



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 9FKS / pdb_00009fks
EMDB ID : EMD-50526
Title : Respiratory supercomplex CIII2-CIV2 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-06-04
Resolution : 4.31 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

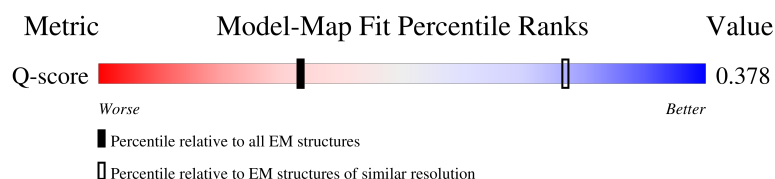
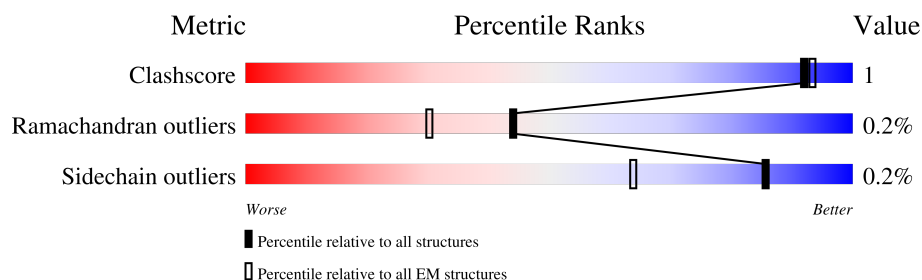
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.31 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	3904 (3.81 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	a	440	<div> <div>21%</div> <div>93%</div> <div>5%</div> </div>
1	d	440	<div> <div>22%</div> <div>95%</div> <div>• •</div> </div>
2	b	450	<div> <div>12%</div> <div>52%</div> <div>47%</div> </div>
2	e	450	<div> <div>12%</div> <div>52%</div> <div>47%</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	195	
3	f	195	
4	g	558	
4	k	558	
5	h	298	
5	l	298	
6	i	274	
6	m	274	
7	j	66	
7	n	66	
8	o	176	
8	p	176	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 34791 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
1	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
2	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
3	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
4	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
5	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 6 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
6	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

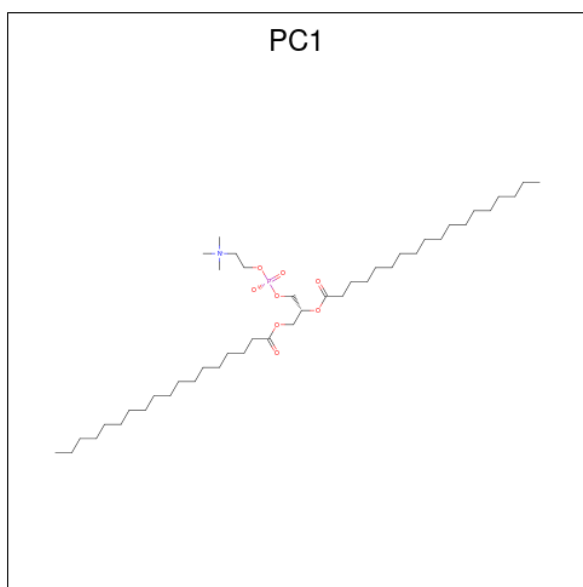
- Molecule 7 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
7	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 8 is a protein called Cytochrome c, class I.

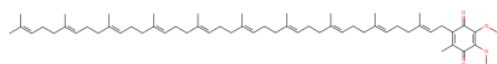
Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		
8	p	45	Total	C	N	O	S	0	0
			330	218	50	60	2		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).

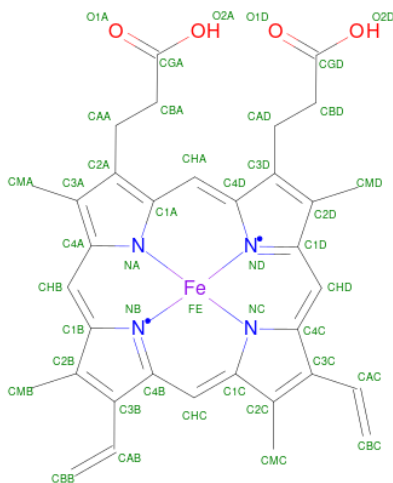


Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	d	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	j	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	n	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	o	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

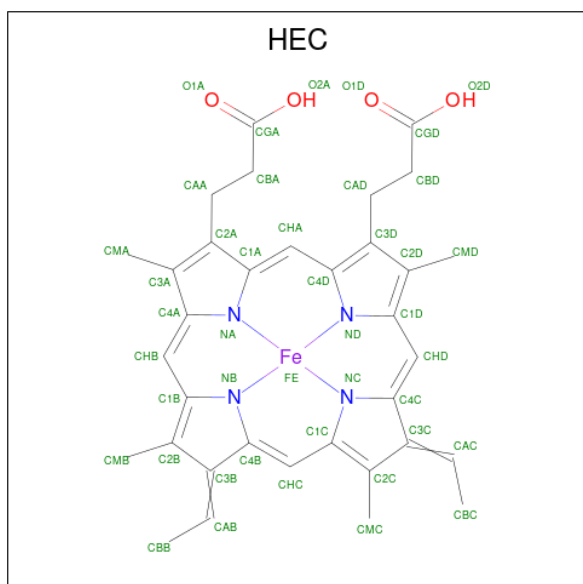


Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
12	b	1	Total Ca 1 1	0
12	e	1	Total Ca 1 1	0
12	g	1	Total Ca 1 1	0
12	k	1	Total Ca 1 1	0

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



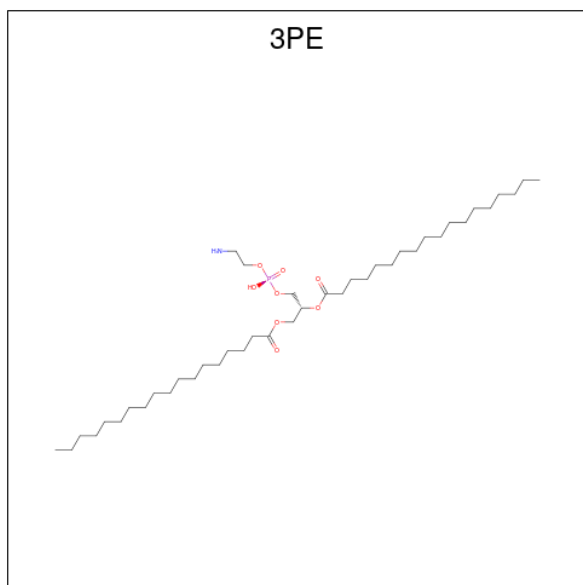
Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 43	C 34	Fe 1	N 4	O 4	0

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

- Molecule 14 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



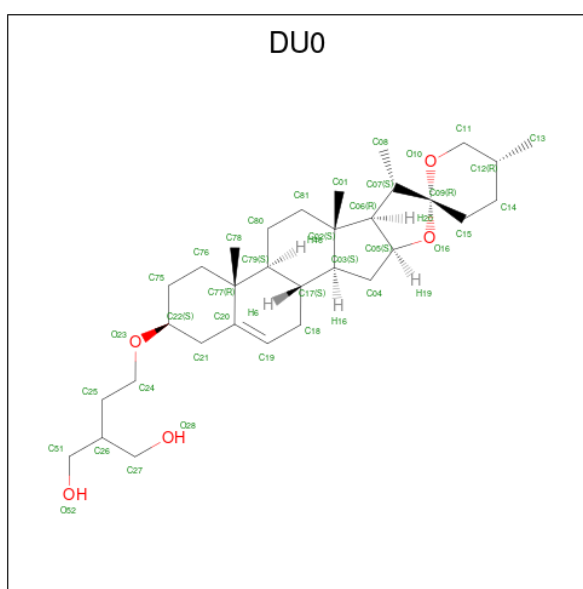
Mol	Chain	Residues	Atoms					AltConf
14	c	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	g	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	n	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 15 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



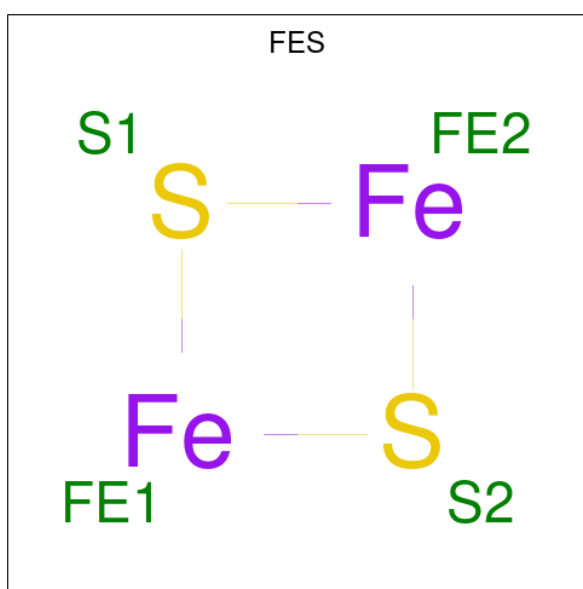
Mol	Chain	Residues	Atoms			AltConf
15	c	1	Total	C	O	0
			37	32	5	
15	c	1	Total	C	O	0
			37	32	5	
15	d	1	Total	C	O	0
			37	32	5	
15	d	1	Total	C	O	0
			37	32	5	
15	f	1	Total	C	O	0
			37	32	5	
15	f	1	Total	C	O	0
			37	32	5	
15	i	1	Total	C	O	0
			37	32	5	

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Mol	Chain	Residues	Atoms			AltConf
15	i	1	Total	C	O	0
			37	32	5	
15	k	1	Total	C	O	0
			37	32	5	
15	m	1	Total	C	O	0
			37	32	5	
15	m	1	Total	C	O	0
			37	32	5	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



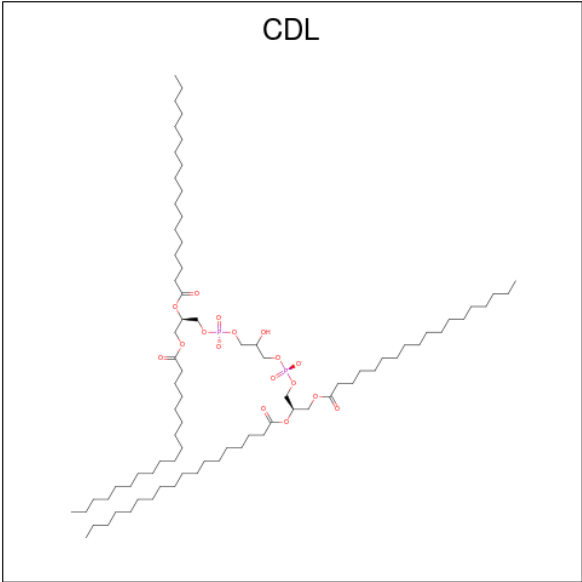
Mol	Chain	Residues	Atoms			AltConf
16	c	1	Total	Fe	S	0
			4	2	2	
16	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $\text{C}_{39}\text{H}_{77}\text{O}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



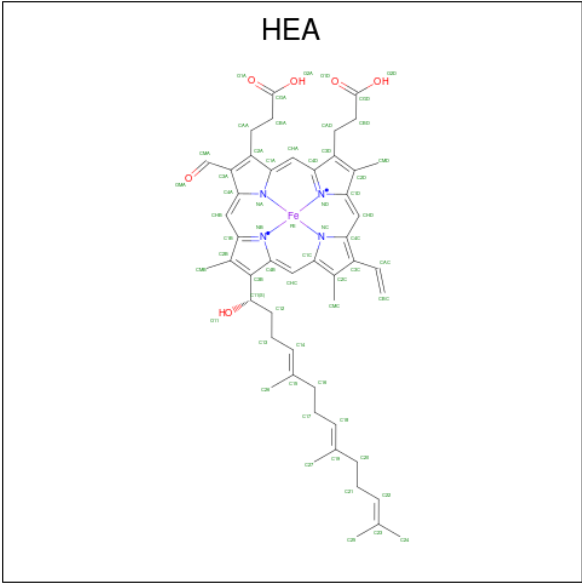
Mol	Chain	Residues	Atoms				AltConf
17	c	1	Total	C	O	P	0
			48	39	8	1	
17	d	1	Total	C	O	P	0
			48	39	8	1	
17	f	1	Total	C	O	P	0
			48	39	8	1	
17	g	1	Total	C	O	P	0
			48	39	8	1	
17	i	1	Total	C	O	P	0
			48	39	8	1	
17	k	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	p	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	d	1	100	81	17	2	0

- Molecule 19 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
19	g	1	60	49	1	4	6	0
19	g	1	60	49	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
19	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
19	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

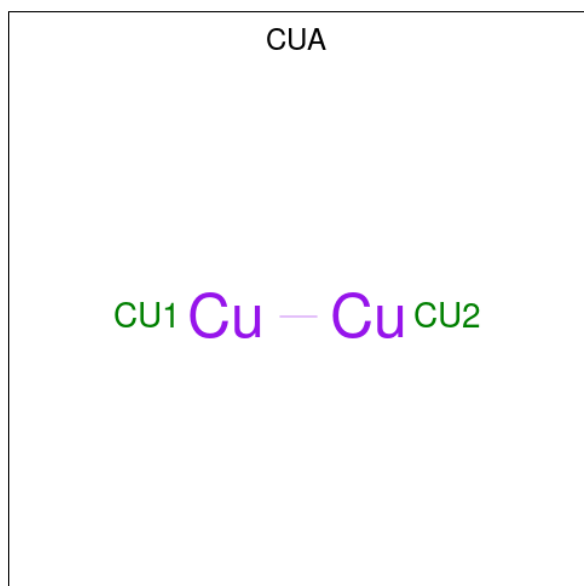
- Molecule 20 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
20	g	1	Total	Cu	0
			1	1	
20	k	1	Total	Cu	0
			1	1	

- Molecule 21 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
21	g	1	Total	Mn	0
			1	1	
21	k	1	Total	Mn	0
			1	1	

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
22	h	1	Total	Cu	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
22	l	1	Total	Cu	0
			2	2	

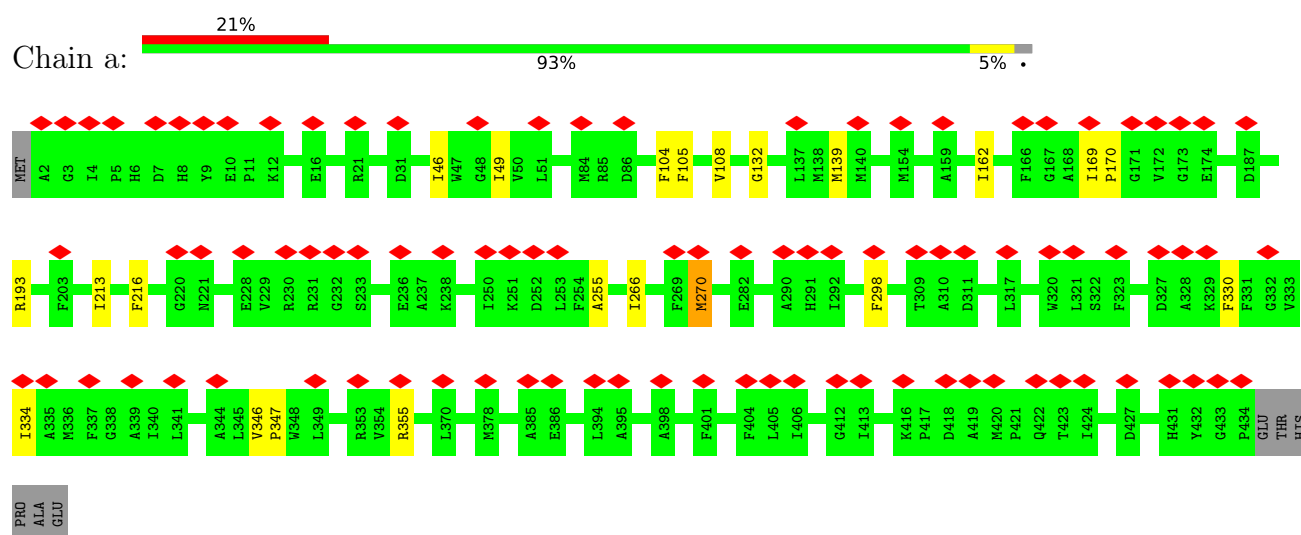
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	i	1	Total	Zn	0
			1	1	
23	m	1	Total	Zn	0
			1	1	

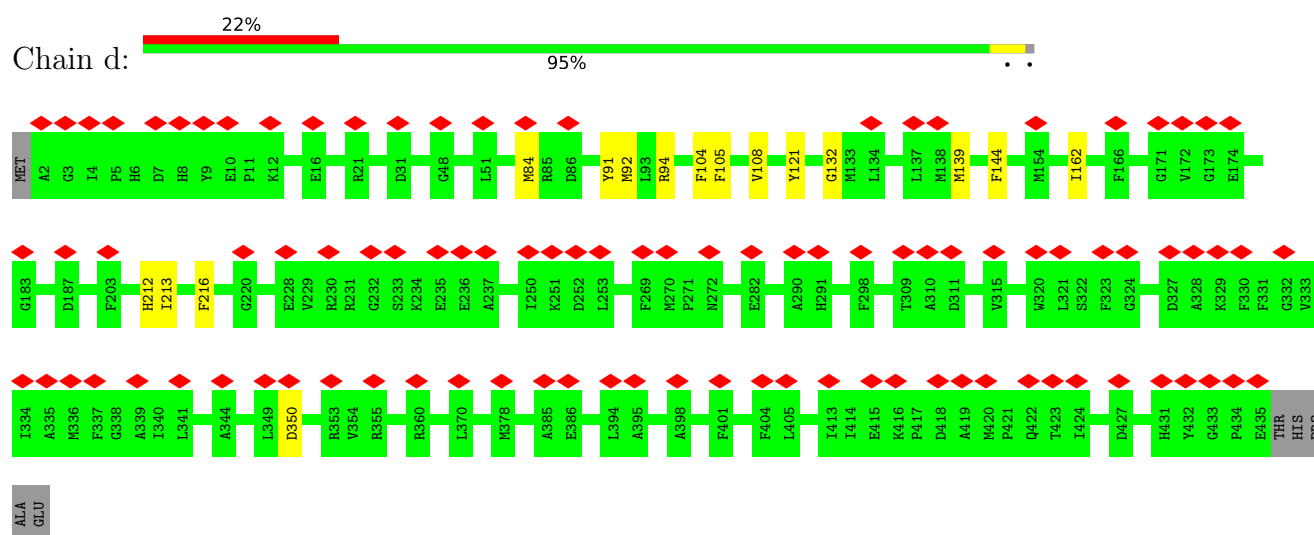
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome b

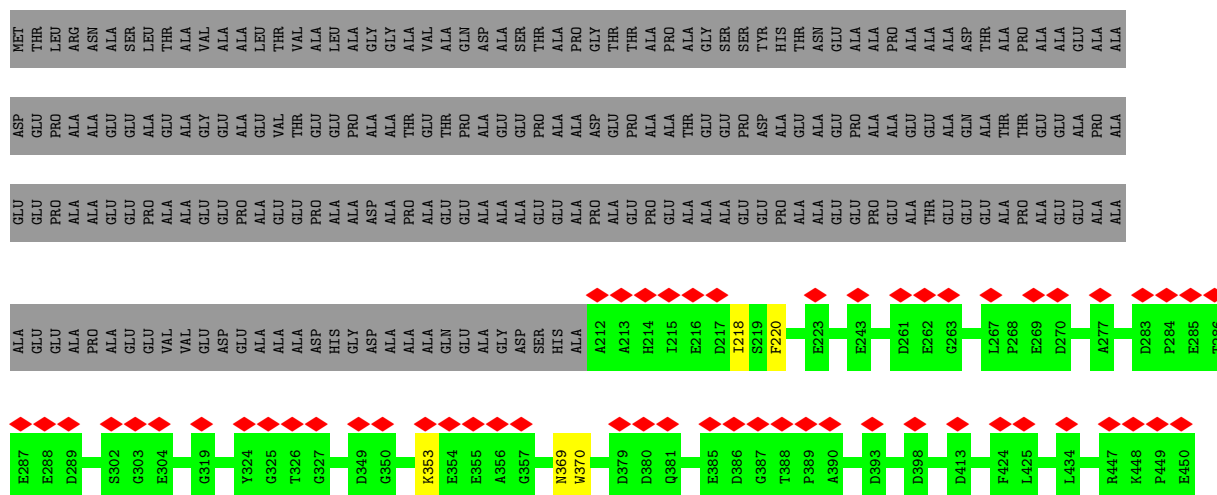


• Molecule 1: Cytochrome b

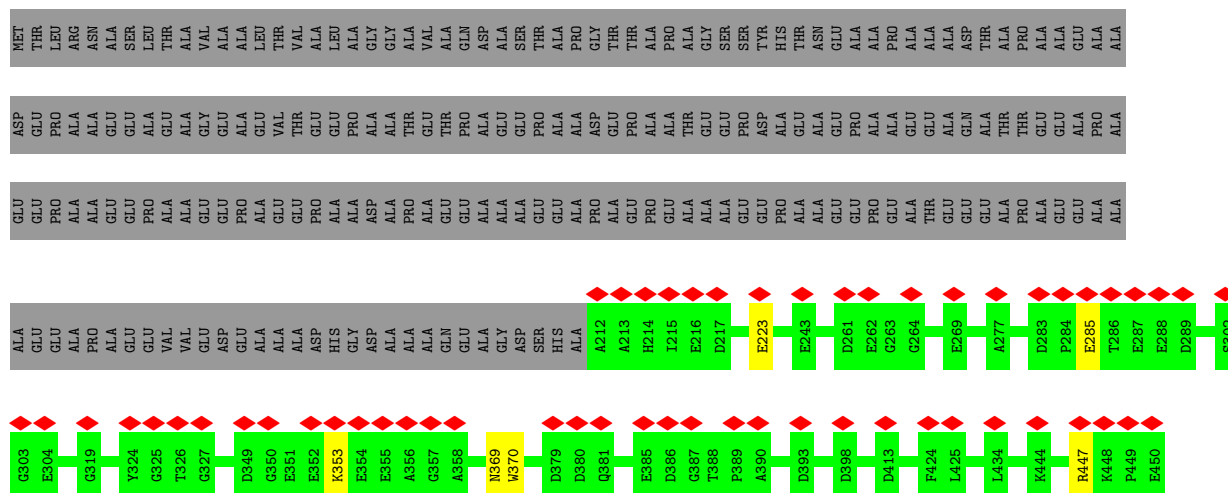


• Molecule 2: Cytochrome c1

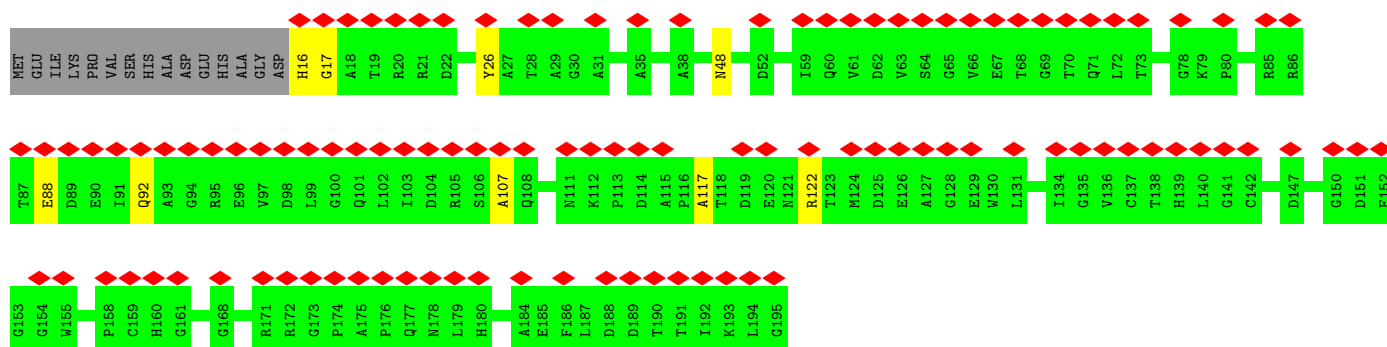
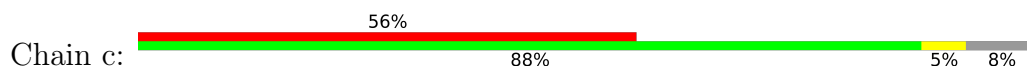




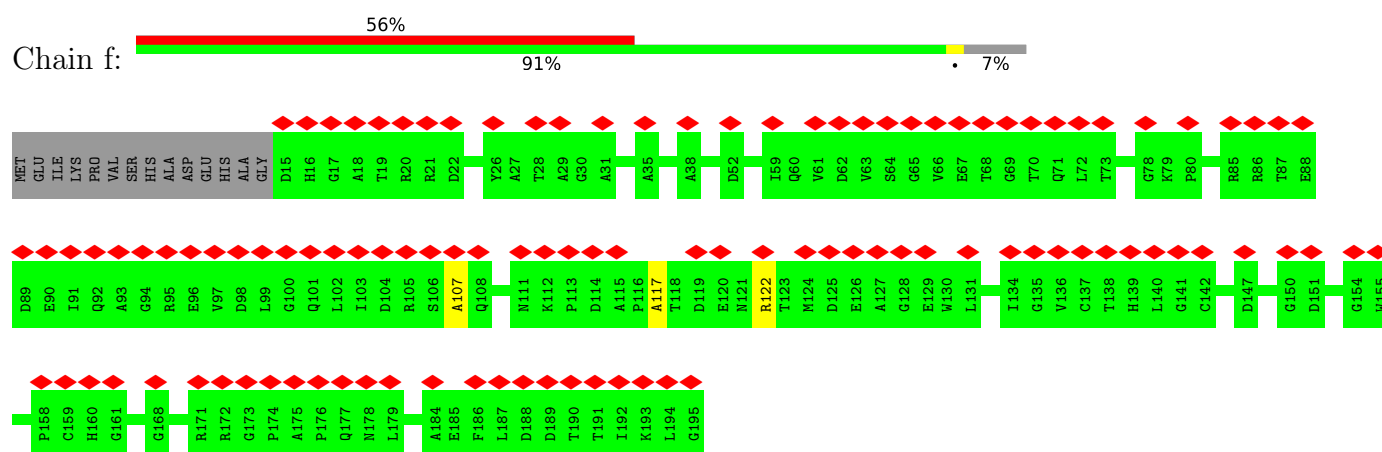
• Molecule 2: Cytochrome c1



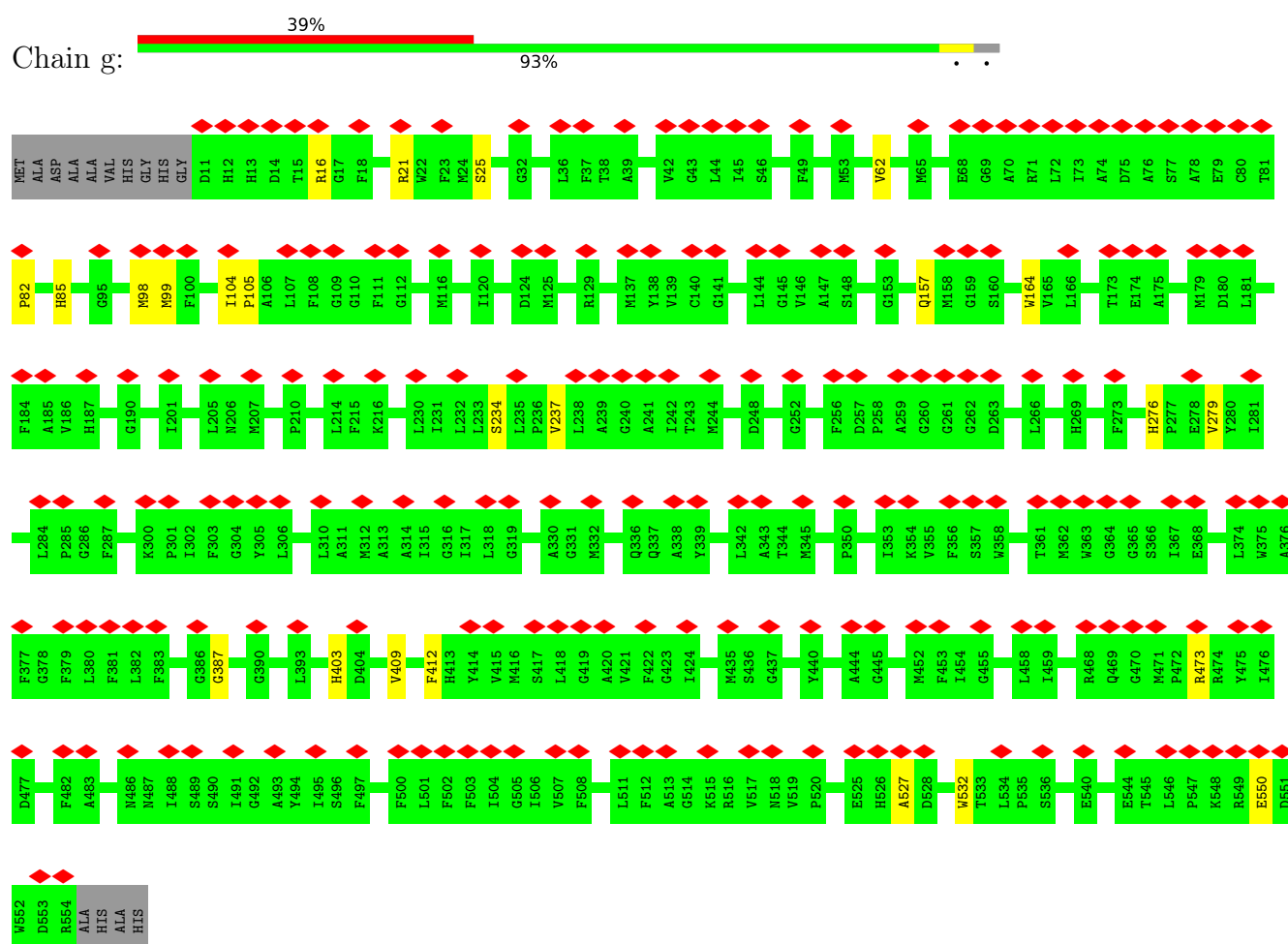
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



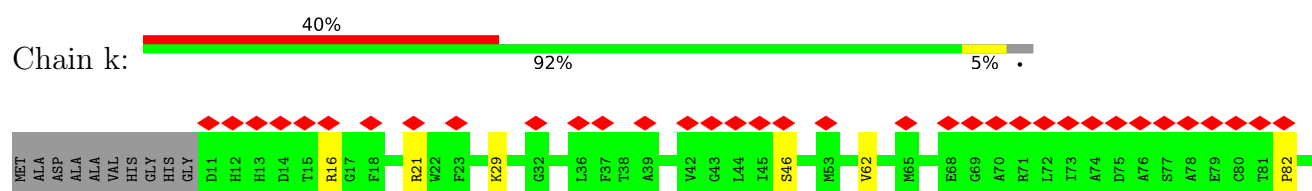
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

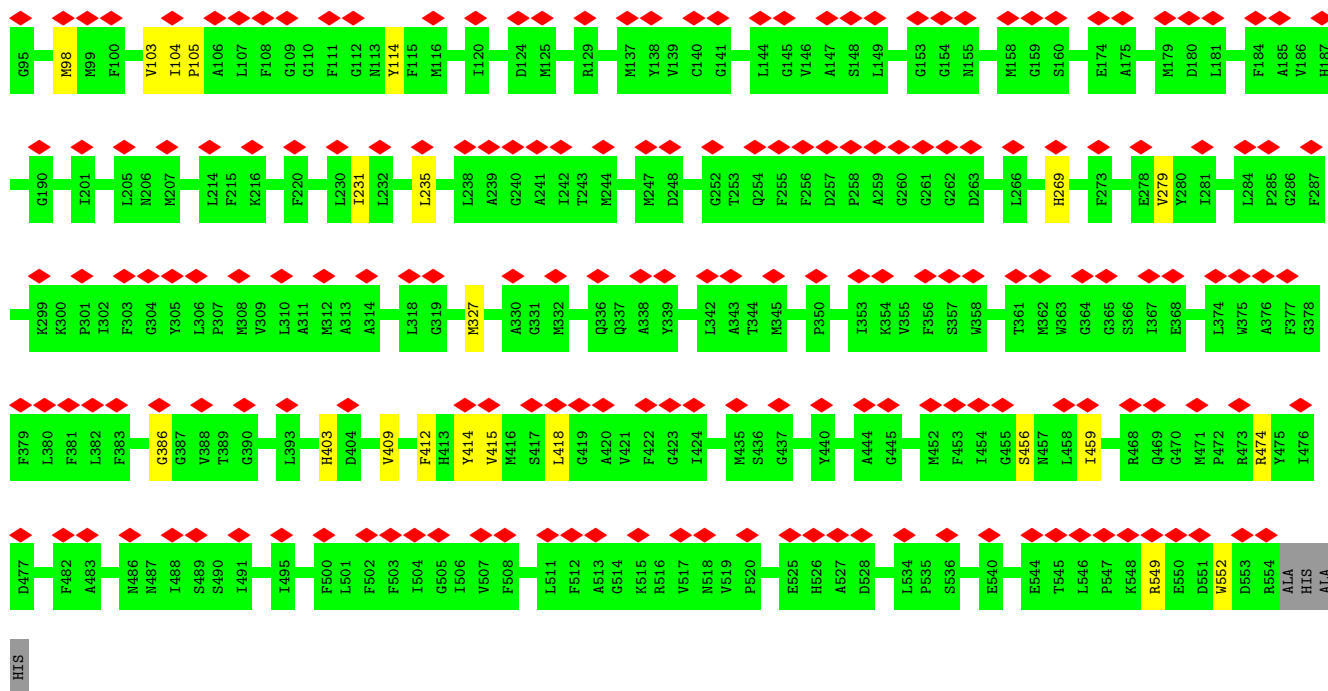


- Molecule 4: Cytochrome c oxidase subunit 1

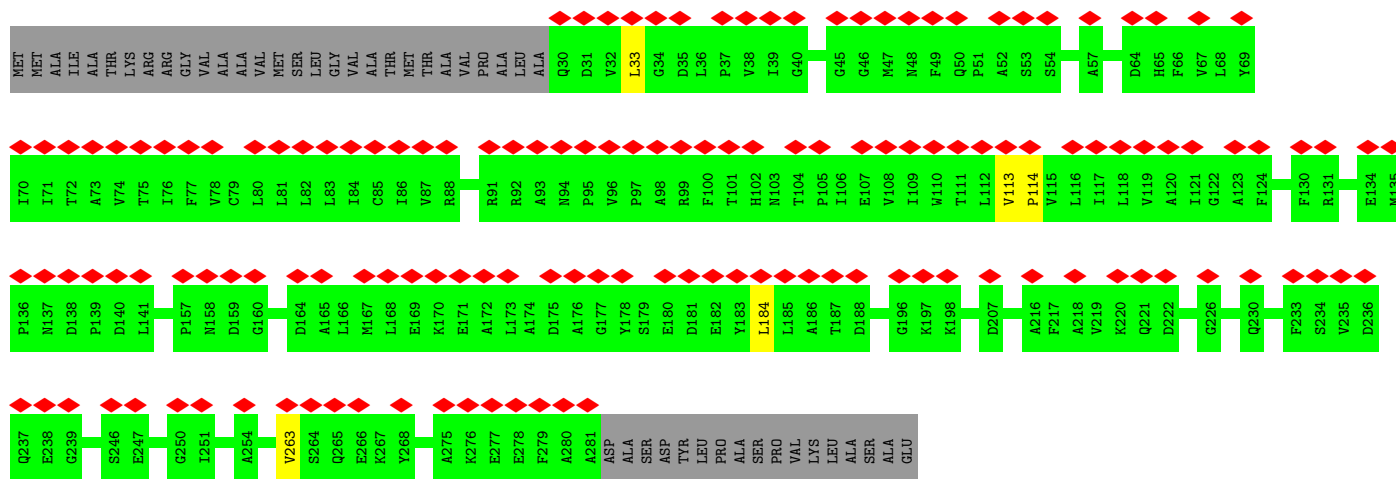
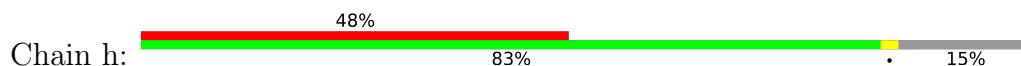


