wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 02:59 AM EST

PDB ID	:	2OZ0
Title	:	Mechanistic and Structural Studies of H373Q Flavocytochrome b2: Effects of Mutating the Active Site Base
Authors	:	Tsai, C.-L.; Gokulan, K.; Sobrado, P.; Sacchettini, J.C.; Fitzpatrick, P.F.
Deposited on	:	2007-02-23
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

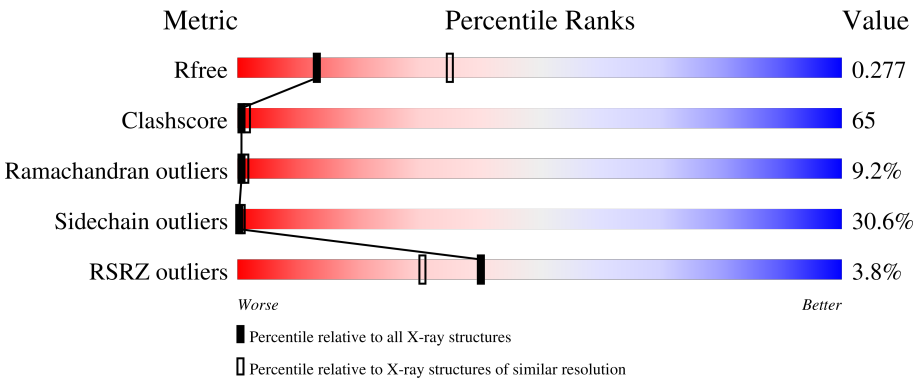
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	511	4%, 16%, 38%, 30%, 13%, •
1	B	511	2%, 11%, 25%, 26%, 16%, 23%

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
3	FMN	A	569	X	-	X	-
3	FMN	B	570	-	-	X	-
4	PYR	B	571	-	X	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7042 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.

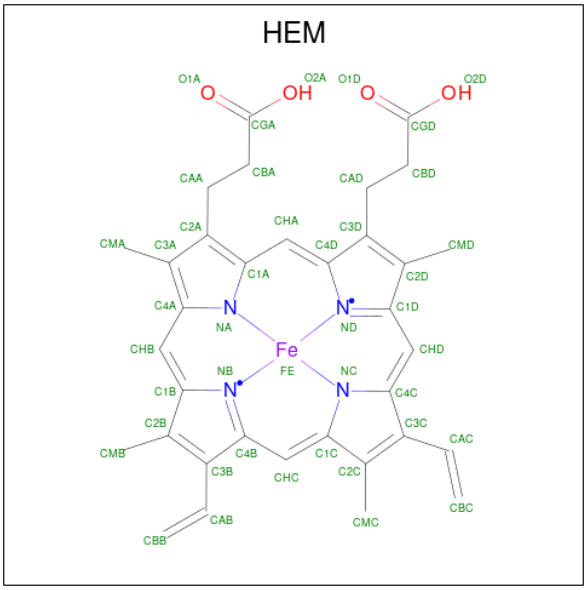
- Molecule 1 is a protein called Cytochrome b2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	492	3833	2441	649	728	15	0	0	0
1	B	396	3081	1953	524	593	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

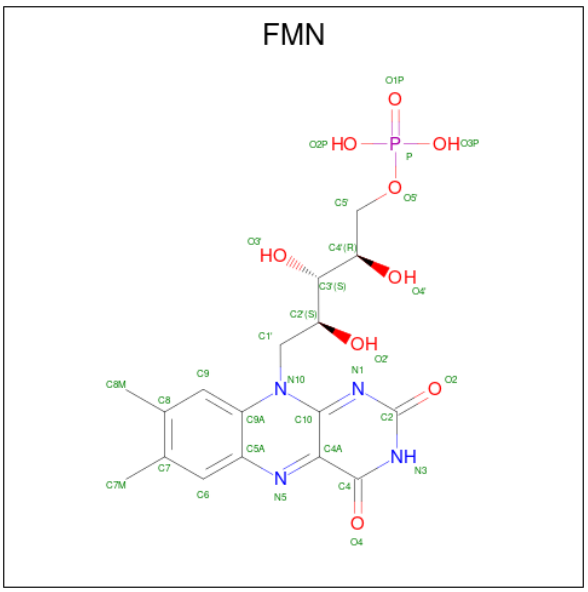
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLN	HIS	engineered mutation	UNP P00175
B	373	GLN	HIS	engineered mutation	UNP P00175

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



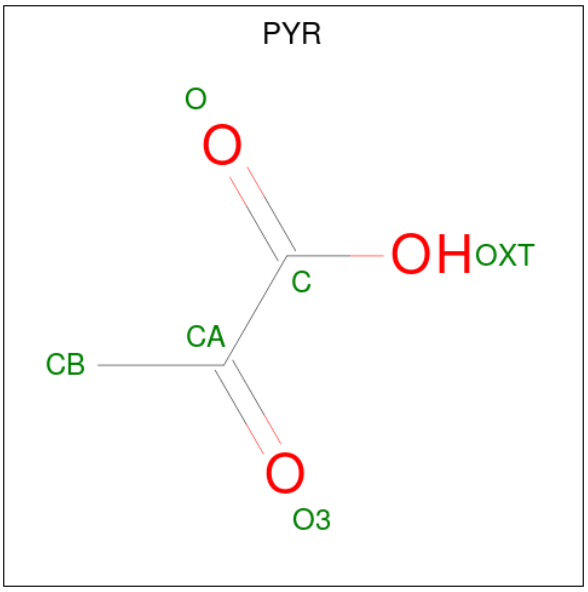
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	B	1	31	17	4	9	1	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is water.

