Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 05:19 PM EDT

PDB ID	:	3BTS
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 (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 (i)) were used in the production of this report:

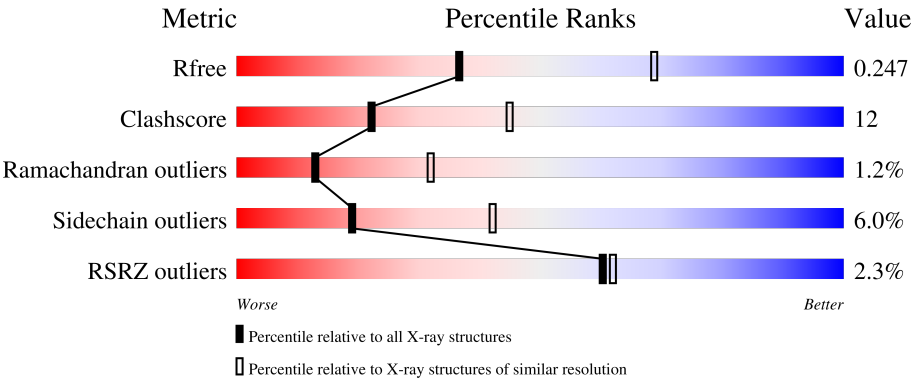
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	% 64% 21% · 12%
1	B	438	3% 63% 23% · 11%
2	E	21	43% 57%
2	F	21	5% 24% 76%

2 Entry composition (i)

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			

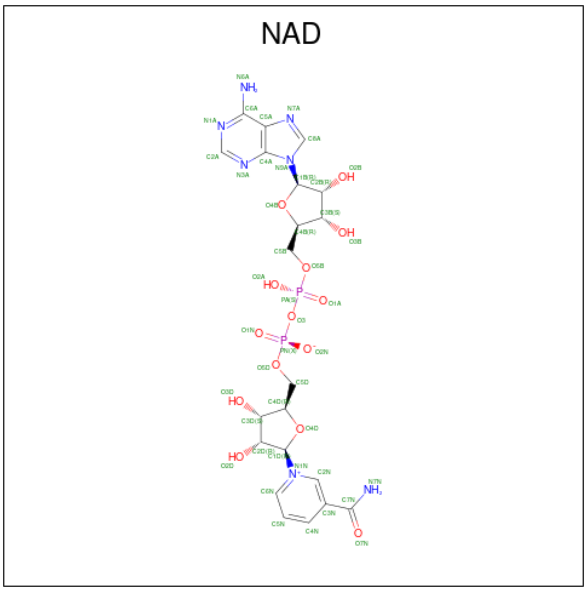
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is water.

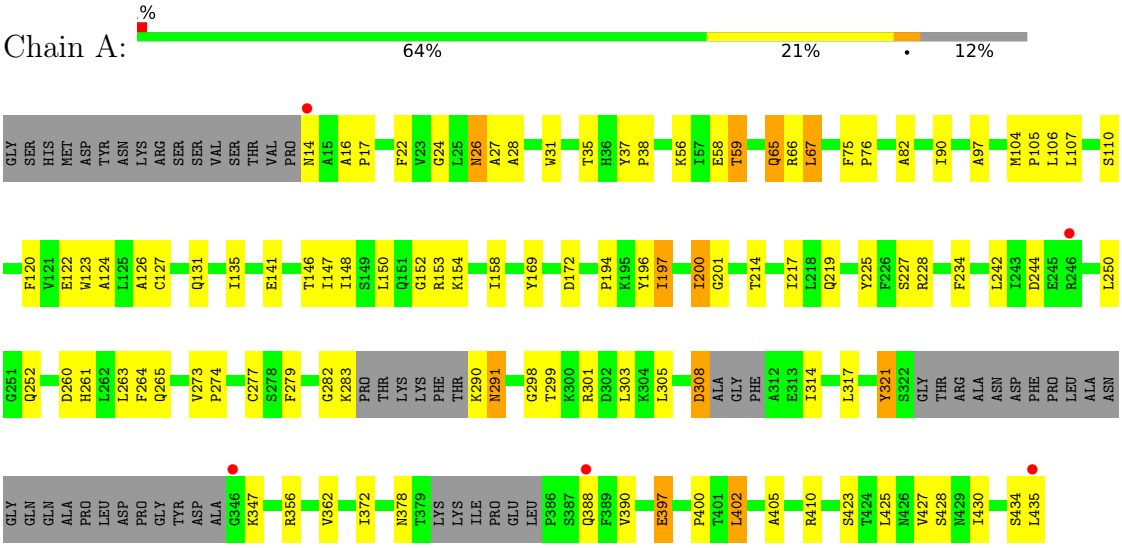
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	56	Total	O	0	0
			56	56		

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 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.

