Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 08:55 AM UTC

PDB ID	:	4WNC / pdb_00004wnc
Title	:	Crystal structure of human wild-type GAPDH at 1.99 angstroms resolution
Authors	:	Garcin, E.D.
Deposited on	:	2014-10-11
Resolution	:	1.99 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:

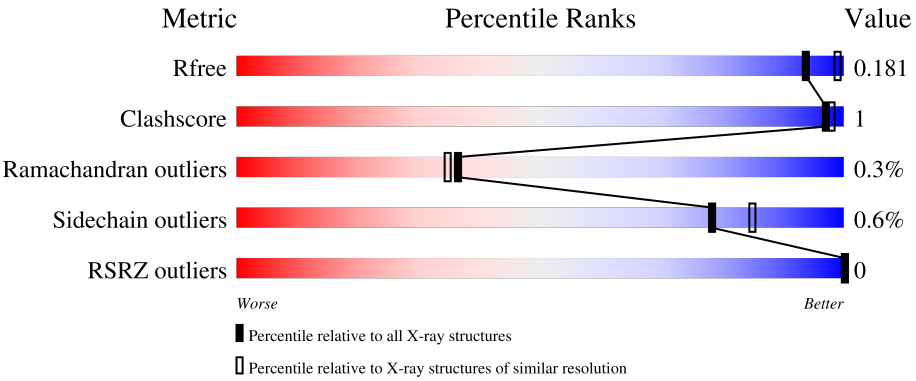
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	335	97%
1	B	335	96%
1	C	335	98%
1	D	335	97%
1	E	335	96%

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Mol	Chain	Length	Quality of chain
1	F	335	97%
1	G	335	97%
1	O	335	97%

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
2	NAD	E	401	X	-	-	-

2 Entry composition (i)

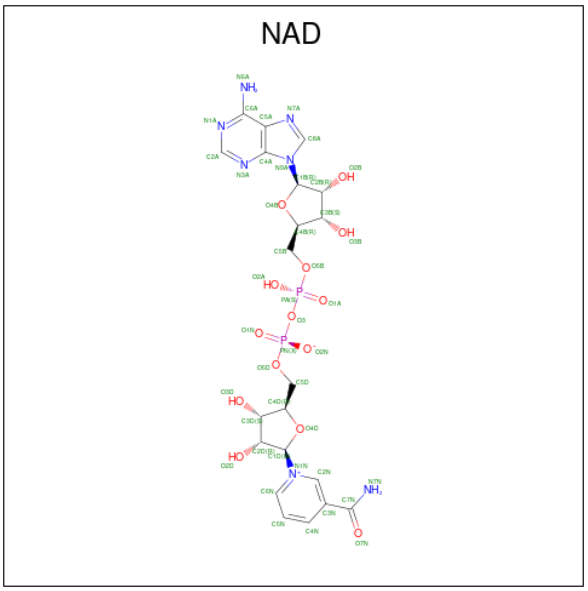
There are 5 unique types of molecules in this entry. The entry contains 43182 atoms, of which 20297 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	O	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	A	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	B	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	C	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	D	333	Total	C	H	N	O	S	0	1	0
			5048	1599	2519	439	478	13			
1	E	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	F	333	Total	C	H	N	O	S	0	1	0
			5043	1598	2517	438	477	13			
1	G	333	Total	C	H	N	O	S	0	0	0
			5037	1596	2514	438	477	12			

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

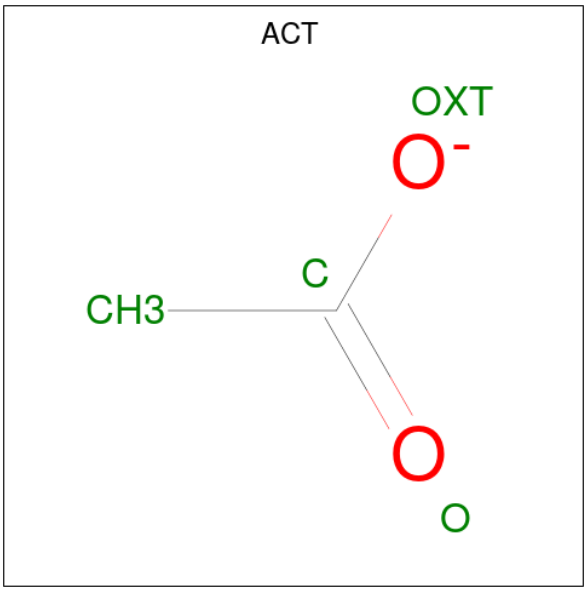


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	O	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	2	Total	Zn	0	0
			2	2		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total C H O 7 2 3 2	0	0
4	C	1	Total C H O 7 2 3 2	0	0

- Molecule 5 is water.

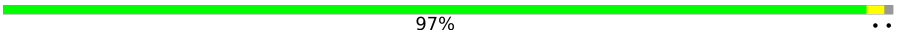
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	320	Total O 320 320	0	0
5	A	352	Total O 352 352	0	0
5	B	336	Total O 336 336	0	0
5	C	289	Total O 289 289	0	0
5	D	322	Total O 322 322	0	0
5	E	277	Total O 277 277	0	0
5	F	246	Total O 246 246	0	0
5	G	257	Total O 257 257	0	0

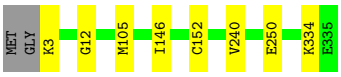
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Glyceraldehyde-3-phosphate dehydrogenase

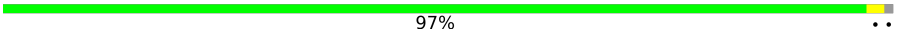
Chain O:





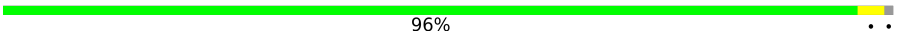
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



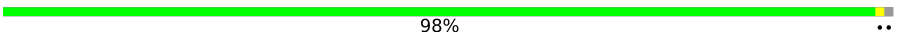
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:



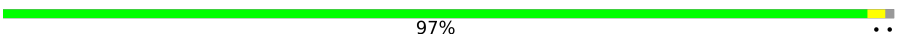
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:



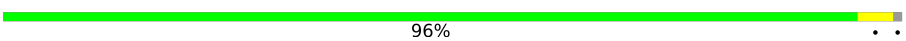
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

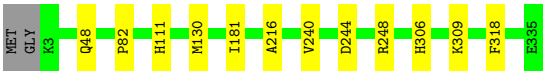
Chain D:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

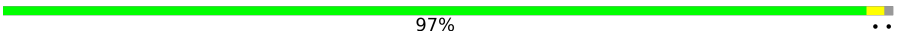
Chain E:

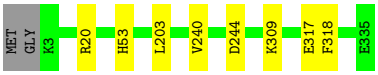




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

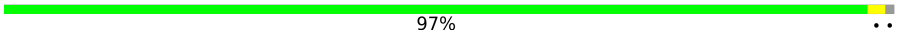
Chain F:





• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.54Å 81.42Å 147.80Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	49.36 – 1.99 49.36 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.36-1.99) 99.4 (49.36-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.139 , 0.179 0.141 , 0.181	Depositor DCC
R_{free} test set	2001 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	43182	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, ACT, ZN

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	0.59	0/2579	0.75	0/3489
1	B	0.60	0/2579	0.76	0/3489
1	C	0.56	0/2579	0.73	0/3489
1	D	0.58	0/2579	0.73	0/3489
1	E	0.58	0/2579	0.74	0/3489
1	F	0.54	0/2579	0.72	0/3489
1	G	0.54	0/2573	0.72	0/3481
1	O	0.58	0/2579	0.74	0/3489
All	All	0.57	0/20626	0.73	0/27904

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	2526	2517	2529	5	0
1	B	2526	2517	2529	7	0
1	C	2526	2517	2529	3	0
1	D	2529	2519	2528	6	0
1	E	2526	2517	2529	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2526	2517	2529	5	0
1	G	2523	2514	2524	4	0
1	O	2526	2517	2529	3	0
2	A	44	26	25	2	0
2	B	44	26	25	2	0
2	C	44	26	25	0	0
2	D	44	26	23	1	0
2	E	44	26	24	1	0
2	O	44	26	24	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	O	1	0	0	0	0
4	C	4	3	3	0	0
4	O	4	3	3	0	0
5	A	352	0	0	1	0
5	B	336	0	0	2	0
5	C	289	0	0	2	0
5	D	322	0	0	3	0
5	E	277	0	0	3	0
5	F	246	0	0	0	0
5	G	257	0	0	3	0
5	O	320	0	0	1	0
All	All	22885	20297	20378	37	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 1.

