



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2021 – 06:06 PM EDT

PDB ID : 5KLN
Title : Crystal structure of 2-aminomuconate 6-semialdehyde dehydrogenase N169A
in complex with NAD⁺
Authors : Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on : 2016-06-24
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

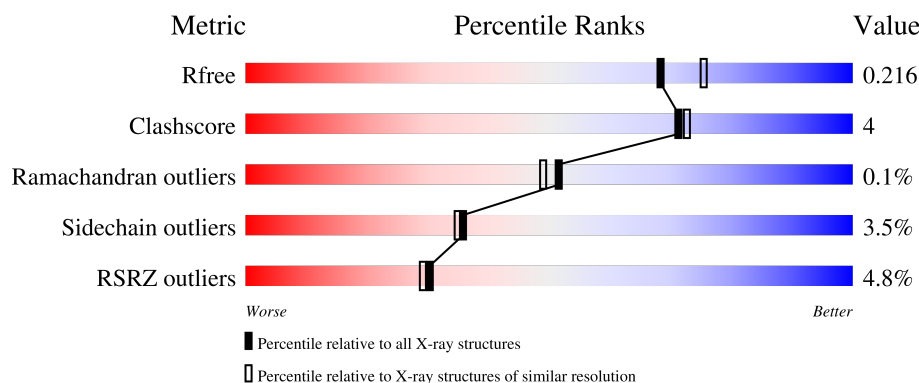
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 $\leq 5\%$. 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	520	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	520	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	C	520	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	520	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16060 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 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3675	2325	637	701	12			
1	D	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	B	483	Total	C	N	O	S	0	2	0
			3690	2332	644	702	12			
1	C	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q83V33
A	-18	GLY	-	expression tag	UNP Q83V33
A	-17	SER	-	expression tag	UNP Q83V33
A	-16	SER	-	expression tag	UNP Q83V33
A	-15	HIS	-	expression tag	UNP Q83V33
A	-14	HIS	-	expression tag	UNP Q83V33
A	-13	HIS	-	expression tag	UNP Q83V33
A	-12	HIS	-	expression tag	UNP Q83V33
A	-11	HIS	-	expression tag	UNP Q83V33
A	-10	HIS	-	expression tag	UNP Q83V33
A	-9	SER	-	expression tag	UNP Q83V33
A	-8	SER	-	expression tag	UNP Q83V33
A	-7	GLY	-	expression tag	UNP Q83V33
A	-6	LEU	-	expression tag	UNP Q83V33
A	-5	VAL	-	expression tag	UNP Q83V33
A	-4	PRO	-	expression tag	UNP Q83V33
A	-3	ARG	-	expression tag	UNP Q83V33
A	-2	GLY	-	expression tag	UNP Q83V33
A	-1	SER	-	expression tag	UNP Q83V33
A	0	HIS	-	expression tag	UNP Q83V33
A	169	ALA	ASN	engineered mutation	UNP Q83V33

Continued on next page...

Continued from previous page...

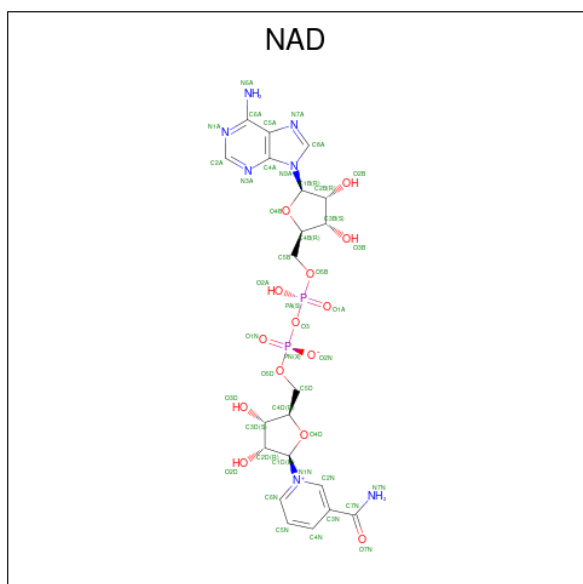
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q83V33
D	-18	GLY	-	expression tag	UNP Q83V33
D	-17	SER	-	expression tag	UNP Q83V33
D	-16	SER	-	expression tag	UNP Q83V33
D	-15	HIS	-	expression tag	UNP Q83V33
D	-14	HIS	-	expression tag	UNP Q83V33
D	-13	HIS	-	expression tag	UNP Q83V33
D	-12	HIS	-	expression tag	UNP Q83V33
D	-11	HIS	-	expression tag	UNP Q83V33
D	-10	HIS	-	expression tag	UNP Q83V33
D	-9	SER	-	expression tag	UNP Q83V33
D	-8	SER	-	expression tag	UNP Q83V33
D	-7	GLY	-	expression tag	UNP Q83V33
D	-6	LEU	-	expression tag	UNP Q83V33
D	-5	VAL	-	expression tag	UNP Q83V33
D	-4	PRO	-	expression tag	UNP Q83V33
D	-3	ARG	-	expression tag	UNP Q83V33
D	-2	GLY	-	expression tag	UNP Q83V33
D	-1	SER	-	expression tag	UNP Q83V33
D	0	HIS	-	expression tag	UNP Q83V33
D	169	ALA	ASN	engineered mutation	UNP Q83V33
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression tag	UNP Q83V33
B	-12	HIS	-	expression tag	UNP Q83V33
B	-11	HIS	-	expression tag	UNP Q83V33
B	-10	HIS	-	expression tag	UNP Q83V33
B	-9	SER	-	expression tag	UNP Q83V33
B	-8	SER	-	expression tag	UNP Q83V33
B	-7	GLY	-	expression tag	UNP Q83V33
B	-6	LEU	-	expression tag	UNP Q83V33
B	-5	VAL	-	expression tag	UNP Q83V33
B	-4	PRO	-	expression tag	UNP Q83V33
B	-3	ARG	-	expression tag	UNP Q83V33
B	-2	GLY	-	expression tag	UNP Q83V33
B	-1	SER	-	expression tag	UNP Q83V33
B	0	HIS	-	expression tag	UNP Q83V33
B	169	ALA	ASN	engineered mutation	UNP Q83V33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression tag	UNP Q83V33
C	-12	HIS	-	expression tag	UNP Q83V33
C	-11	HIS	-	expression tag	UNP Q83V33
C	-10	HIS	-	expression tag	UNP Q83V33
C	-9	SER	-	expression tag	UNP Q83V33
C	-8	SER	-	expression tag	UNP Q83V33
C	-7	GLY	-	expression tag	UNP Q83V33
C	-6	LEU	-	expression tag	UNP Q83V33
C	-5	VAL	-	expression tag	UNP Q83V33
C	-4	PRO	-	expression tag	UNP Q83V33
C	-3	ARG	-	expression tag	UNP Q83V33
C	-2	GLY	-	expression tag	UNP Q83V33
C	-1	SER	-	expression tag	UNP Q83V33
C	0	HIS	-	expression tag	UNP Q83V33
C	169	ALA	ASN	engineered mutation	UNP Q83V33

