



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 05:32 pm GMT

PDB ID : 6T15
EMDB ID : EMD-10318
Title : The III2-IV(5B)1 respiratory supercomplex from *S. cerevisiae*
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.
Deposited on : 2019-10-03
Resolution : 3.29 Å (reported)
Based on initial model : 6HU9

This is a wwPDB EM Validation Summary 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:

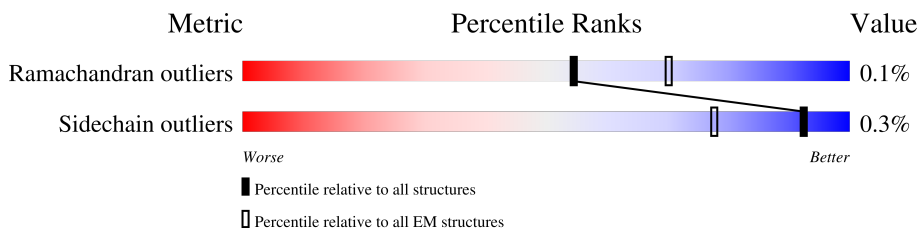
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.29 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	431	100%
1	L	431	100%
2	B	352	100%
2	M	352	99%
3	C	385	100%
3	N	385	99%
4	D	248	100%
4	O	248	100%
5	E	185	98%

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Mol	Chain	Length	Quality of chain
5	P	185	100% 98%
6	F	147	51% 50% 49%
6	Q	147	51% 50% 49%
7	G	127	99%
7	R	127	99% 98%
8	H	94	99% 98%
8	S	94	99% 98%
9	I	66	86% 86% 14%
9	T	66	86% 86% 14%
10	J	77	99%
10	U	77	99%
11	a	534	98%
12	b	236	99%
13	c	269	99%
14	d	130	92% 7%
15	e	134	13% 99%
16	f	108	95%
17	g	59	98%
18	h	51	100%
19	i	55	100%
20	j	82	91% 6%
21	k	131	89% 10%
22	l	66	67% 32%
23	m	224	44% 56%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	HEA	a	602	X	-	-	-
31	HEA	a	603	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 48966 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-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3345	2110	576	653	6	0	0
1	L	431	3345	2110	576	653	6	0	0

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	352	2735	1747	453	534	1	0	0
2	M	352	2735	1747	453	534	1	0	0

- Molecule 3 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	385	3090	2082	484	503	21	0	0
3	N	385	3090	2082	484	503	21	0	0

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6, COMPLEX III SUBUNIT VI, CYTOCHROME C1 NON-HEME 17 KDA PROTEIN, MITOCHONDRIAL HINGE PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			465	310	77	78		
9	T	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

- Molecule 11 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 12 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

- Molecule 13 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	c	269	2146	1430	344	357	15	0	0

- Molecule 14 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	d	121	913	576	151	181	5	0	0

- Molecule 15 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	e	134	1083	694	188	199	2	0	0

- Molecule 16 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	f	104	866	554	141	170	1	0	0

- Molecule 17 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	g	59	484	328	83	73	0	0

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	h	51	409	278	66	64	1	0	0

- Molecule 19 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	i	55	456	300	79	74	3	0	0

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	j	77	642	410	109	118	5	0	0

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	k	118	967	626	167	171	3	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799

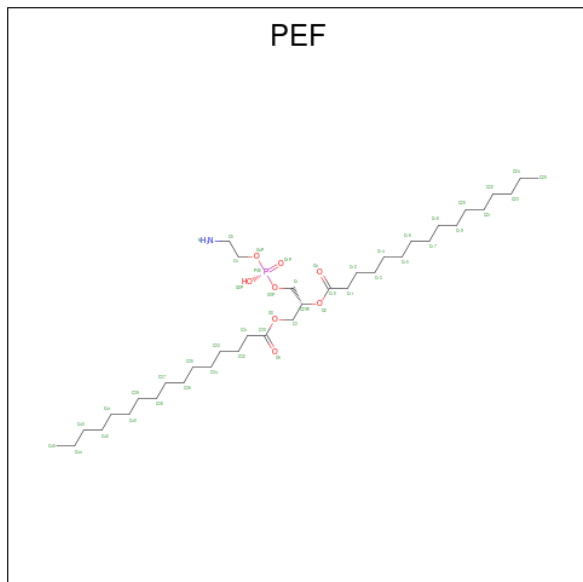
- Molecule 22 is a protein called COX26; SYNONYM: Uncharacterized protein YDR119W-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	l	45	361	238	63	59	1	0	0

- Molecule 23 is a protein called RCF2; SYNONYM: Respiratory supercomplex factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	m	99	799	511	140	144	4	0	0

- Molecule 24 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P).



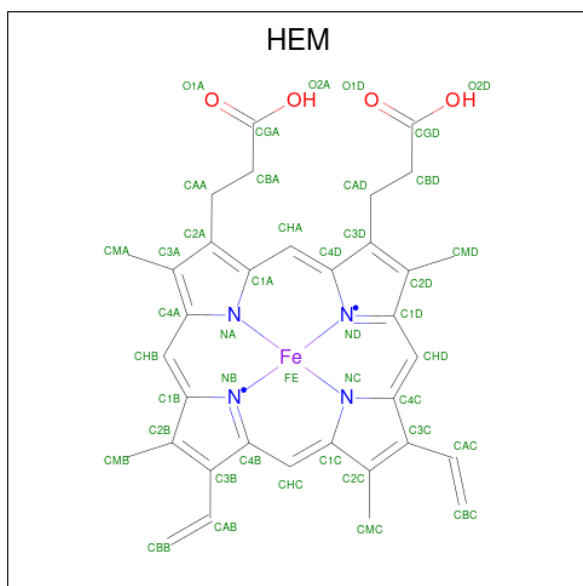
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	A	1	Total 31	C 21	N 1	O 8	P 1	0
24	C	1	Total 83	C 63	N 2	O 16	P 2	0
24	C	1	Total 83	C 63	N 2	O 16	P 2	0
24	E	1	Total 43	C 33	N 1	O 8	P 1	0
24	H	1	Total 32	C 22	N 1	O 8	P 1	0
24	J	1	Total 29	C 19	N 1	O 8	P 1	0
24	L	1	Total 36	C 26	N 1	O 8	P 1	0
24	N	1	Total 83	C 63	N 2	O 16	P 2	0
24	N	1	Total 83	C 63	N 2	O 16	P 2	0
24	P	1	Total 42	C 32	N 1	O 8	P 1	0
24	S	1	Total 36	C 26	N 1	O 8	P 1	0
24	U	1	Total 47	C 37	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	a	1	Total 33	C 23	N 1	O 8	P 1	0
24	b	1	Total 73	C 53	N 2	O 16	P 2	0
24	b	1	Total 73	C 53	N 2	O 16	P 2	0
24	c	1	Total 77	C 57	N 2	O 16	P 2	0
24	c	1	Total 77	C 57	N 2	O 16	P 2	0
24	e	1	Total 42	C 32	N 1	O 8	P 1	0

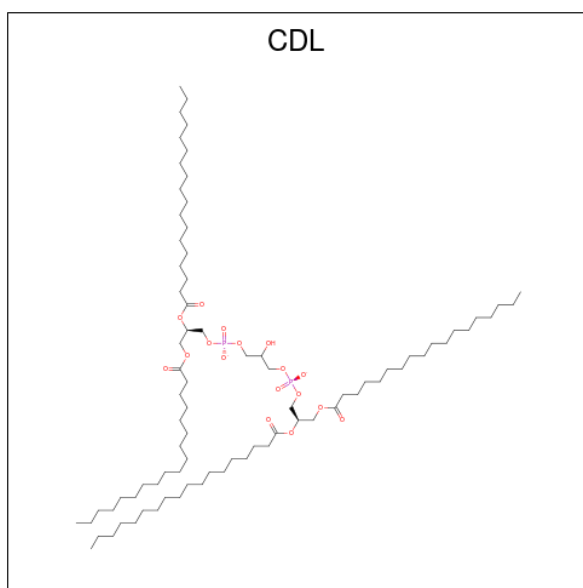
- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
25	C	1	Total 86	C 68	Fe 2	N 8	O 8	0
25	C	1	Total 86	C 68	Fe 2	N 8	O 8	0
25	N	1	Total 86	C 68	Fe 2	N 8	O 8	0
25	N	1	Total 86	C 68	Fe 2	N 8	O 8	0

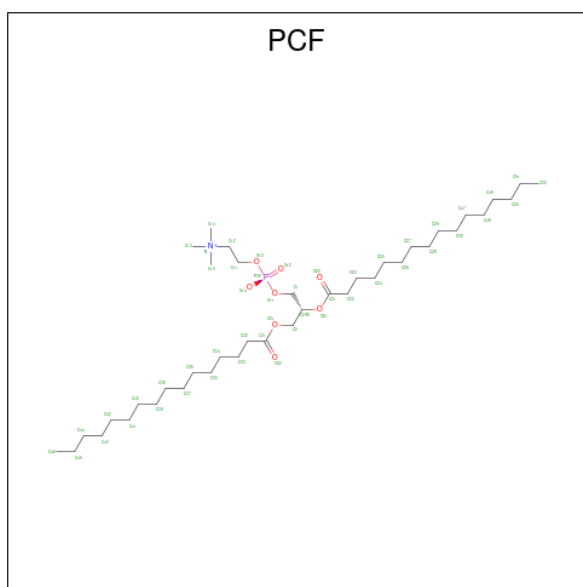
- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	C	1	55	36	17	2	0
26	D	1	67	48	17	2	0
26	H	1	53	34	17	2	0
26	L	1	58	39	17	2	0
26	N	1	66	47	17	2	0
26	O	1	71	52	17	2	0
26	S	1	53	34	17	2	0

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



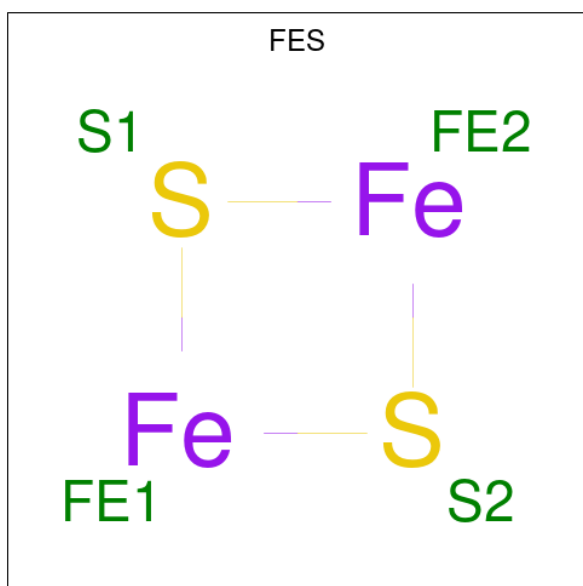
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	C	1	50	40	1	8	1	0
27	I	1	39	29	1	8	1	0
27	N	1	39	29	1	8	1	0
27	S	1	32	22	1	8	1	0
27	T	1	50	40	1	8	1	0
27	e	1	36	26	1	8	1	0

- Molecule 28 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



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

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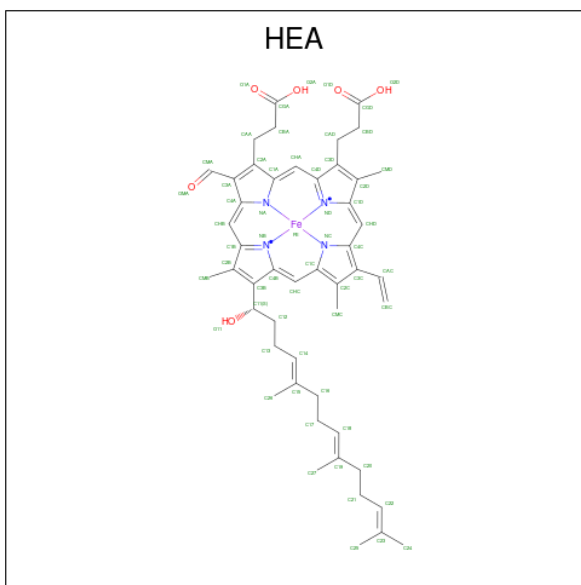
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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
29	P	1	4	2	2	0

- Molecule 30 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
30	a	1	1	1	0

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).

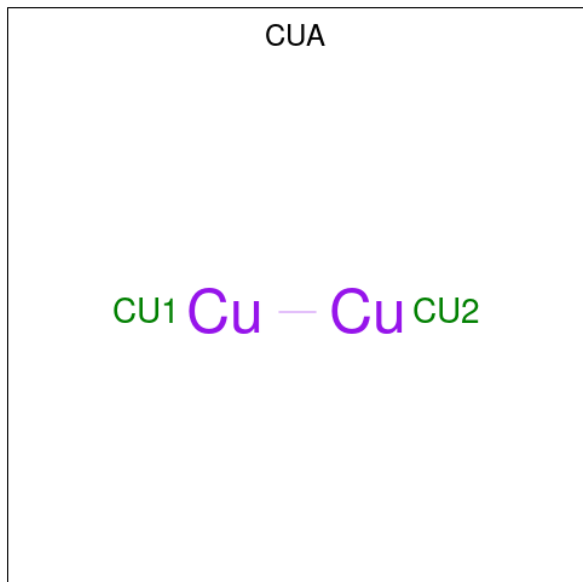


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
31	a	1	120	98	2	8	12	0
31	a	1	120	98	2	8	12	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
32	a	1	1	1	0

- Molecule 33 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
33	b	1	2	2	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	d	1	1	1	0

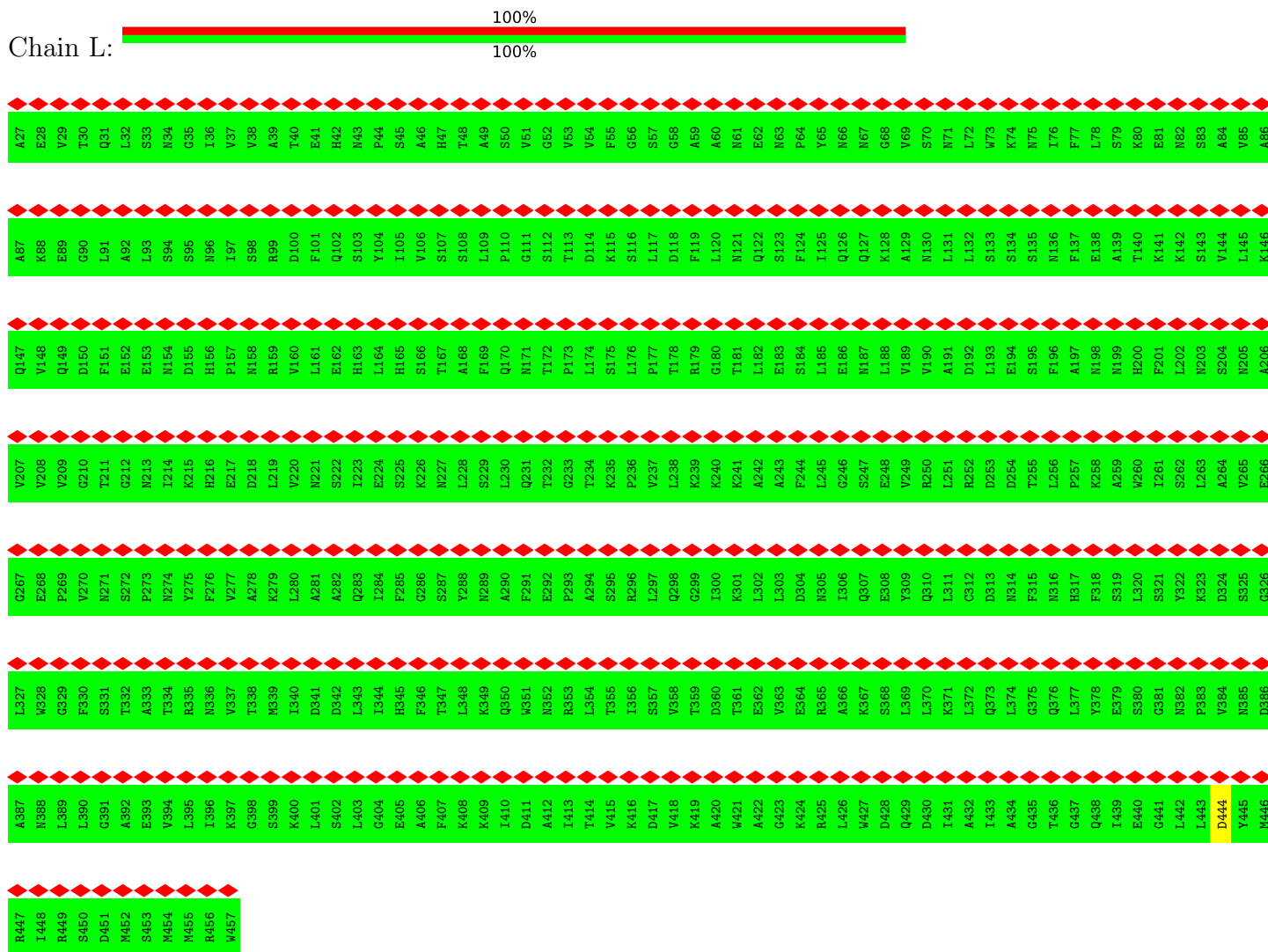
3 Residue-property plots [i](#)

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

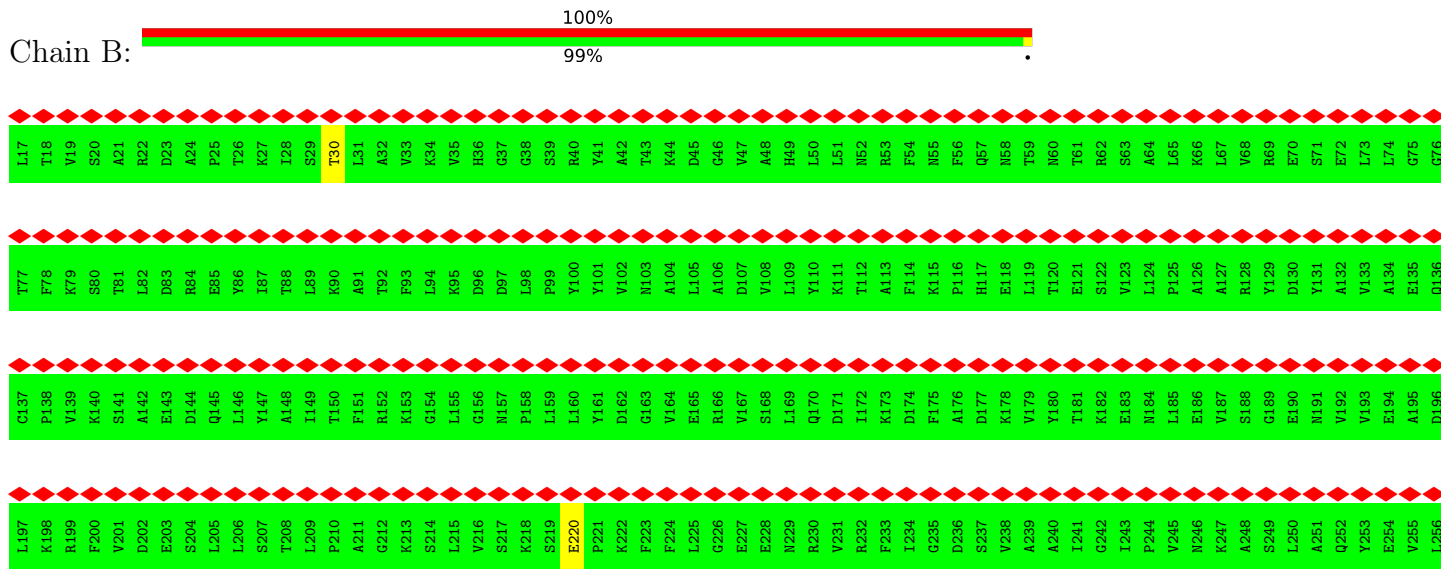
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1



- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1



● Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2



A257 N258 N259 N260 N261 N262 N263 N264 N265 N266 N267 N268 N269 N270 N271 N272 N273 N274 N275 N276 N277 N278 N279 N280 N281 N282 N283 N284 N285 N286 N287 N288 N289 N290 N291 N292 N293 N294 N295 N296 N297 N298 N299 N300 N301 N302 N303 N304 N305 N306 N307 N308 N309 N310 N311 N312 N313 N314 N315 P316

A317 I318 N319 Y320 T321 K322 K323 K324 N325 A326 V327 Q328 N329 E330 E331 V332 S333 S334 P335 I336 E337 L338 N339 F340 D341 A342 V343 K344 D345 F346 K347 L348 G349 K350 F351 N352 Y353 Y354 A355 V356 G357 D358 V359 N360 N361 K362 P363 Y364 L365 D366 E367 L368

● Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2



L17 T18 V19 S20 A21 R22 D23 A24 P25 T26 K27 I28 S29 L29 T30 L31 A32 A33 K34 V35 H36 D37 G38 S39 R40 Y41 Y42 A43 T43 T44 D45 G46 V47 A48 L49 H49 L50 L51 N52 N53 A54 F54 N55 F56 Q57 N58 T59 N60 T61 R62 S63 A64 L65 K66 L67 V68 R69 E70 E71 S71 E72 L73 L74 G75 G76

T77 F78 K79 S80 T81 L82 D83 R84 E85 E86 Y87 T88 L89 K90 K91 A92 T92 T93 L94 K95 D96 D97 L98 P99 Y100 Y101 Y102 N103 A104 L105 A106 D107 V108 L109 H110 K111 T112 A113 F114 K115 P116 H117 L118 T119 L120 T121 E122 V123 L124 P125 K126 A127 A128 Y129 D130 Y131 A132 V133 A134 E135 O136

C137 P138 V139 K140 S141 A142 E143 D144 L205 L206 Y147 T208 L209 P210 A211 R152 K153 G154 L215 V216 S217 K218 S219 E220 P221 F222 F223 V224 L225 G226 E227 S228 L229 A239 A240 G241 I243 V244 N245 E186 V187 S188 L189 E190 N191 Q252 V193 E194 A195 D196

L197 K198 R199 F200 T201 D202 E203 S204 L206 S207 T208 L209 P210 A211 R152 K153 G154 L215 V216 S217 K218 S219 E220 P221 F222 F223 V224 L225 G226 E227 S228 L229 A239 A240 G241 I243 V244 N245 E186 V187 S188 L189 E190 N191 Q252 V193 E194 A195 D196

A257 N258 N259 N260 N261 N262 N263 N264 N265 N266 N267 N268 N269 N270 N271 N272 N273 N274 N275 N276 N277 N278 N279 N280 N281 N282 N283 N284 N285 N286 N287 N288 N289 N290 N291 N292 N293 N294 N295 N296 N297 N298 N299 N300 N301 N302 N303 N304 N305 N306 N307 N308 N309 N310 N311 N312 N313 N314 N315 P316

A317 I318 N319 Y320 T321 K322 K323 K324 N325 A326 V327 Q328 N329 E330 E331 V332 S333 S334 P335 I336 E337 L338 N339 F340 D341 A342 V343 K344 D345 F346 K347 L348 G349 K350 F351 N352 Y353 Y354 A355 V356 G357 D358 V359 N360 N361 K362 P363 Y364 L365 D366 E367 L368

