Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:03 pm BST

PDB ID	:	1GVH
Title	:	The X-ray structure of ferric Escherichia coli flavohemoglobin reveals an unespected geometry of the distal heme pocket
Authors	:	Ilari, A.; Johnson, K.A.; Bonamore, A.; Farina, A.; Boffi, A.
Deposited on	:	2002-02-13
Resolution	:	2.19 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:

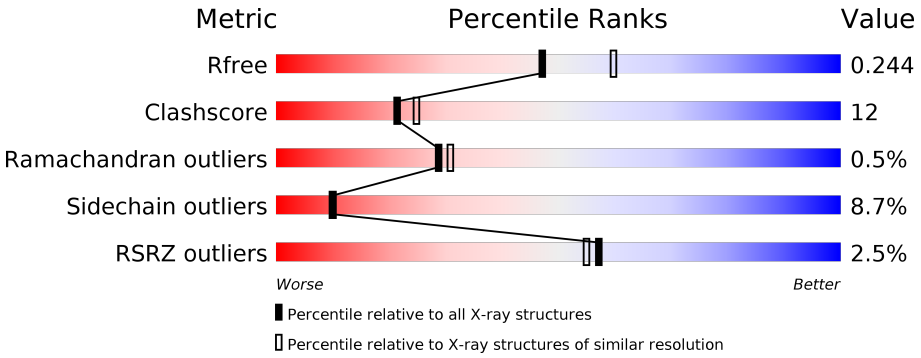
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	3% 66% 26% 7% .

2 Entry composition

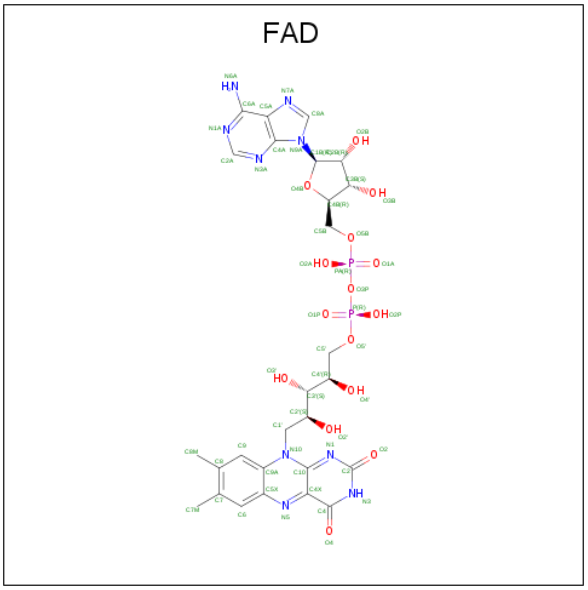
There are 6 unique types of molecules in this entry. The entry contains 3387 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOHEMOPROTEIN.

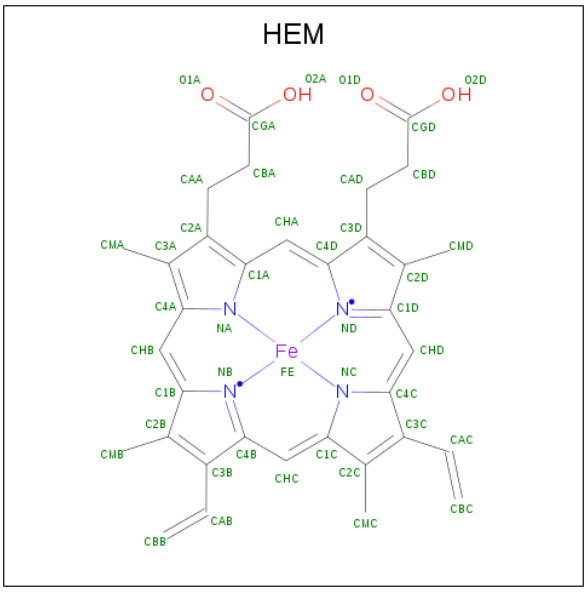
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3097	1972	532	581	12	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

