



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:41 PM UTC

PDB ID : 1P2E / pdb_00001p2e
Title : H61A mutant of flavocytochrome c3
Authors : Rothery, E.L.; Mowat, C.G.; Miles, C.S.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2003-04-15
Resolution : 2.20 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)	:	2.49

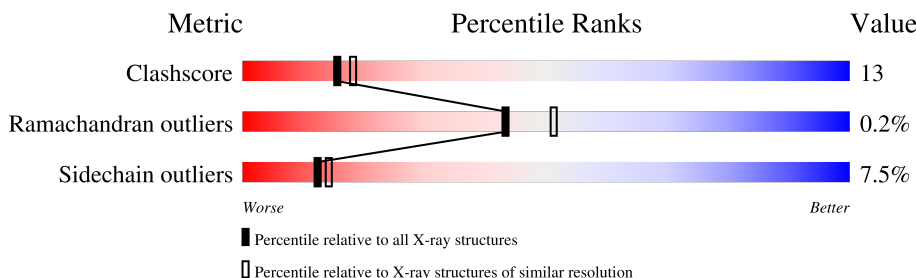
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	

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	805	X	-	-	-
5	FUM	A	806	-	-	X	-
6	ACY	A	811	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4921 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
			4162	2584	729	824	25			

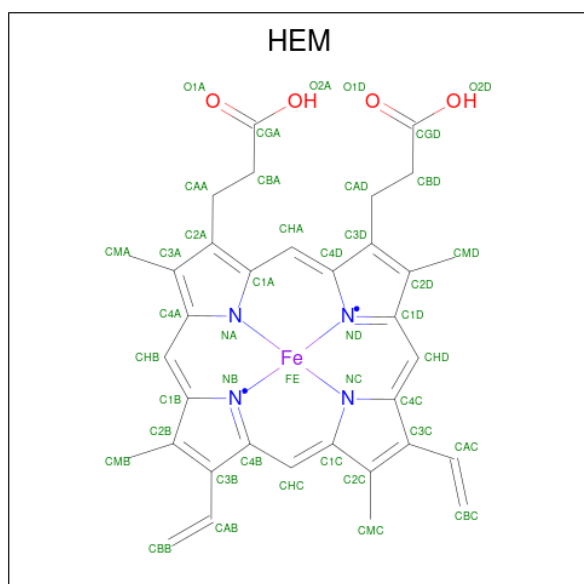
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	HIS	engineered mutation	UNP Q02469

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

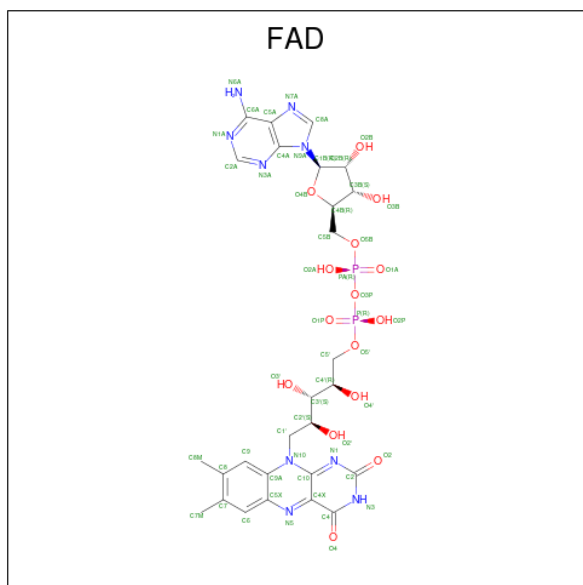
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



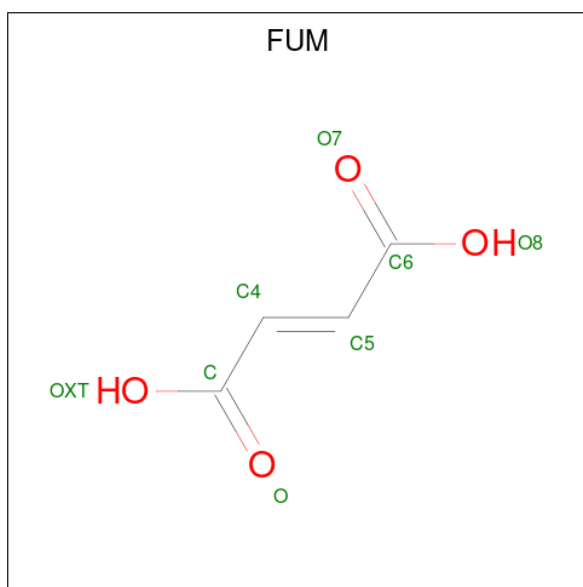
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



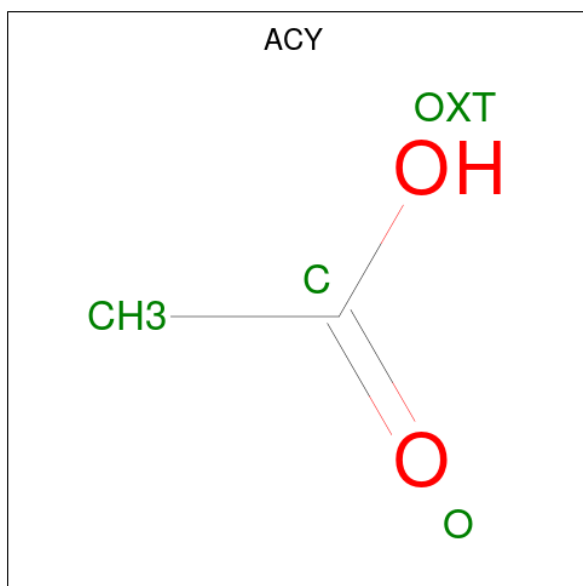
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

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



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

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

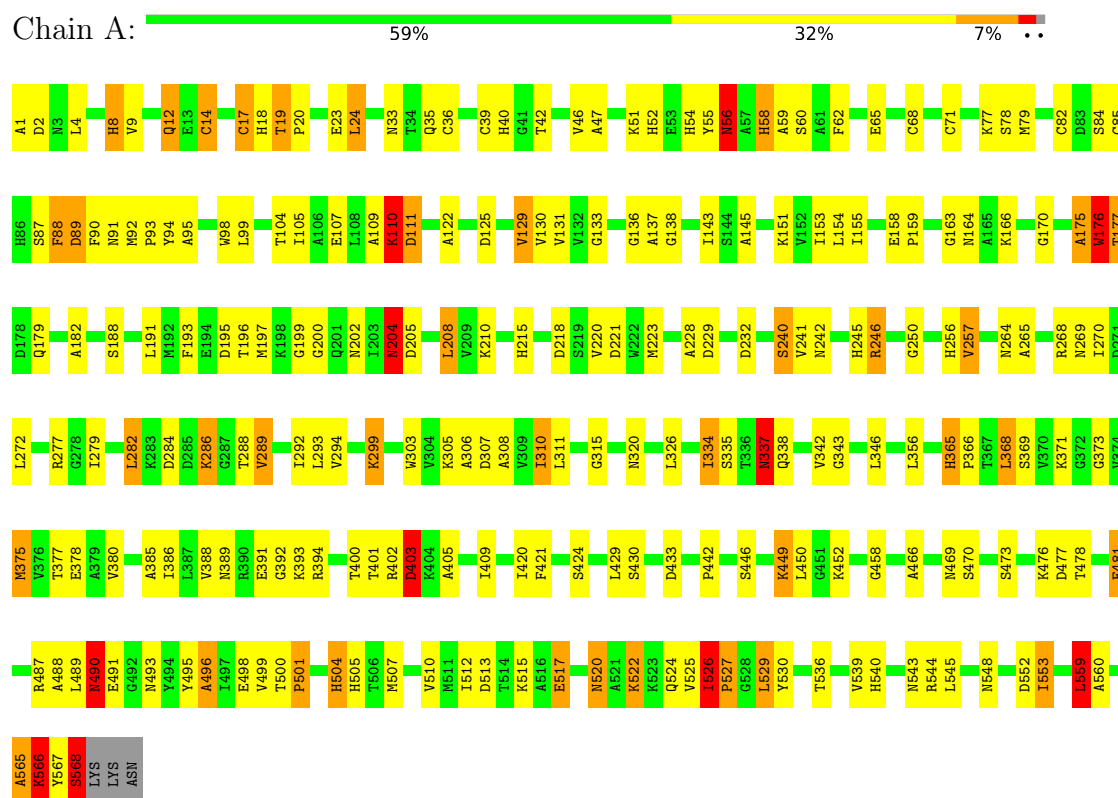
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	521	Total 521	O 521	0	0