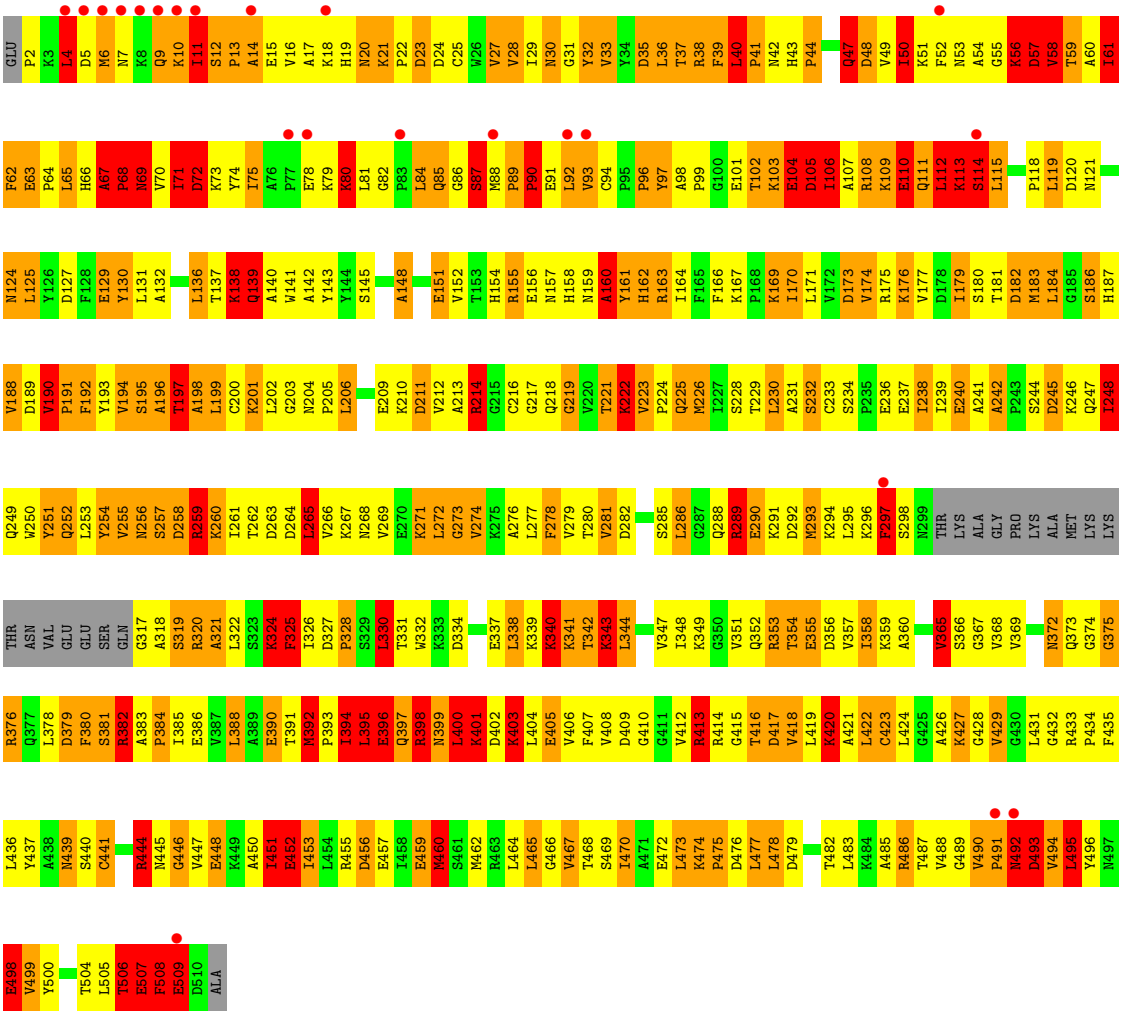
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	7	7	7	0	0
			Total	O		
5	B	10	10	10	0	0