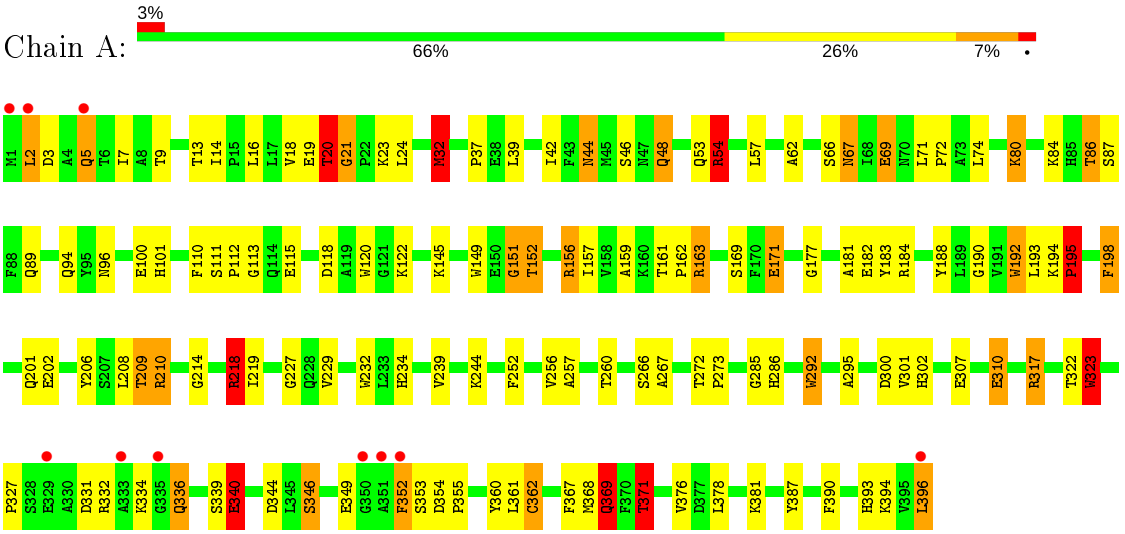
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: FLAVOHEMOPROTEIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α, β, γ	164.86Å 164.86Å 53.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.19 24.44 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.19) 99.5 (24.44-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.95 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.187 , 0.247 0.186 , 0.244	Depositor DCC
R_{free} test set	1148 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 71.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3387	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CL, 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	0.64	1/3175 (0.0%)	1.19	26/4308 (0.6%)

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	56

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	HIS	CG-CD2	7.71	1.48	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	ARG	NE-CZ-NH1	-20.42	110.09	120.30
1	A	317	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	A	156	ARG	NE-CZ-NH1	-10.59	115.01	120.30
1	A	218	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	A	323	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	A	210	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	120	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	A	149	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	292	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	A	232	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	A	163	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	192	TRP	CD1-CG-CD2	7.96	112.67	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ARG	NH1-CZ-NH2	-7.70	110.93	119.40
1	A	149	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	120	TRP	CE2-CD2-CG	-7.24	101.50	107.30
1	A	156	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	292	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	323	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	A	232	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	A	192	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	54	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	323	TRP	CG-CD1-NE1	-6.29	103.81	110.10
1	A	396	LEU	N-CA-CB	6.24	122.88	110.40
1	A	232	TRP	CG-CD1-NE1	-5.75	104.34	110.10
1	A	302	HIS	CA-CB-CG	5.46	122.89	113.60
1	A	163	ARG	NE-CZ-NH2	5.30	122.95	120.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	PHE	Mainchain
1	A	113	GLY	Mainchain
1	A	145	LYS	Mainchain
1	A	151	GLY	Mainchain
1	A	157	ILE	Mainchain
1	A	16	LEU	Mainchain
1	A	161	THR	Mainchain
1	A	162	PRO	Mainchain
1	A	177	GLY	Mainchain
1	A	181	ALA	Mainchain
1	A	184	ARG	Mainchain
1	A	19	GLU	Mainchain
1	A	190	GLY	Mainchain
1	A	194	LYS	Mainchain
1	A	195	PRO	Mainchain
1	A	198	PHE	Mainchain
1	A	20	THR	Mainchain
1	A	201	GLN	Mainchain
1	A	208	LEU	Mainchain
1	A	209	THR	Mainchain
1	A	210	ARG	Sidechain
1	A	214	GLY	Mainchain
1	A	218	ARG	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	A	219	ILE	Mainchain
1	A	23	LYS	Mainchain
1	A	234	HIS	Mainchain
1	A	239	VAL	Mainchain
1	A	252	PHE	Mainchain
1	A	257	ALA	Mainchain
1	A	266	SER	Mainchain
1	A	267	ALA	Mainchain
1	A	292	TRP	Mainchain
1	A	295	ALA	Mainchain
1	A	3	ASP	Mainchain
1	A	317	ARG	Sidechain
1	A	32	MET	Mainchain
1	A	323	TRP	Mainchain
1	A	340	GLU	Mainchain
1	A	344	ASP	Mainchain
1	A	346	SER	Mainchain
1	A	352	PHE	Mainchain
1	A	362	CYS	Mainchain
1	A	369	GLN	Mainchain
1	A	37	PRO	Mainchain
1	A	371	THR	Mainchain
1	A	378	LEU	Mainchain
1	A	390	PHE	Mainchain
1	A	394	LYS	Mainchain
1	A	48	GLN	Mainchain
1	A	5	GLN	Mainchain
1	A	54	ARG	Sidechain
1	A	62	ALA	Mainchain
1	A	66	SER	Mainchain
1	A	7	ILE	Mainchain
1	A	87	SER	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3097	0	3013	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	8	0
3	A	43	0	30	4	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	191	0	0	7	0
All	All	3387	0	3072	75	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 12.

