



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 06:45 PM EDT

PDB ID : 3NTR  
Title : Crystal structure of K97V mutant of myo-inositol dehydrogenase from *Bacillus subtilis* with bound cofactor NAD and inositol  
Authors : Van Straaten, K.E.; Palmer, D.R.J.; Sanders, D.A.R.  
Deposited on : 2010-07-05  
Resolution : 2.65 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

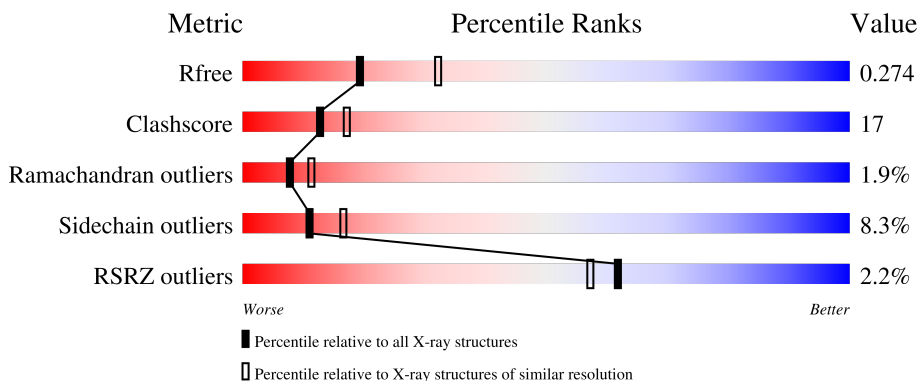
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	344	
1	B	344	

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	INS	A	801	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5444 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.

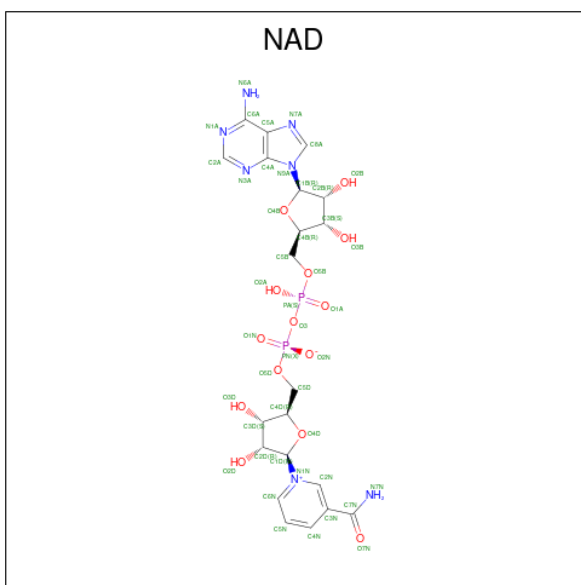
- Molecule 1 is a protein called Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	Total 2638	C 1669	N 443	O 514	S 12	0	0	0
1	B	337	Total 2638	C 1669	N 443	O 514	S 12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	VAL	LYS	engineered mutation	UNP P26935
B	97	VAL	LYS	engineered mutation	UNP P26935

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



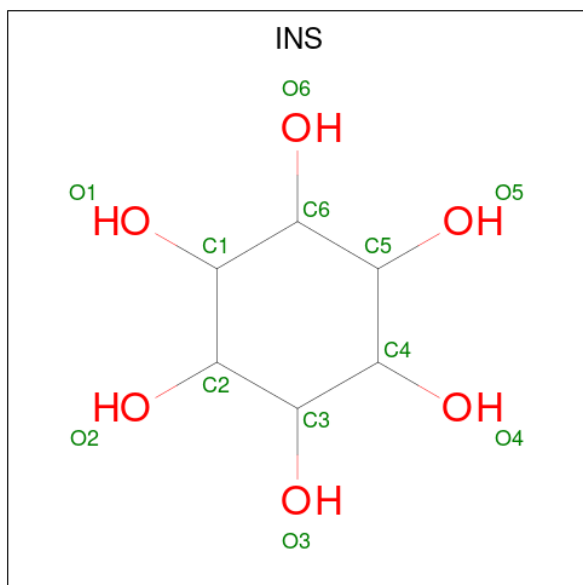
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 3 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (three-letter code: INS) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	6	6	0	0
3	B	1	12	6	6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	31	31	31	0	0
4	B	25	25	25	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.69Å 183.69Å 183.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.65 19.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-2.65) 100.0 (19.81-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.50Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.232 , 0.279 0.226 , 0.274	Depositor DCC
$R_{free}$ test set	1832 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, INS

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	0.48	0/2685	0.62	0/3643
1	B	0.50	0/2685	0.64	0/3643
All	All	0.49	0/5370	0.63	0/7286

There are no bond length outliers.

There are no bond angle outliers.

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	2638	0	2631	76	0
1	B	2638	0	2631	105	0
2	A	44	0	26	4	0
2	B	44	0	26	3	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
4	A	31	0	0	2	0
4	B	25	0	0	8	0
All	All	5444	0	5338	178	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 17.