- Molecule 4: Cytochrome c oxidase subunit 1

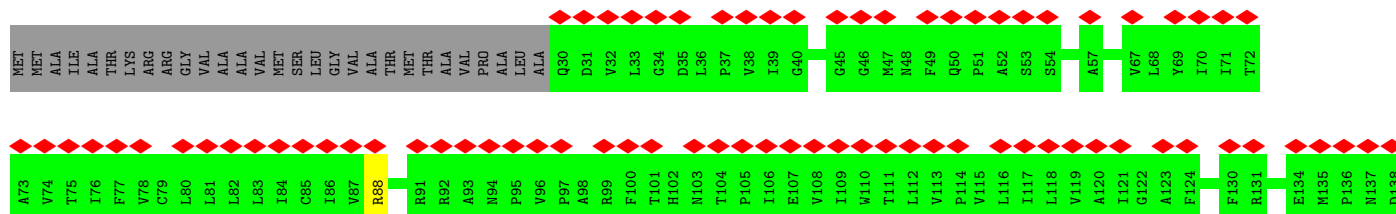
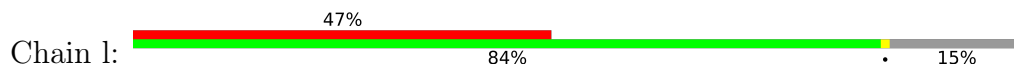


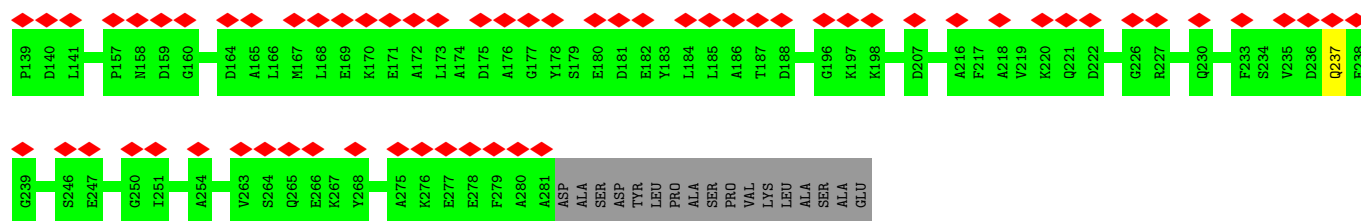


• Molecule 5: Cytochrome c oxidase subunit 2

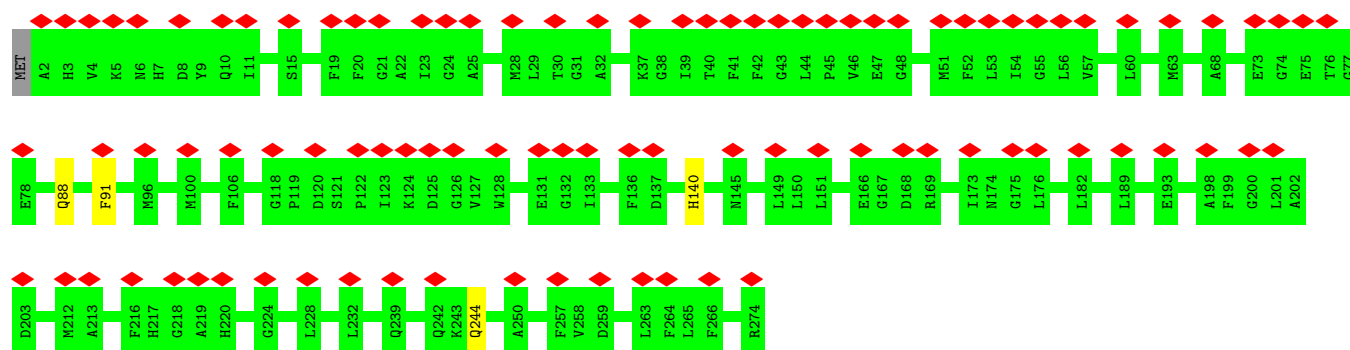


• Molecule 5: Cytochrome c oxidase subunit 2

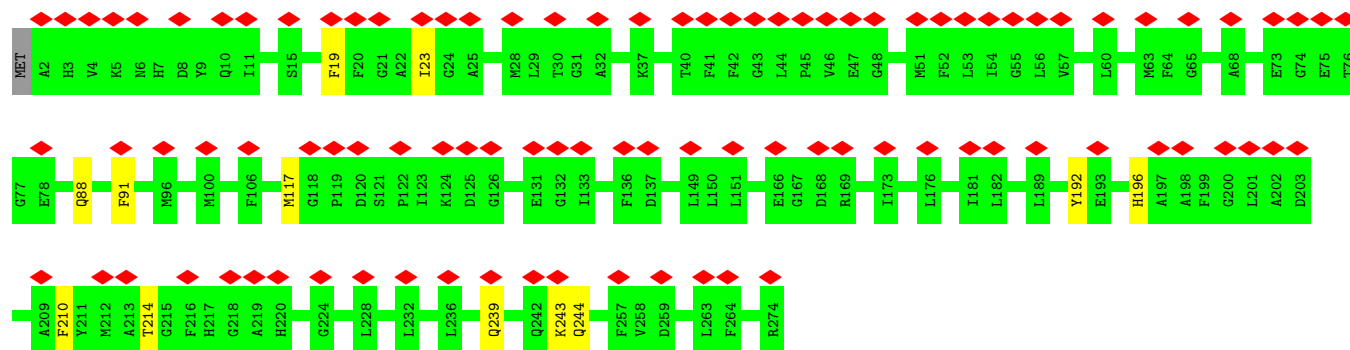




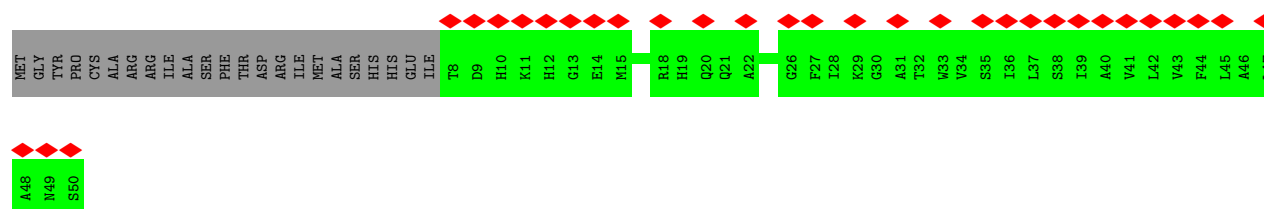
• Molecule 6: cytochrome-c oxidase



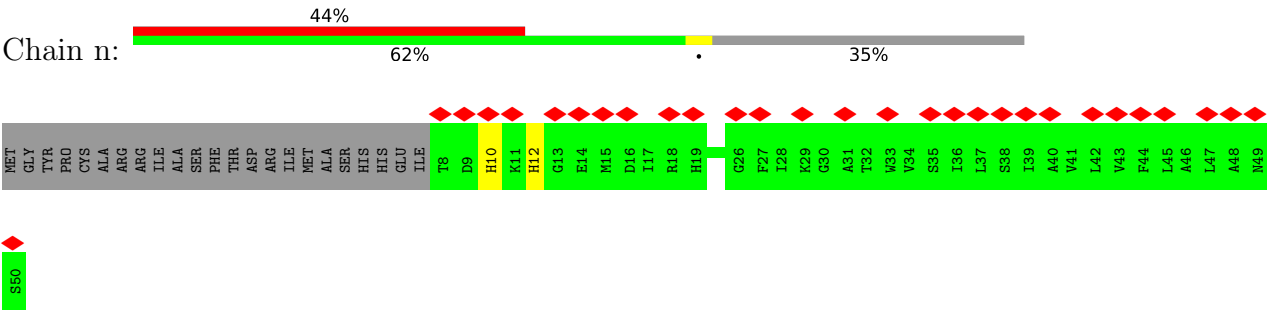
• Molecule 6: cytochrome-c oxidase



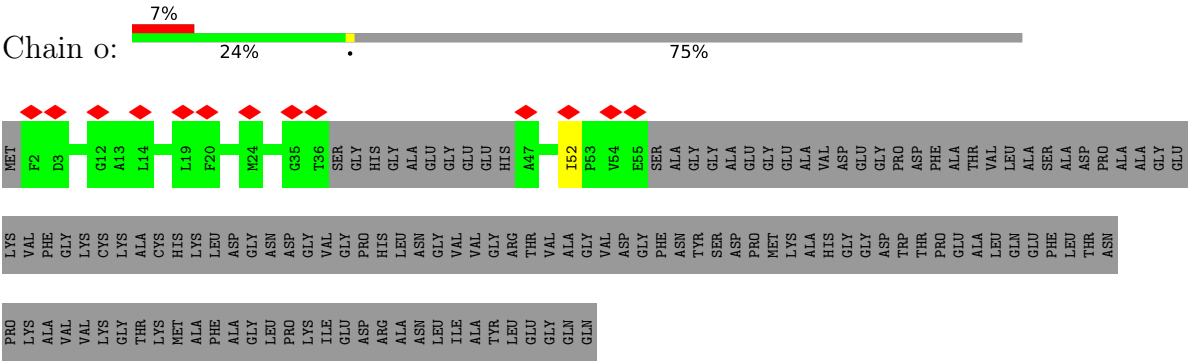
• Molecule 7: Aa3 type cytochrome c oxidase subunit IV



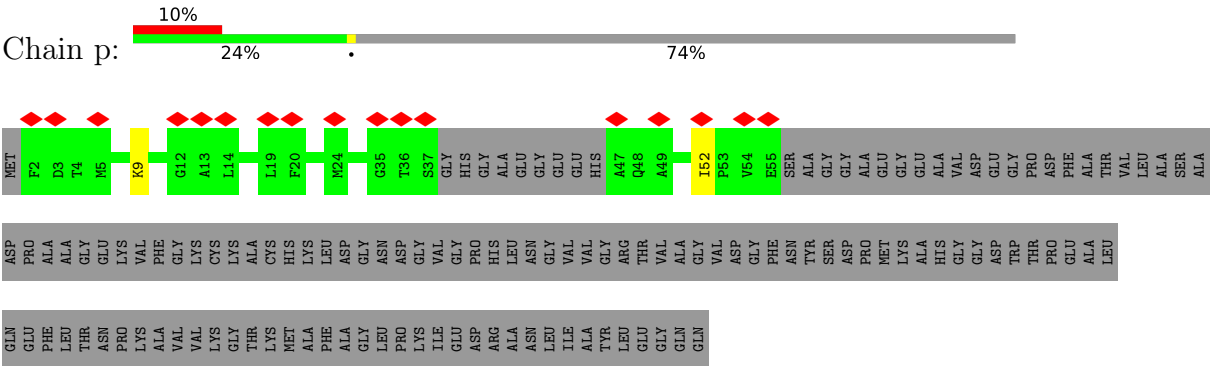
• Molecule 7: Aa3 type cytochrome c oxidase subunit IV



• Molecule 8: Cytochrome c, class I



• Molecule 8: Cytochrome c, class I



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	10322	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, HEC, DU0, ZN, 3PE, HEM, FES, PC1, CUA, MN, HEA, CDL, CA, U10, CU

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	a	0.31	0/3641	0.51	0/4993
1	d	0.31	0/3650	0.49	0/5005
2	b	0.26	0/1906	0.48	0/2592
2	e	0.26	0/1906	0.50	0/2592
3	c	0.21	0/1382	0.48	0/1880
3	f	0.21	0/1390	0.50	0/1891
4	g	0.24	0/4483	0.51	0/6118
4	k	0.25	0/4483	0.51	0/6118
5	h	0.19	0/2033	0.50	0/2787
5	l	0.19	0/2033	0.49	0/2787
6	i	0.24	0/2270	0.46	0/3107
6	m	0.25	0/2270	0.47	0/3107
7	j	0.20	0/339	0.40	0/457
7	n	0.20	0/339	0.47	0/457
8	o	0.23	0/330	0.46	0/448
8	p	0.25	0/336	0.48	0/456
All	All	0.25	0/32791	0.49	0/44795

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
4	g	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	355	ARG	Sidechain
4	g	473	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3504	0	3483	15	0
1	d	3513	0	3489	12	0
2	b	1855	0	1773	2	0
2	e	1855	0	1773	3	0
3	c	1353	0	1297	5	0
3	f	1361	0	1301	1	0
4	g	4322	0	4225	16	0
4	k	4322	0	4225	18	0
5	h	1976	0	1960	2	0
5	l	1976	0	1960	0	0
6	i	2183	0	2144	2	0
6	m	2183	0	2144	8	0
7	j	332	0	331	0	0
7	n	332	0	331	1	0
8	o	324	0	330	1	0
8	p	330	0	335	2	0
9	a	108	0	176	1	0
9	b	54	0	88	0	0
9	d	54	0	88	0	0
9	i	108	0	176	1	0
9	j	54	0	88	0	0
9	m	162	0	264	2	0
9	n	54	0	88	0	0
9	o	54	0	88	0	0
10	a	126	0	180	7	0
10	d	126	0	180	8	0
11	a	86	0	60	1	0
11	d	86	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	b	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	k	1	0	0	0	0
13	b	43	0	30	2	0
13	e	43	0	30	3	0
14	c	51	0	82	0	0
14	e	102	0	164	1	0
14	g	51	0	82	0	0
14	i	153	0	246	0	0
14	k	51	0	82	0	0
14	m	204	0	328	1	0
14	n	51	0	82	0	0
15	c	74	0	0	1	0
15	d	74	0	0	0	0
15	f	74	0	0	0	0
15	i	74	0	0	0	0
15	k	37	0	0	0	0
15	m	74	0	0	0	0
16	c	4	0	0	0	0
16	f	4	0	0	0	0
17	c	48	0	75	0	0
17	d	48	0	75	0	0
17	f	48	0	75	0	0
17	g	48	0	75	0	0
17	i	48	0	75	0	0
17	k	48	0	75	0	0
17	m	144	0	225	0	0
17	p	48	0	75	0	0
18	d	100	0	156	0	0
19	g	120	0	108	7	0
19	k	120	0	108	7	0
20	g	1	0	0	0	0
20	k	1	0	0	0	0
21	g	1	0	0	0	0
21	k	1	0	0	0	0
22	h	2	0	0	0	0
22	l	2	0	0	0	0
23	i	1	0	0	0	0
23	m	1	0	0	1	0
All	All	34791	0	34885	104	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 1.

All (104) 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)
4:g:98:MET:HB3	19:g:603:HEA:CBC	2.15	0.77
1:d:162:ILE:HG13	10:d:508:U10:H3M3	1.76	0.68
14:m:308:3PE:O14	23:m:309:ZN:ZN	1.42	0.68
10:a:506:U10:H452	10:d:508:U10:H253	1.77	0.66
10:a:502:U10:H253	10:d:506:U10:H43	1.77	0.65
1:d:104:PHE:CE2	1:d:139:MET:HE3	2.34	0.63
4:k:98:MET:HB3	19:k:606:HEA:CAC	2.31	0.60
10:a:506:U10:H1M3	10:a:506:U10:H103	1.84	0.60
1:d:108:VAL:HG21	1:d:139:MET:HE1	1.85	0.59
3:c:88:GLU:O	3:c:92:GLN:NE2	2.37	0.57
3:c:48:ASN:HD21	15:c:203:DU0:C19	2.18	0.57
1:d:91:TYR:CE2	1:d:92:MET:HG2	2.41	0.56
4:g:98:MET:SD	19:g:603:HEA:HBC1	2.46	0.56
4:g:16:ARG:HH11	4:g:16:ARG:HG3	1.71	0.55
1:a:104:PHE:CE2	1:a:139:MET:HE3	2.42	0.54
4:k:98:MET:HB3	19:k:606:HEA:HAC	1.89	0.54
1:d:132:GLY:HA3	11:d:504:HEM:HBC2	1.90	0.54
3:c:107:ALA:O	3:c:122:ARG:NH1	2.35	0.53
1:a:330:PHE:CE2	1:a:334:ILE:HD11	2.45	0.52
4:k:549:ARG:HA	4:k:552:TRP:NE1	2.25	0.51
4:k:103:VAL:HG21	19:k:606:HEA:HBC2	1.91	0.51
1:d:162:ILE:CG1	10:d:508:U10:H3M3	2.42	0.50
6:m:88:GLN:HA	6:m:91:PHE:CE2	2.45	0.50
1:a:105:PHE:HA	1:a:108:VAL:HG22	1.94	0.50
4:g:62:VAL:HG21	4:g:82:PRO:HB3	1.93	0.49
4:k:62:VAL:HG21	4:k:82:PRO:HB3	1.94	0.49
1:a:49:ILE:HD11	10:a:506:U10:H4M1	1.95	0.49
4:g:104:ILE:HB	4:g:105:PRO:HD3	1.94	0.49
19:g:603:HEA:HBB	19:g:603:HEA:OMA	2.12	0.49
1:a:193:ARG:HG3	1:a:193:ARG:HH11	1.77	0.48
2:e:285:GLU:H	2:e:285:GLU:CD	2.21	0.48
1:a:213:ILE:HA	1:a:216:PHE:CE2	2.48	0.48
1:d:144:PHE:HB2	10:d:508:U10:H1M3	1.95	0.48
1:d:105:PHE:CE1	1:d:139:MET:HE2	2.48	0.48
1:a:346:VAL:HG12	1:a:347:PRO:HD3	1.97	0.47
13:b:503:HEC:HMC1	13:b:503:HEC:HBC3	1.97	0.47
3:f:107:ALA:O	3:f:122:ARG:NH1	2.36	0.47
4:g:276:HIS:O	4:g:279:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:117:MET:HA	6:m:117:MET:HE2	1.95	0.47
1:a:162:ILE:HD11	10:a:502:U10:C5	2.45	0.47
6:m:244:GLN:CD	9:m:303:PC1:H132	2.40	0.47
6:m:210:PHE:O	6:m:214:THR:HG22	2.15	0.47
19:k:606:HEA:HHB	19:k:606:HEA:OMA	2.15	0.47
4:k:456:SER:HA	4:k:459:ILE:HD12	1.97	0.46
13:e:503:HEC:HBC3	13:e:503:HEC:HMC1	1.97	0.46
4:g:98:MET:HB3	19:g:603:HEA:CAC	2.45	0.46
4:k:409:VAL:HA	4:k:412:PHE:CE2	2.51	0.46
4:k:403:HIS:HD1	19:k:601:HEA:CGA	2.28	0.46
4:k:104:ILE:HB	4:k:105:PRO:HD3	1.98	0.46
4:g:403:HIS:HD1	19:g:605:HEA:CGA	2.29	0.45
6:i:88:GLN:HA	6:i:91:PHE:CE2	2.51	0.45
1:d:213:ILE:HA	1:d:216:PHE:CE2	2.52	0.45
4:g:234:SER:O	4:g:237:VAL:HG22	2.16	0.45
4:g:527:ALA:HB1	4:g:532:TRP:CD1	2.52	0.45
6:i:244:GLN:CD	9:i:307:PC1:H132	2.42	0.45
2:b:353:LYS:HE2	2:b:370:TRP:CE2	2.52	0.45
4:k:474:ARG:H	19:k:606:HEA:CGA	2.29	0.45
8:p:52:ILE:HD12	8:p:52:ILE:N	2.31	0.45
2:e:353:LYS:HE2	2:e:370:TRP:CE2	2.51	0.45
1:d:84:MET:SD	1:d:94:ARG:HD3	2.57	0.44
4:g:409:VAL:HA	4:g:412:PHE:CE2	2.53	0.44
9:a:503:PC1:O12	9:a:503:PC1:H122	2.17	0.44
10:d:508:U10:H172	10:d:508:U10:H151	1.86	0.44
3:c:16:HIS:CG	3:c:17:GLY:H	2.36	0.43
1:d:121:TYR:OH	1:d:350:ASP:OD2	2.30	0.43
8:o:52:ILE:N	8:o:52:ILE:HD12	2.33	0.43
1:d:212:HIS:CD2	11:d:504:HEM:NB	2.87	0.43
4:g:21:ARG:O	4:g:25:SER:HB3	2.18	0.43
13:e:503:HEC:HBB3	13:e:503:HEC:HMB3	2.01	0.43
4:g:387:GLY:HA3	19:g:605:HEA:C15	2.48	0.43
4:k:16:ARG:HH11	4:k:16:ARG:HG3	1.83	0.43
4:g:550:GLU:CD	4:g:550:GLU:H	2.27	0.43
1:a:266:ILE:HA	1:a:270:MET:SD	2.59	0.43
6:m:19:PHE:CZ	6:m:23:ILE:HD11	2.54	0.42
1:a:132:GLY:HA3	11:a:504:HEM:HBC2	2.01	0.42
4:k:16:ARG:HH21	4:k:21:ARG:HG3	1.84	0.42
1:a:162:ILE:HD11	10:a:502:U10:C4	2.49	0.42
10:d:506:U10:H8	10:d:506:U10:H153	2.00	0.42
2:e:223:GLU:HB3	14:e:504:3PE:H122	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:99:MET:HG3	4:g:164:TRP:CZ3	2.55	0.42
6:m:192:TYR:CZ	6:m:196:HIS:CE1	3.08	0.42
13:b:503:HEC:HBB3	13:b:503:HEC:HMB3	2.01	0.42
19:k:601:HEA:HHB	19:k:601:HEA:OMA	2.20	0.42
5:h:33:LEU:HD22	5:h:263:VAL:HG11	2.02	0.41
4:k:231:ILE:HG23	4:k:235:LEU:HD12	2.02	0.41
4:k:414:TYR:CD1	4:k:418:LEU:HD12	2.55	0.41
1:a:46:ILE:HD12	1:a:255:ALA:HB1	2.03	0.41
2:b:218:ILE:HD11	2:b:220:PHE:CZ	2.56	0.41
13:e:503:HEC:HHA	13:e:503:HEC:HBD1	2.03	0.41
1:a:298:PHE:HB3	10:a:502:U10:H71	2.03	0.41
1:a:169:ILE:HA	1:a:170:PRO:HD3	1.95	0.41
4:g:85:HIS:CD2	4:g:157:GLN:HB2	2.55	0.41
3:c:26:TYR:CE2	8:p:9:LYS:HE3	2.56	0.41
19:g:605:HEA:HHB	19:g:605:HEA:OMA	2.20	0.41
6:m:239:GLN:O	9:m:303:PC1:H121	2.20	0.41
10:d:508:U10:H401	10:d:508:U10:H422	1.85	0.41
5:h:113:VAL:HB	5:h:114:PRO:HD3	2.03	0.41
4:k:46:SER:HB2	4:k:98:MET:HE2	2.02	0.41
4:k:29:LYS:HB2	4:k:114:TYR:CE2	2.57	0.40
4:k:269:HIS:CD2	4:k:327:MET:HE1	2.55	0.40
4:k:386:GLY:HA3	4:k:415:VAL:HG13	2.03	0.40
7:n:10:HIS:CE1	7:n:12:HIS:HA	2.57	0.40
1:a:216:PHE:CD1	1:a:216:PHE:C	3.00	0.40
6:m:243:LYS:H	6:m:243:LYS:HD2	1.85	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	a	431/440 (98%)	422 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	432/440 (98%)	417 (96%)	15 (4%)	0	100	100
2	b	237/450 (53%)	231 (98%)	5 (2%)	1 (0%)	30	66
2	e	237/450 (53%)	233 (98%)	3 (1%)	1 (0%)	30	66
3	c	178/195 (91%)	171 (96%)	6 (3%)	1 (1%)	21	58
3	f	179/195 (92%)	173 (97%)	5 (3%)	1 (1%)	21	58
4	g	542/558 (97%)	521 (96%)	21 (4%)	0	100	100
4	k	542/558 (97%)	525 (97%)	17 (3%)	0	100	100
5	h	250/298 (84%)	241 (96%)	8 (3%)	1 (0%)	30	66
5	l	250/298 (84%)	239 (96%)	11 (4%)	0	100	100
6	i	271/274 (99%)	265 (98%)	5 (2%)	1 (0%)	30	66
6	m	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
7	j	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
7	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
8	o	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
8	p	41/176 (23%)	41 (100%)	0	0	100	100
All	All	3983/4914 (81%)	3860 (97%)	117 (3%)	6 (0%)	44	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	369	ASN
3	f	117	ALA
3	c	117	ALA
6	i	140	HIS
2	e	369	ASN
5	h	184	LEU

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	a	360/366 (98%)	359 (100%)	1 (0%)	86	84
1	d	361/366 (99%)	361 (100%)	0	100	100
2	b	192/319 (60%)	192 (100%)	0	100	100
2	e	192/319 (60%)	191 (100%)	1 (0%)	81	81
3	c	139/151 (92%)	139 (100%)	0	100	100
3	f	140/151 (93%)	140 (100%)	0	100	100
4	g	447/454 (98%)	447 (100%)	0	100	100
4	k	447/454 (98%)	446 (100%)	1 (0%)	87	85
5	h	211/243 (87%)	211 (100%)	0	100	100
5	l	211/243 (87%)	209 (99%)	2 (1%)	70	76
6	i	220/221 (100%)	220 (100%)	0	100	100
6	m	220/221 (100%)	220 (100%)	0	100	100
7	j	34/53 (64%)	34 (100%)	0	100	100
7	n	34/53 (64%)	34 (100%)	0	100	100
8	o	33/126 (26%)	33 (100%)	0	100	100
8	p	34/126 (27%)	34 (100%)	0	100	100
All	All	3275/3866 (85%)	3270 (100%)	5 (0%)	85	85

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

Mol	Chain	Res	Type
1	a	270	MET
2	e	447	ARG
4	k	279	VAL
5	l	88	ARG
5	l	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	221	ASN
1	a	272	ASN
2	b	333	ASN
2	b	436	ASN
2	b	445	HIS
3	c	48	ASN

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Mol	Chain	Res	Type
1	d	358	GLN
2	e	362	HIS
2	e	436	ASN
2	e	445	HIS
3	f	121	ASN
4	g	83	ASN
4	g	155	ASN
4	g	157	GLN
4	g	206	ASN
4	g	336	GLN
4	g	457	ASN
5	h	102	HIS
5	h	158	ASN
5	h	244	GLN
6	i	79	HIS
6	i	165	HIS
7	j	21	GLN
4	k	206	ASN
4	k	268	GLN
4	k	269	HIS
4	k	463	GLN
5	l	158	ASN
5	l	202	GLN
5	l	230	GLN
5	l	252	ASN
6	m	79	HIS
6	m	165	HIS
7	n	21	GLN
8	p	33	HIS

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 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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$
15	DU0	i	301	-	42,42,42	0.67	0	64,66,66	0.91	1 (1%)
15	DU0	k	605	-	42,42,42	0.64	0	64,66,66	0.82	2 (3%)
9	PC1	a	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.85	2 (3%)
14	3PE	g	607	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	4 (7%)
17	3PH	m	301	-	47,47,47	1.37	5 (10%)	50,52,52	1.05	5 (10%)
14	3PE	m	313	-	50,50,50	0.95	4 (8%)	53,55,55	1.04	2 (3%)
11	HEM	a	504	1	50,50,50	1.27	5 (10%)	67,82,82	0.88	0
18	CDL	d	501	-	99,99,99	0.91	8 (8%)	105,111,111	0.92	5 (4%)
14	3PE	i	308	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	3 (5%)
17	3PH	i	304	-	47,47,47	1.39	5 (10%)	50,52,52	1.02	5 (10%)
17	3PH	g	601	-	47,47,47	1.39	5 (10%)	50,52,52	1.04	3 (6%)
15	DU0	c	202	-	42,42,42	0.69	0	64,66,66	0.88	2 (3%)
9	PC1	j	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.91	3 (5%)
13	HEC	b	503	2	46,50,50	1.90	6 (13%)	58,82,82	1.62	8 (13%)
15	DU0	i	302	-	42,42,42	0.63	0	64,66,66	0.80	1 (1%)
17	3PH	f	204	-	47,47,47	1.37	5 (10%)	50,52,52	1.06	4 (8%)
15	DU0	d	502	-	42,42,42	0.61	0	64,66,66	0.96	4 (6%)
11	HEM	d	505	1	50,50,50	1.27	6 (12%)	67,82,82	1.03	3 (4%)
19	HEA	g	605	4	67,67,67	1.35	6 (8%)	81,103,103	2.33	27 (33%)
9	PC1	d	503	-	53,53,53	0.93	3 (5%)	59,61,61	0.91	2 (3%)
14	3PE	e	501	-	50,50,50	0.96	4 (8%)	53,55,55	0.98	2 (3%)
15	DU0	m	312	-	42,42,42	0.61	0	64,66,66	0.92	2 (3%)
14	3PE	i	309	-	50,50,50	0.97	4 (8%)	53,55,55	1.06	4 (7%)
17	3PH	k	602	-	47,47,47	1.38	5 (10%)	50,52,52	1.03	6 (12%)
14	3PE	m	306	-	50,50,50	0.97	4 (8%)	53,55,55	1.00	3 (5%)
16	FES	f	202	3	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	3PH	c	205	-	47,47,47	1.38	5 (10%)	50,52,52	1.14	5 (10%)
9	PC1	m	303	-	53,53,53	0.97	3 (5%)	59,61,61	0.85	3 (5%)
14	3PE	m	305	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	3 (5%)
9	PC1	a	503	-	53,53,53	0.95	3 (5%)	59,61,61	0.82	1 (1%)
11	HEM	d	504	1	50,50,50	1.25	4 (8%)	67,82,82	0.93	1 (1%)
9	PC1	b	501	-	53,53,53	0.95	3 (5%)	59,61,61	0.87	1 (1%)
10	U10	a	502	-	63,63,63	0.71	0	78,79,79	0.94	4 (5%)
10	U10	a	506	-	63,63,63	0.68	0	78,79,79	0.72	1 (1%)
14	3PE	e	504	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	4 (7%)
15	DU0	c	203	-	42,42,42	0.66	0	64,66,66	1.10	4 (6%)
15	DU0	f	203	-	42,42,42	0.67	0	64,66,66	0.81	0
9	PC1	m	307	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	3 (5%)
9	PC1	i	303	-	53,53,53	0.97	3 (5%)	59,61,61	0.89	4 (6%)
14	3PE	i	305	-	50,50,50	0.97	4 (8%)	53,55,55	1.17	3 (5%)
9	PC1	o	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	1 (1%)
15	DU0	d	509	-	42,42,42	0.65	0	64,66,66	0.90	1 (1%)
14	3PE	k	608	-	50,50,50	0.96	4 (8%)	53,55,55	0.98	4 (7%)
15	DU0	f	201	-	42,42,42	0.68	0	64,66,66	0.97	3 (4%)
17	3PH	m	302	-	47,47,47	1.37	5 (10%)	50,52,52	1.00	4 (8%)
17	3PH	m	304	-	47,47,47	1.38	5 (10%)	50,52,52	1.10	6 (12%)
17	3PH	p	1000	-	47,47,47	1.38	5 (10%)	50,52,52	1.02	4 (8%)
19	HEA	k	606	4	67,67,67	1.37	7 (10%)	81,103,103	2.35	29 (35%)
22	CUA	h	301	5	0,1,1	-	-	-	-	-
9	PC1	m	310	-	53,53,53	0.95	3 (5%)	59,61,61	0.95	3 (5%)
22	CUA	l	301	5	0,1,1	-	-	-	-	-
19	HEA	k	601	4	67,67,67	1.35	6 (8%)	81,103,103	2.28	28 (34%)
9	PC1	n	102	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	3 (5%)
14	3PE	n	101	-	50,50,50	0.98	4 (8%)	53,55,55	0.92	2 (3%)
9	PC1	i	307	-	53,53,53	0.96	3 (5%)	59,61,61	0.85	3 (5%)
10	U10	d	506	-	63,63,63	0.66	0	78,79,79	1.01	3 (3%)
16	FES	c	204	3	0,4,4	-	-	-	-	-
15	DU0	m	311	-	42,42,42	0.68	0	64,66,66	0.88	2 (3%)
17	3PH	d	507	-	47,47,47	1.38	5 (10%)	50,52,52	1.00	4 (8%)
14	3PE	m	308	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	2 (3%)
19	HEA	g	603	4	67,67,67	1.38	7 (10%)	81,103,103	2.33	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	a	505	1	50,50,50	1.27	6 (12%)	67,82,82	0.94	3 (4%)
10	U10	d	508	-	63,63,63	0.66	0	78,79,79	1.12	4 (5%)
14	3PE	c	201	-	50,50,50	0.96	4 (8%)	53,55,55	1.18	4 (7%)
13	HEC	e	503	2	46,50,50	1.90	6 (13%)	58,82,82	1.53	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	DU0	i	301	-	-	2/10/98/98	0/6/6/6
15	DU0	k	605	-	-	0/10/98/98	0/6/6/6
9	PC1	a	501	-	-	11/57/57/57	-
14	3PE	g	607	-	-	11/54/54/54	-
17	3PH	m	301	-	-	2/49/49/49	-
14	3PE	m	313	-	-	12/54/54/54	-
11	HEM	a	504	1	-	5/14/54/54	-
18	CDL	d	501	-	-	24/110/110/110	-
14	3PE	i	308	-	-	7/54/54/54	-
17	3PH	i	304	-	-	10/49/49/49	-
17	3PH	g	601	-	-	5/49/49/49	-
15	DU0	c	202	-	-	2/10/98/98	0/6/6/6
9	PC1	j	1001	-	-	16/57/57/57	-
13	HEC	b	503	2	-	8/14/54/54	-
15	DU0	i	302	-	-	2/10/98/98	0/6/6/6
17	3PH	f	204	-	-	15/49/49/49	-
15	DU0	d	502	-	-	1/10/98/98	0/6/6/6
11	HEM	d	505	1	-	8/14/54/54	-
19	HEA	g	605	4	-	2/36/76/76	-
9	PC1	d	503	-	-	15/57/57/57	-
14	3PE	e	501	-	-	12/54/54/54	-
15	DU0	m	312	-	-	0/10/98/98	0/6/6/6
14	3PE	i	309	-	-	10/54/54/54	-
17	3PH	k	602	-	-	7/49/49/49	-
14	3PE	m	306	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3PH	c	205	-	-	4/49/49/49	-
16	FES	f	202	3	-	-	0/1/1/1
9	PC1	m	303	-	-	12/57/57/57	-
14	3PE	m	305	-	-	5/54/54/54	-
9	PC1	a	503	-	-	13/57/57/57	-
11	HEM	d	504	1	-	8/14/54/54	-
9	PC1	b	501	-	-	13/57/57/57	-
10	U10	a	502	-	-	8/63/87/87	0/1/1/1
10	U10	a	506	-	-	13/63/87/87	0/1/1/1
14	3PE	e	504	-	-	11/54/54/54	-
15	DU0	c	203	-	-	3/10/98/98	0/6/6/6
15	DU0	f	203	-	-	1/10/98/98	0/6/6/6
9	PC1	m	307	-	-	18/57/57/57	-
9	PC1	i	303	-	-	7/57/57/57	-
14	3PE	i	305	-	-	14/54/54/54	-
9	PC1	o	1001	-	-	12/57/57/57	-
15	DU0	d	509	-	-	1/10/98/98	0/6/6/6
14	3PE	k	608	-	-	11/54/54/54	-
15	DU0	f	201	-	-	0/10/98/98	0/6/6/6
17	3PH	m	302	-	-	14/49/49/49	-
17	3PH	m	304	-	-	8/49/49/49	-
17	3PH	p	1000	-	-	5/49/49/49	-
19	HEA	k	606	4	-	6/36/76/76	-
9	PC1	m	310	-	-	7/57/57/57	-
19	HEA	k	601	4	-	4/36/76/76	-
9	PC1	n	102	-	-	16/57/57/57	-
14	3PE	n	101	-	-	11/54/54/54	-
9	PC1	i	307	-	-	9/57/57/57	-
10	U10	d	506	-	-	9/63/87/87	0/1/1/1
19	HEA	g	603	4	-	3/36/76/76	-
15	DU0	m	311	-	-	3/10/98/98	0/6/6/6
17	3PH	d	507	-	-	14/49/49/49	-
14	3PE	m	308	-	-	12/54/54/54	-
16	FES	c	204	3	-	-	0/1/1/1
11	HEM	a	505	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U10	d	508	-	-	11/63/87/87	0/1/1/1
14	3PE	c	201	-	-	16/54/54/54	-
13	HEC	e	503	2	-	8/14/54/54	-