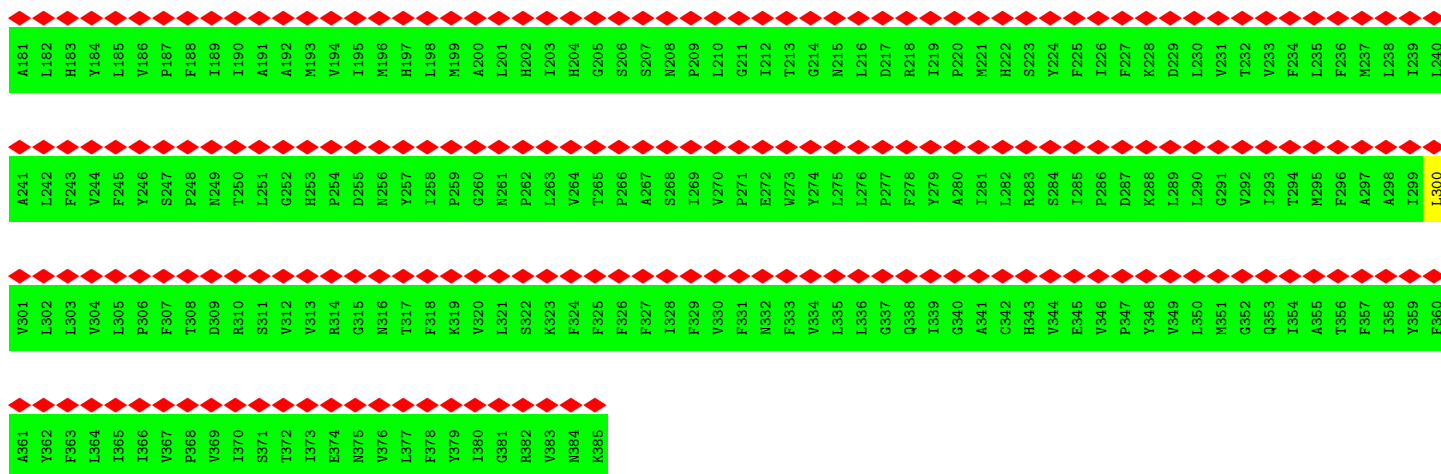
● Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2



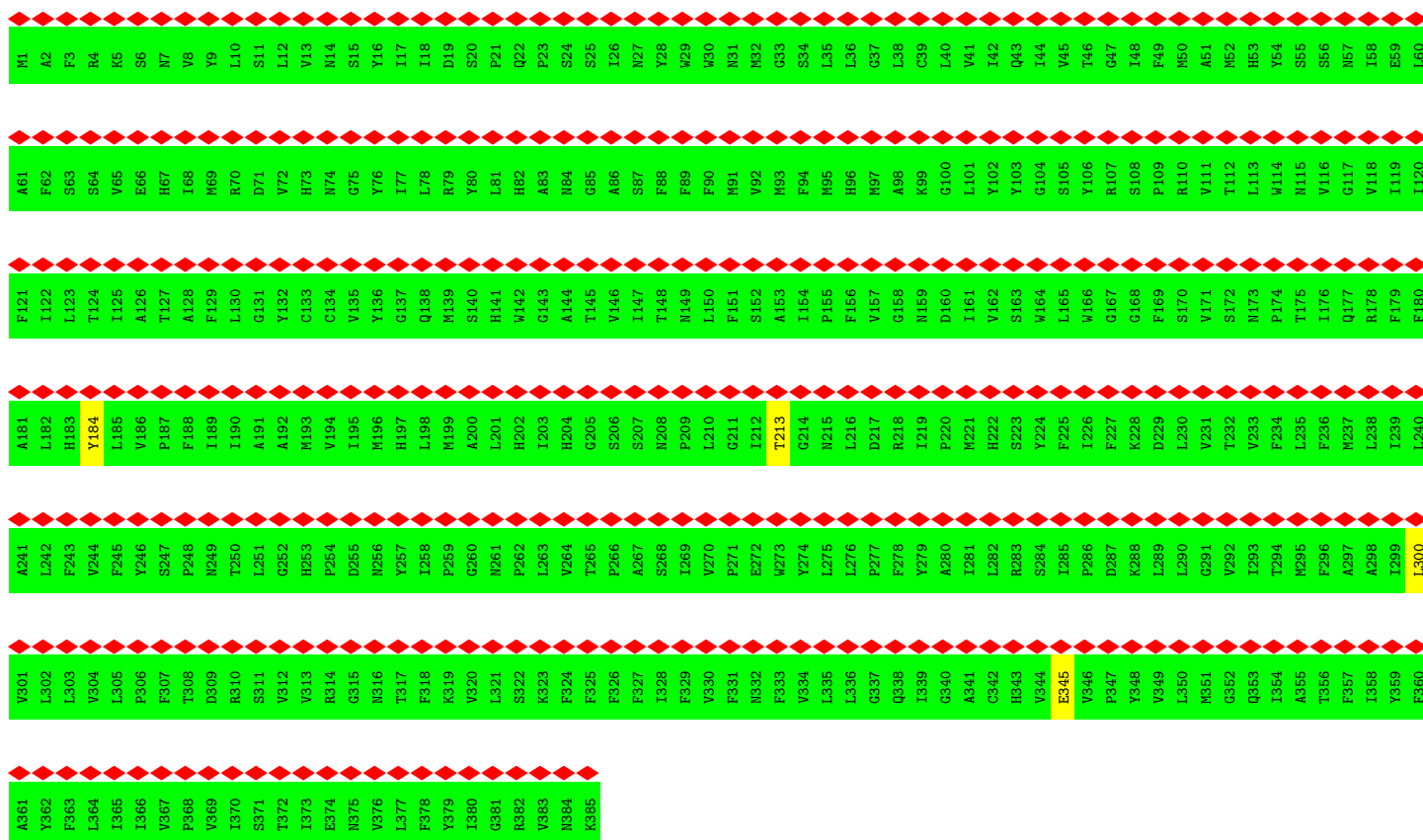
M1 A2 F3 R4 K5 S6 M7 V8 Y9 L10 S11 L12 V13 M14 S15 Y16 I17 I18 D19 S20 P21 Q22 P23 S24 S25 I26 M27 Y28 M29 W30 N31 K32 G33 L35 L36 G37 L38 C39 L40 L41 L42 Q43 L44 W45 T46 O47 I48 F49 M50 A51 M52 H53 Y54 M55 S56 M57 L58 E59 L60

A61 F62 S63 S64 V65 E66 T67 I68 M69 R70 D71 V72 H73 M74 G75 Y76 I77 L78 R79 Y80 L81 H82 A83 N84 G85 A86 S87 F88 M89 F90 M91 V92 M93 I94 M95 F96 M97 G98 A99 G100 L101 L102 Y103 G104 S105 L106 R107 S108 F109 R110 V111 T112 L113 W114 M115 V116 G117 L118 I119 I120

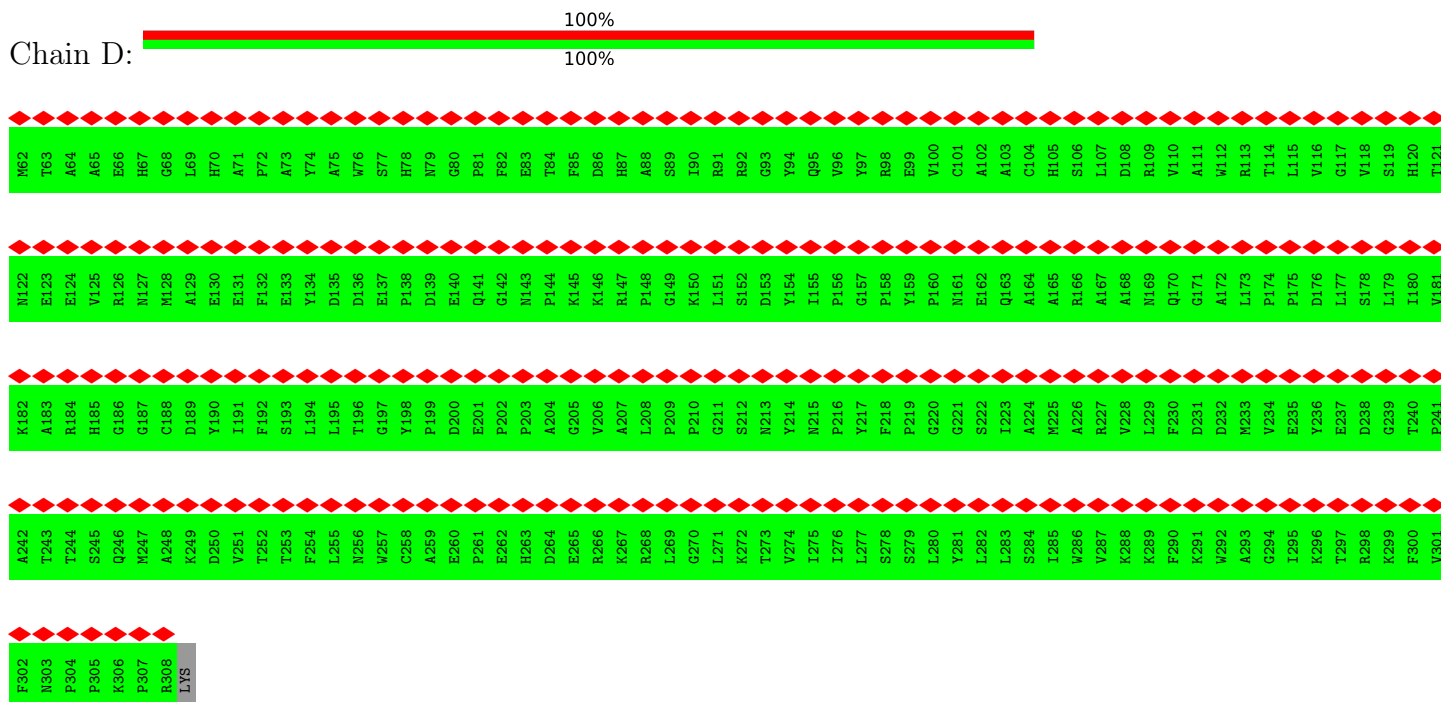
F121 I122 L123 T124 I125 A126 T127 A128 F129 L130 G131 Y132 C133 M134 V135 Y136 I137 M139 S140 H141 W142 G143 A144 T145 I146 L147 T148 M149 L150 F151 S152 A153 P155 F156 V157 G158 N159 D160 I161 V162 S163 W164 L165 L166 R167 G168 F169 S170 V171 S172 M173 P174 T175 I176 G177 R178 F179 F180



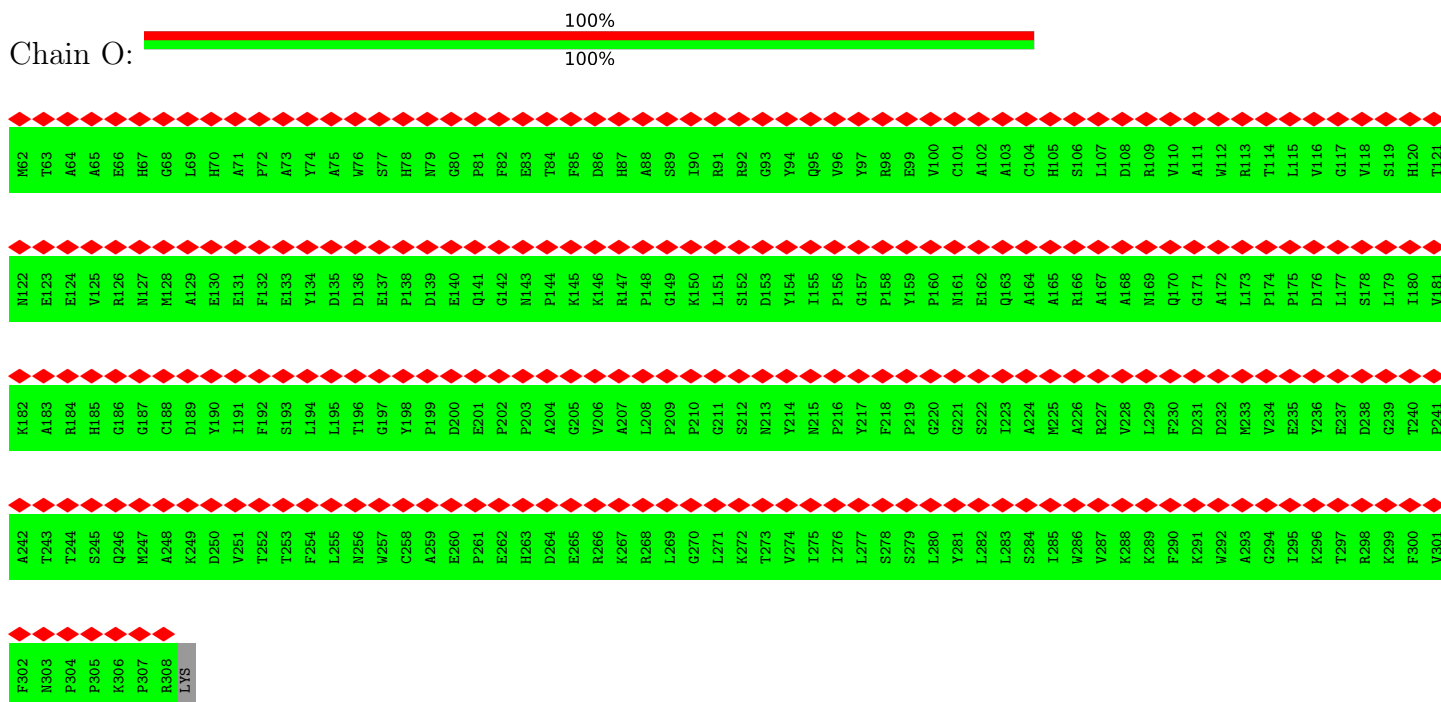
- Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2



- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1



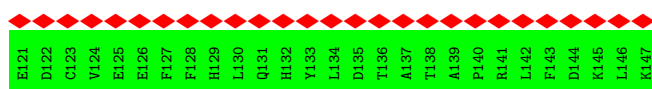
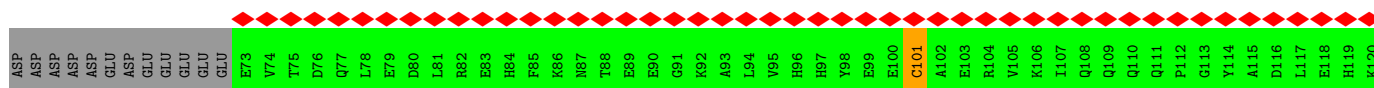
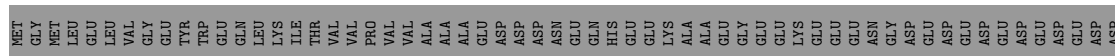
- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1



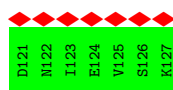
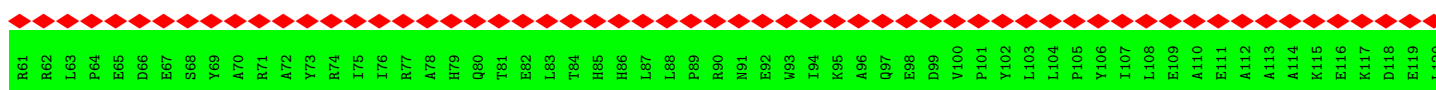
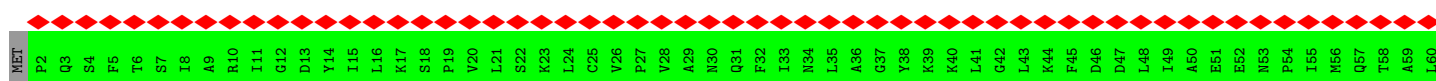
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT



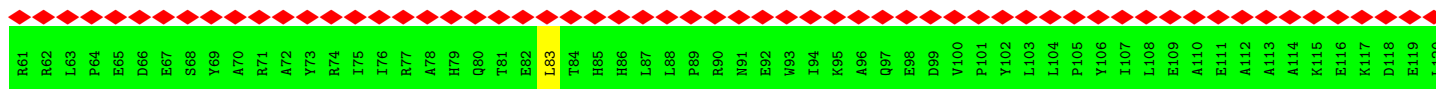
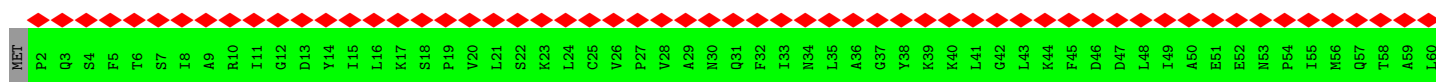
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6, COMPLEX III SUBUNIT VI, CYTOCHROME C1 NON-HEME 17 KDA PROTEIN, MITOCHONDRIAL HINGE PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN

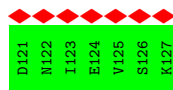


- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

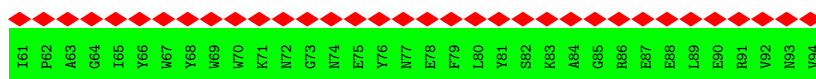
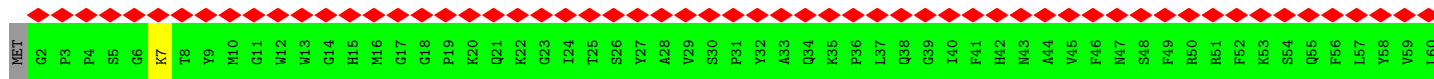


- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

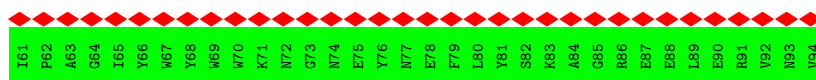
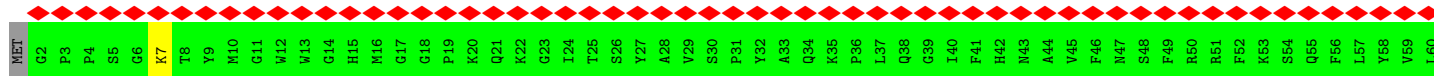




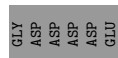
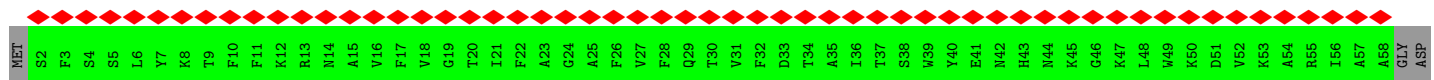
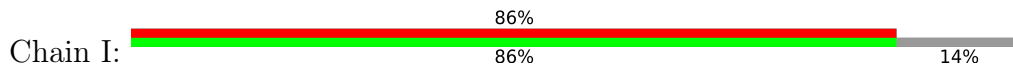
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



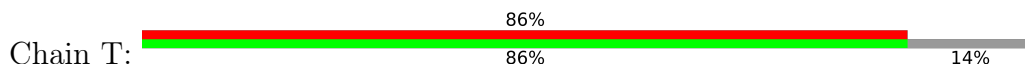
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

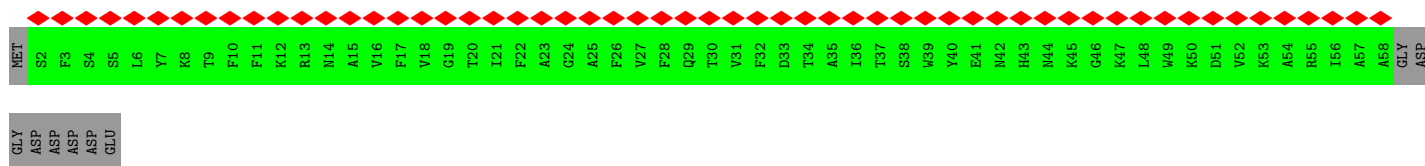


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

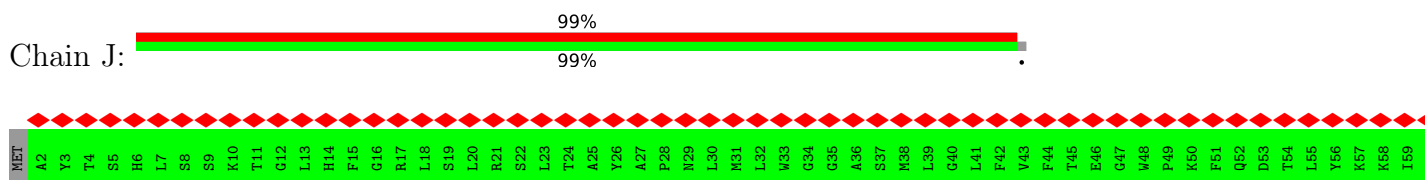


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

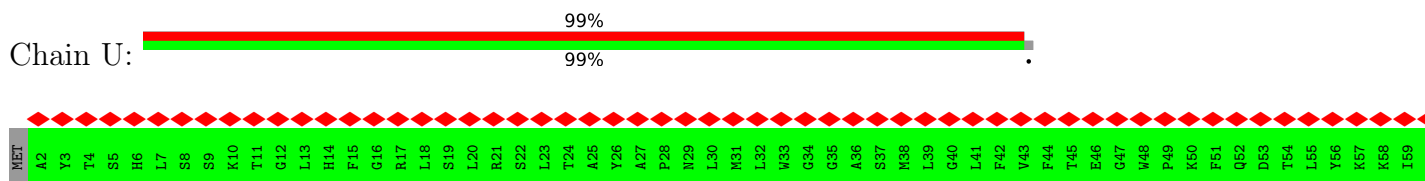




- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10,COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN



- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10,COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN



- Molecule 11: CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1

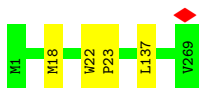


- Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2



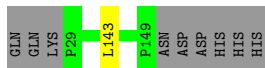
- Molecule 13: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

Chain c:  99%



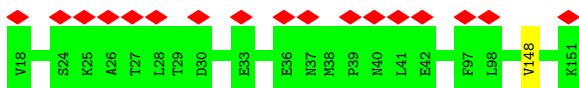
- Molecule 14: CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4

Chain d:  92% 7%



- Molecule 15: CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B

Chain e:  13% 99%



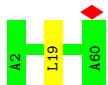
- Molecule 16: CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6

Chain f:  95%



- Molecule 17: CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7

Chain g:  98%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9

Chain i:  100%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73042	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 ($e^-/\text{\AA}^2$)	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.004	Depositor
Minimum map value	-1.391	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.424	Depositor
Map size (Å)	402.432, 402.432, 402.432	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: HEC, HEA, FES, MG, HEM, PEF, CUA, CU, CDL, ZN, PCF

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	0.29	0/3406	0.52	0/4615
1	L	0.30	0/3406	0.55	0/4615
2	B	0.31	0/2781	0.54	0/3764
2	M	0.31	0/2781	0.54	0/3764
3	C	0.34	0/3192	0.56	1/4354 (0.0%)
3	N	0.34	0/3192	0.56	1/4354 (0.0%)
4	D	0.30	0/2012	0.46	0/2740
4	O	0.31	0/2012	0.46	0/2740
5	E	0.31	0/1444	0.60	1/1957 (0.1%)
5	P	0.33	0/1444	0.66	2/1957 (0.1%)
6	F	0.36	0/647	0.66	1/870 (0.1%)
6	Q	0.38	1/647 (0.2%)	0.57	0/870
7	G	0.31	0/1040	0.54	0/1408
7	R	0.28	0/1040	0.52	1/1408 (0.1%)
8	H	0.29	0/804	0.46	0/1088
8	S	0.30	0/804	0.49	0/1088
9	I	0.29	0/479	0.45	0/646
9	T	0.29	0/479	0.45	0/646
10	J	0.30	0/619	0.58	0/841
10	U	0.31	0/619	0.57	0/841
11	a	0.35	0/4290	0.64	6/5857 (0.1%)
12	b	0.34	0/1941	0.64	2/2653 (0.1%)
13	c	0.34	0/2218	0.59	1/3036 (0.0%)
14	d	0.31	0/932	0.58	0/1269
15	e	0.31	0/1111	0.57	0/1503
16	f	0.36	0/884	0.54	0/1196
17	g	0.35	0/500	0.67	1/681 (0.1%)
18	h	0.34	0/424	0.60	0/569
19	i	0.33	0/468	0.49	0/626
20	j	0.37	0/664	0.58	0/899
21	k	0.29	0/1002	0.54	0/1364
22	l	0.30	0/372	0.59	0/502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	m	0.34	0/813	0.58	0/1093
All	All	0.32	1/48467 (0.0%)	0.56	17/65814 (0.0%)

