



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:02 PM GMT

PDB ID : 5FX2  
Title : COMPARISON OF THE CRYSTAL STRUCTURES OF A FLAVODOXIN  
IN ITS THREE OXIDATION STATES AT CRYOGENIC TEMPERATURES  
Authors : Watt, W.; Watenpaugh, K.D.  
Deposited on : 1991-10-17  
Resolution : 1.90 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  
<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

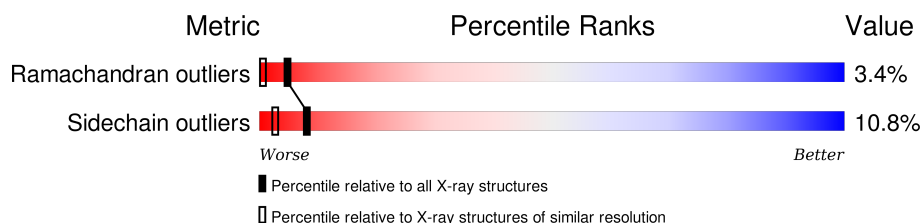
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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	147	

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	149	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1377 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 FLAVODOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	1102	0	0
			1102	684	181	233	4			

- 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).



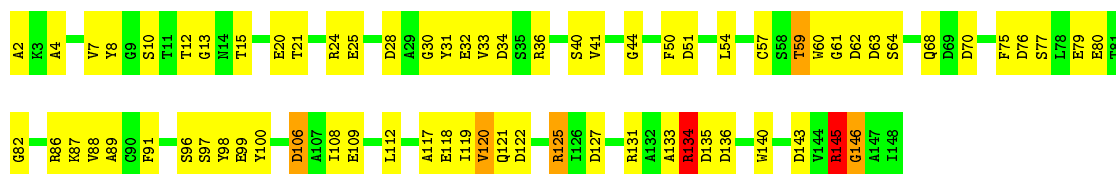
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: FLAVODOXIN

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.36 Å 51.36 Å 139.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 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

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	1.59	7/1119 (0.6%)	3.00	99/1514 (6.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	GLU	CD-OE1	7.13	1.33	1.25
1	A	80	GLU	CD-OE1	-6.45	1.18	1.25
1	A	100	TYR	CG-CD2	5.89	1.46	1.39
1	A	125	ARG	CD-NE	-5.44	1.37	1.46
1	A	146	GLY	N-CA	5.32	1.54	1.46
1	A	21	THR	CB-OG1	5.15	1.53	1.43
1	A	30	GLY	C-O	5.11	1.31	1.23

