



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 08:15 AM EDT

PDB ID : 1LJ1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

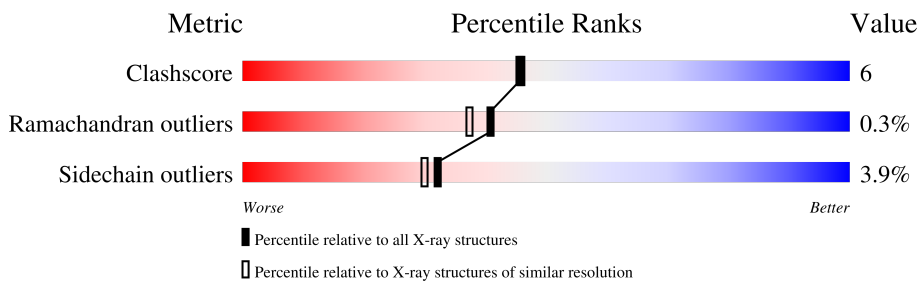
1 Overall quality at a glance

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	86% 11% ...
1	B	571	85% 12% ..

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 (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		

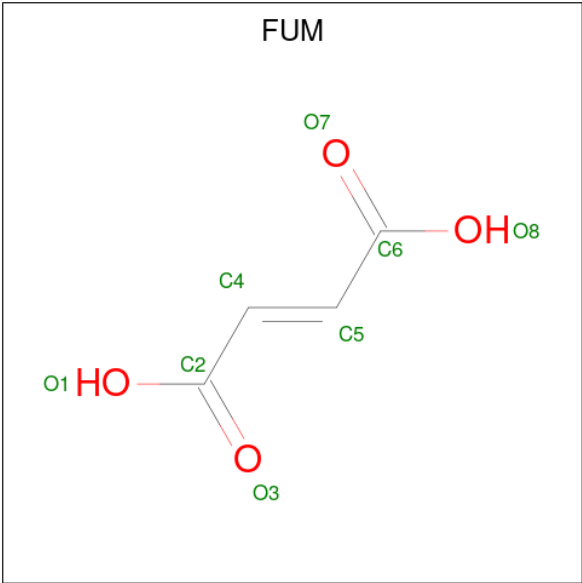
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).





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

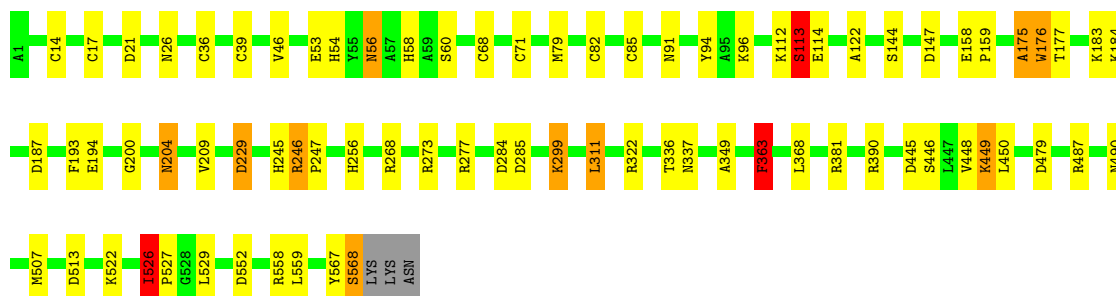
3 Residue-property plots [i](#)

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.

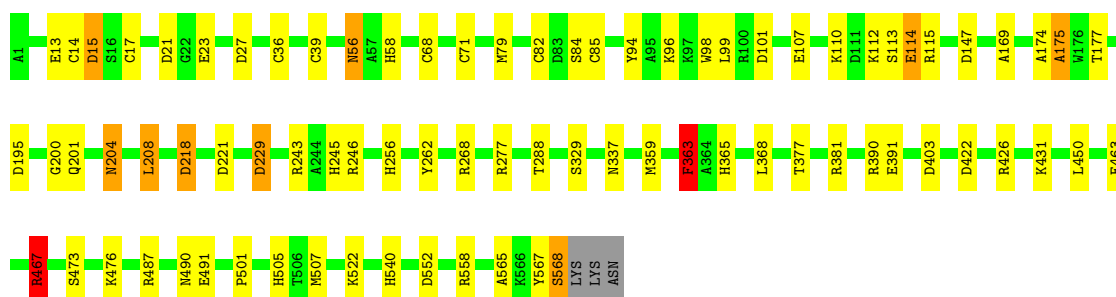
- Molecule 1: flavocytochrome c3

Chain A:  86% 11% ...



- Molecule 1: flavocytochrome c3

Chain B:  85% 12% ..



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: 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	0.67	1/4258 (0.0%)	1.41	34/5764 (0.6%)
1	B	0.67	0/4275	1.43	46/5782 (0.8%)
All	All	0.67	1/8533 (0.0%)	1.42	80/11546 (0.7%)

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	-5.47	1.35	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	22.09	176.91	121.70
1	B	175	ALA	O-C-N	-13.96	100.37	122.70
1	B	381	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	B	390	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	B	558	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	390	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	A	176	TRP	N-CA-CB	9.63	127.94	110.60
1	B	115	ARG	NE-CZ-NH1	9.17	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	N-CA-CB	9.13	122.88	110.10
1	B	15	ASP	CB-CG-OD2	-9.02	110.18	118.30
1	B	218	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	A	21	ASP	CB-CG-OD1	7.87	125.38	118.30
1	A	381	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	175	ALA	CA-C-N	7.76	134.28	117.20
1	A	113	SER	N-CA-CB	-7.44	99.33	110.50
1	A	268	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	229	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	390	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	487	ARG	NE-CZ-NH2	6.87	123.74	120.30
1	B	403	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	390	ARG	CD-NE-CZ	6.81	133.14	123.60
1	A	390	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	285	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	218	ASP	OD1-CG-OD2	6.75	136.13	123.30
1	A	526	ILE	CA-CB-CG2	6.74	124.38	110.90
1	A	558	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	558	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	390	ARG	CG-CD-NE	6.70	125.87	111.80
1	A	552	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	322	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	B	277	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	218	ASP	CB-CA-C	-6.47	97.46	110.40
1	B	467	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	112	LYS	C-N-CA	6.44	137.80	121.70
1	A	268	ARG	CD-NE-CZ	6.40	132.56	123.60
1	B	174	ALA	N-CA-CB	6.36	119.01	110.10
1	B	15	ASP	N-CA-CB	6.32	121.98	110.60
1	A	526	ILE	CB-CA-C	6.31	124.22	111.60
1	A	187	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	15	ASP	OD1-CG-OD2	6.00	134.70	123.30
1	B	268	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	363	PHE	CB-CG-CD2	5.89	124.92	120.80
1	B	218	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	B	381	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	391	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	B	221	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	277	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	568	SER	CA-C-O	-5.58	108.39	120.10
1	A	273	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	229	ASP	CB-CG-OD1	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	ARG	CG-CD-NE	-5.57	100.11	111.80
1	B	359	MET	CG-SD-CE	5.55	109.08	100.20
1	B	27	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	94	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	B	195	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	491	GLU	OE1-CD-OE2	-5.47	116.74	123.30
1	B	505	HIS	CA-CB-CG	5.45	122.87	113.60
1	B	422	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	277	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	567	TYR	C-N-CA	5.38	135.16	121.70
1	B	208	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	94	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	479	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	147	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	558	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	568	SER	N-CA-C	5.30	125.30	111.00
1	B	467	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	284	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	284	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	147	ASP	CB-CG-OD1	5.21	122.98	118.30
1	B	114	GLU	N-CA-CB	5.18	119.93	110.60
1	B	262	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	363	PHE	CB-CG-CD2	5.12	124.38	120.80
1	B	426	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	246	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	21	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	243	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	122	ALA	N-CA-CB	-5.01	103.09	110.10
1	A	445	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	513	ASP	CB-CG-OD1	5.00	122.80	118.30

