



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:06 PM GMT

PDB ID : 1LDC  
Title : X-RAY STRUCTURE OF TWO COMPLEXES OF THE Y143F FLAVO-CYTOCHROME B2 MUTANT CRYSTALLIZED IN THE PRESENCE OF LACTATE OR PHENYL-LACTATE  
Authors : Tegoni, M.; Cambillau, C.  
Deposited on : 1995-04-13  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

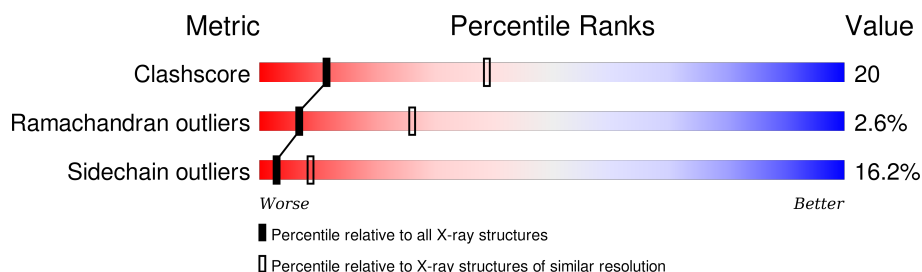
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	
1	B	511	

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
2	FMN	A	570	X	-	-	-
2	FMN	B	570	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8726 atoms, of which 1765 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	H	N	O	S	0	0	0
			4530	2373	809	629	705	14			
1	B	382	Total	C	H	N	O	S	0	0	0
			3648	1893	666	507	571	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	PHE	TYR	ENGINEERED MUTATION	UNP P00175
B	143	PHE	TYR	ENGINEERED MUTATION	UNP P00175

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



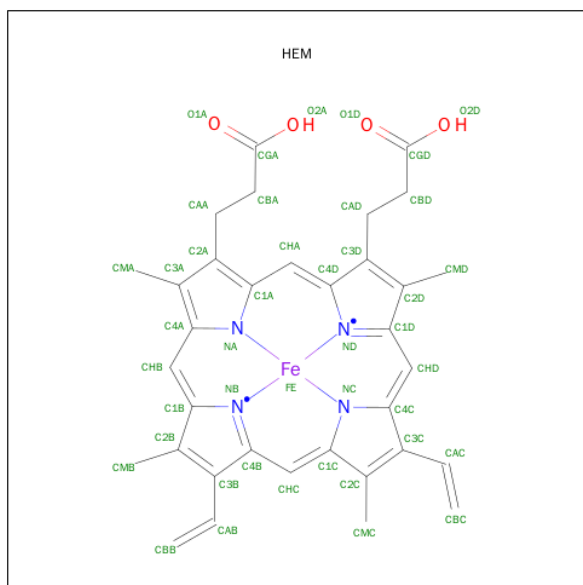
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

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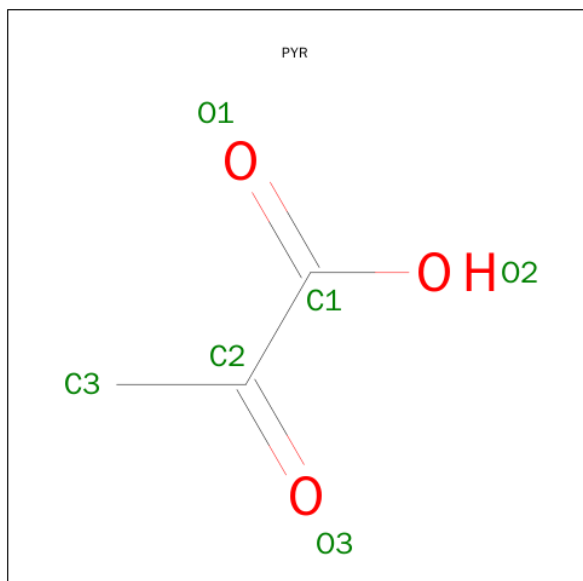
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

- 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	C	Fe	H	N	O	0	0
			47	34	1	4	4	4		

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



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

- Molecule 5 is water.

