



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:17 AM JST

PDB ID : 5XMJ / pdb_00005xmj
Title : Crystal structure of quinol:fumarate reductase from *Desulfovibrio gigas*
Authors : Guan, H.H.; Hsieh, Y.C.; Lin, P.R.; Chen, C.J.
Deposited on : 2017-05-15
Resolution : 3.60 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 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:

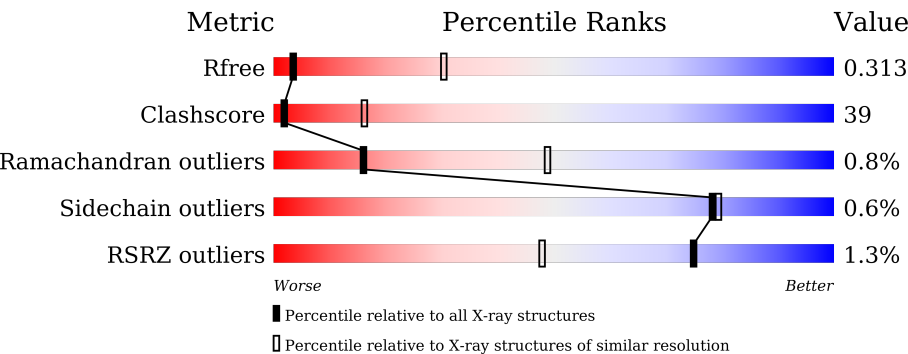
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	627	47% 51% ..
1	E	627	44% 55% .
1	I	627	42% 55% ..
1	M	627	43% 54% ..
2	B	264	51% 39% 9%
2	F	264	47% 43% 9%

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Mol	Chain	Length	Quality of chain
2	J	264	
2	N	264	
3	C	218	
3	G	218	
3	K	218	
3	O	218	

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
10	LMT	C	303	-	-	X	-
10	LMT	O	301	-	-	X	-
11	MQ7	C	304	-	-	X	-
5	FUM	A	702	-	-	X	-
5	FUM	E	702	-	-	X	-
5	FUM	M	702	-	-	X	-
6	F3S	F	301	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34118 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	622	Total	C	N	O	S	0	0	0
			4769	2976	854	903	36			
1	E	622	Total	C	N	O	S	0	0	0
			4767	2975	853	903	36			
1	I	622	Total	C	N	O	S	0	0	0
			4767	2975	853	903	36			
1	M	622	Total	C	N	O	S	0	0	0
			4769	2976	854	903	36			

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur subunit.

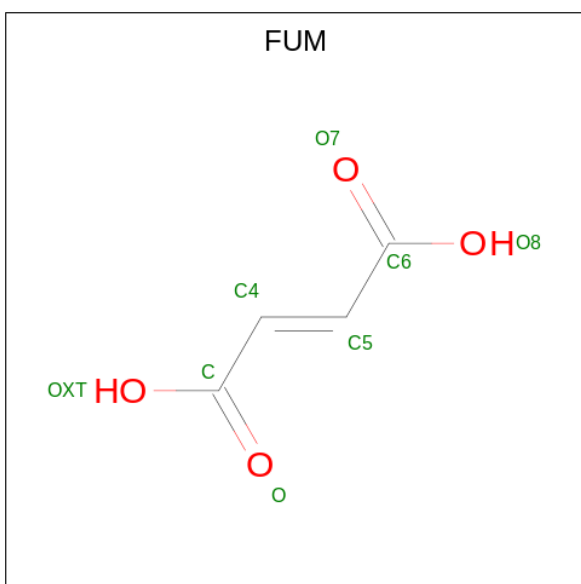
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			1879	1171	325	355	28			
2	F	240	Total	C	N	O	S	0	0	0
			1879	1171	325	355	28			
2	J	240	Total	C	N	O	S	0	0	0
			1879	1171	325	355	28			
2	N	240	Total	C	N	O	S	0	0	0
			1879	1171	325	355	28			

- Molecule 3 is a protein called fumarate reductase respiratory complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1693	1130	282	265	16			
3	G	212	Total	C	N	O	S	0	0	0
			1693	1130	282	265	16			
3	K	212	Total	C	N	O	S	0	0	0
			1693	1130	282	265	16			
3	O	212	Total	C	N	O	S	0	0	0
			1693	1130	282	265	16			

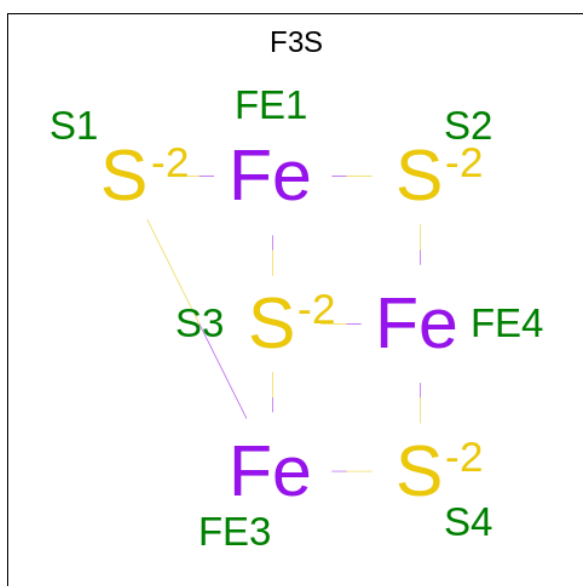
- # FAD

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



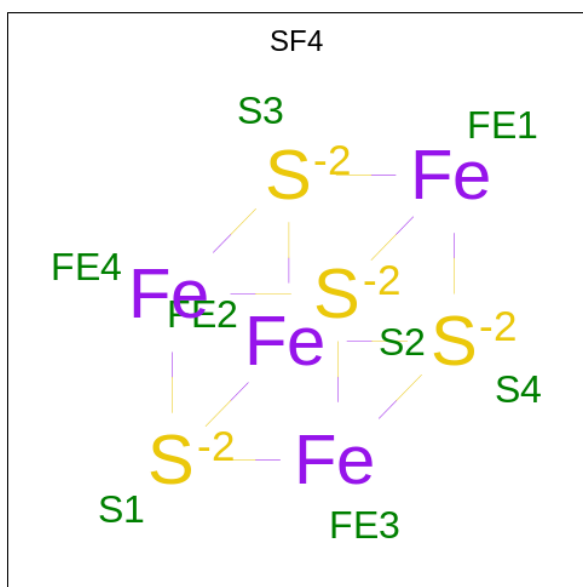
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	E	1	Total	C	O	0	0
			8	4	4		
5	I	1	Total	C	O	0	0
			8	4	4		
5	M	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



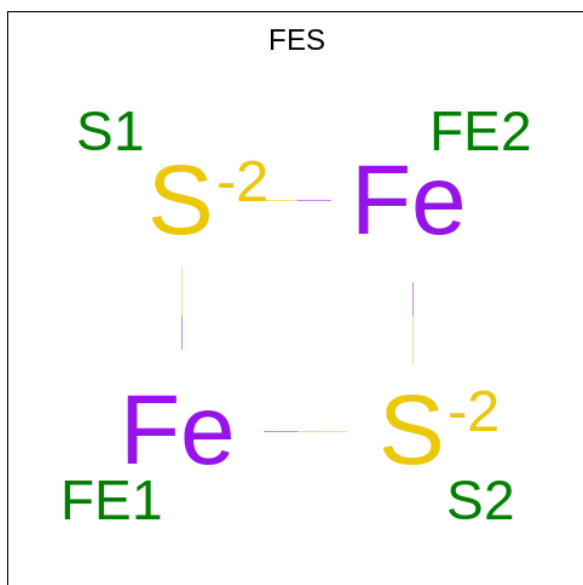
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			7	3	4		
6	F	1	Total	Fe	S	0	0
			7	3	4		
6	J	1	Total	Fe	S	0	0
			7	3	4		
6	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



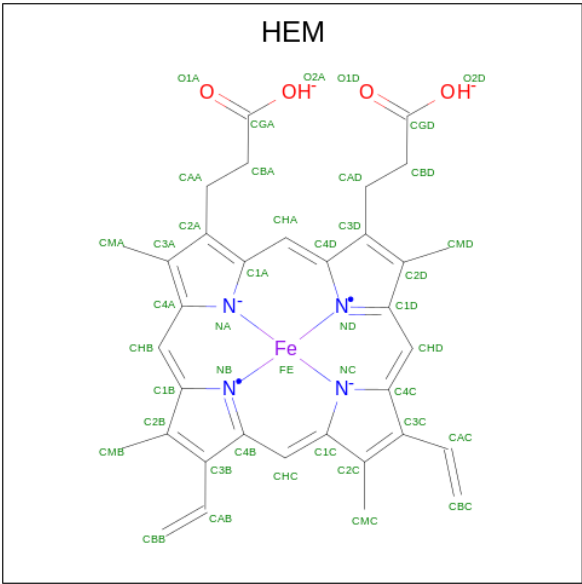
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	J	1	Total	Fe	S	0	0
			8	4	4		
7	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		
8	J	1	Total	Fe	S	0	0
			4	2	2		
8	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



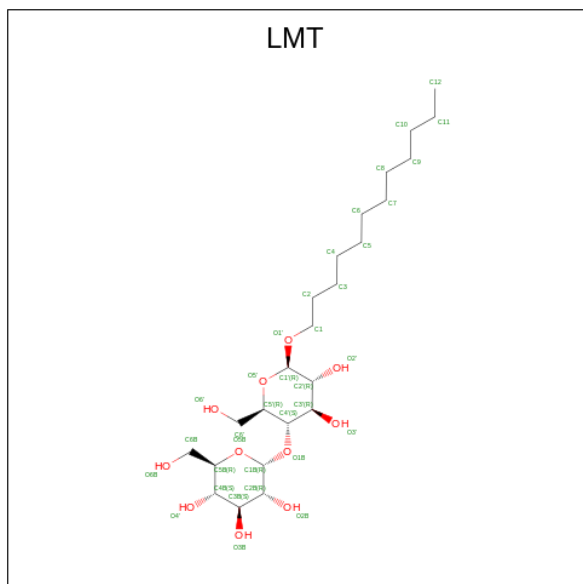
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	K	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	K	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	O	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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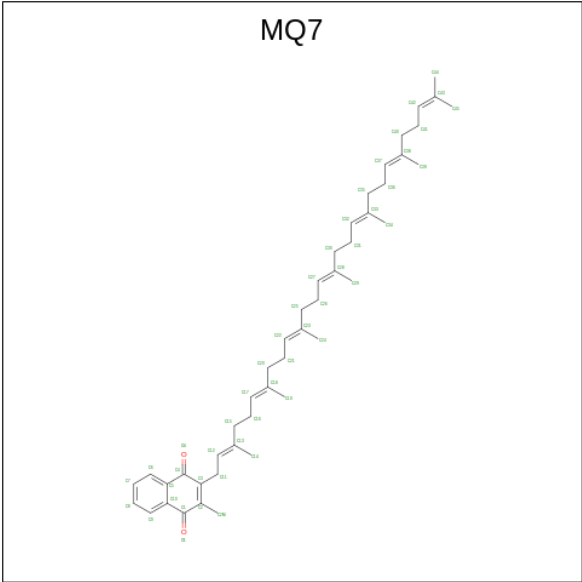
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	O	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O		
			35	24	11		
10	O	1	Total	C	O		
			35	24	11		
						0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).