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	55	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	28	1
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	8	0	2	0	0
5	B	8	0	2	0	0
6	A	804	0	0	7	1
6	B	826	0	0	9	0
All	All	10489	0	8523	112	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 (112) 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:B:39:CYS:HG	3:B:802:HEM:CAC	1.78	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.58	0.92
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: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:82:CYS:HG	3:B:804:HEM:CAB	1.89	0.83
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.95	0.79
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:71:CYS:HG	3:B:803:HEM:CAC	1.97	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
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: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:A:39:CYS:SG	3:A:802:HEM:C3C	3.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:SER:OG	1:A:449:LYS:HD3	2.12	0.50
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.03	0.49
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:79:MET:CE	1:B:96:LYS:HE3	2.44	0.48
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.01	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: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:HG2	1:A:194:GLU:O	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
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:79:MET:CE	1:A:96:LYS:HE3	2.46	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:79:MET:HE2	1:B:96:LYS:HE3	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.12	0.42
1:B:476:LYS:NZ	6:B:2547:HOH:O	2.53	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: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:CB	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%)	34 30
1	B	566/571 (99%)	545 (96%)	20 (4%)	1 (0%)	47 44
All	All	1132/1142 (99%)	1088 (96%)	41 (4%)	3 (0%)	41 37

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%)	416 (96%)	16 (4%)	34	32
1	B	438/444 (99%)	420 (96%)	18 (4%)	30	28
All	All	870/888 (98%)	836 (96%)	34 (4%)	32	30

All (34) 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
1	A	144	SER
1	A	204	ASN
1	A	299	LYS
1	A	311	LEU
1	A	337	ASN
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	56	ASN
1	B	99	LEU
1	B	112	LYS

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Mol	Chain	Res	Type
1	B	113	SER
1	B	204	ASN
1	B	208	LEU
1	B	218	ASP
1	B	246	ARG
1	B	288	THR
1	B	337	ASN
1	B	363	PHE
1	B	450	LEU
1	B	467	ARG
1	B	473	SER
1	B	490	ASN
1	B	522	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	10	GLN
1	B	56	ASN
1	B	116	GLN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	490	ASN
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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	804	1	27,50,50	1.91	5 (18%)	17,82,82	2.13	8 (47%)
3	HEM	A	801	1	27,50,50	2.08	7 (25%)	17,82,82	2.40	7 (41%)
4	FAD	B	1800	-	51,58,58	2.10	11 (21%)	60,89,89	2.14	11 (18%)
4	FAD	A	1700	-	51,58,58	2.00	14 (27%)	60,89,89	2.31	14 (23%)
5	FUM	A	1701	-	1,7,7	0.73	0	2,8,8	3.44	2 (100%)
3	HEM	A	803	1	27,50,50	1.92	7 (25%)	17,82,82	1.81	5 (29%)
5	FUM	B	1801	-	1,7,7	0.52	0	2,8,8	1.28	0
3	HEM	A	802	1	27,50,50	1.97	6 (22%)	17,82,82	2.36	6 (35%)
3	HEM	B	801	1	27,50,50	2.23	9 (33%)	17,82,82	2.06	8 (47%)
3	HEM	B	802	1	27,50,50	1.95	6 (22%)	17,82,82	2.35	9 (52%)
3	HEM	A	804	1	27,50,50	2.03	5 (18%)	17,82,82	2.13	8 (47%)
3	HEM	B	803	1	27,50,50	2.10	6 (22%)	17,82,82	2.29	6 (35%)