All (178) 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:199:LYS:HE2	1:A:207:LEU:O	1.66	0.95
1:B:199:LYS:HE2	1:B:207:LEU:O	1.67	0.94
1:A:39:GLU:HG2	1:A:43:LYS:HE2	1.53	0.91
1:B:182:HIS:HE1	4:B:348:HOH:O	1.62	0.81
1:B:75:TRP:HA	1:B:75:TRP:CE3	2.17	0.78
1:B:182:HIS:HD2	4:B:369:HOH:O	1.65	0.77
1:B:75:TRP:HB3	1:B:77:PRO:HD2	1.67	0.74
1:B:34:THR:HG22	1:B:61:LEU:HD13	1.69	0.74
1:B:35:ASP:HB2	1:B:41:ALA:HB2	1.69	0.74
1:A:34:THR:HG22	1:A:61:LEU:HD13	1.70	0.73
1:B:310:VAL:HG11	1:B:329:LEU:HD23	1.69	0.73
1:A:174:LEU:HD13	1:A:227:ILE:HD11	1.72	0.72
1:B:126:MET:HG3	1:B:280:TYR:CE1	2.25	0.72
1:B:181:LEU:O	1:B:185:VAL:HG22	1.89	0.71
1:B:318:ALA:HB2	1:B:325:GLU:HG2	1.71	0.70
1:B:174:LEU:HD13	1:B:227:ILE:HD11	1.72	0.70
1:B:75:TRP:HA	1:B:75:TRP:HE3	1.57	0.69
1:A:181:LEU:O	1:A:185:VAL:HG22	1.93	0.68
1:B:130:ASP:O	1:B:134:VAL:HG23	1.96	0.66
1:A:310:VAL:HG11	1:A:329:LEU:HD23	1.78	0.65
1:A:318:ALA:HB2	1:A:325:GLU:HG2	1.77	0.65
1:B:174:LEU:O	1:B:174:LEU:HG	1.97	0.65
1:A:126:MET:HG3	1:A:280:TYR:CE1	2.32	0.64
1:B:140:LEU:HD12	1:B:184:LEU:HD22	1.80	0.64
1:A:170:VAL:HG11	1:A:315:CYS:HB3	1.81	0.63
1:A:6:GLY:O	1:A:70:VAL:HA	1.99	0.63
1:A:64:ASP:OD1	1:A:66:ASN:HB2	1.98	0.63
1:B:48:TYR:O	1:B:50:LEU:HD23	1.99	0.63
1:B:170:VAL:HG11	1:B:315:CYS:HB3	1.80	0.62
1:B:182:HIS:CE1	4:B:348:HOH:O	2.42	0.62
1:A:35:ASP:OD1	2:A:400:NAD:H1B	1.99	0.62
1:A:126:MET:HE3	2:A:400:NAD:O7N	2.00	0.61
1:B:57:ASN:HA	4:B:355:HOH:O	1.99	0.61
1:A:30:ILE:HB	1:A:50:LEU:HD13	1.82	0.60
1:B:64:ASP:OD1	1:B:66:ASN:HB2	2.02	0.60
1:A:58:ASP:OD1	1:A:58:ASP:N	2.33	0.59
1:B:310:VAL:HG11	1:B:329:LEU:CD2	2.33	0.58
1:B:58:ASP:OD1	1:B:58:ASP:N	2.34	0.58
1:B:6:GLY:O	1:B:70:VAL:HA	2.04	0.58
1:A:48:TYR:O	1:A:50:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:OE1	1:A:56:PRO:HA	2.05	0.57
1:A:182:HIS:HD2	4:A:352:HOH:O	1.86	0.56
1:B:35:ASP:CB	1:B:41:ALA:HB2	2.35	0.56
1:B:126:MET:HE3	2:B:400:NAD:O7N	2.06	0.56
1:B:119:ARG:HH21	1:B:336:TYR:HA	1.71	0.56
1:B:336:TYR:O	1:B:337:GLN:HB3	2.06	0.56
1:A:174:LEU:HG	1:A:174:LEU:O	2.05	0.56
1:A:151:ILE:HG12	1:A:241:ILE:HG12	1.88	0.55
1:B:38:GLN:OE1	1:B:56:PRO:HA	2.07	0.55
1:B:147:GLU:HB2	1:B:244:GLU:CD	2.26	0.55
1:A:11:GLY:O	1:A:15:LYS:HD3	2.07	0.55
1:A:128:ARG:HD2	1:A:300:PRO:HG3	1.88	0.55
1:B:116:VAL:HG12	1:B:116:VAL:O	2.07	0.55
1:A:119:ARG:HH21	1:A:336:TYR:HA	1.71	0.54
1:B:42:GLN:OE1	1:B:54:VAL:HG21	2.08	0.54
1:A:140:LEU:HD12	1:A:184:LEU:HD22	1.90	0.54
1:A:70:VAL:N	1:A:92:TYR:O	2.30	0.54
1:A:197:PRO:HB3	1:B:222:VAL:HG23	1.90	0.54
1:B:128:ARG:HD2	1:B:300:PRO:HG3	1.88	0.54
1:A:130:ASP:O	1:A:134:VAL:HG23	2.08	0.54
1:A:83:VAL:O	1:A:87:ILE:HG13	2.08	0.53