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	L	0	1
2	B	0	1
3	N	0	1
5	E	0	1
5	P	0	1
11	a	0	4
13	c	0	1
14	d	0	1
21	k	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	101	CYS	CB-SG	-5.00	1.73	1.81

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	156	LEU	CA-CB-CG	7.14	131.73	115.30
12	b	172	ASP	CB-CG-OD2	7.14	124.72	118.30
5	E	156	LEU	CA-CB-CG	6.23	129.62	115.30
11	a	200	LEU	CA-CB-CG	6.18	129.52	115.30
3	C	300	LEU	CA-CB-CG	6.17	129.48	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	GLU	Peptide
5	E	167	ILE	Peptide
1	L	444	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	N	345	GLU	Peptide
5	P	125	GLU	Peptide

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	429/431 (100%)	397 (92%)	32 (8%)	0	100	100
1	L	429/431 (100%)	394 (92%)	35 (8%)	0	100	100
2	B	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
2	M	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
3	C	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
3	N	383/385 (100%)	357 (93%)	26 (7%)	0	100	100
4	D	245/248 (99%)	239 (98%)	6 (2%)	0	100	100
4	O	245/248 (99%)	241 (98%)	4 (2%)	0	100	100
5	E	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
5	P	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
6	F	73/147 (50%)	68 (93%)	5 (7%)	0	100	100
6	Q	73/147 (50%)	70 (96%)	3 (4%)	0	100	100
7	G	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
8	S	91/94 (97%)	85 (93%)	6 (7%)	0	100	100
9	I	55/66 (83%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	55/66 (83%)	55 (100%)	0	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	490 (92%)	40 (8%)	2 (0%)	34	66
12	b	234/236 (99%)	214 (92%)	20 (8%)	0	100	100
13	c	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	34	66
14	d	119/130 (92%)	101 (85%)	18 (15%)	0	100	100
15	e	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
16	f	102/108 (94%)	96 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
18	h	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
20	j	75/82 (92%)	67 (89%)	8 (11%)	0	100	100
21	k	116/131 (88%)	103 (89%)	13 (11%)	0	100	100
22	l	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
23	m	97/224 (43%)	91 (94%)	6 (6%)	0	100	100
All	All	5890/6303 (93%)	5521 (94%)	366 (6%)	3 (0%)	54	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	a	121	SER
11	a	521	PRO
13	c	23	PRO

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	370/370 (100%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	300 (100%)	1 (0%)	92	96
2	M	301/301 (100%)	301 (100%)	0	100	100
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	336 (99%)	2 (1%)	86	91
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	150 (99%)	1 (1%)	84	90
5	P	151/151 (100%)	151 (100%)	0	100	100
6	F	68/131 (52%)	67 (98%)	1 (2%)	65	81
6	Q	68/131 (52%)	67 (98%)	1 (2%)	65	81
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	76 (99%)	1 (1%)	69	82
8	S	77/78 (99%)	76 (99%)	1 (1%)	69	82
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	65 (100%)	0	100	100
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	446 (100%)	1 (0%)	93	97
12	b	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	227 (100%)	1 (0%)	91	95
14	d	102/111 (92%)	102 (100%)	0	100	100
15	e	115/115 (100%)	114 (99%)	1 (1%)	78	87
16	f	92/96 (96%)	91 (99%)	1 (1%)	73	85
17	g	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
20	j	69/73 (94%)	67 (97%)	2 (3%)	42	69
21	k	104/113 (92%)	104 (100%)	0	100	100
22	l	36/53 (68%)	35 (97%)	1 (3%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	m	84/191 (44%)	84 (100%)	0	100	100
All	All	5087/5385 (94%)	5072 (100%)	15 (0%)	92	96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	7	LYS
20	j	41	LYS
11	a	244	VAL
22	l	65	LYS
16	f	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
10	U	29	ASN
13	c	47	ASN
11	a	99	ASN
11	a	482	ASN
23	m	149	GLN

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](#)

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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
25	HEM	C	602	3	41,50,50	1.37	4 (9%)	45,82,82	1.83	11 (24%)
24	PEF	c	301	-	35,35,46	1.08	2 (5%)	38,40,51	1.14	3 (7%)
24	PEF	A	501	1	30,30,46	1.17	2 (6%)	33,35,51	1.12	3 (9%)
24	PEF	H	602	-	31,31,46	1.16	2 (6%)	34,36,51	1.24	4 (11%)
26	CDL	N	603	26	65,65,99	1.12	4 (6%)	71,77,111	1.16	6 (8%)
27	PCF	e	202	15	35,35,49	1.13	2 (5%)	41,43,57	1.06	3 (7%)
24	PEF	P	302	-	41,41,46	1.00	2 (4%)	44,46,51	1.04	3 (6%)
31	HEA	a	602	11	57,67,67	2.04	16 (28%)	61,103,103	2.63	27 (44%)
26	CDL	D	402	-	66,66,99	1.12	4 (6%)	72,78,111	1.19	6 (8%)
24	PEF	c	302	-	40,40,46	1.02	2 (5%)	43,45,51	1.04	1 (2%)
24	PEF	L	502	1	35,35,46	1.08	2 (5%)	38,40,51	1.14	4 (10%)
26	CDL	O	402	26	70,70,99	1.09	4 (5%)	76,82,111	1.22	6 (7%)
24	PEF	N	605	-	38,38,46	1.08	2 (5%)	41,43,51	0.99	2 (4%)
24	PEF	E	302	-	42,42,46	1.01	2 (4%)	45,47,51	1.10	3 (6%)
24	PEF	S	102	-	35,35,46	1.08	2 (5%)	38,40,51	1.11	3 (7%)
24	PEF	e	201	-	41,41,46	1.03	2 (4%)	44,46,51	0.97	2 (4%)
26	CDL	H	601	-	52,52,99	1.26	4 (7%)	58,64,111	1.26	5 (8%)
24	PEF	b	303	-	32,32,46	1.12	2 (6%)	35,37,51	1.23	4 (11%)
24	PEF	U	101	-	46,46,46	0.96	2 (4%)	49,51,51	1.03	2 (4%)
24	PEF	b	302	-	39,39,46	1.04	2 (5%)	42,44,51	1.05	2 (4%)
33	CUA	b	301	12	0,1,1	-	-	-	-	-
24	PEF	C	605	-	42,42,46	1.01	2 (4%)	45,47,51	1.15	3 (6%)
24	PEF	J	101	-	28,28,46	1.22	2 (7%)	31,33,51	1.18	2 (6%)
27	PCF	N	606	-	38,38,49	1.10	2 (5%)	44,46,57	1.05	3 (6%)
27	PCF	I	101	24	38,38,49	1.07	2 (5%)	44,46,57	1.08	4 (9%)
27	PCF	C	606	-	49,49,49	0.96	2 (4%)	55,57,57	1.00	4 (7%)
26	CDL	L	501	-	57,57,99	1.21	4 (7%)	63,69,111	1.20	4 (6%)
25	HEM	N	601	3	41,50,50	1.34	4 (9%)	45,82,82	1.88	11 (24%)
29	FES	P	301	5	0,4,4	-	-	-	-	-
24	PEF	C	604	27	39,39,46	1.04	2 (5%)	42,44,51	1.10	3 (7%)
27	PCF	T	101	-	49,49,49	0.97	2 (4%)	55,57,57	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	HEM	N	602	3	41,50,50	1.35	4 (9%)	45,82,82	1.85	11 (24%)
26	CDL	S	101	-	52,52,99	1.26	4 (7%)	58,64,111	1.25	7 (12%)
28	HEC	D	401	4	32,50,50	2.54	12 (37%)	24,82,82	2.79	9 (37%)
28	HEC	O	401	4	32,50,50	2.52	12 (37%)	24,82,82	2.85	9 (37%)
24	PEF	a	605	11	32,32,46	1.16	2 (6%)	35,37,51	1.19	3 (8%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
31	HEA	a	603	11	57,67,67	2.03	16 (28%)	61,103,103	2.66	27 (44%)
27	PCF	S	103	8	31,31,49	1.19	2 (6%)	37,39,57	1.09	4 (10%)
25	HEM	C	601	3	41,50,50	1.34	5 (12%)	45,82,82	1.93	12 (26%)
26	CDL	C	603	1,3	54,54,99	1.16	4 (7%)	60,66,111	1.24	5 (8%)
24	PEF	N	604	-	43,43,46	0.97	2 (4%)	46,48,51	1.05	3 (6%)

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
25	HEM	C	602	3	-	4/12/54/54	-
24	PEF	c	301	-	-	10/39/39/50	-
24	PEF	A	501	1	-	7/34/34/50	-
24	PEF	H	602	-	-	6/35/35/50	-
26	CDL	N	603	26	-	11/76/76/110	-
27	PCF	e	202	15	-	7/39/39/53	-
24	PEF	P	302	-	-	13/45/45/50	-
31	HEA	a	602	11	2/2/7/16	10/32/76/76	-
26	CDL	D	402	-	-	29/77/77/110	-
24	PEF	c	302	-	-	11/44/44/50	-
24	PEF	L	502	1	-	15/39/39/50	-
26	CDL	O	402	26	-	19/81/81/110	-
24	PEF	N	605	-	-	10/42/42/50	-
24	PEF	E	302	-	-	14/46/46/50	-
24	PEF	S	102	-	-	10/39/39/50	-
24	PEF	e	201	-	-	13/45/45/50	-
26	CDL	H	601	-	-	19/63/63/110	-
24	PEF	b	303	-	-	14/36/36/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEF	U	101	-	-	14/50/50/50	-
24	PEF	b	302	-	-	19/43/43/50	-
24	PEF	C	605	-	-	13/46/46/50	-
24	PEF	J	101	-	-	15/32/32/50	-
27	PCF	N	606	-	-	11/42/42/53	-
27	PCF	I	101	24	-	6/42/42/53	-
27	PCF	C	606	-	-	15/53/53/53	-
26	CDL	L	501	-	-	19/68/68/110	-
25	HEM	N	601	3	-	8/12/54/54	-
29	FES	P	301	5	-	-	0/1/1/1
24	PEF	C	604	27	-	9/43/43/50	-
27	PCF	T	101	-	-	9/53/53/53	-
25	HEM	N	602	3	-	4/12/54/54	-
26	CDL	S	101	-	-	23/63/63/110	-
31	HEA	a	603	11	2/2/7/16	4/32/76/76	-
28	HEC	D	401	4	-	0/10/54/54	-
24	PEF	a	605	11	-	6/36/36/50	-
28	HEC	O	401	4	-	3/10/54/54	-
29	FES	E	301	5	-	-	0/1/1/1
27	PCF	S	103	8	-	8/35/35/53	-
25	HEM	C	601	3	-	8/12/54/54	-
26	CDL	C	603	1,3	-	21/64/64/110	-
24	PEF	N	604	-	-	9/47/47/50	-

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C2B-C3B	7.64	1.48	1.40
28	D	401	HEC	C2B-C3B	7.62	1.48	1.40
28	D	401	HEC	C3C-C2C	7.50	1.48	1.40
28	O	401	HEC	C3C-C2C	7.36	1.48	1.40
31	a	602	HEA	C3B-C2B	5.41	1.46	1.34

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	HEC	CMB-C2B-C3B	7.99	135.22	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	401	HEC	CMB-C2B-C3B	7.61	134.76	125.82
31	a	603	HEA	C3D-C4D-ND	6.65	116.80	110.36
28	D	401	HEC	CMC-C2C-C3C	6.56	133.53	125.82
31	a	603	HEA	C2D-C1D-ND	6.36	117.38	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	a	602	HEA	NB
31	a	602	HEA	ND
31	a	603	HEA	NB
31	a	603	HEA	ND

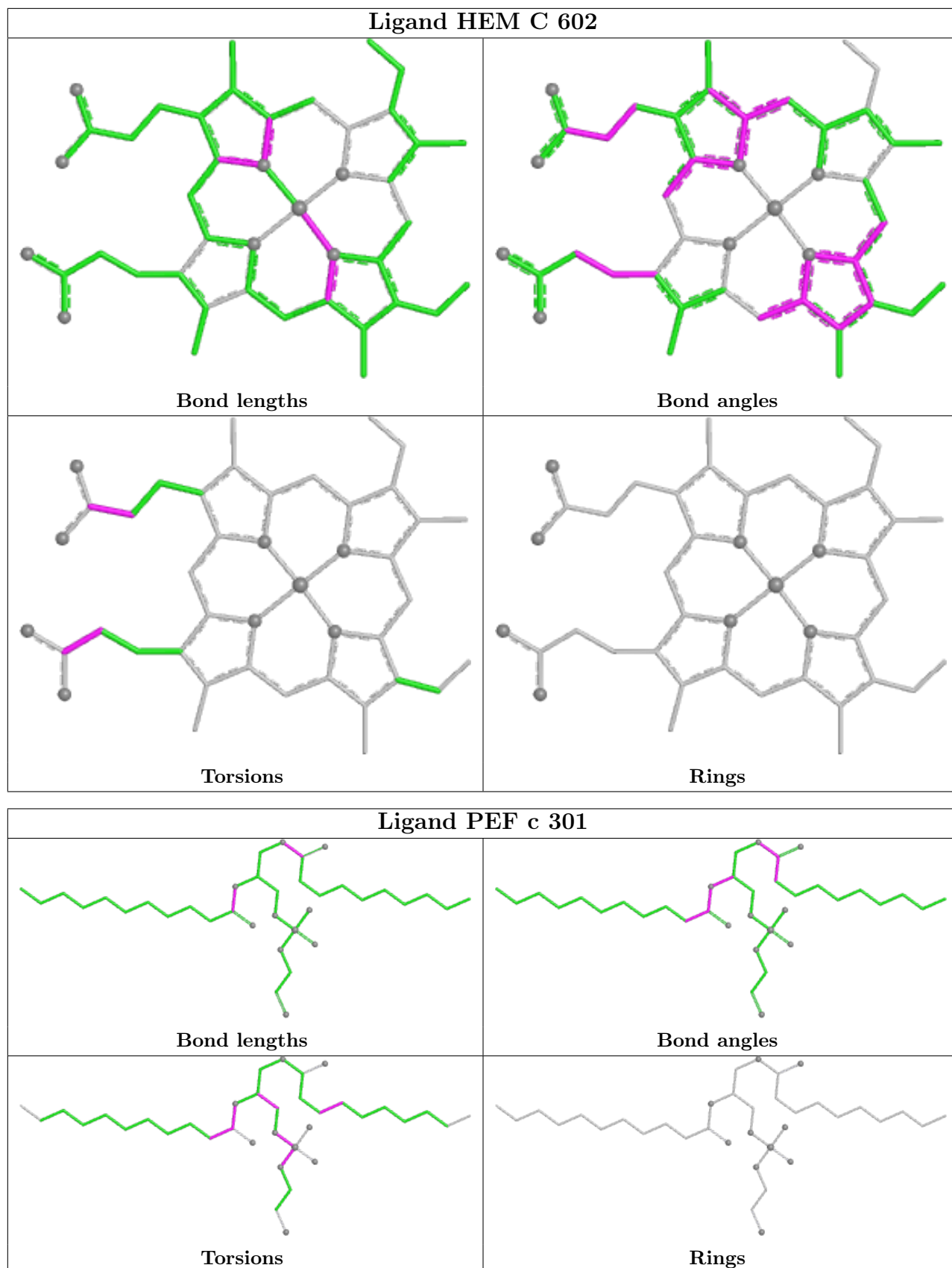
5 of 446 torsion outliers are listed below:

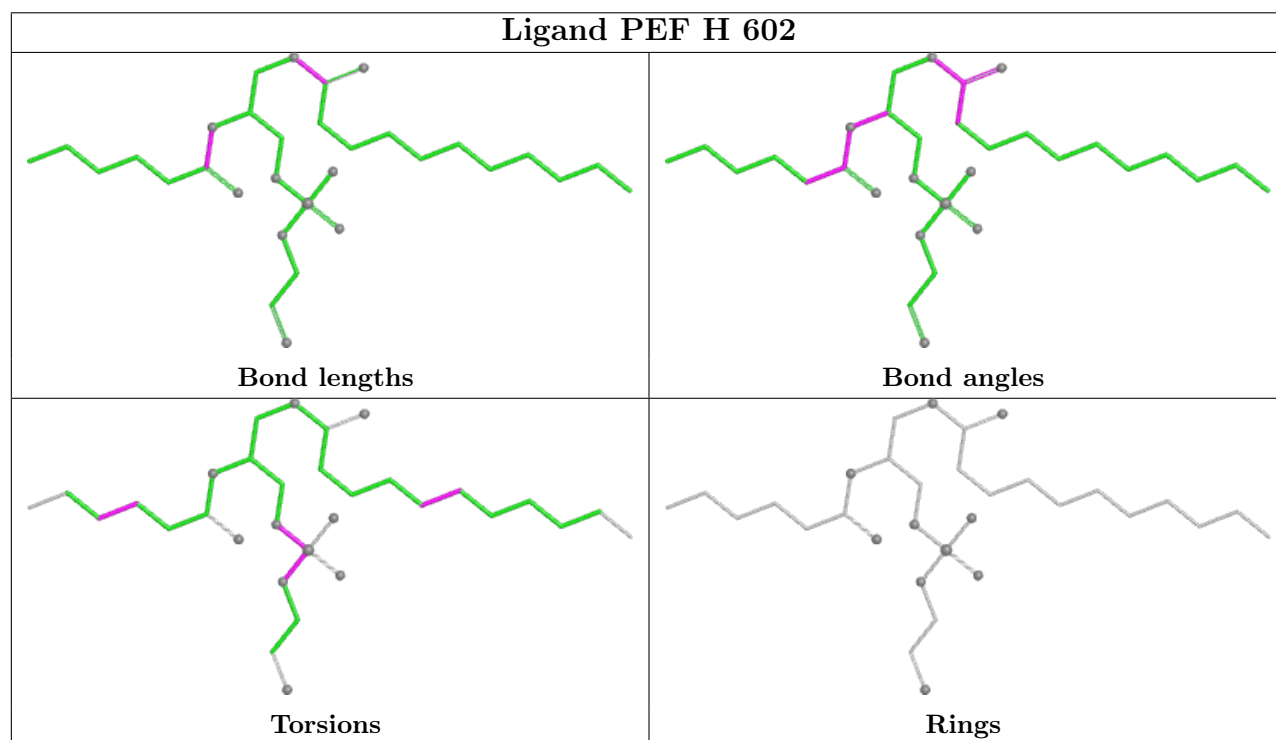
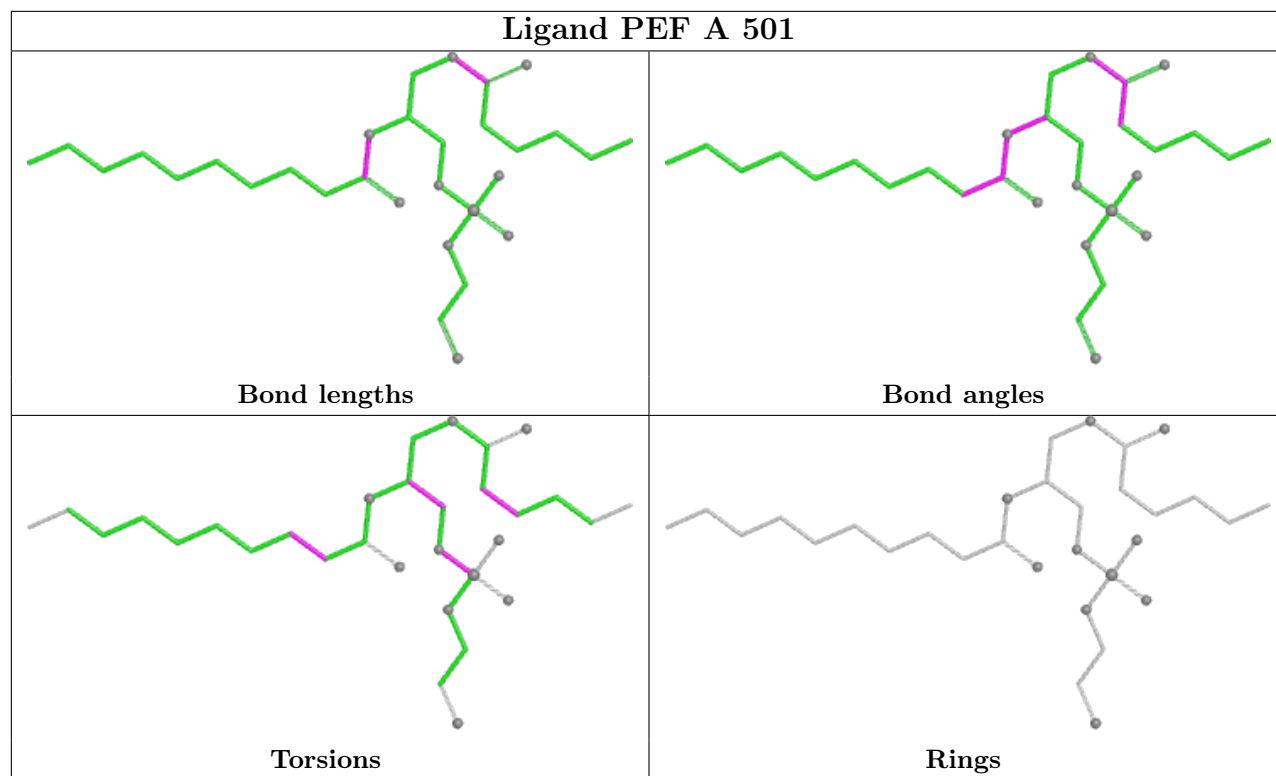
Mol	Chain	Res	Type	Atoms
24	A	501	PEF	C1-O3P-P-O1P
24	A	501	PEF	C1-O3P-P-O2P
24	A	501	PEF	C1-O3P-P-O4P
24	C	605	PEF	C11-C10-O2-C2
24	C	605	PEF	O4-C10-O2-C2

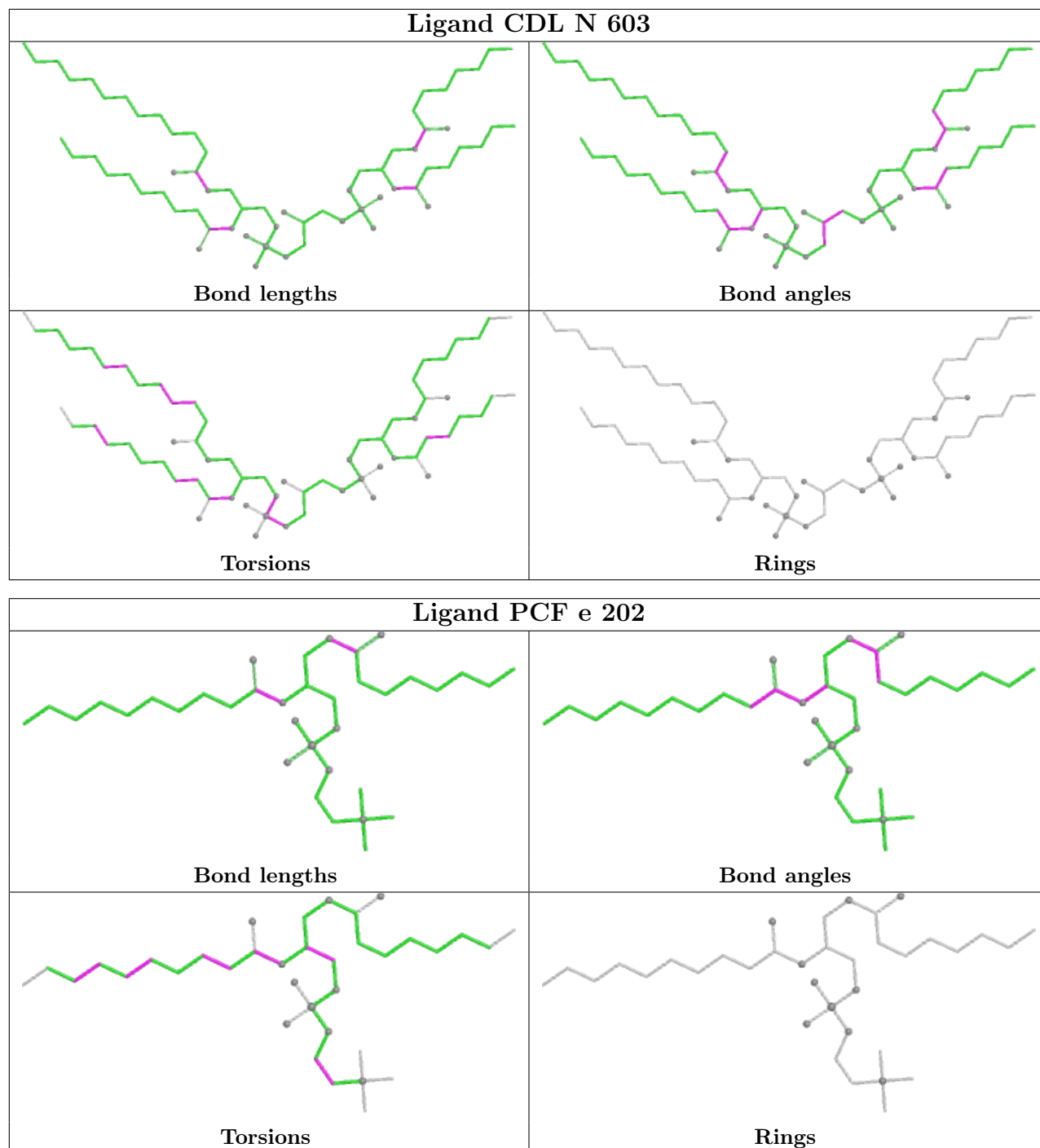
There are no ring outliers.

