



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 08:07 am GMT

PDB ID : 1F3P
Title : FERREDOXIN REDUCTASE (BPHA4)-NADH COMPLEX
Authors : Senda, T.; Yamada, T.; Sakurai, N.; Kubota, M.; Nishizaki, T.; Masai, E.;
Fukuda, M.; Mitsuidagger, Y.
Deposited on : 2000-06-06
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

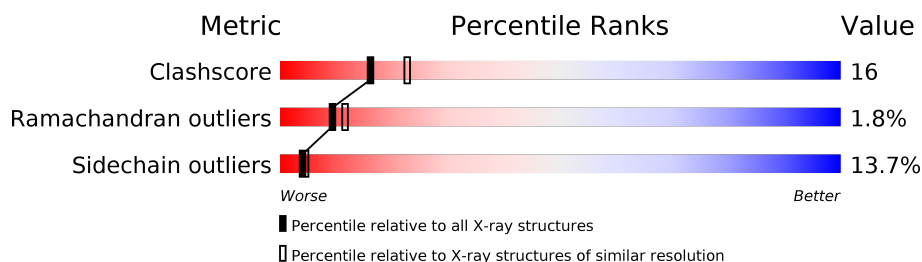
1 Overall quality at a glance

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	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (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.

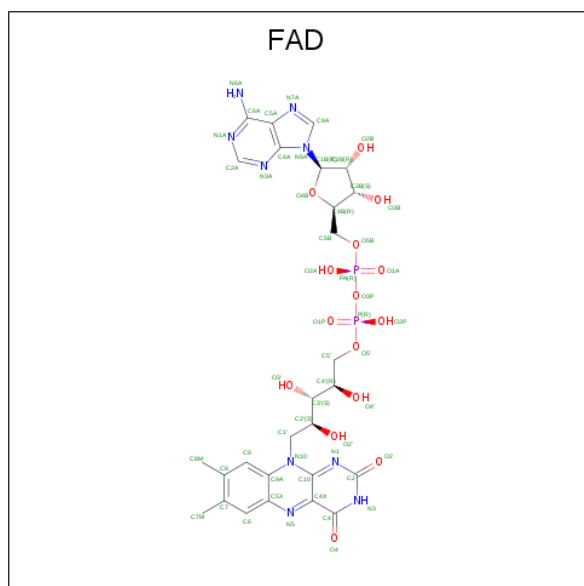
Mol	Chain	Length	Quality of chain
1	A	408	

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 FERREDONIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			2976	1865	544	559	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

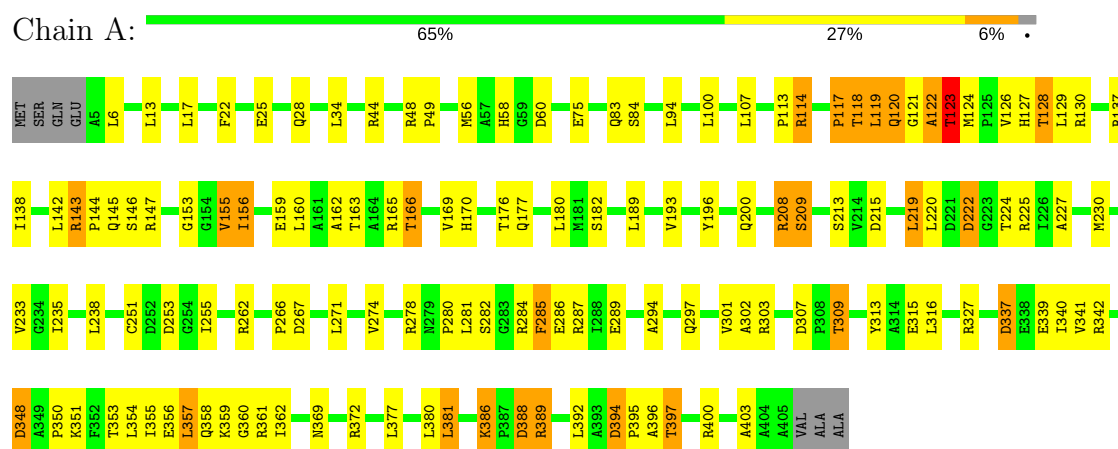
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total	0	0
			81 O 81 81		

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 the various outlier classes 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: FERREDOXIN REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.90Å 98.90Å 170.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (38.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3154	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: FAD, NAD

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	0.37	0/3028	0.63	1/4129 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	THR	N-CA-C	-5.49	96.18	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	2976	0	2995	95	0
2	A	53	0	31	0	0
3	A	44	0	25	6	0
4	A	81	0	0	3	0
All	All	3154	0	3051	95	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 16.