3 Residue-property plots (i)

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

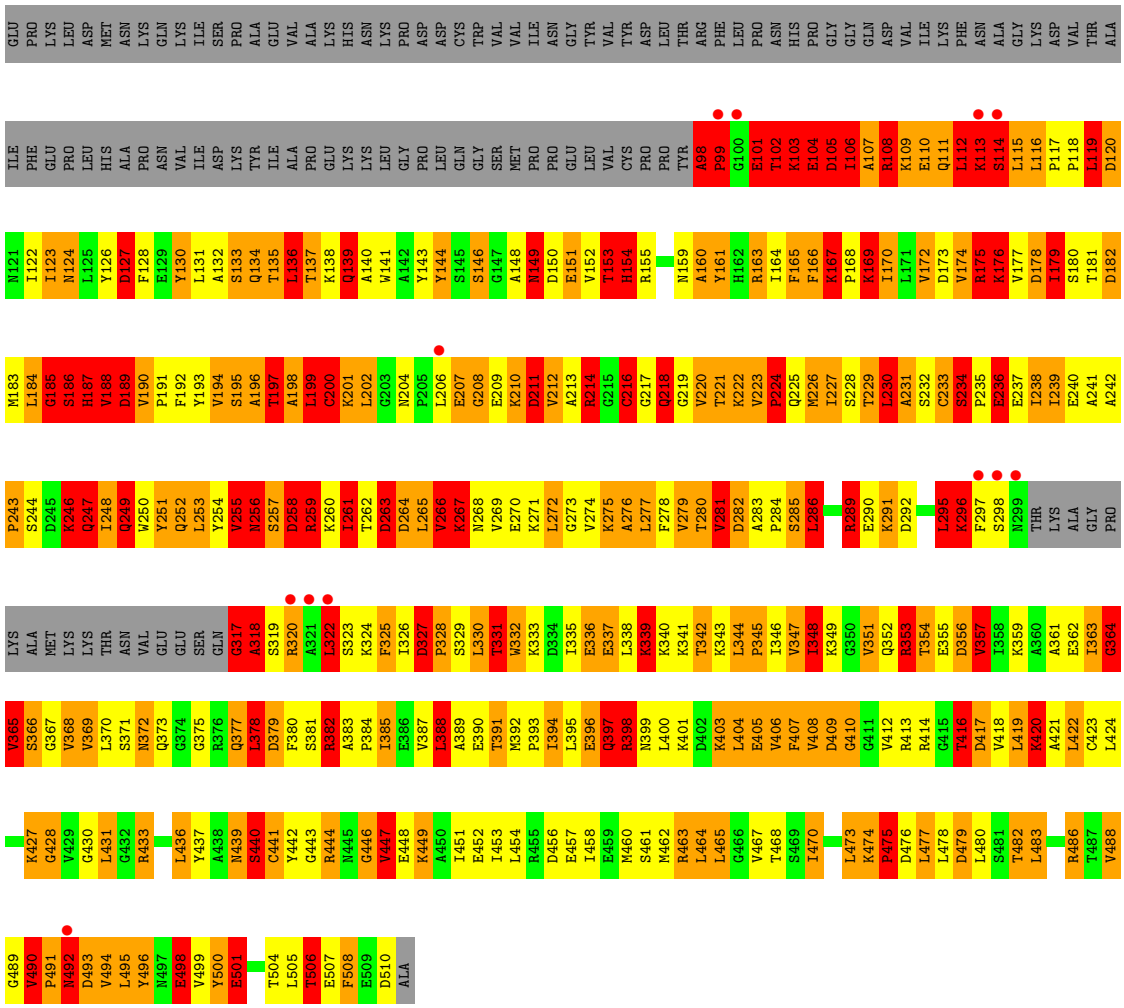
• Molecule 1: Cytochrome b2

Chain A: 4% 16% 38% 30% 13%



• Molecule 1: Cytochrome b2

Chain B: 2% 11% 25% 26% 16% 23%


GLU PRO LYS LEU ASP MET ASN LYS GLN LYS ILE SER PRO ALA GLU VAL ALA LYS HIS ASN LYS PRO ASP ASP CYS TRP VAL VAL ILE ASN GLY TYR VAL TYR ASP LEU THR ARG PHE LEU PRO ASN HIS PRO GLY GLY GLN ASP VAL ILE LYS PHE ASN ALA GLY LYS ASP VAL THR ALA
ILE PHE GLU PRO LEU HIS ALA PRO ASN VAL ILE ASP LYS TYR ILE ALA PRO GLU LYS LYS LEU GLY PRO LEU GLN GLY SER MET PRO PRO GLU LEU VAL CYS PRO PRO TYR A98 P99 G100 E101 T102 K103 E104 D105 I106 A107 R108 K109 E110 Q111 L112 K113 S114 L115 L116 P117 P118 L119 D120
N121 I122 I123 N124 L125 Y126 D127 F128 E129 Y130 L131 A132 S133 Q134 T135 L136 T137 K138 Q139 A140 W141 A142 Y143 Y144 S145 S146 G147 A148 N149 D150 E151 V152 T153 H154 R155 N159 A160 Y161 H162 R163 I164 F165 F166 K167 P168 K169 I170 L171 V172 D173 V174 R175 K176 V177 D178 I179 S180 T181 D182
M183 L184 G185 S186 H187 V188 D189 V190 P191 F192 Y193 V194 S195 A196 T197 A198 L199 C200 K201 L202 G203 N204 P205 L206 E207 G208 E209 K210 D211 V212 A213 R214 G215 C216 G217 Q218 G219 V220 T221 K222 V223 P224 Q225 M226 I227 S228 T229 L230 A231 S232 C233 S234 P235 E236 E237 I238 I239 E240 A241 A242
P243 S244 D245 K246 Q247 I248 Q249 W250 Y251 Q252 L253 Y254 V255 N256 S257 D258 R259 K260 I261 T262 D263 D264 L265 V266 K267 N268 V269 E270 K271 L272 G273 V274 K275 A276 L277 F278 V279 T280 V281 D282 A283 P284 S285 L286 R289 E290 K291 D292 L295 K296 F297 S298 N299 THR LYS ALA GLY PRO
LYS ALA MET LYS LYS THR ASN VAL GLU GLU SER GLN G317 A318 S319 R320 A321 L322 S323 K324 F325 I326 D327 P328 S329 L330 T331 W332 K333 D334 I335 E336 E337 L338 K339 K340 K341 T342 K343 L344 P345 I346 V347 I348 K349 G350 V351 Q352 R353 T354 E355 D356 V357 I358 K359 A360 A361 E362 I363 G364
V365 S366 G367 V368 V369 L370 S371 N372 Q373 G374 G375 R376 Q377 L378 D379 F380 S381 R382 A383 P384 I385 E386 V387 L388 A389 E390 T391 M392 P393 I394 L395 E396 Q397 R398 N399 L400 K401 D402 K403 L404 E405 V406 F407 V408 D409 G410 G411 V412 R413 R414 G415 T416 D417 V418 L419 K420 A421 L422 C423 L424
K427 G428 V429 G430 L431 G432 R433 L436 Y437 A438 N439 S440 C441 Y442 G443 R444 N445 G446 V447 E448 K449 A450 I451 E452 I453 L454 R455 D456 E457 I458 E459 M460 S461 M462 R463 L464 L465 G466 V467 T468 S469 I470 L473 K474 P475 D476 L477 L478 D479 L480 S481 T482 L483 R486 T487 V488
G489 V490 P491 N492 D493 V494 L495 Y496 N497 E498 V499 Y500 E501 T504 L505 T506 E507 F508 E509 D510 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.69Å 163.69Å 112.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.34 – 2.45	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-2.80) 64.2 (48.34-2.45)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.278 0.226 , 0.277	Depositor DCC
R_{free} test set	2123 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PYR, HEM

