



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:49 PM EDT

PDB ID : 1P2E  
Title : H61A mutant of flavocytochrome c3  
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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](mailto: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.

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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

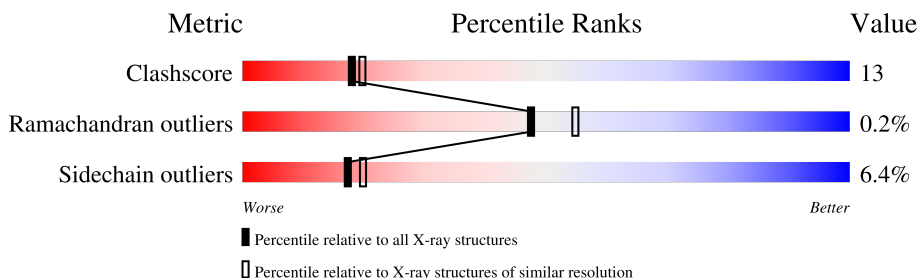
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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  $\geq 3$ , 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	-

## 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			

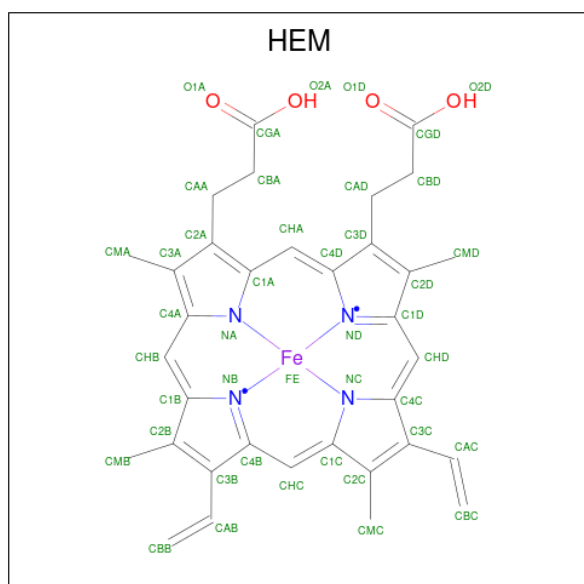
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

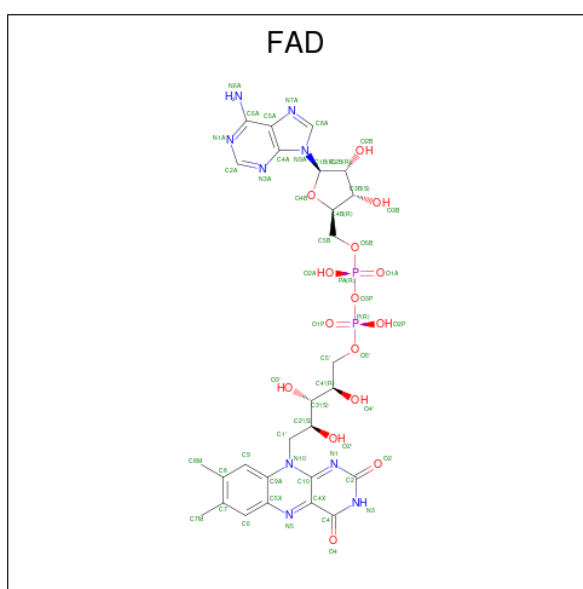
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

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



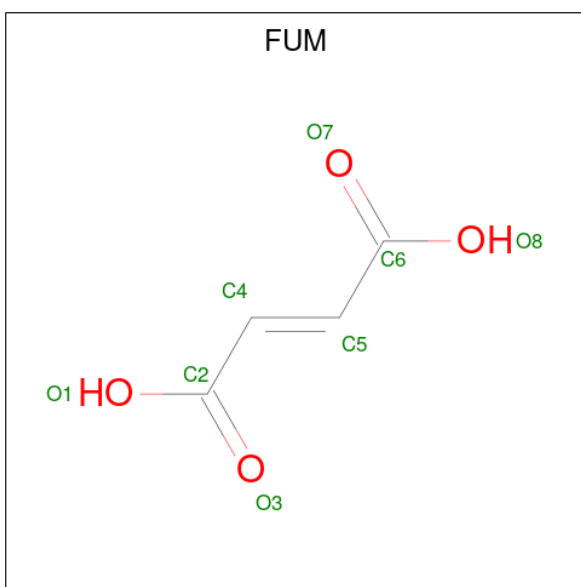
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



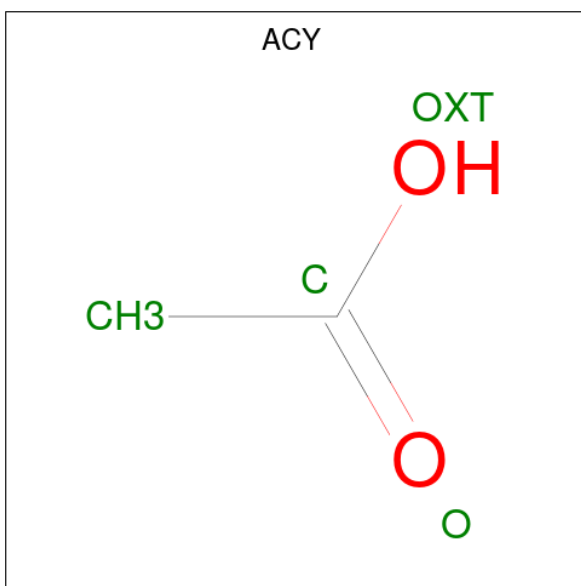
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

