



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:45 AM UTC

PDB ID : 3BTS / pdb_00003bts
Title : Crystal structure of a ternary complex of the transcriptional repressor Gal80p (Gal80S0 [G301R]) and the acidic activation domain of Gal4p (aa 854-874) from *Saccharomyces cerevisiae* with NAD
Authors : Kumar, P.R.; Joshua-Tor, L.
Deposited on : 2007-12-30
Resolution : 2.70 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

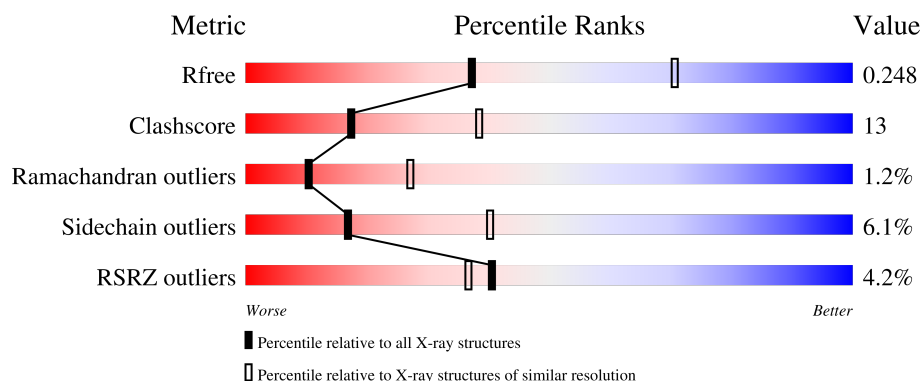
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	438	3% 63% 21% • 12%
1	B	438	3% 62% 23% • 11%
2	E	21	14% 43% 57%
2	F	21	24% 24% 76%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6432 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	3	0
			3050	1958	513	566	13			
1	B	390	Total	C	N	O	S	0	3	0
			3097	1990	519	576	12			

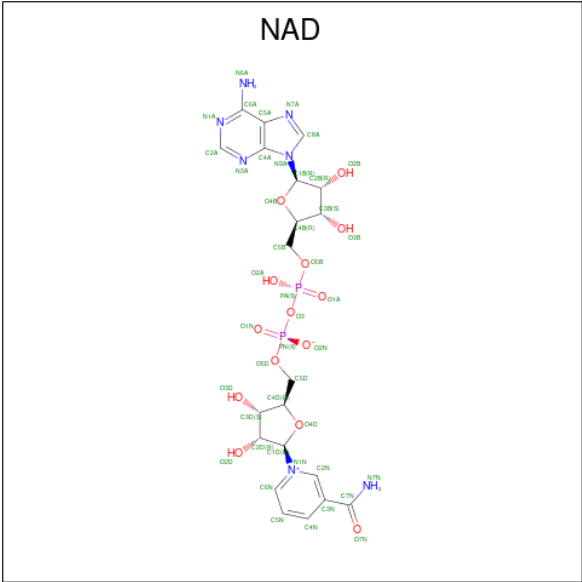
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P04387
A	-1	SER	-	expression tag	UNP P04387
A	0	HIS	-	expression tag	UNP P04387
A	301	ARG	GLY	engineered mutation	UNP P04387
B	-2	GLY	-	expression tag	UNP P04387
B	-1	SER	-	expression tag	UNP P04387
B	0	HIS	-	expression tag	UNP P04387
B	301	ARG	GLY	engineered mutation	UNP P04387

- Molecule 2 is a protein called Regulatory protein GAL4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			45	27	9	9			
2	F	5	Total	C	N	O	0	0	0
			25	15	5	5			

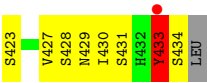
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



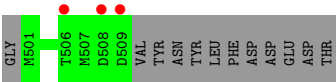
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

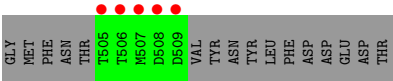
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	56	Total	O	0	0
			56	56		



● Molecule 2: Regulatory protein GAL4



● Molecule 2: Regulatory protein GAL4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.07Å 103.43Å 106.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 2.70 46.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.57-2.70) 99.4 (46.57-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.175 , 0.232 0.194 , 0.248	Depositor DCC
R_{free} test set	1395 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.42	0/3114	0.80	3/4214 (0.1%)
1	B	0.39	0/3164	0.81	3/4286 (0.1%)
2	E	0.36	0/44	0.57	0/60
2	F	0.26	0/24	0.50	0/32
All	All	0.40	0/6346	0.80	6/8592 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	TYR	N-CA-C	8.88	129.70	110.80
1	A	314	ILE	N-CA-C	5.53	116.54	109.30
1	A	20	VAL	N-CA-C	5.29	115.48	107.80
1	A	321	TYR	N-CA-C	5.17	114.96	108.45
1	B	193	SER	CA-C-N	5.00	126.09	119.84
1	B	193	SER	C-N-CA	5.00	126.09	119.84