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



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	45.35Å 87.08Å 79.68Å 90.00° 109.38° 90.00°	Depositor
Resolution (Å)	17.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4921	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: ACY, HEM, NA, FAD, 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	1.05	1/4231 (0.0%)	2.28	201/5731 (3.5%)

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	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	-7.82	1.36	1.46

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	CA-C-N	19.93	159.60	121.54
1	A	175	ALA	C-N-CA	19.93	159.60	121.54
1	A	202	ASN	CA-CB-CG	-11.23	101.37	112.60
1	A	389	ASN	OD1-CG-ND2	11.03	133.63	122.60
1	A	8	HIS	CA-CB-CG	10.75	124.55	113.80
1	A	481	GLU	CB-CG-CD	10.44	130.35	112.60
1	A	493	ASN	CA-CB-CG	-10.42	102.18	112.60
1	A	525	VAL	CA-C-N	-10.39	115.53	122.60
1	A	525	VAL	C-N-CA	-10.39	115.53	122.60
1	A	56	ASN	CA-CB-CG	10.13	122.73	112.60
1	A	490	ASN	OD1-CG-ND2	-10.01	112.59	122.60
1	A	195	ASP	CA-CB-CG	9.97	122.57	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PRO	CB-CA-C	9.52	122.98	111.46
1	A	90	PHE	CA-C-O	-9.29	110.59	121.46
1	A	221	ASP	CA-CB-CG	9.02	121.62	112.60
1	A	552	ASP	CA-CB-CG	8.93	121.53	112.60
1	A	33	ASN	OD1-CG-ND2	8.71	131.31	122.60
1	A	52	HIS	CA-CB-CG	8.47	122.27	113.80
1	A	394	ARG	CD-NE-CZ	8.41	136.18	124.40
1	A	337	ASN	N-CA-C	8.16	121.06	110.53
1	A	92	MET	CA-C-O	-8.12	111.95	120.23
1	A	277	ARG	NE-CZ-NH1	-8.10	113.40	121.50
1	A	385	ALA	CA-C-O	-7.92	112.68	121.87
1	A	566	LYS	CA-C-O	7.92	129.13	120.82
1	A	90	PHE	CA-C-N	-7.50	111.11	123.04
1	A	90	PHE	C-N-CA	-7.50	111.11	123.04
1	A	215	HIS	CA-CB-CG	7.47	121.27	113.80
1	A	540	HIS	CA-CB-CG	-7.44	106.36	113.80
1	A	526	ILE	CA-CB-CG2	7.42	123.12	110.50
1	A	466	ALA	CA-C-O	-7.38	112.66	120.63
1	A	377	THR	CA-C-O	7.36	129.24	121.15
1	A	54	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	89	ASP	CA-C-O	-7.26	113.00	120.84
1	A	177	THR	N-CA-C	7.26	120.35	110.55
1	A	303	TRP	CA-C-O	7.22	129.56	121.11
1	A	289	VAL	N-CA-CB	7.21	121.38	110.13
1	A	487	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	A	241	VAL	CA-C-O	-7.10	114.68	121.64
1	A	269	ASN	CA-CB-CG	-7.08	105.52	112.60
1	A	58	HIS	CA-CB-CG	-7.04	106.76	113.80
1	A	59	ALA	CA-C-O	-7.04	111.61	120.20
1	A	277	ARG	NH1-CZ-NH2	7.04	128.45	119.30
1	A	18	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	137	ALA	O-C-N	6.96	130.09	122.15
1	A	405	ALA	CA-C-O	-6.93	113.08	120.42
1	A	420	ILE	CA-C-O	-6.83	113.12	120.36
1	A	277	ARG	CD-NE-CZ	6.82	133.94	124.40
1	A	380	VAL	CA-C-O	-6.79	113.89	120.95
1	A	526	ILE	CB-CA-C	6.72	118.74	110.95
1	A	35	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	264	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	402	ARG	CA-C-N	6.67	129.11	120.44
1	A	402	ARG	C-N-CA	6.67	129.11	120.44
1	A	500	THR	CA-C-N	6.60	126.51	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	THR	C-N-CA	6.60	126.51	119.85
1	A	143	ILE	CA-C-O	6.55	127.79	120.85
1	A	272	LEU	CA-C-O	-6.54	113.13	120.32
1	A	145	ALA	N-CA-C	-6.51	104.27	111.36
1	A	54	HIS	N-CA-C	6.49	120.91	112.92
1	A	40	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	565	ALA	CA-C-N	6.42	128.78	120.44
1	A	565	ALA	C-N-CA	6.42	128.78	120.44
1	A	424	SER	N-CA-CB	6.40	119.52	110.12
1	A	65	GLU	CA-C-O	-6.38	114.29	120.92
1	A	130	VAL	CA-C-O	-6.35	113.75	120.48
1	A	179	GLN	CG-CD-NE2	-6.34	106.89	116.40
1	A	515	LYS	CA-C-O	6.34	126.98	119.56
1	A	193	PHE	CA-C-O	6.33	127.67	120.90
1	A	196	THR	CA-C-O	-6.31	114.37	121.00
1	A	218	ASP	CA-CB-CG	6.30	118.91	112.60
1	A	373	GLY	O-C-N	-6.30	115.13	122.31
1	A	95	ALA	O-C-N	-6.28	115.40	122.75
1	A	9	VAL	O-C-N	-6.23	114.78	122.57
1	A	129	VAL	CA-C-N	-6.23	115.47	123.19
1	A	129	VAL	C-N-CA	-6.23	115.47	123.19
1	A	306	ALA	CA-C-O	-6.22	114.57	121.23
1	A	368	LEU	O-C-N	6.21	130.01	123.06
1	A	403	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	110	LYS	CG-CD-CE	6.18	125.51	111.30
1	A	315	GLY	N-CA-C	6.17	121.67	112.41
1	A	242	ASN	CA-C-O	-6.16	113.44	120.58
1	A	154	LEU	CA-C-O	-6.15	113.56	120.32
1	A	510	VAL	CB-CA-C	-6.08	102.01	111.26
1	A	433	ASP	CA-C-O	-6.04	111.95	119.38
1	A	430	SER	CA-C-O	-6.02	113.30	120.10
1	A	151	LYS	CA-C-O	6.00	127.32	120.54
1	A	515	LYS	O-C-N	-5.99	115.15	122.34
1	A	208	LEU	N-CA-CB	-5.98	101.30	110.16
1	A	246	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	495	TYR	CA-C-O	-5.96	114.15	121.06
1	A	517	GLU	O-C-N	5.92	129.96	123.22
1	A	488	ALA	O-C-N	-5.89	116.31	122.96
1	A	1	ALA	O-C-N	5.88	132.41	123.00