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	p	1000	3PH	P-O11	7.47	1.83	1.60
17	g	601	3PH	P-O11	7.47	1.83	1.60
17	k	602	3PH	P-O11	7.43	1.83	1.60
17	i	304	3PH	P-O11	7.43	1.83	1.60
17	m	304	3PH	P-O11	7.36	1.83	1.60
17	c	205	3PH	P-O11	7.35	1.83	1.60
17	d	507	3PH	P-O11	7.31	1.83	1.60
17	f	204	3PH	P-O11	7.30	1.83	1.60
17	m	302	3PH	P-O11	7.21	1.83	1.60
17	m	301	3PH	P-O11	7.20	1.83	1.60
13	b	503	HEC	CAC-C3C	6.19	1.55	1.35
13	e	503	HEC	CAC-C3C	6.18	1.55	1.35
13	e	503	HEC	CAB-C3B	6.12	1.54	1.35
13	b	503	HEC	CAB-C3B	6.07	1.54	1.35
13	e	503	HEC	C3D-C2D	5.03	1.52	1.38
13	b	503	HEC	C3D-C2D	4.97	1.51	1.38
19	k	606	HEA	C3B-C2B	4.17	1.44	1.34
19	g	605	HEA	C3B-C2B	4.16	1.44	1.34
19	k	601	HEA	C3B-C2B	4.15	1.44	1.34
19	g	603	HEA	C3B-C2B	4.07	1.44	1.34
19	g	603	HEA	C3D-C2D	3.71	1.44	1.36
14	c	201	3PE	P-O14	-3.61	1.38	1.50
14	e	504	3PE	P-O14	-3.61	1.38	1.50
14	e	501	3PE	P-O14	-3.60	1.38	1.50
14	i	309	3PE	P-O14	-3.60	1.38	1.50
14	i	305	3PE	P-O14	-3.59	1.38	1.50
14	n	101	3PE	P-O14	-3.59	1.38	1.50
14	g	607	3PE	P-O14	-3.57	1.38	1.50
14	m	308	3PE	P-O14	-3.57	1.38	1.50
14	m	306	3PE	P-O14	-3.57	1.38	1.50
14	m	313	3PE	P-O14	-3.57	1.38	1.50
14	k	608	3PE	P-O14	-3.57	1.38	1.50
19	k	606	HEA	C3D-C2D	3.56	1.44	1.36
9	n	102	PC1	P-O14	-3.50	1.38	1.50
14	m	305	3PE	P-O14	-3.49	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	303	PC1	P-O14	-3.49	1.38	1.50
9	m	303	PC1	P-O14	-3.49	1.38	1.50
14	i	308	3PE	P-O14	-3.49	1.38	1.50
9	b	501	PC1	P-O14	-3.47	1.38	1.50
9	a	503	PC1	P-O14	-3.45	1.38	1.50
9	d	503	PC1	P-O14	-3.45	1.38	1.50
9	j	1001	PC1	P-O14	-3.42	1.39	1.50
9	a	501	PC1	P-O14	-3.41	1.39	1.50
9	i	307	PC1	P-O14	-3.40	1.39	1.50
9	o	1001	PC1	P-O14	-3.40	1.39	1.50
9	m	310	PC1	P-O14	-3.38	1.39	1.50
9	n	102	PC1	P-O13	3.37	1.72	1.59
9	m	307	PC1	P-O14	-3.34	1.39	1.50
9	a	501	PC1	P-O13	3.31	1.72	1.59
9	a	503	PC1	P-O13	3.31	1.72	1.59
9	m	307	PC1	P-O13	3.30	1.72	1.59
19	k	601	HEA	C3D-C2D	3.30	1.43	1.36
19	g	605	HEA	C3D-C2D	3.26	1.43	1.36
9	j	1001	PC1	P-O13	3.24	1.72	1.59
9	b	501	PC1	P-O13	3.22	1.72	1.59
9	o	1001	PC1	P-O13	3.22	1.72	1.59
9	i	307	PC1	P-O13	3.20	1.71	1.59
9	m	303	PC1	P-O13	3.18	1.71	1.59
9	i	303	PC1	P-O13	3.14	1.71	1.59
9	m	303	PC1	P-O12	-3.14	1.40	1.55
9	a	501	PC1	P-O12	-3.13	1.40	1.55
9	i	307	PC1	P-O12	-3.12	1.40	1.55
9	d	503	PC1	P-O12	-3.10	1.41	1.55
9	i	303	PC1	P-O12	-3.09	1.41	1.55
9	m	310	PC1	P-O13	3.09	1.71	1.59
9	b	501	PC1	P-O12	-3.08	1.41	1.55
9	j	1001	PC1	P-O12	-3.07	1.41	1.55
9	m	310	PC1	P-O12	-3.06	1.41	1.55
9	a	503	PC1	P-O12	-3.06	1.41	1.55
9	n	102	PC1	P-O12	-3.06	1.41	1.55
19	k	606	HEA	C3A-C2A	3.06	1.44	1.37
9	m	307	PC1	P-O12	-3.05	1.41	1.55
9	o	1001	PC1	P-O12	-3.02	1.41	1.55
19	g	605	HEA	C3A-C2A	2.95	1.43	1.37
9	d	503	PC1	P-O13	2.92	1.70	1.59
14	n	101	3PE	P-O12	-2.91	1.41	1.55
19	k	601	HEA	C3A-C2A	2.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	606	HEA	C1D-ND	-2.90	1.35	1.40
14	c	201	3PE	P-O12	-2.89	1.42	1.55
14	e	501	3PE	P-O12	-2.88	1.42	1.55
14	g	607	3PE	P-O12	-2.88	1.42	1.55
14	m	308	3PE	P-O12	-2.86	1.42	1.55
19	g	603	HEA	C3A-C2A	2.86	1.43	1.37
14	k	608	3PE	P-O12	-2.86	1.42	1.55
14	i	305	3PE	P-O12	-2.86	1.42	1.55
14	e	504	3PE	P-O12	-2.85	1.42	1.55
14	i	309	3PE	P-O12	-2.84	1.42	1.55
19	g	603	HEA	C1D-ND	-2.83	1.35	1.40
14	m	305	3PE	P-O12	-2.83	1.42	1.55
14	i	308	3PE	P-O12	-2.83	1.42	1.55
14	m	313	3PE	P-O12	-2.82	1.42	1.55
19	k	601	HEA	C1D-ND	-2.81	1.35	1.40
19	g	605	HEA	C1D-ND	-2.81	1.35	1.40
14	m	306	3PE	P-O12	-2.80	1.42	1.55
19	g	603	HEA	C11-C3B	-2.80	1.48	1.51
19	g	605	HEA	C4B-C3B	2.66	1.49	1.44
11	a	504	HEM	CAB-C3B	2.65	1.54	1.47
11	d	504	HEM	CAB-C3B	2.63	1.54	1.47
17	d	507	3PH	P-O14	-2.63	1.45	1.54
11	a	504	HEM	C3C-C2C	-2.62	1.31	1.37
17	c	205	3PH	P-O14	-2.61	1.45	1.54
17	f	204	3PH	P-O14	-2.61	1.45	1.54
11	a	505	HEM	CAB-C3B	2.60	1.54	1.47
17	m	301	3PH	P-O14	-2.60	1.45	1.54
17	c	205	3PH	P-O13	-2.59	1.45	1.54
11	d	505	HEM	C3B-C2B	-2.59	1.31	1.37
17	g	601	3PH	P-O13	-2.58	1.45	1.54
17	m	301	3PH	P-O13	-2.57	1.45	1.54
11	d	505	HEM	C3C-C2C	-2.57	1.31	1.37
17	i	304	3PH	P-O14	-2.57	1.45	1.54
17	i	304	3PH	P-O13	-2.56	1.45	1.54
17	m	304	3PH	P-O13	-2.55	1.45	1.54
17	k	602	3PH	P-O13	-2.55	1.45	1.54
17	g	601	3PH	P-O14	-2.55	1.45	1.54
17	k	602	3PH	P-O14	-2.54	1.45	1.54
19	k	606	HEA	C11-C3B	-2.54	1.48	1.51
17	m	302	3PH	P-O13	-2.54	1.45	1.54
17	m	302	3PH	P-O14	-2.54	1.45	1.54
17	p	1000	3PH	P-O14	-2.53	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	m	304	3PH	P-O14	-2.53	1.45	1.54
14	n	101	3PE	P-O11	2.52	1.69	1.59
17	f	204	3PH	P-O13	-2.52	1.45	1.54
17	d	507	3PH	P-O13	-2.52	1.45	1.54
11	a	505	HEM	C2A-C3A	-2.51	1.32	1.38
19	k	601	HEA	C4B-C3B	2.51	1.49	1.44
17	p	1000	3PH	P-O13	-2.50	1.45	1.54
14	i	309	3PE	P-O13	2.50	1.69	1.59
18	d	501	CDL	OB8-CB7	2.49	1.40	1.33
14	m	306	3PE	P-O13	2.49	1.69	1.59
18	d	501	CDL	OB6-CB4	-2.48	1.40	1.46
11	d	505	HEM	C2A-C3A	-2.47	1.32	1.38
11	d	504	HEM	C3C-C2C	-2.47	1.32	1.37
14	m	308	3PE	P-O13	2.47	1.69	1.59
11	a	505	HEM	C3C-C2C	-2.46	1.32	1.37
19	g	603	HEA	C4A-NA	-2.43	1.35	1.39
14	m	305	3PE	P-O11	2.42	1.68	1.59
18	d	501	CDL	OA6-CA5	2.41	1.41	1.34
17	m	301	3PH	O11-C1	-2.40	1.35	1.44
14	m	313	3PE	P-O13	2.40	1.68	1.59
18	d	501	CDL	OA8-CA7	2.40	1.40	1.33
14	i	308	3PE	P-O13	2.40	1.68	1.59
14	m	305	3PE	P-O13	2.38	1.68	1.59
11	d	505	HEM	CAB-C3B	2.37	1.53	1.47
14	m	306	3PE	P-O11	2.37	1.68	1.59
18	d	501	CDL	OB8-CB6	-2.37	1.39	1.45
14	i	308	3PE	P-O11	2.37	1.68	1.59
19	g	605	HEA	C4A-NA	-2.37	1.35	1.39
14	m	308	3PE	P-O11	2.36	1.68	1.59
17	d	507	3PH	O11-C1	-2.36	1.35	1.44
11	a	504	HEM	C2A-C3A	-2.35	1.32	1.38
14	k	608	3PE	P-O11	2.35	1.68	1.59
14	c	201	3PE	P-O11	2.34	1.68	1.59
19	k	601	HEA	C4A-NA	-2.34	1.35	1.39
14	e	501	3PE	P-O11	2.34	1.68	1.59
17	m	302	3PH	O11-C1	-2.33	1.35	1.44
11	a	504	HEM	CAC-C3C	2.33	1.53	1.47
11	d	504	HEM	CAC-C3C	2.32	1.53	1.47
17	m	304	3PH	O11-C1	-2.32	1.35	1.44
19	k	606	HEA	C4A-NA	-2.32	1.35	1.39
14	i	305	3PE	P-O11	2.31	1.68	1.59
14	g	607	3PE	P-O11	2.31	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	205	3PH	P-O12	-2.31	1.43	1.50
17	d	507	3PH	P-O12	-2.31	1.43	1.50
11	a	505	HEM	CAC-C3C	2.30	1.53	1.47
17	f	204	3PH	O11-C1	-2.30	1.35	1.44
14	e	504	3PE	P-O13	2.30	1.68	1.59
11	d	504	HEM	C2A-C3A	-2.29	1.32	1.38
14	e	501	3PE	P-O13	2.29	1.68	1.59
14	n	101	3PE	P-O13	2.28	1.68	1.59
14	k	608	3PE	P-O13	2.28	1.68	1.59
14	i	309	3PE	P-O11	2.28	1.68	1.59
17	k	602	3PH	O11-C1	-2.28	1.36	1.44
14	i	305	3PE	P-O13	2.27	1.68	1.59
17	i	304	3PH	O11-C1	-2.26	1.36	1.44
17	m	302	3PH	P-O12	-2.26	1.43	1.50
17	i	304	3PH	P-O12	-2.26	1.43	1.50
17	p	1000	3PH	P-O12	-2.26	1.43	1.50
18	d	501	CDL	OA6-CA4	-2.25	1.41	1.46
11	d	505	HEM	CAC-C3C	2.23	1.53	1.47
17	g	601	3PH	O11-C1	-2.23	1.36	1.44
17	m	301	3PH	P-O12	-2.22	1.43	1.50
19	g	603	HEA	C4B-NB	-2.22	1.36	1.40
17	g	601	3PH	P-O12	-2.21	1.43	1.50
17	f	204	3PH	P-O12	-2.21	1.43	1.50
17	p	1000	3PH	O11-C1	-2.21	1.36	1.44
17	c	205	3PH	O11-C1	-2.21	1.36	1.44
14	c	201	3PE	P-O13	2.21	1.68	1.59
14	g	607	3PE	P-O13	2.21	1.68	1.59
17	k	602	3PH	P-O12	-2.20	1.43	1.50
14	e	504	3PE	P-O11	2.19	1.68	1.59
17	m	304	3PH	P-O12	-2.19	1.43	1.50
18	d	501	CDL	OB6-CB5	2.14	1.40	1.34
11	a	505	HEM	C3B-C2B	-2.12	1.32	1.37
11	a	505	HEM	C3D-C2D	-2.10	1.32	1.36
14	m	313	3PE	P-O11	2.10	1.67	1.59
19	k	606	HEA	C4B-NB	-2.10	1.36	1.40
13	b	503	HEC	C3B-C2B	-2.09	1.34	1.41
18	d	501	CDL	OA8-CA6	-2.09	1.40	1.45
13	b	503	HEC	C3C-C2C	-2.08	1.34	1.41
13	e	503	HEC	C3B-C2B	-2.08	1.34	1.41
13	b	503	HEC	CMC-C2C	2.07	1.55	1.50
11	d	505	HEM	C3D-C2D	-2.06	1.32	1.36
13	e	503	HEC	C3C-C2C	-2.04	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	504	HEM	C3B-C2B	-2.03	1.33	1.37
13	e	503	HEC	CMC-C2C	2.02	1.54	1.50

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	606	HEA	C3A-C2A-C1A	-7.01	100.41	107.05
19	g	605	HEA	C3A-C2A-C1A	-6.80	100.61	107.05
19	g	603	HEA	C3A-C2A-C1A	-6.77	100.64	107.05
19	k	601	HEA	C3A-C2A-C1A	-6.68	100.72	107.05
13	b	503	HEC	CBB-CAB-C3B	-6.09	115.27	127.43
13	e	503	HEC	CBB-CAB-C3B	-5.98	115.49	127.43
13	b	503	HEC	CBC-CAC-C3C	-5.29	116.87	127.43
13	e	503	HEC	CBC-CAC-C3C	-5.11	117.21	127.43
19	g	605	HEA	C3D-C4D-ND	5.03	115.21	110.35
19	k	606	HEA	C2A-C1A-NA	4.97	115.12	110.32
19	k	601	HEA	C3D-C4D-ND	4.93	115.12	110.35
19	g	605	HEA	C2A-C1A-NA	4.88	115.03	110.32
19	k	606	HEA	CMC-C2C-C3C	4.82	137.88	126.55
19	k	601	HEA	C2A-C1A-NA	4.74	114.90	110.32
19	g	603	HEA	CMC-C2C-C3C	4.73	137.68	126.55
19	g	605	HEA	CMC-C2C-C3C	4.72	137.65	126.55
19	g	603	HEA	CMD-C2D-C1D	-4.71	117.67	125.03
10	d	508	U10	C6-C1-C2	4.65	122.84	119.17
19	k	606	HEA	CAA-CBA-CGA	-4.65	101.33	113.67
19	k	601	HEA	CMC-C2C-C3C	4.65	137.49	126.55
14	m	313	3PE	O12-P-O14	4.63	133.96	112.44
19	g	605	HEA	CMC-C2C-C1C	-4.62	118.38	125.42
9	d	503	PC1	O12-P-O14	4.61	133.89	112.44
19	k	606	HEA	CMD-C2D-C1D	-4.60	117.85	125.03
9	m	310	PC1	O12-P-O14	4.60	133.82	112.44
9	b	501	PC1	O12-P-O14	4.52	133.49	112.44
9	o	1001	PC1	O12-P-O14	4.52	133.46	112.44
19	k	606	HEA	C3D-C4D-ND	4.51	114.71	110.35
19	g	603	HEA	C2A-C1A-NA	4.48	114.65	110.32
19	g	603	HEA	C3D-C4D-ND	4.48	114.68	110.35
19	g	603	HEA	CMC-C2C-C1C	-4.47	118.62	125.42
19	k	601	HEA	CMC-C2C-C1C	-4.45	118.65	125.42
14	e	504	3PE	O12-P-O14	4.42	133.02	112.44
9	i	303	PC1	O12-P-O14	4.41	132.95	112.44
14	c	201	3PE	C2-O21-C21	4.39	128.30	117.80
9	i	307	PC1	O12-P-O14	4.39	132.85	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	g	607	3PE	O12-P-O14	4.35	132.70	112.44
19	g	603	HEA	CAA-CBA-CGA	-4.35	102.13	113.67
19	k	606	HEA	CBA-CAA-C2A	4.35	124.56	112.53
9	m	303	PC1	O12-P-O14	4.34	132.64	112.44
14	i	305	3PE	O12-P-O14	4.33	132.61	112.44
9	m	307	PC1	O12-P-O14	4.33	132.61	112.44
19	g	605	HEA	CMB-C2B-C1B	-4.32	118.28	125.03
19	k	601	HEA	CMB-C2B-C1B	-4.30	118.32	125.03
14	c	201	3PE	O12-P-O14	4.28	132.37	112.44
19	k	606	HEA	CMC-C2C-C1C	-4.28	118.90	125.42
14	m	305	3PE	O12-P-O14	4.27	132.33	112.44
14	k	608	3PE	O12-P-O14	4.27	132.31	112.44
14	e	501	3PE	O12-P-O14	4.25	132.19	112.44
14	i	308	3PE	O12-P-O14	4.24	132.16	112.44
9	a	503	PC1	O12-P-O14	4.22	132.06	112.44
10	a	502	U10	C6-C1-C2	4.19	122.48	119.17
14	i	309	3PE	O12-P-O14	4.19	131.92	112.44
19	k	606	HEA	CMB-C2B-C1B	-4.18	118.50	125.03
9	j	1001	PC1	O12-P-O14	4.15	131.75	112.44
14	m	308	3PE	O12-P-O14	4.14	131.72	112.44
9	a	501	PC1	O12-P-O14	4.14	131.69	112.44
10	d	506	U10	C7-C6-C5	-4.11	113.74	118.52
9	n	102	PC1	O12-P-O14	4.09	131.45	112.44
14	m	306	3PE	O12-P-O14	4.06	131.31	112.44
14	n	101	3PE	O12-P-O14	4.03	131.21	112.44
19	g	605	HEA	CHA-C4D-C3D	-4.02	118.91	124.77
19	g	603	HEA	CMB-C2B-C1B	-4.01	118.78	125.03
19	g	605	HEA	CHA-C1A-C2A	-3.98	118.59	124.86
19	g	603	HEA	C4D-C3D-C2D	-3.92	101.19	106.89
19	g	605	HEA	C26-C15-C16	3.91	122.01	115.23
19	g	605	HEA	C4D-C3D-C2D	-3.86	101.27	106.89
19	k	601	HEA	CHA-C1A-C2A	-3.84	118.80	124.86
19	k	601	HEA	CHA-C4D-C3D	-3.83	119.19	124.77
19	k	606	HEA	C4D-C3D-C2D	-3.82	101.33	106.89
10	d	506	U10	C6-C1-C2	3.82	122.18	119.17
14	i	305	3PE	O31-C3-C2	3.81	119.36	108.40
13	e	503	HEC	CMC-C2C-C1C	-3.75	119.71	125.42
19	k	601	HEA	C4D-C3D-C2D	-3.74	101.44	106.89
19	g	605	HEA	CAA-CBA-CGA	-3.73	103.77	113.67
19	g	603	HEA	CBA-CAA-C2A	3.73	122.84	112.53
14	i	305	3PE	C2-O21-C21	3.72	126.71	117.80
19	k	601	HEA	CMD-C2D-C1D	-3.70	119.25	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	601	HEA	CAA-CBA-CGA	-3.69	103.88	113.67
19	k	606	HEA	CHA-C1A-C2A	-3.69	119.04	124.86
17	m	304	3PH	O31-C3-C2	3.68	119.01	108.40
13	b	503	HEC	CMC-C2C-C1C	-3.55	120.02	125.42
17	f	204	3PH	O13-P-O11	-3.54	97.45	106.67
19	g	605	HEA	CMD-C2D-C1D	-3.50	119.56	125.03
19	k	606	HEA	CMD-C2D-C3D	3.48	135.55	126.15
19	g	603	HEA	CMD-C2D-C3D	3.45	135.48	126.15
17	c	205	3PH	O31-C3-C2	3.43	118.29	108.40
19	g	603	HEA	CHA-C4D-C3D	-3.43	119.78	124.77
15	c	203	DU0	C22-C21-C20	3.41	116.49	111.45
17	m	301	3PH	O13-P-O11	-3.41	97.78	106.67
19	g	603	HEA	CAA-C2A-C1A	3.37	131.70	124.85
19	k	606	HEA	C3C-C2C-C1C	-3.36	103.20	107.17
9	n	102	PC1	C2-O21-C21	3.36	125.84	117.80
19	g	605	HEA	CAD-C3D-C4D	3.34	130.52	124.70
19	k	606	HEA	CHA-C4D-C3D	-3.32	119.93	124.77
17	d	507	3PH	O13-P-O11	-3.31	98.04	106.67
14	m	306	3PE	C2-O21-C21	3.31	125.72	117.80
19	g	603	HEA	CMB-C2B-C3B	3.28	136.62	130.28
10	a	506	U10	C6-C1-C2	3.28	121.75	119.17
19	g	603	HEA	CHA-C1A-C2A	-3.27	119.70	124.86
19	k	601	HEA	CAD-C3D-C4D	3.25	130.36	124.70
17	p	1000	3PH	O13-P-O11	-3.24	98.23	106.67
19	k	606	HEA	CAD-C3D-C4D	3.22	130.32	124.70
19	k	606	HEA	C26-C15-C16	3.22	120.81	115.23
19	g	605	HEA	C27-C19-C20	3.18	120.75	115.23
19	k	606	HEA	CMB-C2B-C3B	3.17	136.41	130.28
17	f	204	3PH	O31-C31-O32	-3.15	115.75	123.63
19	k	601	HEA	CAA-C2A-C1A	3.14	131.24	124.85
19	k	601	HEA	C26-C15-C16	3.12	120.64	115.23
14	i	309	3PE	C2-O21-C21	3.11	125.23	117.80
19	g	605	HEA	CAA-C2A-C1A	3.08	131.11	124.85
17	p	1000	3PH	O31-C31-O32	-3.05	116.00	123.63
17	k	602	3PH	O13-P-O11	-3.04	98.73	106.67
19	k	601	HEA	CMD-C2D-C3D	3.01	134.30	126.15
19	g	603	HEA	C27-C19-C20	3.00	120.43	115.23
18	d	501	CDL	OB6-CB5-C51	2.98	117.93	111.48
19	g	603	HEA	C3C-C2C-C1C	-2.98	103.66	107.17
19	g	603	HEA	CAD-C3D-C4D	2.97	129.87	124.70
19	k	601	HEA	C17-C18-C19	-2.96	120.85	127.62
19	g	603	HEA	C13-C14-C15	-2.94	120.89	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	603	HEA	CHB-C1B-C2B	-2.93	120.41	125.03
19	k	601	HEA	C13-C12-C11	-2.90	109.76	114.39
19	k	606	HEA	C12-C13-C14	2.88	119.73	112.16
13	b	503	HEC	CAA-CBA-CGA	-2.87	106.04	113.67
17	i	304	3PH	O13-P-O11	-2.87	99.19	106.67
19	g	605	HEA	C4B-C3B-C2B	-2.85	102.64	107.44
19	k	601	HEA	CAD-CBD-CGD	-2.83	106.16	113.67
17	m	302	3PH	O13-P-O11	-2.83	99.30	106.67
19	k	601	HEA	CMB-C2B-C3B	2.81	135.71	130.28
17	c	205	3PH	O31-C31-O32	-2.80	116.61	123.63
19	k	601	HEA	C3C-C2C-C1C	-2.80	103.86	107.17
19	g	605	HEA	CMD-C2D-C3D	2.80	133.71	126.15
19	g	603	HEA	C13-C12-C11	-2.79	109.93	114.39
17	g	601	3PH	O31-C31-O32	-2.77	116.69	123.63
17	i	304	3PH	O31-C31-O32	-2.77	116.70	123.63
17	m	304	3PH	O13-P-O11	-2.75	99.50	106.67
17	c	205	3PH	O13-P-O11	-2.74	99.54	106.67
19	g	605	HEA	C3C-C2C-C1C	-2.72	103.97	107.17
19	k	606	HEA	CAA-C2A-C1A	2.71	130.37	124.85
18	d	501	CDL	OA8-CA6-CA4	2.71	116.21	108.40
19	g	605	HEA	CMB-C2B-C3B	2.71	135.51	130.28
19	g	605	HEA	C3B-C4B-NB	2.70	112.94	109.84
19	g	605	HEA	CBA-CAA-C2A	2.70	119.98	112.53
19	k	601	HEA	C4B-C3B-C2B	-2.67	102.94	107.44
17	m	302	3PH	O31-C31-O32	-2.65	117.01	123.63
15	c	203	DU0	C76-C75-C22	2.64	114.64	110.33
14	i	309	3PE	O31-C31-O32	-2.64	117.03	123.63
19	g	605	HEA	CAD-CBD-CGD	-2.63	106.68	113.67
17	k	602	3PH	O31-C31-O32	-2.62	117.07	123.63
15	c	203	DU0	C76-C77-C79	2.61	112.20	108.74
19	g	603	HEA	CHC-C1C-C2C	-2.60	119.87	127.43
17	g	601	3PH	O13-P-O11	-2.59	99.90	106.67
19	g	605	HEA	C25-C23-C24	2.59	120.56	114.59
19	g	603	HEA	C2B-C1B-NB	2.57	112.88	109.90
15	f	201	DU0	O23-C24-C25	-2.57	103.37	108.77
17	d	507	3PH	O31-C31-O32	-2.56	117.22	123.63
9	j	1001	PC1	C2-O21-C21	2.55	123.89	117.80
19	g	605	HEA	CHC-C1C-C2C	-2.54	120.06	127.43
15	d	502	DU0	O10-C09-C15	2.53	112.97	110.76
9	m	310	PC1	O31-C31-O32	-2.52	117.32	123.63
19	k	601	HEA	C25-C23-C24	2.52	120.38	114.59
19	k	601	HEA	CHB-C1B-C2B	-2.51	121.06	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	601	HEA	CBA-CAA-C2A	2.51	119.47	112.53
19	k	606	HEA	CHB-C1B-C2B	-2.50	121.09	125.03
19	k	606	HEA	C3B-C4B-NB	2.49	112.70	109.84
19	k	606	HEA	C27-C19-C20	2.49	119.54	115.23
15	m	312	DU0	C75-C22-C21	-2.48	107.52	110.97
19	k	601	HEA	CHC-C1C-C2C	-2.48	120.24	127.43
10	d	508	U10	C7-C6-C5	-2.47	115.64	118.52
19	k	606	HEA	CHC-C1C-C2C	-2.47	120.25	127.43
17	m	304	3PH	O31-C31-O32	-2.47	117.45	123.63
13	e	503	HEC	C4D-ND-C1D	2.46	109.83	105.82
19	k	601	HEA	C3B-C4B-NB	2.45	112.66	109.84
13	b	503	HEC	C4D-ND-C1D	2.45	109.81	105.82
17	k	602	3PH	O21-C21-O22	-2.44	118.00	123.70
9	i	307	PC1	O31-C31-O32	-2.40	117.61	123.63
10	d	508	U10	C41-C39-C38	2.39	126.54	121.17
19	g	605	HEA	C16-C15-C14	-2.39	115.80	121.17
17	m	302	3PH	O14-P-O13	2.39	116.76	107.80
14	m	313	3PE	O12-P-O11	-2.38	96.78	107.57
19	g	603	HEA	C3B-C4B-NB	2.38	112.57	109.84
11	d	505	HEM	CHD-C4C-NC	2.37	127.04	124.45
19	g	605	HEA	CHB-C1B-C2B	-2.37	121.28	125.03
15	m	311	DU0	C04-C03-C02	-2.36	101.05	103.85
11	d	504	HEM	CAD-CBD-CGD	-2.35	107.42	113.67
17	g	601	3PH	O14-P-O11	-2.34	100.57	106.67
15	m	311	DU0	C22-C21-C20	2.34	114.90	111.45
15	i	301	DU0	C04-C03-C02	-2.33	101.08	103.85
14	c	201	3PE	O12-P-O11	-2.33	96.98	107.57
17	m	302	3PH	O14-P-O11	-2.33	100.59	106.67
9	m	307	PC1	O12-P-O13	-2.33	97.00	107.57
15	f	201	DU0	O10-C09-O16	-2.33	104.34	109.88
14	n	101	3PE	O31-C31-O32	-2.33	117.81	123.63
9	j	1001	PC1	O12-P-O13	-2.32	97.04	107.57
17	m	301	3PH	O14-P-O11	-2.32	100.61	106.67
10	d	508	U10	C22-C23-C24	-2.32	122.31	127.62
17	m	301	3PH	O31-C31-O32	-2.32	117.83	123.63
18	d	501	CDL	CA4-OA6-CA5	2.31	123.33	117.80
14	g	607	3PE	O31-C31-O32	-2.31	117.86	123.63
14	m	305	3PE	O31-C31-O32	-2.31	117.86	123.63
15	f	201	DU0	C77-C79-C17	-2.31	109.34	112.71
15	d	502	DU0	C22-C21-C20	2.31	114.86	111.45
14	g	607	3PE	O21-C21-O22	-2.30	118.32	123.70
13	b	503	HEC	CBD-CAD-C3D	-2.30	106.18	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	503	HEC	CHC-C4B-NB	2.29	126.95	124.45
14	e	504	3PE	O12-P-O11	-2.28	97.22	107.57
17	m	304	3PH	O14-P-O11	-2.28	100.73	106.67
13	e	503	HEC	CBD-CAD-C3D	-2.25	106.30	112.53
19	k	601	HEA	C12-C11-C3B	2.24	115.63	112.12
13	e	503	HEC	CAA-CBA-CGA	-2.24	107.71	113.67
14	m	305	3PE	O12-P-O11	-2.24	97.41	107.57
14	m	308	3PE	O31-C31-O32	-2.24	118.03	123.63
14	i	308	3PE	O12-P-O11	-2.24	97.43	107.57
9	m	303	PC1	O31-C31-O32	-2.23	118.04	123.63
18	d	501	CDL	OA8-CA7-C31	2.23	118.63	111.83
17	p	1000	3PH	O14-P-O11	-2.23	100.87	106.67
9	d	503	PC1	C2-O21-C21	2.22	123.12	117.80
19	k	606	HEA	CBD-CAD-C3D	-2.22	106.40	112.53
15	d	502	DU0	O10-C11-C12	-2.21	109.33	112.17
11	a	505	HEM	CHD-C4C-NC	2.21	126.86	124.45
19	k	606	HEA	C4B-C3B-C2B	-2.20	103.74	107.44
14	e	501	3PE	O31-C31-O32	-2.20	118.12	123.63
15	c	202	DU0	C77-C79-C17	-2.20	109.50	112.71
14	i	308	3PE	O31-C31-O32	-2.20	118.13	123.63
10	a	502	U10	C7-C6-C1	-2.19	121.14	124.89
14	k	608	3PE	O12-P-O11	-2.18	97.69	107.57
15	c	203	DU0	O10-C09-O16	-2.17	104.71	109.88
19	k	601	HEA	CHB-C1B-NB	2.17	126.76	124.42
14	e	504	3PE	O21-C21-O22	-2.17	118.64	123.70
17	c	205	3PH	O21-C21-O22	-2.17	118.64	123.70
15	i	302	DU0	C08-C07-C09	-2.16	111.45	114.94
17	k	602	3PH	O14-P-O11	-2.16	101.04	106.67
18	d	501	CDL	OA6-CA5-C11	2.16	116.14	111.48
17	m	304	3PH	O14-P-O13	2.15	115.87	107.80
9	i	303	PC1	O21-C21-O22	-2.15	118.68	123.70
9	i	303	PC1	O31-C31-O32	-2.15	118.25	123.63
9	m	307	PC1	O31-C31-O32	-2.15	118.25	123.63
14	g	607	3PE	O12-P-O11	-2.15	97.84	107.57
17	d	507	3PH	O14-P-O13	2.14	115.84	107.80
17	m	301	3PH	O14-P-O13	2.14	115.83	107.80
17	c	205	3PH	O14-P-O13	2.14	115.83	107.80
14	k	608	3PE	O21-C21-O22	-2.14	118.70	123.70
17	k	602	3PH	O32-C31-C32	2.14	132.14	123.78
19	g	603	HEA	CHB-C1B-NB	2.13	126.72	124.42
10	d	506	U10	C27-C28-C29	-2.13	122.75	127.62
13	b	503	HEC	CAD-C3D-C4D	2.13	129.10	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	304	3PH	C2-O21-C21	2.12	122.87	117.80
17	d	507	3PH	O21-C21-O22	-2.12	118.75	123.70
14	e	504	3PE	O31-C31-O32	-2.10	118.36	123.63
14	k	608	3PE	O31-C31-O32	-2.10	118.36	123.63
17	f	204	3PH	O14-P-O13	2.10	115.66	107.80
17	i	304	3PH	O31-C3-C2	2.09	114.42	108.40
15	k	605	DU0	O10-C11-C12	-2.09	109.49	112.17
15	k	605	DU0	O10-C09-O16	-2.08	104.92	109.88
17	i	304	3PH	O14-P-O13	2.08	115.59	107.80
9	a	501	PC1	C3-C2-C1	-2.07	106.95	111.78
17	m	304	3PH	O21-C21-O22	-2.07	118.86	123.70
11	d	505	HEM	CAA-CBA-CGA	-2.07	108.17	113.67
17	f	204	3PH	O21-C21-O22	-2.07	118.86	123.70
9	m	310	PC1	O12-P-O13	-2.07	98.18	107.57
19	k	606	HEA	CBC-CAC-C3C	-2.07	117.18	127.53
19	k	606	HEA	C2B-C1B-NB	2.07	112.29	109.90
17	k	602	3PH	O14-P-O13	2.07	115.55	107.80
19	g	605	HEA	CHC-C1C-NC	2.06	127.60	123.86
10	a	502	U10	C1M-C1-C6	-2.06	121.07	124.45
9	i	303	PC1	O12-P-O13	-2.05	98.26	107.57
9	n	102	PC1	O31-C31-O32	-2.05	118.50	123.63
15	d	509	DU0	C08-C07-C09	-2.05	111.63	114.94
15	c	202	DU0	O10-C09-O16	-2.05	105.00	109.88
19	k	606	HEA	C25-C23-C24	2.05	119.30	114.59
17	p	1000	3PH	O14-P-O13	2.04	115.47	107.80
11	a	505	HEM	CBD-CAD-C3D	-2.04	106.88	112.53
19	k	606	HEA	CHB-C1B-NB	2.04	126.62	124.42
11	d	505	HEM	C3B-C2B-C1B	2.04	107.94	106.41
14	i	309	3PE	O12-P-O11	-2.04	98.32	107.57
17	m	301	3PH	C2-O21-C21	2.04	122.68	117.80
9	m	303	PC1	O12-P-O13	-2.04	98.34	107.57
14	c	201	3PE	O21-C2-C1	2.03	115.64	108.34
11	a	505	HEM	CAA-CBA-CGA	-2.03	108.28	113.67
15	d	502	DU0	C08-C07-C09	-2.02	111.68	114.94
14	m	306	3PE	O12-P-O11	-2.02	98.41	107.57
10	a	502	U10	C27-C26-C24	2.02	119.87	113.19
15	m	312	DU0	C75-C76-C77	2.02	117.08	112.78
9	i	307	PC1	O12-P-O13	-2.02	98.43	107.57
19	g	603	HEA	C4B-C3B-C2B	-2.01	104.05	107.44

There are no chirality outliers.

