



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 10:02 PM EST

PDB ID : 1KSU
Title : Crystal Structure of His505Tyr Mutant Flavocytochrome c3 from *Shewanella frigidimarina*
Authors : Pankhurst, K.L.; Mowat, C.G.; Miles, C.S.; Leys, D.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2002-01-14
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

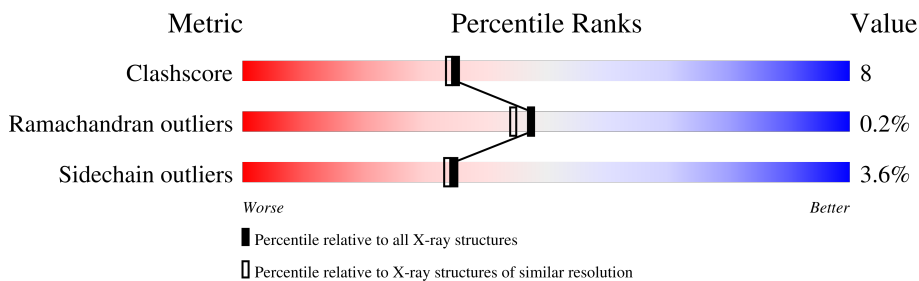
1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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	
1	B	571	

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
4	FAD	A	2805	X	-	-	-
4	FAD	B	3805	X	-	-	-
5	FUM	A	2806	-	X	-	-
5	FUM	B	3806	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10753 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 c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4202	2608	738	831	25	0	0	0
1	B	568	4216	2617	742	832	25	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	TYR	HIS	engineered mutation	UNP Q02469
B	505	TYR	HIS	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: 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 (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



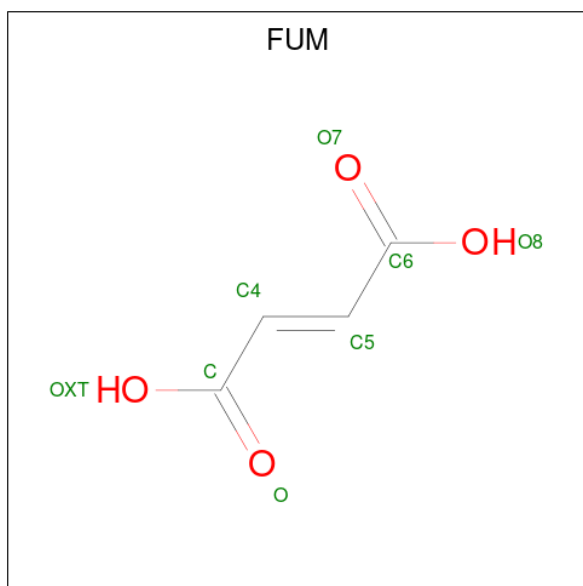
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is FUMARIC ACID (three-letter code: 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.

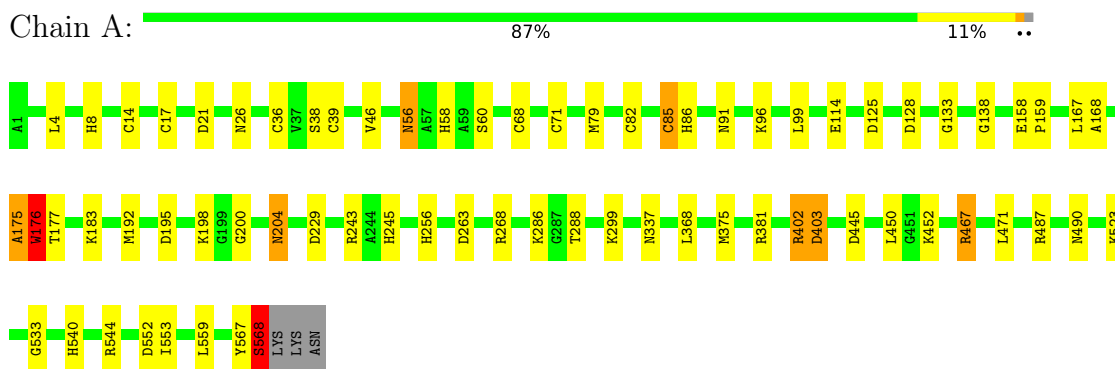
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	932	Total 932	O 932	0	0
6	B	935	Total 935	O 935	0	0

3 Residue-property plots [i](#)

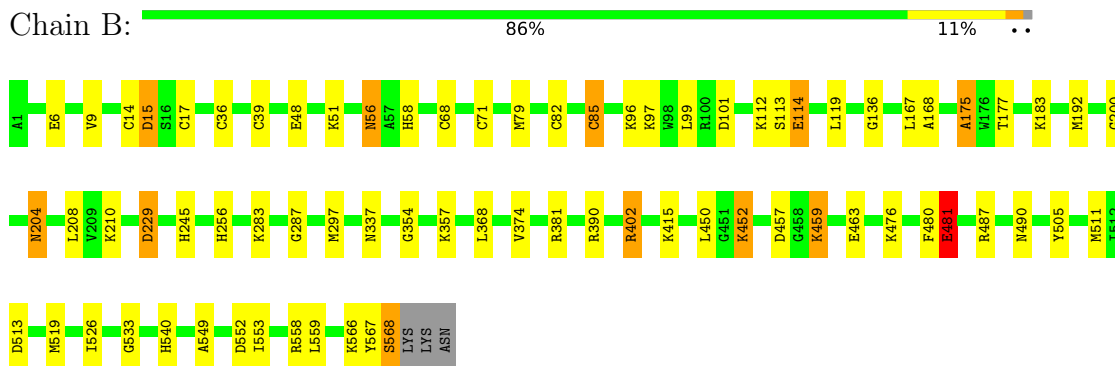
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 c



- Molecule 1: flavocytochrome c



4 Data and refinement statistics

Xtrriage (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	76.99Å 87.27Å 89.37Å 90.00° 104.43° 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}	0.167 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FUM, FAD, NA

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	0.60	1/4272 (0.0%)	1.29	24/5779 (0.4%)
1	B	0.58	0/4286	1.26	21/5794 (0.4%)
All	All	0.59	1/8558 (0.0%)	1.28	45/11573 (0.4%)

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	2
1	B	0	2
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	-5.74	1.34	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	18.36	167.60	121.70
1	A	467	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	B	175	ALA	O-C-N	-11.50	104.30	122.70
1	A	487	ARG	NE-CZ-NH2	11.50	126.05	120.30
1	A	381	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	487	ARG	NE-CZ-NH1	-10.65	114.97	120.30
1	B	390	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	B	481	GLU	OE1-CD-OE2	-10.48	110.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	B	402	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	B	558	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	B	390	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	15	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	A	381	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	176	TRP	N-CA-CB	7.74	124.54	110.60
1	A	567	TYR	C-N-CA	7.31	139.98	121.70
1	A	402	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	263	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	B	402	ARG	NH1-CZ-NH2	6.64	126.70	119.40
1	A	445	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	175	ALA	N-CA-CB	6.39	119.05	110.10
1	B	101	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	B	558	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	229	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	15	ASP	N-CA-CB	5.69	120.84	110.60
1	A	375	MET	CG-SD-CE	-5.63	91.19	100.20
1	B	487	ARG	CG-CD-NE	-5.61	100.01	111.80
1	A	243	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	175	ALA	CA-C-N	5.55	129.41	117.20
1	A	21	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	487	ARG	CG-CD-NE	-5.49	100.27	111.80
1	A	85	CYS	CA-CB-SG	-5.38	104.32	114.00
1	A	195	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	125	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	268	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	487	ARG	CB-CA-C	-5.21	99.97	110.40
1	B	114	GLU	N-CA-CB	5.08	119.74	110.60
1	B	15	ASP	OD1-CG-OD2	5.07	132.93	123.30
1	A	403	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	268	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	85	CYS	CA-CB-SG	-5.05	104.91	114.00
1	B	452	LYS	N-CA-CB	5.03	119.65	110.60
1	B	381	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	568	SER	N-CA-C	5.02	124.55	111.00
1	B	175	ALA	N-CA-CB	5.00	117.10	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	175	ALA	Peptide
1	B	175	ALA	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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	4202	0	4124	61	0
1	B	4216	0	4160	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	28	0
3	B	172	0	120	32	0
4	A	53	0	30	5	0
4	B	53	0	30	6	0
5	A	8	0	1	3	0
5	B	8	0	1	1	0
6	A	932	0	0	8	0
6	B	935	0	0	18	0
All	All	10753	0	8586	143	0

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 8.

