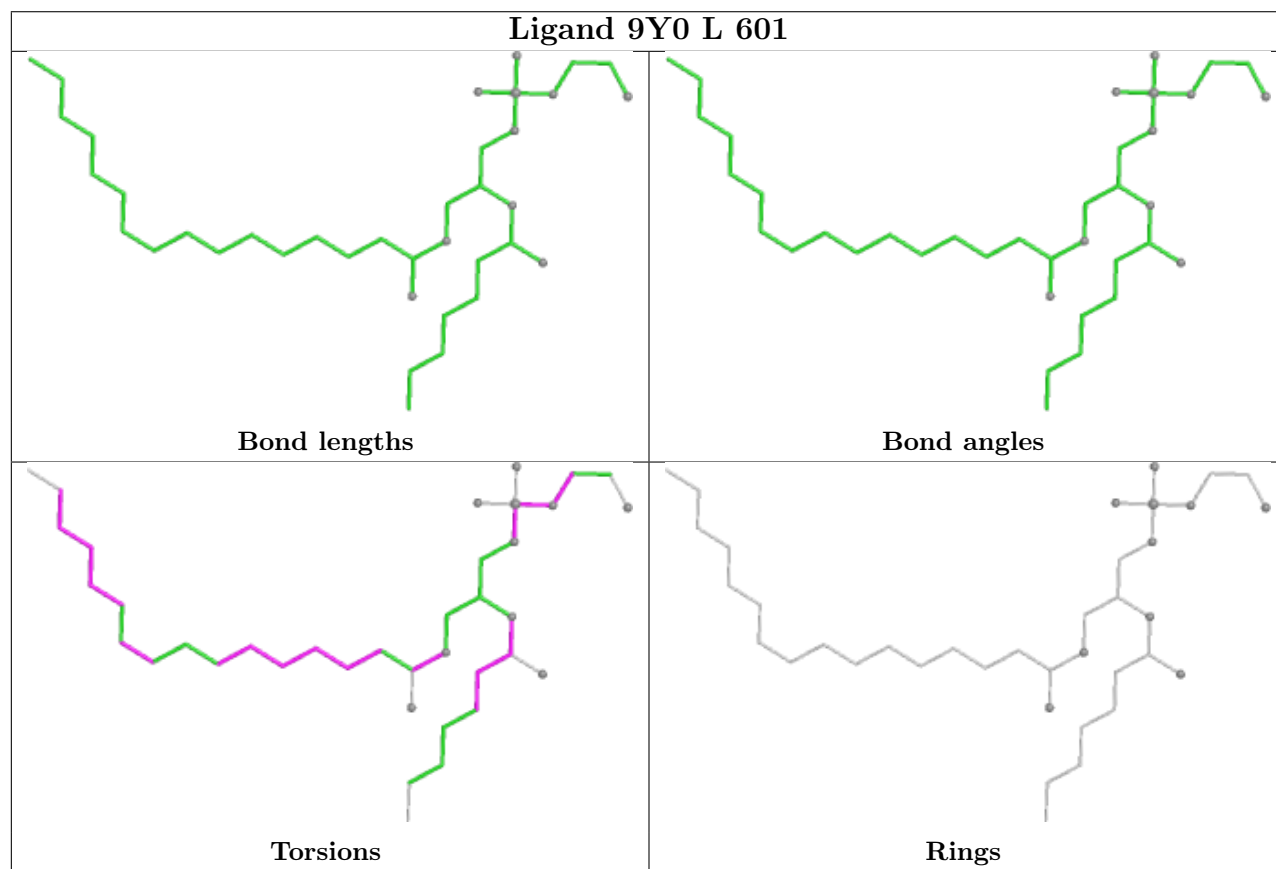
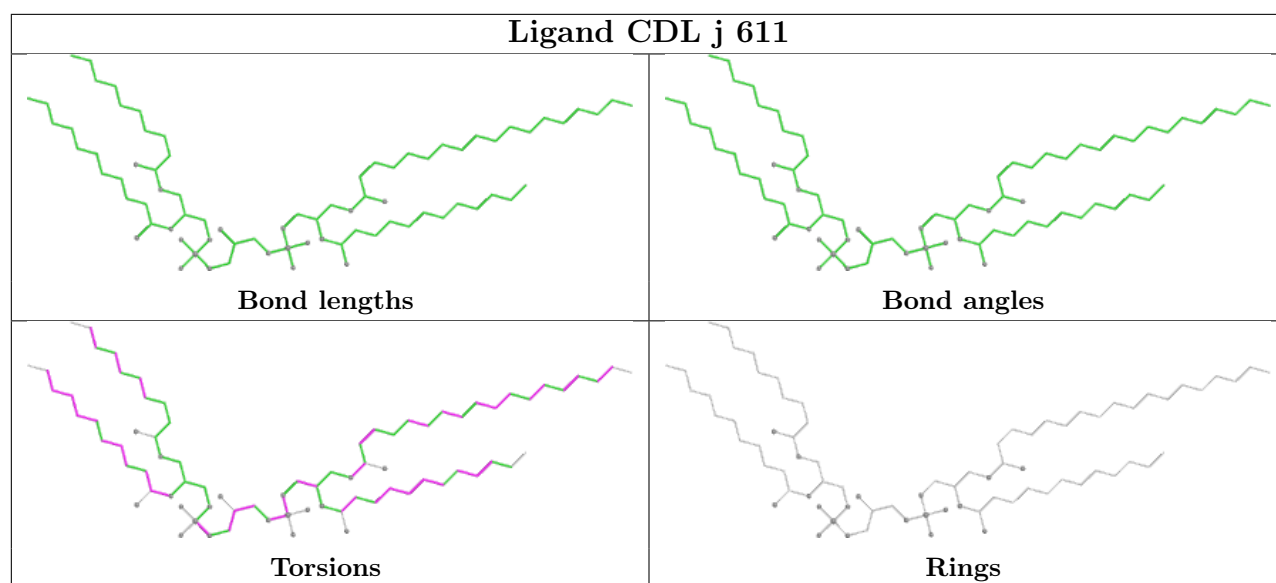


