



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:42 am BST

PDB ID : 1E7P
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINOGENES
Authors : Lancaster, C.R.D.; Kroeger, A.
Deposited on : 2000-09-01
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

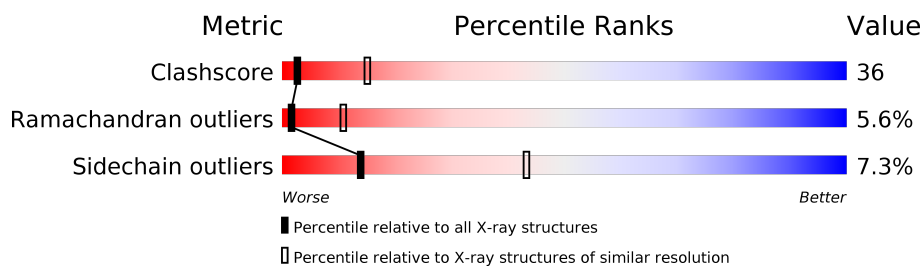
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)


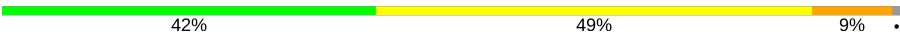
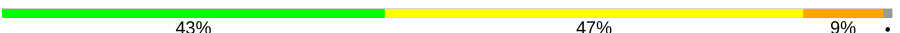

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	656	
1	D	656	
1	G	656	
1	J	656	
2	B	239	
2	E	239	
2	H	239	
2	K	239	

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Mol	Chain	Length	Quality of chain
3	C	256	 42% 48% 9%
3	F	256	 42% 49% 9%
3	I	256	 43% 47% 9%
3	L	256	 43% 48% 9%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLA	A	702	-	-	X	-
5	MLA	D	702	-	-	X	-
5	MLA	G	702	-	-	X	-
5	MLA	J	702	-	-	X	-
8	F3S	B	302	-	-	X	-
8	F3S	E	302	-	-	X	-
8	F3S	H	302	-	-	X	-
8	F3S	K	302	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	D	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	G	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	J	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	E	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	H	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	K	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			

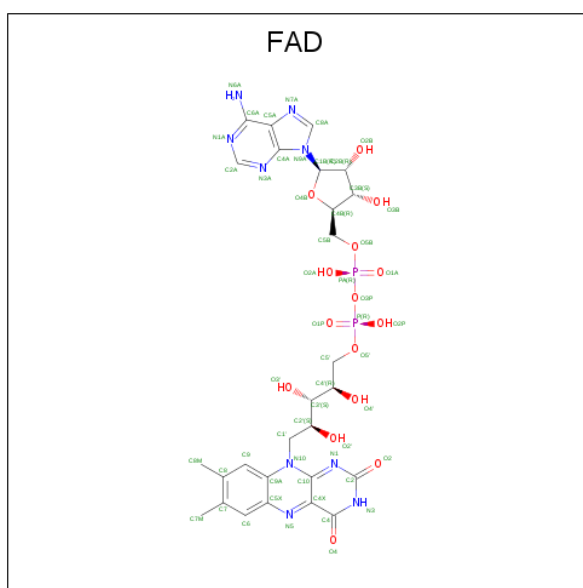
- Molecule 3 is a protein called Fumarate reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	F	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	I	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	L	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			

There are 4 discrepancies between the modelled and reference sequences:

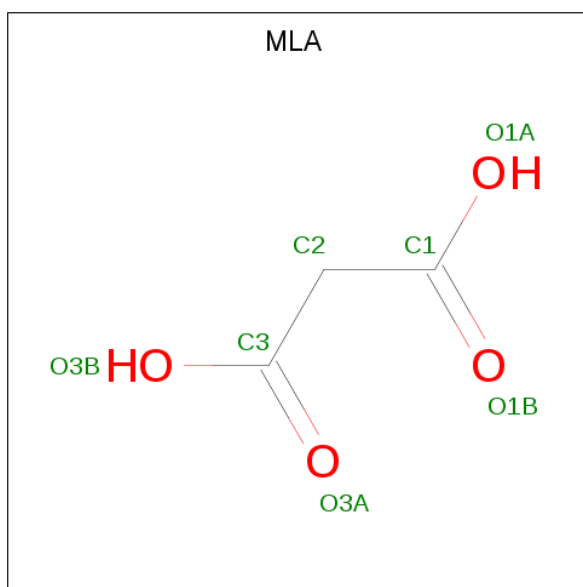
Chain	Residue	Modelled	Actual	Comment	Reference
C	66	GLN	GLU	engineered mutation	UNP P17413
F	66	GLN	GLU	engineered mutation	UNP P17413
I	66	GLN	GLU	engineered mutation	UNP P17413
L	66	GLN	GLU	engineered mutation	UNP P17413

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	J	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: $\text{C}_3\text{H}_4\text{O}_4$).

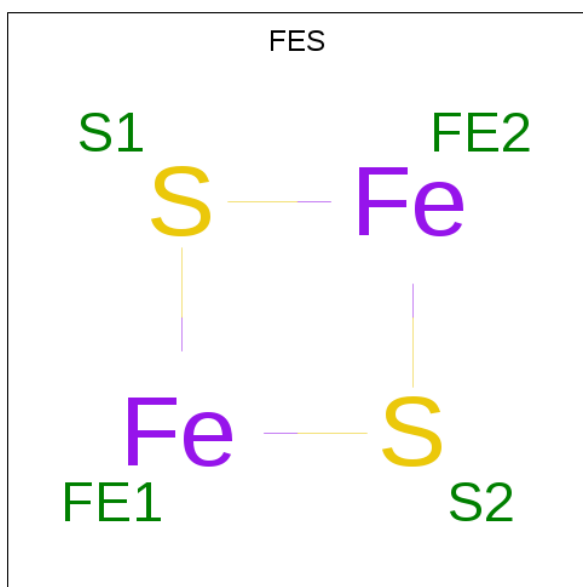


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		
5	G	1	Total	C	O	0	0
			7	3	4		
5	J	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

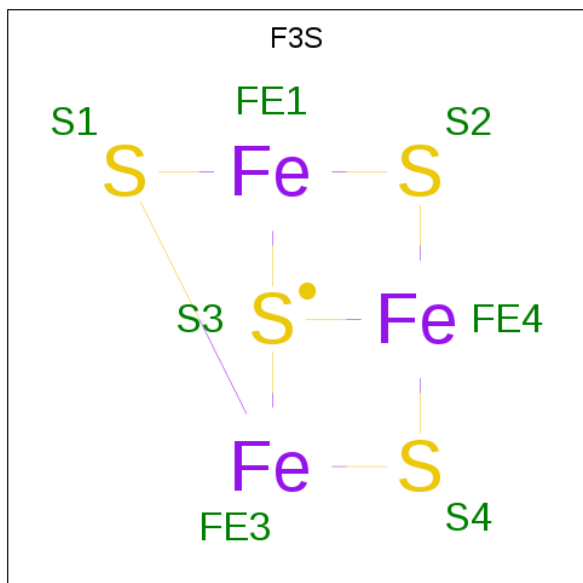
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Na	0	0
			1	1		
6	J	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



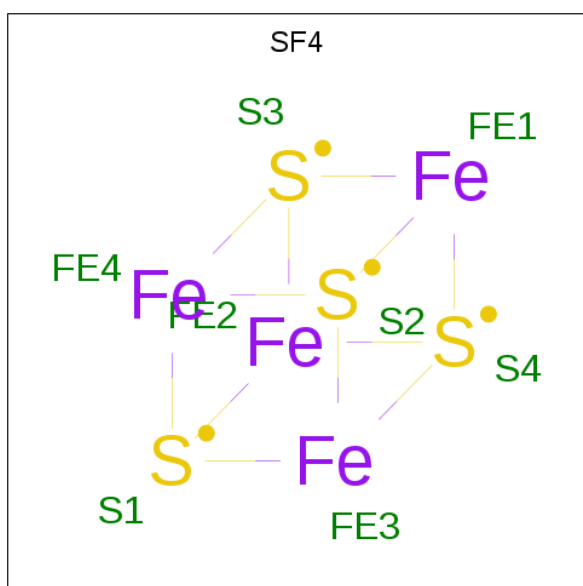
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		
7	H	1	Total	Fe	S	0	0
			4	2	2		
7	K	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



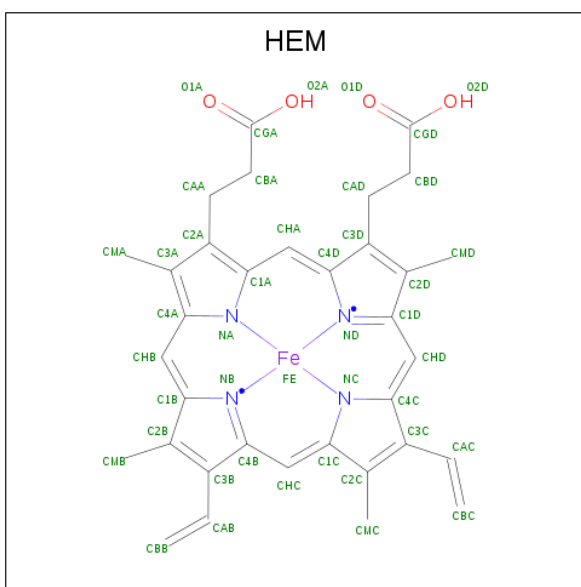
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		
8	H	1	Total	Fe	S	0	0
			7	3	4		
8	K	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



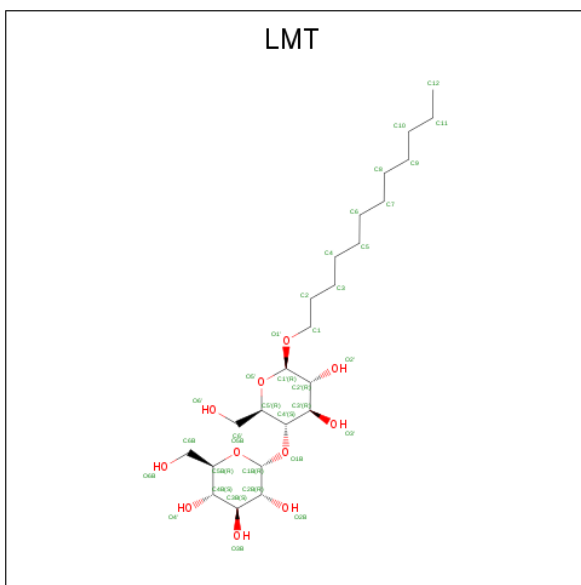
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	K	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



