



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:57 PM EDT

PDB ID : 1LJ1 / pdb_00001lj1
Title : Crystal structure of Q363F/R402A mutant flavocytochrome c3
Authors : Mowat, C.G.; Pankhurst, K.L.; Miles, C.S.; Leys, D.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2002-04-18
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

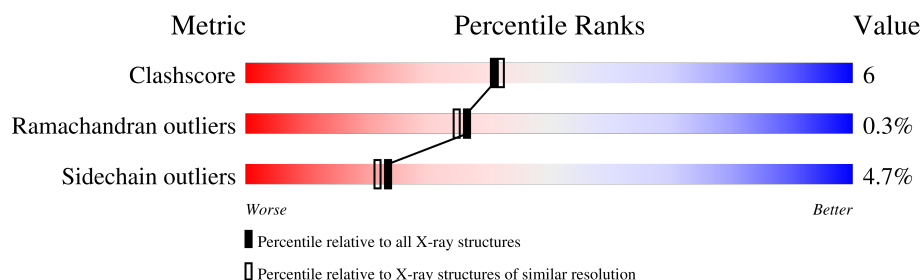
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	 81% 15% ...
1	B	571	 83% 13% ..

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	FUM	A	1701	-	X	-	-
5	FUM	B	1801	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10489 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 flavocytochrome c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4187	2602	730	830	25			
1	B	568	Total	C	N	O	S	0	0	0
			4204	2611	738	830	25			

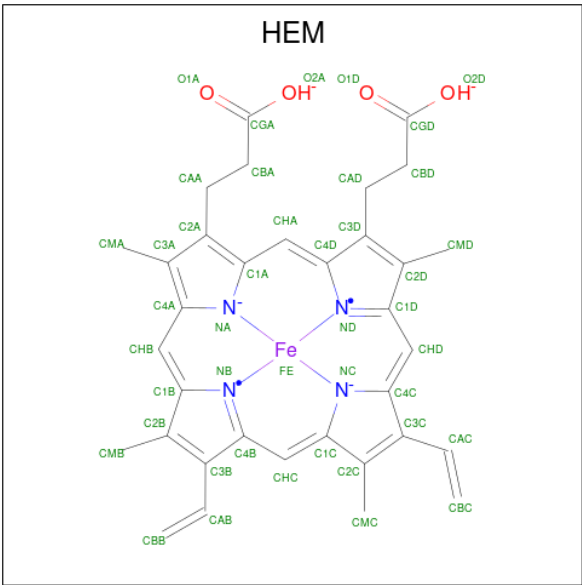
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	PHE	GLN	engineered mutation	UNP Q02469
A	402	ALA	ARG	engineered mutation	UNP Q02469
B	363	PHE	GLN	engineered mutation	UNP Q02469
B	402	ALA	ARG	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

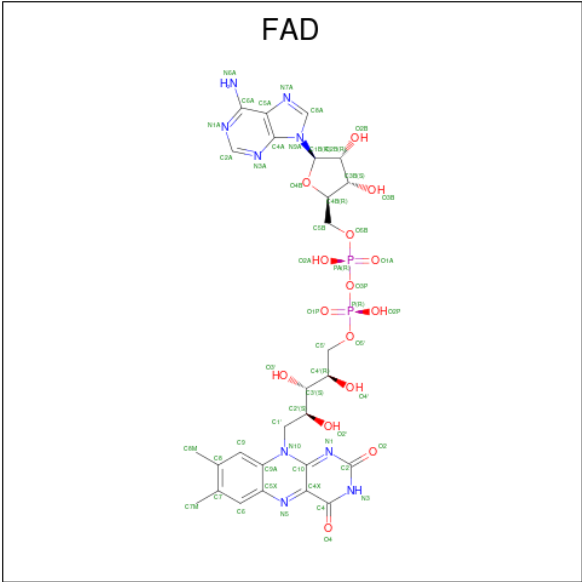
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



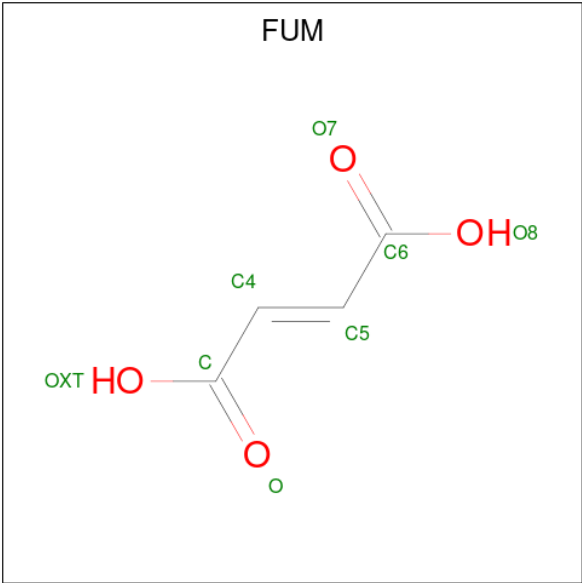
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

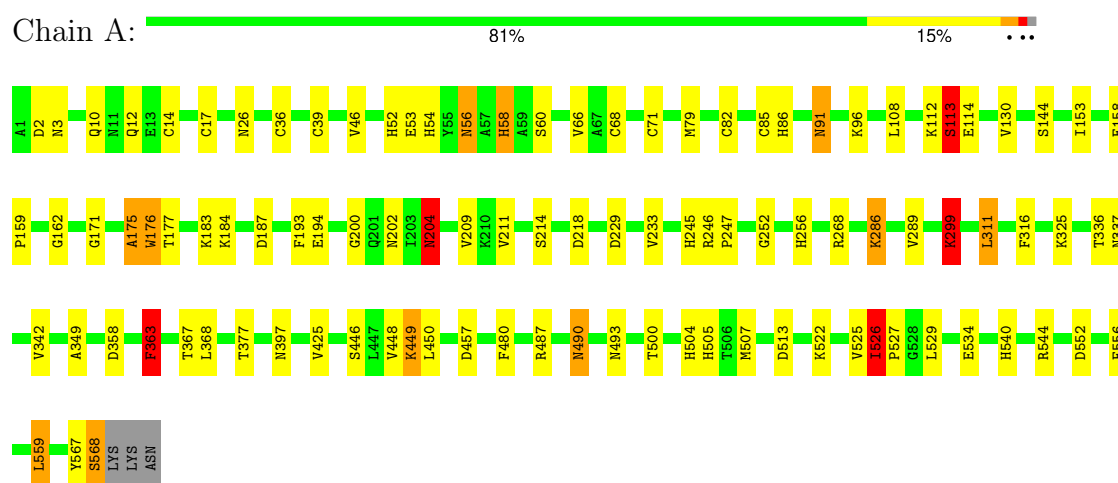
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	804	Total 804	O 804	0	0
6	B	826	Total 826	O 826	0	0

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. 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: flavocytochrome c3



• Molecule 1: flavocytochrome c3



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	77.97Å 88.28Å 90.09Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10489	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: NA, FAD, HEM, FUM

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	0.86	1/4258 (0.0%)	1.83	74/5764 (1.3%)
1	B	0.84	0/4275	1.73	69/5782 (1.2%)
All	All	0.85	1/8533 (0.0%)	1.78	143/11546 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-8.36	1.35	1.46