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	3050	0	3046	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3097	0	3091	89	0
2	E	45	0	17	0	0
2	F	25	0	9	0	0
3	A	44	0	26	2	0
3	B	44	0	26	1	0
4	A	71	0	0	3	0
4	B	56	0	0	0	0
All	All	6432	0	6215	157	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 13.

All (157) 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:B:403:MET:HE1	1:B:434:SER:HB3	1.51	0.91
1:B:153:ARG:HD2	1:B:400:PRO:HG3	1.65	0.76
1:B:344:ASP:N	1:B:345:ALA:HA	2.04	0.72
1:A:158:ILE:HD11	1:A:314:ILE:HD12	1.72	0.70
1:A:26:ASN:HD22	1:A:27:ALA:N	1.90	0.69
1:B:277[B]:CYS:SG	1:B:279:PHE:HE2	2.15	0.69
1:B:26:ASN:HD22	1:B:27:ALA:N	1.92	0.68
1:B:277[B]:CYS:HG	1:B:279:PHE:HE2	1.41	0.68
1:A:277[B]:CYS:SG	1:A:279:PHE:HE2	2.15	0.68
1:A:26:ASN:ND2	1:A:28:ALA:H	1.92	0.68
1:B:26:ASN:ND2	1:B:28:ALA:H	1.92	0.68
1:B:126:ALA:HB1	1:B:131:GLN:HE21	1.59	0.67
1:B:26:ASN:HD22	1:B:26:ASN:C	2.03	0.67
1:A:126:ALA:HB1	1:A:131:GLN:HE21	1.61	0.66
1:B:97:ALA:HA	1:B:127:CYS:SG	2.35	0.66
1:A:291:ASN:HB2	1:A:308:ASP:HA	1.78	0.66
1:A:26:ASN:HD22	1:A:26:ASN:C	2.05	0.65
1:A:97:ALA:HA	1:A:127:CYS:SG	2.38	0.64
1:B:403:MET:CE	1:B:434:SER:HB3	2.26	0.63
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.80	0.63
1:A:301:ARG:HG2	1:A:321:TYR:HB3	1.80	0.62
1:A:305:LEU:HD22	1:A:314:ILE:HD13	1.80	0.62
1:B:277[B]:CYS:SG	1:B:279:PHE:CE2	2.91	0.62
1:B:155:SER:HB3	1:B:158:ILE:HG12	1.83	0.61
1:A:277[B]:CYS:SG	1:A:279:PHE:CE2	2.93	0.61
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.83	0.60
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.37	0.59
1:B:146:THR:C	1:B:147:ILE:HG13	2.28	0.59
1:A:158:ILE:CD1	1:A:314:ILE:HD12	2.33	0.58
1:B:303:LEU:C	1:B:303:LEU:HD23	2.28	0.58
1:B:191:VAL:HA	1:B:242:LEU:HD22	1.85	0.58
1:A:194:PRO:HB3	1:A:196:TYR:CE1	2.38	0.58
1:A:131:GLN:O	1:A:135:ILE:HG13	2.04	0.58
1:A:14:ASN:C	1:A:16:ALA:H	2.12	0.57
1:A:90:ILE:HD13	1:A:106:LEU:HD21	1.85	0.57
1:A:146:THR:C	1:A:147:ILE:HG13	2.31	0.56
1:B:427:VAL:HB	1:B:430:ILE:HD12	1.87	0.56
1:A:261[A]:HIS:HE1	1:B:174:ASN:OD1	1.89	0.56
1:A:56:LYS:HB3	1:A:58:GLU:OE1	2.05	0.56
1:B:347:LYS:NZ	1:B:347:LYS:HB3	2.21	0.55
1:B:136:TYR:CE2	1:B:434:SER:HB2	2.42	0.55
1:A:227:SER:HA	1:A:428:SER:HB3	1.89	0.54
1:B:90:ILE:HD13	1:B:106:LEU:HD21	1.89	0.54
1:A:59:THR:HG22	4:A:499:HOH:O	2.08	0.54
1:B:58:GLU:H	1:B:58:GLU:CD	2.16	0.54
1:A:58:GLU:H	1:A:58:GLU:CD	2.16	0.54
1:B:313:GLU:HA	1:B:314:ILE:O	2.08	0.54
1:B:131:GLN:O	1:B:135:ILE:HG13	2.09	0.53
1:B:160:ARG:NH2	1:B:353[B]:TYR:HE1	2.08	0.52
1:A:263:LEU:HD13	1:B:265:GLN:HB2	1.91	0.52
