



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:29 AM UTC

PDB ID : 8Y4B / pdb_00008y4b
Title : Crystal structure of L-2-keto-3-deoxyfuconate 4-dehydrogenase bound to L-2,4-DKDF and NADH
Authors : Akagashi, M.; Watanabe, S.
Deposited on : 2024-01-30
Resolution : 1.67 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

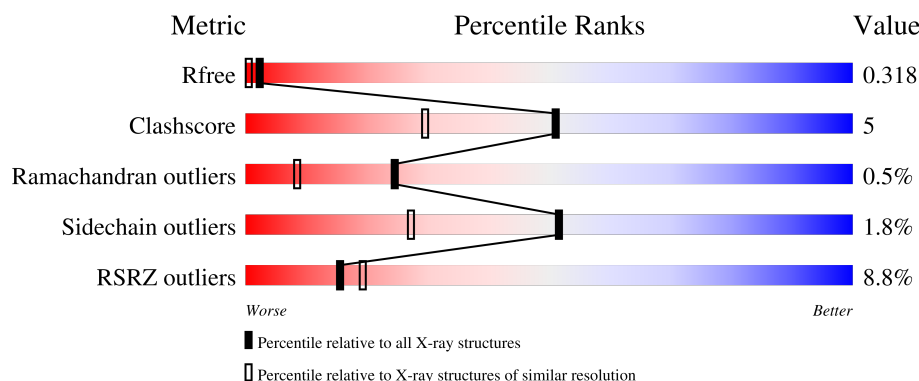
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	264	4% 84% 9% 6%
1	B	264	8% 78% 16% 6%
1	C	264	11% 80% 14% • 5%
1	D	264	10% 84% 9% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7801 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 SDR family oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1807	1128	319	352	8			
1	B	249	Total	C	N	O	S	0	0	0
			1785	1115	315	347	8			
1	C	250	Total	C	N	O	S	0	1	0
			1824	1139	321	356	8			
1	D	248	Total	C	N	O	S	7	1	0
			1805	1128	319	350	8			

There are 44 discrepancies between the modelled and reference sequences:

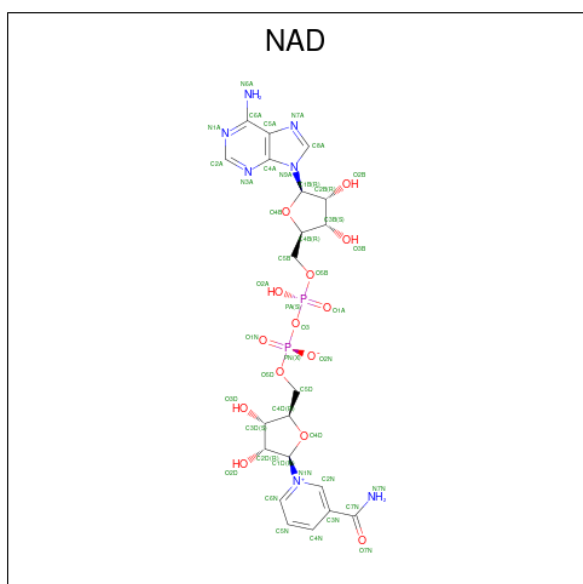
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A4P7ABK7
A	-8	ARG	-	expression tag	UNP A0A4P7ABK7
A	-7	GLY	-	expression tag	UNP A0A4P7ABK7
A	-6	SER	-	expression tag	UNP A0A4P7ABK7
A	-5	HIS	-	expression tag	UNP A0A4P7ABK7
A	-4	HIS	-	expression tag	UNP A0A4P7ABK7
A	-3	HIS	-	expression tag	UNP A0A4P7ABK7
A	-2	HIS	-	expression tag	UNP A0A4P7ABK7
A	-1	HIS	-	expression tag	UNP A0A4P7ABK7
A	0	HIS	-	expression tag	UNP A0A4P7ABK7
A	1	GLY	-	expression tag	UNP A0A4P7ABK7
B	-9	MET	-	initiating methionine	UNP A0A4P7ABK7
B	-8	ARG	-	expression tag	UNP A0A4P7ABK7
B	-7	GLY	-	expression tag	UNP A0A4P7ABK7
B	-6	SER	-	expression tag	UNP A0A4P7ABK7
B	-5	HIS	-	expression tag	UNP A0A4P7ABK7
B	-4	HIS	-	expression tag	UNP A0A4P7ABK7
B	-3	HIS	-	expression tag	UNP A0A4P7ABK7
B	-2	HIS	-	expression tag	UNP A0A4P7ABK7
B	-1	HIS	-	expression tag	UNP A0A4P7ABK7
B	0	HIS	-	expression tag	UNP A0A4P7ABK7