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	CA-C-N	28.99	176.91	121.54
1	A	175	ALA	C-N-CA	28.99	176.91	121.54
1	B	175	ALA	O-C-N	-17.93	100.37	122.96
1	A	526	ILE	CB-CA-C	11.17	124.22	111.04
1	A	176	TRP	N-CA-CB	10.32	127.94	110.49
1	A	91	ASN	OD1-CG-ND2	9.81	132.41	122.60
1	A	113	SER	CA-C-N	9.29	132.73	120.28
1	A	113	SER	C-N-CA	9.29	132.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ASN	CA-CB-CG	9.13	121.73	112.60
1	B	162	GLY	N-CA-C	9.11	125.53	114.69
1	B	505	HIS	CA-CB-CG	9.07	122.87	113.80
1	B	218	ASP	CA-CB-CG	-9.07	103.53	112.60
1	A	363	PHE	CA-CB-CG	8.97	122.77	113.80
1	B	363	PHE	CA-CB-CG	8.94	122.74	113.80
1	A	337	ASN	N-CA-C	8.63	122.20	110.55
1	A	112	LYS	CA-C-N	8.51	137.80	121.54
1	A	112	LYS	C-N-CA	8.51	137.80	121.54
1	B	171	GLY	N-CA-C	8.50	121.07	110.96
1	A	490	ASN	OD1-CG-ND2	-8.45	114.15	122.60
1	A	91	ASN	CA-CB-CG	-8.38	104.22	112.60
1	A	526	ILE	CA-CB-CG2	8.17	124.38	110.50
1	B	337	ASN	N-CA-C	8.16	122.60	110.52
1	B	218	ASP	CB-CA-C	-8.03	97.46	110.79
1	A	112	LYS	CA-C-O	7.96	129.83	120.92
1	A	457	ASP	CA-C-N	7.86	128.70	119.98
1	A	457	ASP	C-N-CA	7.86	128.70	119.98
1	A	171	GLY	N-CA-C	7.85	120.30	110.96
1	A	187	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	552	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	567	TYR	CA-C-N	7.48	135.16	121.70
1	B	567	TYR	C-N-CA	7.48	135.16	121.70
1	A	52	HIS	CA-CB-CG	7.34	121.14	113.80
1	A	58	HIS	CA-CB-CG	-7.30	106.50	113.80
1	B	568	SER	CA-C-O	-7.30	108.39	120.80
1	B	15	ASP	N-CA-CB	7.14	121.98	110.42
1	A	500	THR	O-C-N	-7.13	116.45	121.65
1	B	337	ASN	CA-CB-CG	7.08	119.68	112.60
1	B	175	ALA	CA-C-O	-7.06	113.60	121.51
1	B	35	GLN	CA-C-O	-7.05	112.95	120.42
1	A	377	THR	CA-C-O	7.04	129.02	121.55
1	B	367	THR	N-CA-C	7.00	118.41	108.54
1	B	377	THR	CA-C-N	6.99	130.35	120.28
1	B	377	THR	C-N-CA	6.99	130.35	120.28
1	A	480	PHE	CA-CB-CG	-6.63	107.17	113.80
1	B	552	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	113	SER	N-CA-CB	-6.60	99.33	110.49
1	A	504	HIS	CA-CB-CG	6.59	120.39	113.80
1	A	175	ALA	N-CA-CB	6.57	122.88	111.13
1	B	490	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	513	ASP	CA-CB-CG	6.51	119.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	CA-C-O	-6.48	113.36	120.81
1	A	108	LEU	CA-C-N	6.43	129.54	120.28
1	A	108	LEU	C-N-CA	6.43	129.54	120.28
1	A	505	HIS	CA-C-N	-6.41	114.02	123.11
1	A	505	HIS	C-N-CA	-6.41	114.02	123.11
1	B	377	THR	CA-C-O	6.39	128.22	121.19
1	B	381	ARG	CA-C-N	6.38	127.17	120.03
1	B	381	ARG	C-N-CA	6.38	127.17	120.03
1	B	390	ARG	CG-CD-NE	6.31	125.87	112.00
1	B	62	PHE	CA-CB-CG	6.30	120.10	113.80
1	B	390	ARG	CD-NE-CZ	6.24	133.14	124.40
1	A	544	ARG	CA-C-O	-6.23	113.95	121.05
1	A	525	VAL	CA-C-N	-6.21	115.77	122.85
1	A	525	VAL	C-N-CA	-6.21	115.77	122.85
1	A	86	HIS	CA-CB-CG	6.20	120.00	113.80
1	B	202	ASN	CA-CB-CG	-6.20	106.40	112.60
1	A	316	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	457	ASP	CA-C-N	6.03	126.67	119.98
1	B	457	ASP	C-N-CA	6.03	126.67	119.98
1	A	397	ASN	CA-CB-CG	6.00	118.60	112.60
1	B	435	TYR	CA-C-O	5.98	126.84	119.97
1	B	90	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	355	ALA	CA-C-O	-5.89	114.33	121.28
1	A	10	GLN	CG-CD-NE2	5.84	125.16	116.40
1	A	268	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	367	THR	N-CA-C	5.80	118.74	107.71
1	B	77	LYS	CA-C-O	-5.79	115.41	121.55
1	A	358	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	325	LYS	CA-C-O	-5.77	114.43	120.55
1	B	113	SER	CA-C-O	-5.75	114.14	120.69
1	A	493	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	162	GLY	N-CA-C	5.71	121.48	114.69
1	A	505	HIS	CA-CB-CG	5.71	119.51	113.80
1	A	204	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	2	ASP	CA-CB-CG	-5.70	106.90	112.60
1	A	526	ILE	O-C-N	-5.69	117.79	121.37
1	B	501	PRO	CA-C-N	5.68	127.20	121.35
1	B	501	PRO	C-N-CA	5.68	127.20	121.35
1	B	221	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	135	GLY	O-C-N	-5.65	117.37	122.96
1	B	568	SER	CA-CB-OG	-5.58	99.93	111.10
1	B	114	GLU	N-CA-CB	5.58	119.93	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	GLN	CG-CD-NE2	5.58	124.77	116.40
1	B	310	ILE	CA-C-O	5.57	126.61	120.48
1	A	211	VAL	N-CA-C	-5.57	104.94	110.62
1	B	71	CYS	CA-C-N	-5.56	115.61	122.84
1	B	71	CYS	C-N-CA	-5.56	115.61	122.84
1	B	218	ASP	O-C-N	5.55	128.01	122.12
1	B	558	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	B	218	ASP	OD1-CG-OD2	5.51	136.13	122.90
1	B	130	VAL	CA-C-O	-5.48	114.67	120.48
1	A	218	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	342	VAL	N-CA-C	5.43	118.11	112.90
1	A	233	VAL	O-C-N	-5.42	117.45	123.20
1	B	487	ARG	CG-CD-NE	-5.40	100.11	112.00
1	B	170	GLY	CA-C-O	-5.39	114.58	120.40
1	A	252	GLY	O-C-N	-5.38	118.80	122.62
1	B	15	ASP	CA-C-O	-5.38	112.08	119.12
1	B	73	SER	CA-C-O	-5.35	115.49	121.81
1	A	3	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	556	PHE	CA-C-O	-5.33	113.84	119.97
1	B	381	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	299	LYS	N-CA-C	5.32	119.83	113.23
1	B	45	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	130	VAL	CA-C-O	-5.32	114.84	120.48
1	B	390	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	559	LEU	CA-C-O	5.29	126.38	120.82
1	B	201	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	B	216	SER	N-CA-C	5.28	116.72	111.07
1	B	390	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	A	153	ILE	N-CA-CB	5.23	118.62	111.41
1	A	337	ASN	CB-CG-ND2	5.22	124.24	116.40
1	A	113	SER	O-C-N	-5.20	115.67	122.59
1	A	66	VAL	CB-CA-C	5.20	117.01	111.35
1	B	559	LEU	CA-C-O	5.19	126.27	120.82
1	A	112	LYS	O-C-N	-5.18	116.15	122.11
1	A	425	VAL	CA-C-O	-5.17	115.69	121.17
1	A	214	SER	N-CA-C	5.12	117.76	111.82
1	B	458	GLY	N-CA-C	5.11	118.87	112.73
1	B	568	SER	N-CA-C	5.11	125.30	111.00
1	B	299	LYS	N-CA-C	5.09	119.77	113.50
1	B	113	SER	N-CA-C	-5.09	101.67	109.76
1	A	202	ASN	CA-CB-CG	-5.08	107.52	112.60
1	B	185	ILE	O-C-N	5.08	128.32	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	286	LYS	CB-CA-C	-5.08	102.85	111.02
1	B	504	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	258	VAL	CA-C-O	-5.07	115.48	120.85
1	B	488	ALA	CA-C-O	-5.07	115.27	121.05
1	A	534	GLU	O-C-N	-5.05	115.49	122.46
1	A	487	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	540	HIS	CA-CB-CG	-5.03	108.77	113.80
1	B	75	HIS	N-CA-C	5.00	119.08	112.92

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ALA	Peptide
1	B	101	ASP	Mainchain
1	B	175	ALA	Mainchain,Peptide

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	4187	0	4084	56	0
1	B	4204	0	4133	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	27	0
3	B	172	0	120	27	1
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
6	A	804	0	0	7	1
6	B	826	0	0	8	0
All	All	10489	0	8521	113	1

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 6.

All (113) 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:A:36:CYS:SG	3:A:802:HEM:CAB	2.45	1.05
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.46	1.04
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.47	1.02
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.53	0.96
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.53	0.96
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.53	0.95
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.54	0.95
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.55	0.95
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.56	0.94
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.56	0.94
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.56	0.94
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.56	0.93
1:A:14:CYS:HG	3:A:801:HEM:CAB	1.82	0.93
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.57	0.92
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.58	0.92
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.83	0.91
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.59	0.90
1:B:229:ASP:H	1:B:256:HIS:HE1	1.20	0.89
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.62	0.88
1:A:79:MET:HE3	1:A:96:LYS:HE3	1.57	0.86
1:A:204:ASN:HD22	1:A:204:ASN:H	1.21	0.86
1:A:229:ASP:H	1:A:256:HIS:HE1	1.22	0.85
1:B:79:MET:HE3	1:B:96:LYS:HE3	1.57	0.84
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.94	0.80
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.21	0.78
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.21	0.77
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.49	0.76
1:B:204:ASN:H	1:B:204:ASN:HD22	1.34	0.75
1:A:567:TYR:O	1:A:568:SER:HB2	1.86	0.74
1:B:169:ALA:HB1	6:B:2450:HOH:O	1.88	0.73
1:A:229:ASP:H	1:A:256:HIS:CE1	2.06	0.73
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.33	0.68
1:B:17:CYS:SG	3:B:801:HEM:HAC	2.33	0.68
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.32	0.68
1:B:229:ASP:H	1:B:256:HIS:CE1	2.09	0.66
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.35	0.66
1:A:204:ASN:H	1:A:204:ASN:ND2	1.94	0.65
1:B:431:LYS:HG2	6:B:2450:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.39	0.62
1:B:39:CYS:SG	3:B:802:HEM:HAC	2.37	0.62
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.83	0.60
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.39	0.60
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.41	0.59
1:B:71:CYS:HG	3:B:803:HEM:CAC	2.14	0.59
1:A:113:SER:HB2	6:A:2175:HOH:O	2.02	0.59
1:B:368:LEU:HB2	6:B:2235:HOH:O	2.01	0.58
1:A:17:CYS:SG	3:A:801:HEM:HAC	2.43	0.58
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.67	0.58
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.44	0.56
1:B:107:GLU:O	1:B:110:LYS:HG2	2.06	0.56
1:A:336:THR:HG22	1:A:368:LEU:HD11	1.87	0.56
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.87	0.55
1:A:336:THR:CG2	1:A:368:LEU:HD11	2.37	0.54
1:B:56:ASN:HD22	1:B:58:HIS:H	1.56	0.52
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.93	0.52
3:B:803:HEM:HMB1	3:B:803:HEM:HBB2	1.91	0.52
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.03	0.52
1:B:79:MET:HE3	1:B:96:LYS:CE	2.34	0.51
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.04	0.50
1:A:446:SER:OG	1:A:449:LYS:HD3	2.12	0.50
1:A:522:LYS:HD2	6:A:2318:HOH:O	2.12	0.49
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.95	0.49
1:B:13:GLU:HG3	6:B:2035:HOH:O	2.13	0.48
1:B:463:GLU:HG3	6:B:2589:HOH:O	2.12	0.48
1:A:183:LYS:O	1:A:184:LYS:HB2	2.14	0.48
1:B:56:ASN:ND2	1:B:58:HIS:H	2.12	0.47
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.01	0.47
1:B:467:ARG:NH1	1:B:467:ARG:HG2	2.30	0.47
1:B:85:CYS:SG	3:B:804:HEM:CBC	3.02	0.46
1:A:56:ASN:HD22	1:A:58:HIS:H	1.62	0.46
1:A:194:GLU:O	1:A:194:GLU:HG2	2.10	0.46
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.97	0.46
1:A:39:CYS:SG	3:A:802:HEM:CBC	3.04	0.46
1:B:68:CYS:SG	3:B:803:HEM:CBB	3.02	0.46
1:B:36:CYS:SG	3:B:802:HEM:CBB	3.03	0.46
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.09	0.46
1:B:565:ALA:O	1:B:568:SER:HA	2.16	0.45
3:A:804:HEM:HMB1	3:A:804:HEM:HBB2	1.98	0.45
1:A:26:ASN:HA	1:A:299:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.03	0.45
1:B:204:ASN:H	1:B:204:ASN:ND2	2.06	0.45
1:A:193:PHE:CD2	1:A:209:VAL:HG12	2.52	0.45
1:B:71:CYS:SG	3:B:803:HEM:C3C	3.10	0.45
1:B:201:GLN:HG2	6:B:2534:HOH:O	2.16	0.44
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.10	0.44
6:A:2467:HOH:O	1:B:329:SER:HB3	2.17	0.44
1:A:246:ARG:HB2	1:A:247:PRO:CD	2.48	0.43
1:B:23:GLU:HB3	6:B:2618:HOH:O	2.18	0.43
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.11	0.43
1:A:36:CYS:SG	3:A:802:HEM:CBB	3.03	0.43
1:A:56:ASN:ND2	1:A:58:HIS:H	2.17	0.43
1:A:311:LEU:HD23	1:A:349:ALA:HB2	1.99	0.43
1:A:60:SER:HB3	3:A:804:HEM:CMB	2.49	0.43
1:A:363:PHE:HB2	1:A:507:MET:SD	2.59	0.43
1:B:84:SER:HB3	1:B:98:TRP:CE2	2.53	0.43
1:B:365:HIS:O	1:B:501:PRO:HA	2.19	0.42
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.12	0.42
1:A:56:ASN:HD22	1:A:56:ASN:C	2.27	0.42
1:A:113:SER:HB3	6:A:1971:HOH:O	2.19	0.42
1:B:17:CYS:SG	3:B:801:HEM:C3C	3.12	0.42
1:B:511:MET:HE3	1:B:511:MET:HB2	1.85	0.42
1:B:357:LYS:HB3	1:B:511:MET:HE2	2.02	0.42
1:B:377:THR:HG21	6:B:2450:HOH:O	2.20	0.42
1:A:526:ILE:HA	1:A:527:PRO:HD3	1.94	0.41
4:A:1700:FAD:H4B	6:A:1706:HOH:O	2.19	0.41
1:A:448:VAL:HG23	6:A:1918:HOH:O	2.19	0.41
1:B:36:CYS:SG	3:B:802:HEM:C3B	3.13	0.41
1:A:36:CYS:SG	3:A:802:HEM:C3B	3.12	0.41
1:A:113:SER:HB2	1:A:114:GLU:H	1.55	0.41
1:A:256:HIS:HD2	6:A:2277:HOH:O	2.04	0.41
1:B:540:HIS:HE1	1:B:552:ASP:OD2	2.04	0.41
1:A:53:GLU:HG2	1:A:54:HIS:CE1	2.56	0.41
1:B:363:PHE:HB2	1:B:507:MET:SD	2.61	0.40