All (75) 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:48:GLN:HG3	2:A:1397:FAD:H3B	1.47	0.96
1:A:368:MET:CE	1:A:387:TYR:HB2	1.98	0.94
1:A:369:GLN:NE2	1:A:396:LEU:HD13	1.88	0.87
1:A:368:MET:HE2	1:A:387:TYR:HB2	1.58	0.86
1:A:209:THR:OG1	1:A:218:ARG:HD2	1.74	0.85
1:A:53:GLN:HB3	3:A:1398:HEM:HBD2	1.63	0.80
1:A:86:THR:HG23	6:A:2119:HOH:O	1.82	0.80
1:A:369:GLN:CD	1:A:396:LEU:HD13	2.04	0.77
1:A:368:MET:HE1	1:A:387:TYR:HB2	1.67	0.76
1:A:71:LEU:N	1:A:72:PRO:HD2	2.01	0.75
1:A:71:LEU:HA	1:A:74:LEU:HD12	1.70	0.71
1:A:229:VAL:N	2:A:1397:FAD:O1P	2.23	0.70
1:A:361:LEU:C	1:A:368:MET:HE3	2.16	0.66
1:A:2:LEU:HD11	1:A:122:LYS:HB3	1.78	0.65
1:A:44:ASN:ND2	1:A:46:SER:H	2.00	0.60
1:A:272:THR:OG1	1:A:273:PRO:HD3	2.03	0.58
1:A:396:LEU:OXT	1:A:396:LEU:HG	2.02	0.58
1:A:96:ASN:O	1:A:100:GLU:HG3	2.06	0.55
1:A:171:GLU:OE2	1:A:218:ARG:HB2	2.07	0.55
1:A:322:THR:HG23	6:A:2156:HOH:O	2.07	0.55
1:A:256:VAL:HB	1:A:260:THR:HB	1.88	0.55
1:A:206:TYR:HH	2:A:1397:FAD:HO4'	1.50	0.54
1:A:89:GLN:NE2	1:A:151:GLY:HA2	2.22	0.54
1:A:195:PRO:HD2	1:A:198:PHE:CD1	2.43	0.53
1:A:332:ARG:NH2	1:A:340:GLU:OE1	2.42	0.53
1:A:188:TYR:CD2	2:A:1397:FAD:HM72	2.45	0.52
1:A:32:MET:HG2	1:A:101:HIS:CD2	2.44	0.52
1:A:48:GLN:CG	2:A:1397:FAD:H3B	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:O	1:A:371:THR:HB	2.11	0.51
1:A:57:LEU:HD23	1:A:57:LEU:C	2.30	0.51
1:A:163:ARG:HD3	1:A:169:SER:OG	2.11	0.51
1:A:71:LEU:N	1:A:72:PRO:CD	2.74	0.51
1:A:42:ILE:HD13	1:A:94:GLN:HE22	1.75	0.51
1:A:361:LEU:O	1:A:368:MET:HE1	2.10	0.51
1:A:111:SER:N	1:A:112:PRO:HD3	2.26	0.51
1:A:369:GLN:OE1	1:A:396:LEU:HD13	2.11	0.51
1:A:67:ASN:HA	1:A:69:GLU:OE1	2.11	0.50
1:A:331:ASP:HA	1:A:336:GLN:HE22	1.77	0.50
1:A:396:LEU:HD11	6:A:2169:HOH:O	2.12	0.50
1:A:44:ASN:HD21	1:A:46:SER:HB3	1.77	0.49
1:A:195:PRO:HD2	1:A:198:PHE:CG	2.47	0.49
1:A:369:GLN:HE22	1:A:396:LEU:HD13	1.74	0.49
1:A:361:LEU:O	1:A:368:MET:CE	2.61	0.48
2:A:1397:FAD:H5'1	6:A:2188:HOH:O	2.12	0.48
1:A:227:GLY:HA3	2:A:1397:FAD:O2P	2.14	0.48
1:A:42:ILE:HD13	1:A:94:GLN:NE2	2.29	0.48
1:A:53:GLN:HE22	3:A:1398:HEM:HAA1	1.78	0.47
1:A:192:TRP:CD1	1:A:192:TRP:N	2.83	0.47
1:A:152:THR:HG21	1:A:244:LYS:HD3	1.97	0.47
1:A:171:GLU:OE2	1:A:218:ARG:HG3	2.15	0.46
1:A:361:LEU:C	1:A:368:MET:CE	2.83	0.46
1:A:336:GLN:H	1:A:336:GLN:HE21	1.64	0.46
1:A:54:ARG:NE	6:A:2028:HOH:O	2.48	0.46
1:A:323:TRP:CD1	1:A:339:SER:HB2	2.50	0.46
1:A:14:ILE:O	1:A:18:VAL:HG13	2.15	0.46
1:A:362:CYS:N	1:A:368:MET:HE3	2.30	0.46
1:A:229:VAL:HB	2:A:1397:FAD:O1P	2.16	0.46
1:A:182:GLU:HG2	1:A:183:TYR:H	1.80	0.45
1:A:44:ASN:HA	1:A:202:GLU:OE2	2.17	0.45
1:A:327:PRO:HG3	1:A:340:GLU:HB2	1.98	0.44
1:A:86:THR:CG2	6:A:2119:HOH:O	2.51	0.44
1:A:193:LEU:HD12	1:A:229:VAL:HG13	2.00	0.43
1:A:369:GLN:HG3	1:A:396:LEU:HD22	2.00	0.43
1:A:360:TYR:C	1:A:361:LEU:HD12	2.39	0.43
1:A:80:LYS:HE2	6:A:2181:HOH:O	2.19	0.43
1:A:20:THR:O	1:A:21:GLY:C	2.57	0.43
1:A:307:GLU:O	1:A:310:GLU:HG3	2.19	0.42
1:A:84:LYS:HE3	3:A:1398:HEM:HAD1	2.02	0.42
1:A:354:ASP:OD2	1:A:355:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG21	1:A:244:LYS:NZ	2.36	0.41
1:A:285:GLY:O	1:A:286:HIS:C	2.58	0.41
1:A:9:THR:O	1:A:13:THR:HG23	2.21	0.41
1:A:39:LEU:HD22	3:A:1398:HEM:HBC1	2.02	0.41
1:A:159:ALA:HB3	1:A:171:GLU:HB2	2.02	0.40
1:A:381:LYS:HD3	1:A:381:LYS:HA	1.93	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	394/396 (100%)	379 (96%)	13 (3%)	2 (0%)	29 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLY
1	A	195	PRO