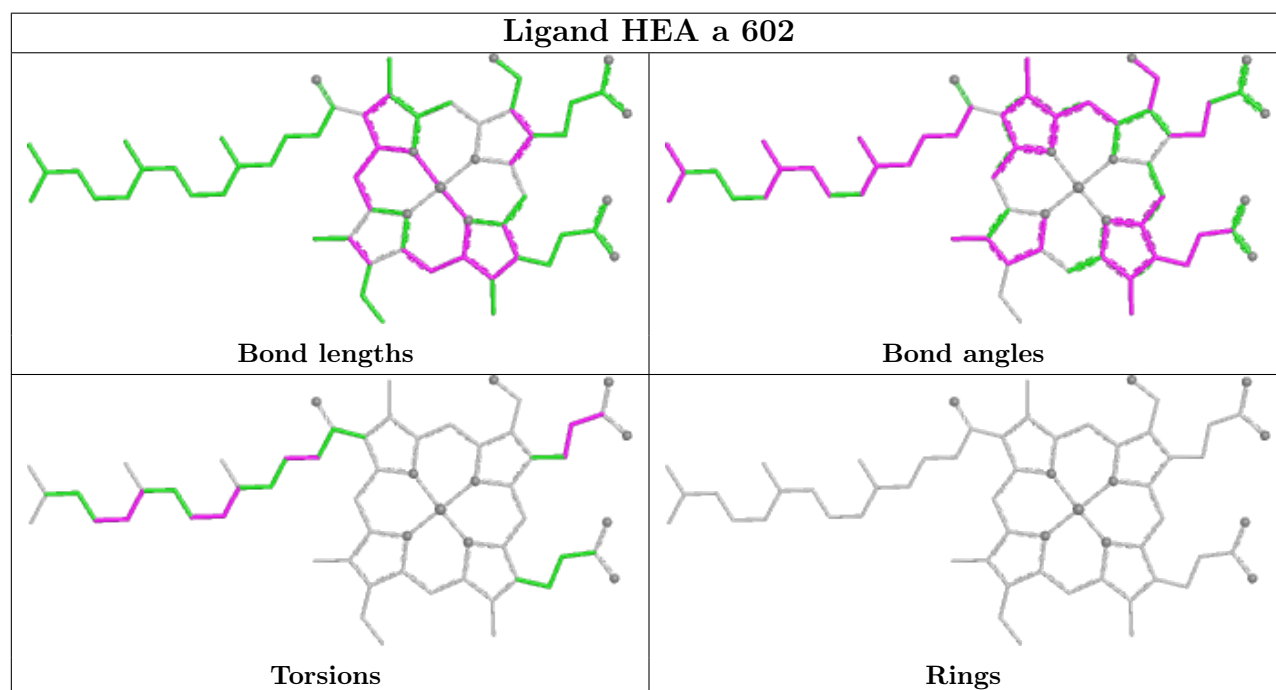
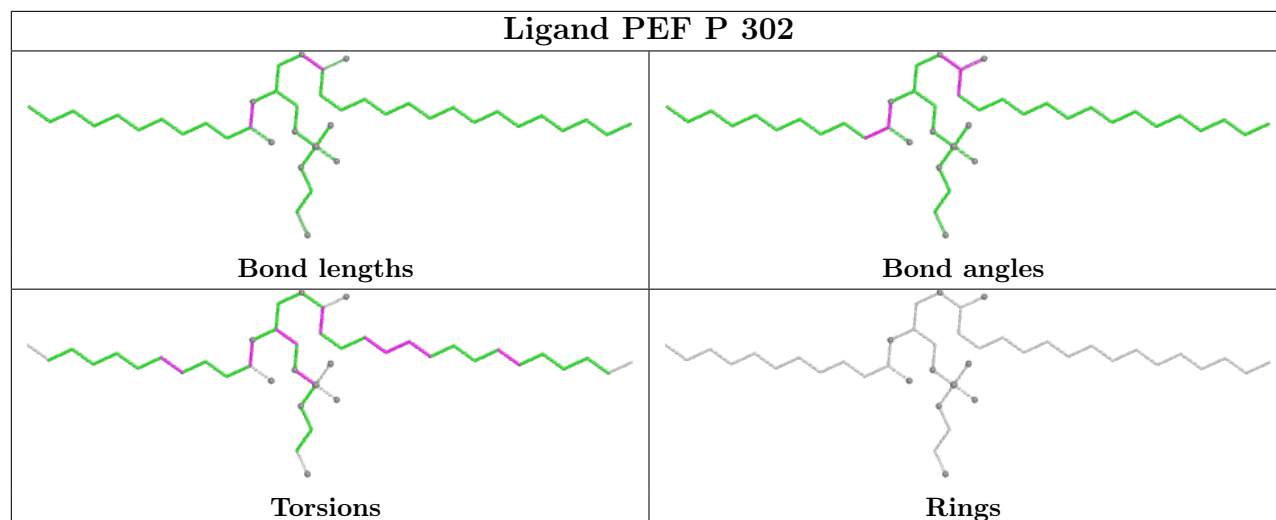
No monomer is involved in short contacts.

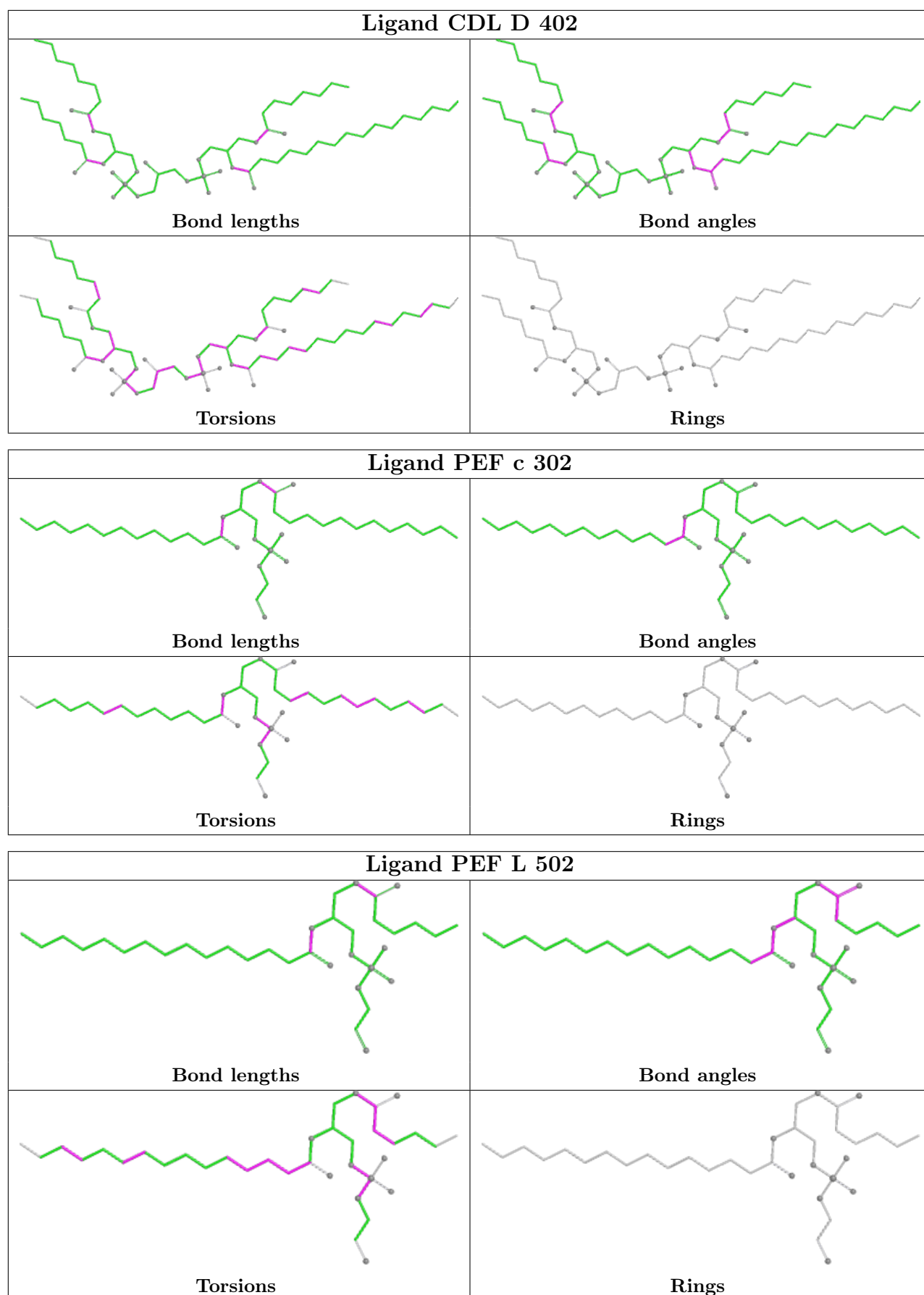
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

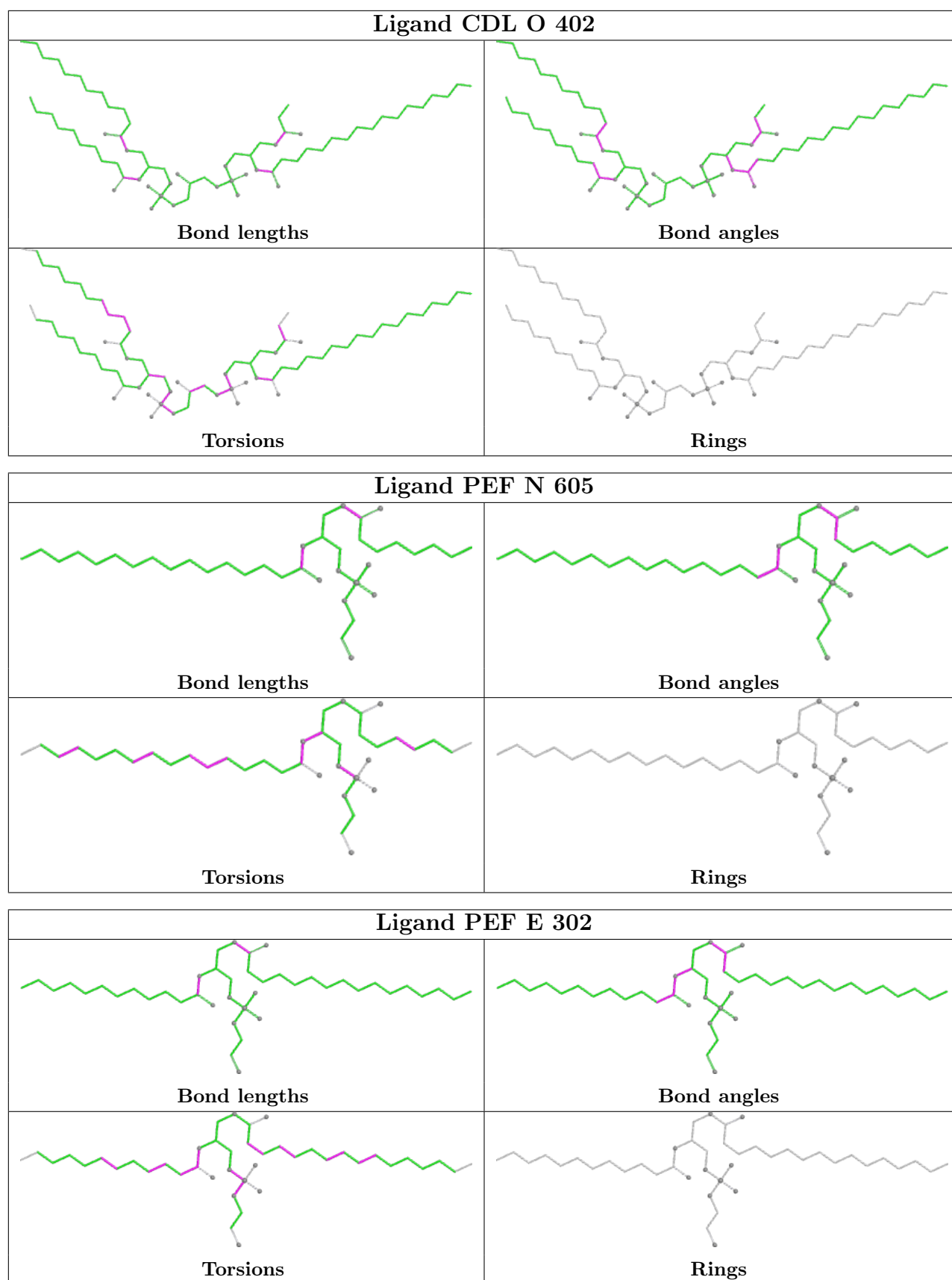


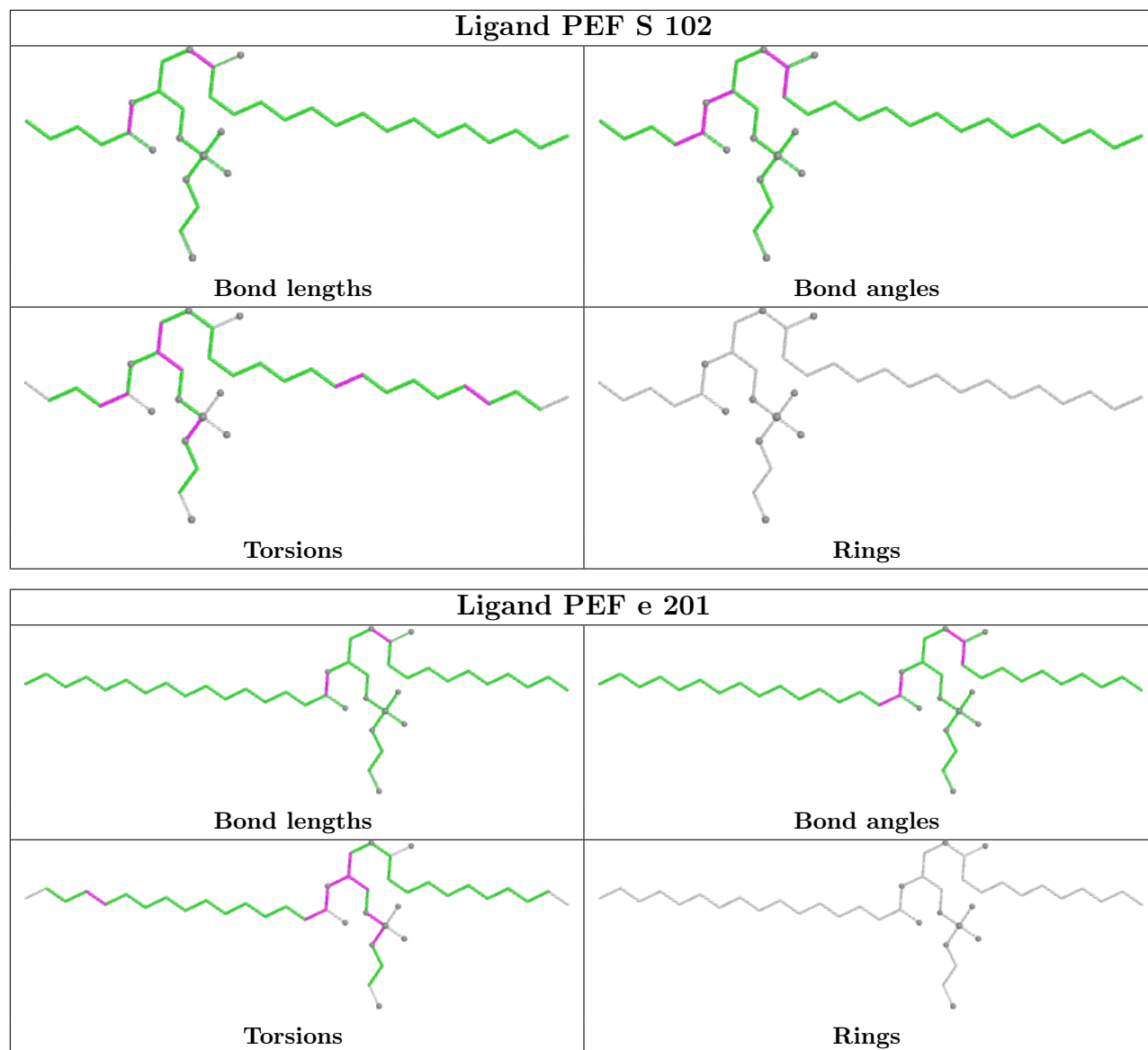


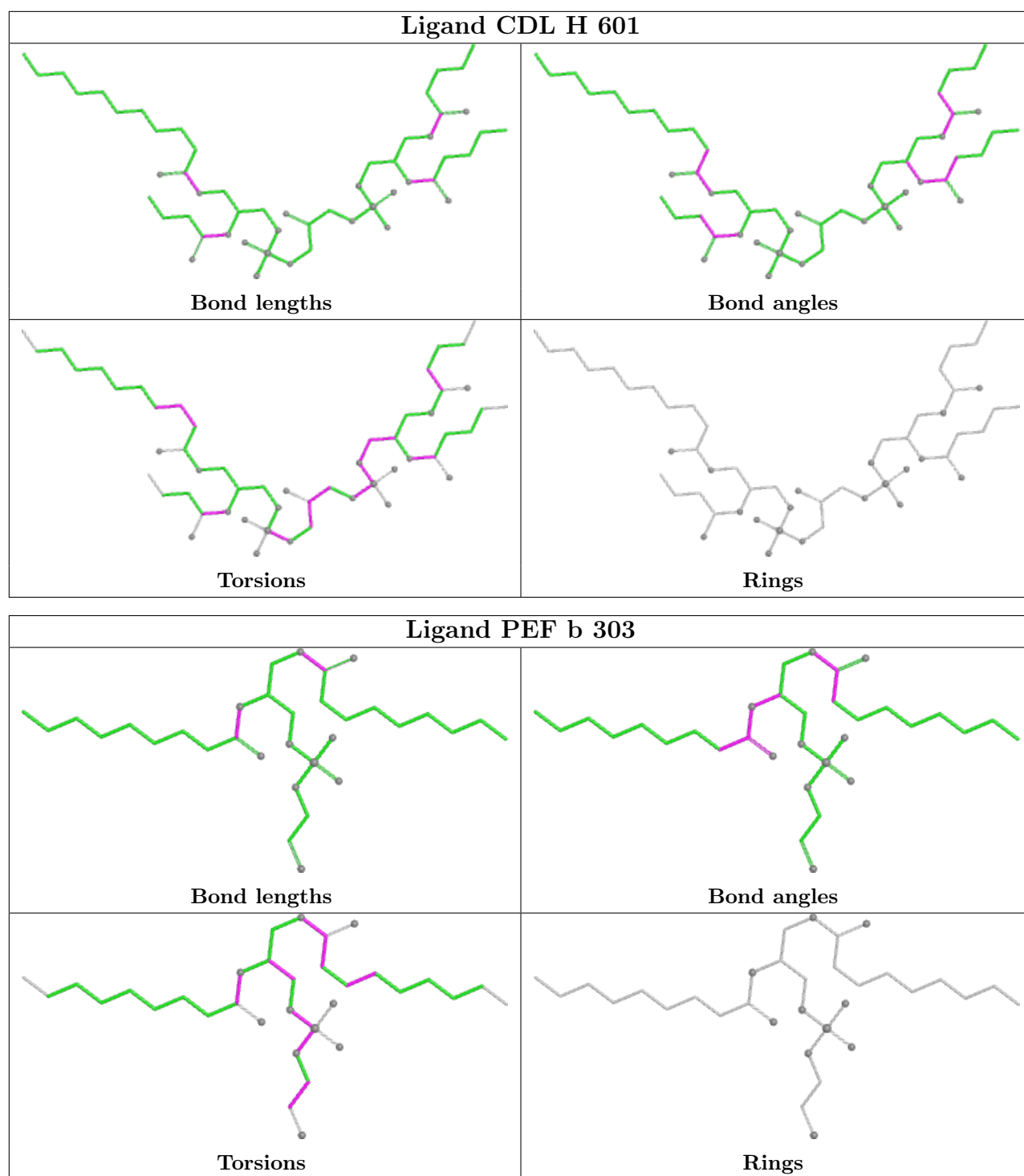


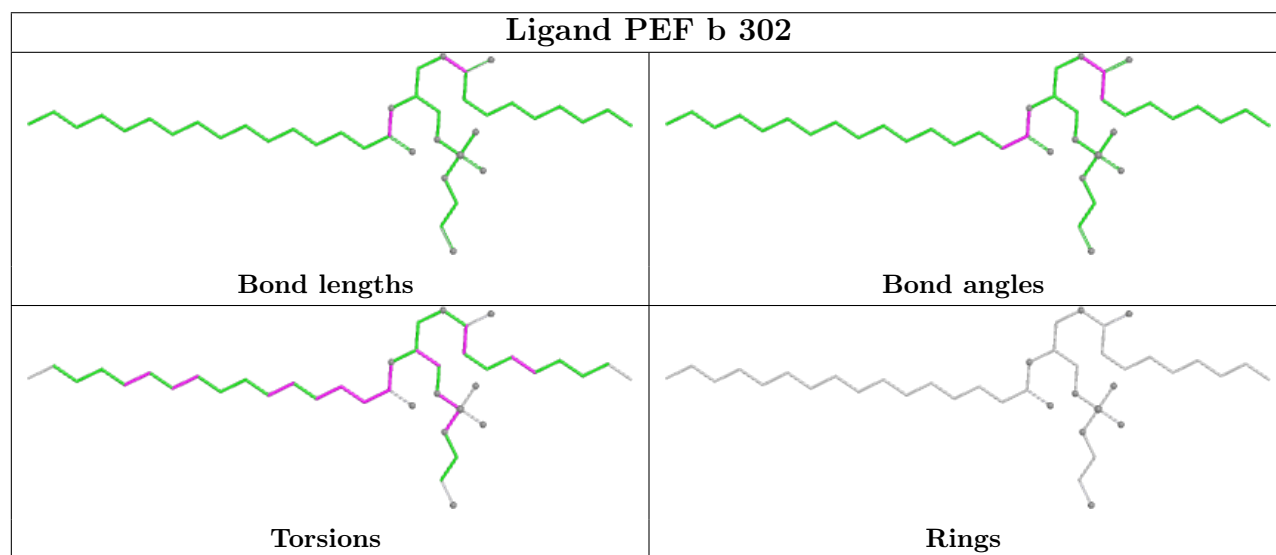
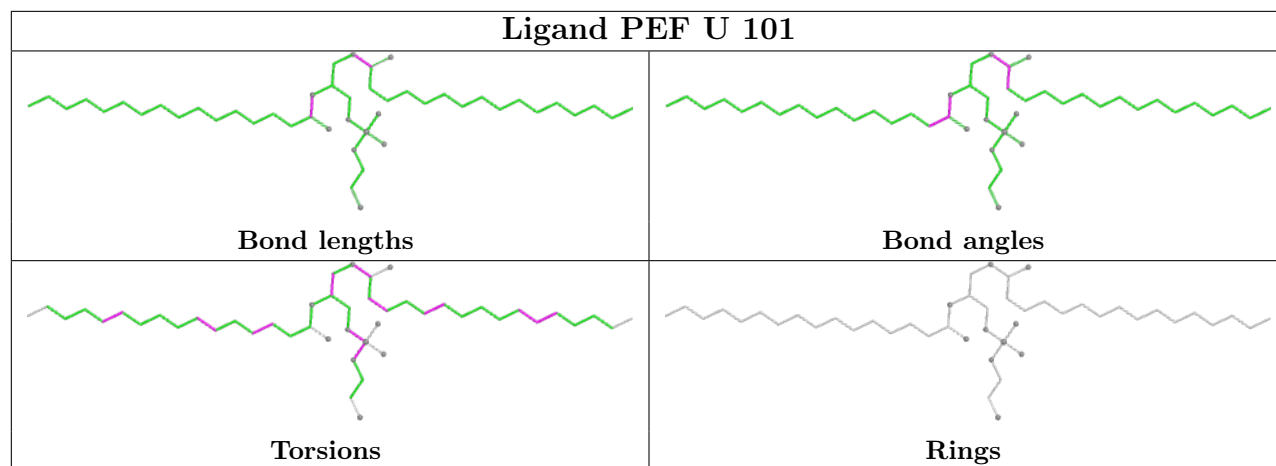