1:B:65:GLN:HG3	1:B:66:ARG:N	2.25	0.52
1:B:397:GLU:CD	1:B:397:GLU:H	2.18	0.52
1:B:382:ILE:HD12	1:B:385:LEU:HD11	1.91	0.52
1:A:147:ILE:HD13	1:A:372:ILE:CD1	2.39	0.51
1:A:410:ARG:HB3	1:A:435:LEU:CD1	2.40	0.51
1:A:397:GLU:H	1:A:397:GLU:CD	2.18	0.51
1:B:56:LYS:HB3	1:B:58:GLU:OE1	2.11	0.51
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.92	0.51
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.92	0.51
1:B:264:PHE:HB3	1:B:277[B]:CYS:HB3	1.92	0.50
1:B:24:GLY:HA2	3:B:436:NAD:O4B	2.12	0.49
1:B:26:ASN:HD22	1:B:28:ALA:H	1.60	0.49
1:B:290:LYS:O	1:B:291:ASN:C	2.56	0.49
1:A:305:LEU:HB3	1:A:314:ILE:HD13	1.95	0.49
1:A:214:THR:O	1:A:217:ILE:HG12	2.13	0.48
1:A:26:ASN:HD22	1:A:28:ALA:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:HG3	1:A:66:ARG:N	2.27	0.48
1:A:234:PHE:HE2	1:B:267:THR:CG2	2.26	0.48
1:A:225:TYR:HB3	4:A:442:HOH:O	2.12	0.48
1:A:290:LYS:O	1:A:291:ASN:C	2.55	0.48
1:B:189:ARG:O	1:B:242:LEU:HA	2.14	0.48
1:B:214:THR:O	1:B:217:ILE:HG12	2.14	0.48
1:B:227:SER:HA	1:B:428:SER:HB3	1.96	0.48
1:B:123:TRP:CG	1:B:124:ALA:HA	2.49	0.48
1:A:423:SER:HA	1:B:423:SER:HA	1.96	0.48
1:A:234:PHE:HE2	1:B:267:THR:HG22	1.79	0.48
1:A:82:ALA:O	1:A:110:SER:HA	2.14	0.47
1:A:123:TRP:CG	1:A:124:ALA:HA	2.49	0.47
1:B:234:PHE:HB2	1:B:261[A]:HIS:HB2	1.95	0.47
1:B:219:GLN:HE21	1:B:225:TYR:HA	1.80	0.47
1:A:264:PHE:HB3	1:A:277[B]:CYS:HB3	1.96	0.47
1:A:427:VAL:O	1:A:430:ILE:HG12	2.14	0.47
1:B:403:MET:HE1	1:B:434:SER:CB	2.34	0.47
1:B:308:ASP:O	1:B:309:ALA:C	2.56	0.46
1:A:234:PHE:HB2	1:A:261[A]:HIS:HB2	1.98	0.46
1:B:242:LEU:HD12	1:B:252:GLN:HB3	1.98	0.46
1:A:152:GLY:C	1:A:154:LYS:H	2.23	0.46
1:B:244:ASP:HB3	1:B:250:LEU:HD21	1.97	0.46
1:A:265:GLN:HB2	1:B:263:LEU:HD13	1.97	0.46
1:A:169:TYR:O	1:A:301:ARG:HD2	2.16	0.45
1:A:244:ASP:HB3	1:A:250:LEU:HD21	1.97	0.45
1:A:26:ASN:ND2	1:A:26:ASN:C	2.74	0.45
1:A:232:MET:HE3	1:B:265:GLN:HG3	1.98	0.45
1:A:172:ASP:O	1:A:298:GLY:HA2	2.17	0.45
1:A:136:TYR:CZ	1:A:403:MET:HE2	2.52	0.45
1:B:273:VAL:HA	1:B:274:PRO:HD3	1.85	0.45
1:A:299:THR:HG22	1:B:187:TYR:HE1	1.81	0.45
1:A:234:PHE:CE2	1:B:267:THR:CG2	2.99	0.45
1:B:147:ILE:HG12	1:B:399:PHE:CE2	2.51	0.45
1:A:219:GLN:HE21	1:A:225:TYR:HA	1.82	0.45
1:A:148:ILE:HG12	1:A:405:ALA:HB2	1.99	0.45
1:B:430:ILE:O	1:B:431:SER:CB	2.65	0.44
1:A:299:THR:HG22	1:B:187:TYR:CE1	2.52	0.44
1:A:273:VAL:HA	1:A:274:PRO:HD3	1.80	0.44
1:B:82:ALA:O	1:B:110:SER:HA	2.17	0.44
1:A:228:ARG:HA	1:A:425:LEU:O	2.17	0.44
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:O	1:B:193:SER:C	2.60	0.43