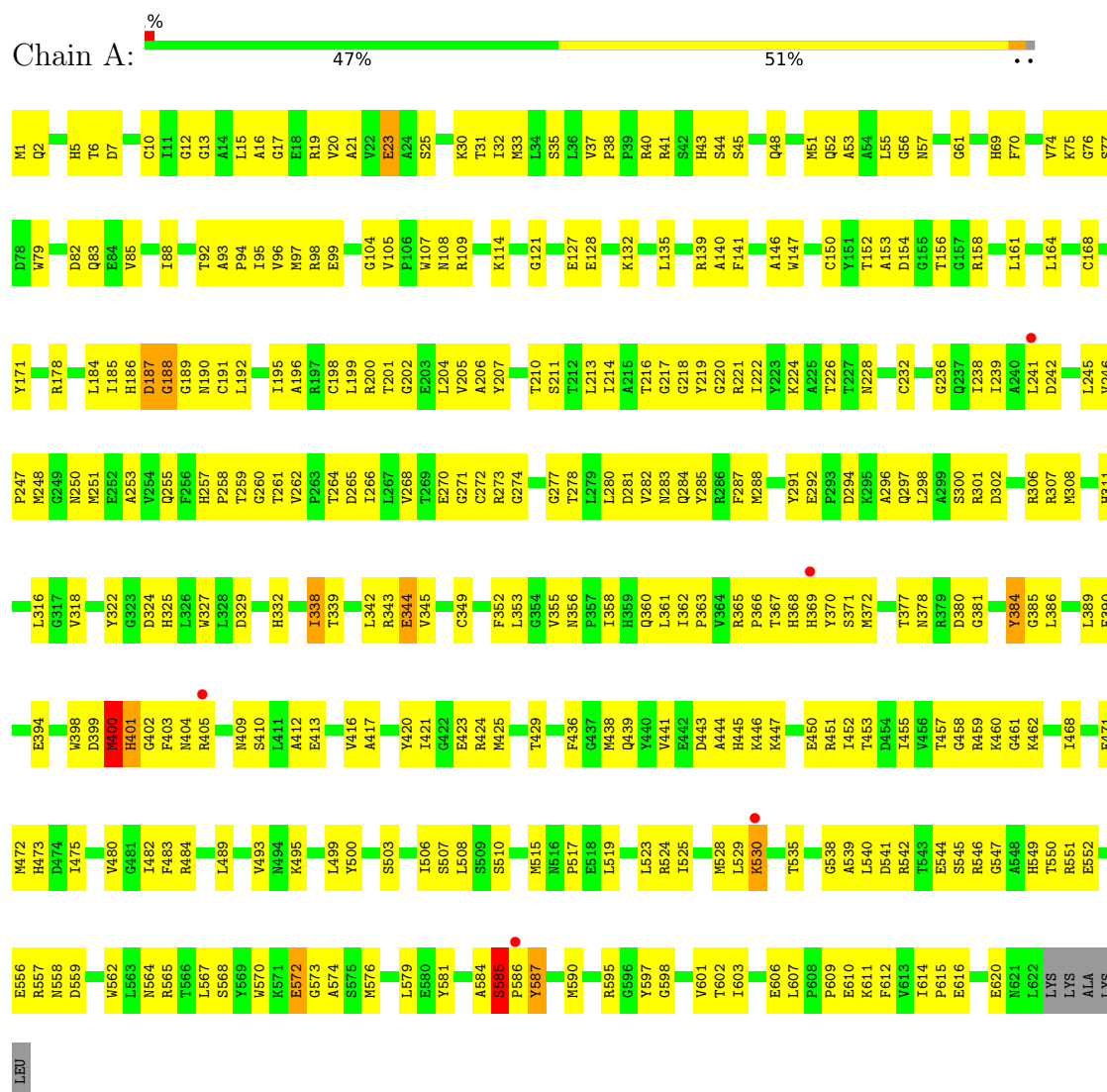


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			24	22	2		

3 Residue-property plots

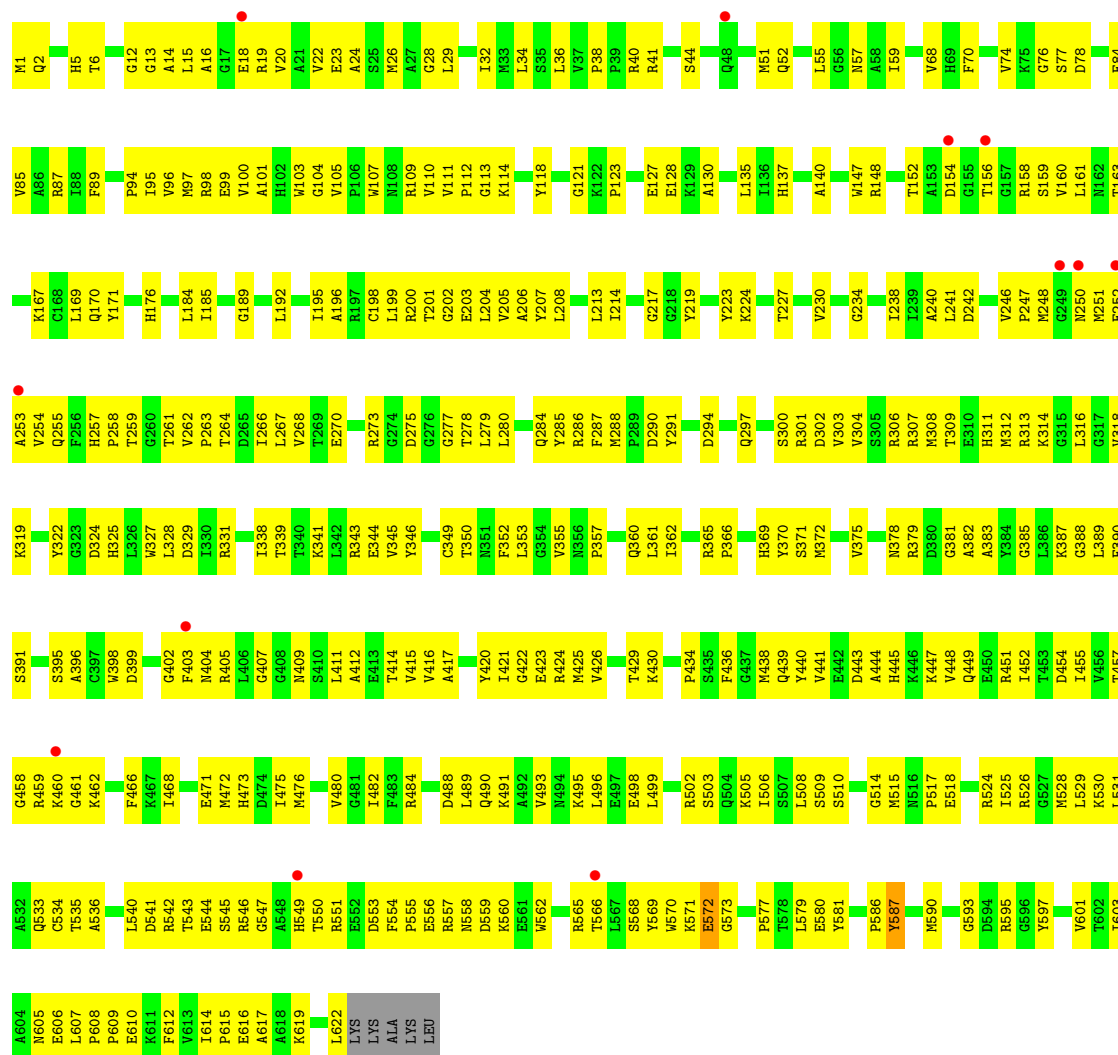
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: fumarate reductase flavoprotein subunit

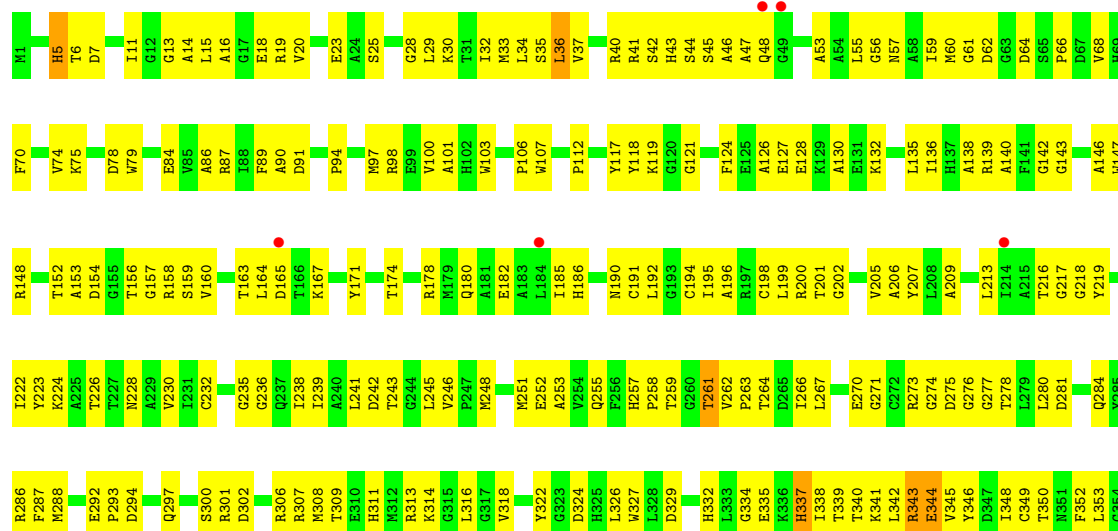


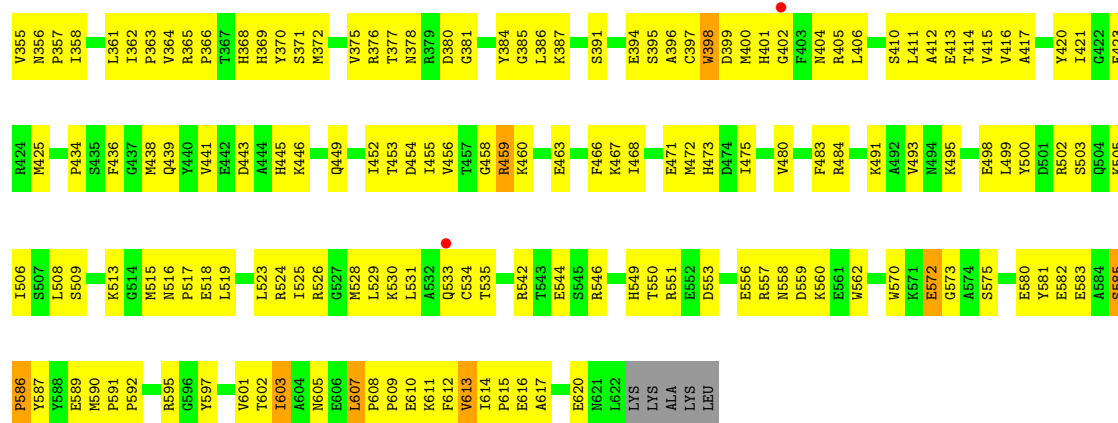
- Molecule 1: fumarate reductase flavoprotein subunit



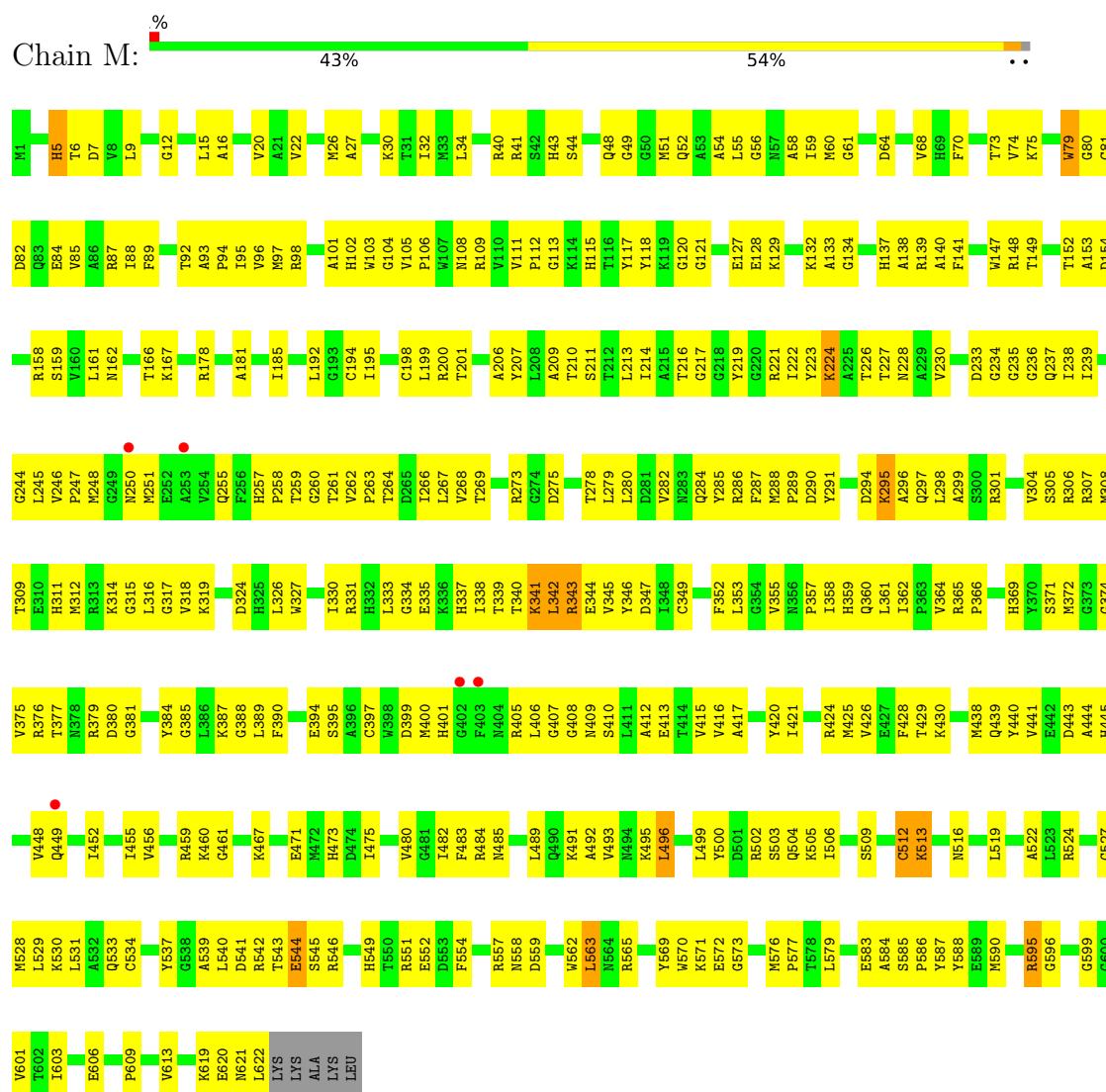


• Molecule 1: fumarate reductase flavoprotein subunit



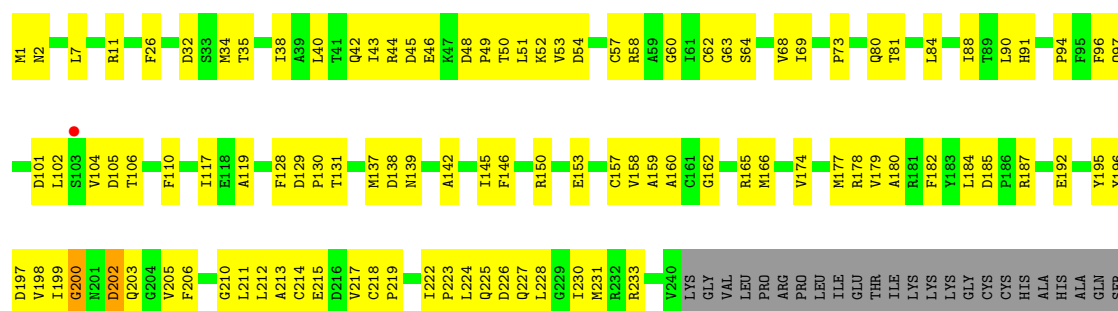


● Molecule 1: fumarate reductase flavoprotein subunit

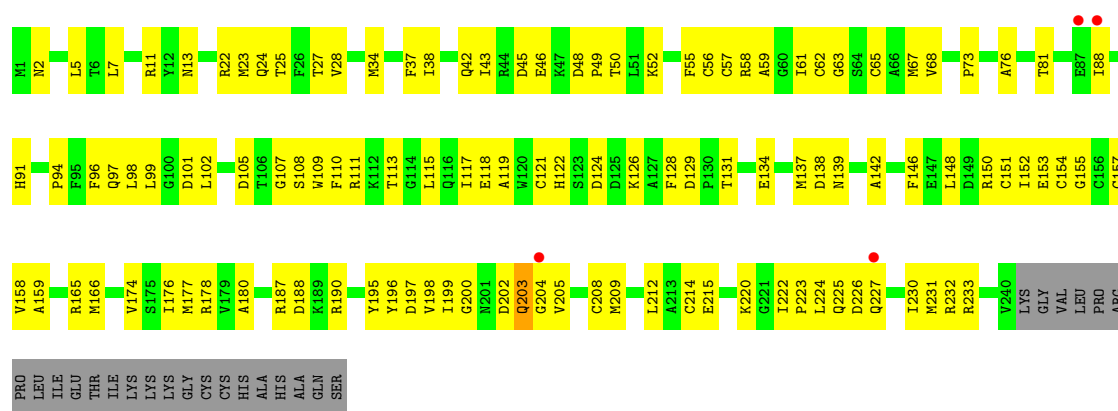


● Molecule 2: Succinate dehydrogenase iron-sulfur subunit

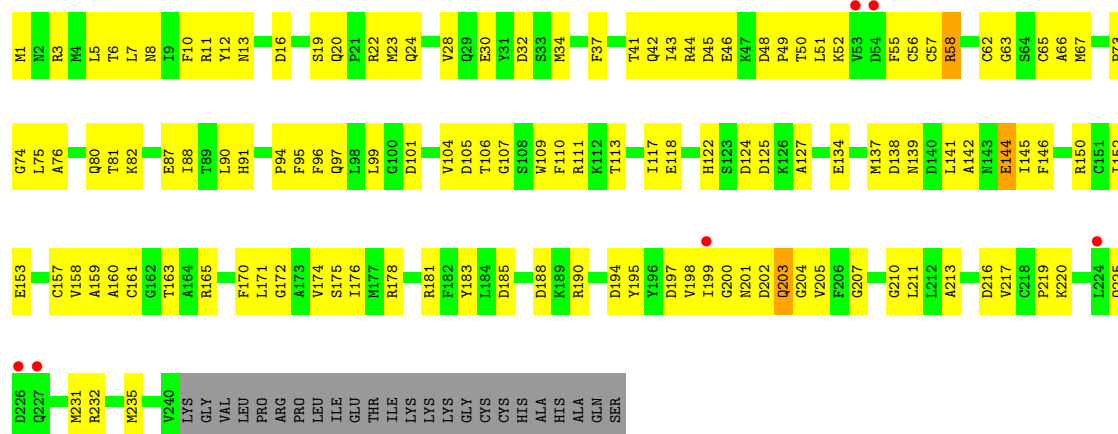




• Molecule 2: Succinate dehydrogenase iron-sulfur subunit

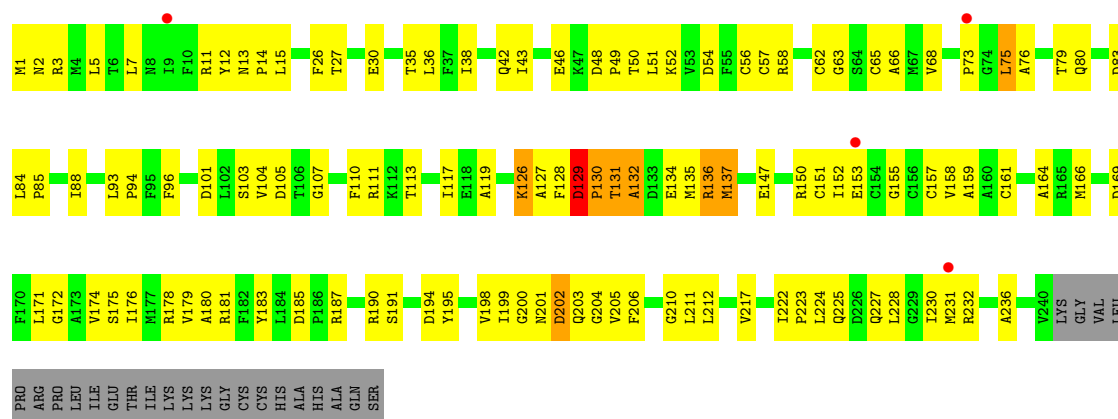


• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



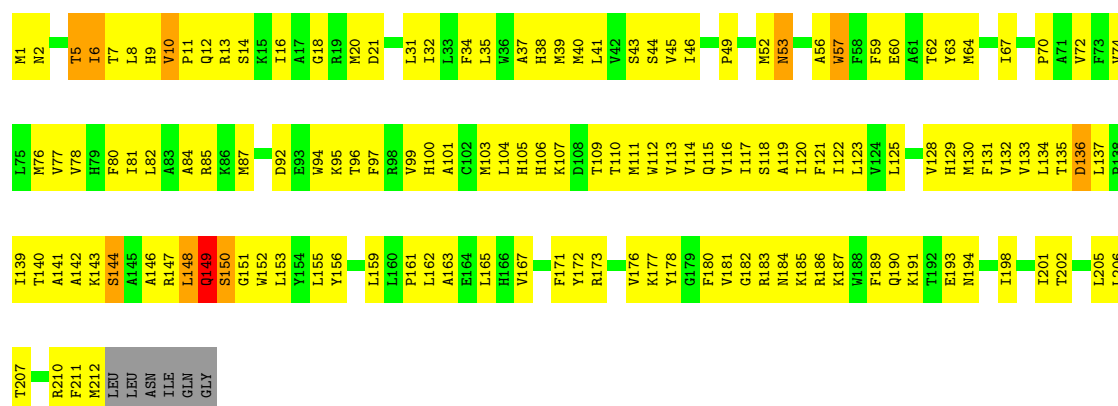
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit





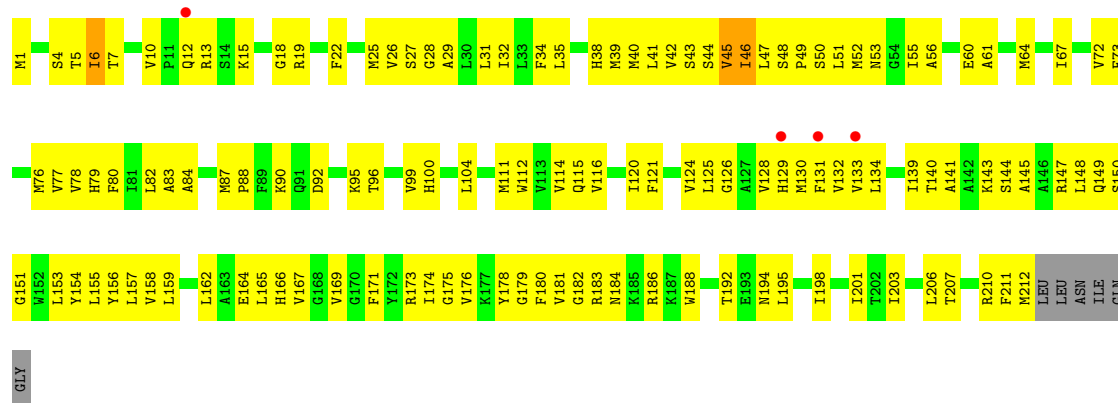
• Molecule 3: fumarate reductase respiratory complex

Chain C: 33% 60%



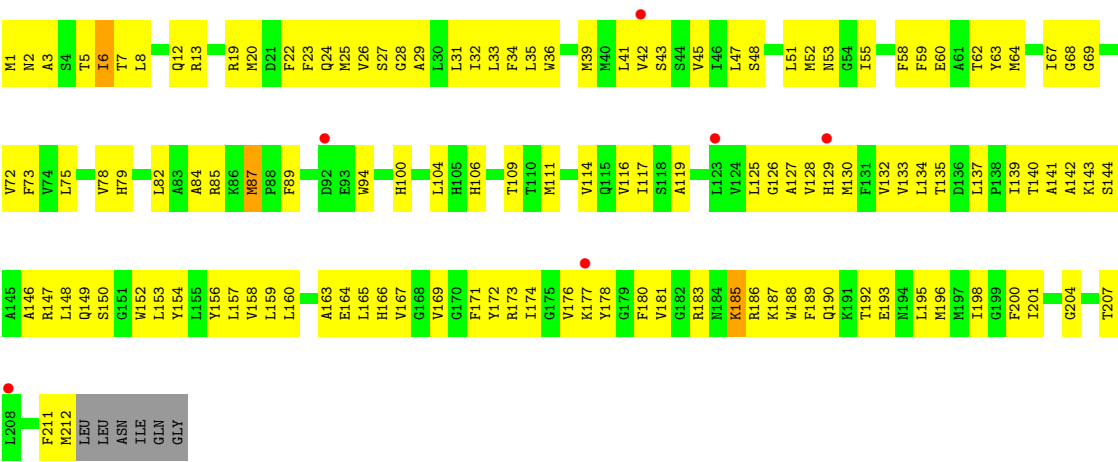
• Molecule 3: fumarate reductase respiratory complex

Chain G: 2% 39% 57%

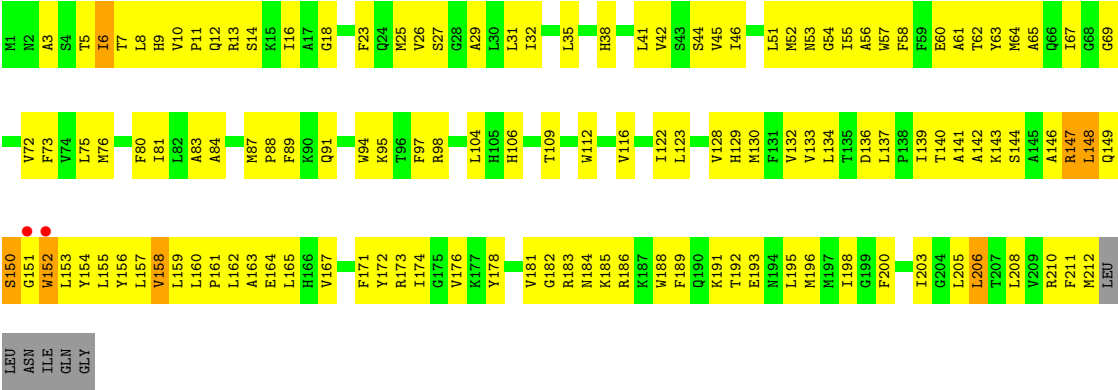


• Molecule 3: fumarate reductase respiratory complex

Chain K: 3% 39% 57%



● Molecule 3: fumarate reductase respiratory complex



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.14Å 131.77Å 195.43Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	29.80 – 3.60 29.80 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.80-3.60) 98.1 (29.80-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.232 , 0.313 0.235 , 0.313	Depositor DCC
R_{free} test set	3515 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	120.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 15.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34118	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FAD, MQ7, FUM, HEM, SF4, F3S, FES

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	0.70	0/4868	1.07	16/6581 (0.2%)
1	E	0.54	0/4866	0.91	2/6579 (0.0%)
1	I	0.60	2/4866 (0.0%)	0.95	8/6579 (0.1%)
1	M	0.55	3/4868 (0.1%)	0.98	9/6581 (0.1%)
2	B	0.66	0/1915	1.02	2/2587 (0.1%)
2	F	0.57	0/1915	0.96	1/2587 (0.0%)
2	J	0.53	0/1915	0.86	0/2587
2	N	0.64	0/1915	1.07	9/2587 (0.3%)
3	C	0.62	0/1739	1.05	9/2355 (0.4%)
3	G	0.51	0/1739	0.95	5/2355 (0.2%)
3	K	0.61	2/1739 (0.1%)	0.94	2/2355 (0.1%)
3	O	0.59	0/1739	1.02	9/2355 (0.4%)
All	All	0.60	7/34084 (0.0%)	0.98	72/46088 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	459	ARG	CA-C	12.41	1.58	1.52
3	K	183	ARG	NE-CZ	-8.63	1.23	1.33
1	M	595	ARG	NE-CZ	-6.41	1.26	1.33
1	I	337	HIS	CE1-NE2	-6.10	1.26	1.32
3	K	183	ARG	CZ-NH1	-6.02	1.24	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	459	ARG	CA-C-O	-8.79	114.76	119.77
1	M	79	TRP	N-CA-C	-8.07	101.18	111.02
1	A	400	MET	N-CA-C	-7.98	103.34	113.23
3	O	158	VAL	N-CA-C	-7.75	103.89	112.80
1	M	295	LYS	CA-C-N	7.66	135.49	121.70

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	4769	0	4681	317	0
1	E	4767	0	4674	359	0
1	I	4767	0	4674	396	1
1	M	4769	0	4681	421	1
2	B	1879	0	1821	101	0
2	F	1879	0	1823	128	1
2	J	1879	0	1821	135	0
2	N	1879	0	1821	149	0
3	C	1693	0	1775	235	0
3	G	1693	0	1775	165	0
3	K	1693	0	1775	166	1
3	O	1693	0	1775	186	0
4	A	53	0	28	2	0
4	E	53	0	29	4	0
4	I	53	0	31	17	0
4	M	53	0	31	13	0
5	A	8	0	1	7	0
5	E	8	0	1	5	0
5	I	8	0	1	3	0
5	M	8	0	1	5	0
6	B	7	0	0	0	0
6	F	7	0	0	3	0
6	J	7	0	0	0	0
6	N	7	0	0	0	0
7	B	8	0	0	1	0
7	F	8	0	0	0	0
7	J	8	0	0	0	0
7	N	8	0	0	1	0
8	B	4	0	0	1	0
8	F	4	0	0	1	0
8	J	4	0	0	0	0
8	N	4	0	0	1	0
9	C	86	0	60	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	86	0	60	20	0
9	K	86	0	60	25	0
9	O	86	0	60	20	0
10	C	35	0	46	31	0
10	O	35	0	46	24	0
11	C	24	0	23	21	0
All	All	34118	0	33574	2653	2

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 39.

The worst 5 of 2653 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:M:43:HIS:NE2	4:M:701:FAD:C8M	1.76	1.46
3:C:10:VAL:HG22	3:C:11:PRO:CD	1.42	1.45
1:M:43:HIS:NE2	4:M:701:FAD:HM81	1.12	1.39
1:M:43:HIS:CD2	4:M:701:FAD:HM83	1.58	1.36
1:I:43:HIS:NE2	4:I:701:FAD:C8M	1.89	1.35

All (2) 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)
3:K:187:LYS:NZ	1:M:285:TYR:OH[1_454]	1.97	0.23
2:F:27:THR:OG1	1:I:575:SER:OG[2_545]	2.19	0.01

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	620/627 (99%)	556 (90%)	59 (10%)	5 (1%)	16	49
1	E	620/627 (99%)	558 (90%)	61 (10%)	1 (0%)	43	72
1	I	620/627 (99%)	552 (89%)	63 (10%)	5 (1%)	16	49
1	M	620/627 (99%)	550 (89%)	65 (10%)	5 (1%)	16	49
2	B	238/264 (90%)	216 (91%)	21 (9%)	1 (0%)	30	61
2	F	238/264 (90%)	209 (88%)	28 (12%)	1 (0%)	30	61
2	J	238/264 (90%)	215 (90%)	21 (9%)	2 (1%)	16	49
2	N	238/264 (90%)	207 (87%)	25 (10%)	6 (2%)	4	28
3	C	210/218 (96%)	180 (86%)	25 (12%)	5 (2%)	4	29
3	G	210/218 (96%)	181 (86%)	27 (13%)	2 (1%)	12	45
3	K	210/218 (96%)	180 (86%)	29 (14%)	1 (0%)	24	57
3	O	210/218 (96%)	181 (86%)	28 (13%)	1 (0%)	24	57
All	All	4272/4436 (96%)	3785 (89%)	452 (11%)	35 (1%)	16	49

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	149	GLN
3	C	150	SER
1	E	587	TYR
1	I	343	ARG
1	I	613	VAL

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	495/500 (99%)	489 (99%)	6 (1%)	63	73
1	E	494/500 (99%)	494 (100%)	0	100	100
1	I	494/500 (99%)	490 (99%)	4 (1%)	73	77
1	M	495/500 (99%)	492 (99%)	3 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	208/228 (91%)	208 (100%)	0	100	100
2	F	208/228 (91%)	208 (100%)	0	100	100
2	J	208/228 (91%)	207 (100%)	1 (0%)	81	80
2	N	208/228 (91%)	205 (99%)	3 (1%)	59	71
3	C	180/185 (97%)	178 (99%)	2 (1%)	65	74
3	G	180/185 (97%)	179 (99%)	1 (1%)	78	79
3	K	180/185 (97%)	180 (100%)	0	100	100
3	O	180/185 (97%)	178 (99%)	2 (1%)	65	74
All	All	3530/3652 (97%)	3508 (99%)	22 (1%)	78	79

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	5	HIS
2	N	75	LEU
1	M	513	LYS
2	N	83	ASP
3	C	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	351	ASN
2	J	91	HIS
2	N	8	ASN
1	I	445	HIS
2	J	8	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	G	301	3	50,50,50	2.00	6 (12%)	66,82,82	1.56	12 (18%)
5	FUM	A	702	-	7,7,7	1.53	1 (14%)	8,8,8	1.23	2 (25%)
7	SF4	F	302	2	0,12,12	-	-	-	-	-
4	FAD	E	701	1	56,58,58	2.58	16 (28%)	81,89,89	2.37	21 (25%)
9	HEM	K	302	3	50,50,50	1.77	9 (18%)	66,82,82	1.13	3 (4%)
8	FES	F	303	2	0,4,4	-	-	-	-	-
8	FES	B	303	2	0,4,4	-	-	-	-	-
7	SF4	N	302	2	0,12,12	-	-	-	-	-
6	F3S	B	301	2	0,9,9	-	-	-	-	-
9	HEM	O	303	3	50,50,50	1.82	6 (12%)	66,82,82	1.53	11 (16%)
8	FES	J	303	2	0,4,4	-	-	-	-	-
6	F3S	J	301	2	0,9,9	-	-	-	-	-
10	LMT	O	301	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
5	FUM	M	702	-	7,7,7	1.37	0	8,8,8	1.19	1 (12%)
9	HEM	C	302	3	50,50,50	1.73	11 (22%)	66,82,82	1.34	10 (15%)
5	FUM	I	702	-	7,7,7	1.20	0	8,8,8	1.65	2 (25%)
8	FES	N	303	2	0,4,4	-	-	-	-	-
7	SF4	B	302	2	0,12,12	-	-	-	-	-
9	HEM	O	302	3	50,50,50	1.67	7 (14%)	66,82,82	1.39	9 (13%)
4	FAD	M	701	-	56,58,58	2.60	15 (26%)	81,89,89	2.42	24 (29%)
4	FAD	I	701	-	56,58,58	2.77	20 (35%)	81,89,89	2.41	29 (35%)
9	HEM	C	301	3	50,50,50	1.58	8 (16%)	66,82,82	1.25	7 (10%)
4	FAD	A	701	1	56,58,58	2.58	19 (33%)	81,89,89	2.52	31 (38%)
10	LMT	C	303	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	G	302	3	50,50,50	2.19	7 (14%)	66,82,82	1.19	6 (9%)
9	HEM	K	301	3	50,50,50	2.01	8 (16%)	66,82,82	2.26	18 (27%)
6	F3S	N	301	2	0,9,9	-	-	-	-	-
6	F3S	F	301	2	0,9,9	-	-	-	-	-
11	MQ7	C	304	-	25,25,49	2.99	11 (44%)	31,34,63	1.60	4 (12%)
7	SF4	J	302	2	0,12,12	-	-	-	-	-
5	FUM	E	702	-	7,7,7	1.62	1 (14%)	8,8,8	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	G	301	3	-	2/14/54/54	-
5	FUM	A	702	-	-	4/5/5/5	-
7	SF4	F	302	2	-	-	0/6/5/5
4	FAD	E	701	1	-	13/34/50/50	0/6/6/6
9	HEM	K	302	3	-	2/14/54/54	-
8	FES	F	303	2	-	-	0/1/1/1
8	FES	B	303	2	-	-	0/1/1/1
6	F3S	B	301	2	-	-	0/3/3/3
7	SF4	N	302	2	-	-	0/6/5/5
9	HEM	O	303	3	-	1/14/54/54	-
8	FES	J	303	2	-	-	0/1/1/1
6	F3S	J	301	2	-	-	0/3/3/3
10	LMT	O	301	-	-	10/21/61/61	0/2/2/2
5	FUM	M	702	-	-	4/5/5/5	-
9	HEM	C	302	3	-	1/14/54/54	-
5	FUM	I	702	-	-	2/5/5/5	-
8	FES	N	303	2	-	-	0/1/1/1
9	HEM	O	302	3	-	10/14/54/54	-
7	SF4	B	302	2	-	-	0/6/5/5
4	FAD	M	701	-	-	13/34/50/50	0/6/6/6
4	FAD	I	701	-	-	16/34/50/50	0/6/6/6
9	HEM	C	301	3	-	6/14/54/54	-
4	FAD	A	701	1	-	17/34/50/50	0/6/6/6
10	LMT	C	303	-	-	13/21/61/61	0/2/2/2
9	HEM	G	302	3	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	K	301	3	-	6/14/54/54	-
6	F3S	N	301	2	-	-	0/3/3/3
6	F3S	F	301	2	-	-	0/3/3/3
11	MQ7	C	304	-	-	5/13/33/61	0/2/2/2
7	SF4	J	302	2	-	-	0/6/5/5
5	FUM	E	702	-	-	4/5/5/5	-