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	321/321 (100%)	293 (91%)	28 (9%)	10 10

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	5	GLN
1	A	20	THR
1	A	24	LEU
1	A	32	MET
1	A	44	ASN
1	A	67	ASN
1	A	69	GLU
1	A	80	LYS
1	A	86	THR
1	A	115	GLU
1	A	118	ASP
1	A	152	THR
1	A	156	ARG
1	A	171	GLU
1	A	300	ASP
1	A	301	VAL
1	A	310	GLU
1	A	334	LYS
1	A	336	GLN
1	A	340	GLU
1	A	346	SER
1	A	349	GLU
1	A	352	PHE
1	A	353	SER
1	A	369	GLN
1	A	371	THR
1	A	376	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	53	GLN
1	A	67	ASN
1	A	70	ASN
1	A	89	GLN
1	A	142	ASN
1	A	235	ASN
1	A	271	GLN
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	369	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	FAD	A	1397	-	51,58,58	3.04	21 (41%)	60,89,89	2.74	18 (30%)
3	HEM	A	1398	1	27,50,50	1.79	9 (33%)	17,82,82	1.12	2 (11%)

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
2	FAD	A	1397	-	-	12/30/50/50	0/6/6/6
3	HEM	A	1398	1	-	1/6/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1397	FAD	C1'-N10	-8.08	1.39	1.48
2	A	1397	FAD	C4X-N5	7.41	1.43	1.33
2	A	1397	FAD	C9A-N10	7.35	1.48	1.38
2	A	1397	FAD	C2A-N3A	6.58	1.42	1.32
2	A	1397	FAD	C4A-N3A	6.22	1.44	1.35
2	A	1397	FAD	C5X-N5	5.06	1.43	1.35
2	A	1397	FAD	C4-N3	5.00	1.41	1.33
2	A	1397	FAD	C10-N1	4.78	1.39	1.33
2	A	1397	FAD	C2'-C3'	-4.17	1.45	1.53
2	A	1397	FAD	C5'-C4'	-3.68	1.46	1.51
3	A	1398	HEM	C3C-C2C	-3.67	1.35	1.40
3	A	1398	HEM	C3C-CAC	-3.42	1.40	1.47
2	A	1397	FAD	C4X-C10	3.40	1.42	1.38
2	A	1397	FAD	C5A-C4A	-3.36	1.32	1.40
2	A	1397	FAD	C8A-N7A	-2.85	1.29	1.34
2	A	1397	FAD	C4'-C3'	-2.66	1.48	1.53
3	A	1398	HEM	C3B-CAB	-2.64	1.42	1.47
2	A	1397	FAD	P-O1P	-2.59	1.41	1.50
2	A	1397	FAD	P-O5'	-2.56	1.48	1.59
3	A	1398	HEM	C1C-C2C	2.54	1.48	1.42
2	A	1397	FAD	C9A-C5X	2.54	1.47	1.42
3	A	1398	HEM	C4B-NB	2.52	1.41	1.36
3	A	1398	HEM	CBC-CAC	2.42	1.45	1.29
3	A	1398	HEM	CBB-CAB	2.39	1.45	1.29
3	A	1398	HEM	C3B-C2B	-2.27	1.37	1.40
2	A	1397	FAD	O5'-C5'	-2.13	1.36	1.44
2	A	1397	FAD	C2B-C3B	-2.11	1.47	1.53
2	A	1397	FAD	C4-C4X	-2.06	1.37	1.41
2	A	1397	FAD	C6-C7	2.05	1.42	1.37
3	A	1398	HEM	C1D-ND	2.04	1.40	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1397	FAD	C4-N3-C2	12.79	125.94	115.14
2	A	1397	FAD	P-O3P-PA	6.68	155.74	132.83
2	A	1397	FAD	C4X-C4-N3	-6.61	114.39	123.43
2	A	1397	FAD	O3'-C3'-C2'	6.02	123.35	108.81
2	A	1397	FAD	C5X-C9A-N10	-4.65	114.34	117.72
2	A	1397	FAD	O4'-C4'-C3'	4.54	120.14	109.10
2	A	1397	FAD	C1'-N10-C9A	-3.61	115.45	118.29
2	A	1397	FAD	C1B-N9A-C4A	3.44	132.68	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1397	FAD	C1'-N10-C10	3.08	121.17	118.41
2	A	1397	FAD	O4'-C4'-C5'	2.56	115.66	109.92
3	A	1398	HEM	CBA-CAA-C2A	-2.47	107.93	112.49
2	A	1397	FAD	C10-C4X-N5	2.39	122.91	121.26
2	A	1397	FAD	N3A-C2A-N1A	-2.36	124.99	128.68
2	A	1397	FAD	O5B-C5B-C4B	-2.36	100.87	108.99
2	A	1397	FAD	C1'-C2'-C3'	2.34	116.33	109.79
2	A	1397	FAD	O2A-PA-O1A	2.14	122.82	112.24
2	A	1397	FAD	C6-C5X-C9A	-2.08	116.32	119.05
2	A	1397	FAD	O4B-C4B-C5B	2.05	116.11	109.37
3	A	1398	HEM	C3B-C4B-NB	2.03	111.83	109.21
2	A	1397	FAD	C5B-C4B-C3B	2.01	122.73	115.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1397	FAD	C5B-O5B-PA-O1A
2	A	1397	FAD	C1'-C2'-C3'-O3'
2	A	1397	FAD	C1'-C2'-C3'-C4'
2	A	1397	FAD	O2'-C2'-C3'-O3'
2	A	1397	FAD	O2'-C2'-C3'-C4'
2	A	1397	FAD	O4'-C4'-C5'-O5'
2	A	1397	FAD	C5'-O5'-P-O3P
3	A	1398	HEM	C3D-CAD-CBD-CGD
2	A	1397	FAD	C3'-C4'-C5'-O5'
2	A	1397	FAD	C5B-O5B-PA-O3P
2	A	1397	FAD	C5'-O5'-P-O2P
2	A	1397	FAD	O4B-C4B-C5B-O5B
2	A	1397	FAD	C2'-C3'-C4'-O4'

There are no ring outliers.