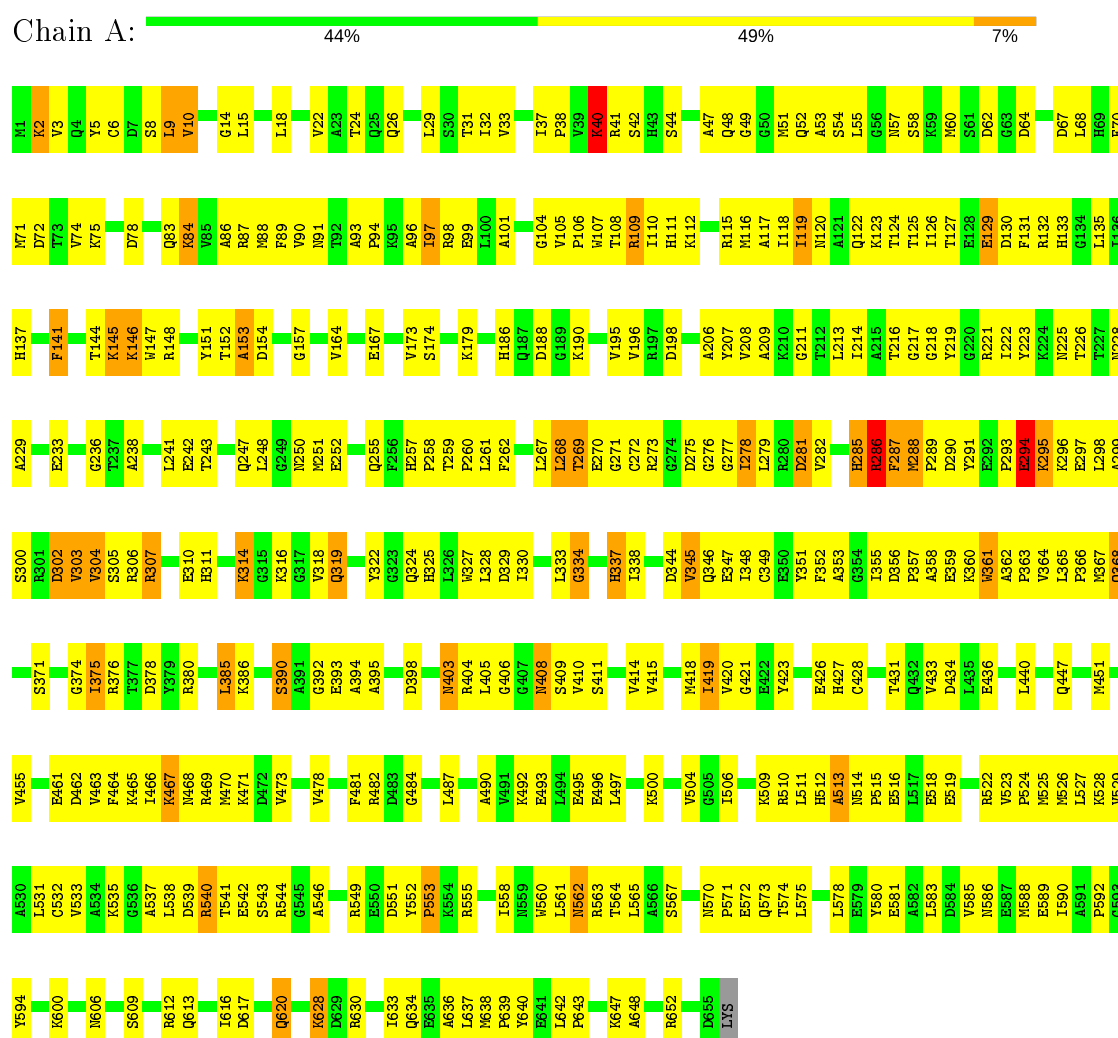
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 35	C 24	O 11	17	0
11	F	1	Total 35	C 24	O 11	17	0
11	I	1	Total 35	C 24	O 11	17	0
11	L	1	Total 35	C 24	O 11	17	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

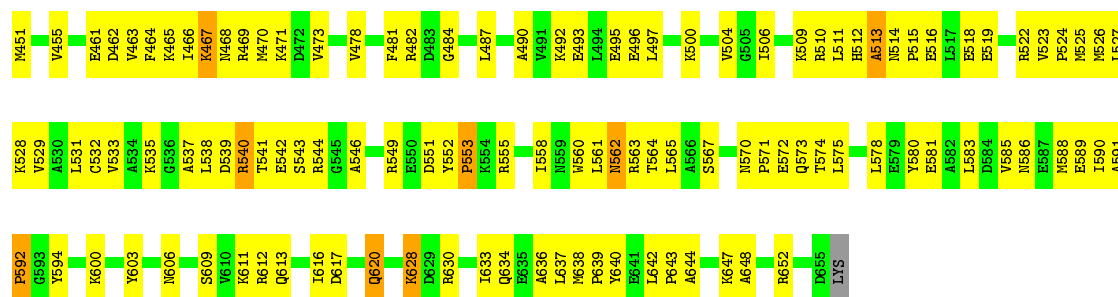
Note EDS was not executed.

- Molecule 1: Fumarate reductase flavoprotein subunit



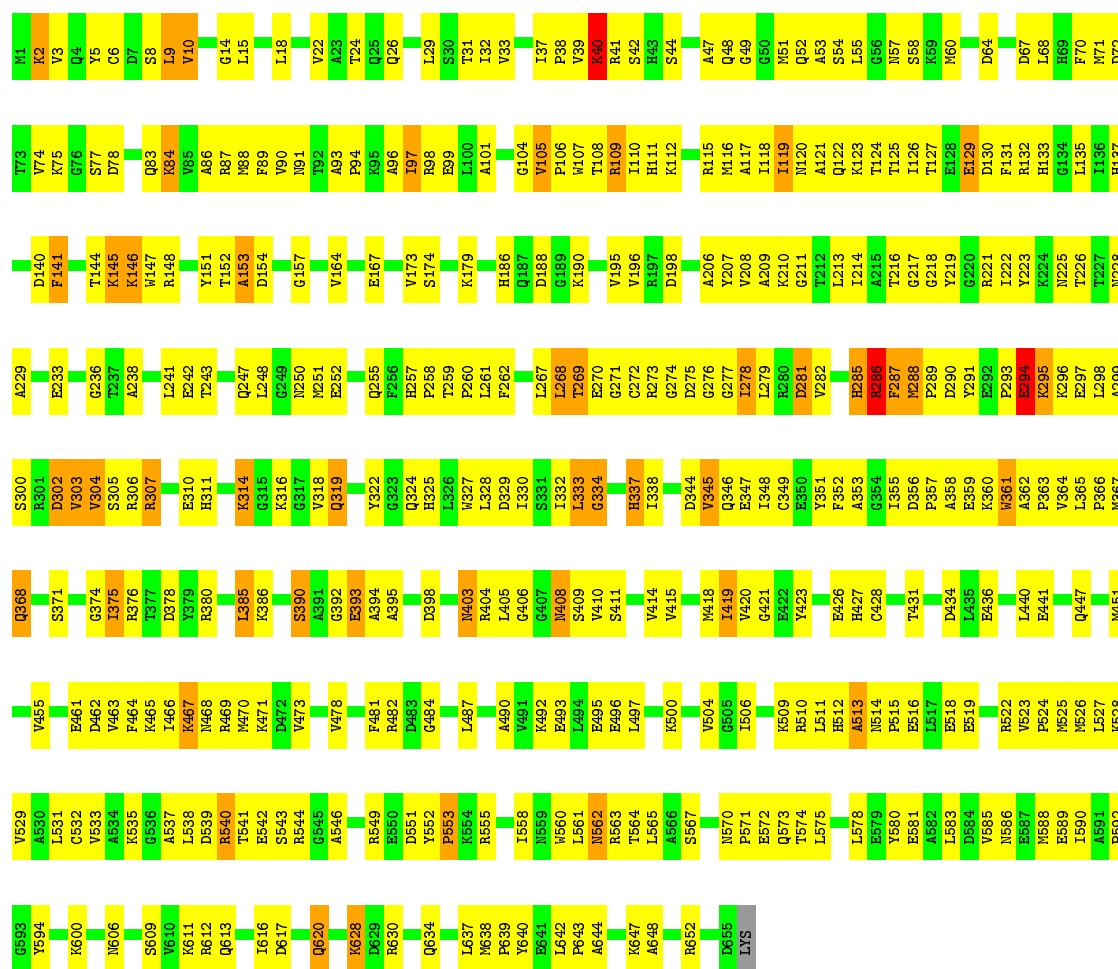
- Molecule 1: Fumarate reductase flavoprotein subunit





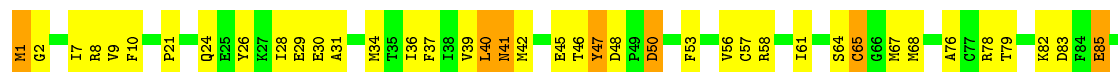
• Molecule 1: Fumarate reductase flavoprotein subunit

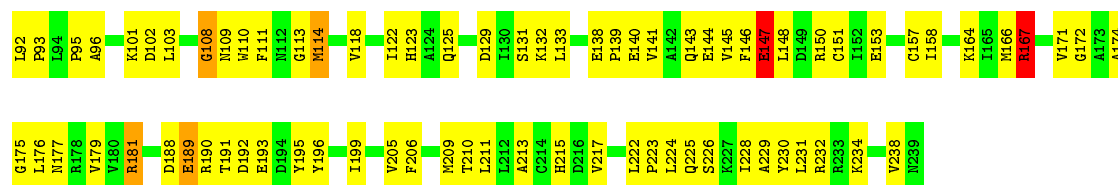
Chain J: 43% 50% 7%



• Molecule 2: Fumarate reductase iron-sulfur subunit

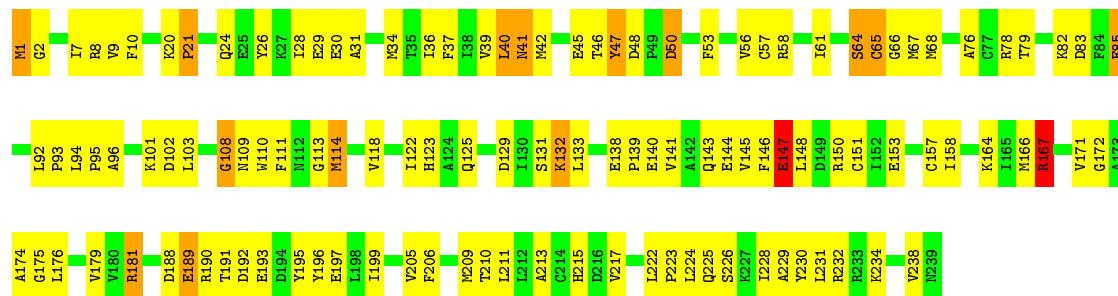
Chain B: 51% 43% 5%





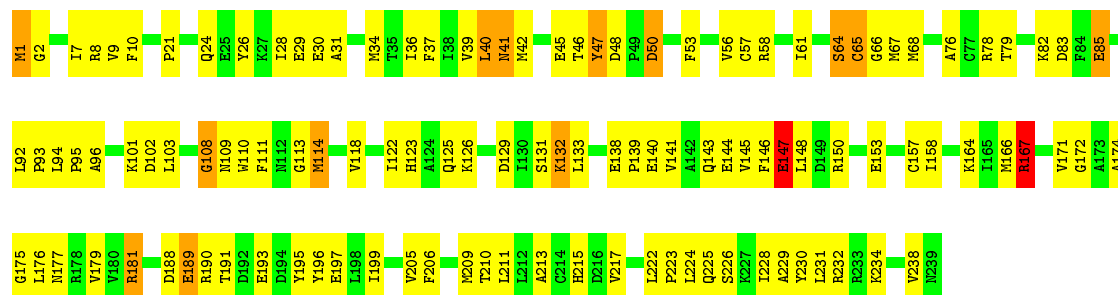
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain E: 50% 43% 6%