1:A:242:LEU:HD12	1:A:252:GLN:HB3	2.00	0.43
1:B:175:SER:C	1:B:176:ILE:HG13	2.43	0.43
1:B:403:MET:HE1	1:B:433:TYR:O	2.18	0.43
1:B:403:MET:CE	1:B:433:TYR:O	2.66	0.43
1:B:408:LEU:O	1:B:412:ILE:HG12	2.17	0.43
1:A:24:GLY:HA2	3:A:436:NAD:O4B	2.17	0.43
1:B:200:ILE:HG12	1:B:201:GLY:N	2.32	0.43
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.54	0.43
1:A:200:ILE:HG12	1:A:201:GLY:N	2.33	0.43
1:B:433:TYR:O	1:B:434:SER:HB3	2.19	0.43
1:A:430:ILE:HG22	1:A:435:LEU:HD12	2.00	0.43
1:A:234:PHE:CE2	1:B:267:THR:HG22	2.54	0.43
1:B:46:GLN:HB3	1:B:377:PHE:HE1	1.84	0.42
1:A:303:LEU:HD21	1:A:317:LEU:HD11	2.00	0.42
1:B:148:ILE:HG12	1:B:405:ALA:HB2	2.00	0.42
1:B:155:SER:HB3	1:B:158:ILE:CG1	2.48	0.42
1:B:170:ILE:HA	1:B:301:ARG:HB2	2.01	0.42
1:B:357:ASN:HD22	1:B:357:ASN:HA	1.62	0.42
1:A:153:ARG:CD	1:A:400:PRO:HG3	2.50	0.42
1:B:120:PHE:CD1	1:B:120:PHE:C	2.96	0.42
1:B:136:TYR:CZ	1:B:403:MET:HE2	2.54	0.42
1:A:16:ALA:HA	1:A:17:PRO:HD3	1.90	0.42
1:A:120:PHE:C	1:A:120:PHE:CD1	2.97	0.42
1:A:261[A]:HIS:CE1	1:B:174:ASN:OD1	2.71	0.42
1:A:153:ARG:HD2	1:A:400:PRO:HG3	2.02	0.42
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.83	0.42
1:B:429:ASN:O	1:B:430:ILE:C	2.63	0.42
1:A:303:LEU:C	1:A:303:LEU:HD23	2.45	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.81	0.41
1:B:392:GLN:HB2	1:B:399:PHE:O	2.19	0.41
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.91	0.41
1:A:147:ILE:HD13	1:A:372:ILE:HD13	2.01	0.41
1:A:402:LEU:HD12	1:A:402:LEU:HA	1.89	0.41
1:B:113:ASN:HA	1:B:114:PRO:HD3	1.89	0.41
1:A:265:GLN:NE2	4:A:445:HOH:O	2.48	0.41
1:B:27:ALA:HB2	1:B:67:LEU:CD2	2.50	0.41
1:B:193:SER:HA	1:B:194:PRO:HD3	1.79	0.41
1:B:151:GLN:H	1:B:151:GLN:HG3	1.49	0.41
1:A:75:PHE:HA	1:A:76:PRO:HD3	1.76	0.41
1:B:190:PRO:C	1:B:192:LYS:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB2	1:A:67:LEU:CD2	2.51	0.40
1:A:197:ILE:O	1:A:197:ILE:HG13	2.21	0.40
1:B:154:LYS:HD3	1:B:154:LYS:HA	1.90	0.40
1:B:176:ILE:HD13	1:B:218:LEU:HD11	2.03	0.40
1:B:265:GLN:HA	1:B:275:VAL:O	2.21	0.40
1:A:122:GLU:OE1	3:A:436:NAD:H2N	2.21	0.40
1:A:31:TRP:CZ2	1:A:35:THR:HG21	2.56	0.40
1:B:158:ILE:CD1	1:B:217:ILE:HD12	2.52	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	377/438 (86%)	358 (95%)	16 (4%)	3 (1%)	16	37
1	B	385/438 (88%)	360 (94%)	19 (5%)	6 (2%)	7	20
2	E	7/21 (33%)	4 (57%)	3 (43%)	0	100	100
2	F	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
All	All	772/918 (84%)	724 (94%)	39 (5%)	9 (1%)	10	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	ILE
1	A	282	GLY
1	A	291	ASN
1	A	434	SER
1	B	291	ASN
1	B	433	TYR
1	B	381	LYS