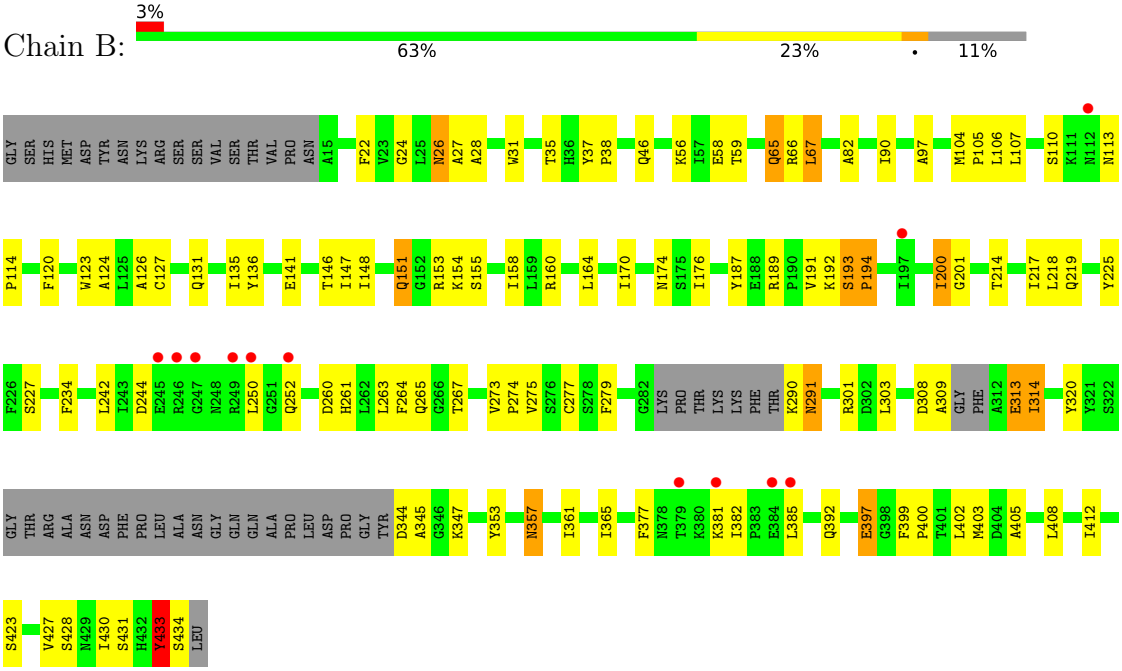
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain A:



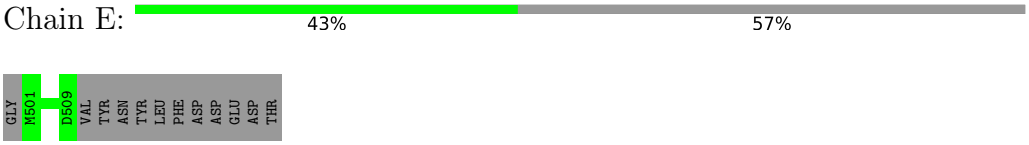
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain B:



• Molecule 2: Regulatory protein GAL4

Chain E:



• Molecule 2: Regulatory protein GAL4

Chain F:

4 Data and refinement statistics (i)

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 46.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.57-2.70) 99.4 (46.55-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.175 , 0.232 0.194 , 0.247	Depositor DCC
R_{free} test set	1395 reflections (5.11%)	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)	0.29 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.32	0/3114	0.52	0/4214
1	B	0.31	0/3164	0.52	1/4286 (0.0%)
2	E	0.23	0/44	0.27	0/60
2	F	0.21	0/24	0.26	0/32
All	All	0.32	0/6346	0.52	1/8592 (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	B	433	TYR	N-CA-C	6.93	129.70	111.00

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	3050	0	3046	76	0
1	B	3097	0	3091	82	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	71	0	0	3	0
4	B	56	0	0	0	0
All	All	6432	0	6215	147	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 12.

