



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:02 AM UTC

PDB ID : 5NNO / pdb_00005nno
Title : Structure of TbALDH3 complexed with NAD and AN3057 aldehyde
Authors : Zoltner, M.; Zhang, N.; Horn, D.; Field, M.C.
Deposited on : 2017-04-10
Resolution : 2.50 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

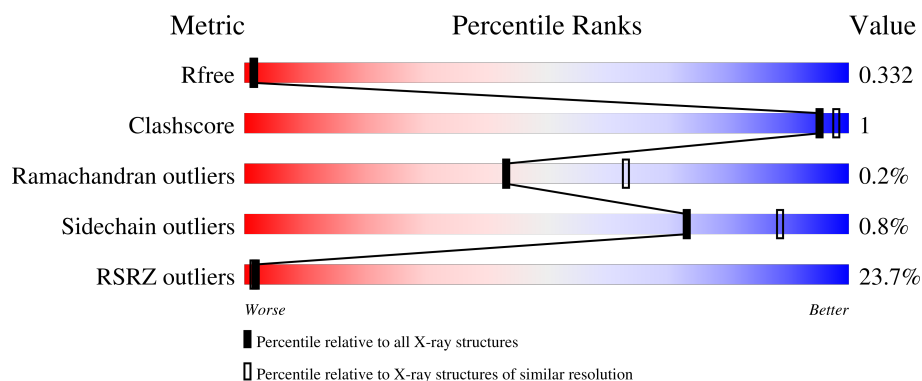
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	546	23% 85% 11%
1	B	546	19% 85% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7941 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	5	0
			3801	2413	662	709	17			
1	B	484	Total	C	N	O	S	0	6	0
			3814	2425	661	711	17			

There are 12 discrepancies between the modelled and reference sequences:

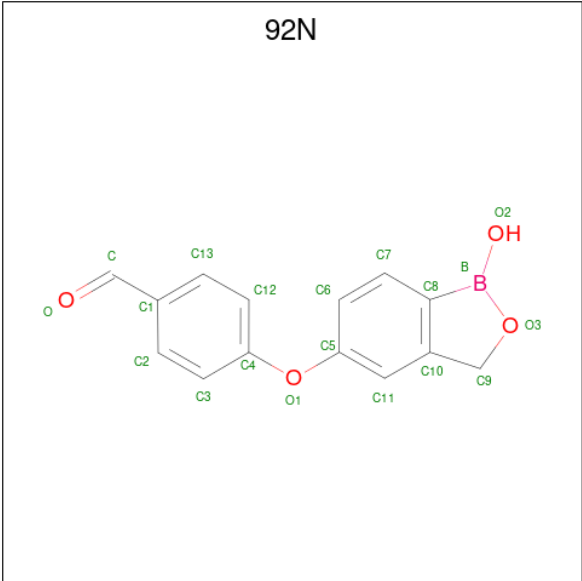
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP C9ZQX6
A	2	SER	-	expression tag	UNP C9ZQX6
A	3	MET	-	expression tag	UNP C9ZQX6
A	4	ALA	-	expression tag	UNP C9ZQX6
A	259	SER	CYS	conflict	UNP C9ZQX6
A	394	ALA	SER	conflict	UNP C9ZQX6
B	1	GLY	-	expression tag	UNP C9ZQX6
B	2	SER	-	expression tag	UNP C9ZQX6
B	3	MET	-	expression tag	UNP C9ZQX6
B	4	ALA	-	expression tag	UNP C9ZQX6
B	259	SER	CYS	conflict	UNP C9ZQX6
B	394	ALA	SER	conflict	UNP C9ZQX6

- 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	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is 4-[(1-oxidanyl-3 {H}-2,1-benzoxaborol-5-yl)oxy]benzaldehyde (CCD ID: 92N) (formula: C₁₄H₁₁BO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	B	C	O	0	0
			19	1	14	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	B	C	O	0	0
			19	1	14	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	94	Total	O	0	0
			94	94		

LYS
SER
PRO
ARG
SER
ASN
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.17Å 62.52Å 92.97Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	46.56 – 2.50 46.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.9 (46.56-2.50) 98.8 (46.56-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.234 , 0.278 0.272 , 0.332	Depositor DCC
R_{free} test set	1820 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	1.998	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.862 for H, K, L 0.138 for L, -K, H	Depositor
Outliers	0 of 35943 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7941	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.48% 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, 92N

