



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:04 AM UTC

PDB ID : 2NPX / pdb_00002npx
Title : NADH BINDING SITE AND CATALYSIS OF NADH PEROXIDASE
Authors : Stehle, T.; Claiborne, A.; Schulz, G.E.
Deposited on : 1992-05-29
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

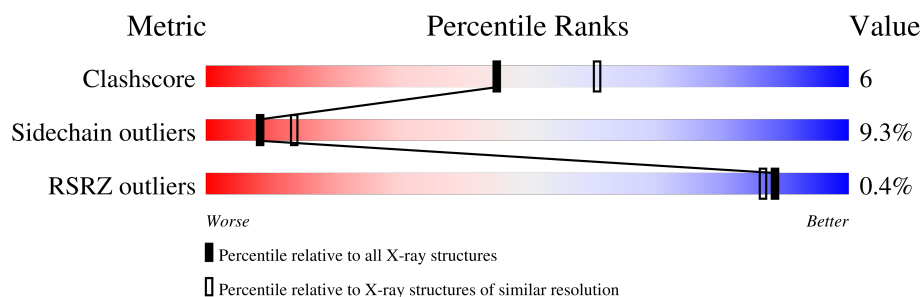
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	447	 74% 19% 5%

2 Entry composition [i](#)

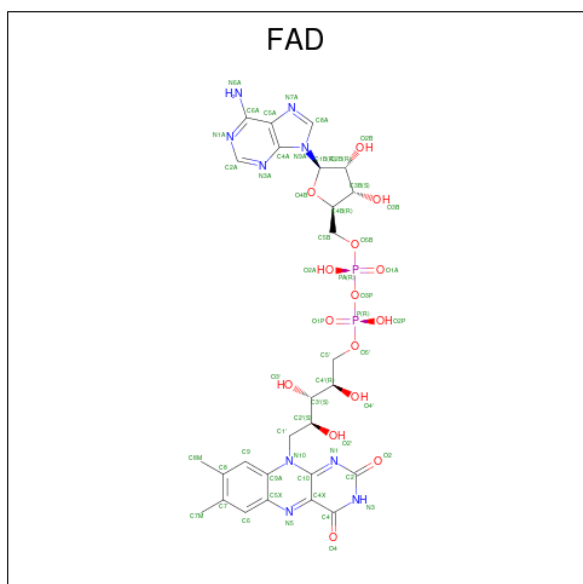
There are 4 unique types of molecules in this entry. The entry contains 3927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADH PEROXIDASE.

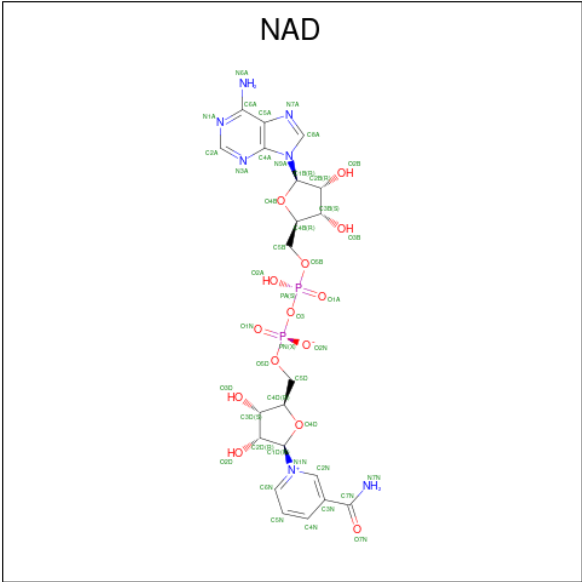
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3493	2225	573	683	12			

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



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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.