All (37) 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)
2:E:401:NAD:O4D	2:E:401:NAD:C1D	1.64	1.26
1:O:3:LYS:N	5:O:723:HOH:O	2.17	0.78
1:C:244:ASP:OD2	5:C:648:HOH:O	2.05	0.73
1:D:3:LYS:N	5:D:727:HOH:O	2.21	0.72
1:G:3:LYS:NZ	5:G:401:HOH:O	2.23	0.71
1:G:244:ASP:OD2	5:G:514:HOH:O	2.13	0.66
1:E:244:ASP:OD2	5:E:661:HOH:O	2.13	0.66
1:E:306:HIS:ND1	5:E:764:HOH:O	2.30	0.64
1:E:48:GLN:NE2	5:E:636:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LYS:NZ	5:D:501:HOH:O	2.35	0.56
1:B:215:LYS:NZ	5:B:827:HOH:O	2.40	0.55
1:C:48:GLN:NE2	5:C:656:HOH:O	2.35	0.53
1:G:84:LYS:NZ	5:G:616:HOH:O	2.37	0.51
1:A:130:MET:HE1	1:A:216:ALA:HB1	1.93	0.50
1:D:251:LYS:NZ	5:D:502:HOH:O	2.44	0.50
1:O:105:MET:HE2	1:O:146:ILE:HB	1.94	0.49
1:D:130:MET:HE1	1:D:216:ALA:HB1	1.96	0.47
1:F:244:ASP:C	1:F:244:ASP:OD1	2.58	0.47
1:B:3:LYS:N	5:B:503:HOH:O	2.48	0.46
1:B:248:ARG:HD2	1:C:248:ARG:HD2	1.98	0.46
1:B:203:LEU:HG	1:F:203:LEU:HG	2.00	0.43
1:F:244:ASP:OD1	1:F:309:LYS:HG3	2.18	0.43
1:E:130:MET:HE1	1:E:216:ALA:HB1	2.00	0.43
1:B:181:ILE:HD11	1:F:203:LEU:HD13	2.00	0.43
1:F:53:HIS:NE2	1:F:317:GLU:OE1	2.46	0.42
1:G:244:ASP:OD1	1:G:309:LYS:HG3	2.19	0.42
1:A:3:LYS:NZ	5:A:501:HOH:O	2.35	0.41
1:O:12:GLY:HA3	2:O:401:NAD:O5B	2.20	0.41
1:A:248:ARG:HD2	1:E:248:ARG:HD2	2.02	0.41
1:A:36:PRO:HD3	2:A:401:NAD:C2A	2.50	0.41
1:A:12:GLY:HA3	2:A:401:NAD:O5B	2.20	0.41
1:B:36:PRO:HD3	2:B:401:NAD:C2A	2.51	0.41
1:E:244:ASP:OD1	1:E:309:LYS:HG3	2.21	0.41
1:E:82:PRO:HB3	1:E:111:HIS:CE1	2.56	0.40
1:D:12:GLY:HA3	2:D:401:NAD:O5B	2.21	0.40
1:B:12:GLY:HA3	2:B:401:NAD:O5B	2.21	0.40
1:D:203:LEU:HD22	1:E:181:ILE:HD13	2.04	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	332/335 (99%)	319 (96%)	12 (4%)	1 (0%)	36	35
1	B	332/335 (99%)	320 (96%)	10 (3%)	2 (1%)	21	17
1	C	332/335 (99%)	318 (96%)	13 (4%)	1 (0%)	36	35
1	D	332/335 (99%)	320 (96%)	11 (3%)	1 (0%)	36	35
1	E	332/335 (99%)	318 (96%)	13 (4%)	1 (0%)	36	35
1	F	332/335 (99%)	321 (97%)	10 (3%)	1 (0%)	36	35
1	G	331/335 (99%)	322 (97%)	8 (2%)	1 (0%)	36	35
1	O	332/335 (99%)	320 (96%)	11 (3%)	1 (0%)	36	35
All	All	2655/2680 (99%)	2558 (96%)	88 (3%)	9 (0%)	36	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	240	VAL
1	A	240	VAL
1	C	240	VAL
1	D	240	VAL
1	E	240	VAL
1	F	240	VAL
1	G	240	VAL
1	B	240	VAL
1	B	169	GLY

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	271/271 (100%)	271 (100%)	0	100	100
1	B	271/271 (100%)	270 (100%)	1 (0%)	84	89
1	C	271/271 (100%)	268 (99%)	3 (1%)	65	73
1	D	271/271 (100%)	271 (100%)	0	100	100
1	E	271/271 (100%)	270 (100%)	1 (0%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	271/271 (100%)	269 (99%)	2 (1%)	76 82
1	G	270/271 (100%)	266 (98%)	4 (2%)	57 64
1	O	271/271 (100%)	267 (98%)	4 (2%)	57 64
All	All	2167/2168 (100%)	2152 (99%)	15 (1%)	78 82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	152[A]	CYS
1	O	152[B]	CYS
1	O	250	GLU
1	O	334	LYS
1	B	250	GLU
1	C	244	ASP
1	C	318	PHE
1	C	335	GLU
1	E	318	PHE
1	F	20	ARG
1	F	318	PHE
1	G	20	ARG
1	G	105	MET
1	G	244	ASP
1	G	318	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	279	HIS
1	O	330	HIS
1	A	57	HIS
1	A	64	ASN
1	A	279	HIS
1	A	280	GLN
1	B	113	GLN
1	C	204	GLN
1	C	225	ASN
1	C	239	ASN
1	C	279	HIS
1	C	287	ASN
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	330	HIS
1	E	225	ASN
1	E	239	ASN
1	E	279	HIS
1	E	287	ASN
1	E	322	ASN
1	F	24	ASN
1	F	48	GLN
1	F	64	ASN
1	F	225	ASN
1	F	280	GLN
1	G	24	ASN
1	G	64	ASN
1	G	204	GLN
1	G	306	HIS

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)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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	O	401	-	46,48,48	3.59	16 (34%)	64,73,73	1.88	17 (26%)
2	NAD	B	401	-	46,48,48	3.62	17 (36%)	64,73,73	1.71	11 (17%)
2	NAD	C	401	-	46,48,48	3.69	17 (36%)	64,73,73	1.74	13 (20%)
2	NAD	D	401	-	46,48,48	3.58	17 (36%)	64,73,73	1.90	16 (25%)
4	ACT	C	404	3	3,3,3	0.90	0	3,3,3	1.25	0
4	ACT	O	403	3	3,3,3	0.82	0	3,3,3	1.42	0
2	NAD	A	401	-	46,48,48	3.63	17 (36%)	64,73,73	1.68	12 (18%)
2	NAD	E	401	-	46,48,48	3.78	17 (36%)	64,73,73	1.91	14 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	401	-	-	7/30/62/62	0/5/5/5
2	NAD	B	401	-	-	7/30/62/62	0/5/5/5
2	NAD	C	401	-	-	11/30/62/62	0/5/5/5
2	NAD	D	401	-	-	6/30/62/62	0/5/5/5
2	NAD	A	401	-	-	7/30/62/62	0/5/5/5
2	NAD	E	401	-	1/1/11/11	10/30/62/62	0/5/5/5