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	301	HEM	FE-NB	9.72	2.25	1.94
9	G	302	HEM	FE-NA	9.21	2.26	1.95
4	E	701	FAD	O4B-C1B	8.70	1.62	1.42
4	I	701	FAD	O4B-C1B	8.56	1.62	1.42
11	C	304	MQ7	C3-C2	8.56	1.50	1.35

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	FAD	C7M-C7-C6	-8.74	103.33	119.49
4	I	701	FAD	C5A-C4A-N3A	-8.27	115.96	126.75
4	M	701	FAD	C7M-C7-C6	-8.13	104.46	119.49
4	A	701	FAD	C7M-C7-C6	-8.11	104.50	119.49
4	E	701	FAD	C7M-C7-C8	7.69	136.50	120.74

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	FAD	C5B-O5B-PA-O3P
4	A	701	FAD	C2'-C3'-C4'-C5'
4	A	701	FAD	O3'-C3'-C4'-C5'
4	E	701	FAD	C5B-O5B-PA-O1A
4	E	701	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

25 monomers are involved in 228 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	301	HEM	10	0

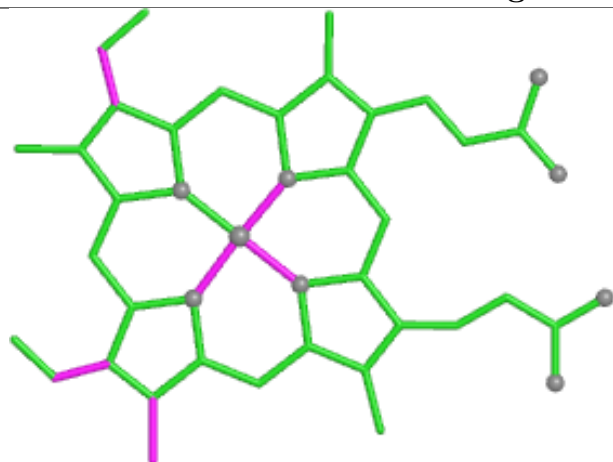
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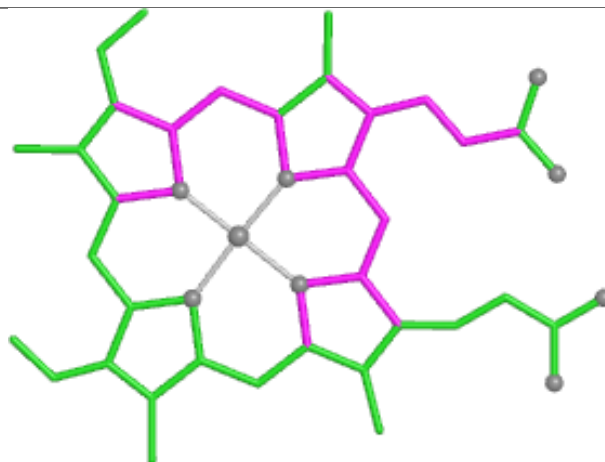
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	FUM	7	0
4	E	701	FAD	4	0
9	K	302	HEM	13	0
8	F	303	FES	1	0
8	B	303	FES	1	0
7	N	302	SF4	1	0
9	O	303	HEM	9	0
10	O	301	LMT	24	0
5	M	702	FUM	5	0
9	C	302	HEM	8	0
5	I	702	FUM	3	0
8	N	303	FES	1	0
7	B	302	SF4	1	0
9	O	302	HEM	11	0
4	M	701	FAD	13	0
4	I	701	FAD	17	0
9	C	301	HEM	15	0
4	A	701	FAD	2	0
10	C	303	LMT	31	0
9	G	302	HEM	10	0
9	K	301	HEM	12	0
6	F	301	F3S	3	0
11	C	304	MQ7	21	0
5	E	702	FUM	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.

