



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:12 PM GMT

PDB ID : 1EP2
Title : CRYSTAL STRUCTURE OF LACTOCOCCUS LACTIS DIHYDROOROTATE DEHYDROGENASE B COMPLEXED WITH OROTATE
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Deposited on : 2000-03-27
Resolution : 2.40 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

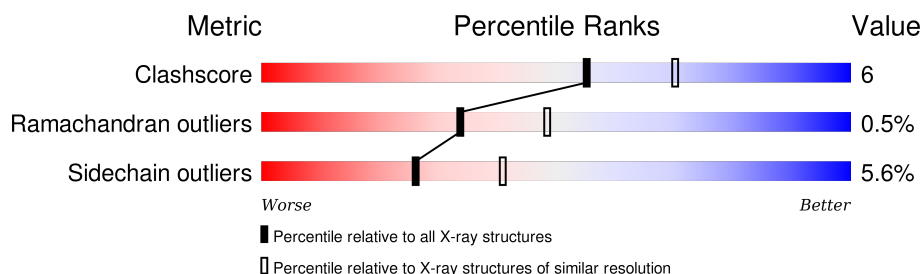
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	311	
2	B	261	

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	501	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4498 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 DIHYDROOROTATE DEHYDROGENASE B (PYRD SUB-UNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2264	1446	375	429	14			

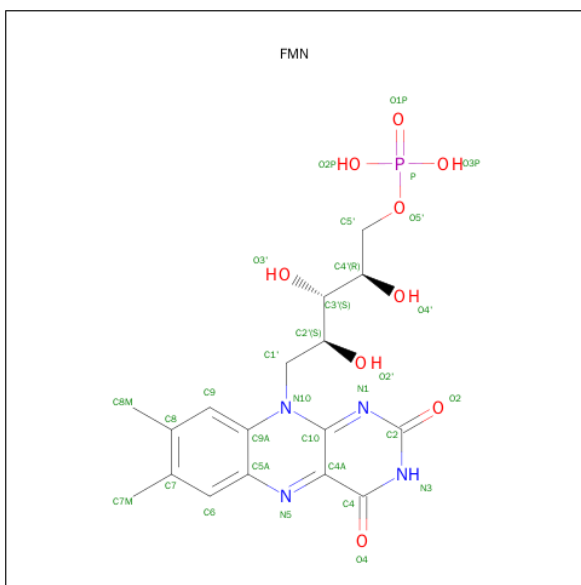
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ALA	ARG	CONFLICT	UNP P54322
A	255	ASP	VAL	CONFLICT	UNP P54322
A	266	ALA	ARG	CONFLICT	UNP P54322

- Molecule 2 is a protein called DIHYDROOROTATE DEHYDROGENASE B (PYRK SUB-UNIT).

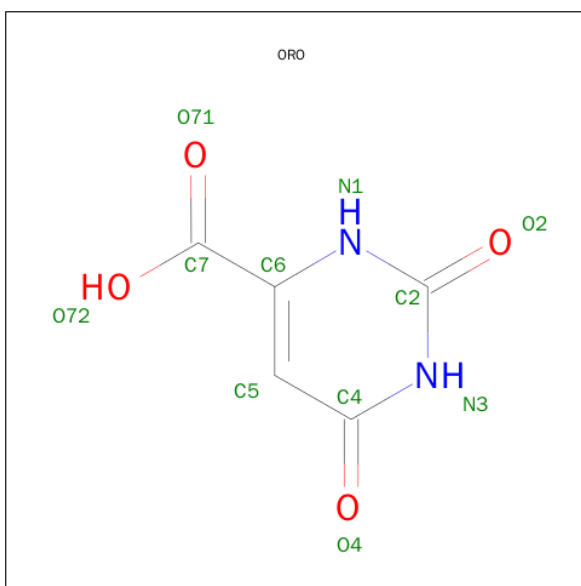
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			1991	1261	326	385	19			

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



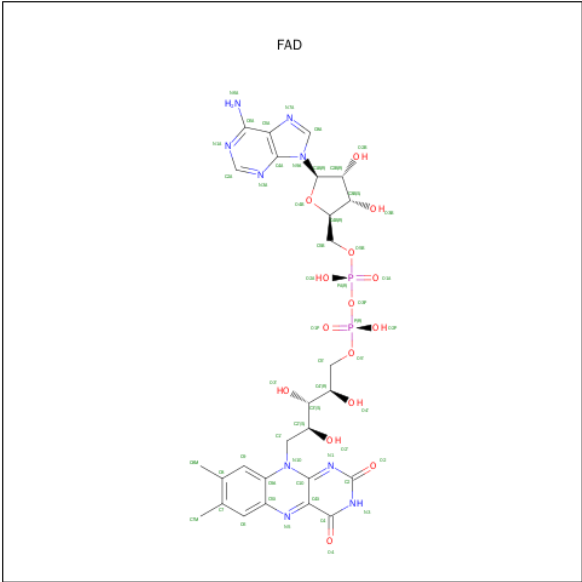
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