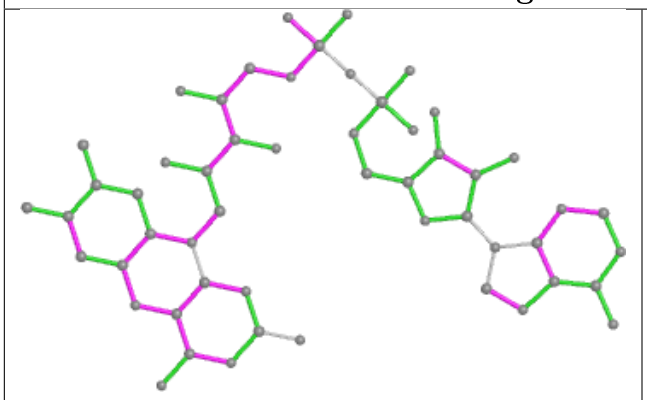
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1397	FAD	8	0
3	A	1398	HEM	4	0

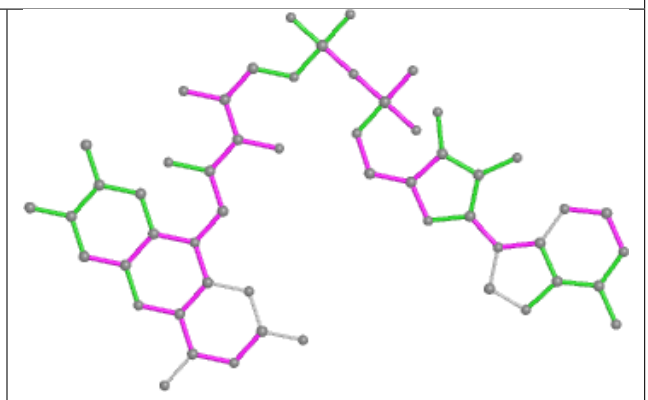
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

