



Full wwPDB EM Validation Report ⓘ

Apr 1, 2023 – 08:56 am BST

PDB ID : 8B6J
EMDB ID : EMD-15868
Title : Cryo-EM structure of cytochrome bc1 complex (complex-III) from respiratory supercomplex of *Tetrahymena thermophila*
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2022-09-27
Resolution : 2.80 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:

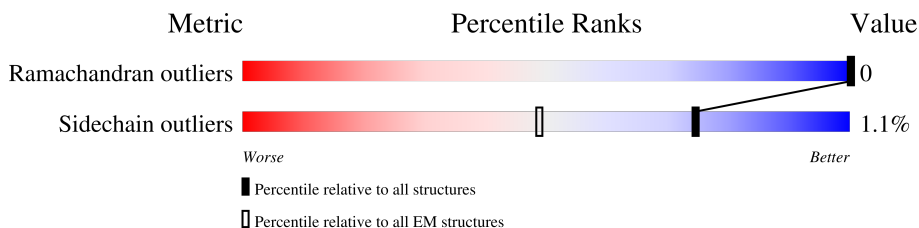
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	513	 93% 6%
1	a	513	 93% 6%
2	B	482	 95% 5%
2	b	482	 94% 5%
3	C	426	 99%
3	c	426	 98%
4	D	319	 92% 8%
4	d	319	 92% 8%
5	E	269	 90% 9%

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Mol	Chain	Length	Quality of chain
5	e	269	47% 90% 9%
6	F	86	23% 100%
6	f	86	22% 98%
7	G	328	13% 99%
7	g	328	16% 98%
8	H	130	5% 98%
8	h	130	17% 98%
9	I	119	24% 96%
9	i	119	14% 97%
10	J	66	74% 100%
10	j	66	71% 100%
11	K	62	8% 94% 6%
11	k	62	11% 94% 6%
12	L	41	76% 22%
12	l	41	10% 78% 22%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 94062 atoms, of which 47043 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 Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	482	Total	C	H	N	O	S	0	0
			7587	2437	3740	671	734	5		
1	a	482	Total	C	H	N	O	S	0	0
			7587	2437	3740	671	734	5		

- Molecule 2 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	460	Total	C	H	N	O	S	0	0
			7118	2240	3555	609	708	6		
2	b	460	Total	C	H	N	O	S	0	0
			7118	2240	3555	609	708	6		

- Molecule 3 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	426	Total	C	H	N	O	S	0	0
			7075	2417	3485	541	610	22		
3	c	426	Total	C	H	N	O	S	0	0
			7074	2417	3484	541	610	22		

- Molecule 4 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	295	Total	C	H	N	O	S	0	0
			4832	1627	2343	418	431	13		
4	d	295	Total	C	H	N	O	S	0	0
			4832	1627	2343	418	431	13		

- Molecule 5 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	245	3893	1251	1927	344	362	9	0	0
5	e	245	3891	1251	1925	344	362	9	0	0

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	86	1372	432	686	116	128	10	0	0
6	f	85	1352	427	674	115	127	9	0	0

- Molecule 7 is a protein called UQCRTT1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	327	5474	1789	2706	482	491	6	0	0
7	g	327	5474	1789	2706	482	491	6	0	0

- Molecule 8 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	129	2138	708	1040	195	187	8	0	0
8	h	129	2138	708	1040	195	187	8	0	0

- Molecule 9 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	117	1998	664	1003	164	166	1	0	0
9	i	117	1998	664	1003	164	166	1	0	0

- Molecule 10 is a protein called UQCRTT3/UP1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
10	J	66	596	198	266	66	66		0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
10	j	66	596	198	266	66	66	0	0

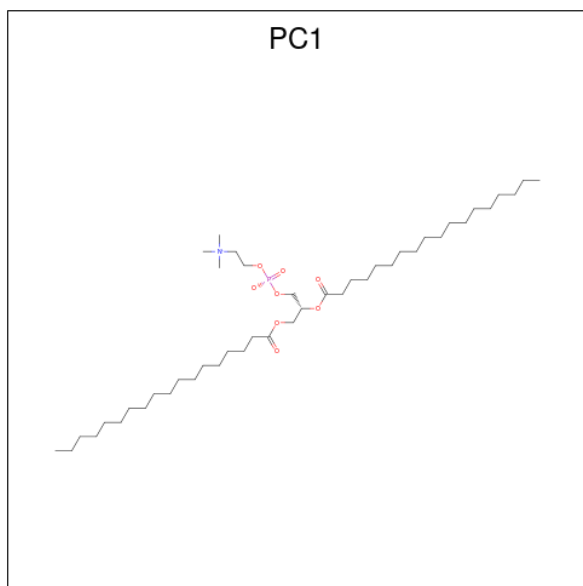
- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	58	1004	341	503	79	79	2	0	0
11	k	58	1004	341	503	79	79	2	0	0

- Molecule 12 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	l	32	535	178	273	41	42	1	0	0
12	L	32	535	178	273	41	42	1	0	0

- Molecule 13 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
13	A	1	142	44	88	1	8	1	0

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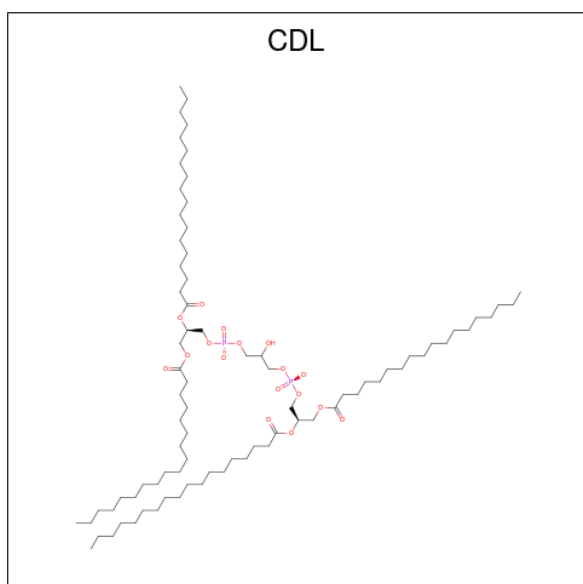
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
13	A	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	E	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	E	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	K	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	d	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	g	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	k	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



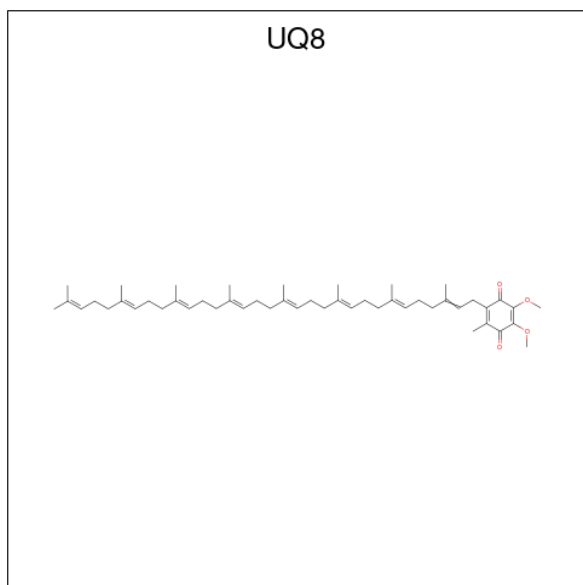
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Fe	H	N		O
14	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
14	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
14	c	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
14	c	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



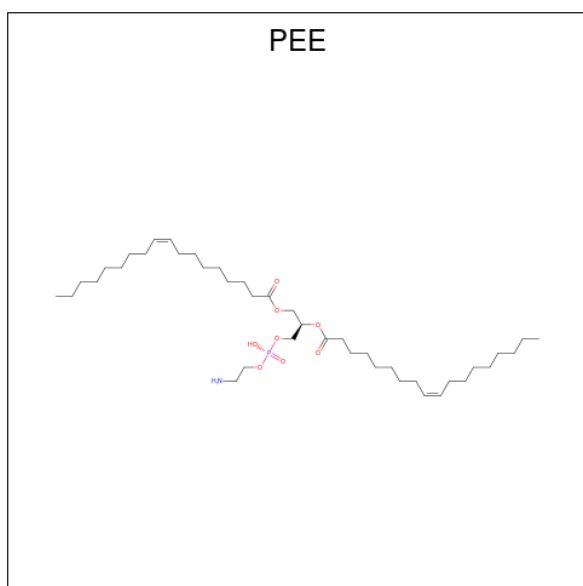
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	D	1	Total 256	C 81	H 156	O 17	P 2	0
15	E	1	Total 256	C 81	H 156	O 17	P 2	0
15	H	1	Total 256	C 81	H 156	O 17	P 2	0
15	H	1	Total 256	C 81	H 156	O 17	P 2	0
15	a	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	g	1	Total 256	C 81	H 156	O 17	P 2	0
15	h	1	Total 256	C 81	H 156	O 17	P 2	0
15	h	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 16 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	C	1	53	49	4	0
16	C	1	53	49	4	0
16	c	1	53	49	4	0

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



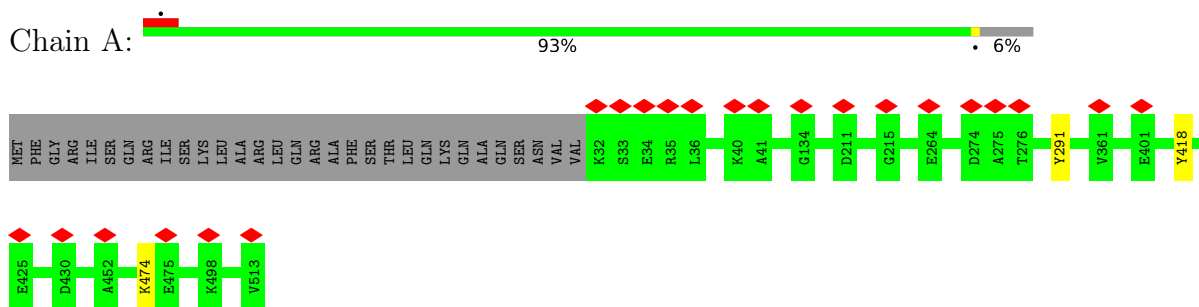


Mol	Chain	Residues	Atoms			AltConf
19	E	1	Total	Fe	S	0
			4	2	2	
19	e	1	Total	Fe	S	0
			4	2	2	

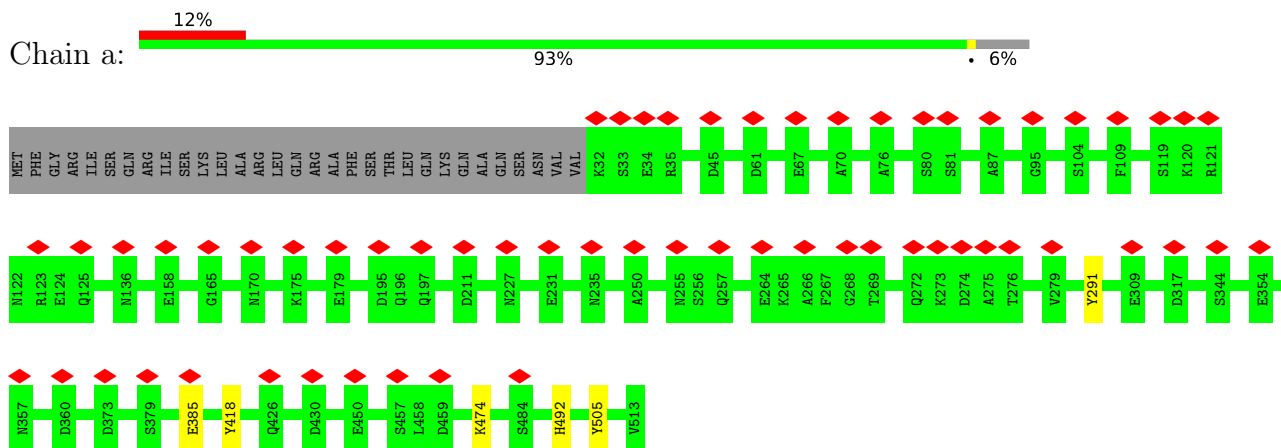
3 Residue-property plots [i](#)

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

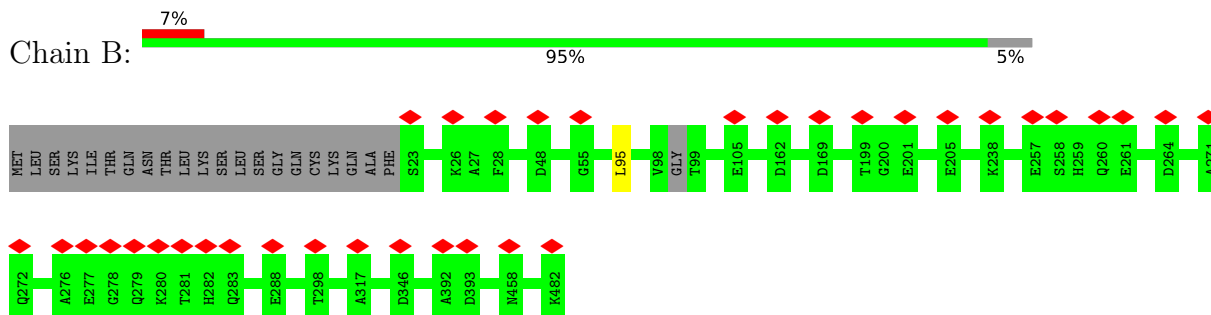
- Molecule 1: Peptidase M16 inactive domain protein



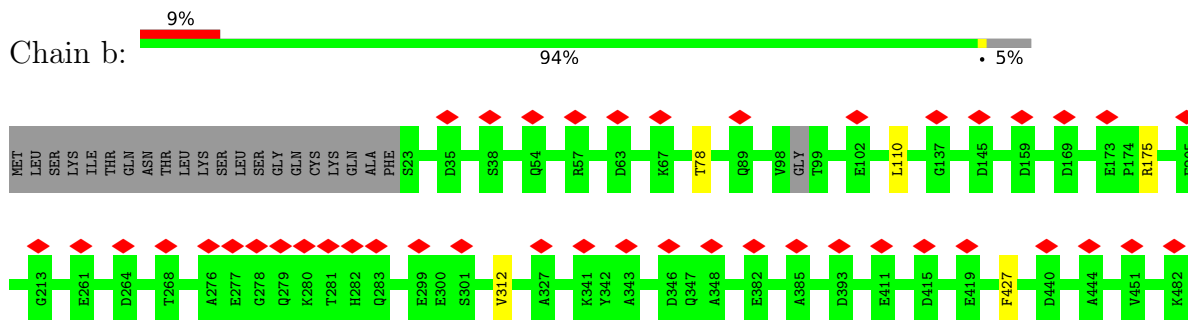
- Molecule 1: Peptidase M16 inactive domain protein



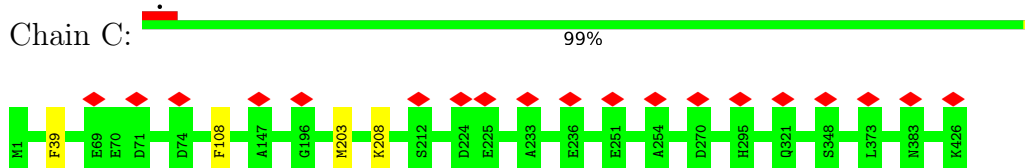
- Molecule 2: M16 family peptidase, putative



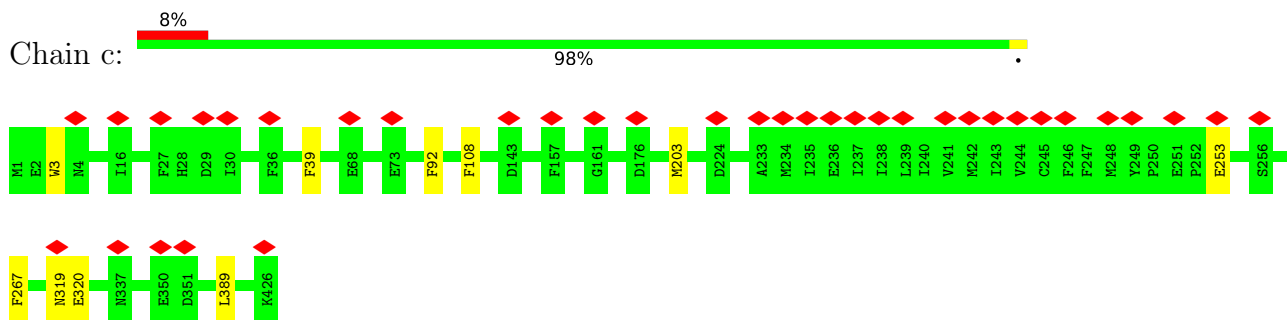
• Molecule 2: M16 family peptidase, putative



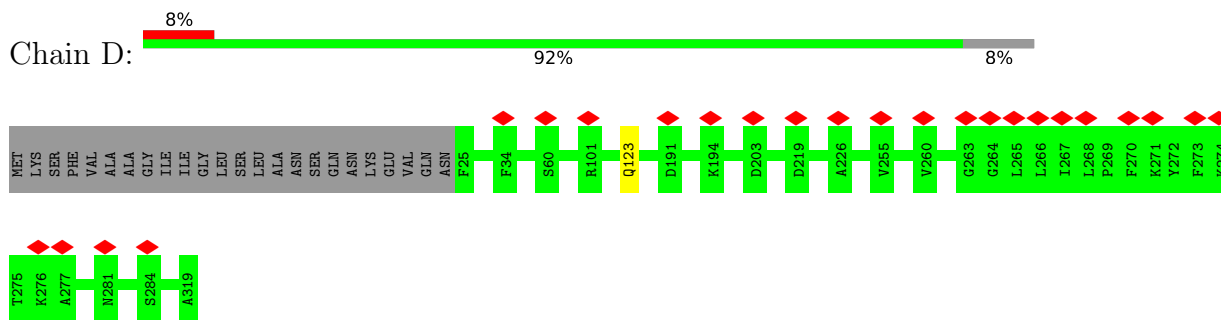
• Molecule 3: Apocytochrome b



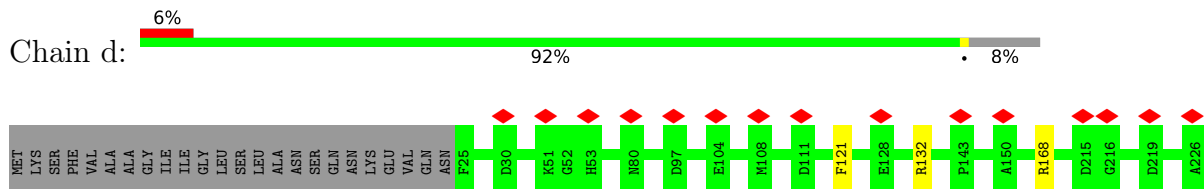
• Molecule 3: Apocytochrome b

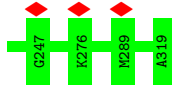


• Molecule 4: Cytochrome protein c1

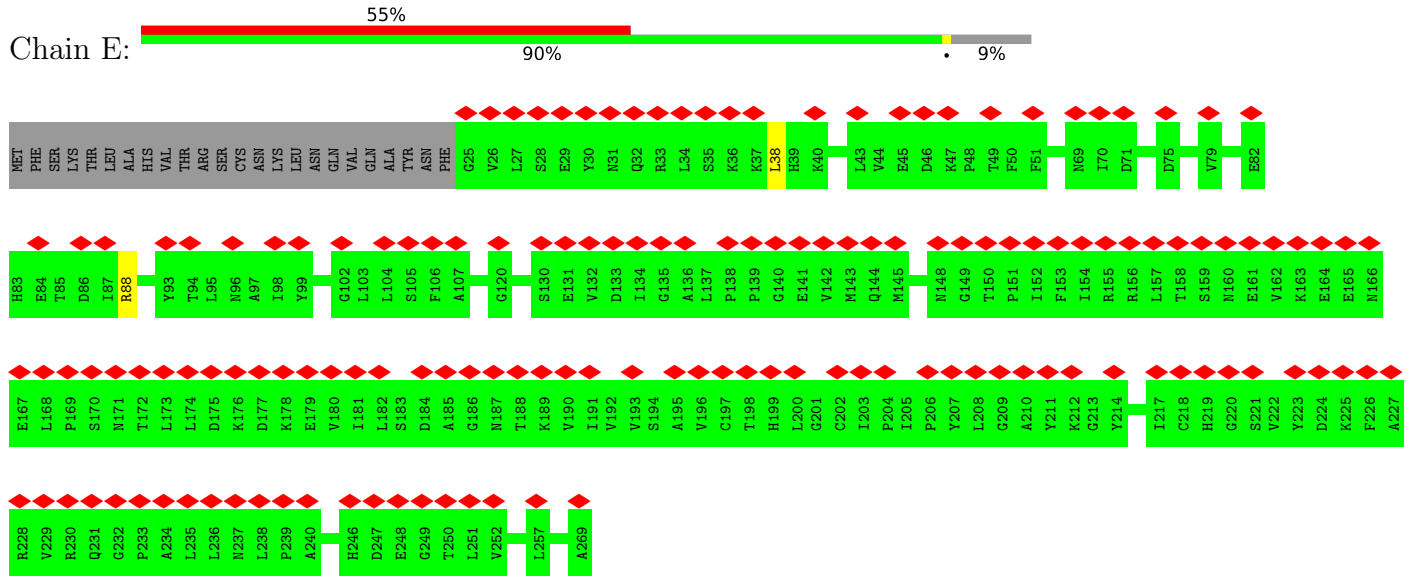


• Molecule 4: Cytochrome protein c1

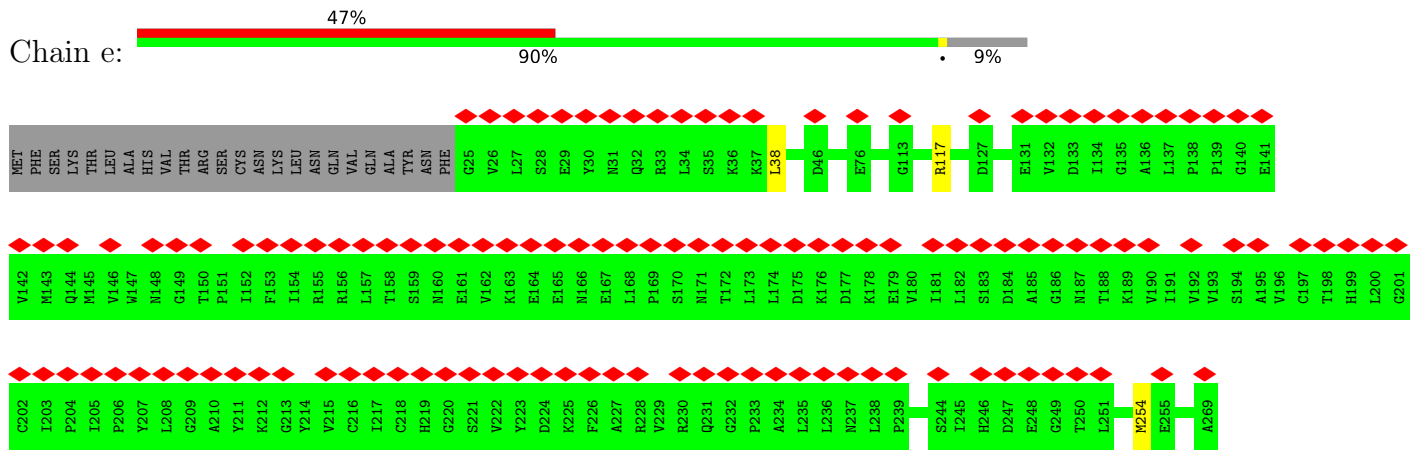




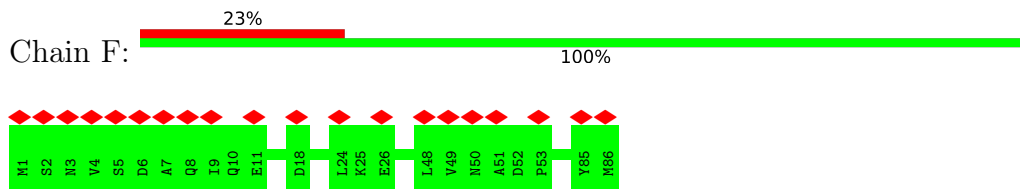
- Molecule 5: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



- Molecule 5: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

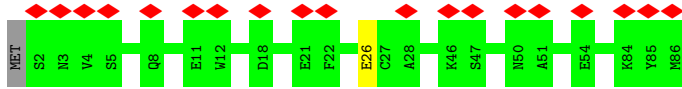


- Molecule 6: Ubiquinol-cytochrome C reductase hinge protein

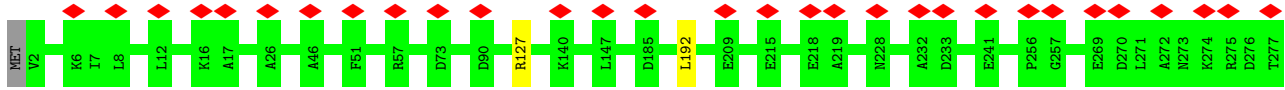


- Molecule 6: Ubiquinol-cytochrome C reductase hinge protein

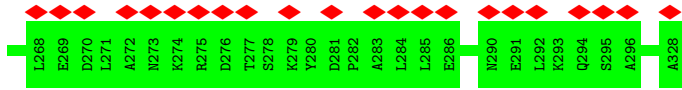
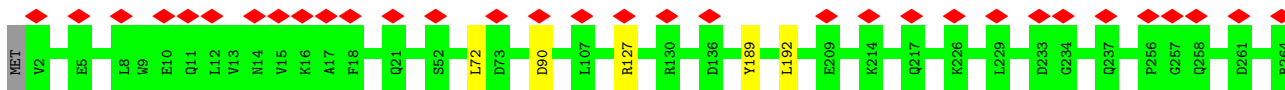




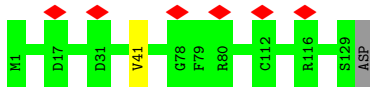
- Molecule 7: UQCRTT1



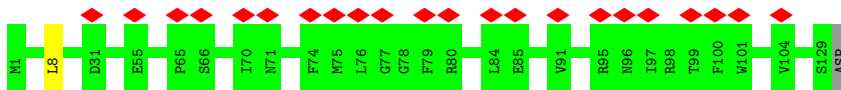
- Molecule 7: UQCRTT1



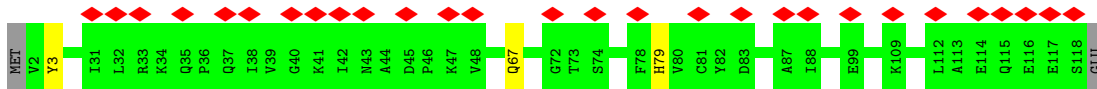
- Molecule 8: Transmembrane protein, putative



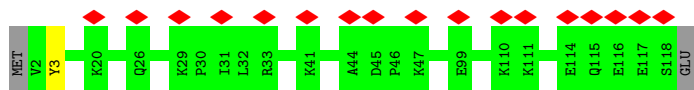
- Molecule 8: Transmembrane protein, putative



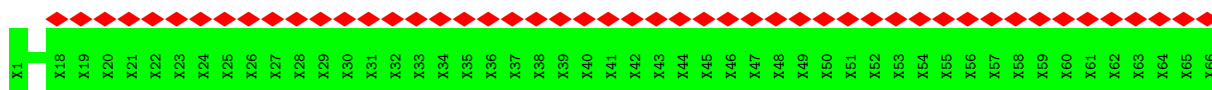
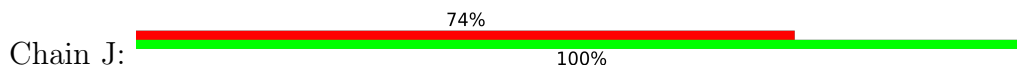
- Molecule 9: Transmembrane protein, putative