All (1) 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:B:802:HEM:CBC	6:A:2362:HOH:O[2_656]	2.08	0.12

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	566/571 (99%)	543 (96%)	21 (4%)	2 (0%)	30	27
1	B	566/571 (99%)	545 (96%)	20 (4%)	1 (0%)	43	42
All	All	1132/1142 (99%)	1088 (96%)	41 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	B	114	GLU
1	A	176	TRP

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 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	432/444 (97%)	415 (96%)	17 (4%)	28	28
1	B	438/444 (99%)	414 (94%)	24 (6%)	19	17
All	All	870/888 (98%)	829 (95%)	41 (5%)	23	22

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	91	ASN
1	A	113	SER

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Mol	Chain	Res	Type
1	A	144	SER
1	A	204	ASN
1	A	286	LYS
1	A	289	VAL
1	A	299	LYS
1	A	311	LEU
1	A	363	PHE
1	A	449	LYS
1	A	450	LEU
1	A	490	ASN
1	A	526	ILE
1	A	529	LEU
1	A	559	LEU
1	A	568	SER
1	B	15	ASP
1	B	21	ASP
1	B	36	CYS
1	B	56	ASN
1	B	99	LEU
1	B	110	LYS
1	B	112	LYS
1	B	113	SER
1	B	204	ASN
1	B	208	LEU
1	B	210	LYS
1	B	218	ASP
1	B	288	THR
1	B	337	ASN
1	B	363	PHE
1	B	368	LEU
1	B	390	ARG
1	B	450	LEU
1	B	467	ARG
1	B	473	SER
1	B	476	LYS
1	B	490	ASN
1	B	522	LYS
1	B	566	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	56	ASN
1	A	173	ASN
1	A	201	GLN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	275	ASN
1	A	389	ASN
1	A	412	GLN
1	A	490	ASN
1	A	540	HIS
1	B	10	GLN
1	B	12	GLN
1	B	54	HIS
1	B	56	ASN
1	B	116	GLN
1	B	201	GLN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	269	ASN
1	B	275	ASN
1	B	490	ASN
1	B	505	HIS
1	B	540	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
4	FAD	A	1700	-	58,58,58	1.45	8 (13%)	85,89,89	1.44	9 (10%)
5	FUM	B	1801	-	7,7,7	2.98	4 (57%)	8,8,8	1.74	2 (25%)
3	HEM	A	802	1	50,50,50	1.32	8 (16%)	67,82,82	1.27	9 (13%)
3	HEM	B	802	1	50,50,50	1.25	5 (10%)	67,82,82	1.29	9 (13%)
3	HEM	B	804	1	50,50,50	1.31	6 (12%)	67,82,82	1.04	4 (5%)
3	HEM	A	803	1	50,50,50	1.35	8 (16%)	67,82,82	1.03	2 (2%)
4	FAD	B	1800	-	58,58,58	1.58	11 (18%)	85,89,89	1.35	8 (9%)
5	FUM	A	1701	-	7,7,7	2.52	4 (57%)	8,8,8	1.96	3 (37%)
3	HEM	B	803	1	50,50,50	1.34	7 (14%)	67,82,82	1.26	7 (10%)
3	HEM	B	801	1	50,50,50	1.49	11 (22%)	67,82,82	1.09	4 (5%)
3	HEM	A	801	1	50,50,50	1.41	8 (16%)	67,82,82	1.21	9 (13%)
3	HEM	A	804	1	50,50,50	1.33	8 (16%)	67,82,82	0.91	1 (1%)