1	A	469	ASN	CB-CG-ND2	5.87	125.21	116.40
1	A	307	ASP	O-C-N	5.86	130.18	122.33
1	A	512	ILE	N-CA-CB	5.85	122.29	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ARG	CA-C-O	-5.85	114.34	121.36
1	A	366	PRO	CA-C-N	-5.84	113.75	123.33
1	A	366	PRO	C-N-CA	-5.84	113.75	123.33
1	A	504	HIS	N-CA-CB	-5.84	97.05	110.83
1	A	498	GLU	O-C-N	-5.83	116.22	123.04
1	A	536	THR	CA-C-N	5.82	128.36	122.66
1	A	536	THR	C-N-CA	5.82	128.36	122.66
1	A	402	ARG	CA-CB-CG	-5.80	102.49	114.10
1	A	155	ILE	O-C-N	-5.80	116.94	123.03
1	A	33	ASN	CA-C-O	5.79	126.56	120.42
1	A	305	LYS	O-C-N	-5.79	116.27	123.04
1	A	210	LYS	CA-C-O	-5.78	114.42	120.55
1	A	24	LEU	CA-C-O	-5.77	114.11	120.69
1	A	19	THR	CA-C-N	5.76	125.88	119.32
1	A	19	THR	C-N-CA	5.76	125.88	119.32
1	A	92	MET	O-C-N	5.75	129.46	121.64
1	A	35	GLN	CG-CD-NE2	5.74	125.02	116.40
1	A	501	PRO	CA-C-N	5.74	126.91	121.46
1	A	501	PRO	C-N-CA	5.74	126.91	121.46
1	A	326	LEU	N-CA-CB	-5.73	101.66	110.20
1	A	507	MET	CA-C-O	-5.73	112.34	119.38
1	A	473	SER	CA-C-O	-5.69	114.52	120.55
1	A	179	GLN	CB-CG-CD	5.66	122.22	112.60
1	A	568	SER	CA-C-O	-5.64	111.21	120.80
1	A	89	ASP	N-CA-CB	-5.64	101.08	110.39
1	A	458	GLY	N-CA-C	5.64	119.50	112.73
1	A	176	TRP	CB-CA-C	5.63	121.63	110.42
1	A	520	ASN	O-C-N	-5.62	114.64	121.83
1	A	14	CYS	CB-CA-C	-5.60	101.15	110.68
1	A	110	LYS	CB-CG-CD	5.60	124.19	111.30
1	A	164	ASN	CA-CB-CG	5.60	118.20	112.60
1	A	487	ARG	CG-CD-NE	-5.59	99.70	112.00
1	A	89	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	51	LYS	O-C-N	-5.59	116.07	122.89
1	A	310	ILE	CA-C-O	5.58	126.50	120.53
1	A	279	ILE	CB-CA-C	-5.57	106.15	111.44
1	A	539	VAL	N-CA-C	5.57	115.77	110.53
1	A	122	ALA	O-C-N	-5.53	115.35	121.66
1	A	293	LEU	O-C-N	-5.53	116.91	123.22
1	A	51	LYS	CA-C-O	5.52	127.34	121.16
1	A	170	GLY	CA-C-N	-5.50	113.10	121.62
1	A	170	GLY	C-N-CA	-5.50	113.10	121.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LYS	CG-CD-CE	-5.50	98.66	111.30
1	A	342	VAL	CA-C-N	-5.49	113.90	122.51
1	A	342	VAL	C-N-CA	-5.49	113.90	122.51
1	A	197	MET	CA-C-O	5.48	126.77	120.90
1	A	375	MET	CG-SD-CE	5.48	112.96	100.90
1	A	505	HIS	CA-C-N	-5.48	115.33	123.11
1	A	505	HIS	C-N-CA	-5.48	115.33	123.11
1	A	188	SER	CA-C-O	-5.47	115.06	120.26
1	A	409	ILE	CA-C-N	-5.45	112.43	120.28
1	A	409	ILE	C-N-CA	-5.45	112.43	120.28
1	A	520	ASN	CA-C-O	5.40	128.25	121.50
1	A	268	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	338	GLN	O-C-N	-5.39	115.89	121.60
1	A	111	ASP	CA-C-N	5.38	127.49	120.28
1	A	111	ASP	C-N-CA	5.38	127.49	120.28
1	A	391	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	365	HIS	CA-C-O	5.37	124.54	119.76
1	A	205	ASP	CA-C-O	5.37	123.59	119.46
1	A	60	SER	CA-C-O	-5.36	115.71	121.45
1	A	182	ALA	CA-C-O	5.36	126.02	119.05
1	A	543	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	553	ILE	N-CA-CB	5.36	118.62	110.58
1	A	282	LEU	CA-C-O	-5.34	114.61	120.43
1	A	91	ASN	N-CA-CB	-5.34	103.47	111.64
1	A	93	PRO	CA-C-N	5.33	131.42	123.05
1	A	93	PRO	C-N-CA	5.33	131.42	123.05
1	A	33	ASN	CB-CG-OD1	-5.33	110.14	120.80
1	A	559	LEU	N-CA-CB	-5.33	102.29	110.12
1	A	2	ASP	CA-C-O	-5.32	113.04	119.27
1	A	488	ALA	CA-C-O	-5.32	115.35	121.47
1	A	469	ASN	CA-C-O	5.32	126.18	120.55
1	A	109	ALA	CB-CA-C	-5.30	101.66	110.68
1	A	153	ILE	N-CA-CB	5.29	118.72	111.41
1	A	496	ALA	CA-C-O	-5.26	114.61	120.66
1	A	491	GLU	CA-C-O	5.25	126.03	120.36
1	A	223	MET	CA-C-O	5.25	126.12	120.55
1	A	220	VAL	N-CA-C	5.25	115.97	110.62
1	A	320	ASN	CA-C-O	-5.24	114.18	120.10
1	A	204	ASN	CA-C-O	-5.21	115.81	121.44
1	A	392	GLY	CA-C-O	5.20	126.34	119.58
1	A	389	ASN	CB-CG-ND2	-5.18	108.63	116.40
1	A	87	SER	CA-C-O	-5.15	115.25	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	105	ILE	N-CA-CB	-5.14	103.55	110.54
1	A	78	SER	CA-C-O	5.13	127.09	121.40
1	A	289	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	378	GLU	CA-C-O	-5.12	113.29	119.49
1	A	548	ASN	CA-C-O	-5.12	112.96	119.31
1	A	240	SER	CA-CB-OG	-5.11	100.88	111.10
1	A	369	SER	O-C-N	-5.08	116.56	122.96
1	A	12	GLN	CA-CB-CG	5.07	124.23	114.10
1	A	504	HIS	N-CA-C	5.07	119.92	113.18
1	A	88	PHE	CA-C-N	-5.06	115.82	122.85
1	A	88	PHE	C-N-CA	-5.06	115.82	122.85
1	A	385	ALA	O-C-N	5.06	128.56	122.79
1	A	449	LYS	CB-CA-C	-5.06	102.25	110.85
1	A	310	ILE	CA-C-N	5.05	129.14	122.42
1	A	310	ILE	C-N-CA	5.05	129.14	122.42
1	A	505	HIS	CA-C-O	-5.03	114.35	120.54
1	A	131	VAL	CA-C-N	-5.03	116.27	123.11
1	A	131	VAL	C-N-CA	-5.03	116.27	123.11
1	A	257	VAL	CA-C-O	-5.01	115.74	120.95
1	A	91	ASN	OD1-CG-ND2	5.00	127.60	122.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	CYS	Mainchain
1	A	175	ALA	Peptide,Mainchain
1	A	228	ALA	Mainchain