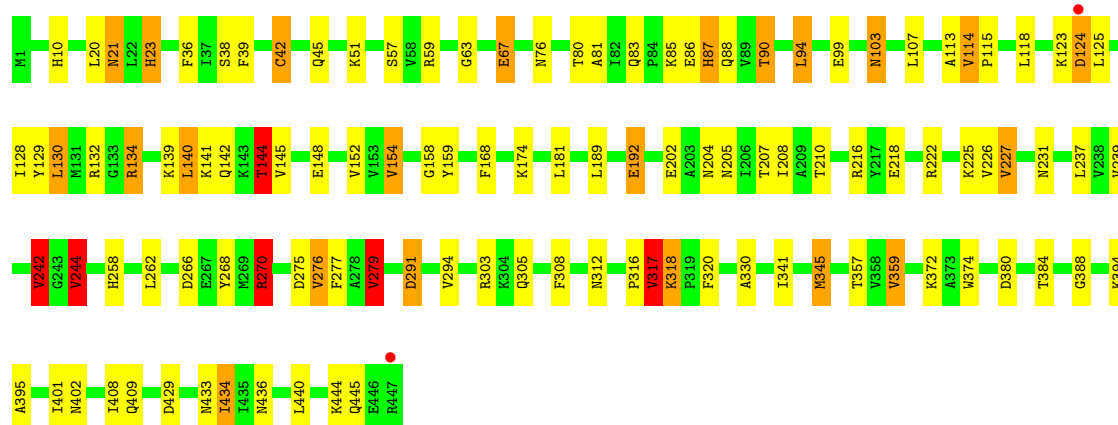
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	337	Total	O	0	0
			337	337		

3 Residue-property plots

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 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.

• Molecule 1: NADH PEROXIDASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.20Å 134.50Å 145.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 98.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 93.1 (98.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.42Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.159 , (Not available) 0.147 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3927	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, OCS, 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	1.03	10/3547 (0.3%)	1.77	66/4807 (1.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	ILE	CA-CB	7.69	1.64	1.54
1	A	276	VAL	CA-CB	7.33	1.63	1.54
1	A	152	VAL	CA-CB	-6.57	1.46	1.54
1	A	10	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	227	VAL	CA-CB	6.27	1.61	1.54
1	A	23	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	258	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	154	VAL	CA-CB	5.58	1.61	1.54
1	A	87	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	341	ILE	CA-CB	5.24	1.60	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	VAL	N-CA-CB	-12.91	97.28	112.39
1	A	317	VAL	N-CA-CB	-10.90	99.35	112.33
1	A	38	SER	N-CA-C	9.12	123.98	111.39
1	A	244	VAL	N-CA-CB	-9.00	96.69	111.44
1	A	279	VAL	N-CA-CB	-8.44	96.75	112.36
1	A	124	ASP	N-CA-C	7.92	122.10	107.60
1	A	205	ASN	CA-CB-CG	7.57	120.17	112.60
1	A	242	VAL	CB-CA-C	7.56	120.89	112.19
1	A	21	ASN	CA-CB-CG	7.35	119.95	112.60
1	A	266	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	114	VAL	N-CA-CB	-7.25	101.05	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	LEU	N-CA-C	-7.05	101.03	110.55
1	A	291	ASP	CA-CB-CG	-6.83	105.77	112.60
1	A	433	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	317	VAL	CB-CA-C	6.75	117.91	110.62
1	A	270	ARG	CB-CG-CD	-6.69	95.92	111.30
1	A	168	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	402	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	205	ASN	N-CA-C	6.36	120.14	111.17
1	A	303	ARG	NE-CZ-NH1	6.31	127.81	121.50
1	A	128	ILE	N-CA-C	-6.31	98.04	107.37
1	A	244	VAL	CB-CA-C	6.27	120.16	110.50
1	A	374	TRP	CB-CG-CD1	-6.12	117.71	126.90
1	A	279	VAL	CB-CA-C	6.04	120.51	110.30
1	A	144	THR	N-CA-CB	-5.92	101.11	110.22
1	A	202	GLU	CA-CB-CG	-5.90	102.31	114.10
1	A	67	GLU	CA-CB-CG	-5.81	102.47	114.10
1	A	57	SER	N-CA-C	-5.81	106.23	113.38
1	A	10	HIS	N-CA-C	5.78	117.58	111.28
1	A	395	ALA	O-C-N	-5.75	116.47	122.96
1	A	244	VAL	O-C-N	-5.73	116.97	123.10
1	A	436	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	103	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	226	VAL	N-CA-C	-5.61	99.56	107.75
1	A	445	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	444	LYS	CB-CA-C	-5.58	102.12	110.88
1	A	320	PHE	CA-C-N	5.56	125.65	119.87
1	A	320	PHE	C-N-CA	5.56	125.65	119.87
1	A	158	GLY	N-CA-C	-5.55	104.67	112.60
1	A	429	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	330	ALA	O-C-N	-5.47	117.09	123.27
1	A	359	VAL	O-C-N	-5.45	117.16	122.99
1	A	303	ARG	CB-CG-CD	5.44	123.81	111.30
1	A	409	GLN	O-C-N	-5.44	116.36	122.12
1	A	308	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	142	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	434	ILE	CA-CB-CG1	-5.27	101.44	110.40
1	A	318	LYS	O-C-N	-5.25	117.55	121.23
1	A	434	ILE	CA-CB-CG2	5.24	119.41	110.50
1	A	239	VAL	N-CA-C	-5.24	100.83	108.17
1	A	231	ASN	N-CA-C	5.23	116.48	108.42
1	A	10	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	207	THR	CA-CB-OG1	-5.16	101.86	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	THR	N-CA-CB	-5.16	102.36	110.30
1	A	80	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	258	HIS	CB-CG-CD2	-5.13	124.52	131.20
1	A	436	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	204	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	23	HIS	CA-C-N	5.06	124.85	119.28
1	A	23	HIS	C-N-CA	5.06	124.85	119.28
1	A	139	LYS	CB-CG-CD	-5.06	99.66	111.30
1	A	394	LYS	N-CA-C	-5.06	106.62	112.89
1	A	434	ILE	N-CA-CB	-5.06	103.66	110.54
1	A	107	LEU	O-C-N	-5.06	117.40	123.27
1	A	374	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	A	374	TRP	CE2-CD2-CG	-5.01	101.19	107.20