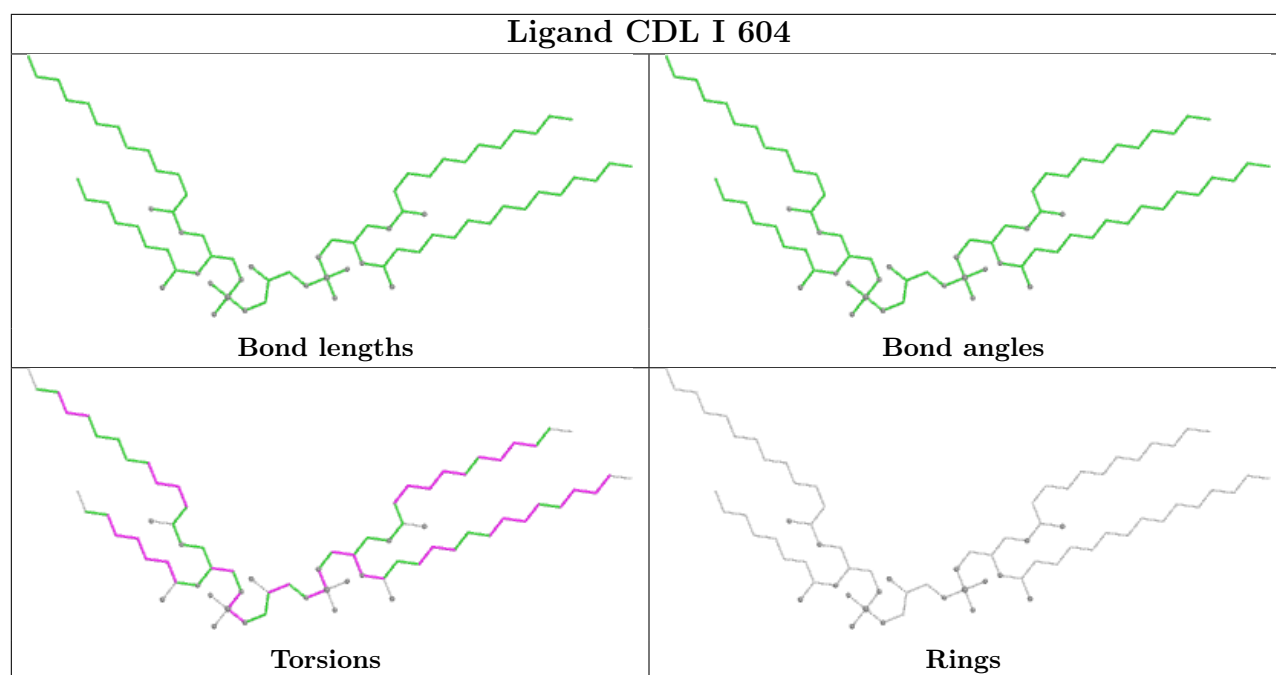


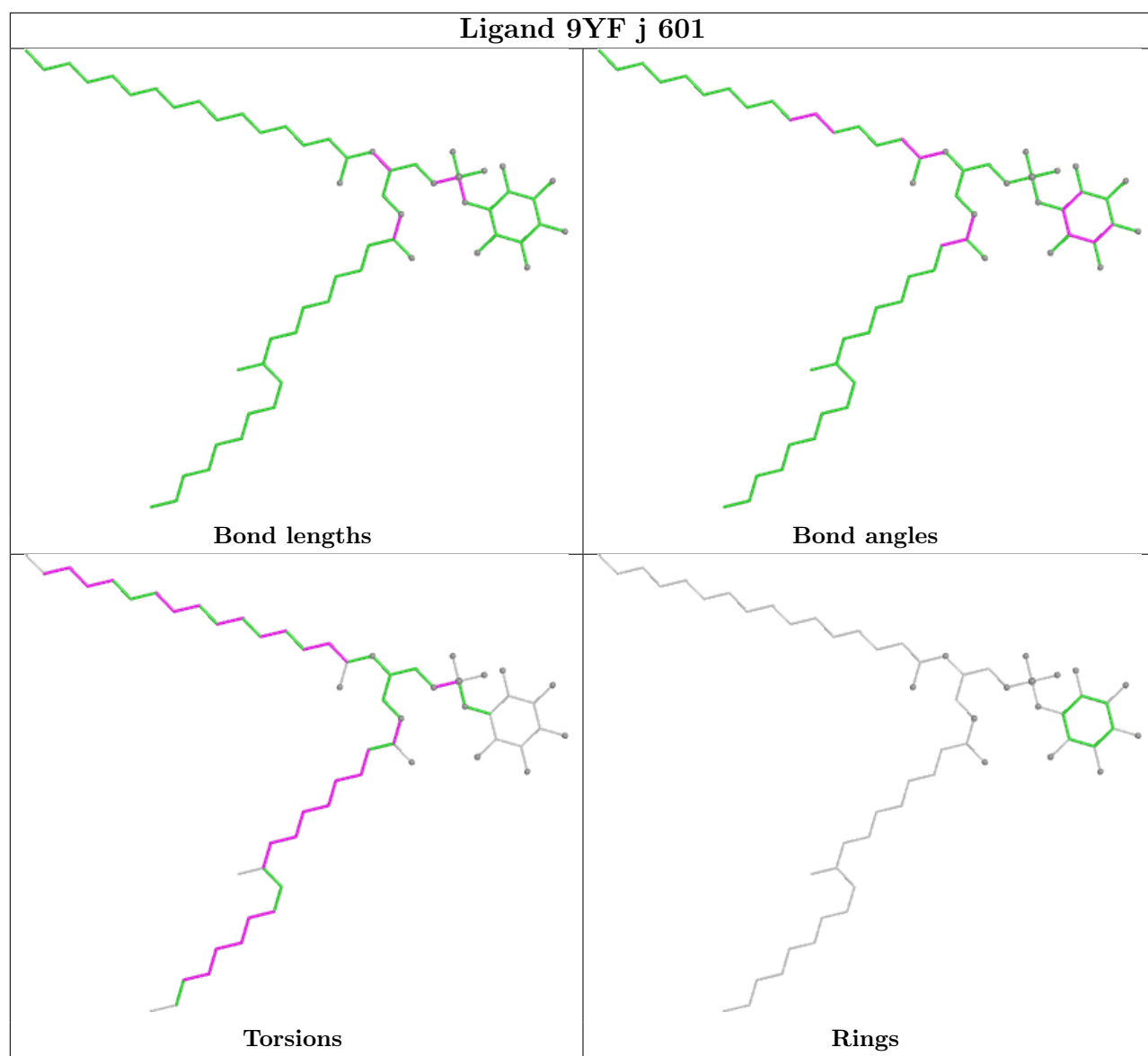




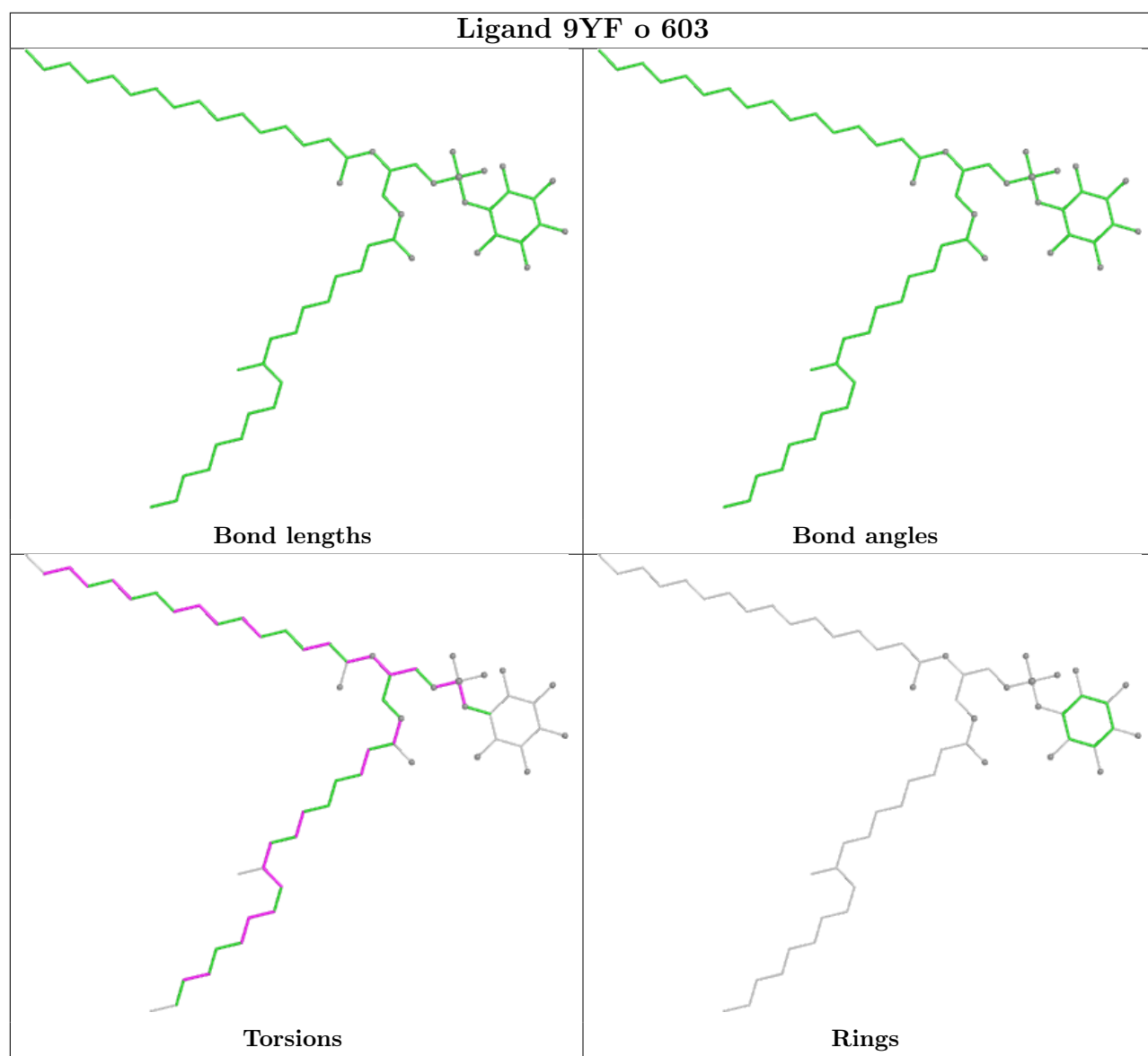


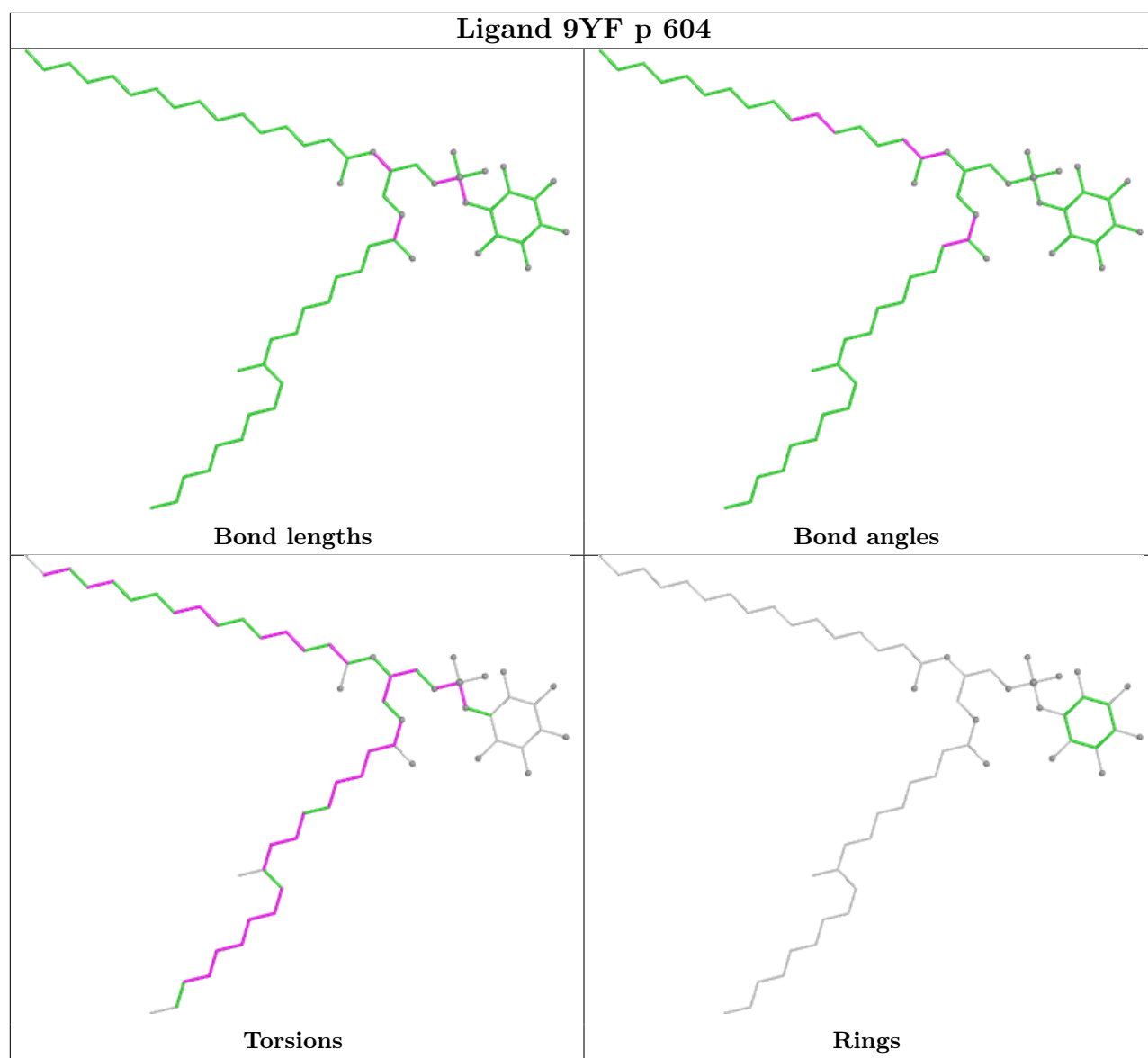


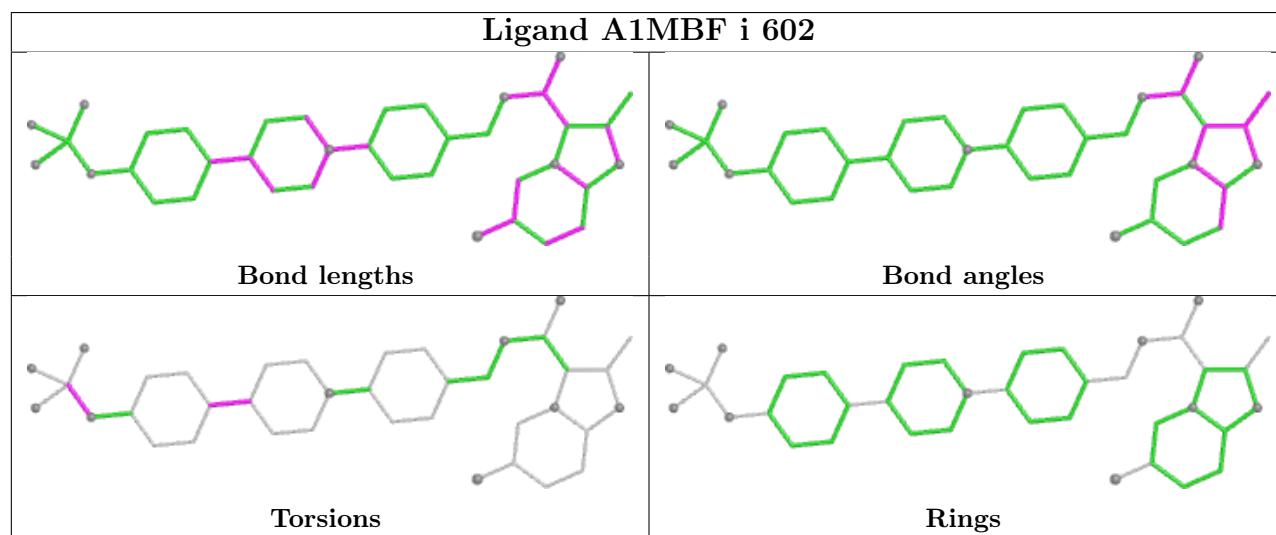
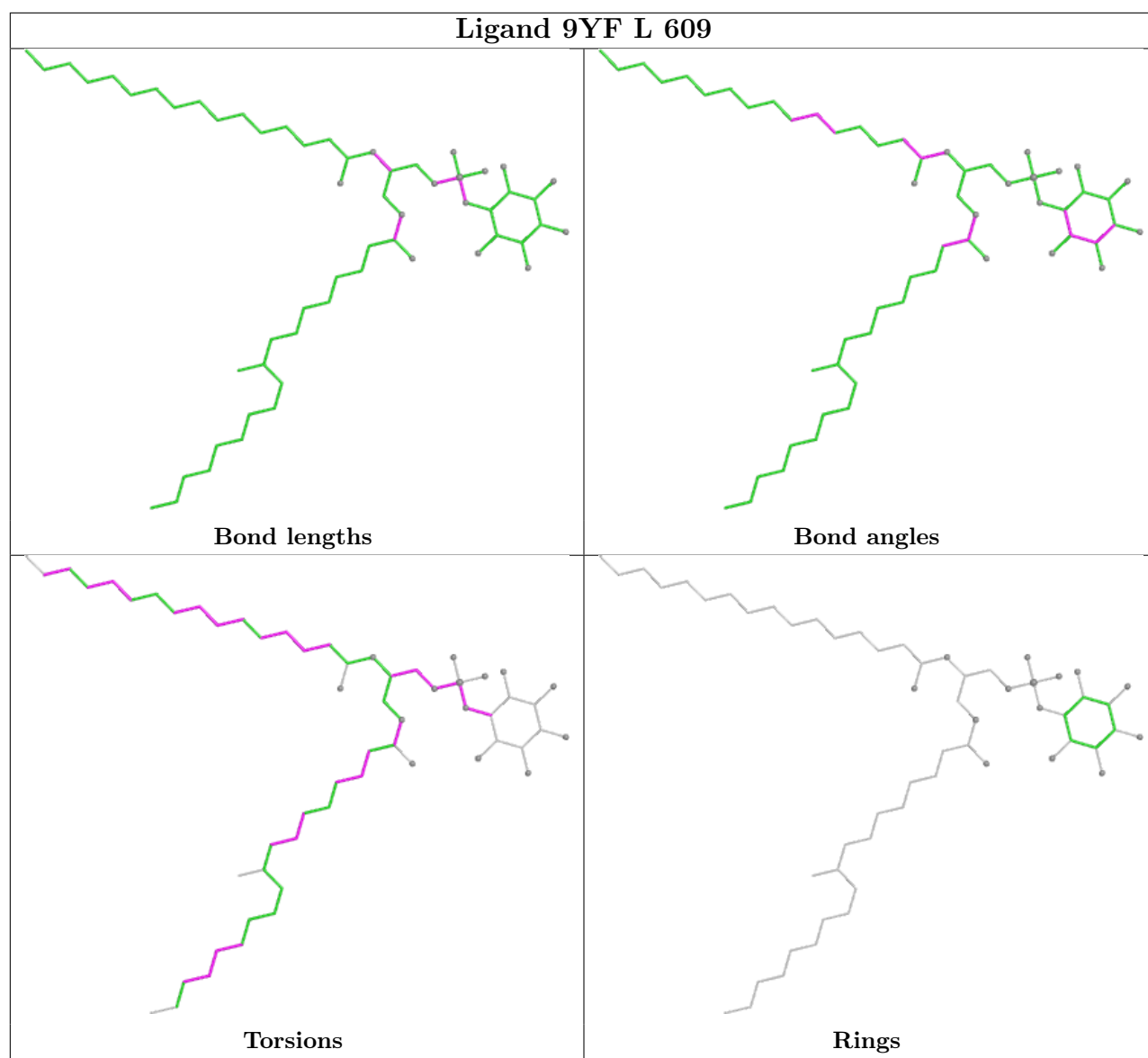


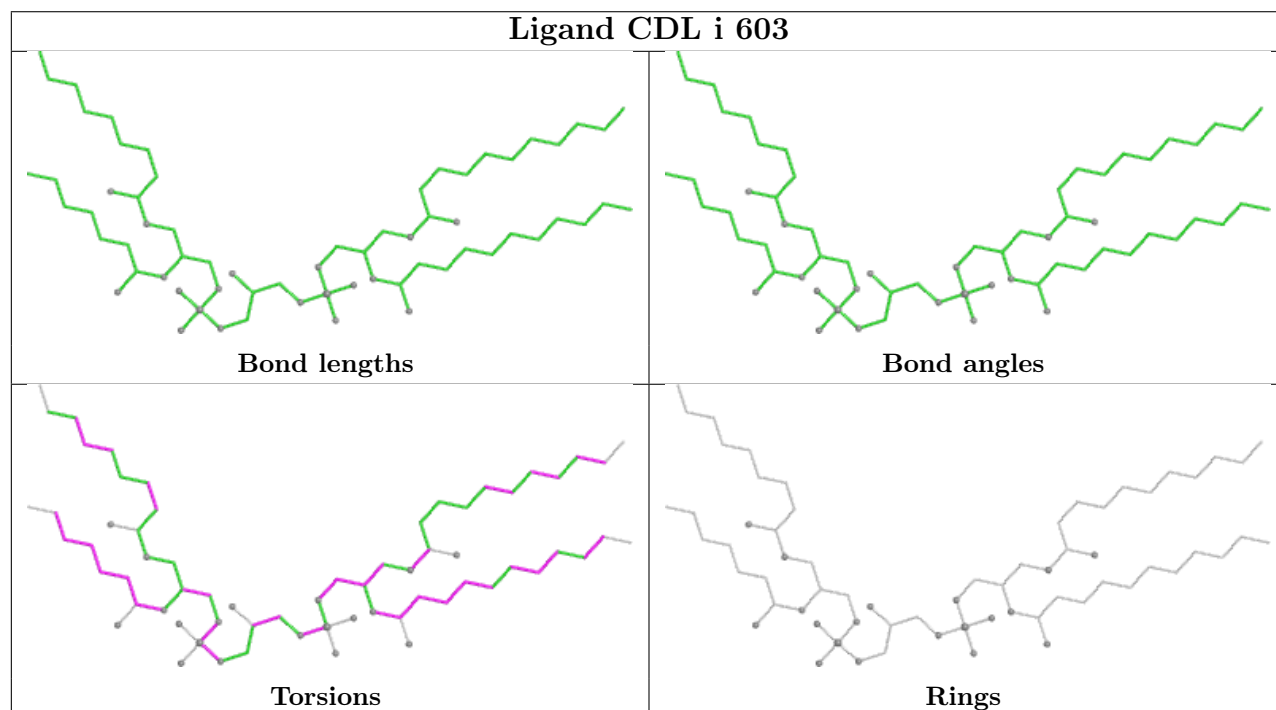
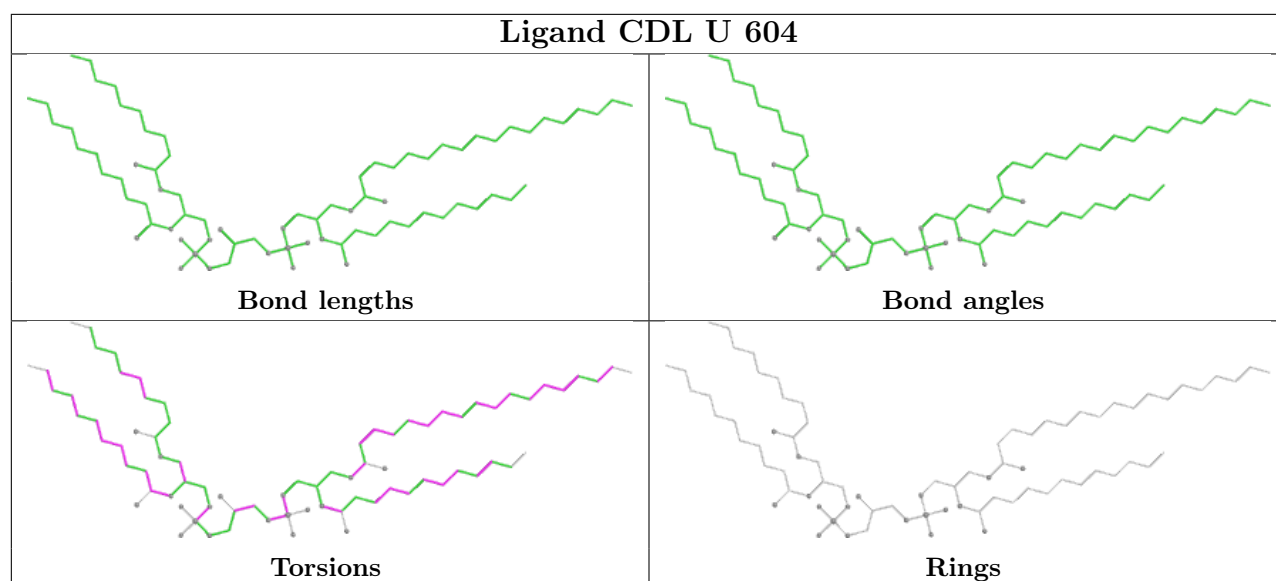