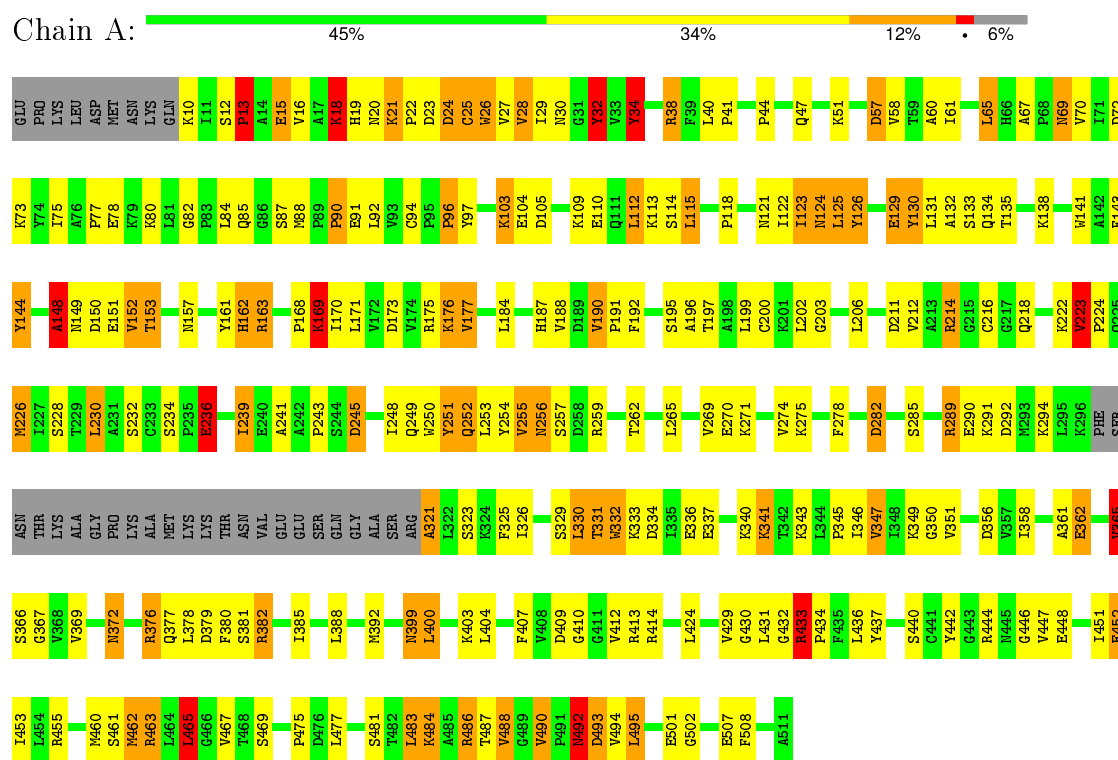
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	130	Total	H	O	0	0
			386	256	130		
5	B	11	Total	H	O	0	0
			33	22	11		

### 3 Residue-property plots

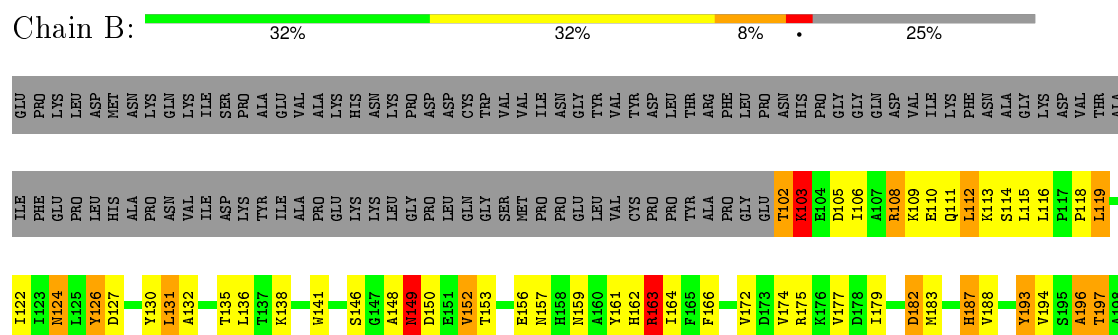
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: L-LACTATE DEHYDROGENASE



#### • Molecule 1: L-LACTATE DEHYDROGENASE



L199	A276	K341	V412	L483
C200	L277	T342	R413	R486
R201	F278	K343	R414	T487
L202	V279	L344	G415	V488
G203	D282	P345	T416	G489
R204	A283	D417	V418	V490
P205	L286	V247	L419	F491
L206	L287	K348	K420	D492
K210	Q288	K349	A421	D493
D211	Q289	V351	V429	V494
V212	Q288	T354	G430	V500
A213	E290	L431	L431	P503
R214	M293	V357	F435	T504
C216	K294	L358	I436	E507
G217	L295	A361	Y437	P508
K222	K296	G364	A438	E509
V223	PIE	V365	M439	D510
P224	SER	S366	C441	A511
Q225	THR	G367	Y442	
L226	LYS	V368	G443	
T229	ALA	R444	R444	
L230	GLY	L370	M445	
C233	PRO	S371	G446	
E236	LYS	N372	V447	
E237	LYS	R373	E448	
P243	THR	G375	K449	
S244	ASN	R376	A450	
Q247	VAL	Q377	I451	
T248	GLU	L378	E452	
Q249	GLU	D379	I453	
M250	SER	F380	R455	
Y251	GLN	S381	D456	
Q252	ALA	R382	E457	
L253	GLY	A383	I458	
R255	SER	P384	E459	
V255	ARG	I385	M460	
D256	ALA	E386	S461	
S257	LEU	V387	M462	
D258	SER	L388	R463	
R259	LYS	T391	L464	
K260	I326	I394	L465	
D263	D327	R398	G466	
K267	P328	K399	V467	
N268	S329	L400	T468	
E270	L330	K403	S469	
K271	W332	V406	E472	
V274	E336	F407	L473	
K275	E337	D408	K474	
	L338	D409	L477	
	K339		L478	
	K340		D479	
			L480	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.50 Å   164.50 Å   114.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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: FMN, HEM, PYR

