



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:23 PM GMT

PDB ID : 3FX2  
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

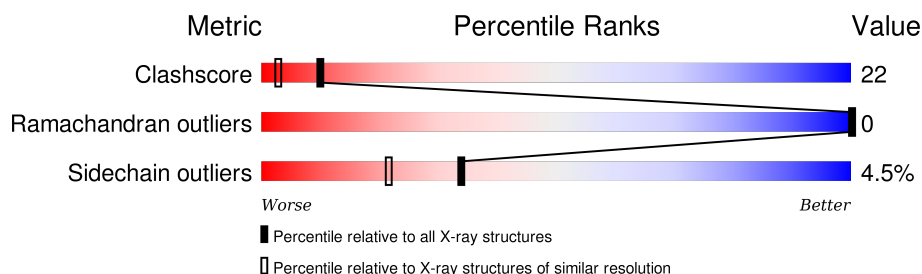
# 1 Overall quality at a glance

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))
Clashscore	102246	5398 (1.90-1.90)
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 1386 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	0	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).

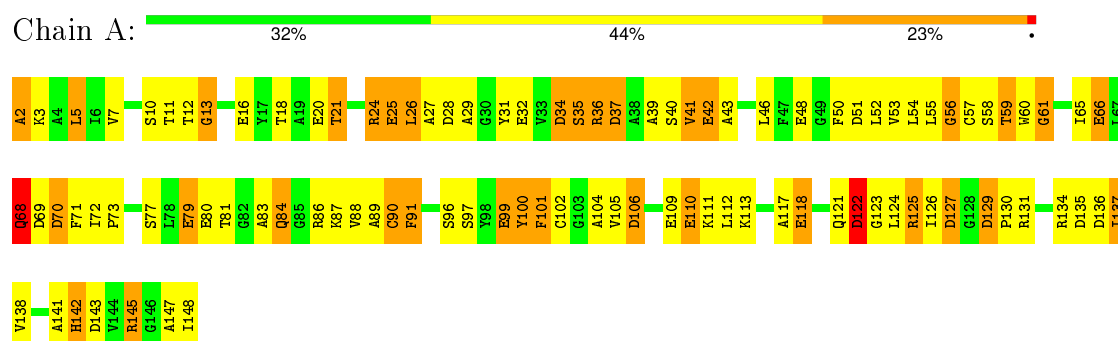


### 3 Residue-property plots [i](#)

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



## 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, $\alpha$ , $\beta$ , $\gamma$	50.72Å 50.72Å 139.04Å 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, $R_{free}$	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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	1.95	22/1119 (2.0%)	2.85	87/1514 (5.7%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	CD-NE	-10.44	1.28	1.46
1	A	40	SER	CB-OG	9.28	1.54	1.42
1	A	61	GLY	N-CA	8.89	1.59	1.46
1	A	145	ARG	CZ-NH1	8.65	1.44	1.33
1	A	25	GLU	CD-OE1	8.05	1.34	1.25
1	A	59	THR	CB-OG1	7.70	1.58	1.43
1	A	131	ARG	CZ-NH2	7.41	1.42	1.33
1	A	101	PHE	C-O	6.21	1.35	1.23
1	A	90	CYS	CB-SG	-6.14	1.71	1.82
1	A	58	SER	CB-OG	-6.12	1.34	1.42
1	A	68	GLN	CD-NE2	-6.00	1.17	1.32
1	A	20	GLU	CD-OE1	-5.79	1.19	1.25
1	A	66	GLU	CD-OE1	-5.79	1.19	1.25
1	A	11	THR	CB-OG1	5.75	1.54	1.43
1	A	79	GLU	CA-CB	-5.71	1.41	1.53
1	A	60	TRP	N-CA	5.66	1.57	1.46
1	A	56	GLY	CA-C	5.59	1.60	1.51
1	A	69	ASP	C-O	5.52	1.33	1.23
1	A	13	GLY	C-O	5.51	1.32	1.23
1	A	87	LYS	CE-NZ	5.48	1.62	1.49
1	A	16	GLU	CD-OE2	-5.18	1.20	1.25
1	A	57	CYS	C-O	5.05	1.32	1.23