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
4	FAD	A	1700	-	-	7/34/50/50	0/6/6/6
5	FUM	B	1801	-	-	2/5/5/5	-
3	HEM	A	802	1	-	2/14/54/54	-
3	HEM	B	802	1	-	4/14/54/54	-
3	HEM	B	804	1	-	7/14/54/54	-
3	HEM	A	803	1	-	3/14/54/54	-
4	FAD	B	1800	-	-	7/34/50/50	0/6/6/6
5	FUM	A	1701	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	803	1	-	3/14/54/54	-
3	HEM	B	801	1	-	2/14/54/54	-
3	HEM	A	801	1	-	5/14/54/54	-
3	HEM	A	804	1	-	5/14/54/54	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1801	FUM	O-C	5.20	1.35	1.23
4	A	1700	FAD	C2'-C3'	5.03	1.62	1.53
5	A	1701	FUM	O-C	4.38	1.33	1.23
4	B	1800	FAD	C9-C8	4.28	1.45	1.39
5	B	1801	FUM	O7-C6	4.13	1.33	1.23
4	B	1800	FAD	C2'-C3'	3.91	1.60	1.53
4	A	1700	FAD	C6-C5X	3.66	1.45	1.40
4	B	1800	FAD	C6-C5X	3.38	1.45	1.40
4	B	1800	FAD	C5'-C4'	3.33	1.56	1.51
5	B	1801	FUM	OXT-C	-3.32	1.21	1.30
5	A	1701	FUM	O7-C6	3.22	1.30	1.23
3	B	802	HEM	CAC-C3C	3.19	1.55	1.47
3	B	804	HEM	CAC-C3C	3.19	1.55	1.47
3	B	801	HEM	CAB-C3B	3.18	1.55	1.47
3	B	801	HEM	CMC-C2C	3.11	1.57	1.50
4	B	1800	FAD	O4'-C4'	3.10	1.49	1.43
3	B	803	HEM	CAB-C3B	3.06	1.55	1.47
3	A	801	HEM	FE-ND	3.06	2.04	1.94
3	B	804	HEM	FE-NB	3.01	2.04	1.94
3	A	802	HEM	CAC-C3C	2.98	1.55	1.47
3	A	803	HEM	CAB-C3B	2.97	1.55	1.47
5	A	1701	FUM	O8-C6	-2.91	1.23	1.30
3	A	804	HEM	CAB-C3B	2.87	1.55	1.47
4	B	1800	FAD	C1'-N10	2.85	1.54	1.47
3	B	802	HEM	CMA-C3A	2.83	1.56	1.50
3	A	804	HEM	CAC-C3C	2.81	1.54	1.47
3	A	801	HEM	CAB-C3B	2.77	1.54	1.47
4	A	1700	FAD	C9-C8	2.73	1.43	1.39
3	A	802	HEM	CMD-C2D	2.72	1.56	1.50
3	B	801	HEM	FE-ND	2.71	2.03	1.94
3	A	802	HEM	FE-ND	2.69	2.03	1.94
3	B	802	HEM	CAB-C3B	2.69	1.54	1.47
3	B	801	HEM	CMA-C3A	2.68	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	CMD-C2D	2.66	1.56	1.50
3	A	801	HEM	CAC-C3C	2.65	1.54	1.47
3	B	804	HEM	CAB-C3B	2.65	1.54	1.47
3	A	803	HEM	CAC-C3C	2.64	1.54	1.47
3	A	803	HEM	CMB-C2B	2.64	1.56	1.50
3	B	803	HEM	CMB-C2B	2.63	1.56	1.50
3	A	804	HEM	CMB-C2B	2.63	1.56	1.50
4	B	1800	FAD	PA-O3P	2.62	1.62	1.59
4	B	1800	FAD	O4-C4	-2.60	1.18	1.23
5	B	1801	FUM	O8-C6	-2.59	1.23	1.30
3	B	801	HEM	CAC-C3C	2.59	1.54	1.47
3	A	801	HEM	FE-NB	2.58	2.02	1.94
3	A	801	HEM	CMA-C3A	2.58	1.56	1.50
3	A	803	HEM	CMD-C2D	2.55	1.56	1.50
3	A	803	HEM	FE-NA	2.53	2.03	1.95
4	A	1700	FAD	C9-C9A	2.53	1.43	1.39
3	B	801	HEM	FE-NC	2.51	2.03	1.95
3	B	801	HEM	CMB-C2B	2.50	1.55	1.50
3	A	803	HEM	FE-NC	2.50	2.03	1.95
3	A	803	HEM	CMA-C3A	2.46	1.55	1.50
4	A	1700	FAD	C8M-C8	2.43	1.55	1.51
5	A	1701	FUM	OXT-C	-2.43	1.24	1.30
3	B	803	HEM	CAC-C3C	2.38	1.53	1.47
4	B	1800	FAD	C4-N3	2.38	1.43	1.38
4	A	1700	FAD	C1'-C2'	-2.38	1.49	1.52
3	B	803	HEM	C2A-C3A	-2.37	1.32	1.38
3	A	804	HEM	FE-NB	2.37	2.02	1.94
3	B	803	HEM	CMD-C2D	2.36	1.55	1.50
4	B	1800	FAD	C9-C9A	2.35	1.43	1.39
3	A	802	HEM	CMA-C3A	2.34	1.55	1.50
3	B	803	HEM	C3B-C2B	-2.33	1.32	1.37
4	A	1700	FAD	O4-C4	-2.30	1.19	1.23
3	B	802	HEM	CMD-C2D	2.28	1.55	1.50
3	A	802	HEM	CMC-C2C	2.27	1.55	1.50
3	B	803	HEM	CMA-C3A	2.26	1.55	1.50
3	A	801	HEM	C2A-C3A	-2.26	1.33	1.38
3	A	804	HEM	CMD-C2D	2.26	1.55	1.50
3	B	801	HEM	CMD-C2D	2.26	1.55	1.50
3	A	804	HEM	FE-ND	2.24	2.01	1.94
4	B	1800	FAD	C9A-N10	-2.24	1.37	1.41
3	A	802	HEM	CAB-C3B	2.24	1.53	1.47
4	A	1700	FAD	C1'-N10	2.22	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEM	FE-NA	2.18	2.02	1.95
3	A	801	HEM	CMC-C2C	2.18	1.55	1.50
3	B	801	HEM	C3C-C2C	-2.17	1.32	1.37
3	A	804	HEM	CMA-C3A	2.17	1.55	1.50
3	B	801	HEM	C2A-C3A	-2.16	1.33	1.38
3	A	803	HEM	C2A-C3A	-2.15	1.33	1.38
3	B	802	HEM	FE-ND	2.13	2.01	1.94
3	B	801	HEM	FE-NB	2.08	2.01	1.94
3	B	804	HEM	CMA-C3A	2.08	1.55	1.50
3	B	804	HEM	FE-ND	2.08	2.01	1.94
3	A	804	HEM	CAA-C2A	2.03	1.56	1.51
3	B	804	HEM	FE-NA	2.02	2.01	1.95
3	A	802	HEM	CAA-C2A	2.02	1.56	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1800	FAD	O4'-C4'-C3'	-5.32	96.80	109.25
4	A	1700	FAD	O5'-C5'-C4'	-5.31	95.19	109.36
4	B	1800	FAD	O5'-C5'-C4'	-5.01	95.98	109.36
4	A	1700	FAD	O4'-C4'-C3'	-4.35	99.06	109.25
3	B	803	HEM	CAD-CBD-CGD	4.24	124.90	113.67
4	A	1700	FAD	O4B-C1B-C2B	-3.83	98.42	106.62
4	B	1800	FAD	O2'-C2'-C3'	-3.68	100.62	109.25
4	A	1700	FAD	O3'-C3'-C2'	-3.57	100.81	108.93
5	A	1701	FUM	O-C-C4	-3.34	110.84	121.06
3	A	802	HEM	CAA-CBA-CGA	3.26	122.31	113.67
3	B	801	HEM	O2D-CGD-CBD	3.14	123.92	114.00
3	B	802	HEM	CBD-CAD-C3D	3.11	121.14	112.53
3	A	802	HEM	O1D-CGD-CBD	-2.97	113.68	123.09
3	B	803	HEM	O2A-CGA-O1A	2.97	130.97	123.33
3	B	803	HEM	CHD-C4C-NC	2.97	127.69	124.45
3	B	804	HEM	O1D-CGD-CBD	-2.90	113.91	123.09
4	B	1800	FAD	O2-C2-N3	-2.86	113.09	118.58
4	A	1700	FAD	C5'-C4'-C3'	2.82	117.55	112.22
3	B	802	HEM	C3B-C4B-NB	-2.82	107.44	109.47
5	B	1801	FUM	OXT-C-C4	2.81	126.47	116.16
4	B	1800	FAD	O4B-C1B-C2B	-2.75	100.74	106.62
3	B	802	HEM	C1B-NB-C4B	2.72	108.43	105.21
3	A	801	HEM	CAA-CBA-CGA	2.72	120.88	113.67
3	B	801	HEM	CHC-C4B-NB	2.67	127.30	124.42
3	B	803	HEM	C3B-C2B-C1B	2.61	108.37	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	HEM	CMD-C2D-C1D	-2.54	121.06	125.03
3	B	802	HEM	CHC-C1C-NC	-2.54	121.68	124.45
4	A	1700	FAD	O2'-C2'-C3'	-2.51	103.37	109.25
3	A	802	HEM	O2D-CGD-CBD	2.50	121.90	114.00
3	B	801	HEM	CAA-CBA-CGA	2.50	120.29	113.67
3	A	802	HEM	CHC-C1C-NC	-2.47	121.76	124.45
4	B	1800	FAD	O2A-PA-O1A	2.45	123.83	112.44
3	A	802	HEM	C1B-NB-C4B	2.42	108.08	105.21
4	A	1700	FAD	O2A-PA-O1A	2.41	123.67	112.44
3	B	802	HEM	CAC-C3C-C4C	-2.39	119.11	124.82
3	B	803	HEM	CAA-C2A-C1A	-2.36	120.34	124.94
3	A	803	HEM	CAD-CBD-CGD	2.32	119.82	113.67
3	B	804	HEM	CMB-C2B-C1B	-2.31	121.42	125.03
3	B	803	HEM	O1A-CGA-CBA	-2.31	115.78	123.09
3	A	803	HEM	O2A-CGA-O1A	2.29	129.23	123.33
4	B	1800	FAD	C4-N3-C2	-2.28	121.59	125.64
3	B	801	HEM	O2D-CGD-O1D	-2.28	117.47	123.33
3	A	804	HEM	CMD-C2D-C1D	-2.26	121.51	125.03
3	B	803	HEM	C2A-C1A-NA	-2.25	107.65	110.15
3	A	801	HEM	C3B-C2B-C1B	2.25	108.10	106.41
5	A	1701	FUM	C4-C5-C6	-2.22	115.76	127.05
5	B	1801	FUM	O-C-C4	-2.22	114.27	121.06
3	B	802	HEM	CMB-C2B-C1B	-2.17	121.64	125.03
3	B	804	HEM	CBD-CAD-C3D	2.15	118.48	112.53
3	B	802	HEM	O2D-CGD-CBD	2.15	120.78	114.00
3	A	802	HEM	C3B-C2B-C1B	2.15	108.02	106.41
3	A	801	HEM	O1A-CGA-CBA	-2.14	116.32	123.09
3	B	802	HEM	CHC-C1C-C2C	2.12	129.90	125.49
3	A	801	HEM	O2A-CGA-CBA	2.12	120.68	114.00
3	A	801	HEM	C1B-NB-C4B	2.12	107.71	105.21
4	A	1700	FAD	O4B-C1B-N9A	-2.11	104.03	108.09
3	A	801	HEM	CMB-C2B-C1B	-2.10	121.75	125.03
3	B	804	HEM	O2D-CGD-CBD	2.10	120.63	114.00
4	B	1800	FAD	C4-C4X-N5	2.10	121.10	118.21
3	A	802	HEM	C2B-C1B-NB	-2.08	107.45	109.84
3	A	801	HEM	C3B-C4B-NB	-2.06	107.99	109.47
3	A	802	HEM	C4D-ND-C1D	2.05	107.63	105.21
3	B	802	HEM	CBC-CAC-C3C	-2.04	117.32	127.53
5	A	1701	FUM	OXT-C-C4	2.04	123.65	116.16
4	A	1700	FAD	N3-C2-N1	2.02	123.79	119.50
3	A	801	HEM	CHA-C4D-ND	-2.01	121.88	124.37
3	A	801	HEM	CAD-CBD-CGD	2.01	118.99	113.67