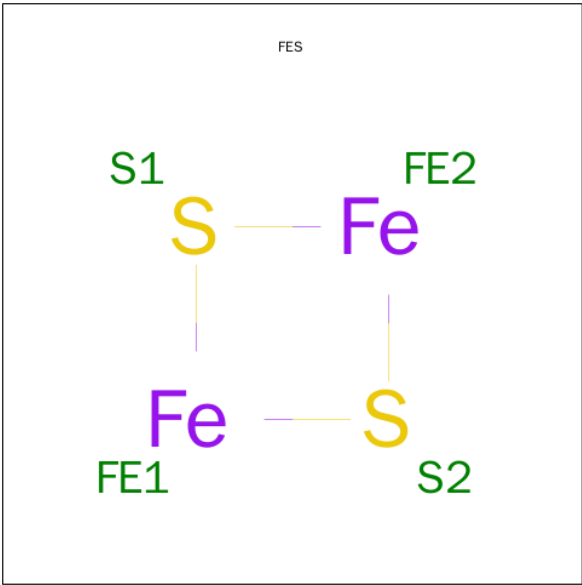
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			11	5	2	4			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is water.

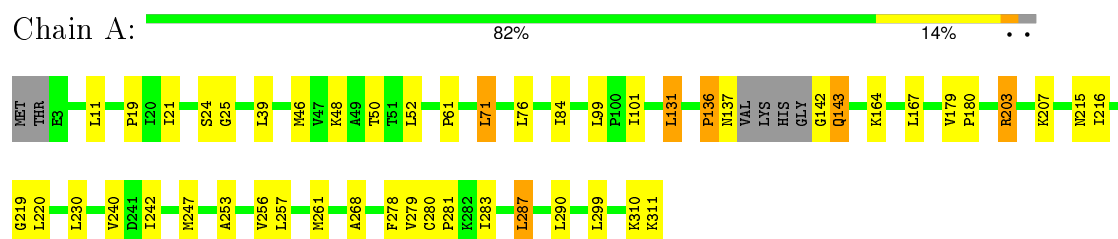
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total 108	O 108	0	0
7	B	36	Total 36	O 36	0	0

3 Residue-property plots

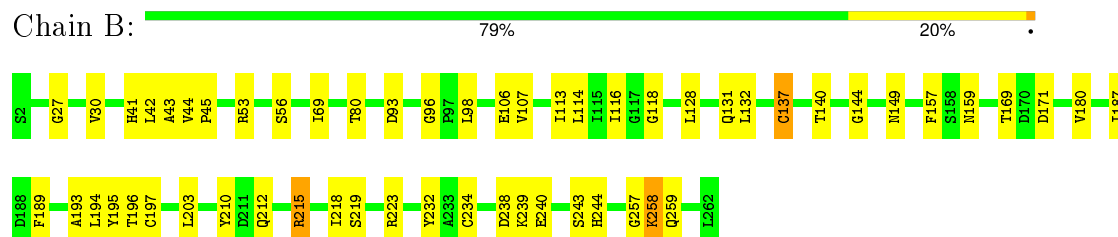
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 2: DIHYDROOROTATE DEHYDROGENASE B (PYRK SUBUNIT)



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	202.42Å 202.42Å 80.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.50 – 2.40	Depositor
% Data completeness (in resolution range)	86.0 (38.50-2.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4498	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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, ORO, FES, FAD

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	0.43	0/2303	0.66	0/3129
2	B	0.38	0/2021	0.70	2/2724 (0.1%)
All	All	0.40	0/4324	0.68	2/5853 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	GLY	N-CA-C	5.44	126.70	113.10
2	B	137	CYS	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2264	0	2331	26	0
2	B	1991	0	2017	30	0
3	A	31	0	17	0	0
4	A	11	0	3	0	0
5	B	53	0	31	3	0
6	B	4	0	0	0	0
7	A	108	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	36	0	0	1	0
All	All	4498	0	4399	55	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 6.