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	3493	0	3489	42	0
2	A	53	0	31	2	0
3	A	44	0	26	2	0
4	A	337	0	0	7	0
All	All	3927	0	3546	42	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 (42) 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:279:VAL:HG22	1:A:305:GLN:HB3	1.73	0.69
1:A:87:HIS:HE1	1:A:275:ASP:OD2	1.84	0.61
1:A:45:GLN:HG3	4:A:1153:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HG2	4:A:1101:HOH:O	2.02	0.58
1:A:81:ALA:HB3	1:A:90:THR:HG23	1.87	0.57
1:A:268:TYR:HB2	1:A:270:ARG:HD2	1.87	0.55
1:A:88:GLN:HG2	1:A:103:ASN:OD1	2.08	0.53
1:A:192:GLU:HG3	1:A:357:THR:HG21	1.91	0.52
1:A:294:VAL:HG11	1:A:345:MET:HE1	1.91	0.51
1:A:312:ASN:ND2	1:A:317:VAL:H	2.09	0.51
1:A:115:PRO:HB2	1:A:130:LEU:HG	1.93	0.50
1:A:216:ARG:HD3	4:A:987:HOH:O	2.12	0.49
1:A:208:ILE:HG22	1:A:210:THR:HG23	1.95	0.48
1:A:144:THR:HG22	1:A:145:VAL:HG13	1.96	0.48
1:A:39:PHE:CD1	1:A:134:ARG:HG2	2.49	0.47
1:A:388:GLY:HA2	1:A:408:ILE:HD11	1.98	0.46
1:A:312:ASN:HD21	1:A:318:LYS:N	2.13	0.45
1:A:23:HIS:HE1	4:A:933:HOH:O	1.99	0.45
1:A:277:PHE:CD1	1:A:277:PHE:N	2.84	0.45
1:A:181:LEU:HD13	4:A:1146:HOH:O	2.17	0.45
1:A:132:ARG:HD3	4:A:1095:HOH:O	2.16	0.44
1:A:270:ARG:NH2	1:A:316:PRO:HG3	2.32	0.44
1:A:42:OCS:OD2	2:A:449:FAD:C10	2.65	0.44
1:A:401:ILE:HA	1:A:401:ILE:HD12	1.70	0.44
1:A:113:ALA:HB1	1:A:244:VAL:HG13	2.00	0.43
1:A:76:ASN:O	1:A:94:LEU:HB2	2.18	0.43
1:A:141:LYS:O	1:A:144:THR:HB	2.18	0.43
1:A:380:ASP:O	1:A:384:THR:HA	2.19	0.42
1:A:312:ASN:HD21	1:A:318:LYS:H	1.68	0.42
1:A:85:LYS:O	1:A:87:HIS:HD2	2.03	0.42
1:A:359:VAL:HG12	1:A:372:LYS:HE3	2.01	0.42
1:A:372:LYS:HE2	1:A:372:LYS:HB3	1.88	0.41
1:A:83:GLN:HE22	1:A:90:THR:HG22	1.84	0.41
1:A:242:VAL:HG22	3:A:818:NAD:C5A	2.50	0.41
1:A:218:GLU:HB2	1:A:225:LYS:HB2	2.02	0.41
1:A:23:HIS:CE1	4:A:933:HOH:O	2.74	0.40
1:A:42:OCS:OD2	2:A:449:FAD:C4X	2.69	0.40
1:A:129:TYR:HD2	1:A:140:LEU:HD13	1.86	0.40
1:A:36:PHE:CD2	1:A:39:PHE:HB2	2.57	0.40
1:A:159:TYR:HB3	3:A:818:NAD:C5N	2.52	0.40
1:A:312:ASN:HD22	1:A:317:VAL:H	1.68	0.40
1:A:63:GLY:O	1:A:67:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	375/375 (100%)	340 (91%)	35 (9%)	8 14