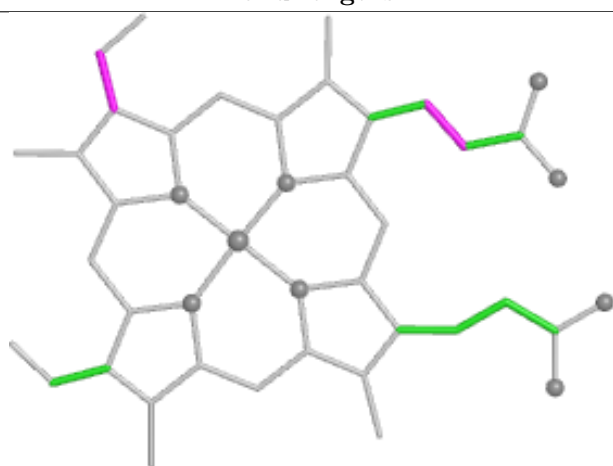
Ligand HEM G 301



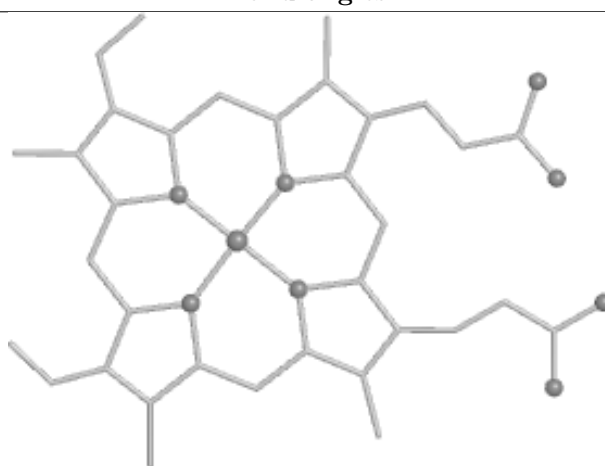
Bond lengths



Bond angles

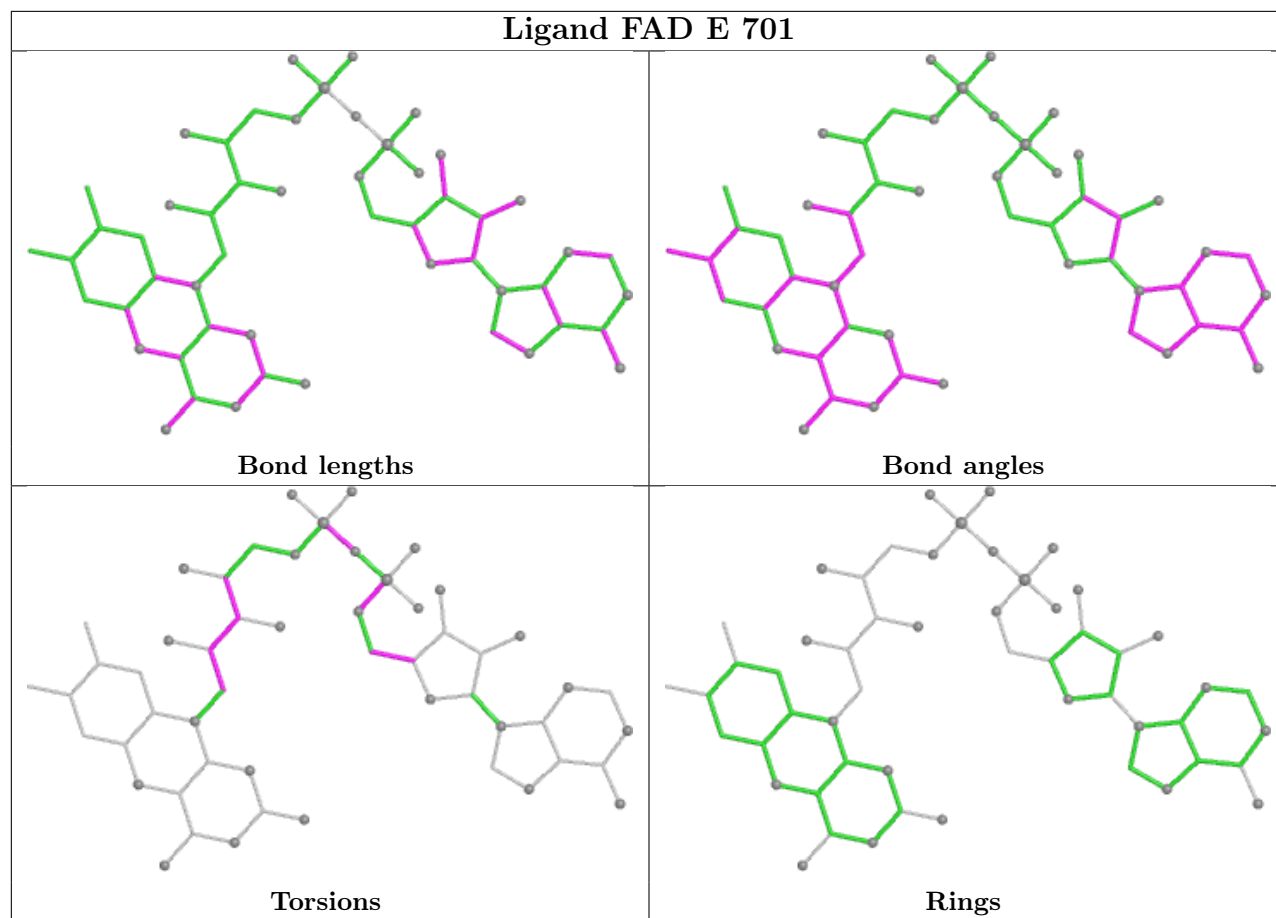


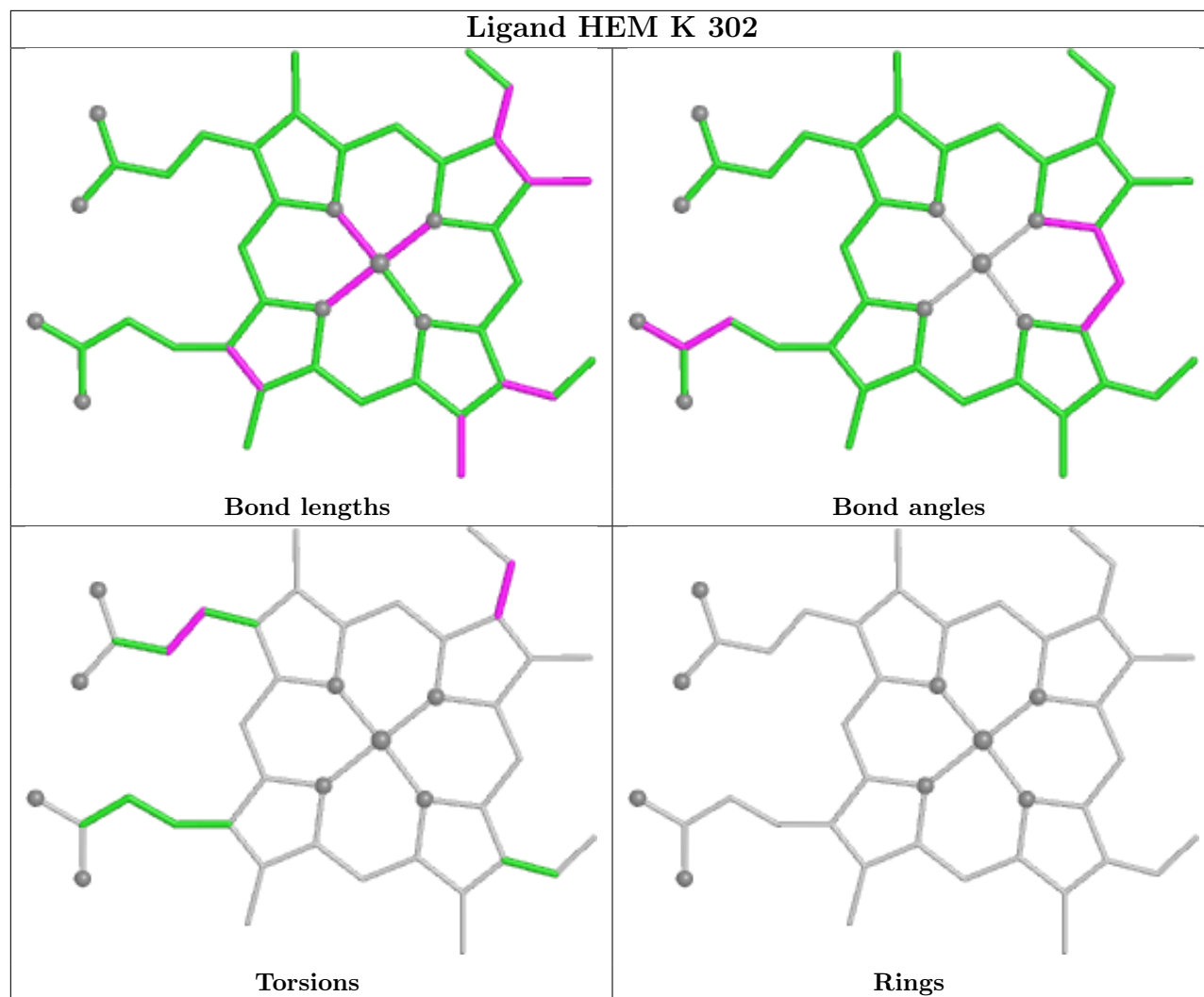
Torsions

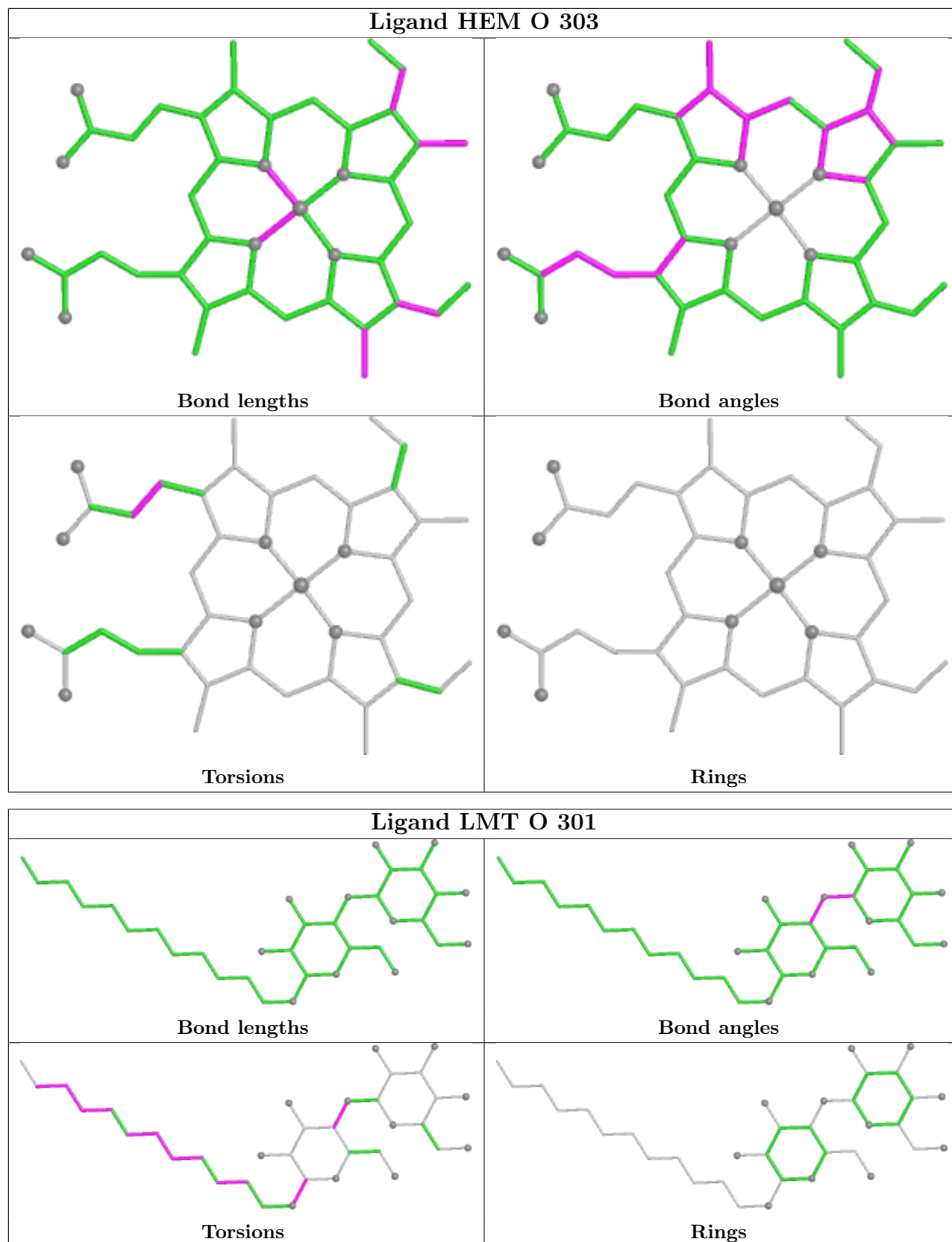


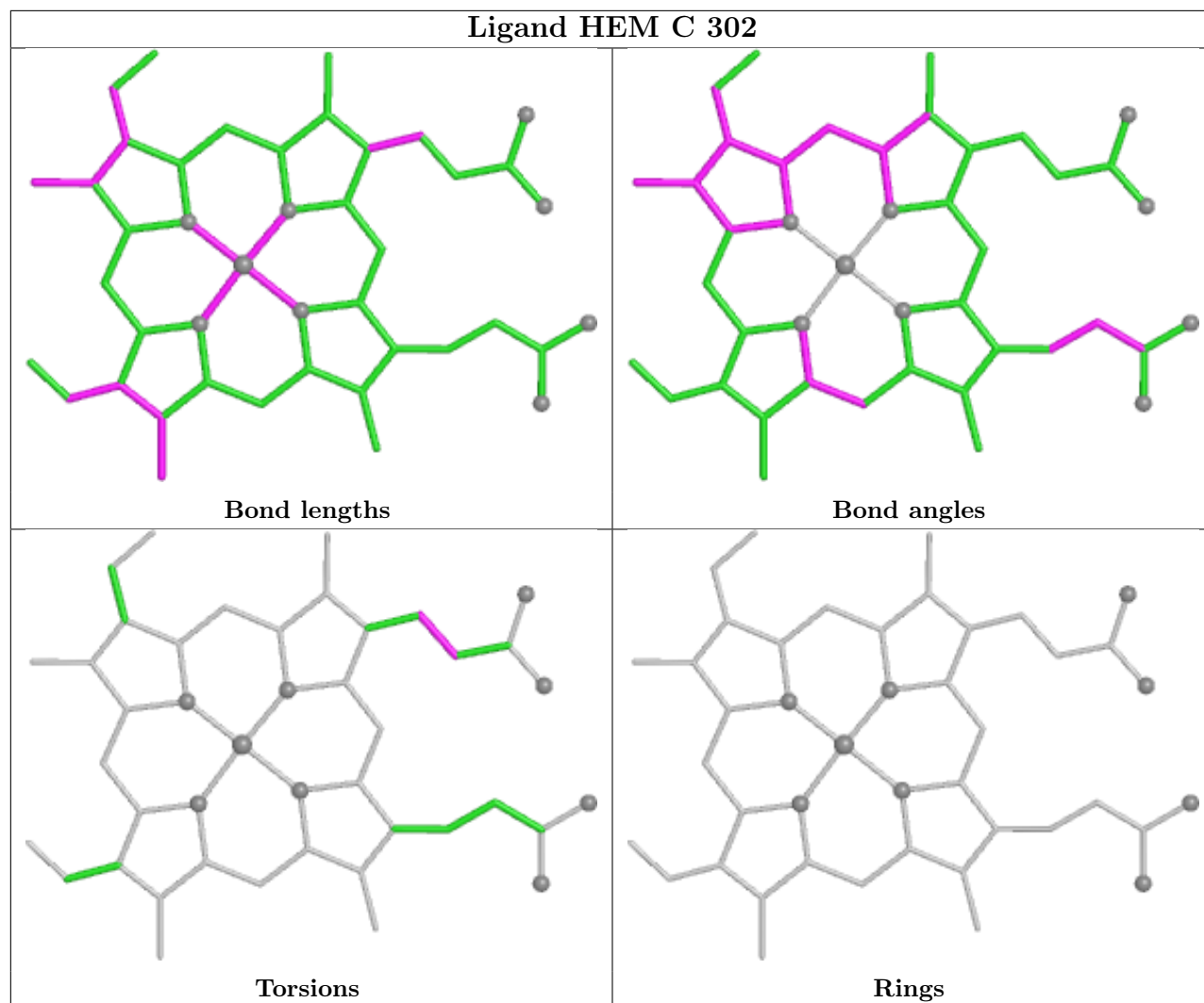
Rings

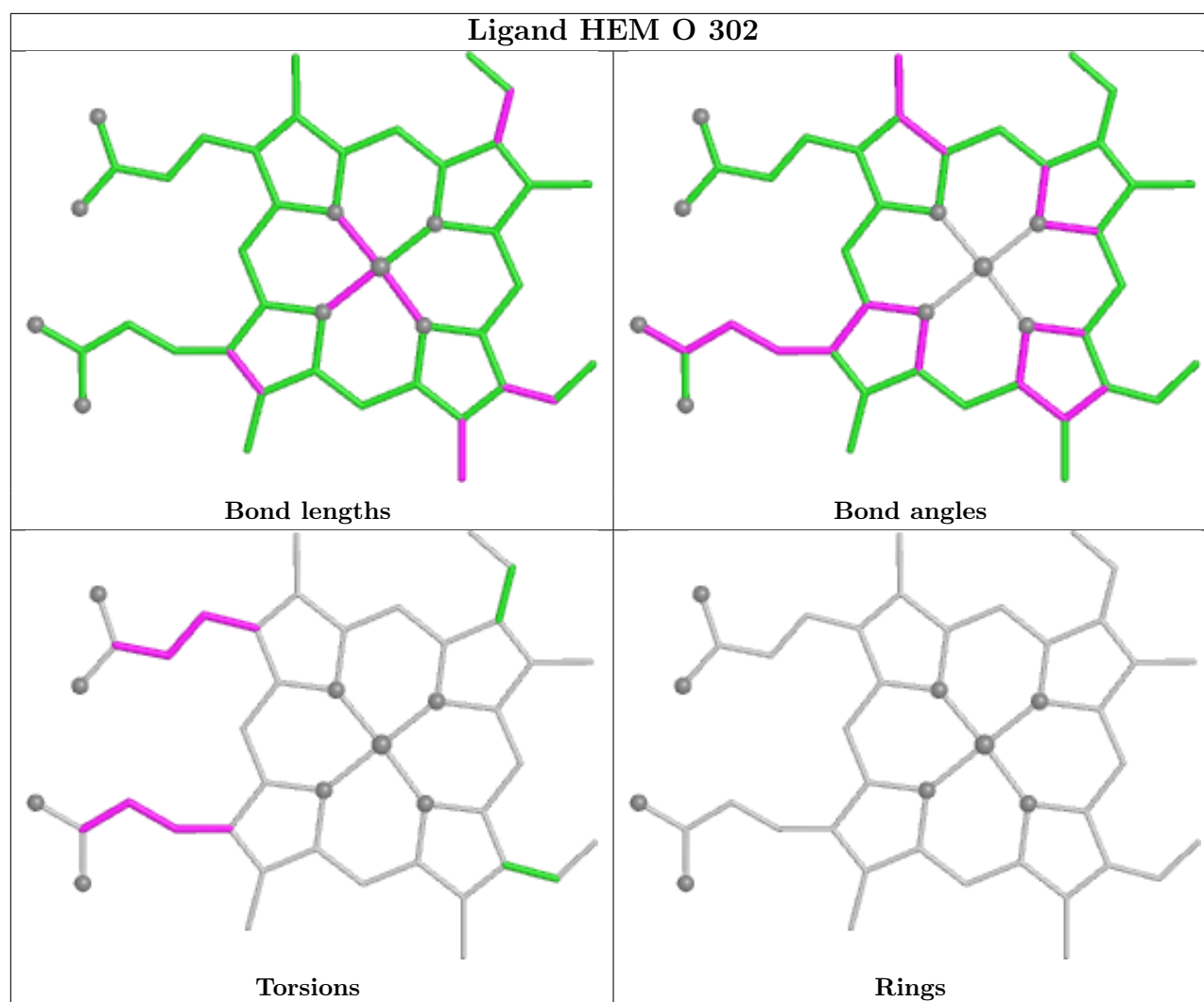
Ligand FAD E 701

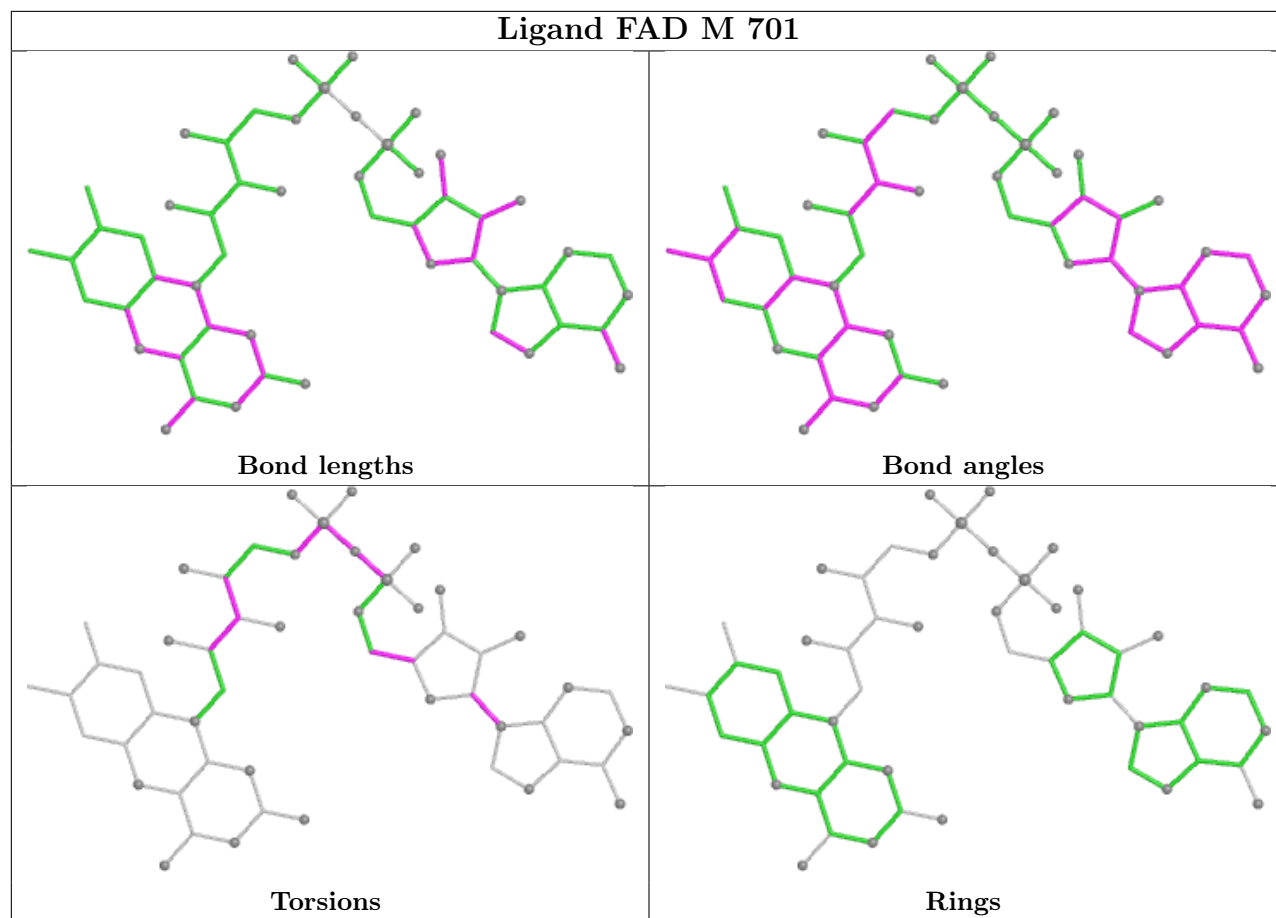




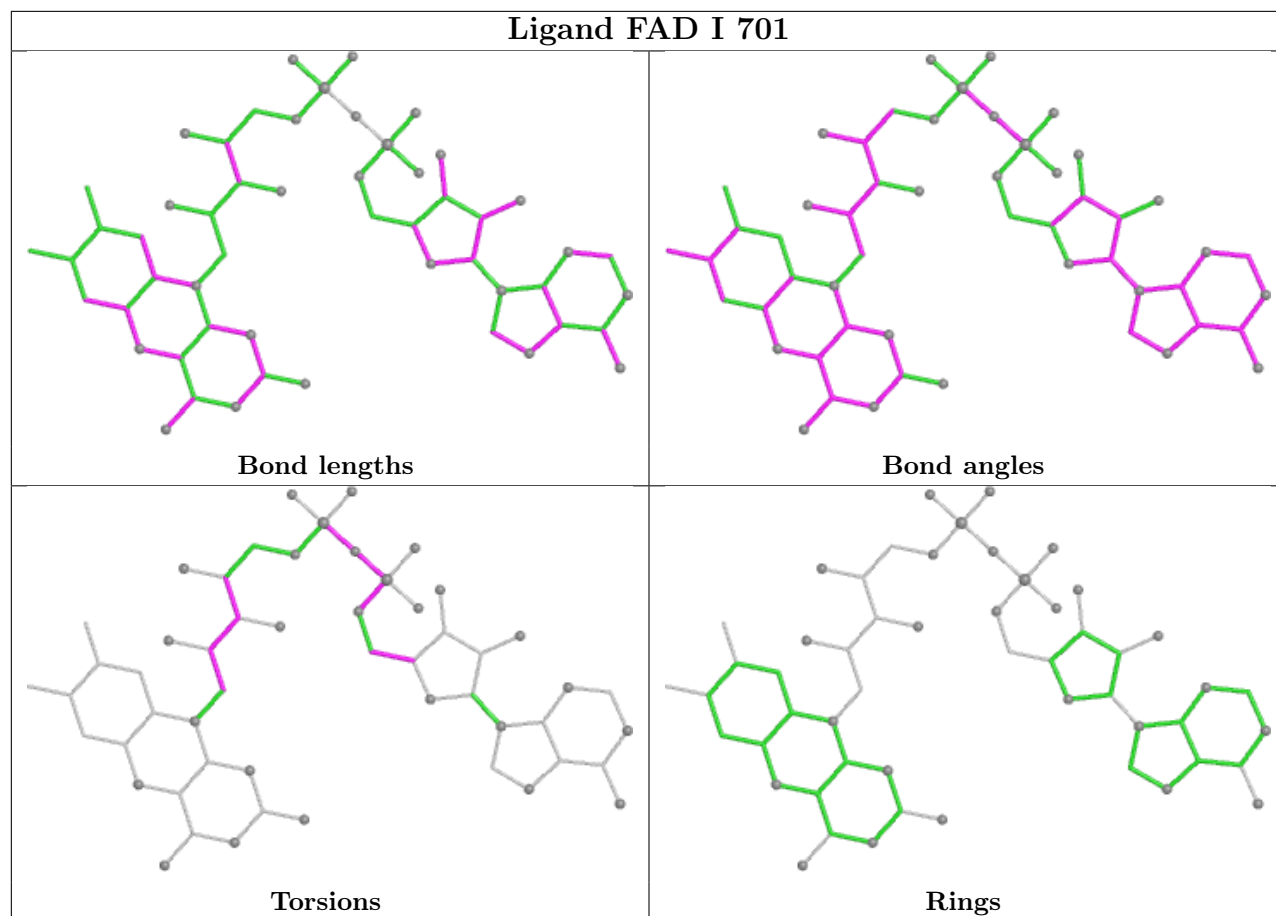


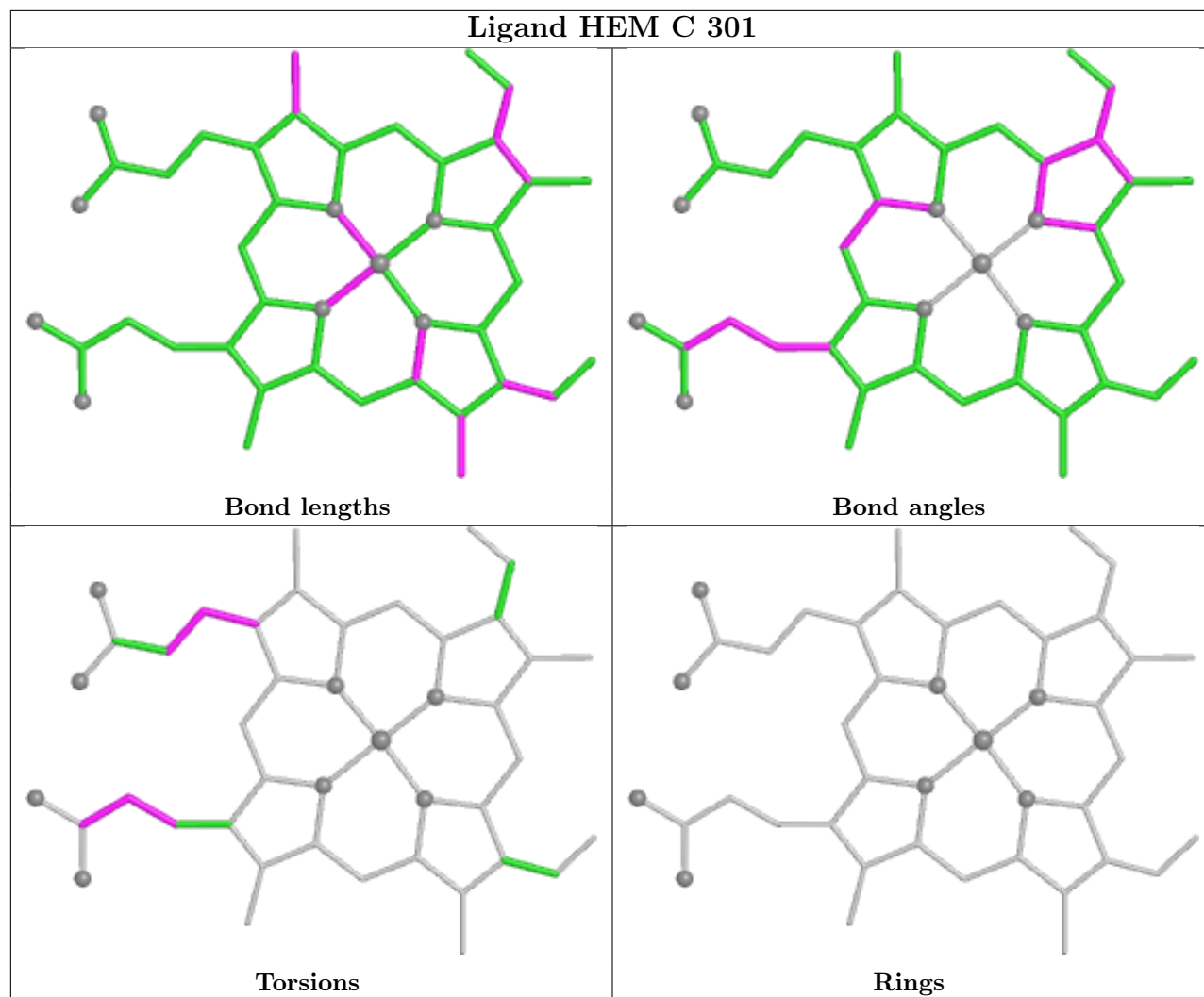




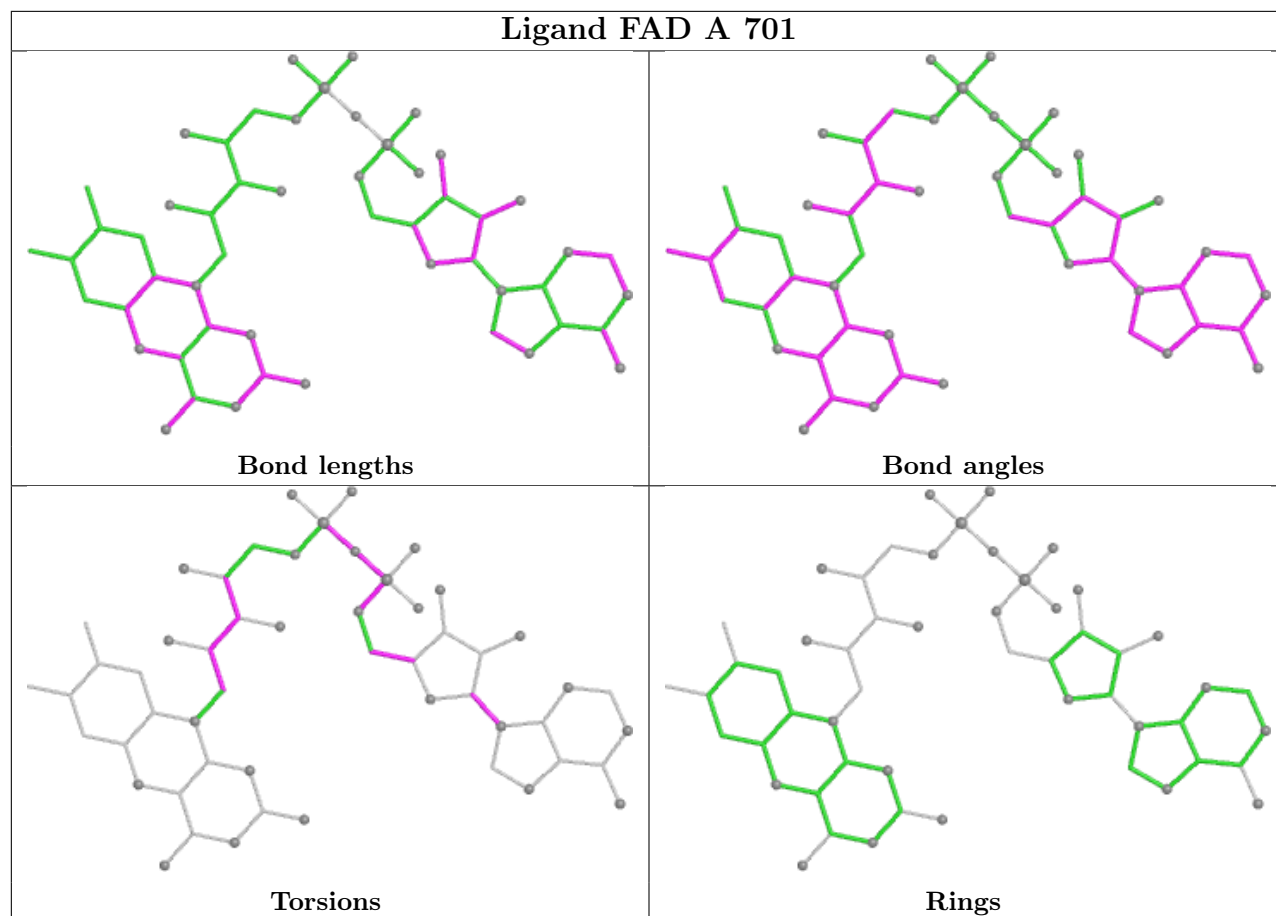


Ligand FAD I 701

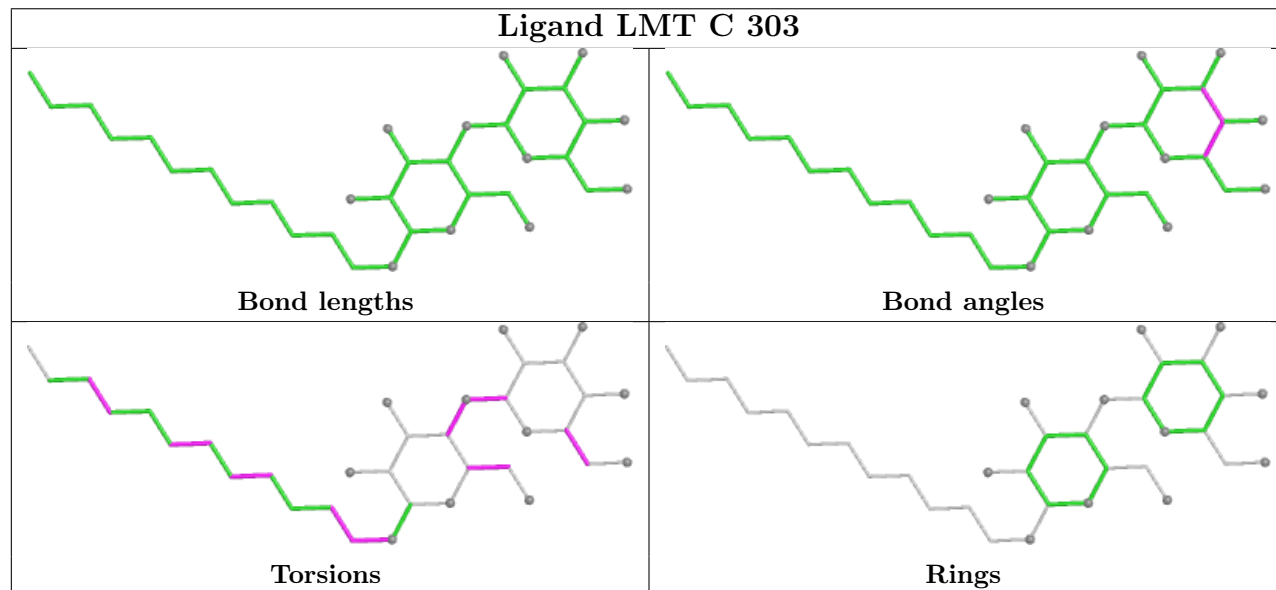


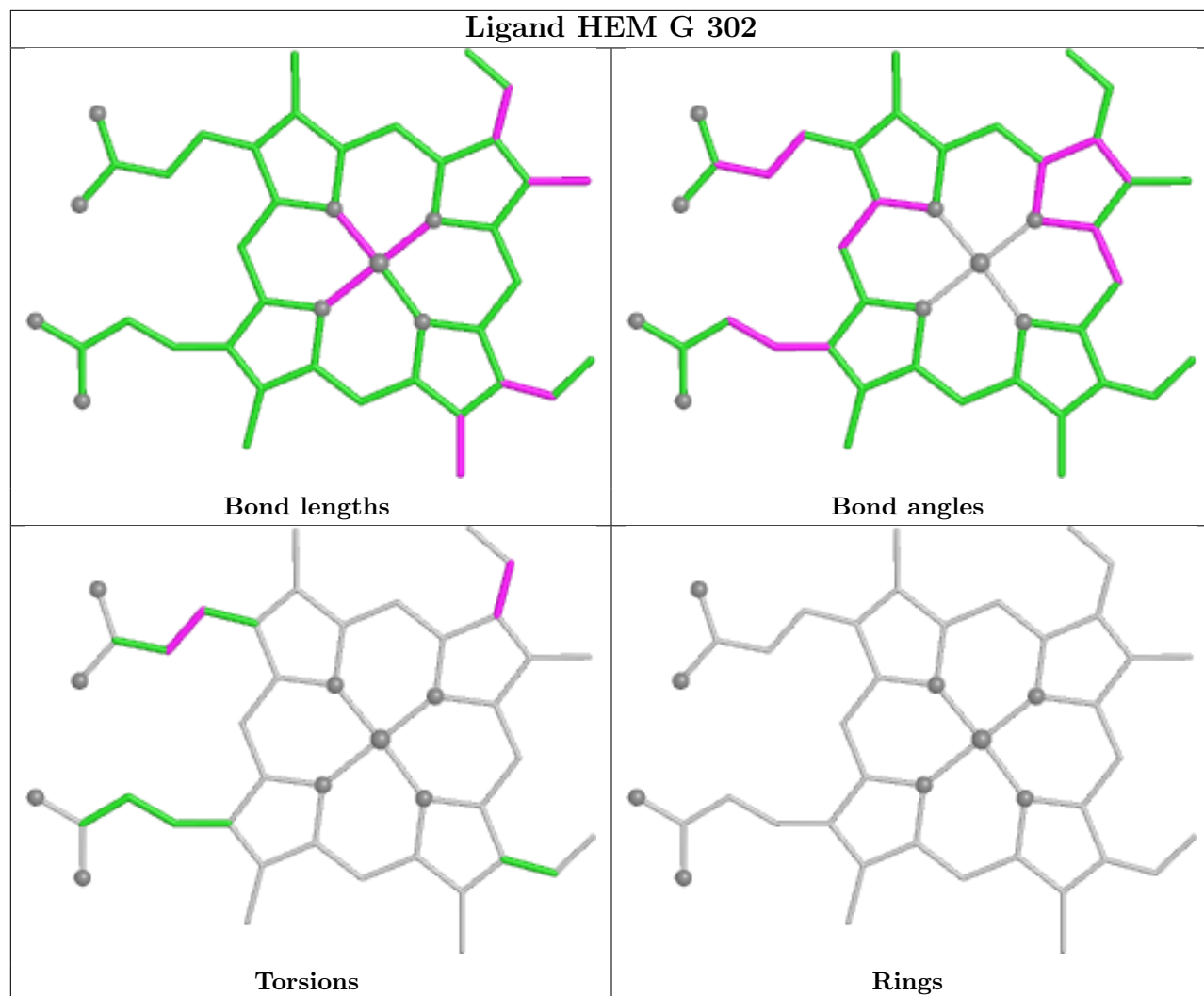


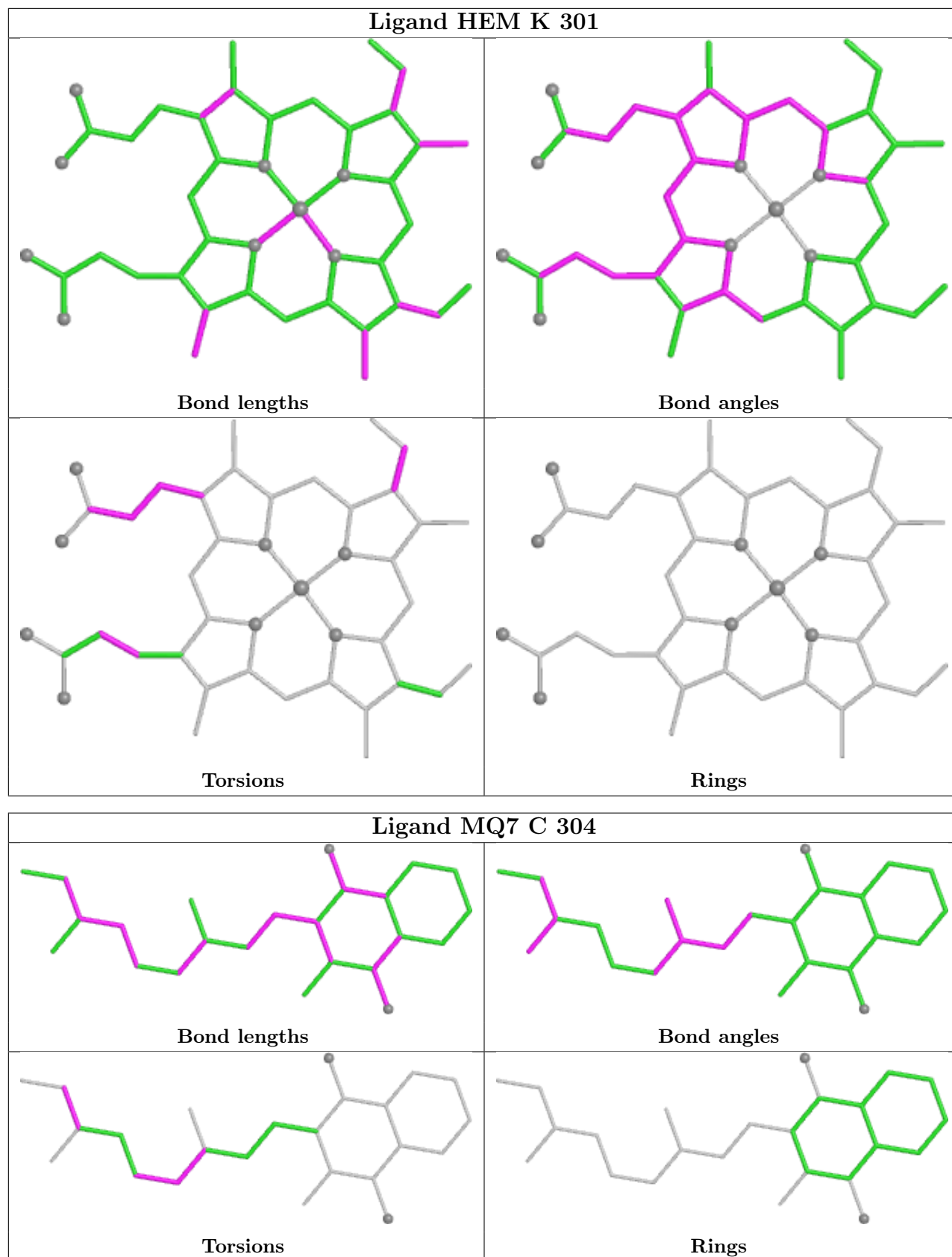
Ligand FAD A 701



Ligand LMT C 303







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	622/627 (99%)	-0.48	5 (0%) 82 58	34, 66, 101, 137	0