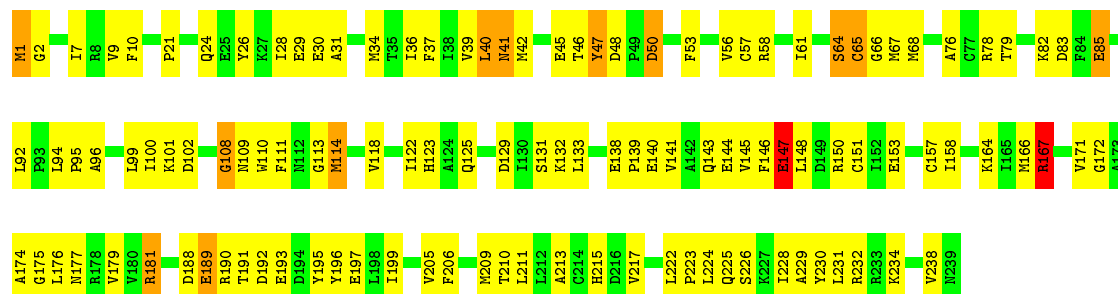
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain H: 51% 43% 5%



• Molecule 2: Fumarate reductase iron-sulfur subunit

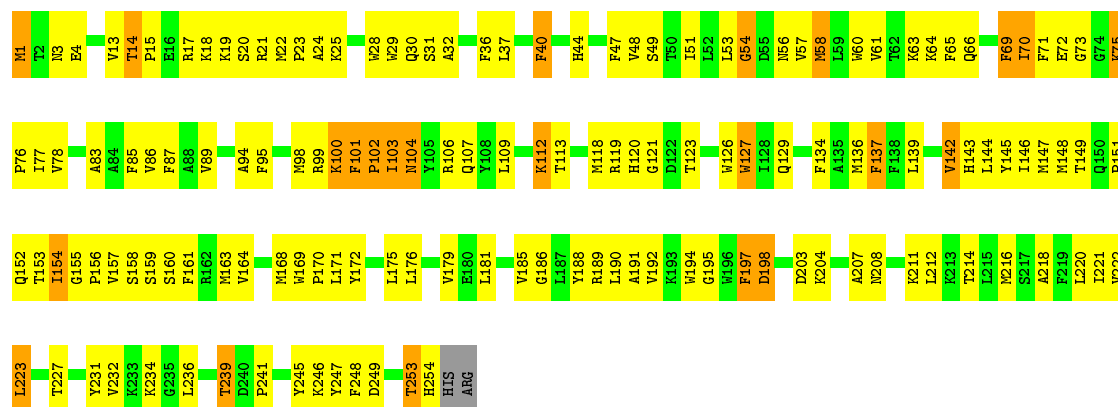
Chain K: 51% 44% 5%



• Molecule 3: Fumarate reductase cytochrome b subunit

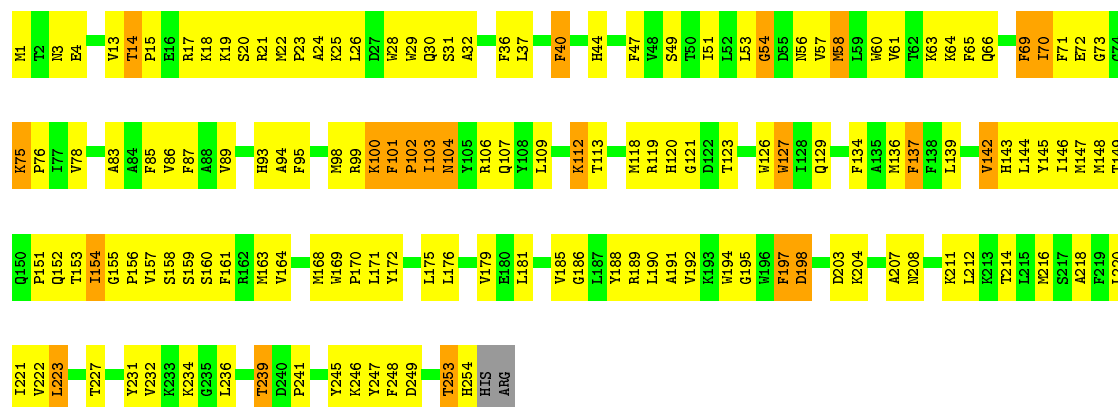
Chain C: 42% 48% 9%





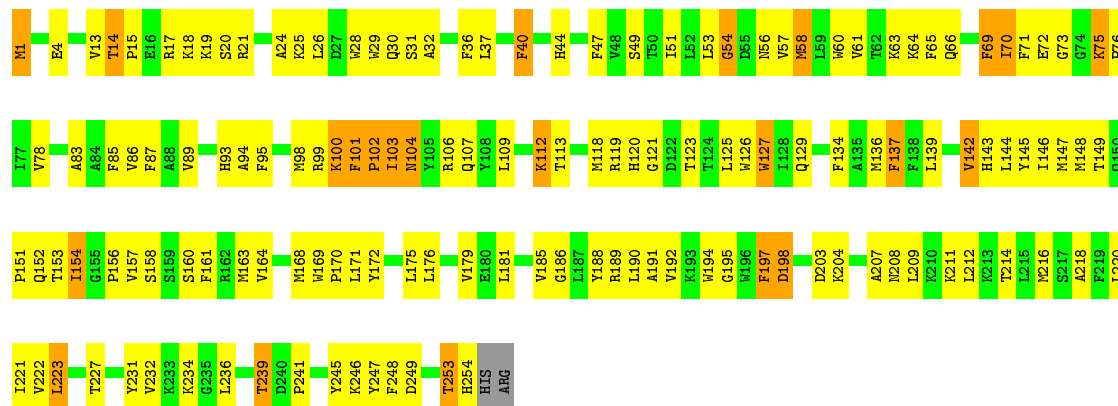
• Molecule 3: Fumarate reductase cytochrome b subunit

Chain F: 42% 49% 9% .



• Molecule 3: Fumarate reductase cytochrome b subunit

Chain I: 43% 47% 9% .



• Molecule 3: Fumarate reductase cytochrome b subunit

Chain L: 43% 48% 9% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.07Å 290.24Å 153.61Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	80.8 (30.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	37072	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, NA, SF4, LMT, F3S, FES, HEM, FAD

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	0.57	0/5189	0.73	0/6996
1	D	0.58	0/5189	0.73	0/6996
1	G	0.58	0/5189	0.73	0/6996
1	J	0.58	0/5189	0.73	0/6996
2	B	0.47	0/1931	0.70	1/2604 (0.0%)
2	E	0.47	0/1931	0.70	1/2604 (0.0%)
2	H	0.47	0/1931	0.70	1/2604 (0.0%)
2	K	0.47	0/1931	0.70	1/2604 (0.0%)
3	C	0.60	0/2146	0.67	1/2904 (0.0%)
3	F	0.60	0/2146	0.67	1/2904 (0.0%)
3	I	0.60	0/2146	0.67	1/2904 (0.0%)
3	L	0.60	0/2146	0.67	1/2904 (0.0%)
All	All	0.56	0/37064	0.71	8/50016 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	102	PRO	N-CA-C	-5.31	98.30	112.10
3	F	102	PRO	N-CA-C	-5.30	98.31	112.10
3	C	102	PRO	N-CA-C	-5.30	98.32	112.10
3	I	102	PRO	N-CA-C	-5.30	98.32	112.10
2	H	167	ARG	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5093	0	5069	407	11
1	D	5093	0	5069	408	16
1	G	5093	0	5069	416	13
1	J	5093	0	5069	413	14
2	B	1894	0	1861	105	0
2	E	1894	0	1861	106	0
2	H	1894	0	1861	107	0
2	K	1894	0	1861	103	0
3	C	2080	0	2103	163	0
3	F	2080	0	2103	163	0
3	I	2080	0	2103	166	0
3	L	2080	0	2103	162	0
4	A	53	0	29	4	0
4	D	53	0	29	4	0
4	G	53	0	29	4	0
4	J	53	0	29	4	0
5	A	7	0	2	5	0
5	D	7	0	2	5	0
5	G	7	0	2	6	0
5	J	7	0	2	5	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
7	H	4	0	0	0	0
7	K	4	0	0	0	0
8	B	7	0	0	2	0
8	E	7	0	0	2	0
8	H	7	0	0	2	0
8	K	7	0	0	2	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
9	H	8	0	0	0	0
9	K	8	0	0	0	0
10	C	86	0	60	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	86	0	60	12	0
10	I	86	0	60	11	0
10	L	86	0	60	11	0
11	C	35	0	46	3	0
11	F	35	0	46	3	0
11	I	35	0	46	3	0
11	L	35	0	46	3	0
All	All	37072	0	36680	2632	27

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 2632 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:THR:HG21	1:D:236:GLY:HA3	1.32	1.12
1:J:327:TRP:HB3	1:J:361:TRP:HB2	1.30	1.11
1:G:216:THR:HG21	1:G:236:GLY:HA3	1.32	1.09
3:L:152:GLN:HE21	3:L:153:THR:HG23	1.18	1.07
1:G:327:TRP:HB3	1:G:361:TRP:HB2	1.30	1.06

The worst 5 of 27 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:TYR:C	1:G:122:GLN:NE2[1_455]	0.81	1.39
1:A:122:GLN:NE2	1:J:581:GLU:N[1_554]	0.84	1.36
1:D:581:GLU:N	1:G:122:GLN:NE2[1_455]	1.03	1.17
1:A:122:GLN:NE2	1:J:580:TYR:C[1_554]	1.10	1.10
1:A:122:GLN:OE1	1:J:581:GLU:CA[1_554]	1.30	0.90

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 X-ray entries followed by that with respect to entries of similar resolution.

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	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	1	8
1	D	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	1	8
1	G	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	1	8
1	J	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	1	8
2	B	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	E	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	H	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	K	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
3	C	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
3	F	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
3	I	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
3	L	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
All	All	4568/4604 (99%)	3556 (78%)	758 (17%)	254 (6%)	2	11

5 of 254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	THR
1	A	288	MET
1	A	294	GLU
1	A	319	GLN
1	A	333	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	532/533 (100%)	497 (93%)	35 (7%)	16	47
1	D	532/533 (100%)	497 (93%)	35 (7%)	16	47
1	G	532/533 (100%)	497 (93%)	35 (7%)	16	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	532/533 (100%)	497 (93%)	35 (7%)	16	47
2	B	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	E	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	H	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	K	211/211 (100%)	199 (94%)	12 (6%)	20	52
3	C	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	F	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	I	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	L	221/223 (99%)	198 (90%)	23 (10%)	7	27
All	All	3856/3868 (100%)	3576 (93%)	280 (7%)	14	43