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	NAD	O4D-C1D	17.76	1.64	1.40
2	B	401	NAD	O4D-C1D	16.64	1.62	1.40
2	A	401	NAD	O4D-C1D	16.55	1.62	1.40
2	C	401	NAD	O4D-C1D	16.53	1.62	1.40
2	D	401	NAD	O4D-C1D	15.91	1.61	1.40
2	O	401	NAD	O4D-C1D	15.85	1.61	1.40
2	E	401	NAD	O4B-C1B	8.18	1.60	1.42
2	C	401	NAD	O4B-C1B	8.09	1.60	1.42
2	O	401	NAD	O4B-C1B	8.07	1.60	1.42
2	D	401	NAD	O4B-C1B	7.55	1.59	1.42
2	B	401	NAD	O4B-C1B	7.54	1.59	1.42
2	A	401	NAD	O4B-C1B	7.30	1.58	1.42
2	O	401	NAD	O4B-C4B	-7.15	1.29	1.45
2	E	401	NAD	C2B-C1B	-6.81	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2B-C1B	-6.80	1.32	1.53
2	C	401	NAD	C2B-C1B	-6.79	1.32	1.53
2	A	401	NAD	O4B-C4B	-6.78	1.29	1.45
2	B	401	NAD	C2B-C1B	-6.73	1.32	1.53
2	E	401	NAD	O4B-C4B	-6.71	1.30	1.45
2	C	401	NAD	O4B-C4B	-6.66	1.30	1.45
2	D	401	NAD	C2B-C1B	-6.66	1.32	1.53
2	B	401	NAD	O4B-C4B	-6.58	1.30	1.45
2	D	401	NAD	O4B-C4B	-6.53	1.30	1.45
2	C	401	NAD	O4D-C4D	-6.22	1.31	1.45
2	O	401	NAD	C2B-C1B	-6.14	1.34	1.53
2	E	401	NAD	O4D-C4D	-5.87	1.31	1.45
2	B	401	NAD	O4D-C4D	-5.79	1.32	1.45
2	A	401	NAD	O4D-C4D	-5.78	1.32	1.45
2	O	401	NAD	O4D-C4D	-5.77	1.32	1.45
2	D	401	NAD	O4D-C4D	-5.73	1.32	1.45
2	C	401	NAD	C7N-N7N	5.42	1.42	1.33
2	E	401	NAD	C7N-N7N	5.30	1.42	1.33
2	A	401	NAD	C7N-N7N	5.28	1.42	1.33
2	D	401	NAD	C7N-N7N	5.28	1.42	1.33
2	B	401	NAD	C7N-N7N	5.23	1.42	1.33
2	O	401	NAD	C7N-N7N	4.99	1.42	1.33
2	O	401	NAD	C6A-N6A	4.19	1.44	1.34
2	B	401	NAD	C6A-N6A	4.09	1.44	1.34
2	O	401	NAD	C2N-N1N	4.05	1.39	1.35
2	A	401	NAD	C2N-N1N	4.04	1.39	1.35
2	A	401	NAD	C6A-N6A	4.01	1.44	1.34
2	C	401	NAD	C6A-N6A	3.94	1.44	1.34
2	D	401	NAD	C6A-N6A	3.86	1.44	1.34
2	D	401	NAD	C2N-N1N	3.85	1.39	1.35
2	C	401	NAD	O3D-C3D	-3.79	1.33	1.43
2	E	401	NAD	C6A-N6A	3.75	1.43	1.34
2	B	401	NAD	C2N-N1N	3.73	1.39	1.35
2	D	401	NAD	O3D-C3D	-3.60	1.34	1.43
2	O	401	NAD	O3D-C3D	-3.55	1.34	1.43
2	C	401	NAD	C2N-N1N	3.54	1.38	1.35
2	E	401	NAD	C2N-N1N	3.51	1.38	1.35
2	B	401	NAD	O3D-C3D	-3.50	1.34	1.43
2	A	401	NAD	O3D-C3D	-3.39	1.34	1.43
2	E	401	NAD	O3D-C3D	-3.37	1.34	1.43
2	C	401	NAD	O2D-C2D	3.15	1.50	1.43
2	O	401	NAD	O2B-C2B	3.12	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2A-N1A	3.04	1.39	1.33
2	C	401	NAD	C3N-C7N	3.03	1.55	1.50
2	O	401	NAD	C3N-C7N	3.01	1.55	1.50
2	A	401	NAD	C2A-N3A	2.97	1.39	1.33
2	C	401	NAD	C2A-N3A	2.96	1.39	1.33
2	B	401	NAD	C2A-N1A	2.95	1.39	1.33
2	D	401	NAD	O2B-C2B	2.93	1.50	1.43
2	C	401	NAD	O2B-C2B	2.93	1.50	1.43
2	E	401	NAD	O2B-C2B	2.91	1.50	1.43
2	A	401	NAD	C3N-C7N	2.88	1.54	1.50
2	E	401	NAD	O2D-C2D	2.85	1.50	1.43
2	B	401	NAD	C2A-N3A	2.84	1.39	1.33
2	D	401	NAD	C2A-N1A	2.84	1.39	1.33
2	D	401	NAD	C3N-C7N	2.82	1.54	1.50
2	E	401	NAD	C3N-C7N	2.79	1.54	1.50
2	D	401	NAD	O2D-C2D	2.76	1.49	1.43
2	O	401	NAD	C2A-N1A	2.70	1.38	1.33
2	B	401	NAD	C8A-N7A	2.69	1.36	1.31
2	O	401	NAD	C2A-N3A	2.68	1.38	1.33
2	E	401	NAD	C2A-N3A	2.67	1.38	1.33
2	O	401	NAD	C5A-N7A	-2.61	1.34	1.39
2	D	401	NAD	C2A-N3A	2.58	1.38	1.33
2	E	401	NAD	C5A-N7A	-2.57	1.34	1.39
2	B	401	NAD	C3N-C7N	2.55	1.54	1.50
2	O	401	NAD	O2D-C2D	2.51	1.49	1.43
2	C	401	NAD	C8A-N7A	2.49	1.36	1.31
2	E	401	NAD	C8A-N7A	2.49	1.36	1.31
2	A	401	NAD	O2B-C2B	2.48	1.49	1.43
2	C	401	NAD	C2A-N1A	2.46	1.38	1.33
2	D	401	NAD	C8A-N7A	2.45	1.36	1.31
2	C	401	NAD	C5A-N7A	-2.44	1.34	1.39
2	A	401	NAD	O2D-C2D	2.43	1.49	1.43
2	E	401	NAD	C2A-N1A	2.43	1.38	1.33
2	A	401	NAD	C5A-N7A	-2.40	1.34	1.39
2	O	401	NAD	C8A-N7A	2.37	1.36	1.31
2	B	401	NAD	O2B-C2B	2.31	1.48	1.43
2	B	401	NAD	C5A-N7A	-2.20	1.35	1.39
2	D	401	NAD	C5A-N7A	-2.15	1.35	1.39
2	B	401	NAD	O2D-C2D	2.07	1.48	1.43
2	A	401	NAD	O3B-C3B	-2.05	1.37	1.43
2	C	401	NAD	O3B-C3B	-2.03	1.37	1.43
2	E	401	NAD	O3B-C3B	-2.02	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C8A-N7A	2.02	1.35	1.31
2	D	401	NAD	PN-O3	2.01	1.61	1.59
2	B	401	NAD	C2N-C3N	2.01	1.42	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAD	N3A-C2A-N1A	-6.14	119.29	128.58