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	CD-NE-CZ	34.05	171.26	123.60
1	A	79	GLU	CA-CB-CG	16.14	148.90	113.40
1	A	86	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	A	36	ARG	NE-CZ-NH2	12.46	126.53	120.30
1	A	145	ARG	CB-CG-CD	-12.13	80.05	111.60
1	A	24	ARG	NE-CZ-NH2	-12.13	114.24	120.30
1	A	131	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	A	89	ALA	N-CA-CB	10.85	125.30	110.10
1	A	145	ARG	CG-CD-NE	10.71	134.29	111.80
1	A	37	ASP	CB-CG-OD2	10.46	127.72	118.30
1	A	145	ARG	NE-CZ-NH1	-9.83	115.38	120.30
1	A	122	ASP	CB-CA-C	9.51	129.42	110.40
1	A	145	ARG	NE-CZ-NH2	9.27	124.93	120.30
1	A	54	LEU	CB-CG-CD2	-9.22	95.32	111.00
1	A	136	ASP	O-C-N	8.76	136.72	122.70
1	A	143	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	A	69	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	A	106	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	35	SER	CB-CA-C	8.32	125.92	110.10
1	A	48	GLU	CB-CG-CD	8.12	136.13	114.20
1	A	26	LEU	CB-CG-CD2	8.12	124.80	111.00
1	A	122	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	51	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	A	143	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	56	GLY	O-C-N	7.53	134.75	122.70
1	A	100	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	137	ILE	O-C-N	7.25	134.30	122.70
1	A	118	GLU	CA-CB-CG	7.22	129.28	113.40
1	A	122	ASP	CB-CG-OD2	7.19	124.78	118.30
1	A	27	ALA	CB-CA-C	7.17	120.85	110.10
1	A	79	GLU	CG-CD-OE2	-7.13	104.05	118.30
1	A	37	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	142	HIS	CA-CB-CG	-7.05	101.61	113.60
1	A	127	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	86	ARG	NH1-CZ-NH2	6.94	127.03	119.40
1	A	106	ASP	OD1-CG-OD2	-6.84	110.30	123.30
1	A	84	GLN	N-CA-CB	-6.77	98.41	110.60
1	A	29	ALA	N-CA-CB	6.77	119.57	110.10
1	A	25	GLU	OE1-CD-OE2	6.74	131.38	123.30
1	A	91	PHE	CZ-CE2-CD2	-6.72	112.04	120.10
1	A	91	PHE	CG-CD2-CE2	6.71	128.18	120.80
1	A	121	GLN	CA-CB-CG	6.68	128.09	113.40
1	A	110	GLU	CG-CD-OE1	6.67	131.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	GLU	CG-CD-OE1	6.64	131.58	118.30
1	A	25	GLU	CB-CA-C	-6.62	97.17	110.40
1	A	79	GLU	OE1-CD-OE2	6.53	131.14	123.30
1	A	54	LEU	O-C-N	6.45	133.01	122.70
1	A	125	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	135	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	141	ALA	CA-C-O	6.22	133.17	120.10
1	A	71	PHE	CZ-CE2-CD2	-6.20	112.66	120.10
1	A	106	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	70	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	60	TRP	C-N-CA	-6.14	109.40	122.30
1	A	58	SER	N-CA-CB	6.10	119.65	110.50
1	A	136	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	2	ALA	O-C-N	6.03	132.35	122.70
1	A	24	ARG	CD-NE-CZ	6.02	132.02	123.60
1	A	59	THR	O-C-N	5.96	132.24	122.70
1	A	129	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	12	THR	O-C-N	5.91	133.25	123.20
1	A	66	GLU	CA-CB-CG	-5.86	100.51	113.40
1	A	111	LYS	O-C-N	5.85	132.06	122.70
1	A	7	VAL	CA-CB-CG1	-5.82	102.16	110.90
1	A	68	GLN	CA-CB-CG	5.78	126.12	113.40
1	A	84	GLN	CG-CD-NE2	-5.73	102.95	116.70
1	A	121	GLN	O-C-N	5.66	131.75	122.70
1	A	48	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	A	91	PHE	C-N-CA	-5.59	110.56	122.30
1	A	131	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	32	GLU	CG-CD-OE1	-5.46	107.38	118.30
1	A	104	ALA	N-CA-CB	5.45	117.73	110.10
1	A	122	ASP	CA-CB-CG	5.37	125.21	113.40
1	A	42	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	A	97	SER	CB-CA-C	5.34	120.25	110.10
1	A	89	ALA	O-C-N	5.33	131.23	122.70
1	A	34	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	48	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	A	39	ALA	C-N-CA	5.30	134.96	121.70
1	A	5	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	134	ARG	N-CA-CB	5.26	120.07	110.60
1	A	25	GLU	CB-CG-CD	-5.22	100.11	114.20
1	A	21	THR	CA-CB-CG2	5.22	119.71	112.40
1	A	18	THR	OG1-CB-CG2	5.21	121.98	110.00
1	A	28	ASP	CB-CG-OD2	-5.13	113.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLU	CA-C-N	-5.13	105.91	117.20
1	A	100	TYR	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