1	E	622/627 (99%)	-0.30	12 (1%) 66 39	47, 95, 142, 168	0
1	I	622/627 (99%)	-0.36	7 (1%) 78 52	45, 93, 154, 198	0
1	M	622/627 (99%)	-0.31	5 (0%) 82 58	48, 117, 178, 257	0
2	B	240/264 (90%)	-0.51	1 (0%) 88 70	43, 69, 109, 128	0
2	F	240/264 (90%)	-0.31	4 (1%) 69 41	53, 90, 143, 323	0
2	J	240/264 (90%)	-0.34	6 (2%) 58 34	55, 97, 153, 204	0
2	N	240/264 (90%)	-0.35	4 (1%) 69 41	44, 84, 171, 232	0
3	C	212/218 (97%)	-0.45	0 100 100	53, 84, 130, 177	0
3	G	212/218 (97%)	-0.30	4 (1%) 66 39	66, 109, 164, 206	0
3	K	212/218 (97%)	-0.21	6 (2%) 55 31	70, 122, 171, 190	0
3	O	212/218 (97%)	-0.35	2 (0%) 81 56	55, 100, 156, 178	0
All	All	4296/4436 (96%)	-0.36	56 (1%) 75 48	34, 92, 159, 323	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	252	GLU	8.4
2	J	226	ASP	7.6
1	E	403	PHE	7.1
1	M	253	ALA	6.8
1	M	402	GLY	5.7