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	21	ASN
1	A	51	LYS
1	A	59	ARG
1	A	86	GLU
1	A	90	THR
1	A	94	LEU
1	A	99	GLU
1	A	114	VAL
1	A	118	LEU
1	A	123	LYS
1	A	124	ASP
1	A	130	LEU
1	A	134	ARG
1	A	140	LEU
1	A	144	THR
1	A	148	GLU
1	A	154	VAL
1	A	174	LYS
1	A	189	LEU
1	A	192	GLU
1	A	222	ARG
1	A	227	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	LEU
1	A	242	VAL
1	A	244	VAL
1	A	262	LEU
1	A	270	ARG
1	A	276	VAL
1	A	279	VAL
1	A	291	ASP
1	A	317	VAL
1	A	345	MET
1	A	434	ILE
1	A	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	83	GLN
1	A	87	HIS
1	A	142	GLN
1	A	205	ASN
1	A	247	ASN
1	A	288	ASN
1	A	301	ASN
1	A	312	ASN
1	A	371	GLN
1	A	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	OCS	A	42	1	6,8,9	1.34	1 (16%)	7,11,13	4.27	5 (71%)

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
1	OCS	A	42	1	-	0/4/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	OCS	OD2-SG	-2.79	1.36	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	OCS	OD3-SG-CB	7.04	117.27	106.76
1	A	42	OCS	OD1-SG-CB	7.02	117.24	106.76
1	A	42	OCS	OD2-SG-OD1	-3.26	103.23	111.40
1	A	42	OCS	OD2-SG-OD3	-3.18	103.44	111.40
1	A	42	OCS	OD3-SG-OD1	-2.26	106.47	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	42	OCS	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	NAD	A	818	-	46,48,48	2.04	11 (23%)	64,73,73	1.55	14 (21%)
2	FAD	A	449	-	58,58,58	1.22	5 (8%)	85,89,89	1.18	6 (7%)