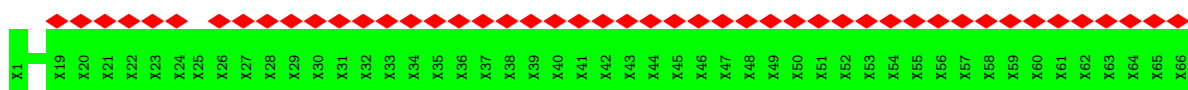
- Molecule 9: Transmembrane protein, putative



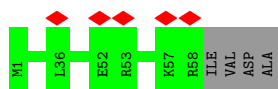
• Molecule 10: UQCRTT3/UP1



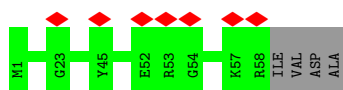
• Molecule 10: UQCRTT3/UP1



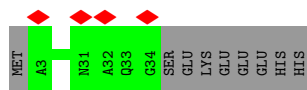
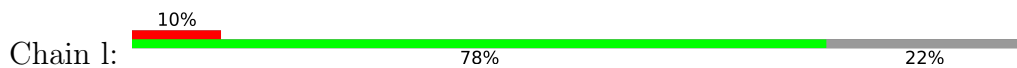
• Molecule 11: Transmembrane protein, putative



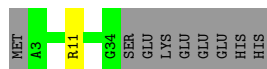
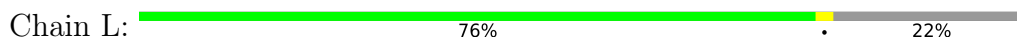
• Molecule 11: Transmembrane protein, putative



• Molecule 12: UQCRTT2



• Molecule 12: UQCRTT2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.090	Depositor
Minimum map value	-2.921	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, FES, HEM, CDL, PEE, PC1, HEC

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	0.25	0/3933	0.49	0/5338
1	a	0.25	0/3933	0.47	0/5338
2	B	0.25	0/3616	0.45	0/4897
2	b	0.24	0/3616	0.44	0/4897
3	C	0.26	0/3716	0.42	0/5046
3	c	0.26	0/3716	0.42	0/5046
4	D	0.27	0/2580	0.47	0/3491
4	d	0.27	0/2580	0.47	0/3491
5	E	0.24	0/2015	0.47	0/2732
5	e	0.24	0/2015	0.47	0/2732
6	F	0.25	0/700	0.45	0/942
6	f	0.25	0/692	0.45	0/932
7	G	0.25	0/2846	0.48	0/3839
7	g	0.25	0/2846	0.48	0/3839
8	H	0.26	0/1133	0.49	0/1524
8	h	0.27	0/1133	0.51	0/1524
9	I	0.25	0/1029	0.40	0/1397
9	i	0.25	0/1029	0.40	0/1397
11	K	0.27	0/522	0.43	0/712
11	k	0.26	0/522	0.43	0/712
12	L	0.27	0/269	0.40	0/366
12	l	0.27	0/269	0.40	0/366
All	All	0.25	0/44710	0.46	0/60558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/513 (94%)	465 (97%)	15 (3%)	0	100	100
1	a	480/513 (94%)	466 (97%)	14 (3%)	0	100	100
2	B	456/482 (95%)	447 (98%)	9 (2%)	0	100	100
2	b	456/482 (95%)	447 (98%)	9 (2%)	0	100	100
3	C	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
3	c	424/426 (100%)	414 (98%)	10 (2%)	0	100	100
4	D	293/319 (92%)	288 (98%)	5 (2%)	0	100	100
4	d	293/319 (92%)	290 (99%)	3 (1%)	0	100	100
5	E	243/269 (90%)	237 (98%)	6 (2%)	0	100	100
5	e	243/269 (90%)	240 (99%)	3 (1%)	0	100	100
6	F	84/86 (98%)	84 (100%)	0	0	100	100
6	f	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
7	G	325/328 (99%)	320 (98%)	5 (2%)	0	100	100
7	g	325/328 (99%)	322 (99%)	3 (1%)	0	100	100
8	H	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	I	115/119 (97%)	115 (100%)	0	0	100	100
9	i	115/119 (97%)	115 (100%)	0	0	100	100
11	K	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
11	k	56/62 (90%)	56 (100%)	0	0	100	100
12	L	30/41 (73%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5265/5550 (95%)	5158 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/440 (93%)	408 (99%)	3 (1%)	84	95
1	a	411/440 (93%)	405 (98%)	6 (2%)	65	89
2	B	389/409 (95%)	388 (100%)	1 (0%)	92	98
2	b	389/409 (95%)	384 (99%)	5 (1%)	69	91
3	C	386/386 (100%)	382 (99%)	4 (1%)	76	93
3	c	386/386 (100%)	376 (97%)	10 (3%)	46	79
4	D	255/274 (93%)	254 (100%)	1 (0%)	91	97
4	d	255/274 (93%)	252 (99%)	3 (1%)	71	92
5	E	215/237 (91%)	213 (99%)	2 (1%)	78	94
5	e	215/237 (91%)	212 (99%)	3 (1%)	67	90
6	F	76/76 (100%)	76 (100%)	0	100	100
6	f	75/76 (99%)	74 (99%)	1 (1%)	69	91
7	G	288/289 (100%)	286 (99%)	2 (1%)	84	95
7	g	288/289 (100%)	283 (98%)	5 (2%)	60	87
8	H	117/118 (99%)	116 (99%)	1 (1%)	78	94
8	h	117/118 (99%)	116 (99%)	1 (1%)	78	94
9	I	107/109 (98%)	104 (97%)	3 (3%)	43	77
9	i	107/109 (98%)	106 (99%)	1 (1%)	78	94
11	K	53/56 (95%)	53 (100%)	0	100	100
11	k	53/56 (95%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	27/36 (75%)	26 (96%)	1 (4%)	34	68
12	l	27/36 (75%)	27 (100%)	0	100	100
All	All	4647/4860 (96%)	4594 (99%)	53 (1%)	74	92

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	TYR
1	A	418	TYR
1	A	474	LYS
2	B	95	LEU
3	C	39	PHE
3	C	108	PHE
3	C	203	MET
3	C	208	LYS
4	D	123	GLN
5	E	38	LEU
5	E	88	ARG
7	G	127	ARG
7	G	192	LEU
8	H	41	VAL
9	I	3	TYR
9	I	67	GLN
9	I	79	HIS
1	a	291	TYR
1	a	385	GLU
1	a	418	TYR
1	a	474	LYS
1	a	492	HIS
1	a	505	TYR
2	b	78	THR
2	b	110	LEU
2	b	175	ARG
2	b	312	VAL
2	b	427	PHE
3	c	3	TRP
3	c	39	PHE
3	c	92	PHE
3	c	108	PHE
3	c	203	MET
3	c	253	GLU

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Mol	Chain	Res	Type
3	c	267	PHE
3	c	319	ASN
3	c	320	GLU
3	c	389	LEU
4	d	121	PHE
4	d	132	ARG
4	d	168	ARG
5	e	38	LEU
5	e	117	ARG
5	e	254	MET
6	f	26	GLU
7	g	72	LEU
7	g	90	ASP
7	g	127	ARG
7	g	189	TYR
7	g	192	LEU
8	h	8	LEU
9	i	3	TYR
12	L	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

43 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	FES	e	301	5	0,4,4	-	-	-		
18	HEC	D	401	4	32,50,50	2.24	3 (9%)	24,82,82	1.41	4 (16%)
13	PC1	A	1202	-	53,53,53	0.29	0	59,61,61	0.28	0
13	PC1	C	509	-	53,53,53	0.28	0	59,61,61	0.27	0
13	PC1	E	303	-	53,53,53	0.28	0	59,61,61	0.26	0
13	PC1	c	506	-	53,53,53	0.28	0	59,61,61	0.28	0
15	CDL	C	505	-	99,99,99	0.29	0	105,111,111	0.26	0
15	CDL	H	1301	-	99,99,99	0.30	0	105,111,111	0.24	0
16	UQ8	c	508	-	53,53,53	0.50	0	64,67,67	0.69	3 (4%)
17	PEE	L	401	-	50,50,50	0.76	2 (4%)	53,55,55	0.45	0
18	HEC	d	802	4	32,50,50	2.23	3 (9%)	24,82,82	1.42	3 (12%)
13	PC1	k	301	-	53,53,53	0.37	0	59,61,61	0.36	0
14	HEM	C	502	3	41,50,50	1.44	3 (7%)	45,82,82	1.25	3 (6%)
15	CDL	H	1302	-	99,99,99	0.30	0	105,111,111	0.26	0
13	PC1	c	505	-	53,53,53	0.28	0	59,61,61	0.27	0
13	PC1	c	504	-	53,53,53	0.29	0	59,61,61	0.26	0
13	PC1	E	302	-	53,53,53	0.28	0	59,61,61	0.26	0
15	CDL	g	801	-	99,99,99	0.30	0	105,111,111	0.25	0
15	CDL	h	402	-	99,99,99	0.30	0	105,111,111	0.24	0
17	PEE	C	512	-	50,50,50	0.76	2 (4%)	53,55,55	0.44	0
13	PC1	c	510	-	53,53,53	0.29	0	59,61,61	0.28	0
15	CDL	c	509	-	99,99,99	0.29	0	105,111,111	0.25	0
15	CDL	C	503	-	99,99,99	0.30	0	105,111,111	0.25	0
13	PC1	C	507	-	53,53,53	0.29	0	59,61,61	0.26	0
13	PC1	d	801	-	53,53,53	0.28	0	59,61,61	0.26	0
13	PC1	K	901	-	53,53,53	0.28	0	59,61,61	0.28	0
16	UQ8	C	511	-	53,53,53	0.51	0	64,67,67	0.67	2 (3%)
15	CDL	E	304	-	99,99,99	0.29	0	105,111,111	0.25	0
14	HEM	C	501	3	41,50,50	1.44	3 (7%)	45,82,82	1.37	5 (11%)
15	CDL	C	504	-	99,99,99	0.30	0	105,111,111	0.25	0
14	HEM	c	501	3	41,50,50	1.45	3 (7%)	45,82,82	1.35	6 (13%)
14	HEM	c	502	3	41,50,50	1.44	3 (7%)	45,82,82	1.31	4 (8%)
13	PC1	A	1201	-	53,53,53	0.28	0	59,61,61	0.26	0
15	CDL	D	402	-	99,99,99	0.30	0	105,111,111	0.24	0
15	CDL	h	401	-	99,99,99	0.30	0	105,111,111	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CDL	c	507	-	99,99,99	0.30	0	105,111,111	0.25	0
15	CDL	a	1201	-	99,99,99	0.30	0	105,111,111	0.24	0
15	CDL	c	503	-	99,99,99	0.30	0	105,111,111	0.25	0
16	UQ8	C	510	-	53,53,53	0.53	0	64,67,67	0.75	3 (4%)
13	PC1	C	508	-	53,53,53	0.28	0	59,61,61	0.28	0
13	PC1	g	802	-	53,53,53	0.29	0	59,61,61	0.25	0
15	CDL	C	506	-	99,99,99	0.29	0	105,111,111	0.25	0
19	FES	E	301	5	0,4,4	-	-	-	-	-

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
19	FES	e	301	5	-	-	0/1/1/1
18	HEC	D	401	4	-	0/10/54/54	-
13	PC1	A	1202	-	-	15/57/57/57	-
13	PC1	C	509	-	-	12/57/57/57	-
13	PC1	E	303	-	-	10/57/57/57	-
13	PC1	c	506	-	-	13/57/57/57	-
15	CDL	C	505	-	-	25/110/110/110	-
15	CDL	H	1301	-	-	24/110/110/110	-
16	UQ8	c	508	-	-	14/51/75/75	0/1/1/1
17	PEE	L	401	-	-	11/54/54/54	-
18	HEC	d	802	4	-	2/10/54/54	-
13	PC1	k	301	-	-	23/57/57/57	-
14	HEM	C	502	3	-	7/12/54/54	-
15	CDL	H	1302	-	-	19/110/110/110	-
13	PC1	c	505	-	-	8/57/57/57	-
13	PC1	c	504	-	-	19/57/57/57	-
13	PC1	E	302	-	-	20/57/57/57	-
15	CDL	g	801	-	-	22/110/110/110	-
15	CDL	h	402	-	-	22/110/110/110	-
17	PEE	C	512	-	-	17/54/54/54	-
13	PC1	c	510	-	-	15/57/57/57	-
15	CDL	c	509	-	-	20/110/110/110	-
15	CDL	C	503	-	-	29/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PC1	C	507	-	-	22/57/57/57	-
13	PC1	d	801	-	-	15/57/57/57	-
13	PC1	K	901	-	-	11/57/57/57	-
16	UQ8	C	511	-	-	7/51/75/75	0/1/1/1
15	CDL	E	304	-	-	27/110/110/110	-
14	HEM	C	501	3	-	5/12/54/54	-
15	CDL	C	504	-	-	30/110/110/110	-
14	HEM	c	501	3	-	0/12/54/54	-
14	HEM	c	502	3	-	0/12/54/54	-
13	PC1	A	1201	-	-	14/57/57/57	-
15	CDL	D	402	-	-	21/110/110/110	-
15	CDL	h	401	-	-	24/110/110/110	-
15	CDL	c	507	-	-	29/110/110/110	-
15	CDL	a	1201	-	-	34/110/110/110	-
15	CDL	c	503	-	-	31/110/110/110	-
16	UQ8	C	510	-	-	16/51/75/75	0/1/1/1
13	PC1	C	508	-	-	25/57/57/57	-
13	PC1	g	802	-	-	13/57/57/57	-
15	CDL	C	506	-	-	25/110/110/110	-
19	FES	E	301	5	-	-	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	C2B-C3B	-6.66	1.33	1.40
18	d	802	HEC	C2B-C3B	-6.65	1.33	1.40
18	D	401	HEC	C3C-C2C	-6.60	1.33	1.40
18	d	802	HEC	C3C-C2C	-6.54	1.33	1.40
18	d	802	HEC	C3D-C2D	5.38	1.53	1.37
18	D	401	HEC	C3D-C2D	5.35	1.53	1.37
14	c	502	HEM	C3C-C2C	-4.39	1.34	1.40
14	c	501	HEM	C3C-C2C	-4.28	1.34	1.40
14	C	501	HEM	C3C-C2C	-4.26	1.34	1.40
14	C	502	HEM	C3C-C2C	-4.07	1.34	1.40
17	C	512	PEE	C18-C19	3.59	1.52	1.31
14	c	501	HEM	C3C-CAC	3.55	1.55	1.47
17	L	401	PEE	C18-C19	3.54	1.52	1.31
17	L	401	PEE	C39-C38	3.53	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	512	PEE	C39-C38	3.53	1.52	1.31
14	C	501	HEM	C3C-CAC	3.48	1.54	1.47
14	C	502	HEM	C3C-CAC	3.47	1.54	1.47
14	c	502	HEM	C3C-CAC	3.19	1.54	1.47
14	C	502	HEM	CAB-C3B	2.88	1.55	1.47
14	c	502	HEM	CAB-C3B	2.88	1.55	1.47
14	C	501	HEM	CAB-C3B	2.85	1.55	1.47
14	c	501	HEM	CAB-C3B	2.85	1.55	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	501	HEM	C4D-ND-C1D	2.89	108.06	105.07
14	c	501	HEM	C4D-ND-C1D	2.87	108.04	105.07
14	C	502	HEM	C1B-NB-C4B	2.85	108.02	105.07
14	c	502	HEM	C1B-NB-C4B	2.85	108.01	105.07
14	C	502	HEM	C4D-ND-C1D	2.84	108.00	105.07
16	c	508	UQ8	C7-C8-C9	2.76	131.39	126.79
14	C	501	HEM	C1B-NB-C4B	2.73	107.90	105.07
16	C	510	UQ8	C7-C8-C9	2.70	131.29	126.79
14	c	502	HEM	C4D-ND-C1D	2.64	107.80	105.07
14	c	501	HEM	C4B-CHC-C1C	2.64	126.04	122.56
14	c	501	HEM	C1B-NB-C4B	2.57	107.73	105.07
16	c	508	UQ8	C8-C7-C6	2.53	118.86	112.05
16	C	510	UQ8	C8-C7-C6	2.51	118.80	112.05
14	C	501	HEM	C4B-CHC-C1C	2.42	125.75	122.56
16	C	510	UQ8	C17-C18-C19	-2.36	121.98	127.66
14	c	501	HEM	CBA-CAA-C2A	-2.33	108.64	112.62
16	C	511	UQ8	C8-C7-C6	2.29	118.22	112.05
14	C	501	HEM	C4C-CHD-C1D	2.28	125.56	122.56
18	d	802	HEC	CBA-CAA-C2A	-2.27	108.79	112.60
18	d	802	HEC	CMC-C2C-C1C	-2.26	124.99	128.46
16	C	511	UQ8	C7-C8-C9	2.20	130.45	126.79
18	D	401	HEC	C1D-C2D-C3D	-2.19	105.47	107.00
14	c	502	HEM	C3B-C2B-C1B	2.19	108.11	106.49
14	c	501	HEM	C4C-CHD-C1D	2.14	125.38	122.56
18	D	401	HEC	CMB-C2B-C1B	-2.14	125.17	128.46
14	C	502	HEM	C3D-C4D-ND	-2.14	107.78	110.17
18	d	802	HEC	C1D-C2D-C3D	-2.09	105.54	107.00
14	C	501	HEM	C3B-C2B-C1B	2.08	108.03	106.49
18	D	401	HEC	CBA-CAA-C2A	-2.07	109.11	112.60
18	D	401	HEC	CBD-CAD-C3D	-2.04	109.14	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	c	501	HEM	CAD-CBD-CGD	-2.02	109.26	113.60
14	c	502	HEM	C3D-C4D-ND	-2.01	107.93	110.17
16	c	508	UQ8	C17-C18-C19	-2.00	122.83	127.66

There are no chirality outliers.