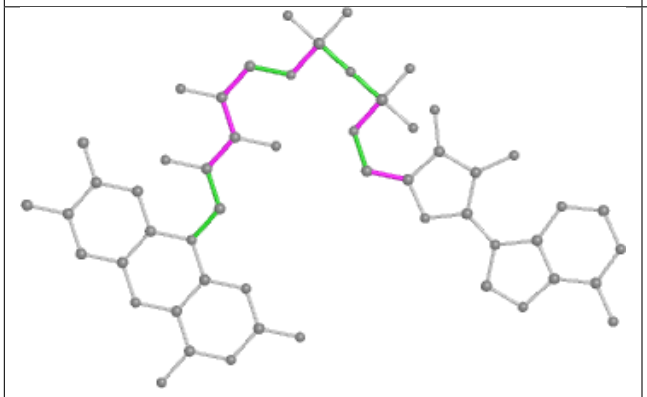
Ligand FAD A 1397



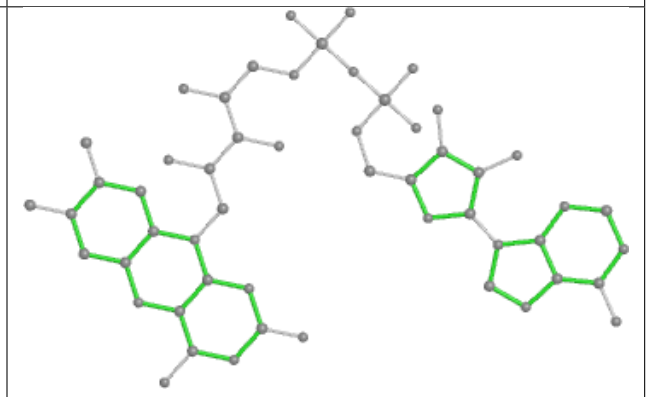
Bond lengths



Bond angles

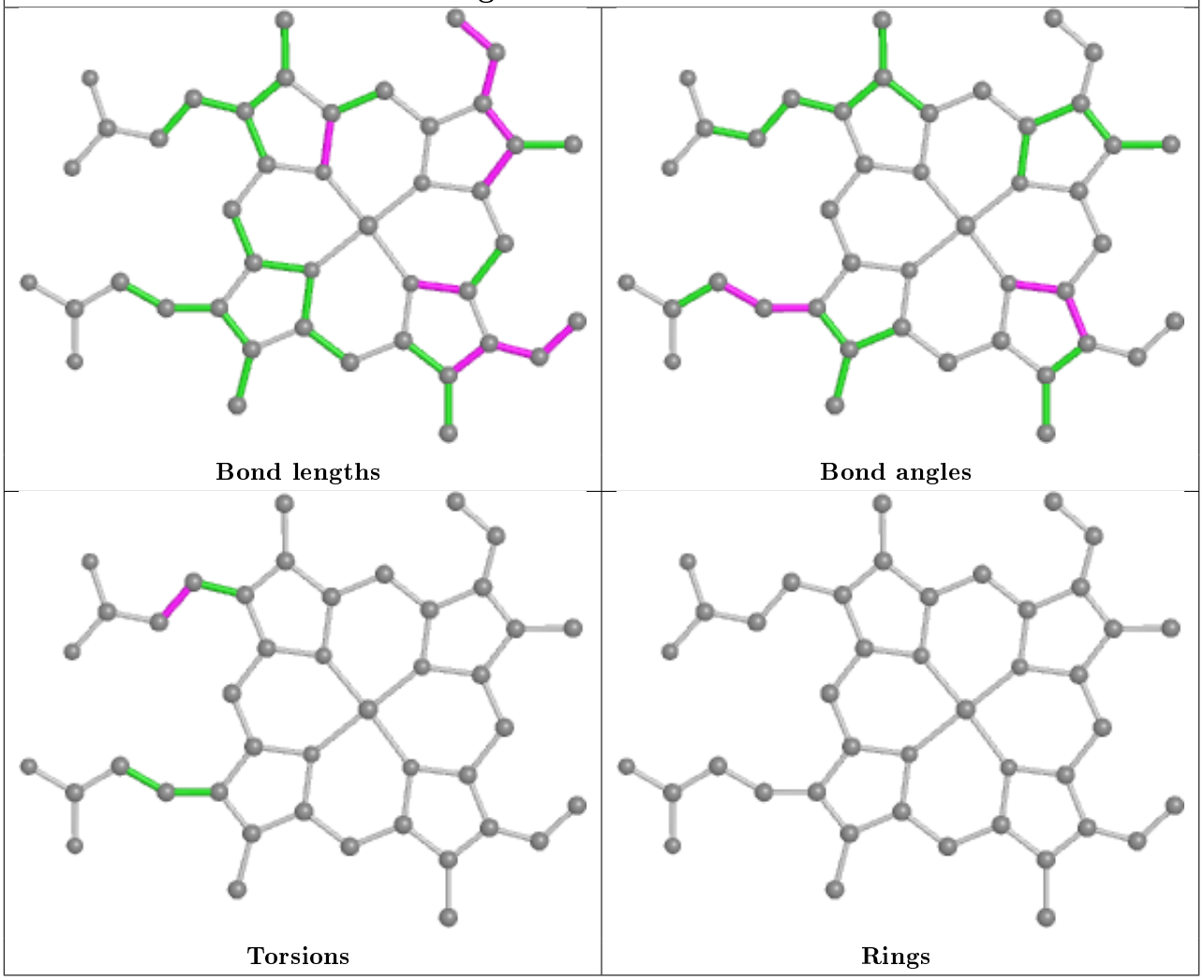


Torsions



Rings

Ligand HEM A 1398



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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	396/396 (100%)	-0.26	10 (2%) 57 55	11, 20, 51, 78	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	LEU	5.4
1	A	351	ALA	3.6
1	A	352	PHE	3.6
1	A	333	ALA	3.6
1	A	5	GLN	2.9