All (143) 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	2.44	1.04
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.44	1.04
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.48	1.02
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.51	0.99
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.77	0.97
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.53	0.96
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.54	0.96
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.55	0.95
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.54	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.57	0.93
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.56	0.93
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.57	0.92
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.58	0.92
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.58	0.91
1:A:229:ASP:H	1:A:256:HIS:HE1	1.18	0.91
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.59	0.91
1:B:229:ASP:H	1:B:256:HIS:HE1	1.18	0.89
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.60	0.88
1:B:71:CYS:HG	3:B:803:HEM:CAC	1.89	0.84
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.91	0.83
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.67	0.83
1:B:287:GLY:HA2	6:B:3981:HOH:O	1.81	0.80
1:B:204:ASN:H	1:B:204:ASN:HD22	1.28	0.79
1:B:229:ASP:H	1:B:256:HIS:CE1	1.99	0.79
1:A:229:ASP:H	1:A:256:HIS:CE1	2.01	0.78
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.25	0.76
1:A:402:ARG:HH22	5:A:2806:FUM:C5	1.99	0.75
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.26	0.74
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.51	0.73
1:B:567:TYR:O	1:B:568:SER:HB2	1.87	0.73
1:B:402:ARG:HH22	5:B:3806:FUM:C5	2.03	0.71
1:B:368:LEU:HB2	6:B:4282:HOH:O	1.91	0.70
1:A:204:ASN:HD22	1:A:204:ASN:H	1.38	0.70
1:A:368:LEU:HB2	6:A:3127:HOH:O	1.92	0.69
1:B:48:GLU:HG3	6:B:4302:HOH:O	1.95	0.67
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.37	0.63
1:B:183:LYS:HE2	6:B:4006:HOH:O	2.01	0.60
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.66	0.60
1:A:168:ALA:HA	4:A:2805:FAD:N5	2.16	0.60
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.84	0.59
1:B:526:ILE:HD11	6:B:4396:HOH:O	2.01	0.59
1:A:168:ALA:HA	4:A:2805:FAD:C5X	2.33	0.59
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.41	0.58
1:A:167:LEU:HB3	4:A:2805:FAD:HM72	1.85	0.57
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.87	0.56
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.41	0.56
1:B:526:ILE:CD1	6:B:4396:HOH:O	2.55	0.55
1:B:457:ASP:OD1	1:B:459:LYS:HG3	2.07	0.55
1:B:568:SER:HA	6:B:4220:HOH:O	2.06	0.55
1:A:114:GLU:HB2	6:A:3045:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:HG2	6:B:4067:HOH:O	2.06	0.55
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.00	0.54
1:B:71:CYS:SG	3:B:803:HEM:C3C	3.01	0.54
1:B:452:LYS:HD2	6:B:4622:HOH:O	2.07	0.53
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.89	0.53
1:A:82:CYS:SG	3:A:804:HEM:HAB	2.46	0.53
1:B:566:LYS:HB3	1:B:566:LYS:NZ	2.24	0.52
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.44	0.52
1:B:79:MET:CE	1:B:96:LYS:HE3	2.39	0.52
1:B:229:ASP:N	1:B:256:HIS:HE1	1.99	0.52
1:A:533:GLY:HA2	1:A:553:ILE:HG22	1.92	0.52
1:B:82:CYS:SG	3:B:804:HEM:C3B	2.97	0.52
1:A:26:ASN:HA	1:A:299:LYS:HE3	1.92	0.51
1:B:505:TYR:HE1	4:B:3805:FAD:O3'	1.94	0.51
1:B:17:CYS:SG	3:B:801:HEM:C3C	3.03	0.51
1:B:204:ASN:H	1:B:204:ASN:ND2	2.03	0.50
1:B:283:LYS:HB2	6:B:3981:HOH:O	2.11	0.50
1:B:549:ALA:HB3	4:B:3805:FAD:N1	2.26	0.50
1:A:204:ASN:H	1:A:204:ASN:ND2	2.07	0.50
1:B:9:VAL:HG23	6:B:4375:HOH:O	2.11	0.50
1:B:85:CYS:SG	3:B:804:HEM:CBC	2.99	0.49
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.47	0.49
1:A:288:THR:HG22	6:A:2921:HOH:O	2.11	0.49
1:B:136:GLY:HA3	1:B:553:ILE:HD12	1.95	0.49
1:B:357:LYS:HB3	1:B:511:MET:HE2	1.94	0.49
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.06	0.49
1:B:357:LYS:HB3	1:B:511:MET:CE	2.43	0.49
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.78	0.49
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.95	0.49
1:B:192:MET:HG3	6:B:4671:HOH:O	2.13	0.48
1:B:533:GLY:HA2	1:B:553:ILE:HG22	1.96	0.48
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.06	0.48
1:B:354:GLY:HA2	6:B:4396:HOH:O	2.13	0.48
1:B:297:MET:HE2	6:B:4585:HOH:O	2.13	0.48
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.06	0.47
1:B:480:PHE:C	1:B:481:GLU:HG3	2.34	0.47
1:A:568:SER:HB3	6:A:3186:HOH:O	2.15	0.47
1:B:168:ALA:HA	4:B:3805:FAD:N5	2.29	0.47
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.49	0.47
1:B:36:CYS:SG	3:B:802:HEM:C3B	3.08	0.47
1:B:505:TYR:CE1	4:B:3805:FAD:O3'	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:HD22	1:B:58:HIS:H	1.62	0.46
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.03	0.46
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.97	0.46
1:B:167:LEU:HB3	4:B:3805:FAD:HM72	1.98	0.46
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.49	0.46
1:A:56:ASN:HD22	1:A:58:HIS:H	1.62	0.46
1:B:559:LEU:C	1:B:559:LEU:HD13	2.37	0.45
1:B:71:CYS:SG	3:B:803:HEM:CBC	3.03	0.45
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.99	0.45
1:A:36:CYS:SG	3:A:802:HEM:CBB	3.03	0.44
1:A:79:MET:CE	1:A:96:LYS:HE3	2.47	0.44
1:A:540:HIS:HE1	1:A:552:ASP:OD2	1.99	0.44
1:A:183:LYS:HA	1:A:183:LYS:HD2	1.87	0.44
1:B:283:LYS:CB	6:B:3981:HOH:O	2.65	0.44
1:A:540:HIS:HD2	6:A:2819:HOH:O	2.00	0.44
1:B:17:CYS:SG	3:B:801:HEM:HAC	2.51	0.44
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.10	0.44
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.53	0.44
1:A:299:LYS:HG2	6:A:3288:HOH:O	2.18	0.43
1:B:71:CYS:HG	3:B:803:HEM:CBC	2.27	0.43
1:A:467:ARG:HH11	1:A:471:LEU:HD11	1.84	0.43
1:B:97:LYS:HE3	6:B:4581:HOH:O	2.18	0.43
1:A:168:ALA:HA	4:A:2805:FAD:C6	2.49	0.43
1:A:36:CYS:SG	3:A:802:HEM:C3B	3.11	0.43
1:B:210:LYS:HD2	6:B:4501:HOH:O	2.18	0.43
1:A:60:SER:HB3	3:A:804:HEM:CMB	2.49	0.43
1:A:402:ARG:HH22	5:A:2806:FUM:C4	2.32	0.43
1:A:402:ARG:HH12	5:A:2806:FUM:C6	2.31	0.43
1:B:168:ALA:HA	4:B:3805:FAD:C5X	2.49	0.43
1:A:38:SER:HB3	6:A:3353:HOH:O	2.18	0.42
1:A:192:MET:HG3	6:A:3645:HOH:O	2.19	0.42
1:B:56:ASN:ND2	1:B:58:HIS:H	2.17	0.42
1:B:68:CYS:SG	3:B:803:HEM:C3B	3.11	0.42
1:A:56:ASN:ND2	1:A:58:HIS:H	2.17	0.42
1:B:6:GLU:HA	1:B:9:VAL:HG22	2.01	0.42
1:B:79:MET:HE2	1:B:96:LYS:HE3	2.00	0.42
1:B:14:CYS:SG	3:B:801:HEM:CBB	3.05	0.42
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.13	0.41
1:B:566:LYS:HG3	6:B:4318:HOH:O	2.20	0.41
1:A:133:GLY:O	1:A:138:GLY:HA3	2.20	0.41
1:B:68:CYS:SG	3:B:803:HEM:CBB	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:CYS:SG	3:A:802:HEM:CBC	3.09	0.41
1:B:79:MET:HE3	1:B:96:LYS:HE3	2.01	0.41
1:B:17:CYS:SG	3:B:801:HEM:CBC	3.08	0.41
1:B:374:VAL:HB	3:B:804:HEM:CMD	2.51	0.41
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.13	0.41
1:A:85:CYS:SG	3:A:804:HEM:HAC	2.54	0.41
1:B:513:ASP:HB3	1:B:519:MET:CE	2.50	0.41
4:A:2805:FAD:H1'1	4:A:2805:FAD:H9	1.66	0.41
1:A:86:HIS:CD2	3:A:804:HEM:NB	2.90	0.40
1:B:36:CYS:SG	3:B:802:HEM:CBB	3.07	0.40
3:B:803:HEM:HBB2	3:B:803:HEM:HMB1	2.03	0.40

There are no symmetry-related clashes.

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%)	546 (96%)	19 (3%)	1 (0%)	47 44
1	B	566/571 (99%)	548 (97%)	17 (3%)	1 (0%)	47 44
All	All	1132/1142 (99%)	1094 (97%)	36 (3%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

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

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	437/445 (98%)	422 (97%)	15 (3%)	37	36
1	B	441/445 (99%)	424 (96%)	17 (4%)	32	30
All	All	878/890 (99%)	846 (96%)	32 (4%)	35	34

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	91	ASN
1	A	99	LEU
1	A	176	TRP
1	A	198	LYS
1	A	204	ASN
1	A	286	LYS
1	A	337	ASN
1	A	403	ASP
1	A	450	LEU
1	A	452	LYS
1	A	490	ASN
1	A	523	LYS
1	A	559	LEU
1	A	568	SER
1	B	15	ASP
1	B	51	LYS
1	B	56	ASN
1	B	99	LEU
1	B	112	LYS
1	B	113	SER
1	B	119	LEU
1	B	204	ASN
1	B	208	LEU
1	B	337	ASN
1	B	415	LYS
1	B	450	LEU