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	1.94	115/3907 (2.9%)	2.38	216/5291 (4.1%)
1	B	1.85	71/3130 (2.3%)	2.45	202/4230 (4.8%)
All	All	1.90	186/7037 (2.6%)	2.41	418/9521 (4.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	57
1	B	4	64
All	All	6	121

The worst 5 of 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CG-CD	12.01	1.81	1.51
1	B	441	CYS	CB-SG	11.82	2.02	1.82
1	A	413	ARG	CG-CD	10.79	1.78	1.51
1	A	266	VAL	CB-CG2	-10.57	1.30	1.52
1	A	421	ALA	CA-CB	-10.42	1.30	1.52

The worst 5 of 418 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	ARG	O-C-N	-25.98	81.14	122.70
1	A	395	LEU	O-C-N	-19.10	92.14	122.70
1	B	317	GLY	C-N-CA	18.27	167.38	121.70
1	A	245	ASP	CB-CG-OD1	-16.45	103.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	GLU	O-C-N	-16.19	96.79	122.70

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	11	ILE	CA
1	A	298	SER	CA
1	B	102	THR	CB
1	B	149	ASN	CA
1	B	272	LEU	CA

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	11	ILE	Peptide
1	A	31	GLY	Peptide
1	A	47	GLN	Peptide
1	A	50	ILE	Peptide

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	3833	0	3888	416	1
1	B	3081	0	3136	511	1
2	A	43	0	30	15	0
3	A	31	0	17	13	0
3	B	31	0	18	15	0
4	B	6	0	0	1	0
5	A	7	0	0	0	0
5	B	10	0	0	1	0
All	All	7042	0	7089	914	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

The worst 5 of 914 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:B:175:ARG:CD	1:B:175:ARG:CG	1.77	1.63
1:A:413:ARG:CD	1:A:413:ARG:CG	1.78	1.61
1:A:343:LYS:CB	1:A:343:LYS:CG	1.79	1.60
1:A:286:LEU:CD1	1:A:286:LEU:CG	1.78	1.59
1:B:106:ILE:CD1	1:B:106:ILE:CG1	1.75	1.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:NH2	1:B:169:LYS:CG[6_555]	2.19	0.01

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	488/511 (96%)	381 (78%)	67 (14%)	40 (8%)	1 2
1	B	392/511 (77%)	273 (70%)	78 (20%)	41 (10%)	0 1
All	All	880/1022 (86%)	654 (74%)	145 (16%)	81 (9%)	1 1

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	ILE
1	A	20	ASN
1	A	37	THR
1	A	48	ASP

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	424/440 (96%)	298 (70%)	126 (30%)	0 1
1	B	340/440 (77%)	232 (68%)	108 (32%)	0 0
All	All	764/880 (87%)	530 (69%)	234 (31%)	0 1

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	LYS
1	B	439	ASN
1	B	139	GLN
1	B	431	LEU
1	B	348	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	497	ASN
1	B	497	ASN
1	B	218	GLN
1	B	373	GLN
1	B	157	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	FMN	B	570	-	33,33,33	1.06	1 (3%)	48,50,50	2.27	15 (31%)
2	HEM	A	560	1	41,50,50	2.53	13 (31%)	45,82,82	3.05	18 (40%)
4	PYR	B	571	-	5,5,5	3.27	3 (60%)	3,6,6	0.76	0
3	FMN	A	569	-	33,33,33	0.96	1 (3%)	48,50,50	2.38	16 (33%)