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	804	1	-	0/6/54/54	-
3	HEM	A	801	1	-	1/6/54/54	-
4	FAD	B	1800	-	-	8/30/50/50	0/6/6/6
4	FAD	A	1700	-	-	6/30/50/50	0/6/6/6
5	FUM	A	1701	-	-	0/0/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	803	1	-	1/6/54/54	-
5	FUM	B	1801	-	-	0/0/5/5	-
3	HEM	A	802	1	-	0/6/54/54	-
3	HEM	B	801	1	-	0/6/54/54	-
3	HEM	B	802	1	-	1/6/54/54	-
3	HEM	A	804	1	-	0/6/54/54	-
3	HEM	B	803	1	-	0/6/54/54	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1800	FAD	C1'-N10	6.34	1.54	1.48
4	B	1800	FAD	C4-N3	5.89	1.43	1.33
4	B	1800	FAD	C4-C4X	5.77	1.51	1.41
3	B	803	HEM	C3B-C2B	-5.73	1.32	1.40
3	B	801	HEM	C3C-C2C	-5.49	1.32	1.40
4	A	1700	FAD	C4-C4X	5.33	1.50	1.41
4	A	1700	FAD	C4X-C10	5.29	1.44	1.38
3	B	801	HEM	C3B-C2B	-5.19	1.33	1.40
3	A	801	HEM	C3B-C2B	-5.09	1.33	1.40
4	A	1700	FAD	C1'-N10	4.86	1.53	1.48
3	A	804	HEM	C3C-C2C	-4.79	1.33	1.40
4	B	1800	FAD	C4X-C10	4.77	1.43	1.38
3	A	802	HEM	C3B-C2B	-4.71	1.33	1.40
3	A	804	HEM	C3B-C2B	-4.69	1.33	1.40
4	A	1700	FAD	C2'-C3'	4.64	1.62	1.53
3	B	802	HEM	C3C-C2C	-4.57	1.34	1.40
3	A	803	HEM	C3C-C2C	-4.55	1.34	1.40
3	A	801	HEM	C3C-C2C	-4.54	1.34	1.40
3	B	804	HEM	C3B-C2B	-4.46	1.34	1.40
4	A	1700	FAD	C4-N3	4.46	1.40	1.33
3	B	803	HEM	C3C-C2C	-4.36	1.34	1.40
3	A	802	HEM	C3C-C2C	-4.32	1.34	1.40
3	B	802	HEM	C3B-C2B	-4.32	1.34	1.40
3	B	804	HEM	C3C-C2C	-4.29	1.34	1.40
3	A	803	HEM	C3B-C2B	-4.23	1.34	1.40
3	B	802	HEM	C3C-CAC	3.95	1.55	1.47
3	B	804	HEM	C3C-CAC	3.95	1.55	1.47
3	B	801	HEM	C3B-CAB	3.90	1.55	1.47
3	B	803	HEM	C3B-CAB	3.74	1.55	1.47
3	A	802	HEM	C3C-CAC	3.68	1.55	1.47
3	A	803	HEM	C3B-CAB	3.62	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1800	FAD	C2'-C3'	3.61	1.60	1.53
3	A	804	HEM	C3B-CAB	3.49	1.55	1.47
3	A	804	HEM	C3C-CAC	3.45	1.54	1.47
3	A	801	HEM	C3B-CAB	3.35	1.54	1.47
3	B	802	HEM	C3B-CAB	3.26	1.54	1.47
4	B	1800	FAD	C2A-N3A	3.26	1.37	1.32
3	A	801	HEM	C3C-CAC	3.25	1.54	1.47
3	A	803	HEM	C3C-CAC	3.24	1.54	1.47
4	B	1800	FAD	C5'-C4'	3.21	1.56	1.51
3	B	804	HEM	C3B-CAB	3.20	1.54	1.47
3	B	801	HEM	C3C-CAC	3.16	1.54	1.47
4	A	1700	FAD	C2A-N3A	3.09	1.37	1.32
3	A	804	HEM	CAA-C2A	3.08	1.56	1.52
3	A	802	HEM	CAA-C2A	3.06	1.56	1.52
4	B	1800	FAD	O4'-C4'	3.06	1.49	1.43
4	B	1800	FAD	C9-C8	3.03	1.45	1.37
3	B	801	HEM	CAA-C2A	2.96	1.56	1.52
3	B	803	HEM	C3C-CAC	2.90	1.53	1.47
3	A	801	HEM	CAA-C2A	2.81	1.56	1.52
3	A	802	HEM	C3B-CAB	2.67	1.53	1.47
4	A	1700	FAD	C2B-C1B	2.56	1.57	1.53
3	B	804	HEM	CAA-C2A	2.47	1.55	1.52
3	B	803	HEM	CAD-C3D	2.42	1.56	1.52
3	B	801	HEM	C4A-NA	2.39	1.41	1.36
4	A	1700	FAD	C6-C5X	2.38	1.45	1.41
3	B	802	HEM	CMA-C3A	2.37	1.56	1.51
4	B	1800	FAD	O4-C4	-2.35	1.18	1.24
3	B	801	HEM	CMC-C2C	2.34	1.57	1.51
4	A	1700	FAD	C8M-C8	2.27	1.55	1.51
3	A	802	HEM	CMD-C2D	2.27	1.56	1.51
3	B	801	HEM	CAD-C3D	2.23	1.56	1.52
3	B	801	HEM	CMA-C3A	2.22	1.56	1.51
4	A	1700	FAD	C9-C8	2.21	1.43	1.37
3	A	801	HEM	CMD-C2D	2.20	1.56	1.51
4	A	1700	FAD	C10-N1	-2.15	1.30	1.33
4	A	1700	FAD	O4-C4	-2.13	1.19	1.24
3	A	801	HEM	CMA-C3A	2.12	1.56	1.51
3	A	803	HEM	CAD-C3D	2.10	1.55	1.52
4	B	1800	FAD	C6-C5X	2.10	1.45	1.41
3	A	803	HEM	CMD-C2D	2.10	1.56	1.51
4	A	1700	FAD	C5X-N5	2.09	1.38	1.35
3	B	803	HEM	CAA-C2A	2.08	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	HEM	C4A-NA	2.07	1.40	1.36
4	A	1700	FAD	C2-N3	2.05	1.42	1.38
3	A	803	HEM	CMA-C3A	2.01	1.55	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1700	FAD	C4-N3-C2	8.53	122.34	115.14
4	A	1700	FAD	C4X-C4-N3	-7.70	112.89	123.43
4	B	1800	FAD	C4-N3-C2	7.64	121.59	115.14
3	B	803	HEM	CAD-CBD-CGD	7.29	124.90	112.67
4	B	1800	FAD	C4X-C4-N3	-6.39	114.69	123.43
4	B	1800	FAD	C4-C4X-C10	-6.26	115.80	119.95
4	A	1700	FAD	O4B-C1B-C2B	-5.82	98.42	106.93
3	A	802	HEM	CAA-CBA-CGA	5.74	122.31	112.67
4	A	1700	FAD	O5'-C5'-C4'	-5.31	95.19	109.36
4	B	1800	FAD	O4'-C4'-C3'	-5.06	96.80	109.10
4	B	1800	FAD	O5'-C5'-C4'	-5.01	95.98	109.36
3	A	801	HEM	CAA-CBA-CGA	4.89	120.88	112.67
3	A	802	HEM	CMD-C2D-C1D	-4.82	121.06	128.46
3	B	802	HEM	CBD-CAD-C3D	4.70	121.14	112.48
3	B	801	HEM	CAA-CBA-CGA	4.54	120.29	112.67
3	A	804	HEM	CMD-C2D-C1D	-4.53	121.51	128.46
3	A	803	HEM	CAD-CBD-CGD	4.26	119.82	112.67
4	B	1800	FAD	O4B-C1B-C2B	-4.23	100.74	106.93
3	B	802	HEM	CMD-C2D-C1D	-4.15	122.08	128.46
4	A	1700	FAD	O4'-C4'-C3'	-4.13	99.06	109.10
4	A	1700	FAD	C4-C4X-C10	-3.91	117.36	119.95
3	A	801	HEM	CMD-C2D-C1D	-3.89	122.49	128.46
3	B	804	HEM	CMD-C2D-C1D	-3.80	122.63	128.46
3	A	801	HEM	CAD-CBD-CGD	3.76	118.99	112.67
5	A	1701	FUM	C6-C5-C4	-3.71	115.76	123.69
3	B	804	HEM	CMB-C2B-C3B	3.55	131.32	124.68
4	B	1800	FAD	O2'-C2'-C3'	-3.49	100.62	109.10
3	A	804	HEM	CMD-C2D-C3D	3.40	131.35	124.94
4	A	1700	FAD	O3'-C3'-C2'	-3.31	100.81	108.81
3	A	802	HEM	CMD-C2D-C3D	3.30	131.16	124.94
3	B	801	HEM	CMD-C2D-C1D	-3.27	123.44	128.46
3	B	804	HEM	CBD-CAD-C3D	3.26	118.48	112.48
3	B	802	HEM	CMB-C2B-C3B	3.25	130.76	124.68
4	A	1700	FAD	C10-C4X-N5	3.25	123.50	121.26
5	A	1701	FUM	C2-C4-C5	-3.15	116.96	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1700	FAD	C5A-C6A-N6A	3.08	125.03	120.35
3	B	804	HEM	CMA-C3A-C4A	-3.00	123.85	128.46
3	B	804	HEM	CMD-C2D-C3D	3.00	130.60	124.94
3	A	801	HEM	CMA-C3A-C4A	-2.99	123.87	128.46
3	B	804	HEM	CMC-C2C-C3C	2.93	130.16	124.68
3	A	801	HEM	CMB-C2B-C3B	2.92	130.15	124.68
3	B	802	HEM	CMD-C2D-C3D	2.88	130.37	124.94
3	B	802	HEM	CAA-CBA-CGA	2.85	117.45	112.67
3	A	804	HEM	CMC-C2C-C3C	2.85	130.00	124.68
3	A	801	HEM	CMD-C2D-C3D	2.83	130.28	124.94
4	A	1700	FAD	C9A-N10-C10	-2.80	118.24	121.91
4	A	1700	FAD	O2'-C2'-C1'	2.79	116.30	109.59
4	A	1700	FAD	C5'-C4'-C3'	2.77	117.55	112.20
3	B	801	HEM	CBD-CAD-C3D	-2.70	107.50	112.48
3	A	804	HEM	CAA-CBA-CGA	2.69	117.18	112.67
3	A	804	HEM	CBD-CAD-C3D	2.66	117.38	112.48
3	A	803	HEM	CMA-C3A-C4A	-2.64	124.41	128.46
3	B	801	HEM	CMD-C2D-C3D	2.63	129.90	124.94
3	A	802	HEM	CMB-C2B-C3B	2.62	129.58	124.68
3	A	801	HEM	CMC-C2C-C3C	2.61	129.56	124.68
4	B	1800	FAD	C10-C4X-N5	2.56	123.03	121.26
3	B	803	HEM	CMC-C2C-C3C	2.45	129.27	124.68
3	B	804	HEM	CMA-C3A-C2A	2.42	129.50	124.94
3	B	803	HEM	CMA-C3A-C4A	-2.40	124.77	128.46
3	B	801	HEM	CMC-C2C-C3C	2.38	129.14	124.68
4	A	1700	FAD	O2'-C2'-C3'	-2.35	103.37	109.10
3	A	804	HEM	CMA-C3A-C4A	-2.35	124.85	128.46
3	B	802	HEM	CBA-CAA-C2A	2.35	116.82	112.49
4	B	1800	FAD	O2A-PA-O1A	2.34	123.83	112.24
4	A	1700	FAD	O2A-PA-O1A	2.31	123.67	112.24
3	A	802	HEM	CMC-C2C-C3C	2.31	128.99	124.68
3	B	801	HEM	CMA-C3A-C4A	-2.29	124.95	128.46
3	A	802	HEM	CMA-C3A-C4A	-2.26	124.99	128.46
3	B	803	HEM	CMB-C2B-C3B	2.22	128.84	124.68
3	B	802	HEM	CMC-C2C-C3C	2.22	128.83	124.68
3	A	803	HEM	CMD-C2D-C1D	-2.21	125.07	128.46
3	A	803	HEM	CMB-C2B-C3B	2.20	128.79	124.68
4	B	1800	FAD	C4-C4X-N5	2.19	121.10	118.60
3	A	804	HEM	CMB-C2B-C3B	2.19	128.77	124.68
3	B	801	HEM	C4A-C3A-C2A	2.18	108.51	107.00
3	A	804	HEM	CAD-CBD-CGD	2.15	116.28	112.67
3	B	802	HEM	CMA-C3A-C4A	-2.12	125.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	HEM	CBA-CAA-C2A	2.08	116.33	112.49
3	B	804	HEM	CAA-CBA-CGA	2.06	116.13	112.67
3	B	801	HEM	CMB-C2B-C3B	2.05	128.51	124.68
3	B	802	HEM	C4C-C3C-C2C	2.02	108.31	106.90
3	B	803	HEM	CMD-C2D-C1D	-2.01	125.38	128.46
3	A	803	HEM	CMC-C2C-C3C	2.01	128.43	124.68
4	B	1800	FAD	C1B-N9A-C4A	-2.01	123.12	126.64

There are no chirality outliers.