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Mol	Chain	Res	Type
1	B	459	LYS
1	B	476	LYS
1	B	481	GLU
1	B	490	ASN
1	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	56	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	490	ASN
1	A	540	HIS
1	B	35	GLN
1	B	54	HIS
1	B	56	ASN
1	B	91	ASN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	490	ASN
1	B	540	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
3	HEM	B	801	1	41,50,50	1.65	7 (17%)	45,82,82	1.52	8 (17%)
3	HEM	B	803	1	41,50,50	1.49	3 (7%)	45,82,82	1.48	6 (13%)
3	HEM	A	802	1	41,50,50	1.64	5 (12%)	45,82,82	1.50	9 (20%)
3	HEM	A	804	1	41,50,50	1.65	7 (17%)	45,82,82	1.48	4 (8%)
3	HEM	B	802	1	41,50,50	1.53	4 (9%)	45,82,82	1.75	12 (26%)
4	FAD	B	3805	-	53,58,58	1.66	9 (16%)	68,89,89	2.06	16 (23%)
4	FAD	A	2805	-	53,58,58	1.47	10 (18%)	68,89,89	2.13	22 (32%)
3	HEM	B	804	1	41,50,50	1.68	5 (12%)	45,82,82	1.60	8 (17%)
3	HEM	A	801	1	41,50,50	1.61	6 (14%)	45,82,82	1.48	8 (17%)
3	HEM	A	803	1	41,50,50	1.59	8 (19%)	45,82,82	1.40	9 (20%)
5	FUM	A	2806	-	7,7,7	2.54	4 (57%)	8,8,8	2.10	5 (62%)
5	FUM	B	3806	-	7,7,7	2.53	4 (57%)	8,8,8	2.29	6 (75%)

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
3	HEM	B	801	1	-	2/12/54/54	-
3	HEM	B	803	1	-	0/12/54/54	-
3	HEM	A	802	1	-	2/12/54/54	-
3	HEM	A	804	1	-	6/12/54/54	-
3	HEM	B	802	1	-	2/12/54/54	-
4	FAD	B	3805	-	1/1/9/9	11/30/50/50	0/6/6/6
4	FAD	A	2805	-	1/1/9/9	11/30/50/50	0/6/6/6
3	HEM	B	804	1	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	801	1	-	3/12/54/54	-
3	HEM	A	803	1	-	2/12/54/54	-
5	FUM	A	2806	-	-	2/5/5/5	-
5	FUM	B	3806	-	-	2/5/5/5	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	HEM	C3C-C2C	-5.47	1.32	1.40
3	B	803	HEM	C3C-C2C	-5.34	1.33	1.40
3	A	804	HEM	C3C-C2C	-4.98	1.33	1.40
4	B	3805	FAD	C2A-N3A	4.93	1.40	1.32
3	B	801	HEM	C3C-C2C	-4.74	1.33	1.40
3	A	803	HEM	C3C-C2C	-4.67	1.33	1.40
3	A	802	HEM	C3C-C2C	-4.61	1.34	1.40
3	B	802	HEM	C3C-C2C	-4.53	1.34	1.40
4	B	3805	FAD	O2-C2	-4.53	1.15	1.24
3	A	801	HEM	C3C-C2C	-4.31	1.34	1.40
3	A	802	HEM	C3C-CAC	4.20	1.56	1.47
3	B	804	HEM	C3C-CAC	3.98	1.56	1.47
5	B	3806	FUM	O-C	3.83	1.32	1.23
4	B	3805	FAD	C6-C5X	3.74	1.45	1.40
3	B	802	HEM	C3C-CAC	3.72	1.55	1.47
4	A	2805	FAD	O4-C4	-3.72	1.16	1.23
3	A	803	HEM	C3C-CAC	3.55	1.55	1.47
4	B	3805	FAD	C9-C8	3.53	1.44	1.39
3	A	804	HEM	C3C-CAC	3.52	1.55	1.47
5	A	2806	FUM	OXT-C	-3.49	1.21	1.30
3	A	801	HEM	C3C-CAC	3.46	1.54	1.47
5	A	2806	FUM	O7-C6	3.38	1.31	1.23
5	B	3806	FUM	OXT-C	-3.26	1.21	1.30
4	B	3805	FAD	O4-C4	-3.24	1.17	1.23
3	A	801	HEM	CAB-C3B	3.23	1.56	1.47
3	B	803	HEM	C3C-CAC	3.19	1.54	1.47
5	B	3806	FUM	O7-C6	3.19	1.31	1.23
5	A	2806	FUM	O-C	3.15	1.31	1.23
4	A	2805	FAD	C5'-C4'	3.13	1.56	1.51
4	A	2805	FAD	C9-C8	3.12	1.44	1.39
3	A	803	HEM	CAB-C3B	3.11	1.55	1.47
4	A	2805	FAD	C2A-N3A	3.03	1.37	1.32
3	B	801	HEM	CAA-C2A	3.03	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	HEM	CAA-C2A	3.00	1.56	1.52
4	A	2805	FAD	C6-C5X	2.99	1.44	1.40
3	A	804	HEM	CAB-C3B	2.97	1.55	1.47
4	B	3805	FAD	C5'-C4'	2.97	1.56	1.51
5	A	2806	FUM	O8-C6	-2.94	1.22	1.30
3	B	801	HEM	C3C-CAC	2.93	1.53	1.47
3	A	802	HEM	CAA-C2A	2.89	1.56	1.52
3	B	801	HEM	CAB-C3B	2.89	1.55	1.47
3	B	804	HEM	CAA-C2A	2.80	1.56	1.52
3	B	804	HEM	CAB-C3B	2.80	1.55	1.47
5	B	3806	FUM	O8-C6	-2.80	1.23	1.30
4	A	2805	FAD	C2'-C3'	2.76	1.58	1.53
4	B	3805	FAD	C1'-C2'	-2.75	1.48	1.52
3	A	804	HEM	CMB-C2B	2.73	1.56	1.50
4	B	3805	FAD	C10-N1	-2.71	1.27	1.33
3	A	801	HEM	CAA-C2A	2.65	1.55	1.52
4	A	2805	FAD	C2B-C1B	2.61	1.57	1.53
3	A	801	HEM	CMD-C2D	2.60	1.56	1.50
3	B	803	HEM	CAB-C3B	2.51	1.54	1.47
4	A	2805	FAD	O2-C2	-2.50	1.19	1.24
3	A	802	HEM	CAB-C3B	2.50	1.54	1.47
4	B	3805	FAD	C9A-N10	-2.49	1.36	1.41
3	A	803	HEM	CMB-C2B	2.48	1.56	1.50
3	A	802	HEM	CMD-C2D	2.43	1.55	1.50
3	A	803	HEM	CAA-C2A	2.42	1.55	1.52
3	A	801	HEM	C3B-C2B	-2.41	1.32	1.37
4	A	2805	FAD	C10-N1	-2.39	1.28	1.33
4	A	2805	FAD	C9A-N10	-2.35	1.37	1.41
3	B	802	HEM	CAB-C3B	2.26	1.53	1.47
3	A	803	HEM	CMD-C2D	2.26	1.55	1.50
3	B	801	HEM	CAD-C3D	2.14	1.56	1.51
3	B	802	HEM	CMD-C2D	2.09	1.55	1.50
3	A	804	HEM	CAD-C3D	2.09	1.56	1.51
3	B	801	HEM	CMD-C2D	2.06	1.55	1.50
3	A	803	HEM	CAD-C3D	2.06	1.56	1.51
3	B	804	HEM	CMA-C3A	2.05	1.55	1.51
3	B	801	HEM	CMB-C2B	2.05	1.55	1.50
3	A	803	HEM	C3B-C2B	-2.03	1.33	1.37
3	A	804	HEM	C3B-C2B	-2.01	1.33	1.37