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	NAD	A	818	-	-	1/30/62/62	0/5/5/5
2	FAD	A	449	-	-	3/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	818	NAD	C4N-C3N	7.68	1.51	1.39
3	A	818	NAD	C5N-C4N	7.09	1.51	1.38
2	A	449	FAD	PA-O3P	3.94	1.63	1.59
3	A	818	NAD	C2N-N1N	3.03	1.38	1.35
3	A	818	NAD	C3N-C7N	-2.95	1.46	1.50
3	A	818	NAD	O4D-C1D	2.69	1.44	1.40
2	A	449	FAD	P-O5'	-2.56	1.49	1.59
3	A	818	NAD	C5A-C4A	2.50	1.43	1.39
3	A	818	NAD	C2N-C3N	2.47	1.42	1.39
2	A	449	FAD	P-O3P	-2.42	1.56	1.59
2	A	449	FAD	C5X-N5	-2.35	1.35	1.39
2	A	449	FAD	PA-O5B	-2.28	1.50	1.59
3	A	818	NAD	PN-O2N	-2.25	1.44	1.55
3	A	818	NAD	PA-O5B	-2.08	1.51	1.59
3	A	818	NAD	O5D-C5D	2.01	1.52	1.44
3	A	818	NAD	PN-O5D	-2.01	1.51	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	818	NAD	C5N-C4N-C3N	-5.27	115.18	120.36
3	A	818	NAD	C6N-N1N-C2N	-3.97	118.50	121.88
2	A	449	FAD	C5A-C4A-N3A	-3.86	121.41	126.72
3	A	818	NAD	C5A-C4A-N3A	-3.40	122.04	126.72
3	A	818	NAD	C3N-C7N-N7N	3.35	121.87	117.74
3	A	818	NAD	C4A-C5A-N7A	-2.96	107.20	110.58
2	A	449	FAD	O4B-C1B-N9A	2.71	113.30	108.09
2	A	449	FAD	N3A-C4A-N9A	2.48	131.39	127.17
3	A	818	NAD	N3A-C4A-N9A	2.48	131.38	127.17
2	A	449	FAD	O4'-C4'-C5'	-2.47	104.53	109.99
3	A	818	NAD	N3A-C2A-N1A	2.44	132.28	128.58
2	A	449	FAD	C4-N3-C2	-2.39	121.41	125.64
3	A	818	NAD	O4B-C1B-N9A	2.31	112.53	108.09
2	A	449	FAD	O2A-PA-O3P	2.29	113.45	107.27
3	A	818	NAD	C5N-C6N-N1N	2.24	123.44	120.38
3	A	818	NAD	C6A-C5A-C4A	2.23	120.22	117.18
3	A	818	NAD	O4B-C1B-C2B	-2.20	101.91	106.62
3	A	818	NAD	C5A-N7A-C8A	2.15	106.83	103.45
3	A	818	NAD	O4D-C4D-C5D	2.02	115.81	109.33
3	A	818	NAD	O7N-C7N-C3N	-2.01	117.14	119.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	449	FAD	O4B-C4B-C5B-O5B
2	A	449	FAD	PA-O3P-P-O5'
2	A	449	FAD	C3B-C4B-C5B-O5B
3	A	818	NAD	O4B-C4B-C5B-O5B

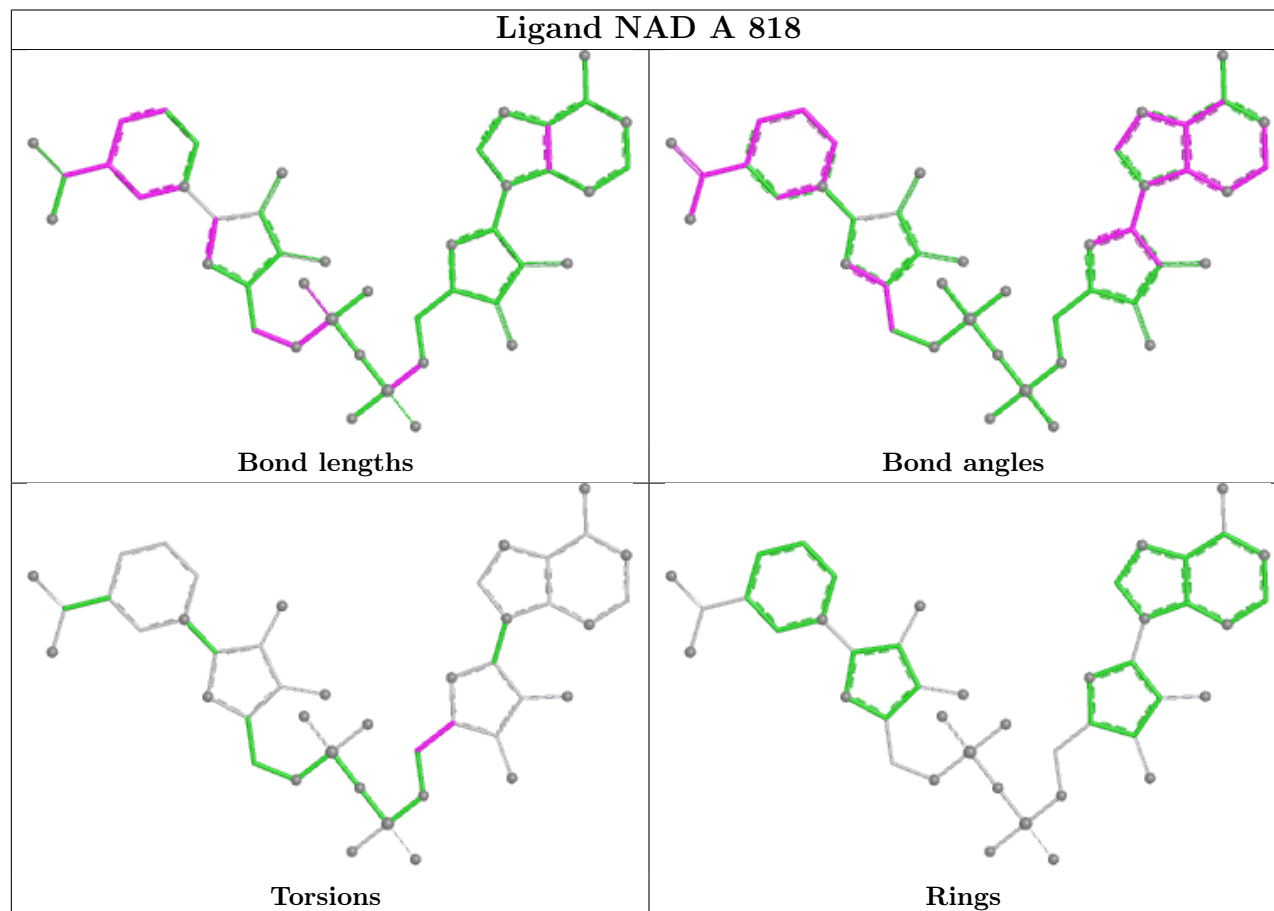
There are no ring outliers.