All (696) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1201	PC1	C11-O13-P-O14
13	A	1202	PC1	C11-O13-P-O14
13	A	1202	PC1	C1-O11-P-O14
13	A	1202	PC1	C1-O11-P-O13
13	A	1202	PC1	O13-C11-C12-N
13	C	508	PC1	C11-O13-P-O12
13	C	508	PC1	C11-O13-P-O14
13	C	508	PC1	O13-C11-C12-N
13	C	509	PC1	C11-O13-P-O14
13	E	302	PC1	C11-O13-P-O14
13	E	302	PC1	C1-O11-P-O14
13	E	303	PC1	C22-C21-O21-C2
13	K	901	PC1	C22-C21-O21-C2
13	c	504	PC1	O13-C11-C12-N
13	c	505	PC1	C22-C21-O21-C2
13	c	506	PC1	C11-O13-P-O14
13	c	510	PC1	O22-C21-O21-C2
13	c	510	PC1	C22-C21-O21-C2
13	d	801	PC1	C1-O11-P-O14
13	g	802	PC1	C11-O13-P-O12
13	g	802	PC1	C22-C21-O21-C2
13	k	301	PC1	C11-O13-P-O11
13	k	301	PC1	O13-C11-C12-N
13	k	301	PC1	O22-C21-O21-C2
14	C	501	HEM	C1A-C2A-CAA-CBA
14	C	501	HEM	C3A-C2A-CAA-CBA
15	C	503	CDL	CA3-OA5-PA1-OA3
15	C	503	CDL	CA3-OA5-PA1-OA4
15	C	503	CDL	CB2-OB2-PB2-OB3
15	C	503	CDL	CB2-OB2-PB2-OB5
15	C	503	CDL	CB3-OB5-PB2-OB3
15	C	504	CDL	CA3-OA5-PA1-OA3
15	C	505	CDL	CA3-OA5-PA1-OA3
15	C	505	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
15	C	505	CDL	CB3-OB5-PB2-OB3
15	C	505	CDL	CB3-OB5-PB2-OB4
15	C	505	CDL	C51-CB5-OB6-CB4
15	C	506	CDL	OA7-CA5-OA6-CA4
15	C	506	CDL	CB3-OB5-PB2-OB3
15	D	402	CDL	CA2-OA2-PA1-OA3
15	D	402	CDL	CA3-OA5-PA1-OA3
15	E	304	CDL	CA2-OA2-PA1-OA3
15	E	304	CDL	CA3-OA5-PA1-OA3
15	E	304	CDL	C11-CA5-OA6-CA4
15	E	304	CDL	CB2-OB2-PB2-OB3
15	E	304	CDL	CB2-OB2-PB2-OB4
15	E	304	CDL	CB2-OB2-PB2-OB5
15	H	1301	CDL	C11-CA5-OA6-CA4
15	H	1301	CDL	CB3-OB5-PB2-OB3
15	H	1301	CDL	CB3-OB5-PB2-OB4
15	H	1302	CDL	CA2-C1-CB2-OB2
15	H	1302	CDL	CA2-OA2-PA1-OA3
15	H	1302	CDL	CA2-OA2-PA1-OA4
15	H	1302	CDL	C11-CA5-OA6-CA4
15	a	1201	CDL	CA2-OA2-PA1-OA3
15	a	1201	CDL	CA3-OA5-PA1-OA4
15	a	1201	CDL	OA7-CA5-OA6-CA4
15	a	1201	CDL	C11-CA5-OA6-CA4
15	c	503	CDL	CA2-C1-CB2-OB2
15	c	503	CDL	CA2-OA2-PA1-OA3
15	c	503	CDL	C11-CA5-OA6-CA4
15	c	507	CDL	CB2-C1-CA2-OA2
15	c	507	CDL	CA2-OA2-PA1-OA5
15	c	507	CDL	C1-CB2-OB2-PB2
15	c	507	CDL	CB3-OB5-PB2-OB3
15	c	509	CDL	CA3-OA5-PA1-OA2
15	c	509	CDL	CA3-OA5-PA1-OA3
15	c	509	CDL	CA3-OA5-PA1-OA4
15	c	509	CDL	C11-CA5-OA6-CA4
15	g	801	CDL	CA3-OA5-PA1-OA3
15	g	801	CDL	CA3-OA5-PA1-OA4
15	g	801	CDL	OB6-CB4-CB6-OB8
15	g	801	CDL	C51-CB5-OB6-CB4
15	h	402	CDL	CB2-OB2-PB2-OB3
15	h	402	CDL	C51-CB5-OB6-CB4
16	C	510	UQ8	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
16	C	510	UQ8	C38-C39-C41-C42
16	C	510	UQ8	C30-C29-C31-C32
16	C	510	UQ8	C28-C29-C31-C32
16	C	511	UQ8	C20-C19-C21-C22
16	C	511	UQ8	C9-C11-C12-C13
16	c	508	UQ8	C1-C6-C7-C8
16	c	508	UQ8	C5-C6-C7-C8
17	C	512	PEE	C4-O4P-P-O2P
17	C	512	PEE	C4-O4P-P-O1P
17	L	401	PEE	C1-O3P-P-O1P
17	L	401	PEE	C1-O3P-P-O4P
17	L	401	PEE	C4-O4P-P-O3P
17	L	401	PEE	C4-O4P-P-O2P
13	c	505	PC1	O32-C31-O31-C3
13	c	506	PC1	O32-C31-O31-C3
15	C	505	CDL	OA9-CA7-OA8-CA6
15	g	801	CDL	OA9-CA7-OA8-CA6
17	C	512	PEE	O5-C30-O3-C3
13	c	506	PC1	C32-C31-O31-C3
15	H	1301	CDL	C71-CB7-OB8-CB6
13	E	302	PC1	O32-C31-O31-C3
13	c	510	PC1	O32-C31-O31-C3
15	H	1301	CDL	OB9-CB7-OB8-CB6
15	H	1302	CDL	OA9-CA7-OA8-CA6
13	E	303	PC1	O22-C21-O21-C2
13	K	901	PC1	O22-C21-O21-C2
13	c	505	PC1	O22-C21-O21-C2
15	C	505	CDL	OB7-CB5-OB6-CB4
15	E	304	CDL	OA7-CA5-OA6-CA4
15	H	1301	CDL	OA7-CA5-OA6-CA4
15	H	1302	CDL	OA7-CA5-OA6-CA4
15	c	503	CDL	OA7-CA5-OA6-CA4
15	g	801	CDL	OB7-CB5-OB6-CB4
15	h	402	CDL	OB7-CB5-OB6-CB4
13	E	303	PC1	C32-C31-O31-C3
13	c	504	PC1	C32-C31-O31-C3
13	c	505	PC1	C32-C31-O31-C3
15	C	505	CDL	C31-CA7-OA8-CA6
15	H	1302	CDL	C31-CA7-OA8-CA6
15	g	801	CDL	C31-CA7-OA8-CA6
17	C	512	PEE	C31-C30-O3-C3
13	k	301	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
15	C	506	CDL	C11-CA5-OA6-CA4
15	a	1201	CDL	C51-CB5-OB6-CB4
16	C	510	UQ8	C25-C24-C26-C27
16	C	510	UQ8	C23-C24-C26-C27
16	C	511	UQ8	C18-C19-C21-C22
13	E	302	PC1	C32-C31-O31-C3
13	c	510	PC1	C32-C31-O31-C3
15	c	507	CDL	C71-CB7-OB8-CB6
17	C	512	PEE	C17-C18-C19-C20
17	C	512	PEE	C37-C38-C39-C40
13	g	802	PC1	O22-C21-O21-C2
15	a	1201	CDL	OB7-CB5-OB6-CB4
15	c	509	CDL	OA7-CA5-OA6-CA4
13	E	303	PC1	O32-C31-O31-C3
13	c	504	PC1	O32-C31-O31-C3
15	c	507	CDL	OB9-CB7-OB8-CB6
15	C	503	CDL	O1-C1-CA2-OA2
15	C	504	CDL	O1-C1-CA2-OA2
15	H	1302	CDL	O1-C1-CB2-OB2
15	a	1201	CDL	O1-C1-CA2-OA2
15	c	507	CDL	O1-C1-CA2-OA2
15	c	509	CDL	O1-C1-CA2-OA2
15	h	401	CDL	O1-C1-CA2-OA2
13	K	901	PC1	C32-C31-O31-C3
15	C	503	CDL	C31-CA7-OA8-CA6
15	E	304	CDL	C31-CA7-OA8-CA6
15	g	801	CDL	C71-CB7-OB8-CB6
15	g	801	CDL	OB9-CB7-OB8-CB6
13	A	1201	PC1	C22-C21-O21-C2
13	C	508	PC1	C22-C21-O21-C2
15	C	505	CDL	C11-CA5-OA6-CA4
13	C	508	PC1	O22-C21-O21-C2
15	C	503	CDL	OA9-CA7-OA8-CA6
16	C	510	UQ8	C20-C19-C21-C22
16	C	510	UQ8	C18-C19-C21-C22
13	K	901	PC1	O32-C31-O31-C3
16	C	510	UQ8	C34-C36-C37-C38
16	C	510	UQ8	C9-C11-C12-C13
16	c	508	UQ8	C9-C11-C12-C13
15	c	509	CDL	C31-CA7-OA8-CA6
15	c	509	CDL	C71-CB7-OB8-CB6
15	E	304	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
13	k	301	PC1	C29-C2A-C2B-C2C
13	A	1201	PC1	O22-C21-O21-C2
15	C	506	CDL	C71-CB7-OB8-CB6
15	a	1201	CDL	C31-CA7-OA8-CA6
15	a	1201	CDL	C71-CB7-OB8-CB6
15	c	503	CDL	C31-CA7-OA8-CA6
15	h	402	CDL	C71-CB7-OB8-CB6
17	L	401	PEE	C31-C30-O3-C3
13	d	801	PC1	C3E-C3F-C3G-C3H
15	C	506	CDL	O1-C1-CB2-OB2
17	L	401	PEE	O5-C30-O3-C3
15	C	506	CDL	CB5-C51-C52-C53
15	D	402	CDL	CA5-C11-C12-C13
15	C	505	CDL	OA7-CA5-OA6-CA4
15	h	402	CDL	CA5-C11-C12-C13
14	C	502	HEM	C3D-CAD-CBD-CGD
15	a	1201	CDL	OA9-CA7-OA8-CA6
15	a	1201	CDL	OB9-CB7-OB8-CB6
15	h	402	CDL	OB9-CB7-OB8-CB6
15	C	506	CDL	OB9-CB7-OB8-CB6
16	C	511	UQ8	C24-C26-C27-C28
15	C	504	CDL	O1-C1-CB2-OB2
15	c	503	CDL	O1-C1-CB2-OB2
15	c	503	CDL	OA9-CA7-OA8-CA6
15	c	509	CDL	OA9-CA7-OA8-CA6
15	c	509	CDL	OB9-CB7-OB8-CB6
13	E	302	PC1	C22-C21-O21-C2
15	h	401	CDL	C11-CA5-OA6-CA4
13	A	1202	PC1	C11-O13-P-O11
13	C	507	PC1	C11-O13-P-O11
13	C	507	PC1	C1-O11-P-O13
13	C	508	PC1	C11-O13-P-O11
13	C	509	PC1	C11-O13-P-O11
13	K	901	PC1	C11-O13-P-O11
13	c	505	PC1	C11-O13-P-O11
13	g	802	PC1	C11-O13-P-O11
15	C	503	CDL	CA3-OA5-PA1-OA2
15	D	402	CDL	CA3-OA5-PA1-OA2
15	D	402	CDL	CB2-OB2-PB2-OB5
15	H	1301	CDL	CB2-OB2-PB2-OB5
15	H	1301	CDL	CB3-OB5-PB2-OB2
15	H	1302	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	H	1302	CDL	CA3-OA5-PA1-OA2
15	a	1201	CDL	CA3-OA5-PA1-OA2
15	c	503	CDL	CA3-OA5-PA1-OA2
15	g	801	CDL	CA3-OA5-PA1-OA2
15	h	402	CDL	CA2-OA2-PA1-OA5
15	h	402	CDL	CB2-OB2-PB2-OB5
17	C	512	PEE	C4-O4P-P-O3P
13	k	301	PC1	C33-C34-C35-C36
13	d	801	PC1	C32-C31-O31-C3
15	C	504	CDL	CA2-C1-CB2-OB2
15	c	509	CDL	CB2-C1-CA2-OA2
13	E	302	PC1	O22-C21-O21-C2
15	h	401	CDL	OA7-CA5-OA6-CA4
15	a	1201	CDL	C23-C24-C25-C26
15	g	801	CDL	C11-CA5-OA6-CA4
15	h	402	CDL	C11-CA5-OA6-CA4
13	c	505	PC1	C24-C25-C26-C27
13	k	301	PC1	C2E-C2F-C2G-C2H
15	a	1201	CDL	C21-C22-C23-C24
13	E	302	PC1	C39-C3A-C3B-C3C
15	h	402	CDL	C14-C15-C16-C17
15	H	1302	CDL	CA6-CA4-OA6-CA5
15	h	402	CDL	CB3-CB4-OB6-CB5
15	g	801	CDL	OA7-CA5-OA6-CA4
15	h	402	CDL	OA7-CA5-OA6-CA4
13	C	507	PC1	C2B-C2C-C2D-C2E
13	c	504	PC1	C24-C25-C26-C27
15	C	504	CDL	C53-C54-C55-C56
15	C	504	CDL	C1-CB2-OB2-PB2
13	A	1201	PC1	C36-C37-C38-C39
15	C	503	CDL	C81-C82-C83-C84
15	c	507	CDL	C12-C13-C14-C15
15	C	504	CDL	CA5-C11-C12-C13
17	C	512	PEE	O2-C2-C3-O3
13	k	301	PC1	C22-C23-C24-C25
15	C	504	CDL	C55-C56-C57-C58
15	c	503	CDL	C36-C37-C38-C39
13	C	508	PC1	C35-C36-C37-C38
15	C	503	CDL	C11-CA5-OA6-CA4
15	C	503	CDL	C41-C42-C43-C44
13	k	301	PC1	C27-C28-C29-C2A
15	h	401	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	d	801	PC1	O32-C31-O31-C3
15	E	304	CDL	C36-C37-C38-C39
13	k	301	PC1	C35-C36-C37-C38
15	C	503	CDL	OA7-CA5-OA6-CA4
15	H	1301	CDL	C33-C34-C35-C36
15	c	509	CDL	C51-CB5-OB6-CB4
15	E	304	CDL	CA5-C11-C12-C13
15	g	801	CDL	C79-C80-C81-C82
15	a	1201	CDL	O1-C1-CB2-OB2
13	c	506	PC1	C25-C26-C27-C28
15	c	509	CDL	C13-C14-C15-C16
15	C	503	CDL	CB2-C1-CA2-OA2
15	a	1201	CDL	CA2-C1-CB2-OB2
15	c	509	CDL	OB7-CB5-OB6-CB4
13	E	302	PC1	C3C-C3D-C3E-C3F
15	C	506	CDL	C22-C23-C24-C25
15	C	504	CDL	CA7-C31-C32-C33
13	C	507	PC1	C3D-C3E-C3F-C3G
13	c	504	PC1	C28-C29-C2A-C2B
15	C	505	CDL	C71-C72-C73-C74
15	c	507	CDL	C75-C76-C77-C78
13	E	302	PC1	C25-C26-C27-C28
13	c	504	PC1	C3C-C3D-C3E-C3F
13	A	1201	PC1	C3B-C3C-C3D-C3E
16	c	508	UQ8	C3-C4-O4-C4M
15	D	402	CDL	OB7-CB5-OB6-CB4
17	C	512	PEE	O4-C10-O2-C2
15	C	506	CDL	C17-C18-C19-C20
15	h	402	CDL	C71-C72-C73-C74
13	k	301	PC1	C3D-C3E-C3F-C3G
15	C	503	CDL	C32-C33-C34-C35
15	h	401	CDL	C73-C74-C75-C76
15	C	505	CDL	C20-C21-C22-C23
13	E	303	PC1	C3C-C3D-C3E-C3F
13	k	301	PC1	C3A-C3B-C3C-C3D
15	D	402	CDL	C51-CB5-OB6-CB4
17	C	512	PEE	C11-C10-O2-C2
15	g	801	CDL	C11-C12-C13-C14
15	h	401	CDL	C57-C58-C59-C60
15	c	507	CDL	CA5-C11-C12-C13
13	C	508	PC1	O21-C2-C3-O31
15	D	402	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
13	d	801	PC1	C25-C26-C27-C28
15	H	1301	CDL	C80-C81-C82-C83
13	E	303	PC1	C33-C34-C35-C36
13	c	504	PC1	C2E-C2F-C2G-C2H
13	k	301	PC1	C36-C37-C38-C39
15	c	503	CDL	C13-C14-C15-C16
14	C	502	HEM	C4D-C3D-CAD-CBD
15	c	509	CDL	C12-C13-C14-C15
13	E	302	PC1	C11-O13-P-O11
13	c	506	PC1	C11-O13-P-O11
13	d	801	PC1	C1-O11-P-O13
15	C	505	CDL	CA3-OA5-PA1-OA2
15	E	304	CDL	CA2-OA2-PA1-OA5
13	K	901	PC1	C3D-C3E-C3F-C3G
15	E	304	CDL	C83-C84-C85-C86
15	c	507	CDL	C43-C44-C45-C46
15	H	1302	CDL	CA5-C11-C12-C13
15	C	503	CDL	C79-C80-C81-C82
13	C	508	PC1	O11-C1-C2-C3
13	E	302	PC1	O11-C1-C2-C3
15	H	1302	CDL	C59-C60-C61-C62
13	C	507	PC1	C38-C39-C3A-C3B
15	C	504	CDL	CB2-C1-CA2-OA2
15	g	801	CDL	CA2-C1-CB2-OB2
16	c	508	UQ8	C28-C29-C31-C32
13	E	302	PC1	C2B-C2C-C2D-C2E
13	k	301	PC1	C2C-C2D-C2E-C2F
15	c	503	CDL	C56-C57-C58-C59
13	A	1202	PC1	C1-C2-C3-O31
13	E	302	PC1	C1-C2-C3-O31
13	g	802	PC1	C1-C2-C3-O31
15	g	801	CDL	CB3-CB4-CB6-OB8
17	C	512	PEE	C1-C2-C3-O3
17	C	512	PEE	C32-C33-C34-C35
15	E	304	CDL	C12-C13-C14-C15
13	C	509	PC1	C28-C29-C2A-C2B
15	D	402	CDL	C14-C15-C16-C17
13	C	508	PC1	C2E-C2F-C2G-C2H
15	a	1201	CDL	C75-C76-C77-C78
16	c	508	UQ8	C30-C29-C31-C32
15	C	503	CDL	CA5-C11-C12-C13
14	C	502	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
13	A	1201	PC1	C3-C2-O21-C21
13	k	301	PC1	C3-C2-O21-C21
15	c	509	CDL	CA6-CA4-OA6-CA5
15	c	509	CDL	CB6-CB4-OB6-CB5
13	C	508	PC1	C3E-C3F-C3G-C3H
13	c	510	PC1	C3D-C3E-C3F-C3G
15	a	1201	CDL	C11-C12-C13-C14
15	c	507	CDL	C31-CA7-OA8-CA6
13	A	1202	PC1	O11-C1-C2-O21
13	c	510	PC1	O11-C1-C2-O21
15	C	504	CDL	OA5-CA3-CA4-OA6
15	a	1201	CDL	OB5-CB3-CB4-OB6
13	c	504	PC1	C39-C3A-C3B-C3C
15	a	1201	CDL	C72-C73-C74-C75
13	E	302	PC1	C3F-C3G-C3H-C3I
15	h	401	CDL	O1-C1-CB2-OB2
13	c	504	PC1	O21-C21-C22-C23
15	c	507	CDL	OB6-CB4-CB6-OB8
15	h	401	CDL	OB6-CB4-CB6-OB8
15	c	507	CDL	C41-C42-C43-C44
15	c	503	CDL	C20-C21-C22-C23
13	c	510	PC1	C3C-C3D-C3E-C3F
15	C	506	CDL	CA2-C1-CB2-OB2
15	c	503	CDL	C51-CB5-OB6-CB4
13	A	1201	PC1	C32-C31-O31-C3
13	C	507	PC1	C32-C31-O31-C3
15	h	401	CDL	C31-CA7-OA8-CA6
15	c	503	CDL	C60-C61-C62-C63
15	D	402	CDL	OB5-CB3-CB4-CB6
15	h	401	CDL	OA5-CA3-CA4-CA6
15	C	504	CDL	C43-C44-C45-C46
15	c	507	CDL	C11-C12-C13-C14
13	C	507	PC1	C26-C27-C28-C29
15	C	504	CDL	C41-C42-C43-C44
13	C	507	PC1	C1-C2-C3-O31
13	C	508	PC1	C1-C2-C3-O31
13	c	506	PC1	C1-C2-C3-O31
13	d	801	PC1	C1-C2-C3-O31
15	C	504	CDL	CB3-CB4-CB6-OB8
15	D	402	CDL	CA3-CA4-CA6-OA8
15	c	507	CDL	CA3-CA4-CA6-OA8
15	c	503	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
13	k	301	PC1	C3E-C3F-C3G-C3H
13	c	504	PC1	C22-C21-O21-C2
13	k	301	PC1	C23-C24-C25-C26
15	C	504	CDL	CA3-OA5-PA1-OA2
15	E	304	CDL	CB3-OB5-PB2-OB2
15	h	401	CDL	CB2-OB2-PB2-OB5
13	c	504	PC1	O11-C1-C2-O21
15	D	402	CDL	OB5-CB3-CB4-OB6
15	c	507	CDL	OA9-CA7-OA8-CA6
15	C	504	CDL	C24-C25-C26-C27
13	A	1202	PC1	O21-C2-C3-O31
13	C	507	PC1	O21-C2-C3-O31
13	E	302	PC1	O21-C2-C3-O31
15	c	507	CDL	OA6-CA4-CA6-OA8
13	C	508	PC1	C2-C1-O11-P
15	c	503	CDL	CB4-CB3-OB5-PB2
15	c	509	CDL	CB4-CB3-OB5-PB2
15	H	1301	CDL	C38-C39-C40-C41
13	A	1201	PC1	C3C-C3D-C3E-C3F
13	c	506	PC1	C22-C21-O21-C2
13	d	801	PC1	C22-C21-O21-C2
13	c	504	PC1	O11-C1-C2-C3
15	a	1201	CDL	OB5-CB3-CB4-CB6
15	a	1201	CDL	C76-C77-C78-C79
13	A	1201	PC1	O32-C31-O31-C3
15	c	503	CDL	OB7-CB5-OB6-CB4
15	C	504	CDL	C71-CB7-OB8-CB6
15	h	401	CDL	OA9-CA7-OA8-CA6
15	C	503	CDL	C71-CB7-OB8-CB6
15	h	401	CDL	C71-CB7-OB8-CB6
14	C	501	HEM	C2A-CAA-CBA-CGA
13	C	507	PC1	O32-C31-O31-C3
16	c	508	UQ8	C19-C21-C22-C23
13	A	1201	PC1	C2-C1-O11-P
13	C	509	PC1	C1-C2-C3-O31
15	h	401	CDL	CA3-CA4-CA6-OA8
15	h	401	CDL	OA5-CA3-CA4-OA6
15	c	507	CDL	C32-C31-CA7-OA8
15	c	503	CDL	C21-C22-C23-C24
13	c	504	PC1	O22-C21-O21-C2
13	c	506	PC1	O22-C21-O21-C2
13	c	506	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
13	g	802	PC1	O21-C2-C3-O31
15	C	504	CDL	OB6-CB4-CB6-OB8
15	c	503	CDL	OA6-CA4-CA6-OA8
15	h	401	CDL	OA6-CA4-CA6-OA8
15	h	402	CDL	OA6-CA4-CA6-OA8
13	A	1202	PC1	C22-C23-C24-C25
15	C	503	CDL	OB9-CB7-OB8-CB6
15	C	503	CDL	C73-C74-C75-C76
13	d	801	PC1	O22-C21-O21-C2
15	C	504	CDL	OB9-CB7-OB8-CB6
15	h	401	CDL	OB9-CB7-OB8-CB6
15	h	401	CDL	CA5-C11-C12-C13
15	a	1201	CDL	C38-C39-C40-C41
13	A	1201	PC1	C11-O13-P-O11
15	C	503	CDL	CB3-OB5-PB2-OB2
15	C	505	CDL	CA2-OA2-PA1-OA5
15	D	402	CDL	CA2-OA2-PA1-OA5
15	E	304	CDL	CA3-OA5-PA1-OA2
15	c	507	CDL	CB3-OB5-PB2-OB2
13	C	507	PC1	C2-C1-O11-P
15	C	503	CDL	C1-CA2-OA2-PA1
15	C	505	CDL	C1-CB2-OB2-PB2
13	A	1202	PC1	C11-O13-P-O12
13	C	507	PC1	C11-O13-P-O14
13	C	507	PC1	C1-O11-P-O14
13	C	509	PC1	C11-O13-P-O12
13	K	901	PC1	C11-O13-P-O14
13	c	505	PC1	C11-O13-P-O14
13	d	801	PC1	C1-O11-P-O12
13	k	301	PC1	C11-O13-P-O12
15	C	504	CDL	CA3-OA5-PA1-OA4
15	C	505	CDL	CA3-OA5-PA1-OA4
15	D	402	CDL	CA3-OA5-PA1-OA4
15	D	402	CDL	CB2-OB2-PB2-OB3
15	E	304	CDL	CA2-OA2-PA1-OA4
15	H	1301	CDL	CB2-OB2-PB2-OB3
15	H	1301	CDL	CB2-OB2-PB2-OB4
15	H	1302	CDL	CA3-OA5-PA1-OA3
15	c	503	CDL	CA3-OA5-PA1-OA3
15	c	503	CDL	CA3-OA5-PA1-OA4
15	c	507	CDL	CA2-OA2-PA1-OA4
15	h	402	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
15	h	402	CDL	CB2-OB2-PB2-OB4
17	L	401	PEE	C4-O4P-P-O1P
13	A	1202	PC1	O11-C1-C2-C3
15	C	504	CDL	OA5-CA3-CA4-CA6
15	C	506	CDL	OA5-CA3-CA4-CA6
16	C	510	UQ8	C24-C26-C27-C28
13	c	510	PC1	C24-C25-C26-C27
13	C	508	PC1	C12-C11-O13-P
17	C	512	PEE	C5-C4-O4P-P
15	C	505	CDL	C12-C13-C14-C15
13	c	506	PC1	C3C-C3D-C3E-C3F
15	C	505	CDL	CA5-C11-C12-C13
15	a	1201	CDL	CB2-C1-CA2-OA2
13	E	302	PC1	O11-C1-C2-O21
15	C	506	CDL	OA5-CA3-CA4-OA6
15	C	503	CDL	C37-C38-C39-C40
15	C	506	CDL	O1-C1-CA2-OA2
15	g	801	CDL	O1-C1-CB2-OB2
13	K	901	PC1	O13-C11-C12-N
13	c	506	PC1	O13-C11-C12-N
13	c	510	PC1	O13-C11-C12-N
13	d	801	PC1	O13-C11-C12-N
13	g	802	PC1	O13-C11-C12-N
15	c	503	CDL	CA3-CA4-CA6-OA8
15	h	402	CDL	CA3-CA4-CA6-OA8
13	C	509	PC1	O21-C2-C3-O31
13	d	801	PC1	O21-C2-C3-O31
16	C	510	UQ8	C1-C6-C7-C8
13	E	302	PC1	C3E-C3F-C3G-C3H
16	C	511	UQ8	C15-C14-C16-C17
13	k	301	PC1	C34-C35-C36-C37
15	H	1301	CDL	C14-C15-C16-C17
15	E	304	CDL	OB9-CB7-OB8-CB6
15	c	507	CDL	C44-C45-C46-C47
15	c	503	CDL	OB9-CB7-OB8-CB6
15	C	506	CDL	CA6-CA4-OA6-CA5
15	a	1201	CDL	CB6-CB4-OB6-CB5
13	c	510	PC1	O11-C1-C2-C3
15	h	401	CDL	CB2-C1-CA2-OA2
15	E	304	CDL	C71-CB7-OB8-CB6
13	c	504	PC1	C3E-C3F-C3G-C3H
15	H	1301	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
15	a	1201	CDL	C73-C74-C75-C76
15	c	507	CDL	C72-C71-CB7-OB8
13	C	508	PC1	C22-C23-C24-C25
15	c	503	CDL	C71-CB7-OB8-CB6
13	A	1201	PC1	O11-C1-C2-O21
13	C	508	PC1	O11-C1-C2-O21
13	C	509	PC1	C3B-C3C-C3D-C3E
15	h	402	CDL	OB6-CB4-CB6-OB8
15	c	509	CDL	C79-C80-C81-C82
13	E	302	PC1	C1-O11-P-O13
15	C	503	CDL	CA2-OA2-PA1-OA5
15	C	506	CDL	CA3-OA5-PA1-OA2
15	a	1201	CDL	CA2-OA2-PA1-OA5
15	c	503	CDL	CA2-OA2-PA1-OA5
13	C	507	PC1	C28-C29-C2A-C2B
15	H	1302	CDL	CB3-CB4-CB6-OB8
15	c	507	CDL	CB3-CB4-CB6-OB8
16	C	510	UQ8	C5-C4-O4-C4M
15	D	402	CDL	C19-C20-C21-C22
15	C	506	CDL	C1-CA2-OA2-PA1
15	c	507	CDL	C54-C55-C56-C57
15	C	505	CDL	C23-C24-C25-C26
15	C	505	CDL	C44-C45-C46-C47
15	a	1201	CDL	C14-C15-C16-C17
13	A	1201	PC1	O11-C1-C2-C3
15	a	1201	CDL	OA5-CA3-CA4-CA6
16	C	510	UQ8	C14-C16-C17-C18
13	C	509	PC1	O11-C1-C2-O21
13	E	303	PC1	O11-C1-C2-O21
13	d	801	PC1	C2B-C2C-C2D-C2E
17	L	401	PEE	C18-C19-C20-C21
15	H	1302	CDL	C14-C15-C16-C17
13	d	801	PC1	C3B-C3C-C3D-C3E
15	C	504	CDL	C11-C12-C13-C14
13	E	303	PC1	C3F-C3G-C3H-C3I
13	c	510	PC1	C29-C2A-C2B-C2C
15	H	1301	CDL	CB3-CB4-CB6-OB8
15	a	1201	CDL	CA3-CA4-CA6-OA8
13	d	801	PC1	C22-C23-C24-C25
13	C	508	PC1	C2F-C2G-C2H-C2I
15	C	503	CDL	C14-C15-C16-C17
13	C	507	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
15	c	507	CDL	CA6-CA4-OA6-CA5
13	C	507	PC1	C37-C38-C39-C3A
15	D	402	CDL	CB3-OB5-PB2-OB2
13	E	303	PC1	C3D-C3E-C3F-C3G
15	H	1302	CDL	OB5-CB3-CB4-OB6
16	C	510	UQ8	C6-C7-C8-C9
13	E	302	PC1	C24-C25-C26-C27
13	C	508	PC1	C2C-C2D-C2E-C2F
13	c	506	PC1	O11-C1-C2-C3
15	c	503	CDL	C17-C18-C19-C20
16	C	511	UQ8	C13-C14-C16-C17
13	C	509	PC1	O22-C21-O21-C2
13	C	508	PC1	C25-C26-C27-C28
13	k	301	PC1	C2F-C2G-C2H-C2I
15	C	503	CDL	OB6-CB4-CB6-OB8
15	a	1201	CDL	OA6-CA4-CA6-OA8
13	c	504	PC1	O22-C21-C22-C23
14	C	502	HEM	CAA-CBA-CGA-O1A
18	d	802	HEC	CAA-CBA-CGA-O2A
14	C	502	HEM	CAA-CBA-CGA-O2A
15	c	503	CDL	C15-C16-C17-C18
16	c	508	UQ8	C20-C19-C21-C22
13	c	505	PC1	C38-C39-C3A-C3B
15	C	504	CDL	C17-C18-C19-C20
17	C	512	PEE	C16-C17-C18-C19
17	L	401	PEE	C36-C37-C38-C39
15	C	506	CDL	CA5-C11-C12-C13
13	c	510	PC1	C2C-C2D-C2E-C2F
13	C	509	PC1	O11-C1-C2-C3
16	C	511	UQ8	C35-C34-C36-C37
16	c	508	UQ8	C12-C11-C9-C10
15	c	507	CDL	C34-C35-C36-C37
17	L	401	PEE	C38-C39-C40-C41
13	k	301	PC1	C37-C38-C39-C3A
15	C	503	CDL	C52-C53-C54-C55
15	c	507	CDL	C17-C18-C19-C20
17	C	512	PEE	C18-C19-C20-C21
15	C	506	CDL	C14-C15-C16-C17
15	C	506	CDL	C72-C71-CB7-OB8
13	c	504	PC1	C3F-C3G-C3H-C3I
16	c	508	UQ8	C40-C39-C41-C42
15	C	504	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
15	H	1301	CDL	C32-C31-CA7-OA8
15	c	503	CDL	C72-C71-CB7-OB8
16	C	510	UQ8	C5-C6-C7-C8
17	L	401	PEE	C16-C17-C18-C19
13	c	504	PC1	C33-C34-C35-C36
18	d	802	HEC	CAA-CBA-CGA-O1A
13	C	507	PC1	C3-C2-O21-C21
15	c	507	CDL	C35-C36-C37-C38
13	k	301	PC1	C39-C3A-C3B-C3C
16	c	508	UQ8	C24-C26-C27-C28
13	g	802	PC1	C38-C39-C3A-C3B
15	c	503	CDL	C73-C74-C75-C76
15	H	1301	CDL	CA3-CA4-CA6-OA8
15	g	801	CDL	CA3-CA4-CA6-OA8
15	h	401	CDL	CB3-CB4-CB6-OB8
13	K	901	PC1	C2E-C2F-C2G-C2H
13	C	508	PC1	O31-C31-C32-C33
15	H	1302	CDL	C32-C31-CA7-OA8
15	h	402	CDL	C52-C51-CB5-OB6
13	A	1202	PC1	C3B-C3C-C3D-C3E
17	C	512	PEE	C36-C37-C38-C39
15	C	504	CDL	C32-C31-CA7-OA8
13	C	507	PC1	O11-C1-C2-C3
15	E	304	CDL	OB5-CB3-CB4-CB6
15	C	504	CDL	C31-C32-C33-C34
15	C	505	CDL	C32-C33-C34-C35
13	g	802	PC1	O21-C21-C22-C23
15	C	506	CDL	C32-C31-CA7-OA8
15	D	402	CDL	C72-C71-CB7-OB8
15	E	304	CDL	OB6-CB4-CB6-OB8
15	H	1301	CDL	OA6-CA4-CA6-OA8
15	D	402	CDL	C11-C12-C13-C14
15	E	304	CDL	C74-C75-C76-C77
15	E	304	CDL	C32-C31-CA7-OA8
15	H	1301	CDL	C11-C12-C13-C14
15	g	801	CDL	CA5-C11-C12-C13
13	C	509	PC1	C22-C21-O21-C2
15	C	504	CDL	C51-CB5-OB6-CB4
15	g	801	CDL	C52-C51-CB5-OB6
17	C	512	PEE	C38-C39-C40-C41
13	A	1202	PC1	O31-C31-C32-C33
13	K	901	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
13	c	506	PC1	C21-C22-C23-C24
13	c	510	PC1	C3B-C3C-C3D-C3E
15	E	304	CDL	C12-C11-CA5-OA6
15	H	1301	CDL	C52-C51-CB5-OB6
13	A	1202	PC1	C27-C28-C29-C2A
16	c	508	UQ8	C36-C37-C38-C39
15	C	506	CDL	C72-C71-CB7-OB9
13	g	802	PC1	C35-C36-C37-C38
13	K	901	PC1	C27-C28-C29-C2A
15	C	504	CDL	C19-C20-C21-C22
16	c	508	UQ8	C12-C11-C9-C8
13	c	510	PC1	C22-C23-C24-C25
15	a	1201	CDL	OA5-CA3-CA4-OA6
15	c	503	CDL	C34-C35-C36-C37
15	c	503	CDL	C72-C71-CB7-OB9
15	h	402	CDL	C52-C51-CB5-OB7
13	c	510	PC1	C1-C2-C3-O31
15	h	402	CDL	CB3-CB4-CB6-OB8
15	C	504	CDL	C32-C31-CA7-OA9
14	C	501	HEM	CAA-CBA-CGA-O2A
13	C	507	PC1	C29-C2A-C2B-C2C
15	C	505	CDL	C62-C63-C64-C65
13	A	1202	PC1	O32-C31-C32-C33
13	g	802	PC1	O22-C21-C22-C23
15	H	1301	CDL	C32-C31-CA7-OA9
13	E	302	PC1	C3D-C3E-C3F-C3G
13	c	504	PC1	C11-O13-P-O14
13	g	802	PC1	C1-O11-P-O14
13	k	301	PC1	C1-O11-P-O14
15	C	506	CDL	CA3-OA5-PA1-OA3
15	D	402	CDL	CB3-OB5-PB2-OB3
15	E	304	CDL	CB3-OB5-PB2-OB3
15	h	401	CDL	CB2-OB2-PB2-OB3
15	h	402	CDL	CA3-OA5-PA1-OA3
13	C	508	PC1	O32-C31-C32-C33
15	H	1302	CDL	C32-C31-CA7-OA9
15	D	402	CDL	C72-C71-CB7-OB9
15	H	1301	CDL	C52-C51-CB5-OB7
13	C	508	PC1	C32-C31-O31-C3
15	g	801	CDL	C52-C51-CB5-OB7
13	E	303	PC1	C23-C24-C25-C26
15	C	505	CDL	C24-C25-C26-C27