2	A	401	NAD	N3A-C2A-N1A	-6.03	119.45	128.58
2	D	401	NAD	N3A-C2A-N1A	-6.02	119.46	128.58
2	O	401	NAD	N3A-C2A-N1A	-5.94	119.59	128.58
2	E	401	NAD	N3A-C2A-N1A	-5.78	119.83	128.58
2	C	401	NAD	C5A-C4A-N3A	-5.74	118.81	126.72
2	C	401	NAD	N3A-C2A-N1A	-5.74	119.89	128.58
2	E	401	NAD	C5A-C4A-N3A	-5.49	119.15	126.72
2	O	401	NAD	C5A-C4A-N3A	-5.14	119.63	126.72
2	B	401	NAD	C5A-C4A-N3A	-4.87	120.01	126.72
2	A	401	NAD	C5A-C4A-N3A	-4.84	120.05	126.72
2	D	401	NAD	O2B-C2B-C1B	4.75	126.44	110.10
2	E	401	NAD	O3D-C3D-C4D	4.62	124.35	111.08
2	D	401	NAD	N9A-C8A-N7A	-4.21	107.96	113.94
2	D	401	NAD	C3B-C2B-C1B	4.16	109.34	101.46
2	E	401	NAD	O3D-C3D-C2D	3.92	124.40	111.82
2	A	401	NAD	N9A-C8A-N7A	-3.90	108.41	113.94
2	D	401	NAD	C5A-C4A-N3A	-3.87	121.39	126.72
2	E	401	NAD	N6A-C6A-N1A	-3.84	109.82	118.38
2	B	401	NAD	N9A-C8A-N7A	-3.76	108.60	113.94
2	C	401	NAD	C2A-N3A-C4A	3.70	120.86	111.83
2	C	401	NAD	N6A-C6A-N1A	-3.67	110.21	118.38
2	O	401	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
2	D	401	NAD	N6A-C6A-N1A	-3.63	110.29	118.38
2	C	401	NAD	N9A-C8A-N7A	-3.63	108.79	113.94
2	O	401	NAD	O4B-C4B-C3B	3.62	112.35	105.15
2	E	401	NAD	C2A-N3A-C4A	3.60	120.62	111.83
2	E	401	NAD	N9A-C8A-N7A	-3.56	108.89	113.94
2	O	401	NAD	C2A-N3A-C4A	3.50	120.37	111.83
2	C	401	NAD	N3A-C4A-N9A	3.48	133.09	127.17
2	B	401	NAD	C2A-N3A-C4A	3.46	120.29	111.83
2	E	401	NAD	C2D-C3D-C4D	3.38	109.14	102.61
2	E	401	NAD	N3A-C4A-N9A	3.36	132.89	127.17
2	A	401	NAD	N3A-C4A-N9A	3.35	132.87	127.17
2	O	401	NAD	O4B-C4B-C5B	3.29	119.88	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	401	NAD	N6A-C6A-N1A	-3.27	111.10	118.38
2	B	401	NAD	N6A-C6A-N1A	-3.27	111.10	118.38
2	A	401	NAD	C2A-N3A-C4A	3.26	119.79	111.83
2	C	401	NAD	C6N-N1N-C2N	-3.22	119.14	121.88
2	B	401	NAD	N3A-C4A-N9A	3.16	132.54	127.17
2	B	401	NAD	C6N-N1N-C2N	-3.13	119.22	121.88
2	D	401	NAD	C2A-N3A-C4A	3.05	119.28	111.83
2	O	401	NAD	N3A-C4A-N9A	3.02	132.30	127.17
2	O	401	NAD	C6N-N1N-C2N	-2.97	119.35	121.88
2	O	401	NAD	C4B-O4B-C1B	-2.90	103.06	109.47
2	D	401	NAD	C4D-O4D-C1D	-2.90	107.27	109.92
2	D	401	NAD	C6N-N1N-C2N	-2.87	119.44	121.88
2	O	401	NAD	C5B-C4B-C3B	2.78	125.21	115.21
2	A	401	NAD	N6A-C6A-N1A	-2.76	112.23	118.38
2	A	401	NAD	C6N-N1N-C2N	-2.74	119.55	121.88
2	D	401	NAD	C4A-N9A-C8A	2.68	108.56	105.74
2	C	401	NAD	C5A-N7A-C8A	2.68	107.66	103.45
2	E	401	NAD	C6N-N1N-C2N	-2.67	119.60	121.88
2	O	401	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	401	NAD	C6A-C5A-C4A	2.60	120.73	117.18
2	E	401	NAD	O2N-PN-O3	2.58	114.23	107.27
2	D	401	NAD	C5A-C6A-N6A	2.57	129.64	123.29
2	E	401	NAD	C5A-C6A-N6A	2.55	129.61	123.29
2	E	401	NAD	C5A-N7A-C8A	2.52	107.42	103.45
2	D	401	NAD	O2B-C2B-C3B	2.52	119.89	111.82
2	O	401	NAD	C5A-N7A-C8A	2.50	107.38	103.45
2	A	401	NAD	C5A-N7A-C8A	2.48	107.34	103.45
2	C	401	NAD	O2N-PN-O3	2.46	113.92	107.27
2	B	401	NAD	C5A-N7A-C8A	2.44	107.28	103.45
2	D	401	NAD	C5A-N7A-C8A	2.42	107.25	103.45
2	C	401	NAD	C6A-C5A-C4A	2.42	120.48	117.18
2	O	401	NAD	C6A-C5A-C4A	2.40	120.46	117.18
2	C	401	NAD	C5A-C6A-N6A	2.34	129.07	123.29
2	A	401	NAD	C4D-O4D-C1D	-2.33	107.79	109.92
2	A	401	NAD	C4A-N9A-C8A	2.30	108.15	105.74
2	O	401	NAD	C5A-C6A-N6A	2.28	128.94	123.29
2	D	401	NAD	N3A-C4A-N9A	2.25	130.99	127.17
2	E	401	NAD	C6A-C5A-C4A	2.22	120.21	117.18
2	B	401	NAD	C5A-C6A-N6A	2.20	128.72	123.29
2	O	401	NAD	C2B-C3B-C4B	-2.15	98.45	102.61
2	B	401	NAD	C6A-C5A-C4A	2.15	120.11	117.18
2	C	401	NAD	C5A-C4A-N9A	2.10	108.10	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAD	C2B-C1B-N9A	2.09	118.49	113.30
2	O	401	NAD	C5A-C4A-N9A	2.07	108.06	105.81
2	C	401	NAD	O7N-C7N-N7N	-2.06	119.63	122.62
2	B	401	NAD	C4A-N9A-C8A	2.06	107.90	105.74
2	A	401	NAD	C5B-C4B-C3B	-2.03	107.91	115.21
2	D	401	NAD	O3B-C3B-C2B	-2.01	105.37	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	401	NAD	C3D