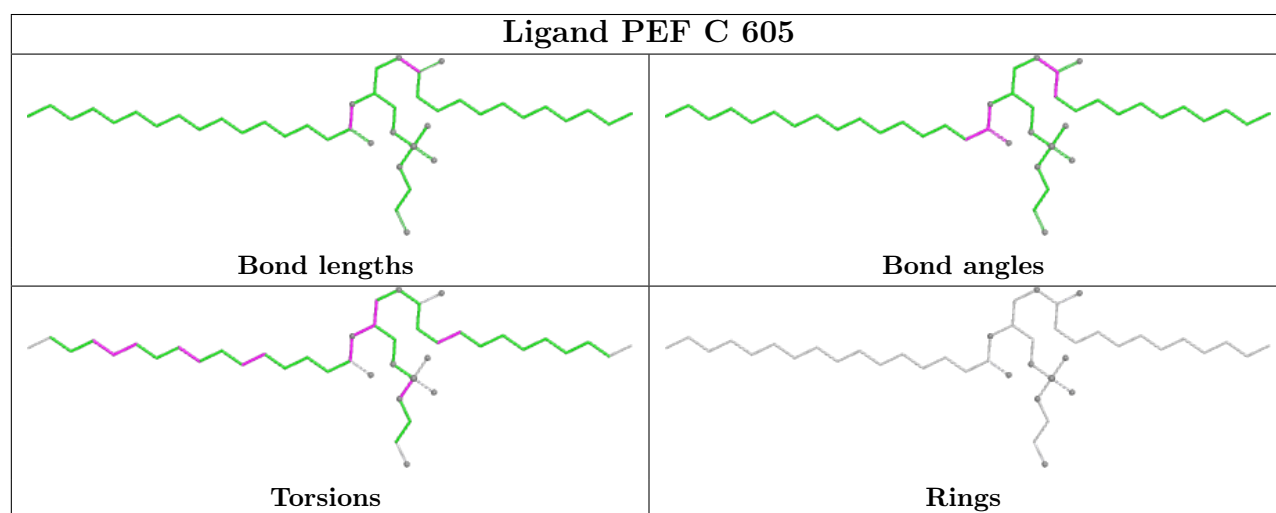
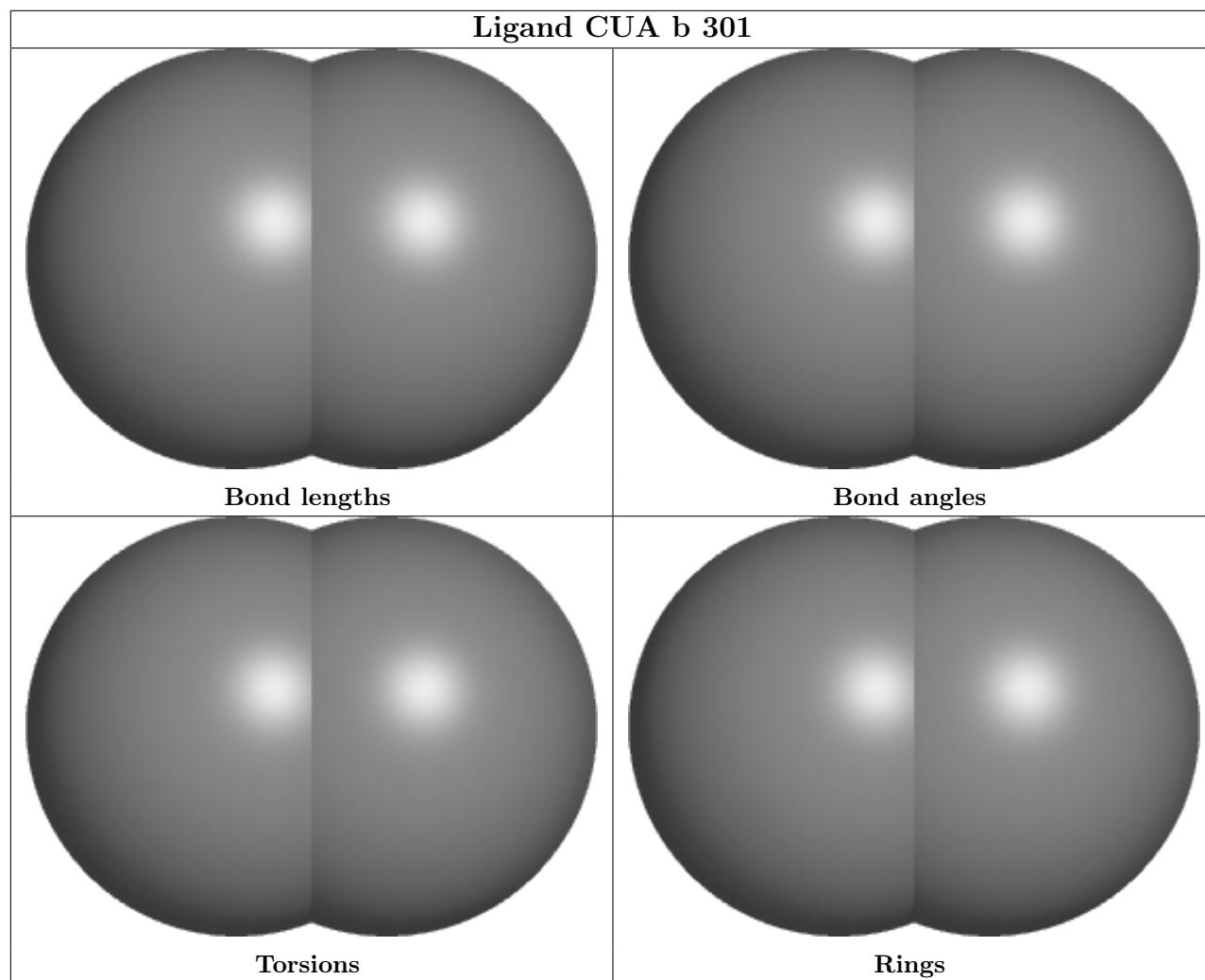


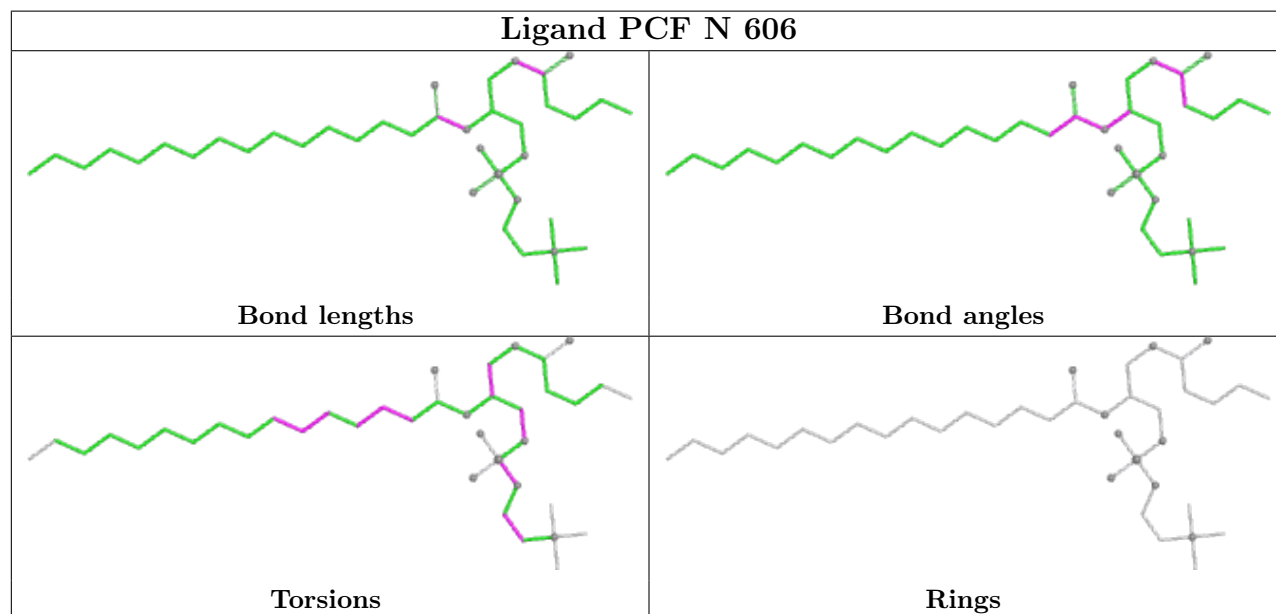
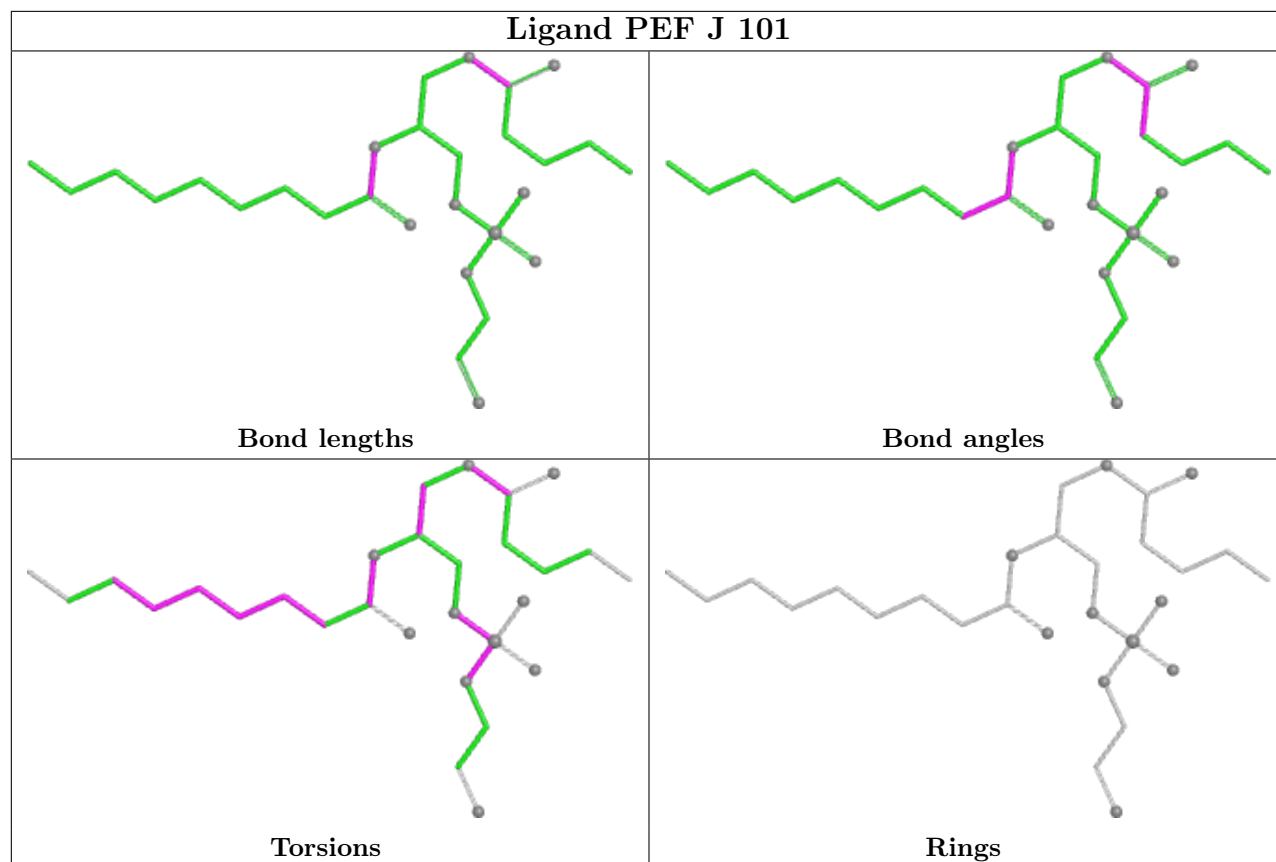