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	FMN	B	570	-	-	4/18/18/18	0/3/3/3
2	HEM	A	560	1	-	8/12/54/54	-
4	PYR	B	571	-	-	4/4/4/4	-
3	FMN	A	569	-	1/1/4/4	3/18/18/18	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3D-C2D	7.41	1.52	1.36
2	A	560	HEM	C3C-C2C	-5.92	1.32	1.40
4	B	571	PYR	CA-C	-5.10	1.36	1.54
2	A	560	HEM	CAA-C2A	5.07	1.59	1.52
4	B	571	PYR	O-C	4.42	1.34	1.22

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	569	FMN	P-O5'-C5'	7.21	138.14	118.30
2	A	560	HEM	C4C-CHD-C1D	6.49	131.12	122.56
2	A	560	HEM	CHC-C4B-NB	6.46	131.44	124.43
3	B	570	FMN	O5'-P-O1P	6.05	123.43	106.47
2	A	560	HEM	CAA-CBA-CGA	5.98	130.53	113.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	569	FMN	C2'

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C1A-C2A-CAA-CBA
2	A	560	HEM	C3D-CAD-CBD-CGD
4	B	571	PYR	O-C-CA-O3
4	B	571	PYR	OXT-C-CA-O3
3	A	569	FMN	O2'-C2'-C3'-C4'

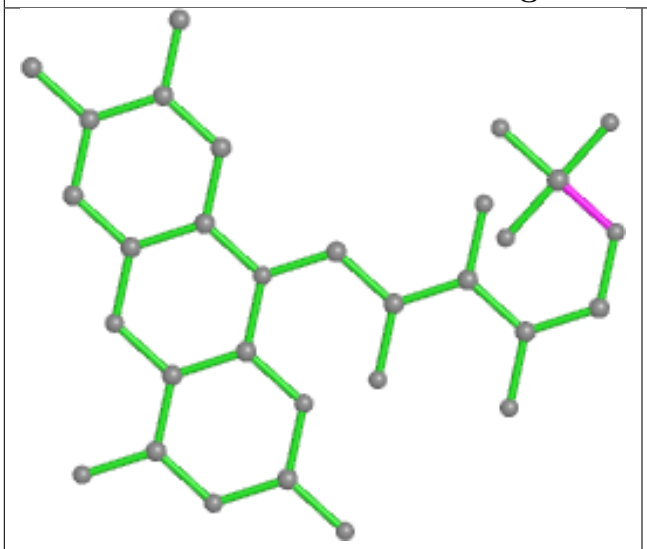
There are no ring outliers.

4 monomers are involved in 44 short contacts:

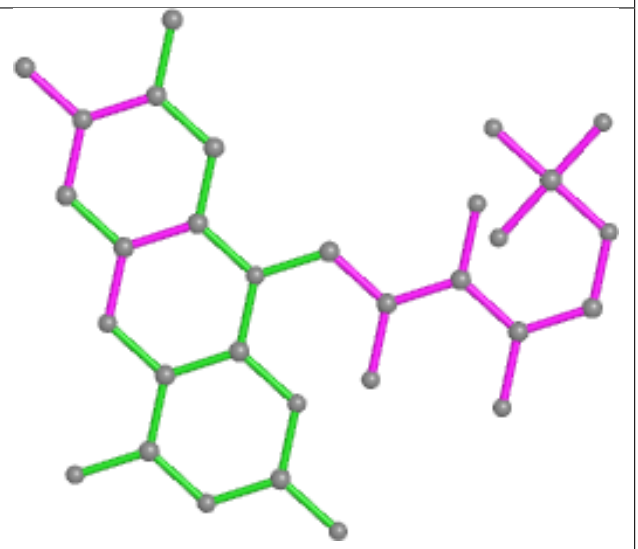
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	570	FMN	15	0
2	A	560	HEM	15	0
4	B	571	PYR	1	0
3	A	569	FMN	13	0

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.