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1800	FAD	C2'-C3'-C4'-O4'
4	B	1800	FAD	O3'-C3'-C4'-O4'
4	B	1800	FAD	PA-O3P-P-O5'
5	A	1701	FUM	OXT-C-C4-C5
5	A	1701	FUM	O-C-C4-C5
5	B	1801	FUM	OXT-C-C4-C5
5	B	1801	FUM	O-C-C4-C5
3	B	802	HEM	C3D-CAD-CBD-CGD
4	A	1700	FAD	C2'-C3'-C4'-O4'
4	A	1700	FAD	C2'-C3'-C4'-C5'
4	B	1800	FAD	C2'-C3'-C4'-C5'
4	B	1800	FAD	O3'-C3'-C4'-C5'
3	A	803	HEM	C2A-CAA-CBA-CGA
4	B	1800	FAD	P-O3P-PA-O1A
3	A	801	HEM	C3D-CAD-CBD-CGD
4	A	1700	FAD	PA-O3P-P-O5'
4	A	1700	FAD	P-O3P-PA-O1A
4	B	1800	FAD	P-O3P-PA-O2A
3	B	803	HEM	C3D-CAD-CBD-CGD
4	A	1700	FAD	P-O3P-PA-O2A
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAD-CBD-CGD-O1D
3	B	801	HEM	CAD-CBD-CGD-O1D
3	B	804	HEM	CAA-CBA-CGA-O2A
3	A	804	HEM	CAA-CBA-CGA-O2A
3	B	804	HEM	CAA-CBA-CGA-O1A
3	A	802	HEM	CAD-CBD-CGD-O2D
3	B	801	HEM	CAD-CBD-CGD-O2D
3	A	801	HEM	CAD-CBD-CGD-O2D
3	B	802	HEM	CAD-CBD-CGD-O1D
3	B	804	HEM	C2B-C3B-CAB-CBB
3	B	803	HEM	CAA-CBA-CGA-O2A
3	A	802	HEM	CAD-CBD-CGD-O1D
3	B	802	HEM	CAD-CBD-CGD-O2D
3	A	801	HEM	C4B-C3B-CAB-CBB
3	B	804	HEM	C4B-C3B-CAB-CBB
3	A	803	HEM	CAA-CBA-CGA-O2A
3	B	804	HEM	C2A-CAA-CBA-CGA
4	A	1700	FAD	O3'-C3'-C4'-C5'
3	A	804	HEM	CAD-CBD-CGD-O2D

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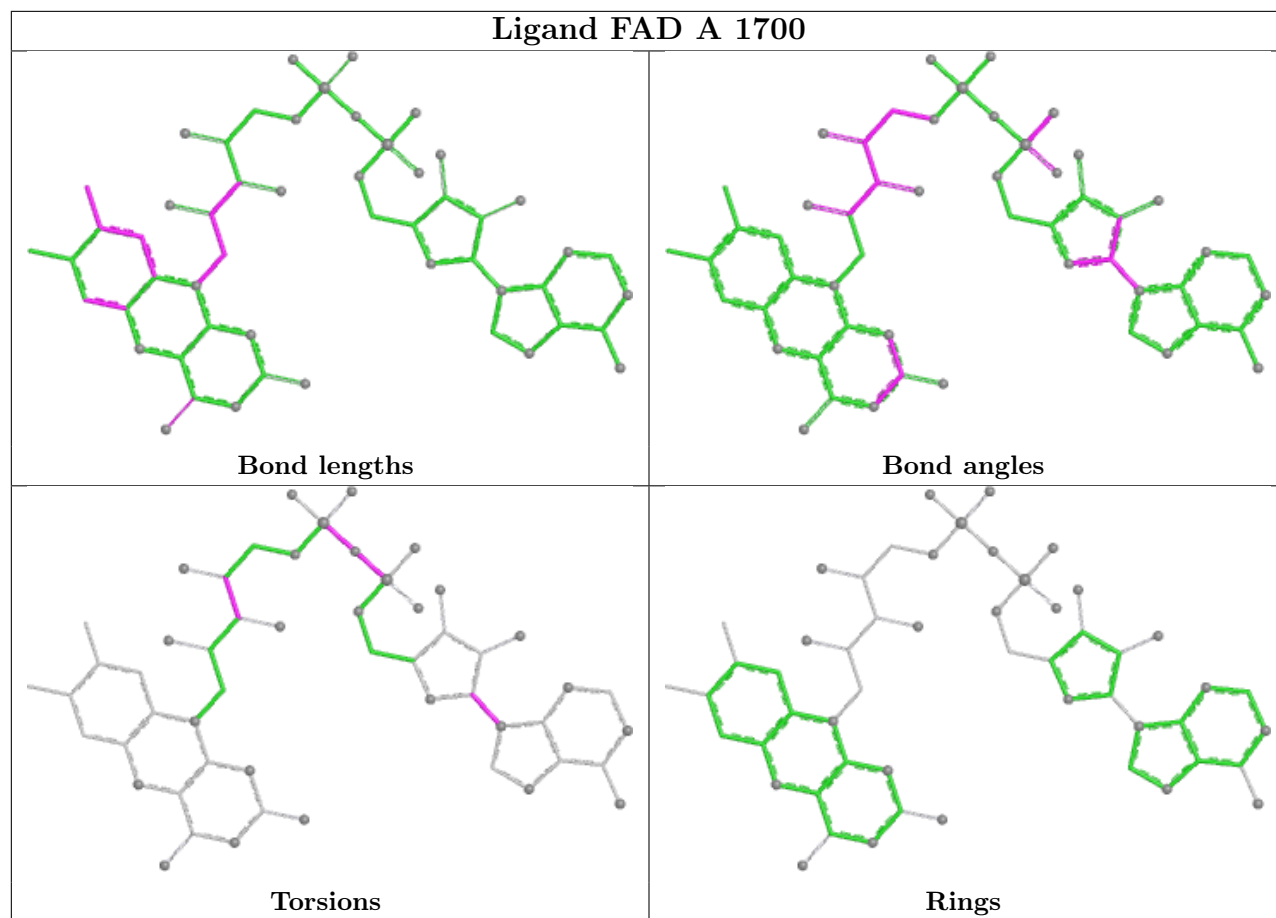
Mol	Chain	Res	Type	Atoms
3	A	804	HEM	C2A-CAA-CBA-CGA
3	A	803	HEM	CAA-CBA-CGA-O1A
3	B	804	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAD-CBD-CGD-O1D
3	B	803	HEM	CAA-CBA-CGA-O1A
4	A	1700	FAD	C2B-C1B-N9A-C8A
3	B	804	HEM	CAD-CBD-CGD-O2D
3	A	801	HEM	C2B-C3B-CAB-CBB
3	B	802	HEM	CAA-CBA-CGA-O2A

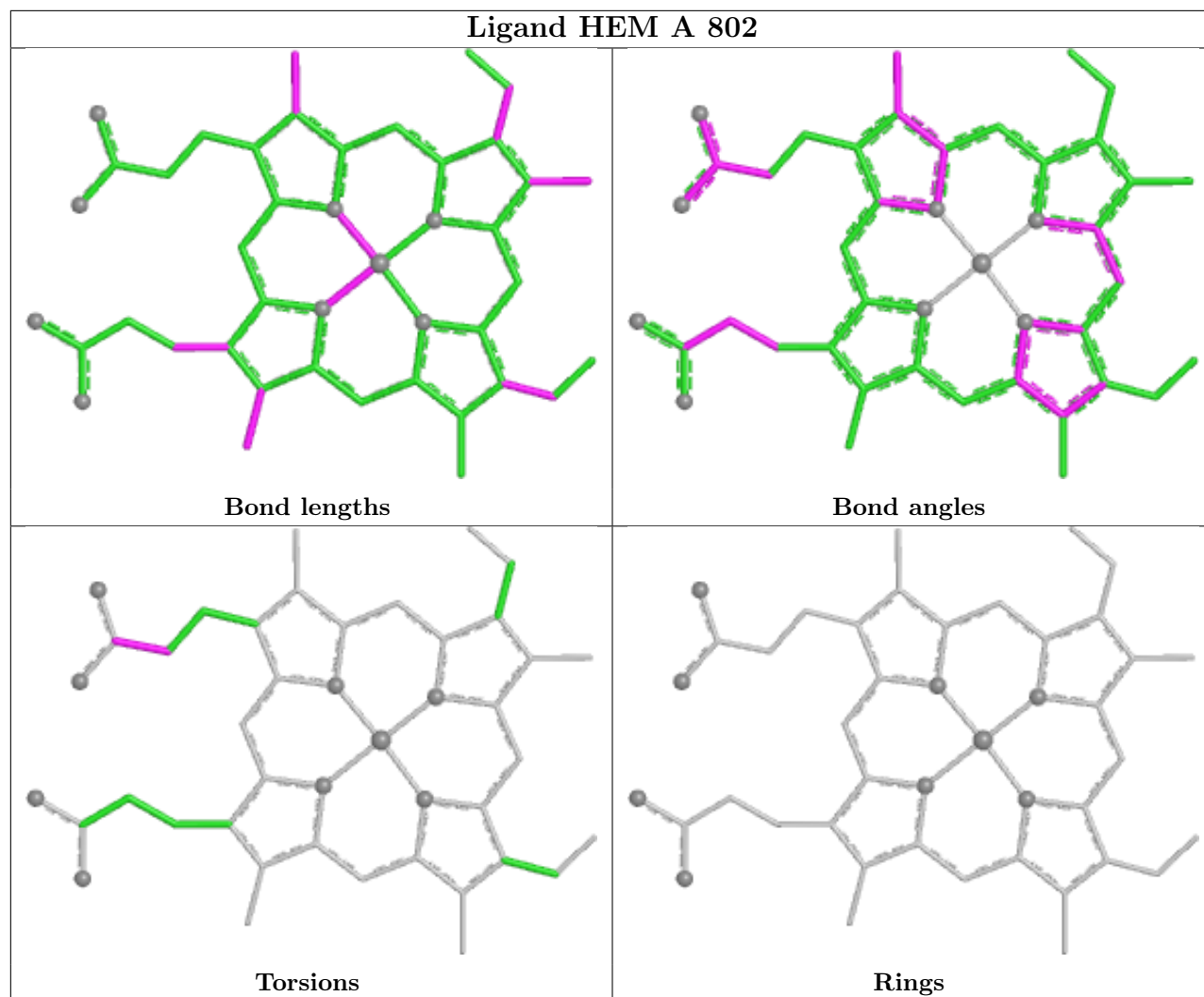
There are no ring outliers.