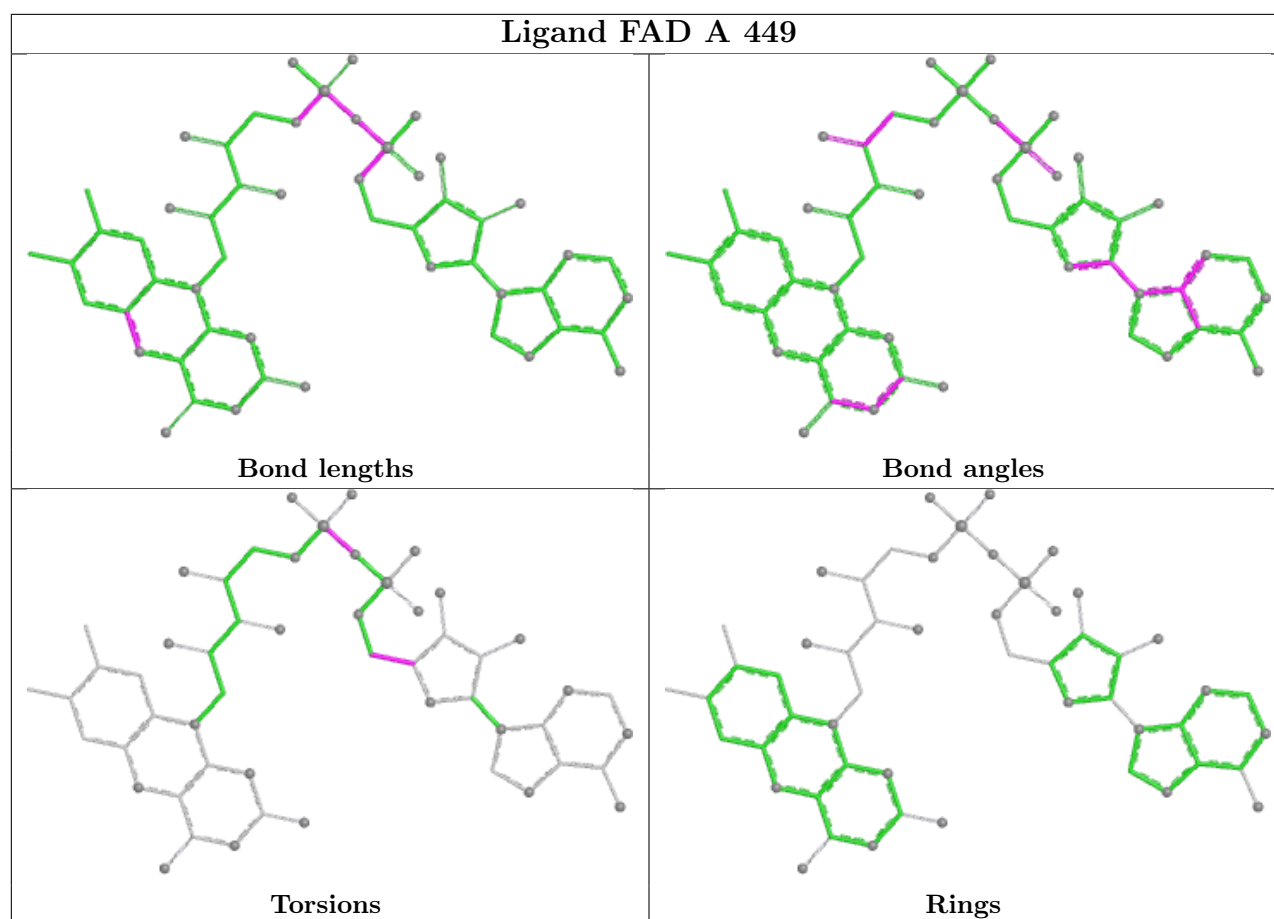
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	818	NAD	2	0
2	A	449	FAD	2	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 than 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.