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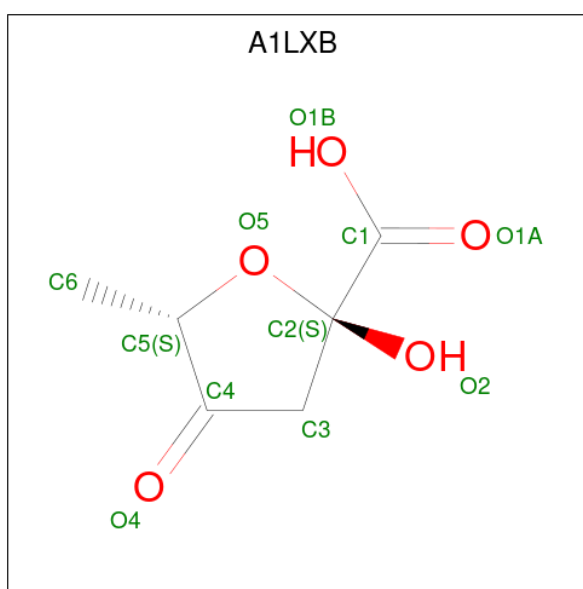
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP A0A4P7ABK7
C	-9	MET	-	initiating methionine	UNP A0A4P7ABK7
C	-8	ARG	-	expression tag	UNP A0A4P7ABK7
C	-7	GLY	-	expression tag	UNP A0A4P7ABK7
C	-6	SER	-	expression tag	UNP A0A4P7ABK7
C	-5	HIS	-	expression tag	UNP A0A4P7ABK7
C	-4	HIS	-	expression tag	UNP A0A4P7ABK7
C	-3	HIS	-	expression tag	UNP A0A4P7ABK7
C	-2	HIS	-	expression tag	UNP A0A4P7ABK7
C	-1	HIS	-	expression tag	UNP A0A4P7ABK7
C	0	HIS	-	expression tag	UNP A0A4P7ABK7
C	1	GLY	-	expression tag	UNP A0A4P7ABK7
D	-9	MET	-	initiating methionine	UNP A0A4P7ABK7
D	-8	ARG	-	expression tag	UNP A0A4P7ABK7
D	-7	GLY	-	expression tag	UNP A0A4P7ABK7
D	-6	SER	-	expression tag	UNP A0A4P7ABK7
D	-5	HIS	-	expression tag	UNP A0A4P7ABK7
D	-4	HIS	-	expression tag	UNP A0A4P7ABK7
D	-3	HIS	-	expression tag	UNP A0A4P7ABK7
D	-2	HIS	-	expression tag	UNP A0A4P7ABK7
D	-1	HIS	-	expression tag	UNP A0A4P7ABK7
D	0	HIS	-	expression tag	UNP A0A4P7ABK7
D	1	GLY	-	expression tag	UNP A0A4P7ABK7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