All (55) 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)
2:B:53:ARG:NH2	5:B:503:FAD:H52A	1.95	0.81
1:A:142:GLY:O	1:A:143:GLN:HB2	1.97	0.64
1:A:136:PRO:HA	1:A:143:GLN:NE2	2.13	0.63
2:B:140:THR:HG21	2:B:189:PHE:CZ	2.33	0.62
2:B:258:LYS:HG3	2:B:259:GLN:H	1.65	0.62
2:B:43:ALA:HB3	2:B:93:ASP:HB3	1.82	0.60
2:B:113:ILE:HD13	2:B:132:LEU:HD13	1.84	0.59
2:B:171:ASP:HB2	7:B:1118:HOH:O	2.02	0.59
1:A:310:LYS:HG3	1:A:311:LYS:H	1.67	0.58
2:B:80:THR:HG23	5:B:503:FAD:O1P	2.04	0.57
1:A:21:ILE:O	1:A:268:ALA:HA	2.07	0.54
1:A:131:LEU:HG	1:A:167:LEU:HD11	1.88	0.54
1:A:61:PRO:HB3	2:B:223:ARG:HG3	1.91	0.51
1:A:50:THR:HG23	1:A:84:ILE:HD12	1.92	0.51
1:A:179:VAL:HB	1:A:180:PRO:HD3	1.92	0.51
1:A:247:MET:HB3	1:A:268:ALA:HB3	1.93	0.50
2:B:197:CYS:SG	2:B:219:SER:HB3	2.52	0.50
2:B:96:GLY:HA2	2:B:98:LEU:HG	1.94	0.49
1:A:253:ALA:HB1	1:A:287:LEU:HD13	1.94	0.49
2:B:203:LEU:HD22	2:B:218:ILE:HG23	1.93	0.48
1:A:279:VAL:O	1:A:283:ILE:HG13	2.14	0.48
2:B:187:ILE:HD11	2:B:210:TYR:OH	2.14	0.48
2:B:238:ASP:O	2:B:240:GLU:N	2.47	0.47
2:B:258:LYS:HD2	2:B:258:LYS:HA	1.79	0.46
1:A:71:LEU:HA	1:A:219:GLY:O	2.15	0.45
2:B:194:LEU:HD23	2:B:195:TYR:N	2.31	0.45
2:B:193:ALA:HB2	2:B:215:ARG:NH2	2.31	0.45
2:B:53:ARG:CZ	5:B:503:FAD:H52A	2.47	0.45
1:A:25:GLY:HA2	1:A:48:LYS:HD3	1.99	0.44
2:B:238:ASP:HB3	2:B:243:SER:OG	2.16	0.44
1:A:19:PRO:HG3	1:A:299:LEU:HD13	1.99	0.44
2:B:232:TYR:N	2:B:232:TYR:CD1	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:SER:O	2:B:69:ILE:HG22	2.17	0.44
2:B:42:LEU:N	2:B:42:LEU:HD12	2.33	0.44
1:A:278:PHE:O	1:A:281:PRO:HD2	2.18	0.43
1:A:280:CYS:HB2	1:A:281:PRO:HD3	2.00	0.43
1:A:164:LYS:HA	1:A:164:LYS:HD3	1.84	0.43
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.89	0.43
1:A:136:PRO:HA	1:A:143:GLN:HE21	1.84	0.43
2:B:107:VAL:HG23	2:B:215:ARG:HH22	1.84	0.43
1:A:24:SER:HA	1:A:46:MET:O	2.19	0.43
1:A:203:ARG:HA	1:A:203:ARG:HD2	1.86	0.42
2:B:234:CYS:SG	2:B:234:CYS:O	2.77	0.42
1:A:137:ASN:HB3	1:A:215:ASN:ND2	2.33	0.42
1:A:215:ASN:O	1:A:216:ILE:HB	2.19	0.42
1:A:240:VAL:HG22	1:A:242:ILE:HG12	2.02	0.42
1:A:257:LEU:O	1:A:261:MET:HG2	2.19	0.42
2:B:116:ILE:HG23	2:B:180:VAL:HG11	2.02	0.42
2:B:27:GLY:O	2:B:30:VAL:HG12	2.20	0.42
1:A:256:VAL:HG21	1:A:283:ILE:HG21	2.01	0.42
2:B:44:VAL:HA	2:B:45:PRO:HD3	1.90	0.42
2:B:232:TYR:HD1	2:B:232:TYR:N	2.18	0.41
2:B:212:GLN:HA	2:B:212:GLN:NE2	2.35	0.41
2:B:243:SER:HB2	2:B:244:HIS:H	1.71	0.41
2:B:118:GLY:HA2	2:B:144:GLY:O	2.21	0.40

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	301/311 (97%)	291 (97%)	8 (3%)	2 (1%)	26	38
2	B	259/261 (99%)	227 (88%)	31 (12%)	1 (0%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	560/572 (98%)	518 (92%)	39 (7%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	PRO
1	A	143	GLN
2	B	239	LYS

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	243/248 (98%)	230 (95%)	13 (5%)	28	44
2	B	219/219 (100%)	206 (94%)	13 (6%)	24	38
All	All	462/467 (99%)	436 (94%)	26 (6%)	26	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	39	LEU
1	A	52	LEU
1	A	71	LEU
1	A	76	LEU
1	A	99	LEU
1	A	101	ILE
1	A	131	LEU
1	A	203	ARG
1	A	207	LYS
1	A	220	LEU
1	A	230	LEU
1	A	287	LEU
2	B	41	HIS
2	B	106	GLU