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Mol	Chain	Res	Type
1	B	192	LYS
1	B	194	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	335/376 (89%)	314 (94%)	21 (6%)	16	39
1	B	339/376 (90%)	319 (94%)	20 (6%)	18	42
All	All	674/752 (90%)	633 (94%)	41 (6%)	17	40

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

Mol	Chain	Res	Type
1	A	59	THR
1	A	65	GLN
1	A	67	LEU
1	A	79	GLU
1	A	150	LEU
1	A	197	ILE
1	A	200	ILE
1	A	252	GLN
1	A	260	ASP
1	A	283	LYS
1	A	308	ASP
1	A	321	TYR
1	A	347	LYS
1	A	356	ARG
1	A	362	VAL
1	A	378	ASN
1	A	388	GLN
1	A	390	VAL
1	A	397	GLU
1	A	402	LEU
1	A	425	LEU

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Mol	Chain	Res	Type
1	B	26	ASN
1	B	59	THR
1	B	65	GLN
1	B	67	LEU
1	B	79	GLU
1	B	151	GLN
1	B	181	ASN
1	B	200	ILE
1	B	252	GLN
1	B	260	ASP
1	B	303	LEU
1	B	313	GLU
1	B	320	TYR
1	B	347	LYS
1	B	349	ILE
1	B	357	ASN
1	B	361	ILE
1	B	365	ILE
1	B	397	GLU
1	B	402	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	71	ASN
1	A	131	GLN
1	A	167	GLN
1	A	174	ASN
1	A	181	ASN
1	A	219	GLN
1	A	265	GLN
1	A	366	HIS
1	A	426	ASN
1	A	429	ASN
1	B	26	ASN
1	B	46	GLN
1	B	71	ASN
1	B	131	GLN
1	B	167	GLN
1	B	213	HIS
1	B	219	GLN

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Mol	Chain	Res	Type
1	B	357	ASN
1	B	370	GLN
1	B	426	ASN

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 oligosaccharides 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	$\# Z > 2$
3	NAD	A	436	-	46,48,48	1.71	4 (8%)	64,73,73	1.54	8 (12%)
3	NAD	B	436	-	46,48,48	1.75	6 (13%)	64,73,73	1.55	9 (14%)

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	436	-	-	6/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	436	-	-	10/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	436	NAD	O7N-C7N	9.19	1.41	1.24
3	B	436	NAD	O7N-C7N	9.16	1.41	1.24
3	B	436	NAD	C2A-N1A	2.68	1.38	1.33
3	B	436	NAD	C2A-N3A	2.63	1.38	1.33
3	A	436	NAD	C2A-N1A	2.61	1.38	1.33
3	A	436	NAD	C2A-N3A	2.47	1.38	1.33
3	B	436	NAD	PN-O3	2.38	1.62	1.59
3	B	436	NAD	PA-O3	2.31	1.62	1.59
3	B	436	NAD	C8A-N7A	2.21	1.35	1.31
3	A	436	NAD	C8A-N7A	2.10	1.35	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	436	NAD	N3A-C2A-N1A	-5.40	120.40	128.58
3	A	436	NAD	N3A-C2A-N1A	-5.20	120.71	128.58
3	A	436	NAD	C5A-C4A-N3A	-4.41	120.64	126.72
3	B	436	NAD	C5A-C4A-N3A	-4.32	120.77	126.72
3	A	436	NAD	N9A-C8A-N7A	-3.85	108.47	113.94
3	B	436	NAD	N9A-C8A-N7A	-3.73	108.64	113.94
3	A	436	NAD	C5A-N7A-C8A	3.44	108.86	103.45
3	B	436	NAD	C2A-N3A-C4A	3.28	119.85	111.83
3	B	436	NAD	C5A-N7A-C8A	3.28	108.61	103.45
3	A	436	NAD	C2A-N3A-C4A	3.27	119.83	111.83
3	B	436	NAD	N3A-C4A-N9A	2.79	131.91	127.17
3	A	436	NAD	N3A-C4A-N9A	2.78	131.90	127.17
3	A	436	NAD	C4A-C5A-N7A	-2.55	107.66	110.58
3	B	436	NAD	C4A-C5A-N7A	-2.38	107.86	110.58
3	B	436	NAD	O2A-PA-O3	2.19	113.20	107.27
3	A	436	NAD	C3B-C2B-C1B	2.04	105.33	101.46
3	B	436	NAD	C3B-C2B-C1B	2.02	105.28	101.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