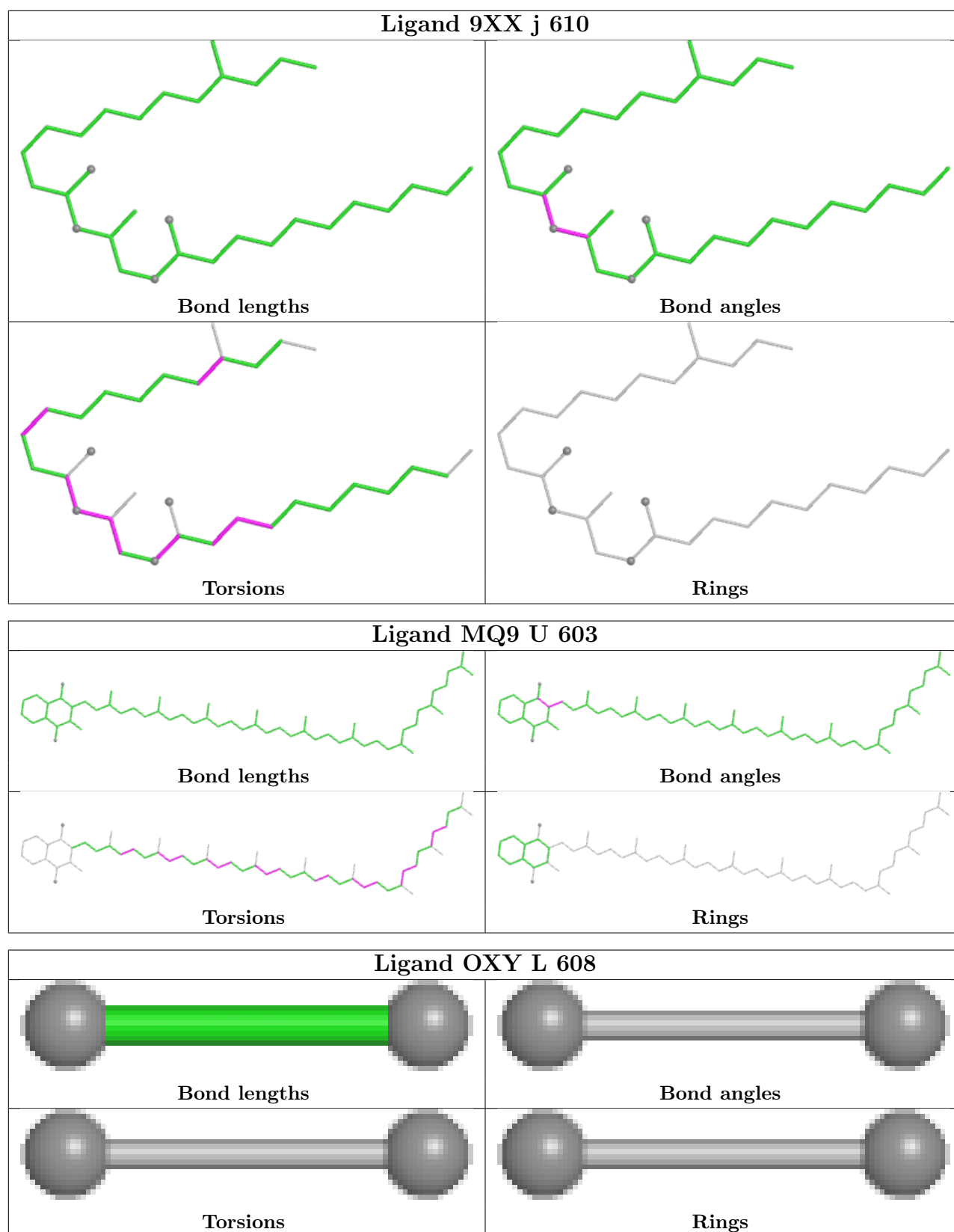


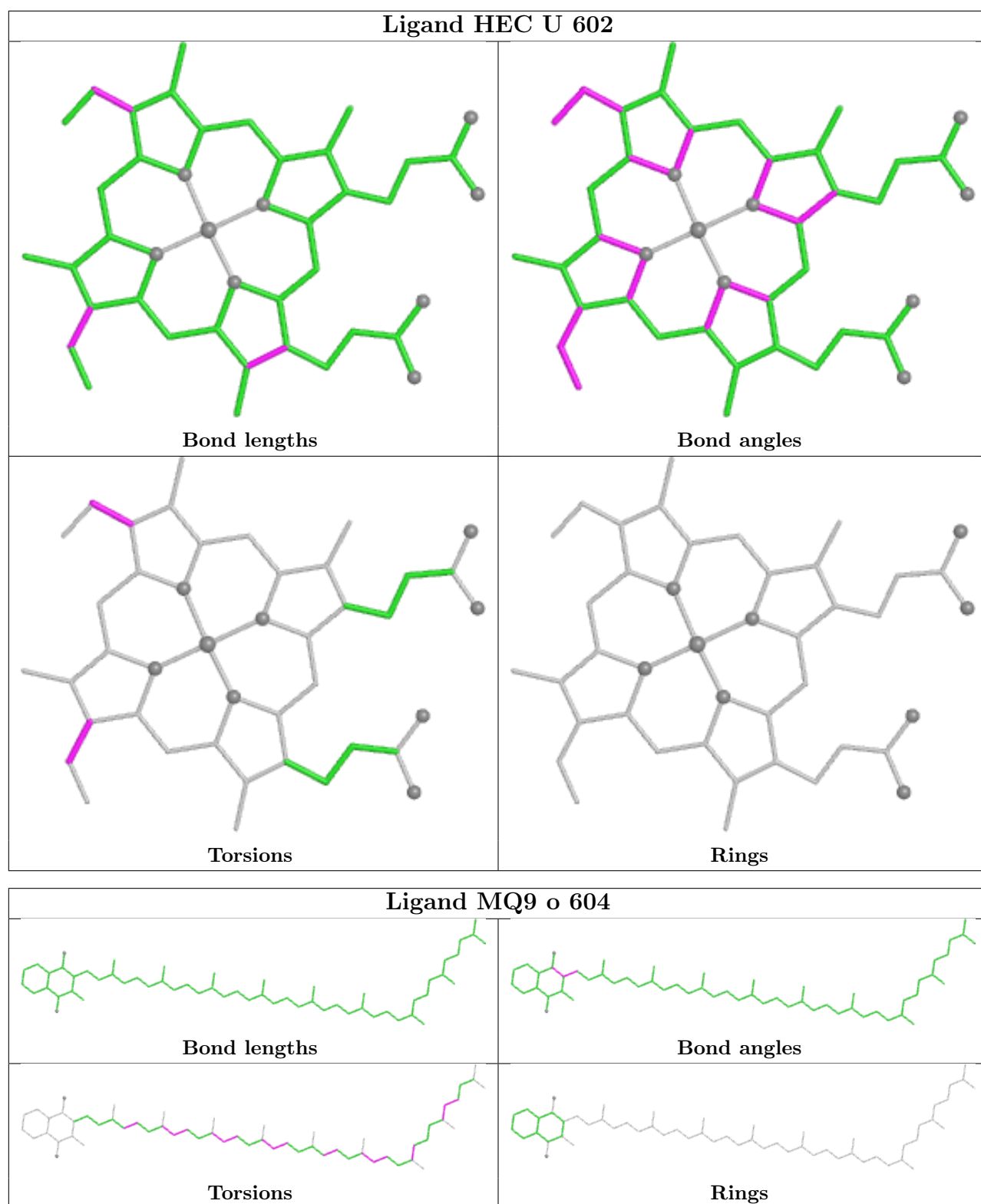


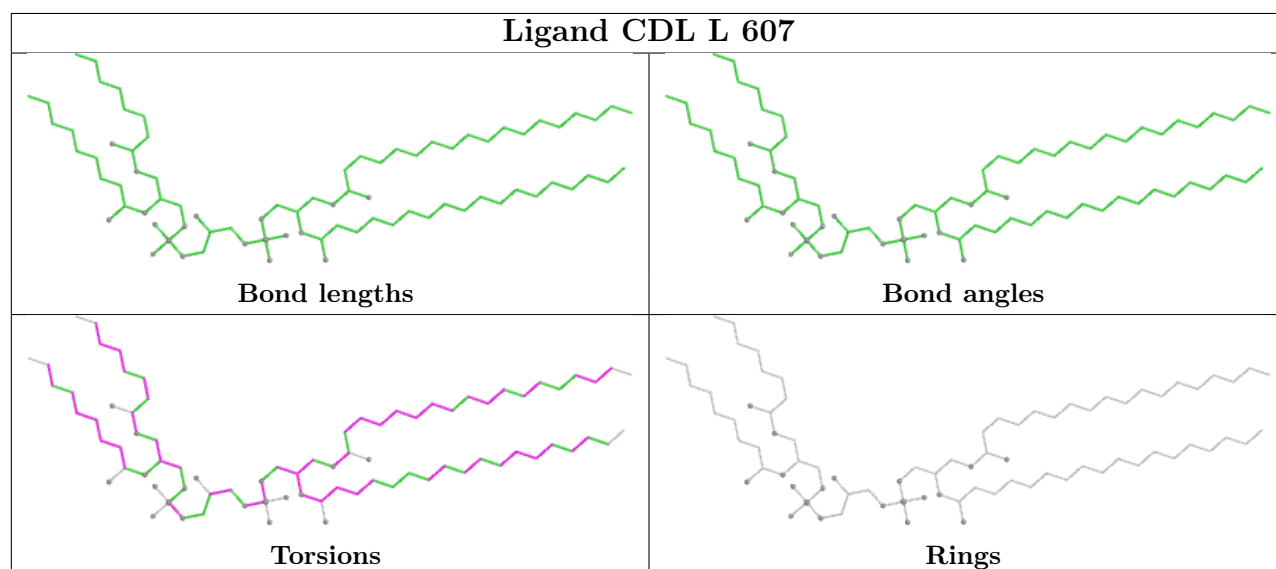
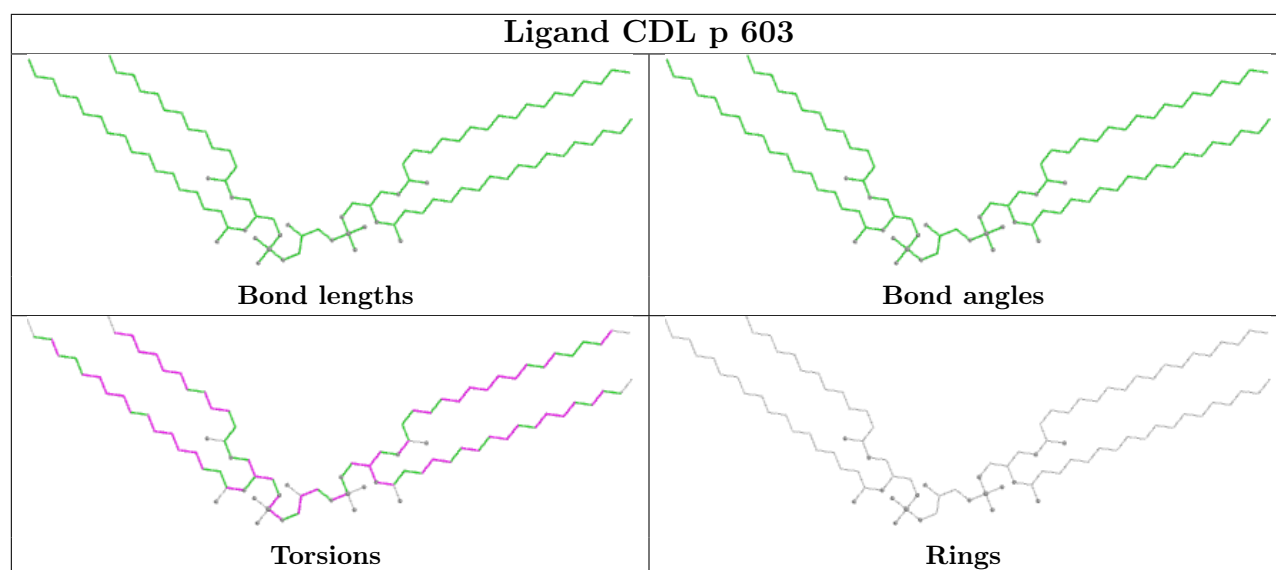