5 of 280 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	78	VAL
1	G	302	ASP
3	L	14	THR
3	F	123	THR
1	G	40	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	225	GLN
1	G	158	HIS
1	J	562	ASN
3	F	3	ASN
1	G	26	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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
8	F3S	B	302	2	0,9,9	0.00	-	-		
8	F3S	E	302	2	0,9,9	0.00	-	-		
10	HEM	L	302	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
10	HEM	I	302	3	27,50,50	1.80	7 (25%)	17,82,82	1.48	2 (11%)
5	MLA	D	702	-	0,6,6	0.00	-	0,7,7	0.00	-
7	FES	B	301	2	0,4,4	0.00	-	-		
9	SF4	H	303	2	0,12,12	0.00	-	-		
9	SF4	B	303	2	0,12,12	0.00	-	-		
4	FAD	G	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)
10	HEM	I	301	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
5	MLA	A	702	-	0,6,6	0.00	-	0,7,7	0.00	-
8	F3S	H	302	2	0,9,9	0.00	-	-		
4	FAD	J	701	1	51,58,58	2.39	15 (29%)	60,89,89	2.14	10 (16%)
7	FES	E	301	2	0,4,4	0.00	-	-		
11	LMT	I	303	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
9	SF4	K	303	2	0,12,12	0.00	-	-		
8	F3S	K	302	2	0,9,9	0.00	-	-		
10	HEM	F	302	3	27,50,50	2.09	8 (29%)	17,82,82	1.65	2 (11%)
7	FES	H	301	2	0,4,4	0.00	-	-		
7	FES	K	301	2	0,4,4	0.00	-	-		
11	LMT	C	303	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	F	303	3	27,50,50	1.81	7 (25%)	17,82,82	1.47	2 (11%)
11	LMT	L	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
9	SF4	E	303	2	0,12,12	0.00	-	-		
4	FAD	D	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	A	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)
10	HEM	C	301	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
11	LMT	F	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	C	302	3	27,50,50	1.81	7 (25%)	17,82,82	1.47	2 (11%)
5	MLA	G	702	-	0,6,6	0.00	-	0,7,7	0.00	-
10	HEM	L	303	3	27,50,50	1.80	7 (25%)	17,82,82	1.47	2 (11%)
5	MLA	J	702	-	0,6,6	0.00	-	0,7,7	0.00	-

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
8	F3S	B	302	2	-	-	0/3/3/3
10	HEM	L	302	3	-	1/6/54/54	-
10	HEM	I	302	3	-	0/6/54/54	-
5	MLA	D	702	-	-	0/0/4/4	-
7	FES	B	301	2	-	-	0/1/1/1
4	FAD	J	701	1	-	9/30/50/50	0/6/6/6
11	LMT	F	301	-	-	10/21/61/61	0/2/2/2
5	MLA	J	702	-	-	0/0/4/4	-
10	HEM	I	301	3	-	1/6/54/54	-
5	MLA	A	702	-	-	0/0/4/4	-
8	F3S	H	302	2	-	-	0/3/3/3
10	HEM	C	301	3	-	1/6/54/54	-
7	FES	E	301	2	-	-	0/1/1/1
9	SF4	H	303	2	-	-	0/6/5/5
11	LMT	I	303	-	-	10/21/61/61	0/2/2/2
9	SF4	K	303	2	-	-	0/6/5/5
9	SF4	E	303	2	-	-	0/6/5/5
8	F3S	K	302	2	-	-	0/3/3/3
10	HEM	F	302	3	-	1/6/54/54	-
7	FES	H	301	2	-	-	0/1/1/1
7	FES	K	301	2	-	-	0/1/1/1
11	LMT	C	303	-	-	10/21/61/61	0/2/2/2
10	HEM	F	303	3	-	0/6/54/54	-
11	LMT	L	301	-	-	10/21/61/61	0/2/2/2
4	FAD	G	701	1	-	9/30/50/50	0/6/6/6
4	FAD	D	701	1	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	701	1	-	9/30/50/50	0/6/6/6
8	F3S	E	302	2	-	-	0/3/3/3
9	SF4	B	303	2	-	-	0/6/5/5
10	HEM	C	302	3	-	0/6/54/54	-
5	MLA	G	702	-	-	0/0/4/4	-
10	HEM	L	303	3	-	0/6/54/54	-

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	701	FAD	C4X-C10	9.34	1.48	1.38
4	A	701	FAD	C4X-C10	9.31	1.48	1.38
4	G	701	FAD	C4X-C10	9.29	1.48	1.38
4	D	701	FAD	C4X-C10	9.23	1.48	1.38
10	F	302	HEM	C3B-CAB	-5.37	1.37	1.47

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	FAD	C1'-N10-C10	9.14	126.60	118.41
4	G	701	FAD	C1'-N10-C10	9.13	126.59	118.41
4	J	701	FAD	C1'-N10-C10	9.12	126.58	118.41
4	A	701	FAD	C1'-N10-C10	9.10	126.56	118.41
4	G	701	FAD	C4-N3-C2	6.92	120.98	115.14

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	701	FAD	C2'-C1'-N10-C9A
4	G	701	FAD	C2'-C1'-N10-C10
4	G	701	FAD	C5'-O5'-P-O1P
4	G	701	FAD	C5'-O5'-P-O3P
4	A	701	FAD	C2'-C1'-N10-C9A

There are no ring outliers.

24 monomers are involved in 102 short contacts:

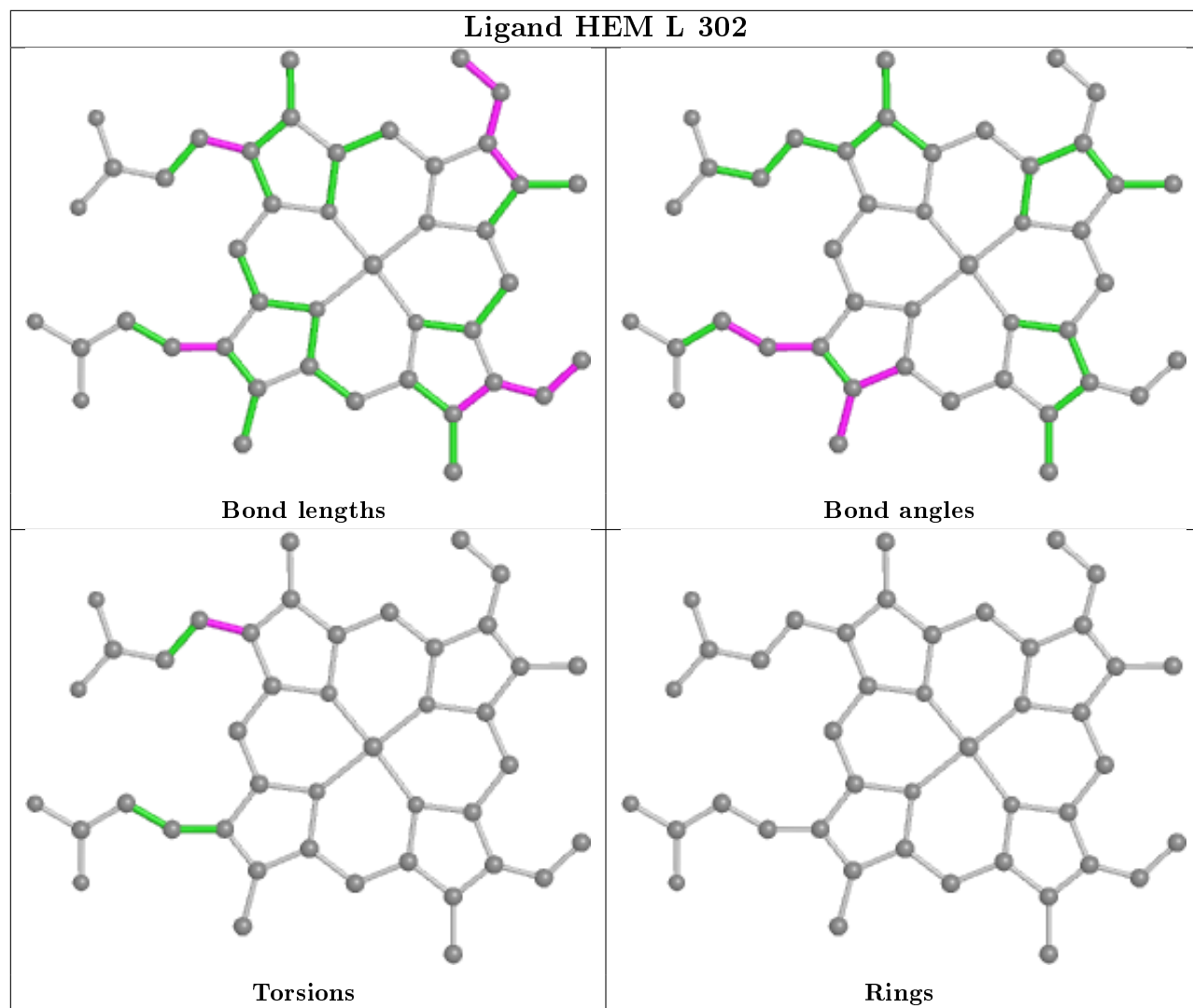
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	302	F3S	2	0
8	E	302	F3S	2	0