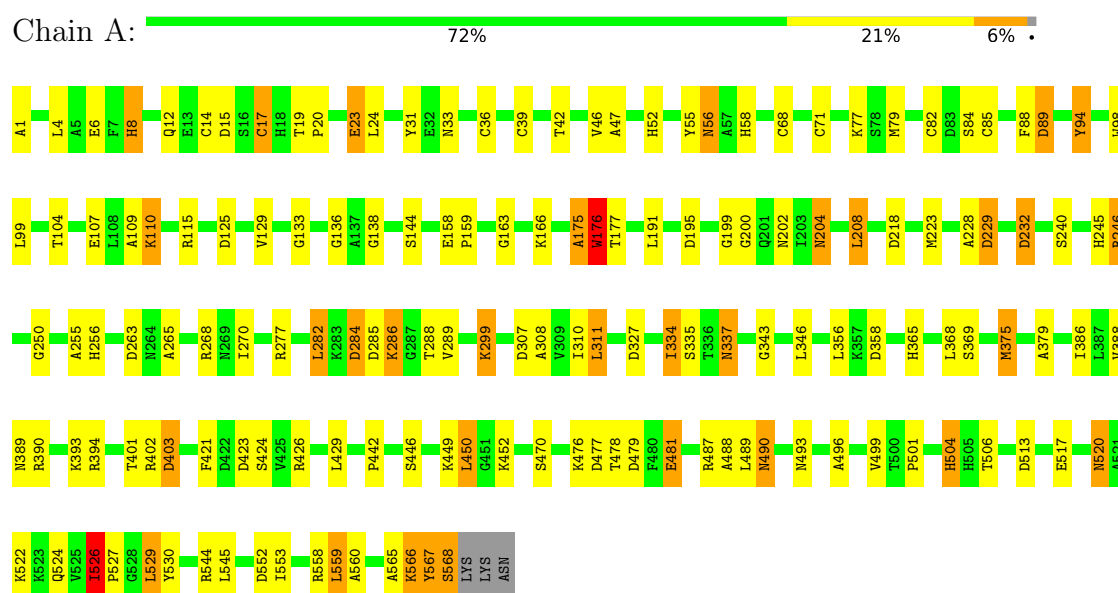
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	521	Total 521	O 521	0	0

### 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: FUM, HEM, NA, FAD, ACY

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	0.80	1/4231 (0.0%)	1.82	75/5731 (1.3%)

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	-5.13	1.36	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	ARG	NE-CZ-NH2	-15.17	112.71	120.30
1	A	175	ALA	C-N-CA	15.16	159.60	121.70
1	A	277	ARG	NE-CZ-NH1	-13.81	113.40	120.30
1	A	268	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	A	487	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	426	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	402	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	263	ASP	CB-CG-OD2	9.97	127.28	118.30
1	A	246	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	A	394	ARG	CD-NE-CZ	8.98	136.18	123.60
1	A	218	ASP	CB-CG-OD1	-8.93	110.27	118.30
1	A	285	ASP	CB-CG-OD2	8.63	126.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	390	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	277	ARG	NH1-CZ-NH2	8.22	128.45	119.40
1	A	481	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	A	375	MET	CG-SD-CE	7.98	112.96	100.20
1	A	504	HIS	N-CA-CB	-7.53	97.05	110.60
1	A	558	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	277	ARG	CD-NE-CZ	7.39	133.94	123.60
1	A	195	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	94	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	423	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	229	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	450	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	229	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	307	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	31	TYR	CG-CD1-CE1	-6.56	116.05	121.30
1	A	327	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	567	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	A	8	HIS	CA-CB-CG	6.44	124.55	113.60
1	A	229	ASP	OD1-CG-OD2	-6.39	111.16	123.30
1	A	390	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	282	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	175	ALA	N-CA-CB	6.16	118.72	110.10
1	A	358	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	A	479	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	526	ILE	CA-CB-CG2	6.11	123.12	110.90
1	A	1	ALA	O-C-N	6.07	132.41	122.70
1	A	424	SER	N-CA-CB	6.01	119.52	110.50
1	A	15	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	481	GLU	CB-CG-CD	5.98	130.35	114.20
1	A	311	LEU	CA-CB-CG	5.93	128.93	115.30
1	A	506	THR	CA-CB-CG2	-5.89	104.15	112.40
1	A	487	ARG	CG-CD-NE	-5.76	99.70	111.80
1	A	33	ASN	CB-CG-OD1	-5.73	110.14	121.60
1	A	15	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	223	MET	CA-CB-CG	5.72	123.02	113.30
1	A	552	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	109	ALA	CB-CA-C	-5.62	101.66	110.10
1	A	176	TRP	CB-CA-C	5.62	121.63	110.40
1	A	255	ALA	CB-CA-C	5.56	118.45	110.10
1	A	23	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	A	307	ASP	OD1-CG-OD2	5.53	133.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	284	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	289	VAL	CA-CB-CG2	5.48	119.12	110.90
1	A	202	ASN	CA-CB-CG	-5.47	101.37	113.40
1	A	402	ARG	NH1-CZ-NH2	5.44	125.39	119.40
1	A	268	ARG	NH1-CZ-NH2	-5.34	113.52	119.40
1	A	6	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	402	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	89	ASP	N-CA-CB	-5.29	101.08	110.60
1	A	379	ALA	N-CA-CB	5.26	117.47	110.10
1	A	232	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	307	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	488	ALA	CB-CA-C	5.20	117.90	110.10
1	A	488	ALA	N-CA-CB	-5.18	102.84	110.10
1	A	218	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	52	HIS	CA-CB-CG	5.10	122.27	113.60
1	A	389	ASN	OD1-CG-ND2	5.10	133.63	121.90
1	A	493	ASN	CA-CB-CG	-5.10	102.18	113.40
1	A	488	ALA	CA-C-N	5.07	128.35	117.20
1	A	520	ASN	O-C-N	-5.04	114.64	122.70
1	A	208	LEU	CB-CG-CD1	5.03	119.56	111.00