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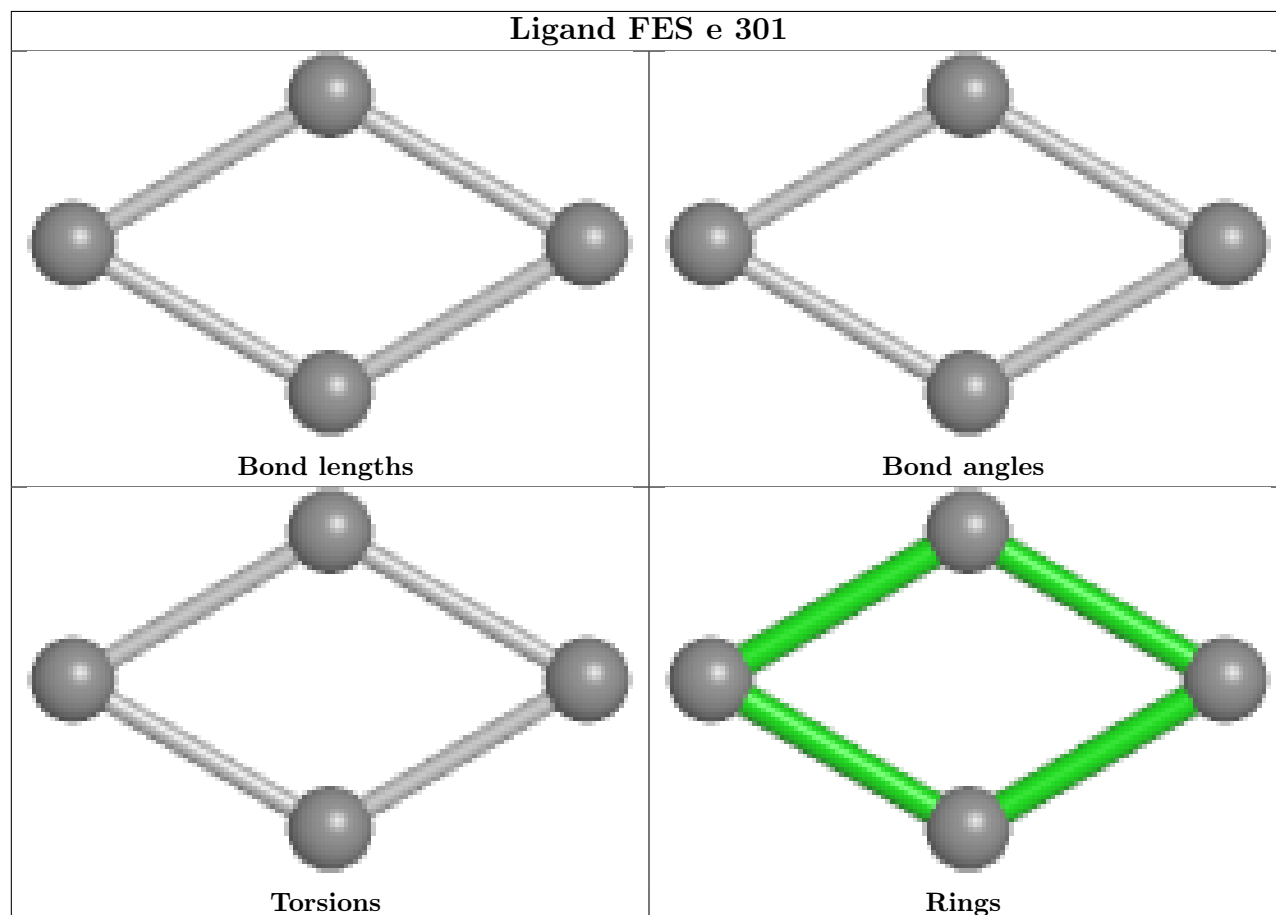
Mol	Chain	Res	Type	Atoms
13	C	507	PC1	C12-C11-O13-P
13	c	504	PC1	C12-C11-O13-P
13	g	802	PC1	C12-C11-O13-P
15	h	401	CDL	CB6-CB4-OB6-CB5
15	g	801	CDL	C39-C40-C41-C42
15	C	506	CDL	C52-C51-CB5-OB6
14	C	501	HEM	CAA-CBA-CGA-O1A
15	C	506	CDL	C32-C31-CA7-OA9
13	C	508	PC1	O21-C21-C22-C23
15	C	505	CDL	C52-C51-CB5-OB6
15	h	401	CDL	C79-C80-C81-C82
13	C	508	PC1	O32-C31-O31-C3
15	E	304	CDL	C12-C11-CA5-OA7
15	C	503	CDL	C78-C79-C80-C81
13	C	509	PC1	O21-C21-C22-C23
15	a	1201	CDL	C32-C31-CA7-OA8
15	h	401	CDL	C12-C11-CA5-OA6
16	c	508	UQ8	C26-C27-C28-C29
14	C	502	HEM	CAD-CBD-CGD-O2D
13	C	507	PC1	C31-C32-C33-C34
15	E	304	CDL	C32-C31-CA7-OA9
15	H	1301	CDL	C1-CA2-OA2-PA1
13	C	507	PC1	O11-C1-C2-O21
13	C	508	PC1	O22-C21-C22-C23
15	C	504	CDL	C13-C14-C15-C16
15	C	505	CDL	C52-C51-CB5-OB7
15	C	506	CDL	C52-C51-CB5-OB7
15	a	1201	CDL	C32-C31-CA7-OA9
13	A	1201	PC1	O31-C31-C32-C33
15	C	503	CDL	C76-C77-C78-C79
15	c	509	CDL	C14-C15-C16-C17
14	C	502	HEM	CAD-CBD-CGD-O1D

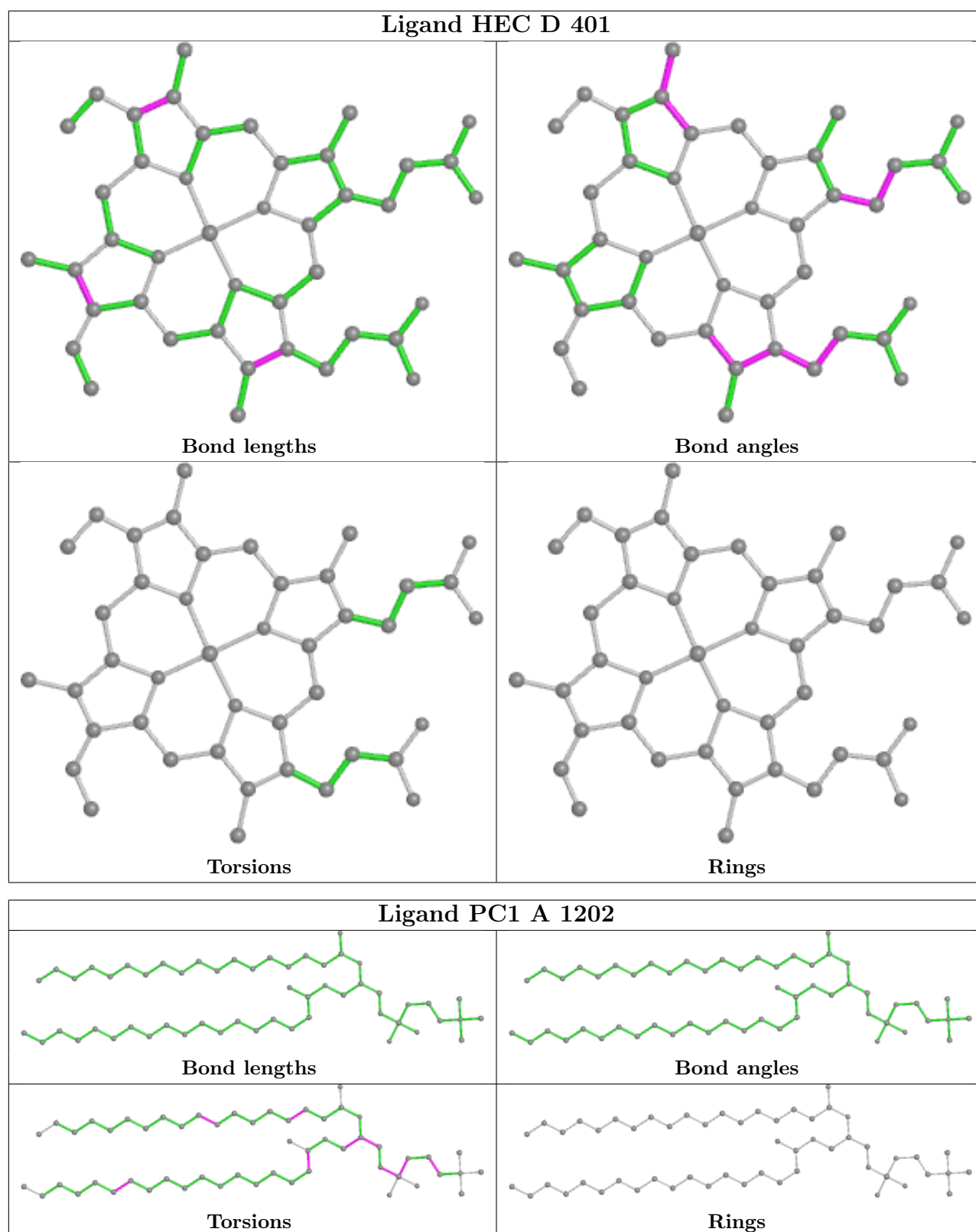
There are no ring outliers.

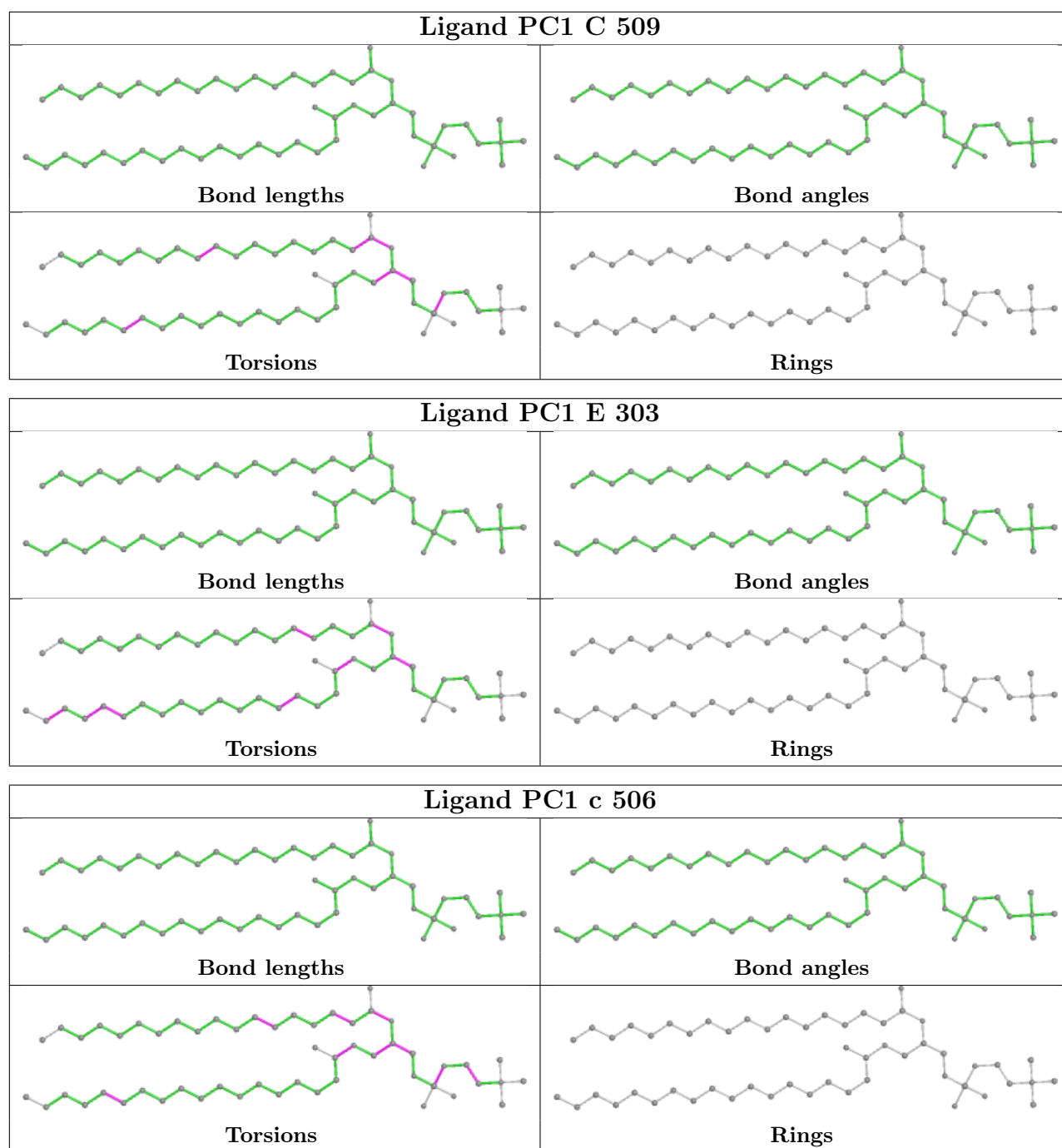
No monomer is involved in short contacts.

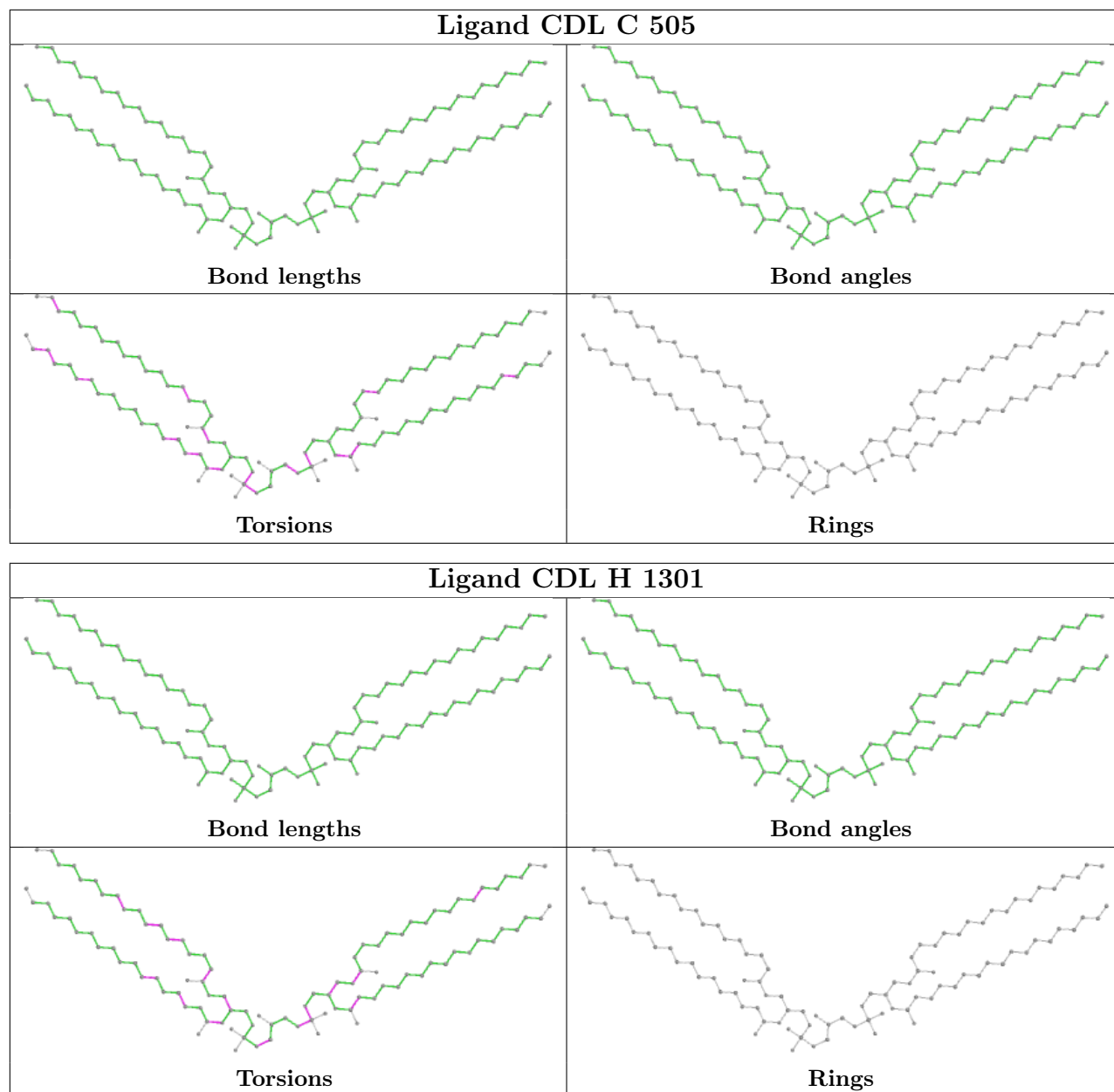
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

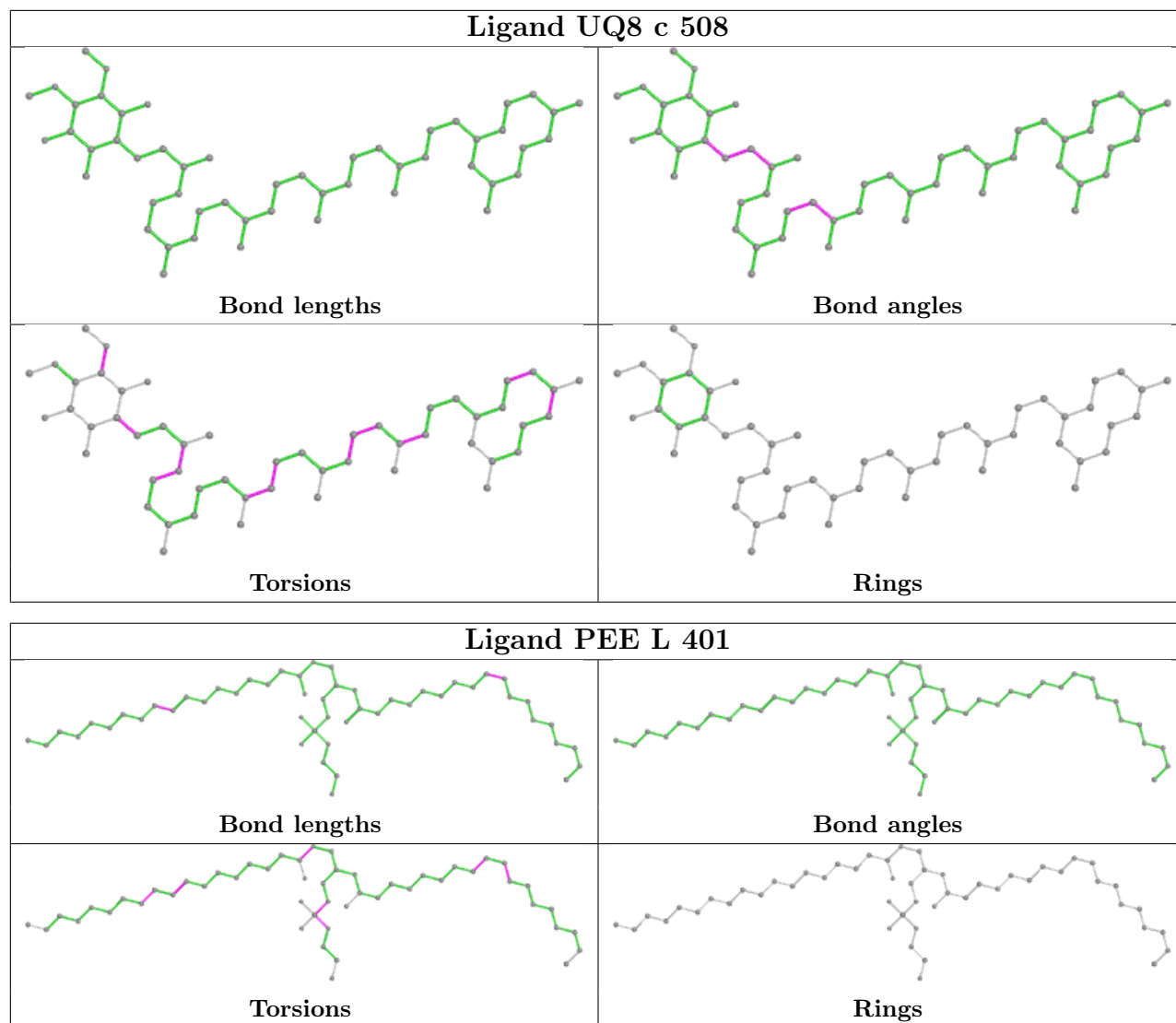
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

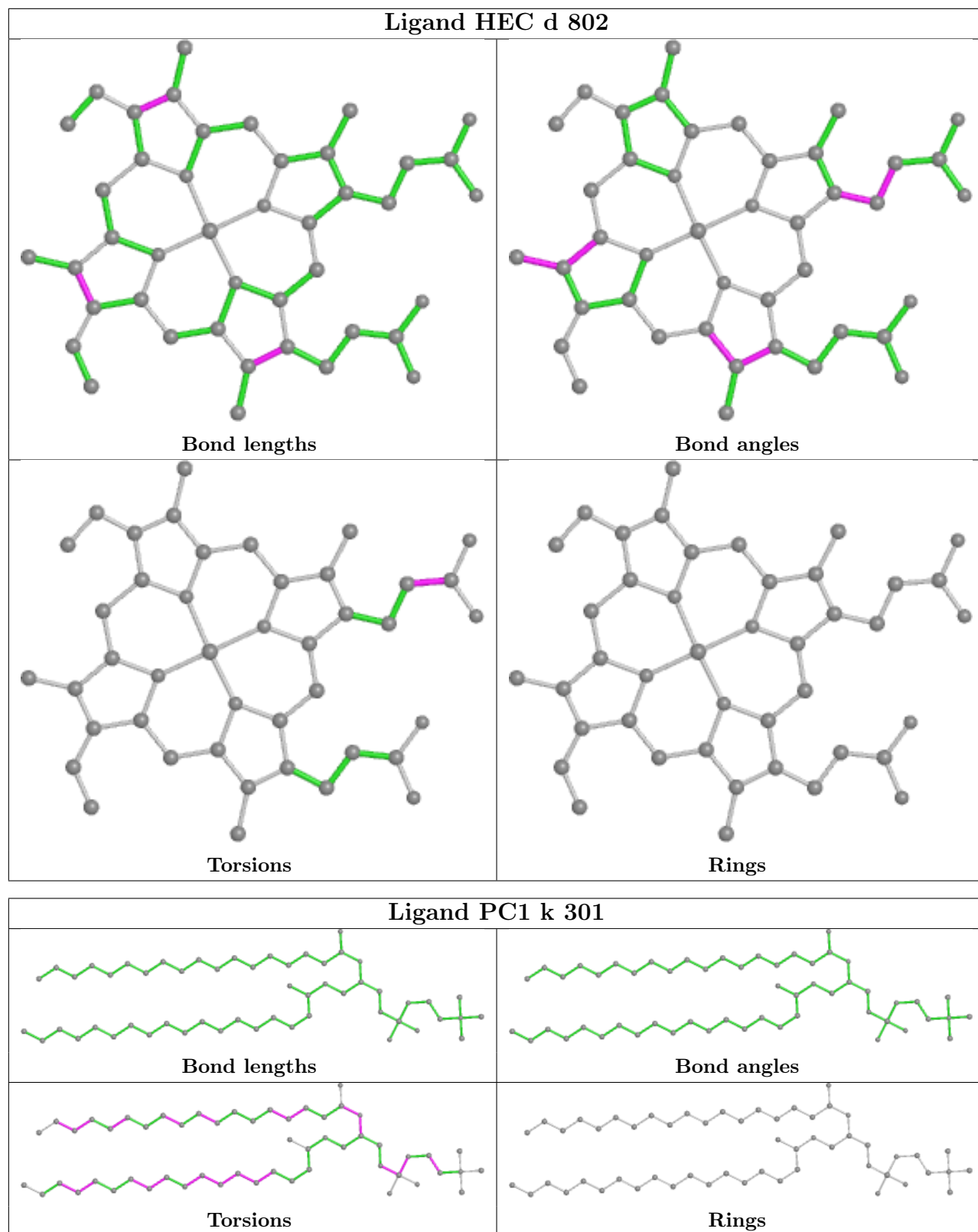


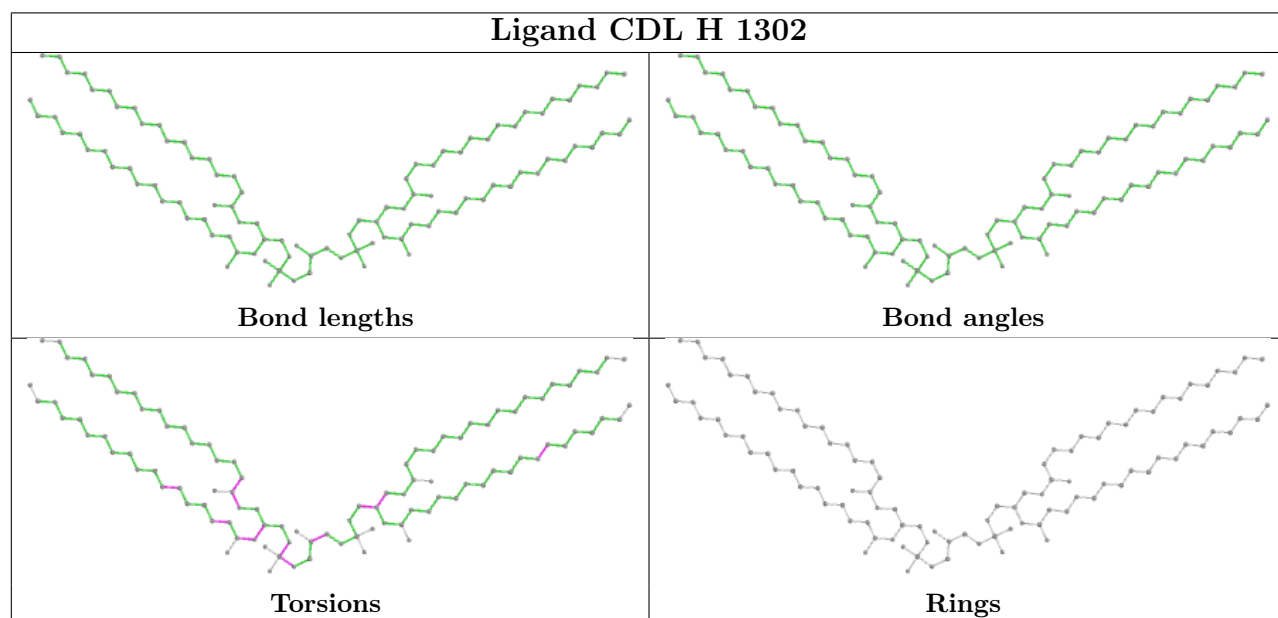
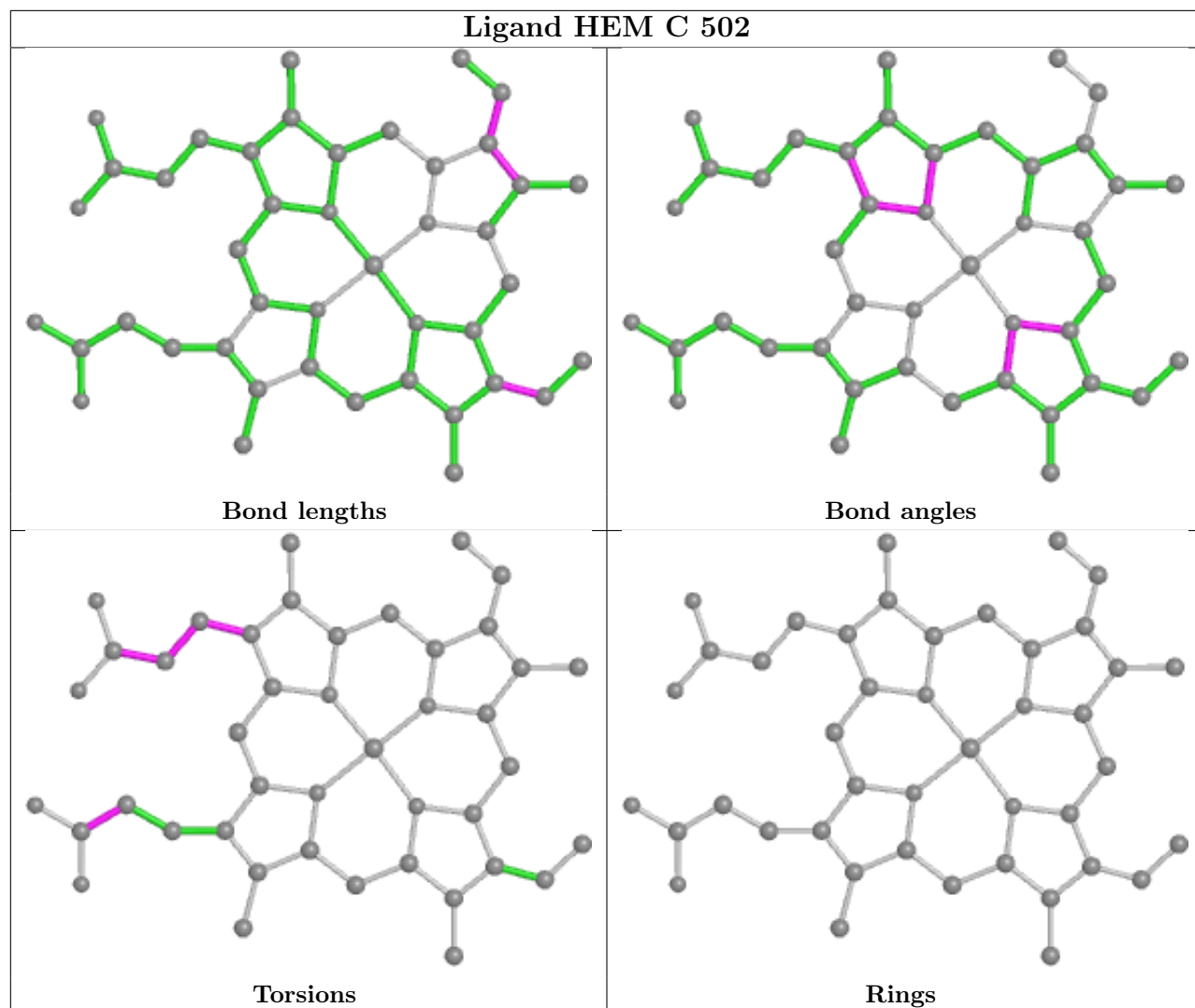