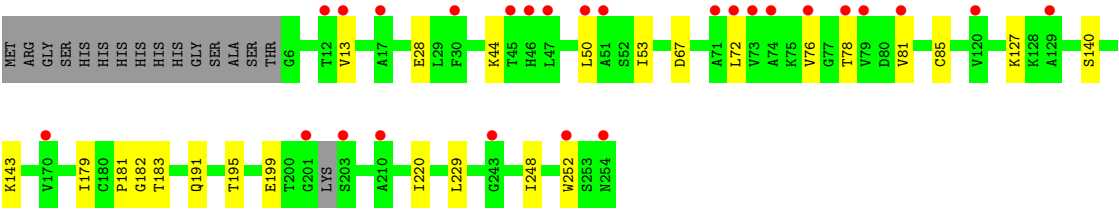
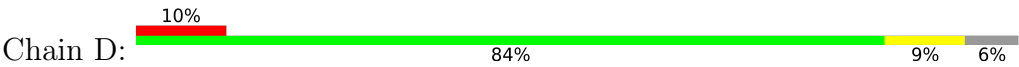
- Molecule 3 is L-2,4-diketo-3-deoxyfuconate (CCD ID: A1LXB) (formula: C₆H₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	90	Total	O	0	0
			90	90		
4	C	105	Total	O	0	0
			105	105		
4	D	86	Total	O	0	0
			86	86		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.87Å 119.54Å 129.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 1.67 44.32 – 1.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.32-1.67) 100.0 (44.32-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.67Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???), REFMAC 5	Depositor
R, R_{free}	0.266 , 0.317 0.271 , 0.318	Depositor DCC
R_{free} test set	5467 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7801	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: A1LXB, 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	0.33	0/1829	0.54	0/2471
1	B	0.32	0/1808	0.54	0/2451
1	C	0.29	0/1847	0.53	0/2501
1	D	0.29	0/1827	0.51	0/2472
All	All	0.31	0/7311	0.53	0/9895

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 [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	1807	0	1819	11	1
1	B	1785	0	1769	26	0
1	C	1824	0	1827	22	1
1	D	1805	0	1812	15	0
2	A	44	0	26	2	0
2	B	44	0	26	5	0
2	C	44	0	26	4	0
2	D	44	0	26	2	0
3	D	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	112	0	0	1	0
4	B	90	0	0	2	0
4	C	105	0	0	3	0
4	D	86	0	0	3	0
All	All	7801	0	7331	77	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 5.