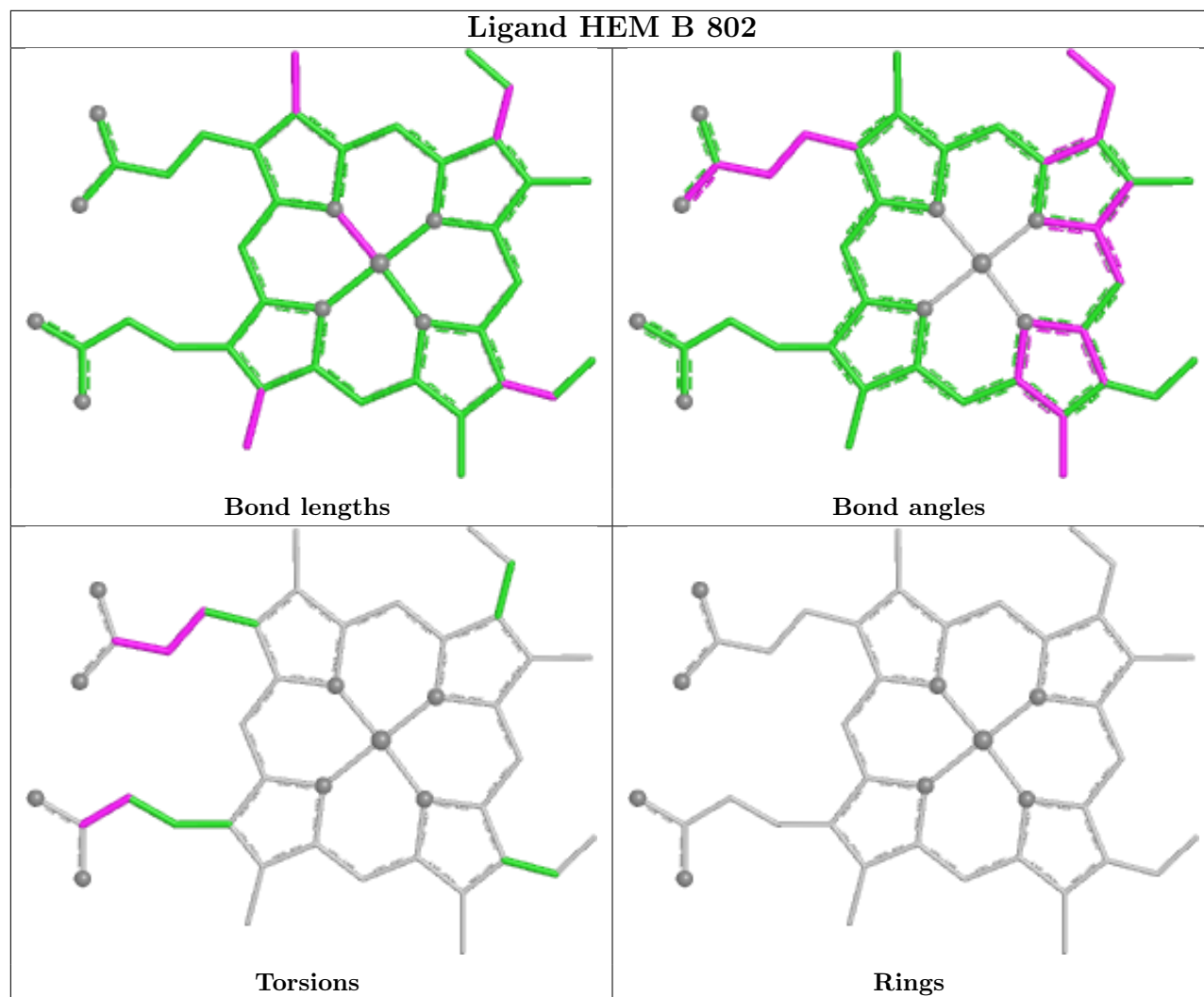
9 monomers are involved in 56 short contacts:

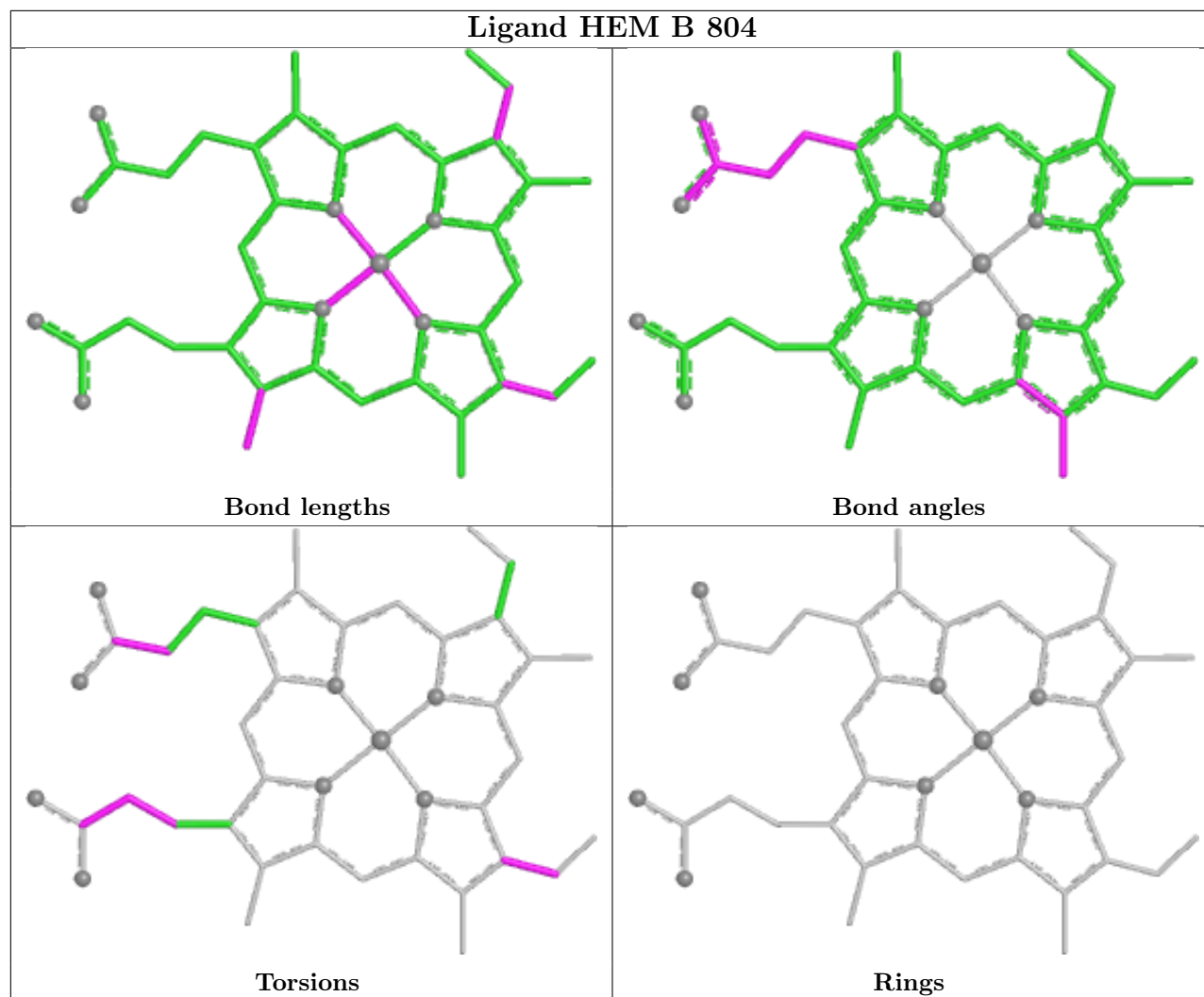
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1700	FAD	1	0
3	A	802	HEM	7	0
3	B	802	HEM	7	1
3	B	804	HEM	7	0
3	A	803	HEM	5	0
3	B	803	HEM	8	0
3	B	801	HEM	5	0
3	A	801	HEM	6	0
3	A	804	HEM	9	0

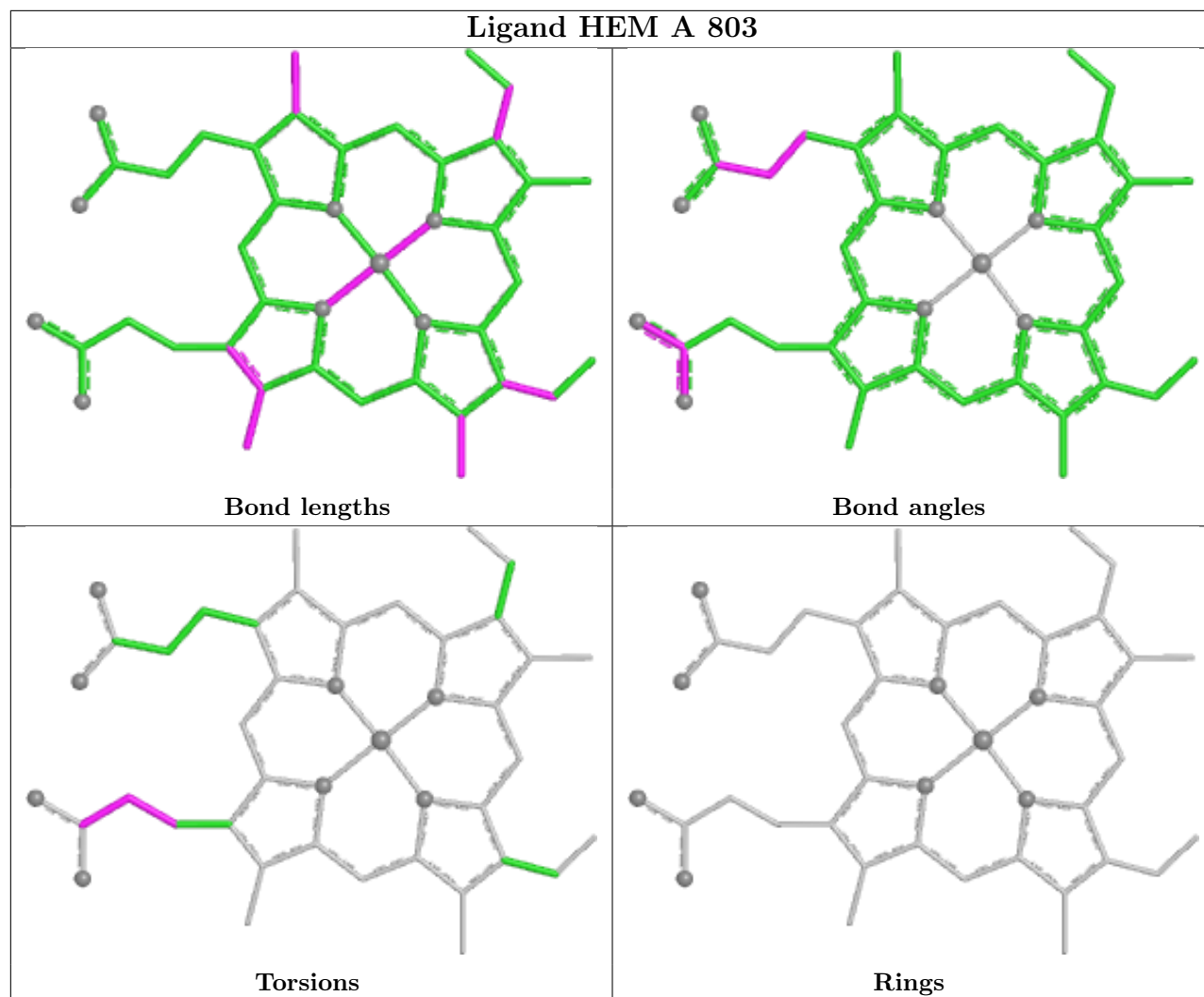
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