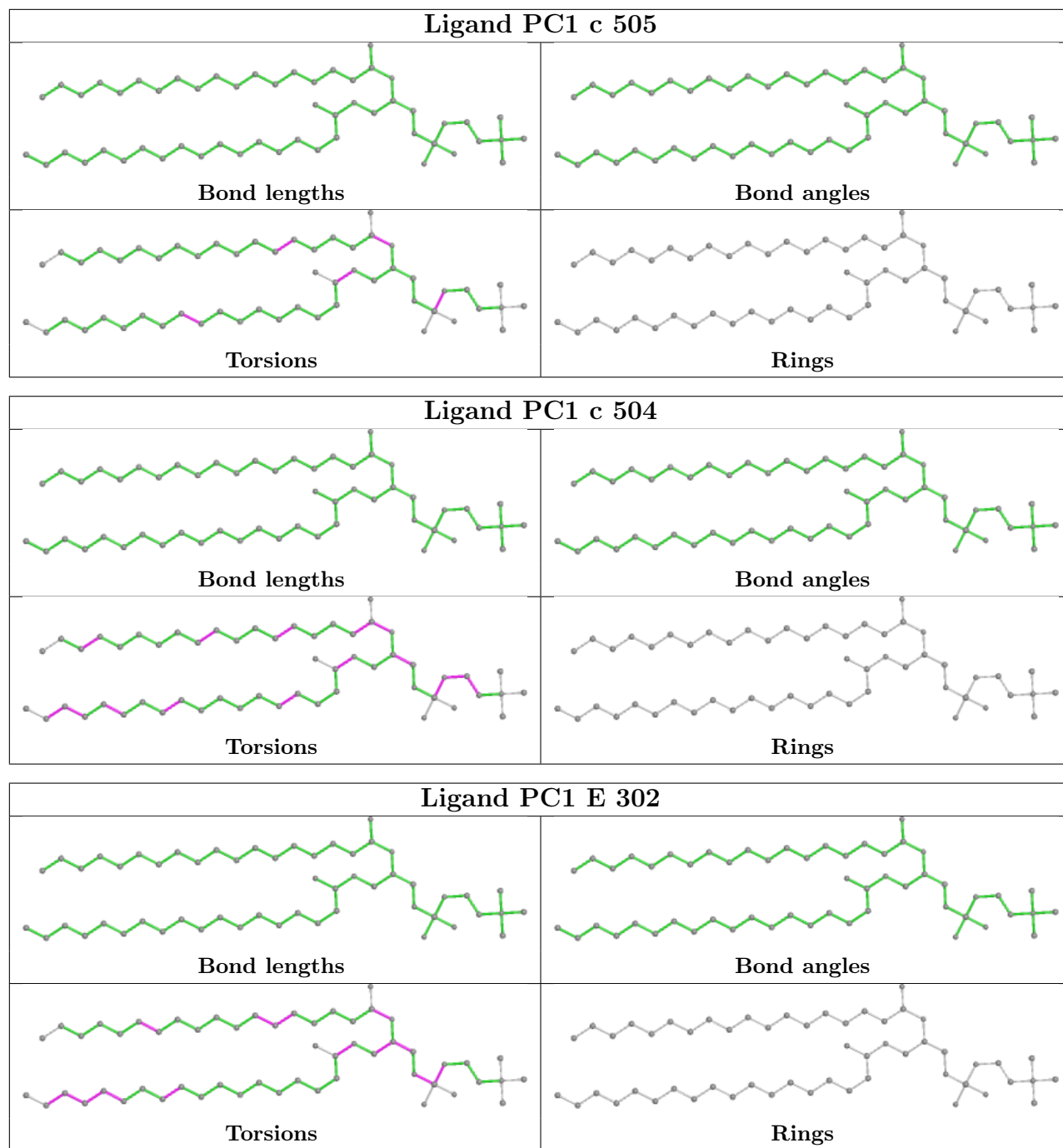


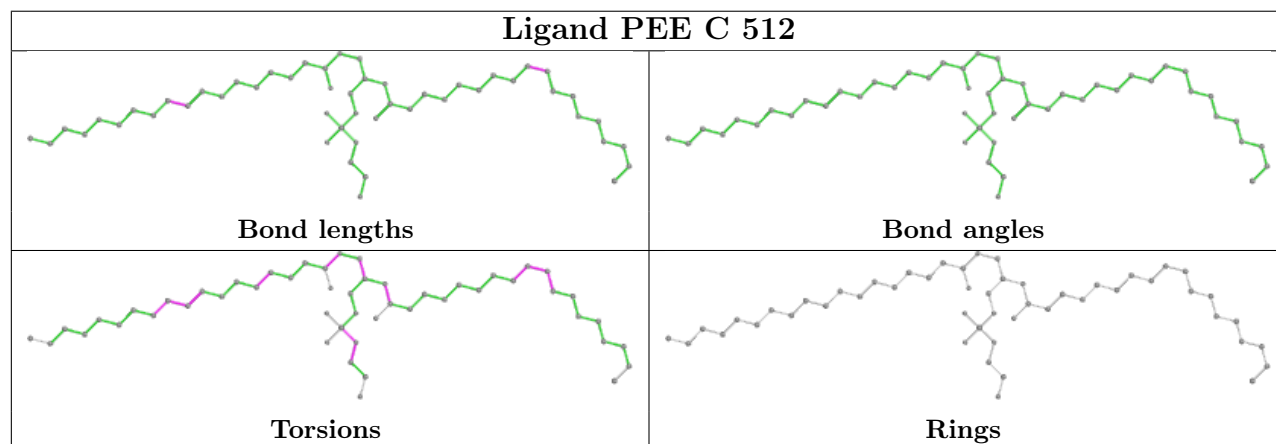
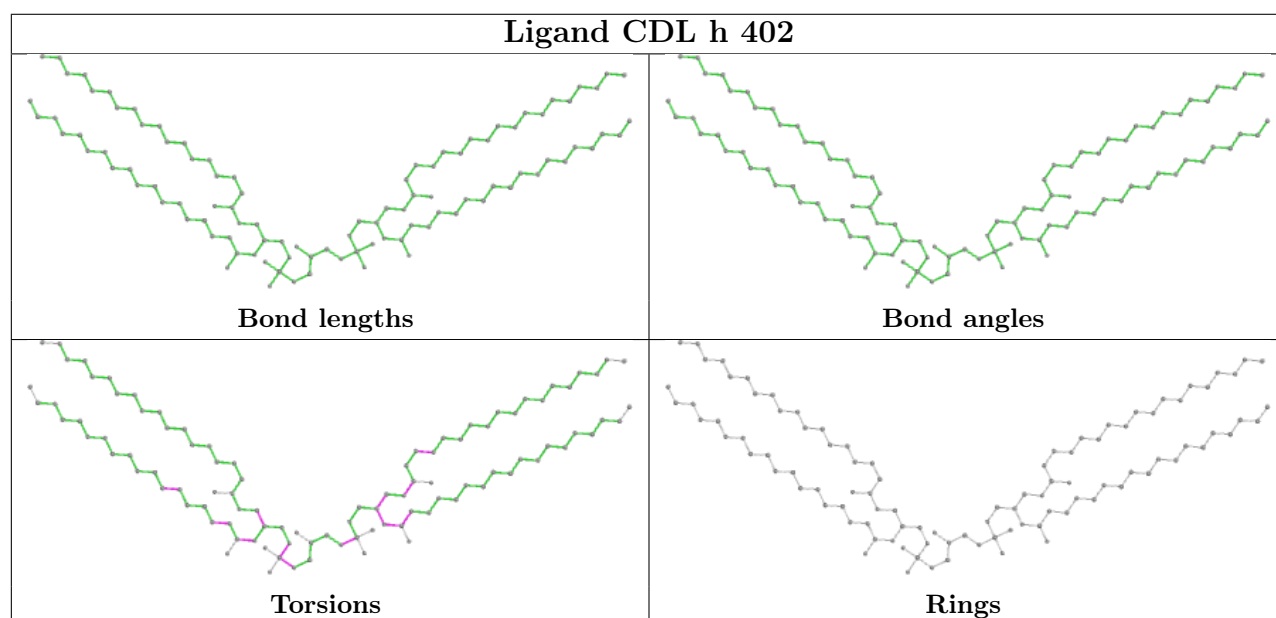
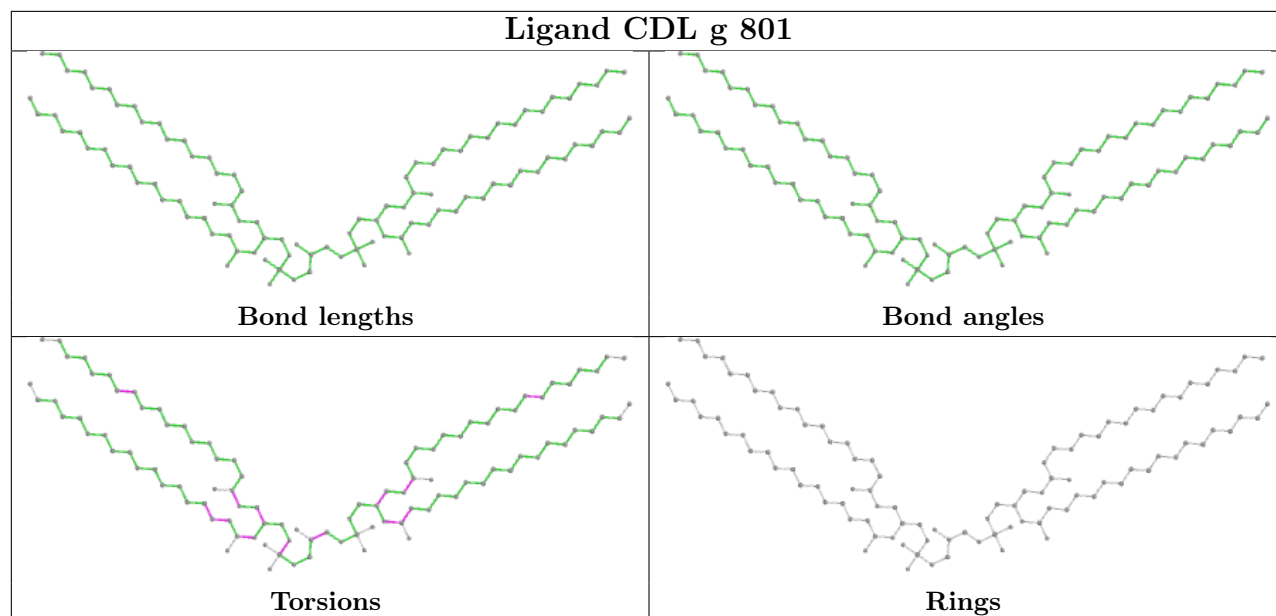


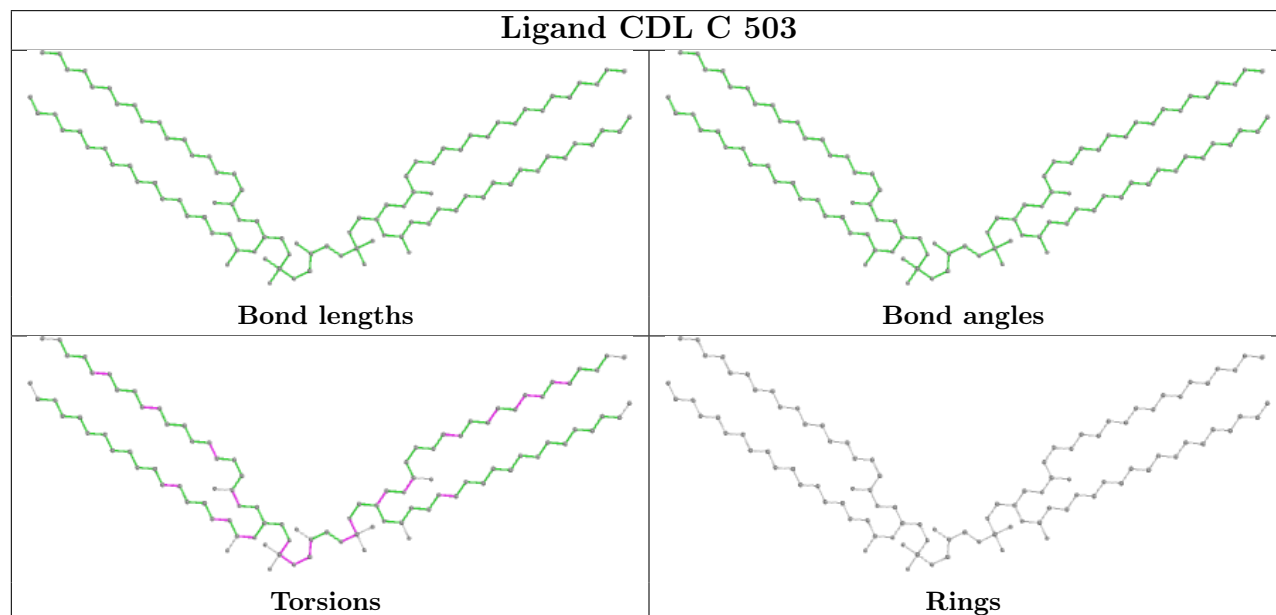
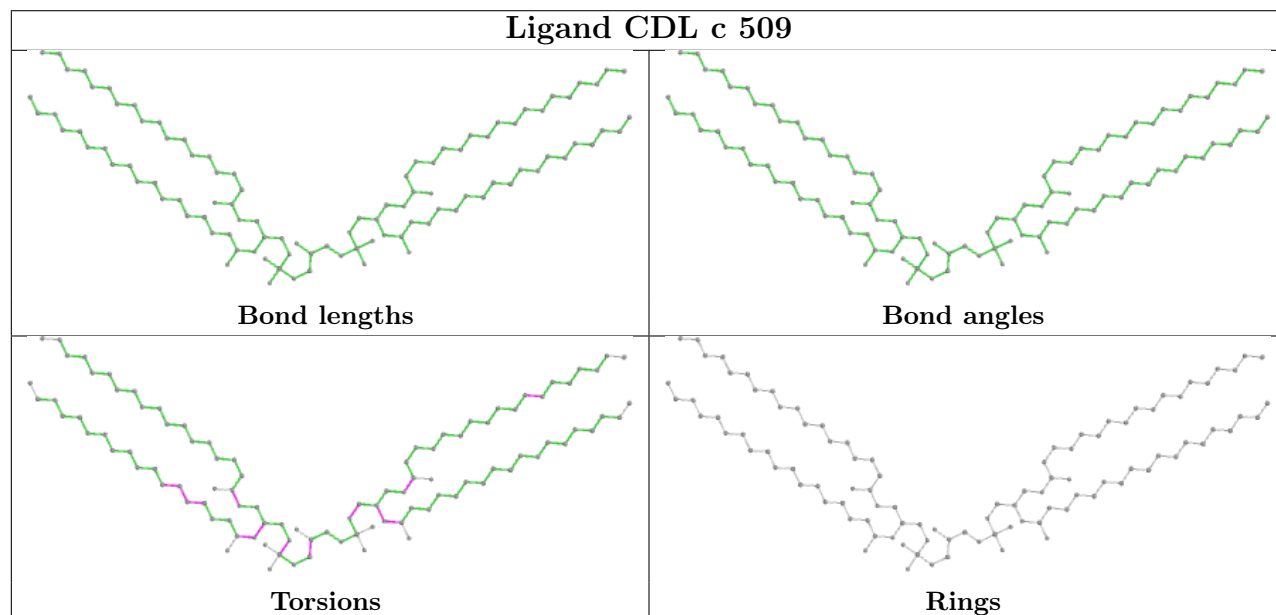
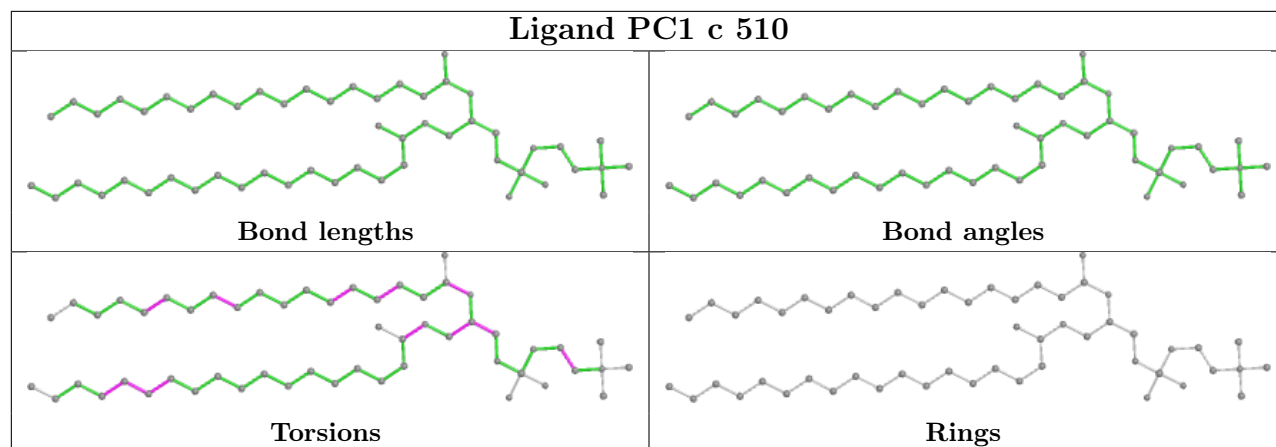


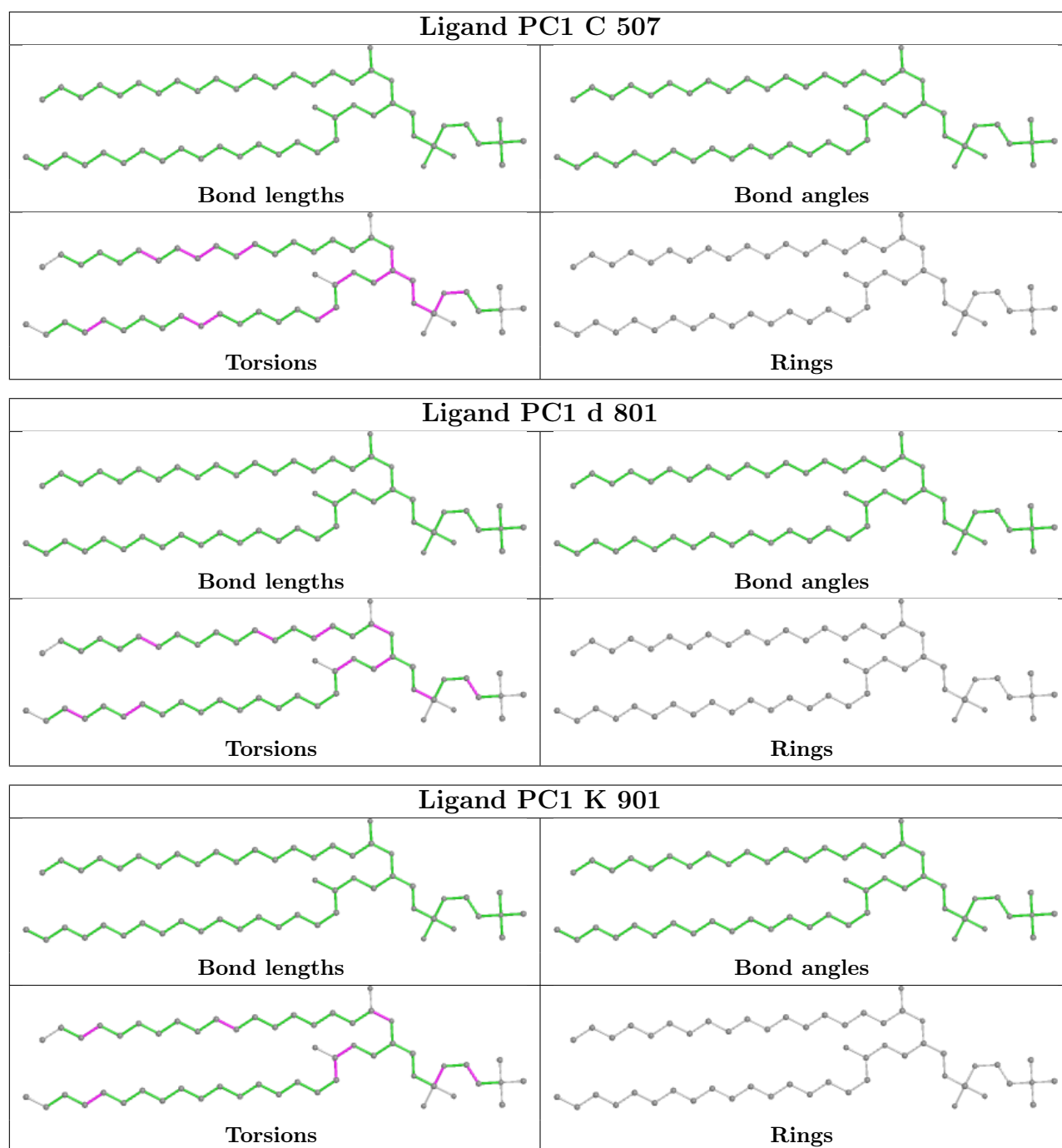


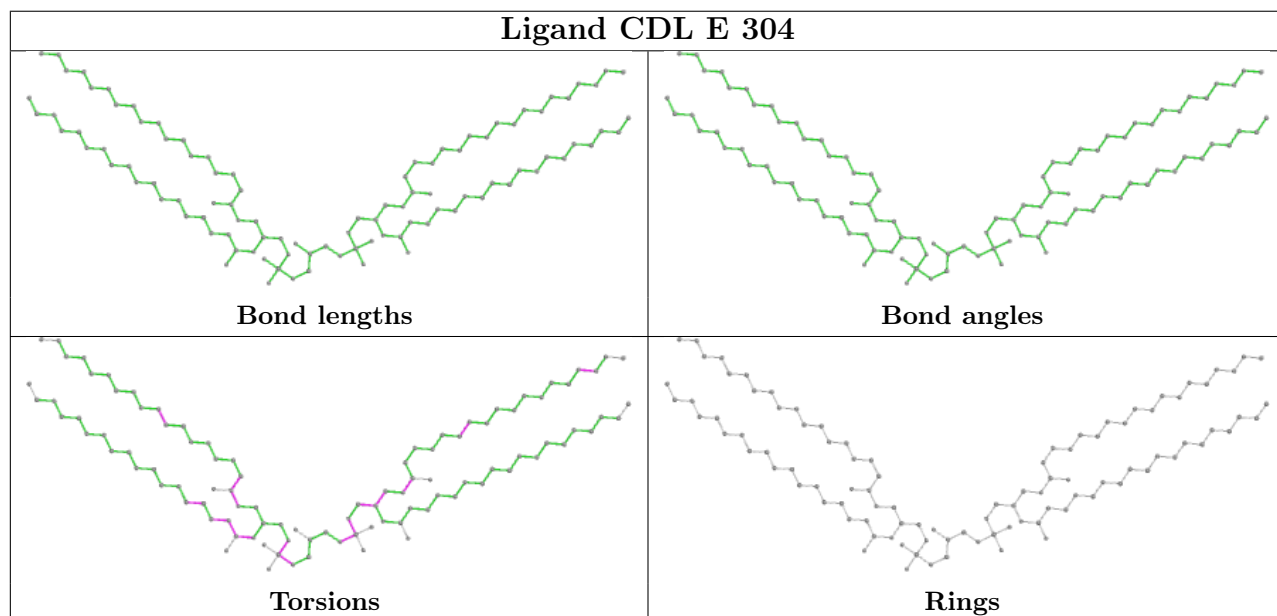
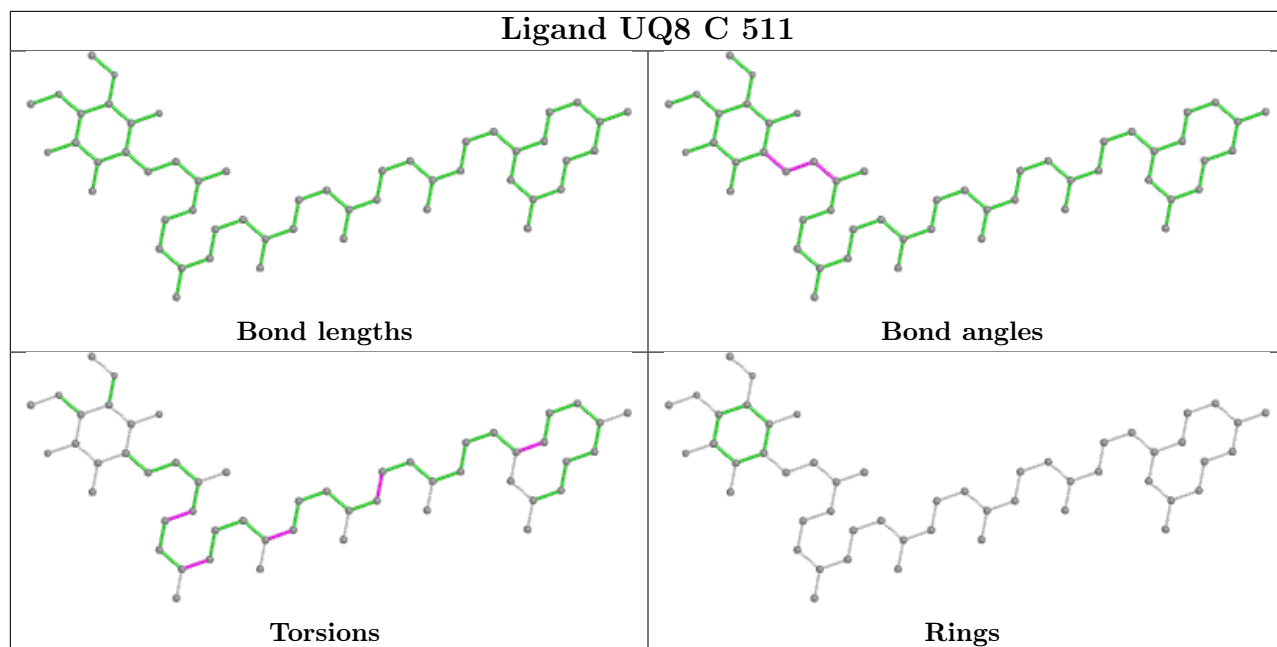