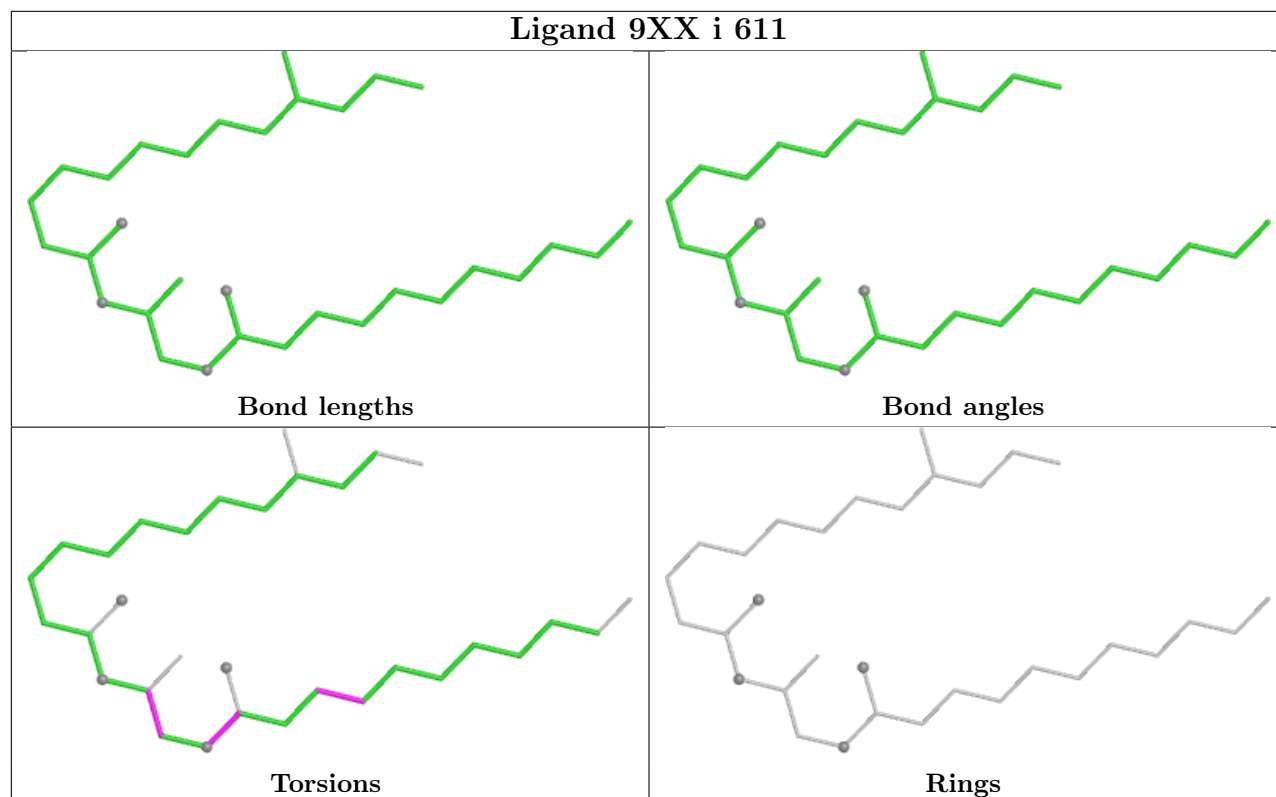




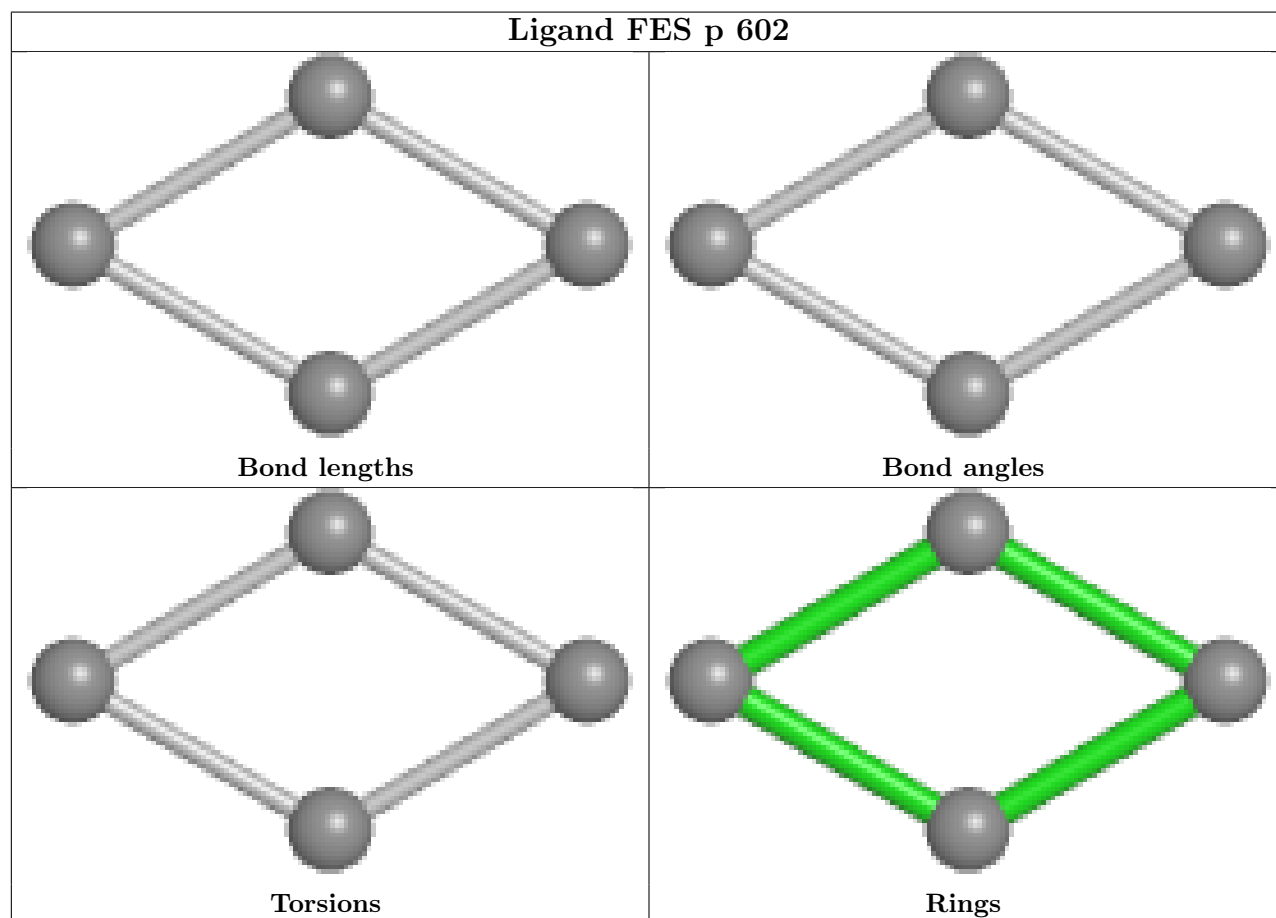




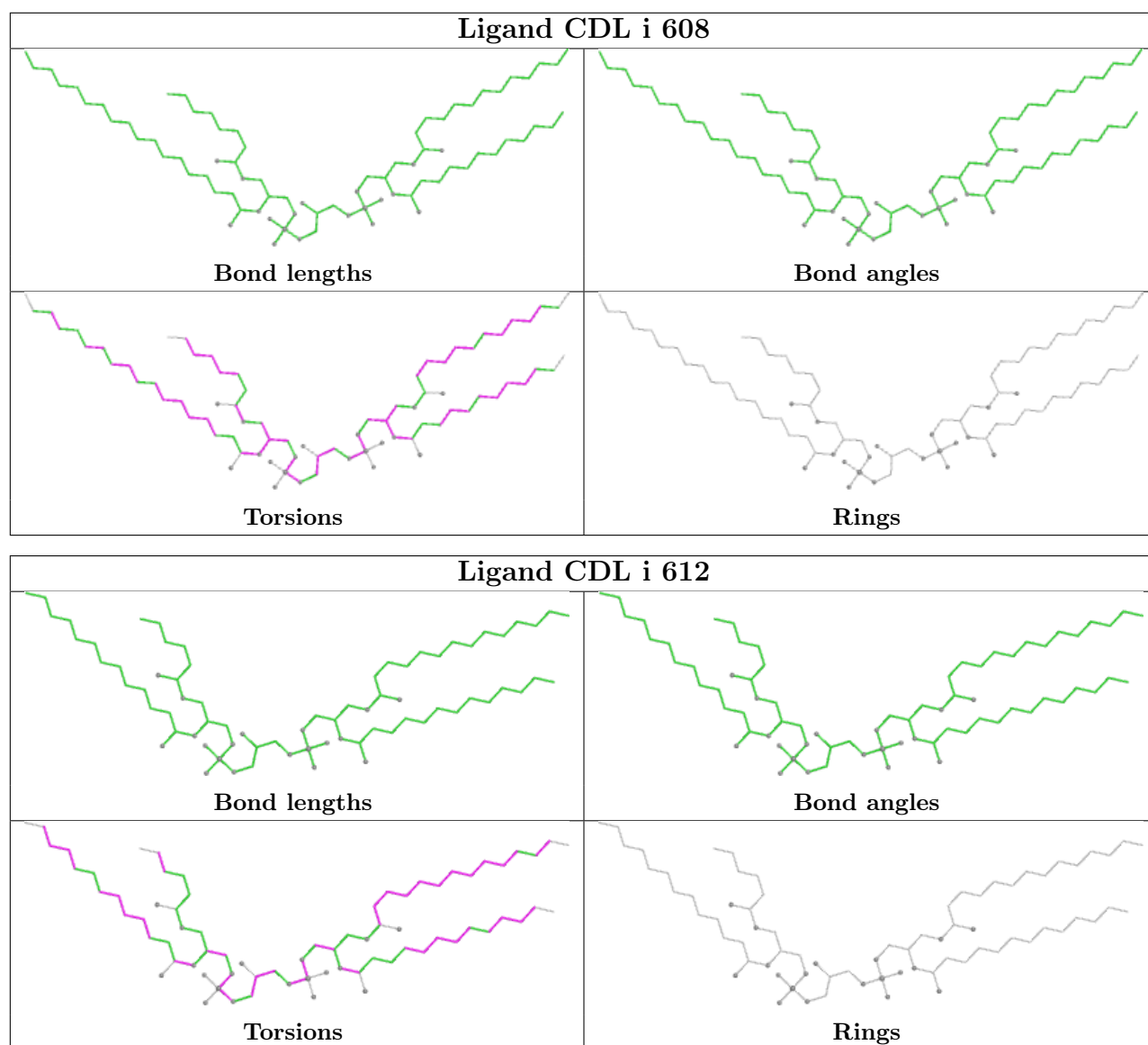
## Ligand 9XX i 611



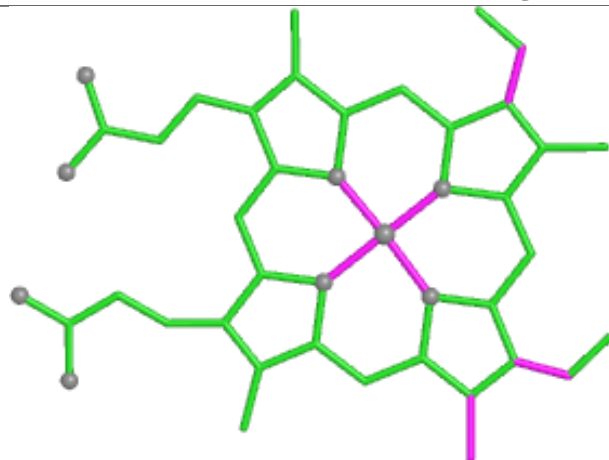
## Ligand FES p 602



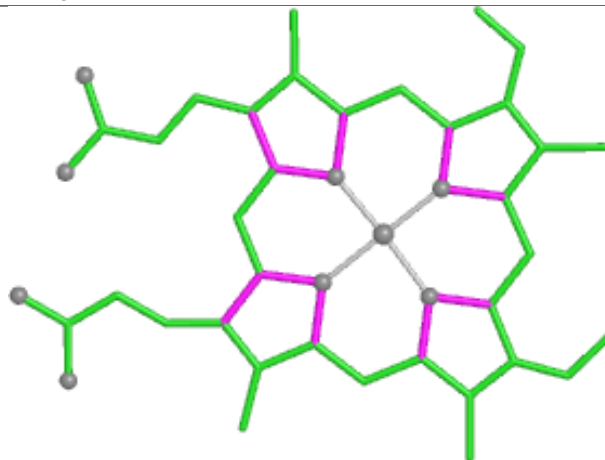




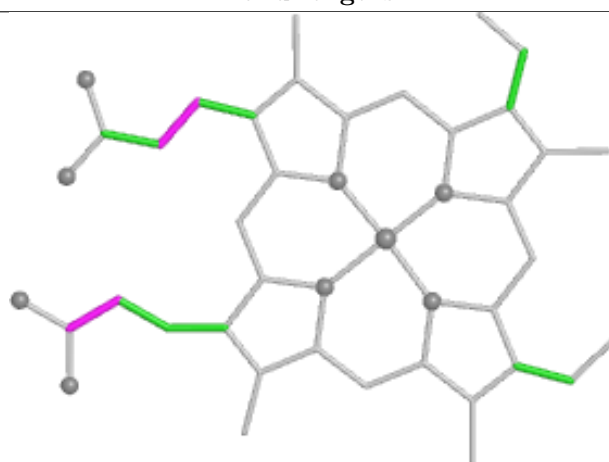
## Ligand HEM j 604



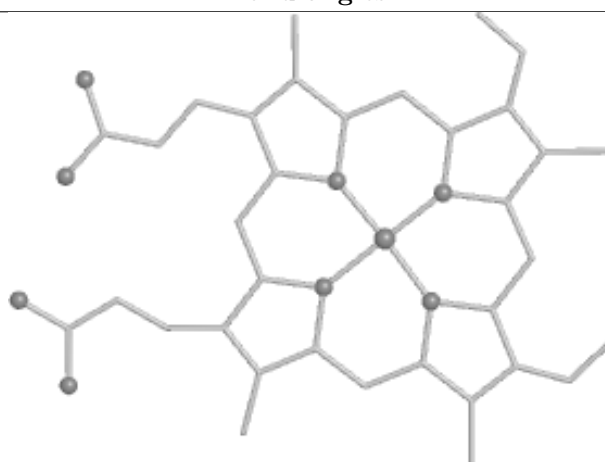
Bond lengths



Bond angles

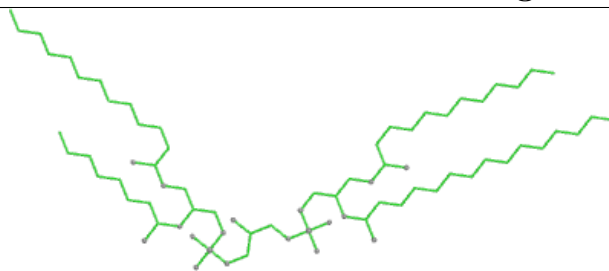


Torsions

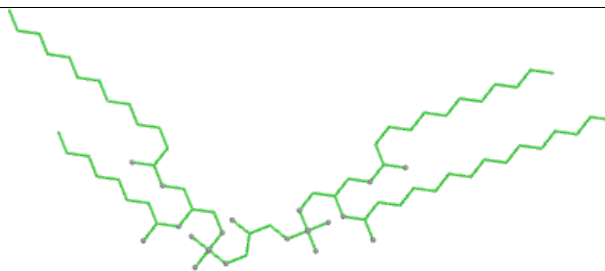


Rings

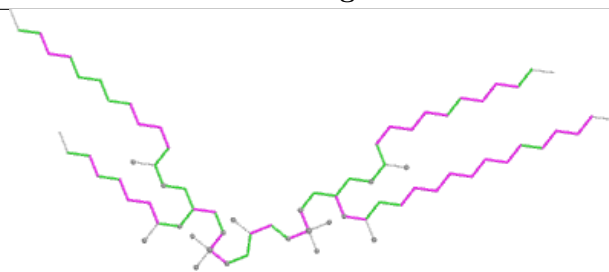
## Ligand CDL L 606



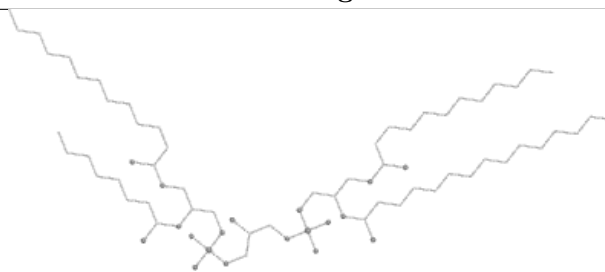
Bond lengths



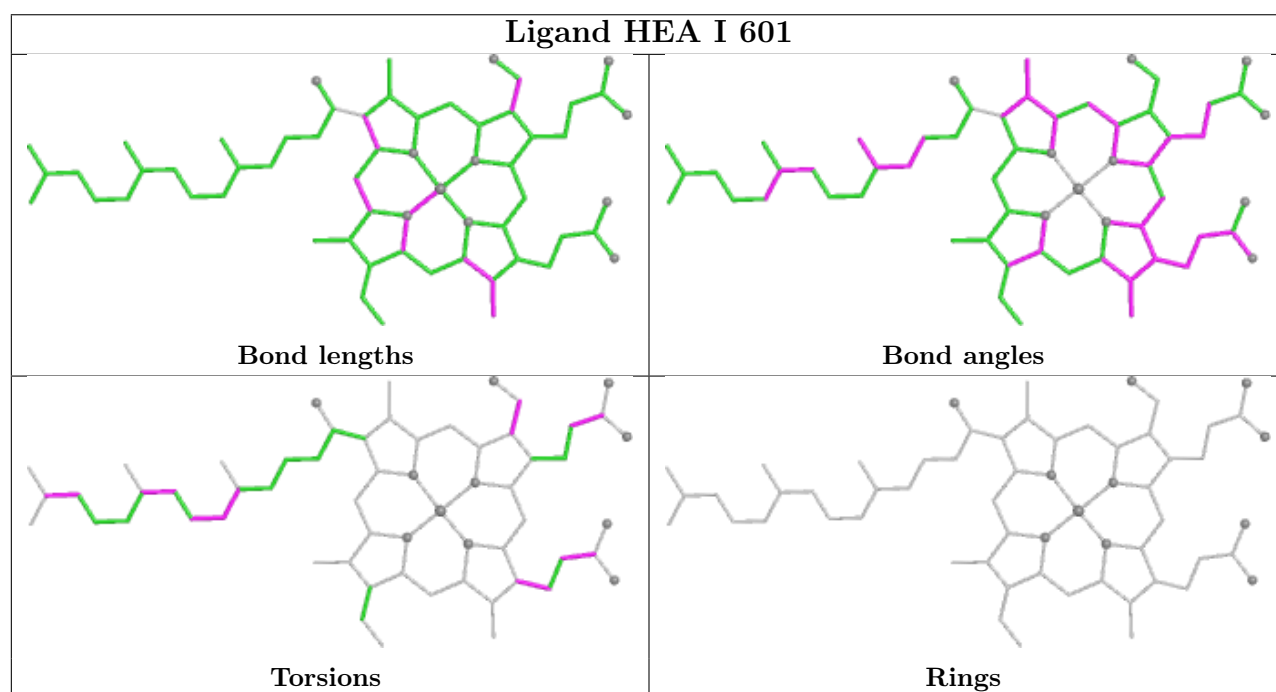
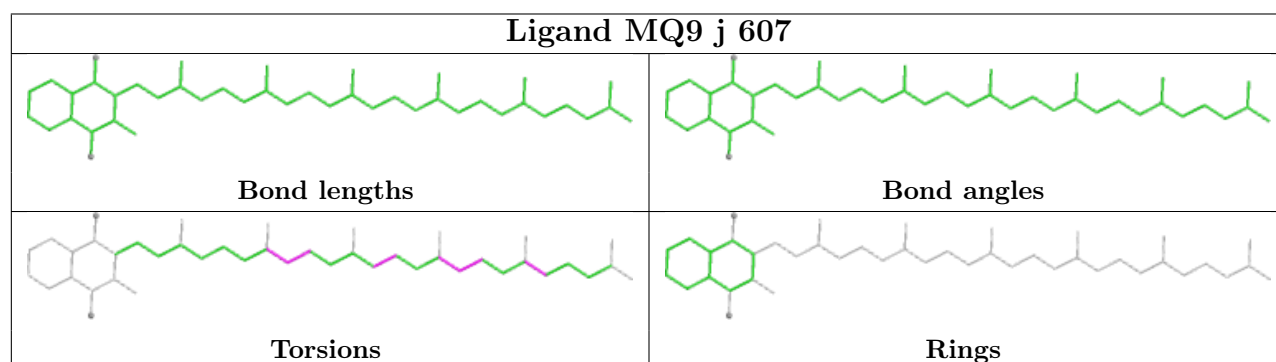
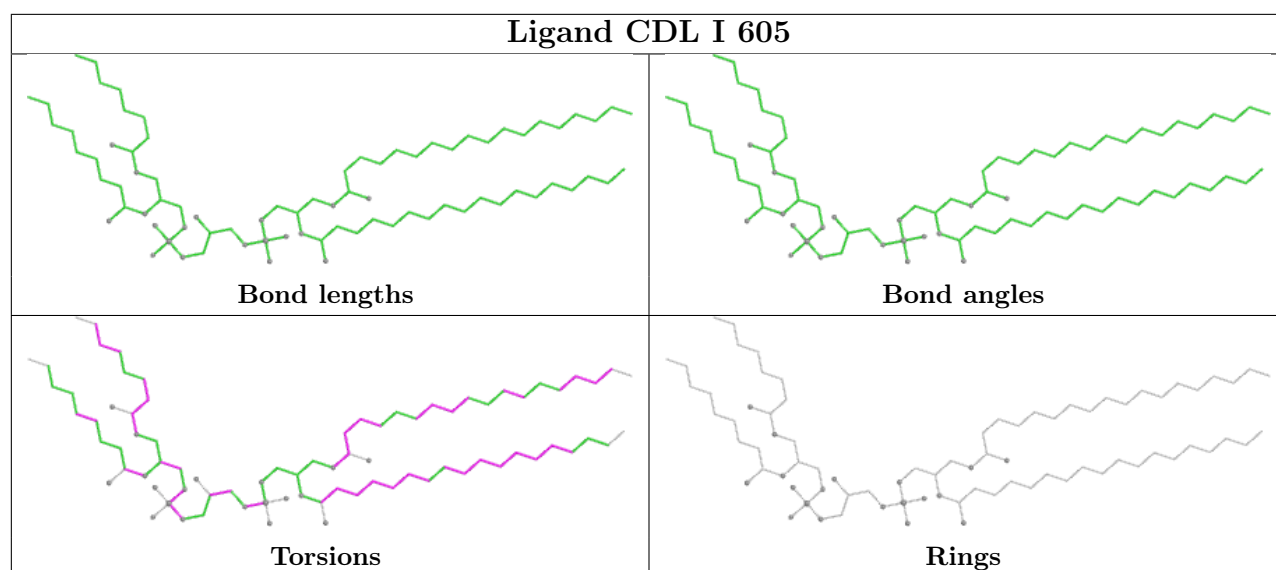
Bond angles

