Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 08:33 PM EDT

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

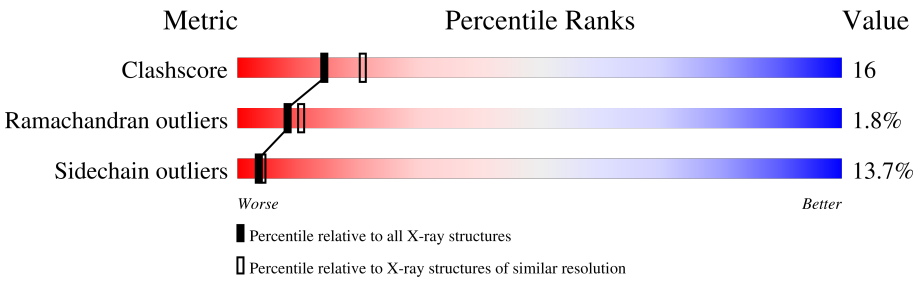
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	408	65% 27% 6% •

2 Entry composition (i)

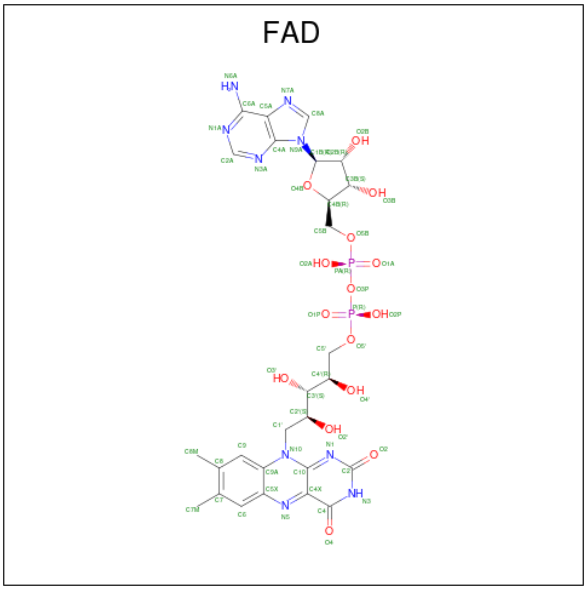
There are 4 unique types of molecules in this entry. The entry contains 3154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FERREDOXIN REDUCTASE.

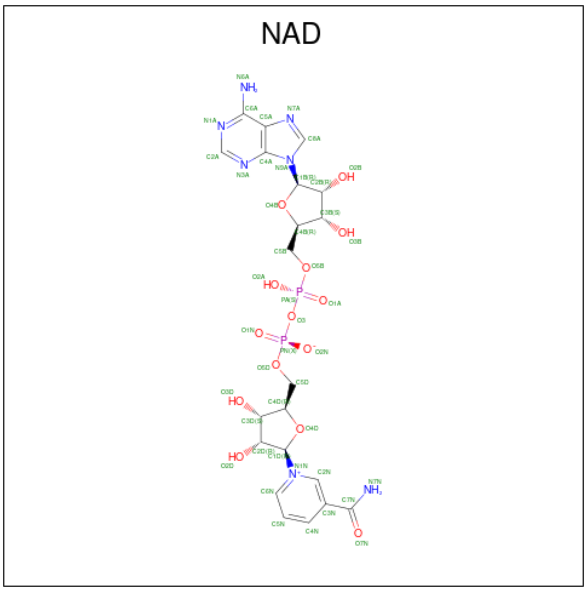
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	2976	1865	544	559	8	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	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
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0

- Molecule 4 is water.

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

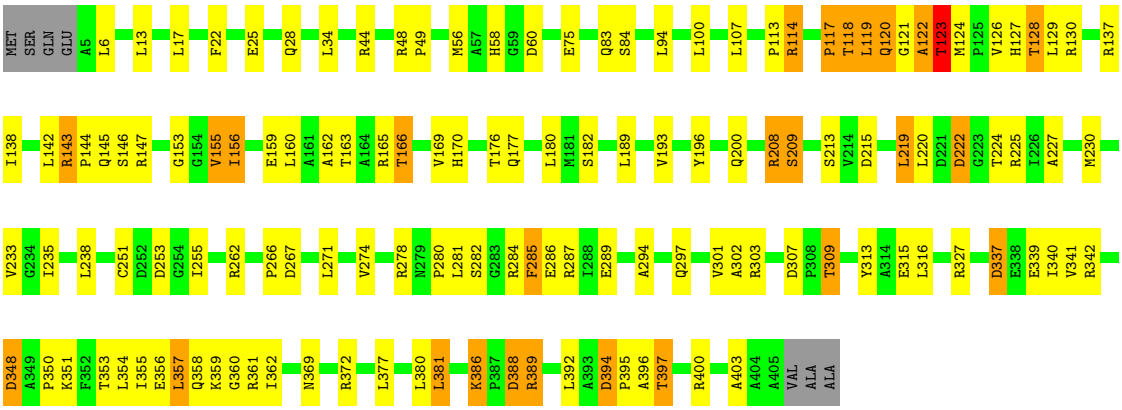
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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