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



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

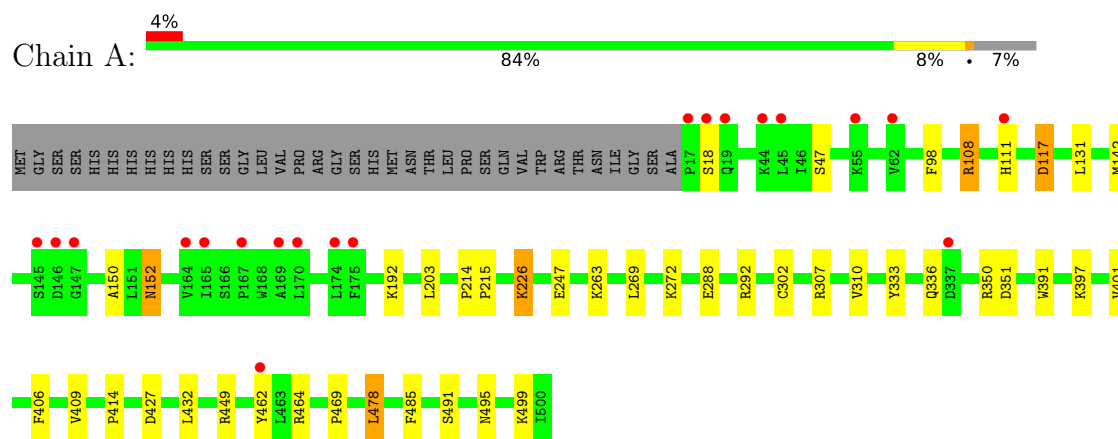
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	313	Total	O	0	0
			313	313		
4	D	241	Total	O	0	0
			241	241		
4	B	327	Total	O	0	0
			327	327		
4	C	298	Total	O	0	0
			298	298		

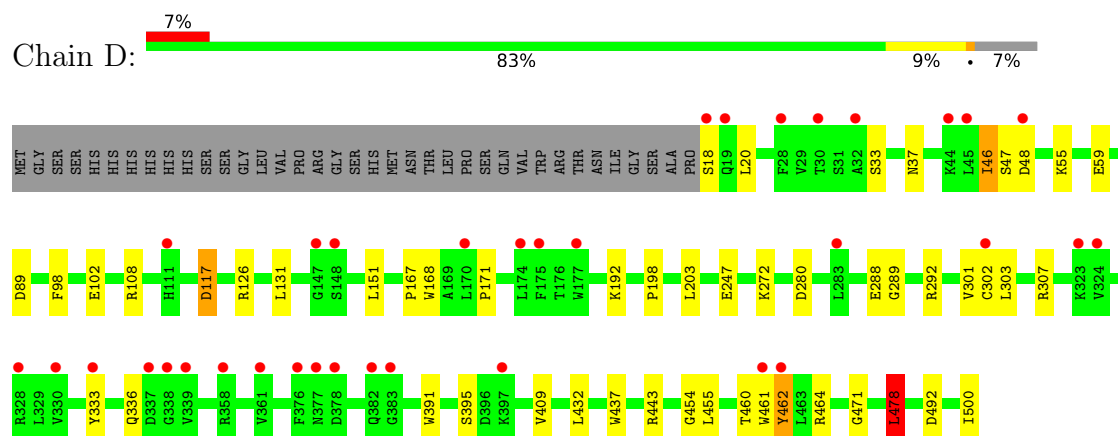
3 Residue-property plots [i](#)

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.

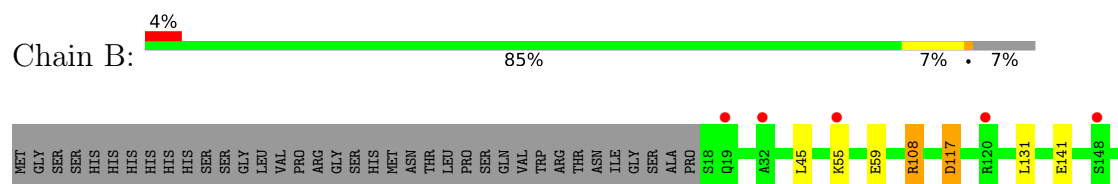
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

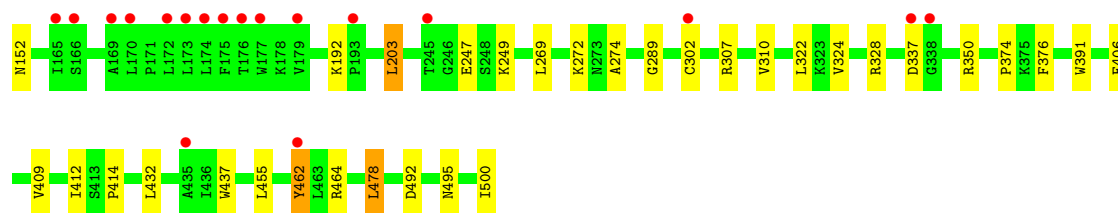


- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

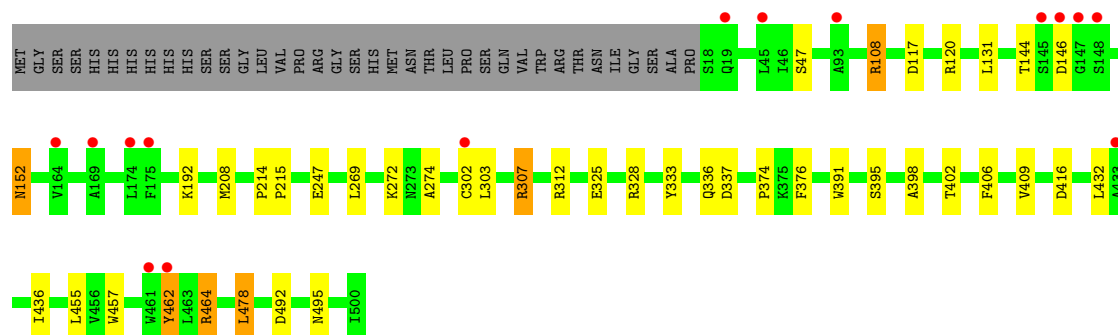
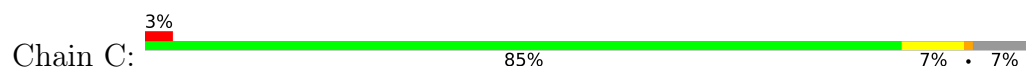


- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase





● Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.70Å 140.99Å 173.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 1.99 34.54 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.54-1.99) 96.4 (34.54-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX phenix.refine: 1.7.3_928	Depositor
R, R_{free}	0.187 , 0.222 0.183 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16060	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: NA, 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	0.41	0/3755	0.57	1/5105 (0.0%)
1	B	0.42	0/3769	0.58	1/5122 (0.0%)
1	C	0.42	0/3747	0.58	3/5094 (0.1%)
1	D	0.37	0/3747	0.54	1/5094 (0.0%)
All	All	0.40	0/15018	0.57	6/20415 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	LEU	CA-CB-CG	7.93	133.55	115.30
1	D	478	LEU	CA-CB-CG	7.04	131.50	115.30
1	C	478	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	307	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	478	LEU	CA-CB-CG	6.26	129.71	115.30
1	C	307	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	3675	0	3612	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3690	0	3628	25	0
1	C	3668	0	3604	19	0
1	D	3668	0	3604	29	0
2	A	44	0	26	3	0
2	B	44	0	26	2	0
2	C	44	0	26	3	0
2	D	44	0	26	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	313	0	0	6	0
4	B	327	0	0	1	0
4	C	298	0	0	1	0
4	D	241	0	0	4	0
All	All	16060	0	14552	103	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 4.