All (17) 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'
4	A	1700	FAD	C2'-C3'-C4'-O4'
4	B	1800	FAD	O3'-C3'-C4'-C5'
4	A	1700	FAD	C2'-C3'-C4'-C5'
4	B	1800	FAD	C2'-C3'-C4'-C5'
4	B	1800	FAD	P-O3P-PA-O1A
4	A	1700	FAD	PA-O3P-P-O5'
4	A	1700	FAD	P-O3P-PA-O1A
4	B	1800	FAD	P-O3P-PA-O2A
4	A	1700	FAD	P-O3P-PA-O2A
3	A	801	HEM	C3D-CAD-CBD-CGD
3	A	803	HEM	C2A-CAA-CBA-CGA
4	A	1700	FAD	O4B-C4B-C5B-O5B
4	B	1800	FAD	O4B-C4B-C5B-O5B
3	B	802	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

9 monomers are involved in 57 short contacts:

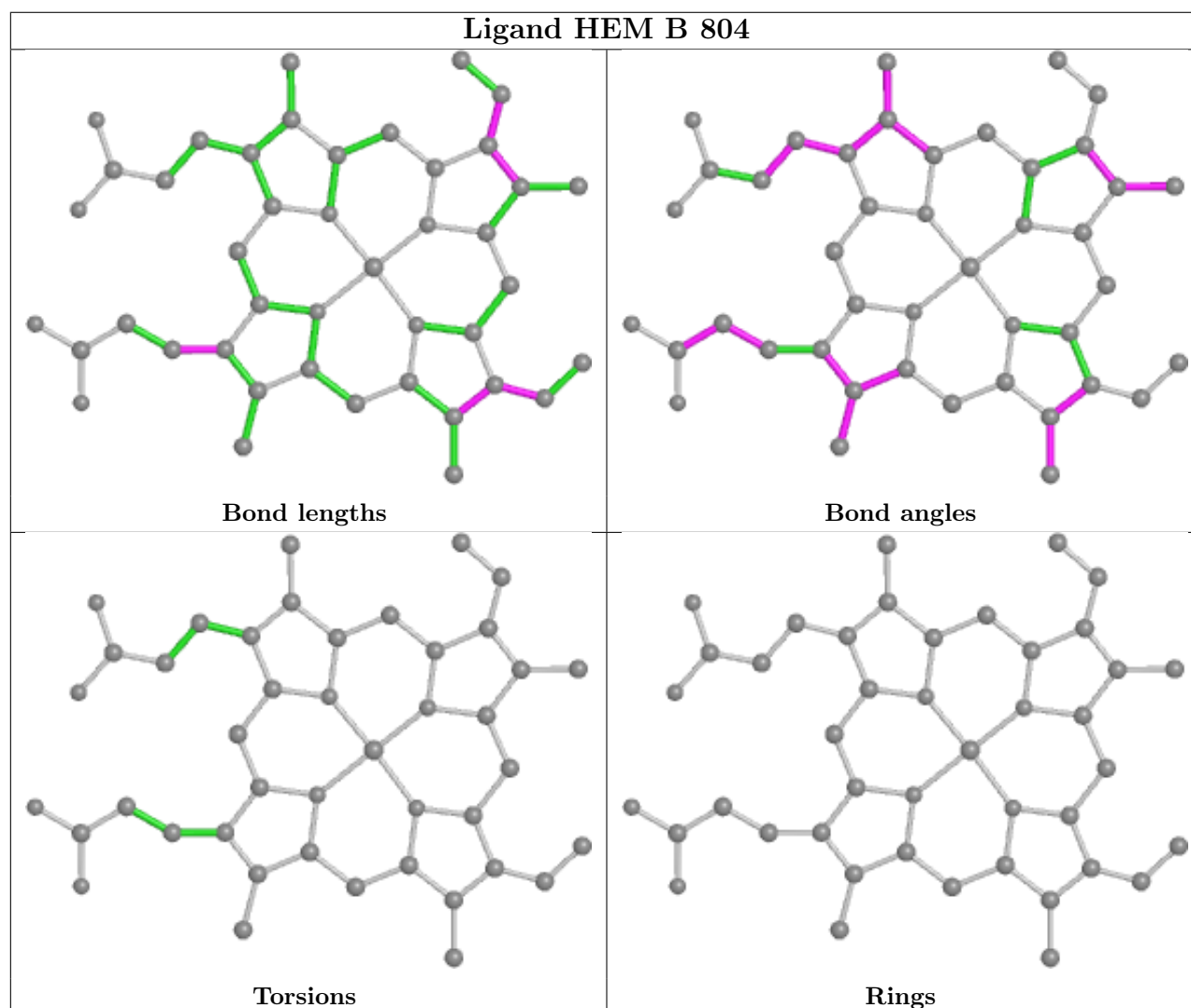
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	HEM	7	0
3	A	801	HEM	6	0
4	A	1700	FAD	1	0
3	A	803	HEM	5	0
3	A	802	HEM	7	0
3	B	801	HEM	5	0
3	B	802	HEM	8	1