1	A	350	GLY	2.8
1	A	335	GLY	2.6
1	A	1	MET	2.5
1	A	2	LEU	2.3
1	A	329	GLU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

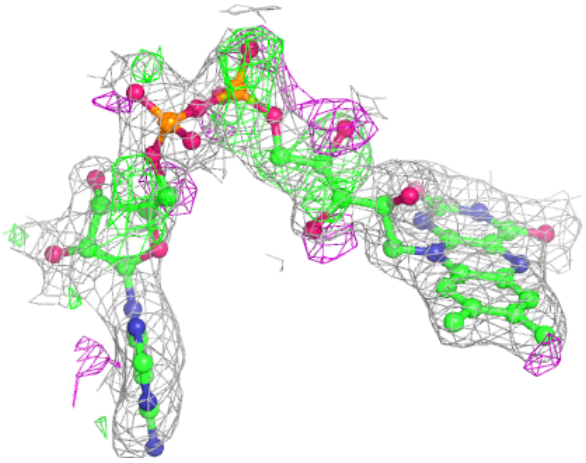
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

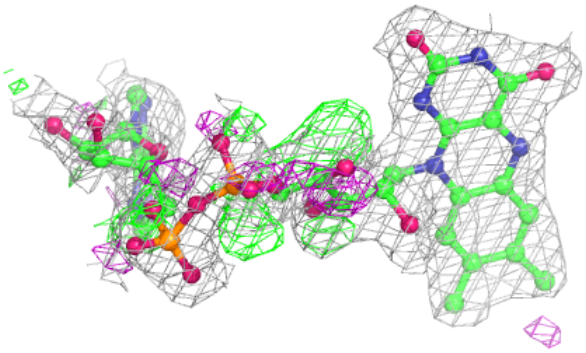
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	1397	53/53	0.93	0.15	8,21,58,61	0
3	HEM	A	1398	43/43	0.97	0.12	10,16,38,43	0
4	NA	A	1399	1/1	0.97	0.12	11,11,11,11	0
5	CL	A	1401	1/1	0.98	0.14	6,6,6,6	0
4	NA	A	1400	1/1	0.99	0.05	2,2,2,2	0