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	Mainchain,Peptide
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	110	0
2	A	1	0	0	0	0
3	A	172	0	120	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	31	6	0
5	A	8	0	2	6	0
6	A	4	0	3	0	0
7	A	521	0	0	7	0
All	All	4921	0	4202	116	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 (116) 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:82:CYS:HG	3:A:804:HEM:CAB	1.90	0.84
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:71:CYS:HG	3:A:803:HEM:CAC	1.97	0.77
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: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: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:375:MET:HE2	5:A:806:FUM:H5	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:HIS:CD2	1:A:375:MET:HE3	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:375:MET:HE3	1:A:504:HIS:CE1	2.37	0.60
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: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:HE1	5:A:806:FUM:H5	1.89	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: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:375:MET:HE2	5:A:806:FUM:C5	2.42	0.50
1:A:47:ALA:HA	1:A:58:HIS:HB2	1.93	0.50
1:A:566:LYS:HB3	1:A:566:LYS:HZ1	1.75	0.49
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: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

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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:375:MET:CE	1:A:504:HIS:CE1	2.98	0.47
1:A:526:ILE:CG1	1:A:529:LEU:HB2	2.44	0.47
1:A:365:HIS:CD2	1:A:375:MET:HE2	2.47	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:79:MET:HE1	7:A:1025:HOH:O	2.15	0.46
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
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:375:MET:HE2	5:A:806:FUM:C6	2.47	0.44
1:A:204:ASN:ND2	1:A:204:ASN:N	2.50	0.44
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:365:HIS:NE2	1:A:375:MET:HE2	2.34	0.43
1:A:17:CYS:SG	3:A:801:HEM:HAC	2.53	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:401:THR:HB	1:A:403:ASP:OD1	2.19	0.42
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:HA	1:A:393:LYS:O	2.21	0.41
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%)	47 55

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%)	398 (94%)	27 (6%)	17 20

All (27) 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	125	ASP
1	A	144	SER
1	A	176	TRP
1	A	204	ASN
1	A	208	LEU
1	A	282	LEU
1	A	286	LYS
1	A	299	LYS
1	A	311	LEU
1	A	334	ILE
1	A	335	SER
1	A	337	ASN
1	A	369	SER
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	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

### 5.3.3 RNA ⓘ

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 [i](#)

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	$\# Z  > 2$
5	FUM	A	806	-	1,7,7	0.21	0	2,8,8	3.06	2 (100%)
3	HEM	A	804	1,6	27,50,50	2.19	7 (25%)	17,82,82	2.55	9 (52%)
4	FAD	A	805	-	51,58,58	2.03	11 (21%)	60,89,89	4.60	30 (50%)
6	ACY	A	811	3	1,3,3	6.61	1 (100%)	0,3,3	-	-
3	HEM	A	803	1	27,50,50	1.96	6 (22%)	17,82,82	2.35	6 (35%)
3	HEM	A	801	1	27,50,50	2.17	7 (25%)	17,82,82	3.19	12 (70%)
3	HEM	A	802	1	27,50,50	2.01	6 (22%)	17,82,82	2.15	7 (41%)

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
5	FUM	A	806	-	-	0/0/5/5	-
3	HEM	A	804	1,6	-	0/6/54/54	-
4	FAD	A	805	-	3/3/9/9	9/30/50/50	0/6/6/6
3	HEM	A	803	1	-	2/6/54/54	-
3	HEM	A	801	1	-	1/6/54/54	-
3	HEM	A	802	1	-	1/6/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	811	ACY	CH3-C	6.61	1.57	1.48
3	A	801	HEM	C3B-C2B	-5.95	1.32	1.40
4	A	805	FAD	C4-C4X	5.89	1.51	1.41
4	A	805	FAD	C2A-N3A	5.72	1.41	1.32
3	A	804	HEM	C3C-C2C	-5.38	1.32	1.40
3	A	802	HEM	C3C-C2C	-5.15	1.33	1.40
3	A	804	HEM	C3B-C2B	-4.89	1.33	1.40
4	A	805	FAD	C4-N3	4.65	1.41	1.33
3	A	803	HEM	C3B-C2B	-4.63	1.33	1.40
3	A	801	HEM	C3C-C2C	-4.48	1.34	1.40
4	A	805	FAD	C4X-C10	4.40	1.43	1.38
3	A	804	HEM	C3B-CAB	4.37	1.56	1.47
3	A	803	HEM	C3C-C2C	-4.31	1.34	1.40
3	A	802	HEM	C3B-C2B	-4.23	1.34	1.40
4	A	805	FAD	C10-N1	-4.14	1.28	1.33
3	A	801	HEM	C3C-CAC	4.02	1.56	1.47
4	A	805	FAD	C6-C5X	3.88	1.47	1.41
3	A	802	HEM	C3C-CAC	3.86	1.55	1.47
3	A	804	HEM	C3C-CAC	3.78	1.55	1.47
3	A	803	HEM	C3B-CAB	3.73	1.55	1.47
3	A	801	HEM	C3B-CAB	3.56	1.55	1.47
3	A	802	HEM	CAA-C2A	3.36	1.57	1.52
3	A	803	HEM	CAA-C2A	3.31	1.56	1.52
4	A	805	FAD	C8A-N7A	-3.15	1.29	1.34
3	A	804	HEM	CAA-C2A	2.76	1.56	1.52
4	A	805	FAD	C2B-C1B	2.69	1.57	1.53
3	A	801	HEM	C1B-C2B	2.65	1.48	1.42
3	A	801	HEM	CMA-C3A	2.57	1.57	1.51
3	A	802	HEM	C3B-CAB	2.45	1.52	1.47
4	A	805	FAD	O4-C4	-2.31	1.18	1.24
3	A	803	HEM	CAD-C3D	2.30	1.56	1.52
4	A	805	FAD	C6-C7	2.26	1.43	1.37
3	A	801	HEM	CAD-C3D	2.20	1.56	1.52
3	A	803	HEM	C3C-CAC	2.16	1.52	1.47
3	A	802	HEM	CAD-C3D	2.13	1.56	1.52
3	A	804	HEM	C4D-C3D	2.11	1.47	1.42
4	A	805	FAD	C9A-C5X	-2.06	1.38	1.42
3	A	804	HEM	C1D-ND	2.02	1.40	1.36