All (513) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	a	501	PC1	C1-O11-P-O12
9	a	501	PC1	O13-C11-C12-N
9	a	503	PC1	C11-O13-P-O11
9	b	501	PC1	C1-O11-P-O13
9	b	501	PC1	O13-C11-C12-N
9	b	501	PC1	C2-C1-O11-P
9	d	503	PC1	C11-O13-P-O12
9	d	503	PC1	C11-O13-P-O11
9	d	503	PC1	C1-O11-P-O12
9	i	303	PC1	O21-C2-C3-O31
9	i	307	PC1	C1-O11-P-O14
9	i	307	PC1	C1-O11-P-O13
9	j	1001	PC1	C12-C11-O13-P
9	m	303	PC1	C1-O11-P-O13
9	m	307	PC1	C11-O13-P-O14
9	m	307	PC1	C11-O13-P-O11
9	m	307	PC1	C1-O11-P-O12
9	m	307	PC1	C1-O11-P-O13
9	m	307	PC1	C12-C11-O13-P
9	m	307	PC1	C2-C1-O11-P
9	m	310	PC1	O21-C2-C3-O31
9	n	102	PC1	C11-O13-P-O12
9	n	102	PC1	C1-O11-P-O14
9	n	102	PC1	C1-O11-P-O13
9	n	102	PC1	C12-C11-O13-P
9	n	102	PC1	C2-C1-O11-P
9	o	1001	PC1	C11-O13-P-O12
9	o	1001	PC1	C11-O13-P-O11
11	a	504	HEM	C2C-C3C-CAC-CBC
11	a	504	HEM	C4C-C3C-CAC-CBC
11	d	504	HEM	C2C-C3C-CAC-CBC
11	d	504	HEM	C4C-C3C-CAC-CBC
11	d	505	HEM	C2B-C3B-CAB-CBB
11	d	505	HEM	C4B-C3B-CAB-CBB
11	d	505	HEM	C2C-C3C-CAC-CBC
11	d	505	HEM	C4C-C3C-CAC-CBC
13	b	503	HEC	C2B-C3B-CAB-CBB
13	b	503	HEC	C4B-C3B-CAB-CBB
13	b	503	HEC	C2C-C3C-CAC-CBC
13	b	503	HEC	C4C-C3C-CAC-CBC
13	e	503	HEC	C2B-C3B-CAB-CBB
13	e	503	HEC	C4B-C3B-CAB-CBB
13	e	503	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	e	503	HEC	C4C-C3C-CAC-CBC
14	c	201	3PE	C11-O13-P-O11
14	c	201	3PE	C12-C11-O13-P
14	e	501	3PE	C1-O11-P-O13
14	e	501	3PE	C1-O11-P-O14
14	e	501	3PE	C11-O13-P-O14
14	e	501	3PE	C12-C11-O13-P
14	e	504	3PE	C11-O13-P-O12
14	e	504	3PE	O13-C11-C12-N
14	g	607	3PE	C11-O13-P-O12
14	i	305	3PE	C11-O13-P-O12
14	i	305	3PE	C12-C11-O13-P
14	i	309	3PE	C2-C1-O11-P
14	k	608	3PE	C11-O13-P-O11
14	m	305	3PE	C11-O13-P-O12
14	m	306	3PE	C11-O13-P-O12
14	m	306	3PE	C12-C11-O13-P
14	m	308	3PE	C1-O11-P-O12
14	m	308	3PE	C1-O11-P-O13
14	m	308	3PE	C1-O11-P-O14
14	m	308	3PE	C11-O13-P-O12
14	m	308	3PE	C12-C11-O13-P
14	m	313	3PE	C12-C11-O13-P
14	n	101	3PE	C2-C1-O11-P
15	f	203	DU0	C75-C22-O23-C24
15	i	302	DU0	C25-C24-O23-C22
17	d	507	3PH	C2-C1-O11-P
17	d	507	3PH	O21-C2-C3-O31
17	f	204	3PH	C1-O11-P-O13
17	f	204	3PH	C1-O11-P-O14
17	f	204	3PH	C2-C1-O11-P
17	g	601	3PH	C2-C1-O11-P
17	g	601	3PH	O21-C2-C3-O31
17	m	302	3PH	C1-O11-P-O13
17	m	302	3PH	C1-O11-P-O14
17	m	302	3PH	C1-O11-P-O12
17	m	302	3PH	C2-C1-O11-P
18	d	501	CDL	OA6-CA4-CA6-OA8
18	d	501	CDL	CB3-OB5-PB2-OB2
18	d	501	CDL	CB3-OB5-PB2-OB3
18	d	501	CDL	CB3-OB5-PB2-OB4
18	d	501	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
10	a	506	U10	C34-C36-C37-C38
10	d	508	U10	C49-C51-C52-C53
9	j	1001	PC1	C2-C1-O11-P
9	m	310	PC1	C2-C1-O11-P
17	p	1000	3PH	C2-C1-O11-P
18	d	501	CDL	O1-C1-CB2-OB2
17	m	302	3PH	O11-C1-C2-O21
9	o	1001	PC1	O21-C2-C3-O31
14	n	101	3PE	C28-C29-C2A-C2B
10	a	502	U10	C39-C41-C42-C43
10	d	508	U10	C34-C36-C37-C38
15	c	203	DU0	C75-C22-O23-C24
9	a	503	PC1	C3A-C3B-C3C-C3D
9	m	303	PC1	C2D-C2E-C2F-C2G
14	c	201	3PE	C3D-C3E-C3F-C3G
9	i	307	PC1	C32-C33-C34-C35
9	a	501	PC1	C33-C34-C35-C36
9	d	503	PC1	C22-C23-C24-C25
17	f	204	3PH	C37-C38-C39-C3A
14	e	501	3PE	C28-C29-C2A-C2B
9	d	503	PC1	C1-C2-C3-O31
14	g	607	3PE	C2D-C2E-C2F-C2G
17	c	205	3PH	C26-C27-C28-C29
17	m	302	3PH	C39-C3A-C3B-C3C
9	a	501	PC1	C3B-C3C-C3D-C3E
9	b	501	PC1	C2A-C2B-C2C-C2D
14	n	101	3PE	C3B-C3C-C3D-C3E
14	c	201	3PE	C29-C2A-C2B-C2C
18	d	501	CDL	C22-C23-C24-C25
9	m	310	PC1	C3C-C3D-C3E-C3F
14	e	501	3PE	C3C-C3D-C3E-C3F
9	a	503	PC1	C26-C27-C28-C29
17	i	304	3PH	C37-C38-C39-C3A
9	a	503	PC1	C34-C35-C36-C37
9	d	503	PC1	C3E-C3F-C3G-C3H
14	m	313	3PE	C38-C39-C3A-C3B
17	d	507	3PH	C2C-C2D-C2E-C2F
17	k	602	3PH	C32-C33-C34-C35
14	k	608	3PE	C21-C22-C23-C24
14	i	305	3PE	C3C-C3D-C3E-C3F
14	i	305	3PE	C25-C26-C27-C28
14	m	313	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	i	301	DU0	O23-C24-C25-C26
9	b	501	PC1	C27-C28-C29-C2A
14	c	201	3PE	C23-C24-C25-C26
14	e	501	3PE	C24-C25-C26-C27
14	k	608	3PE	C28-C29-C2A-C2B
10	a	502	U10	C25-C24-C26-C27
10	a	506	U10	C30-C29-C31-C32
11	a	505	HEM	C2C-C3C-CAC-CBC
14	c	201	3PE	C28-C29-C2A-C2B
9	m	307	PC1	C3E-C3F-C3G-C3H
9	b	501	PC1	C34-C35-C36-C37
11	a	505	HEM	C4C-C3C-CAC-CBC
14	e	504	3PE	C28-C29-C2A-C2B
14	g	607	3PE	C21-C22-C23-C24
9	a	503	PC1	C2D-C2E-C2F-C2G
17	i	304	3PH	C2-C1-O11-P
9	m	303	PC1	C2A-C2B-C2C-C2D
9	b	501	PC1	C37-C38-C39-C3A
9	i	303	PC1	C36-C37-C38-C39
14	n	101	3PE	C33-C34-C35-C36
14	i	305	3PE	C2C-C2D-C2E-C2F
9	i	303	PC1	C29-C2A-C2B-C2C
14	m	305	3PE	C2B-C2C-C2D-C2E
17	f	204	3PH	O11-C1-C2-C3
17	i	304	3PH	O11-C1-C2-C3
9	i	307	PC1	C2D-C2E-C2F-C2G
9	i	303	PC1	C1-C2-C3-O31
9	m	310	PC1	C1-C2-C3-O31
9	n	102	PC1	C1-C2-C3-O31
9	o	1001	PC1	C1-C2-C3-O31
14	m	308	3PE	C1-C2-C3-O31
18	d	501	CDL	CA3-CA4-CA6-OA8
15	c	202	DU0	C24-C25-C26-C51
9	m	307	PC1	C3C-C3D-C3E-C3F
10	a	502	U10	C23-C24-C26-C27
10	a	506	U10	C28-C29-C31-C32
9	a	503	PC1	C2-C1-O11-P
9	i	303	PC1	C2-C1-O11-P
14	e	504	3PE	C33-C34-C35-C36
14	c	201	3PE	C1-C2-O21-C21
14	i	308	3PE	C21-C22-C23-C24
17	m	304	3PH	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
19	k	601	HEA	C18-C19-C20-C21
9	m	303	PC1	C29-C2A-C2B-C2C
17	m	304	3PH	C39-C3A-C3B-C3C
9	a	503	PC1	C3C-C3D-C3E-C3F
17	d	507	3PH	C37-C38-C39-C3A
10	d	506	U10	C19-C21-C22-C23
9	a	503	PC1	C31-C32-C33-C34
9	o	1001	PC1	C2E-C2F-C2G-C2H
10	d	508	U10	C45-C44-C46-C47
19	k	601	HEA	C27-C19-C20-C21
14	e	501	3PE	C2-C1-O11-P
14	m	306	3PE	C2-C1-O11-P
17	m	304	3PH	C2-C1-O11-P
9	d	503	PC1	C32-C33-C34-C35
14	m	306	3PE	O11-C1-C2-C3
17	m	302	3PH	O11-C1-C2-C3
9	o	1001	PC1	C37-C38-C39-C3A
10	a	506	U10	C35-C34-C36-C37
17	k	602	3PH	C22-C23-C24-C25
9	m	303	PC1	C32-C33-C34-C35
9	a	501	PC1	C39-C3A-C3B-C3C
17	d	507	3PH	C1-C2-C3-O31
10	d	508	U10	C43-C44-C46-C47
17	m	302	3PH	C37-C38-C39-C3A
17	d	507	3PH	C36-C37-C38-C39
14	m	306	3PE	O11-C1-C2-O21
14	m	313	3PE	O11-C1-C2-O21
17	i	304	3PH	O11-C1-C2-O21
9	m	310	PC1	C3A-C3B-C3C-C3D
14	c	201	3PE	C2-C1-O11-P
14	i	305	3PE	C2-C1-O11-P
14	m	308	3PE	C2-C1-O11-P
9	b	501	PC1	O21-C2-C3-O31
18	d	501	CDL	OB6-CB4-CB6-OB8
10	d	506	U10	C25-C24-C26-C27
10	a	506	U10	C33-C34-C36-C37
17	i	304	3PH	C34-C35-C36-C37
17	p	1000	3PH	C37-C38-C39-C3A
17	i	304	3PH	C21-C22-C23-C24
17	i	304	3PH	C33-C34-C35-C36
9	a	501	PC1	C2B-C2C-C2D-C2E
17	m	304	3PH	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
14	i	309	3PE	O11-C1-C2-C3
14	m	306	3PE	C3A-C3B-C3C-C3D
10	d	508	U10	C1-C6-C7-C8
14	k	608	3PE	C39-C3A-C3B-C3C
10	d	506	U10	C15-C14-C16-C17
10	d	506	U10	C23-C24-C26-C27
11	a	504	HEM	C2B-C3B-CAB-CBB
15	c	203	DU0	C21-C22-O23-C24
9	j	1001	PC1	O11-C1-C2-O21
17	f	204	3PH	O11-C1-C2-O21
17	g	601	3PH	C1-C2-C3-O31
9	j	1001	PC1	C34-C35-C36-C37
17	f	204	3PH	C2C-C2D-C2E-C2F
9	a	501	PC1	C12-C11-O13-P
9	a	503	PC1	C12-C11-O13-P
9	b	501	PC1	C12-C11-O13-P
9	i	307	PC1	C12-C11-O13-P
9	m	303	PC1	C12-C11-O13-P
9	o	1001	PC1	C12-C11-O13-P
14	e	504	3PE	C12-C11-O13-P
14	i	308	3PE	C12-C11-O13-P
14	i	309	3PE	C12-C11-O13-P
14	k	608	3PE	C12-C11-O13-P
14	m	305	3PE	C12-C11-O13-P
18	d	501	CDL	C39-C40-C41-C42
9	n	102	PC1	O21-C2-C3-O31
9	a	501	PC1	C21-C22-C23-C24
9	n	102	PC1	C32-C33-C34-C35
9	d	503	PC1	C2-C1-O11-P
9	a	503	PC1	O13-C11-C12-N
9	d	503	PC1	O13-C11-C12-N
9	i	303	PC1	O13-C11-C12-N
9	i	307	PC1	O13-C11-C12-N
9	j	1001	PC1	O13-C11-C12-N
9	m	303	PC1	O13-C11-C12-N
9	m	307	PC1	O13-C11-C12-N
9	n	102	PC1	O13-C11-C12-N
14	c	201	3PE	C32-C33-C34-C35
17	f	204	3PH	C26-C27-C28-C29
9	m	307	PC1	C27-C28-C29-C2A
17	k	602	3PH	C34-C35-C36-C37
18	d	501	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
14	k	608	3PE	C25-C26-C27-C28
9	j	1001	PC1	O11-C1-C2-C3
14	c	201	3PE	O11-C1-C2-C3
14	m	313	3PE	O11-C1-C2-C3
18	d	501	CDL	C1-CB2-OB2-PB2
10	a	506	U10	C20-C19-C21-C22
10	d	508	U10	C35-C34-C36-C37
9	i	307	PC1	O11-C1-C2-O21
14	i	309	3PE	O11-C1-C2-O21
9	m	307	PC1	C31-C32-C33-C34
17	d	507	3PH	C3D-C3E-C3F-C3G
14	i	305	3PE	C31-C32-C33-C34
18	d	501	CDL	C31-C32-C33-C34
9	d	503	PC1	O21-C2-C3-O31
14	m	308	3PE	O21-C2-C3-O31
17	p	1000	3PH	O21-C2-C3-O31
15	c	202	DU0	C24-C25-C26-C27
10	d	506	U10	C13-C14-C16-C17
14	m	308	3PE	C2C-C2D-C2E-C2F
14	g	607	3PE	C25-C26-C27-C28
9	a	503	PC1	C11-O13-P-O14
9	b	501	PC1	C1-O11-P-O14
9	d	503	PC1	C1-O11-P-O13
9	m	303	PC1	C1-O11-P-O14
9	m	307	PC1	C11-O13-P-O12
9	m	307	PC1	C1-O11-P-O14
9	m	310	PC1	C1-O11-P-O14
9	n	102	PC1	C11-O13-P-O11
10	d	508	U10	C4-C3-O3-C3M
14	c	201	3PE	C11-O13-P-O14
14	e	501	3PE	C11-O13-P-O12
14	e	504	3PE	C11-O13-P-O11
14	g	607	3PE	C11-O13-P-O11
14	g	607	3PE	C11-O13-P-O14
14	i	309	3PE	C1-O11-P-O13
14	i	309	3PE	C1-O11-P-O14
14	k	608	3PE	C11-O13-P-O14
14	m	313	3PE	C11-O13-P-O14
14	m	313	3PE	O13-C11-C12-N
14	e	504	3PE	C34-C35-C36-C37
10	a	502	U10	C40-C39-C41-C42
14	e	504	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
17	g	601	3PH	C29-C2A-C2B-C2C
17	m	302	3PH	C32-C33-C34-C35
14	i	308	3PE	C2-C1-O11-P
17	c	205	3PH	C2-C1-O11-P
18	d	501	CDL	C1-CA2-OA2-PA1
9	j	1001	PC1	C25-C26-C27-C28
14	i	308	3PE	C3C-C3D-C3E-C3F
14	m	313	3PE	C28-C29-C2A-C2B
18	d	501	CDL	OA5-CA3-CA4-CA6
9	m	303	PC1	C37-C38-C39-C3A
14	m	306	3PE	C23-C24-C25-C26
9	d	503	PC1	C3A-C3B-C3C-C3D
9	a	501	PC1	C2C-C2D-C2E-C2F
9	m	307	PC1	C34-C35-C36-C37
9	o	1001	PC1	C2D-C2E-C2F-C2G
17	p	1000	3PH	C23-C24-C25-C26
14	g	607	3PE	C37-C38-C39-C3A
9	o	1001	PC1	C39-C3A-C3B-C3C
17	c	205	3PH	C25-C26-C27-C28
10	a	502	U10	C46-C47-C48-C49
18	d	501	CDL	C53-C54-C55-C56
14	n	101	3PE	C2A-C2B-C2C-C2D
9	m	307	PC1	C29-C2A-C2B-C2C
10	d	506	U10	C34-C36-C37-C38
18	d	501	CDL	CA2-C1-CB2-OB2
9	m	307	PC1	C39-C3A-C3B-C3C
14	n	101	3PE	C2D-C2E-C2F-C2G
15	m	311	DU0	C25-C24-O23-C22
17	k	602	3PH	O11-C1-C2-O21
14	m	308	3PE	O11-C1-C2-C3
17	f	204	3PH	C25-C26-C27-C28
11	d	504	HEM	C4B-C3B-CAB-CBB
17	m	304	3PH	C23-C24-C25-C26
14	e	504	3PE	C25-C26-C27-C28
9	j	1001	PC1	O21-C2-C3-O31
9	m	307	PC1	C32-C33-C34-C35
14	e	504	3PE	C35-C36-C37-C38
14	m	313	3PE	C27-C28-C29-C2A
10	a	506	U10	C18-C19-C21-C22
10	a	502	U10	C2-C3-O3-C3M
10	d	508	U10	C44-C46-C47-C48
14	g	607	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
9	n	102	PC1	C3-C2-O21-C21
14	i	305	3PE	C1-C2-O21-C21
14	i	309	3PE	C1-C2-O21-C21
18	d	501	CDL	CA3-CA4-OA6-CA5
11	a	505	HEM	CAD-CBD-CGD-O1D
11	d	504	HEM	CAD-CBD-CGD-O2D
14	g	607	3PE	C28-C29-C2A-C2B
19	g	605	HEA	CAD-CBD-CGD-O1D
17	f	204	3PH	C23-C24-C25-C26
11	d	504	HEM	CAA-CBA-CGA-O1A
9	m	310	PC1	C3B-C3C-C3D-C3E
11	a	505	HEM	CAD-CBD-CGD-O2D
9	m	303	PC1	C2-C1-O11-P
14	m	313	3PE	C2-C1-O11-P
17	k	602	3PH	C2-C1-O11-P
19	k	606	HEA	C26-C15-C16-C17
14	i	305	3PE	C29-C2A-C2B-C2C
13	e	503	HEC	CAD-CBD-CGD-O1D
14	i	305	3PE	C24-C25-C26-C27
11	d	504	HEM	CAD-CBD-CGD-O1D
11	d	505	HEM	CAD-CBD-CGD-O2D
14	i	305	3PE	C37-C38-C39-C3A
19	k	601	HEA	CAD-CBD-CGD-O2D
10	a	506	U10	C5-C4-O4-C4M
14	m	305	3PE	C3F-C3G-C3H-C3I
17	f	204	3PH	C38-C39-C3A-C3B
10	a	502	U10	C15-C14-C16-C17
10	d	508	U10	C33-C34-C36-C37
19	k	606	HEA	C14-C15-C16-C17
18	d	501	CDL	C18-C19-C20-C21
13	b	503	HEC	CAA-CBA-CGA-O2A
13	e	503	HEC	CAA-CBA-CGA-O1A
9	a	501	PC1	C37-C38-C39-C3A
14	c	201	3PE	C25-C26-C27-C28
11	d	505	HEM	CAD-CBD-CGD-O1D
10	a	506	U10	C46-C47-C48-C49
9	n	102	PC1	C33-C34-C35-C36
13	e	503	HEC	CAD-CBD-CGD-O2D
19	g	605	HEA	CAD-CBD-CGD-O2D
15	d	502	DU0	C25-C24-O23-C22
15	d	509	DU0	C25-C24-O23-C22
14	m	308	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
10	a	506	U10	C15-C14-C16-C17
10	d	508	U10	C15-C14-C16-C17
11	d	504	HEM	CAA-CBA-CGA-O2A
17	m	301	3PH	C2-C1-O11-P
9	a	501	PC1	C38-C39-C3A-C3B
14	n	101	3PE	C31-C32-C33-C34
17	m	301	3PH	C3A-C3B-C3C-C3D
15	c	203	DU0	C24-C25-C26-C51
9	b	501	PC1	O21-C21-C22-C23
13	e	503	HEC	CAA-CBA-CGA-O2A
14	c	201	3PE	O11-C1-C2-O21
10	a	506	U10	C40-C39-C41-C42
19	g	603	HEA	C27-C19-C20-C21
19	g	603	HEA	CAD-CBD-CGD-O2D
14	c	201	3PE	C39-C3A-C3B-C3C
17	k	602	3PH	O11-C1-C2-C3
18	d	501	CDL	OB5-CB3-CB4-CB6
17	f	204	3PH	O21-C2-C3-O31
14	e	501	3PE	C21-C22-C23-C24
17	c	205	3PH	C21-C22-C23-C24
18	d	501	CDL	C81-C82-C83-C84
19	k	601	HEA	CAD-CBD-CGD-O1D
19	k	606	HEA	CAA-CBA-CGA-O2A
9	o	1001	PC1	C32-C33-C34-C35
17	m	304	3PH	C22-C23-C24-C25
14	m	313	3PE	C35-C36-C37-C38
17	d	507	3PH	C1-O11-P-O12
17	f	204	3PH	C1-O11-P-O12
13	b	503	HEC	CAA-CBA-CGA-O1A
11	d	504	HEM	C2B-C3B-CAB-CBB
15	m	311	DU0	C75-C22-O23-C24
9	j	1001	PC1	C3-C2-O21-C21
9	n	102	PC1	C1-C2-O21-C21
14	i	309	3PE	C3-C2-O21-C21
14	i	305	3PE	C2D-C2E-C2F-C2G
14	m	306	3PE	C3C-C3D-C3E-C3F
11	d	505	HEM	CAA-CBA-CGA-O2A
19	k	606	HEA	CAD-CBD-CGD-O2D
9	j	1001	PC1	C3F-C3G-C3H-C3I
15	m	311	DU0	O23-C24-C25-C26
19	g	603	HEA	CAD-CBD-CGD-O1D
10	a	502	U10	C38-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
9	a	503	PC1	C32-C33-C34-C35
17	m	302	3PH	C32-C31-O31-C3
14	m	308	3PE	O11-C1-C2-O21
19	k	606	HEA	CAD-CBD-CGD-O1D
18	d	501	CDL	CB3-CB4-CB6-OB8
17	m	302	3PH	O32-C31-O31-C3
11	a	504	HEM	C4B-C3B-CAB-CBB
14	n	101	3PE	C3A-C3B-C3C-C3D
9	b	501	PC1	C26-C27-C28-C29
14	c	201	3PE	C24-C25-C26-C27
14	k	608	3PE	C3F-C3G-C3H-C3I
17	m	304	3PH	C3E-C3F-C3G-C3H
10	d	508	U10	C5-C6-C7-C8
17	m	302	3PH	C3D-C3E-C3F-C3G
19	k	606	HEA	CAA-CBA-CGA-O1A
9	d	503	PC1	C24-C25-C26-C27
14	e	501	3PE	C27-C28-C29-C2A
17	g	601	3PH	C26-C27-C28-C29
14	i	309	3PE	O21-C2-C3-O31
17	m	302	3PH	C38-C39-C3A-C3B
17	f	204	3PH	C21-C22-C23-C24
9	d	503	PC1	O11-C1-C2-C3
11	a	505	HEM	CAA-CBA-CGA-O2A
15	i	302	DU0	O23-C24-C25-C26
14	m	313	3PE	C29-C2A-C2B-C2C
17	d	507	3PH	C2D-C2E-C2F-C2G
14	e	501	3PE	C29-C2A-C2B-C2C
10	d	506	U10	C39-C41-C42-C43
14	k	608	3PE	C26-C27-C28-C29
17	m	304	3PH	C38-C39-C3A-C3B
10	d	506	U10	C12-C11-C9-C10
9	j	1001	PC1	O21-C21-C22-C23
10	d	506	U10	C12-C11-C9-C8
11	d	505	HEM	CAA-CBA-CGA-O1A
17	m	302	3PH	C29-C2A-C2B-C2C
14	i	308	3PE	C36-C37-C38-C39
14	k	608	3PE	C2A-C2B-C2C-C2D
10	a	506	U10	C12-C11-C9-C10
14	k	608	3PE	C3C-C3D-C3E-C3F
9	a	503	PC1	C3F-C3G-C3H-C3I
17	d	507	3PH	C38-C39-C3A-C3B
17	d	507	3PH	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
13	b	503	HEC	CAD-CBD-CGD-O1D
9	n	102	PC1	O31-C31-C32-C33
17	d	507	3PH	O31-C31-C32-C33
9	n	102	PC1	C29-C2A-C2B-C2C
14	g	607	3PE	C2B-C2C-C2D-C2E
13	b	503	HEC	CAD-CBD-CGD-O2D
14	n	101	3PE	O21-C21-C22-C23
17	i	304	3PH	O21-C2-C3-O31
17	k	602	3PH	O21-C2-C3-O31
17	i	304	3PH	C31-C32-C33-C34
9	j	1001	PC1	C2B-C2C-C2D-C2E
9	j	1001	PC1	O31-C31-C32-C33
9	j	1001	PC1	C1-C2-O21-C21
14	m	306	3PE	C1-C2-O21-C21
14	m	306	3PE	C3-C2-O21-C21
17	i	304	3PH	C1-C2-O21-C21
18	d	501	CDL	CB6-CB4-OB6-CB5
14	i	305	3PE	O31-C31-C32-C33
14	i	308	3PE	C29-C2A-C2B-C2C
14	m	305	3PE	O31-C31-C32-C33
9	o	1001	PC1	C25-C26-C27-C28
11	a	505	HEM	CAA-CBA-CGA-O1A
14	n	101	3PE	C38-C39-C3A-C3B
9	d	503	PC1	O11-C1-C2-O21
9	m	303	PC1	O11-C1-C2-O21
14	g	607	3PE	C3C-C3D-C3E-C3F
9	m	307	PC1	C2C-C2D-C2E-C2F
14	n	101	3PE	O22-C21-C22-C23
10	a	506	U10	C45-C44-C46-C47
14	i	308	3PE	C25-C26-C27-C28
9	m	303	PC1	O21-C21-C22-C23
17	d	507	3PH	O21-C21-C22-C23
15	i	301	DU0	C25-C24-O23-C22
9	n	102	PC1	O32-C31-C32-C33
9	i	307	PC1	C3B-C3C-C3D-C3E
17	p	1000	3PH	C35-C36-C37-C38
14	c	201	3PE	O31-C31-C32-C33
9	i	303	PC1	O22-C21-O21-C2
17	f	204	3PH	O21-C21-C22-C23
18	d	501	CDL	C52-C51-CB5-OB6
9	b	501	PC1	C1-C2-C3-O31
9	j	1001	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
17	d	507	3PH	O32-C31-C32-C33
14	i	305	3PE	C38-C39-C3A-C3B
11	a	504	HEM	CAD-CBD-CGD-O2D
9	i	307	PC1	O11-C1-C2-C3
14	e	504	3PE	C24-C25-C26-C27
9	j	1001	PC1	O32-C31-C32-C33
9	o	1001	PC1	C34-C35-C36-C37
14	i	309	3PE	C38-C39-C3A-C3B

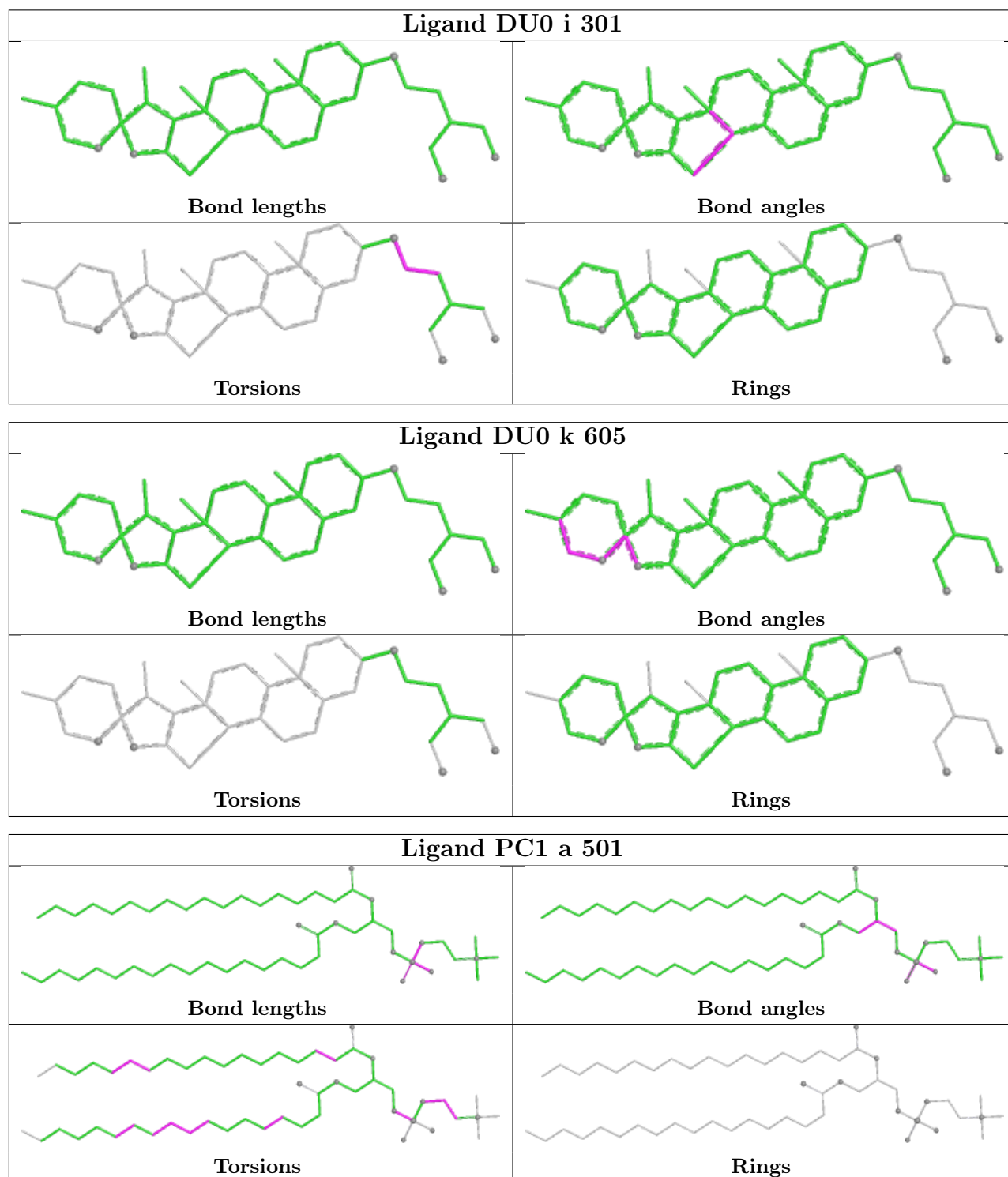
There are no ring outliers.