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N
2	O	401	NAD	C2D-C1D-N1N-C2N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	C5B-O5B-PA-O1A
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	E	401	NAD	C5B-O5B-PA-O1A
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	O	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	C	401	NAD	C3B-C4B-C5B-O5B
2	E	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	C2B-C1B-N9A-C8A
2	B	401	NAD	C2B-C1B-N9A-C8A
2	C	401	NAD	C5B-O5B-PA-O2A
2	E	401	NAD	C5B-O5B-PA-O2A
2	E	401	NAD	C5B-O5B-PA-O3
2	E	401	NAD	PA-O3-PN-O2N
2	E	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	PA-O3-PN-O2N
2	O	401	NAD	O4B-C1B-N9A-C8A
2	C	401	NAD	PA-O3-PN-O1N
2	E	401	NAD	PA-O3-PN-O1N
2	B	401	NAD	O4B-C1B-N9A-C8A
2	B	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	O4B-C1B-N9A-C8A
2	A	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

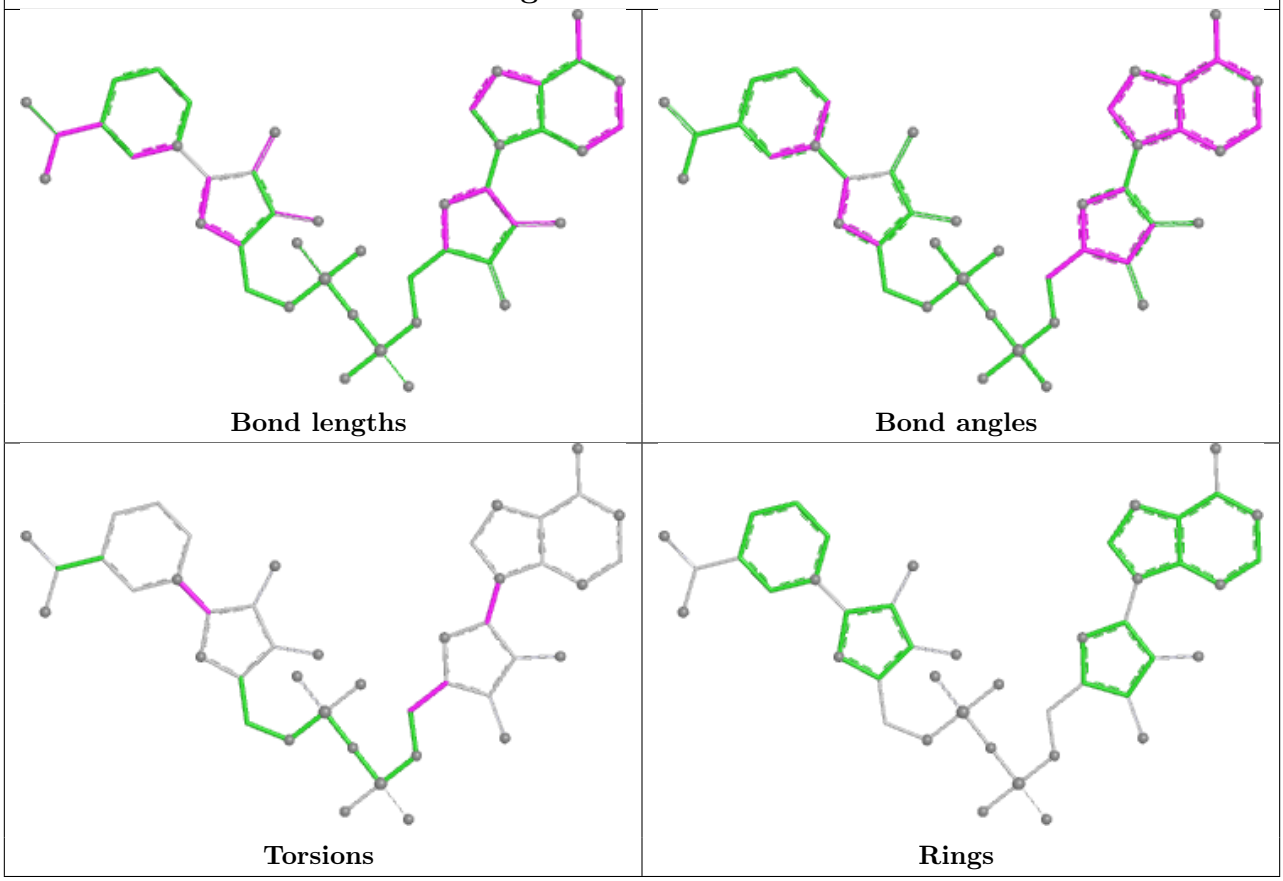
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	401	NAD	1	0
2	B	401	NAD	2	0
2	D	401	NAD	1	0
2	A	401	NAD	2	0
2	E	401	NAD	1	0

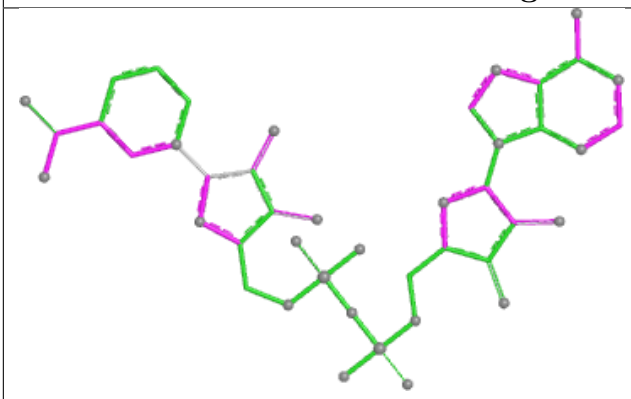
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