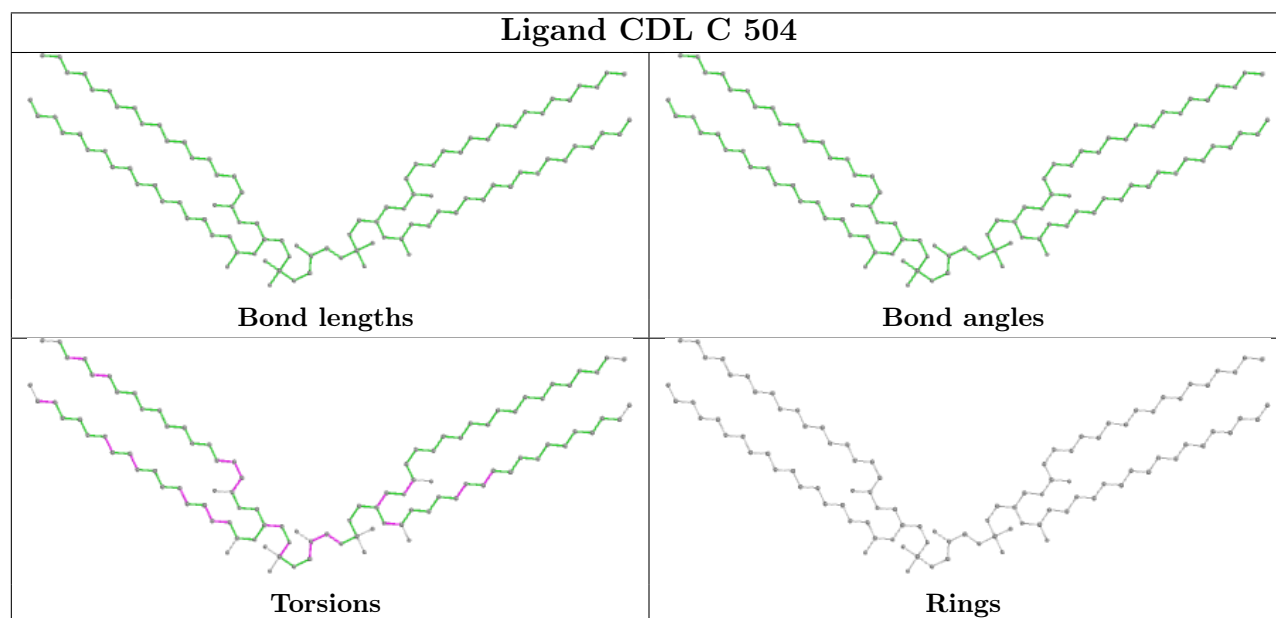
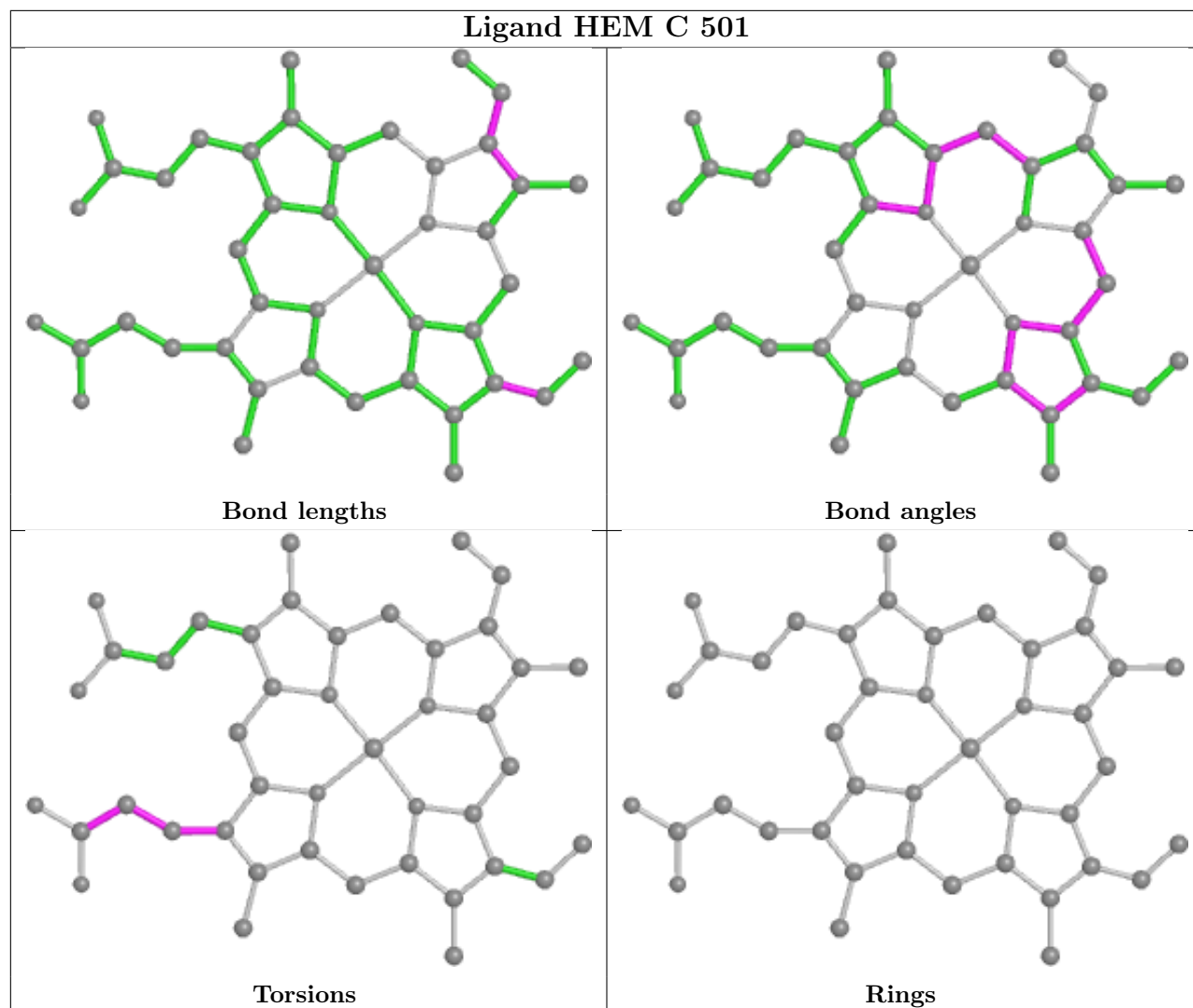


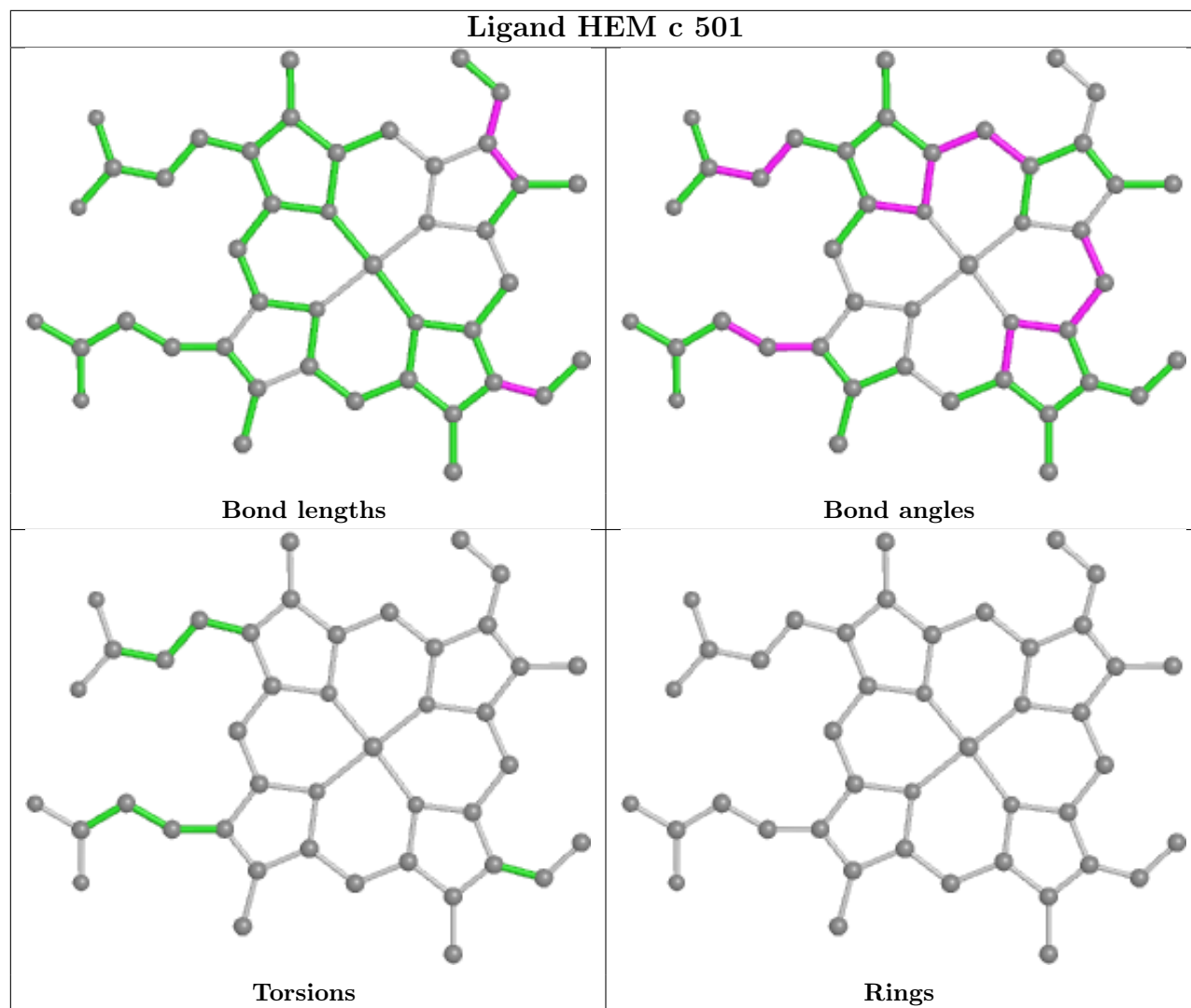


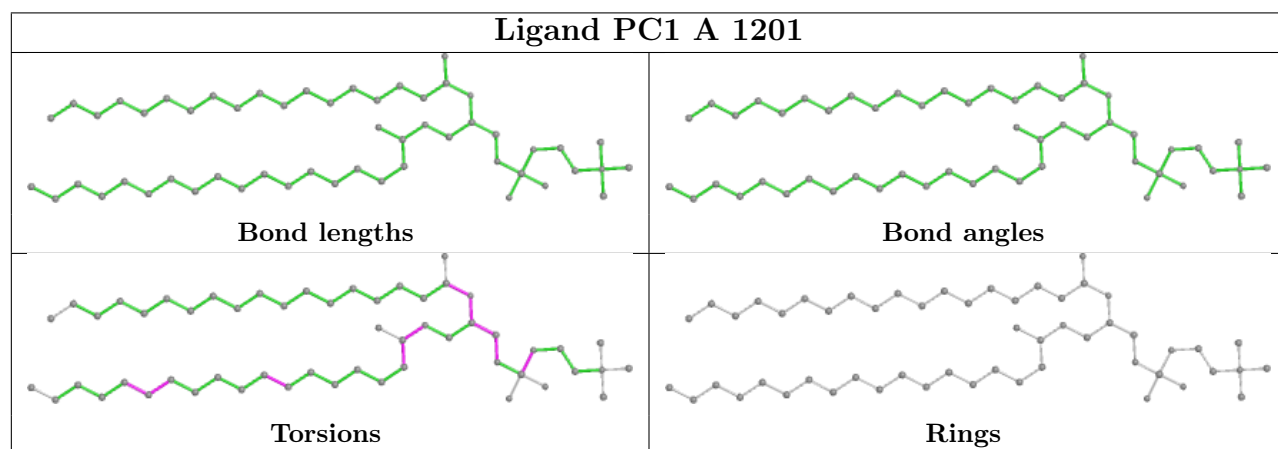
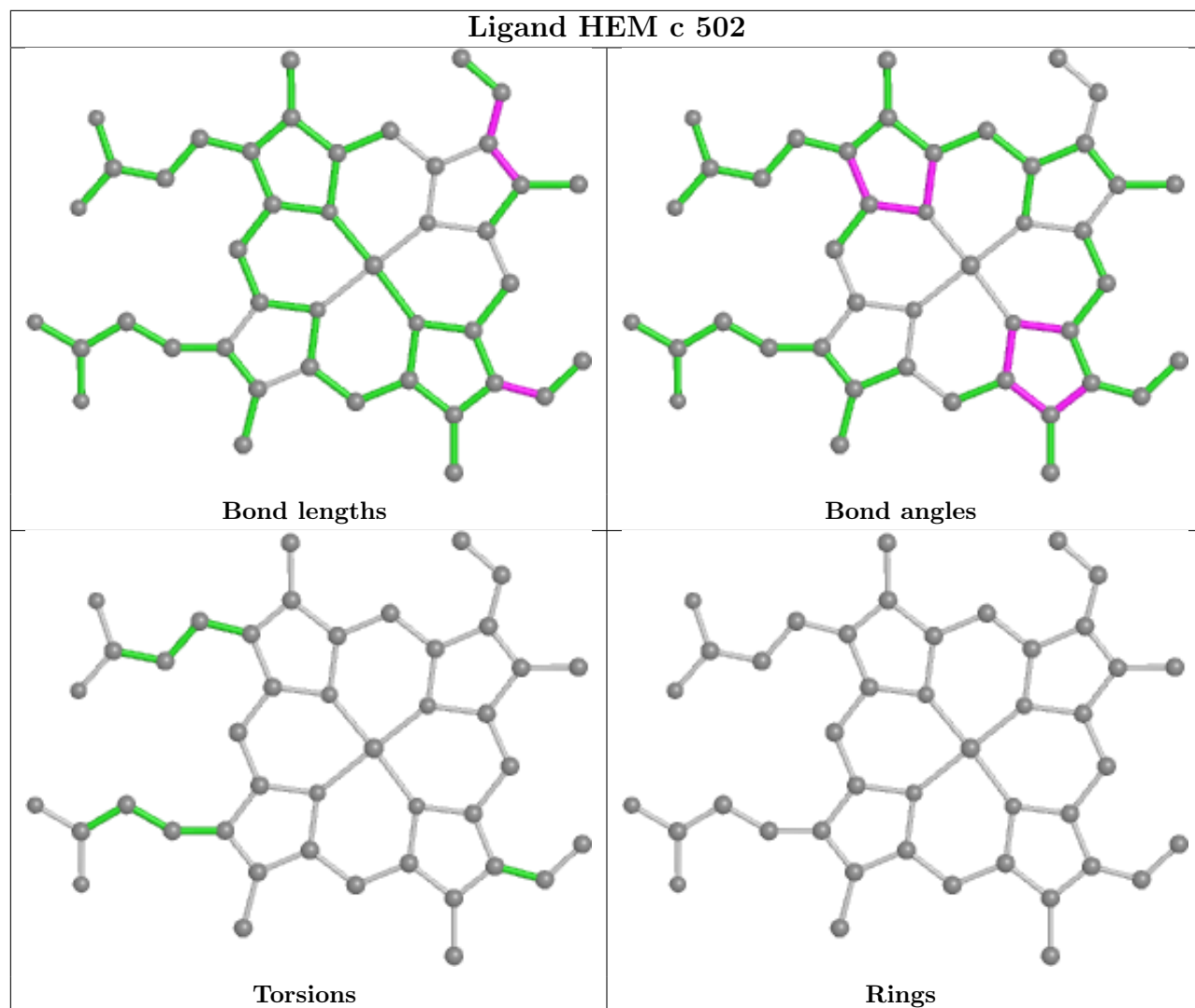


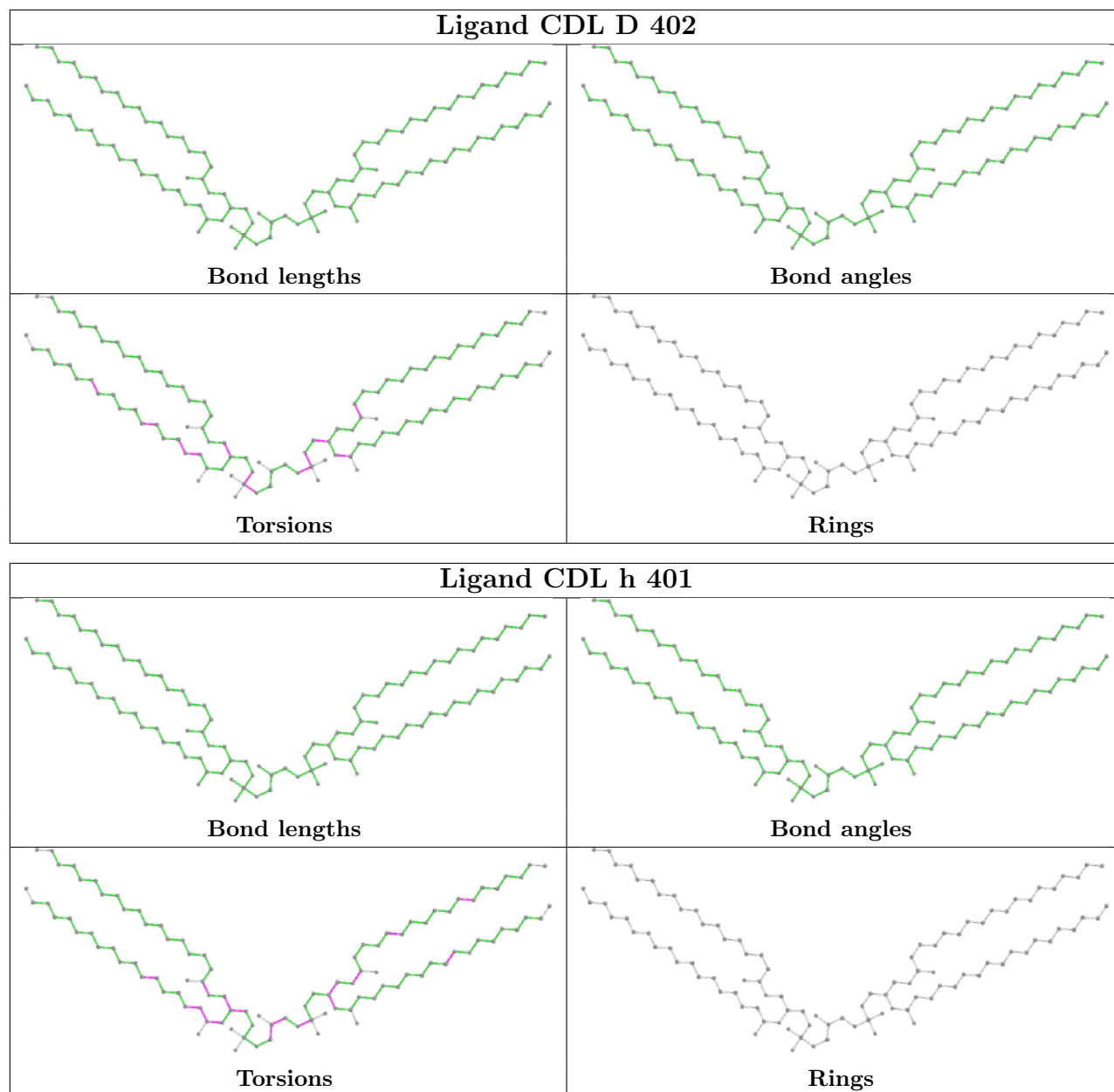


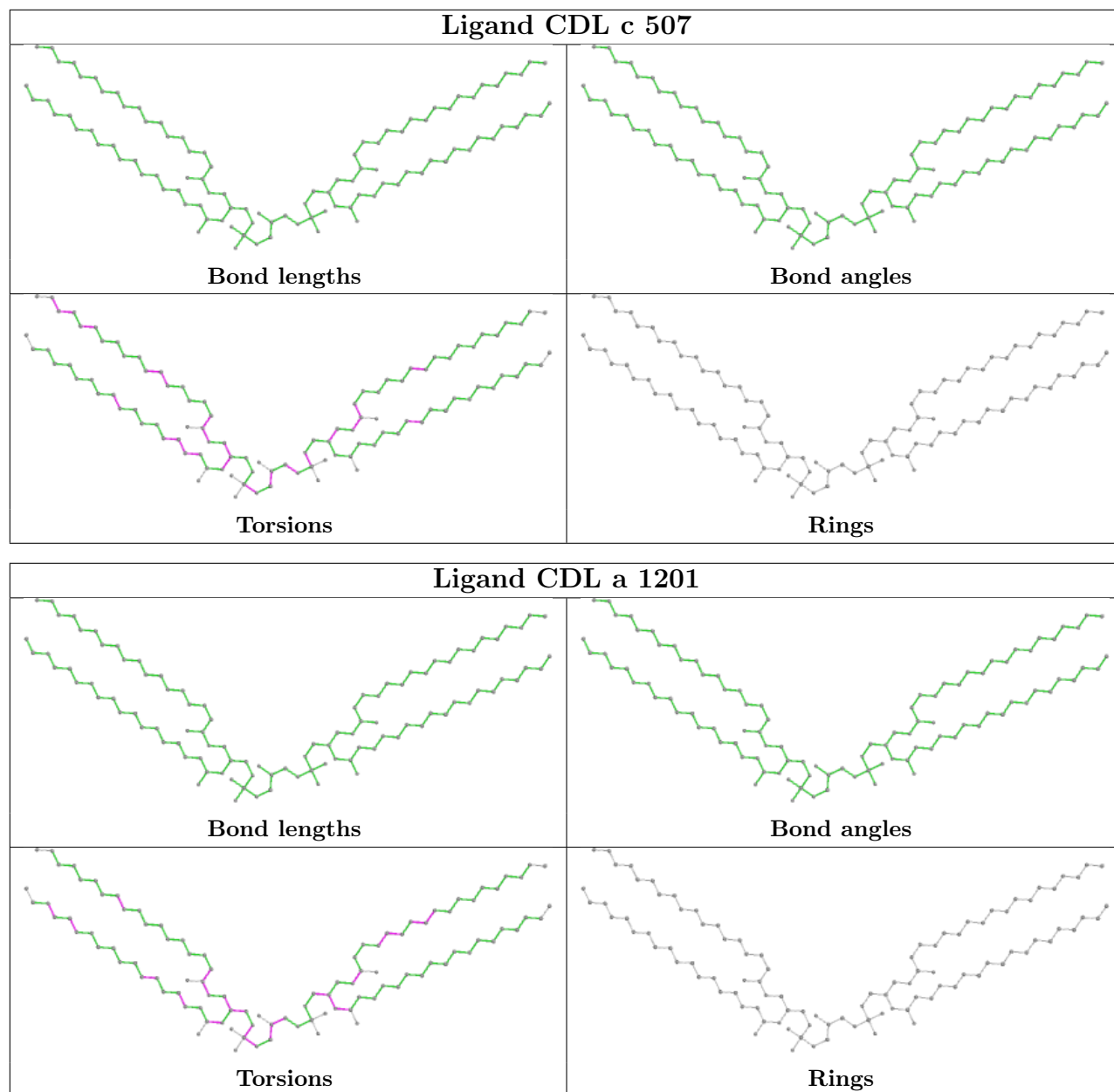


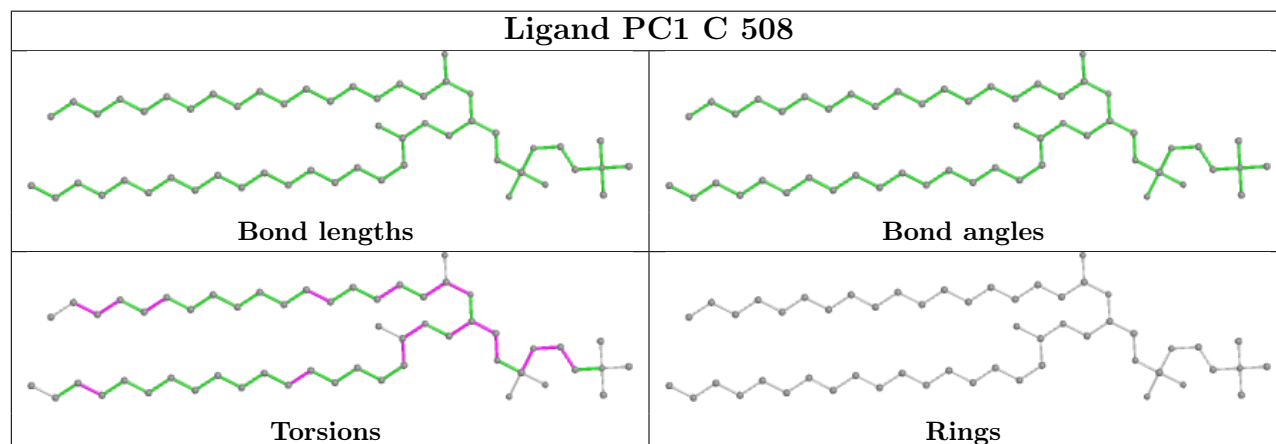
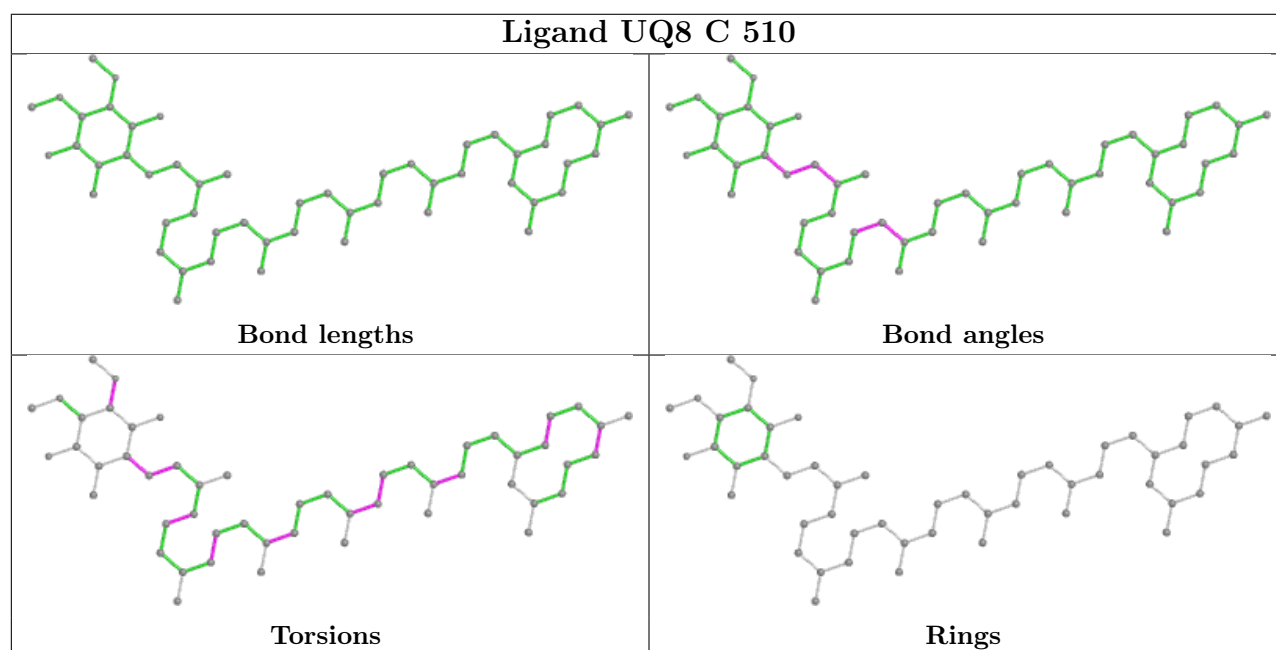
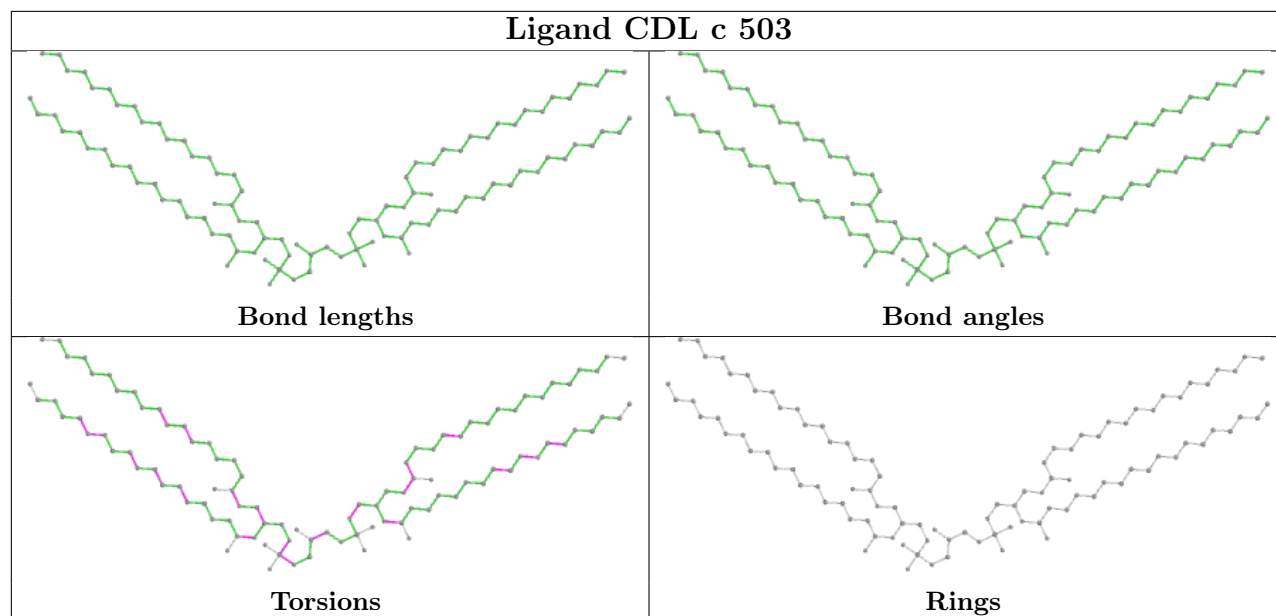