All (95) 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:397:THR:HG22	1:A:400:ARG:H	1.30	0.95
1:A:58:HIS:HD2	1:A:60:ASP:H	1.08	0.93
1:A:388:ASP:O	1:A:389:ARG:HB2	1.77	0.84
1:A:348:ASP:O	1:A:350:PRO:HD3	1.79	0.82
1:A:58:HIS:CD2	1:A:60:ASP:H	1.97	0.81
1:A:147:ARG:HH11	1:A:227:ALA:HB3	1.47	0.79
1:A:208:ARG:HG2	1:A:220:LEU:HD23	1.64	0.77
1:A:147:ARG:NH1	1:A:227:ALA:HB3	1.99	0.77
1:A:280:PRO:HG2	1:A:316:LEU:HD23	1.69	0.74
1:A:94:LEU:HD11	1:A:100:LEU:HG	1.72	0.69
1:A:156:ILE:HG13	3:A:500:NAD:H5N	1.75	0.69
1:A:307:ASP:OD1	1:A:309:THR:HB	1.94	0.68
1:A:25:GLU:OE2	1:A:303:ARG:HD2	1.94	0.68
1:A:348:ASP:C	1:A:350:PRO:HD3	2.16	0.66
1:A:313:TYR:CE2	1:A:315:GLU:HB2	2.33	0.64
1:A:388:ASP:O	1:A:389:ARG:CB	2.46	0.62
1:A:58:HIS:HD2	1:A:60:ASP:N	1.89	0.62
1:A:208:ARG:NE	1:A:222:ASP:HB3	2.14	0.61
1:A:176:THR:HG22	1:A:209:SER:HB3	1.82	0.61
1:A:117:PRO:HA	1:A:120:GLN:OE1	2.02	0.60
1:A:397:THR:HG22	1:A:400:ARG:N	2.10	0.57
1:A:316:LEU:HB2	4:A:545:HOH:O	2.05	0.56
1:A:156:ILE:HG13	3:A:500:NAD:C5N	2.36	0.56
1:A:123:THR:HG21	1:A:215:ASP:HA	1.87	0.56
1:A:280:PRO:HG2	1:A:316:LEU:CD2	2.35	0.55
1:A:113:PRO:HD3	1:A:130:ARG:HD3	1.88	0.55
1:A:34:LEU:HB2	4:A:546:HOH:O	2.07	0.55
1:A:17:LEU:HD23	1:A:294:ALA:HB3	1.88	0.54
1:A:251:CYS:HB3	1:A:255:ILE:HA	1.90	0.54
1:A:122:ALA:HB2	1:A:213:SER:OG	2.08	0.54
1:A:13:LEU:HD12	1:A:107:LEU:HD23	1.89	0.54
1:A:357:LEU:HD22	1:A:357:LEU:N	2.23	0.53
1:A:163:THR:HG23	4:A:556:HOH:O	2.06	0.53
1:A:397:THR:CG2	1:A:400:ARG:H	2.13	0.52
1:A:143:ARG:O	1:A:146:SER:HB3	2.09	0.52
1:A:222:ASP:O	1:A:224:THR:HG23	2.09	0.52
1:A:282:SER:O	1:A:284:ARG:HG2	2.10	0.51
1:A:189:LEU:O	1:A:193:VAL:HG23	2.10	0.51
1:A:340:ILE:HD12	1:A:357:LEU:HD21	1.93	0.51
1:A:119:LEU:HD23	1:A:126:VAL:HG21	1.93	0.50
1:A:119:LEU:HD23	1:A:126:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLY:HA3	1:A:180:LEU:HD23	1.93	0.50
1:A:337:ASP:HB2	1:A:358:GLN:HA	1.93	0.50
1:A:397:THR:HG22	1:A:400:ARG:CB	2.42	0.50
1:A:266:PRO:O	1:A:267:ASP:HB2	2.11	0.49
1:A:400:ARG:O	1:A:403:ALA:HB3	2.13	0.49
1:A:340:ILE:CD1	1:A:392:LEU:HD23	2.42	0.49
1:A:297:GLN:O	1:A:301:VAL:HG23	2.13	0.48
1:A:208:ARG:HE	1:A:222:ASP:HB3	1.77	0.48