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	0.82	0/3870	1.01	1/5246 (0.0%)
1	B	0.82	0/3885	1.01	1/5269 (0.0%)
All	All	0.82	0/7755	1.01	2/10515 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ASP	N-CA-C	5.24	116.68	110.97
1	B	128	ASN	N-CA-C	5.14	117.78	111.82

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	3801	0	3880	8	1
1	B	3814	0	3886	12	1
2	A	44	0	26	1	0
2	B	44	0	26	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
4	A	106	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	94	0	0	0	0
All	All	7941	0	7818	19	1

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 (19) 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:67:ARG:NH1	1:B:128:ASN:O	2.33	0.62
1:A:127:TRP:NE1	2:A:601:NAD:O2N	2.32	0.57
1:B:171[B]:VAL:O	1:B:171[B]:VAL:CG2	2.55	0.55
1:A:47:LEU:HB2	1:A:84:VAL:HG11	1.92	0.52
1:B:66:ARG:NH2	1:B:344:THR:O	2.42	0.52
1:B:47:LEU:HB2	1:B:84:VAL:HG11	1.92	0.51
1:B:85[A]:TRP:CE3	1:B:85[A]:TRP:HA	2.48	0.48
1:B:136:GLN:HB3	1:B:137:PRO:HD3	1.97	0.47
1:A:193[B]:ARG:NH1	1:A:193[B]:ARG:HG2	2.31	0.46
1:B:65:ARG:CZ	1:B:65:ARG:HA	2.47	0.45
1:B:283:ARG:HG2	1:B:287:LEU:HD12	1.98	0.45
1:B:171[B]:VAL:O	1:B:171[B]:VAL:HG23	2.15	0.44
1:A:136:GLN:HB3	1:A:137:PRO:HD3	1.98	0.44
1:A:65[A]:ARG:HA	1:A:65[A]:ARG:CZ	2.47	0.43
1:B:198:LEU:C	1:B:198:LEU:HD23	2.45	0.42
1:B:245:GLU:O	1:B:286:MET:HE1	2.19	0.41
1:A:198:LEU:C	1:A:198:LEU:HD23	2.46	0.41
1:A:245:GLU:O	1:A:286:MET:HE1	2.20	0.41
1:A:419:VAL:HB	1:B:461:ARG:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:NE2	1:B:41:GLN:NE2[1_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	487/546 (89%)	476 (98%)	10 (2%)	1 (0%)	43	63
1	B	488/546 (89%)	475 (97%)	12 (2%)	1 (0%)	43	63
All	All	975/1092 (89%)	951 (98%)	22 (2%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	HIS
1	B	445	HIS

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	417/459 (91%)	412 (99%)	5 (1%)	63	83
1	B	418/459 (91%)	416 (100%)	2 (0%)	81	92
All	All	835/918 (91%)	828 (99%)	7 (1%)	73	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	151	LYS
1	A	300	LEU
1	A	465	LEU