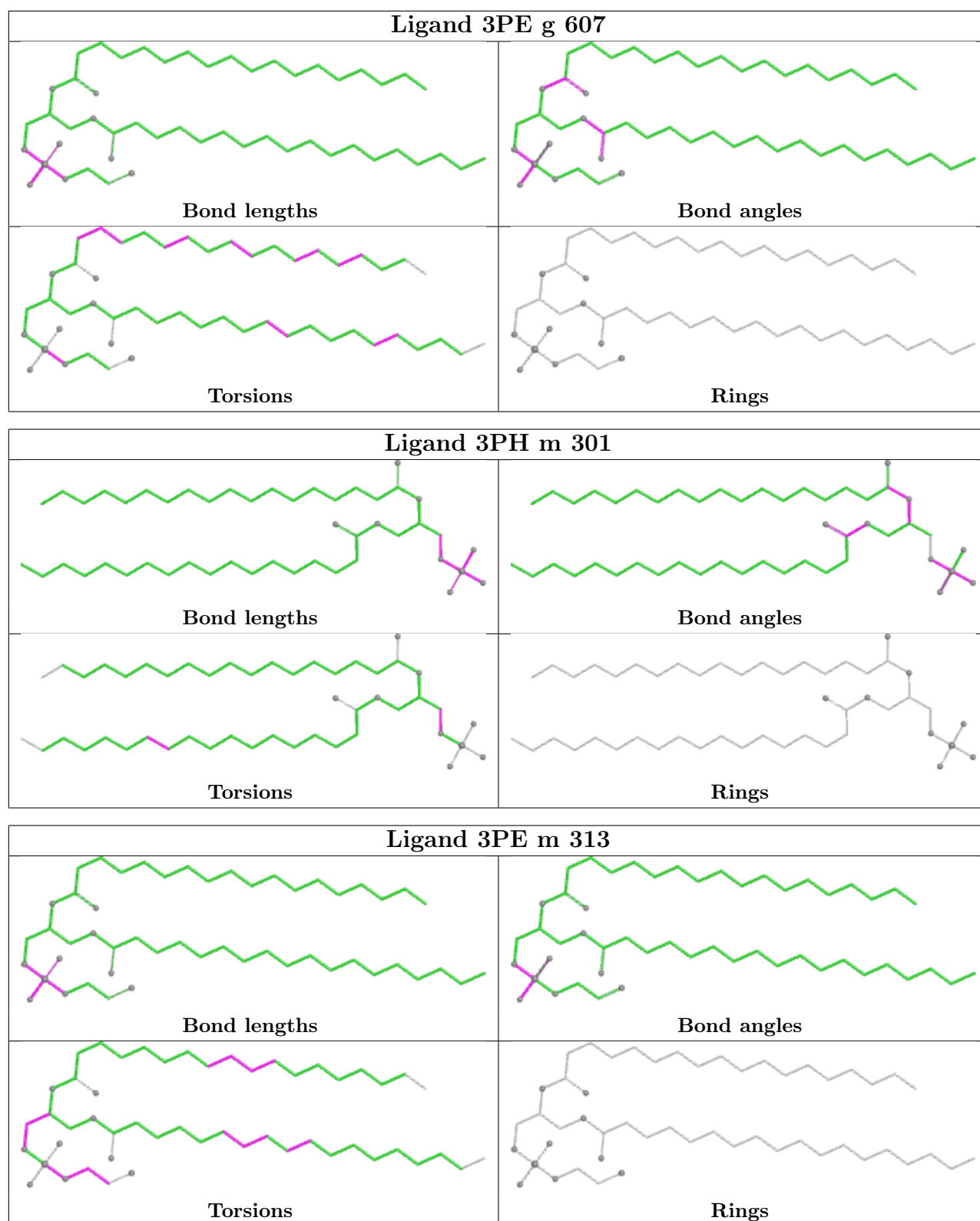
18 monomers are involved in 42 short contacts:

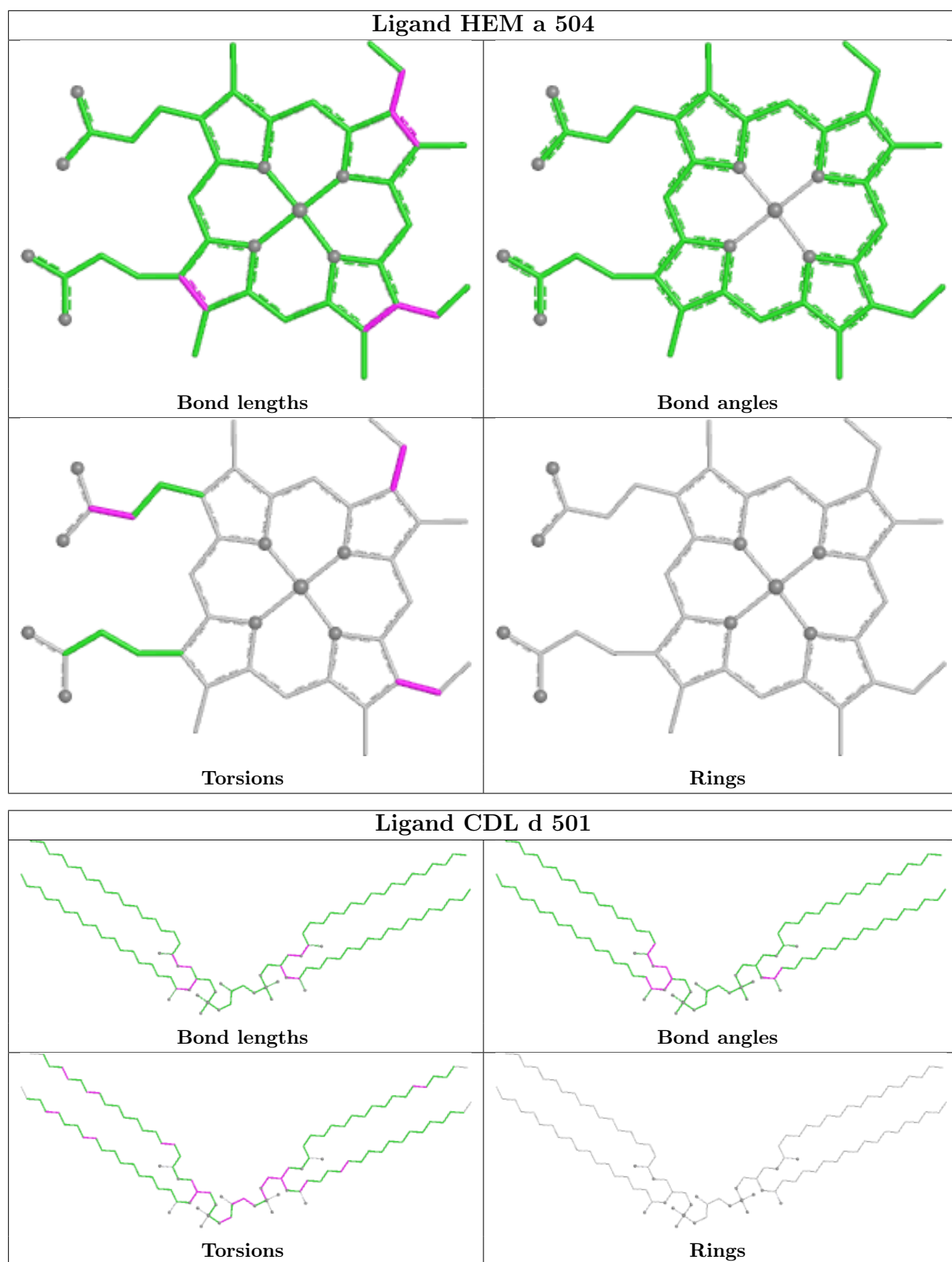
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	a	504	HEM	1	0
13	b	503	HEC	2	0
19	g	605	HEA	3	0
9	m	303	PC1	2	0
9	a	503	PC1	1	0
11	d	504	HEM	2	0
10	a	502	U10	4	0
10	a	506	U10	3	0
14	e	504	3PE	1	0
15	c	203	DU0	1	0
19	k	606	HEA	5	0
19	k	601	HEA	2	0
9	i	307	PC1	1	0
10	d	506	U10	2	0
14	m	308	3PE	1	0
19	g	603	HEA	4	0
10	d	508	U10	6	0
13	e	503	HEC	3	0

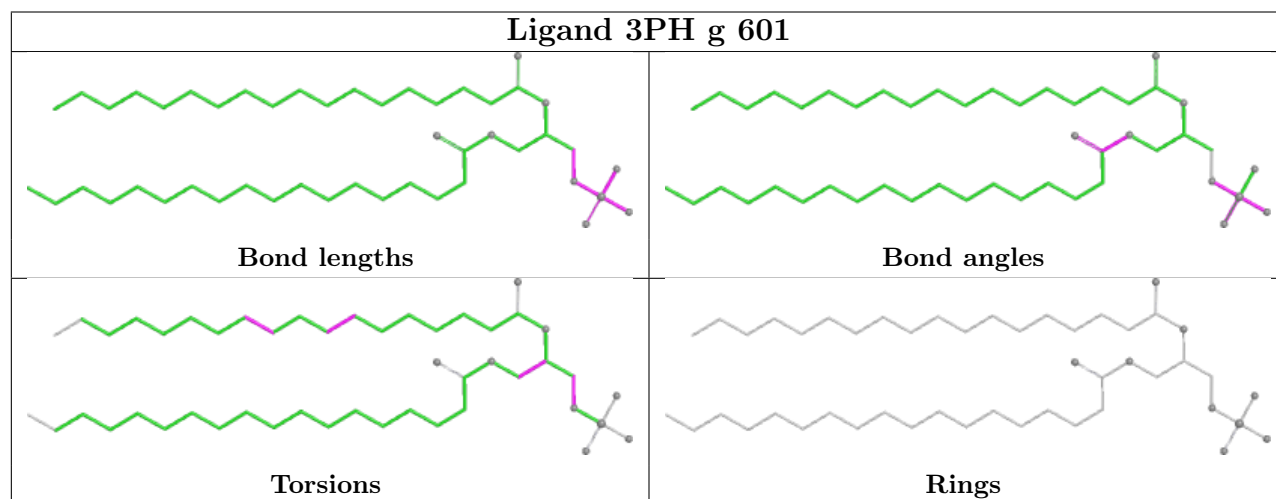
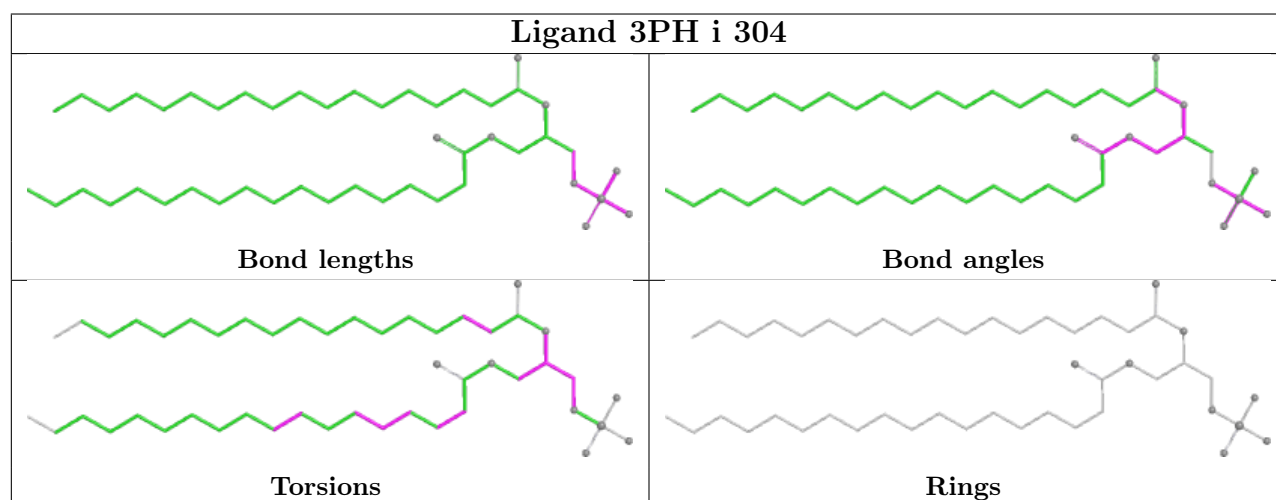
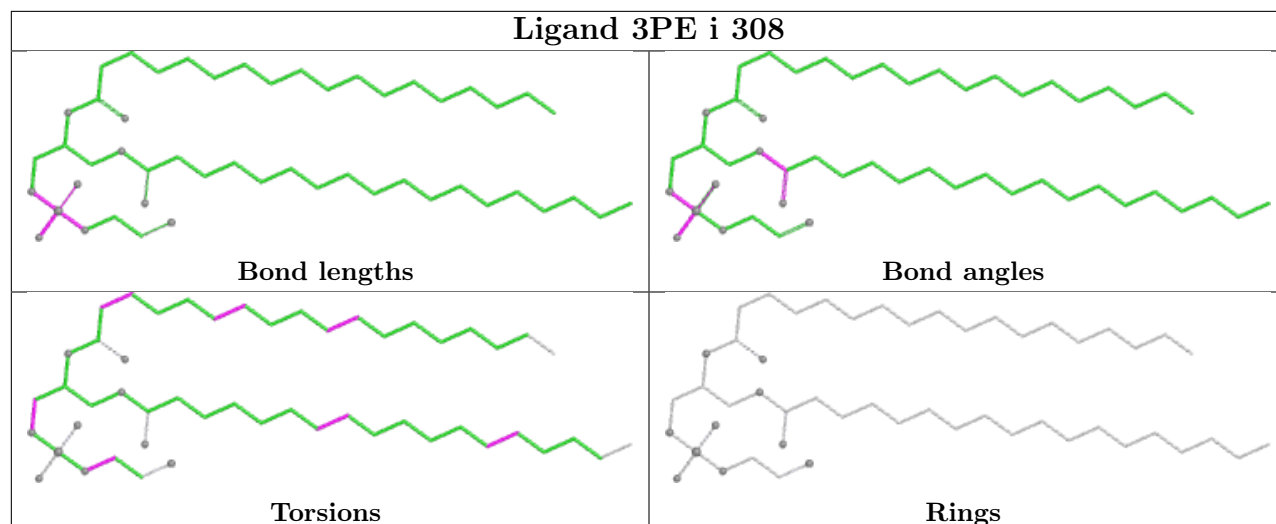
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

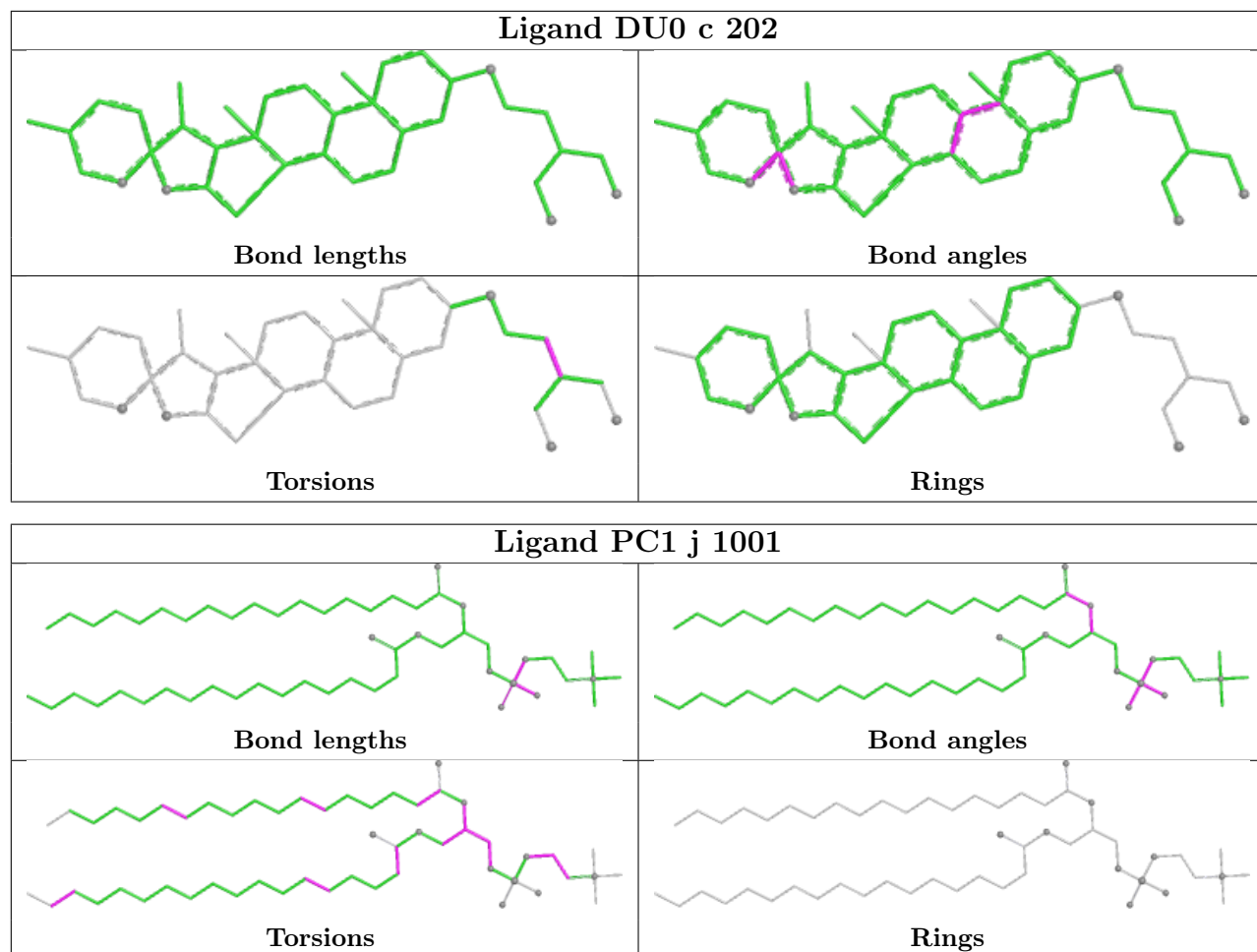
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



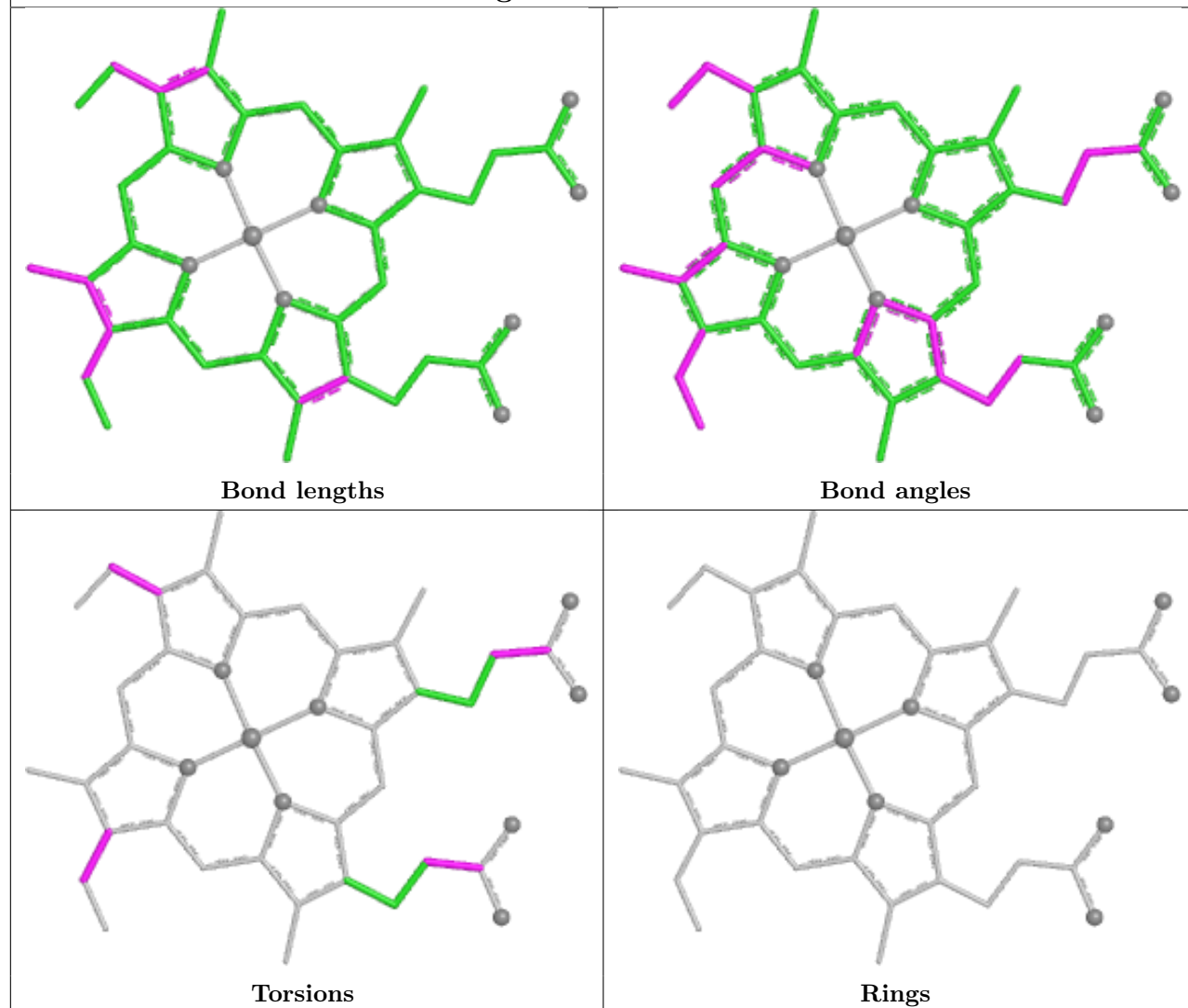




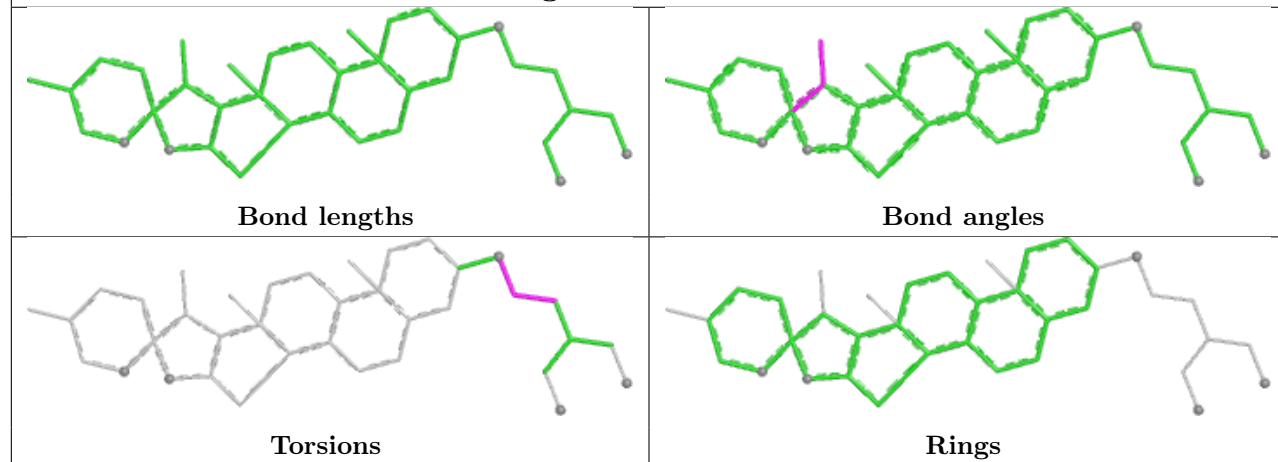


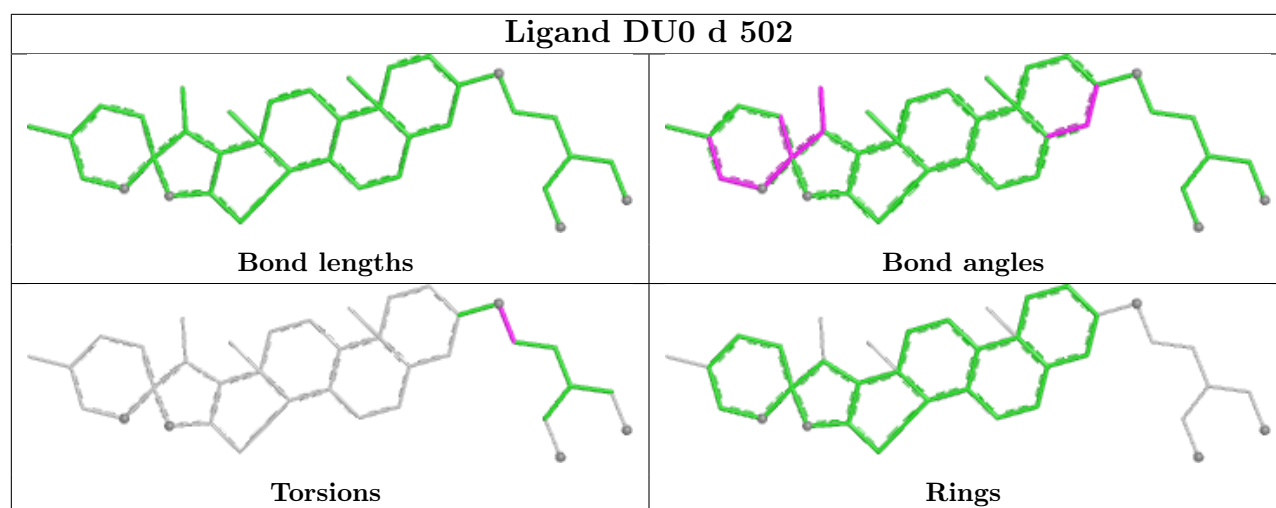
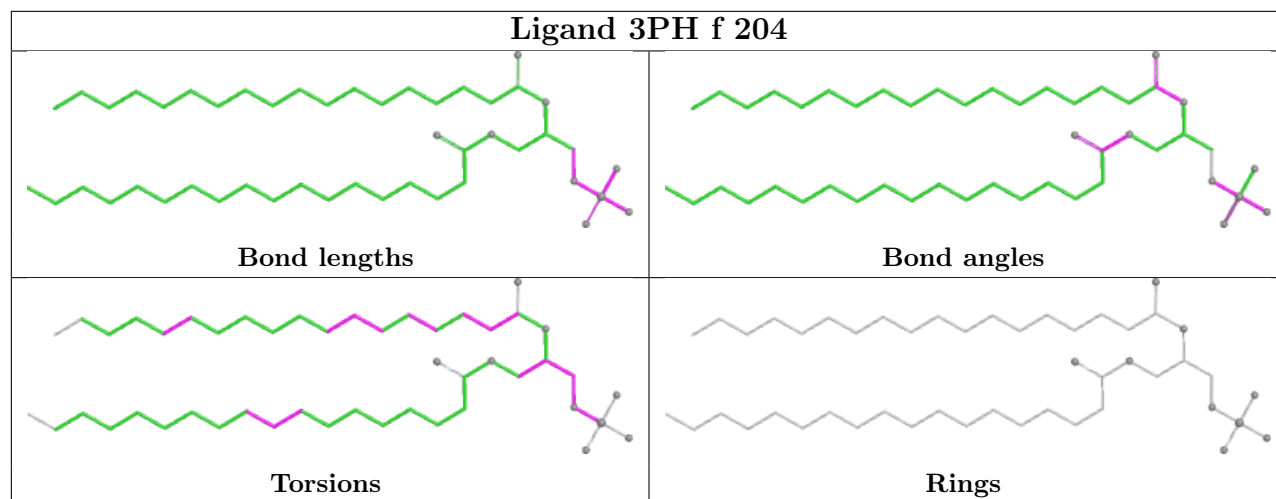


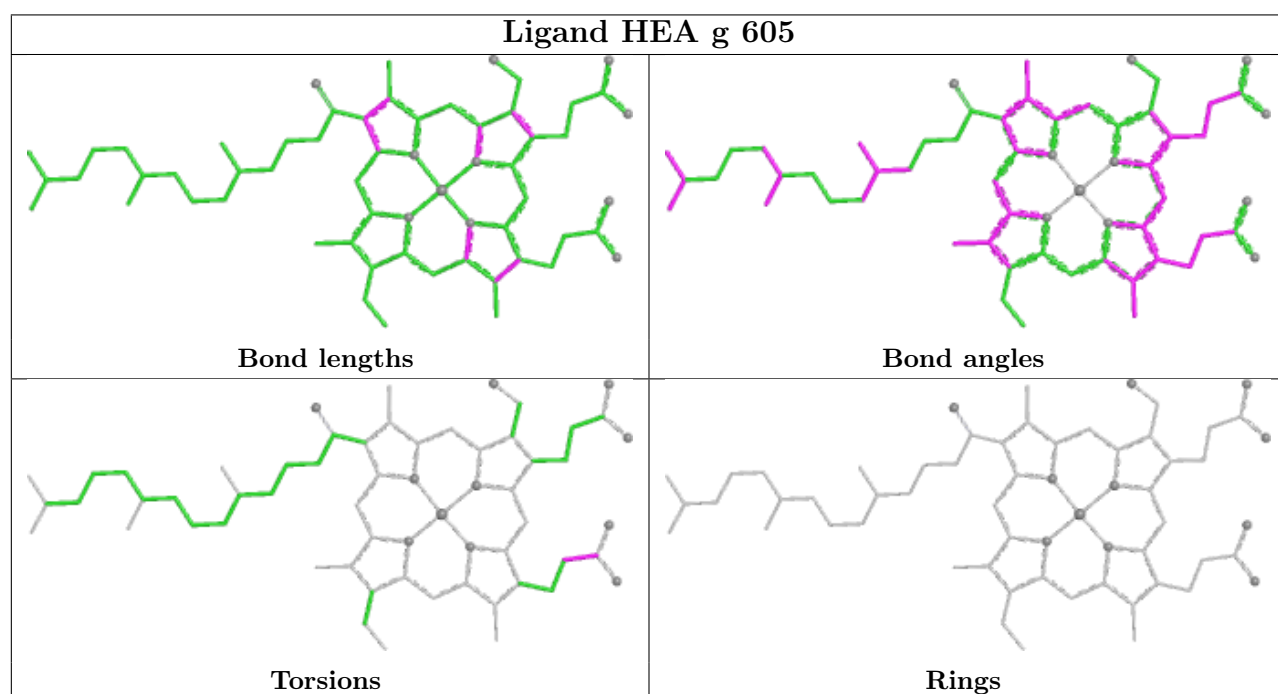
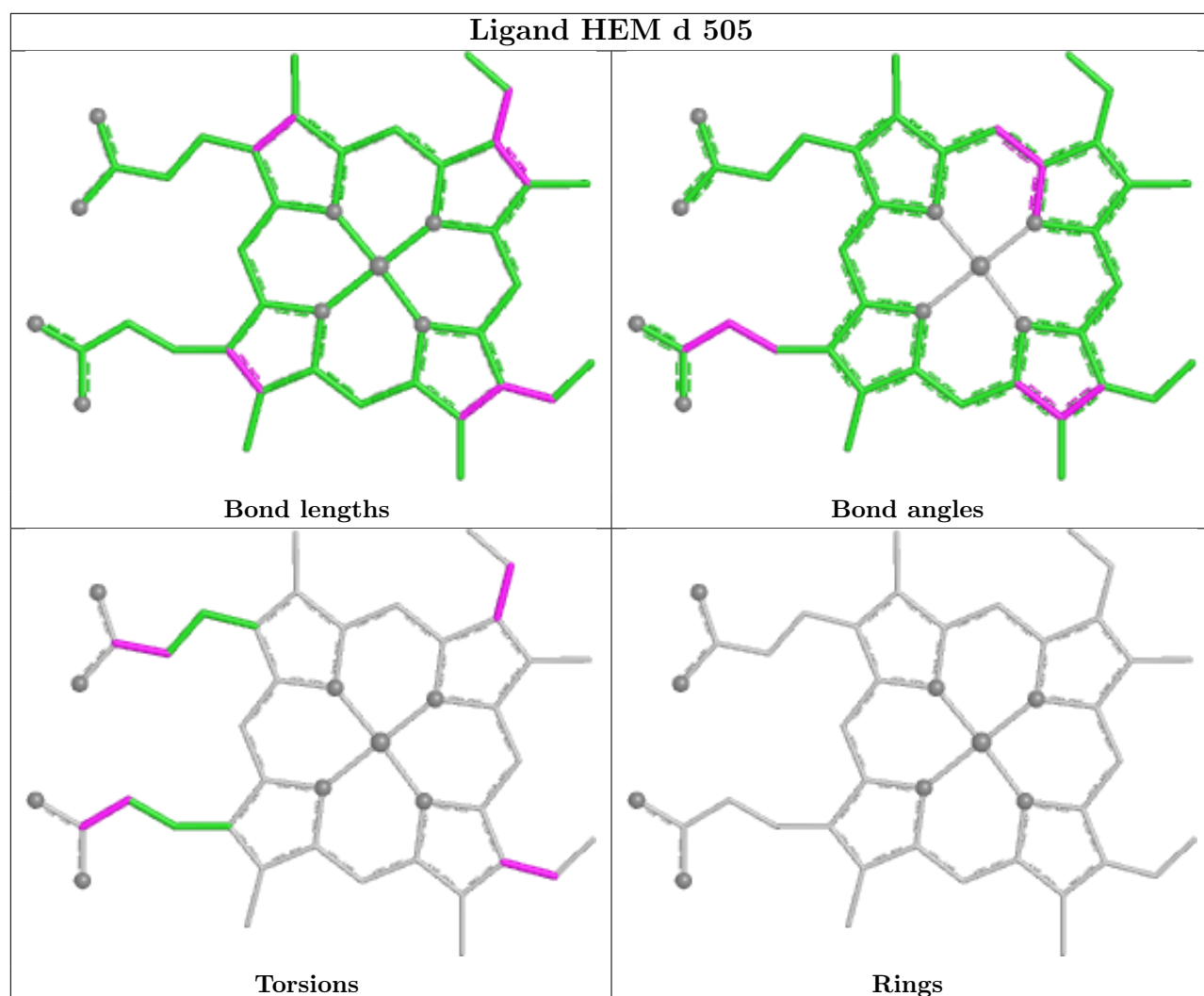
Ligand HEC b 503