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH1	33.64	137.12	120.30
1	A	24	ARG	NE-CZ-NH1	21.17	130.89	120.30
1	A	145	ARG	NE-CZ-NH2	-20.64	109.98	120.30
1	A	28	ASP	CB-CG-OD2	-20.29	100.04	118.30
1	A	24	ARG	NE-CZ-NH2	-19.25	110.67	120.30
1	A	100	TYR	CB-CG-CD1	15.53	130.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	NE-CZ-NH2	13.86	127.23	120.30
1	A	63	ASP	CB-CG-OD1	12.85	129.87	118.30
1	A	89	ALA	CB-CA-C	12.23	128.44	110.10
1	A	100	TYR	CB-CG-CD2	-11.80	113.92	121.00
1	A	36	ARG	NE-CZ-NH2	11.72	126.16	120.30
1	A	86	ARG	NE-CZ-NH1	-10.99	114.81	120.30
1	A	24	ARG	CD-NE-CZ	9.92	137.49	123.60
1	A	80	GLU	CG-CD-OE1	9.84	137.98	118.30
1	A	131	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	80	GLU	CA-CB-CG	9.47	134.23	113.40
1	A	145	ARG	CD-NE-CZ	9.36	136.71	123.60
1	A	80	GLU	OE1-CD-OE2	-8.60	112.98	123.30
1	A	136	ASP	CA-CB-CG	8.52	132.14	113.40
1	A	127	ASP	CB-CG-OD1	8.45	125.90	118.30
1	A	86	ARG	CA-CB-CG	8.27	131.58	113.40
1	A	54	LEU	CB-CA-C	8.24	125.86	110.20
1	A	24	ARG	CA-CB-CG	8.14	131.32	113.40
1	A	70	ASP	CB-CG-OD2	8.08	125.57	118.30
1	A	112	LEU	CB-CA-C	7.96	125.33	110.20
1	A	98	TYR	CB-CG-CD2	7.85	125.71	121.00
1	A	33	VAL	C-N-CA	7.54	140.56	121.70
1	A	118	GLU	CB-CA-C	-7.52	95.36	110.40
1	A	134	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	143	ASP	CB-CG-OD2	7.43	124.98	118.30
1	A	31	TYR	CB-CG-CD2	-7.31	116.62	121.00
1	A	108	ILE	CB-CA-C	7.28	126.15	111.60
1	A	88	VAL	CA-CB-CG1	7.26	121.79	110.90
1	A	118	GLU	OE1-CD-OE2	7.25	132.00	123.30
1	A	134	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	60	TRP	CA-CB-CG	-7.13	100.15	113.70
1	A	98	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	100	TYR	CA-CB-CG	7.03	126.76	113.40
1	A	96	SER	N-CA-CB	7.01	121.02	110.50
1	A	133	ALA	N-CA-CB	-6.98	100.33	110.10
1	A	122	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	135	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	A	145	ARG	NH1-CZ-NH2	-6.96	111.75	119.40
1	A	68	GLN	C-N-CA	6.82	138.76	121.70
1	A	34	ASP	CB-CG-OD1	6.68	124.32	118.30
1	A	119	ILE	CB-CG1-CD1	6.64	132.49	113.90
1	A	108	ILE	C-N-CA	6.62	138.26	121.70
1	A	131	ARG	CD-NE-CZ	6.57	132.80	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	28	ASP	OD1-CG-OD2	6.55	135.75	123.30
1	A	64	SER	CA-CB-OG	6.54	128.84	111.20
1	A	125	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	51	ASP	CB-CA-C	6.32	123.03	110.40
1	A	97	SER	CA-CB-OG	6.31	128.23	111.20
1	A	108	ILE	O-C-N	-6.29	112.64	122.70
1	A	133	ALA	C-N-CA	6.27	137.38	121.70
1	A	87	LYS	CG-CD-CE	6.27	130.71	111.90
1	A	143	ASP	OD1-CG-OD2	-6.22	111.48	123.30
1	A	63	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	8	TYR	CB-CG-CD2	6.07	124.64	121.00
1	A	31	TYR	N-CA-CB	-6.05	99.71	110.60
1	A	57	CYS	CB-CA-C	-6.04	98.32	110.40
1	A	13	GLY	N-CA-C	6.04	128.19	113.10
1	A	15	THR	O-C-N	-6.03	113.06	122.70
1	A	70	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	106	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	122	ASP	O-C-N	6.00	133.41	123.20
1	A	36	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
1	A	131	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	76	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	4	ALA	N-CA-CB	-5.83	101.94	110.10
1	A	121	GLN	CA-CB-CG	5.81	126.18	113.40
1	A	99	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	109	GLU	CG-CD-OE1	5.79	129.89	118.30
1	A	32	GLU	CG-CD-OE2	5.78	129.87	118.30
1	A	143	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	59	THR	CA-CB-OG1	-5.64	97.16	109.00
1	A	140	TRP	CE3-CZ3-CH2	5.60	127.36	121.20
1	A	7	VAL	O-C-N	5.55	131.58	122.70
1	A	2	ALA	C-N-CA	5.50	135.44	121.70
1	A	36	ARG	CG-CD-NE	5.49	123.32	111.80
1	A	134	ARG	C-N-CA	5.47	135.38	121.70
1	A	96	SER	O-C-N	5.41	131.36	122.70
1	A	75	PHE	C-N-CA	5.40	135.21	121.70
1	A	91	PHE	CA-CB-CG	5.40	126.85	113.90
1	A	135	ASP	CB-CA-C	-5.38	99.63	110.40
1	A	79	GLU	CG-CD-OE1	-5.36	107.57	118.30
1	A	97	SER	N-CA-CB	5.26	118.39	110.50
1	A	50	PHE	O-C-N	5.24	131.08	122.70
1	A	13	GLY	C-N-CA	5.23	134.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	VAL	CA-CB-CG2	5.20	118.70	110.90
1	A	70	ASP	C-N-CA	5.17	134.62	121.70
1	A	118	GLU	CA-C-O	-5.09	109.42	120.10
1	A	61	GLY	CA-C-O	5.08	129.74	120.60
1	A	100	TYR	CB-CA-C	5.07	120.55	110.40
1	A	86	ARG	N-CA-CB	5.07	119.72	110.60
1	A	125	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	20	GLU	CB-CG-CD	5.03	127.77	114.20
1	A	63	ASP	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain