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3805	FAD	C5A-C6A-N6A	7.60	131.90	120.35
4	A	2805	FAD	C5A-C6A-N6A	6.99	130.98	120.35
4	A	2805	FAD	O2'-C2'-C3'	-5.94	94.66	109.10
4	B	3805	FAD	C4'-C3'-C2'	5.41	124.61	113.36
4	A	2805	FAD	O4B-C1B-C2B	-5.04	99.57	106.93
4	A	2805	FAD	C4'-C3'-C2'	4.89	123.54	113.36
3	A	804	HEM	C4C-CHD-C1D	4.56	128.58	122.56
3	B	802	HEM	C1B-NB-C4B	4.47	109.69	105.07
4	B	3805	FAD	O3'-C3'-C2'	4.37	119.36	108.81
3	B	803	HEM	CBA-CAA-C2A	4.09	119.60	112.62
4	B	3805	FAD	O5'-C5'-C4'	-4.04	98.58	109.36
3	A	802	HEM	C1B-NB-C4B	3.93	109.13	105.07
4	B	3805	FAD	O4-C4-N3	3.88	127.56	120.12
5	B	3806	FUM	O-C-C4	-3.60	109.75	120.99
4	A	2805	FAD	O3'-C3'-C4'	3.55	117.38	108.81
4	B	3805	FAD	C9-C9A-N10	-3.51	117.09	121.84
4	B	3805	FAD	C5X-C9A-N10	3.43	121.49	117.95
3	A	803	HEM	CMA-C3A-C4A	-3.42	123.20	128.46
3	B	803	HEM	C4B-CHC-C1C	3.42	127.06	122.56
3	A	804	HEM	CMA-C3A-C4A	-3.41	123.22	128.46
4	B	3805	FAD	O4B-C1B-C2B	-3.38	101.98	106.93
3	A	801	HEM	C1B-NB-C4B	3.35	108.53	105.07
3	B	803	HEM	CMA-C3A-C4A	-3.32	123.35	128.46
3	B	803	HEM	CMC-C2C-C3C	3.30	130.86	124.68
3	A	804	HEM	CMC-C2C-C3C	3.29	130.84	124.68
3	B	804	HEM	C2C-C3C-C4C	3.27	109.18	106.90
3	B	804	HEM	CMC-C2C-C3C	3.26	130.78	124.68
3	B	802	HEM	CMA-C3A-C4A	-3.25	123.46	128.46
3	B	802	HEM	CMC-C2C-C3C	3.17	130.62	124.68
3	A	803	HEM	CAD-CBD-CGD	3.03	120.12	113.60
4	A	2805	FAD	O2-C2-N1	-3.02	116.82	121.83
3	B	802	HEM	O2D-CGD-CBD	3.00	123.65	114.03
3	B	801	HEM	C4D-ND-C1D	2.98	108.16	105.07
4	B	3805	FAD	O2'-C2'-C1'	2.94	116.91	109.80
5	A	2806	FUM	C5-C4-C	-2.93	112.22	127.26
4	B	3805	FAD	N6A-C6A-N1A	-2.93	112.50	118.57
4	A	2805	FAD	N6A-C6A-N1A	-2.91	112.54	118.57
3	B	801	HEM	CMA-C3A-C4A	-2.90	124.00	128.46
4	A	2805	FAD	O5'-C5'-C4'	-2.90	101.63	109.36
3	B	804	HEM	O1D-CGD-CBD	-2.84	113.95	123.08
4	A	2805	FAD	C5'-C4'-C3'	-2.84	106.72	112.20
4	B	3805	FAD	O2'-C2'-C3'	-2.79	102.32	109.10
3	B	801	HEM	C1B-NB-C4B	2.75	107.92	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2805	FAD	C9-C9A-N10	-2.74	118.13	121.84
3	B	802	HEM	O1D-CGD-CBD	-2.72	114.34	123.08
4	A	2805	FAD	O4-C4-N3	2.71	125.30	120.12
3	A	803	HEM	CMC-C2C-C3C	2.69	129.72	124.68
5	A	2806	FUM	C4-C5-C6	-2.67	113.53	127.26
4	B	3805	FAD	C2A-N1A-C6A	2.67	123.32	118.75
3	B	801	HEM	C4B-CHC-C1C	2.67	126.08	122.56
3	B	803	HEM	CAD-CBD-CGD	2.64	119.28	113.60
5	B	3806	FUM	C4-C5-C6	-2.63	113.76	127.26
4	A	2805	FAD	C1'-N10-C9A	-2.63	116.13	120.51
3	B	802	HEM	C4B-C3B-C2B	2.62	109.20	107.11
4	B	3805	FAD	C1'-N10-C9A	-2.62	116.15	120.51
3	A	801	HEM	CBB-CAB-C3B	-2.58	114.78	127.62
3	A	802	HEM	C4D-ND-C1D	2.56	107.72	105.07
3	B	804	HEM	CBA-CAA-C2A	-2.55	108.26	112.62
3	B	804	HEM	CMB-C2B-C1B	-2.54	121.17	125.04
3	A	802	HEM	CMC-C2C-C3C	2.54	129.43	124.68
3	B	801	HEM	CHD-C1D-ND	2.54	127.19	124.43
3	B	804	HEM	CBD-CAD-C3D	2.53	119.67	112.63
4	A	2805	FAD	N3-C2-N1	2.53	124.34	119.38
4	B	3805	FAD	O4-C4-C4X	-2.49	119.99	126.60
4	A	2805	FAD	C3B-C2B-C1B	-2.45	97.29	100.98
4	A	2805	FAD	C7M-C7-C6	2.44	123.99	119.49
5	A	2806	FUM	O7-C6-C5	-2.43	113.39	120.99
3	A	802	HEM	C4B-C3B-C2B	2.43	109.05	107.11
3	A	803	HEM	CMA-C3A-C2A	2.43	129.53	124.94
3	B	801	HEM	CMC-C2C-C3C	2.42	129.22	124.68
4	B	3805	FAD	O2A-PA-O5B	-2.42	96.49	107.75
3	B	804	HEM	C4B-CHC-C1C	2.39	125.71	122.56
3	B	802	HEM	C2B-C1B-NB	-2.38	107.02	109.84
3	B	802	HEM	CMB-C2B-C1B	-2.38	121.42	125.04
4	A	2805	FAD	C9A-C5X-N5	-2.35	119.88	122.43
5	B	3806	FUM	OXT-C-C4	2.35	125.03	116.27
4	A	2805	FAD	O2A-PA-O1A	2.33	123.76	112.24
3	A	803	HEM	CBD-CAD-C3D	-2.32	106.18	112.63
3	A	803	HEM	O2D-CGD-O1D	2.29	129.02	123.30
5	B	3806	FUM	C5-C4-C	-2.29	115.48	127.26
5	A	2806	FUM	O-C-C4	-2.29	113.85	120.99
4	A	2805	FAD	C8M-C8-C9	-2.28	115.27	119.49
3	B	802	HEM	CMD-C2D-C1D	-2.27	121.59	125.04
3	A	803	HEM	C3B-C2B-C1B	2.26	108.17	106.49
3	A	802	HEM	CMB-C2B-C1B	-2.26	121.60	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	CHC-C4B-NB	2.25	126.87	124.43
3	B	803	HEM	CMA-C3A-C2A	2.22	129.14	124.94
3	B	802	HEM	CHB-C1B-NB	2.22	127.13	124.38
5	B	3806	FUM	O7-C6-C5	-2.22	114.07	120.99
3	A	804	HEM	CMA-C3A-C2A	2.21	129.12	124.94
4	A	2805	FAD	C10-N1-C2	-2.19	112.52	116.90
5	B	3806	FUM	O8-C6-C5	2.18	124.41	116.27
4	A	2805	FAD	O2'-C2'-C1'	2.17	115.03	109.80
3	A	802	HEM	C2C-C3C-C4C	2.14	108.39	106.90
3	B	802	HEM	CMA-C3A-C2A	2.14	128.97	124.94
5	A	2806	FUM	OXT-C-O	2.13	127.08	122.67
4	A	2805	FAD	C4X-C10-N1	2.12	129.65	124.73
3	A	802	HEM	C4C-CHD-C1D	2.12	125.35	122.56
4	B	3805	FAD	C5A-C6A-N1A	-2.10	115.58	120.35
4	A	2805	FAD	O2A-PA-O5B	-2.09	98.02	107.75
3	B	804	HEM	CMD-C2D-C1D	-2.09	121.86	125.04
3	A	802	HEM	O1A-CGA-CBA	-2.08	116.39	123.08
3	A	801	HEM	CMC-C2C-C3C	2.08	128.56	124.68
3	B	801	HEM	C3D-C4D-ND	-2.07	107.86	110.17
3	A	801	HEM	CHA-C4D-C3D	2.07	129.21	125.33
3	B	802	HEM	C4D-ND-C1D	2.06	107.20	105.07
3	A	801	HEM	C4B-C3B-C2B	2.06	108.75	107.11
3	A	801	HEM	CMB-C2B-C1B	-2.04	121.93	125.04
3	B	801	HEM	C4B-C3B-C2B	2.04	108.73	107.11
3	A	801	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
3	A	802	HEM	C2B-C1B-NB	-2.02	107.45	109.84
3	A	803	HEM	CBB-CAB-C3B	-2.01	117.63	127.62
3	A	803	HEM	C4B-CHC-C1C	2.00	125.20	122.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2805	FAD	C4'
4	B	3805	FAD	C4'

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2805	FAD	C2'-C3'-C4'-C5'
4	A	2805	FAD	O3'-C3'-C4'-O4'
4	A	2805	FAD	O3'-C3'-C4'-C5'
4	A	2805	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
4	B	3805	FAD	C2'-C3'-C4'-C5'
4	B	3805	FAD	O3'-C3'-C4'-O4'
4	B	3805	FAD	O3'-C3'-C4'-C5'
4	B	3805	FAD	PA-O3P-P-O5'
5	A	2806	FUM	OXT-C-C4-C5
5	A	2806	FUM	O-C-C4-C5
4	A	2805	FAD	C2'-C3'-C4'-O4'
4	B	3805	FAD	C2'-C3'-C4'-O4'
5	B	3806	FUM	OXT-C-C4-C5
5	B	3806	FUM	O-C-C4-C5
4	B	3805	FAD	O2'-C2'-C3'-C4'
4	A	2805	FAD	P-O3P-PA-O1A
3	A	801	HEM	C3D-CAD-CBD-CGD
4	A	2805	FAD	P-O3P-PA-O2A
4	B	3805	FAD	P-O3P-PA-O1A
4	B	3805	FAD	P-O3P-PA-O2A
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	803	HEM	CAA-CBA-CGA-O1A
3	A	804	HEM	CAA-CBA-CGA-O2A
3	B	804	HEM	CAA-CBA-CGA-O1A
3	B	804	HEM	CAA-CBA-CGA-O2A
4	A	2805	FAD	C2'-C1'-N10-C10
4	A	2805	FAD	O4'-C4'-C5'-O5'
4	B	3805	FAD	C2'-C1'-N10-C10
3	A	801	HEM	CAD-CBD-CGD-O1D
3	B	802	HEM	CAD-CBD-CGD-O2D
3	B	801	HEM	CAD-CBD-CGD-O1D
3	A	801	HEM	CAD-CBD-CGD-O2D
3	A	803	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAD-CBD-CGD-O2D
3	B	804	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	C2A-CAA-CBA-CGA
3	B	804	HEM	C2A-CAA-CBA-CGA
3	A	802	HEM	CAD-CBD-CGD-O2D
3	B	802	HEM	CAD-CBD-CGD-O1D
3	A	802	HEM	CAD-CBD-CGD-O1D
4	B	3805	FAD	O4'-C4'-C5'-O5'
3	A	804	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAD-CBD-CGD-O2D
3	B	804	HEM	C4B-C3B-CAB-CBB
4	A	2805	FAD	O4B-C4B-C5B-O5B
3	B	804	HEM	CAD-CBD-CGD-O2D