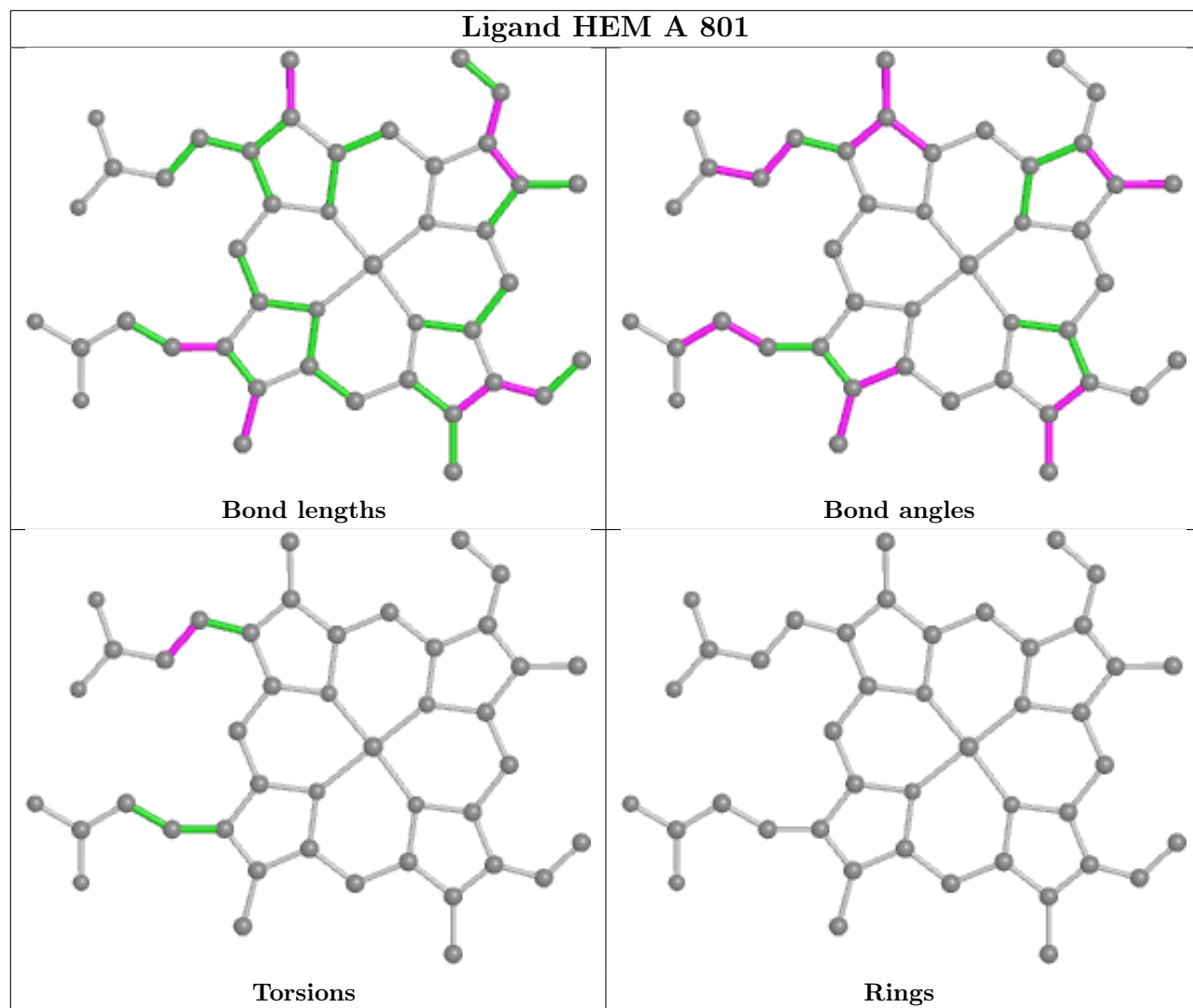
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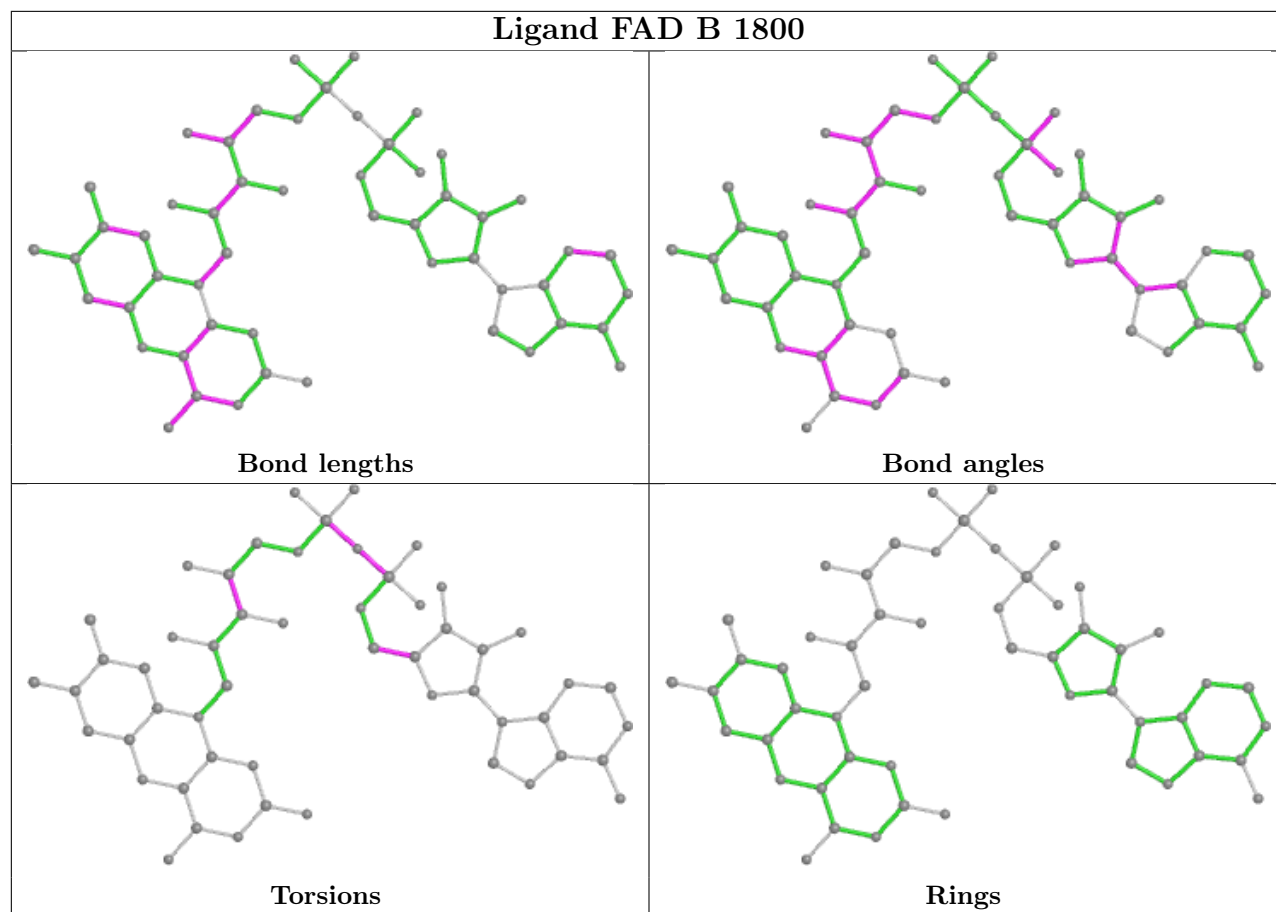
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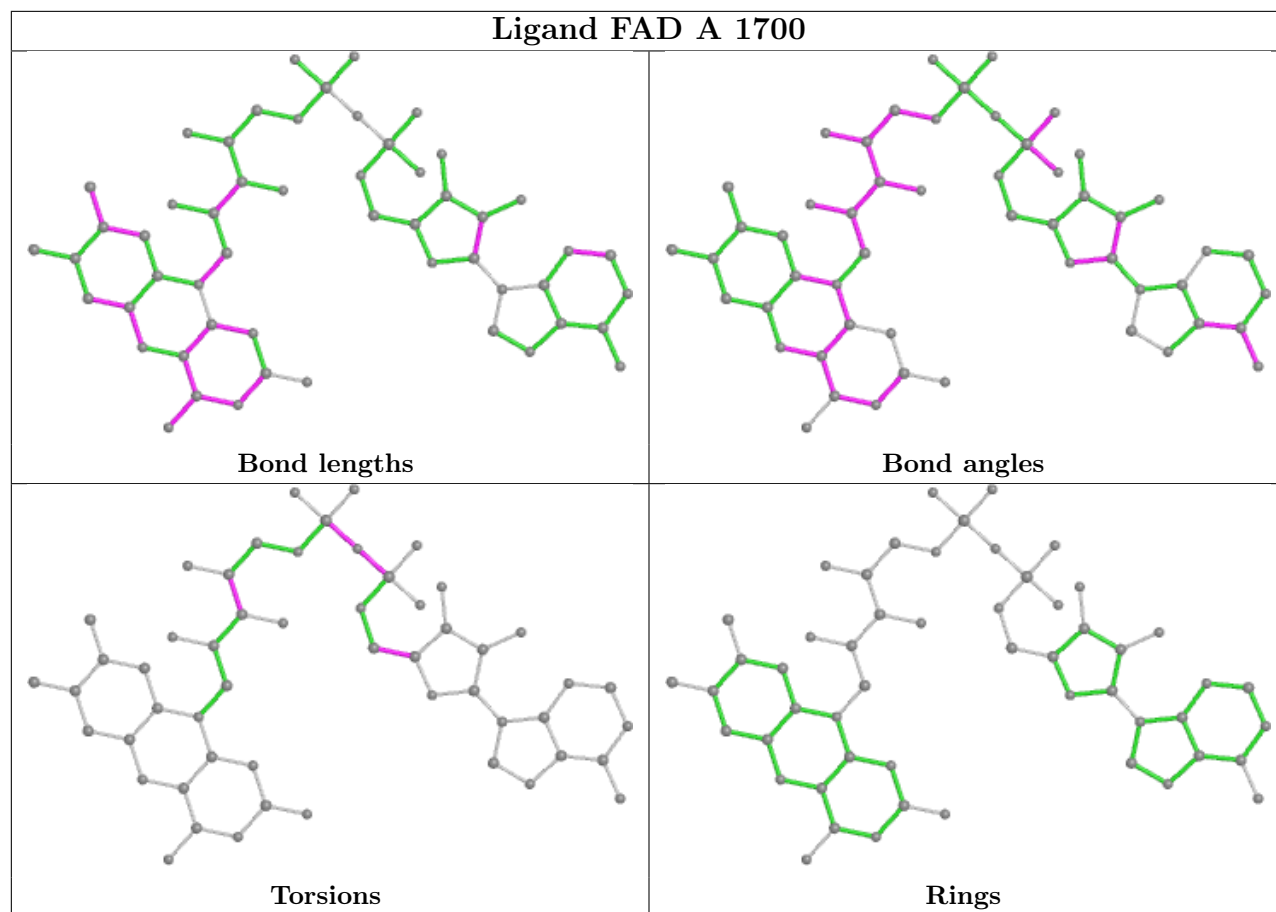
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	HEM	9	0
3	B	803	HEM	8	0