All (103) 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:D:280:ASP:OD2	1:D:443:ARG:NH1	2.16	0.77
1:C:152:ASN:OD1	1:C:495:ASN:ND2	2.18	0.77
1:B:152:ASN:OD1	1:B:495:ASN:ND2	2.21	0.73
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.72	0.72
1:A:449:ARG:NH2	1:B:141:GLU:OE2	2.24	0.71
1:A:247:GLU:OE2	4:A:701:HOH:O	2.08	0.71
1:C:302:CYS:SG	2:C:601:NAD:C4N	2.79	0.70
1:A:350:ARG:NH1	1:A:351:ASP:OD1	2.26	0.69
1:A:288:GLU:OE1	1:A:292:ARG:NH2	2.27	0.67
1:A:302:CYS:SG	2:A:601:NAD:C4N	2.83	0.67
1:B:302:CYS:SG	2:B:601:NAD:C4N	2.84	0.66
1:A:18:SER:HB3	1:A:47:SER:HB3	1.76	0.66
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.78	0.66
1:D:462:TYR:HE1	1:D:464:ARG:HG3	1.62	0.64
1:B:350[B]:ARG:HG2	1:B:350[B]:ARG:HH11	1.62	0.64
1:A:152:ASN:OD1	1:A:495:ASN:ND2	2.30	0.64
1:D:302:CYS:SG	2:D:601:NAD:C4N	2.86	0.64
1:B:247:GLU:OE2	4:B:701:HOH:O	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:TYR:CE1	1:D:464:ARG:HG3	2.35	0.61
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.66	0.61
1:A:491:SER:O	4:A:702:HOH:O	2.16	0.60
1:C:247:GLU:OE2	4:C:701:HOH:O	2.17	0.60
1:A:226:LYS:HE2	2:A:601:NAD:N7A	2.17	0.60
1:A:449:ARG:HH22	1:B:141:GLU:CD	2.05	0.60
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.82	0.60
1:A:292:ARG:NH1	4:A:703:HOH:O	2.24	0.59
1:C:108:ARG:HD3	1:C:117:ASP:OD2	2.03	0.59
1:C:312:ARG:HD2	1:C:416:ASP:OD1	2.03	0.59
1:B:152:ASN:ND2	1:B:495:ASN:OD1	2.26	0.58
1:A:495:ASN:HD22	1:D:455:LEU:HD13	1.69	0.57
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.87	0.57
1:A:397:LYS:NZ	4:A:712:HOH:O	2.38	0.55
1:D:464:ARG:NH2	4:D:701:HOH:O	2.19	0.55
1:D:333:TYR:HB2	1:D:336:GLN:HB2	1.89	0.55
1:D:18:SER:HB3	1:D:47:SER:HB3	1.88	0.55
1:B:117:ASP:N	1:B:117:ASP:OD1	2.38	0.54
1:B:108:ARG:HD3	1:B:117:ASP:OD2	2.07	0.54
1:C:269:LEU:O	2:C:601:NAD:H2N	2.09	0.53
1:D:55:LYS:O	1:D:59:GLU:HG3	2.09	0.53
1:A:269:LEU:O	2:A:601:NAD:H2N	2.10	0.52
1:B:350[B]:ARG:HH11	1:B:350[B]:ARG:CG	2.22	0.52
1:A:333:TYR:HB2	1:A:336:GLN:HB2	1.91	0.52
1:C:303:LEU:HD13	1:C:457:TRP:HH2	1.75	0.51
1:D:37:ASN:O	1:D:46:ILE:HG13	2.10	0.51
1:D:151:LEU:HG	1:D:500:ILE:HD11	1.94	0.50
1:B:55:LYS:HE3	1:B:59:GLU:OE1	2.11	0.50
1:C:333:TYR:HB2	1:C:336:GLN:HB2	1.95	0.49
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.48	0.48
1:A:449:ARG:HG3	1:A:449:ARG:HH21	1.78	0.48
1:D:98:PHE:CE1	1:D:203:LEU:HB3	2.49	0.48
1:D:288:GLU:OE2	1:D:292:ARG:NE	2.47	0.48
1:A:117:ASP:OD1	1:A:117:ASP:N	2.44	0.48
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.49	0.48
1:D:117:ASP:N	1:D:117:ASP:OD1	2.47	0.48
1:D:20:LEU:HD12	1:D:198:PRO:HG2	1.97	0.47
1:D:247:GLU:OE2	4:D:702:HOH:O	2.20	0.47
1:C:144:THR:OG1	1:C:146:ASP:OD1	2.28	0.46
1:B:269:LEU:O	2:B:601:NAD:H2N	2.15	0.46
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:O	1:B:414:PRO:HA	2.16	0.46
1:B:249:LYS:HB3	1:B:249:LYS:HE2	1.74	0.46
1:D:168:TRP:O	1:D:171:PRO:HD3	2.16	0.46
1:D:461:TRP:CE3	1:D:462:TYR:HB2	2.51	0.45
1:B:289:GLY:HA3	1:B:437:TRP:CZ2	2.50	0.45
1:B:350[B]:ARG:HG2	1:B:350[B]:ARG:NH1	2.29	0.45
1:C:398:ALA:O	1:C:402:THR:HG23	2.16	0.45
1:A:397:LYS:NZ	1:A:427:ASP:OD2	2.49	0.45
1:B:274:ALA:HA	1:B:307:ARG:O	2.17	0.45
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.86	0.45
1:C:462:TYR:CE1	1:C:464:ARG:HG3	2.52	0.44
1:D:289:GLY:HA3	1:D:437:TRP:CZ2	2.53	0.44
1:A:111:HIS:HB3	4:A:921:HOH:O	2.17	0.44
1:D:301:VAL:HG12	1:D:303:LEU:H	1.82	0.44
1:C:302:CYS:SG	2:C:601:NAD:C3N	3.06	0.44
1:A:18:SER:CB	1:A:47:SER:HB3	2.47	0.43
1:C:117:ASP:N	1:C:117:ASP:OD1	2.49	0.43
1:D:288:GLU:OE1	4:D:703:HOH:O	2.21	0.43
1:A:397:LYS:HD3	1:A:397:LYS:HA	1.77	0.43
1:A:263:LYS:O	1:D:478:LEU:HD12	2.18	0.43
1:A:142:MET:HG3	1:A:150:ALA:HB3	2.00	0.43
1:B:272:LYS:HG3	1:B:307:ARG:CD	2.49	0.43
1:B:324:VAL:O	1:B:328:ARG:HG3	2.19	0.42
1:A:391:TRP:CH2	1:A:409:VAL:HG21	2.54	0.42
1:D:102:GLU:OE2	1:D:171:PRO:HG2	2.18	0.42
1:D:454:GLY:HA3	1:D:471:GLY:O	2.19	0.42
1:A:310:VAL:O	1:A:414:PRO:HA	2.20	0.42
1:D:89:ASP:OD1	1:D:126:ARG:NH2	2.44	0.42
1:C:214:PRO:HA	1:C:215:PRO:HD3	1.91	0.42
1:A:469:PRO:HB3	1:A:485:PHE:CD2	2.54	0.42
1:A:98:PHE:CE1	1:A:203:LEU:HB3	2.55	0.42
1:A:499:LYS:HB2	1:D:460:THR:HB	2.02	0.42
1:B:322:LEU:HD23	1:B:412:ILE:HD11	2.02	0.42
1:C:374:PRO:HG2	1:C:376:PHE:CE2	2.55	0.41
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.53	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.91	0.41
2:D:601:NAD:O2N	4:D:702:HOH:O	2.22	0.41
1:B:374:PRO:HG2	1:B:376:PHE:CZ	2.55	0.41
1:A:464:ARG:NH1	4:A:708:HOH:O	2.34	0.41
1:A:108:ARG:HD3	1:A:117:ASP:OD2	2.21	0.41
1:C:274:ALA:HA	1:C:307:ARG:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.87	0.40
1:D:302:CYS:SG	2:D:601:NAD:C3N	3.10	0.40
1:B:462:TYR:CE1	1:B:464:ARG:HG3	2.57	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	482/520 (93%)	467 (97%)	15 (3%)	0	100	100
1	B	483/520 (93%)	469 (97%)	14 (3%)	0	100	100
1	C	481/520 (92%)	467 (97%)	14 (3%)	0	100	100
1	D	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	47	44
All	All	1927/2080 (93%)	1869 (97%)	57 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	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	392/423 (93%)	381 (97%)	11 (3%)	43	44
1	B	393/423 (93%)	379 (96%)	14 (4%)	35	34
1	C	391/423 (92%)	374 (96%)	17 (4%)	29	26
1	D	391/423 (92%)	379 (97%)	12 (3%)	40	40
All	All	1567/1692 (93%)	1513 (97%)	54 (3%)	36	36