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Mol	Chain	Res	Type
1	A	483	ARG
1	B	66	ARG
1	B	151	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	48	ASN
1	A	180	ASN
1	A	257	GLN
1	A	305	GLN
1	A	306	GLN
1	A	425	HIS
1	B	16	ASN
1	B	257	GLN
1	B	305	GLN
1	B	306	GLN
1	B	359	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	601	-	46,48,48	1.22	5 (10%)	64,73,73	1.65	12 (18%)
3	92N	A	602	-	21,21,21	0.38	0	27,29,29	1.16	3 (11%)
2	NAD	A	601	-	46,48,48	1.16	4 (8%)	64,73,73	1.94	15 (23%)
3	92N	B	602	-	21,21,21	0.47	0	27,29,29	1.11	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	601	-	-	12/30/62/62	0/5/5/5
3	92N	A	602	-	-	0/6/15/15	0/3/3/3
2	NAD	A	601	-	-	4/30/62/62	0/5/5/5
3	92N	B	602	-	-	0/6/15/15	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	C5A-C4A	4.73	1.47	1.39
2	A	601	NAD	C5A-C4A	4.30	1.46	1.39
2	B	601	NAD	C5A-C6A	2.92	1.49	1.41
2	A	601	NAD	C8A-N7A	2.75	1.37	1.31
2	A	601	NAD	C5A-C6A	2.59	1.48	1.41
2	B	601	NAD	PA-O3	2.45	1.62	1.59
2	B	601	NAD	C8A-N7A	2.40	1.36	1.31
2	B	601	NAD	C5A-N7A	-2.13	1.35	1.39
2	A	601	NAD	PN-O3	2.09	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C4D-O4D-C1D	-7.99	102.61	109.92
2	B	601	NAD	C5A-C4A-N3A	-5.57	119.05	126.72
2	A	601	NAD	C5A-C4A-N3A	-5.53	119.10	126.72
3	A	602	92N	C11-C10-C8	-4.39	119.25	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	N3A-C4A-N9A	4.34	134.55	127.17
2	A	601	NAD	N3A-C4A-N9A	4.33	134.53	127.17
3	B	602	92N	C11-C10-C8	-4.28	119.31	122.09
2	A	601	NAD	N3A-C2A-N1A	-4.10	122.37	128.58
2	B	601	NAD	N3A-C2A-N1A	-4.06	122.43	128.58
2	A	601	NAD	C2A-N3A-C4A	4.03	121.67	111.83
2	B	601	NAD	C2A-N3A-C4A	4.03	121.66	111.83
2	B	601	NAD	C4A-C5A-N7A	-3.69	106.36	110.58
2	A	601	NAD	C4A-C5A-N7A	-3.06	107.08	110.58
2	A	601	NAD	C4A-N9A-C8A	2.93	108.81	105.74
2	B	601	NAD	C4A-N9A-C8A	2.91	108.80	105.74
2	B	601	NAD	C5A-N7A-C8A	2.86	107.94	103.45
2	B	601	NAD	C6A-C5A-N7A	2.57	137.05	132.09
2	A	601	NAD	C6A-C5A-N7A	2.53	136.98	132.09
2	B	601	NAD	C3N-C7N-N7N	2.52	120.84	117.74
3	A	602	92N	O1-C5-C11	2.51	127.01	119.16
2	B	601	NAD	N9A-C8A-N7A	-2.42	110.50	113.94
2	A	601	NAD	C3N-C7N-N7N	2.38	120.67	117.74
2	A	601	NAD	N9A-C8A-N7A	-2.37	110.58	113.94
2	A	601	NAD	C5A-N7A-C8A	2.36	107.15	103.45
2	A	601	NAD	O4D-C4D-C5D	2.33	116.79	109.33
3	B	602	92N	O1-C5-C11	2.14	125.87	119.16
2	B	601	NAD	C2A-N1A-C6A	2.14	122.24	118.73
2	A	601	NAD	O2A-PA-O1A	2.11	122.28	112.44
2	B	601	NAD	C4D-O4D-C1D	2.11	111.86	109.92
3	A	602	92N	C5-O1-C4	2.03	123.43	118.78
2	A	601	NAD	C4A-N9A-C1B	-2.03	121.88	126.63
2	A	601	NAD	O5D-C5D-C4D	2.02	115.88	108.99

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C5D-O5D-PN-O2N
2	B	601	NAD	O4D-C1D-N1N-C6N
2	A	601	NAD	O4B-C4B-C5B-O5B
2	B	601	NAD	O4B-C4B-C5B-O5B
2	B	601	NAD	C3B-C4B-C5B-O5B
2	A	601	NAD	C3B-C4B-C5B-O5B
2	A	601	NAD	O4D-C4D-C5D-O5D