1:B:30:ILE:HB	1:B:50:LEU:HD13	1.90	0.53
1:B:162:ASP:N	1:B:162:ASP:OD1	2.40	0.53
1:A:116:VAL:HG12	1:A:116:VAL:O	2.08	0.53
1:B:75:TRP:HB3	1:B:77:PRO:CD	2.38	0.52
1:B:145:ILE:HG21	1:B:248:ILE:HG23	1.91	0.52
1:A:336:TYR:O	1:A:337:GLN:HB3	2.09	0.52
1:B:228:TYR:CE2	1:B:231:CYS:HA	2.45	0.52
1:B:212:ILE:HG22	1:B:213:VAL:N	2.25	0.52
1:B:157:ASN:ND2	1:B:159:THR:O	2.42	0.51
1:A:162:ASP:N	1:A:162:ASP:OD1	2.44	0.51
1:B:84:LEU:HD22	1:B:112:GLU:HG3	1.93	0.50
1:B:197:PRO:HD3	1:B:211:GLN:HA	1.93	0.50
1:B:36:VAL:HG12	2:B:400:NAD:O2B	2.10	0.50
1:B:11:GLY:HA3	4:B:364:HOH:O	2.11	0.50
1:B:136:LEU:HD23	1:B:248:ILE:HD12	1.92	0.50
1:A:212:ILE:HG22	1:A:213:VAL:N	2.26	0.50
1:B:105:GLY:O	1:B:109:ILE:HG13	2.12	0.49
1:B:151:ILE:HG12	1:B:241:ILE:HG12	1.95	0.49
1:A:68:ASP:OD2	1:A:68:ASP:N	2.46	0.49
1:A:106:CYS:O	1:A:110:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLY:O	1:B:15:LYS:HD3	2.12	0.49
1:A:306:TYR:O	1:A:310:VAL:HG23	2.12	0.49
1:A:145:ILE:HG21	1:A:248:ILE:HG23	1.94	0.48
1:B:196:TYR:CE1	1:B:208:LYS:HD2	2.48	0.48
1:A:318:ALA:HB2	1:A:325:GLU:CG	2.43	0.48
1:A:182:HIS:HB3	1:A:189:TYR:CZ	2.48	0.48
1:A:222:VAL:HG23	1:B:197:PRO:HB3	1.95	0.48
1:B:106:CYS:O	1:B:110:VAL:HG23	2.14	0.48
1:A:84:LEU:HD22	1:A:112:GLU:HG3	1.95	0.48
1:B:76:GLY:N	1:B:77:PRO:HD3	2.29	0.48
1:A:197:PRO:HD3	1:A:211:GLN:HA	1.95	0.48
1:A:310:VAL:HG11	1:A:329:LEU:CD2	2.44	0.48
1:A:182:HIS:HB2	1:A:187:ASP:O	2.14	0.48
1:A:228:TYR:CE2	1:A:231:CYS:HA	2.48	0.47
1:B:129:TYR:CE2	1:B:283:GLU:HG3	2.50	0.47
1:B:318:ALA:HB2	1:B:325:GLU:CG	2.41	0.47
1:A:196:TYR:CE1	1:A:208:LYS:HD2	2.50	0.47
1:B:306:TYR:O	1:B:310:VAL:HG23	2.16	0.47
1:A:62:LEU:HD13	1:A:86:ALA:HA	1.97	0.46
1:A:25:LEU:HB3	1:A:285:GLN:OE1	2.15	0.46
1:B:97:VAL:HG11	1:B:125:PHE:CE1	2.50	0.46
1:B:290:SER:O	1:B:294:LYS:HB2	2.15	0.46
1:A:290:SER:O	1:A:294:LYS:HB2	2.15	0.46
1:B:182:HIS:HB3	1:B:189:TYR:CZ	2.51	0.46
1:A:97:VAL:O	2:A:400:NAD:H1D	2.16	0.46
1:B:5:ILE:HG22	1:B:30:ILE:HD13	1.97	0.46
1:A:75:TRP:O	1:A:78:ALA:HB3	2.16	0.46
1:A:147:GLU:HB2	1:A:244:GLU:CD	2.35	0.46
1:B:13:ILE:HD12	1:B:13:ILE:HA	1.89	0.46
1:B:189:TYR:HD1	1:B:217:THR:HG22	1.81	0.46
1:B:155:HIS:HB2	1:B:177:GLU:OE2	2.16	0.45
1:B:147:GLU:HB2	1:B:244:GLU:OE1	2.17	0.45
1:B:55:TYR:CD2	1:B:61:LEU:HA	2.52	0.45
1:B:321:SER:OG	1:B:323:GLN:HB2	2.17	0.45
1:B:11:GLY:CA	4:B:364:HOH:O	2.64	0.45
1:B:151:ILE:HD13	1:B:181:LEU:HD22	1.99	0.45
1:A:105:GLY:O	1:A:109:ILE:HG13	2.16	0.45
1:B:7:VAL:HG21	1:B:18:ILE:HG12	1.99	0.45
1:A:75:TRP:CE3	1:A:77:PRO:HD2	2.52	0.45
1:A:182:HIS:CD2	4:A:352:HOH:O	2.65	0.45
1:B:68:ASP:OD2	1:B:68:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLY:N	1:B:77:PRO:CD	2.80	0.45