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

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

6.3 Carbohydrates ⓘ

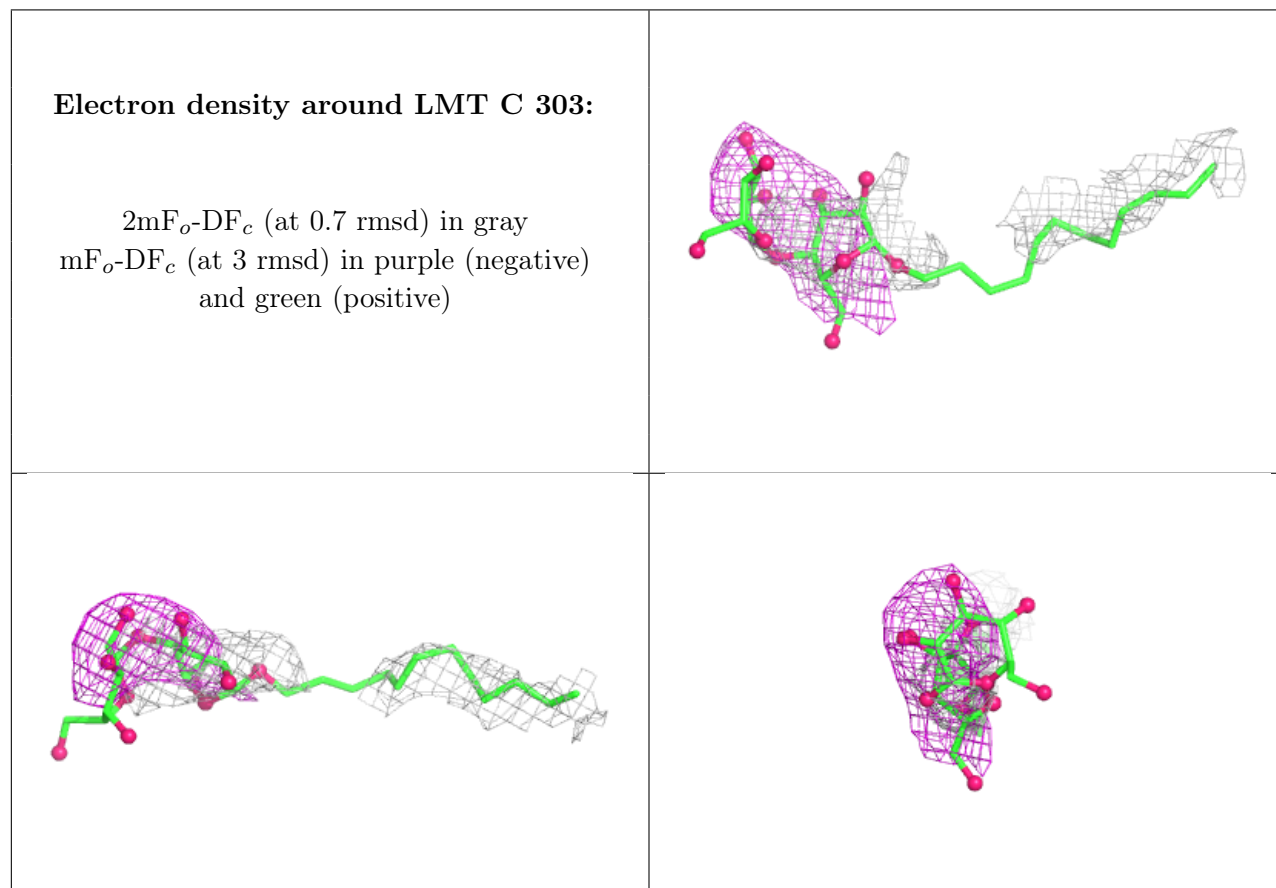
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

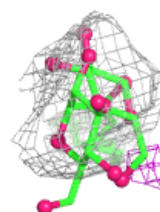
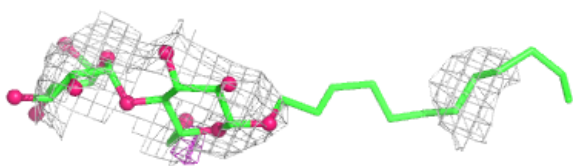
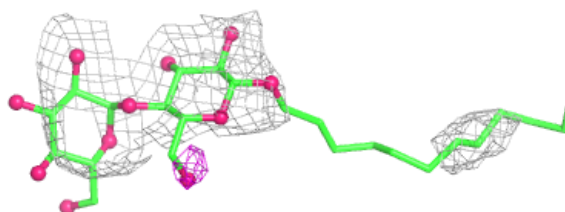
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LMT	C	303	35/35	0.58	0.14	58,92,105,118	0
10	LMT	O	301	35/35	0.72	0.10	56,118,126,130	0
11	MQ7	C	304	24/48	0.81	0.08	112,112,112,112	0
5	FUM	A	702	8/8	0.82	0.14	67,72,80,85	0
5	FUM	M	702	8/8	0.85	0.06	119,124,128,130	0
6	F3S	F	301	7/7	0.88	0.11	45,77,94,97	0
4	FAD	M	701	53/53	0.89	0.08	51,94,119,122	0
9	HEM	K	301	43/43	0.90	0.14	117,130,147,159	0
4	FAD	I	701	53/53	0.91	0.08	57,72,102,107	0
5	FUM	I	702	8/8	0.91	0.11	92,97,107,109	0
9	HEM	G	301	43/43	0.92	0.11	111,125,139,144	0
9	HEM	C	301	43/43	0.93	0.14	69,87,103,126	0
5	FUM	E	702	8/8	0.93	0.14	79,90,95,96	0
4	FAD	A	701	53/53	0.93	0.07	35,51,65,73	0
4	FAD	E	701	53/53	0.94	0.06	46,69,85,93	0
9	HEM	G	302	43/43	0.94	0.11	77,95,104,110	0
9	HEM	O	302	43/43	0.95	0.10	92,104,130,138	0
9	HEM	K	302	43/43	0.95	0.13	83,103,115,123	0
9	HEM	O	303	43/43	0.96	0.09	58,74,86,92	0
9	HEM	C	302	43/43	0.97	0.09	54,71,83,92	0
8	FES	B	303	4/4	0.98	0.04	42,60,69,73	0
8	FES	F	303	4/4	0.98	0.05	60,61,65,101	0
8	FES	J	303	4/4	0.98	0.03	68,73,76,85	0
8	FES	N	303	4/4	0.98	0.03	61,69,71,72	0
6	F3S	J	301	7/7	0.98	0.04	56,76,84,97	0
7	SF4	F	302	8/8	0.99	0.02	36,43,62,67	0
7	SF4	J	302	8/8	0.99	0.02	40,52,55,57	0
7	SF4	N	302	8/8	0.99	0.04	42,63,66,74	0
6	F3S	B	301	7/7	0.99	0.04	25,46,54,70	0
6	F3S	N	301	7/7	0.99	0.03	45,55,65,70	0
7	SF4	B	302	8/8	0.99	0.03	24,29,53,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

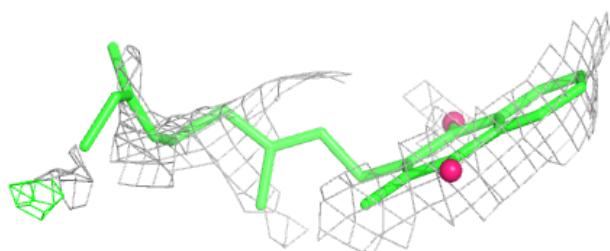
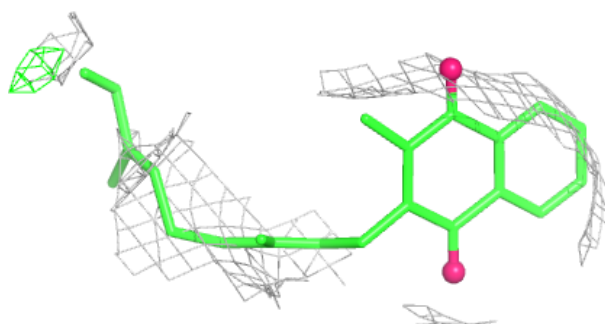


Electron density around LMT O 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

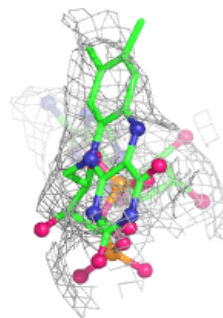
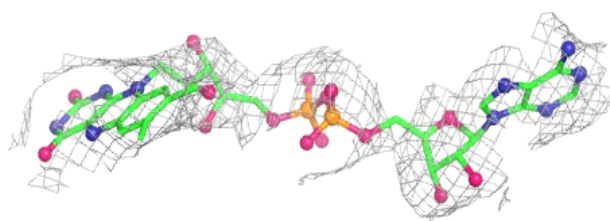
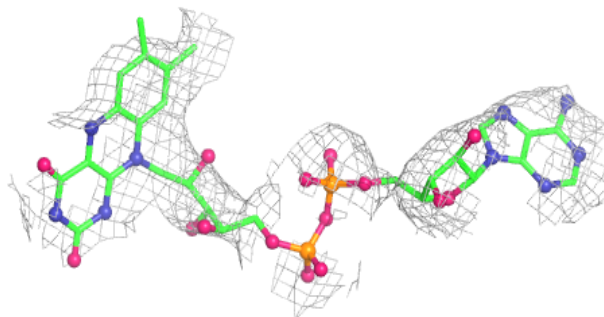
**Electron density around MQ7 C 304:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



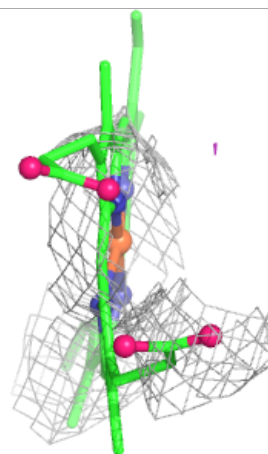
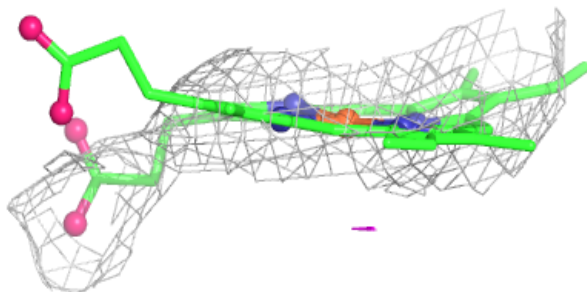
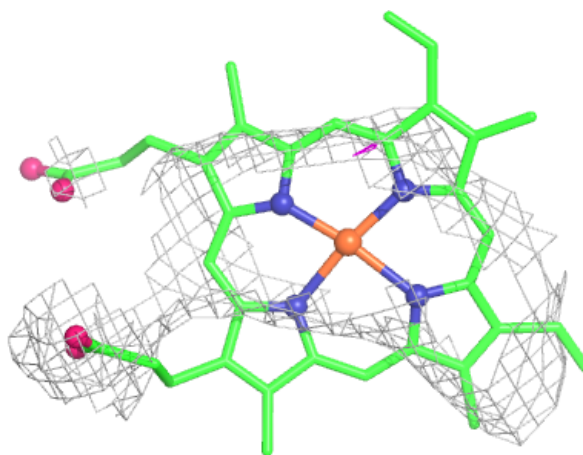
Electron density around FAD M 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



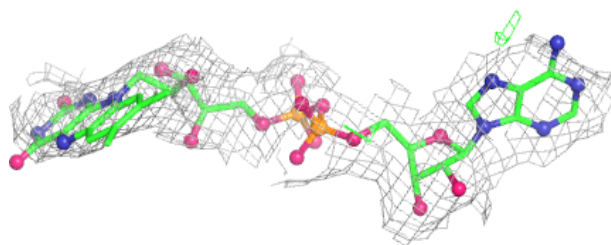
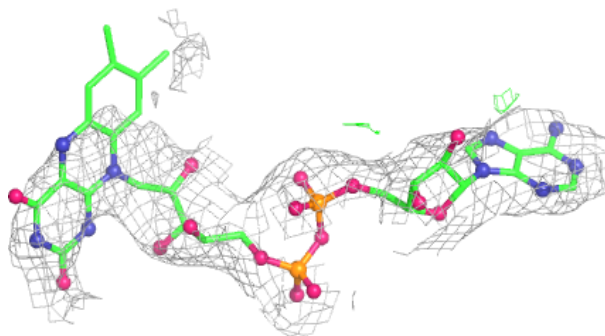
Electron density around HEM K 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



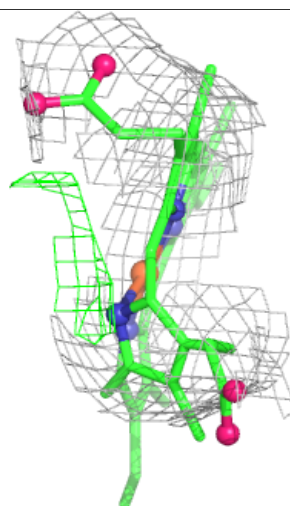
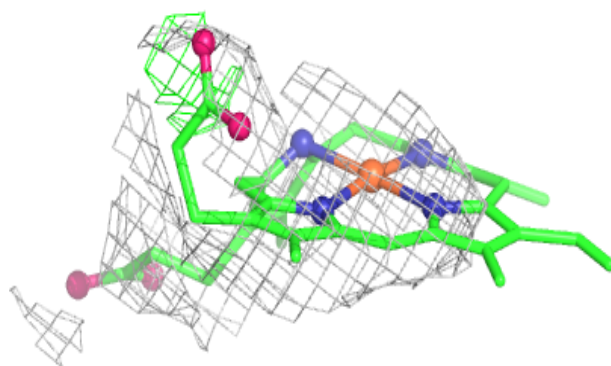
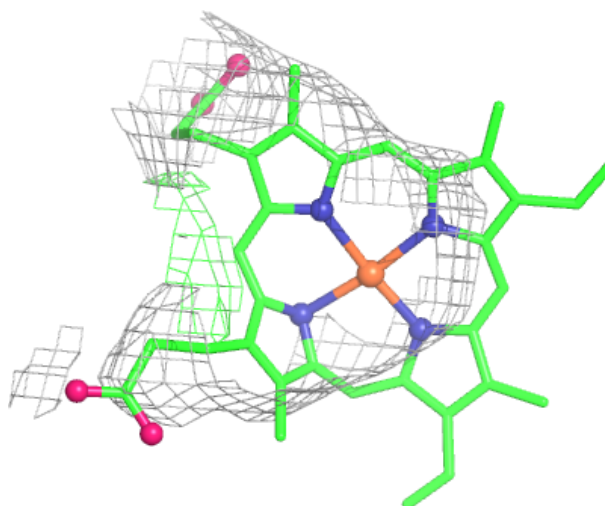
Electron density around FAD I 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