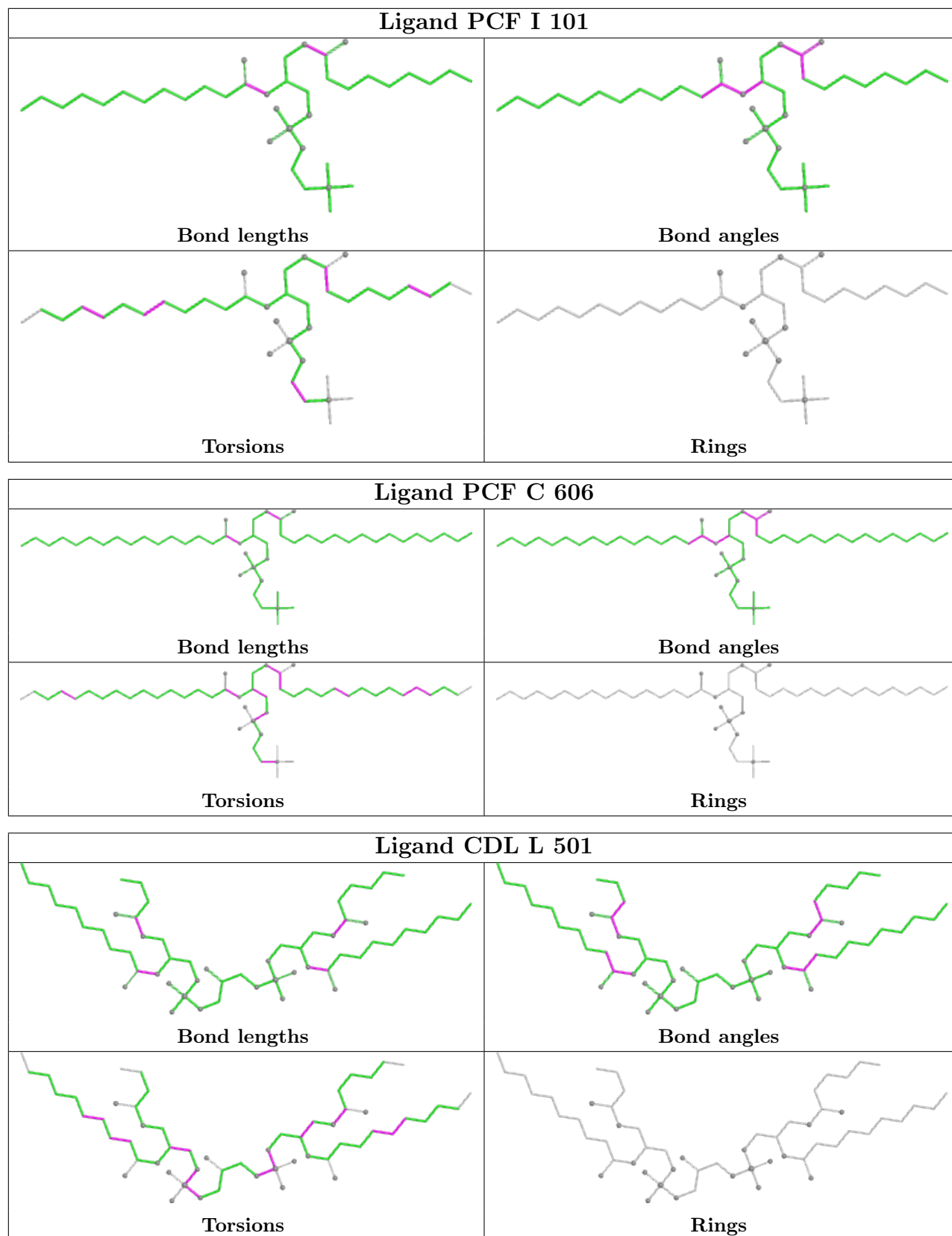


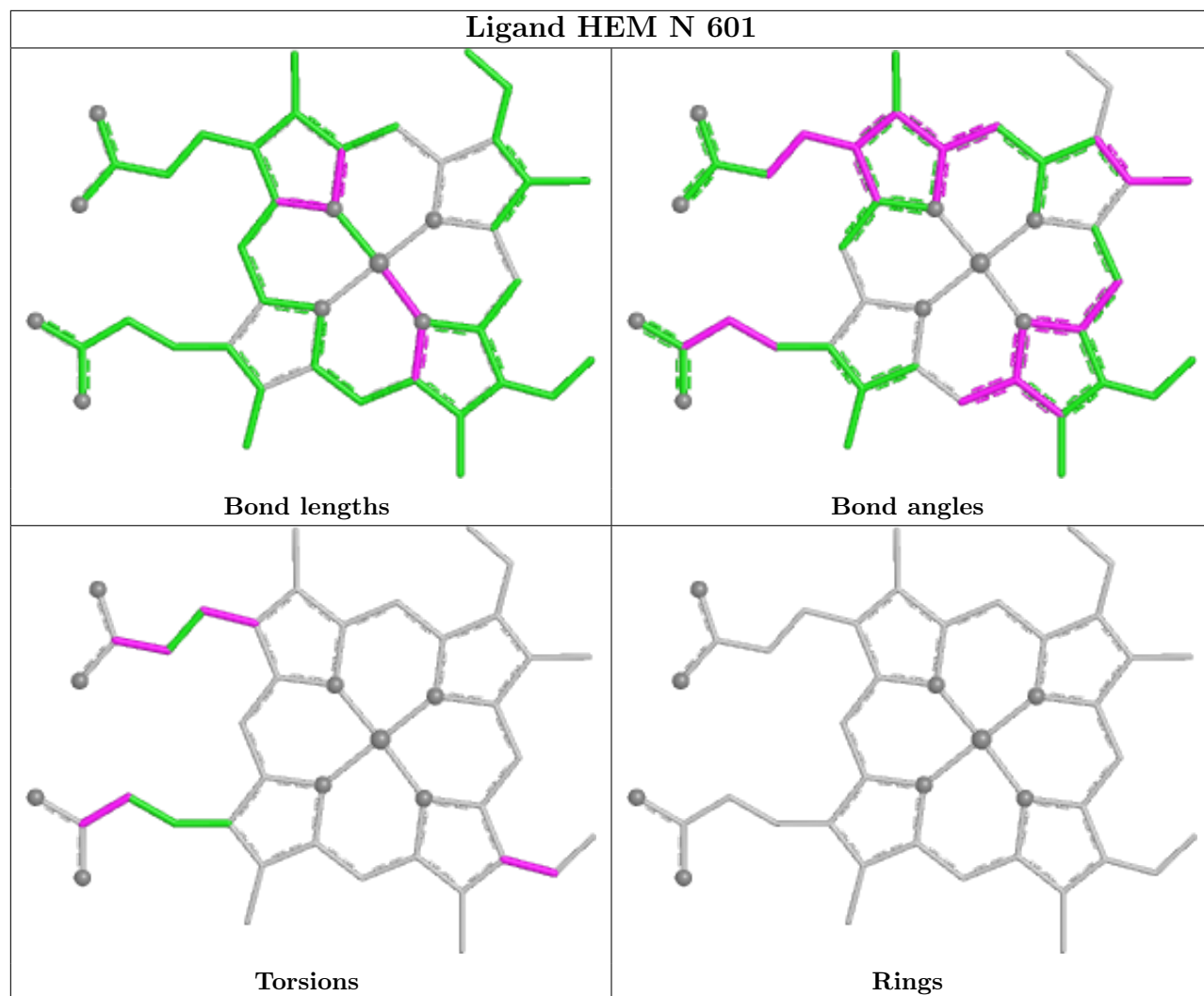


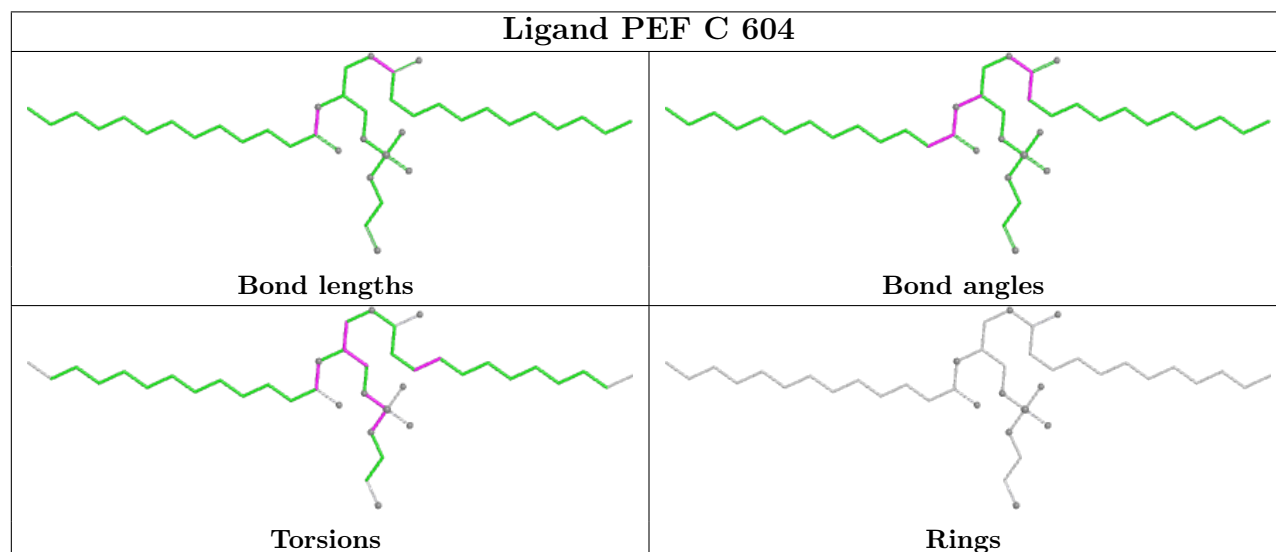
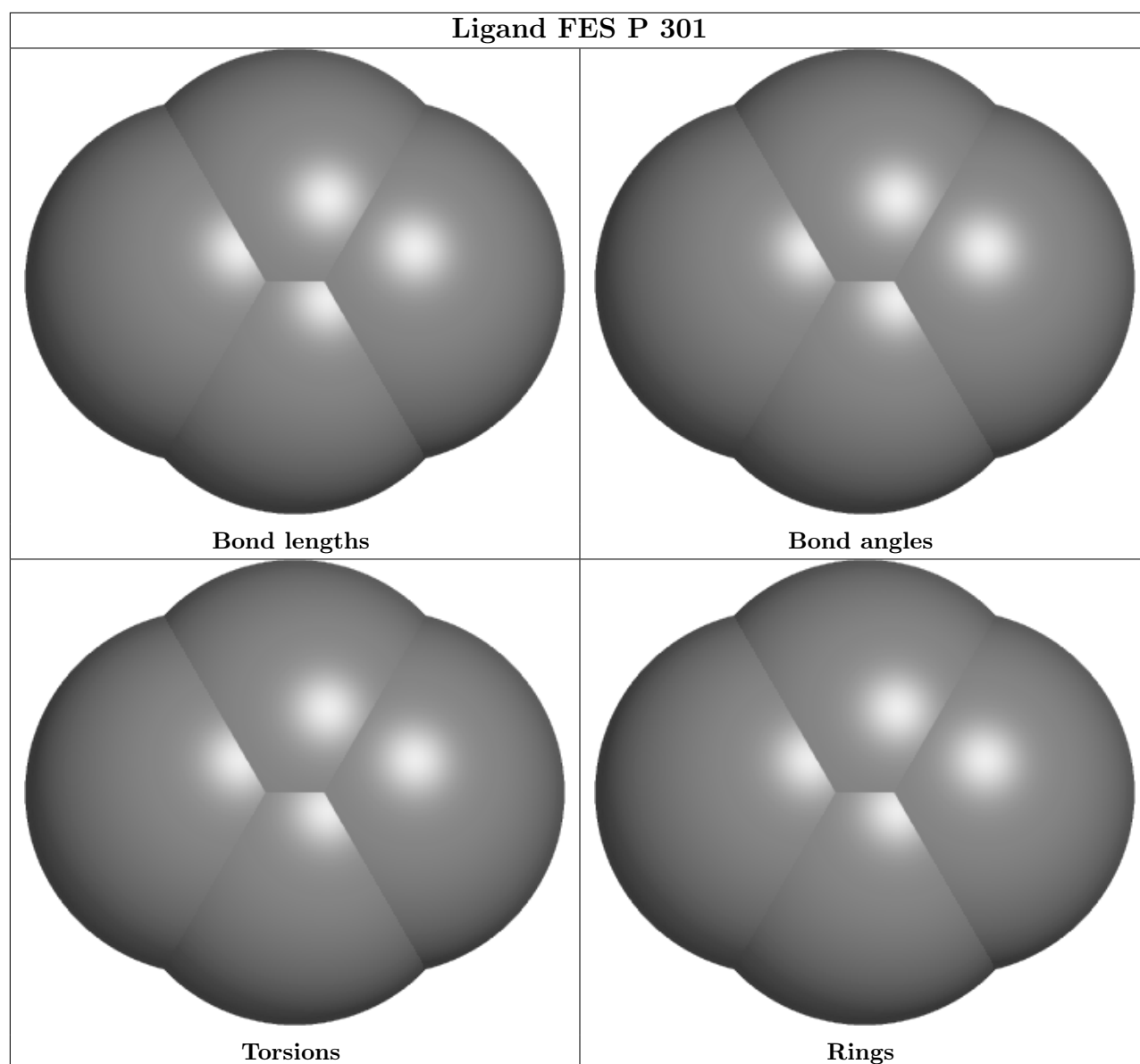


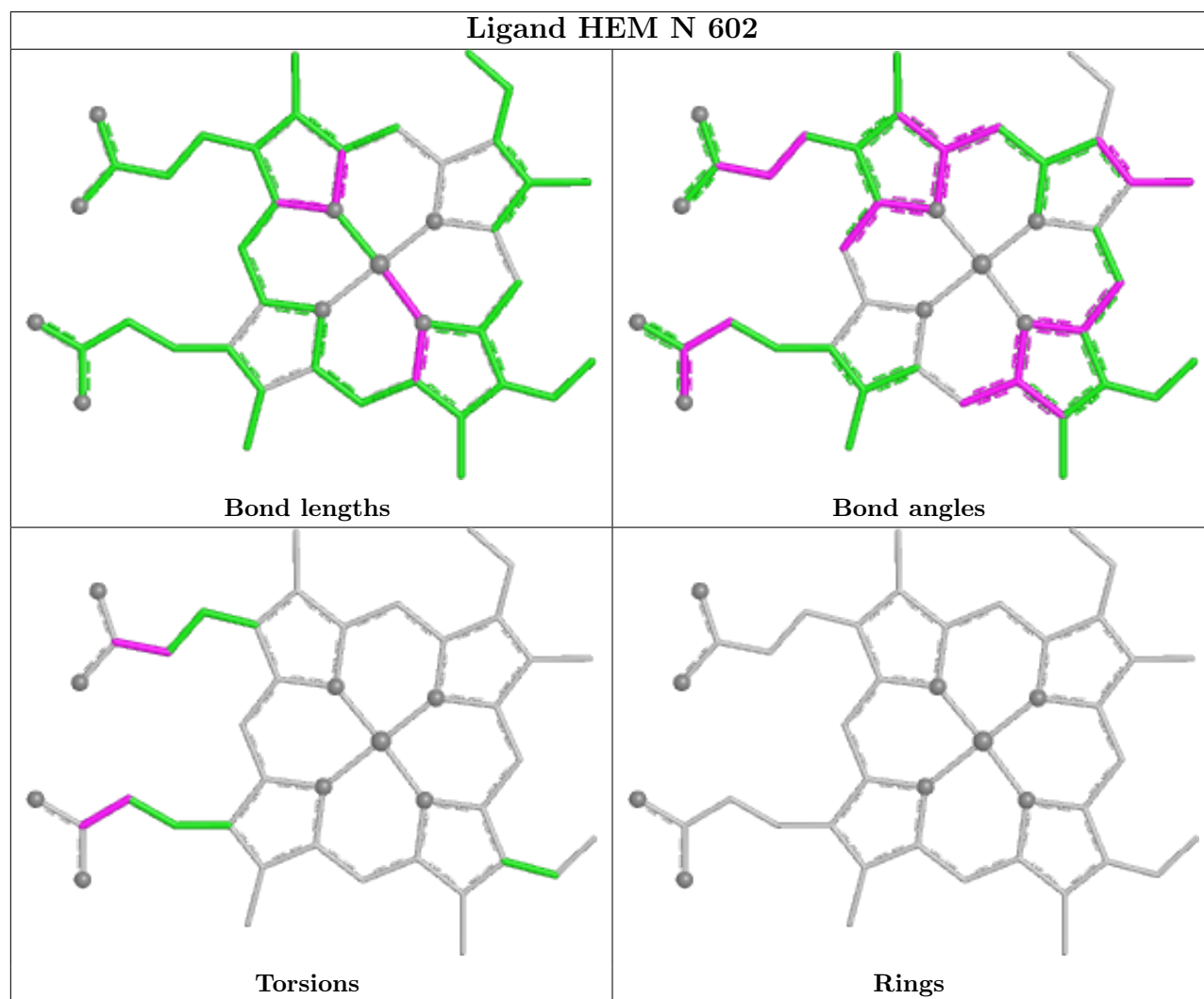
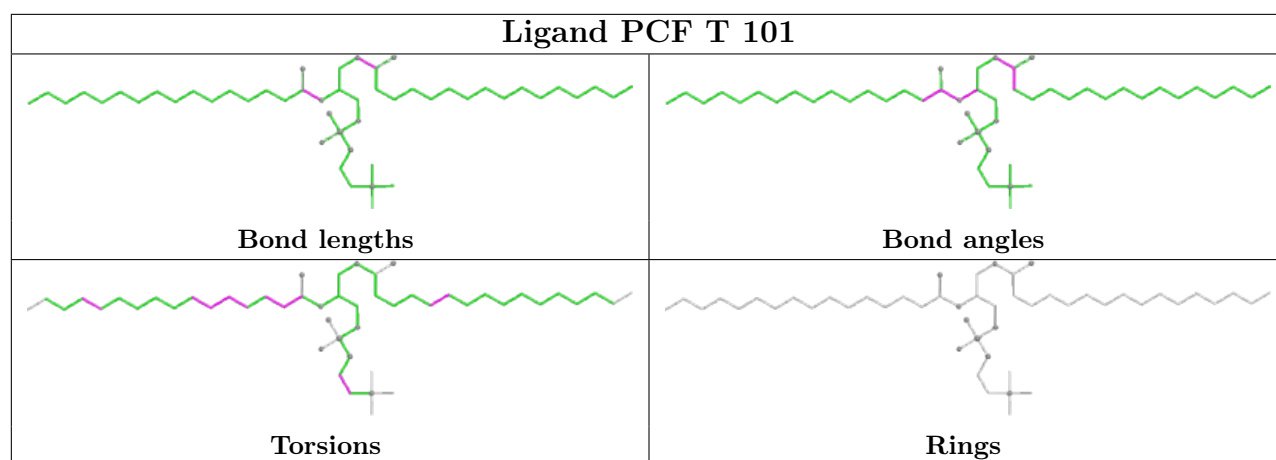