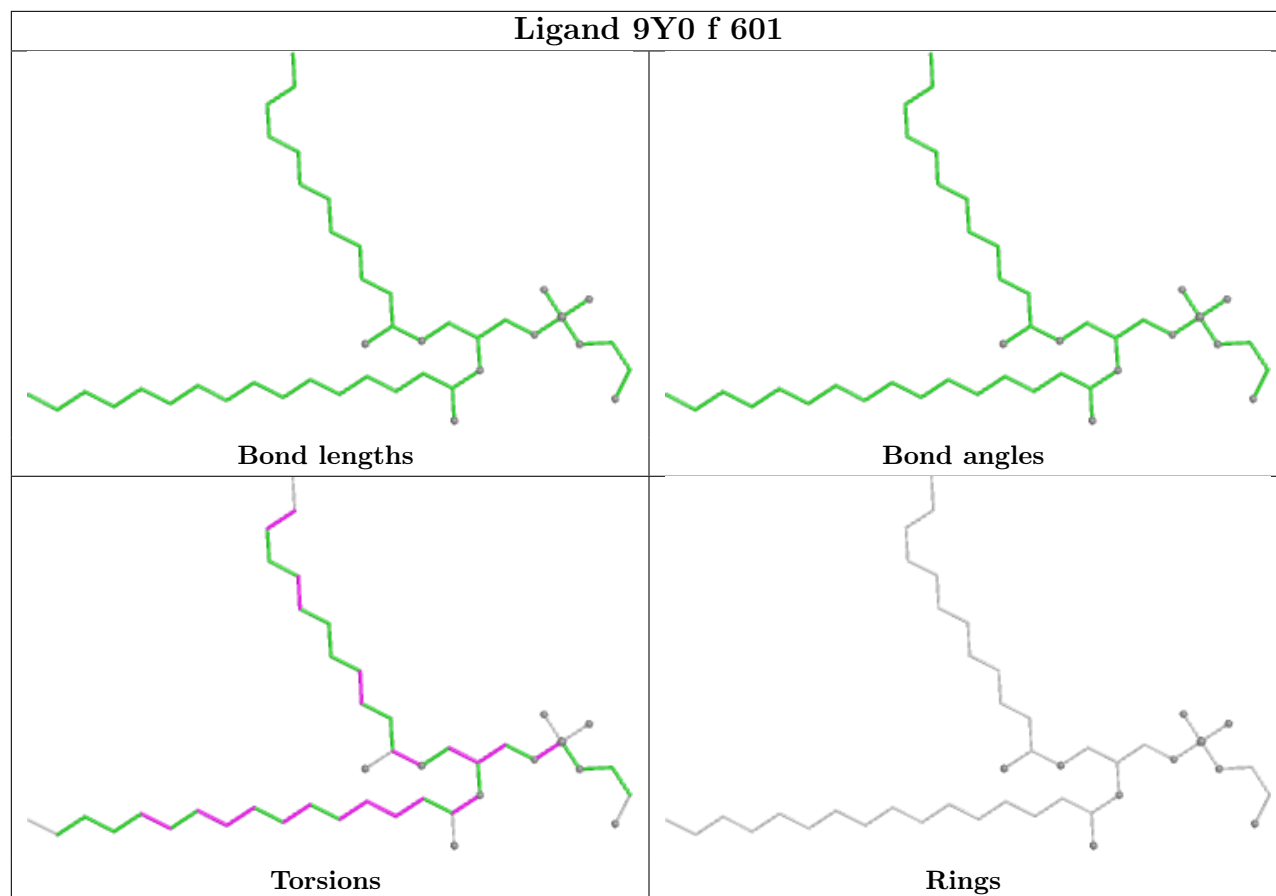


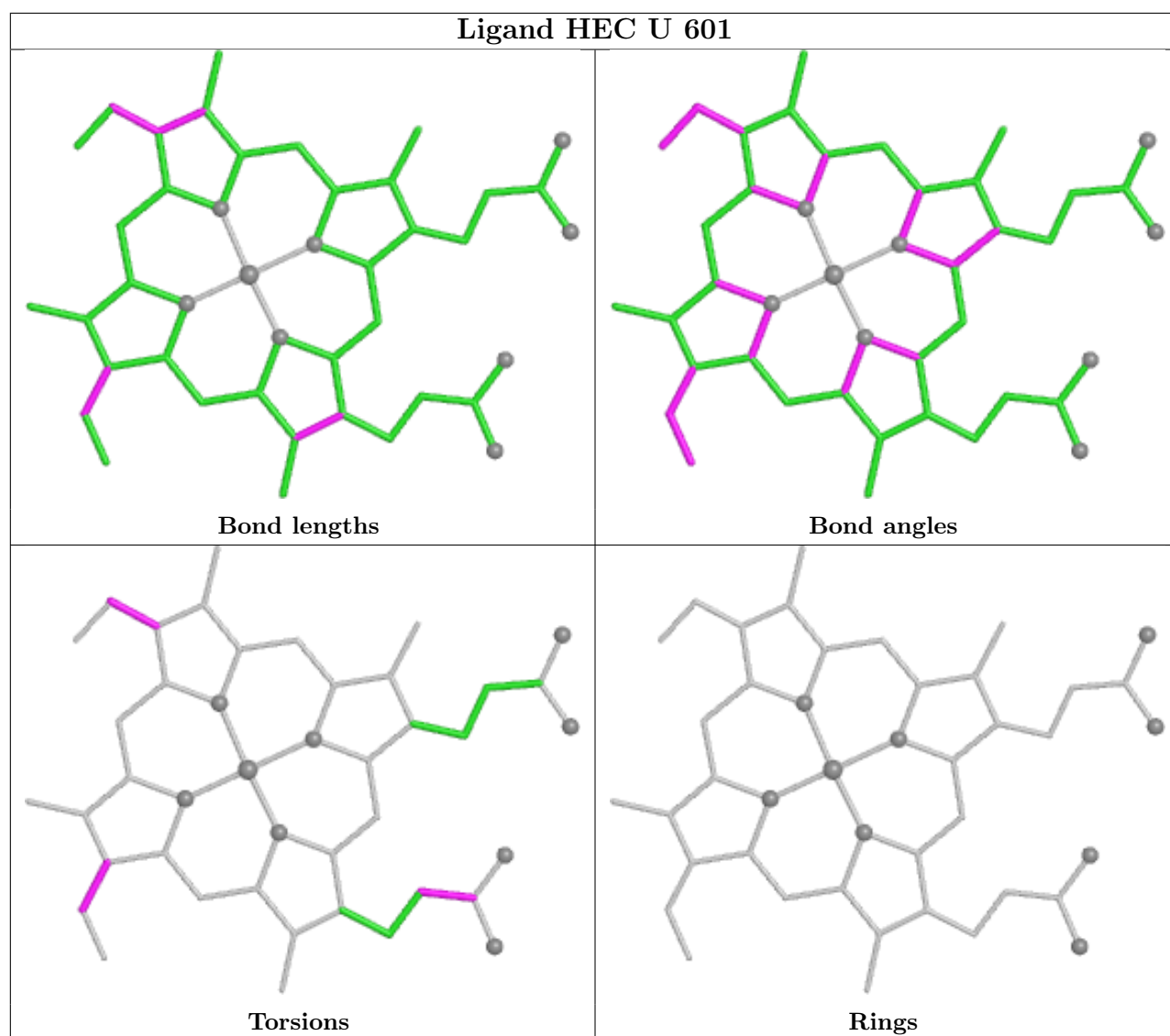
Torsions

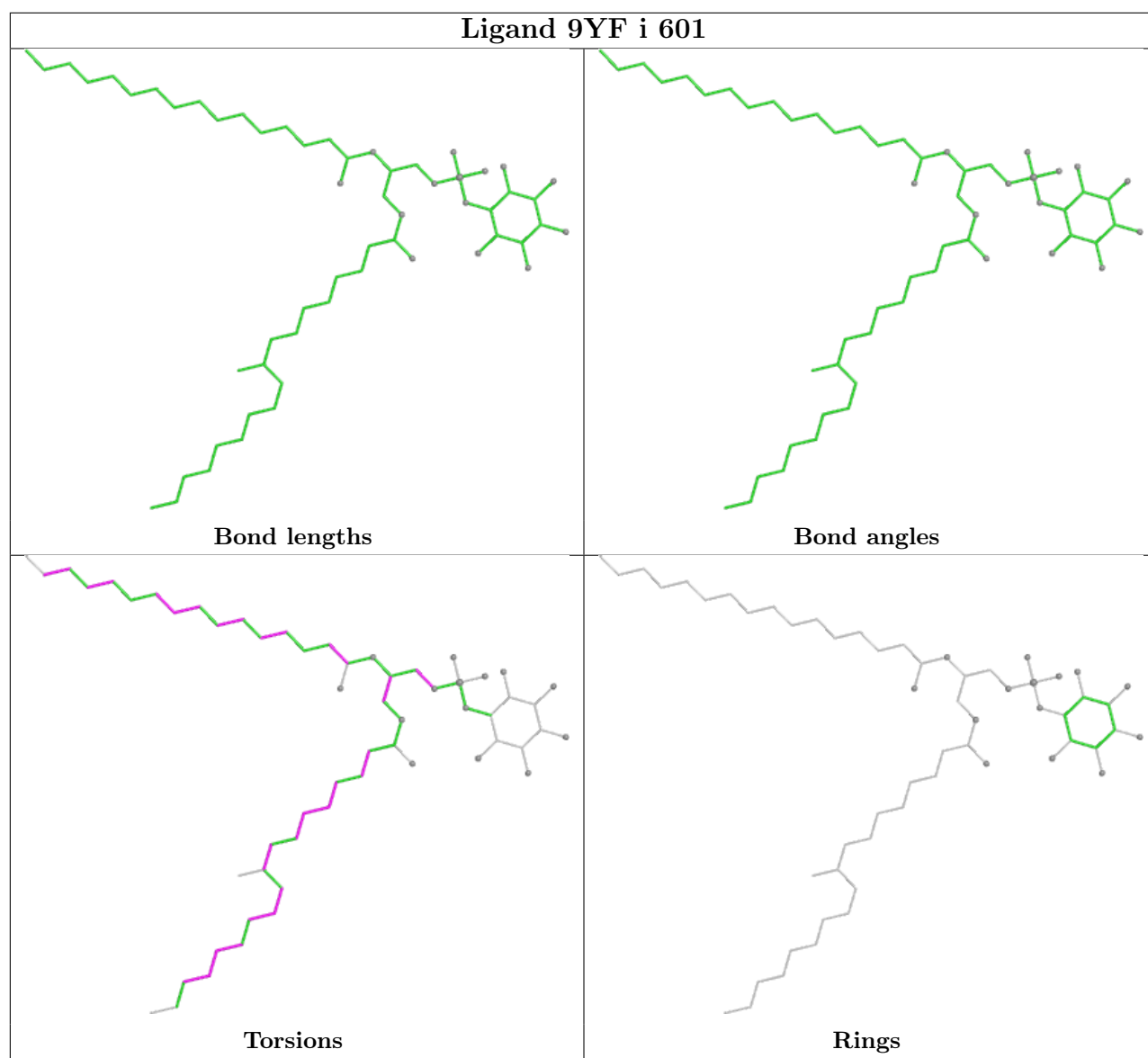


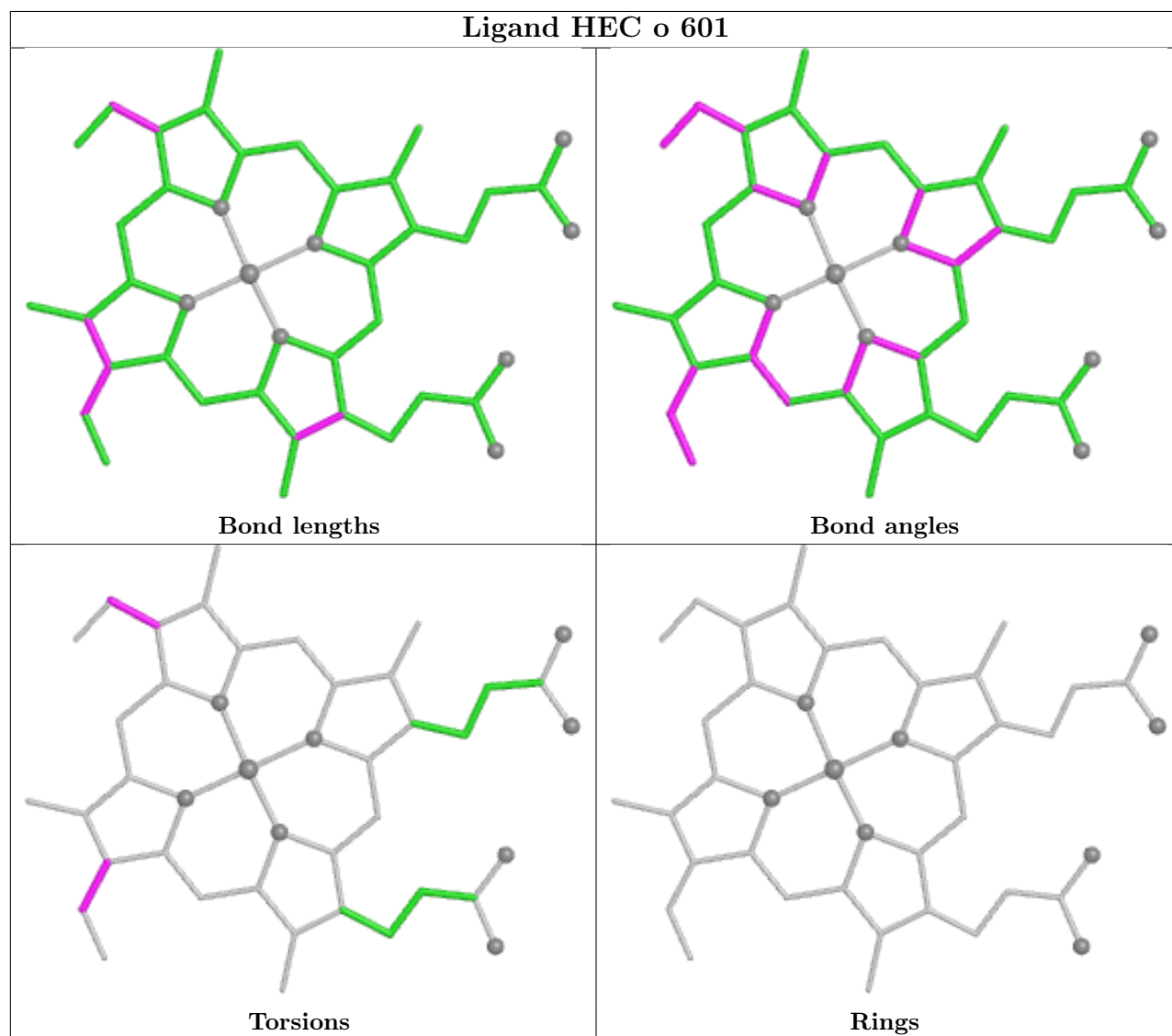
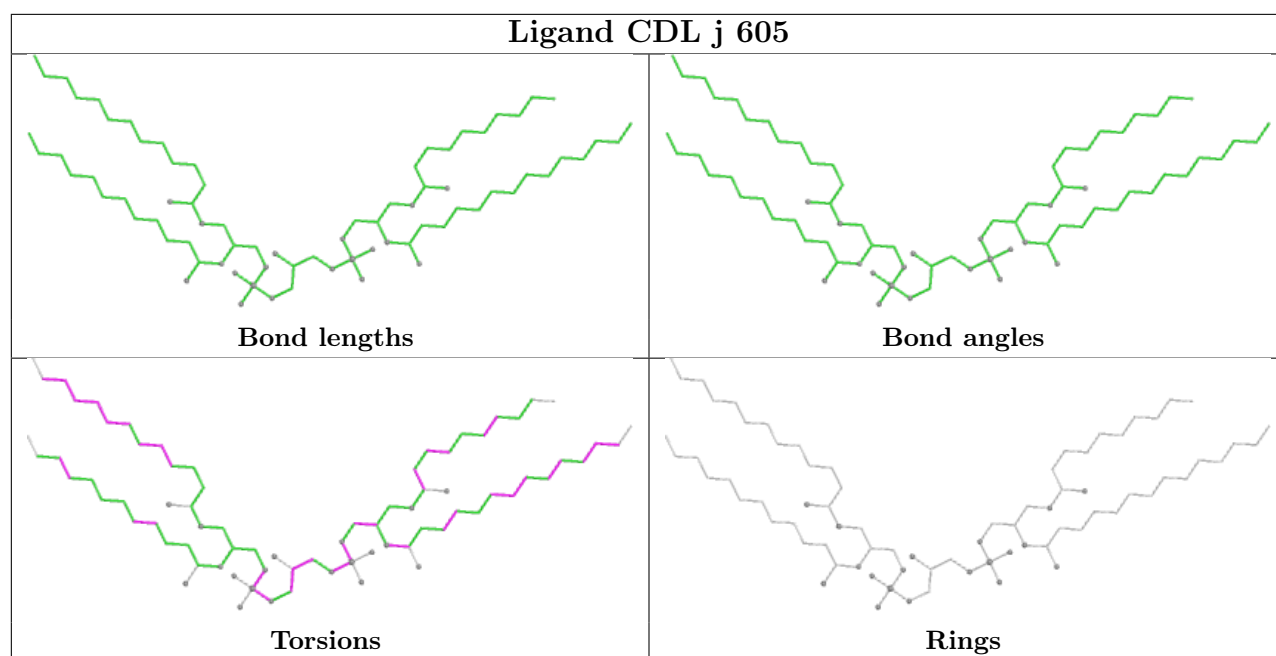
Rings

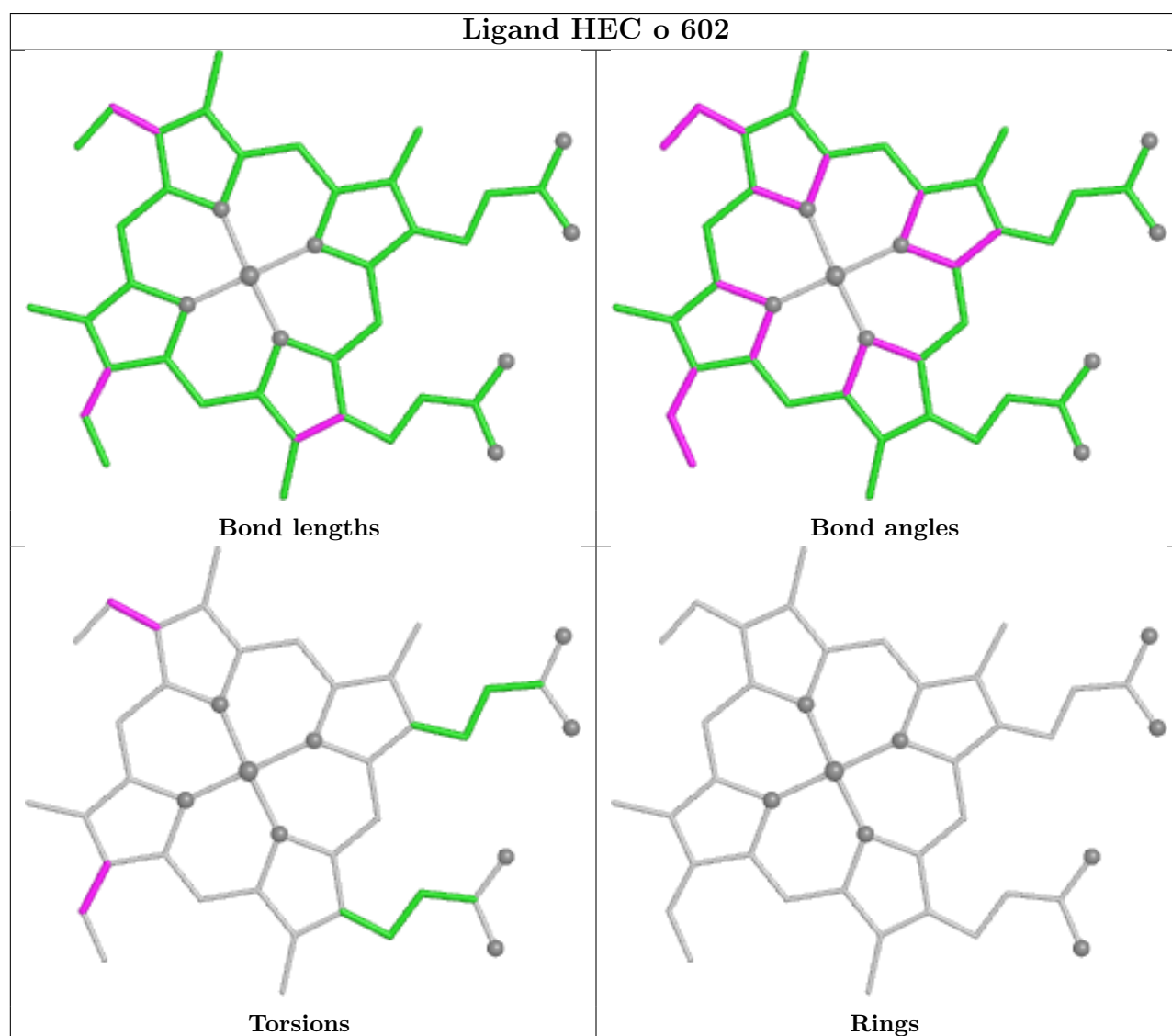
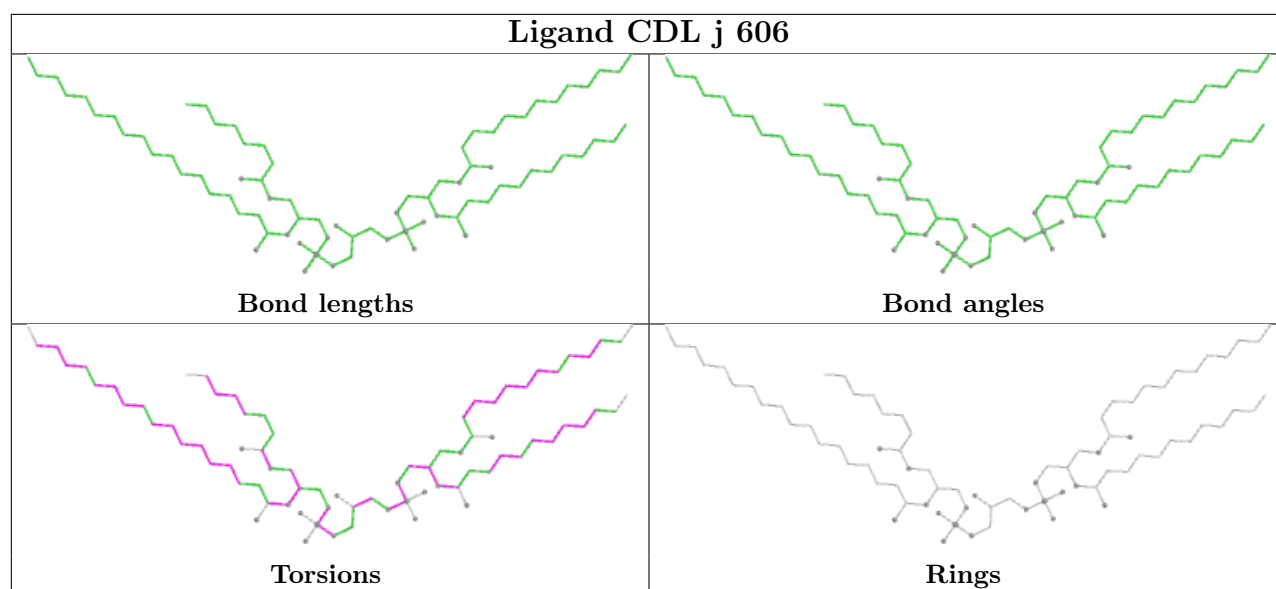