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	4162	0	4046	109	0
2	A	1	0	0	0	0
3	A	172	0	120	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	31	6	0
5	A	8	0	1	4	0
6	A	4	0	3	0	0
7	A	521	0	0	7	0
All	All	4921	0	4201	115	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 13.

All (115) 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:71:CYS:SG	3:A:803:HEM:CAC	2.50	0.99
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.52	0.98
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.54	0.95
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.55	0.95
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.54	0.95
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.56	0.94
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.55	0.94
1:A:204:ASN:HD22	1:A:204:ASN:H	1.02	0.94
1:A:14:CYS:HG	3:A:801:HEM:CAB	1.88	0.87
1:A:229:ASP:H	1:A:256:HIS:HE1	1.20	0.86
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.68	0.80
1:A:204:ASN:H	1:A:204:ASN:ND2	1.80	0.78
1:A:229:ASP:H	1:A:256:HIS:CE1	2.04	0.76
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.26	0.74
1:A:375:MET:HE3	1:A:504:HIS:CE1	2.24	0.73
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.29	0.72
1:A:136:GLY:HA3	1:A:553:ILE:HD12	1.71	0.72
1:A:559:LEU:HG	7:A:1322:HOH:O	1.90	0.72
1:A:567:TYR:O	1:A:568:SER:HB2	1.90	0.71
1:A:375:MET:CE	5:A:806:FUM:H5	2.21	0.71
1:A:566:LYS:HB3	1:A:566:LYS:NZ	2.06	0.71
1:A:375:MET:HE1	5:A:806:FUM:H5	1.76	0.67
1:A:104:THR:OG1	1:A:107:GLU:HG3	1.95	0.66
1:A:23:GLU:HB2	7:A:1289:HOH:O	1.95	0.66
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.76	0.66
1:A:568:SER:HB3	7:A:967:HOH:O	1.96	0.66
1:A:191:LEU:HD21	1:A:240:SER:HB2	1.76	0.66
4:A:805:FAD:H9	4:A:805:FAD:H2'	1.79	0.65
1:A:79:MET:HE1	7:A:1025:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:HIS:CD2	1:A:375:MET:HE2	2.34	0.63
1:A:204:ASN:HD22	1:A:204:ASN:N	1.82	0.62
1:A:375:MET:SD	4:A:805:FAD:C6	2.88	0.62
1:A:365:HIS:CD2	1:A:375:MET:CE	2.83	0.61
1:A:265:ALA:HA	1:A:270:ILE:HD12	1.81	0.61
1:A:288:THR:HG22	1:A:527:PRO:HG2	1.81	0.61
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.41	0.59
1:A:337:ASN:HD22	1:A:337:ASN:N	2.01	0.59
1:A:199:GLY:HA3	1:A:545:LEU:HD21	1.87	0.57
1:A:84:SER:HB3	1:A:98:TRP:CE2	2.41	0.55
1:A:365:HIS:NE2	1:A:375:MET:HE2	2.22	0.55
1:A:229:ASP:N	1:A:256:HIS:HE1	1.99	0.55
1:A:85:CYS:SG	3:A:804:HEM:CBC	2.95	0.54
4:A:805:FAD:H2'	4:A:805:FAD:C9	2.38	0.54
1:A:56:ASN:HD22	1:A:58:HIS:H	1.54	0.54
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.01	0.54
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.01	0.53
1:A:375:MET:SD	4:A:805:FAD:H6	2.49	0.53
1:A:250:GLY:HA3	1:A:429:LEU:HD12	1.90	0.52
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.47	0.52
1:A:526:ILE:O	1:A:526:ILE:HG13	2.06	0.52
1:A:477:ASP:O	1:A:481:GLU:HA	2.11	0.51
1:A:375:MET:HE2	5:A:806:FUM:H5	1.91	0.51
1:A:566:LYS:HB3	1:A:566:LYS:HZ1	1.74	0.51
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.94	0.51
1:A:368:LEU:O	1:A:499:VAL:HA	2.11	0.51
1:A:56:ASN:ND2	1:A:58:HIS:H	2.08	0.51
1:A:421:PHE:HA	1:A:489:LEU:HD22	1.93	0.50
1:A:110:LYS:HD2	7:A:1027:HOH:O	2.12	0.50
1:A:365:HIS:O	1:A:501:PRO:HA	2.12	0.50
1:A:47:ALA:HA	1:A:58:HIS:HB2	1.93	0.50
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.04	0.49
1:A:476:LYS:HG3	1:A:478:THR:HG23	1.94	0.49
1:A:77:LYS:HB3	1:A:94:TYR:O	2.13	0.49
1:A:232:ASP:HB3	1:A:246:ARG:HG2	1.95	0.49
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.95	0.49
1:A:365:HIS:CD2	1:A:375:MET:HE3	2.47	0.48
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.79	0.48
1:A:299:LYS:HB3	1:A:299:LYS:HE2	1.71	0.47
1:A:42:THR:O	1:A:46:VAL:HG23	2.14	0.47
1:A:55:TYR:OH	1:A:89:ASP:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:O	1:A:346:LEU:HB2	2.14	0.47
1:A:526:ILE:CG1	1:A:529:LEU:HB2	2.44	0.47
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.08	0.47
1:A:129:VAL:HG22	1:A:308:ALA:HB3	1.97	0.47
1:A:133:GLY:O	1:A:138:GLY:HA3	2.15	0.47
3:A:803:HEM:CMB	3:A:803:HEM:HBB2	2.45	0.47
1:A:71:CYS:SG	3:A:803:HEM:CBC	3.00	0.46
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.08	0.46
1:A:346:LEU:HD22	1:A:356:LEU:HD22	1.98	0.45
1:A:8:HIS:O	1:A:12:GLN:HG3	2.17	0.45
1:A:375:MET:CE	5:A:806:FUM:C5	2.95	0.45
1:A:4:LEU:HD11	3:A:802:HEM:C3A	2.53	0.45
1:A:526:ILE:HG13	1:A:529:LEU:HB2	1.99	0.45
1:A:490:ASN:ND2	7:A:1141:HOH:O	2.50	0.44
1:A:110:LYS:HE3	1:A:110:LYS:O	2.17	0.44
1:A:520:ASN:ND2	1:A:524:GLN:HB2	2.32	0.44
1:A:559:LEU:HD13	1:A:559:LEU:C	2.43	0.44
4:A:805:FAD:H9	4:A:805:FAD:H1'1	1.55	0.44
1:A:23:GLU:HG2	1:A:24:LEU:N	2.33	0.44
1:A:204:ASN:ND2	1:A:204:ASN:N	2.50	0.44
1:A:490:ASN:HD22	1:A:490:ASN:C	2.26	0.43
1:A:82:CYS:SG	3:A:804:HEM:HAB	2.53	0.43
1:A:284:ASP:OD1	1:A:286:LYS:HG2	2.18	0.43
1:A:17:CYS:SG	3:A:801:HEM:HAC	2.53	0.43
1:A:79:MET:HE3	1:A:79:MET:HB2	1.66	0.43
1:A:334:ILE:HD11	1:A:368:LEU:HD22	2.00	0.43
1:A:82:CYS:SG	3:A:804:HEM:CBB	3.06	0.43
1:A:520:ASN:HB2	7:A:1102:HOH:O	2.19	0.43
1:A:375:MET:CE	1:A:504:HIS:CE1	2.98	0.43
1:A:401:THR:HB	1:A:403:ASP:OD1	2.19	0.42
1:A:559:LEU:HD13	1:A:560:ALA:N	2.34	0.42
3:A:802:HEM:HBC2	3:A:802:HEM:CMC	2.49	0.42
1:A:310:ILE:HG12	1:A:530:TYR:HB2	2.03	0.41
4:A:805:FAD:C9	4:A:805:FAD:C2'	2.87	0.41
1:A:442:PRO:HD2	1:A:496:ALA:O	2.21	0.41
1:A:513:ASP:OD2	1:A:517:GLU:OE1	2.38	0.41
1:A:4:LEU:HG	1:A:8:HIS:CE1	2.56	0.41
1:A:55:TYR:CE2	1:A:88:PHE:HB3	2.55	0.41
1:A:19:THR:HB	1:A:20:PRO:HD2	2.03	0.41
1:A:386:ILE:HD13	1:A:386:ILE:HG21	1.96	0.41
1:A:388:VAL:HA	1:A:393:LYS:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ASP:O	1:A:481:GLU:HG2	2.21	0.41
1:A:565:ALA:O	1:A:568:SER:HA	2.21	0.40
1:A:163:GLY:O	1:A:166:LYS:HG2	2.22	0.40
1:A:446:SER:OG	1:A:449:LYS:HG3	2.22	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%)	538 (95%)	27 (5%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	425/444 (96%)	393 (92%)	32 (8%)	12	14