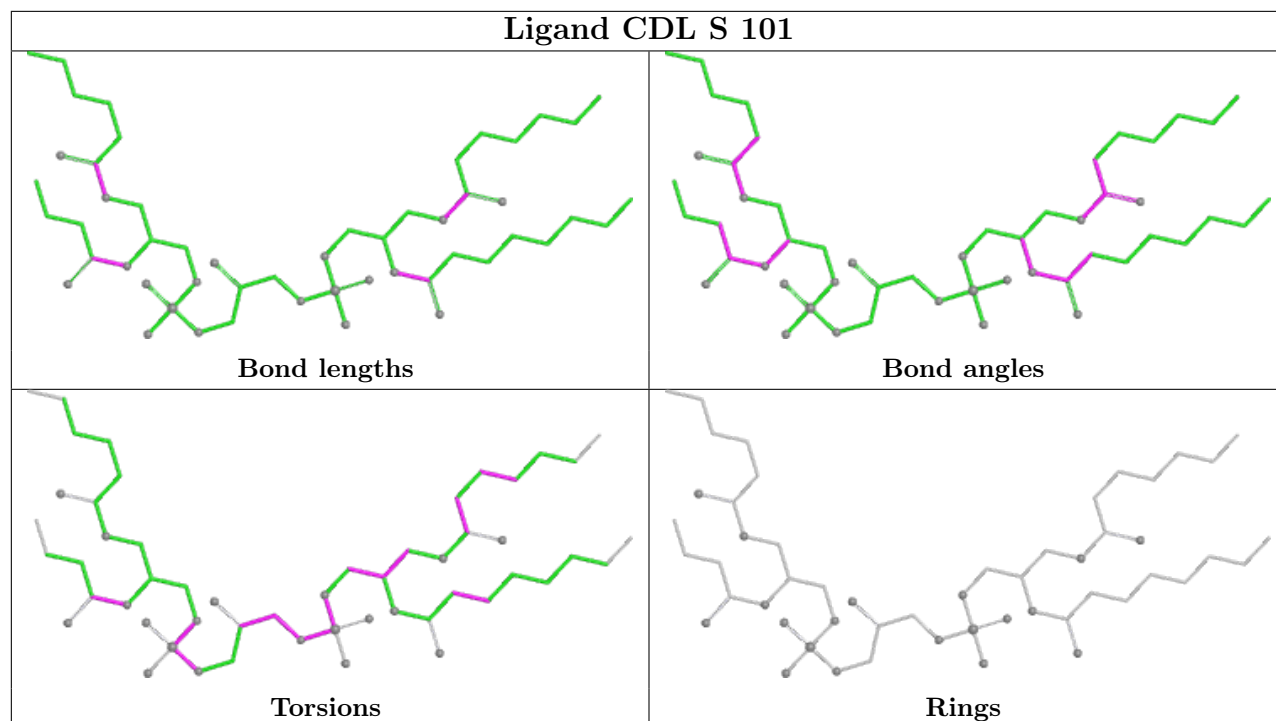


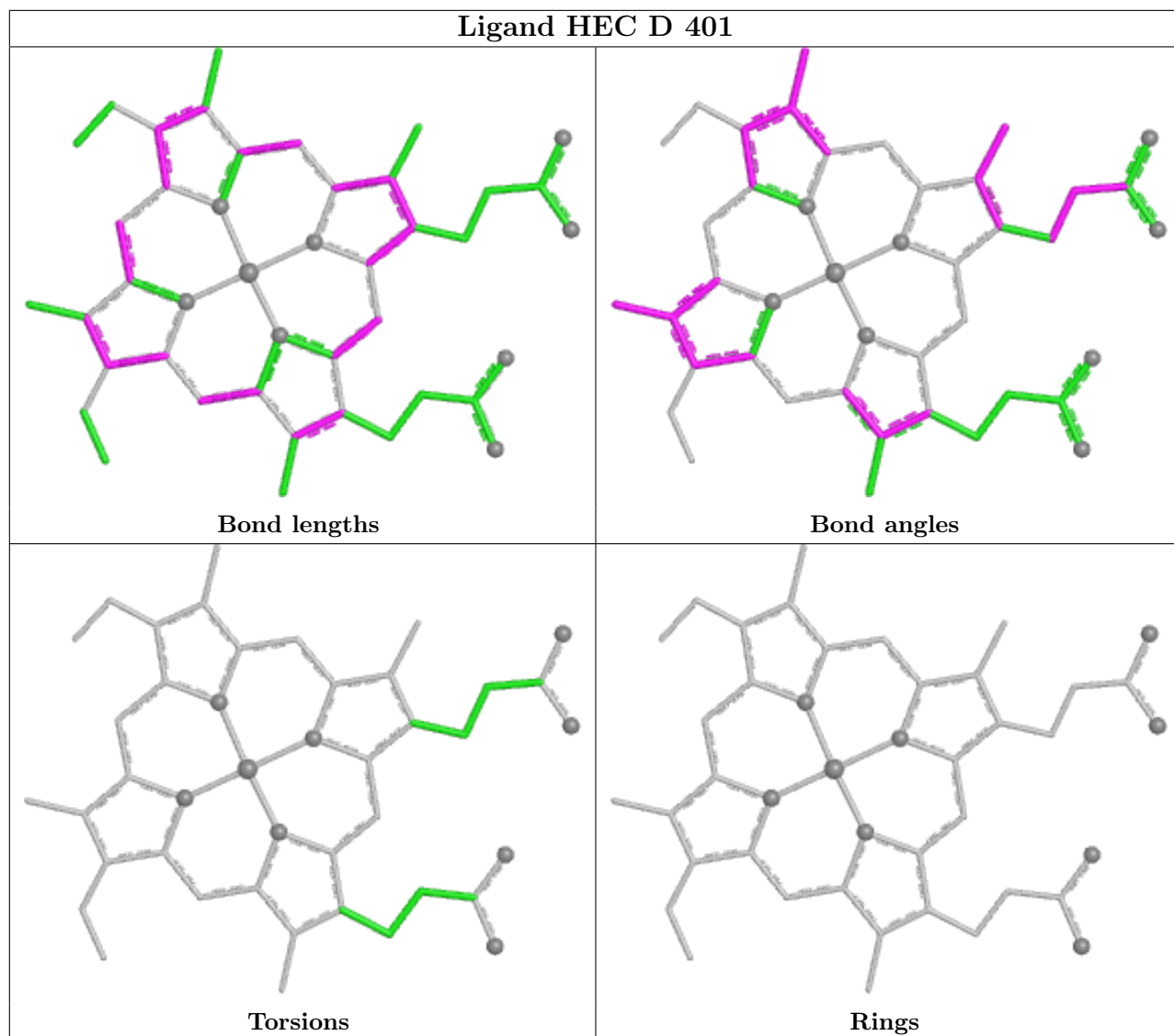


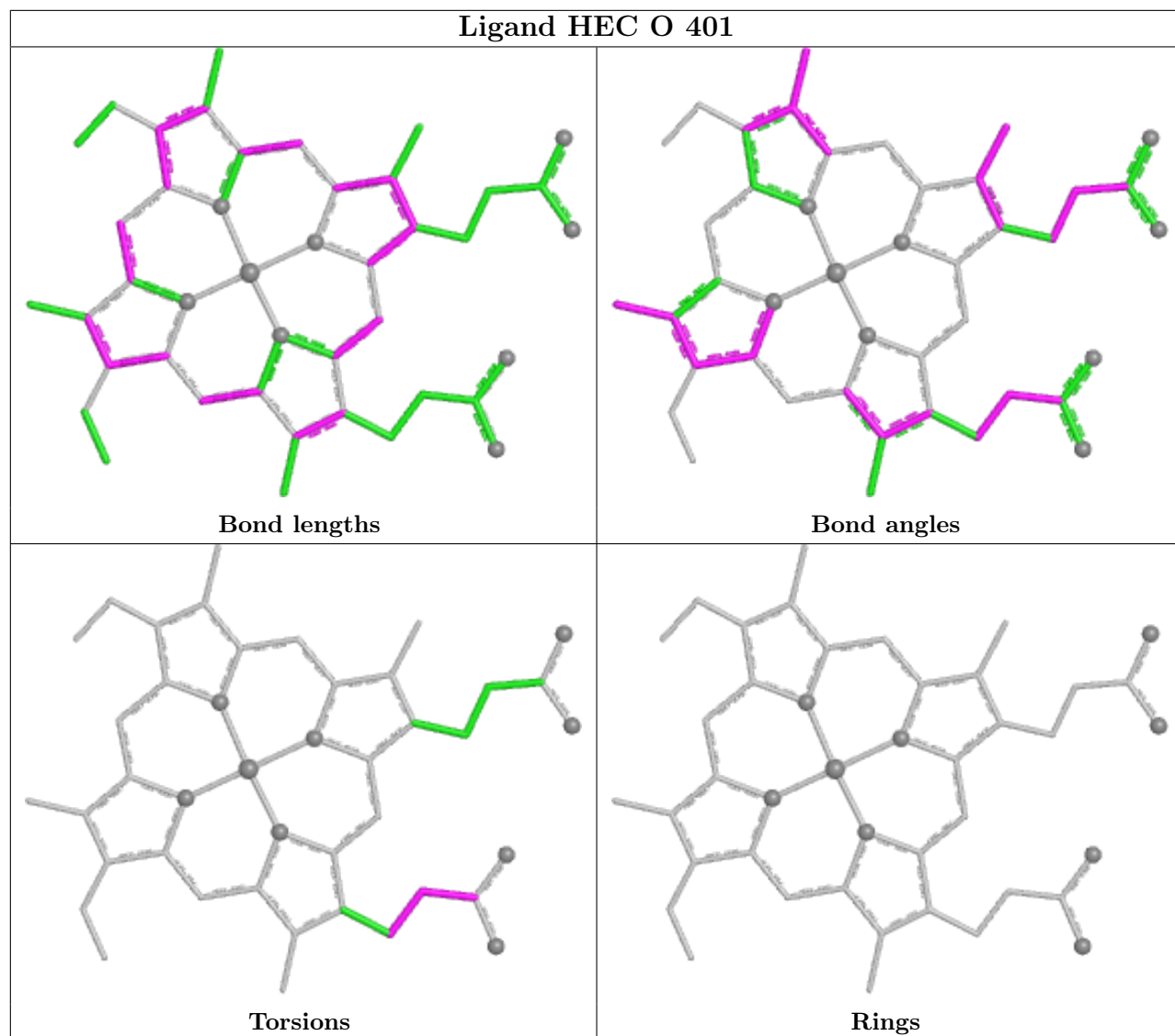


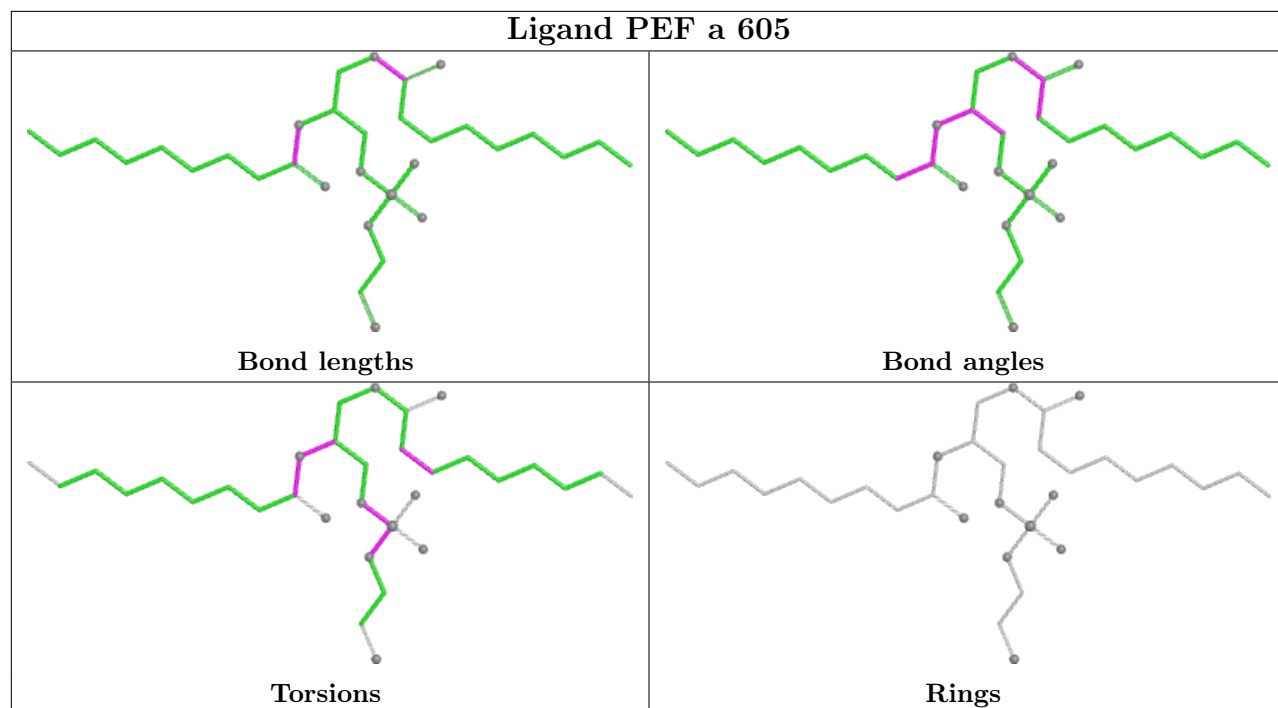


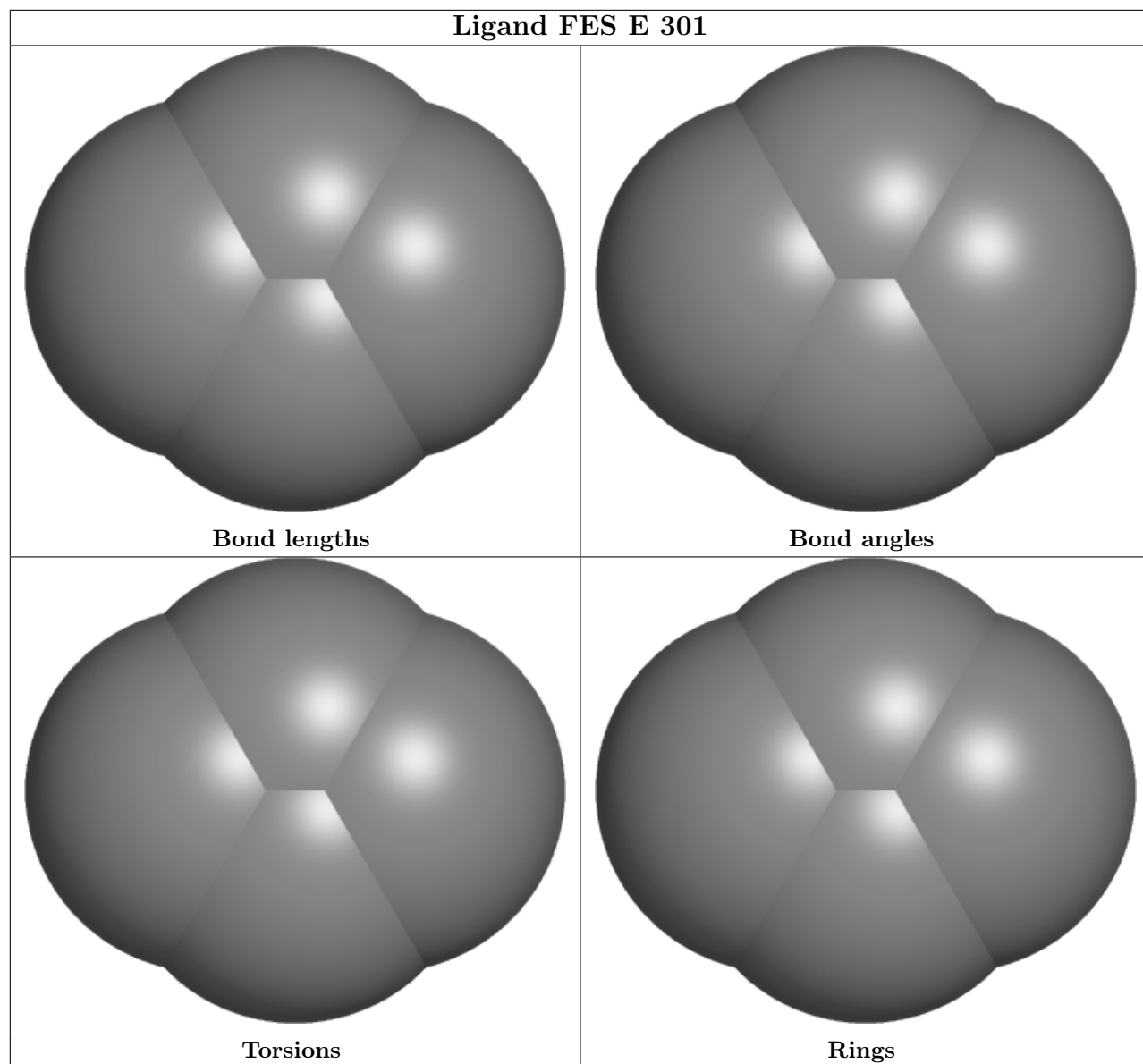


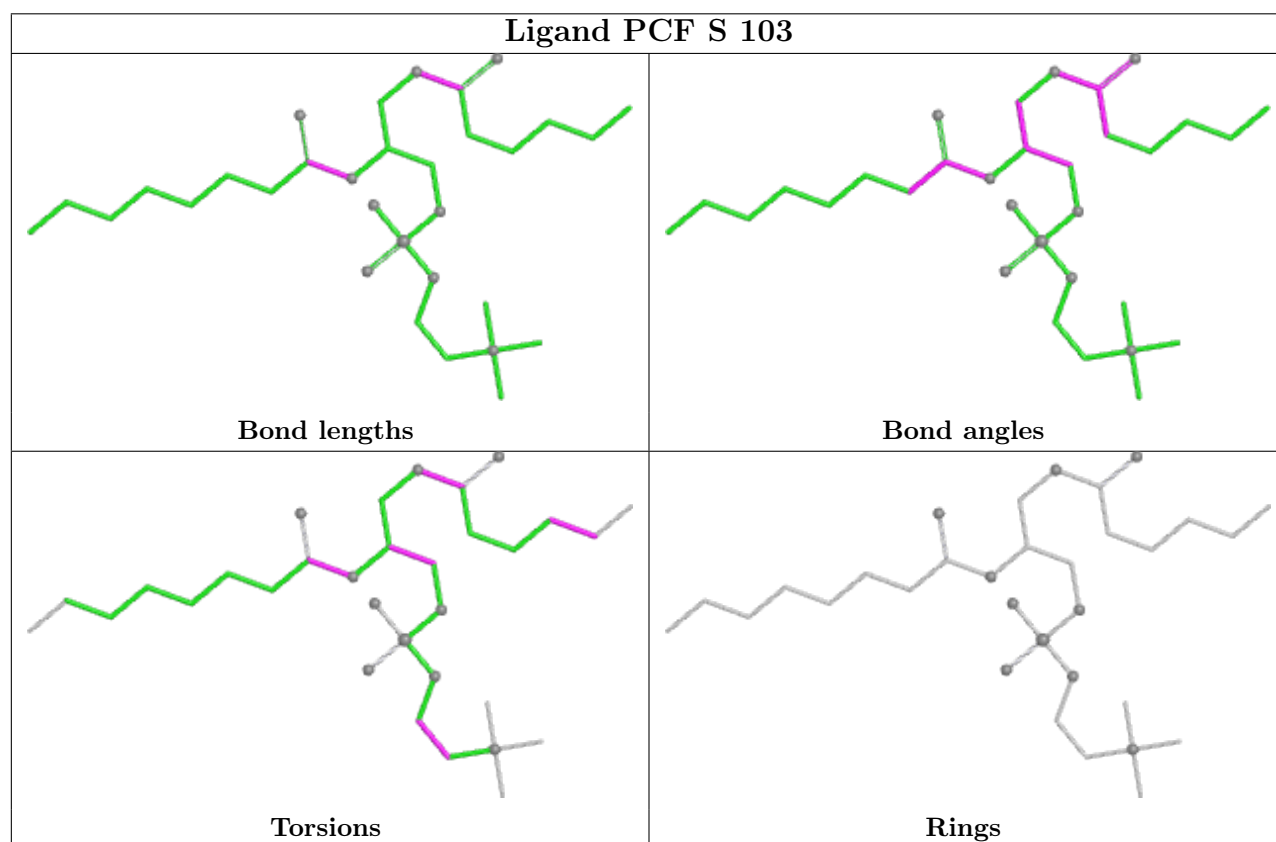
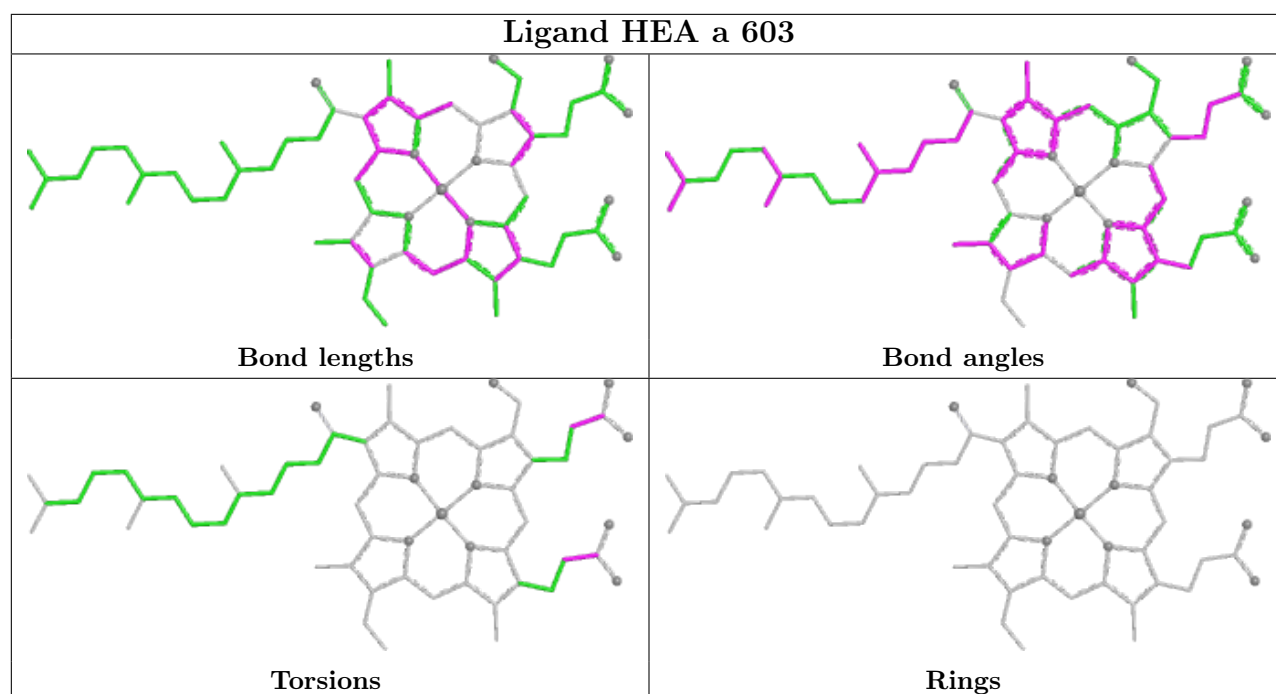


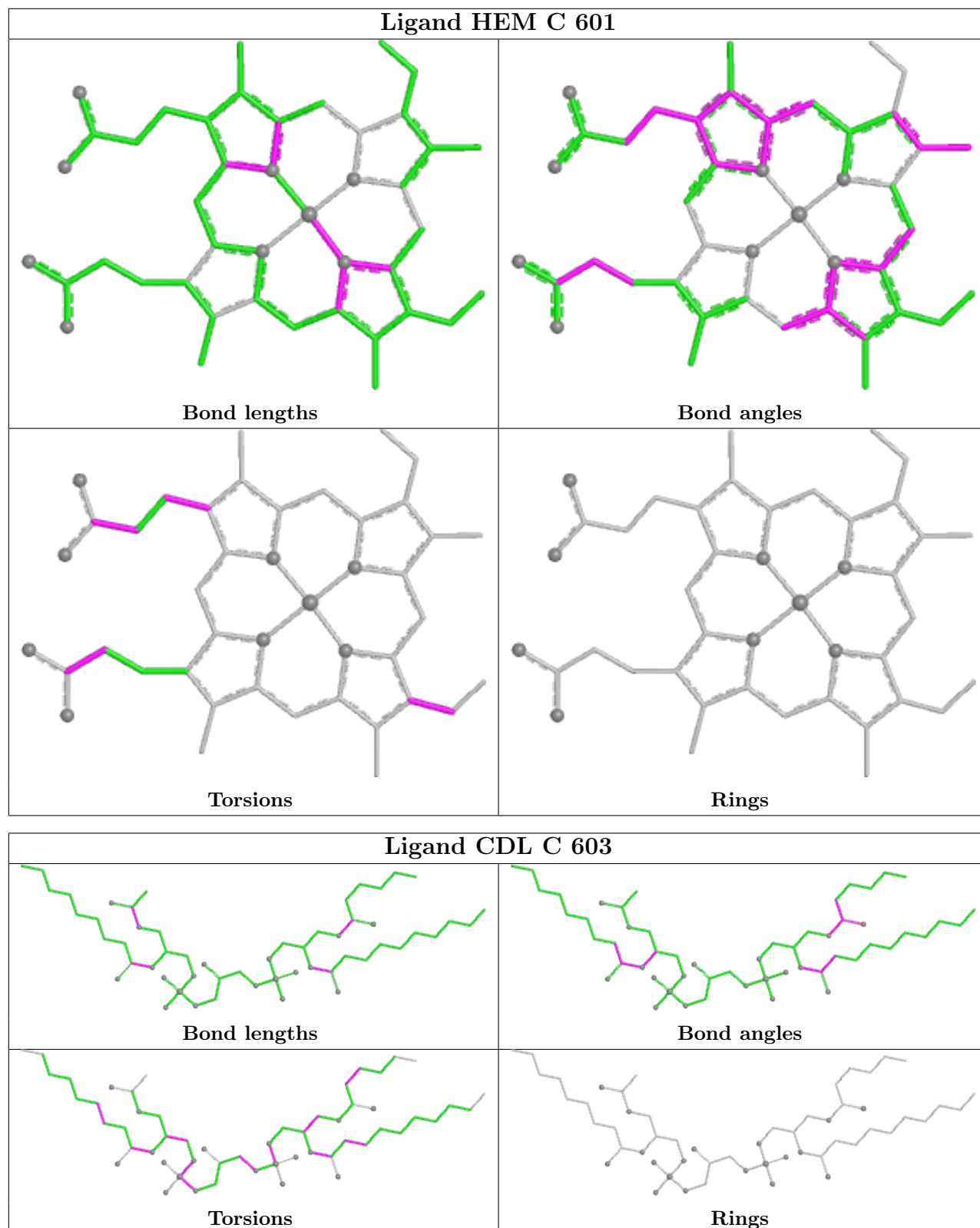


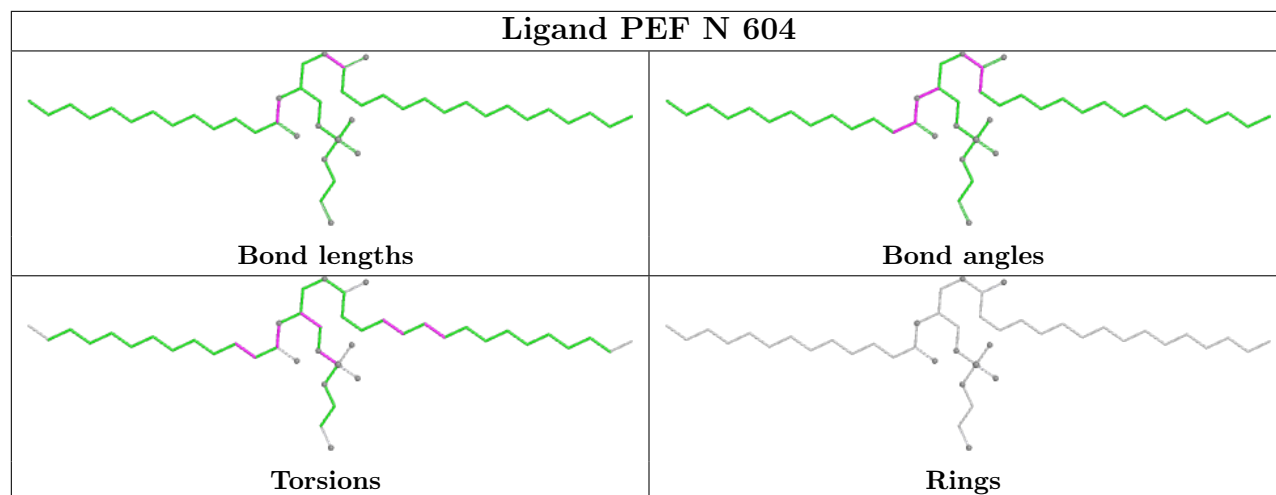












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

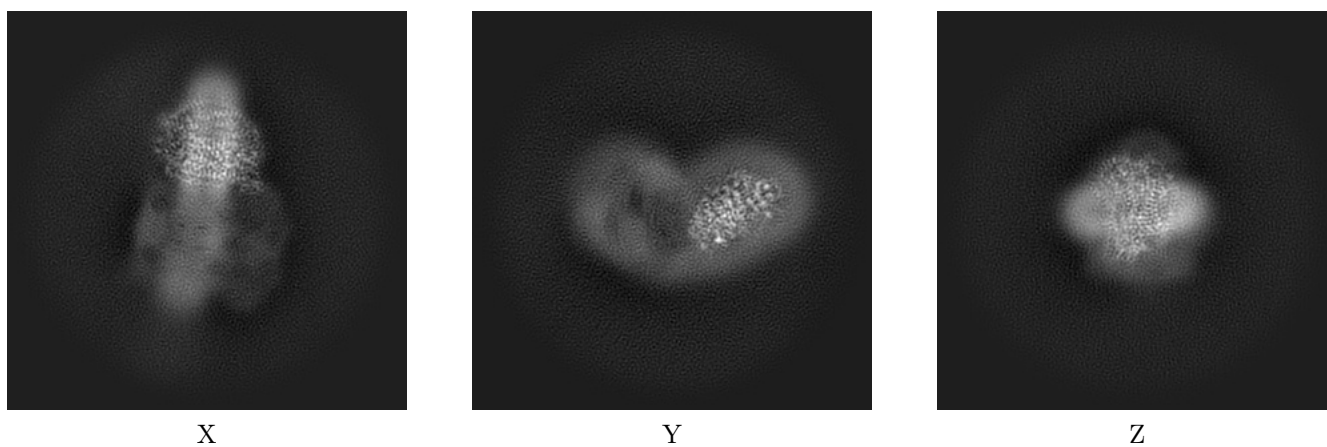
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10318. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

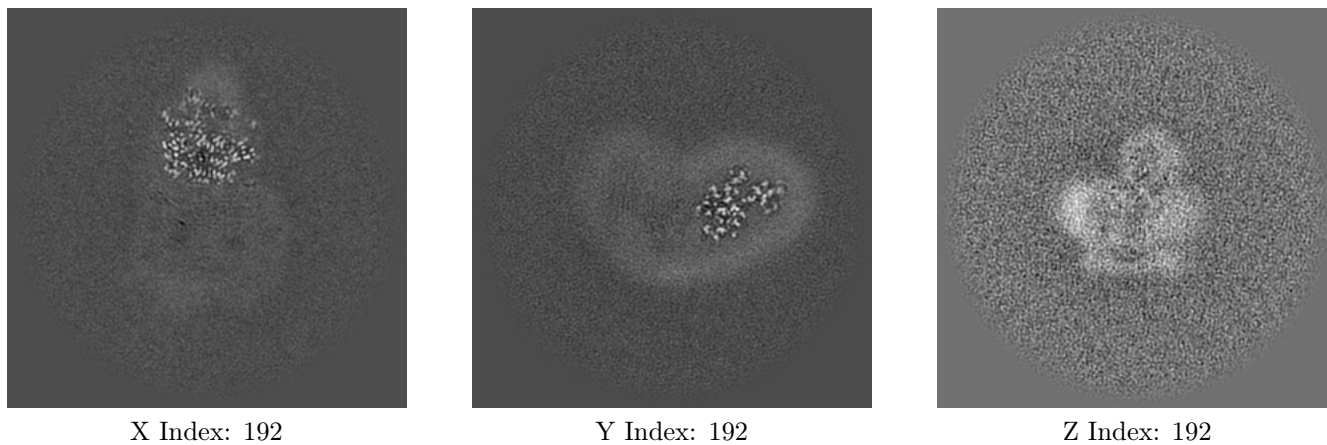
6.1.1 Primary map



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

6.2 Central slices [i](#)

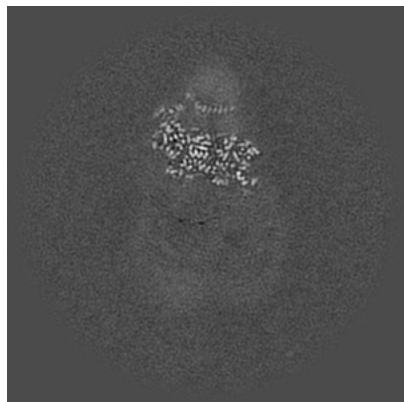
6.2.1 Primary map



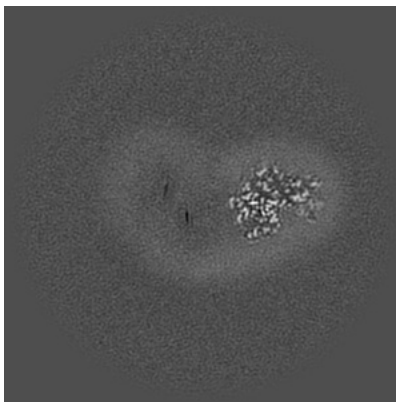
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

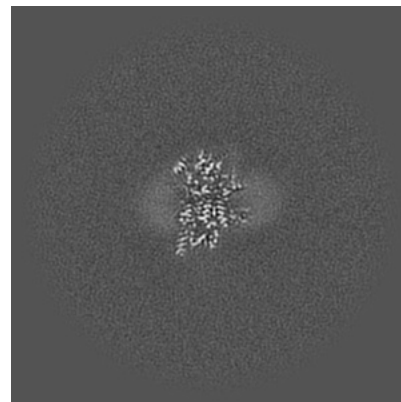
6.3.1 Primary map



X Index: 186



Y Index: 184



Z Index: 241

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.424. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