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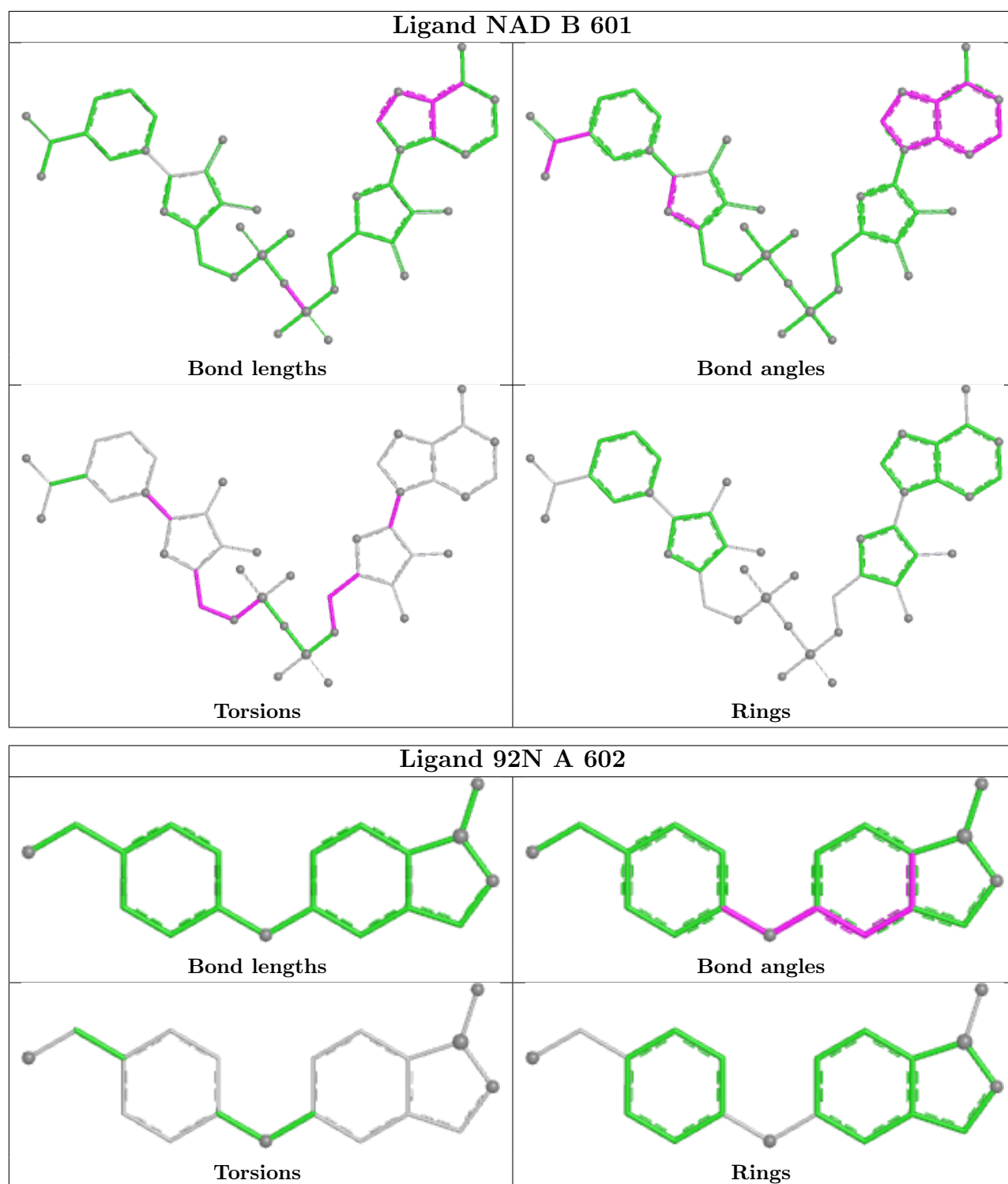
Mol	Chain	Res	Type	Atoms
2	B	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	C4B-C5B-O5B-PA
2	B	601	NAD	O4D-C1D-N1N-C2N
2	B	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	C2B-C1B-N9A-C8A