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

Mol	Chain	Res	Type
1	A	56	ASN
1	A	99	LEU
1	A	110	LYS
1	A	111	ASP
1	A	125	ASP
1	A	176	TRP
1	A	204	ASN
1	A	208	LEU
1	A	257	VAL
1	A	282	LEU
1	A	286	LYS
1	A	289	VAL
1	A	292	ILE
1	A	294	VAL
1	A	299	LYS
1	A	311	LEU
1	A	334	ILE
1	A	335	SER
1	A	337	ASN
1	A	371	LYS
1	A	400	THR
1	A	403	ASP
1	A	450	LEU
1	A	452	LYS
1	A	470	SER
1	A	490	ASN
1	A	522	LYS
1	A	526	ILE
1	A	529	LEU
1	A	559	LEU
1	A	566	LYS
1	A	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) 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	275	ASN
1	A	490	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	A	801	1	50,50,50	1.42	8 (16%)	67,82,82	1.46	11 (16%)
6	ACY	A	811	3	3,3,3	1.35	1 (33%)	3,3,3	2.29	2 (66%)
4	FAD	A	805	-	58,58,58	1.56	7 (12%)	85,89,89	3.20	36 (42%)
3	HEM	A	804	1,6	50,50,50	1.41	6 (12%)	67,82,82	1.28	8 (11%)
3	HEM	A	802	1	50,50,50	1.33	9 (18%)	67,82,82	1.35	11 (16%)
5	FUM	A	806	-	7,7,7	2.21	3 (42%)	8,8,8	1.23	0
3	HEM	A	803	1	50,50,50	1.36	7 (14%)	67,82,82	1.24	7 (10%)

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	A	801	1	-	4/14/54/54	-
4	FAD	A	805	-	3/3/9/9	9/34/50/50	0/6/6/6
3	HEM	A	804	1,6	-	3/14/54/54	-
3	HEM	A	802	1	-	3/14/54/54	-
5	FUM	A	806	-	-	2/5/5/5	-
3	HEM	A	803	1	-	4/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	805	FAD	C6-C5X	5.20	1.47	1.40
4	A	805	FAD	C2A-N3A	4.16	1.41	1.33
3	A	804	HEM	CAB-C3B	3.54	1.56	1.47
5	A	806	FUM	O7-C6	3.30	1.31	1.23
3	A	801	HEM	CAC-C3C	3.25	1.56	1.47
3	A	801	HEM	FE-ND	3.24	2.04	1.94
4	A	805	FAD	C1'-C2'	-3.17	1.48	1.52
3	A	802	HEM	CAC-C3C	3.12	1.55	1.47
5	A	806	FUM	O-C	3.11	1.30	1.23
3	A	804	HEM	CAC-C3C	3.06	1.55	1.47
3	A	803	HEM	CAB-C3B	3.05	1.55	1.47
3	A	801	HEM	CMA-C3A	3.03	1.57	1.50
5	A	806	FUM	OXT-C	-2.96	1.22	1.30
3	A	801	HEM	CAB-C3B	2.93	1.55	1.47
3	A	804	HEM	FE-ND	2.88	2.03	1.94
4	A	805	FAD	C6-C7	2.81	1.43	1.39
3	A	803	HEM	FE-NA	2.76	2.04	1.95
4	A	805	FAD	PA-O3P	2.66	1.62	1.59
3	A	801	HEM	FE-NB	2.59	2.02	1.94
3	A	804	HEM	FE-NB	2.59	2.02	1.94
4	A	805	FAD	C10-N1	-2.58	1.28	1.33
3	A	803	HEM	CMB-C2B	2.56	1.56	1.50
4	A	805	FAD	O4-C4	-2.55	1.18	1.23
3	A	803	HEM	CMC-C2C	2.52	1.55	1.50
3	A	801	HEM	C3B-C2B	-2.48	1.32	1.37
3	A	803	HEM	CMD-C2D	2.41	1.55	1.50
3	A	802	HEM	CMA-C3A	2.37	1.55	1.50
3	A	802	HEM	CMD-C2D	2.35	1.55	1.50
3	A	802	HEM	CMC-C2C	2.35	1.55	1.50
3	A	802	HEM	FE-ND	2.21	2.01	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEM	CAA-C2A	2.19	1.57	1.51
3	A	803	HEM	CAA-C2A	2.16	1.56	1.51
3	A	801	HEM	CMD-C2D	2.16	1.55	1.50
3	A	803	HEM	C2A-C3A	-2.13	1.33	1.38
3	A	804	HEM	C3C-C2C	-2.09	1.32	1.37
3	A	802	HEM	C4D-ND	-2.09	1.36	1.40
3	A	802	HEM	CAB-C3B	2.08	1.52	1.47
3	A	802	HEM	C2A-C3A	-2.06	1.33	1.38
6	A	811	ACY	CH3-C	2.05	1.57	1.49
3	A	804	HEM	CMB-C2B	2.03	1.54	1.50
3	A	801	HEM	O1D-CGD	2.02	1.28	1.22

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	FAD	C5X-C9A-N10	9.95	126.96	117.97
4	A	805	FAD	N3A-C2A-N1A	-9.20	114.65	128.58
4	A	805	FAD	C9-C8-C7	8.67	132.42	119.69
4	A	805	FAD	C4'-C3'-C2'	8.21	127.24	113.57
4	A	805	FAD	C9-C9A-N10	-7.74	111.44	121.85
4	A	805	FAD	C2A-N1A-C6A	7.10	130.39	118.73
4	A	805	FAD	C8M-C8-C9	-5.96	109.07	119.57
4	A	805	FAD	C9A-N10-C10	-5.61	112.20	120.75
4	A	805	FAD	C6-C5X-C9A	4.56	125.31	119.05
4	A	805	FAD	C7M-C7-C6	4.50	127.49	119.57
4	A	805	FAD	C6-C7-C8	-4.40	113.24	119.69
4	A	805	FAD	O4'-C4'-C5'	4.15	119.14	109.99
4	A	805	FAD	C9A-C9-C8	-4.15	110.88	119.22
4	A	805	FAD	C1'-N10-C9A	-3.94	112.97	120.63
4	A	805	FAD	O2'-C2'-C3'	3.94	118.46	109.25
3	A	803	HEM	CAD-CBD-CGD	3.88	123.96	113.67
4	A	805	FAD	O4B-C1B-C2B	-3.84	98.40	106.62
4	A	805	FAD	O5'-C5'-C4'	-3.79	99.24	109.36
3	A	801	HEM	CAA-CBA-CGA	3.72	123.53	113.67
4	A	805	FAD	C4-C4X-N5	-3.47	113.41	118.21
4	A	805	FAD	C9A-C5X-N5	-3.45	118.80	122.45
4	A	805	FAD	O3B-C3B-C2B	3.40	122.70	111.82
4	A	805	FAD	O2-C2-N1	-3.37	116.21	121.80
3	A	802	HEM	C4A-CHB-C1B	-3.36	118.36	126.25
4	A	805	FAD	O4-C4-N3	3.34	126.40	120.11
4	A	805	FAD	N3-C2-N1	3.30	126.51	119.50
4	A	805	FAD	N3A-C4A-N9A	-3.19	121.75	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	CAD-CBD-CGD	3.05	121.74	113.67
3	A	804	HEM	CBD-CAD-C3D	2.98	120.78	112.53
4	A	805	FAD	C6A-C5A-N7A	2.91	137.70	132.09
4	A	805	FAD	O3P-PA-O1A	-2.89	102.01	110.70
3	A	802	HEM	C1B-NB-C4B	2.86	108.59	105.21
6	A	811	ACY	O-C-CH3	-2.85	110.86	122.53
4	A	805	FAD	C5X-C6-C7	-2.79	115.65	120.83
3	A	804	HEM	CHA-C1A-NA	2.77	128.89	123.86
3	A	803	HEM	O2A-CGA-O1A	2.77	130.46	123.33
3	A	804	HEM	CMD-C2D-C1D	-2.74	120.76	125.03
6	A	811	ACY	OXT-C-O	2.73	132.17	122.03
3	A	801	HEM	CMA-C3A-C4A	-2.70	121.31	125.42
3	A	802	HEM	C4C-C3C-C2C	2.68	109.14	106.81
3	A	802	HEM	C3D-C4D-ND	-2.63	107.29	110.17
3	A	802	HEM	C4D-ND-C1D	2.59	108.28	105.21
4	A	805	FAD	C4A-C5A-N7A	-2.54	107.68	110.58
3	A	801	HEM	CAD-C3D-C4D	-2.53	120.29	124.70
4	A	805	FAD	C5X-N5-C4X	-2.52	114.01	118.09
3	A	802	HEM	CMB-C2B-C1B	-2.52	121.09	125.03
3	A	802	HEM	C3B-C2B-C1B	2.52	108.30	106.41
3	A	803	HEM	CBB-CAB-C3B	-2.47	115.19	127.53
4	A	805	FAD	C2B-C1B-N9A	-2.42	107.29	113.30
3	A	801	HEM	C4D-ND-C1D	2.40	108.05	105.21
3	A	801	HEM	C3D-C4D-ND	-2.40	107.54	110.17
3	A	803	HEM	O1A-CGA-CBA	-2.40	115.49	123.09
4	A	805	FAD	O2'-C2'-C1'	2.39	120.04	110.20
3	A	803	HEM	C4A-CHB-C1B	-2.39	120.63	126.25
3	A	801	HEM	CMB-C2B-C1B	-2.35	121.36	125.03
3	A	802	HEM	C2B-C1B-NB	-2.31	107.18	109.84
4	A	805	FAD	O2P-P-O3P	2.31	113.51	107.27
3	A	804	HEM	C2A-C1A-NA	-2.28	107.62	110.15
3	A	804	HEM	O2D-CGD-O1D	2.28	129.19	123.33
4	A	805	FAD	C1'-C2'-C3'	2.27	115.82	109.66
3	A	804	HEM	CMD-C2D-C3D	2.26	132.25	126.15
4	A	805	FAD	C5A-C4A-N9A	2.26	108.27	105.81
3	A	801	HEM	O2A-CGA-CBA	2.26	121.13	114.00
4	A	805	FAD	C5A-C4A-N3A	2.19	129.73	126.72
3	A	801	HEM	CBD-CAD-C3D	-2.17	106.54	112.53
3	A	802	HEM	CMA-C3A-C4A	-2.17	122.12	125.42
3	A	802	HEM	CBC-CAC-C3C	-2.16	116.75	127.53
4	A	805	FAD	C10-N1-C2	-2.15	112.18	116.85
3	A	801	HEM	C4C-C3C-C2C	2.14	108.67	106.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HEM	C2A-C1A-NA	-2.14	107.78	110.15
3	A	801	HEM	CHC-C4B-NB	2.13	126.71	124.42
3	A	804	HEM	CHB-C1B-NB	2.12	126.99	124.37
3	A	803	HEM	CHB-C1B-NB	2.08	126.94	124.37
3	A	802	HEM	CHB-C1B-NB	2.06	126.92	124.37
3	A	804	HEM	CAA-C2A-C1A	-2.05	120.93	124.94