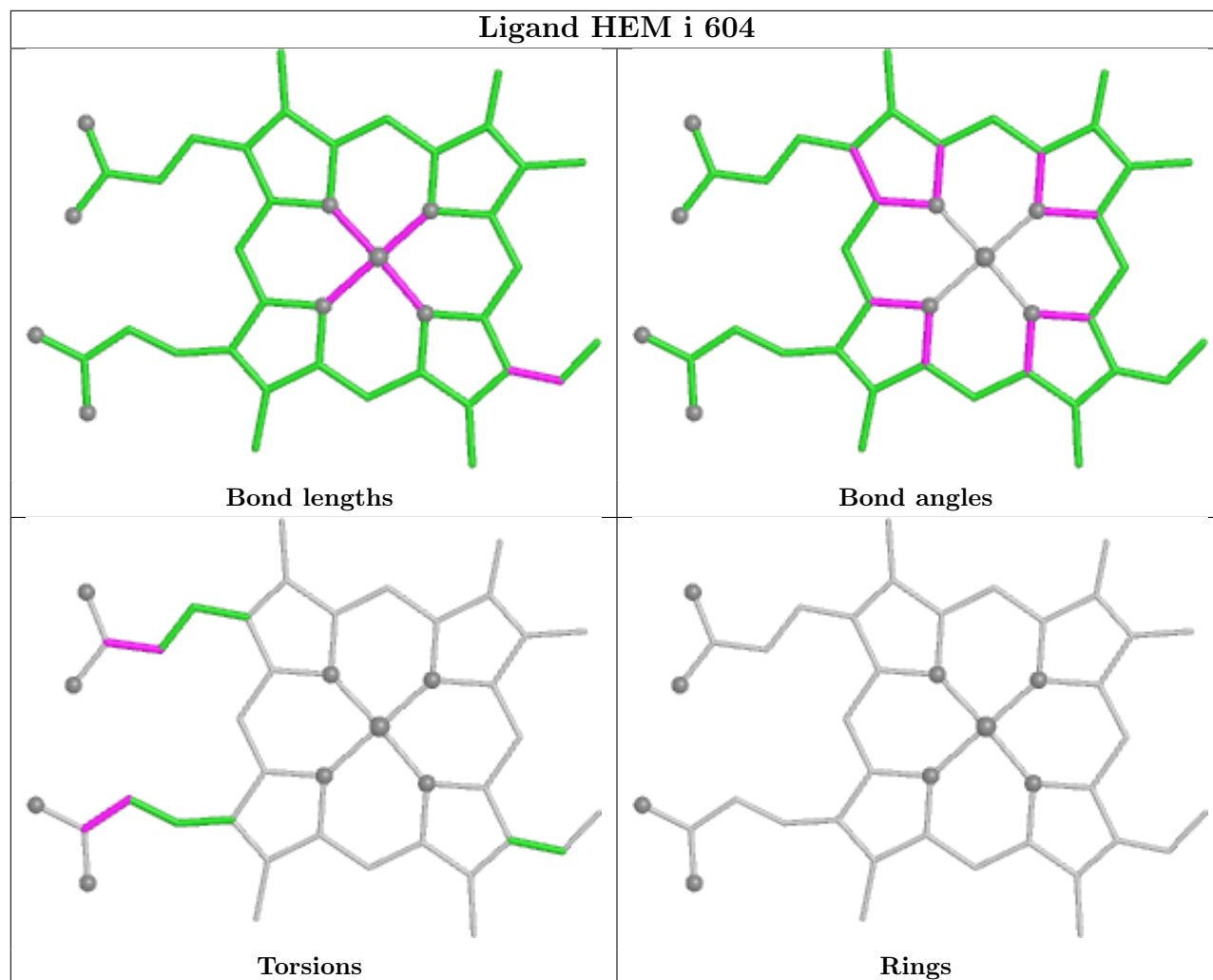


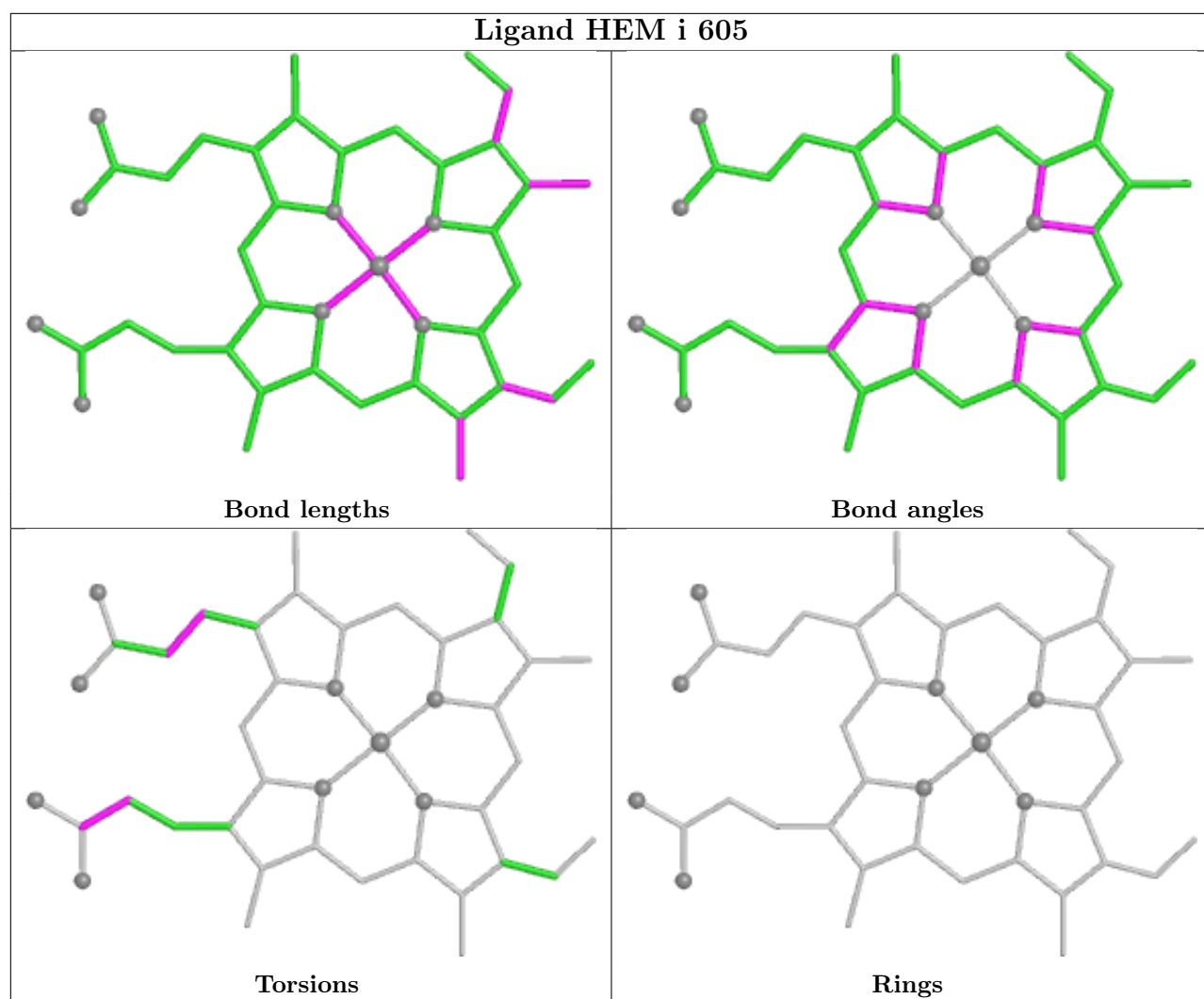


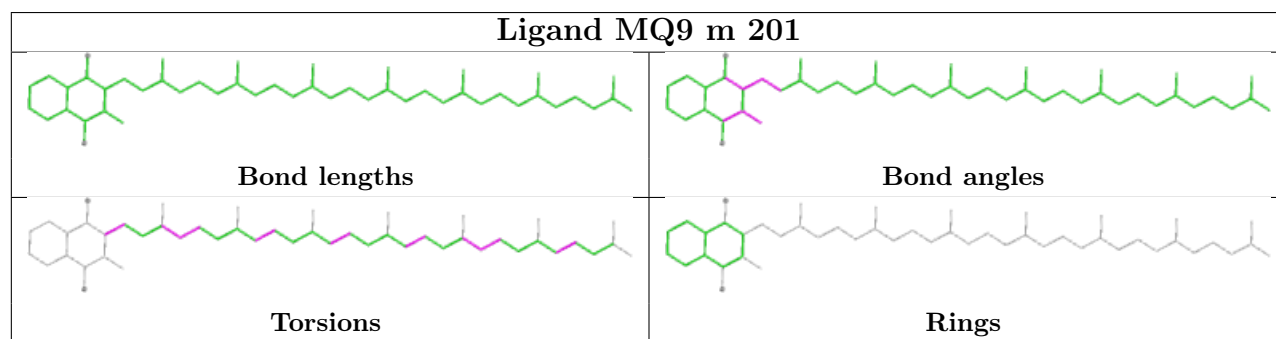
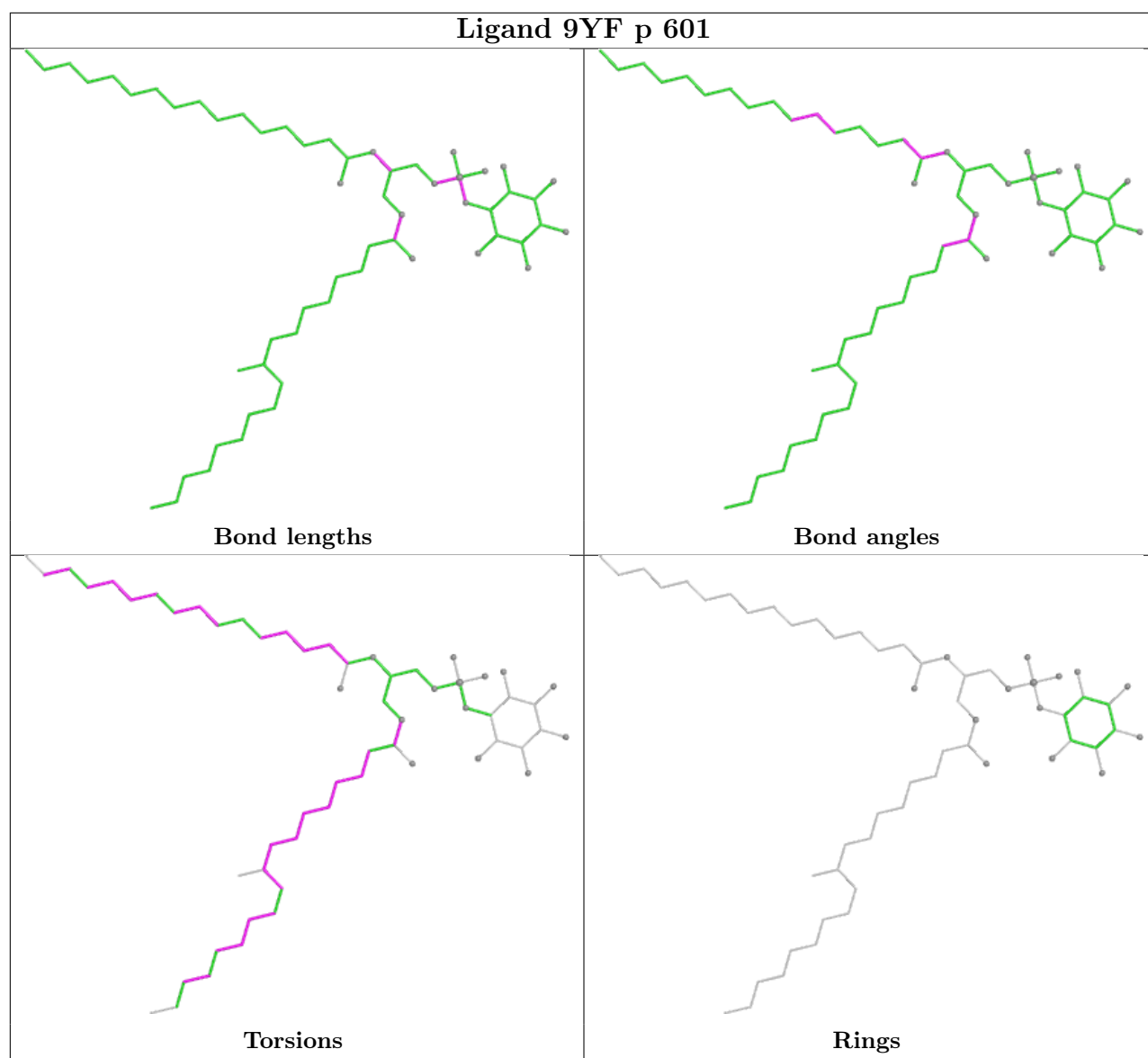


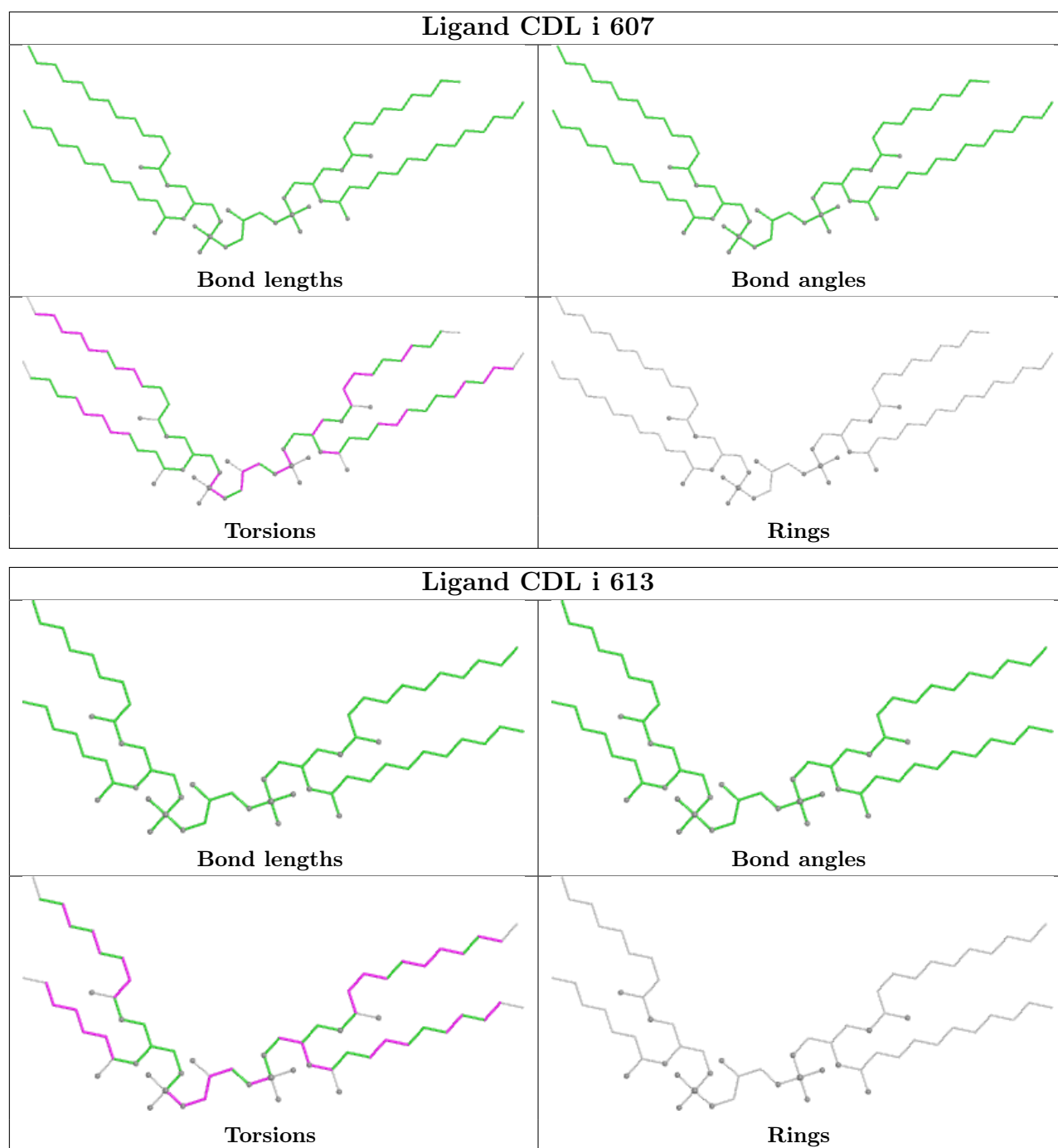


## Ligand HEM i 604









## 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.

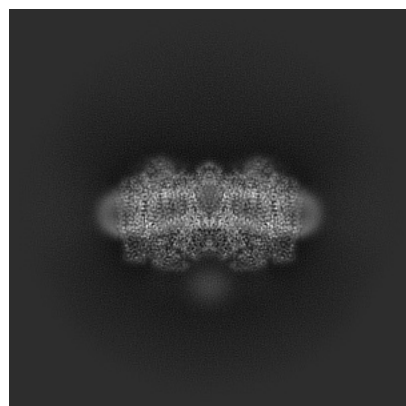
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65879. These allow visual inspection of the internal detail of the map and identification of artifacts.

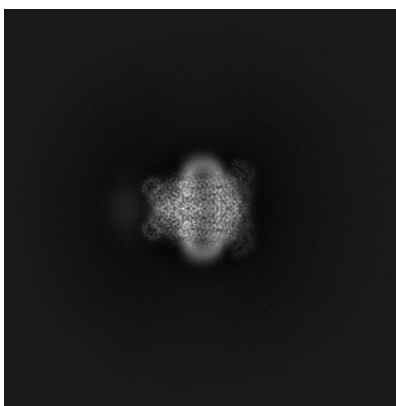
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

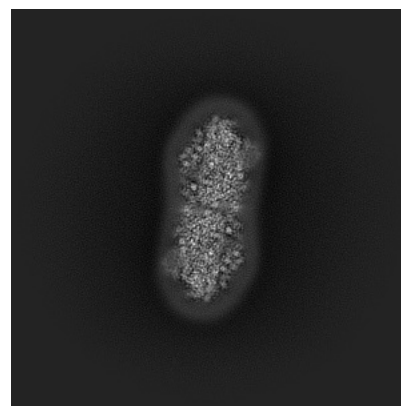
#### 6.1.1 Primary map



X

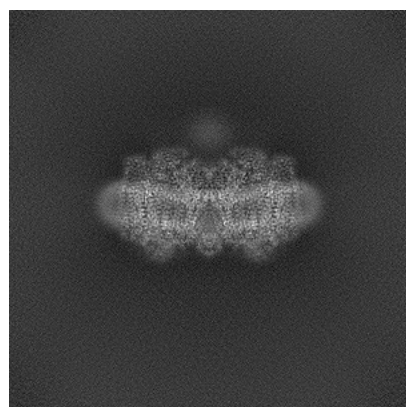


Y

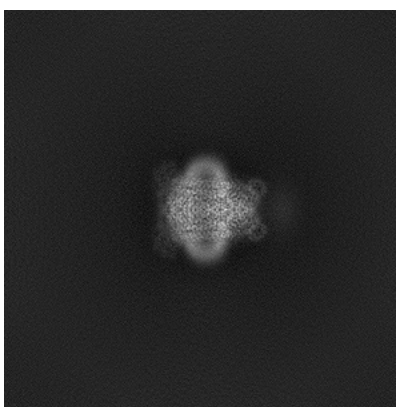


Z

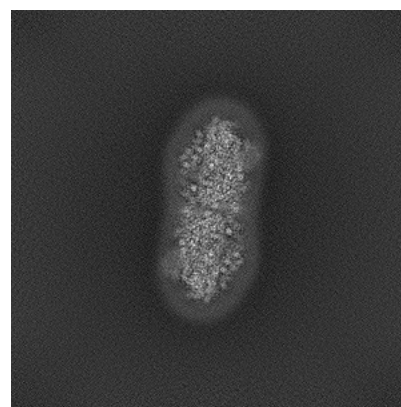
#### 6.1.2 Raw map



X



Y

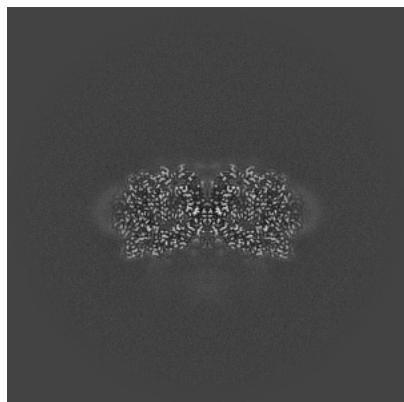


Z

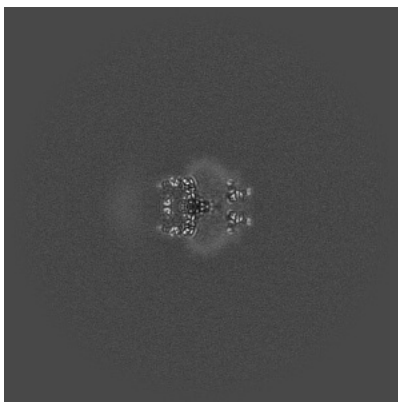
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