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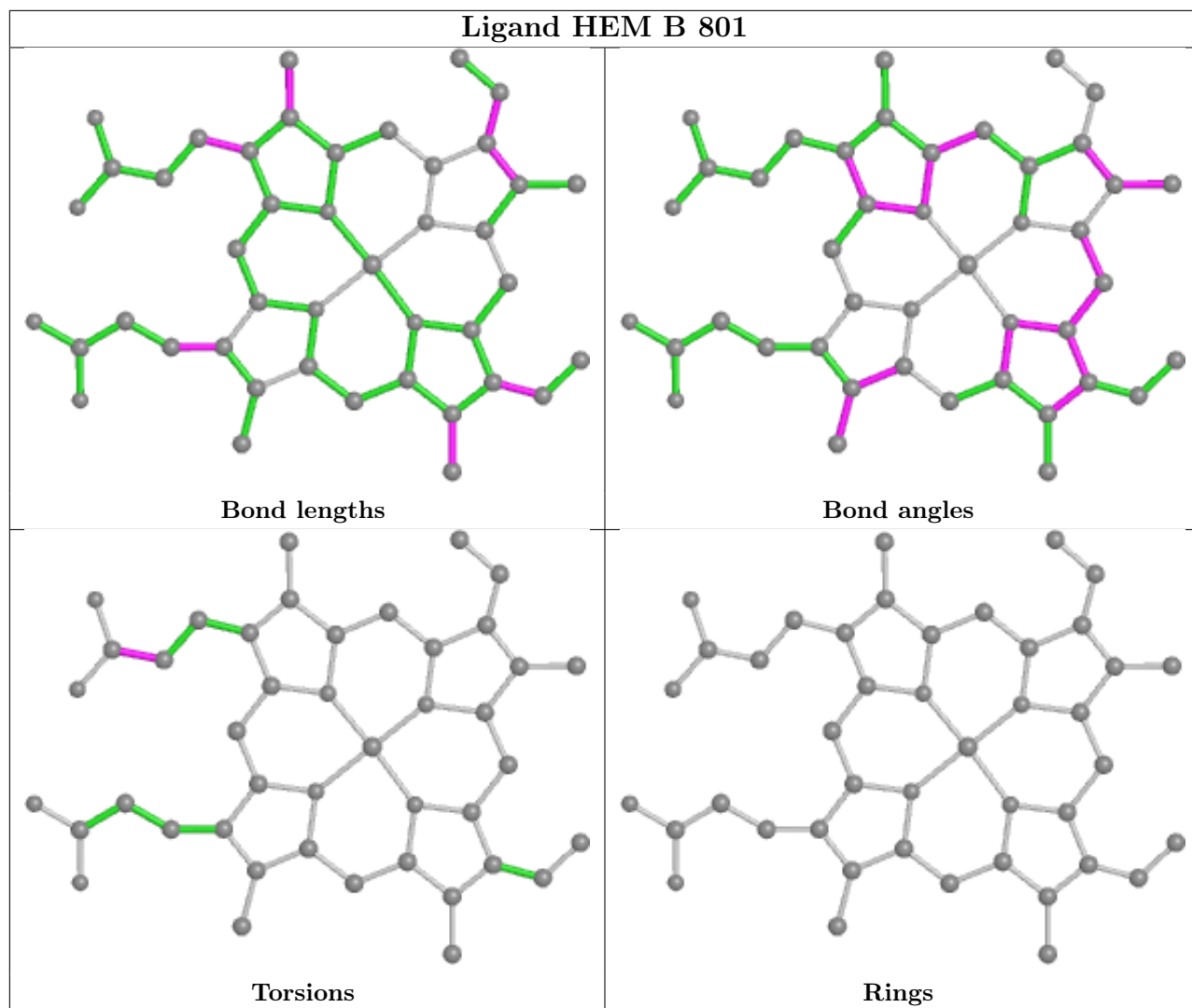
Mol	Chain	Res	Type	Atoms
3	A	804	HEM	C4D-C3D-CAD-CBD
4	A	2805	FAD	C3'-C4'-C5'-O5'
4	B	3805	FAD	O4B-C4B-C5B-O5B

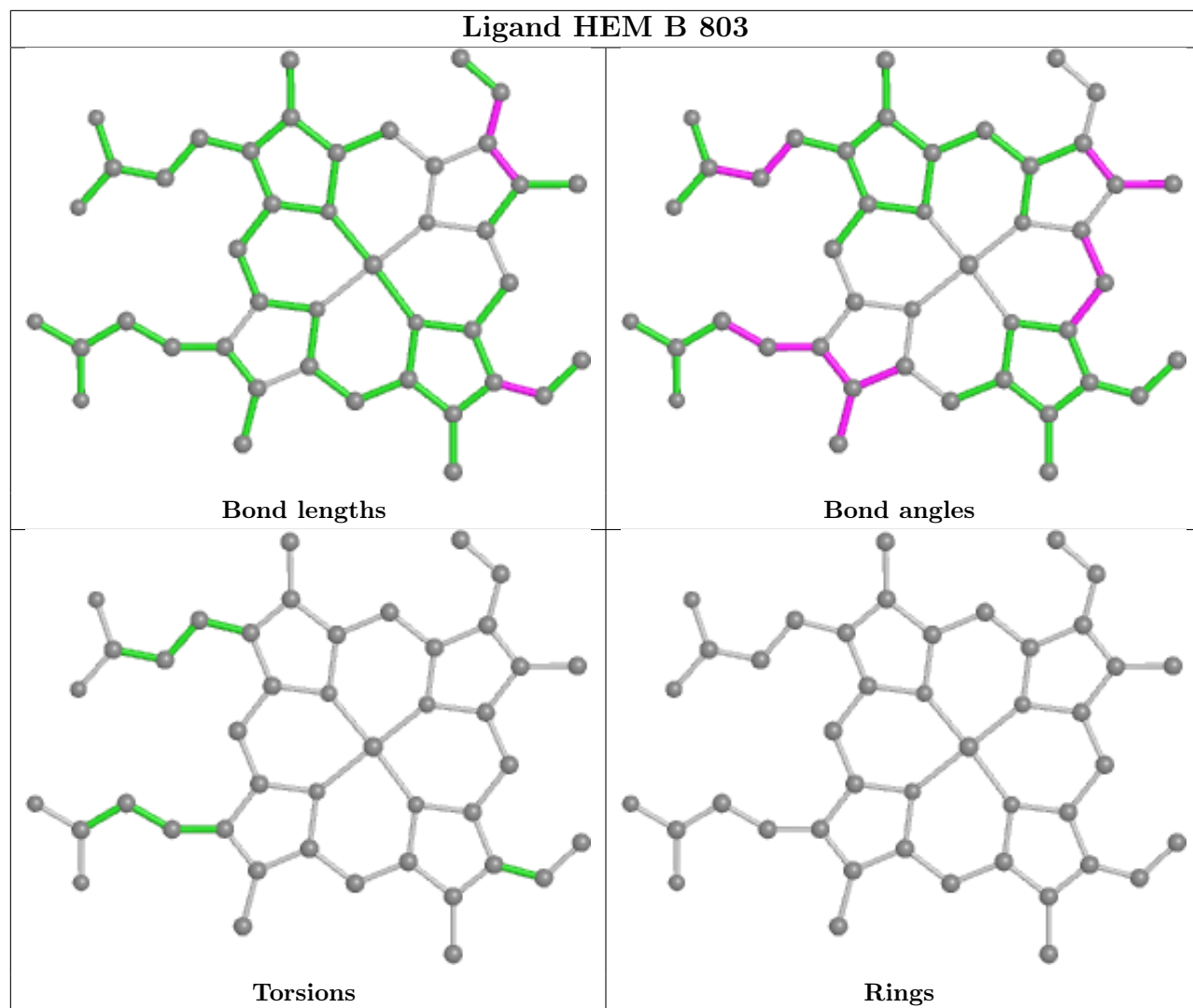
There are no ring outliers.