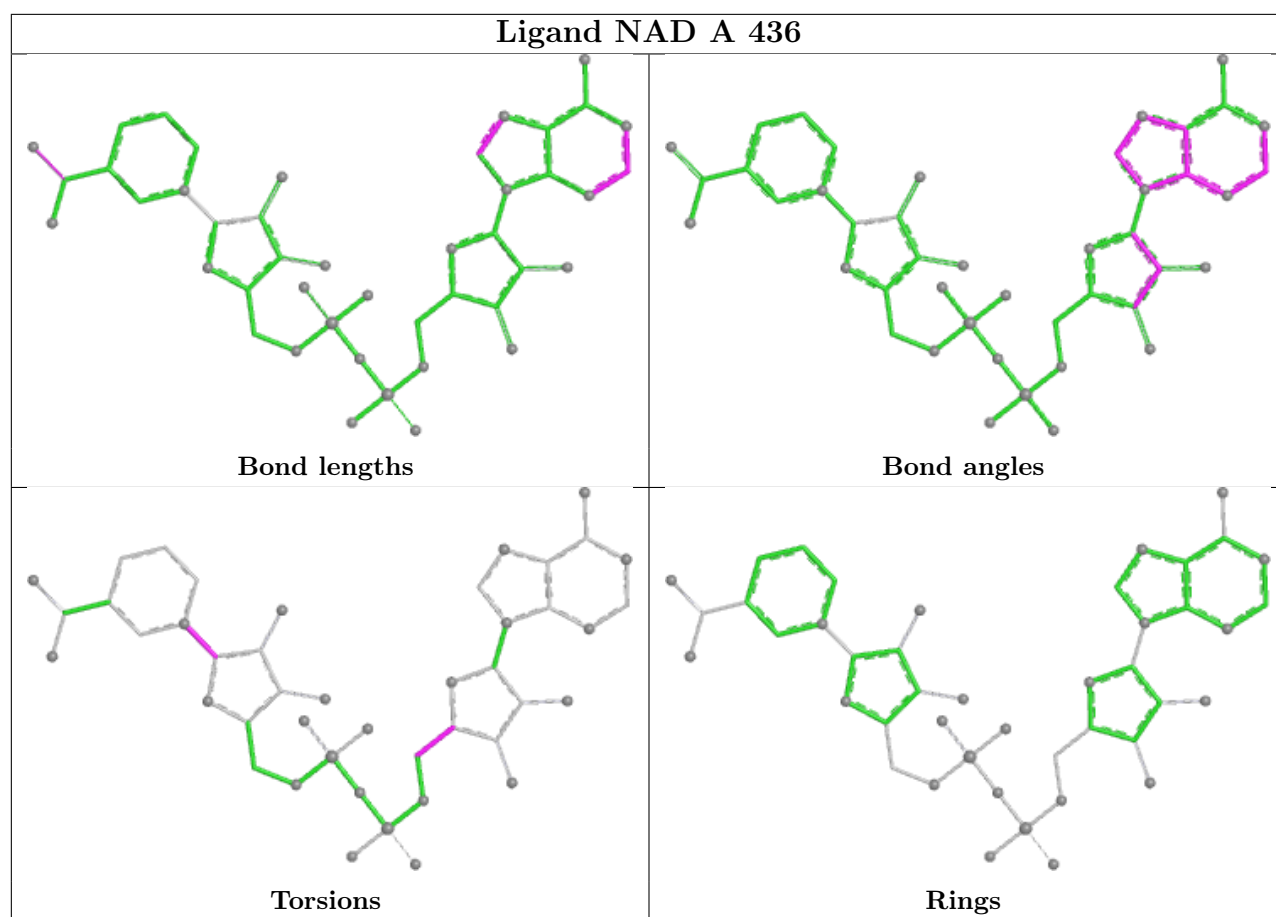
Mol	Chain	Res	Type	Atoms
3	A	436	NAD	O4D-C1D-N1N-C2N
3	A	436	NAD	O4D-C1D-N1N-C6N
3	A	436	NAD	C2D-C1D-N1N-C2N
3	A	436	NAD	C2D-C1D-N1N-C6N
3	B	436	NAD	C5B-O5B-PA-O1A
3	B	436	NAD	C5B-O5B-PA-O3
3	B	436	NAD	O4D-C1D-N1N-C2N
3	B	436	NAD	O4D-C1D-N1N-C6N
3	B	436	NAD	C2D-C1D-N1N-C2N
3	B	436	NAD	C2D-C1D-N1N-C6N
3	A	436	NAD	O4B-C4B-C5B-O5B
3	A	436	NAD	C3B-C4B-C5B-O5B
3	B	436	NAD	C2B-C1B-N9A-C8A
3	B	436	NAD	C5B-O5B-PA-O2A
3	B	436	NAD	C2B-C1B-N9A-C4A
3	B	436	NAD	O4B-C1B-N9A-C8A