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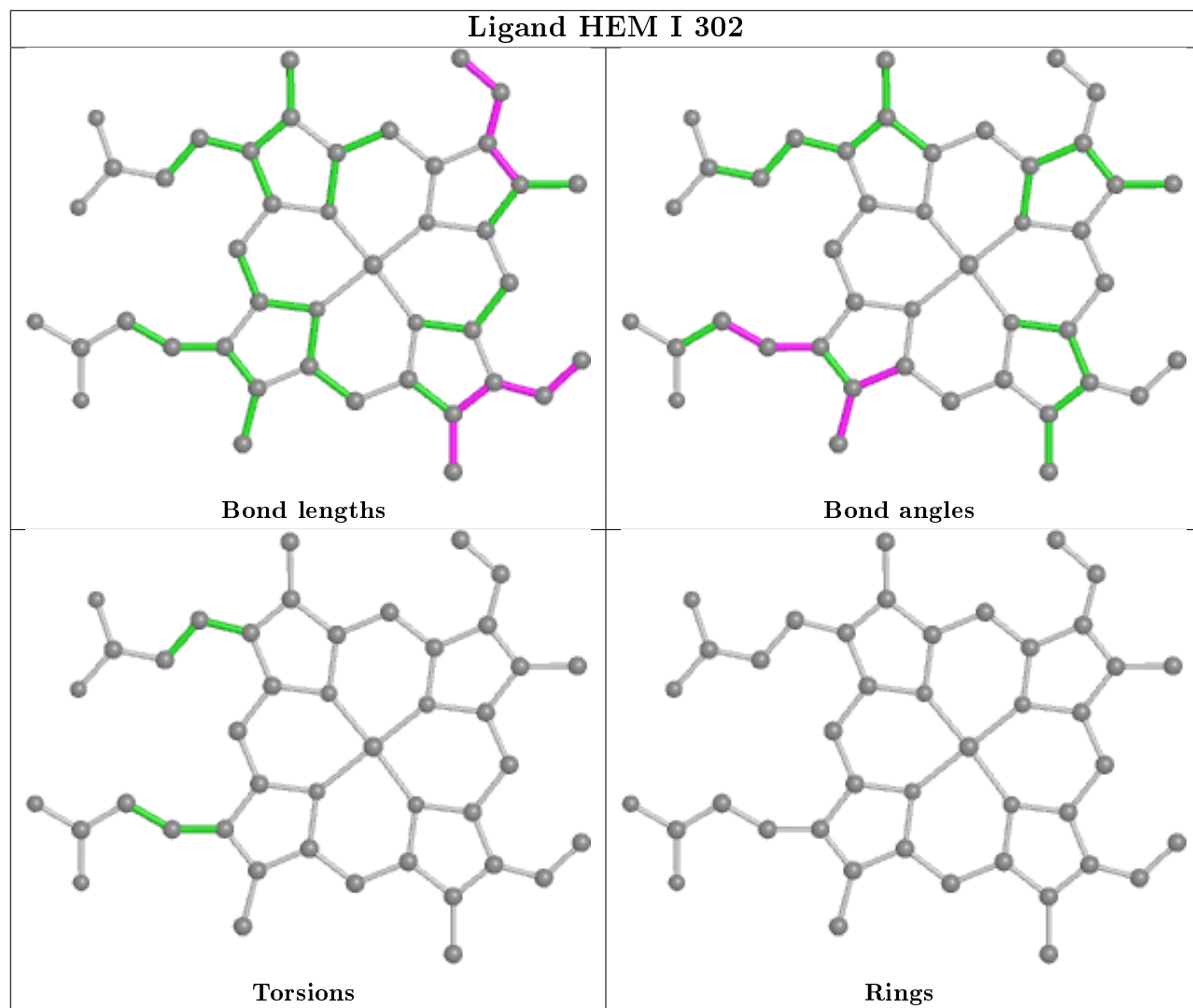
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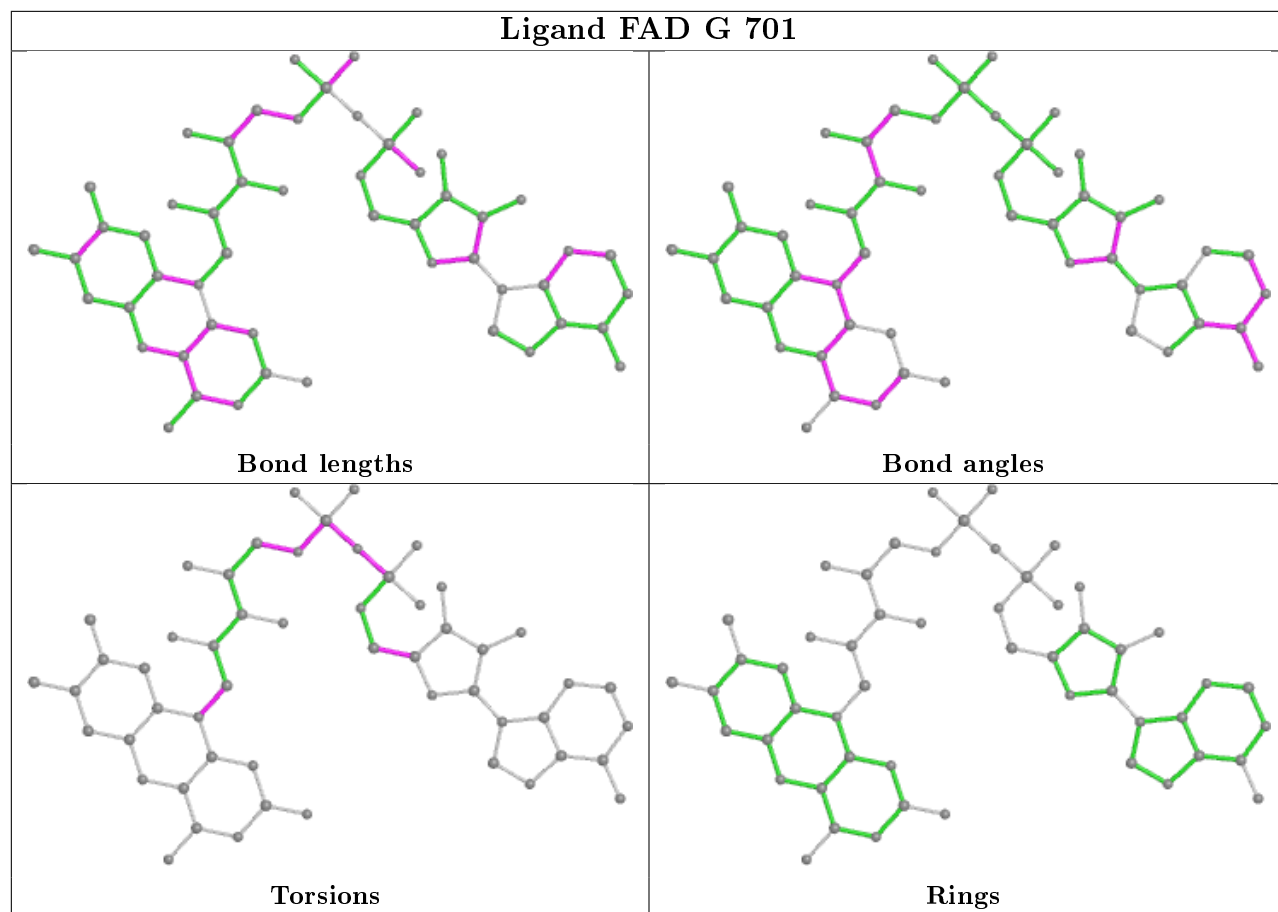
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	302	HEM	4	0
10	I	302	HEM	6	0
5	D	702	MLA	5	0
4	G	701	FAD	4	0
10	I	301	HEM	5	0
5	A	702	MLA	5	0
8	H	302	F3S	2	0
4	J	701	FAD	4	0
11	I	303	LMT	3	0
8	K	302	F3S	2	0
10	F	302	HEM	5	0
11	C	303	LMT	3	0
10	F	303	HEM	7	0
11	L	301	LMT	3	0
4	D	701	FAD	4	0
4	A	701	FAD	4	0
10	C	301	HEM	4	0
11	F	301	LMT	3	0
10	C	302	HEM	7	0
5	G	702	MLA	6	0
10	L	303	HEM	7	0
5	J	702	MLA	5	0