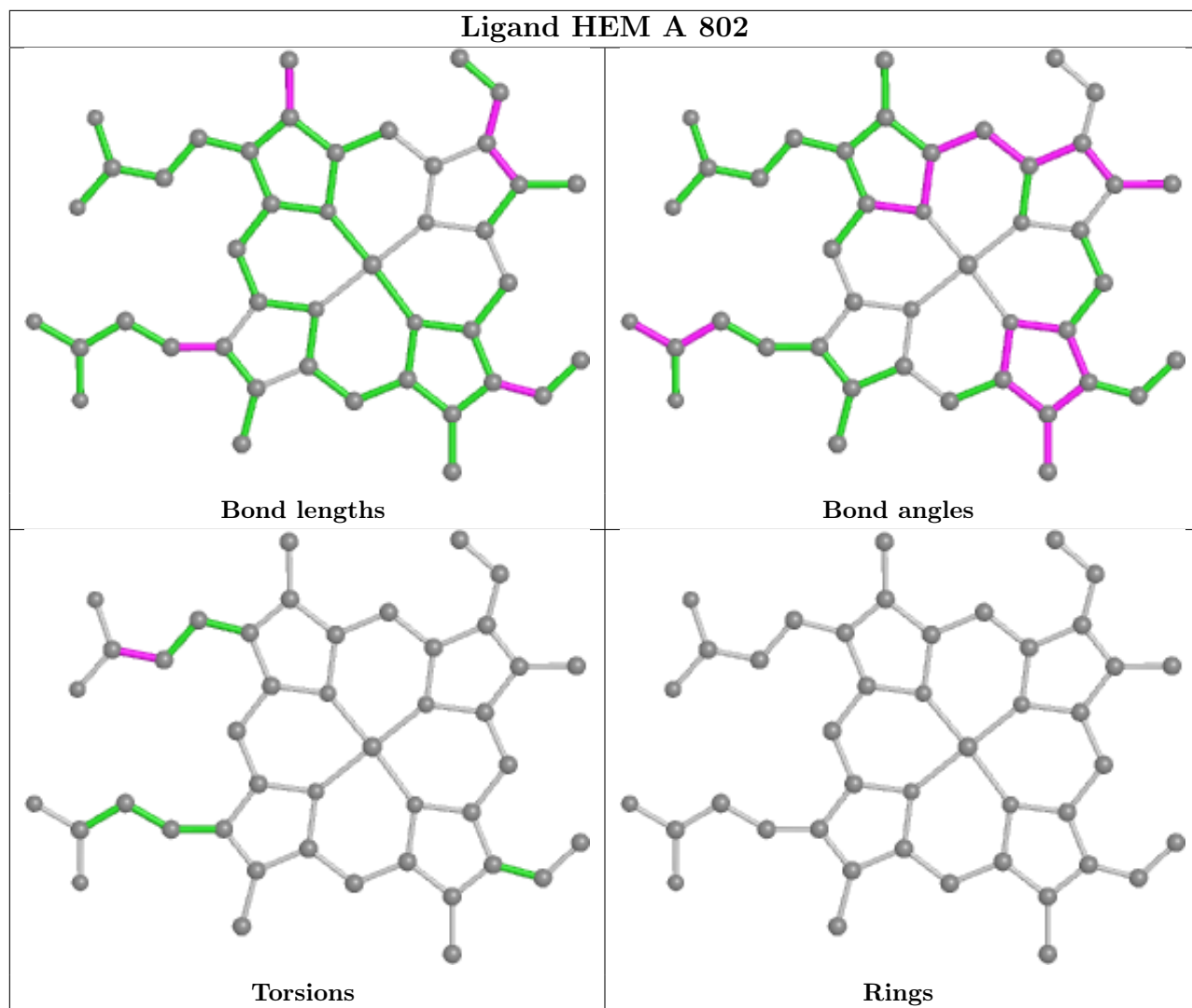
12 monomers are involved in 75 short contacts:

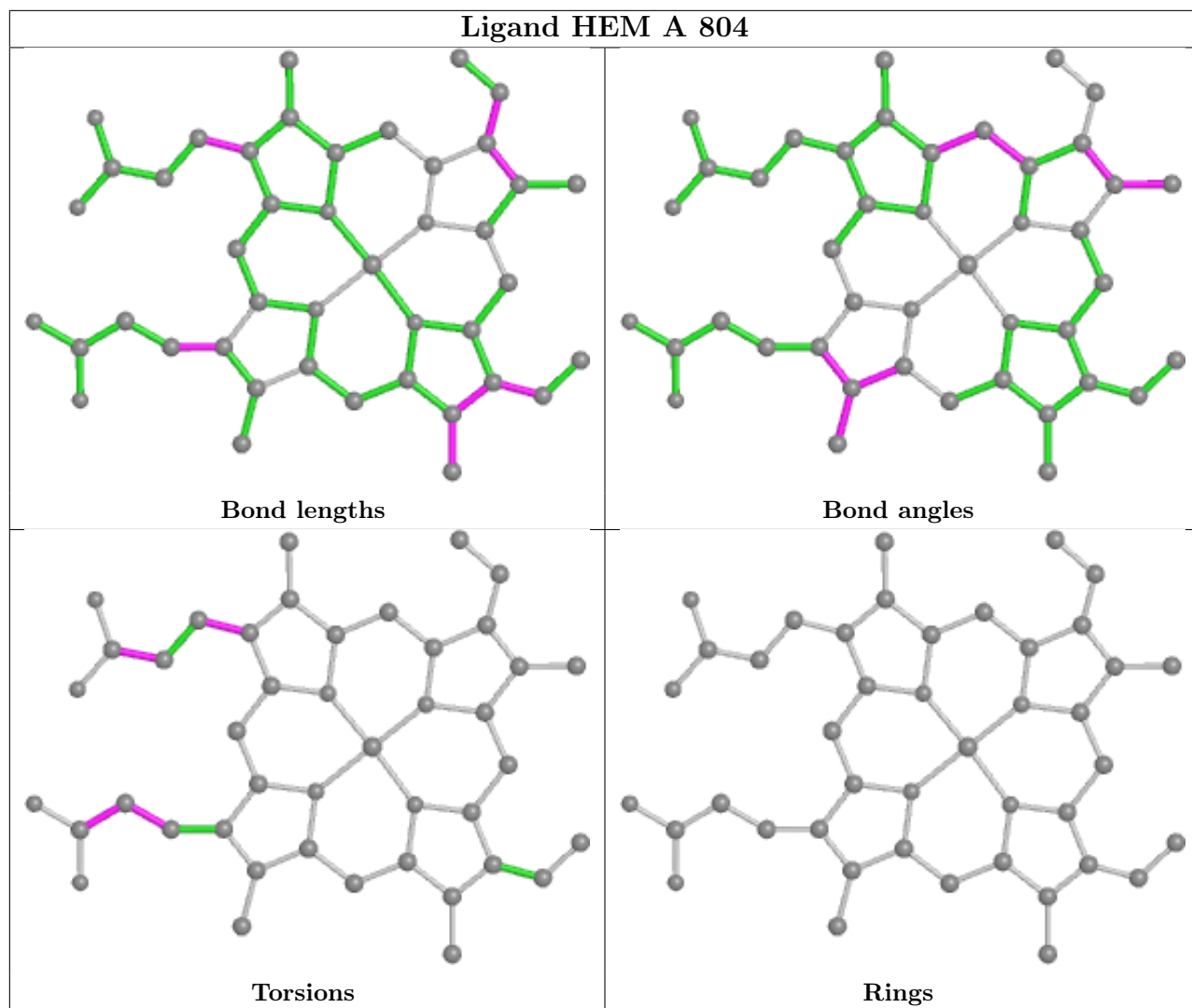
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	HEM	7	0
3	B	803	HEM	11	0
3	A	802	HEM	7	0
3	A	804	HEM	11	0
3	B	802	HEM	6	0
4	B	3805	FAD	6	0
4	A	2805	FAD	5	0
3	B	804	HEM	8	0
3	A	801	HEM	4	0
3	A	803	HEM	6	0
5	A	2806	FUM	3	0
5	B	3806	FUM	1	0

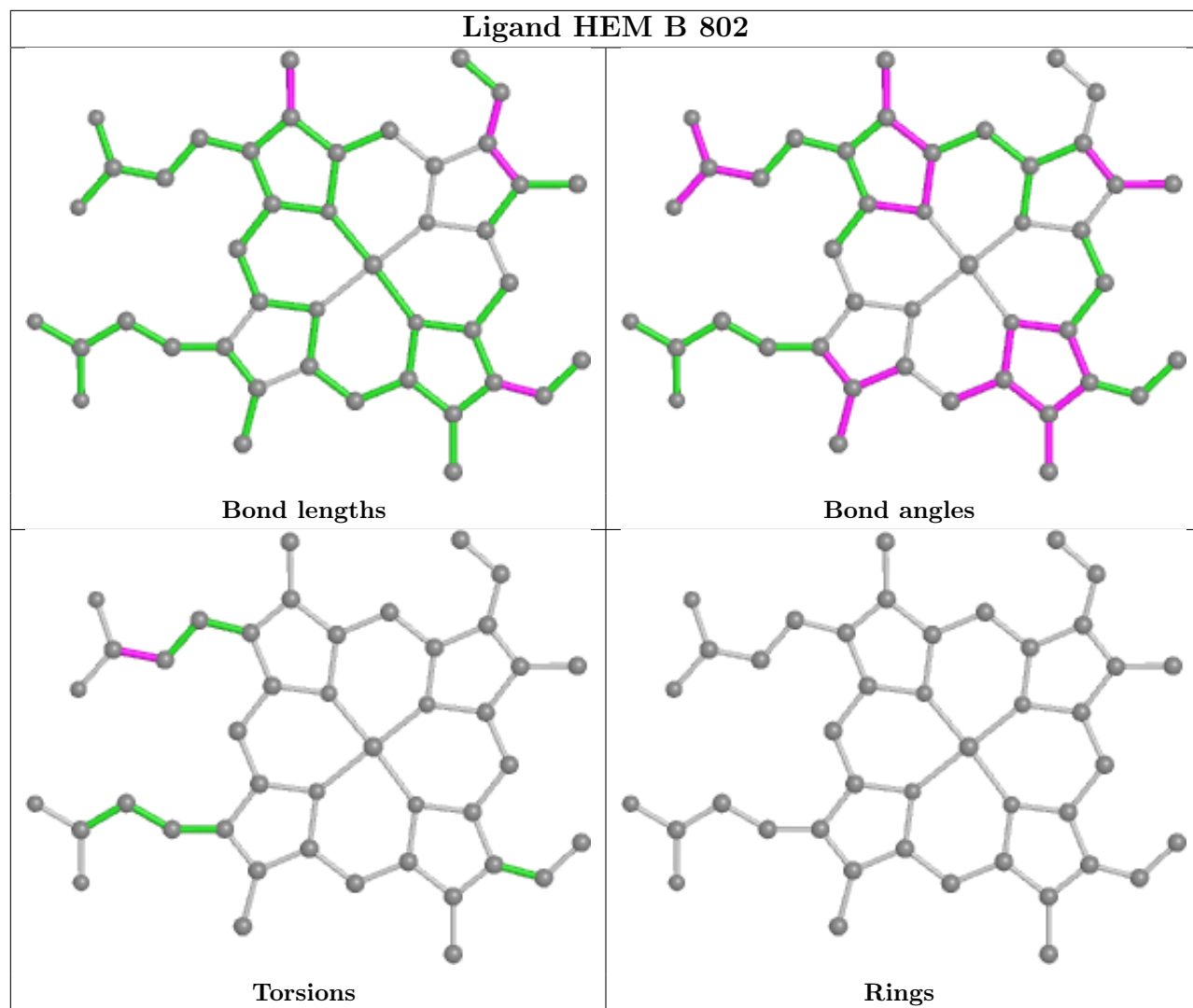
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