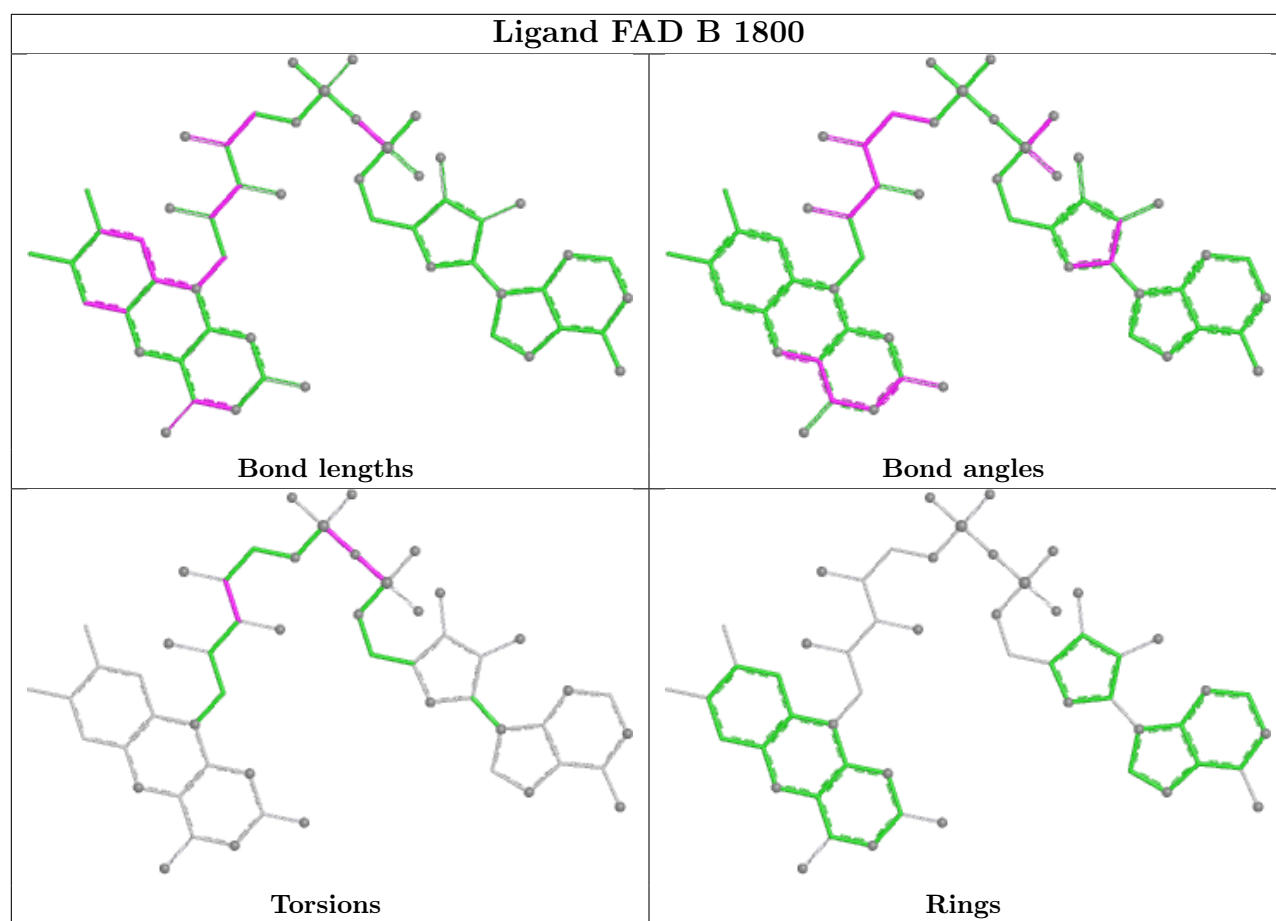


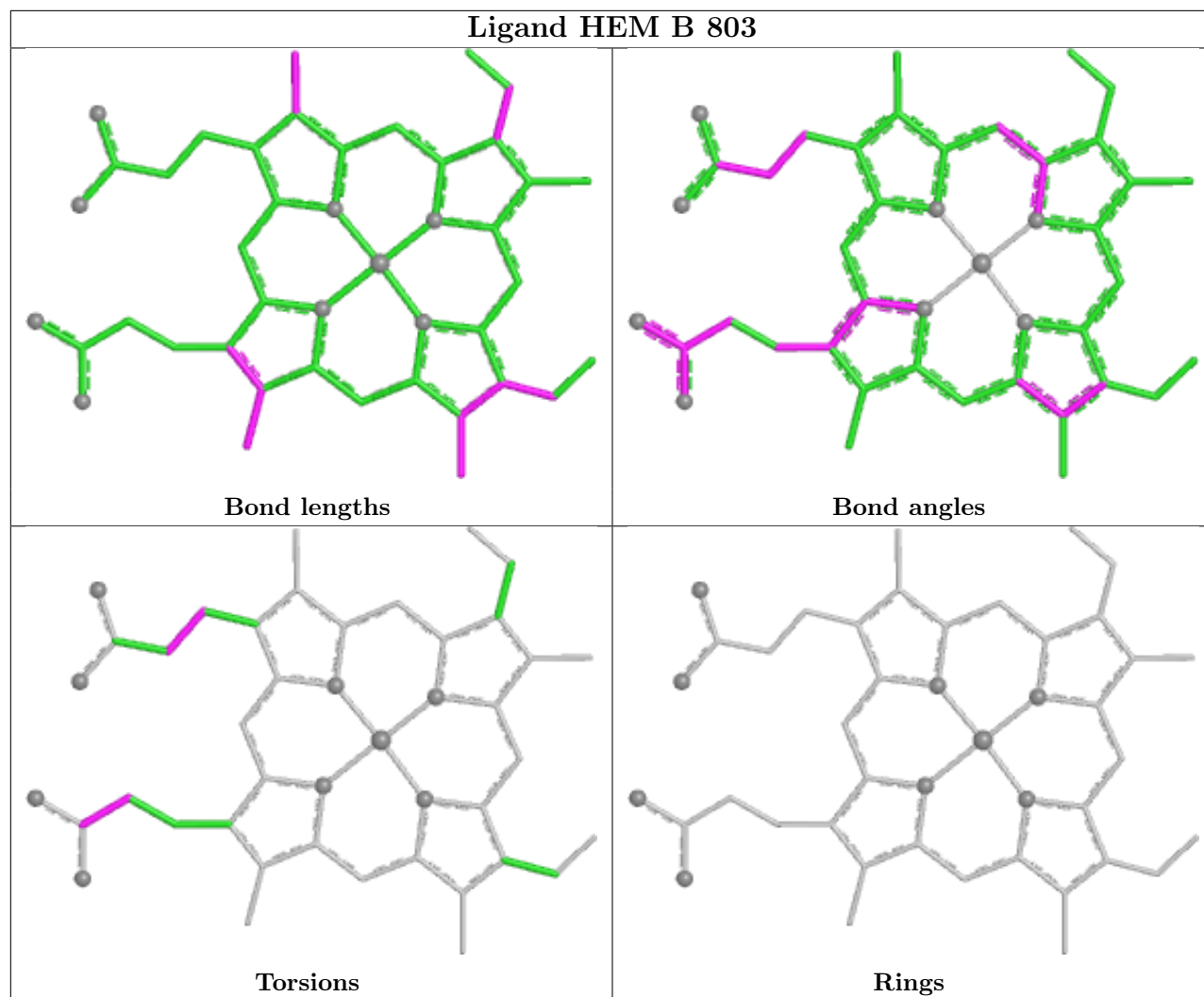


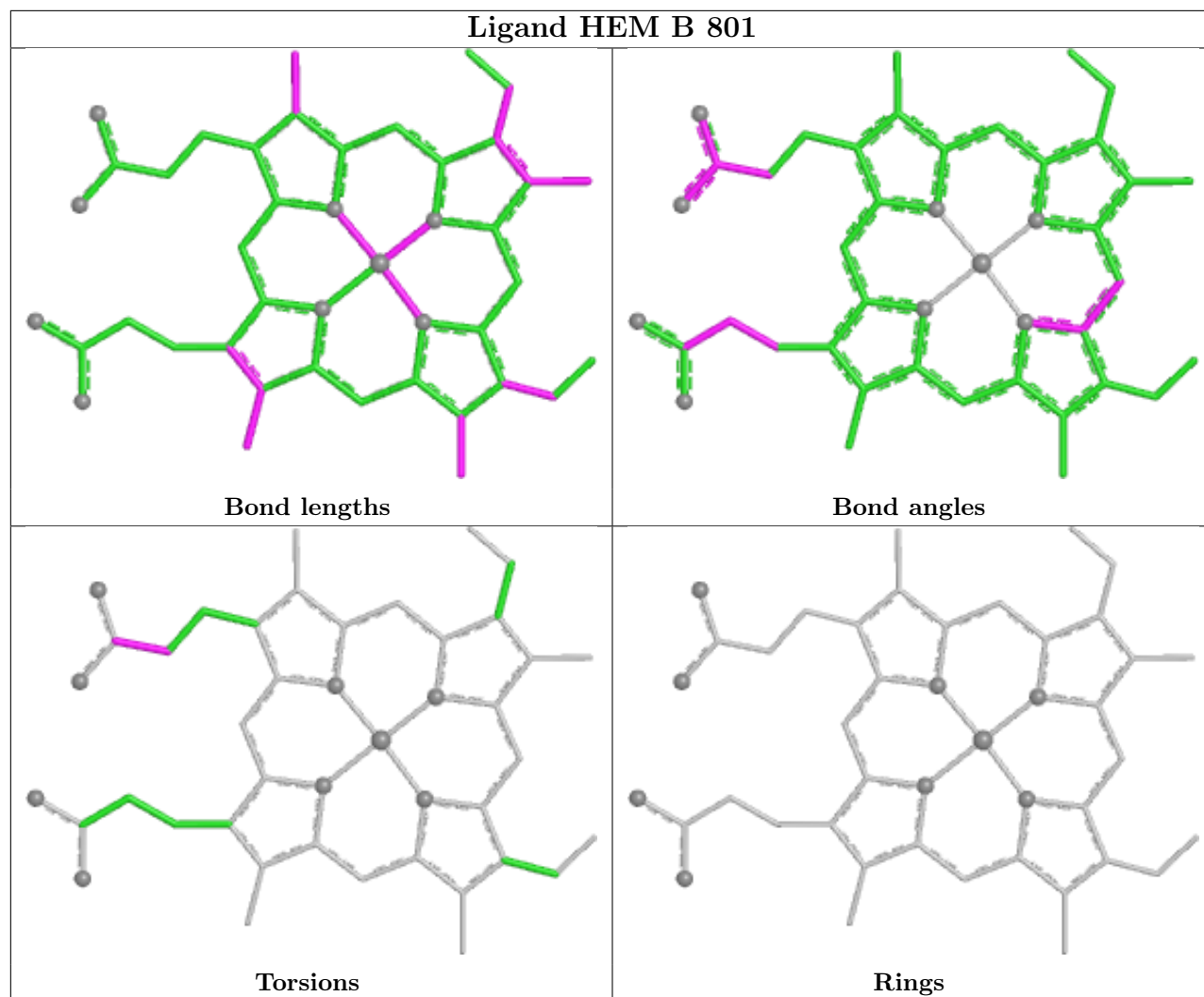


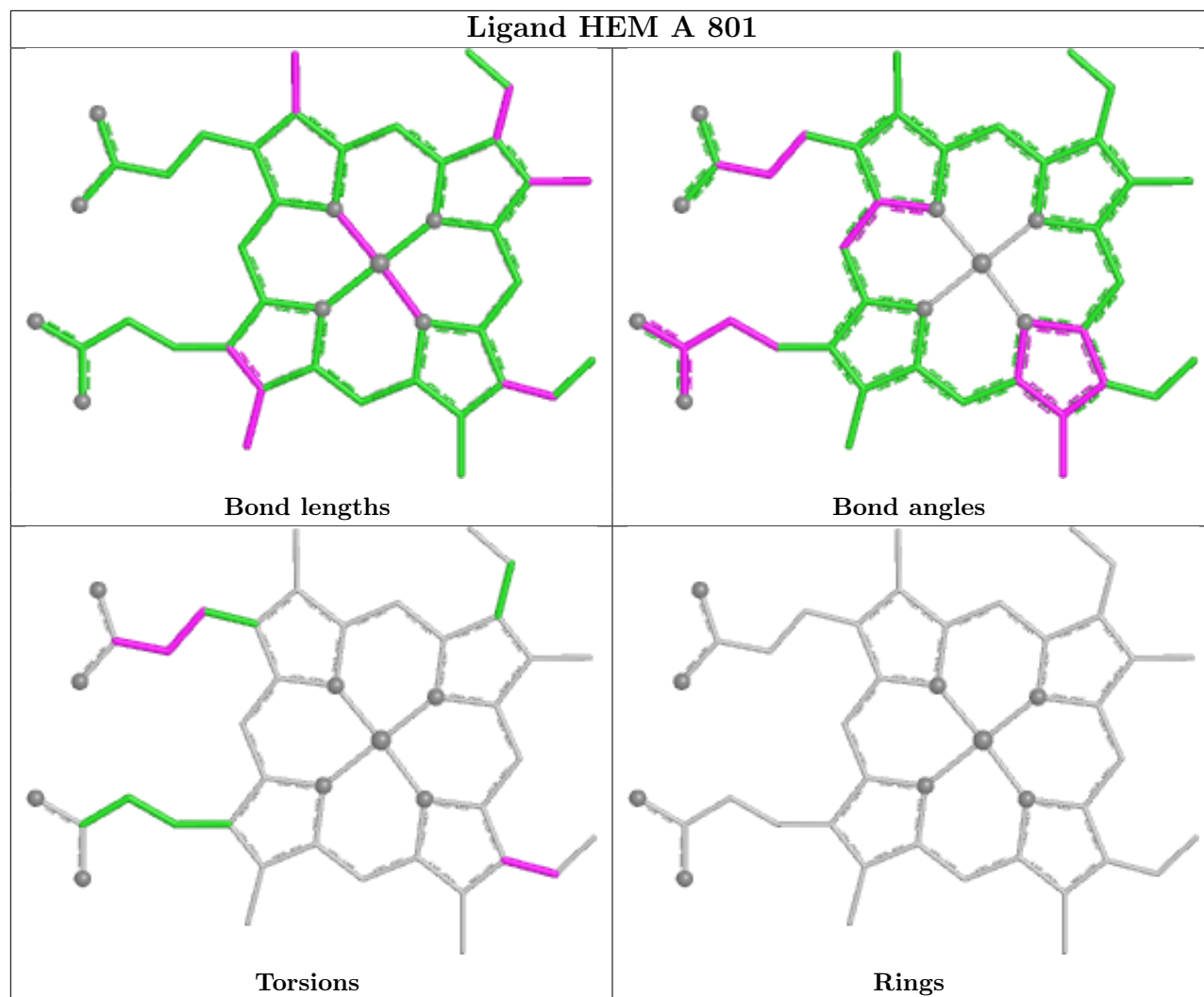