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	117	ASP
1	A	131	LEU
1	A	152	ASN
1	A	192	LYS
1	A	226	LYS
1	A	401	VAL
1	A	406	PHE
1	A	432	LEU
1	A	462	TYR
1	A	478	LEU
1	D	33	SER
1	D	46	ILE
1	D	48	ASP
1	D	108	ARG
1	D	117	ASP
1	D	131	LEU
1	D	192	LYS
1	D	395	SER
1	D	432	LEU
1	D	462	TYR
1	D	478	LEU
1	D	492	ASP
1	B	45	LEU
1	B	108	ARG
1	B	117	ASP
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	337	ASP
1	B	406	PHE
1	B	432	LEU
1	B	455	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	462	TYR
1	B	478	LEU
1	B	492	ASP
1	B	500	ILE
1	C	47	SER
1	C	108	ARG
1	C	120	ARG
1	C	131	LEU
1	C	152	ASN
1	C	192	LYS
1	C	208	MET
1	C	337	ASP
1	C	395	SER
1	C	406	PHE
1	C	432	LEU
1	C	436	ILE
1	C	455	LEU
1	C	462	TYR
1	C	464	ARG
1	C	478	LEU
1	C	492	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	495	ASN
1	C	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	601	-	42,48,48	1.96	10 (23%)	50,73,73	1.24	6 (12%)
2	NAD	D	601	-	42,48,48	2.01	11 (26%)	50,73,73	1.31	5 (10%)
2	NAD	A	601	-	42,48,48	1.92	7 (16%)	50,73,73	1.34	5 (10%)
2	NAD	C	601	-	42,48,48	1.93	7 (16%)	50,73,73	1.30	5 (10%)

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	-	-	3/26/62/62	0/5/5/5
2	NAD	D	601	-	-	1/26/62/62	0/5/5/5
2	NAD	A	601	-	-	4/26/62/62	0/5/5/5
2	NAD	C	601	-	-	2/26/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C7N-N7N	8.12	1.48	1.33
2	A	601	NAD	C7N-N7N	7.94	1.48	1.33
2	B	601	NAD	C7N-N7N	7.83	1.47	1.33
2	C	601	NAD	C7N-N7N	7.60	1.47	1.33
2	C	601	NAD	C2B-C3B	-4.38	1.41	1.53
2	B	601	NAD	C2B-C3B	-4.21	1.41	1.53
2	C	601	NAD	C2D-C1D	-4.10	1.47	1.53
2	D	601	NAD	C2B-C3B	-4.07	1.42	1.53
2	D	601	NAD	C2D-C1D	-4.00	1.47	1.53
2	A	601	NAD	C2B-C3B	-3.98	1.42	1.53
2	A	601	NAD	C2D-C1D	-3.77	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C6A-N6A	3.75	1.47	1.34
2	B	601	NAD	C2D-C1D	-3.71	1.48	1.53
2	A	601	NAD	C6A-N6A	3.66	1.47	1.34
2	B	601	NAD	C6A-N6A	3.60	1.47	1.34
2	C	601	NAD	C6A-N6A	3.58	1.47	1.34
2	B	601	NAD	C2B-C1B	-2.76	1.49	1.53
2	C	601	NAD	C2B-C1B	-2.67	1.49	1.53
2	A	601	NAD	C2B-C1B	-2.56	1.49	1.53
2	D	601	NAD	O2B-C2B	-2.51	1.37	1.43
2	D	601	NAD	O4B-C4B	-2.43	1.39	1.45
2	B	601	NAD	O2B-C2B	-2.42	1.37	1.43
2	C	601	NAD	O2B-C2B	-2.34	1.37	1.43
2	D	601	NAD	C2D-C3D	-2.31	1.47	1.53
2	D	601	NAD	C3D-C4D	-2.28	1.47	1.53
2	C	601	NAD	O4B-C4B	-2.25	1.40	1.45
2	D	601	NAD	C2B-C1B	-2.24	1.50	1.53
2	B	601	NAD	O7N-C7N	2.19	1.28	1.24
2	B	601	NAD	C3N-C7N	-2.17	1.47	1.50
2	D	601	NAD	O2D-C2D	-2.16	1.37	1.43
2	B	601	NAD	C2D-C3D	-2.12	1.47	1.53
2	D	601	NAD	O7N-C7N	2.11	1.28	1.24
2	A	601	NAD	C2D-C3D	-2.07	1.47	1.53
2	A	601	NAD	O4B-C4B	-2.02	1.40	1.45
2	B	601	NAD	O4B-C4B	-2.00	1.40	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C3N-C7N-N7N	4.56	123.22	117.75
2	D	601	NAD	N3A-C2A-N1A	-4.28	121.98	128.68
2	B	601	NAD	N3A-C2A-N1A	-4.03	122.38	128.68
2	A	601	NAD	O7N-C7N-N7N	-3.94	116.99	122.58
2	D	601	NAD	C3N-C7N-N7N	3.80	122.31	117.75
2	A	601	NAD	N3A-C2A-N1A	-3.78	122.77	128.68
2	C	601	NAD	N3A-C2A-N1A	-3.78	122.77	128.68
2	B	601	NAD	O4D-C1D-C2D	-3.62	101.64	106.93
2	C	601	NAD	O7N-C7N-N7N	-3.53	117.56	122.58
2	C	601	NAD	C3N-C7N-N7N	3.34	121.76	117.75
2	D	601	NAD	O7N-C7N-N7N	-3.32	117.86	122.58
2	C	601	NAD	O4D-C1D-C2D	-3.25	102.18	106.93
2	C	601	NAD	O5D-C5D-C4D	3.24	120.14	108.99
2	B	601	NAD	O5D-C5D-C4D	2.72	118.36	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	O5D-C5D-C4D	2.63	118.04	108.99
2	D	601	NAD	O4D-C1D-C2D	-2.45	103.35	106.93
2	B	601	NAD	O7N-C7N-N7N	-2.45	119.10	122.58
2	D	601	NAD	O5B-C5B-C4B	2.33	117.00	108.99
2	B	601	NAD	C3N-C7N-N7N	2.31	120.53	117.75
2	B	601	NAD	O5B-C5B-C4B	2.28	116.84	108.99
2	A	601	NAD	O5B-C5B-C4B	2.25	116.73	108.99

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	NAD	C4D-C5D-O5D-PN
2	C	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C4D-C5D-O5D-PN
2	B	601	NAD	C5B-O5B-PA-O3
2	D	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	C3D-C4D-C5D-O5D
2	A	601	NAD	O4D-C4D-C5D-O5D
2	A	601	NAD	C5B-O5B-PA-O1A
2	C	601	NAD	C5B-O5B-PA-O1A