1:B:126:MET:SD	1:B:126:MET:N	2.89	0.45
1:B:76:GLY:O	1:B:101:THR:HG23	2.18	0.44
1:B:22:THR:HG22	1:B:23:ASN:OD1	2.18	0.44
1:A:157:ASN:ND2	1:A:159:THR:O	2.51	0.44
1:A:334:GLU:C	1:A:336:TYR:H	2.21	0.44
1:A:55:TYR:CD2	1:A:61:LEU:HA	2.52	0.44
1:A:126:MET:SD	1:A:126:MET:N	2.91	0.44
1:B:178:ILE:HG23	1:B:189:TYR:HE2	1.83	0.44
1:B:334:GLU:C	1:B:336:TYR:H	2.21	0.44
1:B:74:SER:O	1:B:75:TRP:O	2.35	0.44
1:B:77:PRO:C	1:B:79:HIS:H	2.21	0.44
1:B:182:HIS:HB2	1:B:187:ASP:O	2.17	0.44
1:B:121:VAL:HG11	1:B:302:ALA:HB2	2.00	0.43
1:B:55:TYR:OH	1:B:64:ASP:OD2	2.36	0.43
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.19	0.43
1:A:321:SER:OG	1:A:323:GLN:HB2	2.19	0.43
1:B:40:ALA:C	1:B:42:GLN:H	2.21	0.43
1:B:145:ILE:CG2	1:B:248:ILE:HG23	2.48	0.43
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.74	0.42
1:A:194:VAL:HG22	1:A:213:VAL:HG22	2.01	0.42
1:A:298:SER:O	1:A:299:GLY:O	2.37	0.42
1:B:194:VAL:HG22	1:B:213:VAL:HG22	2.01	0.42
1:B:203:ALA:HB2	1:B:209:ASP:HB3	2.01	0.42
1:A:203:ALA:HB2	1:A:209:ASP:HB3	2.01	0.42
1:B:176:HIS:HD2	4:B:366:HOH:O	2.01	0.42
1:B:312:THR:O	1:B:316:VAL:HG23	2.20	0.42
1:A:5:ILE:HG22	1:A:30:ILE:HD13	2.02	0.42
1:B:332:LYS:HA	1:B:333:PRO:HD3	1.91	0.42
1:B:272:TRP:CH2	2:B:400:NAD:H5N	2.55	0.41
1:B:310:VAL:HG21	1:B:329:LEU:HD22	2.01	0.41
1:B:166:THR:O	1:B:166:THR:HG22	2.20	0.41
1:B:171:VAL:HG22	1:B:312:THR:CG2	2.49	0.41
1:B:5:ILE:HG13	1:B:69:ALA:HB3	2.02	0.41
1:B:290:SER:OG	1:B:298:SER:HB2	2.20	0.41
1:A:55:TYR:OH	1:A:64:ASP:HB2	2.21	0.41
1:A:13:ILE:HD12	1:A:13:ILE:HA	1.94	0.41
1:A:151:ILE:HD13	1:A:181:LEU:HD22	2.03	0.41
1:A:7:VAL:HG21	1:A:18:ILE:CG1	2.51	0.41
1:A:244:GLU:OE1	1:B:201:LYS:HD3	2.20	0.41
1:B:77:PRO:HD2	1:B:78:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:O	1:B:117:GLY:N	2.54	0.41
1:B:116:VAL:HG11	1:B:120:LEU:HD11	2.02	0.41
1:A:74:SER:O	1:A:79:HIS:NE2	2.53	0.41
1:B:83:VAL:O	1:B:87:ILE:HG13	2.20	0.41
1:B:171:VAL:HG22	1:B:312:THR:HG21	2.02	0.41
1:B:177:GLU:HG3	4:B:354:HOH:O	2.21	0.41
1:A:166:THR:O	1:A:166:THR:HG22	2.21	0.41
1:B:7:VAL:HG21	1:B:18:ILE:CG1	2.50	0.40
1:A:202:ASN:HB2	1:A:230:ASN:HB3	2.03	0.40
1:B:74:SER:O	1:B:79:HIS:NE2	2.55	0.40
1:A:7:VAL:HG21	1:A:18:ILE:HG12	2.04	0.40
1:A:97:VAL:HG22	2:A:400:NAD:H71N	1.87	0.40
1:A:116:VAL:HG11	1:A:120:LEU:HD11	2.04	0.40
1:B:284:ILE:O	1:B:287:PHE:HB3	2.22	0.40
1:B:318:ALA:CB	1:B:325:GLU:HG2	2.47	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	335/344 (97%)	306 (91%)	24 (7%)	5 (2%)	10	15
1	B	335/344 (97%)	297 (89%)	30 (9%)	8 (2%)	6	7
All	All	670/688 (97%)	603 (90%)	54 (8%)	13 (2%)	8	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	TRP
1	A	294	LYS
1	A	299	GLY