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	FAD	C1'-N10-C10	15.00	131.84	118.41
4	A	805	FAD	C5X-C9A-N10	12.76	126.96	117.72
4	A	805	FAD	C4X-C4-N3	-10.21	109.47	123.43
4	A	805	FAD	C4-N3-C2	9.82	123.43	115.14
4	A	805	FAD	N3A-C2A-N1A	-8.98	114.65	128.68
4	A	805	FAD	C10-C4X-N5	7.65	126.55	121.26
4	A	805	FAD	C9-C8-C7	7.42	132.42	119.91
4	A	805	FAD	C9A-N10-C10	-7.42	112.20	121.91
4	A	805	FAD	C2A-N1A-C6A	6.80	130.39	118.75
4	A	805	FAD	C1'-N10-C9A	-6.77	112.97	118.29
3	A	803	HEM	CAD-CBD-CGD	6.73	123.96	112.67
4	A	805	FAD	C4'-C3'-C2'	6.67	127.24	113.36
3	A	801	HEM	CAA-CBA-CGA	6.47	123.53	112.67
4	A	805	FAD	O4B-C1B-C2B	-5.84	98.40	106.93
3	A	801	HEM	CAD-CBD-CGD	5.41	121.74	112.67
3	A	804	HEM	CMD-C2D-C1D	-5.01	120.76	128.46
4	A	805	FAD	C6-C5X-C9A	4.78	125.31	119.05
4	A	805	FAD	C8M-C8-C9	-4.71	109.07	120.34
3	A	801	HEM	CMA-C3A-C4A	-4.65	121.31	128.46
4	A	805	FAD	C4-C4X-N5	-4.54	113.41	118.60
3	A	804	HEM	CBD-CAD-C3D	4.51	120.78	112.48
4	A	805	FAD	O2'-C2'-C1'	4.34	120.04	109.59
3	A	802	HEM	CMA-C3A-C4A	-4.13	122.12	128.46
4	A	805	FAD	O4'-C4'-C5'	4.11	119.14	109.92
4	A	805	FAD	C6-C7-C8	-3.96	113.24	119.91
4	A	805	FAD	C7-C6-C5X	-3.93	115.65	121.22
3	A	804	HEM	CMD-C2D-C3D	3.88	132.25	124.94
4	A	805	FAD	O2'-C2'-C3'	3.85	118.46	109.10
4	A	805	FAD	O5'-C5'-C4'	-3.79	99.24	109.36
3	A	801	HEM	CMD-C2D-C1D	-3.66	122.84	128.46
4	A	805	FAD	C5A-C6A-N6A	3.46	125.61	120.35
5	A	806	FUM	C6-C5-C4	3.45	131.06	123.69
3	A	801	HEM	CMB-C2B-C3B	3.42	131.08	124.68
4	A	805	FAD	O3B-C3B-C2B	3.36	122.70	111.82
3	A	804	HEM	CMB-C2B-C3B	3.34	130.92	124.68
3	A	801	HEM	CBD-CAD-C3D	-3.22	106.54	112.48
3	A	802	HEM	CAD-CBD-CGD	3.21	118.06	112.67
3	A	802	HEM	C4C-C3C-C2C	3.21	109.14	106.90
3	A	802	HEM	CMB-C2B-C3B	3.16	130.60	124.68
3	A	803	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
3	A	804	HEM	CMA-C3A-C4A	-3.09	123.72	128.46
4	A	805	FAD	C7M-C7-C6	2.99	127.49	120.34
3	A	801	HEM	CMC-C2C-C3C	2.99	130.26	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	HEM	CMC-C2C-C3C	2.98	130.25	124.68
4	A	805	FAD	C6-C5X-N5	-2.97	115.78	119.05
3	A	801	HEM	CBA-CAA-C2A	2.85	117.74	112.49
3	A	803	HEM	CMC-C2C-C3C	2.85	130.00	124.68
3	A	804	HEM	CBA-CAA-C2A	-2.84	107.25	112.49
4	A	805	FAD	C4X-N5-C5X	-2.77	114.01	116.77
4	A	805	FAD	C8-C9-C9A	-2.67	110.88	119.19
3	A	801	HEM	CMD-C2D-C3D	2.63	129.90	124.94
5	A	806	FUM	C2-C4-C5	-2.60	118.13	123.69
3	A	801	HEM	CMA-C3A-C2A	2.58	129.80	124.94
3	A	803	HEM	CMD-C2D-C1D	-2.57	124.51	128.46
3	A	801	HEM	C4C-C3C-C2C	2.53	108.67	106.90
3	A	802	HEM	CMA-C3A-C2A	2.45	129.56	124.94
3	A	803	HEM	CMA-C3A-C2A	2.35	129.38	124.94
3	A	801	HEM	C4A-C3A-C2A	2.34	108.63	107.00
3	A	803	HEM	CMD-C2D-C3D	2.31	129.29	124.94
3	A	802	HEM	CMD-C2D-C1D	-2.30	124.94	128.46
4	A	805	FAD	C9A-C5X-N5	-2.28	118.80	122.36
3	A	804	HEM	CMC-C2C-C3C	2.23	128.86	124.68
3	A	804	HEM	CAD-CBD-CGD	-2.21	108.97	112.67
3	A	804	HEM	CMA-C3A-C2A	2.21	129.10	124.94
4	A	805	FAD	C1'-C2'-C3'	2.16	115.82	109.79
4	A	805	FAD	C5A-C6A-N1A	-2.14	115.49	120.35