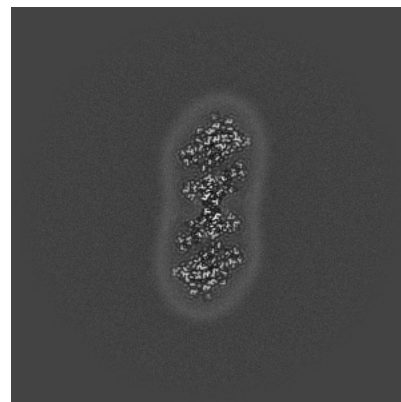
### 6.2.1 Primary map



X Index: 300

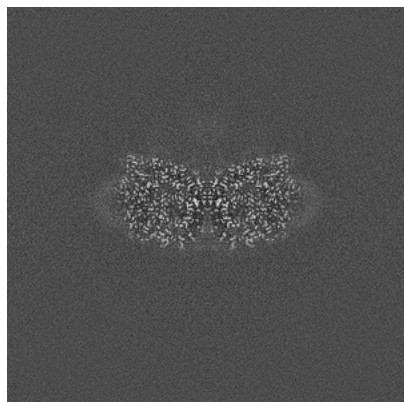


Y Index: 300

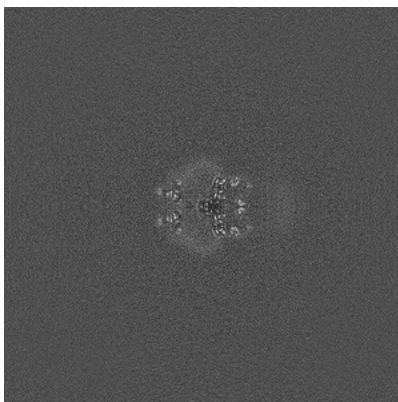


Z Index: 300

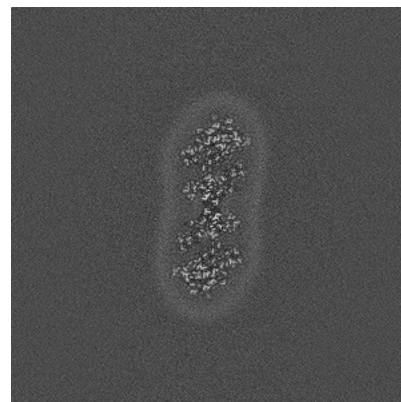
### 6.2.2 Raw map



X Index: 300



Y Index: 300

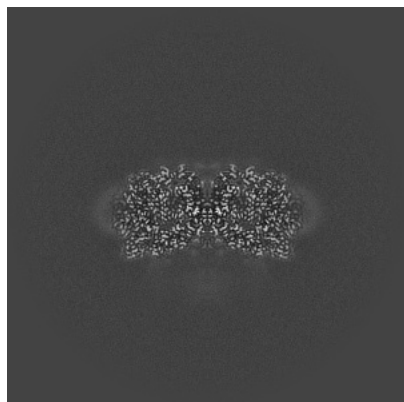


Z Index: 300

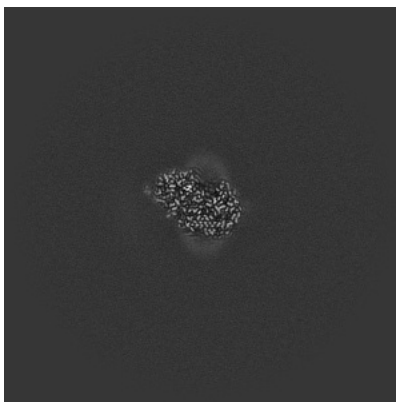
The images above show central slices of the map in three orthogonal directions.

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

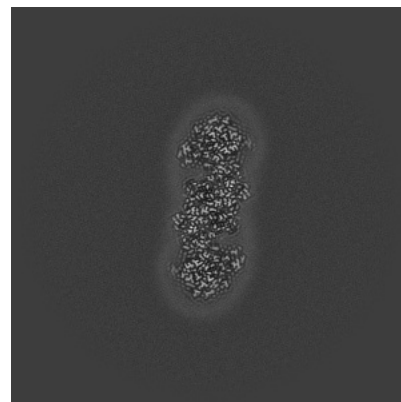
### 6.3.1 Primary map



X Index: 300

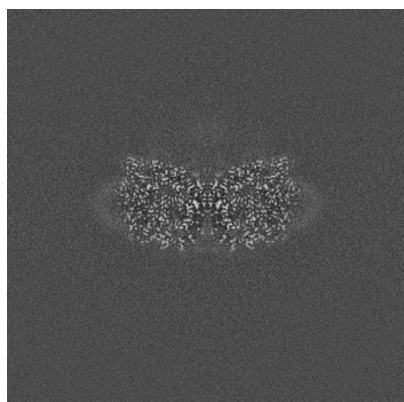


Y Index: 331

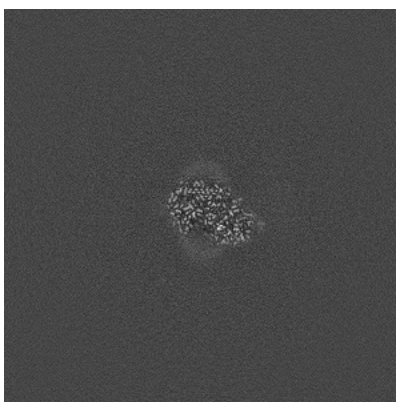


Z Index: 279

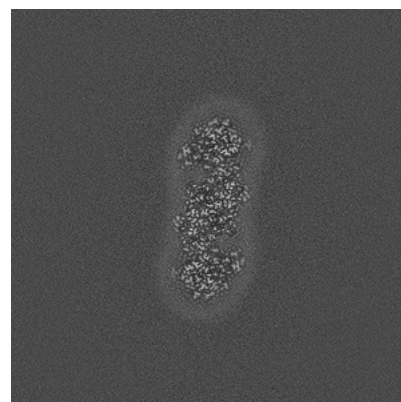
### 6.3.2 Raw map



X Index: 300



Y Index: 269



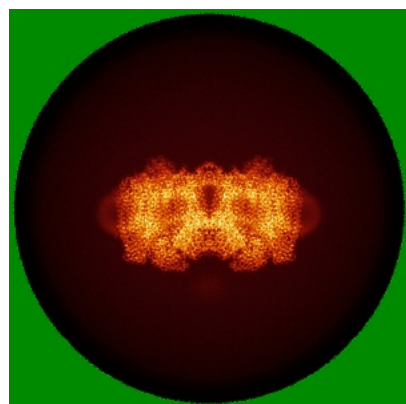
Z Index: 321

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

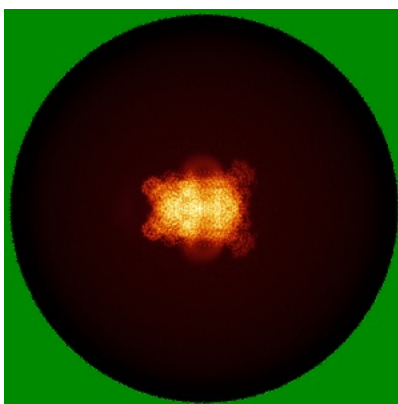


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

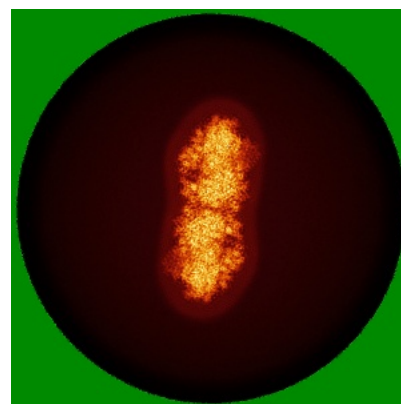
### 6.4.1 Primary map



X

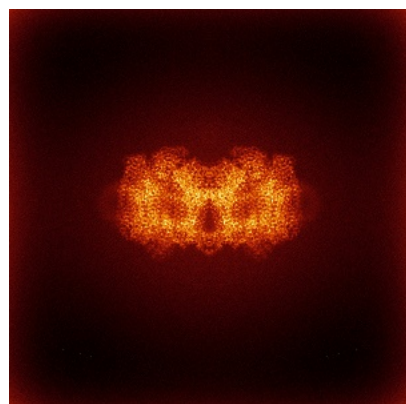


Y

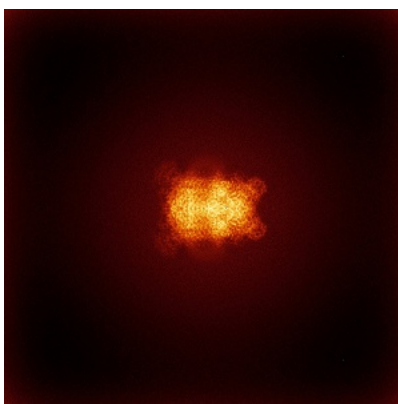


Z

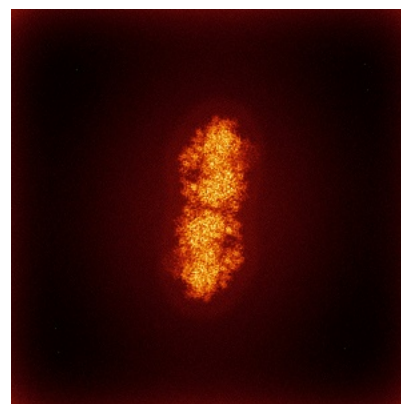
### 6.4.2 Raw map



X



Y



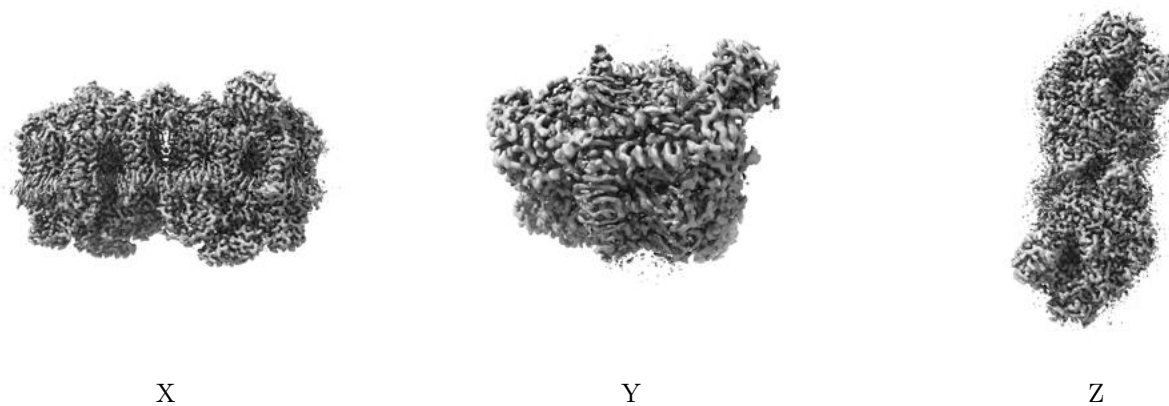
Z

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



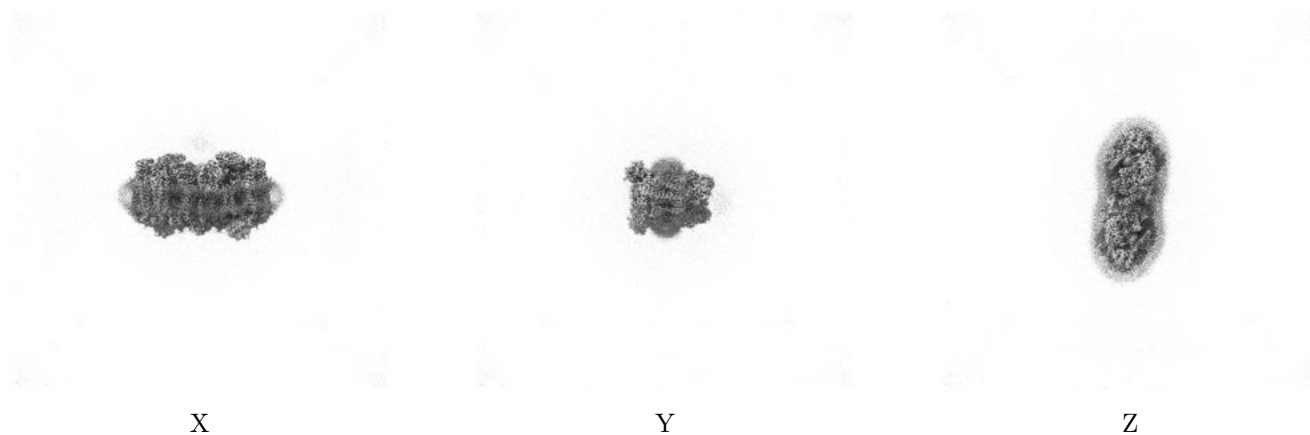
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0332. 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.

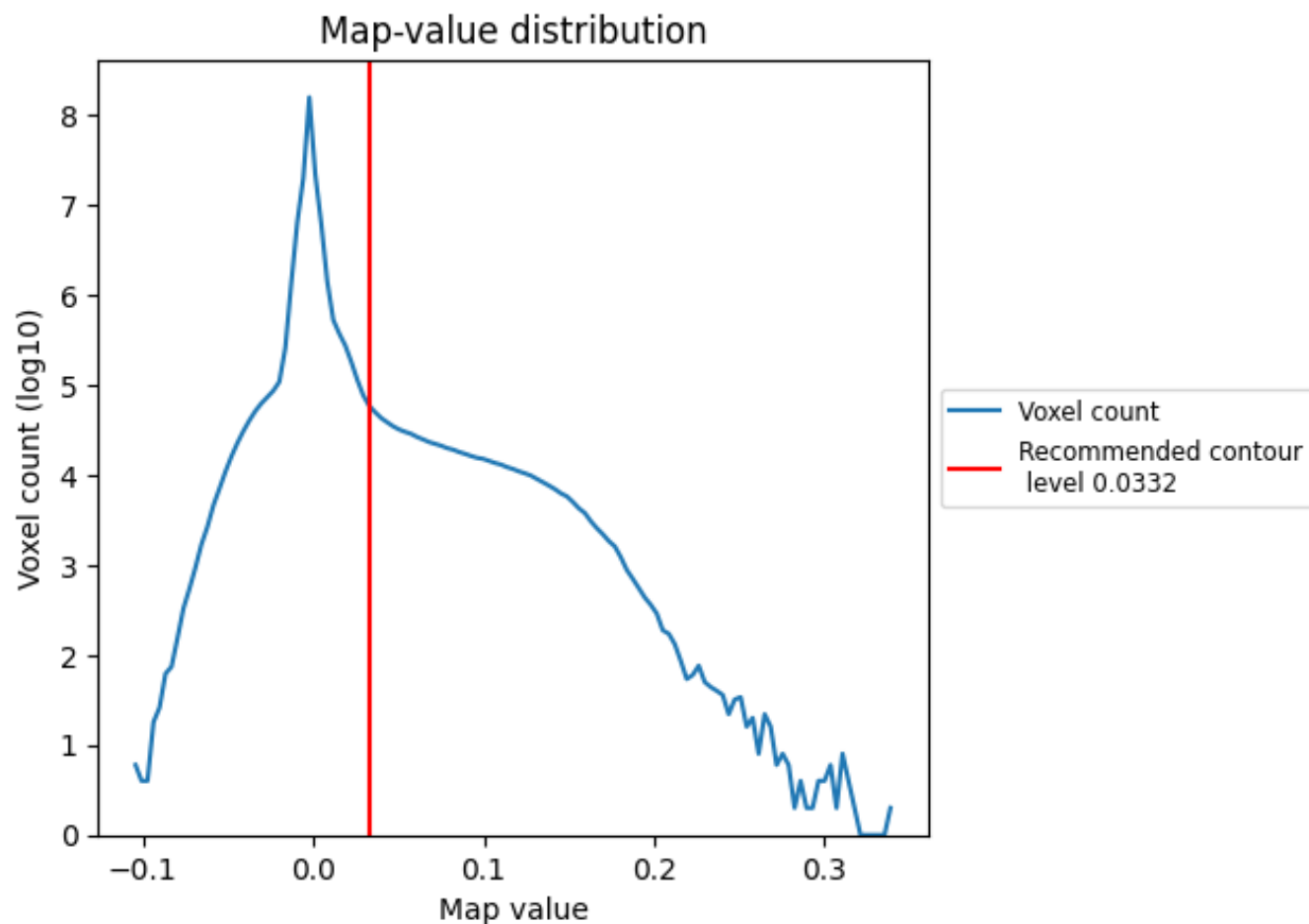
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

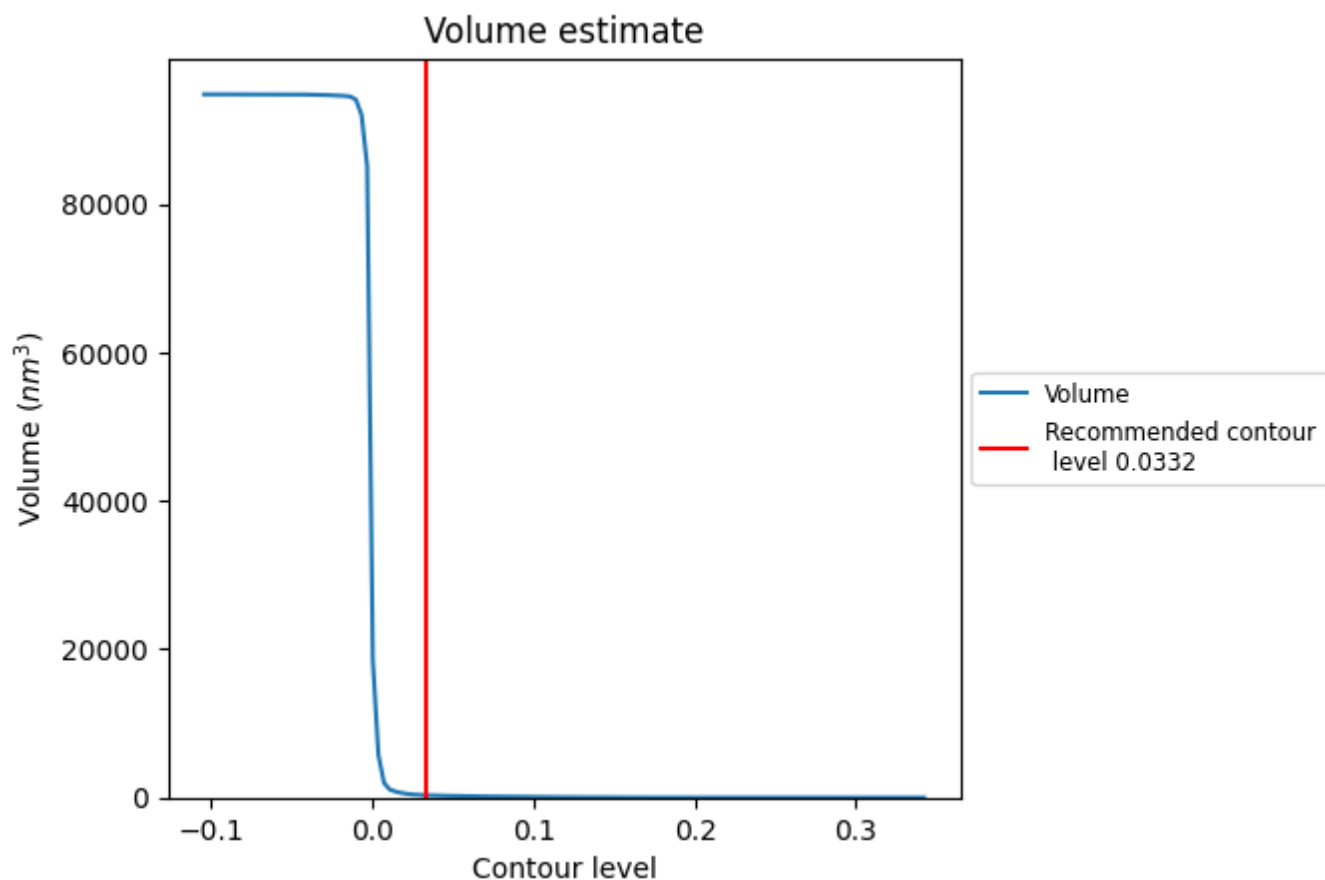
This section contains the results of statistical analysis of the map.