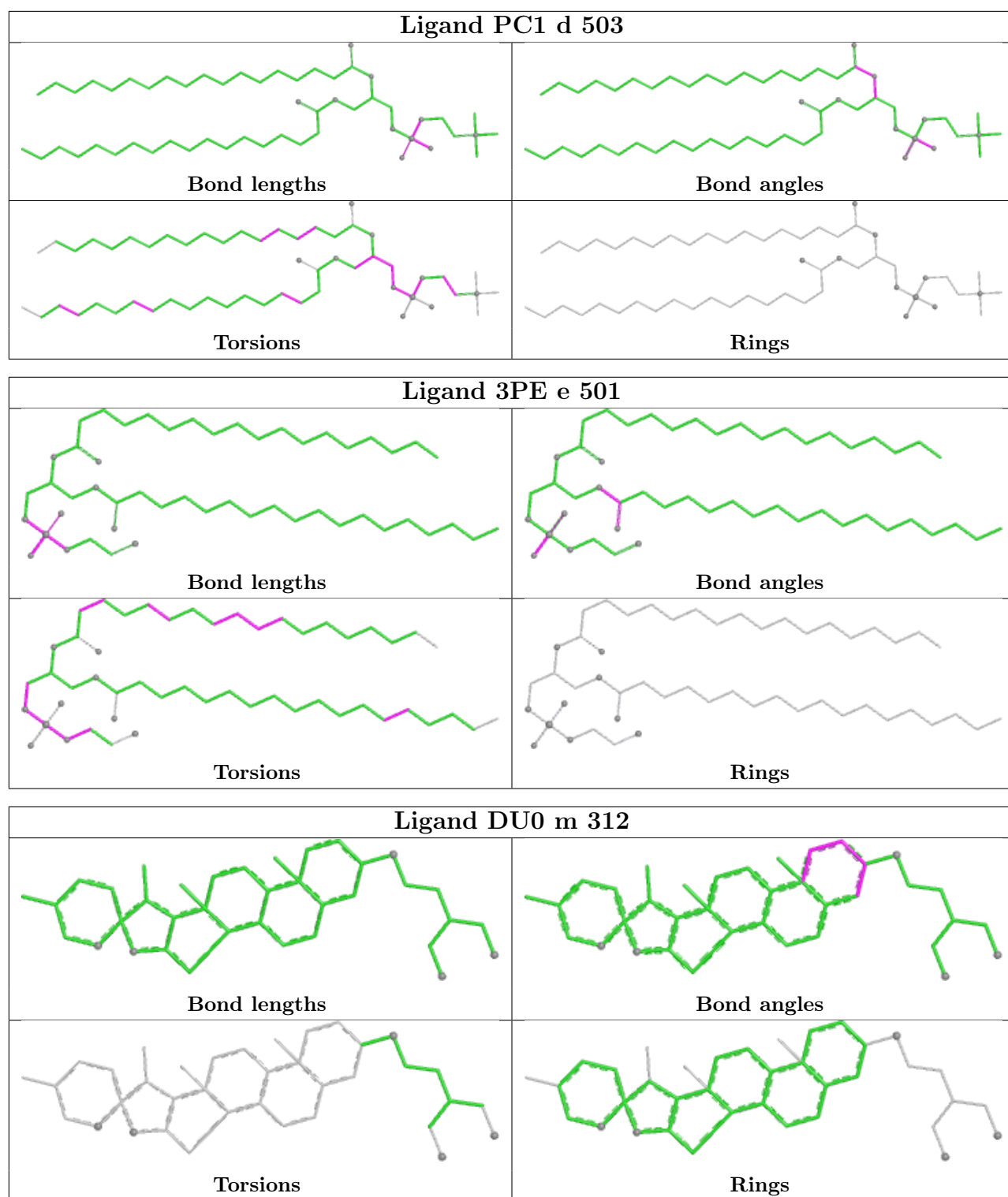


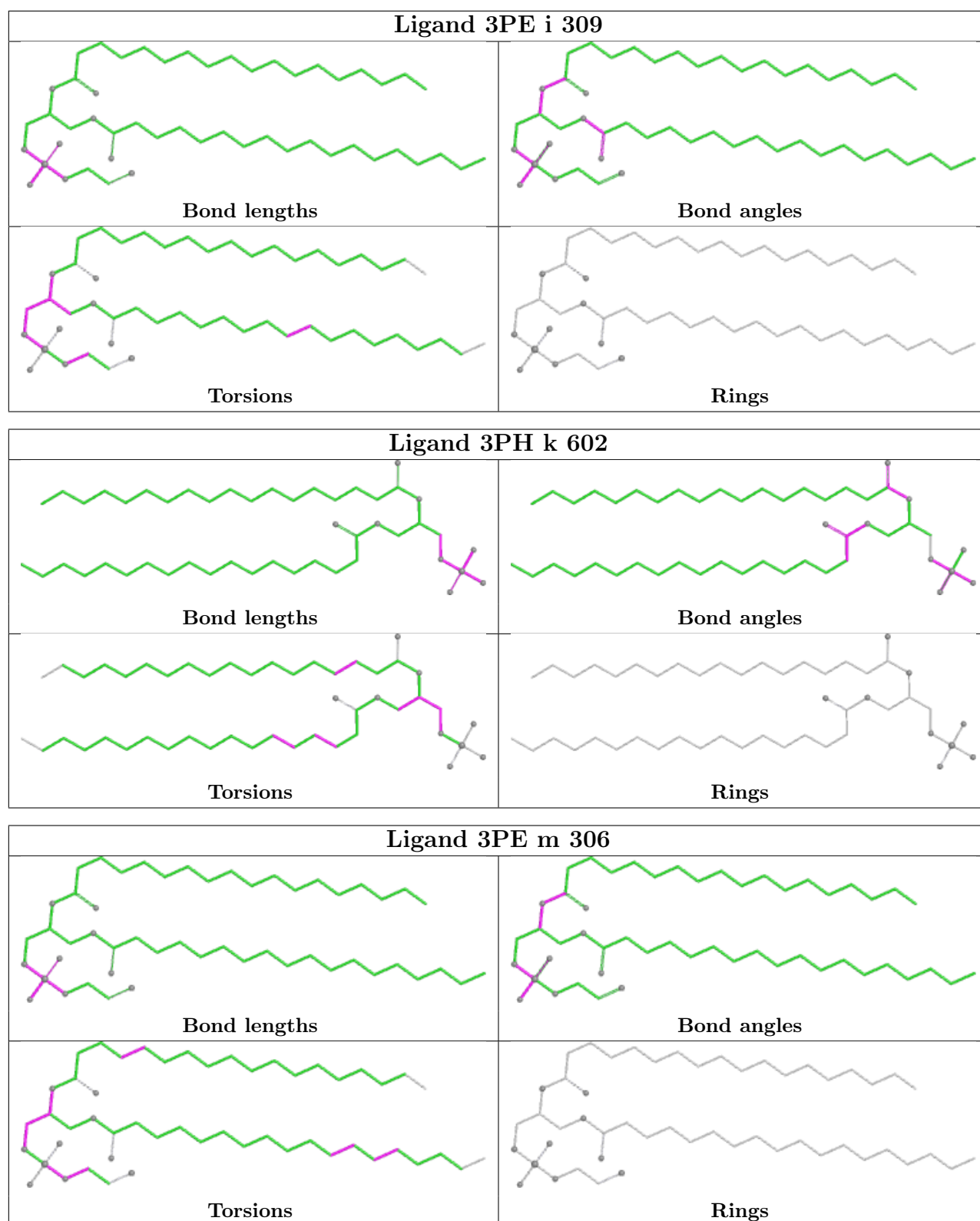
Ligand DU0 i 302

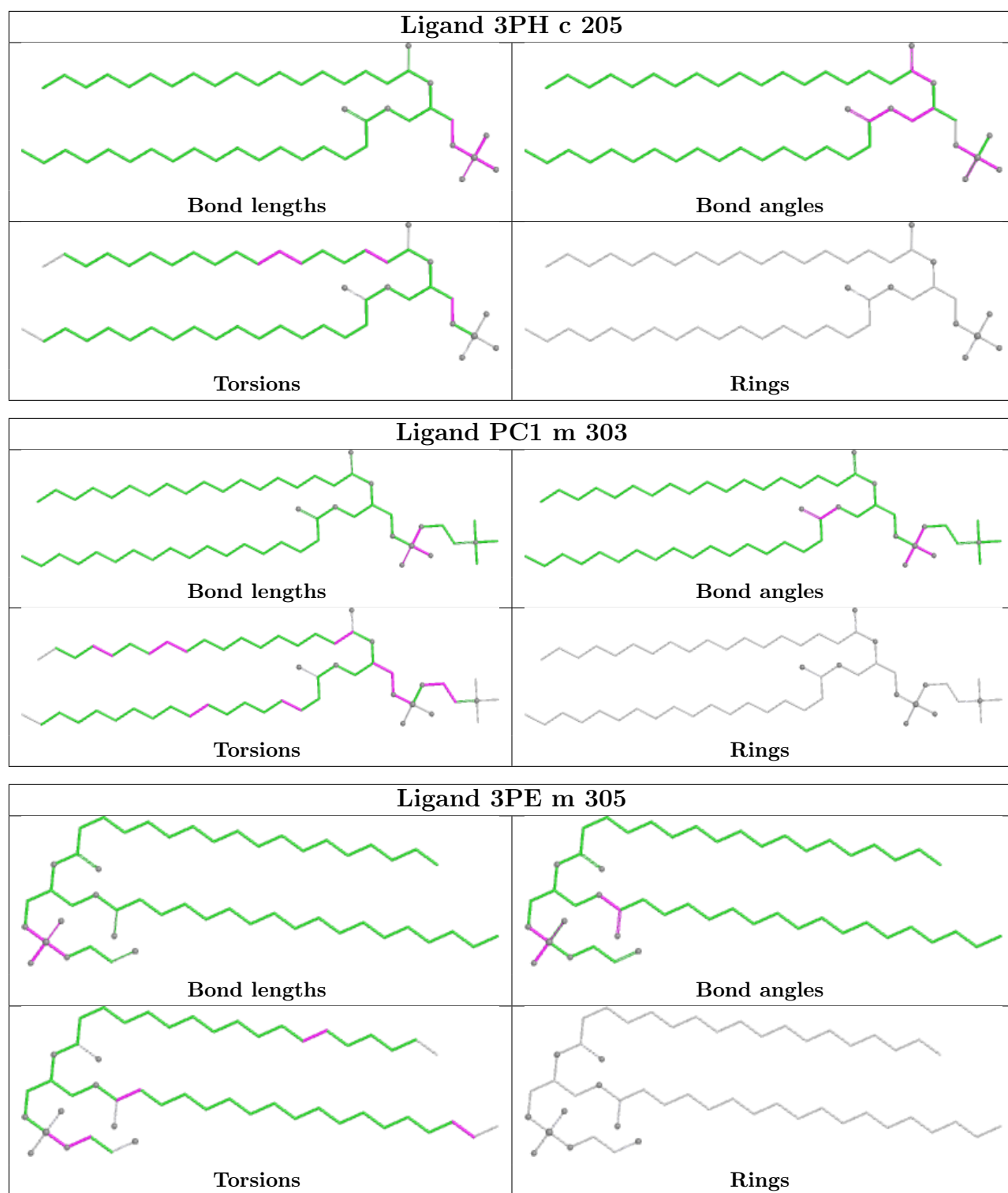


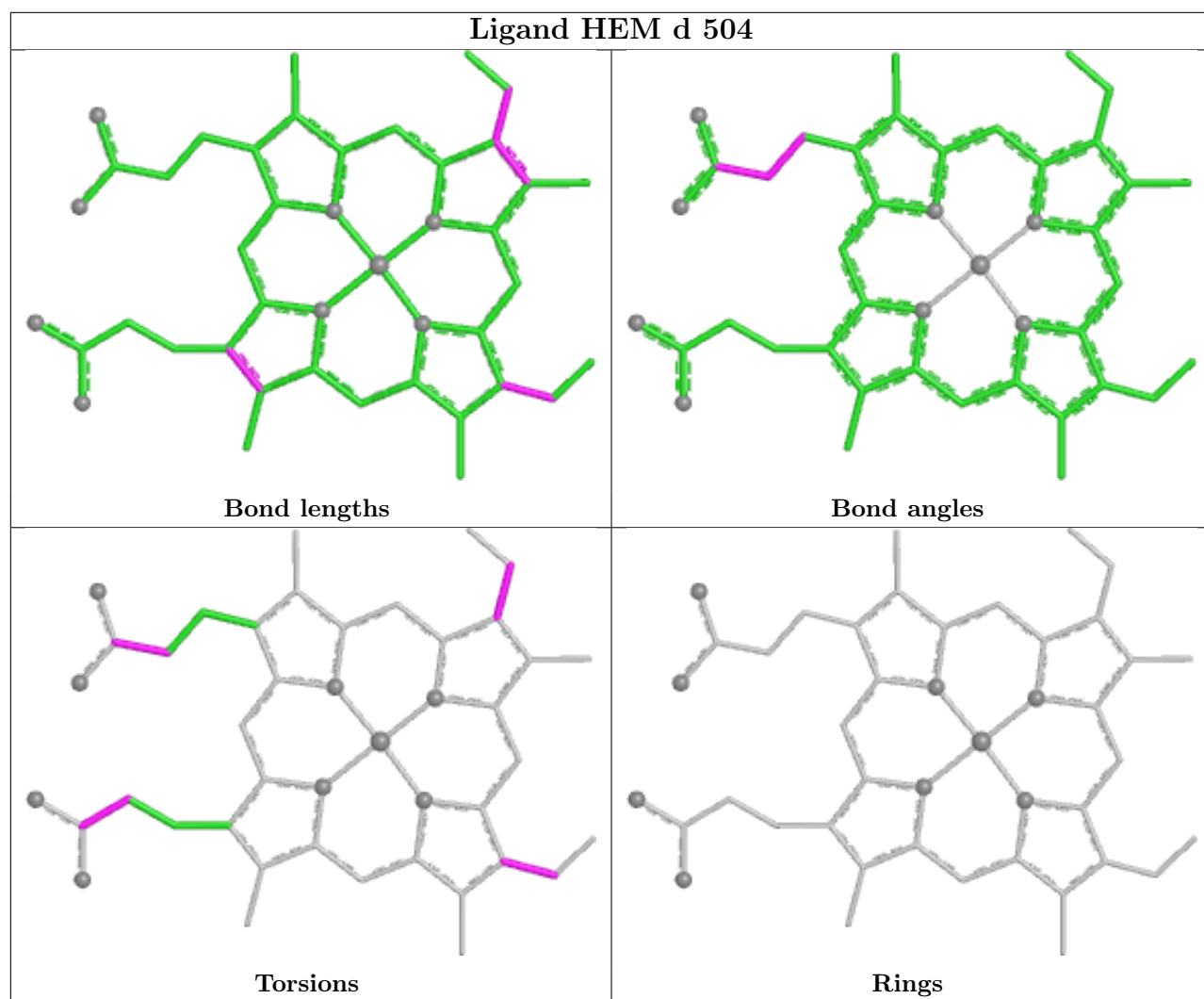
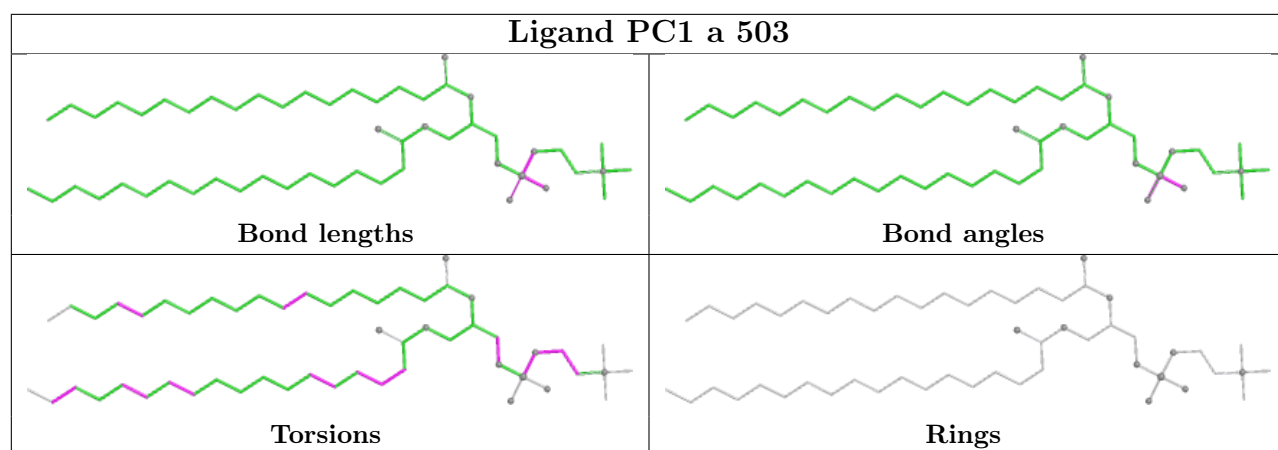


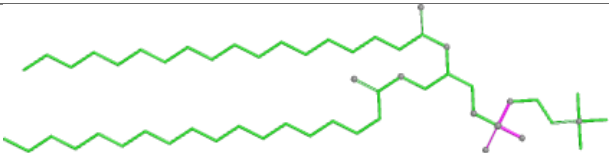
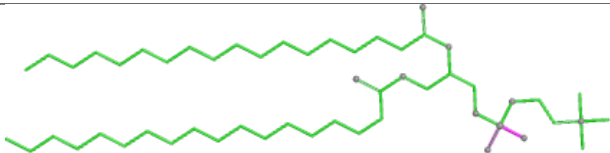
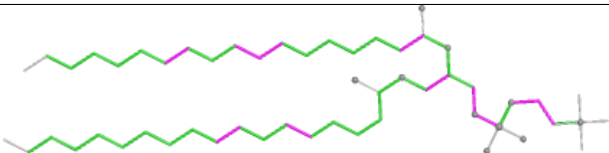
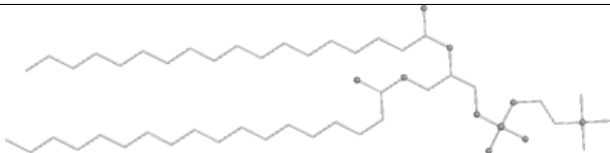
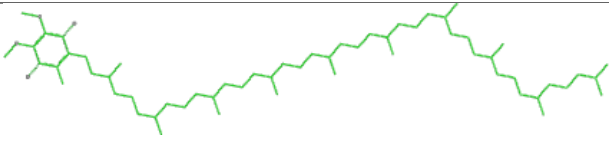
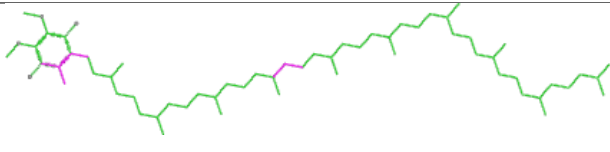


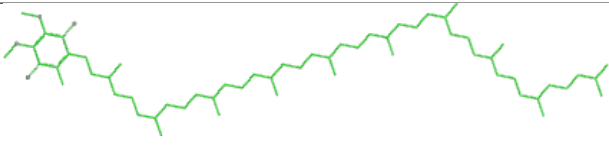
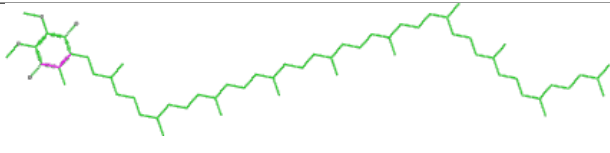
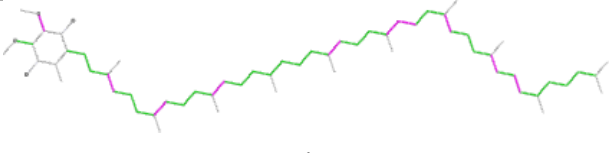
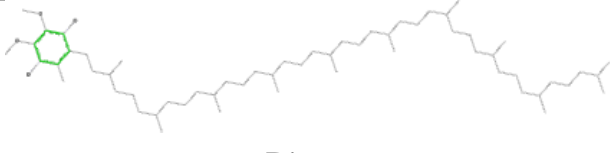


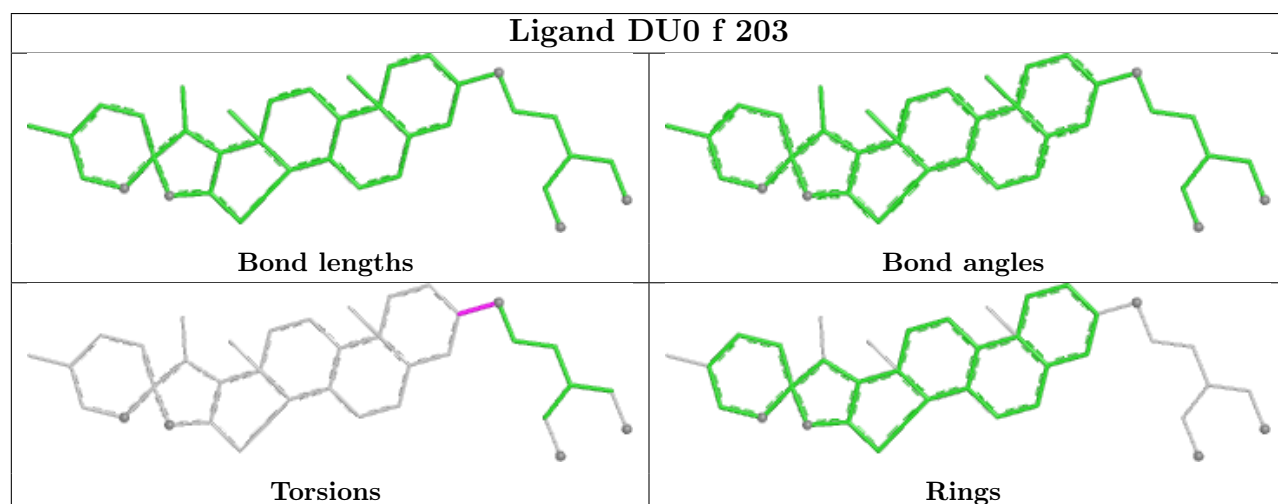
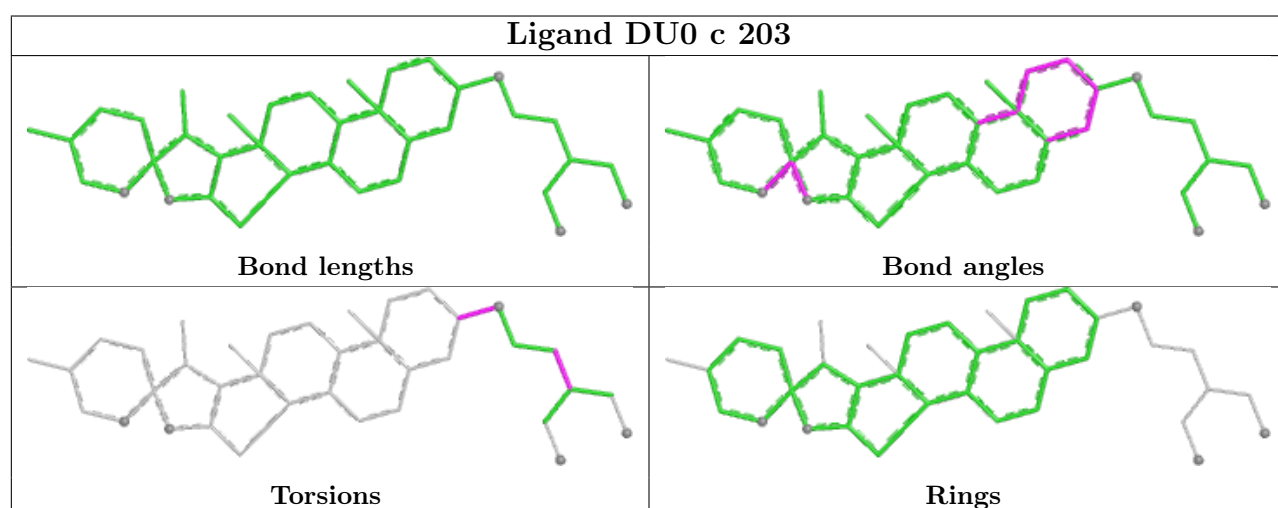
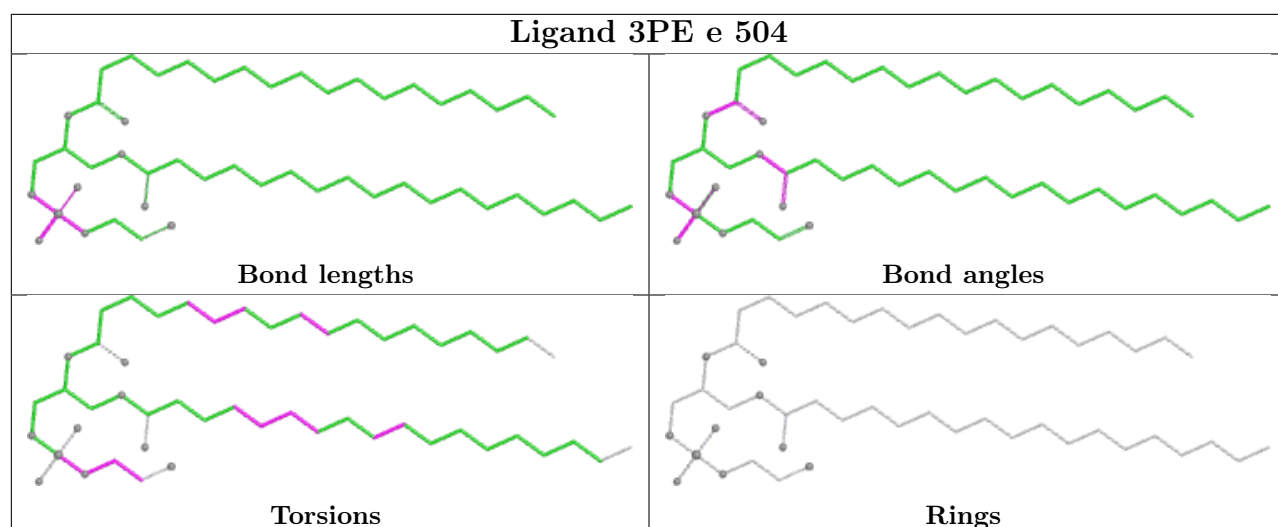


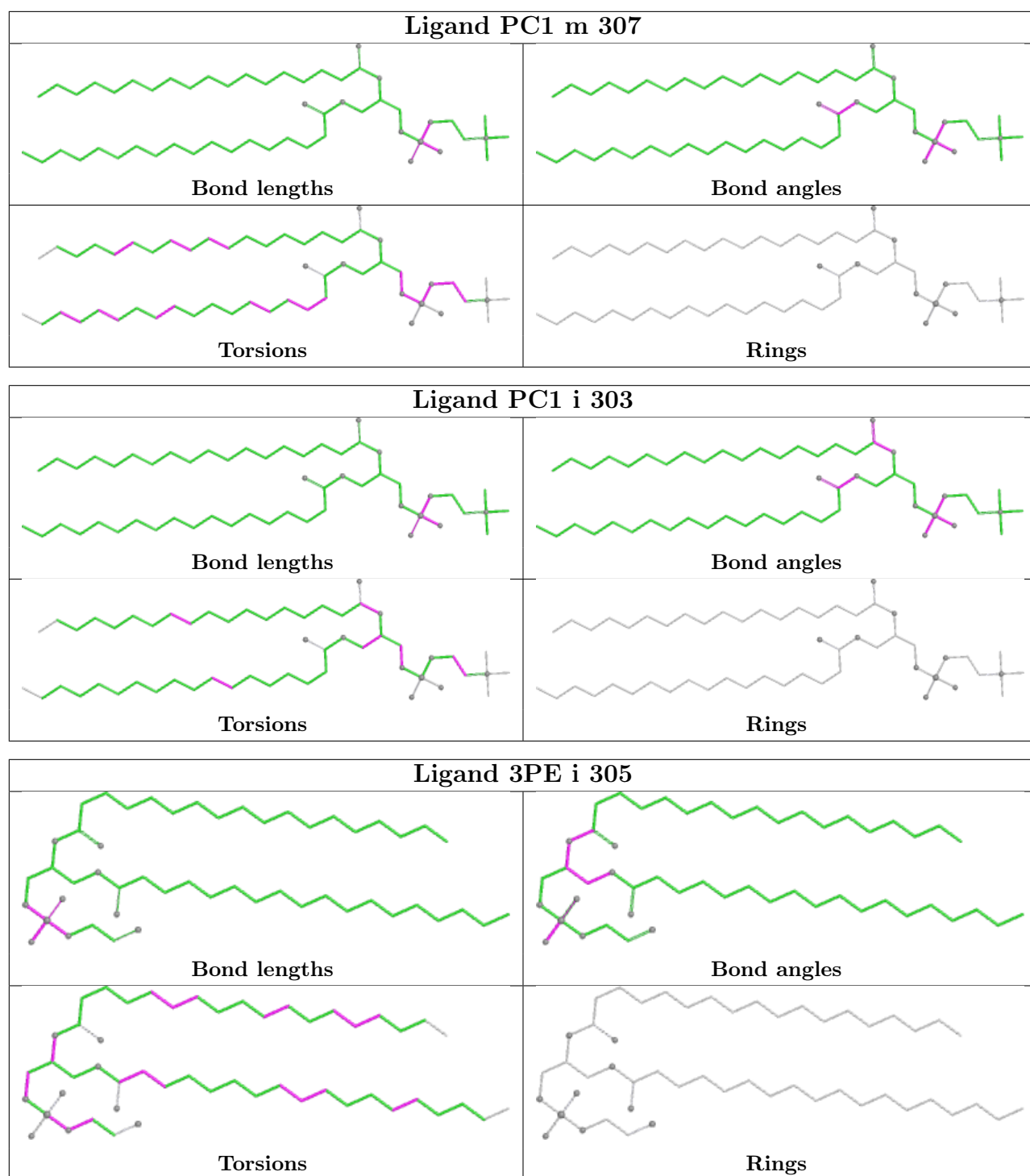


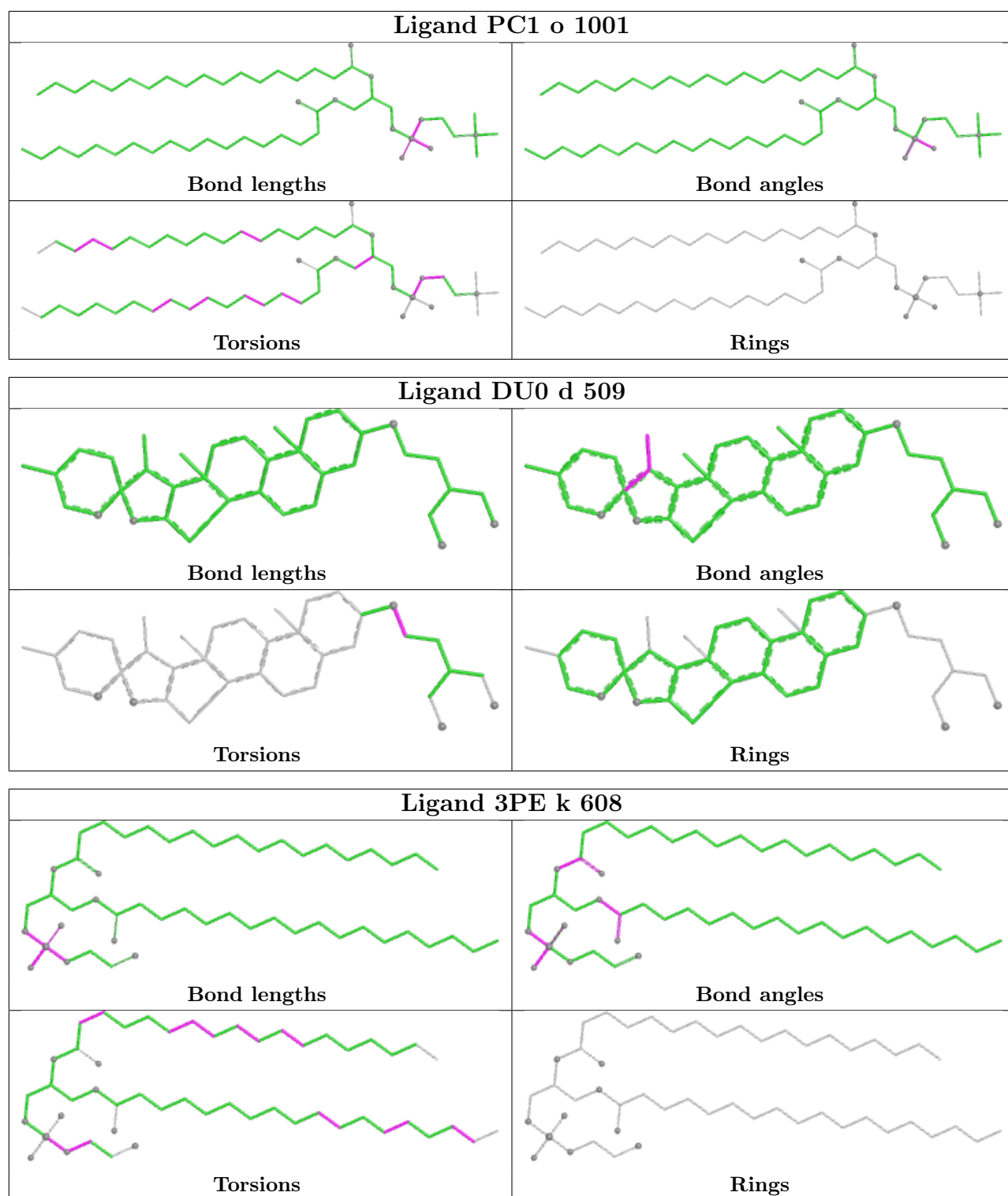


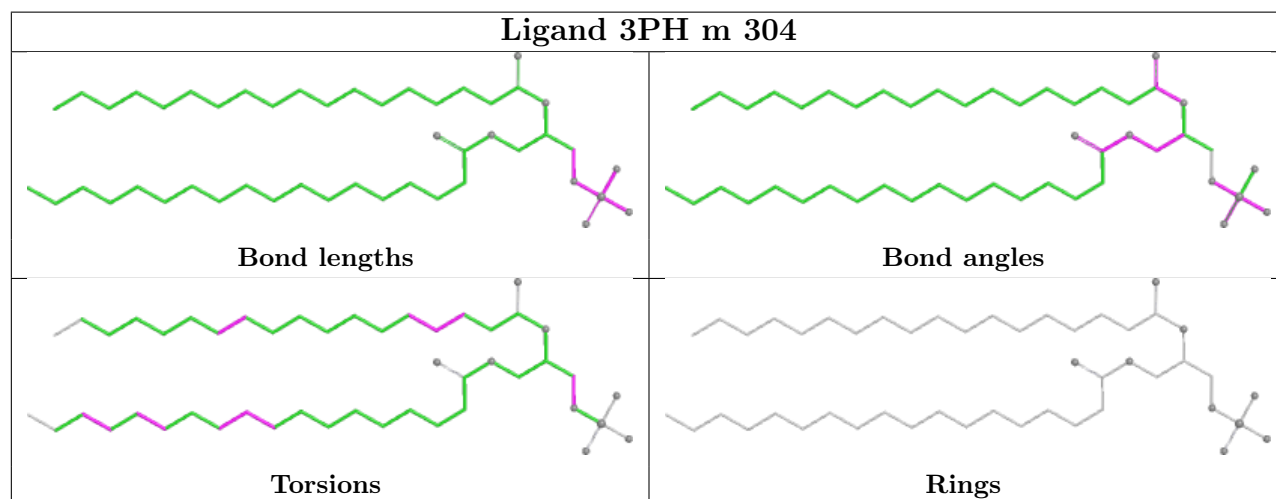
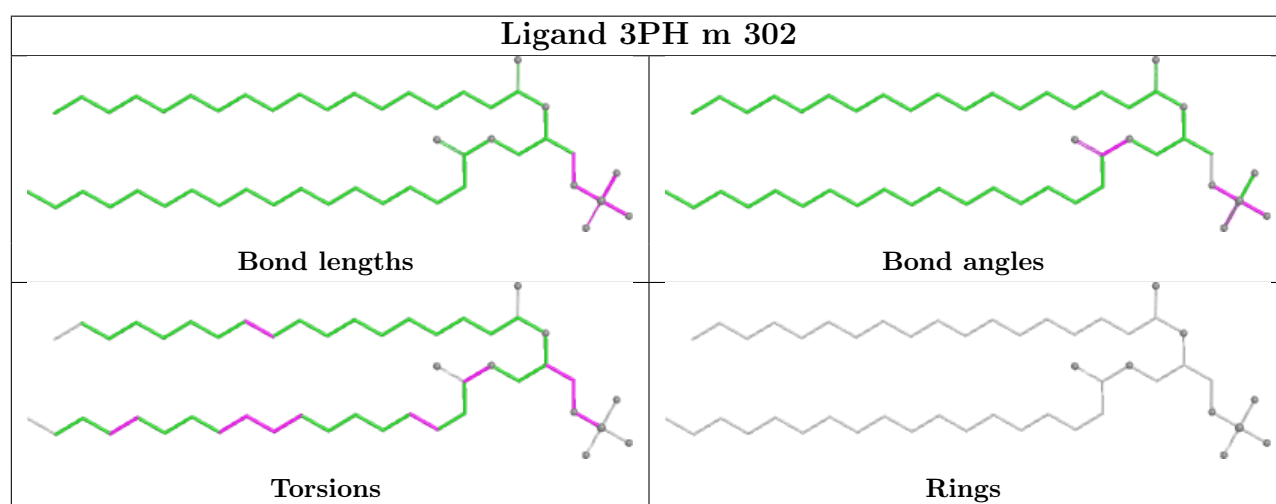
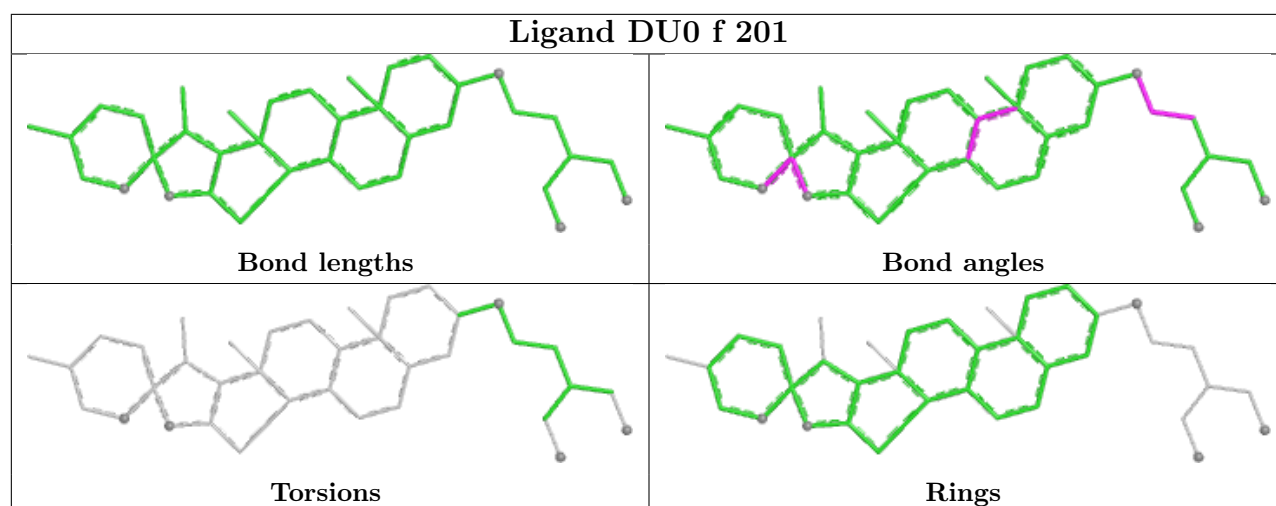