All (147) 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:153:ARG:HD2	1:B:400:PRO:HG3	1.65	0.76
1:B:403:MET:HE1	1:B:434:SER:HB3	1.69	0.74
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: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:B:403:MET:HE3	1:B:433:TYR:O	1.96	0.66
1:A:291:ASN:HB2	1:A:308:ASP:HA	1.78	0.66
1:B:403:MET:CE	1:B:434:SER:HB3	2.26	0.66
1:A:97:ALA:HA	1:A:127:CYS:SG	2.38	0.64
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:26:ASN:HD22	1:B:26:ASN:C	2.03	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
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.83	0.60
1:A:26:ASN:HD22	1:A:26:ASN:C	2.05	0.60
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.37	0.59
1:A:158:ILE:CD1	1:A:314:ILE:HD12	2.33	0.58
1:B:191:VAL:HA	1:B:242:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:ILE:HD13	1:A:106:LEU:HD21	1.85	0.57
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:146:THR:C	1:B:147:ILE:HG13	2.28	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:303:LEU:C	1:B:303:LEU:HD23	2.28	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:A:14:ASN:C	1:A:16:ALA:H	2.12	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:A:146:THR:C	1:A:147:ILE:HG13	2.31	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: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:A:65:GLN:HG3	1:A:66:ARG:N	2.27	0.49
1:B:58:GLU:H	1:B:58:GLU:CD	2.16	0.49
1:A:58:GLU:H	1:A:58:GLU:CD	2.16	0.49
1:B:26:ASN:HD22	1:B:28:ALA:H	1.60	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:397:GLU:CD	1:B:397:GLU:H	2.18	0.47
1:A:397:GLU:H	1:A:397:GLU:CD	2.18	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: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:B:403:MET:HE1	1:B:434:SER:CB	2.44	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:172:ASP:O	1:A:298:GLY:HA2	2.17	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:290:LYS:O	1:A:291:ASN:C	2.55	0.44
1:B:290:LYS:O	1:B:291:ASN:C	2.56	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
1:A:242:LEU:HD12	1:A:252:GLN:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:16:ALA:HA	1:A:17:PRO:HD3	1.90	0.42
1:A:152:GLY:C	1:A:154:LYS:H	2.23	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:308:ASP:O	1:B:309:ALA:C	2.56	0.42
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:B:403:MET:CE	1:B:433:TYR:O	2.66	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: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:26:ASN:ND2	1:A:26:ASN:C	2.74	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%)	19 43
1	B	385/438 (88%)	360 (94%)	19 (5%)	6 (2%)	9 24
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%)	13 32

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
1	B	192	LYS
1	B	194	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	335/376 (89%)	313 (93%)	22 (7%)	16 38
1	B	339/376 (90%)	321 (95%)	18 (5%)	22 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	674/752 (90%)	634 (94%)	40 (6%)	19 43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	26	ASN
1	A	59	THR
1	A	65	GLN
1	A	67	LEU
1	A	120	PHE
1	A	141	GLU
1	A	150	LEU
1	A	197	ILE
1	A	200	ILE
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	B	22	PHE
1	B	26	ASN
1	B	59	THR
1	B	65	GLN
1	B	67	LEU
1	B	120	PHE
1	B	141	GLU
1	B	151	GLN
1	B	193	SER
1	B	200	ILE
1	B	260	ASP
1	B	313	GLU
1	B	320	TYR
1	B	357	ASN
1	B	361	ILE

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Mol	Chain	Res	Type
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	65	GLN
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	252	GLN
1	A	265	GLN
1	A	366	HIS
1	A	376	HIS
1	A	426	ASN
1	A	429	ASN
1	B	26	ASN
1	B	46	GLN
1	B	65	GLN
1	B	71	ASN
1	B	131	GLN
1	B	151	GLN
1	B	167	GLN
1	B	219	GLN
1	B	265	GLN
1	B	357	ASN
1	B	370	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	$\#\|Z\| > 2$
3	NAD	B	436	-	42,48,48	1.75	3 (7%)	50,73,73	1.21	3 (6%)
3	NAD	A	436	-	42,48,48	1.74	3 (7%)	50,73,73	1.18	3 (6%)