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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	446/447 (99%)	-0.78	2 (0%) 88 86	5, 16, 36, 57	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	ASP	2.5
1	A	447	ARG	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	A	42	9/10	0.98	0.06	9,14,16,19	0

6.3 Carbohydrates [i](#)

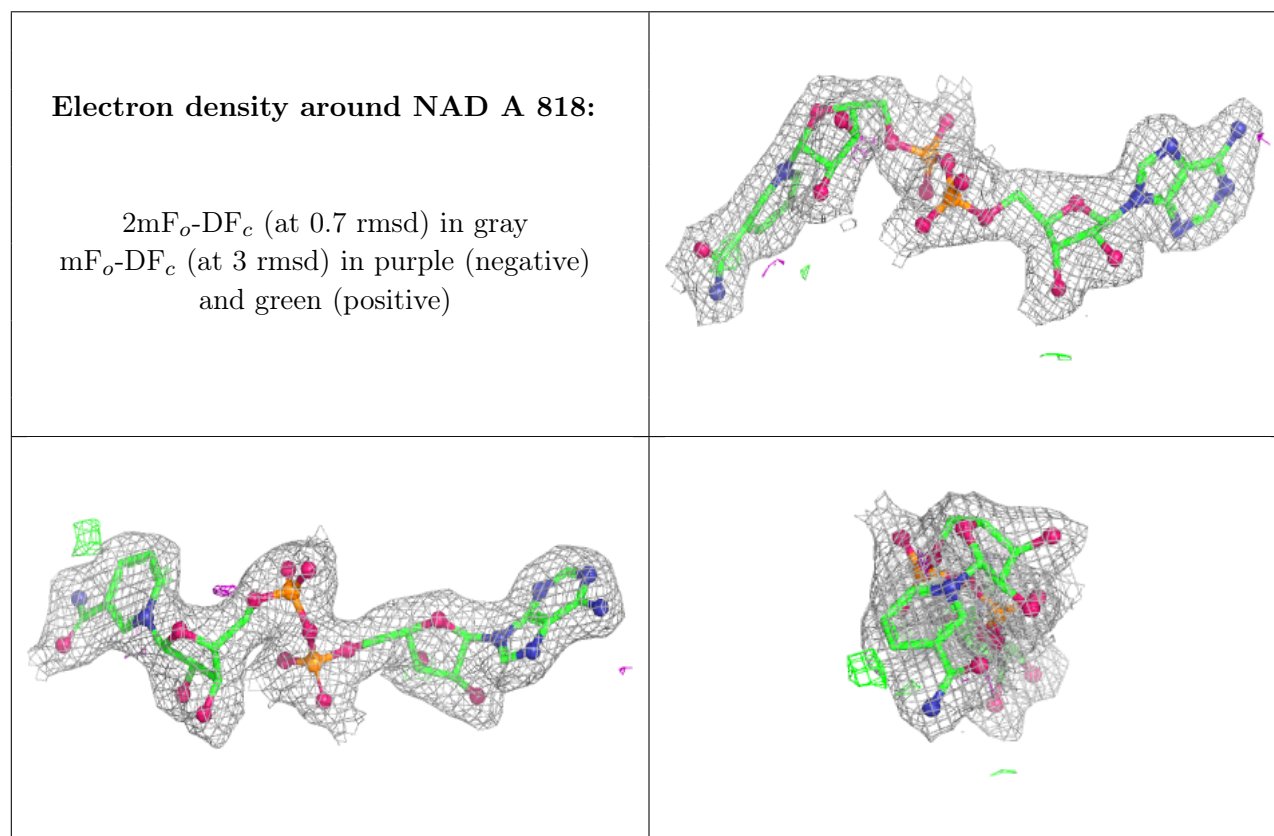
There are no oligosaccharides in this entry.