## 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	1102	0	1027	0	0
2	A	31	0	19	0	0
3	A	244	0	0	0	0
All	All	1377	0	1046	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	145/147 (99%)	127 (88%)	13 (9%)	5 (3%)	5 0

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY
1	A	117	ALA
1	A	134	ARG
1	A	146	GLY
1	A	82	GLY

### 5.3.2 Protein sidechains ⓘ

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	111/111 (100%)	99 (89%)	12 (11%)	8 3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	THR
1	A	40	SER
1	A	41	VAL
1	A	59	THR
1	A	62	ASP
1	A	77	SER
1	A	106	ASP
1	A	120	VAL
1	A	125	ARG
1	A	134	ARG
1	A	145	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

1 ligand is 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	$\# Z  > 2$
2	FMN	A	149	-	32,33,33	2.76	12 (37%)	34,50,50	6.02	17 (50%)

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	FMN	A	149	-	2/2/4/4	0/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C10-N10	-4.82	1.33	1.39
2	A	149	FMN	P-O3P	-4.43	1.39	1.54
2	A	149	FMN	C6-C5A	-2.29	1.38	1.41
2	A	149	FMN	C5'-C4'	-2.19	1.48	1.51
2	A	149	FMN	C2'-C3'	2.23	1.57	1.53
2	A	149	FMN	O3'-C3'	2.24	1.48	1.43
2	A	149	FMN	C9-C8	2.40	1.44	1.37
2	A	149	FMN	C1'-N10	3.24	1.51	1.48
2	A	149	FMN	C4-N3	3.62	1.39	1.33
2	A	149	FMN	P-O1P	4.43	1.64	1.50
2	A	149	FMN	C9A-N10	7.27	1.49	1.38
2	A	149	FMN	C4A-C10	7.69	1.55	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C1'-N10-C9A	-16.53	99.66	118.83
2	A	149	FMN	C5A-C9A-N10	-15.27	106.13	117.58
2	A	149	FMN	C4-C4A-C10	-14.44	110.70	119.94
2	A	149	FMN	C4A-C10-N10	-9.97	113.27	120.52
2	A	149	FMN	N3-C2-N1	-7.83	114.51	127.69
2	A	149	FMN	C6-C5A-C9A	-6.48	111.96	119.11
2	A	149	FMN	C9-C8-C7	-3.38	113.36	119.97
2	A	149	FMN	C4A-C4-N3	-3.27	119.25	123.52
2	A	149	FMN	C7M-C7-C8	-2.30	115.77	120.73
2	A	149	FMN	O2'-C2'-C3'	-2.14	103.46	108.96
2	A	149	FMN	C1'-C2'-C3'	-2.07	103.89	109.82
2	A	149	FMN	O3P-P-O2P	2.26	115.73	107.44
2	A	149	FMN	O4'-C4'-C3'	2.55	115.52	108.96
2	A	149	FMN	C9-C9A-C5A	2.92	124.91	119.65
2	A	149	FMN	C9A-C5A-N5	4.27	129.12	122.18
2	A	149	FMN	C4-C4A-N5	8.78	129.38	118.70
2	A	149	FMN	C4-N3-C2	12.01	125.18	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	149	FMN	C2'
2	A	149	FMN	C3'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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