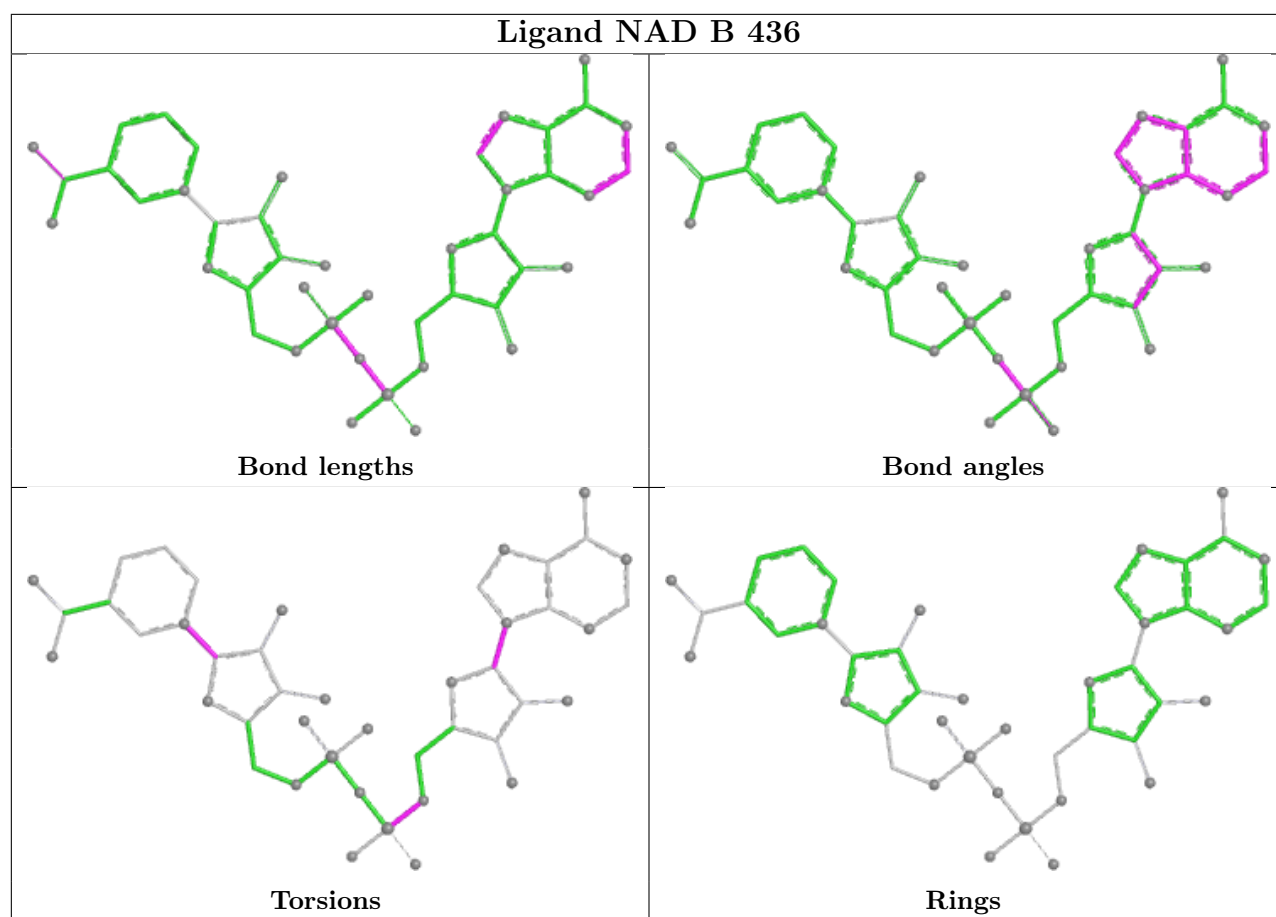
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	436	NAD	2	0
3	B	436	NAD	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	384/438 (87%)	-0.03	14 (3%)	46 42	15, 59, 112, 153	3 (0%)
1	B	390/438 (89%)	0.15	11 (2%)	55 51	18, 67, 123, 197	3 (0%)
2	E	9/21 (42%)	2.20	3 (33%)	1 1	76, 111, 146, 159	0
2	F	5/21 (23%)	4.06	5 (100%)	0 0	150, 153, 158, 166	0
All	All	788/918 (85%)	0.11	33 (4%)	40 37	15, 63, 122, 197	6 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	508	ASP	5.5
2	F	508	ASP	5.4
2	F	505	THR	4.2
2	F	509	ASP	4.1
1	B	282	GLY	3.8
1	B	385	LEU	3.6
2	E	509	ASP	3.5
1	A	346	GLY	3.5
2	F	506	THR	3.4
1	A	387	SER	3.4
1	B	386	PRO	3.4
1	A	250	LEU	3.3
1	A	435	LEU	3.1
2	F	507	MET	3.1
1	A	388	GLN	3.0
1	B	433	TYR	3.0
2	E	506	THR	3.0
1	B	353[A]	TYR	2.8
1	B	397	GLU	2.7
1	A	379	THR	2.5
1	B	74	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	386	PRO	2.4
1	A	433	TYR	2.4
1	B	247	GLY	2.3
1	A	15	ALA	2.3
1	B	196	TYR	2.2
1	B	383	PRO	2.2
1	A	251	GLY	2.2
1	B	15	ALA	2.1
1	A	246	ARG	2.1
1	A	55	PRO	2.1
1	A	312	ALA	2.0
1	A	420	MET	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