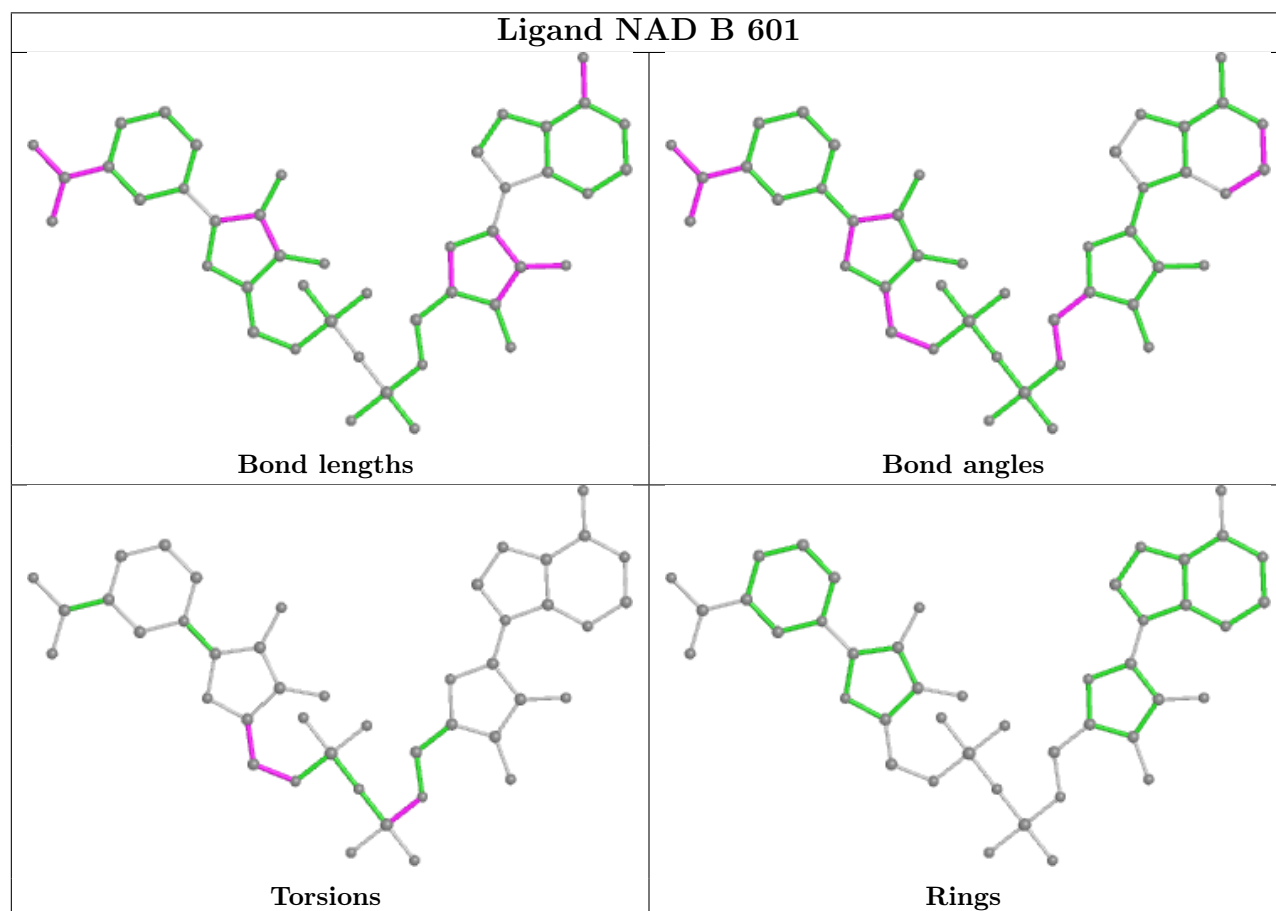
There are no ring outliers.

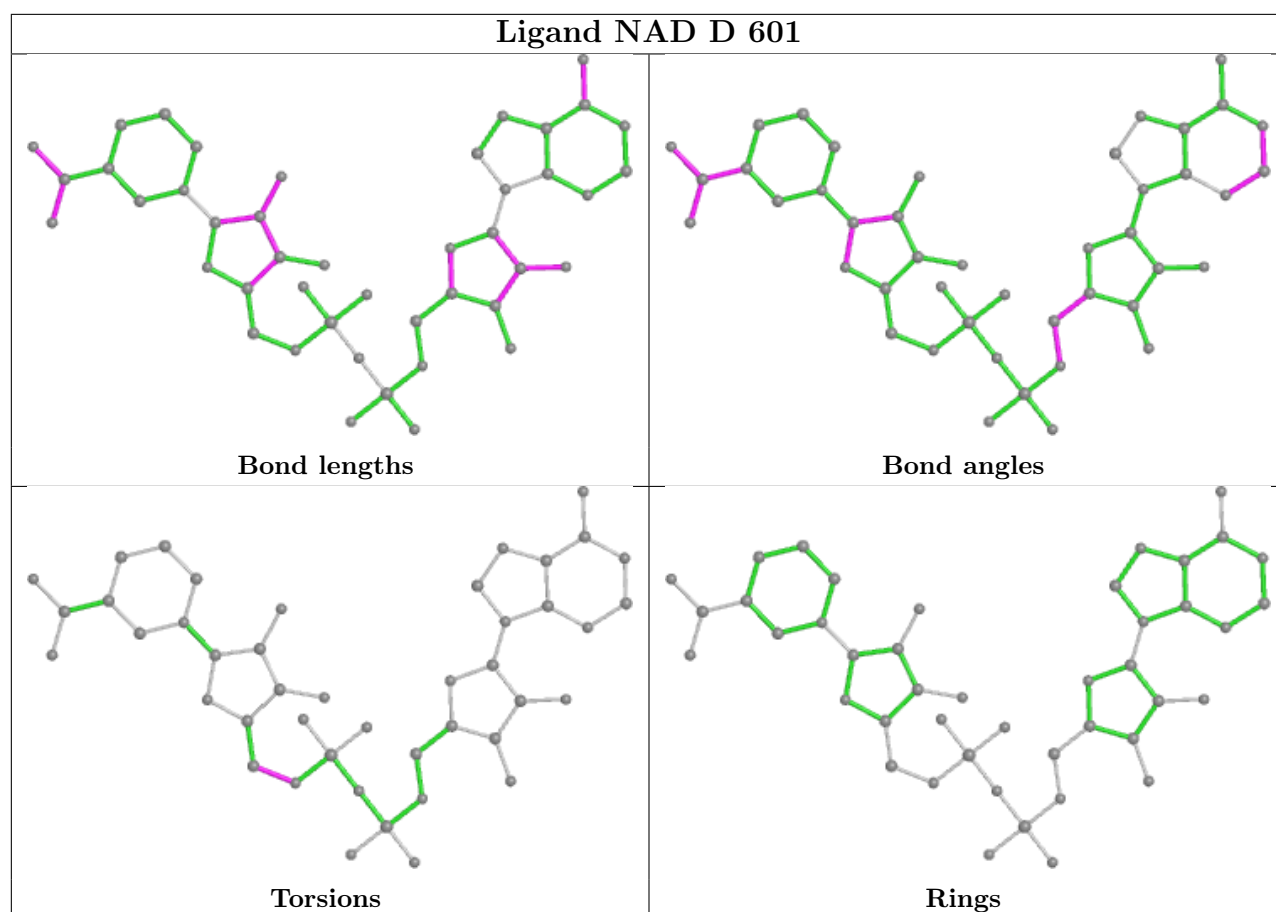
4 monomers are involved in 11 short contacts:

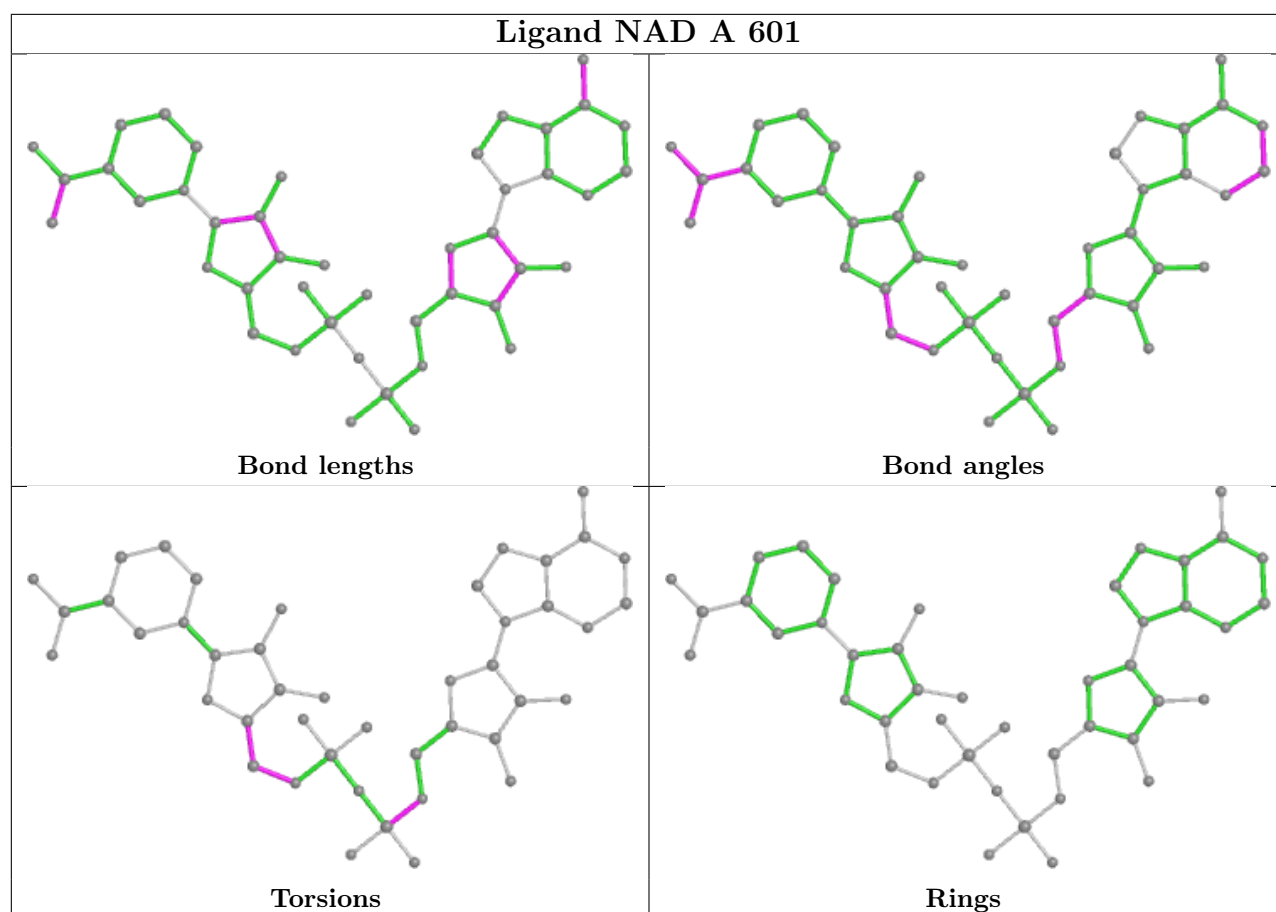
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAD	2	0
2	D	601	NAD	3	0
2	A	601	NAD	3	0
2	C	601	NAD	3	0

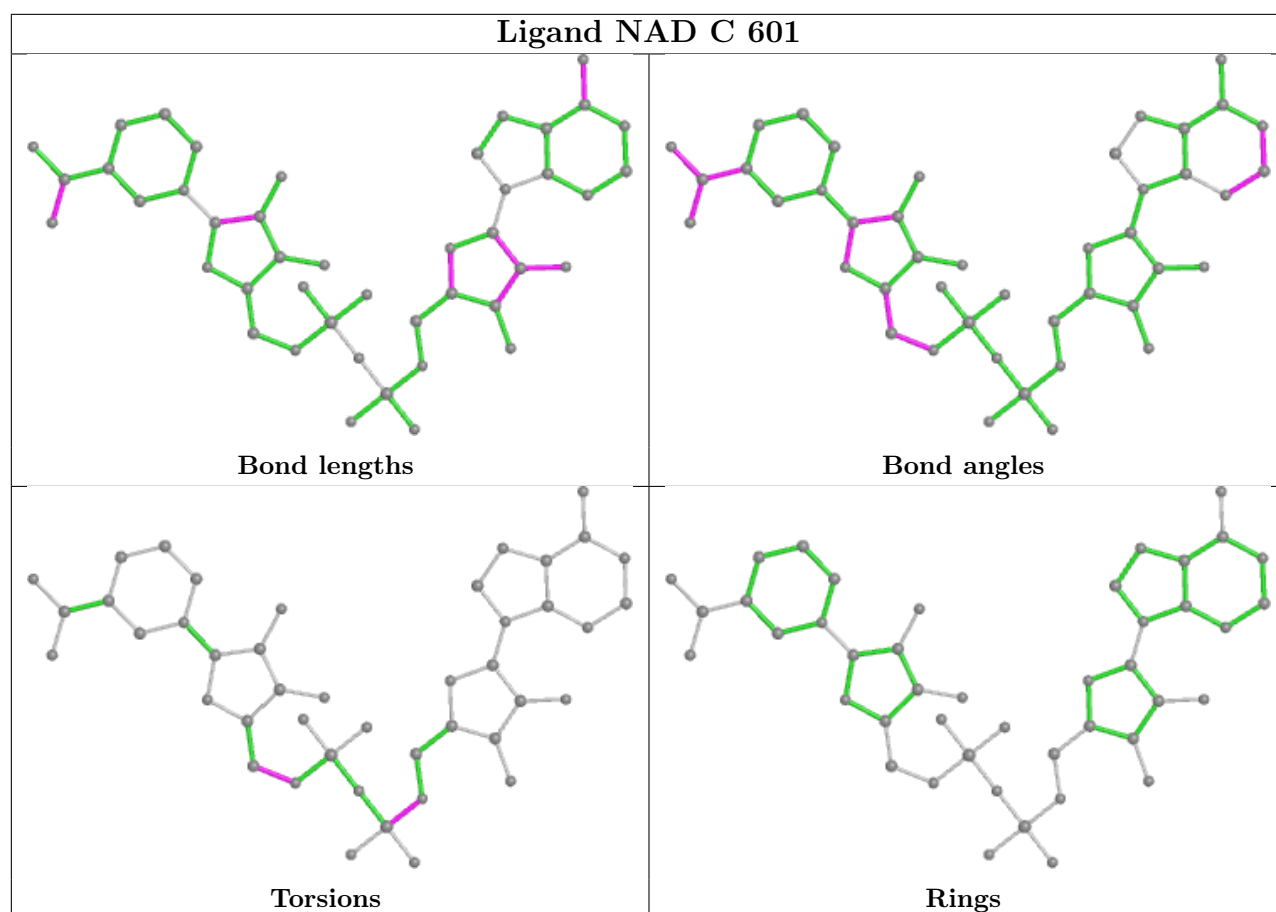
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	484/520 (93%)	0.22	20 (4%) 37 36	25, 36, 49, 70	0
1	B	483/520 (92%)	0.06	23 (4%) 30 29	25, 33, 46, 62	0
1	C	483/520 (92%)	0.11	15 (3%) 49 48	24, 34, 47, 58	0
1	D	483/520 (92%)	0.35	35 (7%) 15 14	27, 41, 57, 71	0
All	All	1933/2080 (92%)	0.18	93 (4%) 30 29	24, 36, 52, 71	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	GLY	4.7
1	A	17	PRO	4.3
1	A	45	LEU	4.2
1	B	174	LEU	3.9
1	D	45	LEU	3.8
1	D	337	ASP	3.5
1	D	361	VAL	3.5
1	C	93	ALA	3.3
1	C	461	TRP	3.3
1	D	462	TYR	3.3
1	A	55	LYS	3.2
1	D	378	ASP	3.2
1	D	111	HIS	3.1
1	D	333	TYR	3.1
1	D	382	GLN	3.1
1	D	28	PHE	3.1
1	A	164	VAL	3.1
1	B	337	ASP	3.0
1	D	376	PHE	3.0
1	D	328	ARG	3.0
1	D	383	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	GLY	2.9
1	B	338	GLY	2.9
1	A	174	LEU	2.9
1	D	44	LYS	2.9
1	C	174	LEU	2.9
1	A	170	LEU	2.9
1	D	174	LEU	2.9
1	C	462	TYR	2.8
1	D	18	SER	2.8
1	A	111	HIS	2.8
1	A	462	TYR	2.8
1	A	175	PHE	2.8
1	A	18	SER	2.7
1	A	145	SER	2.7
1	C	302	CYS	2.7
1	D	330	VAL	2.7
1	C	145	SER	2.6
1	B	170	LEU	2.5
1	C	148	SER	2.5
1	B	175	PHE	2.5
1	B	172	LEU	2.5
1	D	339	VAL	2.5
1	B	169	ALA	2.5
1	B	245	THR	2.5
1	D	32	ALA	2.5
1	D	461	TRP	2.5
1	C	146	ASP	2.5
1	B	32	ALA	2.4
1	B	173	LEU	2.4
1	B	166	SER	2.4
1	D	19	GLN	2.4
1	A	167	PRO	2.4
1	D	148	SER	2.3
1	B	55	LYS	2.3
1	D	177	TRP	2.3
1	D	302	CYS	2.3
1	D	377	ASN	2.3
1	B	179	VAL	2.3
1	B	177	TRP	2.3
1	A	165	ILE	2.3
1	C	164	VAL	2.2
1	D	397	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	169	ALA	2.2
1	D	175	PHE	2.2
1	D	170	LEU	2.2
1	B	462	TYR	2.2
1	C	433	ALA	2.2
1	A	146	ASP	2.2
1	C	147	GLY	2.2
1	A	19	GLN	2.2
1	B	165	ILE	2.1
1	A	62	VAL	2.1
1	D	30	THR	2.1
1	A	337	ASP	2.1
1	D	48	ASP	2.1
1	D	147	GLY	2.1
1	D	283	LEU	2.1
1	A	44	LYS	2.1
1	B	176	THR	2.1
1	D	324	VAL	2.1
1	C	175	PHE	2.1
1	A	169	ALA	2.1
1	D	323	LYS	2.1
1	D	358	ARG	2.0
1	B	435	ALA	2.0
1	B	302	CYS	2.0
1	B	120[A]	ARG	2.0
1	B	193	PRO	2.0
1	B	19	GLN	2.0
1	C	19	GLN	2.0
1	C	45	LEU	2.0
1	B	148	SER	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 ⓘ