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

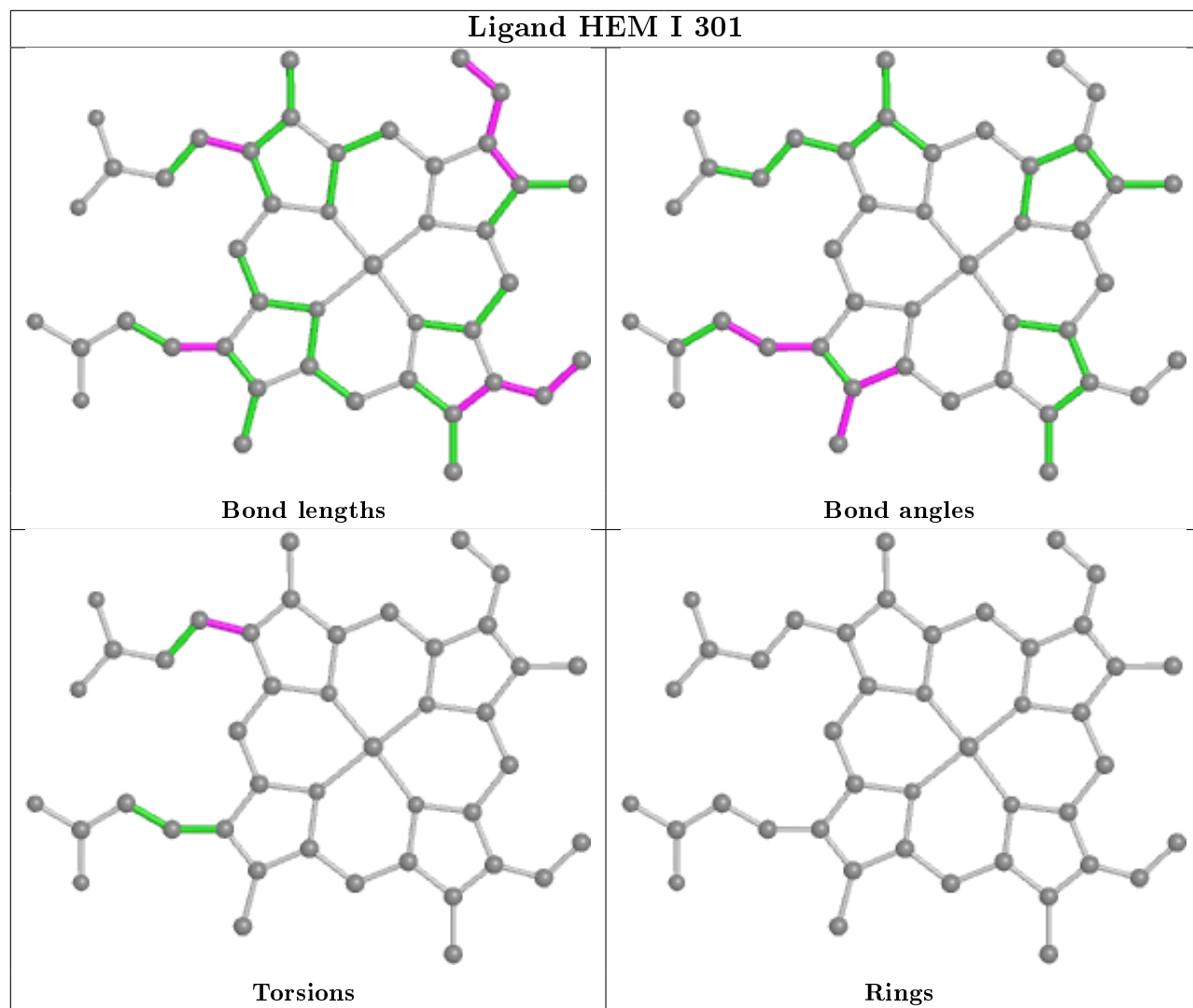


Ligand HEM I 302

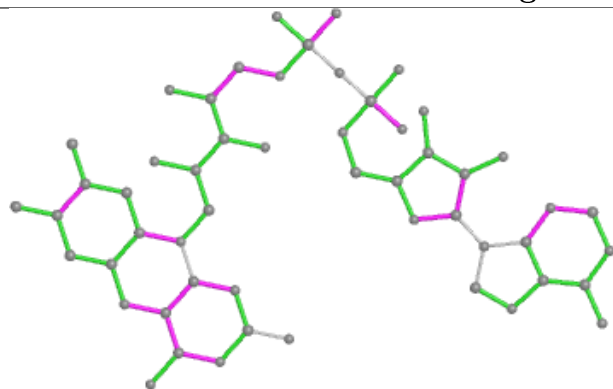




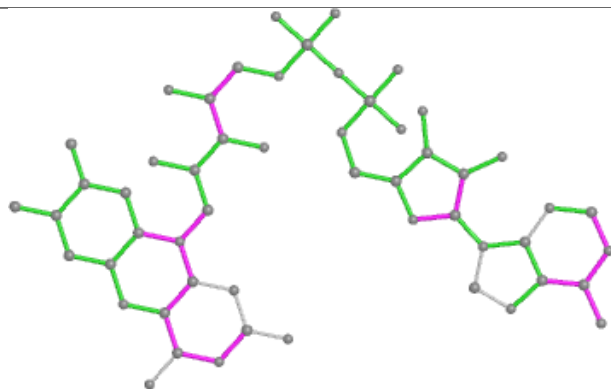
Ligand HEM I 301



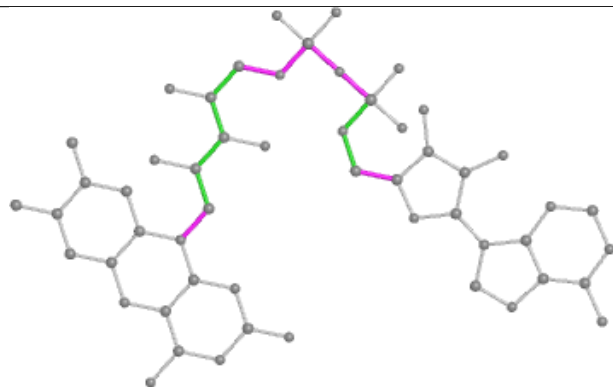
Ligand FAD J 701



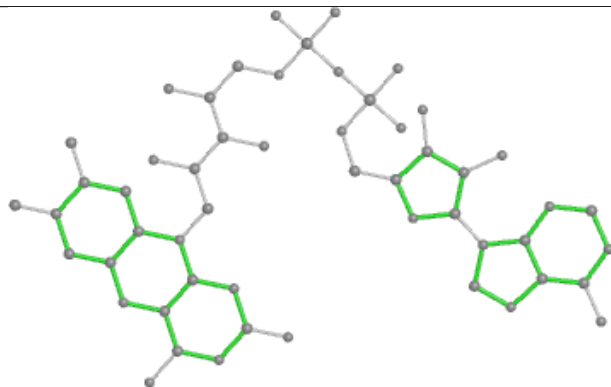
Bond lengths



Bond angles

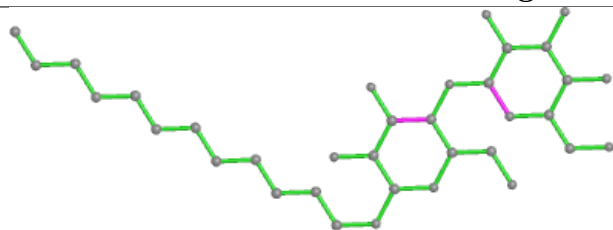


Torsions

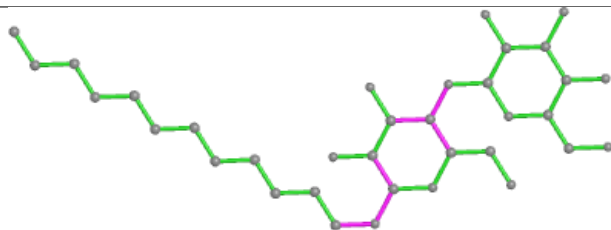


Rings

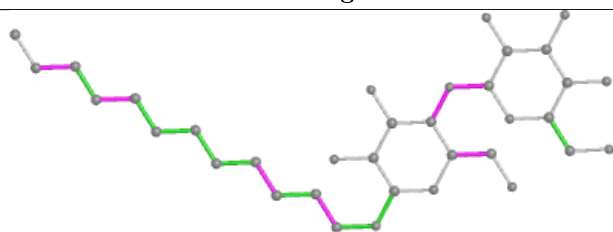
Ligand LMT I 303



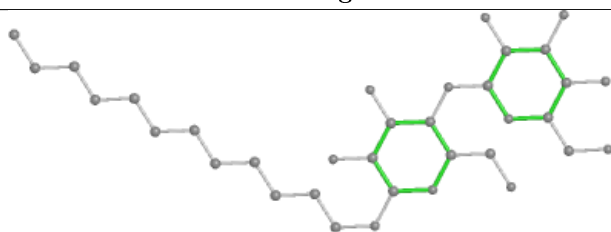
Bond lengths



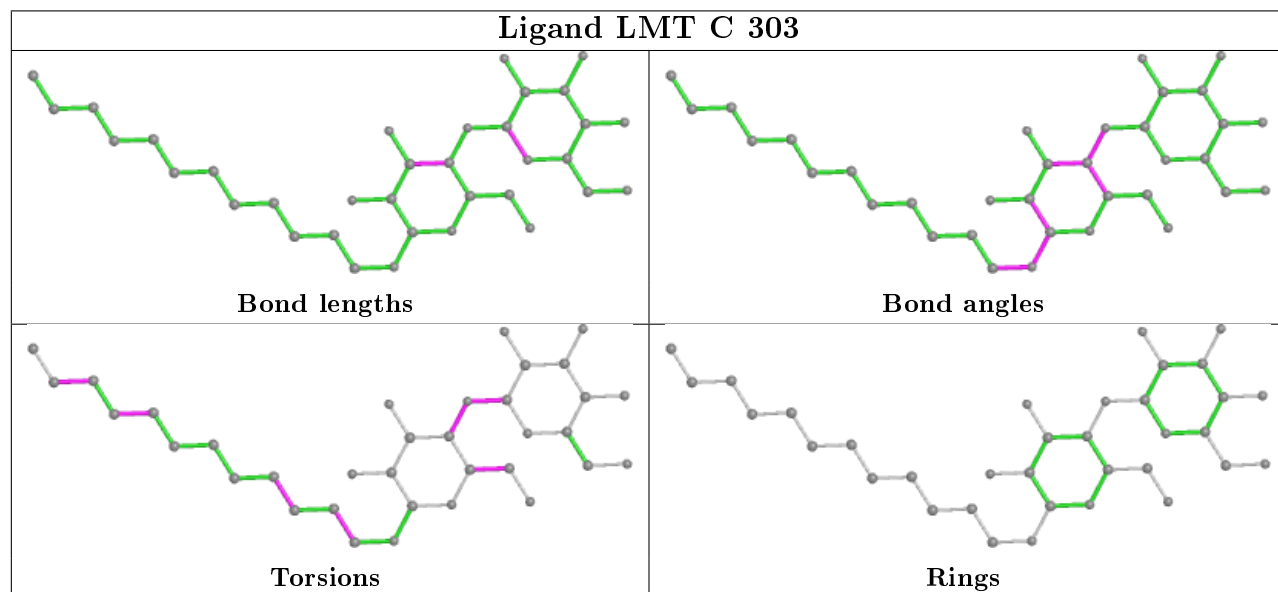
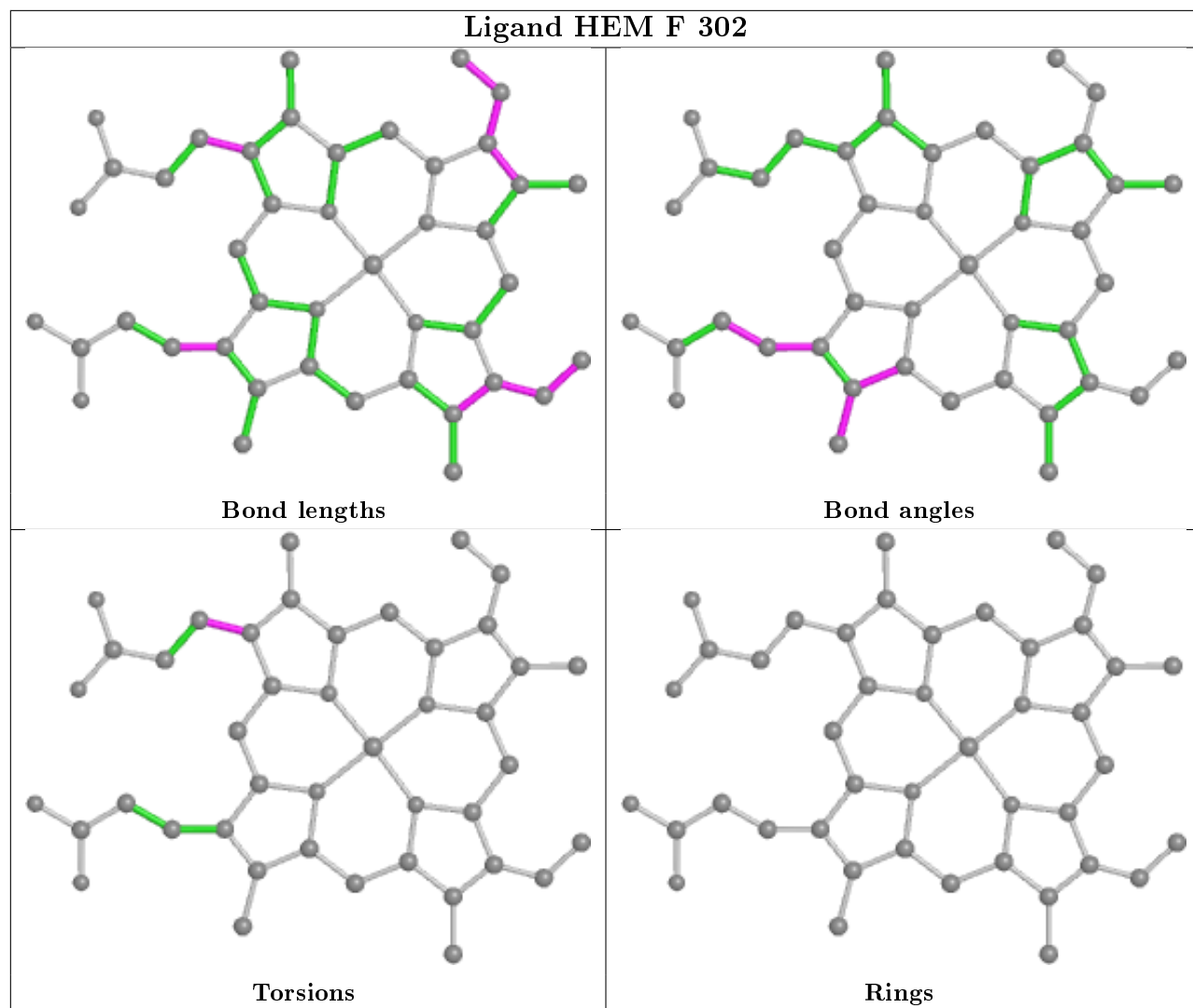
Bond angles