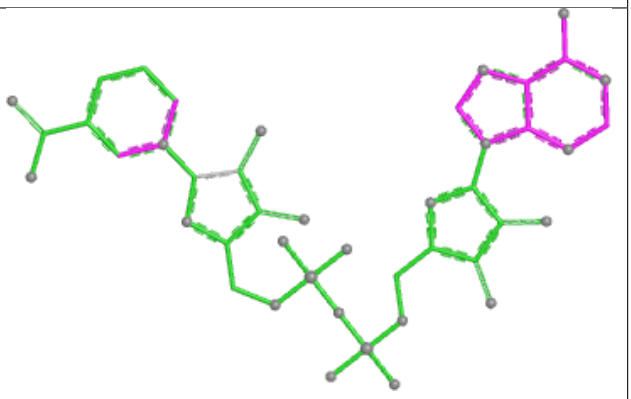
Ligand NAD O 401



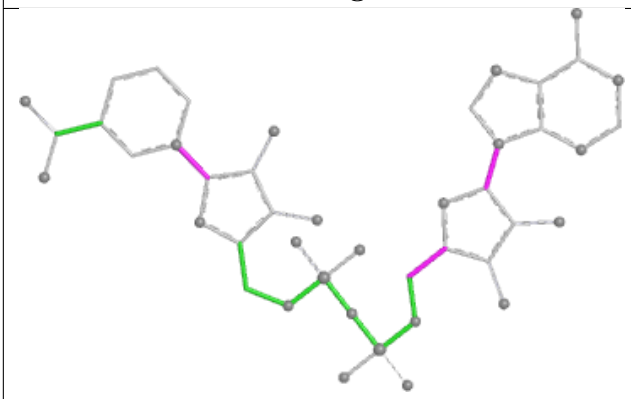
Ligand NAD B 401



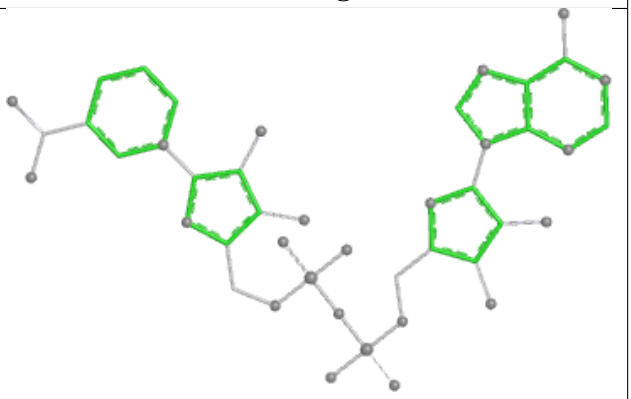
Bond lengths



Bond angles

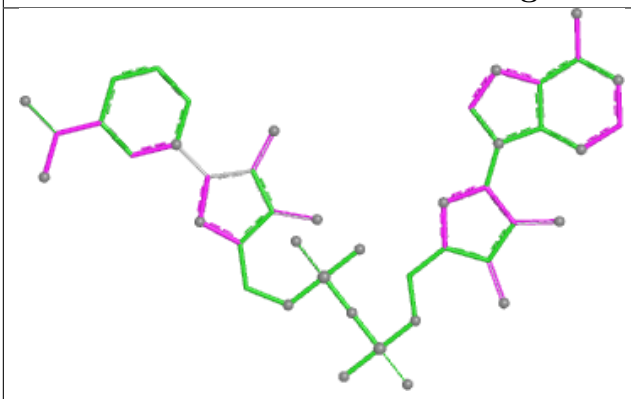


Torsions

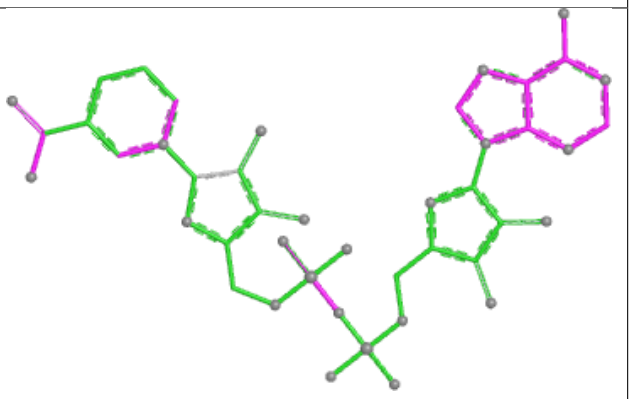


Rings

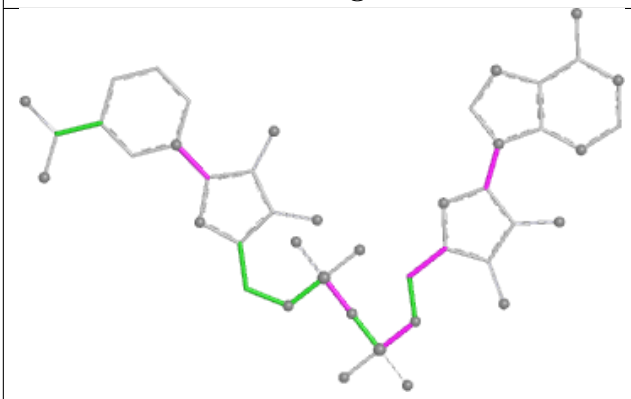
Ligand NAD C 401



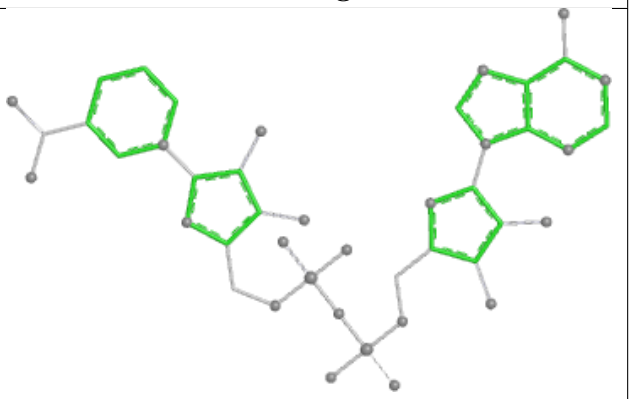
Bond lengths



Bond angles

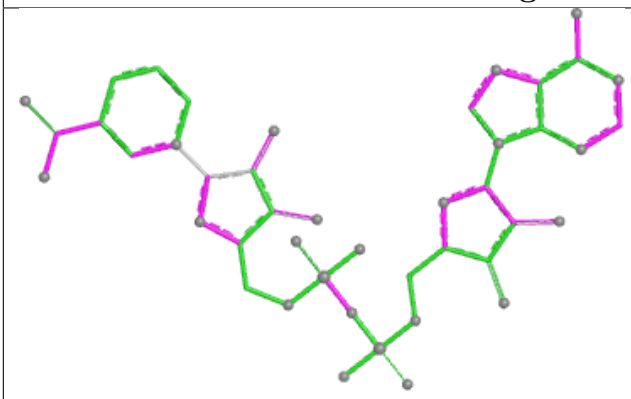


Torsions

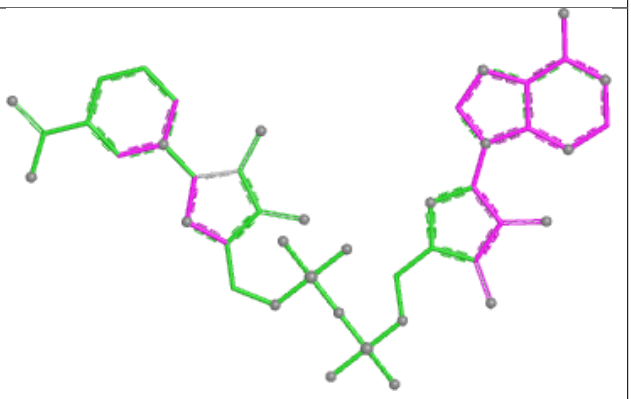


Rings

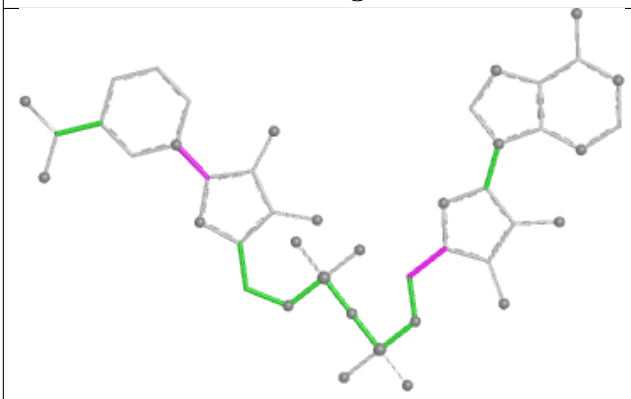
Ligand NAD D 401



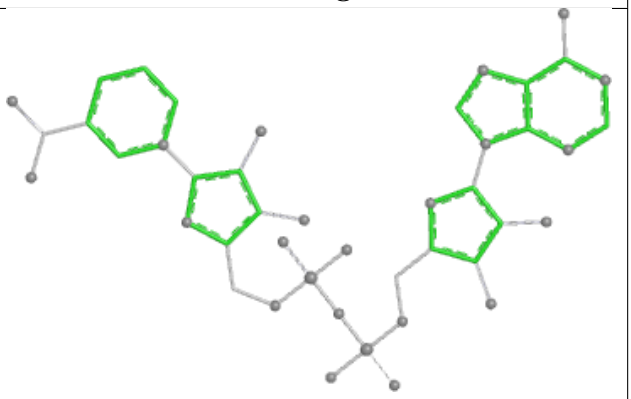
Bond lengths



Bond angles

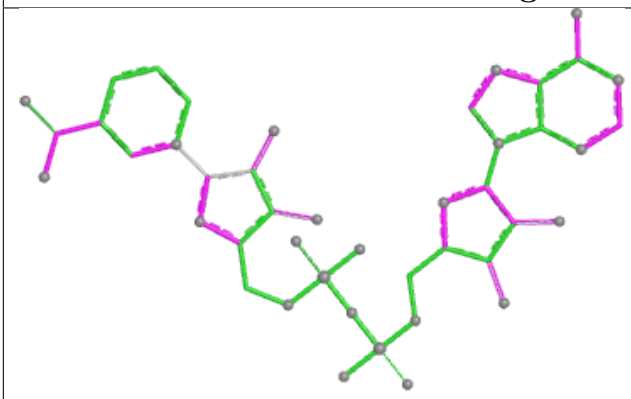


Torsions

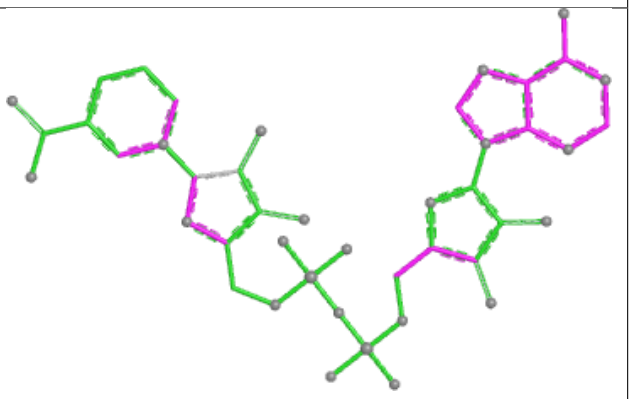


Rings

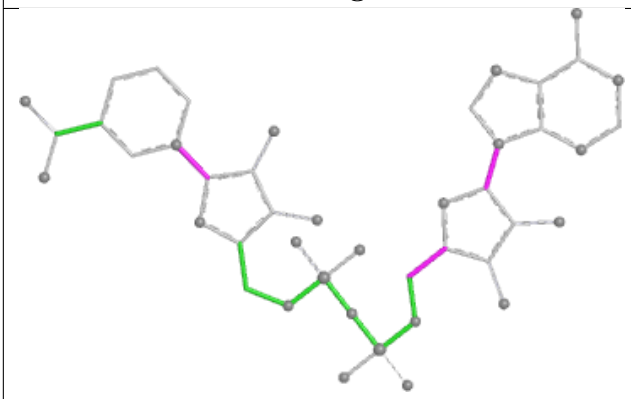
Ligand NAD A 401



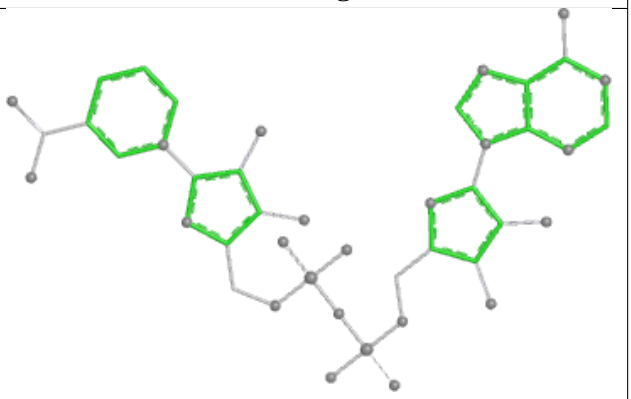
Bond lengths



Bond angles

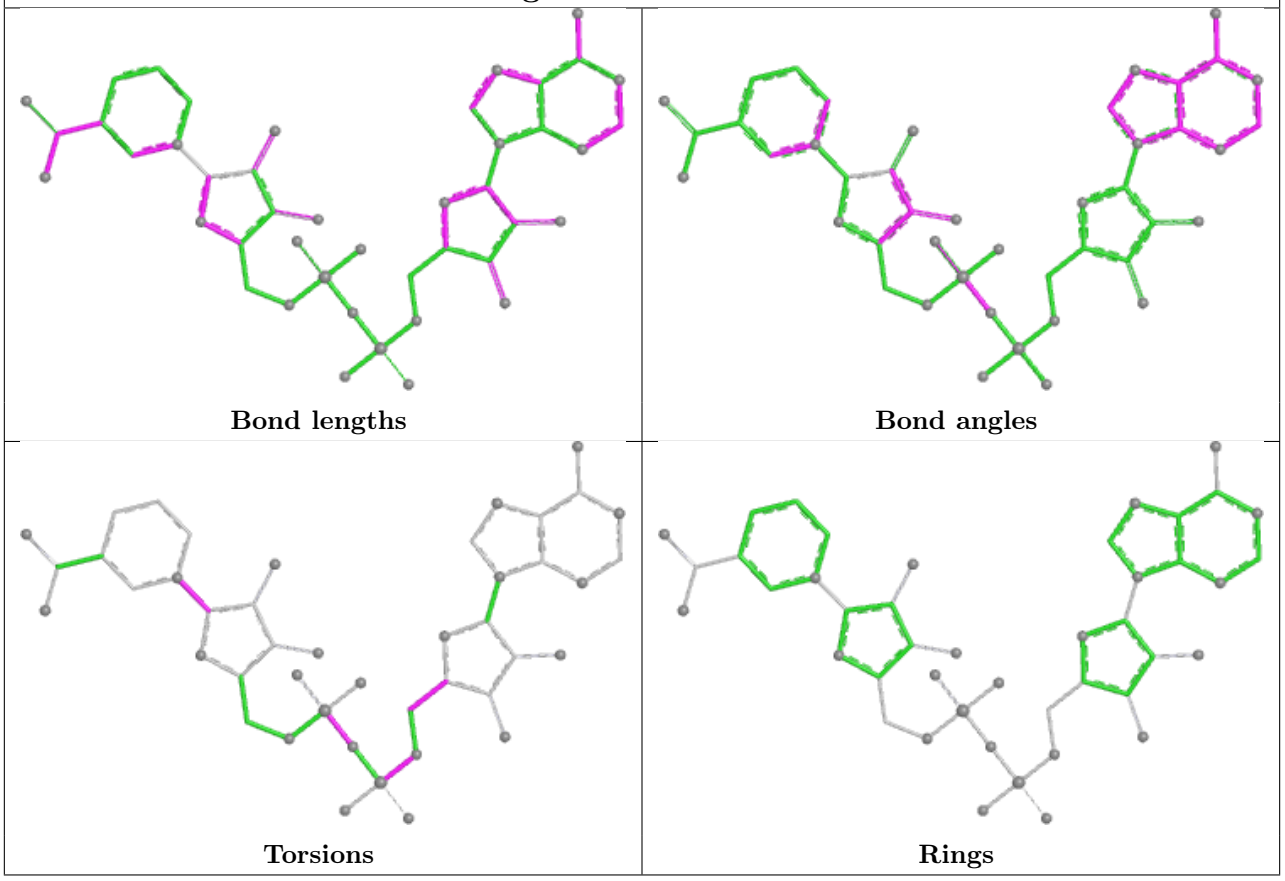


Torsions



Rings

Ligand NAD E 401



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	333/335 (99%)	-1.68	0	100	100	9, 18, 39, 58	1 (0%)
1	B	333/335 (99%)	-1.67	0	100	100	9, 18, 41, 62	1 (0%)
1	C	333/335 (99%)	-1.64	0	100	100	8, 21, 42, 67	1 (0%)
1	D	333/335 (99%)	-1.67	0	100	100	7, 19, 43, 64	1 (0%)
1	E	333/335 (99%)	-1.66	0	100	100	10, 21, 43, 68	1 (0%)