### 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.

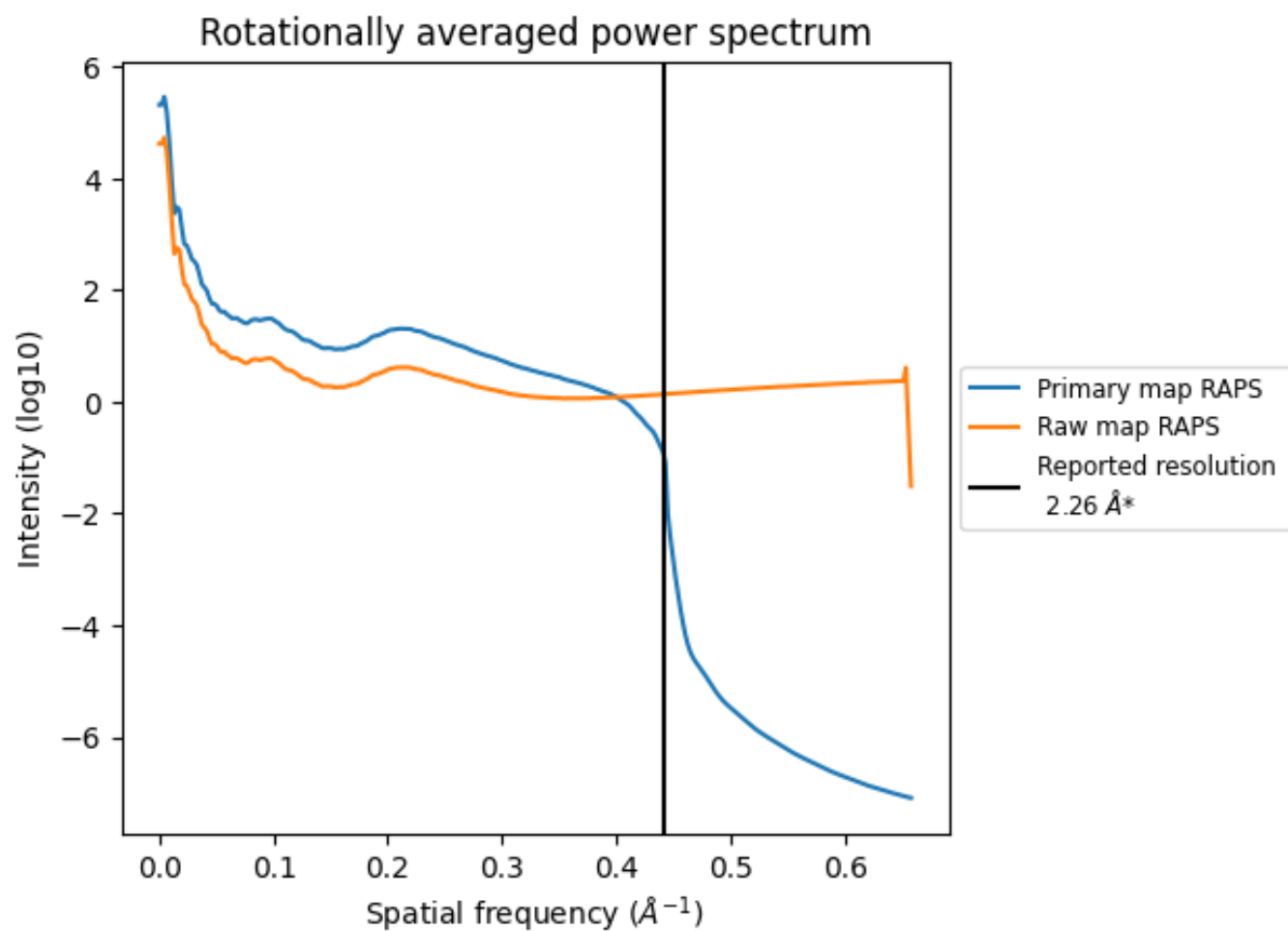
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm<sup>3</sup>; this corresponds to an approximate mass of 285 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

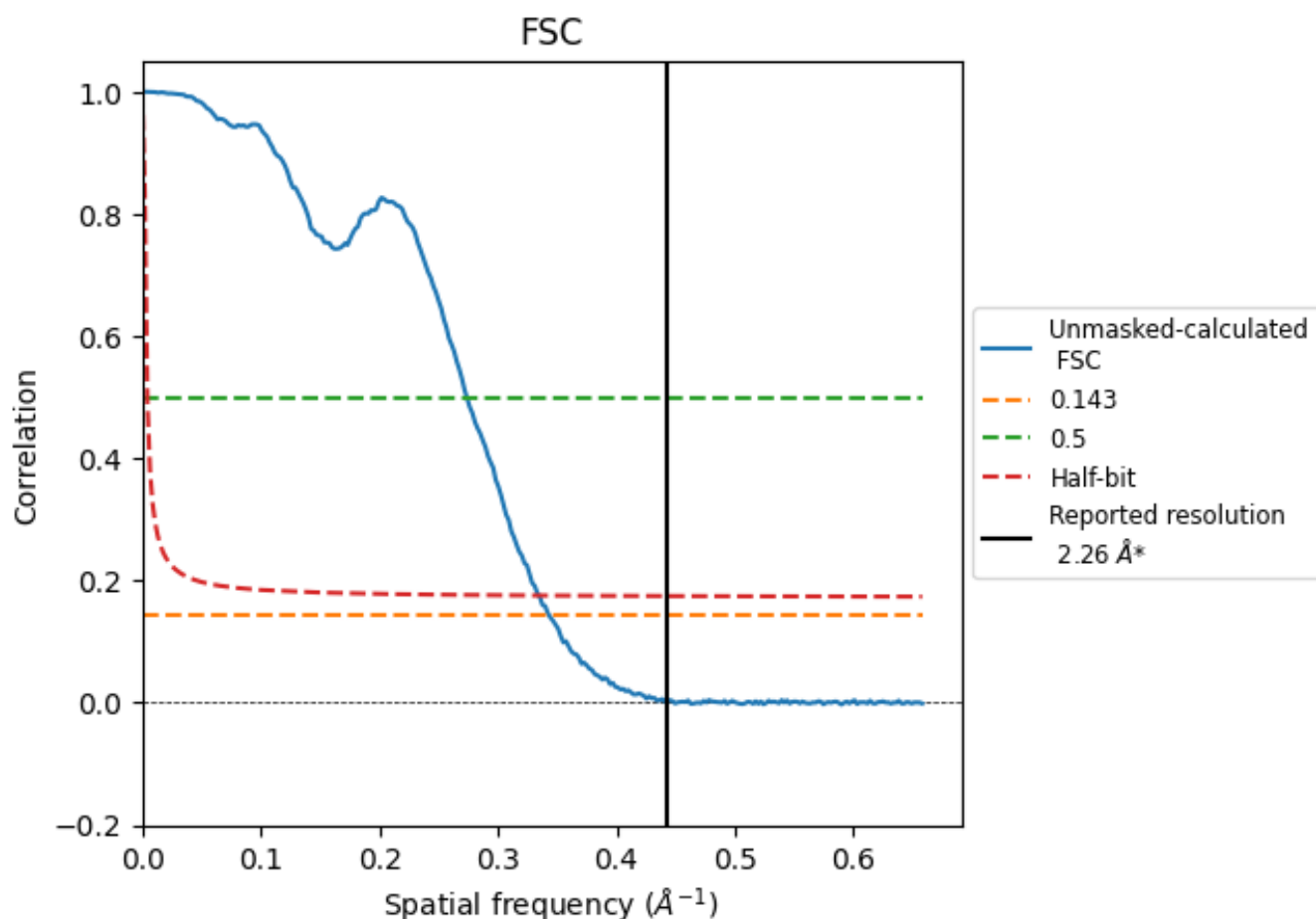


\*Reported resolution corresponds to spatial frequency of 0.442 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.442  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

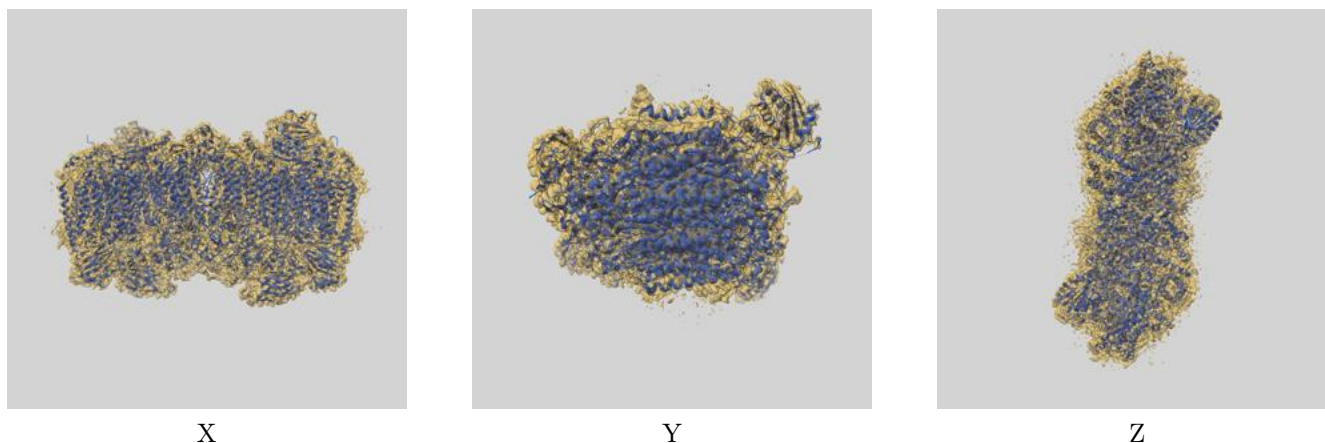
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.91	3.65	2.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.26 by more than 10 %

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

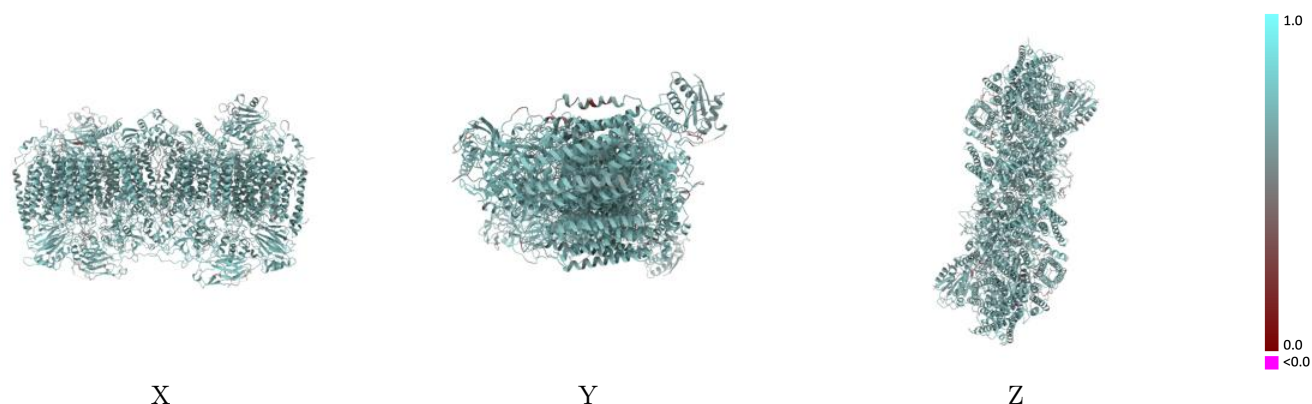
This section contains information regarding the fit between EMDB map EMD-65879 and PDB model 9WCY. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



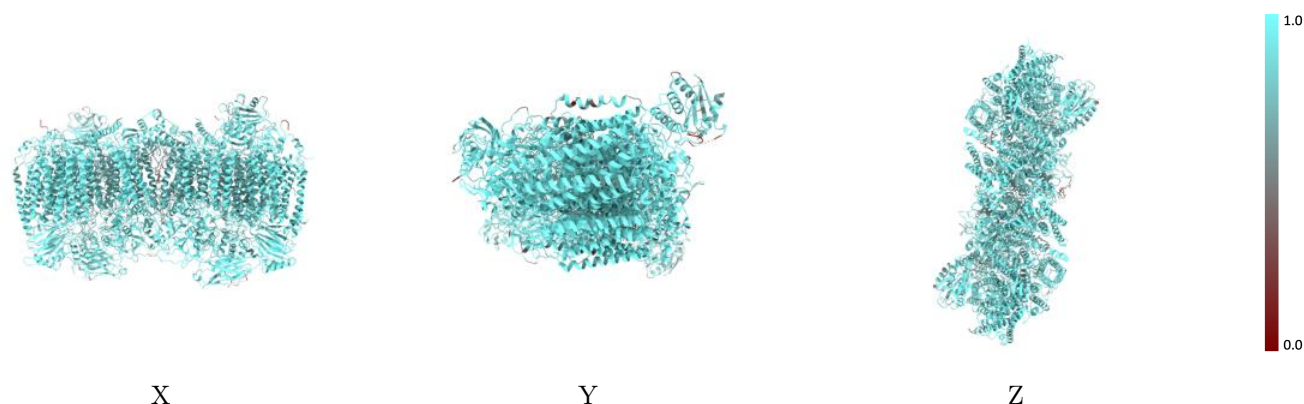
The images above show the 3D surface view of the map at the recommended contour level 0.0332 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

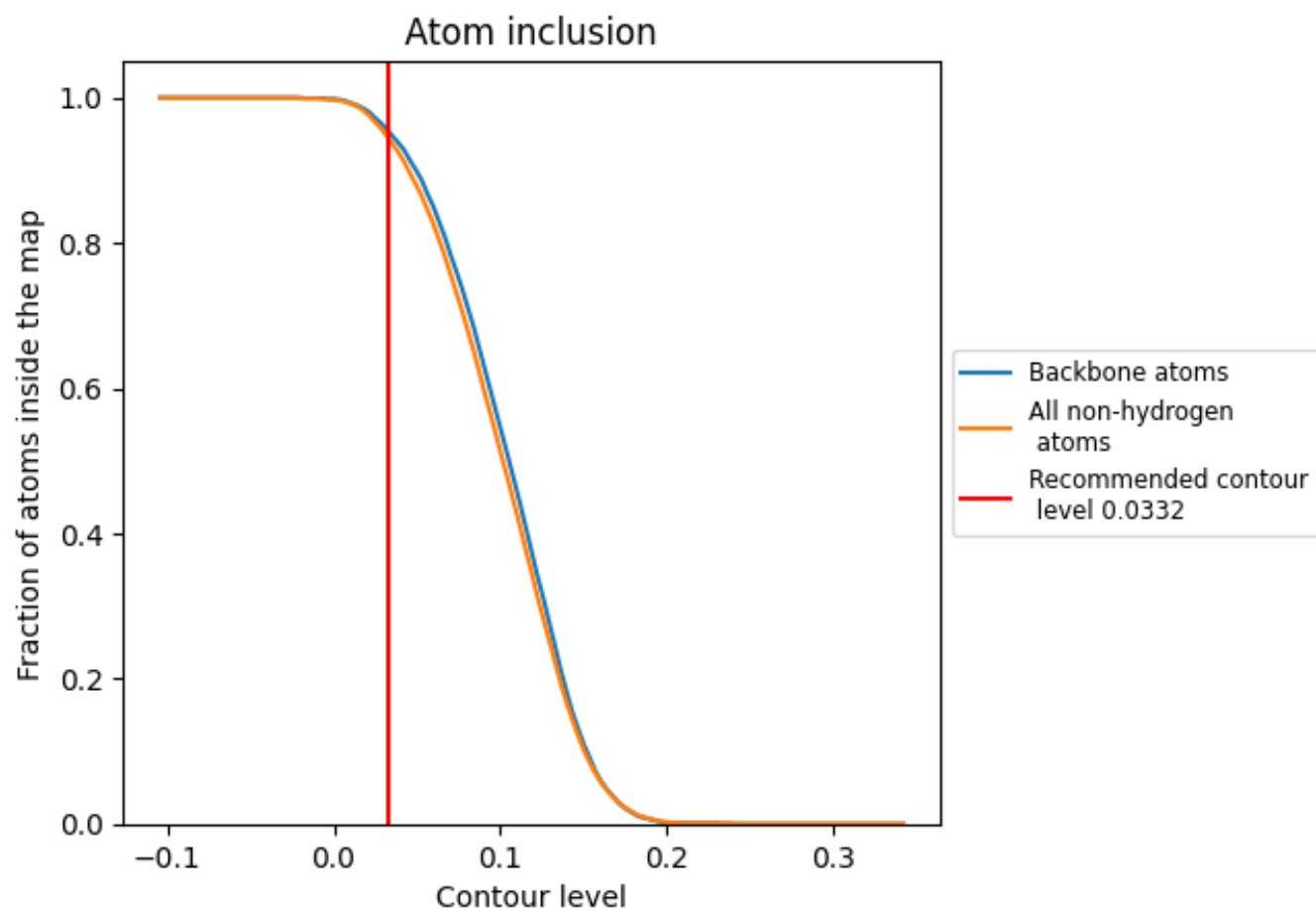
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0332).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0332) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.6610
G	 0.9470	 0.6630
I	 0.9680	 0.6730
J	 0.8360	 0.5880
L	 0.9690	 0.6720
U	 0.9710	 0.6830
V	 0.9610	 0.6780
X	 0.8530	 0.5900
a	 0.8240	 0.5880
b	 0.9300	 0.6490
d	 0.9460	 0.6560
e	 0.9440	 0.6590
f	 0.9540	 0.6410
g	 0.9550	 0.6420
h	 0.8060	 0.5750
i	 0.9340	 0.6660
j	 0.9570	 0.6740
k	 0.8260	 0.6020
l	 0.8290	 0.6050
m	 0.9690	 0.6630
n	 0.9690	 0.6610
o	 0.9600	 0.6800
p	 0.9440	 0.6700
q	 0.9060	 0.6440
r	 0.9040	 0.6310