Chain A: 65% 27% 6% •



4 Data and refinement statistics (i)

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: NAD, 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	0.37	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(^{o})	Ideal(^{o})
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:13:LEU:HD12	1:A:107:LEU:HD23	1.89	0.54
1:A:122:ALA:HB2	1:A:213:SER:OG	2.08	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:114:ARG:HH12	1:A:235:ILE:HD12	1.78	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:155:VAL:HB	3:A:500:NAD:C4N	2.44	0.48
1:A:114:ARG:HG3	1:A:238:LEU:HG	1.96	0.47
1:A:156:ILE:HG13	3:A:500:NAD:C6N	2.44	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:O	1:A:341:VAL:HG12	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:22:PHE:CD1	1:A:302:ALA:HB2	2.53	0.43
1:A:121:GLY:O	1:A:123:THR:N	2.52	0.43
1:A:127:HIS:ND1	1:A:127:HIS:N	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:HG22	1:A:274:VAL:O	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%)	8 10

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 (i)

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%)	3 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

Sometimes 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 monosaccharides 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	-	54,58,58	2.29	15 (27%)	71,89,89	1.37	10 (14%)
3	NAD	A	500	-	42,48,48	2.66	14 (33%)	50,73,73	2.47	17 (34%)

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	-	-	3/30/50/50	0/6/6/6
3	NAD	A	500	-	-	3/26/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	449	FAD	P-O3P	-9.55	1.49	1.59
3	A	500	NAD	C2A-N3A	7.08	1.43	1.32
3	A	500	NAD	C4N-C3N	6.37	1.49	1.39
3	A	500	NAD	O4D-C1D	6.31	1.49	1.40
3	A	500	NAD	C7N-N7N	5.54	1.43	1.33
2	A	449	FAD	O4B-C1B	4.64	1.47	1.40
3	A	500	NAD	C6N-N1N	4.51	1.45	1.35
3	A	500	NAD	C4A-N3A	4.24	1.41	1.35
2	A	449	FAD	PA-O2A	-4.14	1.36	1.55
2	A	449	FAD	O5'-C5'	3.96	1.59	1.44
3	A	500	NAD	O3B-C3B	3.89	1.52	1.43
2	A	449	FAD	C9A-N10	3.72	1.47	1.41
3	A	500	NAD	C2N-N1N	3.68	1.39	1.35
2	A	449	FAD	P-O2P	-3.45	1.39	1.55
2	A	449	FAD	C1'-C2'	3.38	1.57	1.52
3	A	500	NAD	O2B-C2B	-2.99	1.35	1.43
2	A	449	FAD	C2-N3	2.88	1.45	1.39
2	A	449	FAD	C4X-N5	2.83	1.36	1.30
3	A	500	NAD	O4D-C4D	2.75	1.51	1.45
2	A	449	FAD	C2A-N3A	2.65	1.36	1.32
2	A	449	FAD	C6-C5X	2.63	1.44	1.40
2	A	449	FAD	C8-C7	2.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	449	FAD	C9A-C5X	2.46	1.45	1.41
3	A	500	NAD	C3N-C7N	2.43	1.54	1.50
3	A	500	NAD	C1B-N9A	-2.43	1.43	1.49
2	A	449	FAD	O2-C2	-2.35	1.19	1.24
3	A	500	NAD	C3B-C4B	2.08	1.58	1.53
3	A	500	NAD	C5N-C4N	2.03	1.42	1.38
2	A	449	FAD	C2A-N1A	2.02	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	NAD	C5N-C4N-C3N	-7.29	113.20	120.36
3	A	500	NAD	N3A-C2A-N1A	-6.26	120.17	128.67
3	A	500	NAD	O7N-C7N-C3N	5.48	126.30	119.60
2	A	449	FAD	C4B-O4B-C1B	-5.18	105.19	109.92
3	A	500	NAD	O4B-C1B-N9A	-4.49	102.79	108.75
3	A	500	NAD	C6N-C5N-C4N	4.45	125.86	119.45
3	A	500	NAD	C2N-C3N-C4N	4.16	123.10	118.26
3	A	500	NAD	C3N-C7N-N7N	-4.12	112.66	117.74
3	A	500	NAD	C5A-C6A-N1A	-3.52	111.83	120.23
3	A	500	NAD	C2B-C3B-C4B	3.45	109.28	102.61
2	A	449	FAD	O4B-C1B-N9A	-3.20	104.50	108.75
3	A	500	NAD	O2B-C2B-C3B	3.13	121.86	111.82
3	A	500	NAD	O4B-C4B-C5B	-2.99	99.77	109.33
3	A	500	NAD	C1B-N9A-C4A	-2.91	121.53	126.64
3	A	500	NAD	N6A-C6A-N1A	2.90	124.52	118.33
2	A	449	FAD	O5B-PA-O1A	-2.71	98.20	108.94
2	A	449	FAD	C5A-C6A-N6A	2.62	124.30	120.31
3	A	500	NAD	C4B-O4B-C1B	-2.40	107.72	109.92
3	A	500	NAD	C5N-C6N-N1N	-2.37	117.15	120.38
2	A	449	FAD	C5A-C6A-N1A	-2.35	114.62	120.23
2	A	449	FAD	O2A-PA-O3P	2.31	113.53	107.27
2	A	449	FAD	O5'-P-O1P	-2.28	99.88	108.94
3	A	500	NAD	C4D-O4D-C1D	2.26	111.99	109.92
2	A	449	FAD	C5'-C4'-C3'	-2.26	107.96	112.22
3	A	500	NAD	C5A-C6A-N6A	2.19	123.65	120.31
2	A	449	FAD	C4-N3-C2	-2.10	121.92	125.64
2	A	449	FAD	O2A-PA-O1A	2.07	122.09	112.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	NAD	O4D-C4D-C5D-O5D
3	A	500	NAD	C3D-C4D-C5D-O5D
2	A	449	FAD	PA-O3P-P-O5'
2	A	449	FAD	P-O3P-PA-O1A
2	A	449	FAD	P-O3P-PA-O2A
3	A	500	NAD	O4B-C4B-C5B-O5B