1:A:208:ARG:CG	1:A:220:LEU:HD23	2.39	0.48
1:A:281:LEU:HG	1:A:316:LEU:HD22	1.96	0.48
1:A:142:LEU:HD23	1:A:230:MET:CE	2.43	0.48
1:A:196:TYR:O	1:A:200:GLN:HG2	2.13	0.48
1:A:114:ARG:HH12	1:A:235:ILE:HD12	1.78	0.48
1:A:155:VAL:HB	3:A:500:NAD:C4N	2.44	0.48
1:A:156:ILE:HG13	3:A:500:NAD:C6N	2.44	0.47
1:A:114:ARG:HG3	1:A:238:LEU:HG	1.96	0.47
1:A:126:VAL:C	1:A:127:HIS:ND1	2.67	0.47
1:A:165:ARG:HH21	1:A:170:HIS:HA	1.79	0.47
1:A:341:VAL:HG22	1:A:354:LEU:CD2	2.44	0.47
1:A:83:GLN:O	1:A:84:SER:HB3	2.14	0.47
1:A:339:GLU:HA	1:A:355:ILE:O	2.15	0.47
1:A:219:LEU:N	1:A:219:LEU:HD23	2.30	0.47
1:A:337:ASP:CG	1:A:359:LYS:H	2.19	0.46
1:A:394:ASP:O	1:A:396:ALA:N	2.49	0.45
1:A:48:ARG:N	1:A:49:PRO:CD	2.79	0.45
1:A:162:ALA:O	1:A:166:THR:HB	2.17	0.45
1:A:341:VAL:HG12	1:A:341:VAL:O	2.16	0.45
1:A:143:ARG:HG3	1:A:146:SER:HB3	1.98	0.45
1:A:362:ILE:O	1:A:381:LEU:HD23	2.17	0.44
1:A:278:ARG:HB2	1:A:285:PHE:CE1	2.53	0.44
1:A:342:ARG:HB2	1:A:353:THR:HB	1.98	0.44
1:A:156:ILE:HG13	3:A:500:NAD:H6N	1.98	0.44
1:A:377:LEU:HA	1:A:380:LEU:HD12	2.00	0.44
1:A:351:LYS:HD2	1:A:369:ASN:O	2.18	0.43
1:A:222:ASP:CG	1:A:224:THR:HG23	2.39	0.43
1:A:339:GLU:HB2	1:A:356:GLU:OE2	2.18	0.43
1:A:121:GLY:O	1:A:123:THR:N	2.52	0.43
1:A:22:PHE:CD1	1:A:302:ALA:HB2	2.53	0.43
1:A:127:HIS:N	1:A:127:HIS:ND1	2.67	0.42
1:A:360:GLY:O	1:A:386:LYS:HG3	2.20	0.42
1:A:177:GLN:NE2	1:A:177:GLN:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG22	1:A:397:THR:O	2.18	0.42
1:A:233:VAL:HG12	1:A:235:ILE:HG12	2.01	0.42
1:A:381:LEU:HD22	1:A:381:LEU:O	2.20	0.41
1:A:222:ASP:OD1	1:A:224:THR:HG23	2.20	0.41
1:A:117:PRO:O	1:A:120:GLN:N	2.52	0.41
1:A:169:VAL:HG12	1:A:170:HIS:N	2.35	0.41
1:A:114:ARG:NH1	1:A:235:ILE:HG13	2.36	0.41
1:A:122:ALA:O	1:A:123:THR:C	2.58	0.41
1:A:253:ASP:OD2	1:A:287:ARG:NH2	2.54	0.41
1:A:274:VAL:O	1:A:274:VAL:HG22	2.21	0.41
1:A:159:GLU:OE2	3:A:500:NAD:H4N	2.21	0.41
1:A:144:PRO:O	1:A:145:GLN:HB2	2.21	0.40
1:A:127:HIS:HD2	1:A:138:ILE:HG13	1.86	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	399/408 (98%)	361 (90%)	31 (8%)	7 (2%)	9 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	A	395	PRO
1	A	118	THR
1	A	122	ALA
1	A	123	THR
1	A	389	ARG
1	A	117	PRO