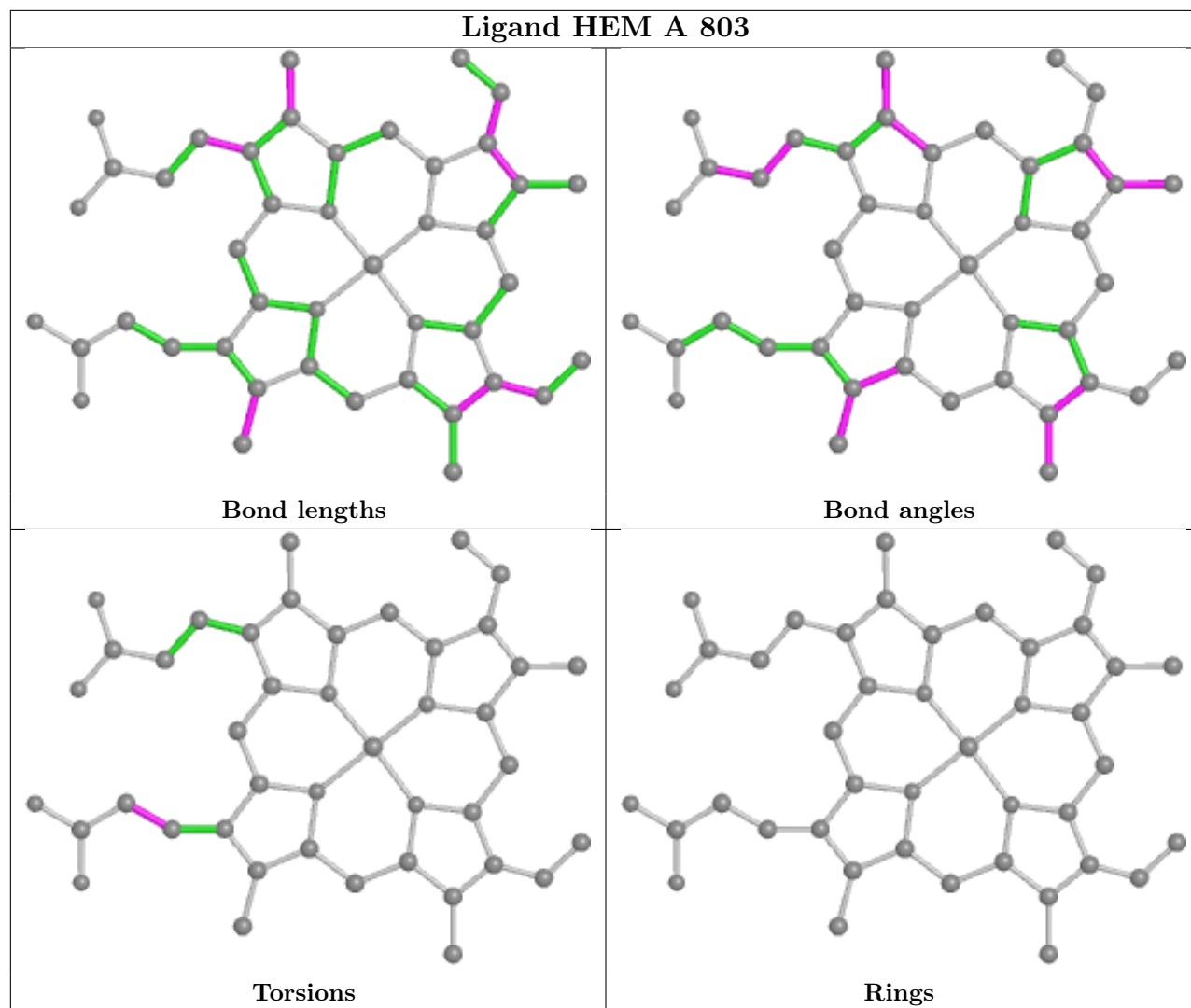
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