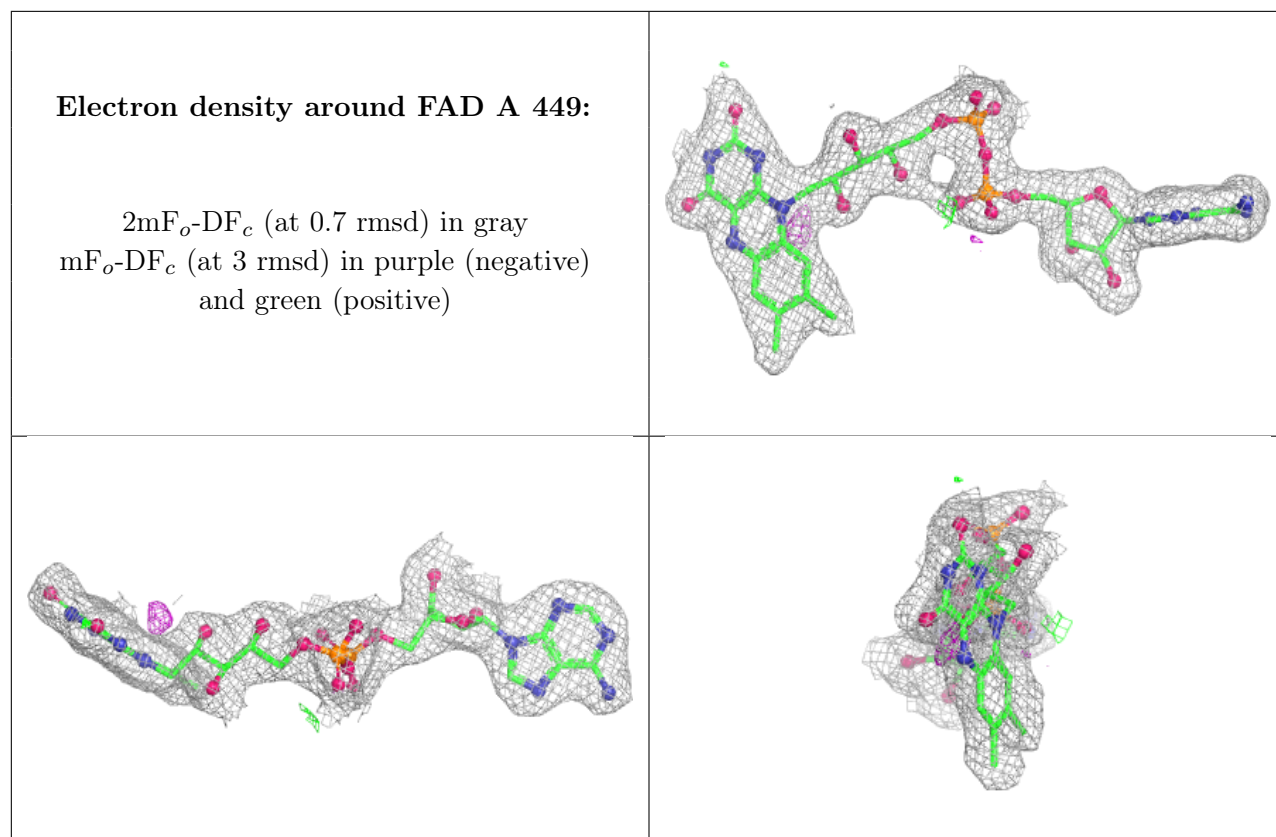
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	A	818	44/44	0.98	0.06	18,21,23,24	0
2	FAD	A	449	53/53	0.99	0.04	6,10,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.