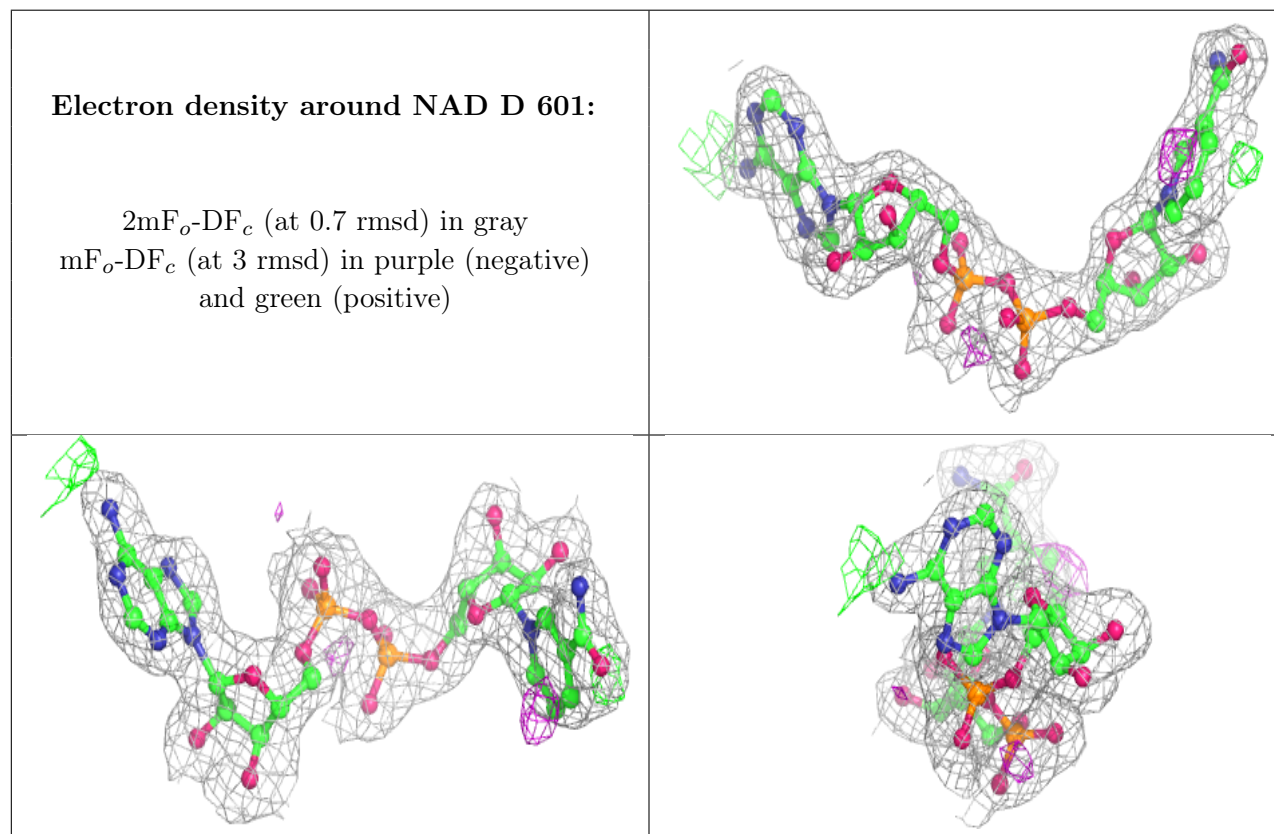
There are no monosaccharides in this entry.

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, 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.