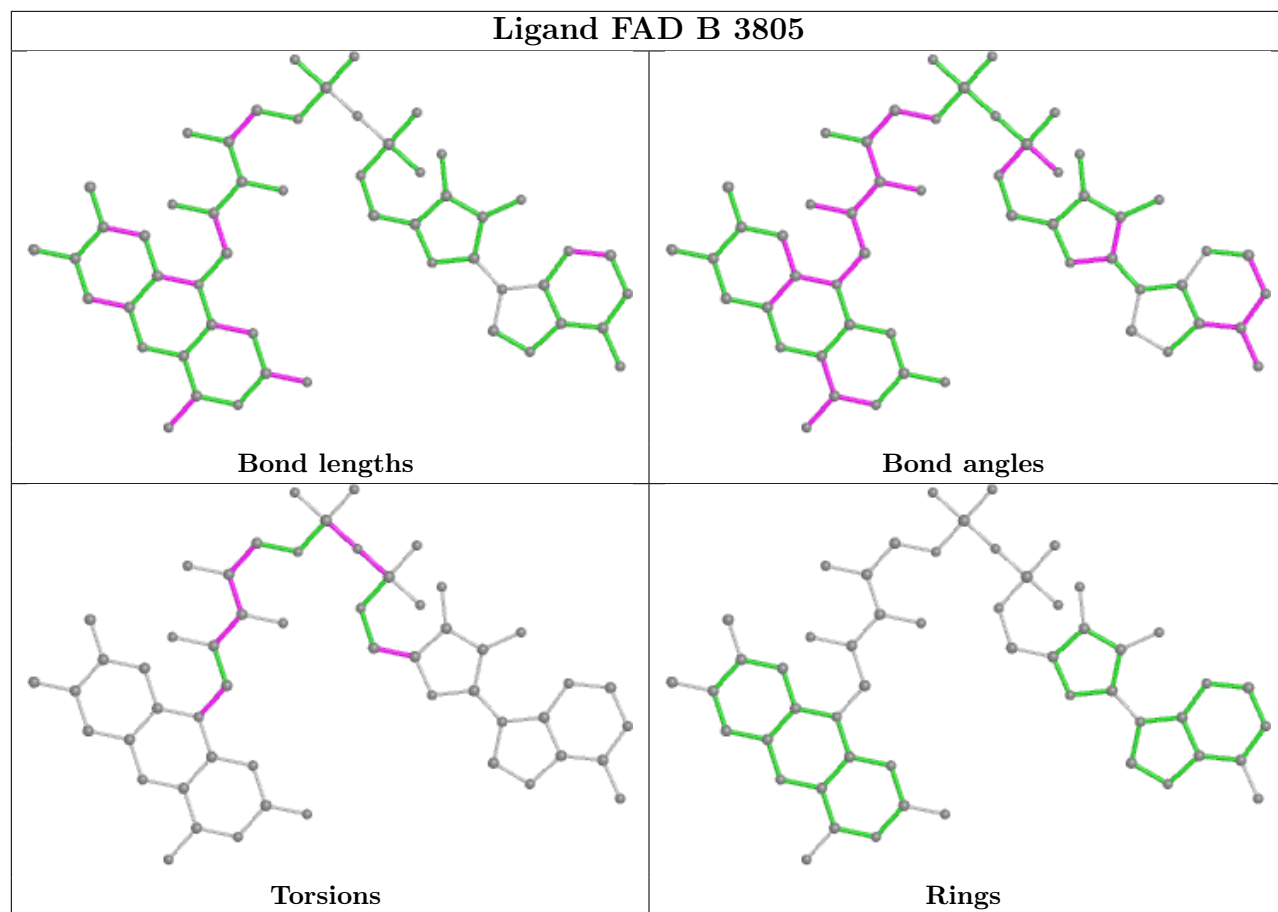


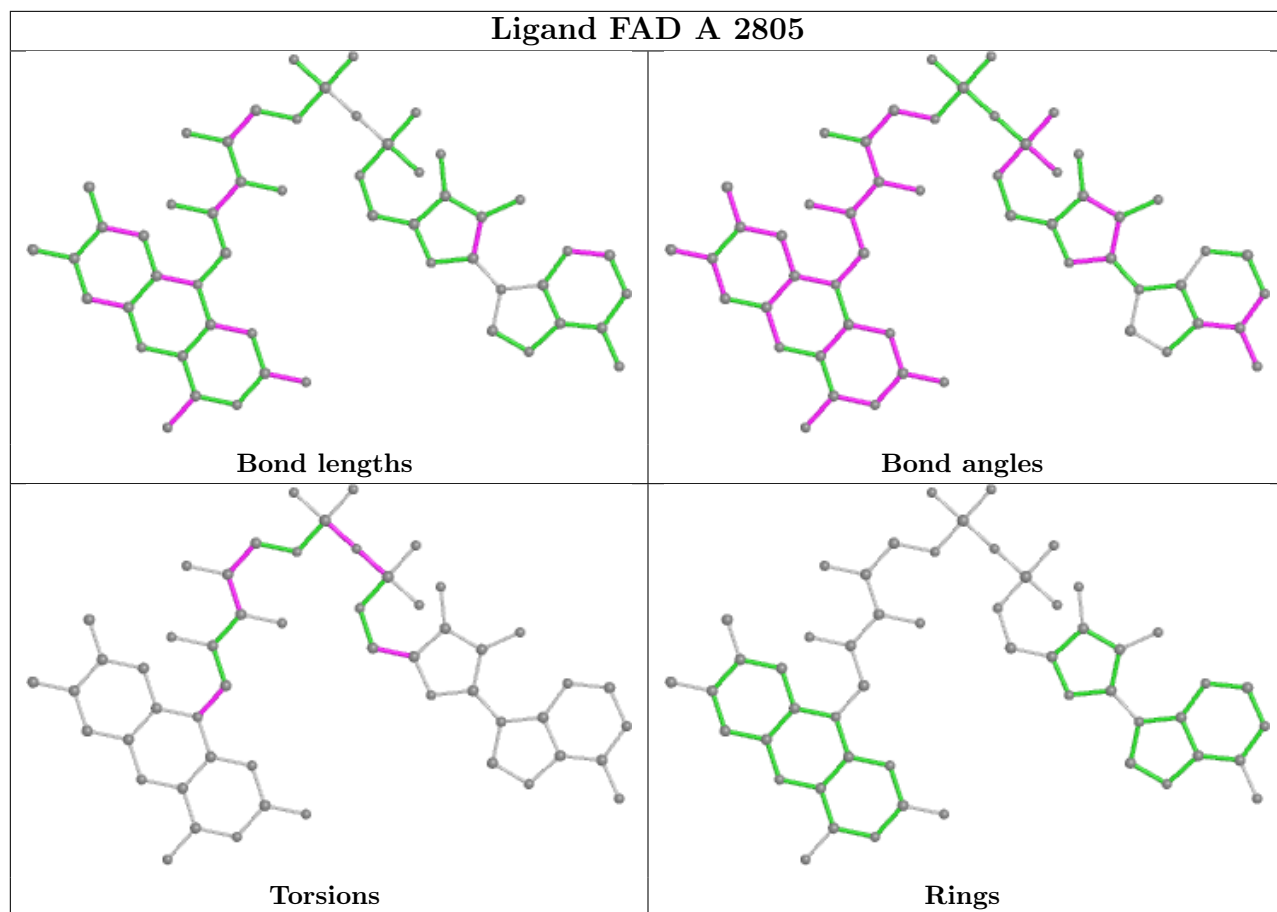


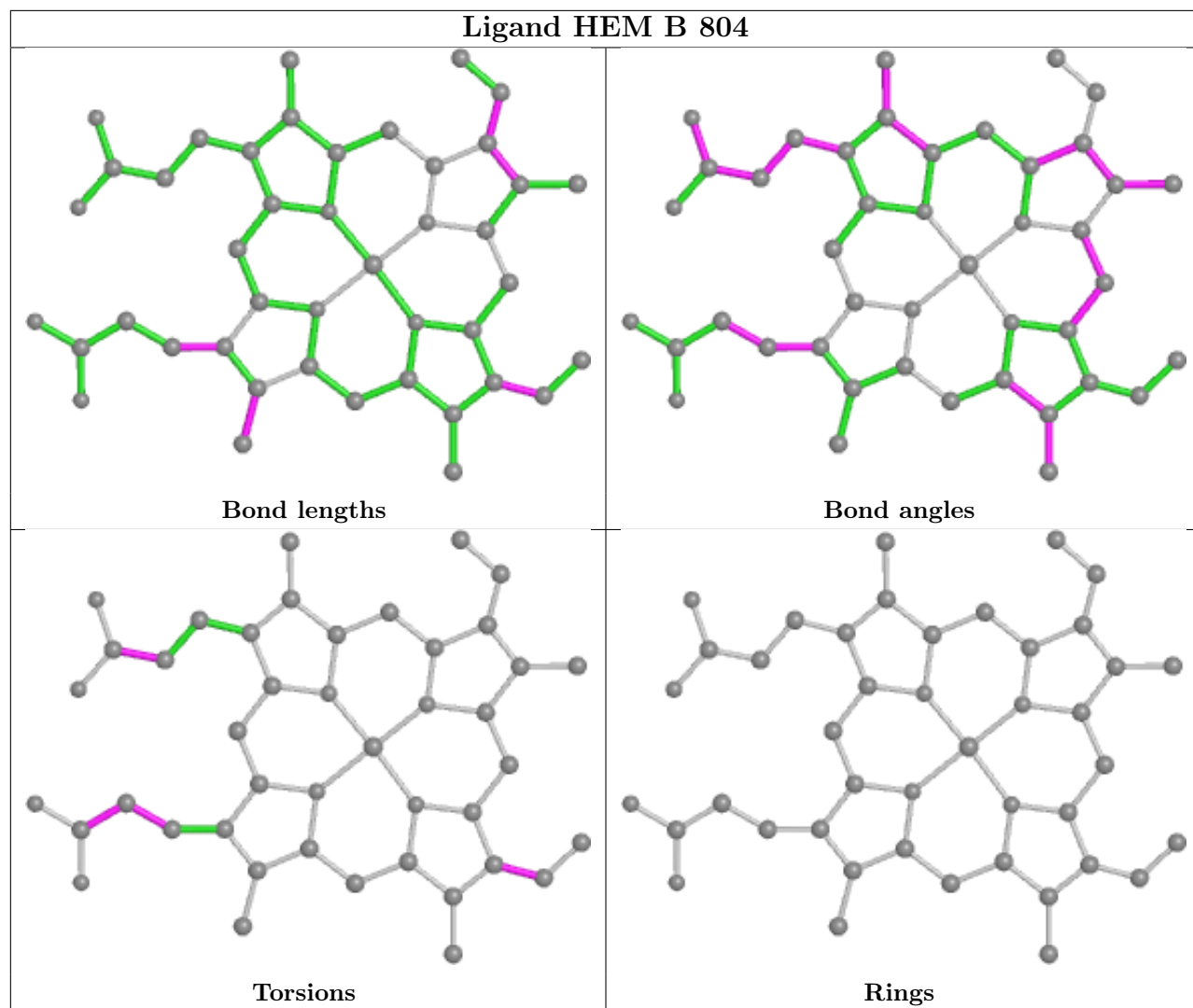


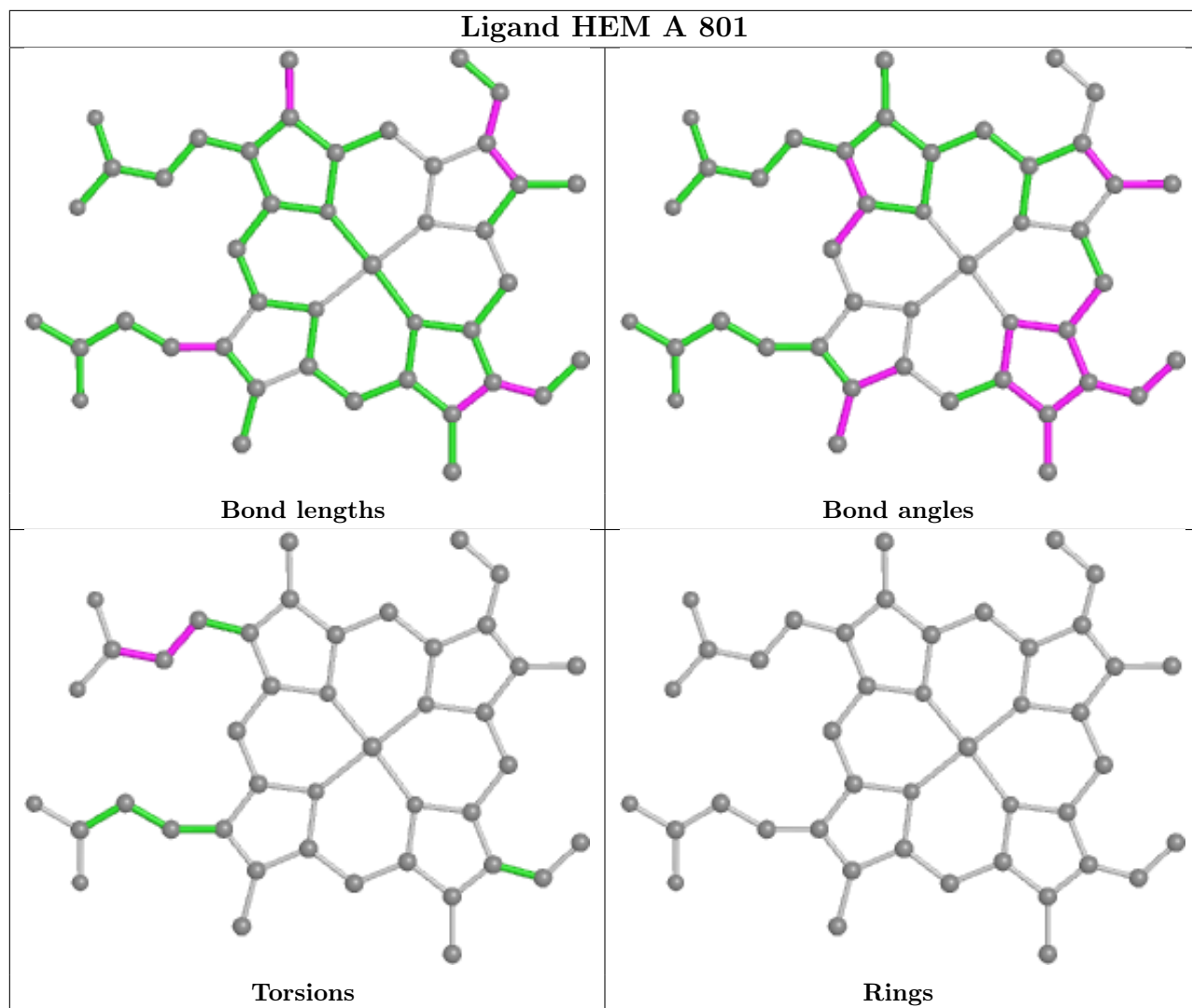