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	B	436	-	-	8/26/62/62	0/5/5/5
3	NAD	A	436	-	-	6/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	436	NAD	O7N-C7N	8.93	1.41	1.24
3	B	436	NAD	O7N-C7N	8.90	1.41	1.24
3	B	436	NAD	C2A-N3A	4.04	1.38	1.32
3	A	436	NAD	C2A-N3A	3.86	1.38	1.32
3	B	436	NAD	C2A-N1A	2.58	1.38	1.33
3	A	436	NAD	C2A-N1A	2.50	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	436	NAD	N3A-C2A-N1A	-5.30	120.40	128.68
3	A	436	NAD	N3A-C2A-N1A	-5.10	120.71	128.68
3	A	436	NAD	C3B-C2B-C1B	2.89	105.33	100.98
3	B	436	NAD	C3B-C2B-C1B	2.86	105.28	100.98
3	A	436	NAD	PN-O3-PA	-2.78	123.28	132.83
3	B	436	NAD	PN-O3-PA	-2.21	125.23	132.83

There are no chirality outliers.

All (14) 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	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	C5B-O5B-PA-O3
3	B	436	NAD	C5B-O5B-PA-O2A
3	B	436	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

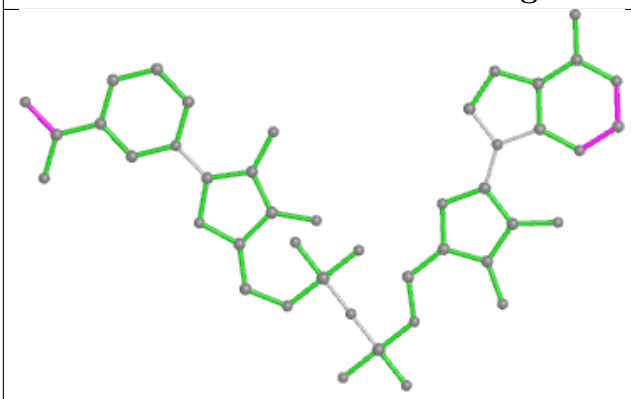
2 monomers are involved in 3 short contacts:

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

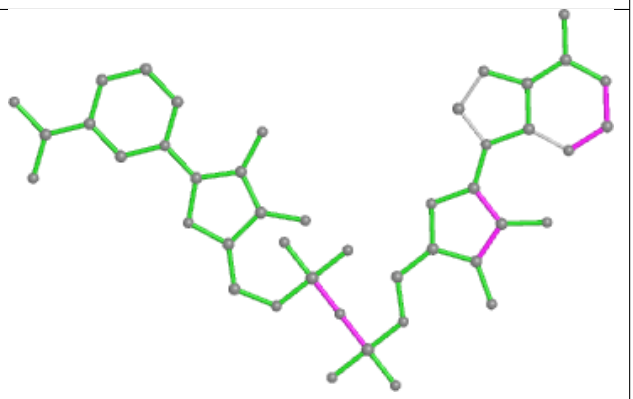
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