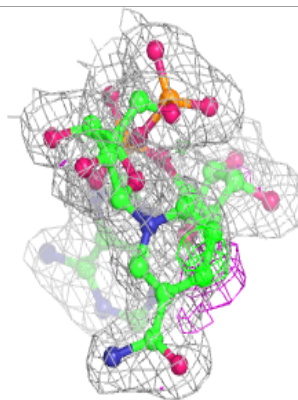
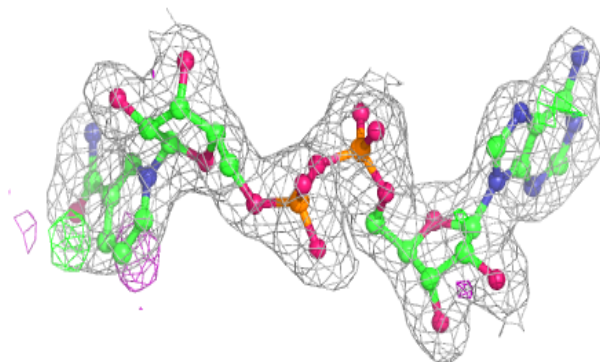
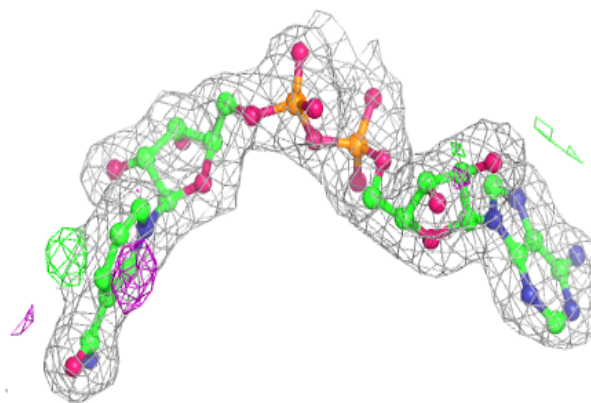
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	D	602	1/1	0.39	0.38	60,60,60,60	0
2	NAD	D	601	44/44	0.95	0.12	34,39,43,46	0
2	NAD	A	601	44/44	0.96	0.11	28,34,39,42	0
2	NAD	C	601	44/44	0.97	0.12	26,30,34,35	0
3	NA	A	602	1/1	0.97	0.22	32,32,32,32	0
2	NAD	B	601	44/44	0.97	0.11	26,31,33,38	0
3	NA	B	602	1/1	0.97	0.21	27,27,27,27	0
3	NA	C	602	1/1	0.98	0.22	30,30,30,30	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.

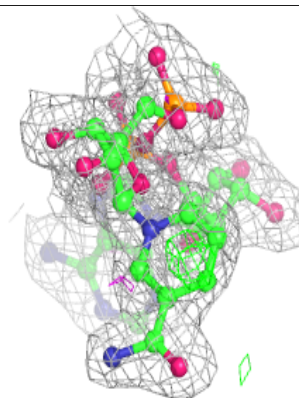
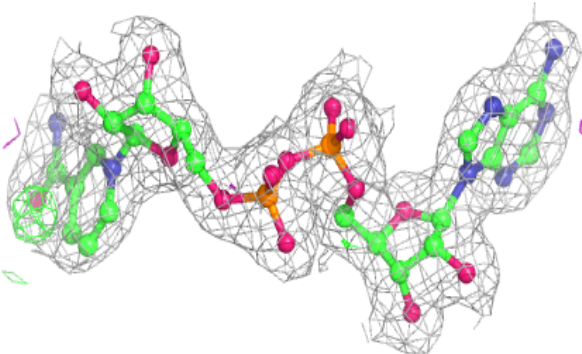
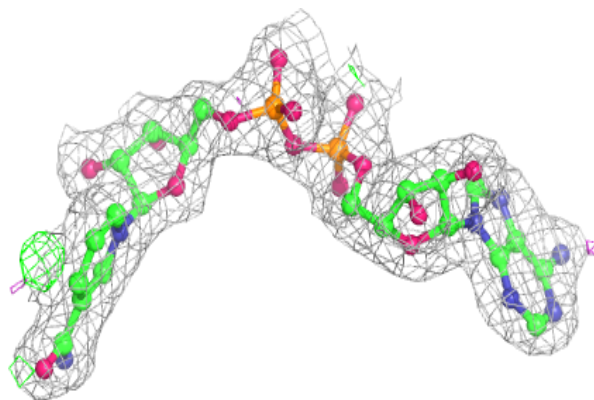


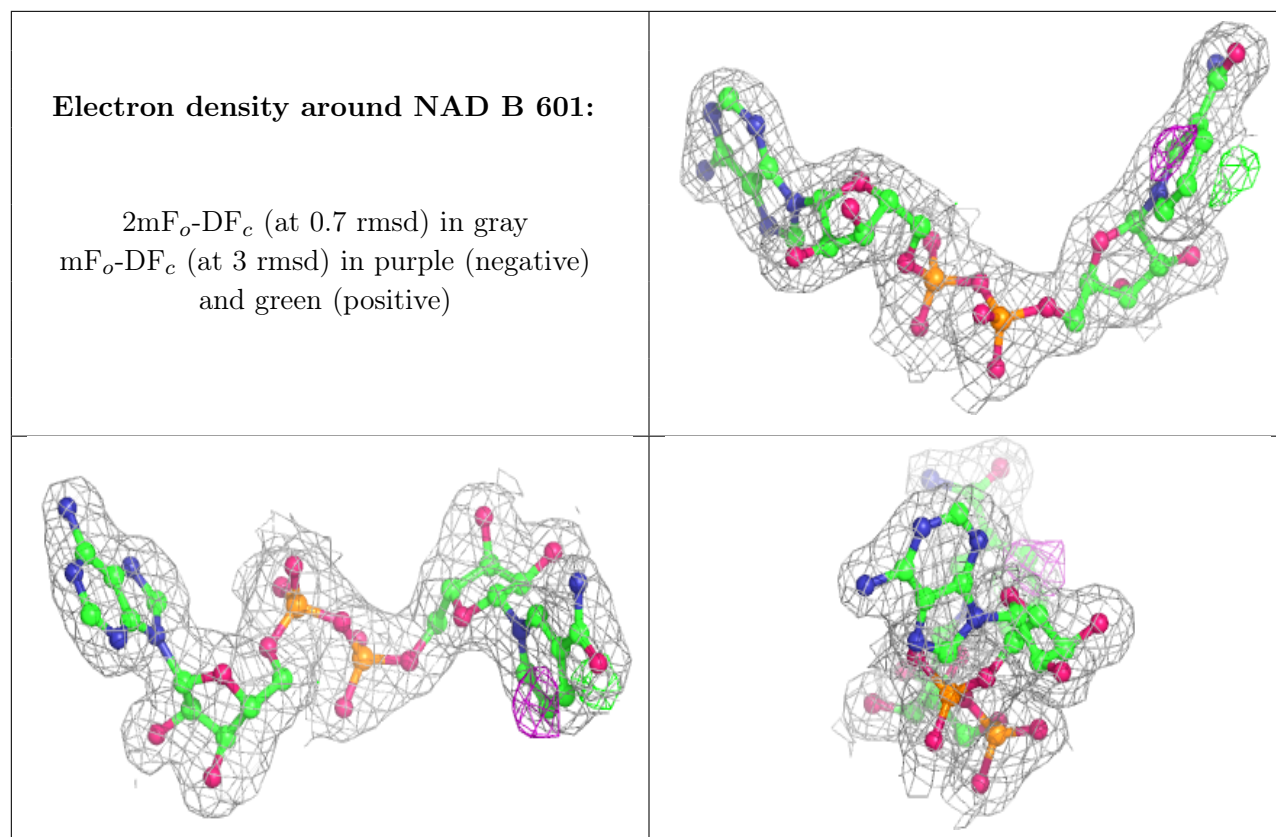
Electron density around NAD A 601:

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

**Electron density around NAD C 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.