All (3) chirality outliers are listed below:

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

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	HEM	C3A-C2A-CAA-CBA
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	O4B-C4B-C5B-O5B
4	A	805	FAD	C2'-C3'-C4'-O4'
3	A	801	HEM	C3D-CAD-CBD-CGD

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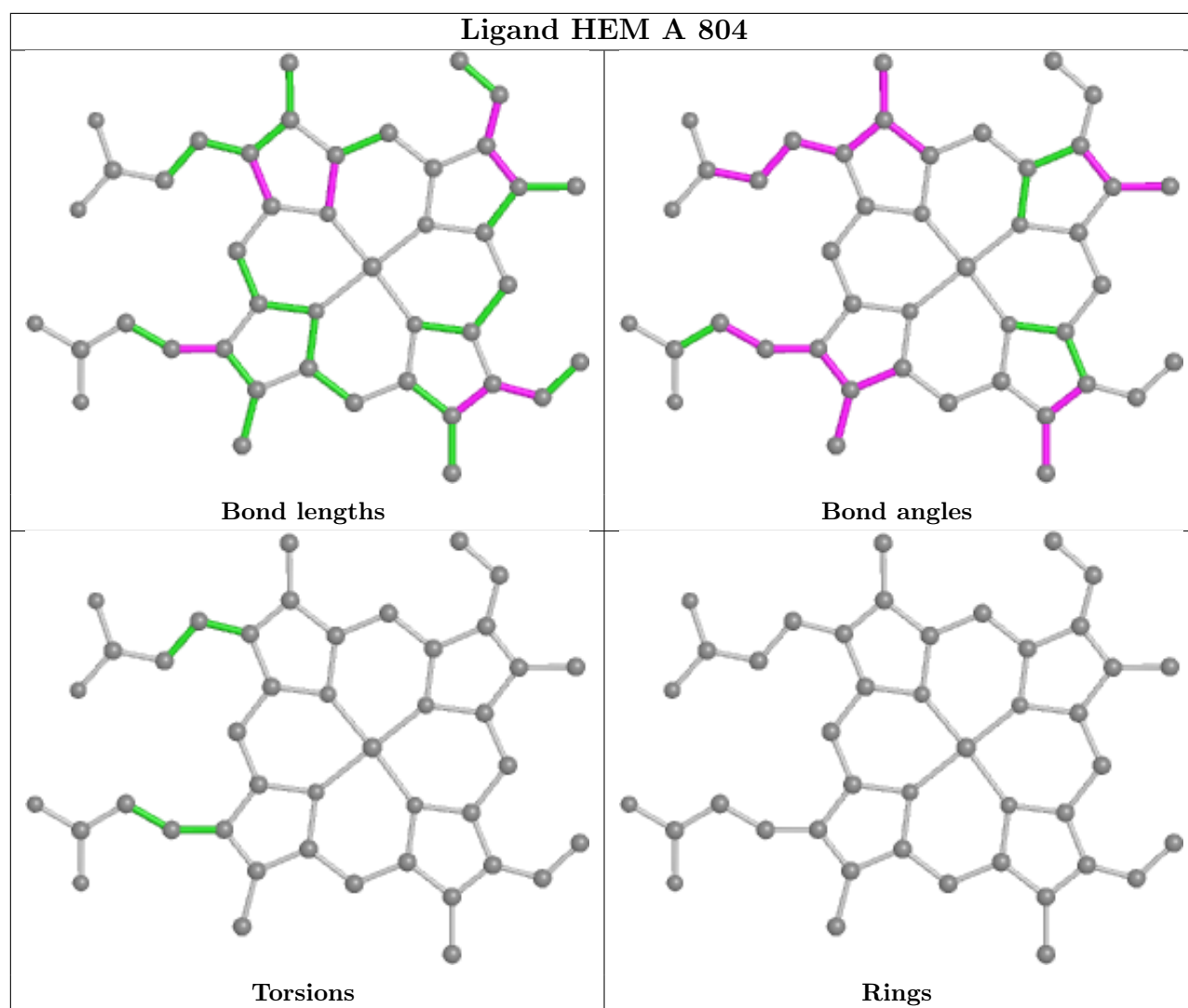
Mol	Chain	Res	Type	Atoms
3	A	803	HEM	C1A-C2A-CAA-CBA
4	A	805	FAD	C3B-C4B-C5B-O5B
4	A	805	FAD	P-O3P-PA-O1A
3	A	802	HEM	C3D-CAD-CBD-CGD
4	A	805	FAD	P-O3P-PA-O2A