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	299/307 (97%)	258 (86%)	41 (14%)	4 4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	28	GLN
1	A	44	ARG
1	A	56	MET
1	A	75	GLU
1	A	114	ARG
1	A	118	THR
1	A	119	LEU
1	A	120	GLN
1	A	123	THR
1	A	124	MET
1	A	128	THR
1	A	129	LEU
1	A	137	ARG
1	A	143	ARG
1	A	155	VAL
1	A	156	ILE
1	A	160	LEU
1	A	166	THR
1	A	182	SER
1	A	208	ARG
1	A	209	SER
1	A	219	LEU
1	A	222	ASP
1	A	225	ARG
1	A	262	ARG
1	A	271	LEU
1	A	285	PHE
1	A	286	GLU
1	A	289	GLU

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Mol	Chain	Res	Type
1	A	309	THR
1	A	327	ARG
1	A	337	ASP
1	A	348	ASP
1	A	357	LEU
1	A	361	ARG
1	A	372	ARG
1	A	381	LEU
1	A	386	LYS
1	A	394	ASP
1	A	397	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	177	GLN
1	A	240	ASN
1	A	323	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](#)

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	FAD	A	449	-	51,58,58	2.22	15 (29%)	57,89,89	1.85	9 (15%)
3	NAD	A	500	-	40,48,48	2.44	11 (27%)	44,73,73	2.93	17 (38%)

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	FAD	A	449	-	-	0/28/50/50	0/6/6/6
3	NAD	A	500	-	-	0/22/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	449	FAD	PA-O2A	-3.90	1.36	1.55
2	A	449	FAD	P-O2P	-3.25	1.39	1.55
3	A	500	NAD	O2B-C2B	-3.02	1.35	1.43
2	A	449	FAD	C2-N1	-2.91	1.32	1.38
3	A	500	NAD	C3B-C4B	2.04	1.58	1.53
3	A	500	NAD	C3N-C7N	2.35	1.54	1.50
2	A	449	FAD	C4X-N5	2.44	1.36	1.33
2	A	449	FAD	C2A-N3A	2.49	1.36	1.32
2	A	449	FAD	C5X-N5	2.50	1.39	1.35
2	A	449	FAD	C8-C7	2.50	1.47	1.40
2	A	449	FAD	C10-N1	2.57	1.36	1.33
2	A	449	FAD	C4-C4X	2.59	1.46	1.41
3	A	500	NAD	O4D-C4D	2.73	1.51	1.45
2	A	449	FAD	C2-N3	3.60	1.45	1.38
2	A	449	FAD	C4-N3	3.80	1.39	1.33
2	A	449	FAD	O5'-C5'	3.81	1.59	1.44
3	A	500	NAD	O3B-C3B	3.91	1.52	1.43
3	A	500	NAD	C6N-N1N	3.95	1.45	1.35
3	A	500	NAD	C4A-N3A	4.04	1.41	1.35
2	A	449	FAD	O4B-C1B	4.12	1.47	1.41
2	A	449	FAD	C4X-C10	4.98	1.49	1.41
3	A	500	NAD	C7N-N7N	5.22	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	C4N-C3N	5.62	1.49	1.39
3	A	500	NAD	O4D-C1D	5.68	1.49	1.41
3	A	500	NAD	C2A-N3A	6.73	1.43	1.32
2	A	449	FAD	C9A-N10	7.27	1.47	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	NAD	N3A-C2A-N1A	-10.15	120.17	128.86
3	A	500	NAD	C5N-C4N-C3N	-6.09	113.20	120.35
2	A	449	FAD	C4X-C4-N3	-4.83	116.60	123.47
2	A	449	FAD	C4B-O4B-C1B	-4.45	105.19	109.83
3	A	500	NAD	C3N-C7N-N7N	-4.39	112.66	117.76
2	A	449	FAD	C4-C4X-C10	-3.04	117.68	119.95
3	A	500	NAD	C1B-N9A-C4A	-2.96	121.53	126.64
3	A	500	NAD	O4B-C4B-C5B	-2.89	99.77	109.39
2	A	449	FAD	O5B-PA-O1A	-2.78	98.20	109.07
2	A	449	FAD	N3A-C2A-N1A	-2.69	126.56	128.86
3	A	500	NAD	C5A-C6A-N1A	-2.60	111.83	119.70
2	A	449	FAD	O5'-P-O1P	-2.35	99.88	109.07
3	A	500	NAD	C5N-C6N-N1N	-2.12	117.15	120.39
3	A	500	NAD	C4B-O4B-C1B	-2.02	107.72	109.83
3	A	500	NAD	C4D-O4D-C1D	2.08	111.99	109.83
2	A	449	FAD	C2A-N1A-C6A	2.19	122.47	118.75
2	A	449	FAD	C1'-N10-C10	2.30	120.75	118.46
3	A	500	NAD	N6A-C6A-N1A	2.87	124.52	118.57
3	A	500	NAD	O2B-C2B-C3B	3.13	121.86	111.83
3	A	500	NAD	C2B-C3B-C4B	3.47	109.28	102.62
3	A	500	NAD	PN-O3-PA	3.49	144.35	132.63
3	A	500	NAD	C2N-C3N-C4N	4.20	123.10	118.26
3	A	500	NAD	C6N-C5N-C4N	4.31	125.86	119.43
3	A	500	NAD	O7N-C7N-C3N	5.33	126.30	119.62
3	A	500	NAD	C2A-N1A-C6A	6.60	129.95	118.75
2	A	449	FAD	C4-N3-C2	7.96	121.92	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAD	6	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.