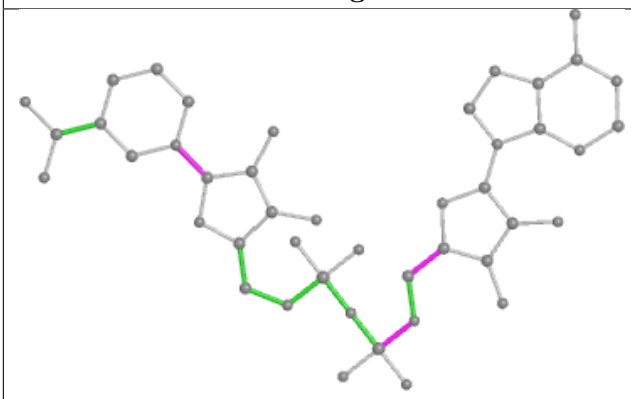
Ligand NAD B 436



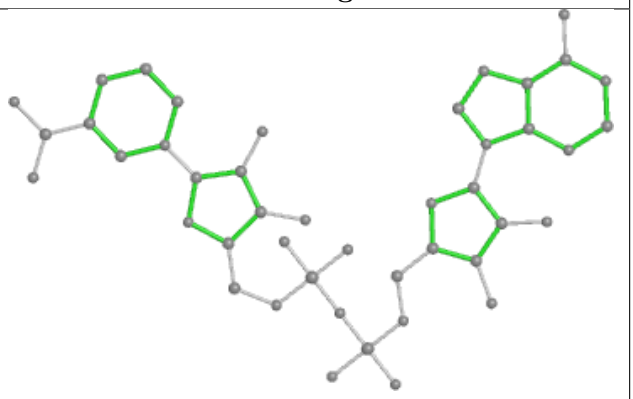
Bond lengths



Bond angles

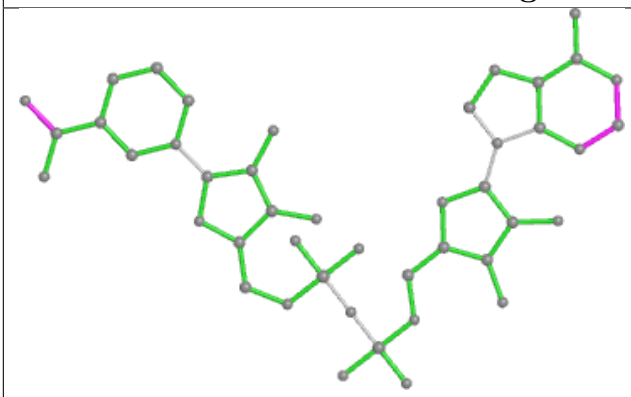


Torsions

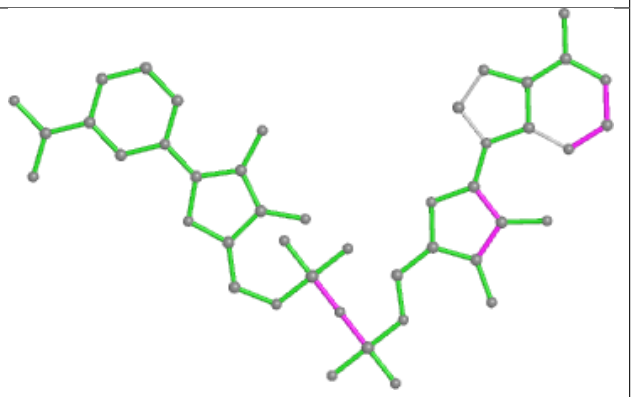


Rings

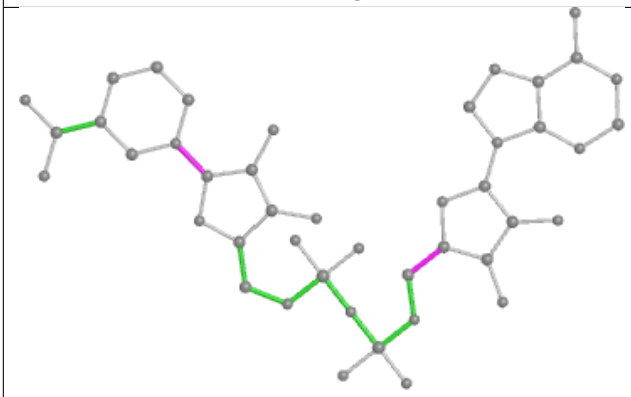
Ligand NAD A 436



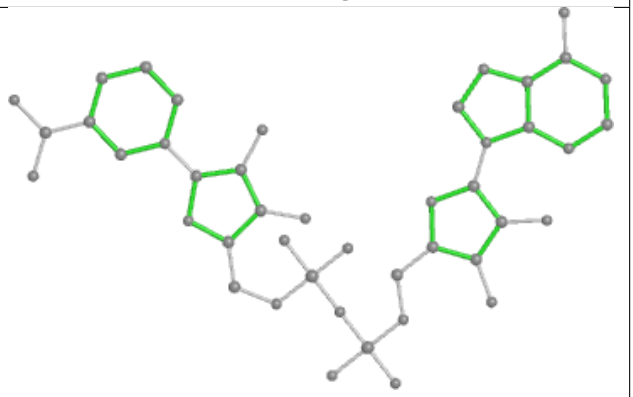
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.15	5 (1%) 77 78	27, 59, 112, 153	0
1	B	390/438 (89%)	0.08	12 (3%) 49 49	32, 67, 123, 197	0
2	E	9/21 (42%)	0.26	0 100 100	76, 111, 146, 159	0
2	F	5/21 (23%)	1.39	1 (20%) 1 0	150, 153, 158, 166	0