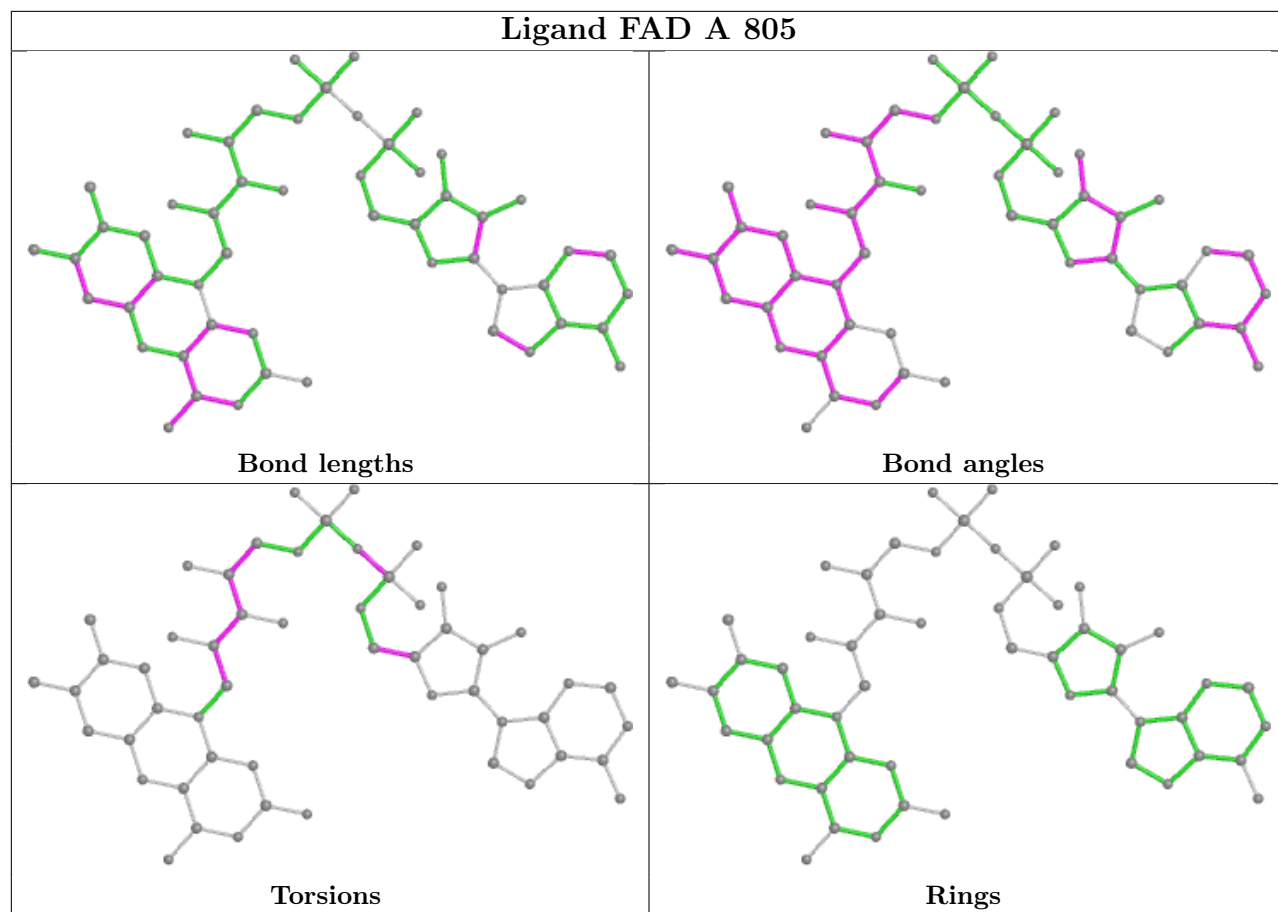
There are no ring outliers.