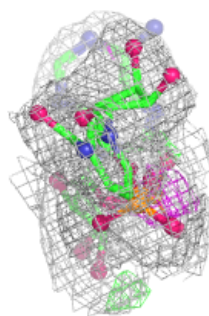
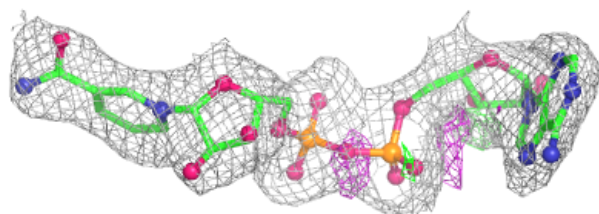
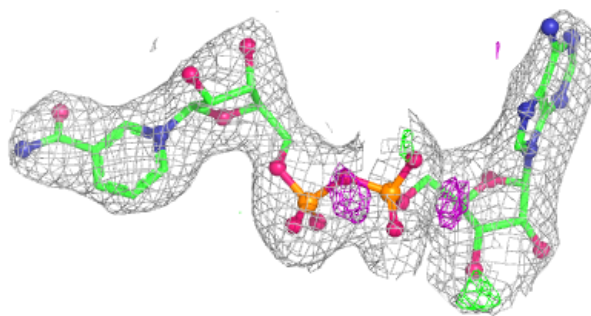
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	436	44/44	0.90	0.11	58,78,121,138	0
3	NAD	A	436	44/44	0.95	0.09	39,53,92,111	0

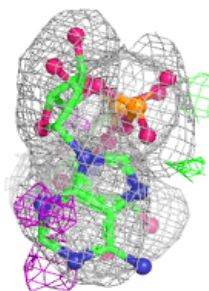
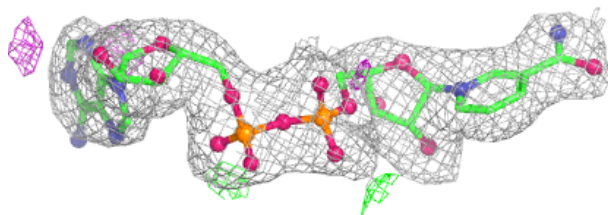
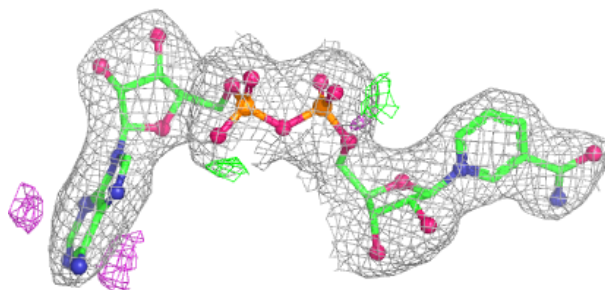
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 436:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD A 436:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.