1	F	333/335 (99%)	-1.54	0	100	100	10, 26, 56, 76	1 (0%)
1	G	333/335 (99%)	-1.53	0	100	100	10, 27, 56, 75	0
1	O	333/335 (99%)	-1.67	0	100	100	8, 18, 43, 62	1 (0%)
All	All	2664/2680 (99%)	-1.63	0	100	100	7, 21, 46, 76	7 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

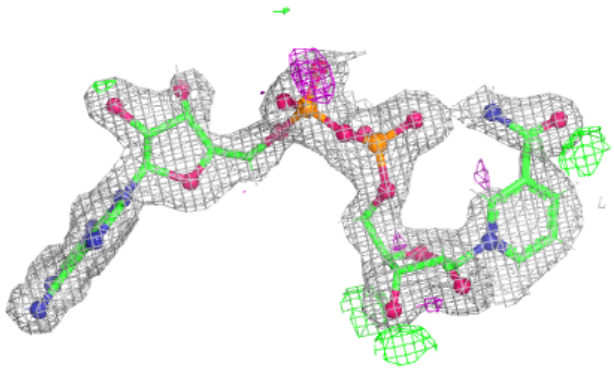
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

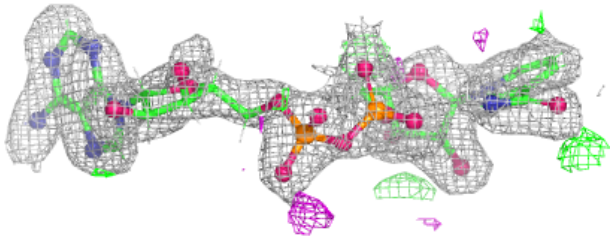
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	401	44/44	0.99	0.03	24,43,61,94	0
2	NAD	E	401	44/44	0.99	0.04	22,41,75,158	0
2	NAD	B	401	44/44	1.00	0.02	12,23,33,37	0
2	NAD	O	401	44/44	1.00	0.02	14,25,35,36	0
2	NAD	D	401	44/44	1.00	0.02	14,23,32,36	0
2	NAD	A	401	44/44	1.00	0.02	12,24,34,37	0
3	ZN	O	402	1/1	1.00	0.01	19,19,19,19	0
3	ZN	A	402	1/1	1.00	0.03	44,44,44,44	0
3	ZN	B	402	1/1	1.00	0.01	28,28,28,28	1
3	ZN	C	402	1/1	1.00	0.01	15,15,15,15	1
3	ZN	C	403	1/1	1.00	0.01	19,19,19,19	0
3	ZN	E	402	1/1	1.00	0.01	18,18,18,18	0
4	ACT	O	403	4/4	1.00	0.03	17,22,36,36	0
4	ACT	C	404	4/4	1.00	0.02	14,22,40,40	0

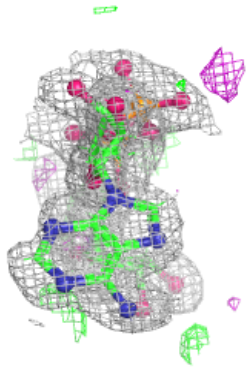
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 401:

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

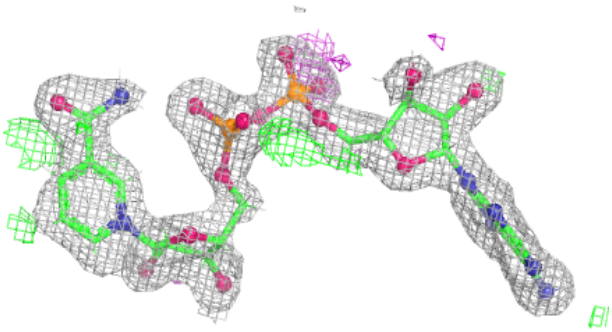


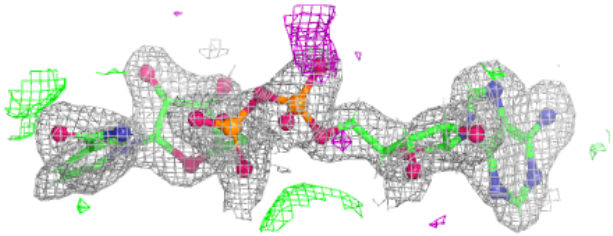


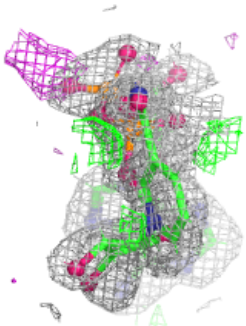


Electron density around NAD E 401:

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

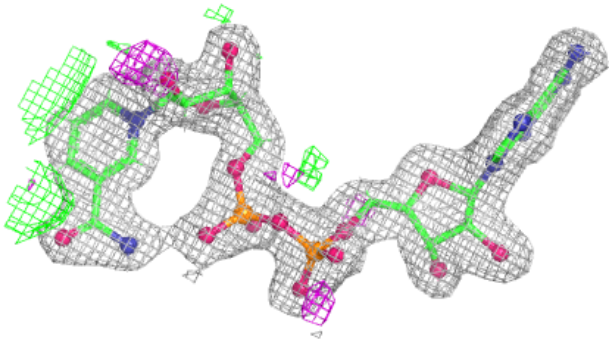


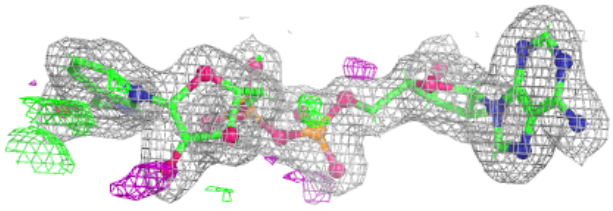


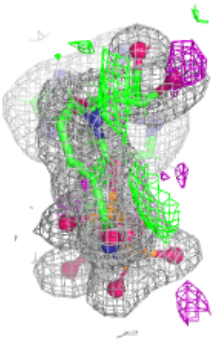


Electron density around NAD B 401:

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

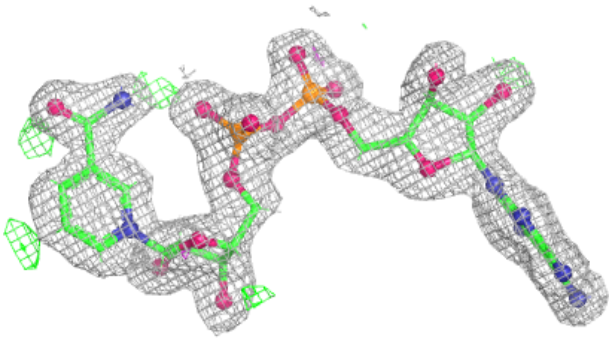


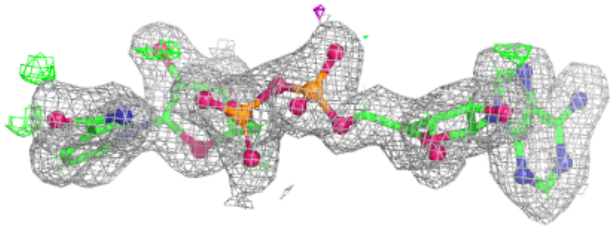


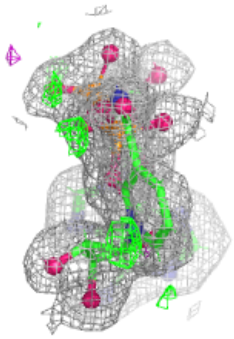


Electron density around NAD O 401:

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

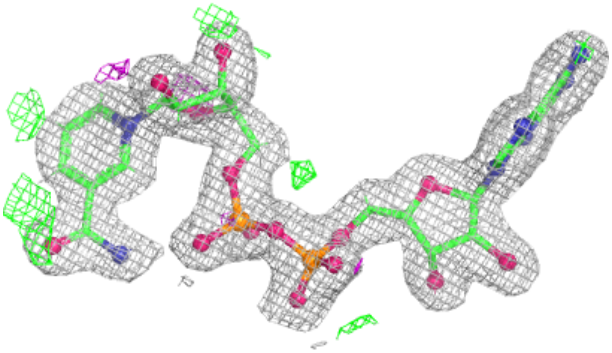


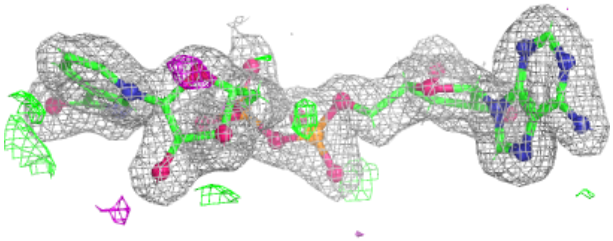


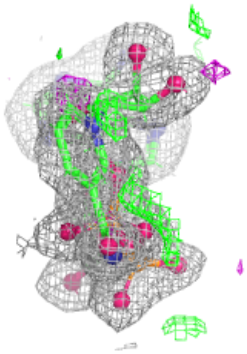


Electron density around NAD D 401:

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

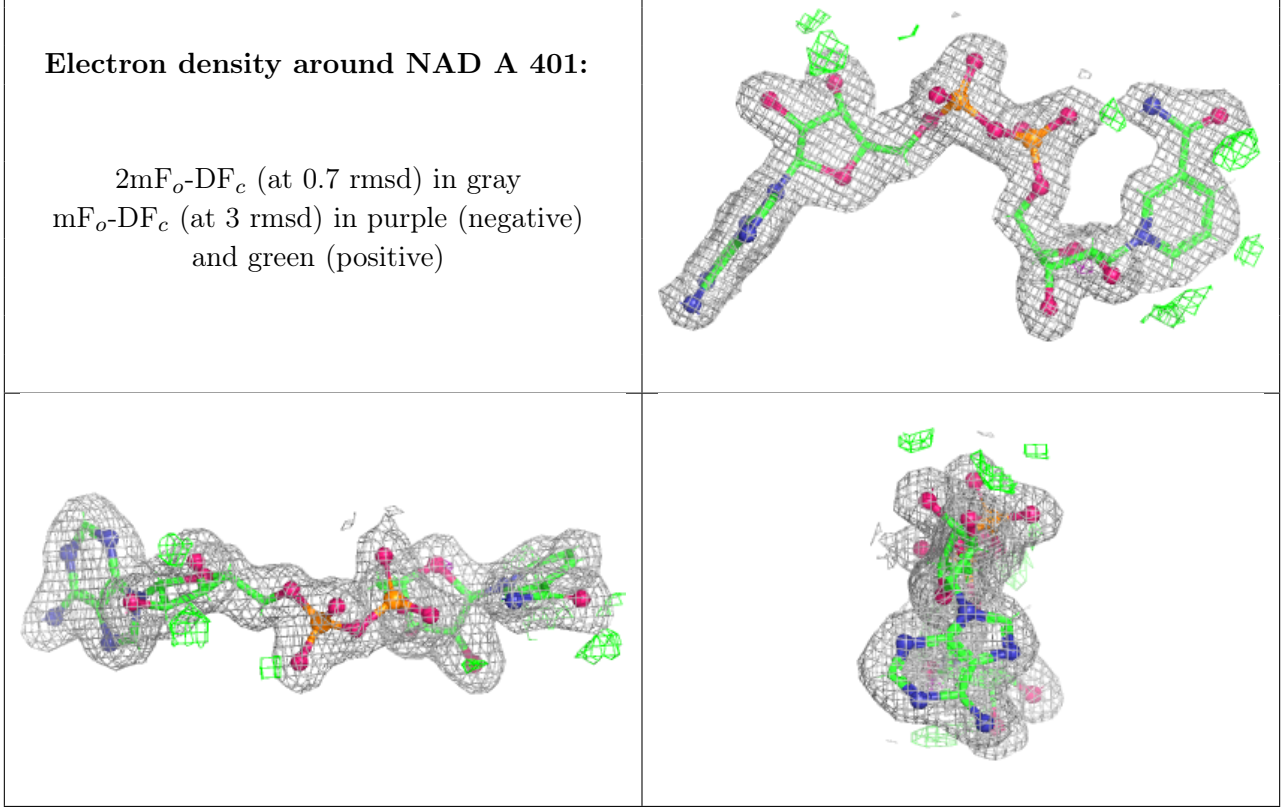






Electron density around NAD A 401:

$2mF_o$-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

There are no such residues in this entry.