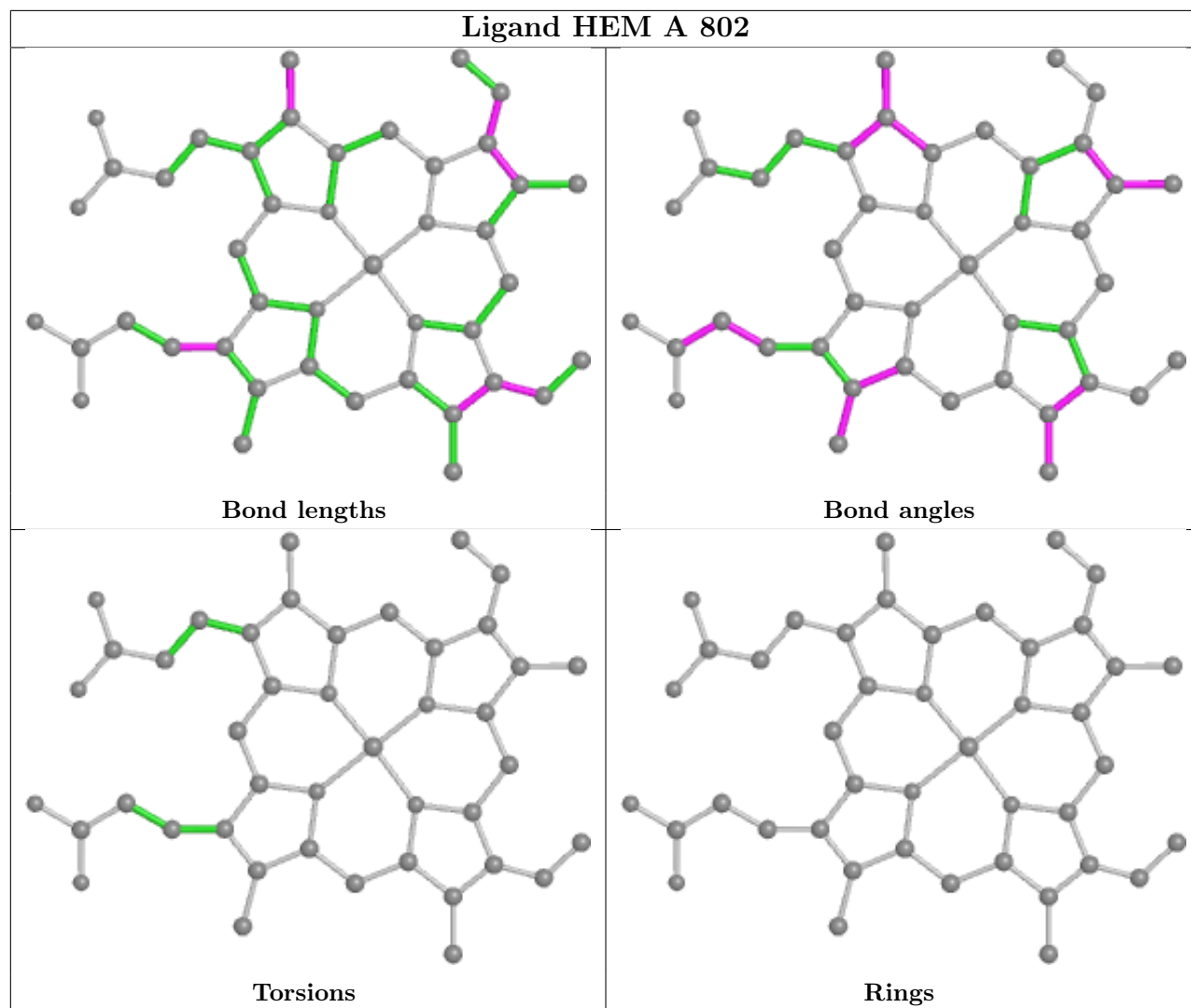


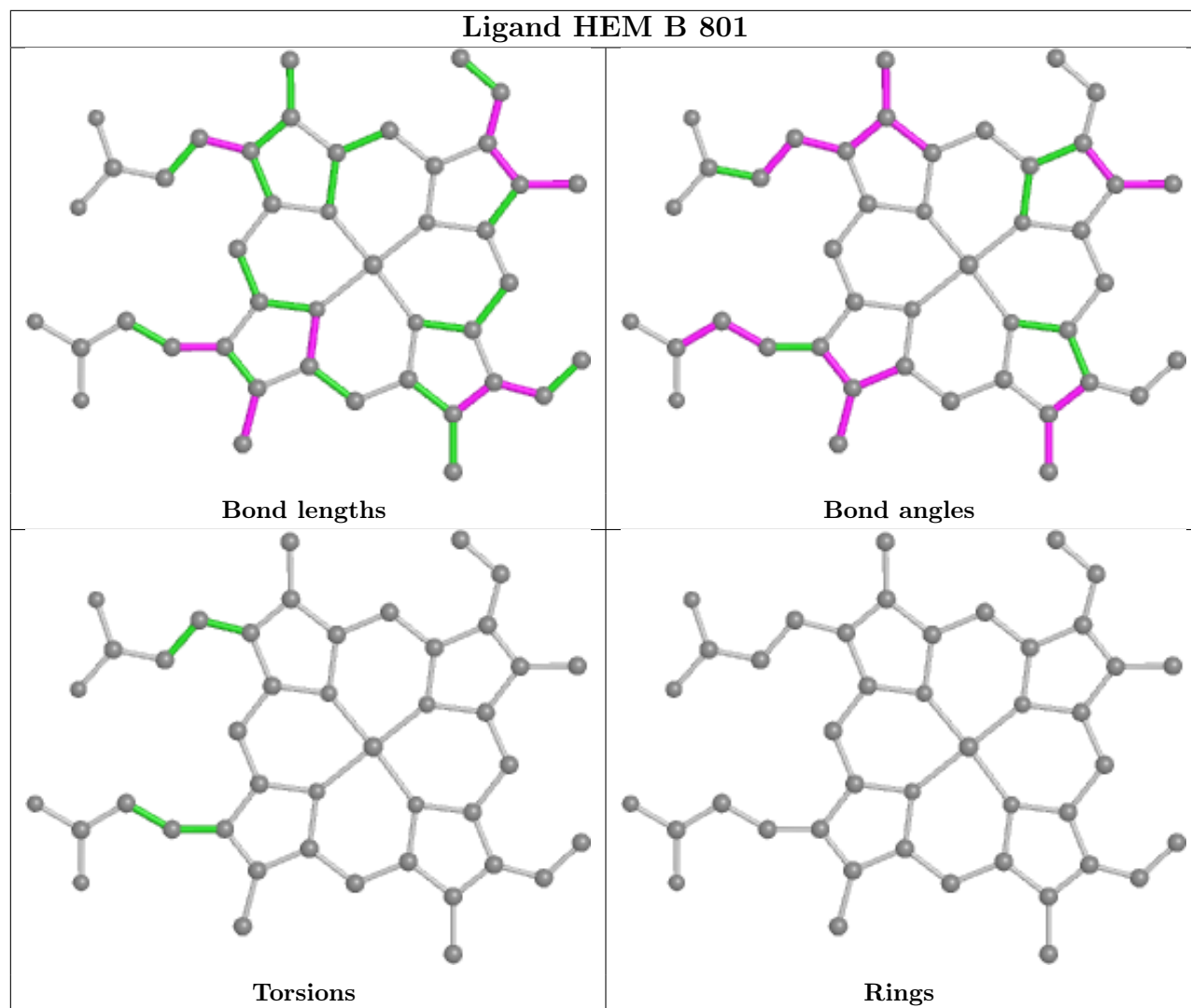


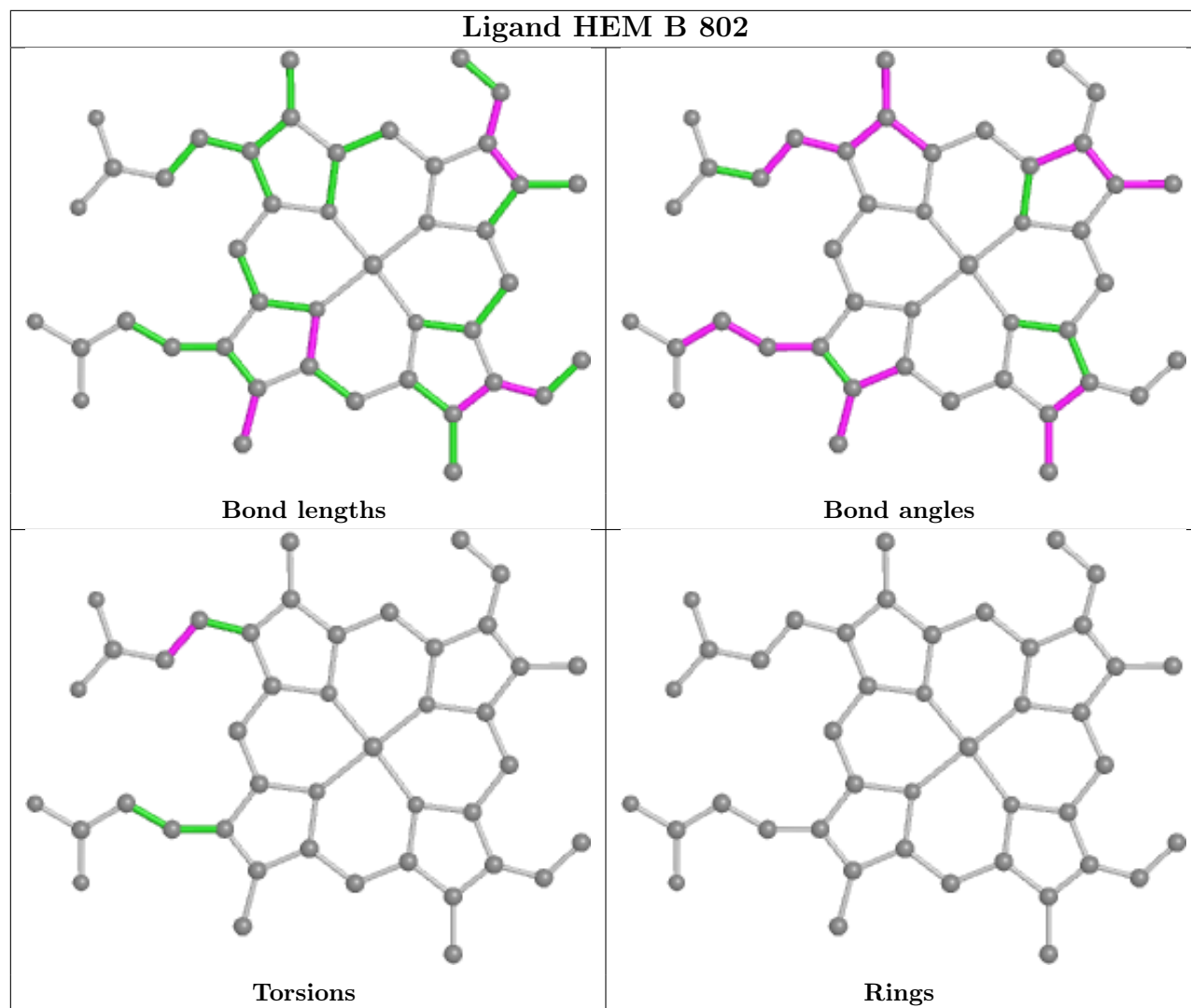


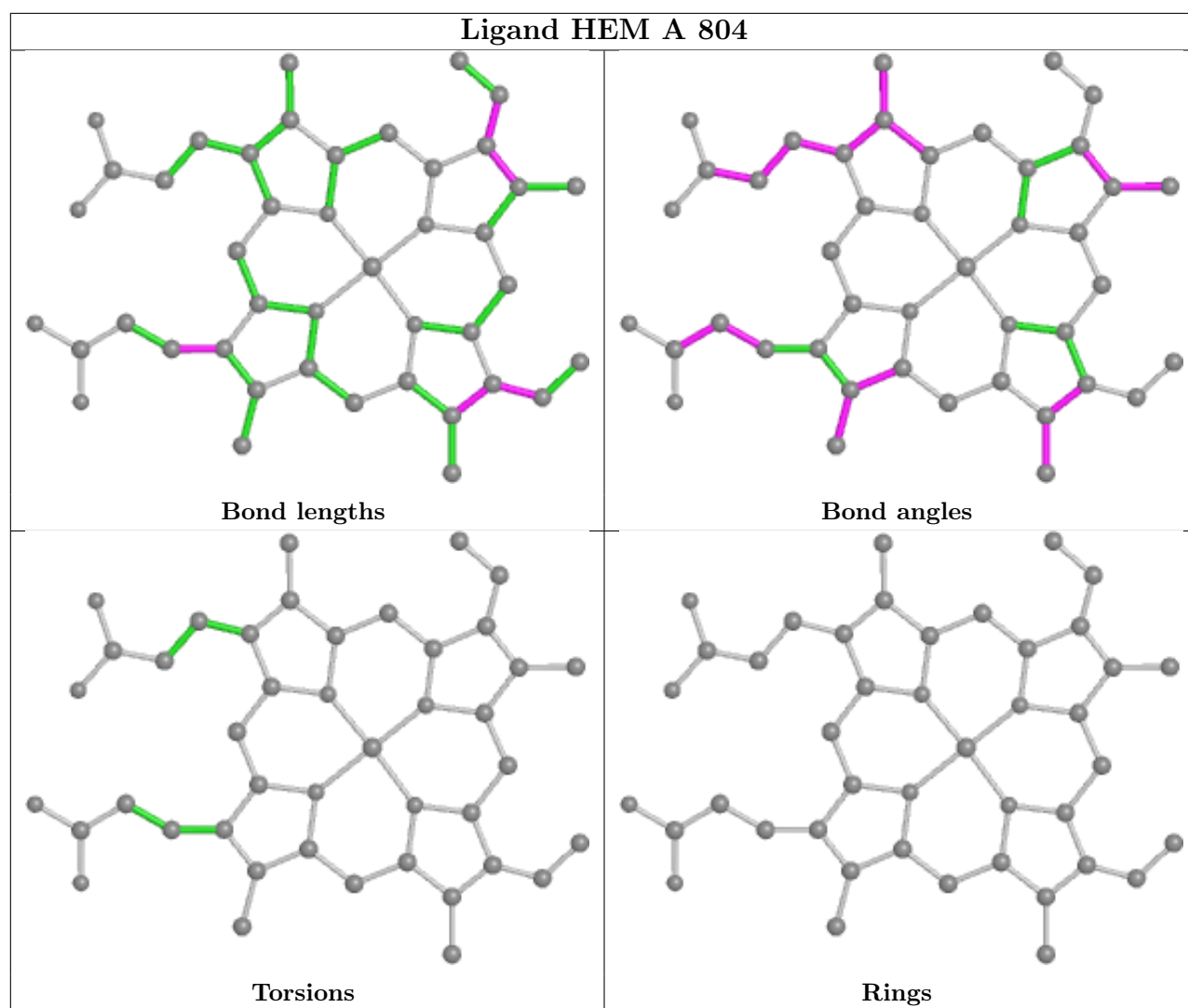