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	1.08	10/3794 (0.3%)	1.95	102/5140 (2.0%)
1	B	1.00	0/3030	1.95	80/4094 (2.0%)
All	All	1.05	10/6824 (0.1%)	1.95	182/9234 (2.0%)

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	6
1	B	0	2
All	All	0	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	LYS	CD-CE	8.02	1.71	1.51
1	A	32	TYR	CE1-CZ	6.87	1.47	1.38
1	A	32	TYR	CG-CD2	6.32	1.47	1.39
1	A	32	TYR	CE2-CZ	6.13	1.46	1.38
1	A	382	ARG	CZ-NH1	5.96	1.40	1.33

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	B	289	ARG	NE-CZ-NH1	18.50	129.55	120.30
1	A	382	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	A	413	ARG	NE-CZ-NH2	-15.36	112.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	ASN	CA-C-N	-13.15	88.26	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	Peptide
1	A	32	TYR	Sidechain
1	A	34	TYR	Sidechain
1	A	433	ARG	Sidechain
1	A	492	ASN	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	3721	809	3783	146	0
1	B	2982	666	3044	139	0
2	A	31	4	16	3	0
2	B	31	4	19	4	0
3	A	43	4	30	8	0
4	A	6	0	3	2	0
4	B	6	0	3	1	0
5	A	130	256	0	13	0
5	B	11	22	0	0	0
All	All	6961	1765	6898	281	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 20.

The worst 5 of 281 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:289:ARG:HH21	1:A:376:ARG:NH2	1.38	1.22
1:A:289:ARG:NH2	1:A:376:ARG:NH2	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG22	1:B:490:VAL:HG11	1.51	0.93
1:A:289:ARG:NH2	1:A:376:ARG:HH22	1.69	0.88
1:B:148:ALA:C	1:B:149:ASN:HD22	1.76	0.87

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	474/511 (93%)	425 (90%)	36 (8%)	13 (3%)	6	25
1	B	378/511 (74%)	331 (88%)	38 (10%)	9 (2%)	7	29
All	All	852/1022 (83%)	756 (89%)	74 (9%)	22 (3%)	7	26

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	104	GLU
1	A	114	SER
1	B	146	SER
1	B	149	ASN

### 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	411/440 (93%)	344 (84%)	67 (16%)	3	8
1	B	330/440 (75%)	277 (84%)	53 (16%)	3	9
All	All	741/880 (84%)	621 (84%)	120 (16%)	3	9

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	B	103	LYS
1	B	429	VAL
1	A	448	GLU
1	A	469	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	GLN
1	A	497	ASN
1	B	372	ASN
1	A	372	ASN
1	B	397	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	HEM	A	560	1	24,50,50	2.72	7 (29%)	16,82,82	2.74	6 (37%)
2	FMN	A	570	-	31,33,33	2.77	10 (32%)	32,50,50	4.28	15 (46%)
4	PYR	A	580	-	2,5,5	1.60	1 (50%)	2,6,6	0.84	0
2	FMN	B	570	-	31,33,33	2.79	9 (29%)	32,50,50	3.68	10 (31%)
4	PYR	B	580	-	2,5,5	1.14	0	2,6,6	1.76	0

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	560	1	-	0/6/54/54	0/0/8/8
2	FMN	A	570	-	2/2/4/4	0/18/18/18	0/3/3/3
4	PYR	A	580	-	-	0/0/4/4	0/0/0/0
2	FMN	B	570	-	2/2/4/4	0/18/18/18	0/3/3/3
4	PYR	B	580	-	-	0/0/4/4	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	570	FMN	C1'-N10	-12.47	1.35	1.48
2	A	570	FMN	C1'-N10	-11.19	1.36	1.48
2	A	570	FMN	C2'-C3'	-5.25	1.43	1.53
3	A	560	HEM	C3B-C2B	-4.60	1.34	1.40
3	A	560	HEM	C3C-CAC	-4.29	1.38	1.47

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	570	FMN	N3-C2-N1	-4.17	112.45	121.28
2	B	570	FMN	N3-C2-N1	-3.24	114.44	121.28
3	A	560	HEM	C3C-CAC-CBC	-3.18	120.01	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	570	FMN	O2'-C2'-C3'	-3.10	100.99	108.96
2	A	570	FMN	C8M-C8-C9	-2.96	111.95	120.33

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	570	FMN	C4'
2	B	570	FMN	C2'
2	A	570	FMN	C4'
2	A	570	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	560	HEM	8	0
2	A	570	FMN	3	0
4	A	580	PYR	2	0
2	B	570	FMN	4	0
4	B	580	PYR	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.