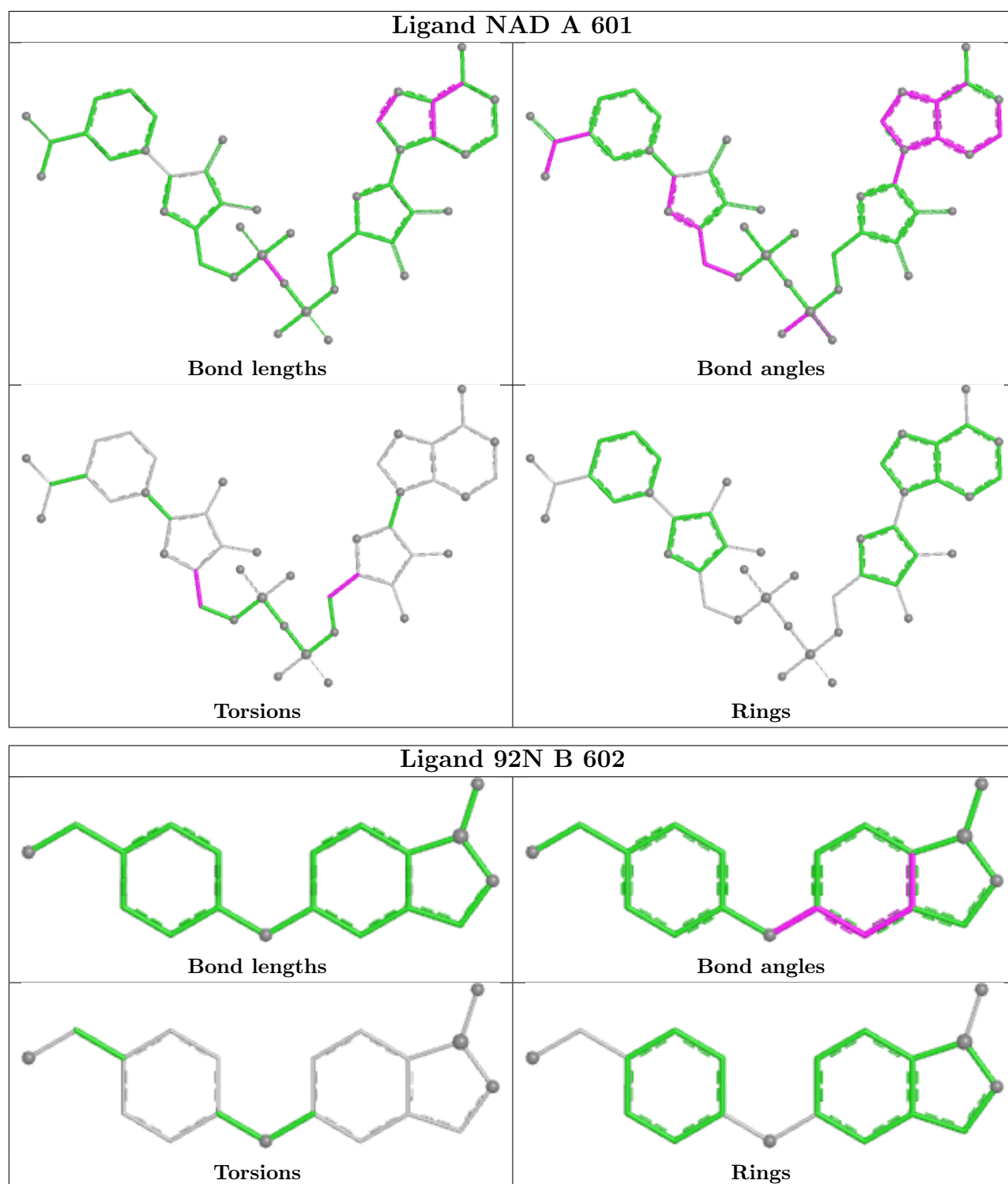
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	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 ⓘ