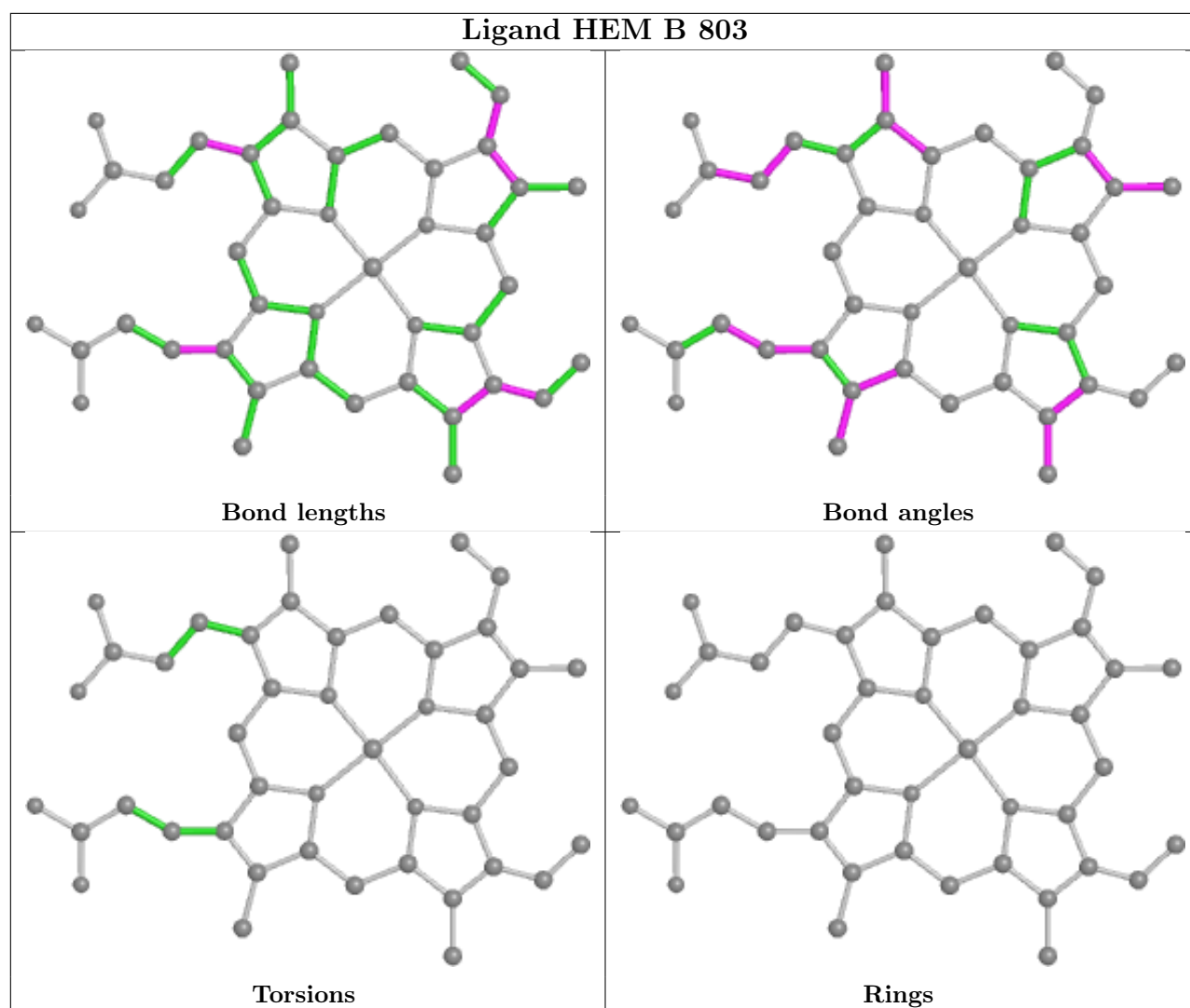












5.7 Other polymers [i](#)

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.