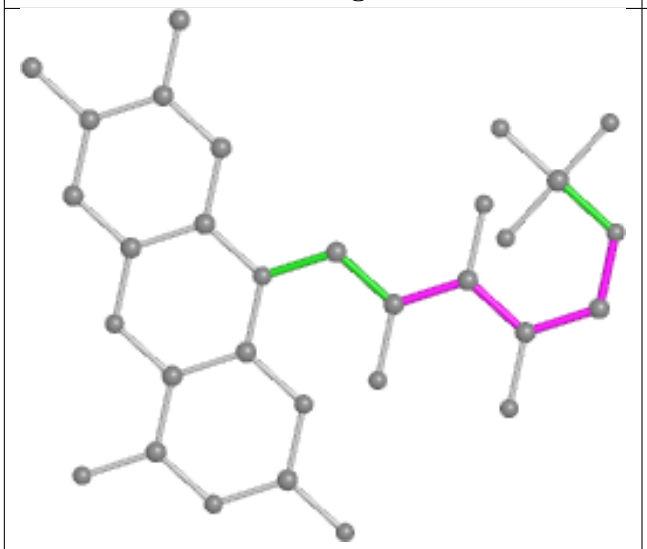
Ligand FMN B 570



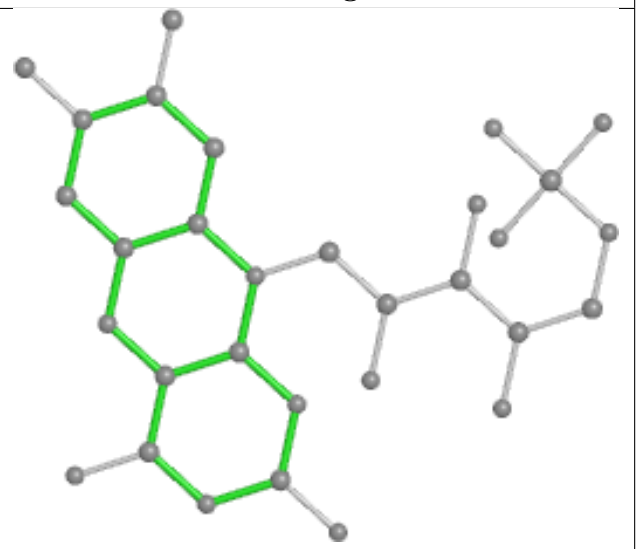
Bond lengths



Bond angles

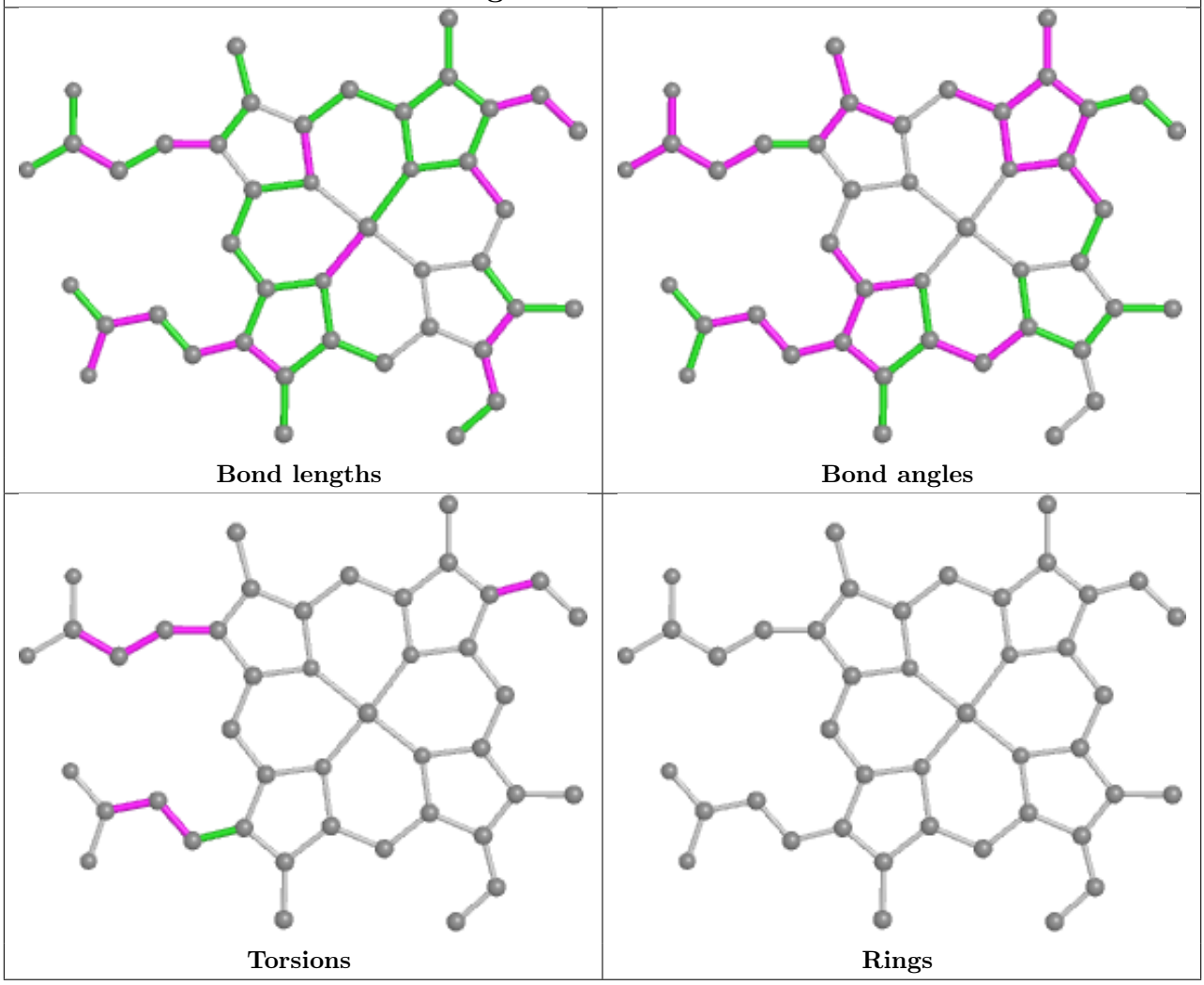


Torsions

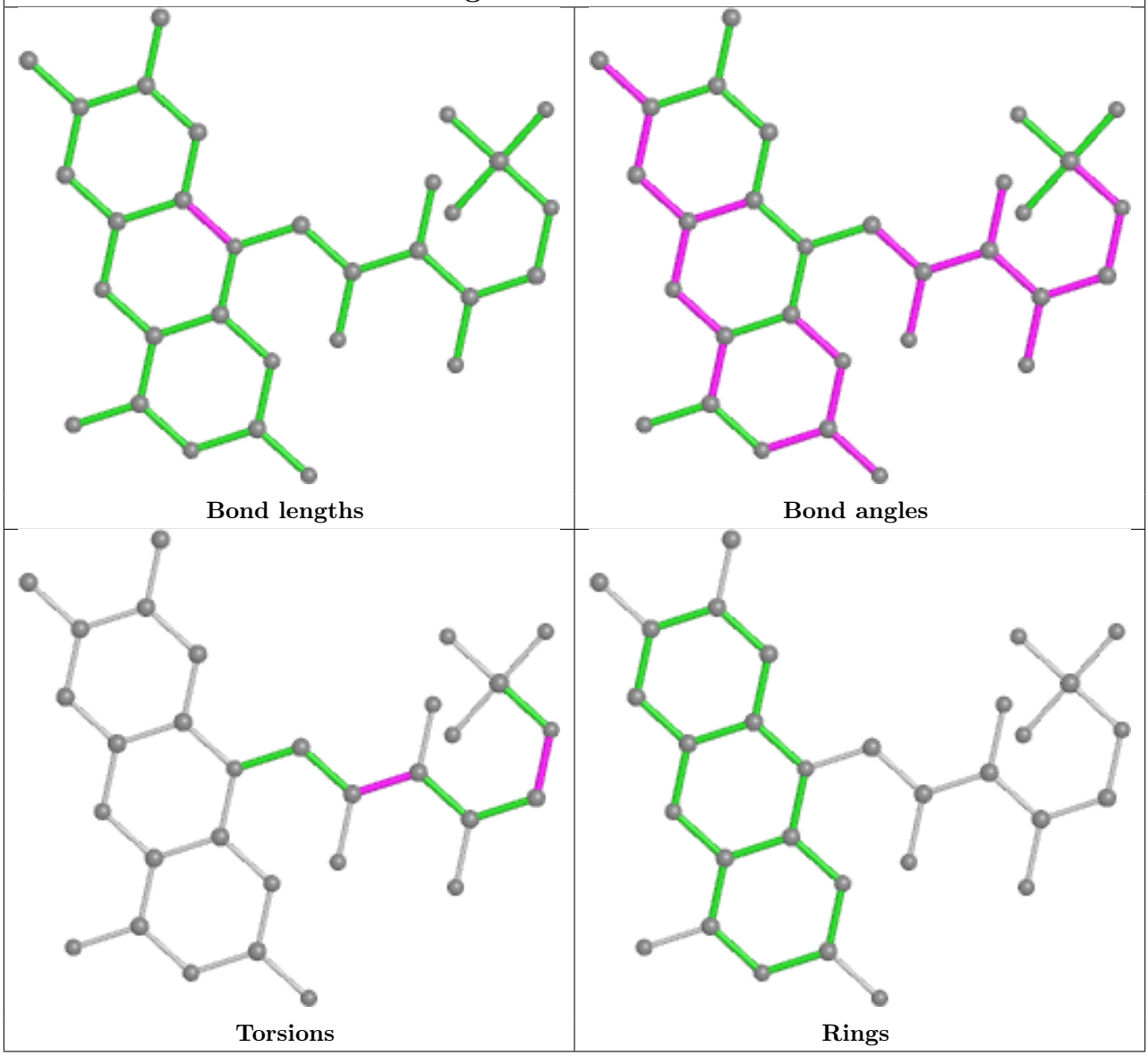


Rings

Ligand HEM A 560



Ligand FMN A 569



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:PRO	C	90:PRO	N	1.19

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	492/511 (96%)	-0.21	22 (4%)	33	23	19, 52, 147, 183	0
1	B	396/511 (77%)	-0.28	12 (3%)	50	40	18, 65, 107, 171	0
All	All	888/1022 (86%)	-0.24	34 (3%)	40	30	18, 58, 138, 183	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASN	8.5
1	A	9	GLN	8.3
1	A	6	MET	6.7
1	B	99	PRO	6.4
1	A	5	ASP	5.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

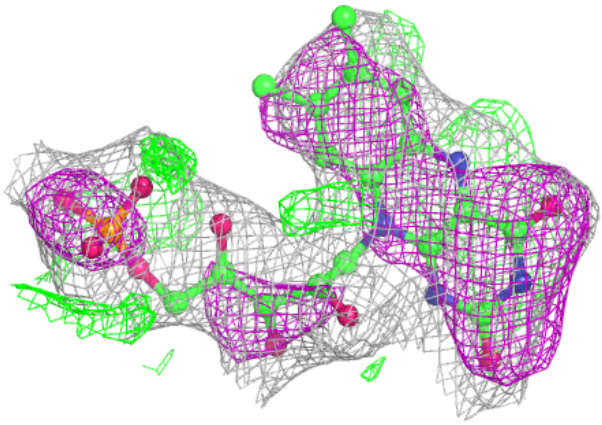
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