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	484/546 (88%)	1.44	124 (25%)	1 1	10, 24, 42, 56	5 (1%)
1	B	484/546 (88%)	1.48	105 (21%)	2 2	10, 24, 51, 76	6 (1%)
All	All	968/1092 (88%)	1.46	229 (23%)	2 1	10, 24, 45, 76	11 (1%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85[A]	TRP	7.2
1	B	467	SER	5.6
1	B	464	PHE	5.5
1	B	466	PHE	5.5
1	B	465	LEU	5.4
1	A	480	ALA	5.2
1	A	471	THR	5.2
1	B	478	THR	5.1
1	B	471	THR	5.0
1	B	469	ILE	4.8
1	A	104	GLY	4.7
1	B	474	PHE	4.6
1	A	474	PHE	4.6
1	A	6	ALA	4.6
1	B	472	VAL	4.5
1	A	484	VAL	4.4
1	B	484	VAL	4.3
1	B	323	GLN	4.1
1	B	475	PRO	4.0
1	A	478	THR	4.0
1	B	355	ILE	4.0
1	B	487	SER	4.0
1	A	103	GLU	3.9
1	A	479	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	470	ASP	3.6
1	B	483	ARG	3.6
1	A	482	SER	3.6
1	A	331	GLY	3.5
1	B	378	ASN	3.5
1	A	234	ASP	3.5
1	B	41	GLN	3.5
1	A	466	PHE	3.5
1	A	321	HIS	3.5
1	A	26[A]	GLU	3.4
1	A	470	ASP	3.4
1	A	8	VAL	3.4
1	A	323	GLN	3.4
1	B	479	THR	3.4
1	A	36	LEU	3.4
1	B	343	ALA	3.4
1	B	359	HIS	3.4
1	A	92	ASP	3.4
1	B	306	GLN	3.4
1	B	364	GLU	3.4
1	A	335	ALA	3.3
1	A	475	PRO	3.3
1	A	101	THR	3.3
1	A	102	MET	3.3
1	B	358	THR	3.3
1	A	476	PRO	3.3
1	B	327	GLU	3.3
1	B	482	SER	3.2
1	B	383	LEU	3.2
1	B	489	LEU	3.2
1	B	330	LYS	3.2
1	B	356	ASP	3.2
1	B	488	LEU	3.2
1	A	98	VAL	3.2
1	A	125	GLY	3.2
1	A	473	ARG	3.2
1	B	26	GLU	3.2
1	B	37	LYS	3.2
1	B	332	GLY	3.1
1	B	373	VAL	3.1
1	B	486	ASN	3.1
1	A	297	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	235	THR	3.1
1	B	477	TYR	3.1
1	B	342	GLU	3.1
1	B	382	ILE	3.0
1	B	360	PRO	3.0
1	A	95	VAL	3.0
1	B	406	ARG	3.0
1	A	273	SER	3.0
1	A	7	GLY	3.0
1	A	377	GLU	2.9
1	B	476	PRO	2.9
1	B	402	LYS	2.9
1	B	481	LYS	2.9
1	B	341	ASP	2.9
1	A	449	SER	2.9
1	B	377	GLU	2.9
1	A	469	ILE	2.9
1	A	238	ASP	2.9
1	B	15	GLU	2.9
1	B	336	VAL	2.8
1	A	358	THR	2.8
1	A	188	ALA	2.8
1	B	105	ALA	2.8
1	A	108	LEU	2.8
1	A	328	PHE	2.8
1	B	357	PRO	2.8
1	B	480	ALA	2.8
1	B	403	ARG	2.8
1	B	361	VAL	2.8
1	B	485	LEU	2.8
1	B	31	ASP	2.8
1	B	86	HIS	2.8
1	A	85	TRP	2.7
1	A	472	VAL	2.7
1	B	292	LEU	2.7
1	A	105	ALA	2.7
1	A	78	LEU	2.7
1	B	429	ASP	2.7
1	A	65[A]	ARG	2.7
1	A	193[A]	ARG	2.7
1	A	322	PHE	2.7
1	A	347	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	344	THR	2.7
1	B	337	GLY	2.6
1	A	361	VAL	2.6
1	A	232	VAL	2.6
1	A	320	SER	2.6
1	A	319	ALA	2.6
1	A	305	GLN	2.6
1	A	106	ALA	2.6
1	B	375	THR	2.6
1	A	385	ILE	2.6
1	A	87	LEU	2.6
1	A	155	LEU	2.6
1	B	468	SER	2.6
1	A	88	ILE	2.5
1	B	363	GLN	2.5
1	A	140	GLY	2.5
1	A	288	GLY	2.5
1	B	181	GLY	2.5
1	A	485	LEU	2.5
1	B	167	LEU	2.5
1	A	481	LYS	2.5
1	B	422	VAL	2.5
1	A	477	TYR	2.5
1	A	184	SER	2.5
1	A	357	PRO	2.5
1	A	15	GLU	2.5
1	B	7	GLY	2.5
1	B	376	TYR	2.5
1	B	367	PHE	2.5
1	A	86	HIS	2.5
1	A	93	GLU	2.4
1	B	379	GLU	2.4
1	B	321	HIS	2.4
1	A	16	ASN	2.4
1	A	141	ALA	2.4
1	A	340	ALA	2.4
1	A	17	ILE	2.4
1	A	334	VAL	2.4
1	A	468	SER	2.4
1	A	333	LYS	2.4
1	A	488	LEU	2.4
1	B	193[A]	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	79	PRO	2.4
1	A	181	GLY	2.4
1	A	363	GLN	2.4
1	B	447	ARG	2.4
1	A	461	ARG	2.3
1	A	381	ASP	2.3
1	A	96	LYS	2.3
1	A	82	ASN	2.3
1	A	27	ALA	2.3
1	A	211	ALA	2.3
1	B	244	ALA	2.3
1	B	473	ARG	2.3
1	A	359	HIS	2.3
1	A	94	TYR	2.3
1	A	44	ARG	2.3
1	B	381	ASP	2.3
1	A	330	LYS	2.3
1	B	48	ASN	2.3
1	A	462	ARG	2.3
1	B	125	GLY	2.3
1	B	273	SER	2.3
1	B	87	LEU	2.3
1	B	89	GLU	2.3
1	A	165	LYS	2.2
1	B	333	LYS	2.2
1	A	356	ASP	2.2
1	B	93	GLU	2.2
1	B	103	GLU	2.2
1	A	483	ARG	2.2
1	B	183	VAL	2.2
1	A	62	HIS	2.2
1	A	345	LEU	2.2
1	A	270	SER	2.2
1	B	366	ILE	2.2
1	A	109	ASP	2.2
1	A	447	ARG	2.2
1	A	100	PRO	2.2
1	A	148	ALA	2.2
1	B	296	LYS	2.2
1	B	351	ILE	2.2
1	A	403	ARG	2.2
1	A	337	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	293	LYS	2.2
1	B	27	ALA	2.1
1	A	119	GLY	2.1
1	A	300	LEU	2.1
1	A	489	LEU	2.1
1	A	61	ILE	2.1
1	A	77	ILE	2.1
1	A	58	CYS	2.1
1	A	55	ASP	2.1
1	A	410	SER	2.1
1	A	487	SER	2.1
1	A	99	LYS	2.1
1	B	8	VAL	2.1
1	A	486	ASN	2.1
1	B	331	GLY	2.1
1	A	79	PRO	2.1
1	A	318	ASN	2.1
1	B	300	LEU	2.1
1	A	164	THR	2.1
1	B	208	ILE	2.1
1	B	370	ILE	2.1
1	A	183	VAL	2.1
1	B	274	VAL	2.1
1	A	14	LEU	2.1
1	A	138	LEU	2.1
1	A	411	ARG	2.1
1	B	281	GLU	2.1
1	B	289	ASP	2.1
1	A	308	LEU	2.0
1	B	82	ASN	2.0
1	A	225	GLY	2.0
1	B	338	GLY	2.0
1	B	455	HIS	2.0
1	B	23	LYS	2.0
1	B	140	GLY	2.0
1	B	30	ASP	2.0
1	B	109	ASP	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