All (77) 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:A:124:MET:HG2	1:A:130:GLY:HA3	1.50	0.94
1:D:78:THR:HG21	1:D:127:LYS:HD2	1.65	0.77
1:D:182:GLY:O	2:D:301:NAD:H4N	1.92	0.69
1:C:61:LEU:HD22	1:C:72:LEU:HD13	1.75	0.69
1:B:163:LYS:NZ	1:B:243:GLY:O	2.26	0.69
1:D:183:THR:HB	1:D:220:ILE:HD12	1.75	0.68
1:D:44:LYS:NZ	4:D:403:HOH:O	2.29	0.64
1:C:78:THR:HG21	1:C:127:LYS:HD2	1.78	0.64
1:C:66:ASP:OD2	1:C:118:ARG:NH2	2.31	0.64
1:B:214:ARG:O	1:B:252:TRP:HD1	1.80	0.63
1:A:203:SER:N	1:A:206:GLU:OE1	2.31	0.61
1:D:28:GLU:HG2	1:D:53:ILE:HD13	1.84	0.60
1:C:185:GLU:OE2	1:C:190:ASN:ND2	2.30	0.60
1:B:44:LYS:HB2	1:B:60:LEU:HD11	1.84	0.59
1:A:47:LEU:HG	1:A:58:THR:HB	1.83	0.59
1:B:13:VAL:HG22	1:B:81:VAL:HB	1.86	0.58
1:A:78:THR:HG21	1:A:127:LYS:HG3	1.86	0.57
1:B:42:ILE:HG23	2:B:301:NAD:C2A	2.35	0.57
1:B:61:LEU:HD22	1:B:72:LEU:HD23	1.87	0.57
1:B:217:MET:HE3	1:B:250:GLY:HA2	1.87	0.56
1:A:44:LYS:O	1:A:48:GLU:HG3	2.05	0.55
1:B:85:CYS:HA	1:B:135:ILE:HD12	1.89	0.55
1:B:84:ASN:HB3	1:B:113:MET:HE2	1.88	0.54
1:B:215:GLN:OE1	4:B:401:HOH:O	2.19	0.53
1:D:13:VAL:HG22	1:D:81:VAL:HB	1.90	0.53
1:B:42:ILE:HG23	2:B:301:NAD:N1A	2.25	0.52
1:C:89:VAL:HG22	1:C:151:TYR:CE1	2.45	0.52
1:D:195:THR:O	1:D:199:GLU:HG3	2.10	0.51
1:A:7:ARG:NE	1:A:237:GLU:OE2	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:NAD:H2A	4:C:443:HOH:O	2.11	0.49
1:B:19:ALA:O	1:B:24:ARG:HD2	2.11	0.49
1:D:179:ILE:HG23	1:D:229:LEU:HD23	1.95	0.49
1:C:63:VAL:HG22	2:C:301:NAD:N1A	2.28	0.48
1:B:42:ILE:HG12	2:B:301:NAD:C4A	2.43	0.48
1:C:183:THR:HB	1:C:220:ILE:HD12	1.96	0.48
1:D:67:ASP:OD1	4:D:401:HOH:O	2.20	0.47
1:B:40:THR:HG22	1:B:59:HIS:HB2	1.97	0.47
1:B:169:PHE:HA	1:B:172:GLN:OE1	2.13	0.47
1:B:163:LYS:HE2	1:B:245:ILE:HD13	1.97	0.47
1:D:143:LYS:HZ3	1:D:252:TRP:CD1	2.32	0.47
1:C:80:ASP:OD1	1:C:127:LYS:NZ	2.46	0.46
1:C:121:LEU:N	1:C:122:PRO:HD2	2.30	0.46
1:A:42:ILE:HG12	2:A:301:NAD:C4A	2.46	0.46
1:A:247:MET:HB3	1:A:247:MET:HE3	1.72	0.46
1:C:13:VAL:HG22	1:C:81:VAL:HB	1.97	0.46
1:C:97:CYS:O	4:C:401:HOH:O	2.21	0.46
1:B:182:GLY:O	2:B:301:NAD:H4N	2.16	0.45
1:C:41:ASP:HB2	1:C:47:LEU:HD13	1.98	0.45
1:C:166:ALA:O	1:C:170:VAL:HB	2.16	0.45
1:D:85:CYS:O	2:D:301:NAD:H4D	2.17	0.45
1:B:222:LYS:HE2	1:B:225:GLU:CD	2.42	0.45
1:B:89:VAL:HG22	1:B:151:TYR:CE1	2.53	0.44
1:C:184:ILE:O	2:C:301:NAD:N7N	2.50	0.44
1:B:127:LYS:HD2	1:B:127:LYS:HA	1.69	0.44
1:C:89:VAL:HG22	1:C:151:TYR:CZ	2.53	0.44
2:A:301:NAD:H2A	4:A:460:HOH:O	2.18	0.43
1:C:44:LYS:HB3	1:C:60:LEU:HD11	2.00	0.43
1:C:182:GLY:O	2:C:301:NAD:H4N	2.17	0.43
1:B:146:ALA:O	4:B:402:HOH:O	2.22	0.43
1:A:161:LEU:C	1:A:161:LEU:HD12	2.43	0.43
1:B:88:TYR:CE2	1:B:90:ALA:HB2	2.54	0.42
1:B:138:ALA:HB1	1:B:252:TRP:CZ3	2.54	0.42
1:D:50:LEU:O	1:D:53:ILE:HG13	2.19	0.42
1:B:159:VAL:HG13	1:B:245:ILE:HD11	2.00	0.42
1:C:65:ASP:O	1:C:69:ILE:HG13	2.19	0.42
1:C:77:GLY:O	4:C:402:HOH:O	2.22	0.42
1:C:41:ASP:O	1:C:60:LEU:HD23	2.20	0.42
1:B:117:ILE:HG12	1:B:132:ILE:HG21	2.01	0.41
1:C:11:LYS:NZ	1:C:236:ASP:OD1	2.47	0.41
1:A:202:LYS:HE2	1:A:202:LYS:HB2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:THR:HB	1:C:61:LEU:HB3	2.02	0.41
1:D:181:PRO:HA	1:D:248:ILE:HG23	2.02	0.41
1:A:181:PRO:HA	1:A:248:ILE:HG23	2.02	0.40
1:D:72:LEU:O	1:D:76:VAL:HG13	2.21	0.40
1:B:187:PRO:O	1:B:190:ASN:HB2	2.22	0.40
2:B:301:NAD:H2N	2:B:301:NAD:H2D	1.92	0.40
1:D:191:GLN:HG3	4:D:455:HOH:O	2.21	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:185:GLU:OE2	1:C:52:SER:OG[3_645]	2.08	0.12