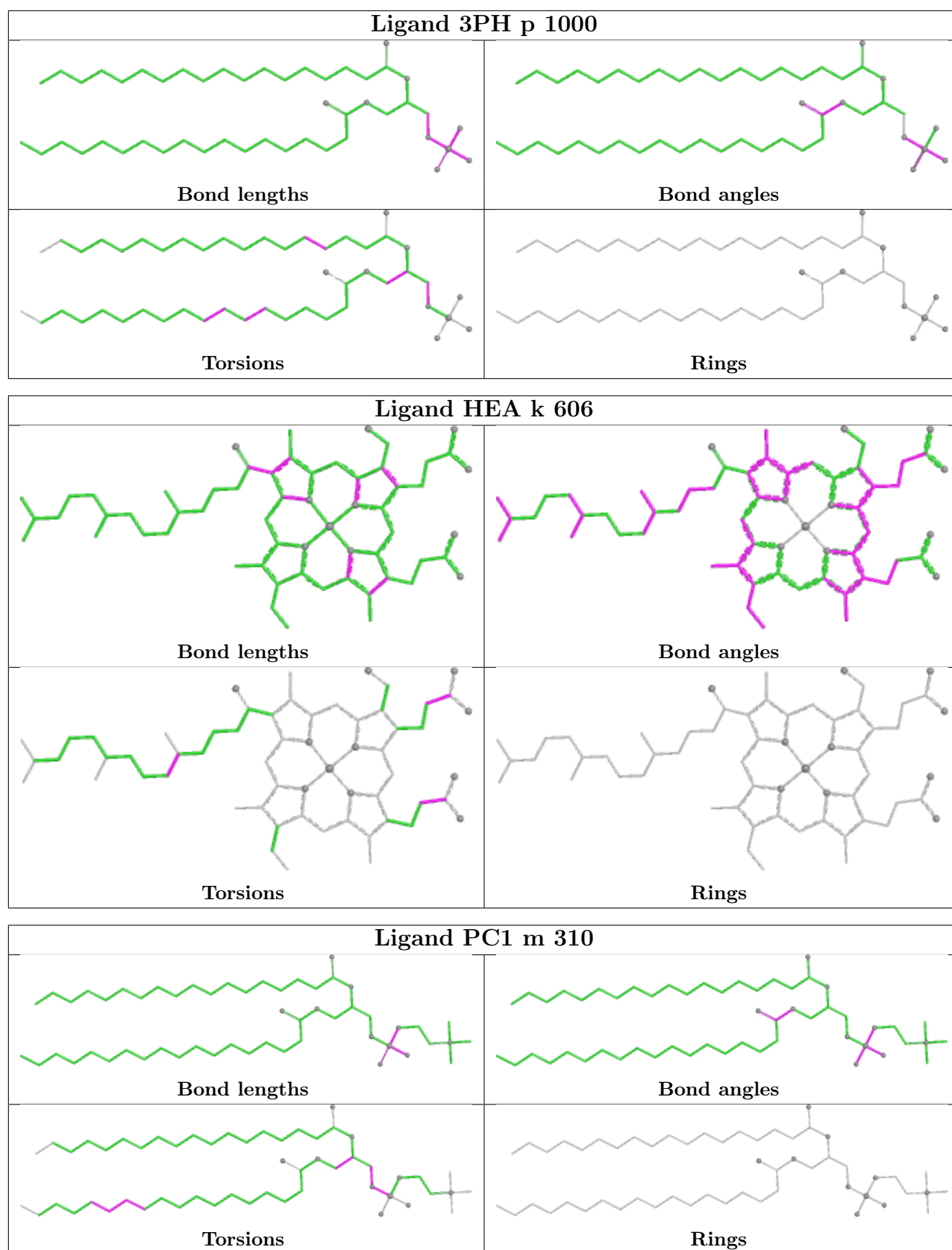
Ligand PC1 b 501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 a 502	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 a 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

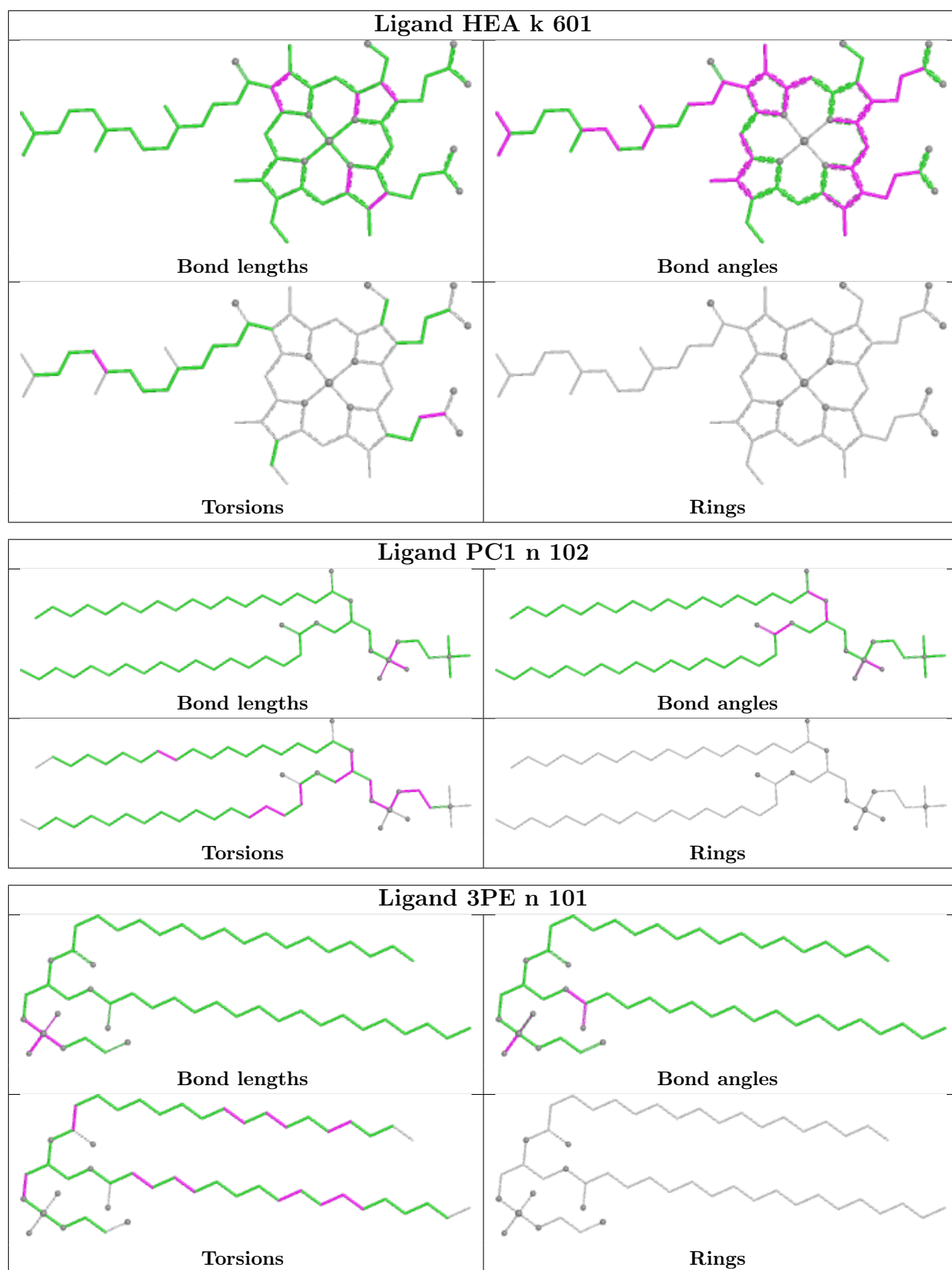


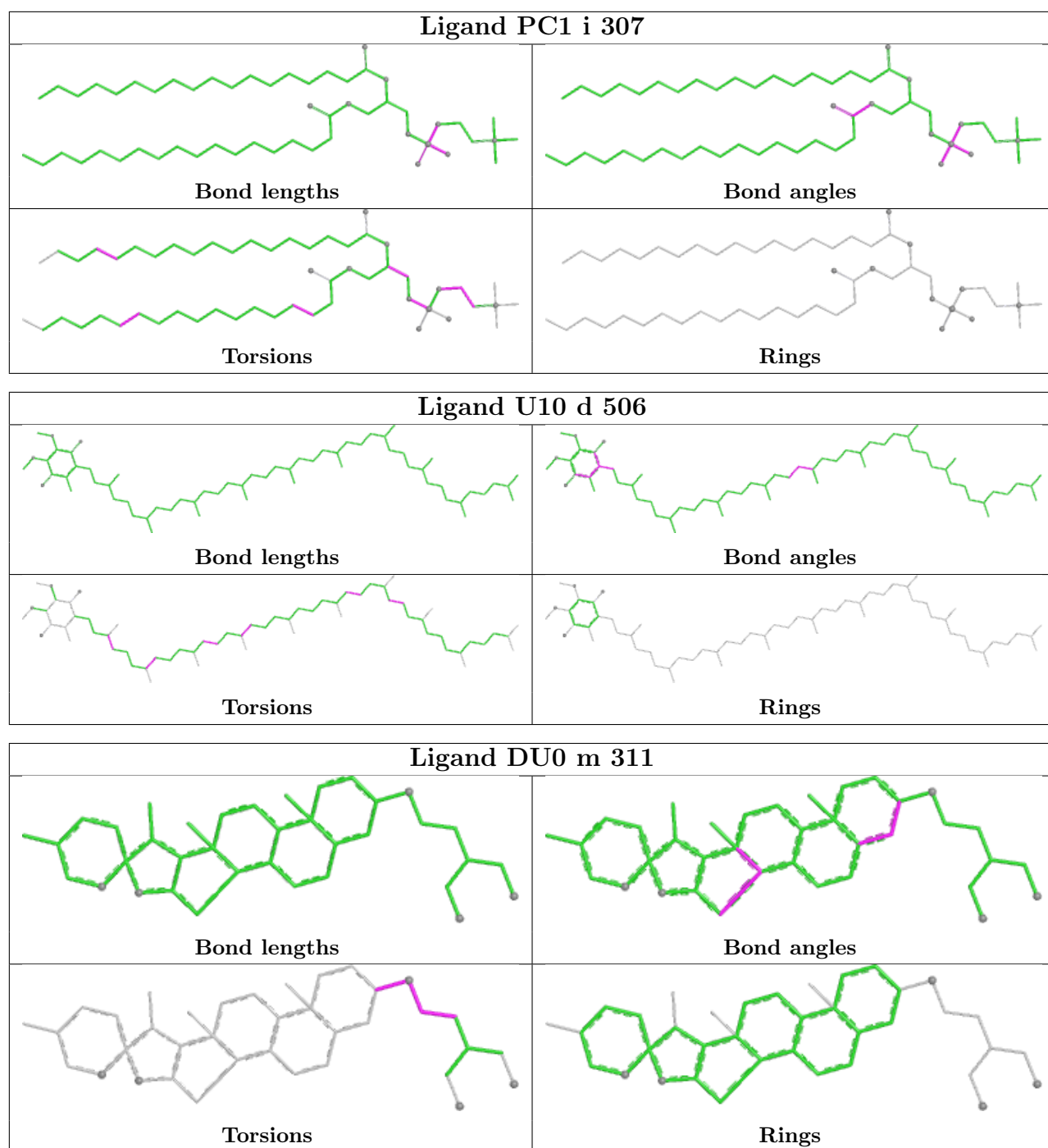


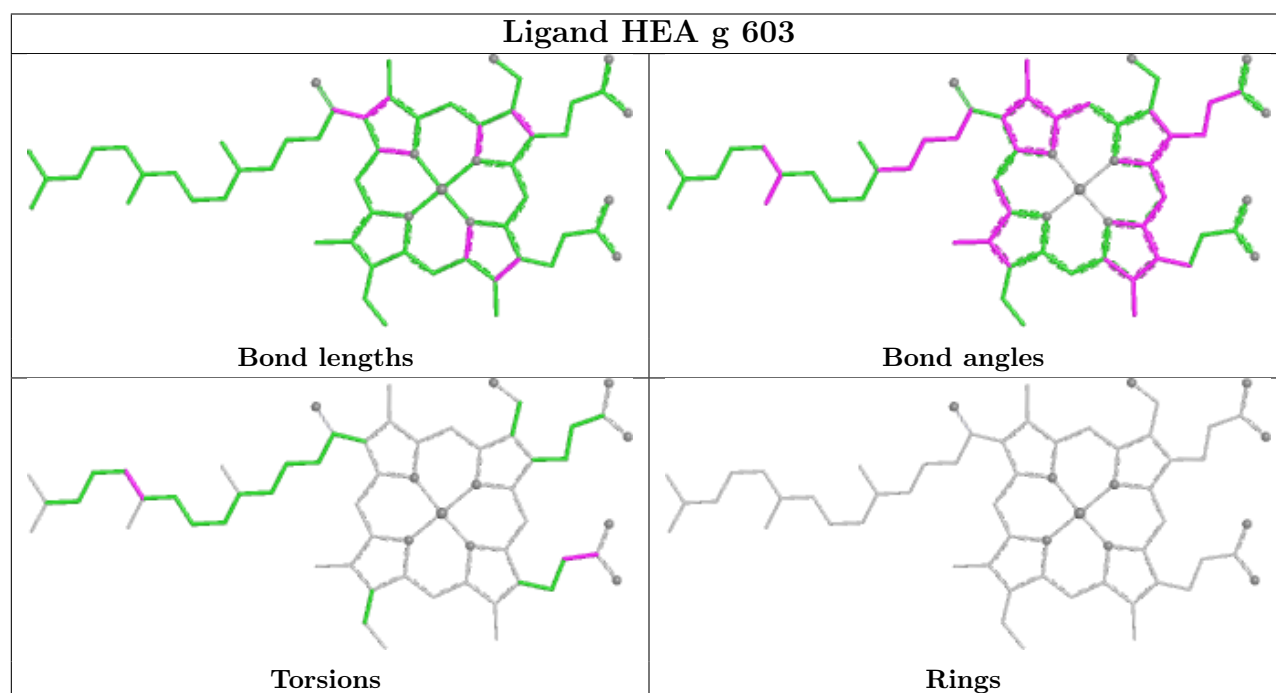
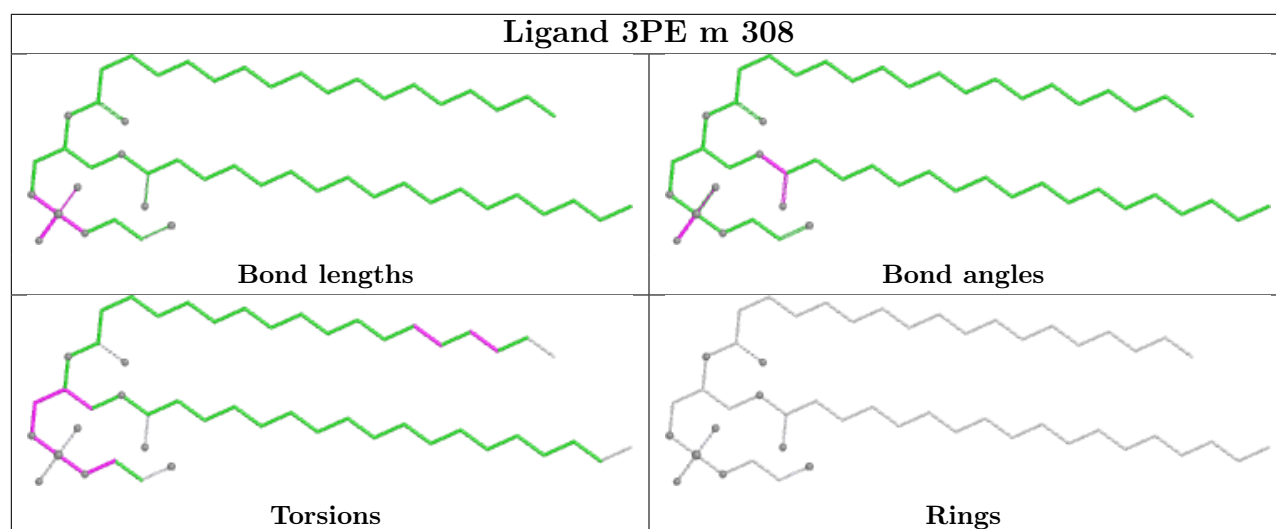
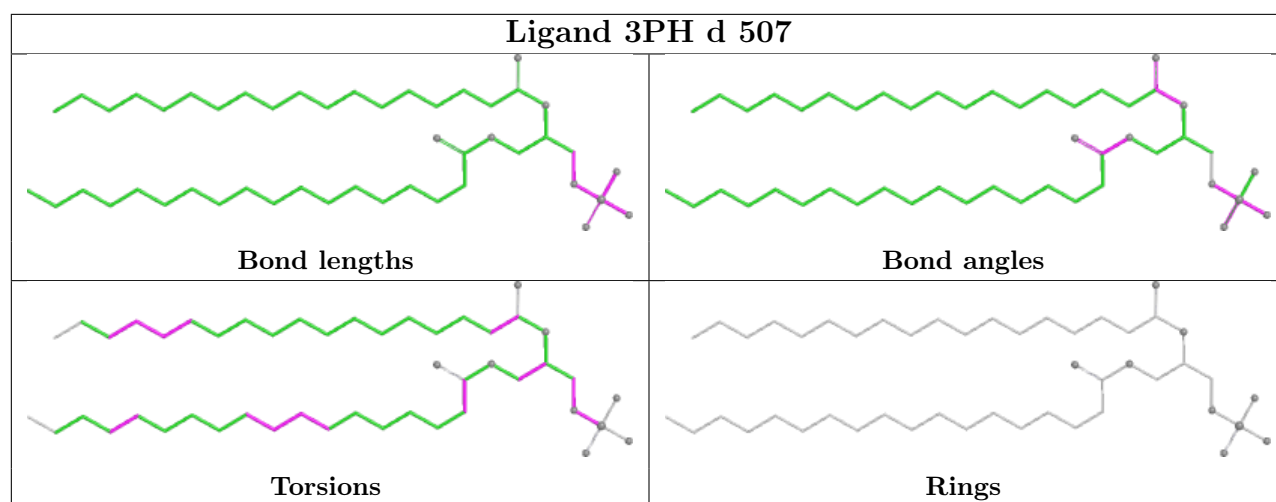




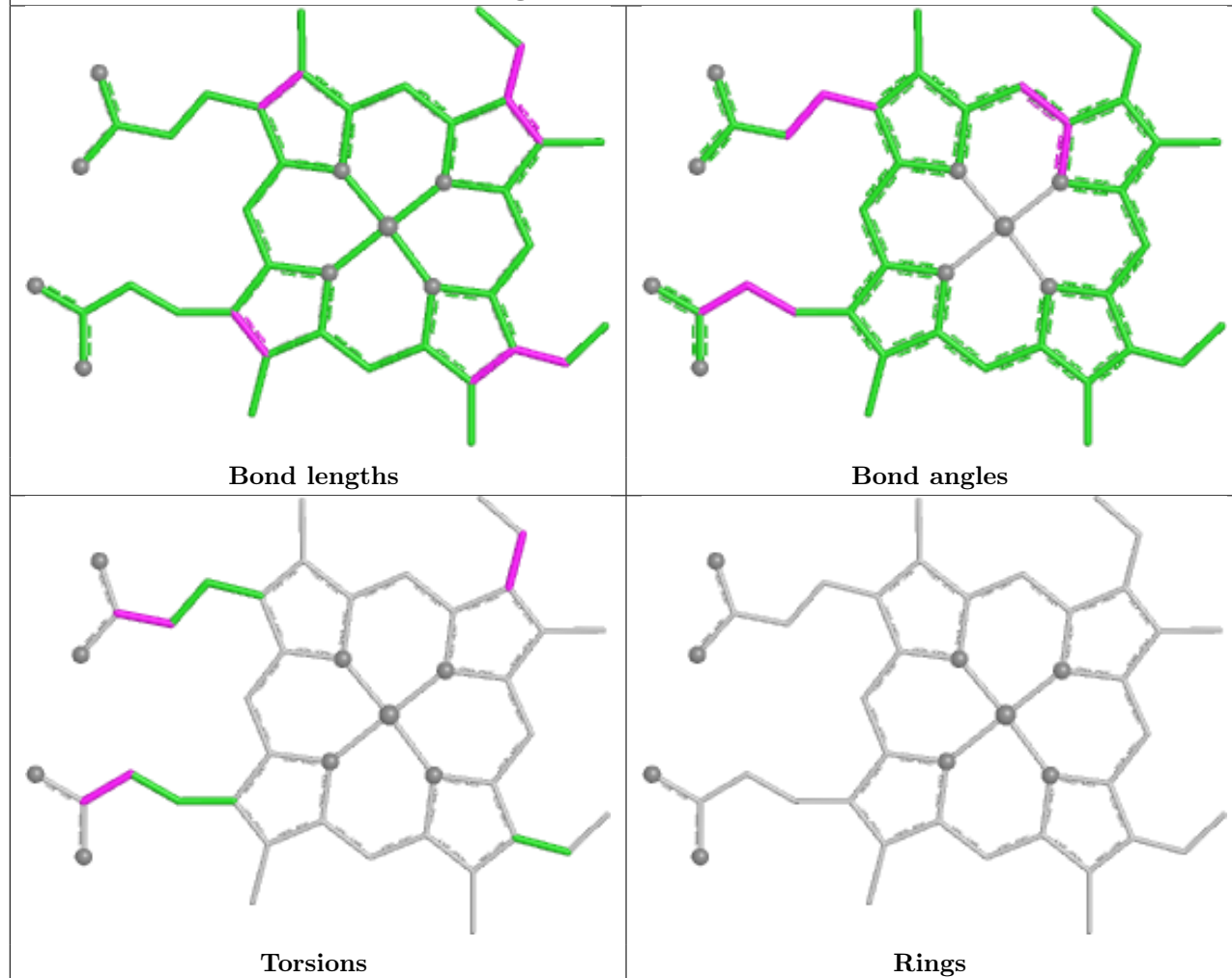




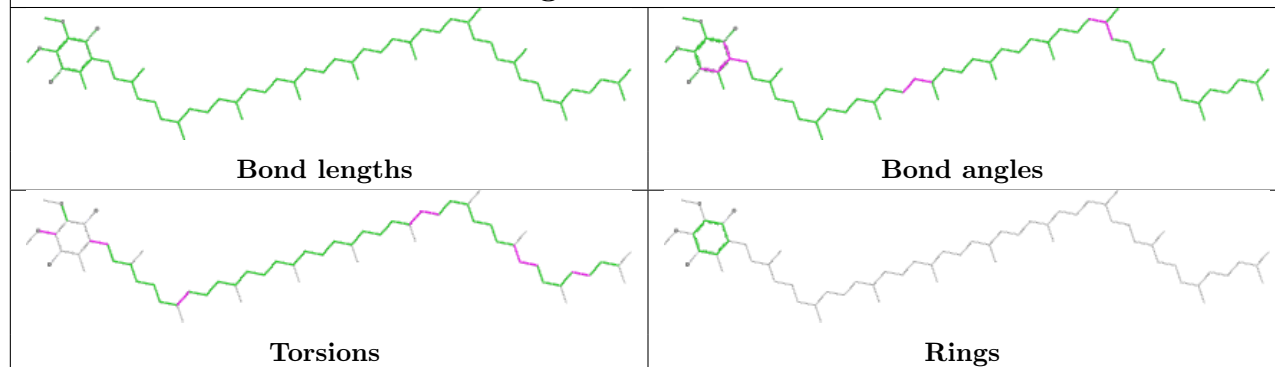


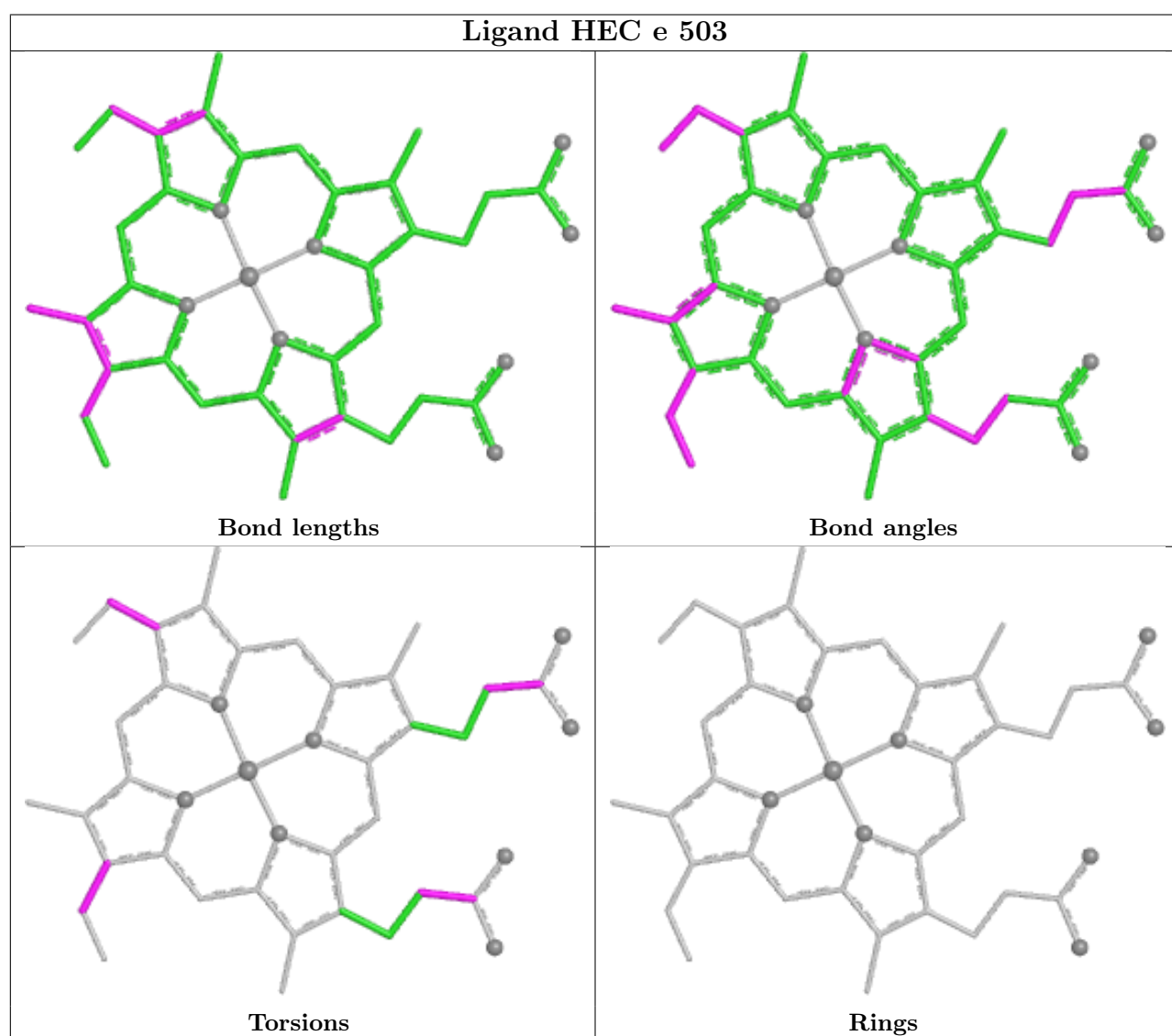
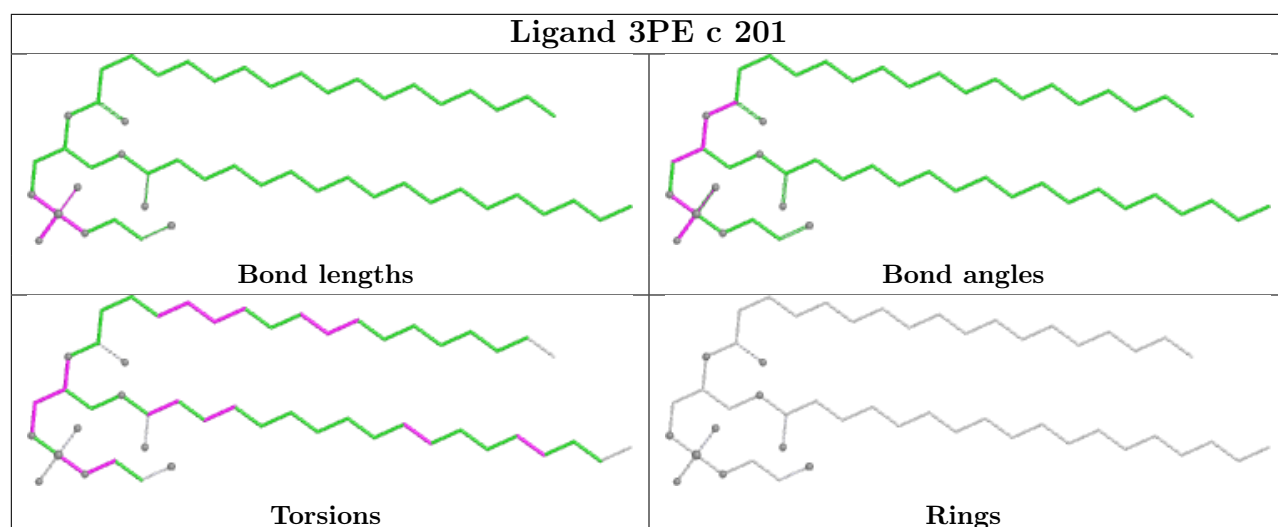


Ligand HEM a 505



Ligand U10 d 508





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

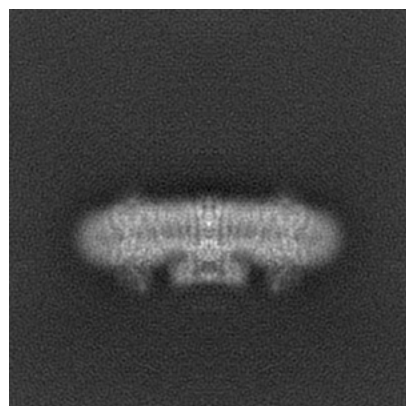
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50526. These allow visual inspection of the internal detail of the map and identification of artifacts.