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	805	FAD	C2'
4	A	805	FAD	C3'
4	A	805	FAD	C4'

All (25) torsion outliers are listed below:

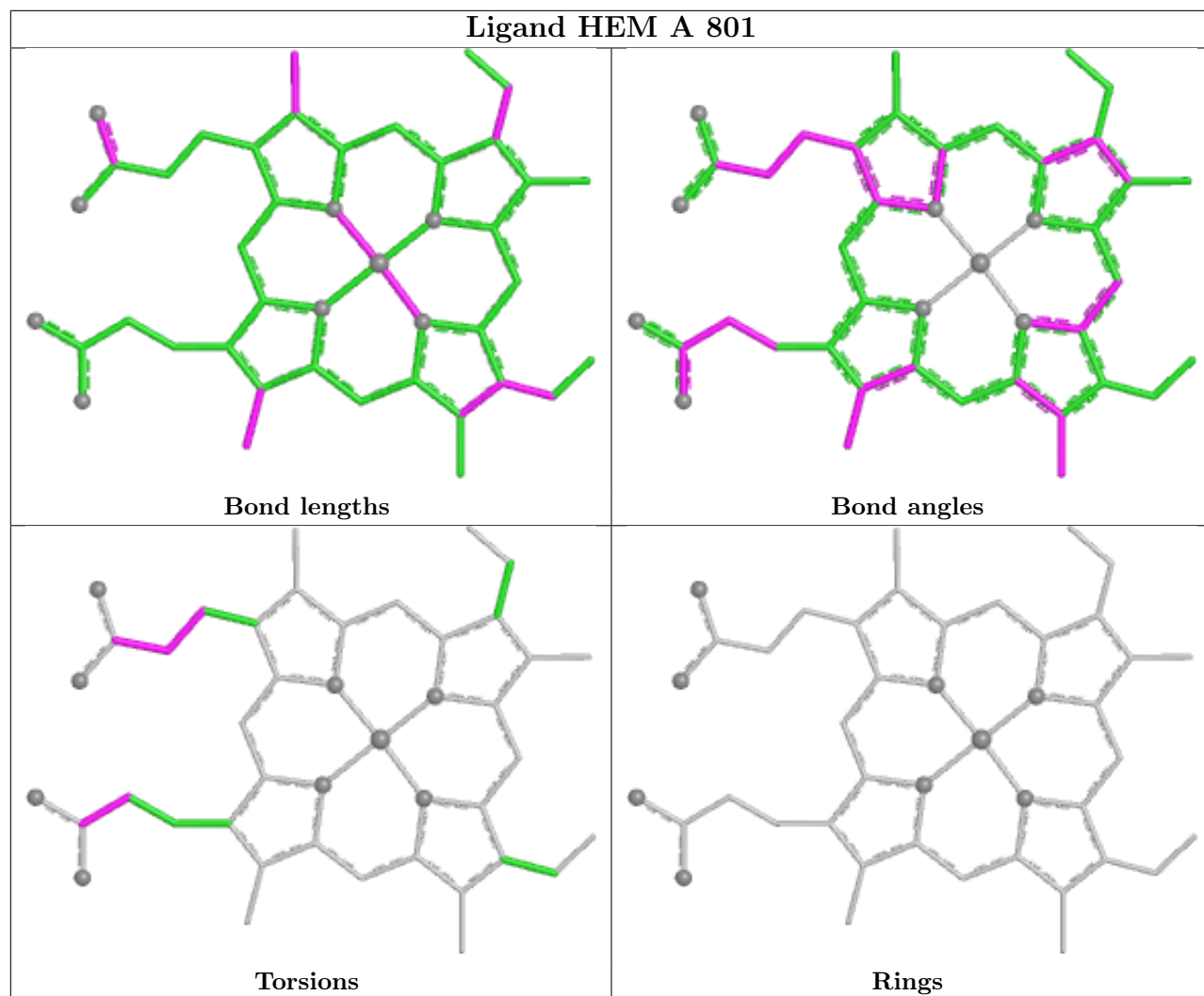
Mol	Chain	Res	Type	Atoms
4	A	805	FAD	N10-C1'-C2'-O2'
4	A	805	FAD	C1'-C2'-C3'-O3'
4	A	805	FAD	C3'-C4'-C5'-O5'
4	A	805	FAD	O4'-C4'-C5'-O5'
4	A	805	FAD	C2'-C3'-C4'-O4'
3	A	802	HEM	C3D-CAD-CBD-CGD
5	A	806	FUM	C4-C5-C6-O7
5	A	806	FUM	C4-C5-C6-O8
3	A	801	HEM	C3D-CAD-CBD-CGD
4	A	805	FAD	O4B-C4B-C5B-O5B
3	A	803	HEM	C3D-CAD-CBD-CGD
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	803	HEM	C3A-C2A-CAA-CBA
4	A	805	FAD	C3B-C4B-C5B-O5B
3	A	802	HEM	CAD-CBD-CGD-O1D
3	A	802	HEM	CAD-CBD-CGD-O2D
3	A	804	HEM	CAA-CBA-CGA-O2A
4	A	805	FAD	P-O3P-PA-O1A
3	A	801	HEM	CAD-CBD-CGD-O2D
3	A	801	HEM	CAD-CBD-CGD-O1D
3	A	803	HEM	CAA-CBA-CGA-O2A
4	A	805	FAD	P-O3P-PA-O2A
3	A	803	HEM	CAA-CBA-CGA-O1A
3	A	804	HEM	C2A-CAA-CBA-CGA
3	A	801	HEM	CAA-CBA-CGA-O2A