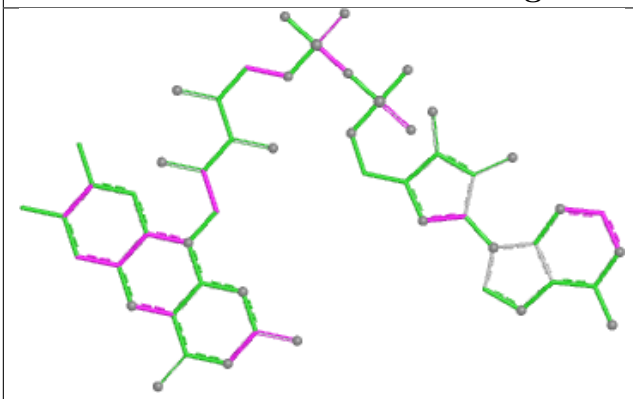
There are no ring outliers.

1 monomer is involved in 6 short contacts:

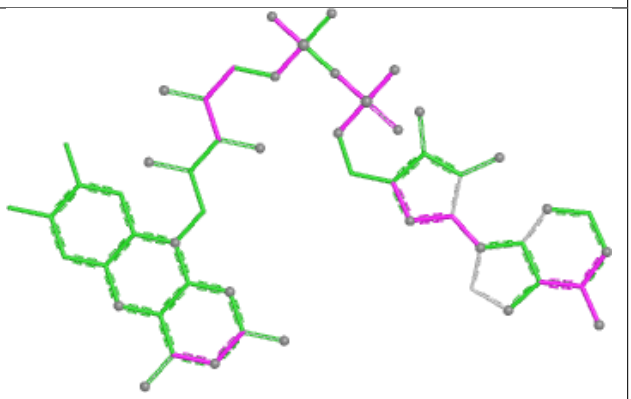
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAD	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

