



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:05 PM GMT

PDB ID : 1OYB
Title : OLD YELLOW ENZYME AT 2 ANGSTROMS RESOLUTION: OVERALL
STRUCTURE, LIGAND BINDING AND COMPARISON WITH RELATED
FLAVOPROTEINS
Authors : Fox, K.M.; Karplus, P.A.
Deposited on : 1994-08-25
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (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

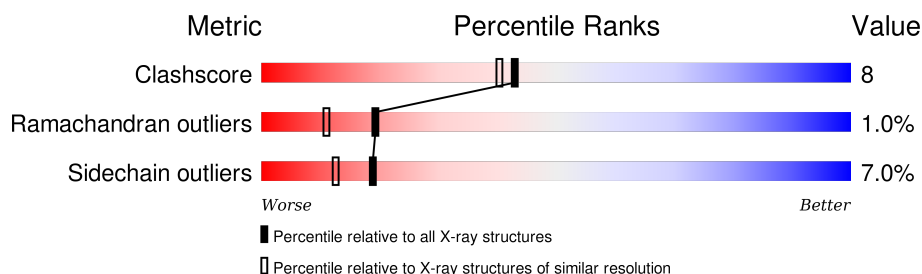
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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	400	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4308 atoms, of which 964 are hydrogens and 0 are deuteriums.

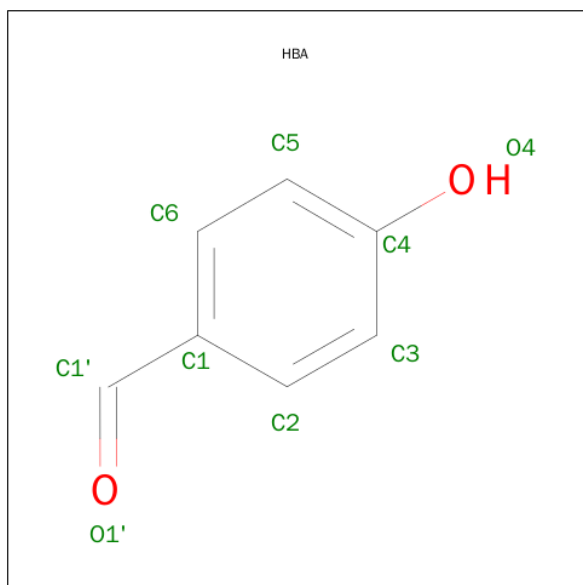
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called OLD YELLOW ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	H	N	O	S	4	0	0
			3886	2027	708	551	594	6			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

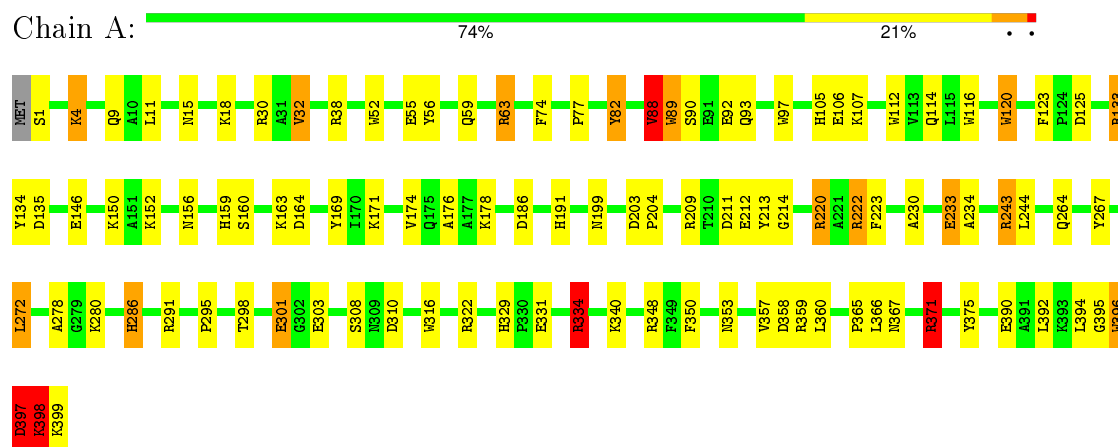
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	126	Total	H	O	0	0
			378	252	126		

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: OLD YELLOW ENZYME



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, α , β , γ	142.88Å 142.88Å 43.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4308	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, HBA

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	1.12	2/3260 (0.1%)	1.87	69/4417 (1.6%)