There are no planarity outliers.

## 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	1102	0	1029	48	0
2	A	31	0	18	0	0
3	A	253	0	0	13	0
All	All	1386	0	1047	48	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 22.

All (48) 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:68:GLN:HE22	1:A:70:ASP:HB2	1.32	0.93
1:A:25:GLU:OE2	3:A:307:HOH:O	1.89	0.91
1:A:79:GLU:OE2	3:A:271:HOH:O	2.03	0.75
1:A:118:GLU:OE1	3:A:392:HOH:O	2.04	0.74
1:A:99:GLU:HG2	3:A:341:HOH:O	1.88	0.74
1:A:24:ARG:HD3	3:A:368:HOH:O	1.87	0.72
1:A:56:GLY:HA2	1:A:91:PHE:O	1.94	0.68
1:A:110:GLU:OE2	3:A:349:HOH:O	2.11	0.67
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.78	0.66
1:A:110:GLU:OE1	3:A:350:HOH:O	2.15	0.64
1:A:42:GLU:O	1:A:46:LEU:HB2	1.99	0.62
1:A:96:SER:OG	1:A:127:ASP:OD2	2.18	0.62
1:A:10:SER:OG	1:A:13:GLY:HA2	2.01	0.59
1:A:113:LYS:NZ	3:A:401:HOH:O	2.31	0.57
1:A:31:TYR:OH	1:A:148:ILE:HD11	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HA	3:A:321:HOH:O	2.06	0.56
1:A:61:GLY:CA	1:A:66:GLU:HG3	2.38	0.54
1:A:5:LEU:HB3	1:A:53:VAL:HG22	1.90	0.53
1:A:90:CYS:O	1:A:123:GLY:HA2	2.07	0.52
1:A:105:VAL:O	1:A:109:GLU:HG3	2.10	0.52
1:A:55:LEU:HD12	1:A:112:LEU:HD11	1.92	0.52
1:A:83:ALA:O	1:A:117:ALA:HB2	2.10	0.51
1:A:126:ILE:HG21	1:A:130:PRO:HB3	1.92	0.51
1:A:10:SER:OG	1:A:13:GLY:CA	2.59	0.51
1:A:31:TYR:CE1	1:A:145:ARG:HG2	2.46	0.50
1:A:43:ALA:O	1:A:81:THR:HA	2.12	0.50
1:A:88:VAL:HG21	1:A:112:LEU:HD13	1.94	0.49
1:A:2:ALA:N	3:A:288:HOH:O	2.44	0.49
1:A:68:GLN:NE2	1:A:70:ASP:HB2	2.15	0.49
1:A:65:ILE:HG13	1:A:100:TYR:CD2	2.48	0.48
1:A:26:LEU:O	1:A:31:TYR:HB2	2.14	0.48
1:A:52:LEU:HD13	1:A:148:ILE:HG21	1.96	0.48
1:A:122:ASP:HB3	3:A:348:HOH:O	2.14	0.47
1:A:77:SER:O	1:A:80:GLU:HG2	2.15	0.47
1:A:124:LEU:HD21	1:A:126:ILE:HD11	1.97	0.46
1:A:130:PRO:HB2	1:A:137:ILE:HD11	1.97	0.45
1:A:5:LEU:HB2	1:A:50:PHE:CD1	2.51	0.45
1:A:72:ILE:CB	1:A:73:PRO:HD3	2.46	0.44
1:A:129:ASP:OD1	1:A:130:PRO:HD2	2.18	0.44
1:A:101:PHE:CZ	1:A:127:ASP:HB2	2.52	0.43
1:A:106:ASP:OD1	1:A:125:ARG:NH2	2.46	0.42
1:A:3:LYS:HE3	3:A:287:HOH:O	2.19	0.42
1:A:59:THR:OG1	1:A:102:CYS:HA	2.19	0.42
1:A:147:ALA:HB2	3:A:321:HOH:O	2.20	0.42
1:A:34:ASP:CG	1:A:36:ARG:HE	2.25	0.40
1:A:138:VAL:O	1:A:142:HIS:HB2	2.21	0.40
1:A:21:THR:HB	1:A:137:ILE:HG21	2.04	0.40
1:A:37:ASP:O	1:A:41:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	138 (95%)	7 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	106 (96%)	5 (4%)	34	21