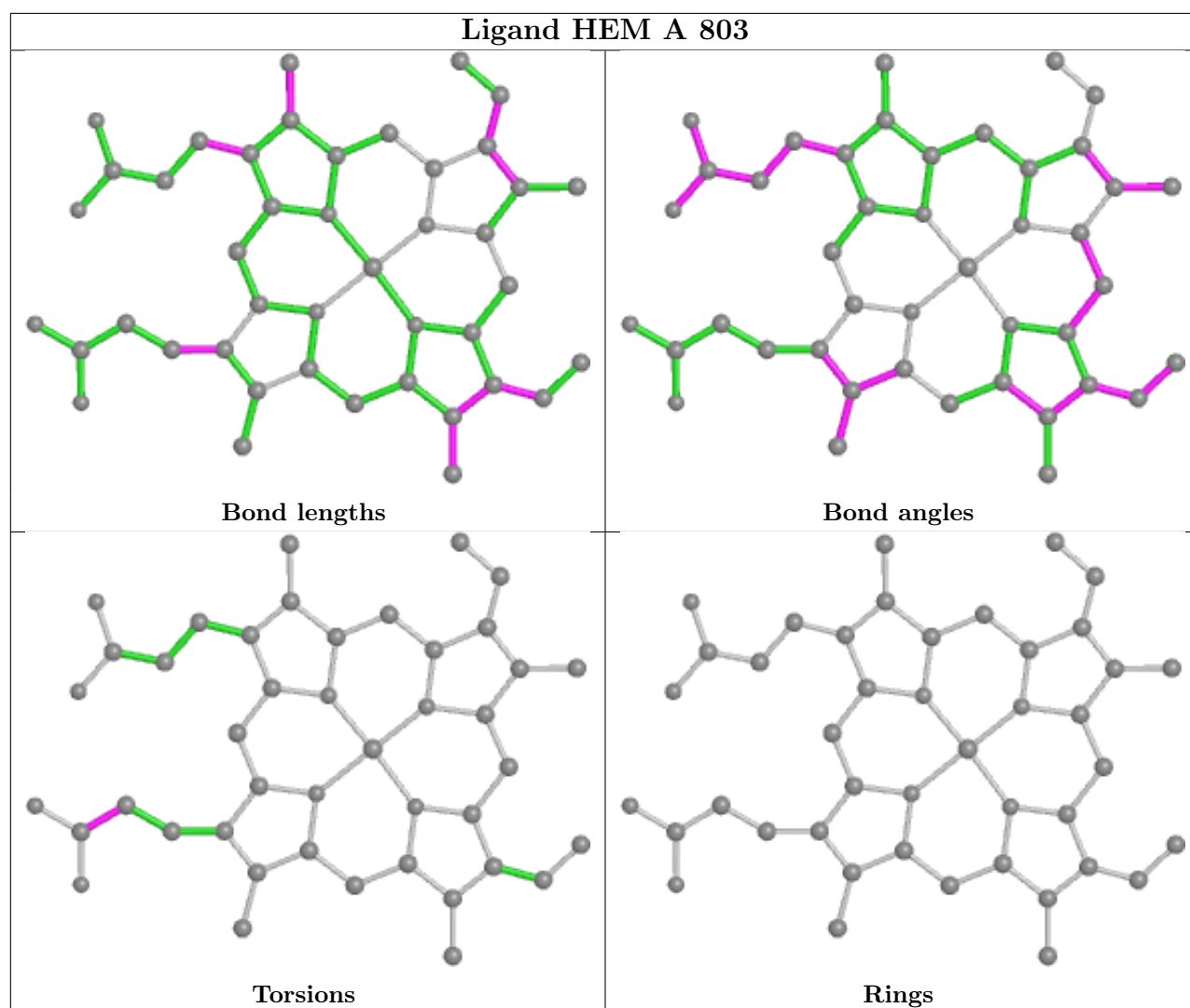












5.7 Other polymers [i](#)

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.