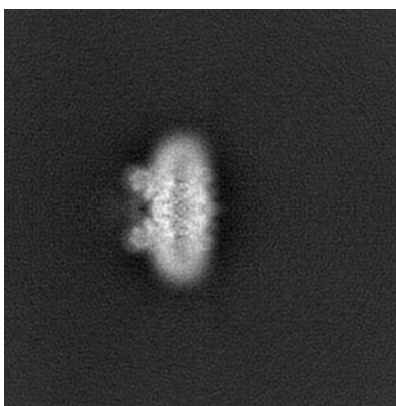
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

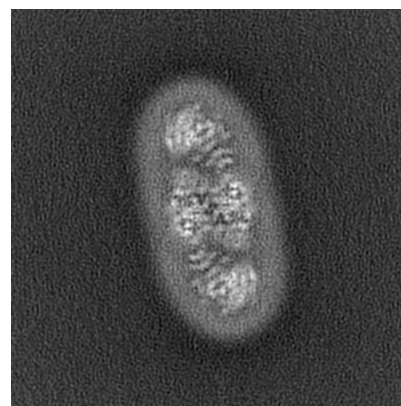
6.1.1 Primary map



X

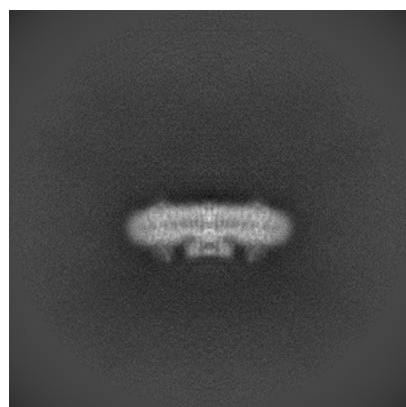


Y

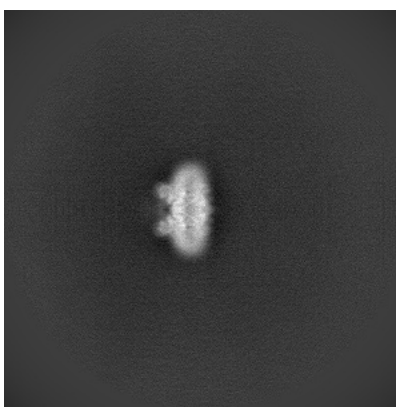


Z

6.1.2 Raw map



X



Y

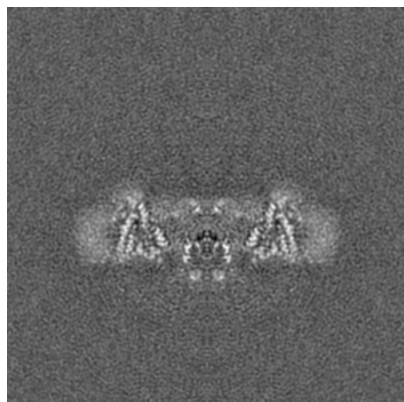


Z

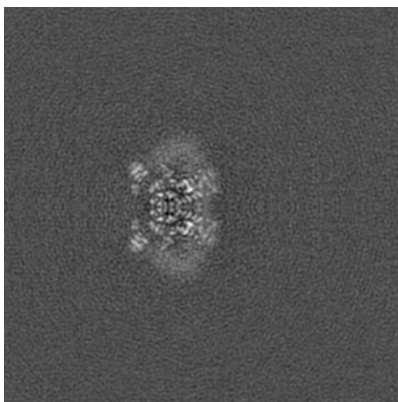
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

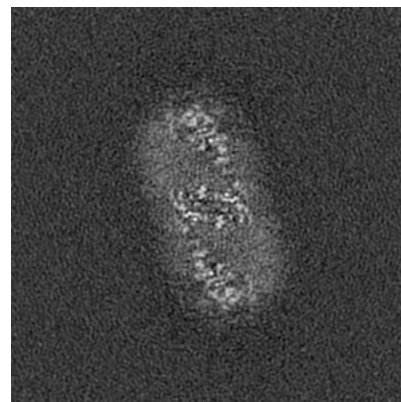
6.2.1 Primary map



X Index: 187

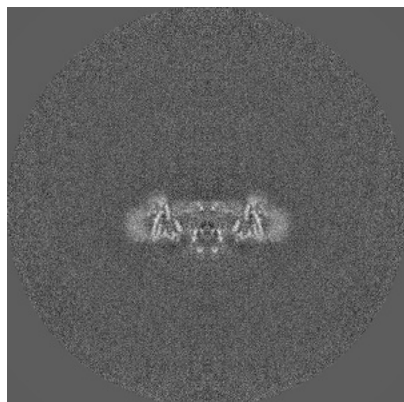


Y Index: 187

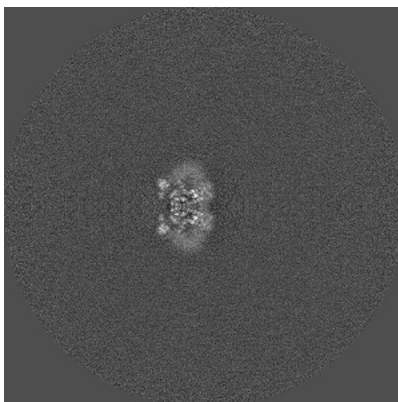


Z Index: 187

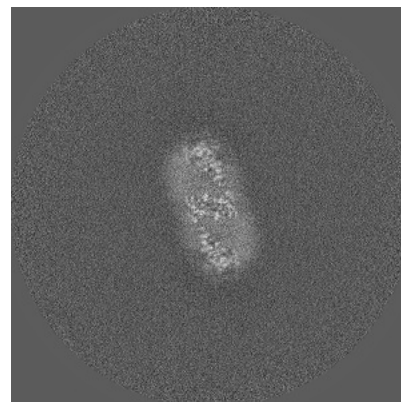
6.2.2 Raw map



X Index: 300



Y Index: 300

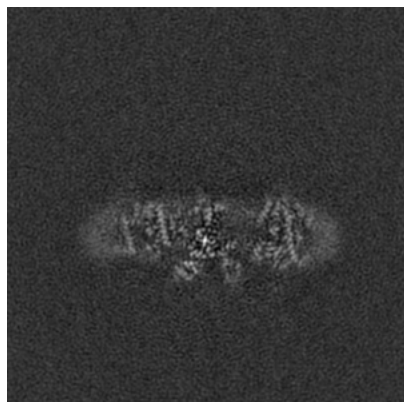


Z Index: 300

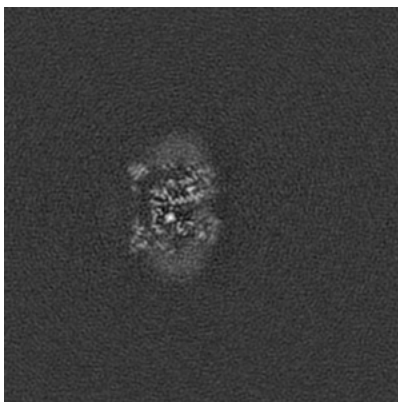
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

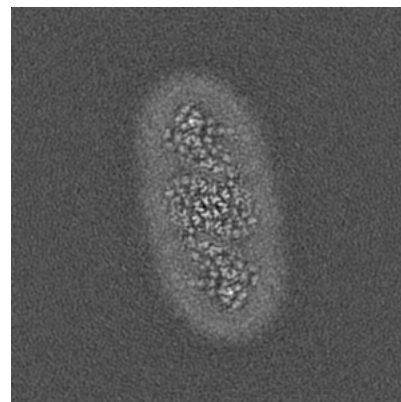
6.3.1 Primary map



X Index: 177

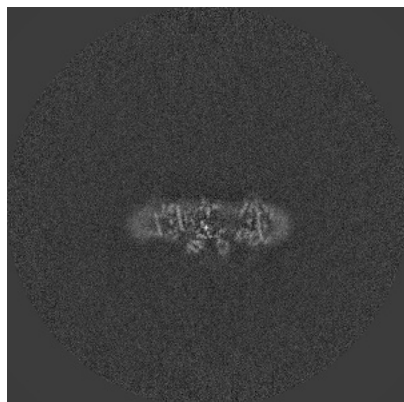


Y Index: 185

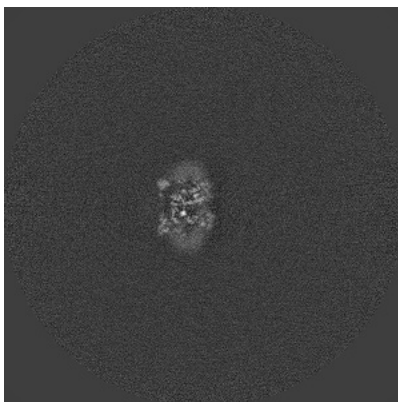


Z Index: 152

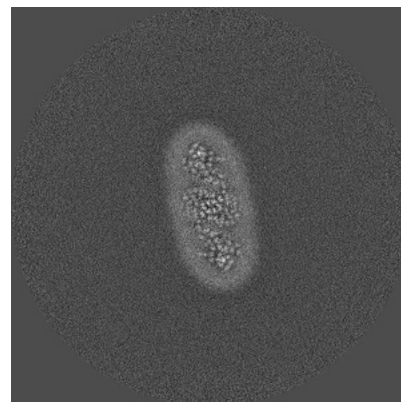
6.3.2 Raw map



X Index: 290



Y Index: 298

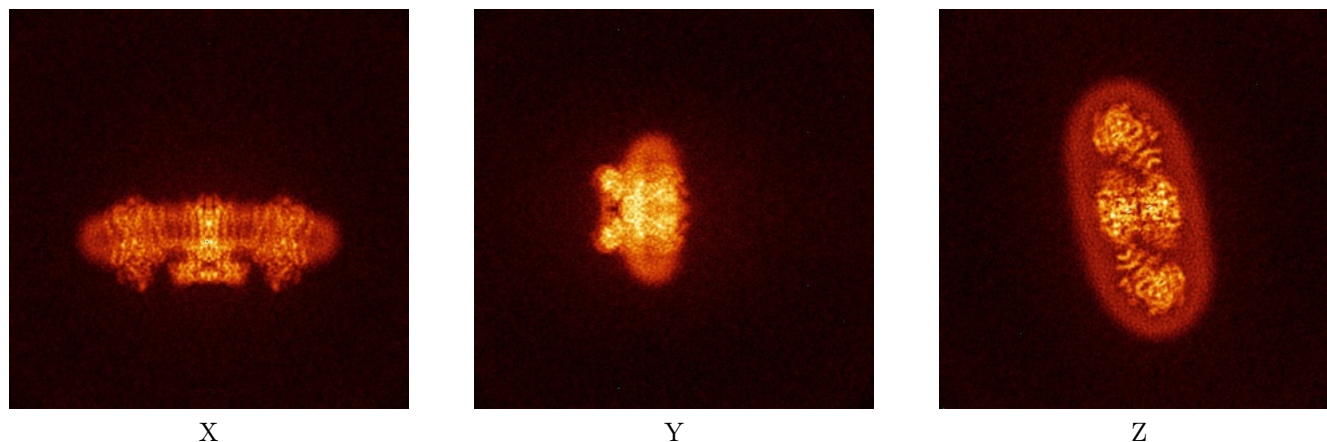


Z Index: 265

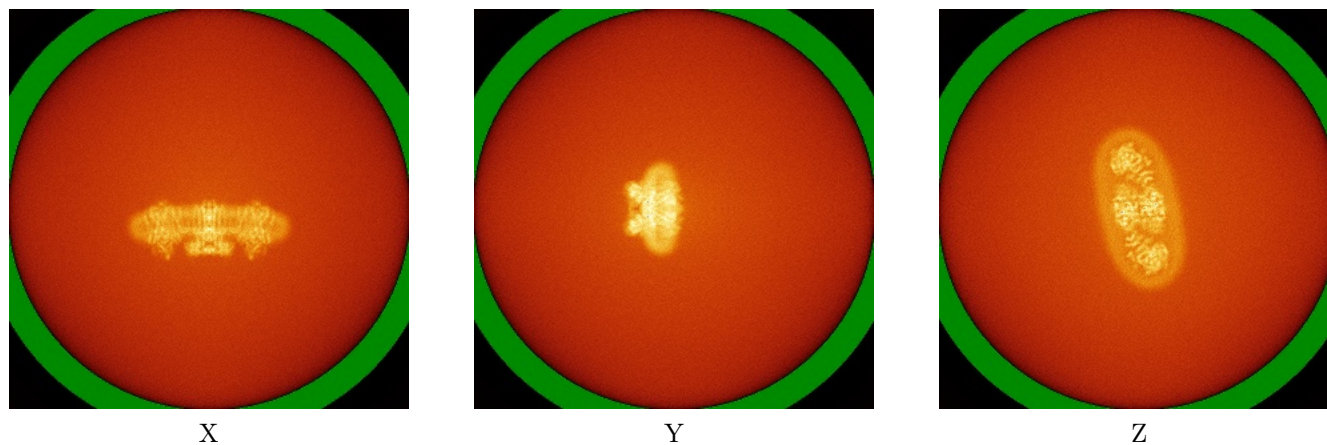
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

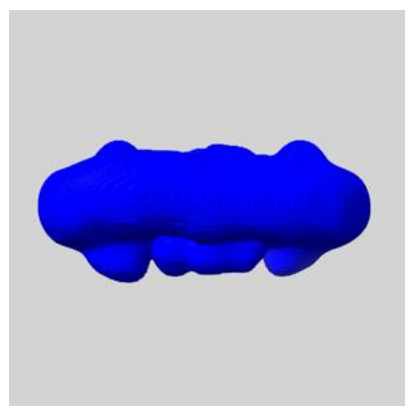
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

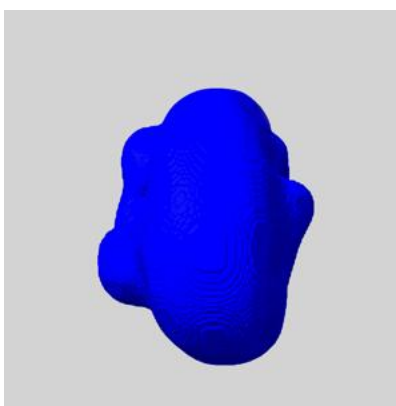
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

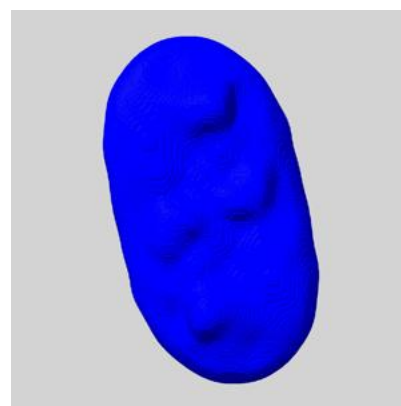
6.6.1 emd_50526_msk_1.map [i](#)



X



Y

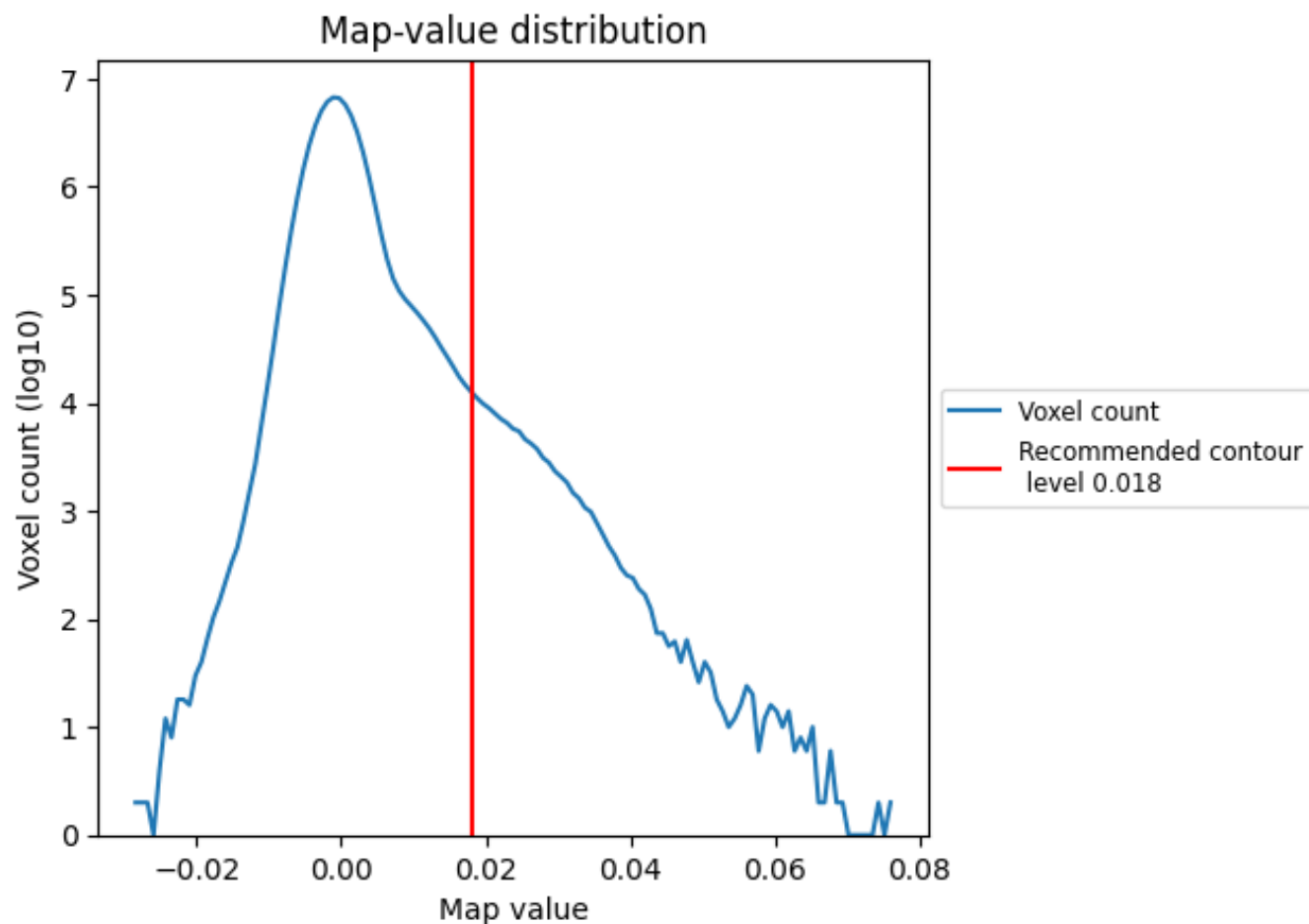


Z

7 Map analysis [i](#)

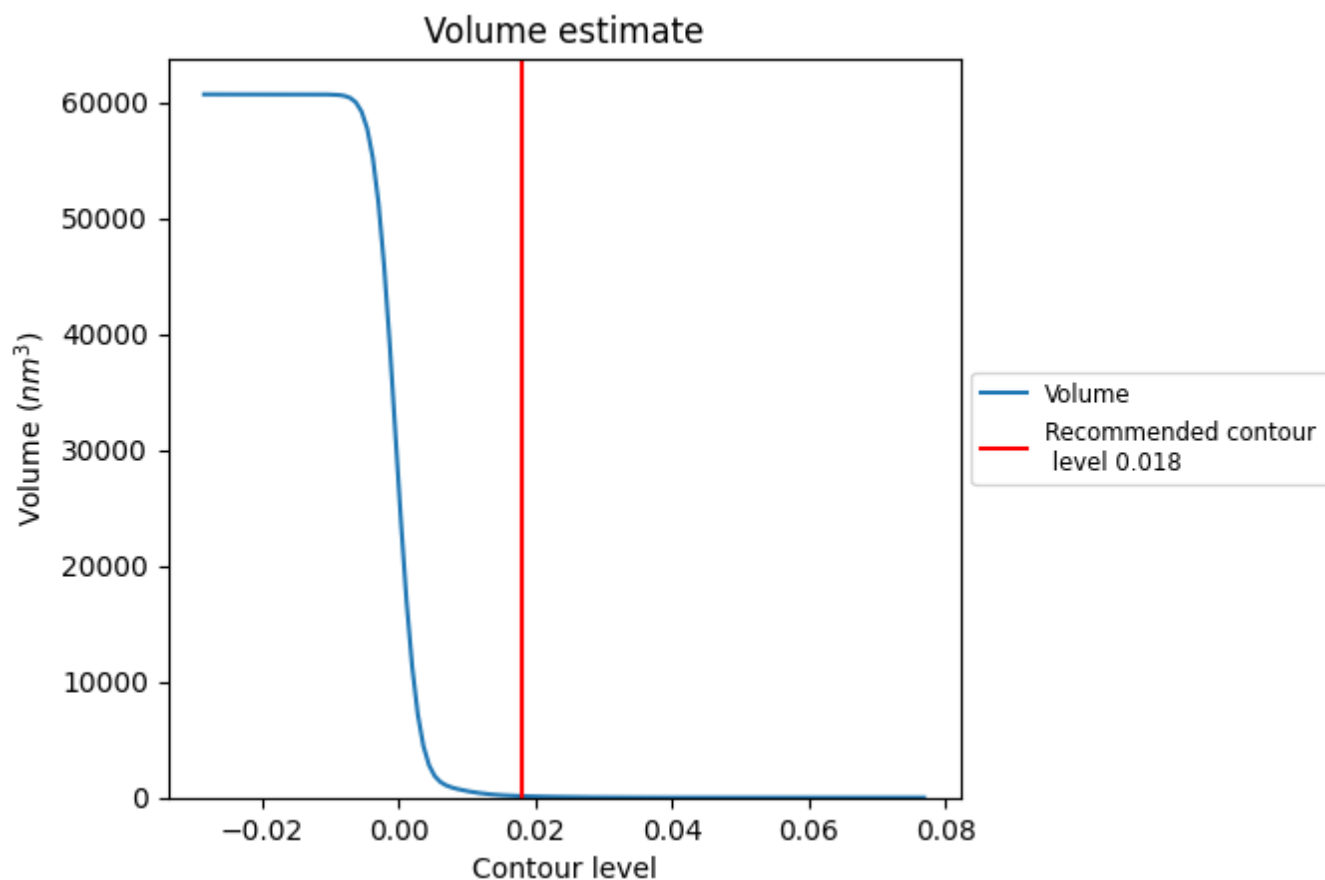
This section contains the results of statistical analysis of the map.

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.

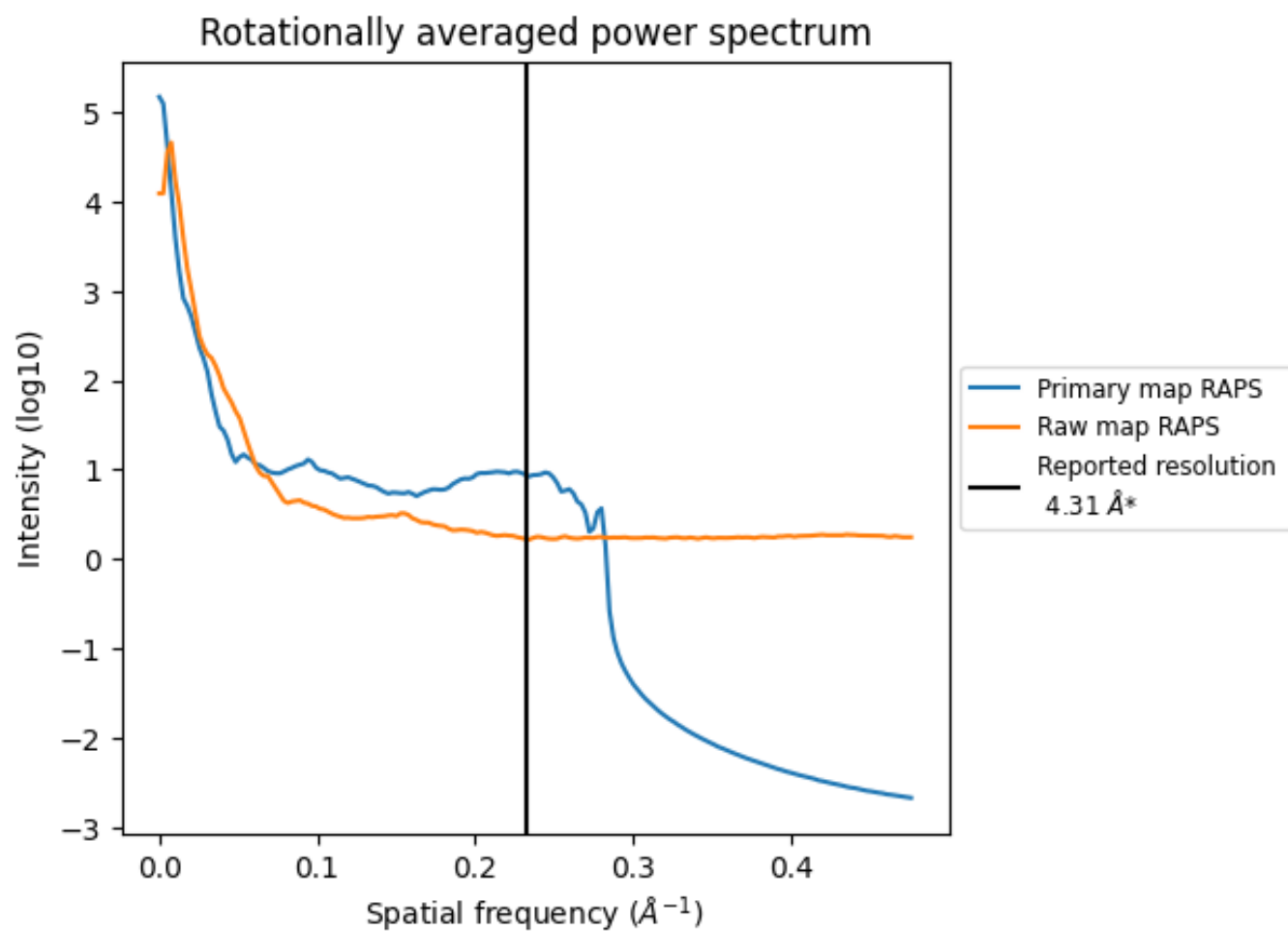
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 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 ⓘ

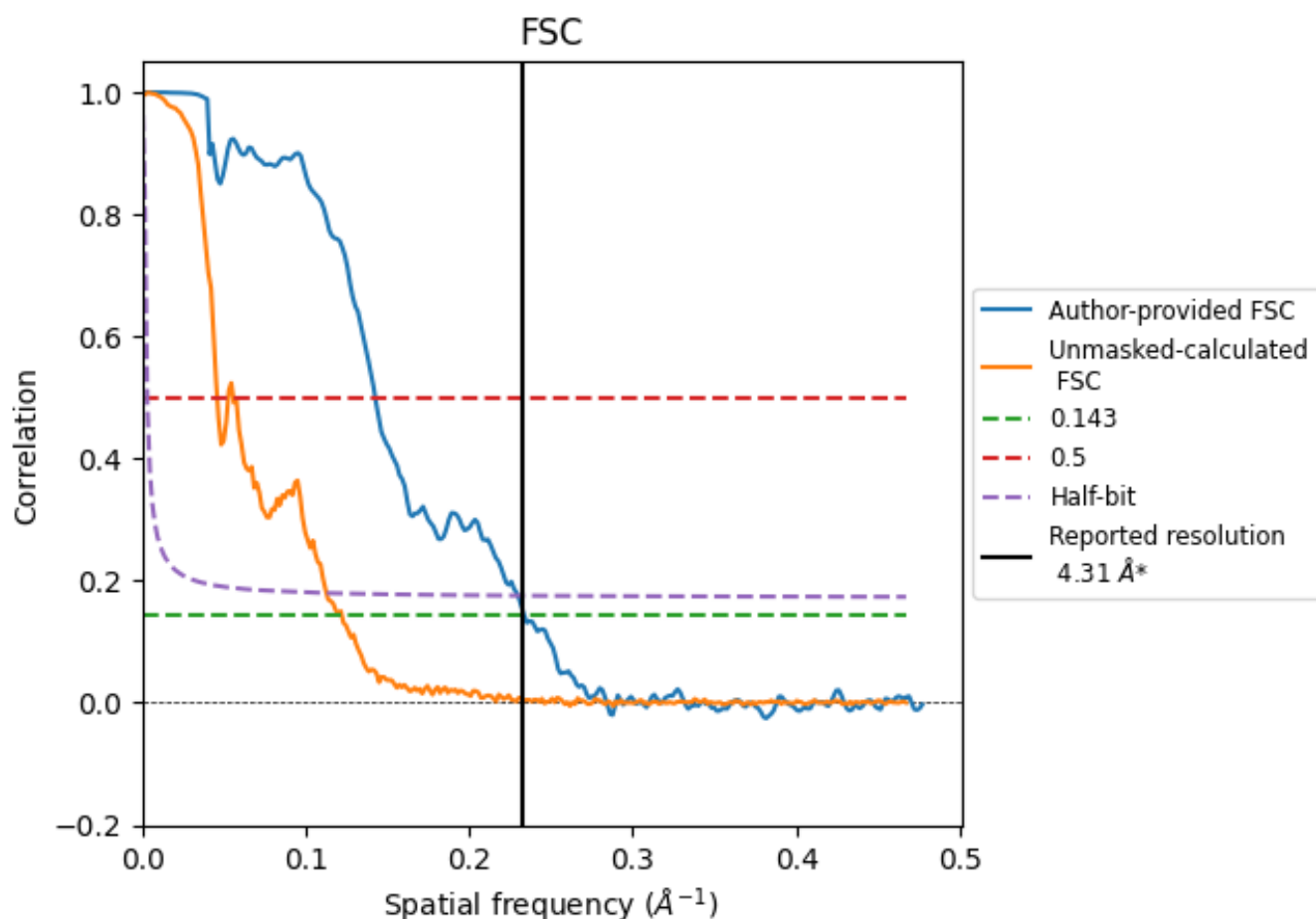


*Reported resolution corresponds to spatial frequency of 0.232 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.232 \AA^{-1}

8.2 Resolution estimates [i](#)

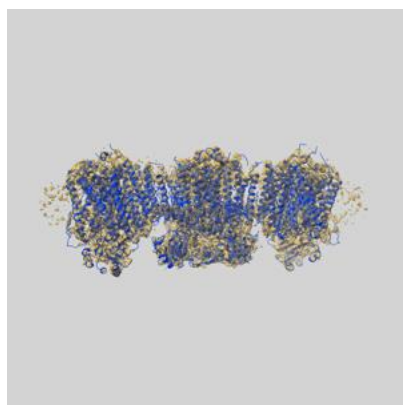
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.31	-	-
Author-provided FSC curve	4.28	7.01	4.35
Unmasked-calculated*	8.19	21.83	8.87

*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 8.19 differs from the reported value 4.31 by more than 10 %

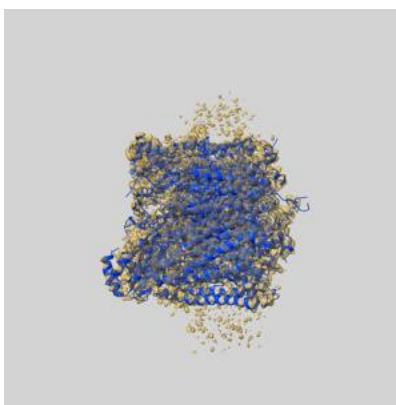
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50526 and PDB model 9FKS. Per-residue inclusion information can be found in section [3](#) on page [16](#).

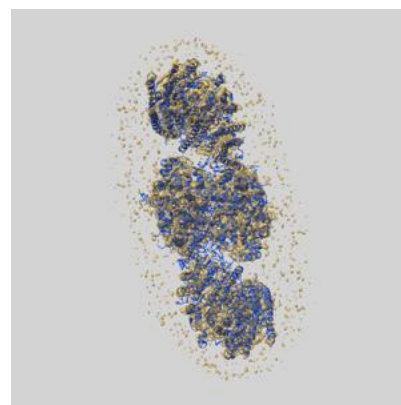
9.1 Map-model overlay [i](#)



X



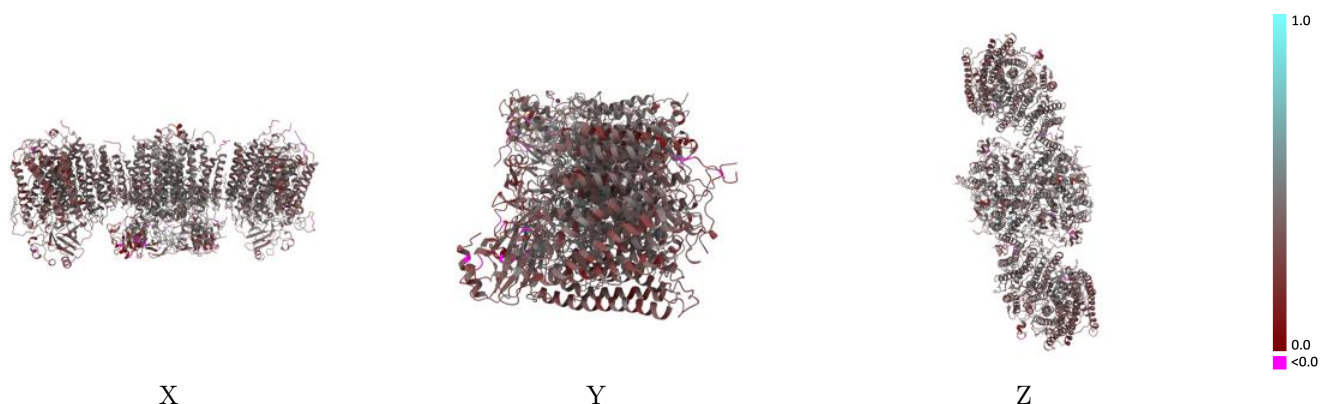
Y



Z

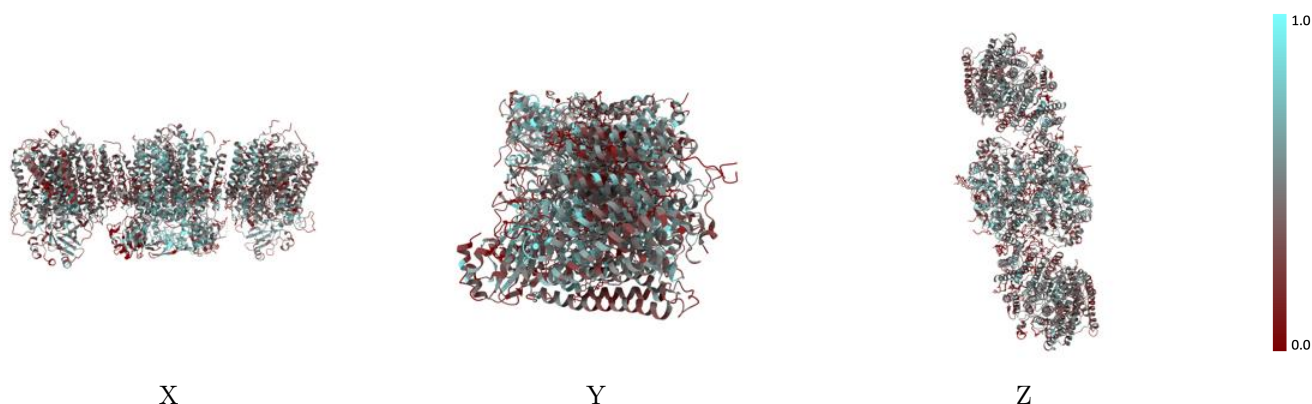
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



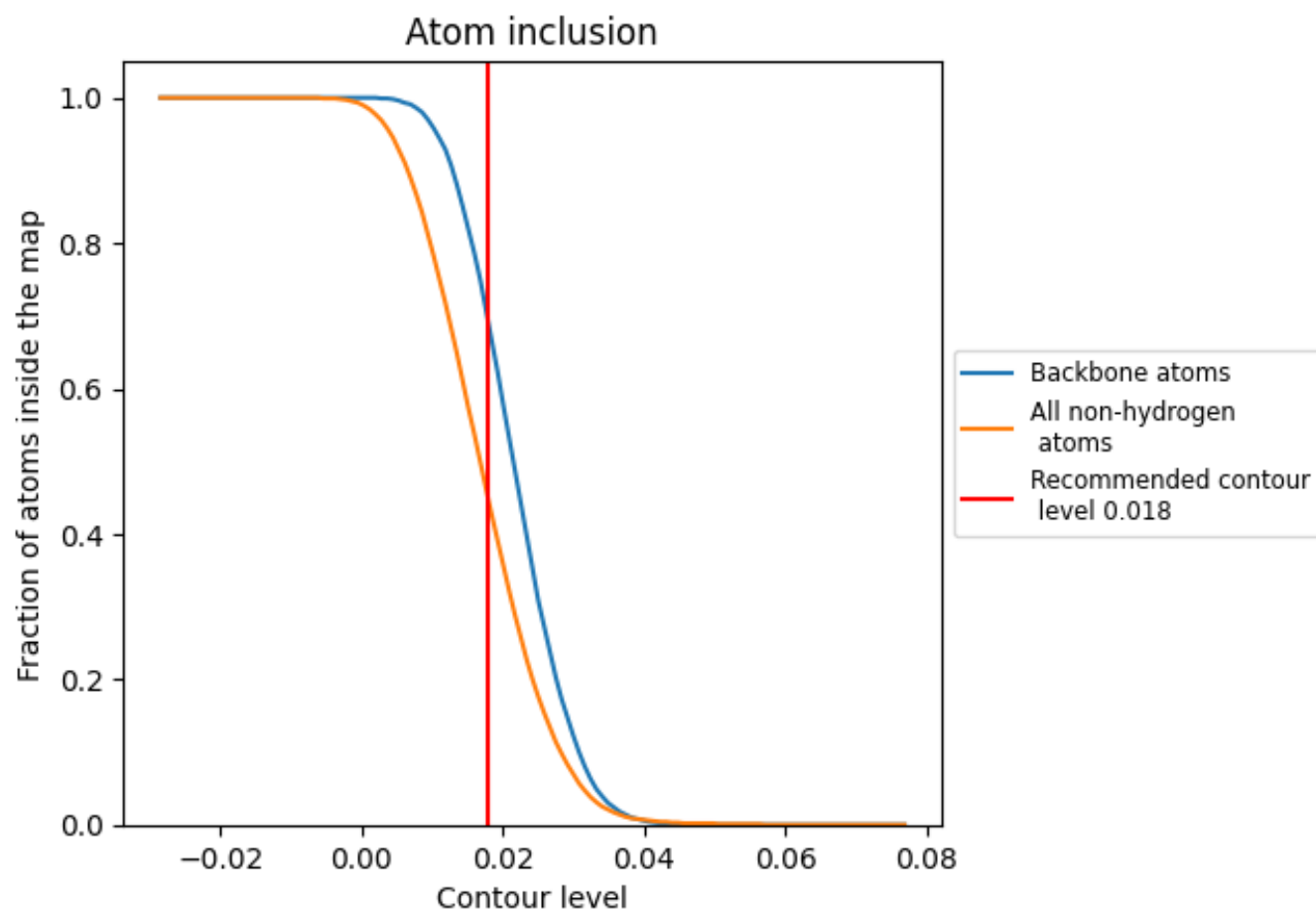
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 44% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4440	<div></div> 0.3780
a	<div></div> 0.5320	<div></div> 0.4210
b	<div></div> 0.5390	<div></div> 0.4010
c	<div></div> 0.3150	<div></div> 0.3070
d	<div></div> 0.5090	<div></div> 0.4190
e	<div></div> 0.5360	<div></div> 0.4060
f	<div></div> 0.3200	<div></div> 0.2990
g	<div></div> 0.4480	<div></div> 0.3670
h	<div></div> 0.3910	<div></div> 0.3430
i	<div></div> 0.4260	<div></div> 0.3910
j	<div></div> 0.2760	<div></div> 0.3450
k	<div></div> 0.4430	<div></div> 0.3680
l	<div></div> 0.3950	<div></div> 0.3370
m	<div></div> 0.3890	<div></div> 0.3850
n	<div></div> 0.2670	<div></div> 0.3390
o	<div></div> 0.3960	<div></div> 0.3840
p	<div></div> 0.3800	<div></div> 0.3950

1.0

0.0

<0.0