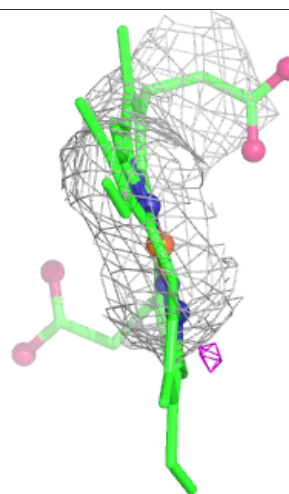
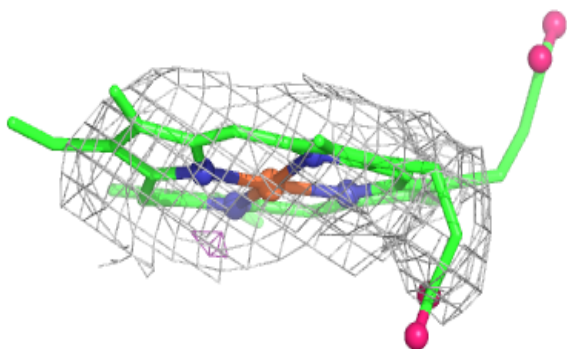
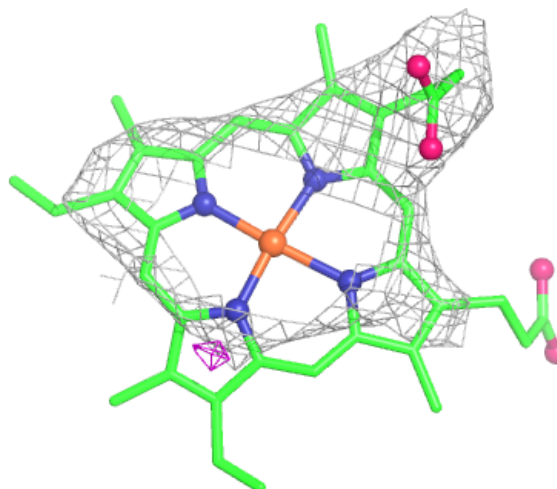
Electron density around HEM G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



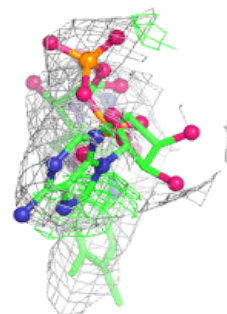
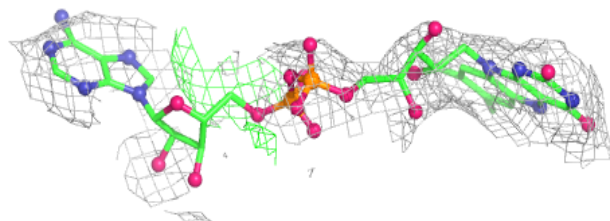
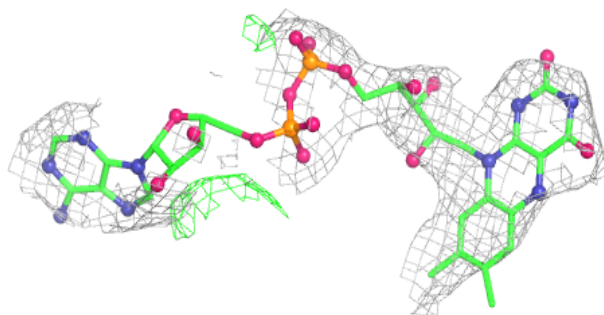
Electron density around HEM C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

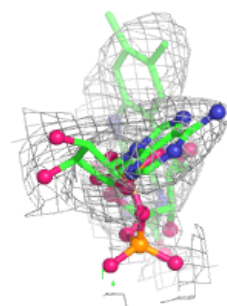
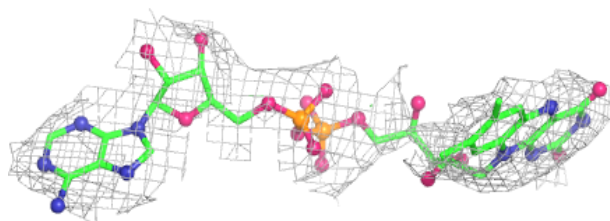
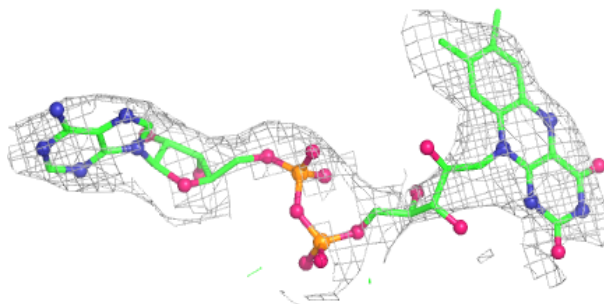


Electron density around FAD A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

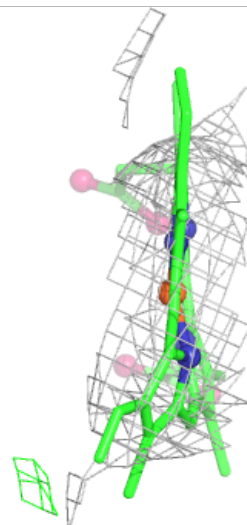
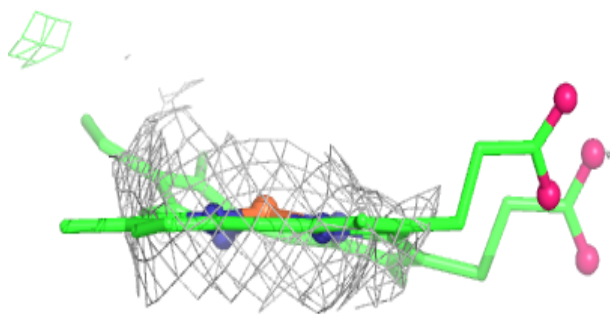
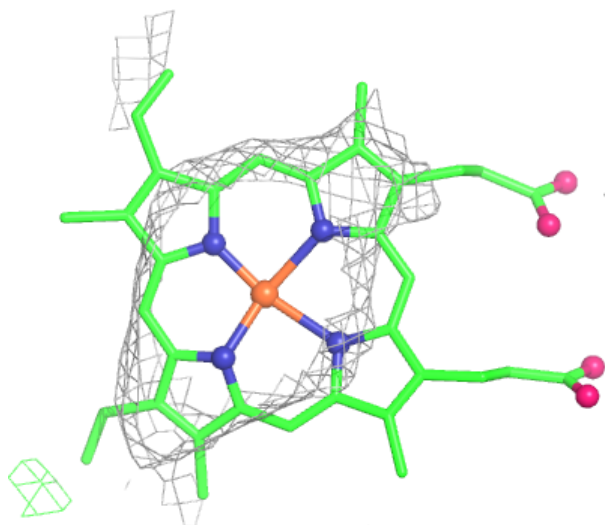
**Electron density around FAD E 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



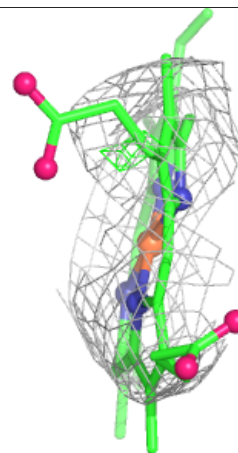
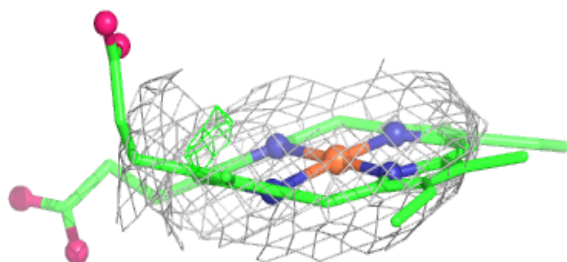
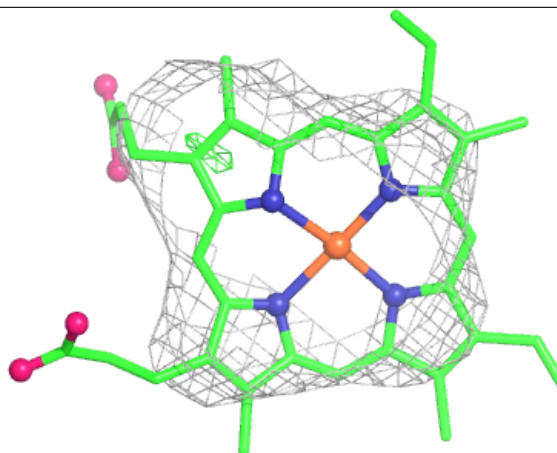
Electron density around HEM G 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



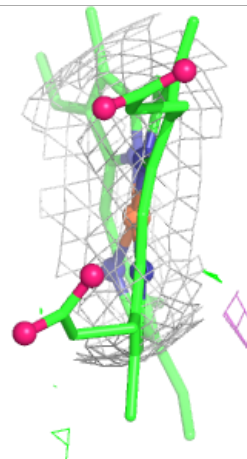
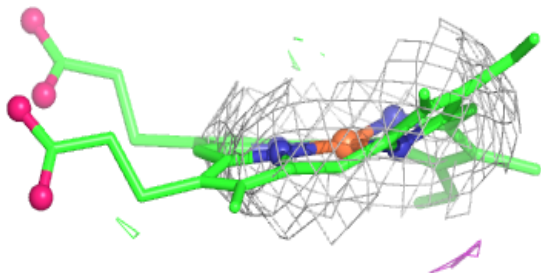
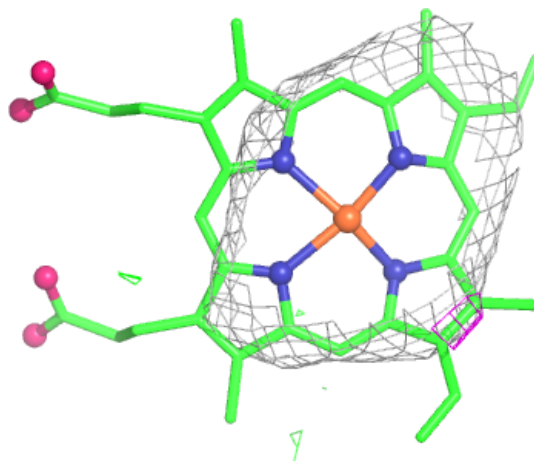
Electron density around HEM O 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



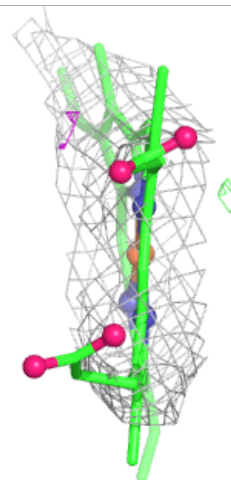
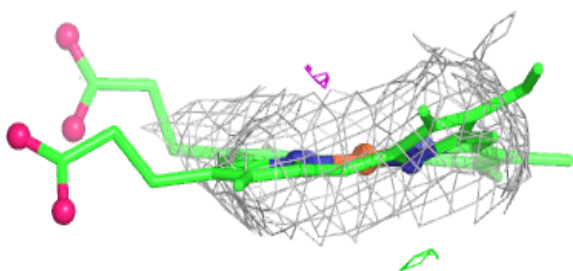
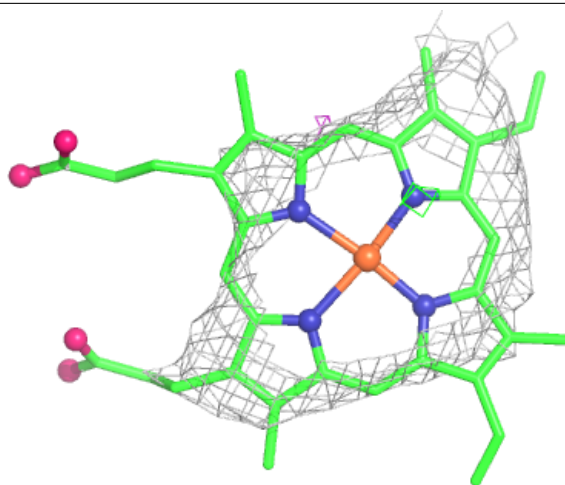
Electron density around HEM K 302:

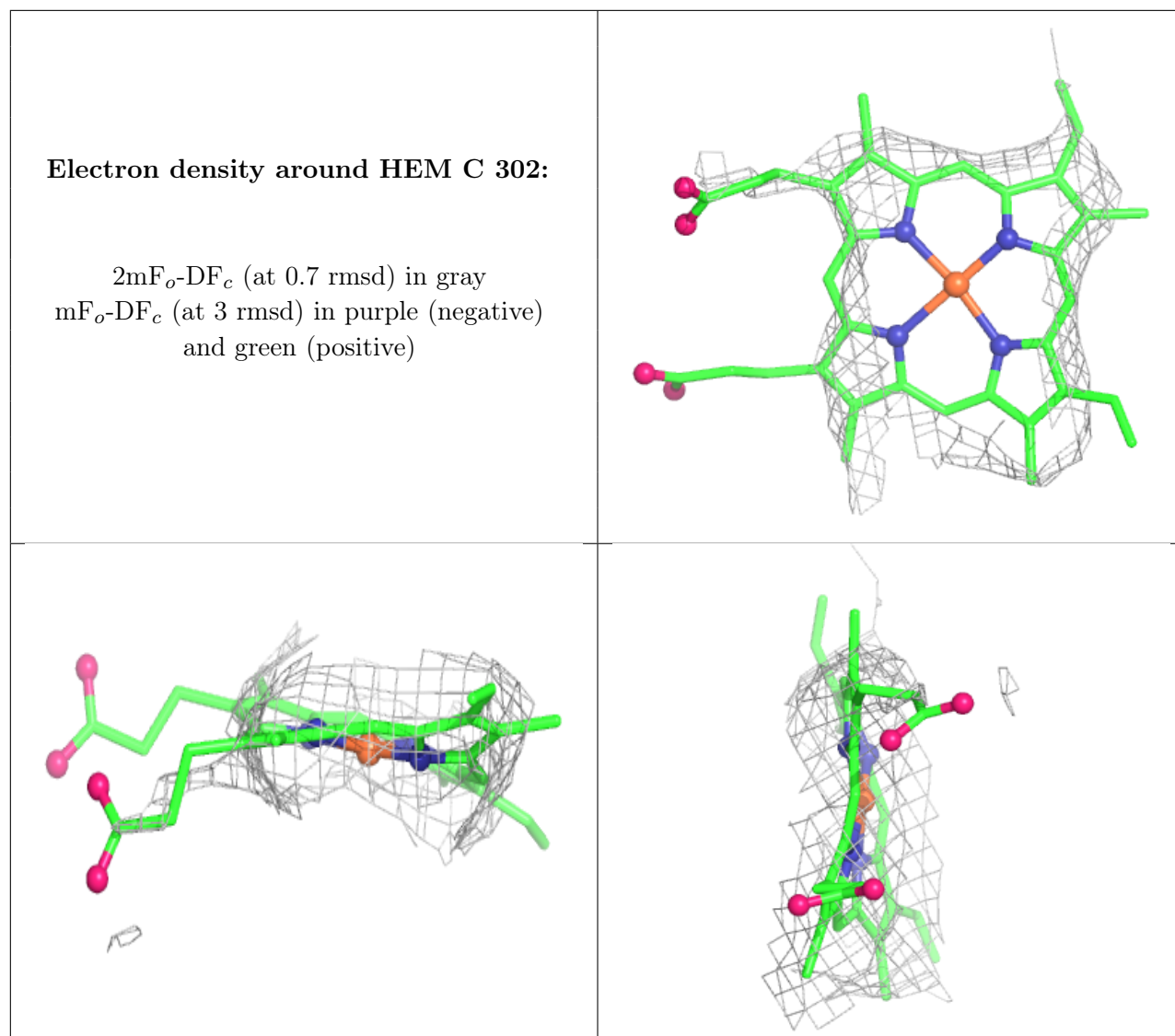
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM O 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.