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Mol	Chain	Res	Type
1	B	294	LYS
1	B	299	GLY
1	B	116	VAL
1	B	277	VAL
1	A	116	VAL
1	A	288	ILE
1	B	41	ALA
1	B	77	PRO
1	B	288	ILE
1	A	277	VAL

### 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	290/297 (98%)	266 (92%)	24 (8%)	11	16
1	B	290/297 (98%)	266 (92%)	24 (8%)	11	16
All	All	580/594 (98%)	532 (92%)	48 (8%)	11	16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	SER
1	A	36	VAL
1	A	38	GLN
1	A	58	ASP
1	A	66	ASN
1	A	67	VAL
1	A	68	ASP
1	A	71	LEU
1	A	81	SER
1	A	120	LEU
1	A	126	MET
1	A	159	THR

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Mol	Chain	Res	Type
1	A	162	ASP
1	A	163	ASN
1	A	170	VAL
1	A	218	LYS
1	A	224	ASN
1	A	231	CYS
1	A	265	SER
1	A	267	ASP
1	A	298	SER
1	A	321	SER
1	A	327	VAL
1	B	5	ILE
1	B	26	SER
1	B	36	VAL
1	B	38	GLN
1	B	58	ASP
1	B	66	ASN
1	B	67	VAL
1	B	68	ASP
1	B	75	TRP
1	B	81	SER
1	B	120	LEU
1	B	126	MET
1	B	159	THR
1	B	162	ASP
1	B	163	ASN
1	B	170	VAL
1	B	185	VAL
1	B	218	LYS
1	B	224	ASN
1	B	265	SER
1	B	267	ASP
1	B	298	SER
1	B	321	SER
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

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](#)

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
2	NAD	A	400	-	42,48,48	1.89	4 (9%)	50,73,73	1.19	4 (8%)
3	INS	A	801	-	12,12,12	0.76	0	18,18,18	1.03	0
2	NAD	B	400	-	42,48,48	1.79	4 (9%)	50,73,73	1.26	5 (10%)
3	INS	B	802	-	12,12,12	0.72	0	18,18,18	1.84	5 (27%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	400	-	-	5/26/62/62	0/5/5/5
3	INS	A	801	-	-	-	0/1/1/1
2	NAD	B	400	-	-	7/26/62/62	0/5/5/5
3	INS	B	802	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NAD	O7N-C7N	9.35	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NAD	O7N-C7N	8.87	1.41	1.24
2	A	400	NAD	C2A-N3A	4.41	1.39	1.32
2	B	400	NAD	C2A-N3A	4.15	1.38	1.32
2	A	400	NAD	C2A-N1A	2.99	1.39	1.33
2	B	400	NAD	C2A-N1A	2.76	1.39	1.33
2	A	400	NAD	C2N-N1N	2.65	1.38	1.35
2	B	400	NAD	C2N-N1N	2.39	1.37	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAD	N3A-C2A-N1A	-5.69	119.79	128.68
2	A	400	NAD	N3A-C2A-N1A	-5.53	120.03	128.68
3	B	802	INS	C5-C6-C1	-3.66	104.43	110.82
3	B	802	INS	C4-C3-C2	3.10	116.24	110.82
3	B	802	INS	C3-C2-C1	3.09	116.21	110.82
3	B	802	INS	C6-C5-C4	-3.07	105.47	110.82
2	A	400	NAD	PN-O3-PA	-2.55	124.08	132.83
2	B	400	NAD	PN-O3-PA	-2.52	124.19	132.83
2	B	400	NAD	C1B-N9A-C4A	-2.51	122.23	126.64
2	B	400	NAD	C3N-C7N-N7N	2.41	120.64	117.75
2	B	400	NAD	C4A-C5A-N7A	-2.28	107.03	109.40
3	B	802	INS	O6-C6-C1	2.27	115.59	110.35
2	A	400	NAD	C4A-C5A-N7A	-2.25	107.06	109.40
2	A	400	NAD	C6N-N1N-C2N	-2.24	119.94	121.97

There are no chirality outliers.

All (12) torsion outliers are listed below:

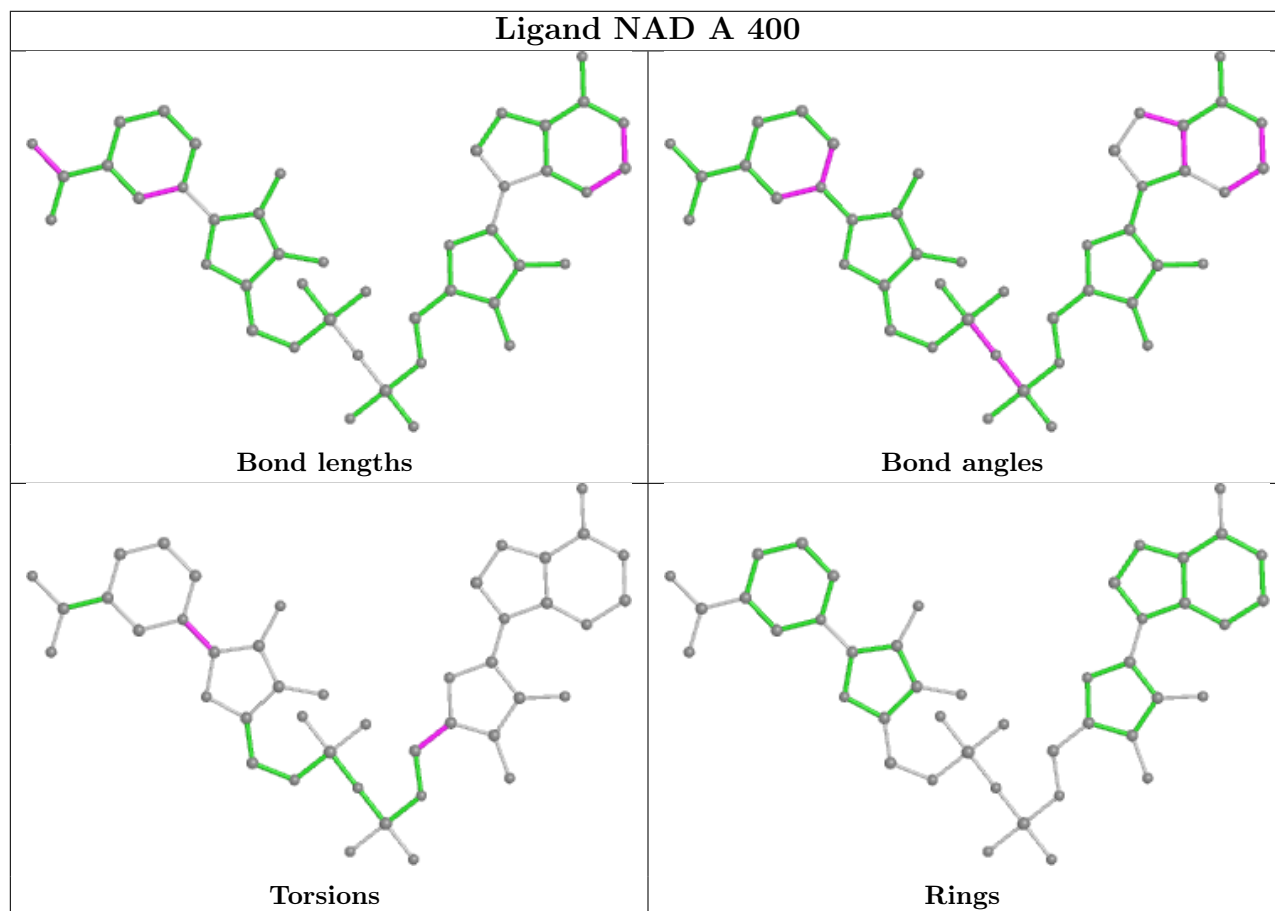
Mol	Chain	Res	Type	Atoms
2	A	400	NAD	O4D-C1D-N1N-C2N
2	A	400	NAD	O4D-C1D-N1N-C6N
2	A	400	NAD	C2D-C1D-N1N-C2N
2	A	400	NAD	C2D-C1D-N1N-C6N
2	B	400	NAD	C5B-O5B-PA-O2A
2	B	400	NAD	O4D-C1D-N1N-C6N
2	B	400	NAD	O4B-C4B-C5B-O5B
2	B	400	NAD	C3B-C4B-C5B-O5B
2	B	400	NAD	C5B-O5B-PA-O3
2	B	400	NAD	C5B-O5B-PA-O1A
2	A	400	NAD	O4B-C4B-C5B-O5B
2	B	400	NAD	C5D-O5D-PN-O1N