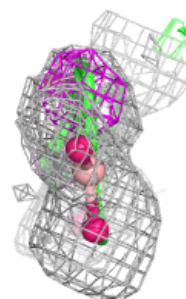
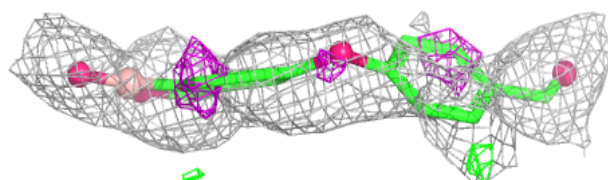
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	92N	B	602	19/19	0.68	0.19	21,25,27,27	0
3	92N	A	602	19/19	0.72	0.19	22,28,29,30	0
2	NAD	B	601	44/44	0.84	0.14	13,21,28,32	0
2	NAD	A	601	44/44	0.85	0.14	11,22,27,29	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.

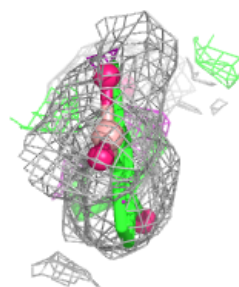
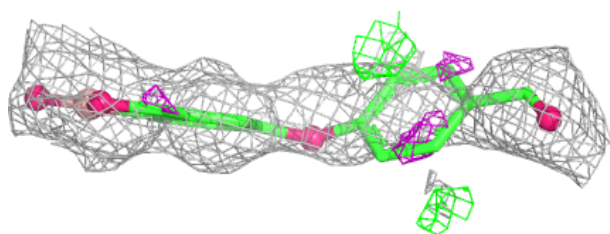
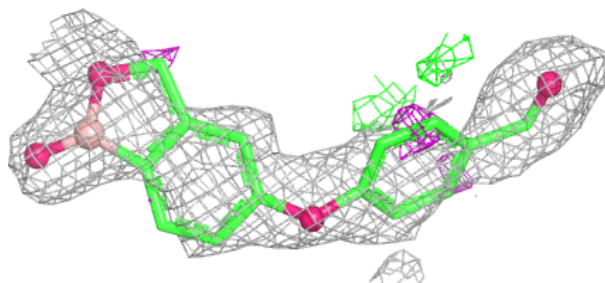
Electron density around 92N B 602:

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

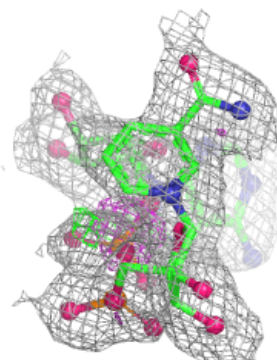
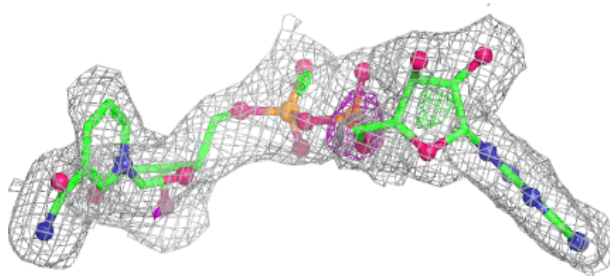
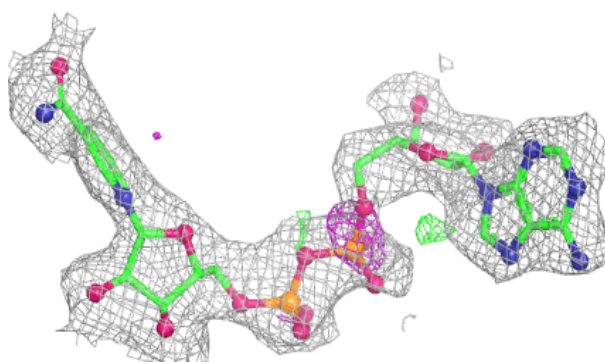


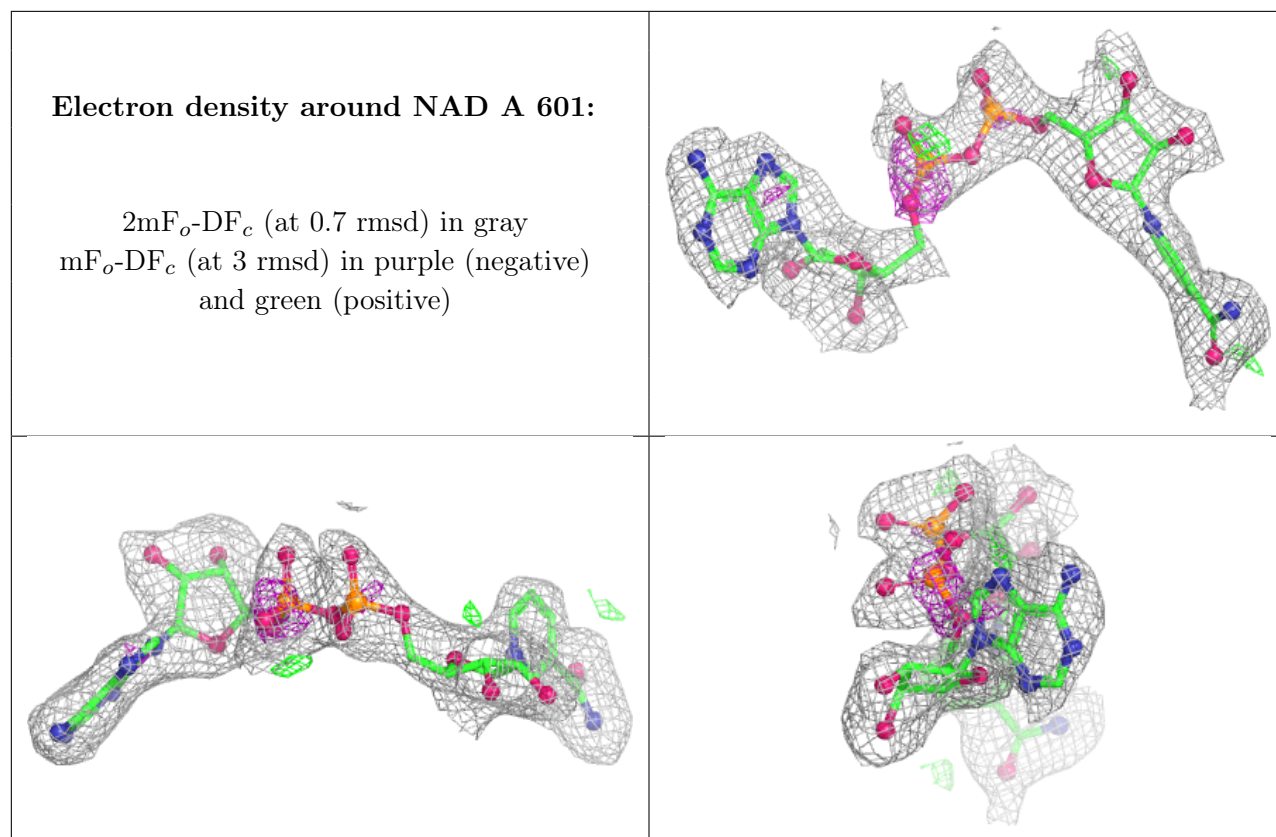
Electron density around 92N A 602:

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

**Electron density around NAD B 601:**

$2mF_o-DF_c$ (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.