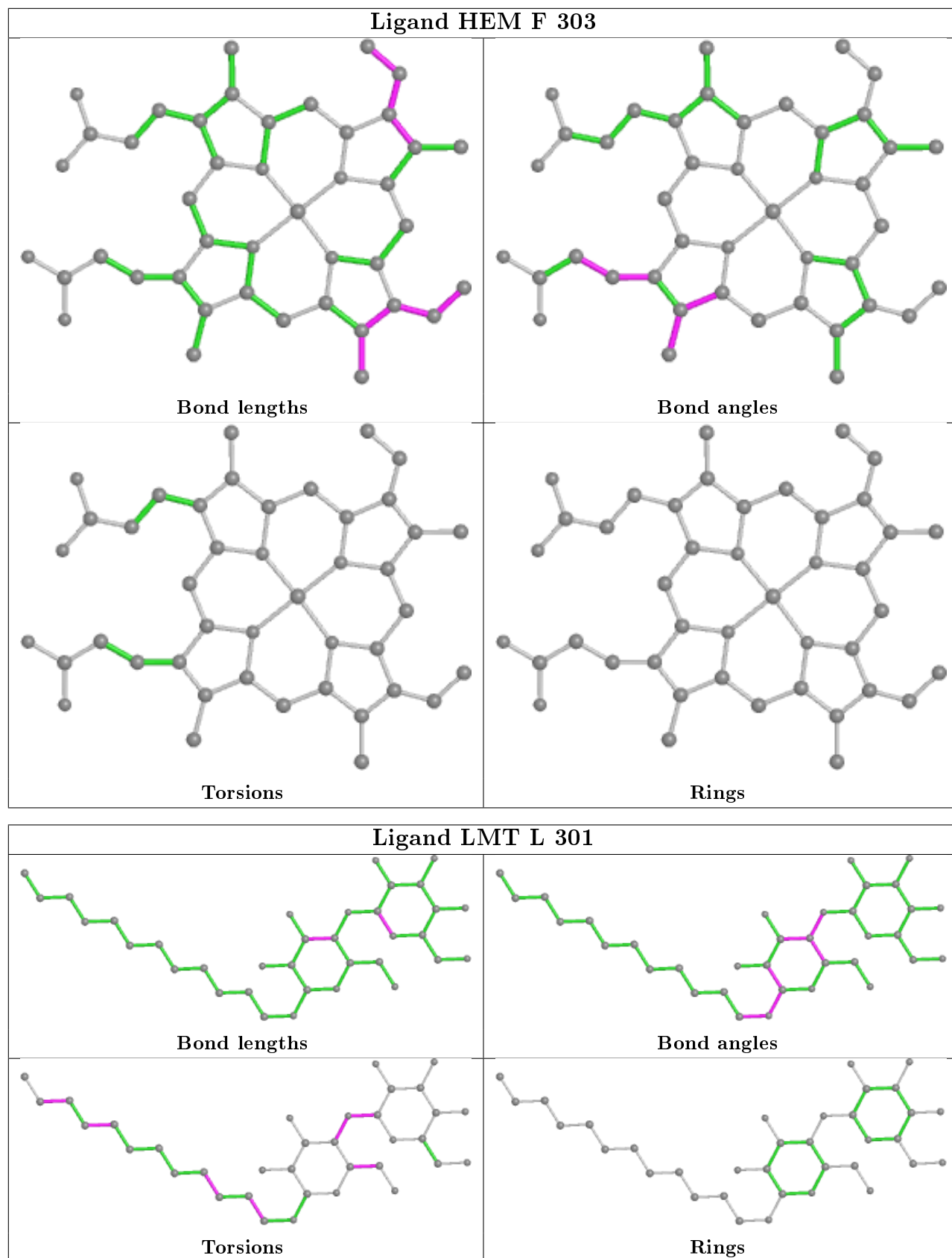


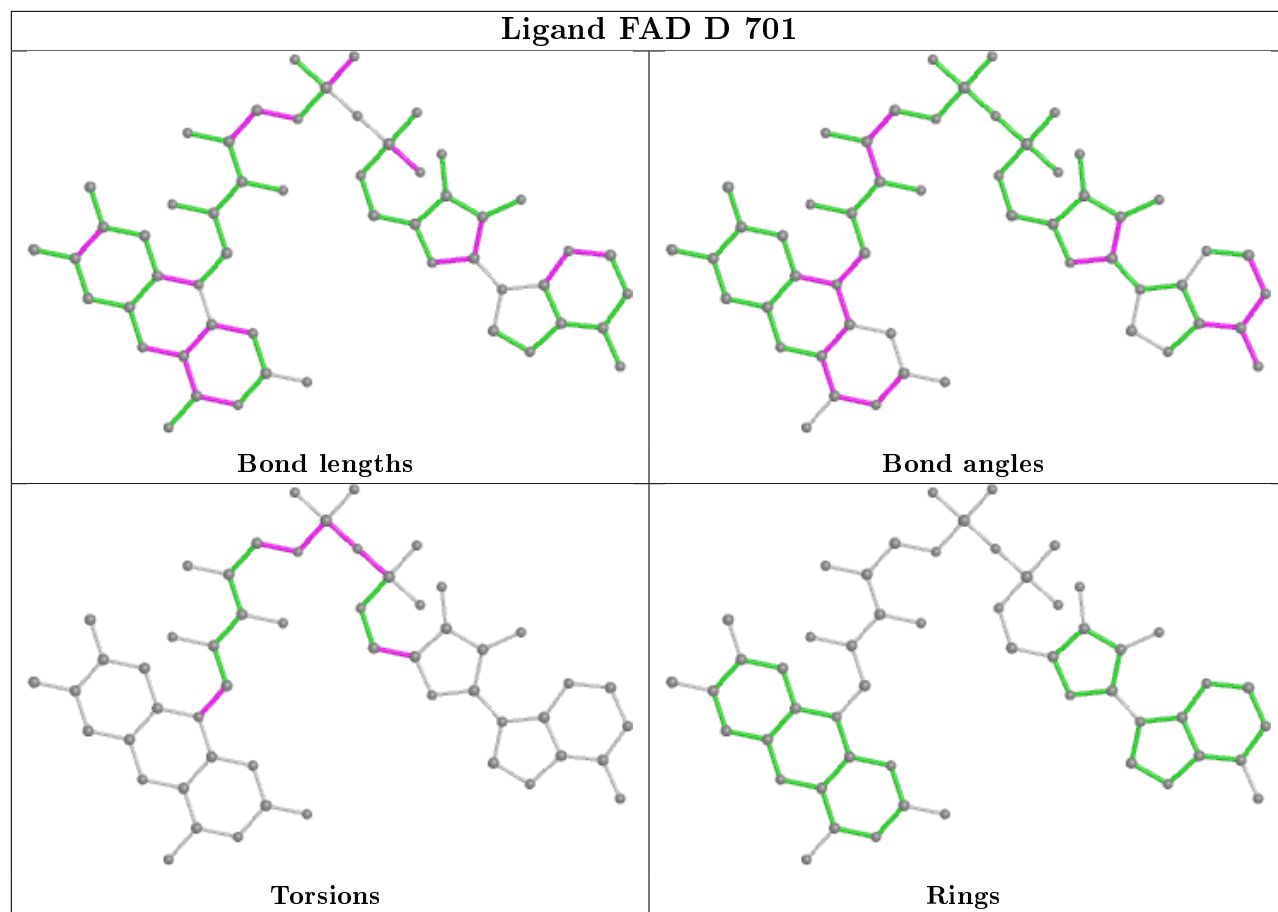
Torsions

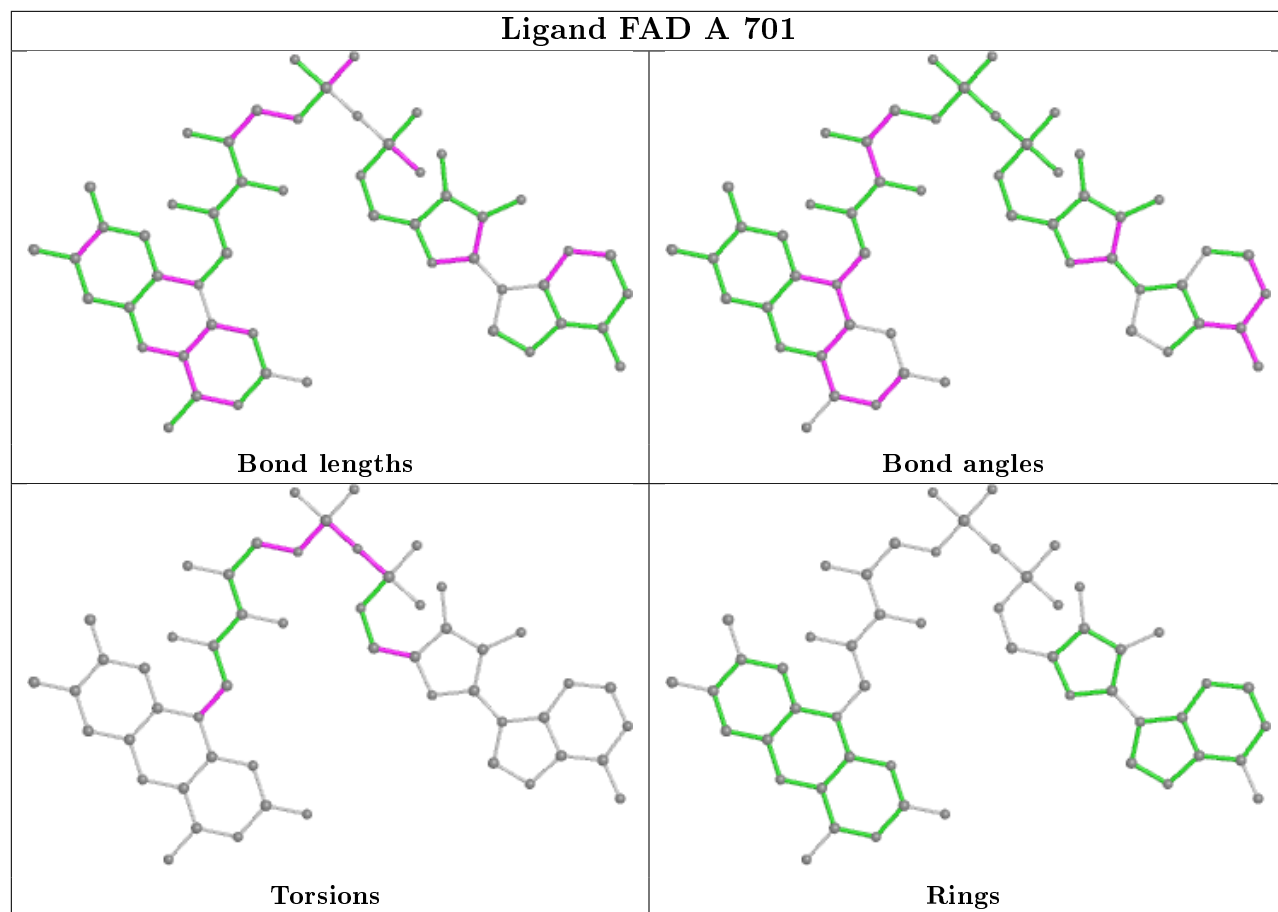


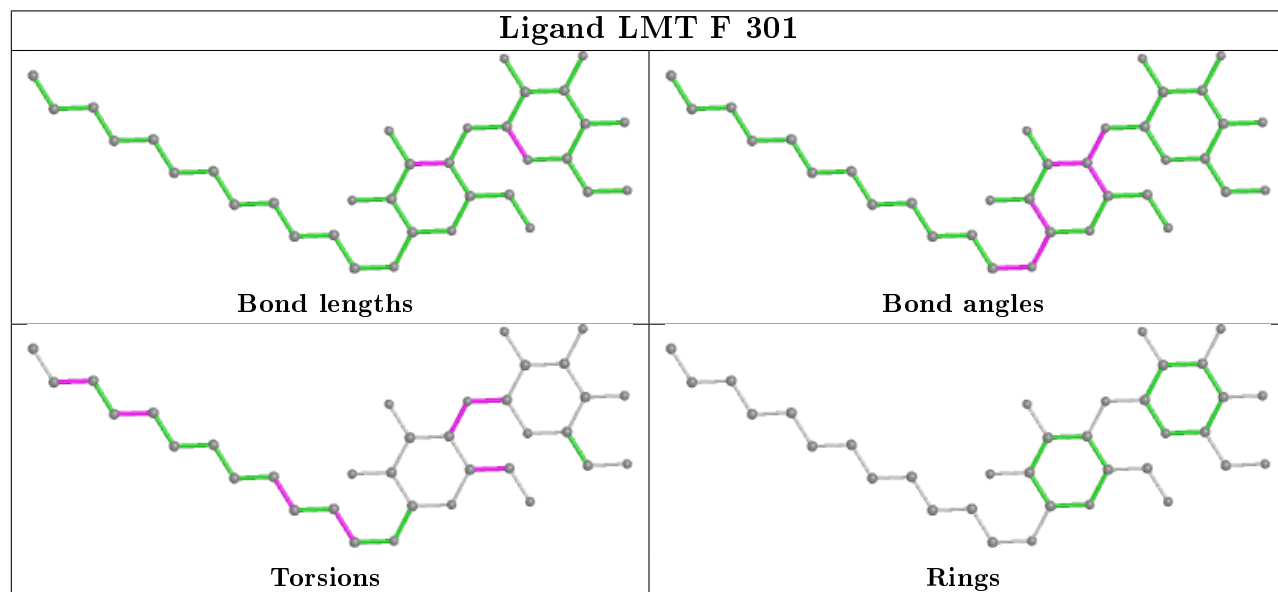