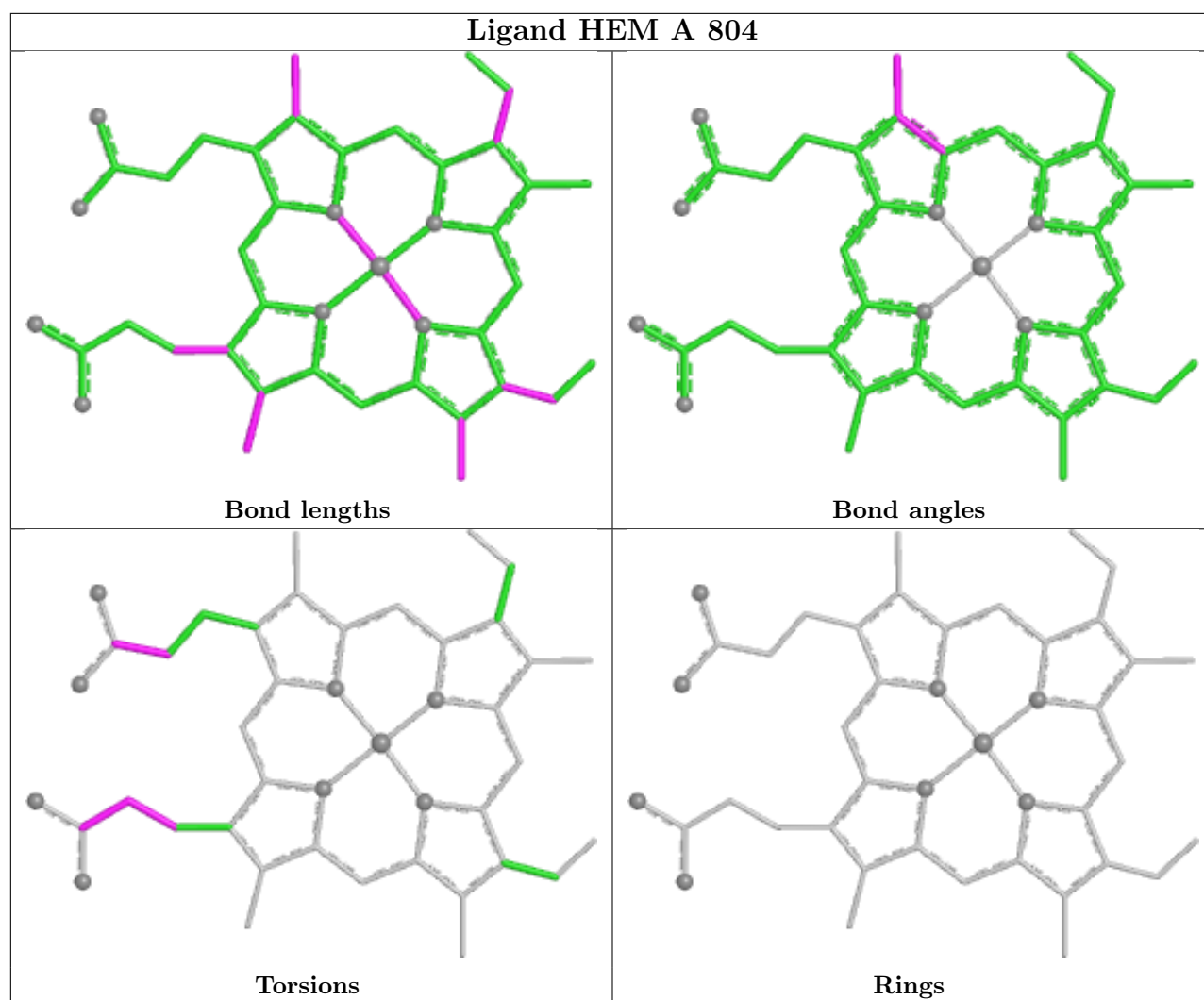












5.7 Other polymers [i](#)

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.