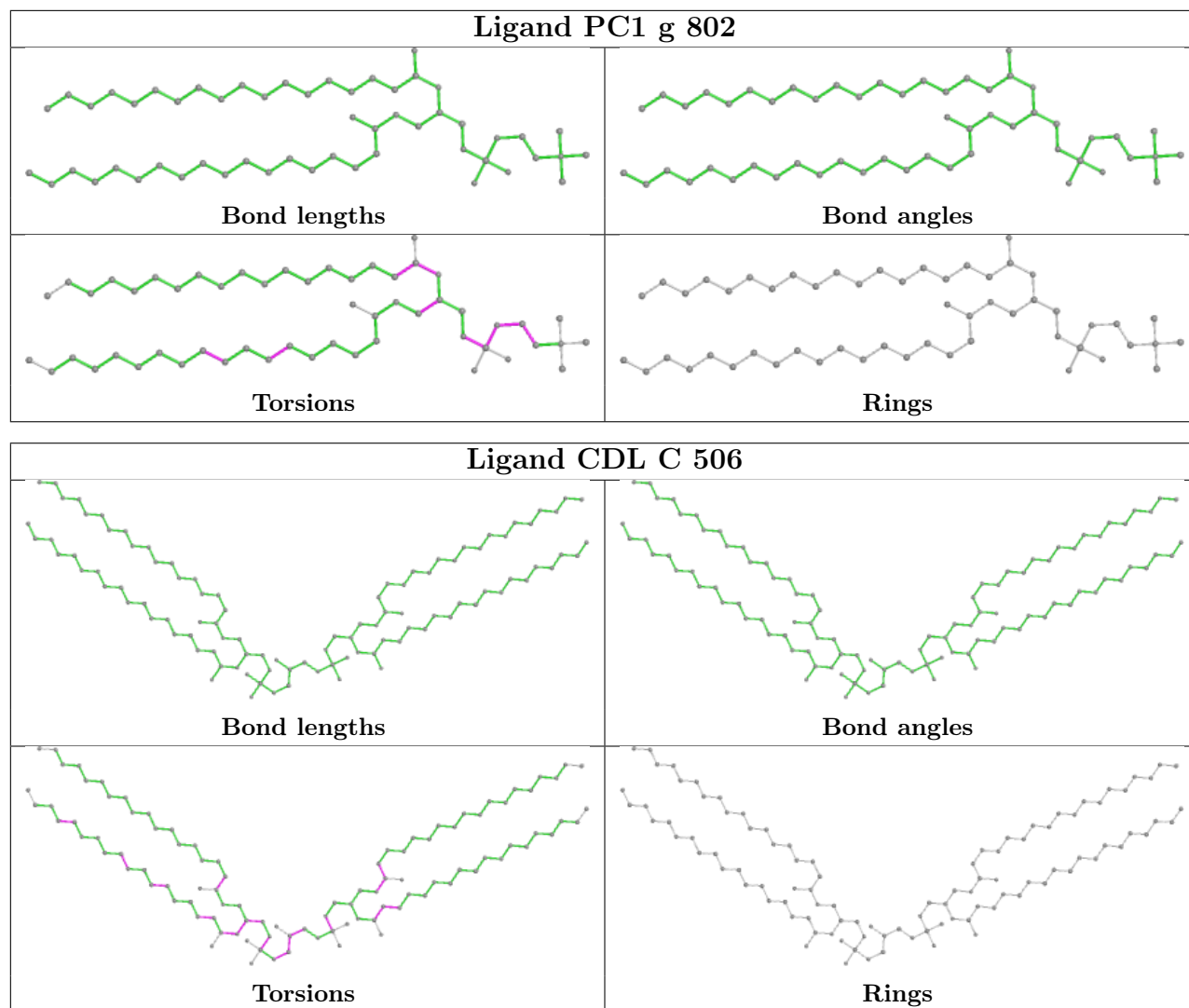


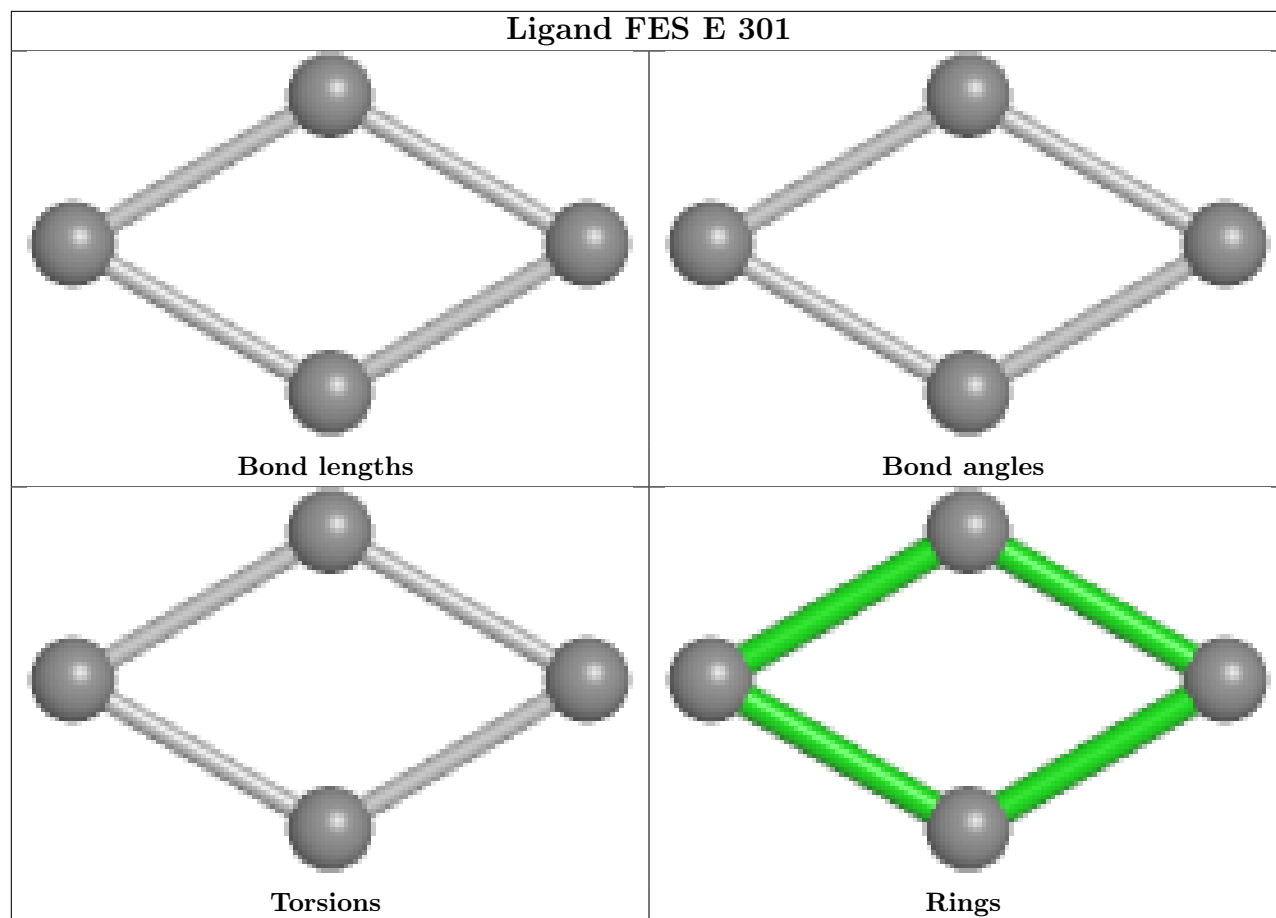












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

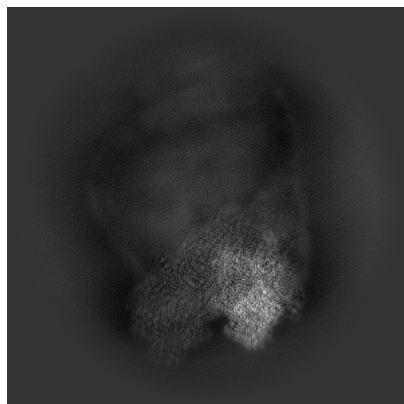
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15868. These allow visual inspection of the internal detail of the map and identification of artifacts.

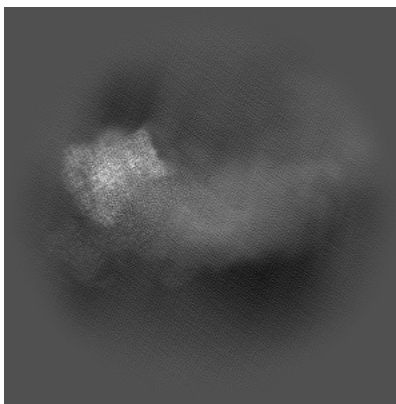
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

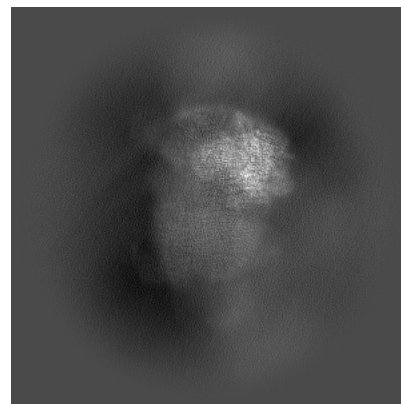
6.1.1 Primary map



X

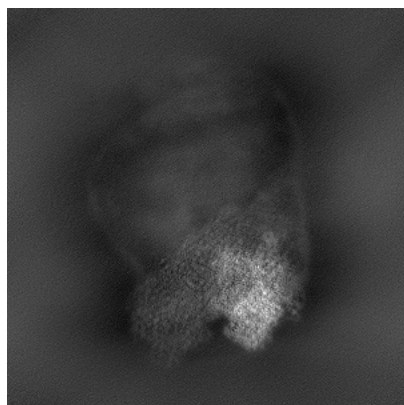


Y

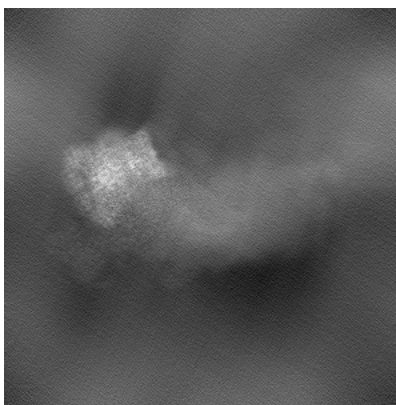


Z

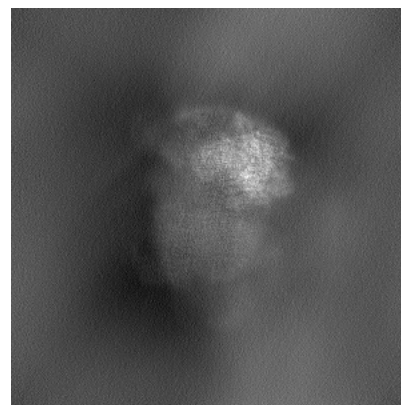
6.1.2 Raw map



X



Y

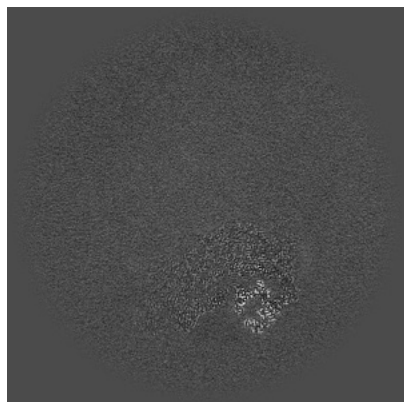


Z

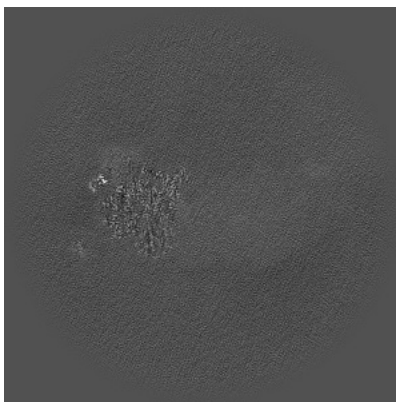
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

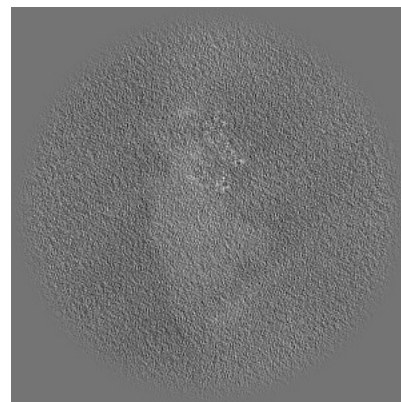
6.2.1 Primary map



X Index: 240

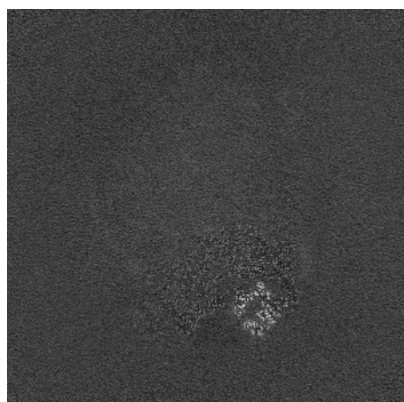


Y Index: 240

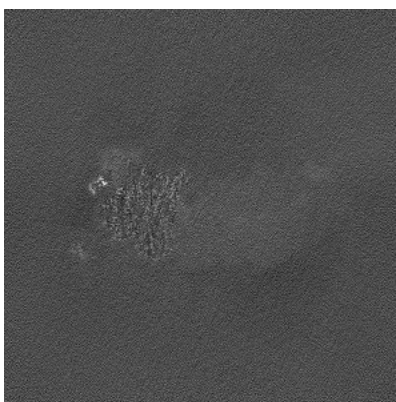


Z Index: 240

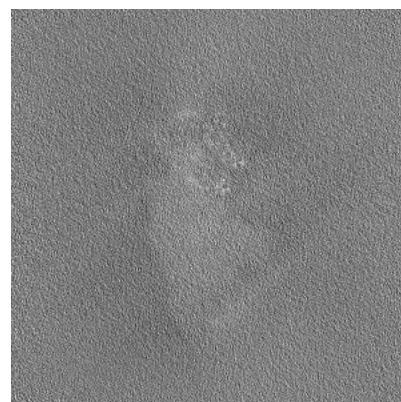
6.2.2 Raw map



X Index: 240



Y Index: 240

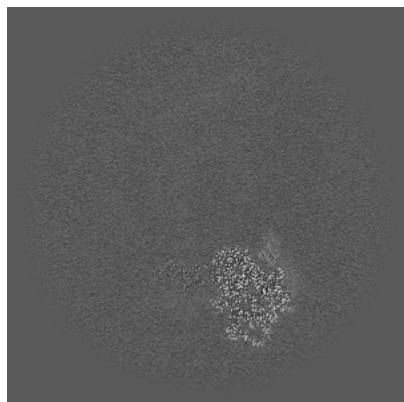


Z Index: 240

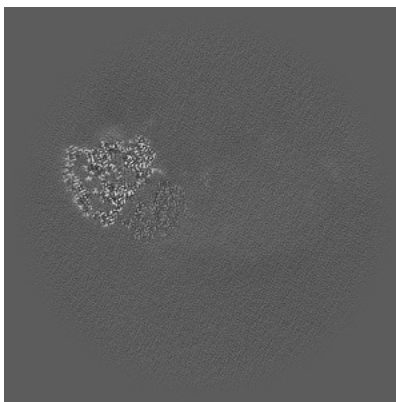
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

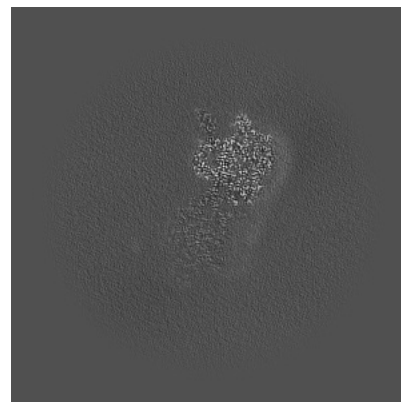
6.3.1 Primary map



X Index: 289

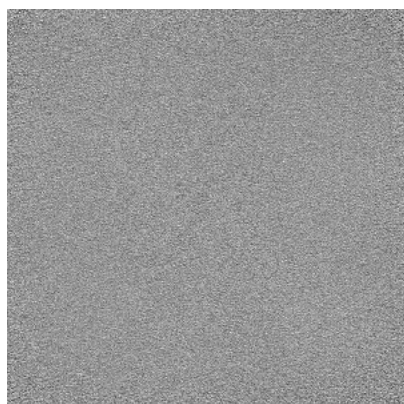


Y Index: 295

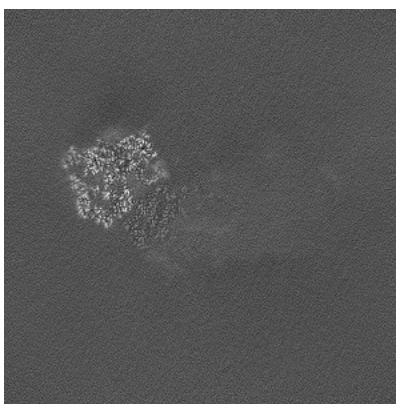


Z Index: 125

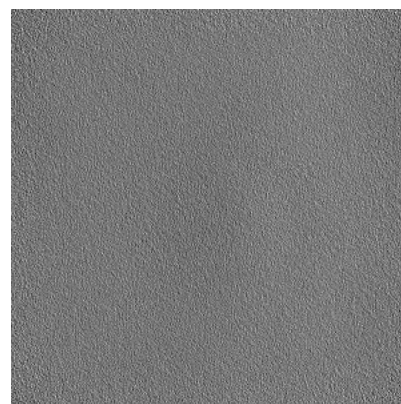
6.3.2 Raw map



X Index: 0



Y Index: 304

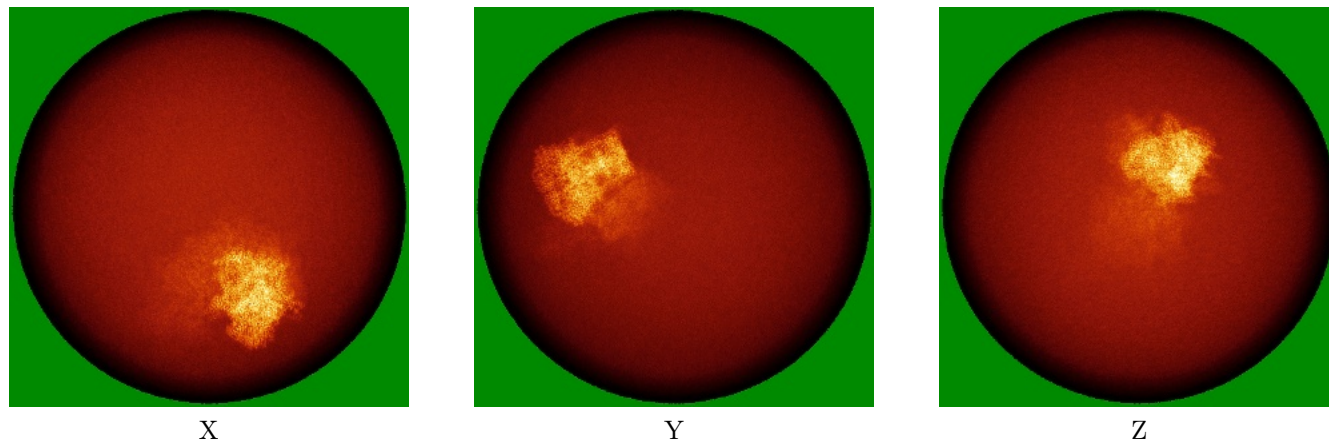


Z Index: 0

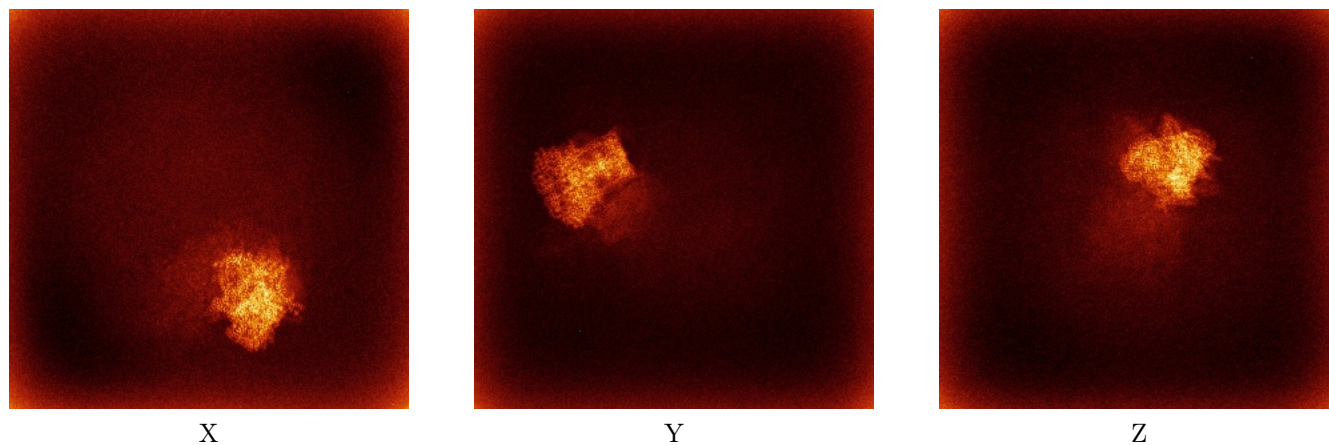
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



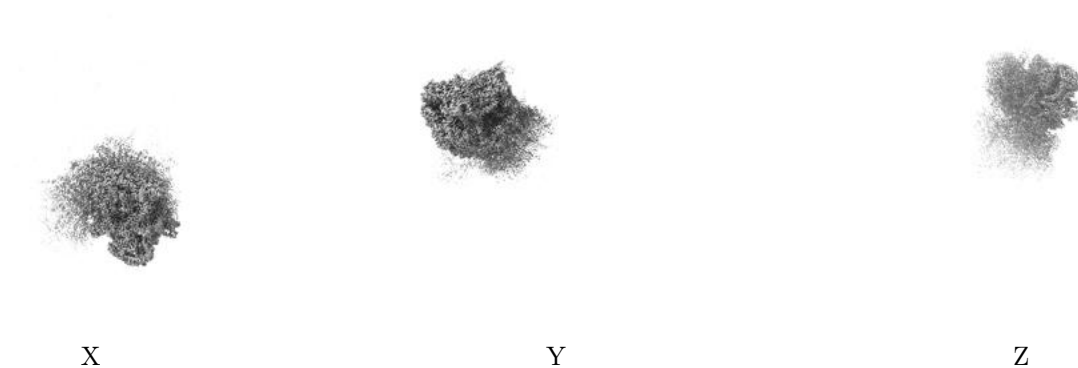
6.4.2 Raw map



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

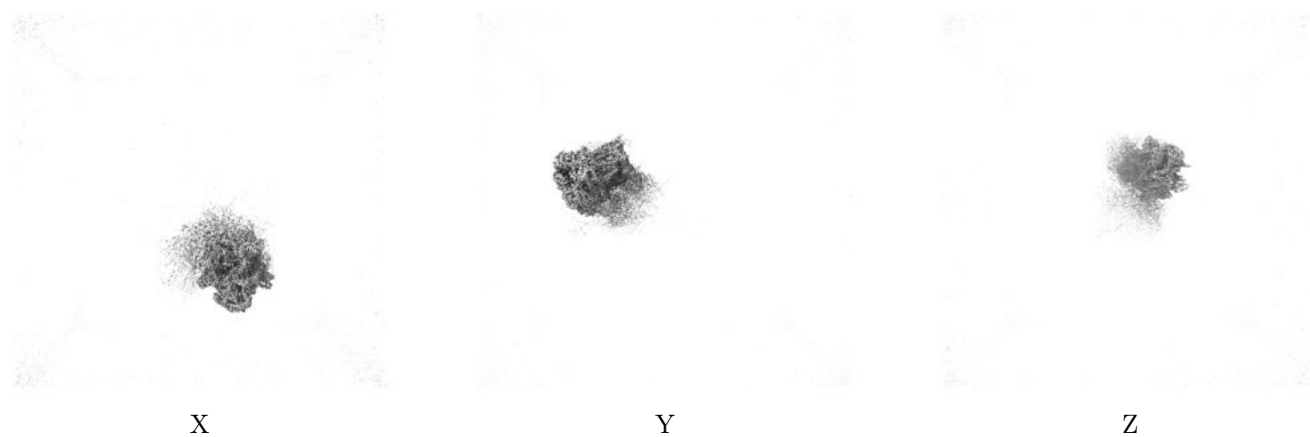
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