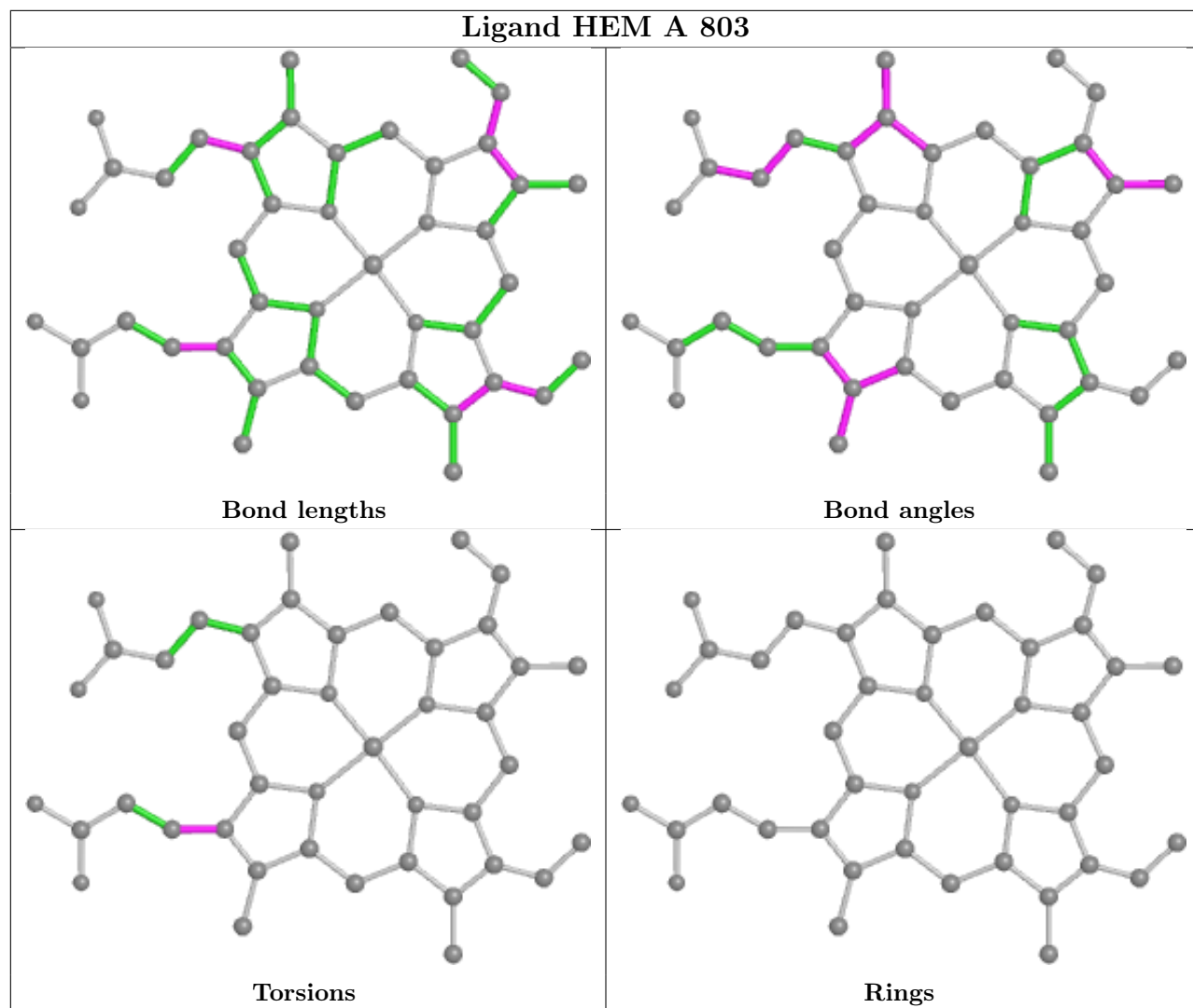
6 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	806	FUM	6	0
3	A	804	HEM	8	0
4	A	805	FAD	6	0
3	A	803	HEM	9	0
3	A	801	HEM	6	0
3	A	802	HEM	6	0

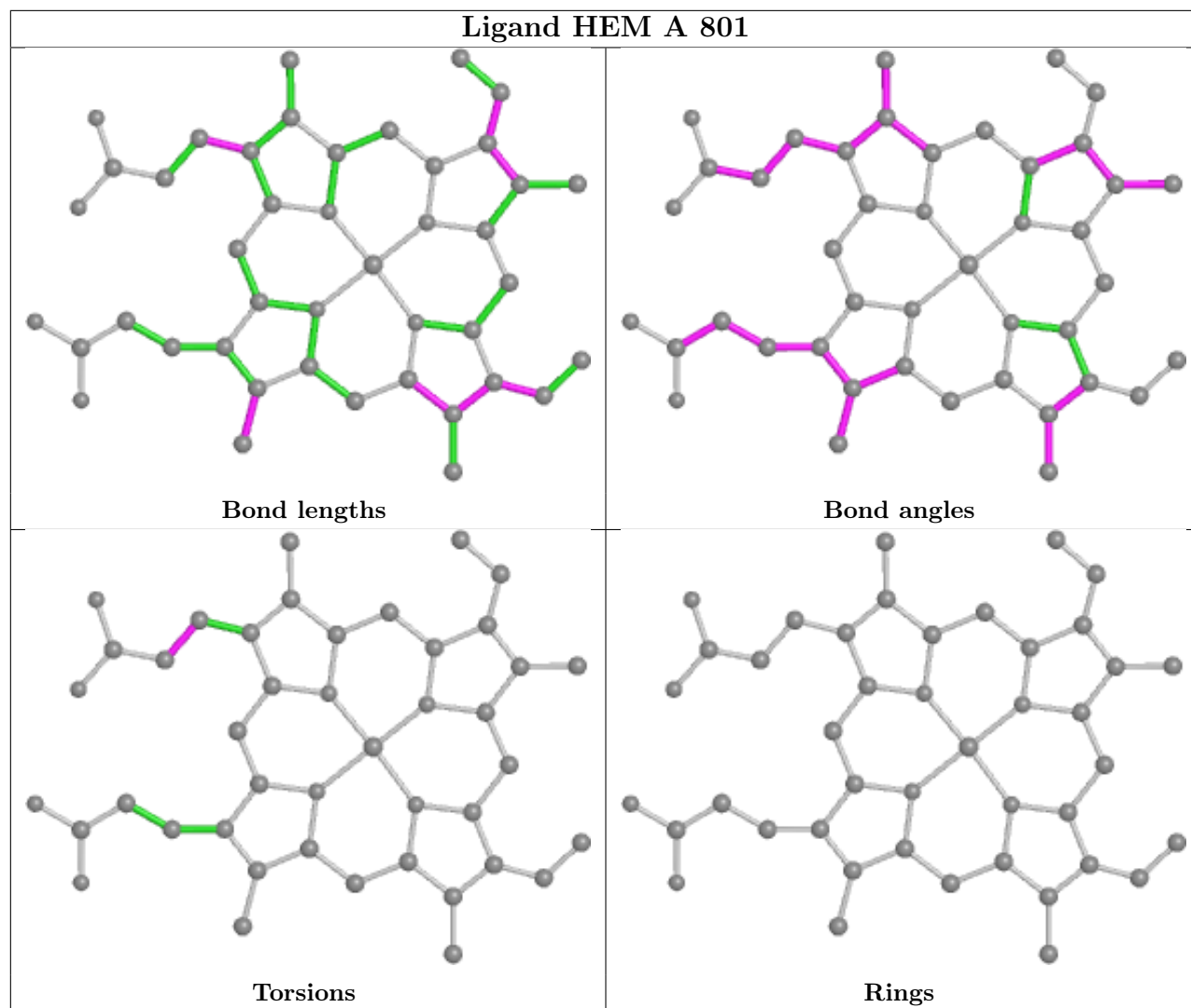
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