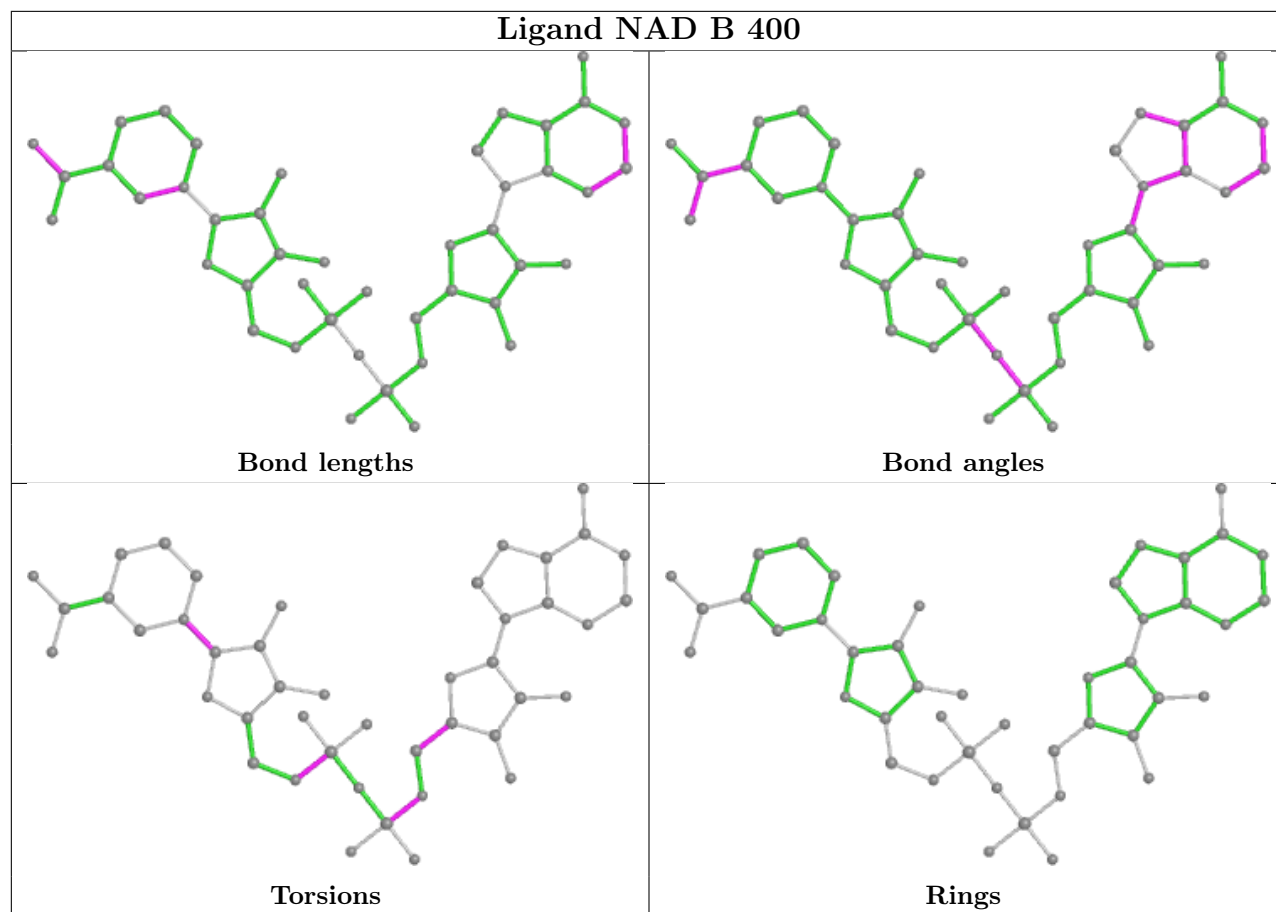
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NAD	4	0
2	B	400	NAD	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	337/344 (97%)	-0.20	9 (2%) 54 50	64, 99, 133, 165	0
1	B	337/344 (97%)	-0.23	6 (1%) 68 65	68, 102, 138, 164	0
All	All	674/688 (97%)	-0.22	15 (2%) 62 57	64, 101, 135, 165	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.5
1	A	6	GLY	3.4
1	A	118	LYS	3.3
1	A	1	MET	3.1
1	B	65	GLU	2.8
1	B	119	ARG	2.7
1	A	320	GLU	2.7
1	A	70	VAL	2.7
1	B	204	LEU	2.6
1	B	7	VAL	2.4
1	A	326	LYS	2.3
1	A	71	LEU	2.3
1	A	94	PHE	2.1
1	A	162	ASP	2.1
1	B	337	GLN	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

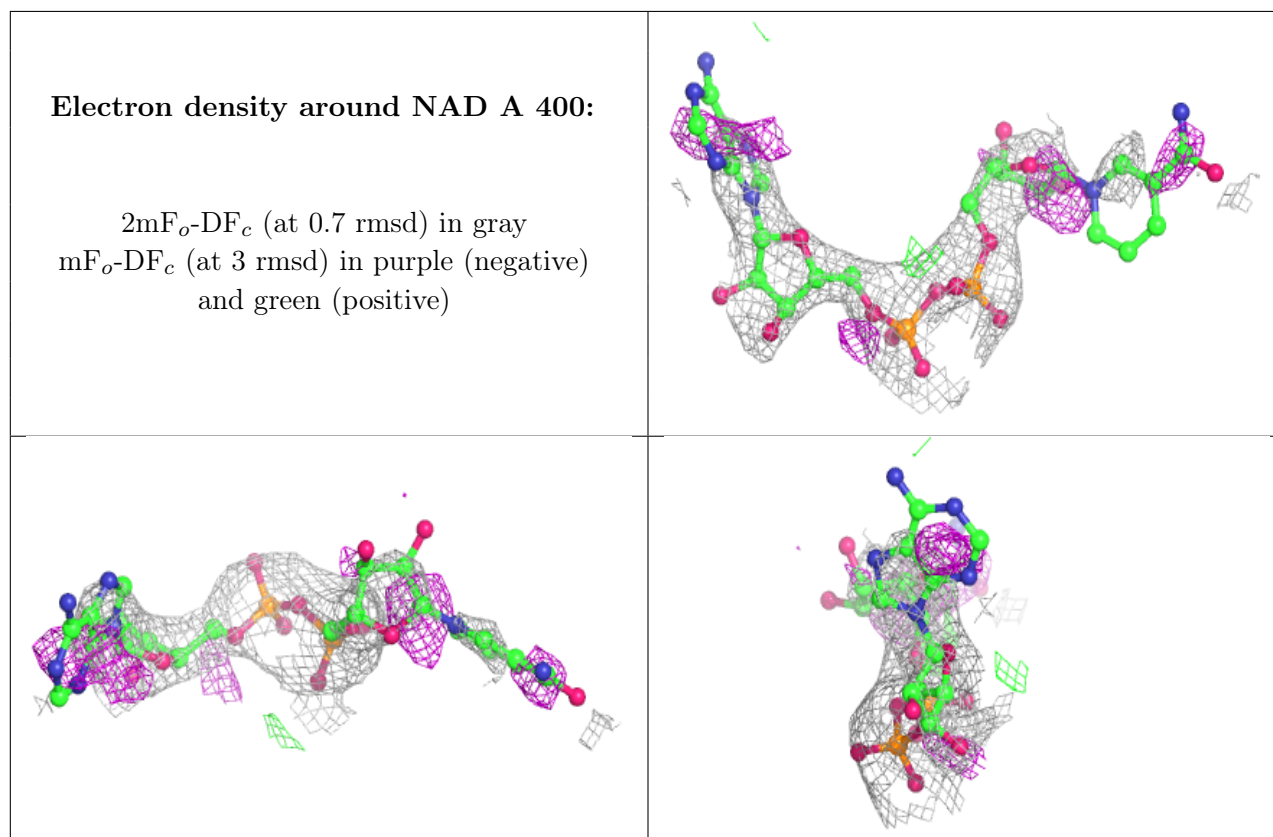
There are no monosaccharides in this entry.