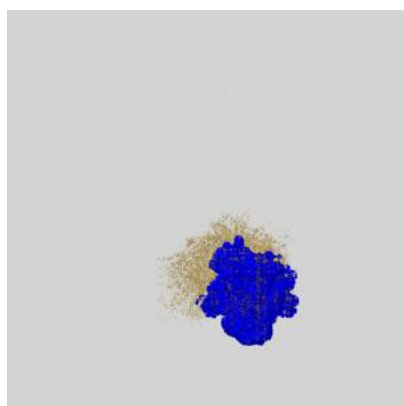
6.6 Mask visualisation [i](#)

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

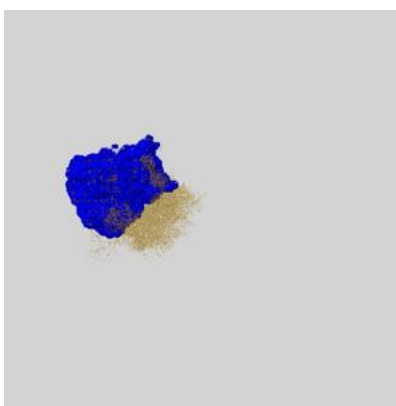
A mask typically either:

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

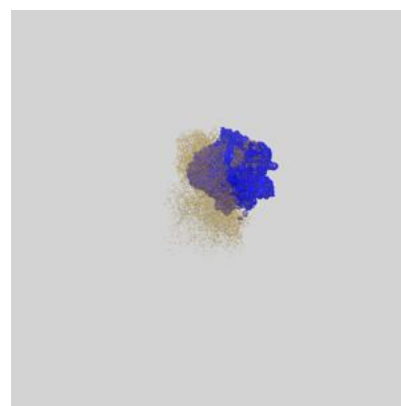
6.6.1 emd_15868_msk_1.map [i](#)



X



Y

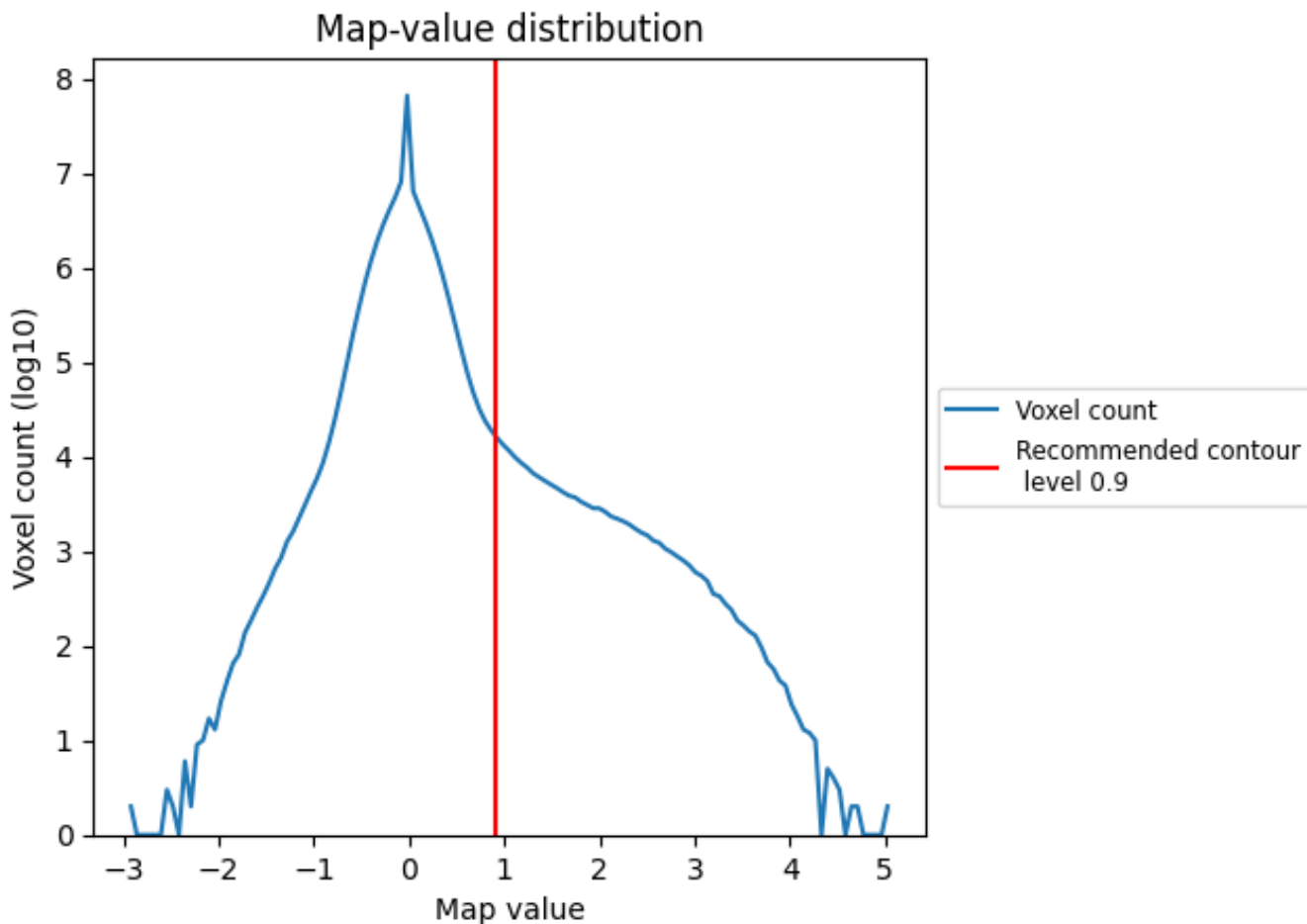


Z

7 Map analysis [i](#)

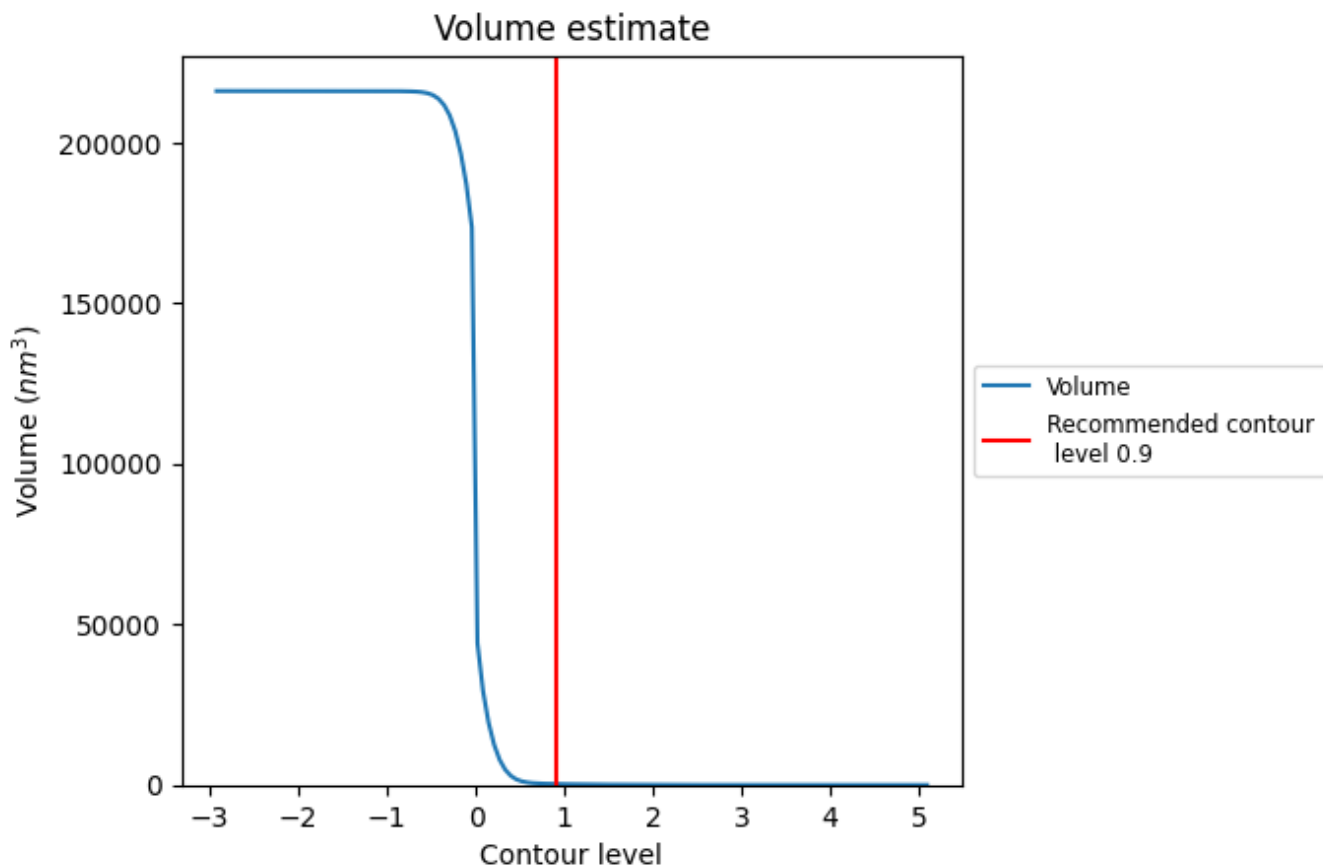
This section contains the results of statistical analysis of the map.

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.

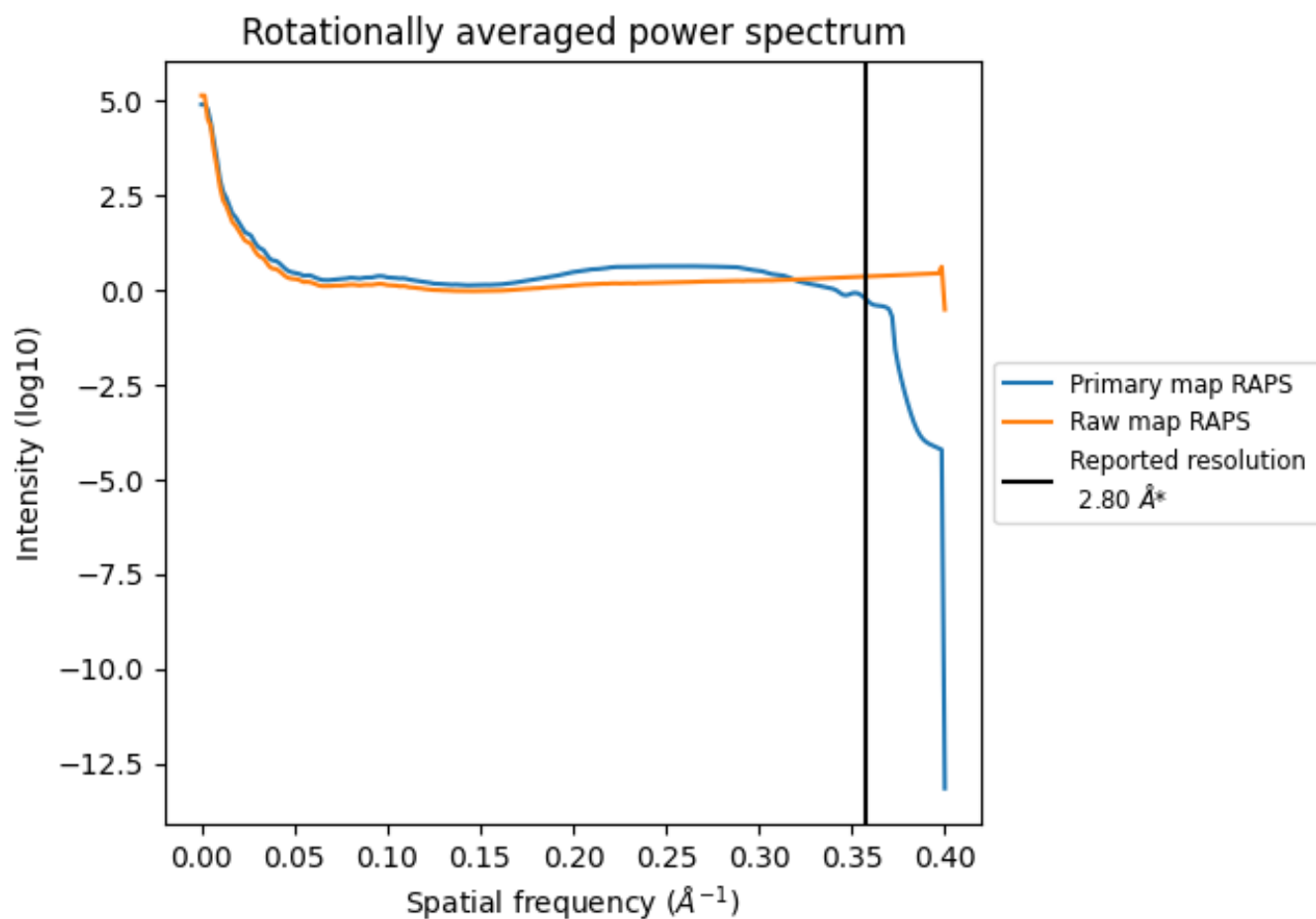
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

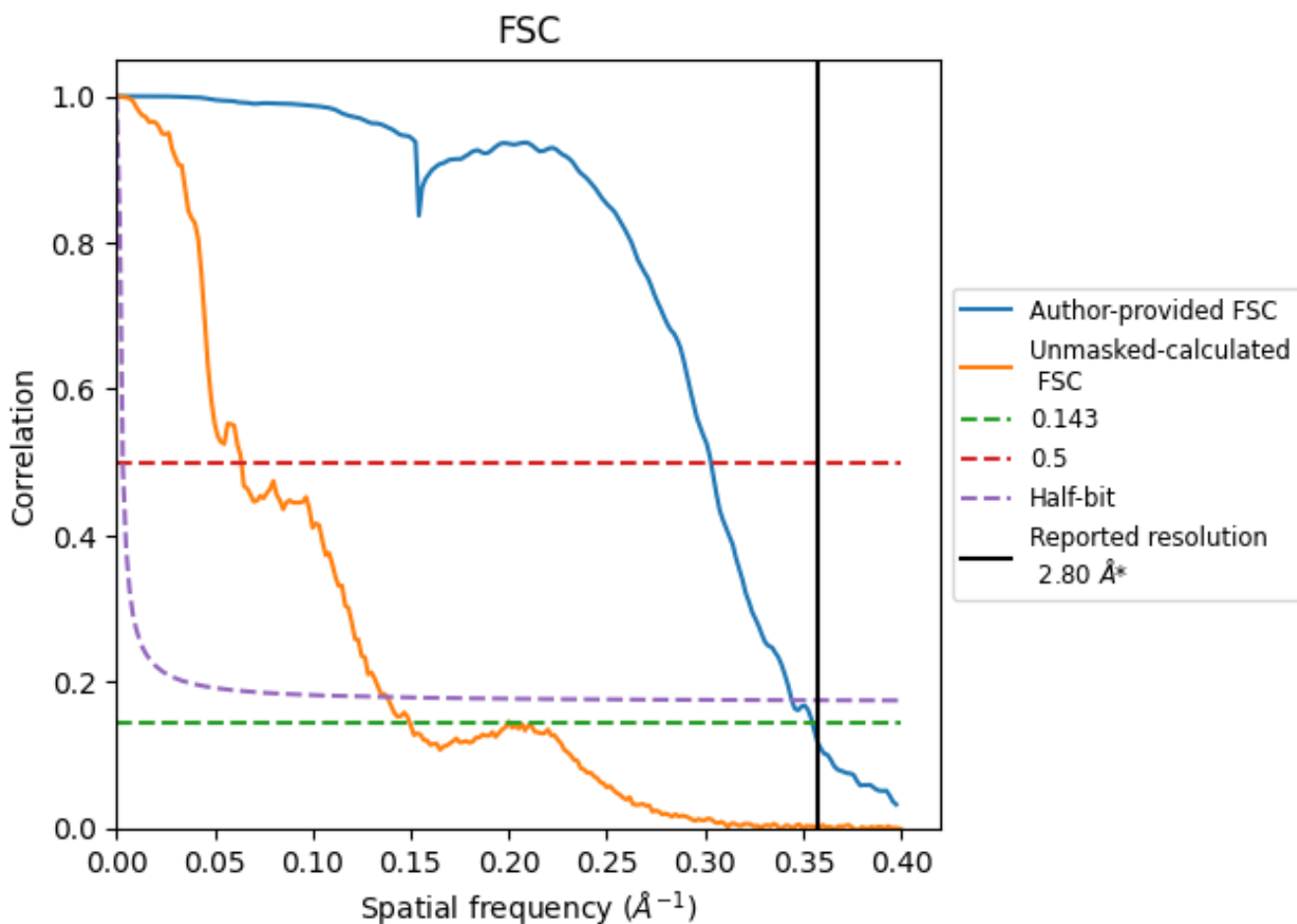


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

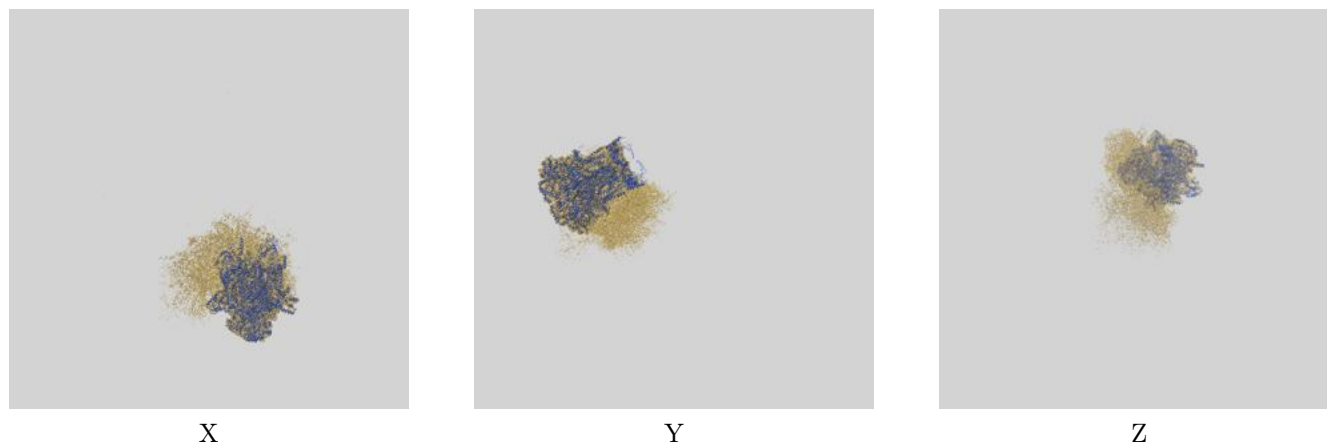
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.30	2.91
Unmasked-calculated*	6.68	15.70	7.25

*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 6.68 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

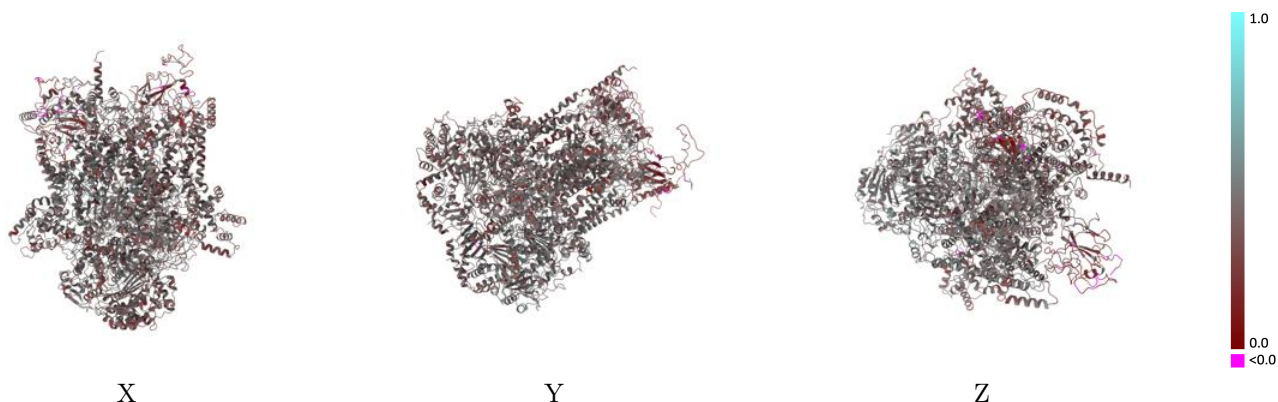
This section contains information regarding the fit between EMDB map EMD-15868 and PDB model 8B6J. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



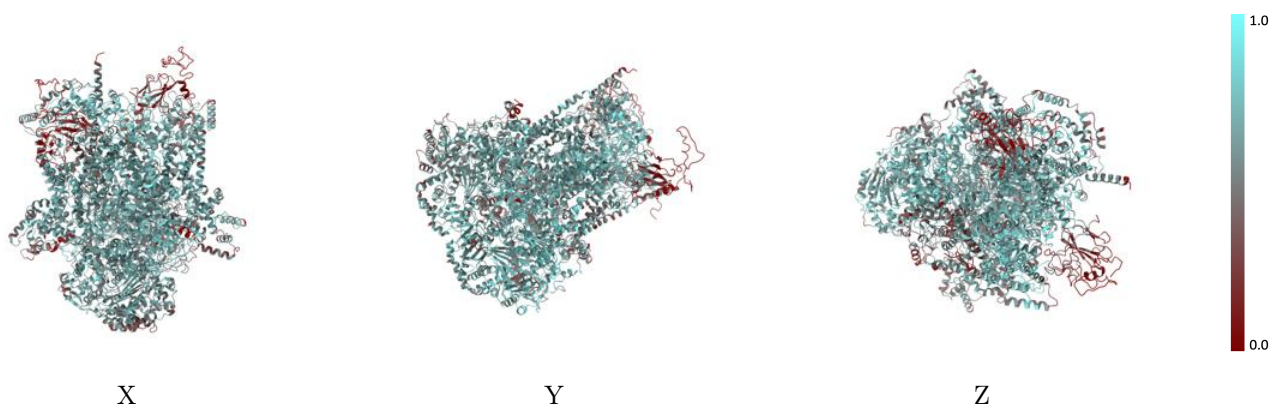
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



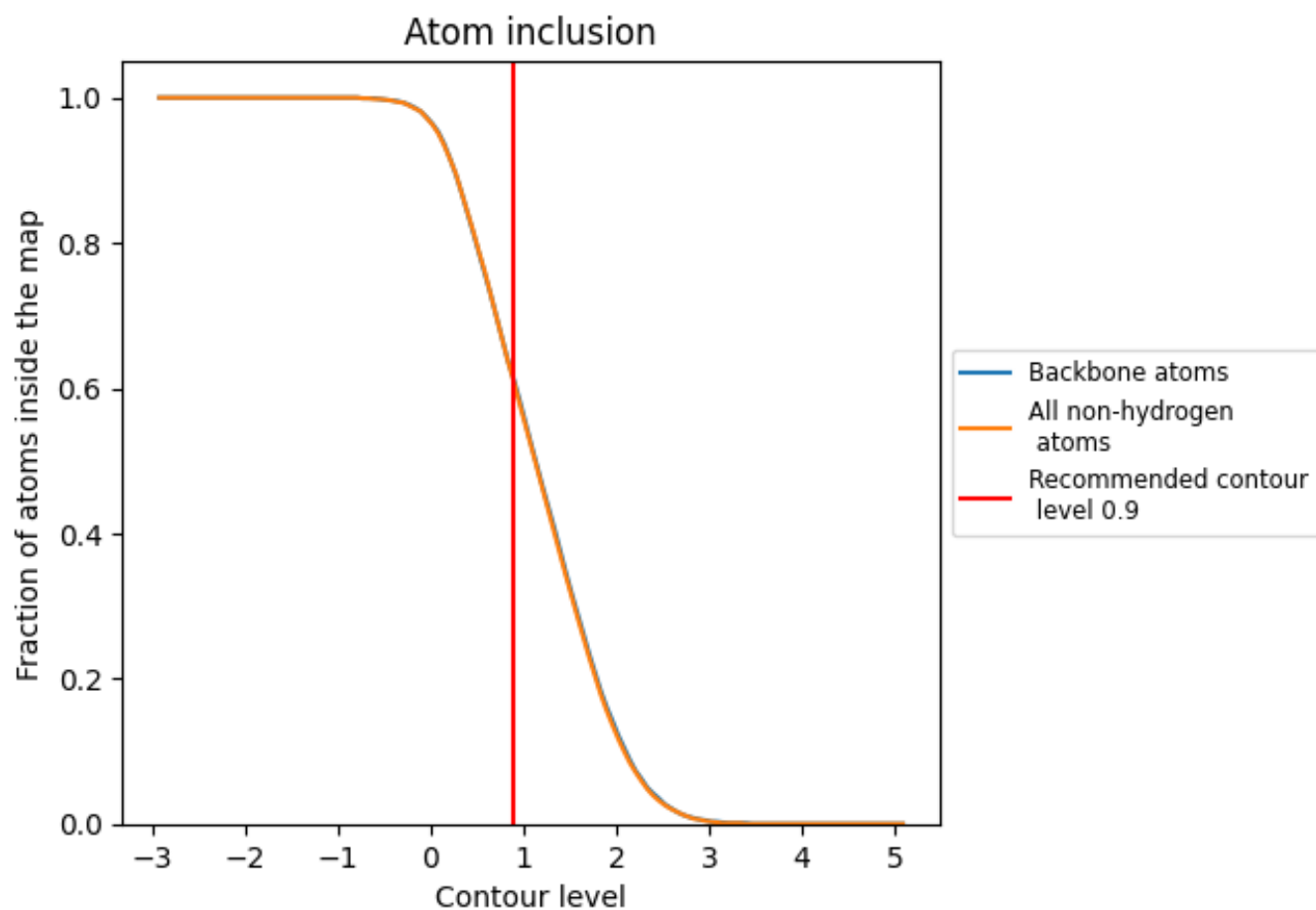
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6080	 0.4020
A	 0.7270	 0.4460
B	 0.6740	 0.4180
C	 0.6400	 0.3960
D	 0.6820	 0.4350
E	 0.3410	 0.3480
F	 0.5350	 0.3750
G	 0.6460	 0.3970
H	 0.6190	 0.3890
I	 0.5680	 0.4450
J	 0.2210	 0.2880
K	 0.6530	 0.4010
L	 0.6240	 0.3650
a	 0.6270	 0.3940
b	 0.6430	 0.4060
c	 0.6280	 0.4190
d	 0.7050	 0.4080
e	 0.4070	 0.3300
f	 0.5410	 0.3350
g	 0.5910	 0.4150
h	 0.5160	 0.4320
i	 0.6070	 0.3770
j	 0.2330	 0.2250
k	 0.6180	 0.3910
l	 0.6590	 0.4440