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	41	VAL
1	A	68	GLN
1	A	84	GLN
1	A	122	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	84	GLN
1	A	121	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 ⓘ

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	3.21	17 (53%)	34,50,50	5.24	20 (58%)

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	-	1/1/4/4	0/18/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C10-N10	-4.24	1.34	1.39
2	A	149	FMN	P-O3P	-3.32	1.43	1.54
2	A	149	FMN	P-O5'	-3.10	1.51	1.59
2	A	149	FMN	C4A-N5	-2.86	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C4-C4A	-2.67	1.35	1.41
2	A	149	FMN	O2'-C2'	-2.55	1.37	1.43
2	A	149	FMN	C2-N1	-2.47	1.33	1.38
2	A	149	FMN	C2'-C3'	-2.20	1.49	1.53
2	A	149	FMN	C8M-C8	2.02	1.55	1.51
2	A	149	FMN	C9-C8	2.08	1.43	1.37
2	A	149	FMN	O4'-C4'	2.96	1.50	1.43
2	A	149	FMN	C7M-C7	3.18	1.57	1.51
2	A	149	FMN	C4'-C3'	5.05	1.63	1.53
2	A	149	FMN	P-O1P	5.13	1.67	1.50
2	A	149	FMN	C4-N3	5.77	1.43	1.33
2	A	149	FMN	C9A-N10	7.68	1.49	1.38
2	A	149	FMN	C4A-C10	8.37	1.56	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C1'-N10-C9A	-14.47	102.04	118.83
2	A	149	FMN	C4-C4A-C10	-13.86	111.07	119.94
2	A	149	FMN	C5A-C9A-N10	-8.37	111.31	117.58
2	A	149	FMN	C4A-C10-N10	-6.97	115.46	120.52
2	A	149	FMN	O4'-C4'-C3'	-5.10	95.84	108.96
2	A	149	FMN	C6-C5A-N5	-4.09	113.82	118.92
2	A	149	FMN	O2P-P-O1P	-4.05	97.40	110.63
2	A	149	FMN	N3-C2-N1	-3.09	122.49	127.69
2	A	149	FMN	C7-C6-C5A	-2.86	116.24	120.90
2	A	149	FMN	O4'-C4'-C5'	-2.58	104.48	110.09
2	A	149	FMN	C7M-C7-C8	-2.55	115.25	120.73
2	A	149	FMN	C4A-C4-N3	-2.16	120.70	123.52
2	A	149	FMN	C1'-C2'-C3'	2.12	115.89	109.82
2	A	149	FMN	O2P-P-O5'	2.75	114.74	106.72
2	A	149	FMN	O2'-C2'-C3'	3.40	117.69	108.96
2	A	149	FMN	O3P-P-O5'	4.42	119.64	106.72
2	A	149	FMN	C4A-N5-C5A	6.38	124.24	116.72
2	A	149	FMN	O2'-C2'-C1'	6.40	125.75	109.93
2	A	149	FMN	C4-N3-C2	8.79	122.49	115.16
2	A	149	FMN	C4-C4A-N5	9.71	130.51	118.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	149	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.