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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ARG	CD-NE	-5.39	1.37	1.46
1	A	32	VAL	CA-CB	5.18	1.65	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-23.47	108.56	120.30
1	A	38	ARG	NE-CZ-NH1	20.57	130.59	120.30
1	A	220	ARG	NE-CZ-NH2	-19.27	110.66	120.30
1	A	220	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	A	397	ASP	CA-C-N	-14.00	86.41	117.20
1	A	133	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	A	334	ARG	NE-CZ-NH1	12.87	126.74	120.30
1	A	133	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	A	222	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	38	ARG	CG-CD-NE	-9.45	91.96	111.80
1	A	371	ARG	NE-CZ-NH1	8.90	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	63	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	116	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	371	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	52	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	63	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	116	TRP	CE2-CD2-CG	-7.29	101.46	107.30
1	A	316	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	97	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	A	222	ARG	CG-CD-NE	-7.27	96.53	111.80
1	A	334	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	30	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	82	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	316	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	A	52	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	88	VAL	N-CA-CB	-6.62	96.93	111.50
1	A	310	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	112	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	A	233	GLU	CA-CB-CG	6.48	127.65	113.40
1	A	38	ARG	CD-NE-CZ	6.42	132.59	123.60
1	A	97	TRP	CD1-CG-CD2	6.37	111.40	106.30
1	A	52	TRP	CG-CD2-CE3	6.35	139.62	133.90
1	A	89	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	A	375	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	A	267	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	A	233	GLU	CB-CG-CD	6.19	130.92	114.20
1	A	396	TRP	CE2-CD2-CG	-6.18	102.36	107.30
1	A	134	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	120	TRP	CA-CB-CG	6.11	125.31	113.70
1	A	398	LYS	N-CA-C	-6.10	94.53	111.00
1	A	301	GLU	CA-CB-CG	-6.07	100.04	113.40
1	A	89	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	A	358	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	322	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	334	ARG	CG-CD-NE	-5.69	99.85	111.80
1	A	348	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	116	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	88	VAL	CA-CB-CG2	-5.59	102.52	110.90
1	A	220	ARG	CB-CG-CD	-5.58	97.09	111.60
1	A	56	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	74	PHE	CB-CG-CD2	-5.52	116.93	120.80
1	A	397	ASP	O-C-N	5.50	131.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	178	LYS	CA-CB-CG	-5.43	101.46	113.40
1	A	303	GLU	N-CA-CB	-5.34	100.99	110.60
1	A	4	LYS	CA-C-N	5.34	128.94	117.20
1	A	396	TRP	CD1-CG-CD2	5.32	110.56	106.30
1	A	89	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	280	LYS	CA-CB-CG	-5.30	101.74	113.40
1	A	291	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	A	316	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	A	396	TRP	C-N-CA	5.19	134.66	121.70
1	A	52	TRP	CB-CG-CD1	-5.16	120.30	127.00
1	A	264	GLN	CG-CD-NE2	5.16	129.07	116.70
1	A	30	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	272	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	A	160	SER	CA-CB-OG	-5.11	97.42	111.20
1	A	88	VAL	CB-CA-C	5.00	120.90	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	TYR	Sidechain
1	A	220	ARG	Sidechain
1	A	397	ASP	Mainchain
1	A	82	TYR	Sidechain

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	3178	708	3093	51	0
2	A	31	4	19	1	0
3	A	9	0	5	1	0
4	A	126	252	0	4	0
All	All	3344	964	3117	52	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 8.