All	All	788/918 (85%)	-0.02	18 (2%) 60 62	27, 63, 122, 197	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	GLY	5.5
1	B	245	GLU	4.4
1	A	435	LEU	3.2
1	B	252	GLN	3.0
1	B	379	THR	3.0
1	B	250	LEU	2.9
1	A	14	ASN	2.8
1	B	246	ARG	2.6
1	A	346	GLY	2.5
1	A	388	GLN	2.5
1	B	197	ILE	2.4
2	F	506	THR	2.4
1	B	384	GLU	2.4
1	B	381	LYS	2.2
1	B	385	LEU	2.1
1	B	112	ASN	2.0
1	B	249	ARG	2.0
1	A	246	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

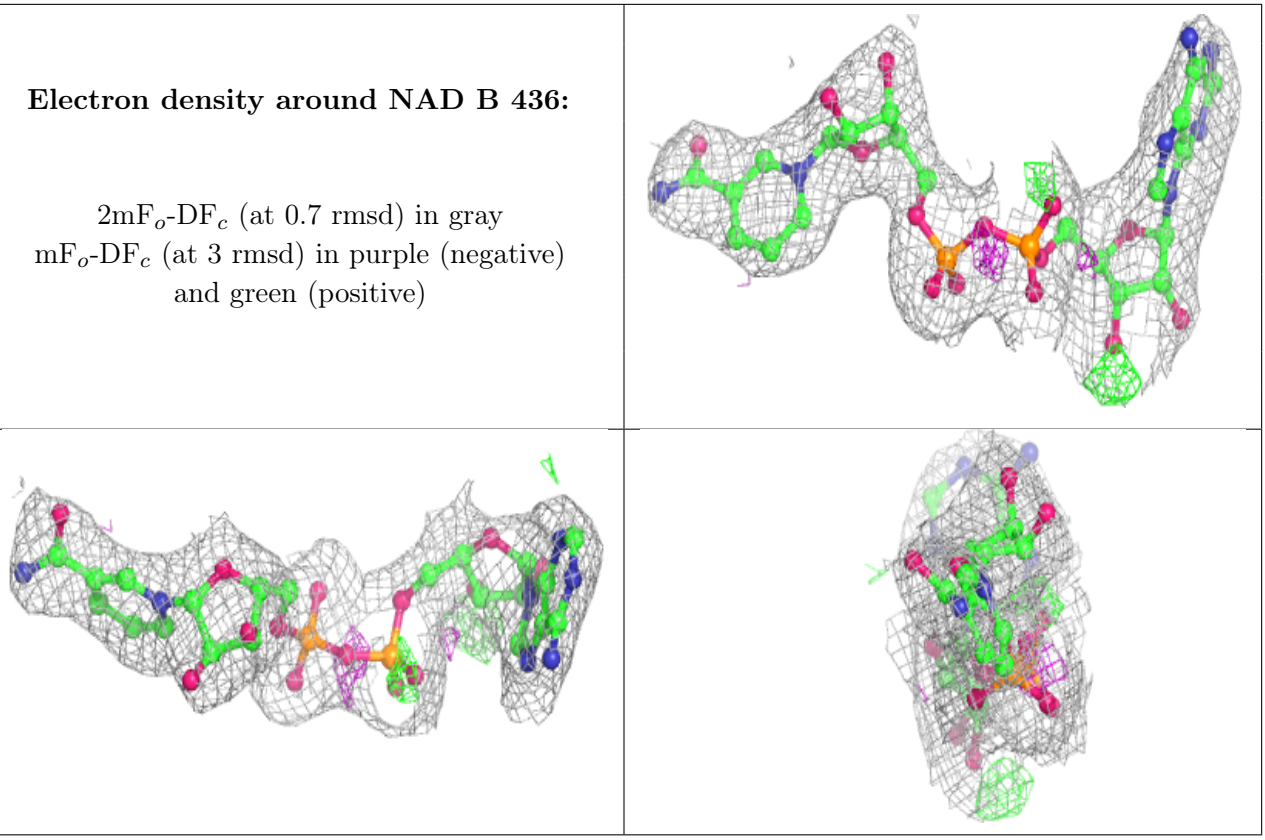
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	NAD	B	436	44/44	0.92	0.15	58,78,121,138	0
3	NAD	A	436	44/44	0.97	0.16	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.