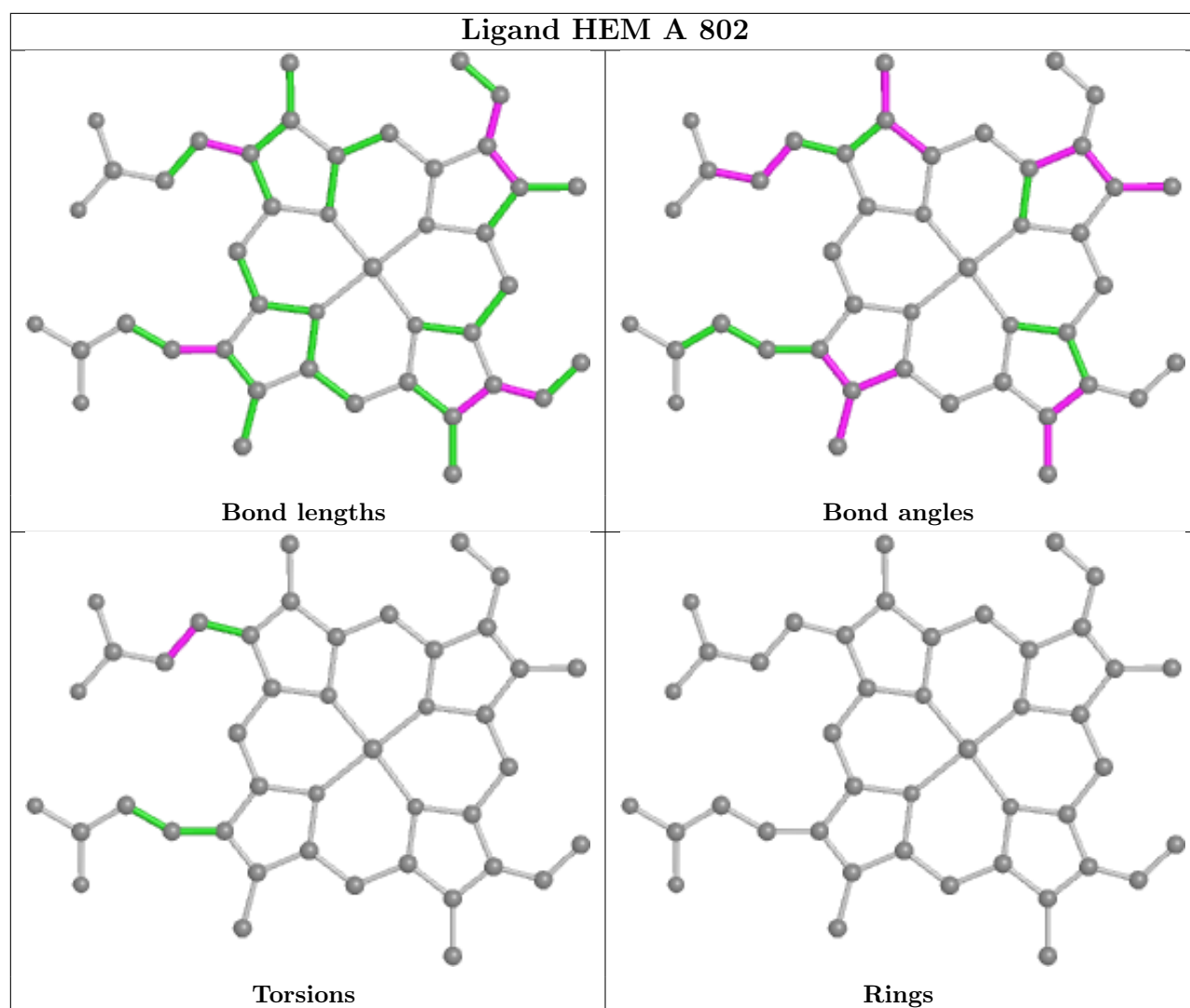












## 5.7 Other polymers [i](#)

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.