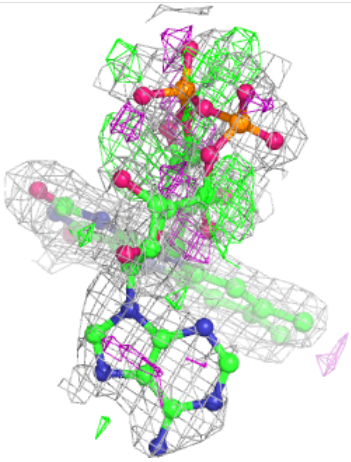
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 1397:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

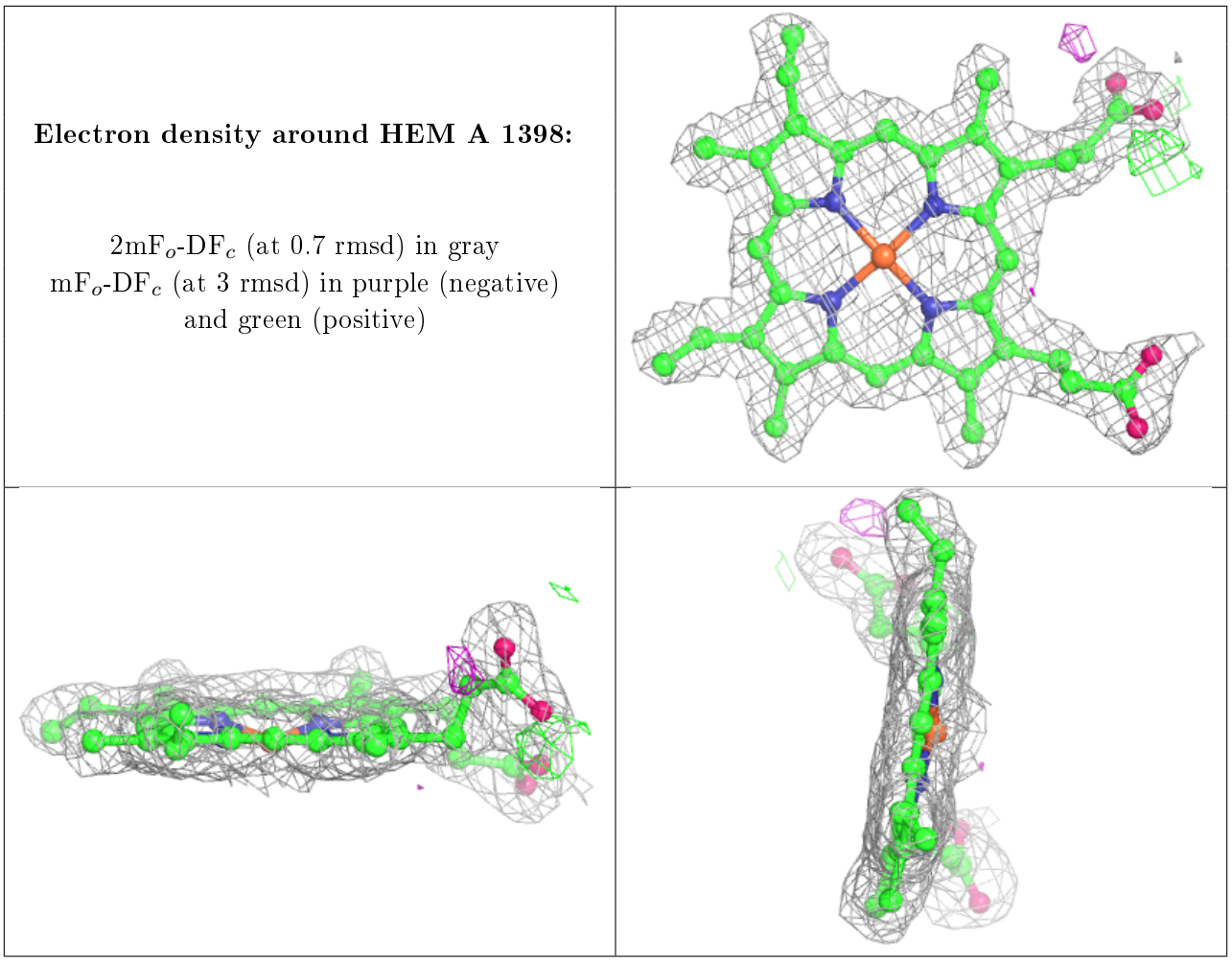






Electron density around HEM A 1398:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.