All (52) 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:114:GLN:HE22	2:A:401:FMN:HN3	1.24	0.81
3:A:402:HBA:H5	4:A:616:HOH:O	1.86	0.75
1:A:353:ASN:HD21	1:A:367:ASN:H	1.38	0.71
1:A:295:PRO:HG3	4:A:616:HOH:O	1.90	0.70
1:A:398:LYS:HZ3	1:A:399:LYS:H	1.47	0.62
1:A:63:ARG:HG2	1:A:357:VAL:HG11	1.84	0.60
1:A:133:ARG:HD2	1:A:135:ASP:OD1	2.01	0.59
1:A:397:ASP:O	1:A:398:LYS:HB2	2.03	0.59
1:A:392:LEU:HD22	1:A:398:LYS:HB3	1.86	0.57
1:A:392:LEU:O	1:A:399:LYS:HA	2.04	0.57
1:A:90:SER:H	1:A:93:GLN:NE2	2.03	0.57
1:A:105:HIS:HE1	1:A:186:ASP:OD2	1.90	0.54
1:A:92:GLU:HG3	4:A:635:HOH:O	2.06	0.54
1:A:230:ALA:O	1:A:233:GLU:HG3	2.08	0.53
1:A:298:THR:O	1:A:301:GLU:HB2	2.09	0.53
1:A:395:GLY:C	1:A:397:ASP:H	2.11	0.53
1:A:63:ARG:HD2	4:A:583:HOH:O	2.08	0.53
1:A:9:GLN:NE2	1:A:334:ARG:HH11	2.08	0.52
1:A:89:TRP:H	1:A:93:GLN:HE22	1.56	0.51
1:A:88:VAL:HG13	1:A:176:ALA:HB1	1.92	0.51
1:A:89:TRP:H	1:A:93:GLN:NE2	2.10	0.50
1:A:353:ASN:ND2	1:A:367:ASN:H	2.09	0.50
1:A:395:GLY:O	1:A:397:ASP:N	2.46	0.48
1:A:55:GLU:O	1:A:59:GLN:HG3	2.13	0.48
1:A:243:ARG:HH21	1:A:286:HIS:CE1	2.30	0.48
1:A:163:LYS:HZ1	1:A:211:ASP:HB2	1.79	0.47
1:A:163:LYS:HZ1	1:A:212:GLU:HG3	1.80	0.47
1:A:15:ASN:HA	1:A:18:LYS:HD3	1.97	0.46
1:A:163:LYS:NZ	1:A:212:GLU:HG3	2.31	0.46
1:A:398:LYS:NZ	1:A:399:LYS:H	2.14	0.46
1:A:398:LYS:NZ	1:A:399:LYS:N	2.64	0.45
1:A:77:PRO:HD3	1:A:89:TRP:CE2	2.51	0.45
1:A:353:ASN:HD21	1:A:367:ASN:N	2.11	0.45
1:A:398:LYS:HZ3	1:A:399:LYS:N	2.15	0.45
1:A:174:VAL:HG13	1:A:234:ALA:HB2	1.99	0.44
1:A:123:PHE:HB3	1:A:125:ASP:OD1	2.18	0.44
1:A:390:GLU:O	1:A:394:LEU:HG	2.18	0.44
1:A:9:GLN:HE21	1:A:334:ARG:HH11	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:HIS:HD2	1:A:331:GLU:OE2	2.02	0.43
1:A:163:LYS:HE3	1:A:211:ASP:OD2	2.19	0.43
1:A:133:ARG:HD3	1:A:159:HIS:CD2	2.53	0.42
1:A:4:LYS:HA	1:A:4:LYS:HD3	1.88	0.42
1:A:213:TYR:CE1	1:A:222:ARG:HG2	2.55	0.42
1:A:88:VAL:CG1	1:A:176:ALA:HB1	2.50	0.41
1:A:209:ARG:HB2	1:A:214:GLY:HA3	2.02	0.41
1:A:146:GLU:O	1:A:150:LYS:HG3	2.21	0.41
1:A:359:ARG:HD3	1:A:365:PRO:O	2.21	0.41
1:A:203:ASP:HA	1:A:204:PRO:HD2	1.98	0.41
1:A:152:LYS:HD2	1:A:152:LYS:HA	1.47	0.41
1:A:371:ARG:H	1:A:371:ARG:CZ	2.33	0.41
1:A:107:LYS:HA	1:A:107:LYS:HD3	1.91	0.41
1:A:163:LYS:NZ	1:A:211:ASP:HB2	2.36	0.41

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	397/400 (99%)	377 (95%)	16 (4%)	4 (1%)	19 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	LYS
1	A	278	ALA
1	A	396	TRP
1	A	397	ASP

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	328/329 (100%)	305 (93%)	23 (7%)	19	12

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	11	LEU
1	A	32	VAL
1	A	88	VAL
1	A	106	GLU
1	A	120	TRP
1	A	156	ASN
1	A	164	ASP
1	A	171	LYS
1	A	191	HIS
1	A	199	ASN
1	A	223	PHE
1	A	244	LEU
1	A	272	LEU
1	A	286	HIS
1	A	308	SER
1	A	334	ARG
1	A	340	LYS
1	A	350	PHE
1	A	360	LEU
1	A	366	LEU
1	A	371	ARG
1	A	398	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	84	ASN
1	A	93	GLN
1	A	105	HIS
1	A	114	GLN
1	A	147	GLN
1	A	156	ASN
1	A	168	GLN
1	A	175	GLN
1	A	179	ASN
1	A	200	GLN
1	A	286	HIS
1	A	329	HIS
1	A	353	ASN
1	A	380	HIS

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](#)

2 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
2	FMN	A	401	-	31,33,33	1.50	6 (19%)	32,50,50	2.12	6 (18%)
3	HBA	A	402	-	9,9,9	2.08	2 (22%)	11,11,11	1.31	1 (9%)

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	401	-	-	0/18/18/18	0/3/3/3
3	HBA	A	402	-	-	0/2/2/2	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HBA	O4-C4	-5.05	1.25	1.37
3	A	402	HBA	C1-C1'	-3.05	1.39	1.47
2	A	401	FMN	C2-N1	-2.84	1.32	1.38
2	A	401	FMN	P-O2P	-2.55	1.46	1.54
2	A	401	FMN	P-O5'	-2.32	1.53	1.59
2	A	401	FMN	C4A-C10	2.60	1.45	1.40
2	A	401	FMN	C4-C4A	2.79	1.46	1.40
2	A	401	FMN	C4-N3	2.85	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C4A-C10-N10	-3.99	117.62	120.52
3	A	402	HBA	O1'-C1'-C1	-2.21	117.37	124.60
2	A	401	FMN	C5A-C9A-N10	2.43	119.40	117.58
2	A	401	FMN	O2P-P-O1P	2.77	119.67	110.63
2	A	401	FMN	C6-C5A-C9A	2.90	122.31	119.11
2	A	401	FMN	C4A-N5-C5A	3.31	120.63	116.72
2	A	401	FMN	C2-N1-C10	8.29	120.46	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FMN	1	0
3	A	402	HBA	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.