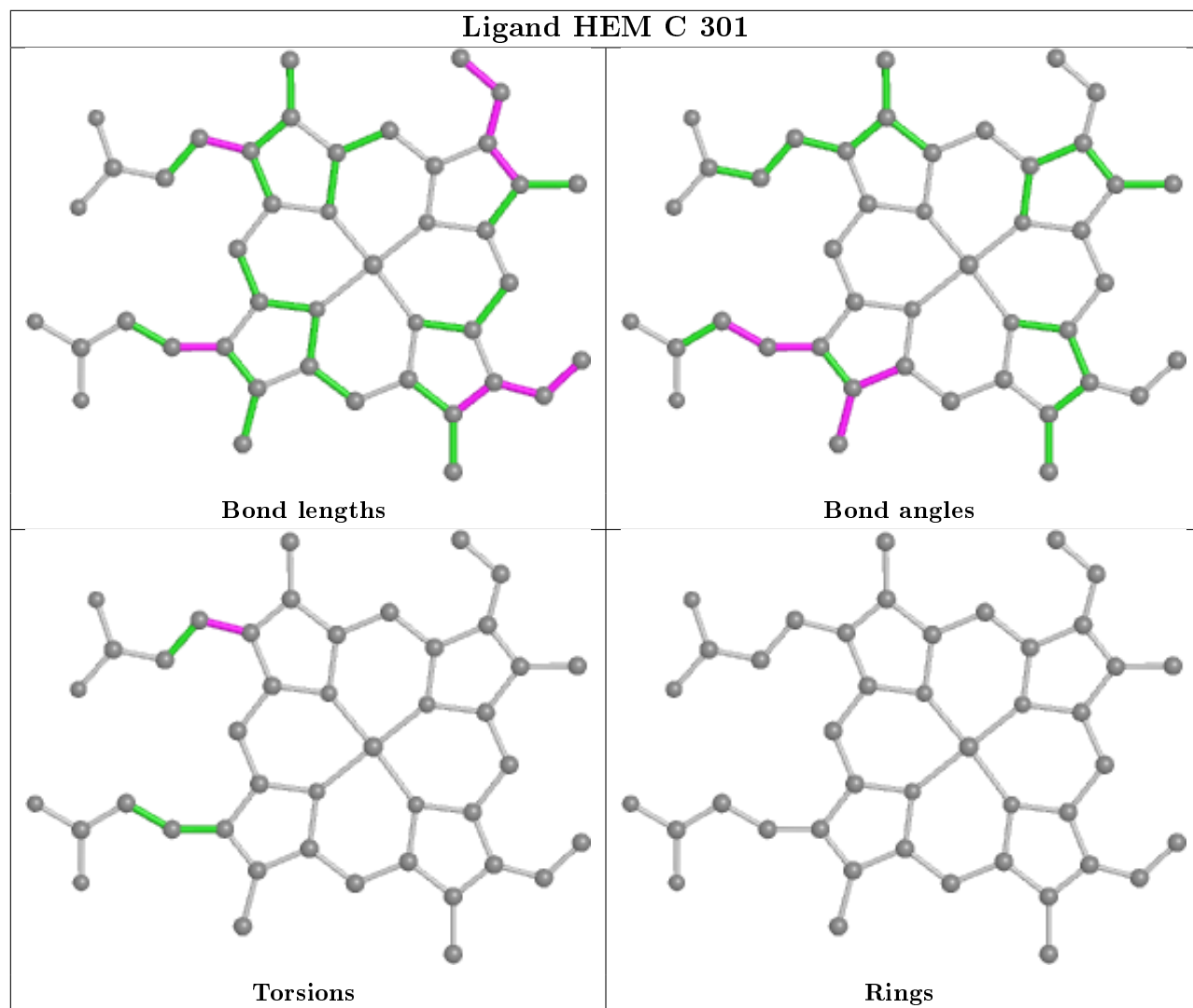
Rings

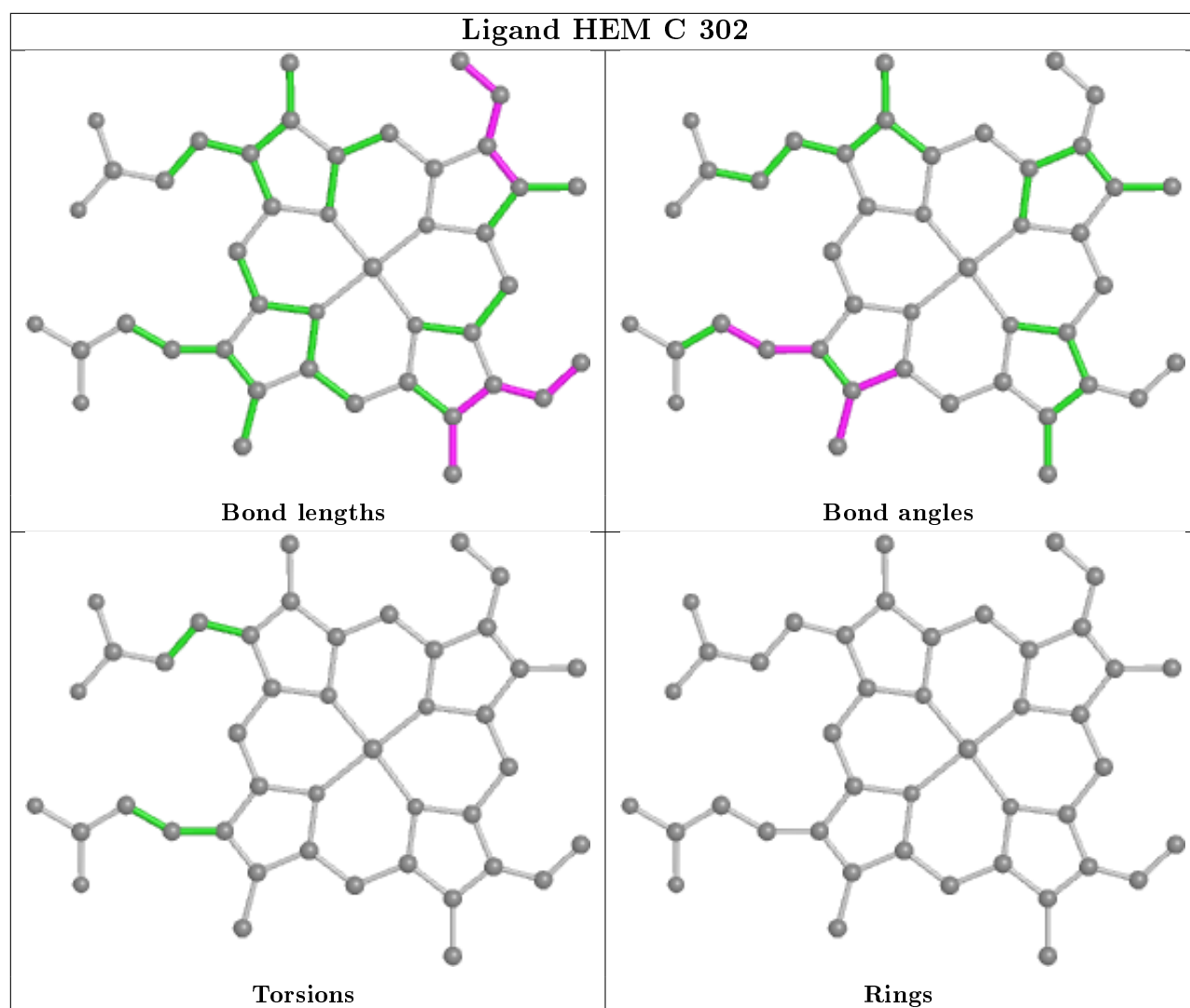


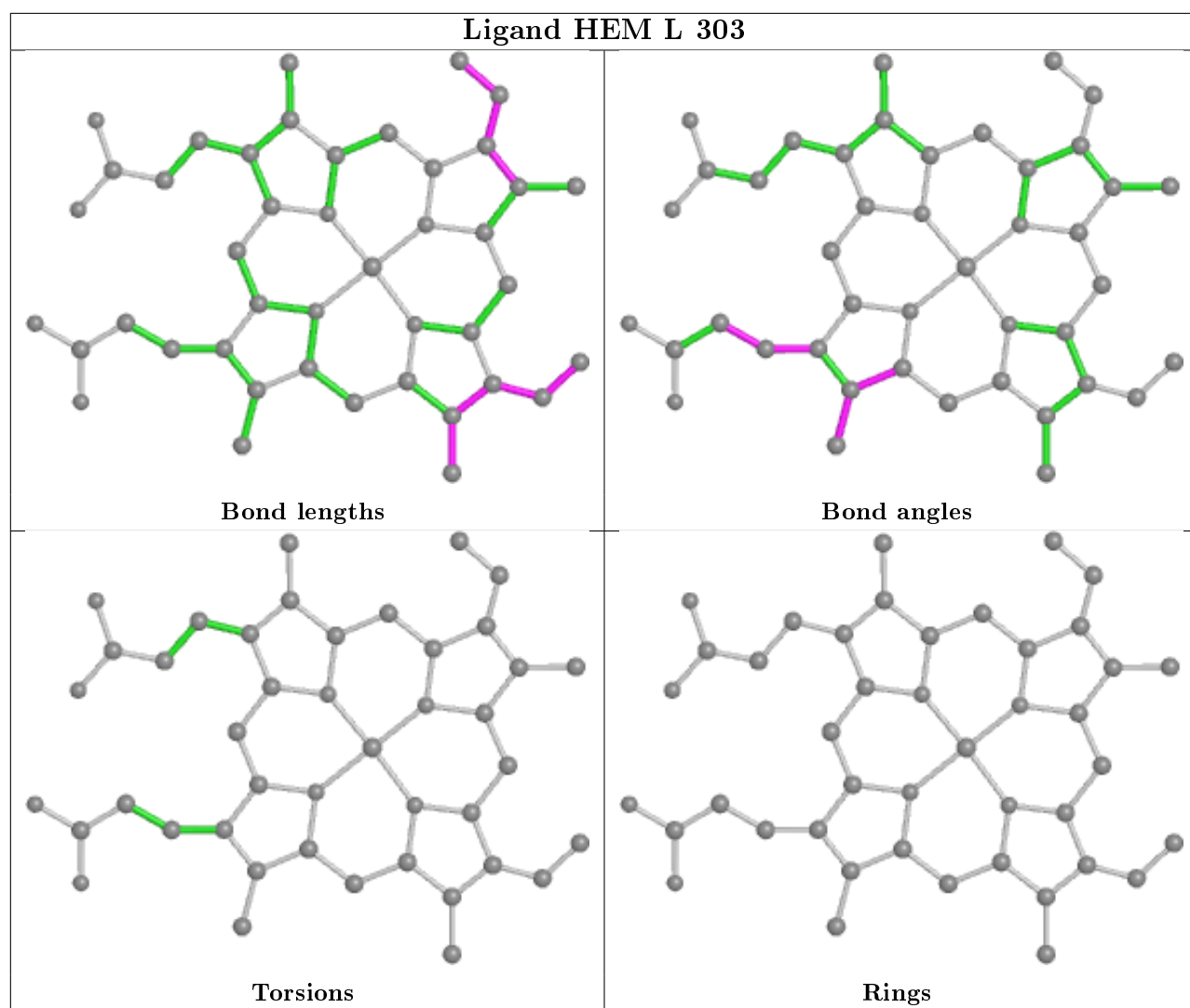












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.