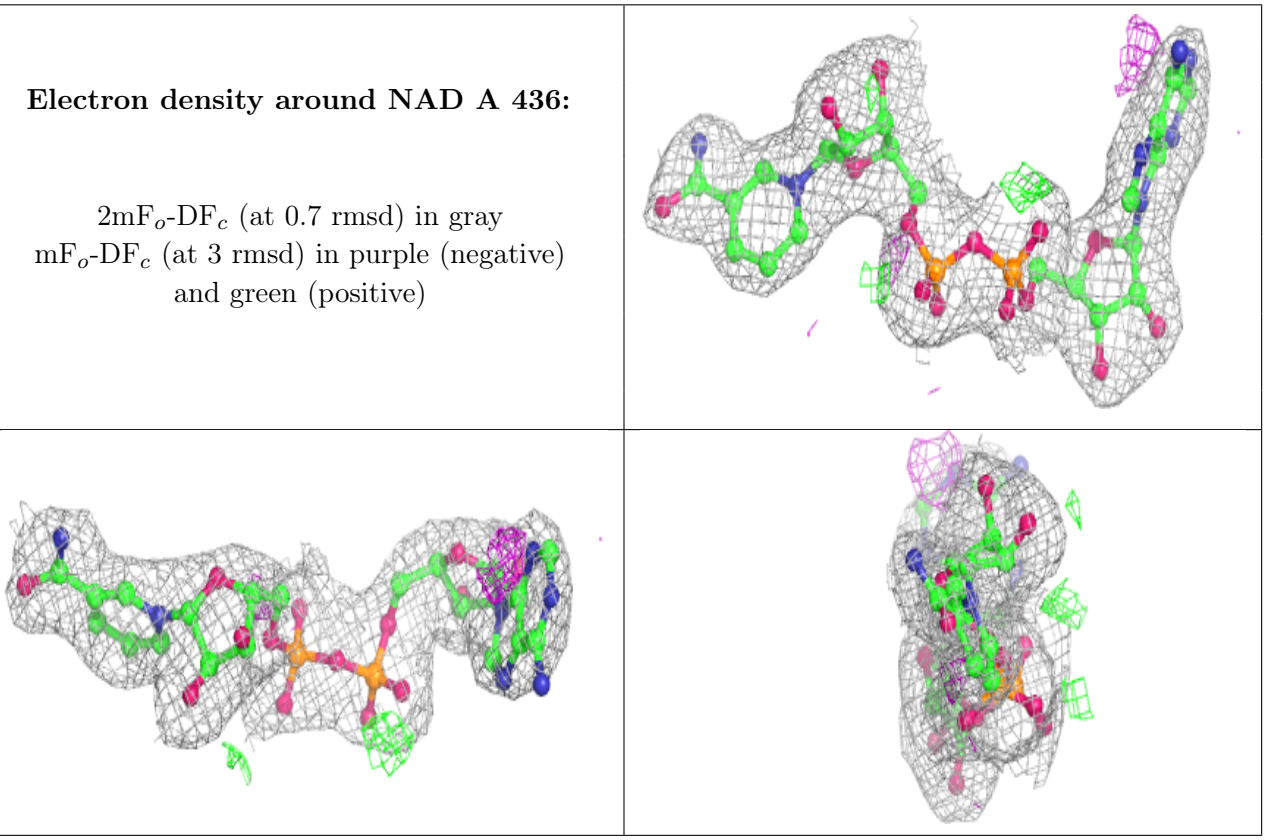
Electron density around NAD B 436:

$2mF_o$-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.