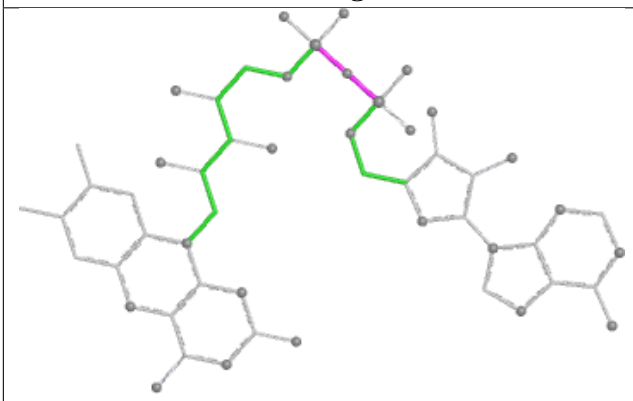
Ligand FAD A 449



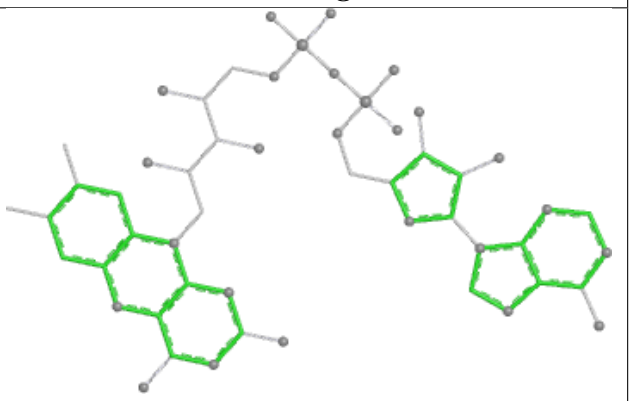
Bond lengths



Bond angles

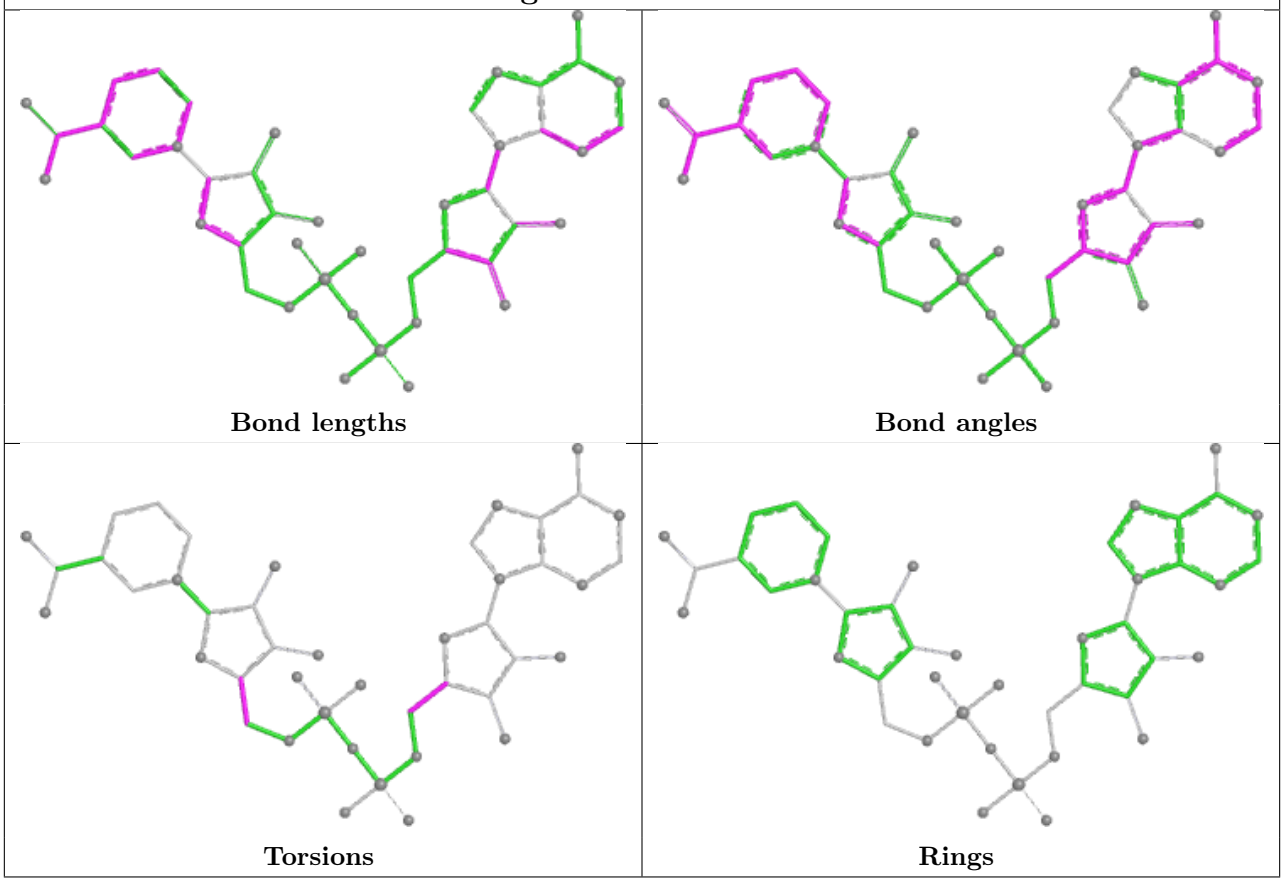


Torsions



Rings

Ligand NAD A 500



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.