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Mol	Chain	Res	Type
2	B	114	LEU
2	B	128	LEU
2	B	131	GLN
2	B	137	CYS
2	B	149	ASN
2	B	157	PHE
2	B	159	ASN
2	B	169	THR
2	B	196	THR
2	B	215	ARG
2	B	258	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	215	ASN
1	A	234	HIS
2	B	159	ASN
2	B	212	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](#)

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	A	501	-	32,33,33	3.08	10 (31%)	34,50,50	3.46	9 (26%)
4	ORO	A	502	-	6,11,11	1.82	2 (33%)	6,15,15	6.97	5 (83%)
5	FAD	B	503	-	52,58,58	1.89	12 (23%)	52,89,89	1.78	8 (15%)
6	FES	B	504	2	0,4,4	0.00	-	0,4,4	0.00	-

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	A	501	-	2/2/4/4	0/18/18/18	0/3/3/3
4	ORO	A	502	-	-	0/0/4/4	0/1/1/1
5	FAD	B	503	-	-	0/30/50/50	0/6/6/6
6	FES	B	504	2	-	0/0/4/4	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	FMN	C1'-N10	-14.23	1.33	1.48
5	B	503	FAD	PA-O2A	-4.84	1.34	1.55
5	B	503	FAD	P-O2P	-3.99	1.38	1.55
3	A	501	FMN	C2'-C3'	-3.69	1.46	1.53
5	B	503	FAD	C10-N10	-3.63	1.34	1.39
3	A	501	FMN	P-O2P	-3.37	1.43	1.54
5	B	503	FAD	C2B-C1B	-3.11	1.48	1.53
3	A	501	FMN	C10-N10	-3.06	1.35	1.39
5	B	503	FAD	C2-N1	-2.66	1.32	1.38
3	A	501	FMN	C5'-C4'	-2.50	1.48	1.51
3	A	501	FMN	C4'-C3'	-2.48	1.48	1.53
3	A	501	FMN	O2'-C2'	-2.39	1.38	1.43
3	A	501	FMN	C9A-N10	2.15	1.41	1.38
3	A	501	FMN	C4-N3	2.46	1.37	1.33
4	A	502	ORO	C6-N1	2.48	1.38	1.34
5	B	503	FAD	C4-N3	2.52	1.37	1.33
5	B	503	FAD	C2-N3	2.79	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	FAD	C9A-N10	2.85	1.42	1.38
5	B	503	FAD	C4X-C10	3.03	1.46	1.40
4	A	502	ORO	C4-N3	3.06	1.38	1.33
5	B	503	FAD	C4-C4X	3.12	1.47	1.41
3	A	501	FMN	C4A-N5	3.68	1.39	1.33
5	B	503	FAD	O5'-C5'	3.91	1.60	1.44
5	B	503	FAD	O4B-C1B	4.71	1.48	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ORO	C5-C4-N3	-8.41	115.12	124.02
3	A	501	FMN	N3-C2-N1	-7.76	114.62	127.69
4	A	502	ORO	N3-C2-N1	-7.42	115.20	127.69
3	A	501	FMN	C4A-C4-N3	-7.04	114.32	123.52
5	B	503	FAD	C4X-C4-N3	-5.46	116.39	123.52
5	B	503	FAD	C4B-O4B-C1B	-3.08	106.37	109.64
5	B	503	FAD	N3A-C2A-N1A	-3.01	126.50	128.87
5	B	503	FAD	N3-C2-N1	-2.93	122.76	127.69
3	A	501	FMN	C4-C4A-N5	-2.91	115.16	118.70
5	B	503	FAD	O4B-C1B-N9A	-2.74	102.93	108.11
5	B	503	FAD	O5B-PA-O1A	-2.17	100.32	109.21
5	B	503	FAD	C2A-N1A-C6A	2.07	122.47	118.77
3	A	501	FMN	C5A-C9A-N10	3.78	120.41	117.58
4	A	502	ORO	C2-N1-C6	3.79	121.99	117.03
3	A	501	FMN	C4-C4A-C10	4.17	122.61	119.94
3	A	501	FMN	C1'-C2'-C3'	4.55	122.82	109.82
4	A	502	ORO	C4-C5-C6	4.93	119.92	116.73
3	A	501	FMN	O4'-C4'-C3'	5.16	122.25	108.96
3	A	501	FMN	O2'-C2'-C1'	5.75	124.13	109.93
5	B	503	FAD	C4-N3-C2	7.19	121.16	115.16
4	A	502	ORO	C4-N3-C2	11.17	125.98	114.21
3	A	501	FMN	C4-N3-C2	12.56	125.64	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	FMN	C4'
3	A	501	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	FAD	3	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 ⓘ

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.