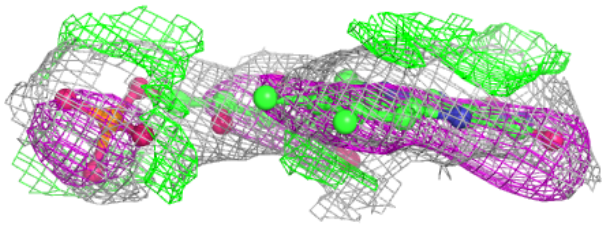
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PYR	B	571	6/6	0.80	0.44	120,125,128,133	0
3	FMN	B	570	31/31	0.87	0.18	16,21,24,26	0
3	FMN	A	569	31/31	0.88	0.17	10,14,17,18	0
2	HEM	A	560	43/43	0.97	0.21	90,98,116,122	0

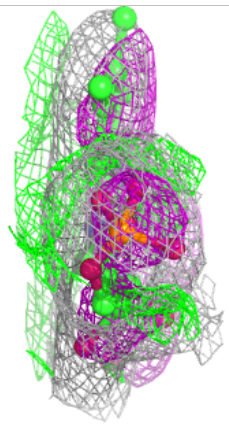
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN B 570:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

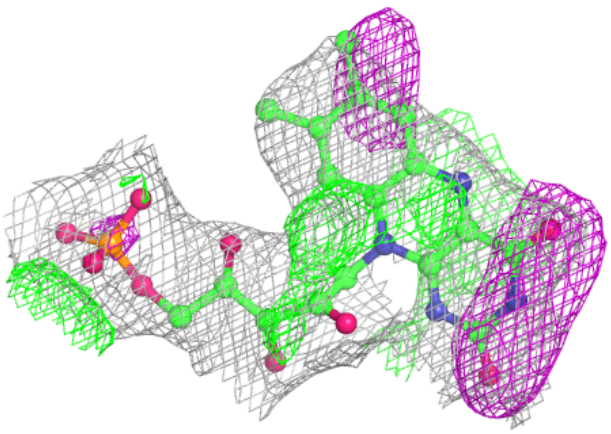


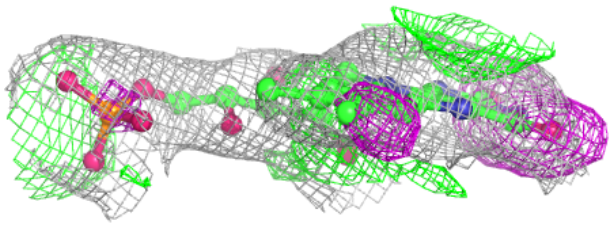


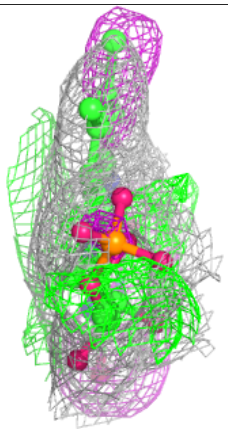


Electron density around FMN A 569:

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

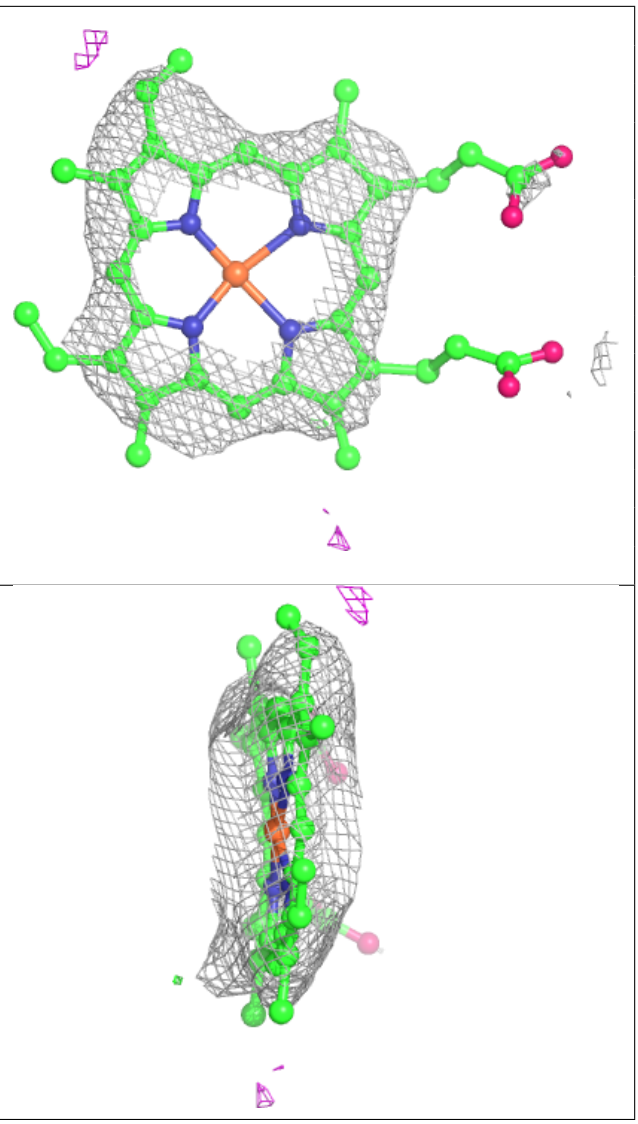






Electron density around HEM A 560:

$2mF_o$-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 (i)

There are no such residues in this entry.