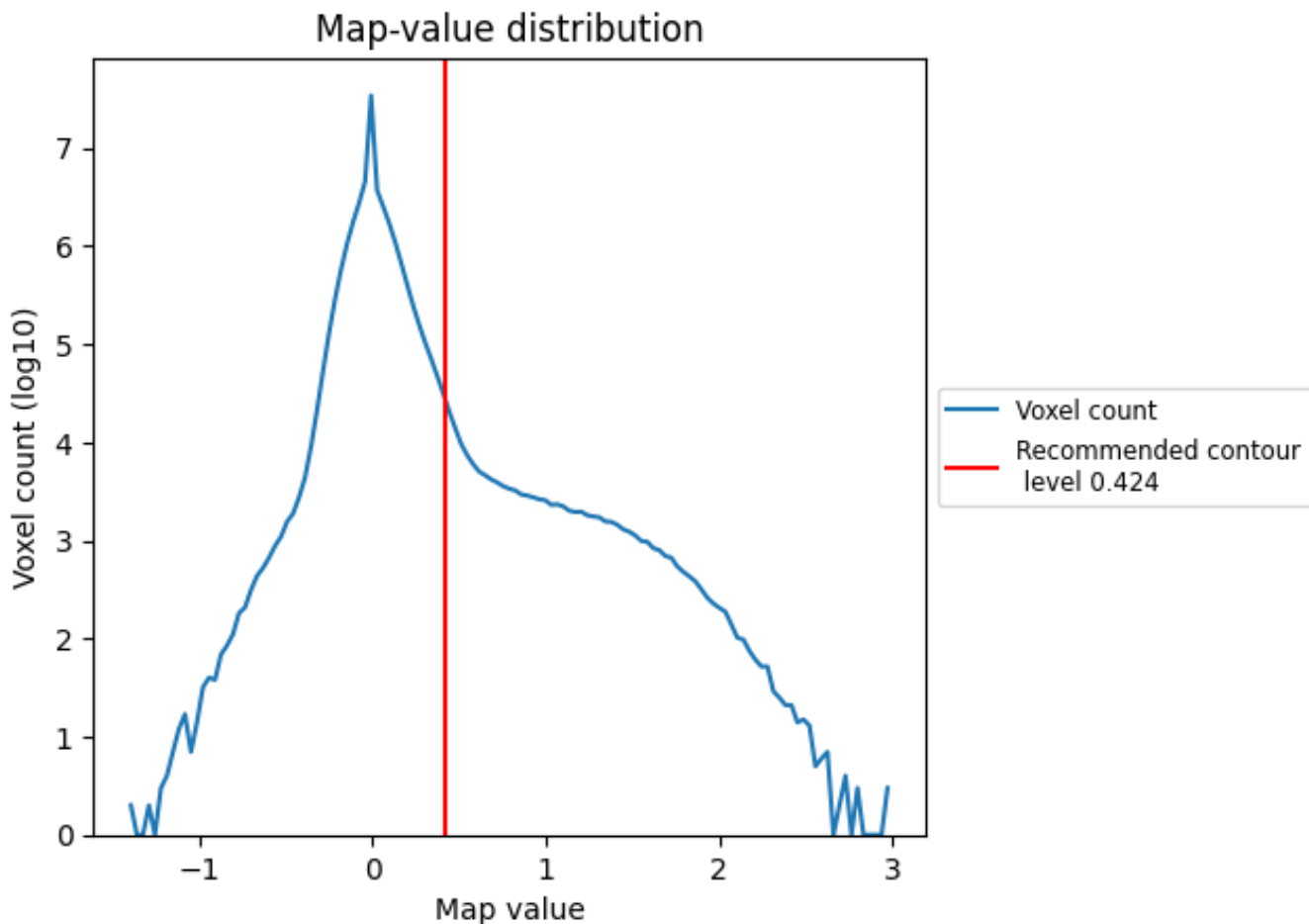
6.5 Mask visualisation

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

7 Map analysis [i](#)

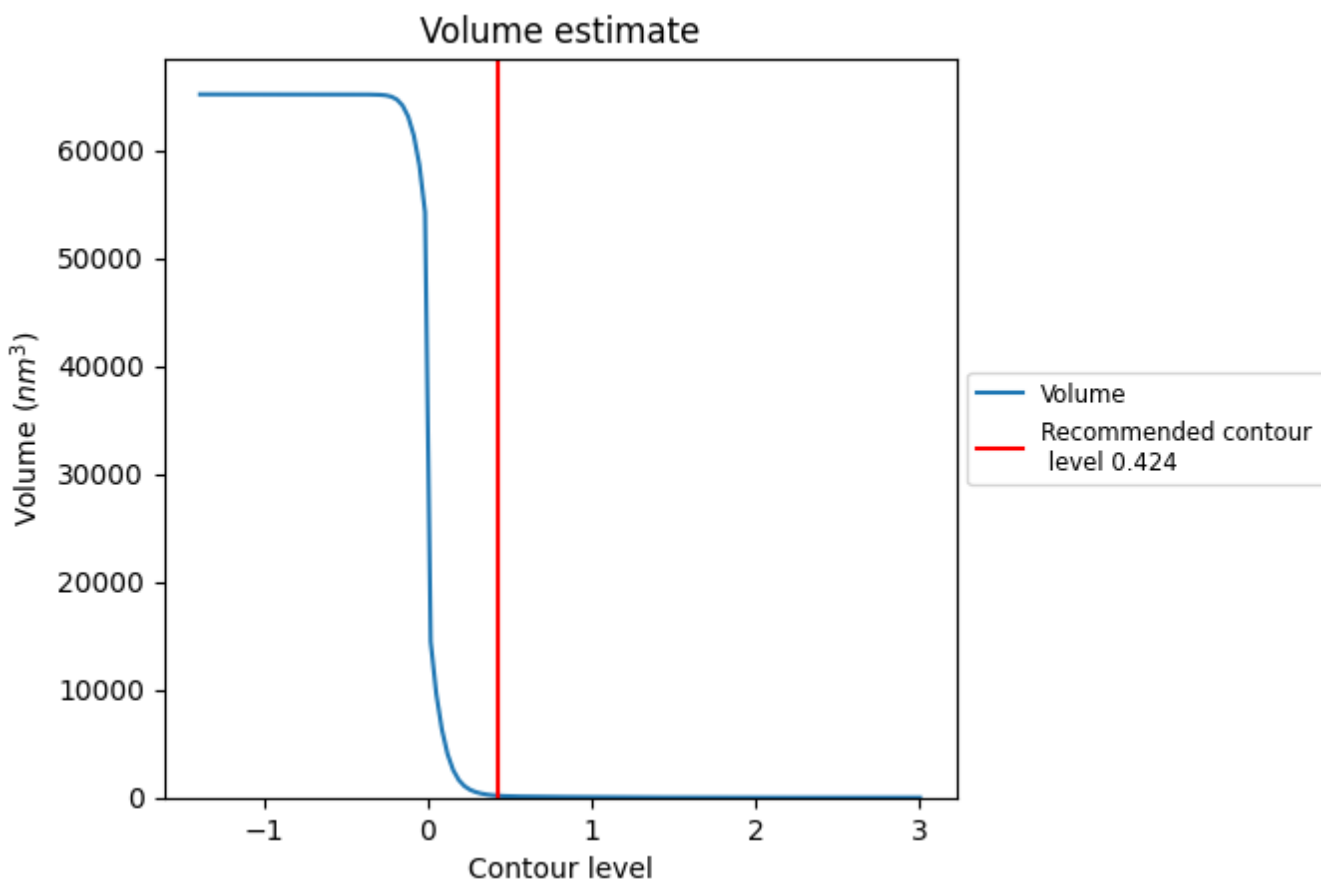
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

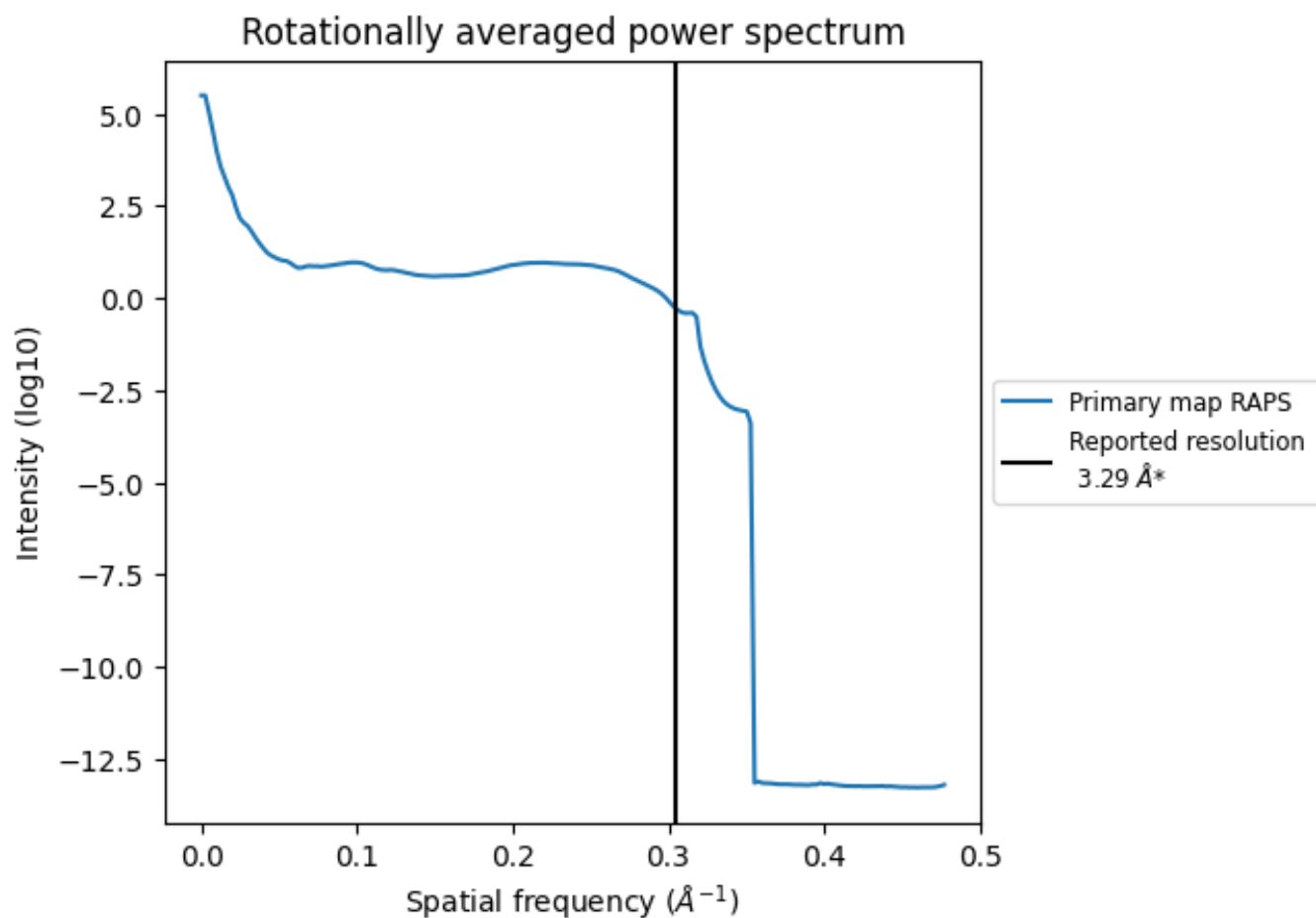
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 174 nm^3 ; this corresponds to an approximate mass of 158 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](#)

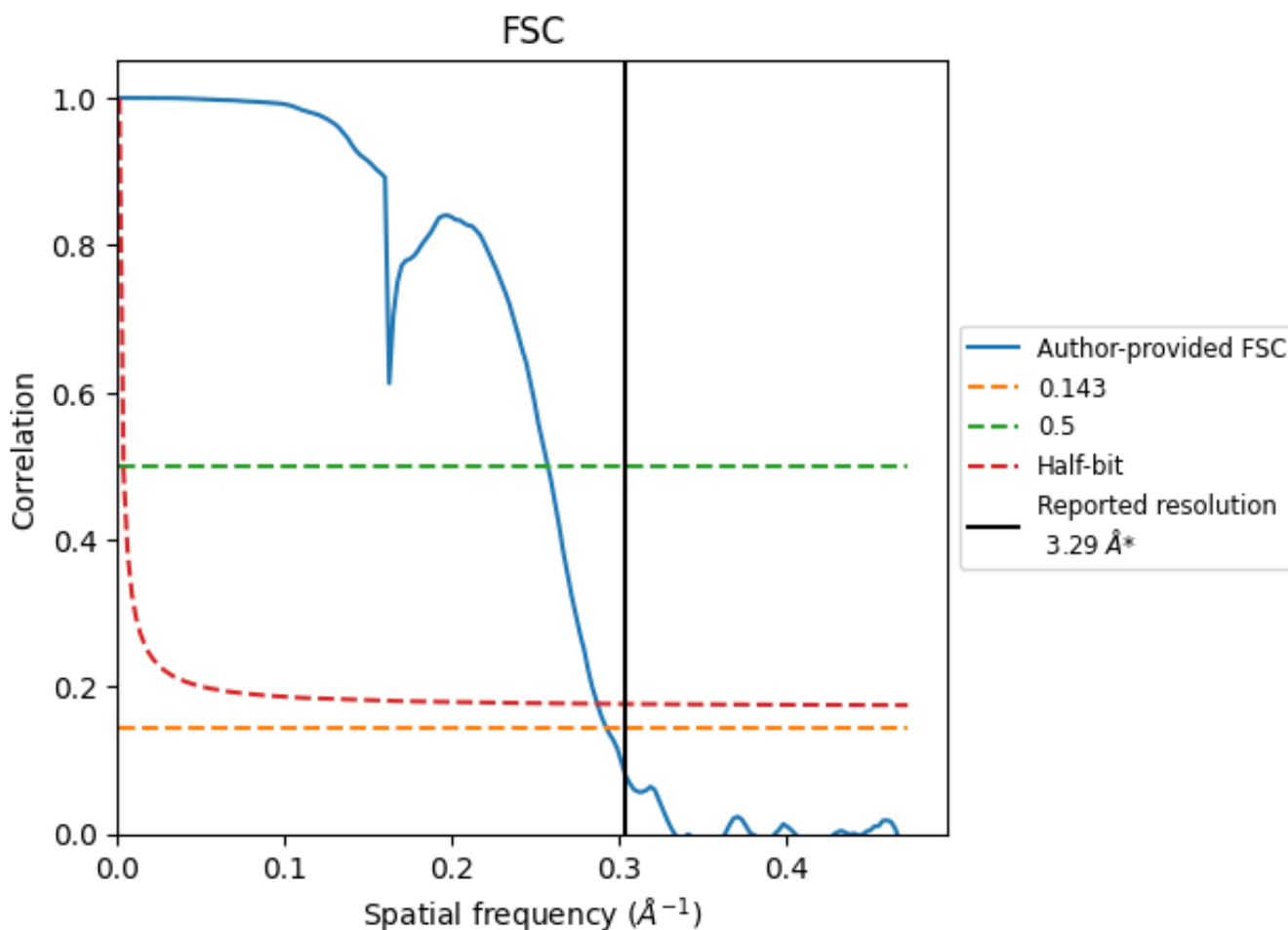


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

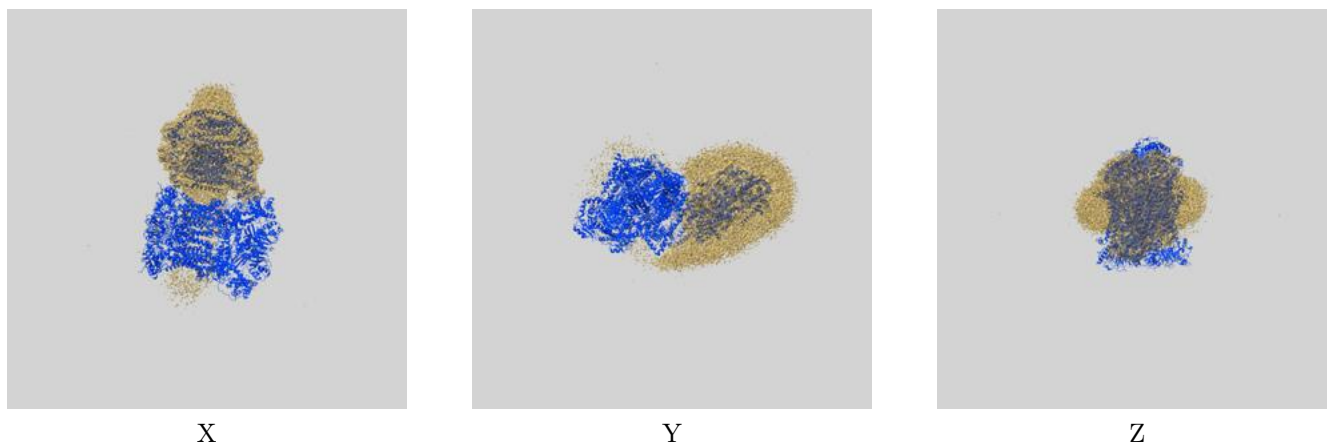
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.41	3.88	3.48
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

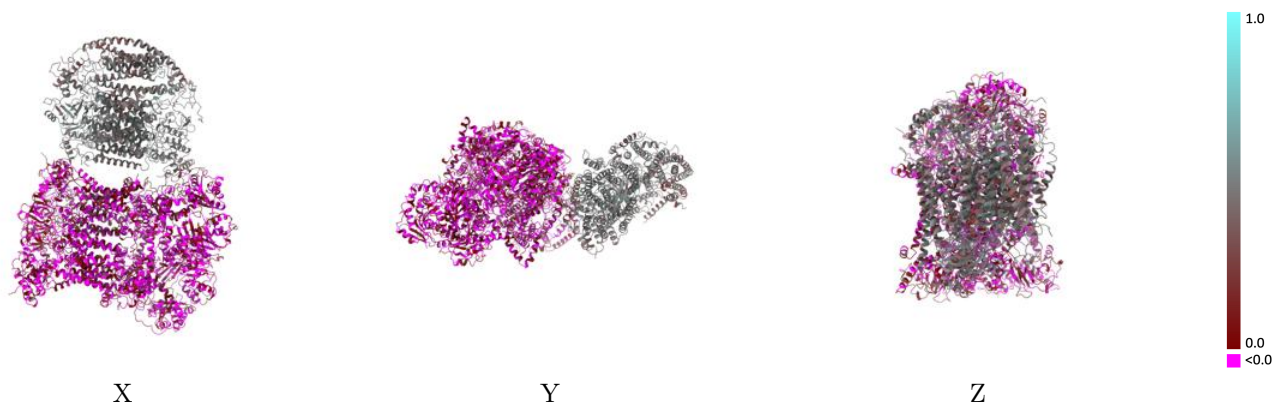
This section contains information regarding the fit between EMDB map EMD-10318 and PDB model 6T15. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



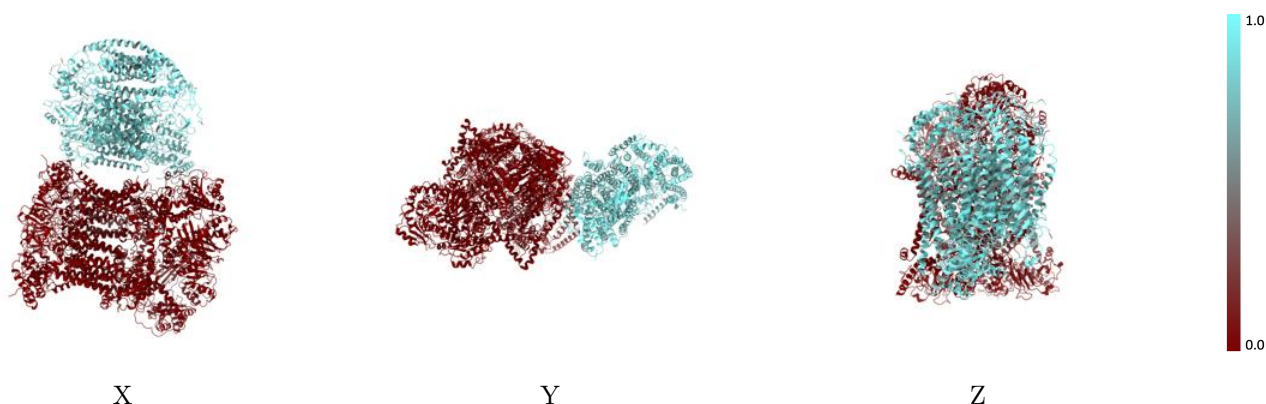
The images above show the 3D surface view of the map at the recommended contour level 0.424 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



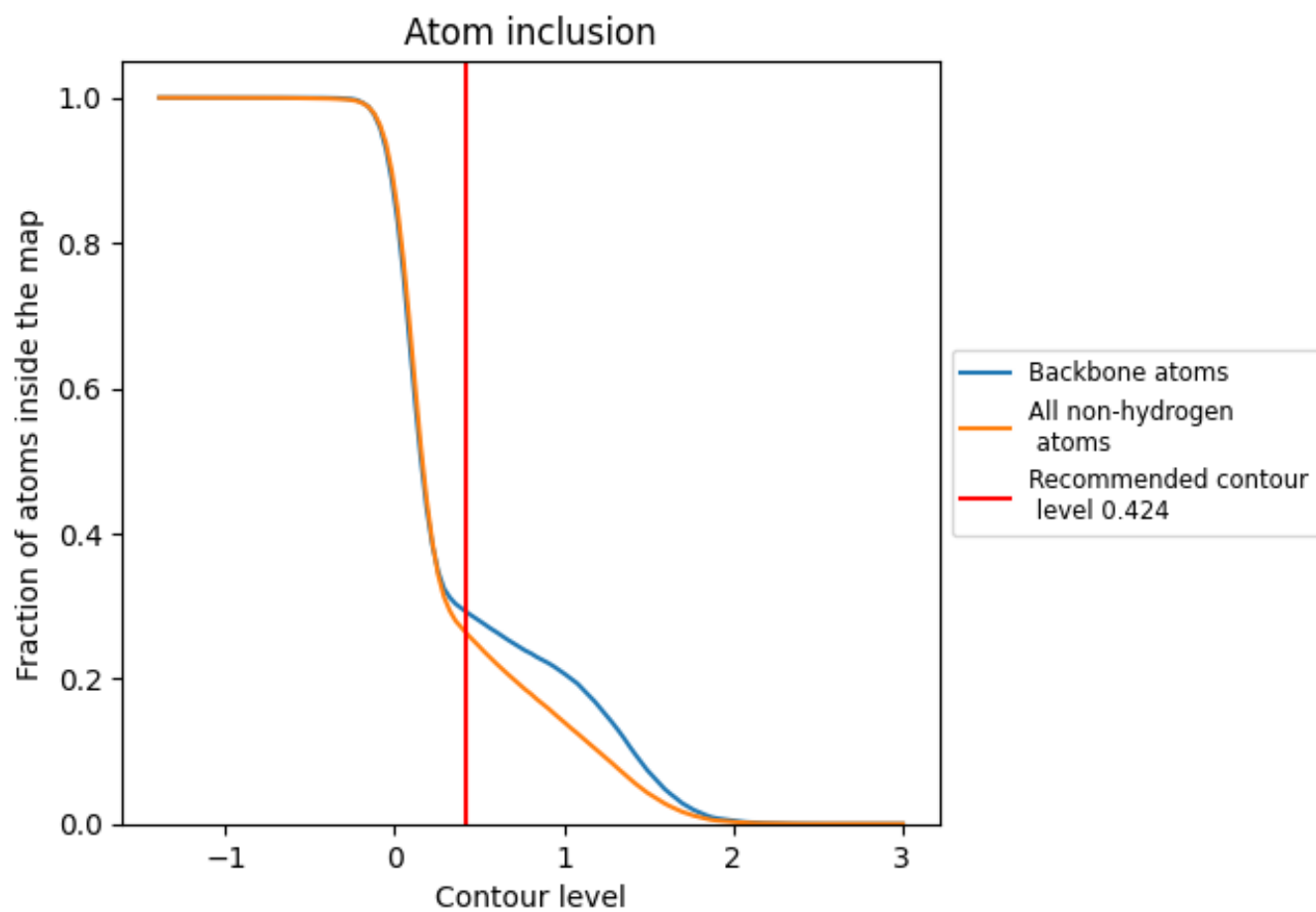
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.424).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 26% 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 (0.424) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2623	 0.1510
A	 0.0003	 -0.0120
B	 0.0000	 -0.0220
C	 0.0012	 -0.0200
D	 0.0000	 -0.0080
E	 0.0028	 0.0720
F	 0.0000	 0.0100
G	 0.0000	 -0.0100
H	 0.0000	 0.0110
I	 0.0000	 0.0150
J	 0.0032	 0.0320
L	 0.0018	 0.0170
M	 0.0004	 -0.0140
N	 0.0006	 0.0040
O	 0.0005	 0.0200
P	 0.0035	 0.0560
Q	 0.0000	 0.0360
R	 0.0000	 -0.0030
S	 0.0046	 0.0550
T	 0.0020	 0.0320
U	 0.0078	 0.0530
a	 0.8288	 0.4840
b	 0.8271	 0.4750
c	 0.8197	 0.4630
d	 0.8744	 0.4750
e	 0.7480	 0.4390
f	 0.8392	 0.4470
g	 0.8517	 0.4730
h	 0.8441	 0.4610
i	 0.8262	 0.4400
j	 0.8399	 0.4460
k	 0.8330	 0.4310
l	 0.8223	 0.4540
m	 0.7724	 0.3910