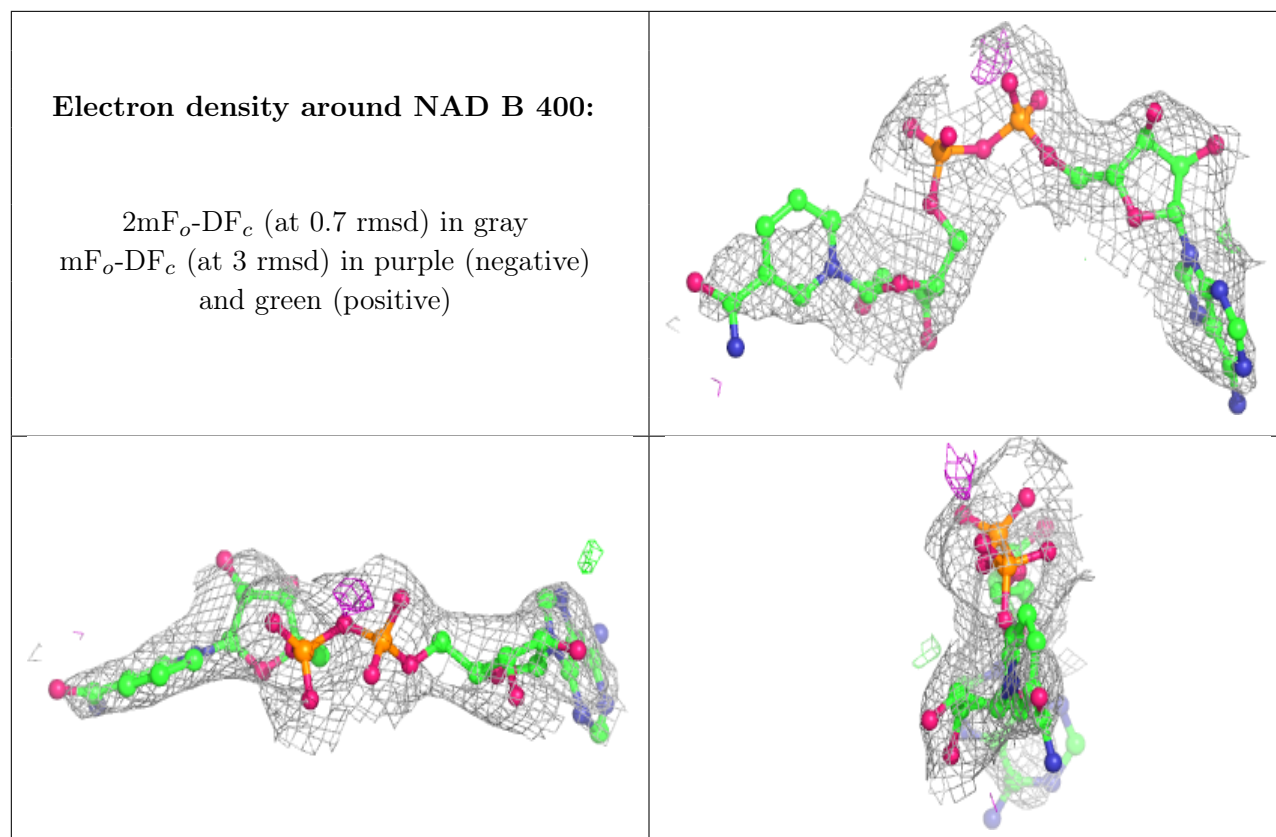
## 6.4 Ligands i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	INS	A	801	12/12	0.61	0.49	79,133,156,157	0
3	INS	B	802	12/12	0.84	0.43	110,127,161,163	0
2	NAD	A	400	44/44	0.92	0.39	98,137,152,154	0
2	NAD	B	400	44/44	0.93	0.17	87,134,149,157	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.