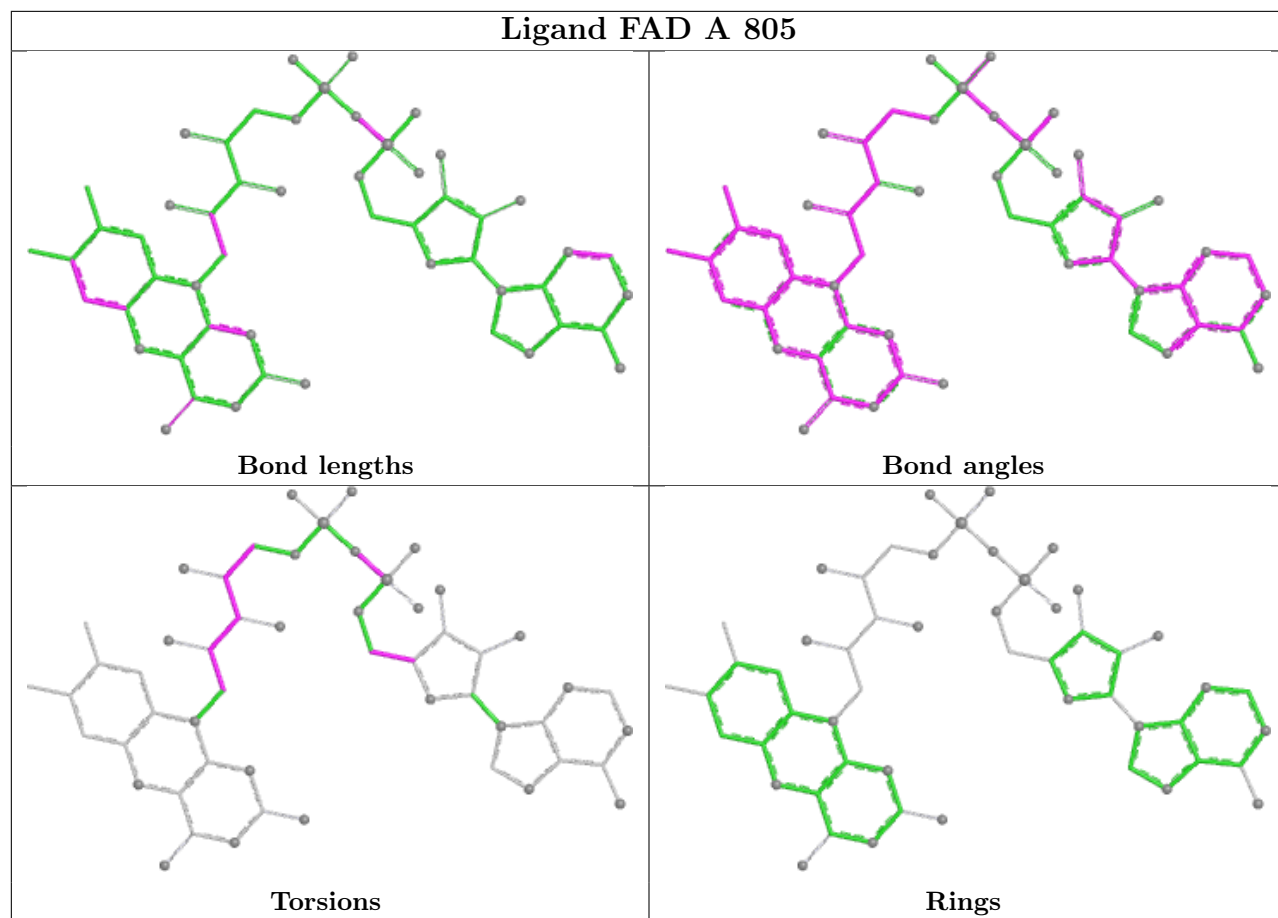
There are no ring outliers.

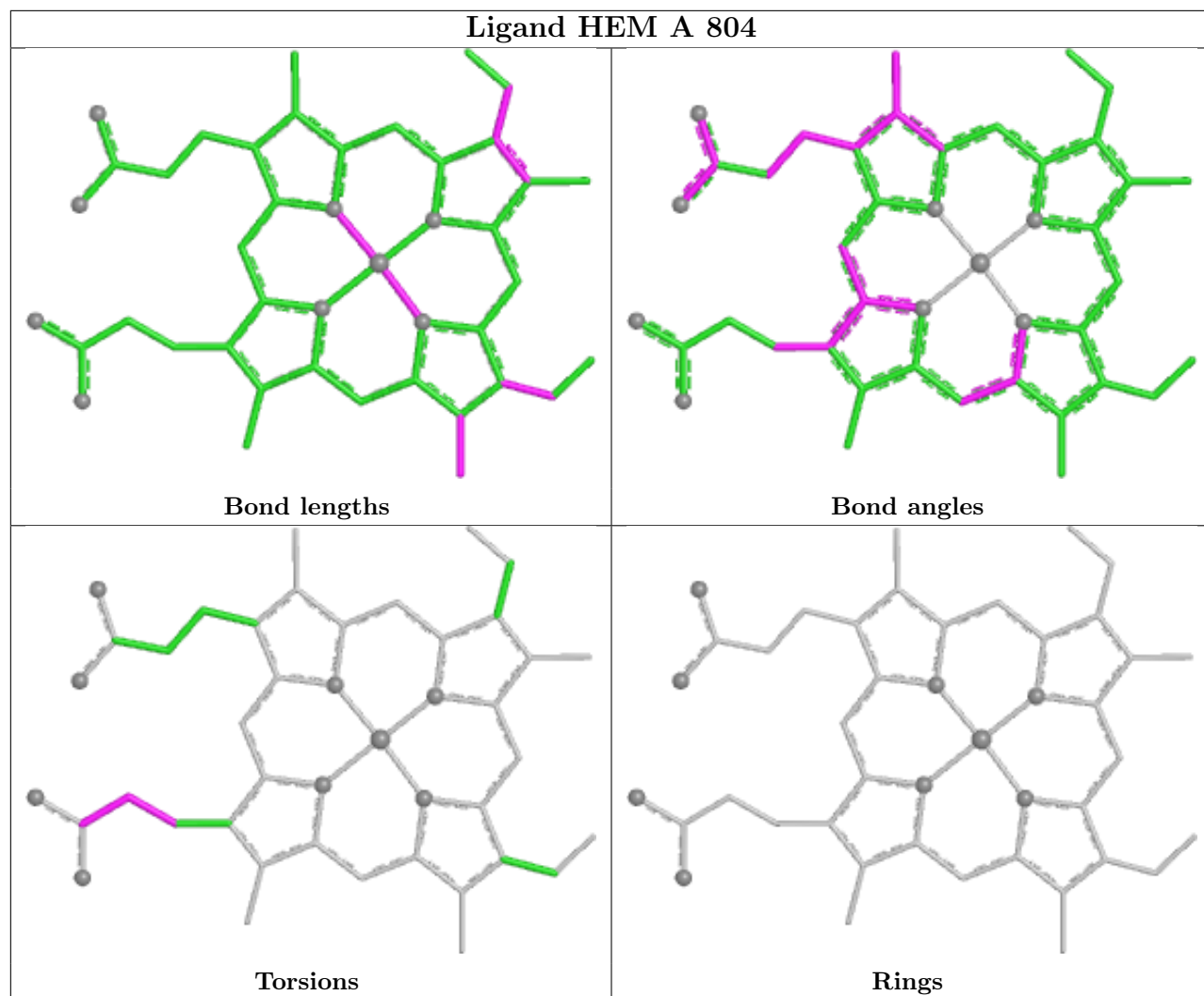
6 monomers are involved in 37 short contacts:

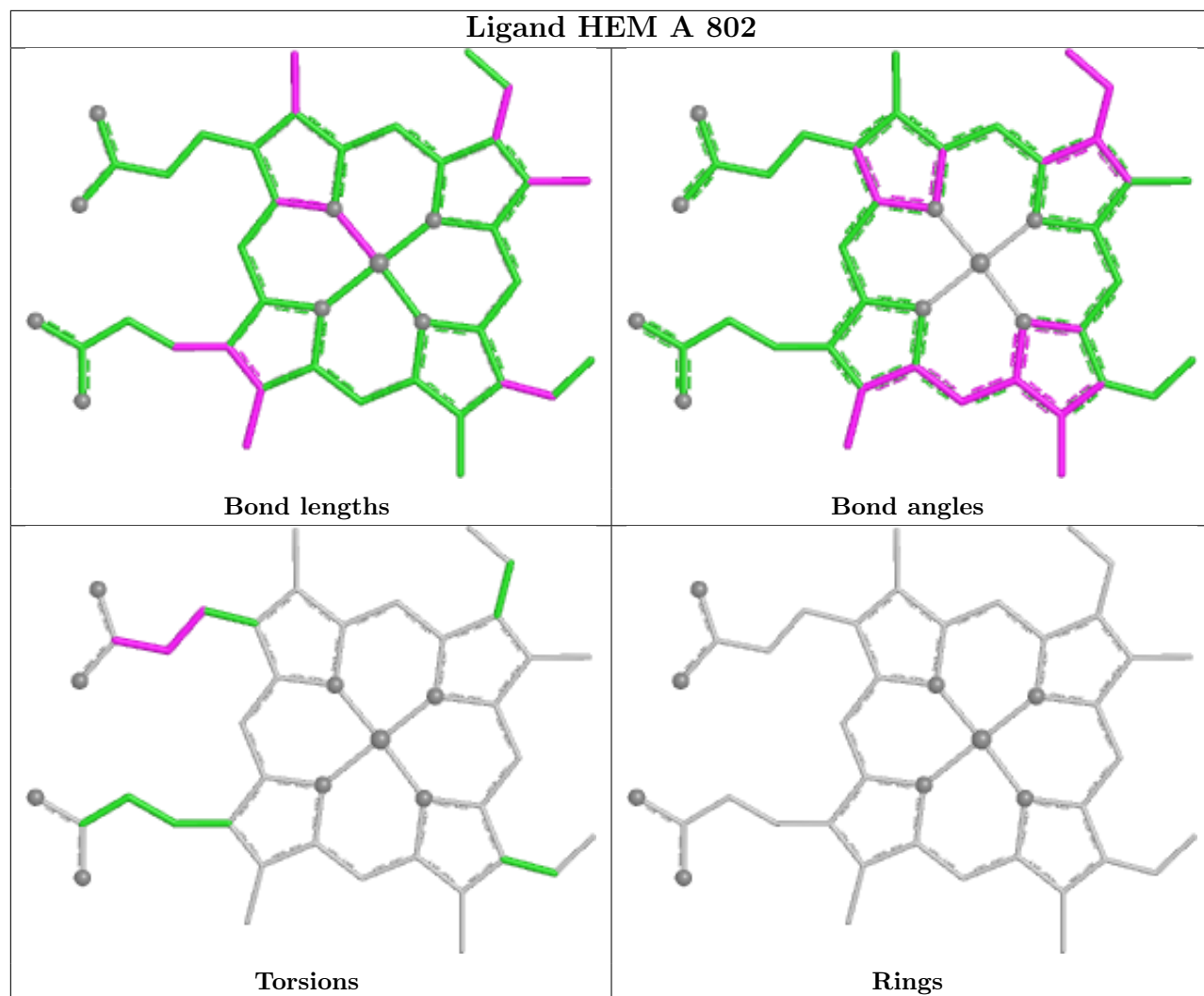
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	HEM	6	0
4	A	805	FAD	6	0
3	A	804	HEM	7	0
3	A	802	HEM	6	0
5	A	806	FUM	4	0
3	A	803	HEM	8	0

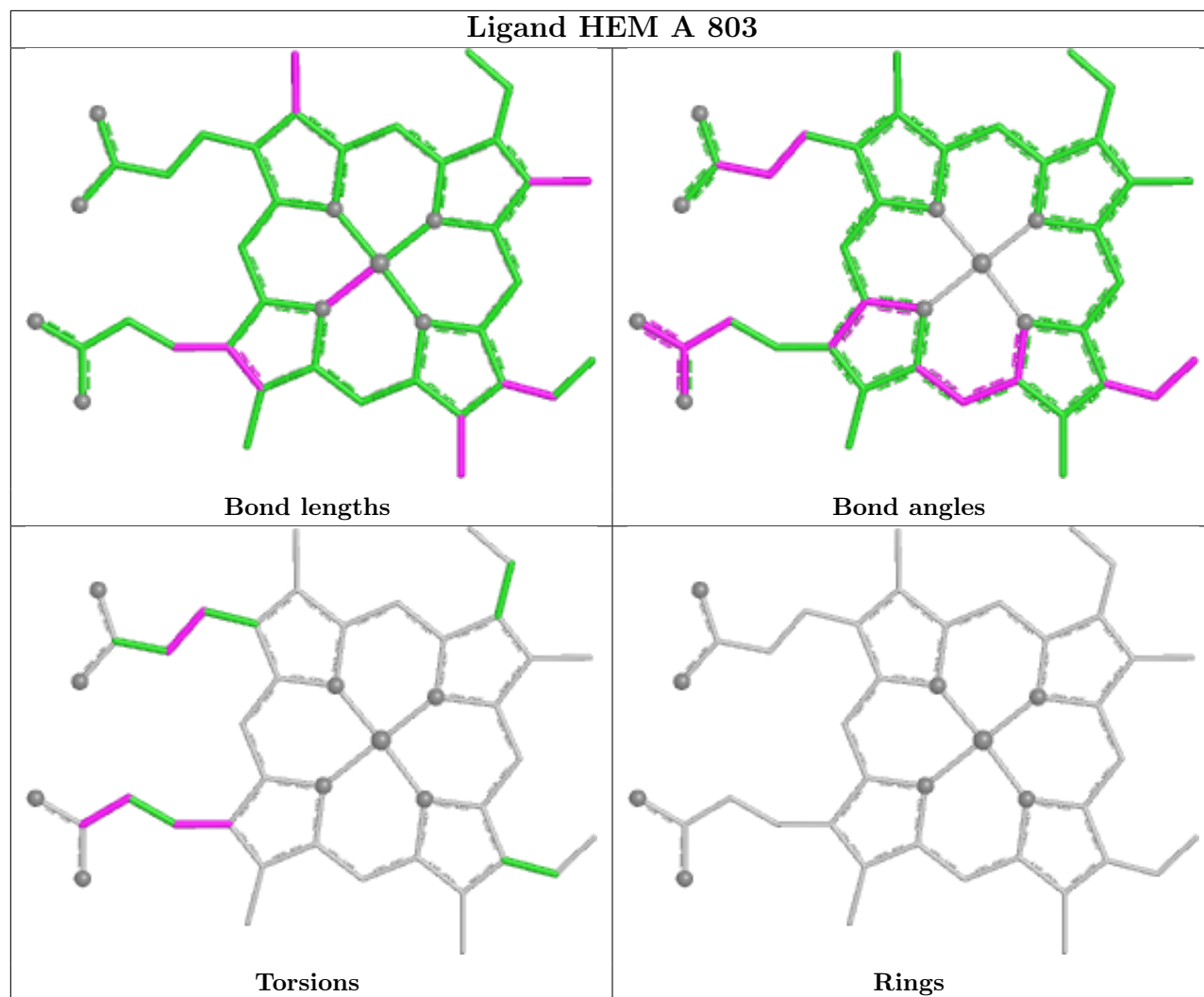
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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