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	244/264 (92%)	237 (97%)	6 (2%)	1 (0%)	30	13
1	B	247/264 (94%)	234 (95%)	12 (5%)	1 (0%)	30	13
1	C	249/264 (94%)	240 (96%)	7 (3%)	2 (1%)	16	4
1	D	245/264 (93%)	235 (96%)	9 (4%)	1 (0%)	30	13
All	All	985/1056 (93%)	946 (96%)	34 (4%)	5 (0%)	24	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	GLY
1	A	140	SER
1	D	140	SER

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Mol	Chain	Res	Type
1	C	140	SER
1	B	140	SER

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	183/197 (93%)	178 (97%)	5 (3%)	39	13
1	B	176/197 (89%)	175 (99%)	1 (1%)	78	67
1	C	184/197 (93%)	177 (96%)	7 (4%)	29	6
1	D	182/197 (92%)	182 (100%)	0	100	100
All	All	725/788 (92%)	712 (98%)	13 (2%)	51	27

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	135	ILE
1	A	198	LYS
1	A	244	SER
1	A	245	ILE
1	B	143	LYS
1	C	5	THR
1	C	14	LEU
1	C	44	LYS
1	C	45	THR
1	C	100	LYS
1	C	183	THR
1	C	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	191	GLN
1	D	147	ASN
1	D	215	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	A	301	-	46,48,48	4.04	17 (36%)	64,73,73	2.34	18 (28%)
3	A1LXB	D	302	-	9,11,11	1.35	2 (22%)	8,17,17	1.96	3 (37%)
2	NAD	C	301	-	46,48,48	4.09	17 (36%)	64,73,73	2.51	19 (29%)
2	NAD	B	301	-	46,48,48	3.93	17 (36%)	64,73,73	2.41	17 (26%)
2	NAD	D	301	-	46,48,48	3.98	18 (39%)	64,73,73	2.43	17 (26%)

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	A	301	-	-	6/30/62/62	0/5/5/5
3	A1LXB	D	302	-	-	1/6/20/20	0/1/1/1
2	NAD	C	301	-	-	5/30/62/62	0/5/5/5
2	NAD	B	301	-	-	9/30/62/62	0/5/5/5
2	NAD	D	301	-	-	5/30/62/62	0/5/5/5

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAD	O4D-C1D	13.28	1.58	1.40
2	D	301	NAD	O4D-C1D	12.31	1.57	1.40
2	B	301	NAD	O4D-C1D	12.12	1.56	1.40
2	A	301	NAD	O4D-C1D	11.60	1.56	1.40
2	A	301	NAD	PN-O3	10.81	1.71	1.59
2	D	301	NAD	C3B-C4B	-9.28	1.29	1.53
2	C	301	NAD	C3B-C4B	-9.03	1.30	1.53
2	D	301	NAD	PN-O3	8.91	1.69	1.59
2	C	301	NAD	PN-O3	8.80	1.69	1.59
2	A	301	NAD	C3B-C4B	-8.72	1.30	1.53
2	B	301	NAD	PN-O3	8.70	1.68	1.59
2	B	301	NAD	C3B-C4B	-8.46	1.31	1.53
2	A	301	NAD	PA-O3	8.37	1.68	1.59
2	C	301	NAD	C3D-C4D	-8.37	1.31	1.53
2	B	301	NAD	C3D-C4D	-8.06	1.32	1.53
2	D	301	NAD	C3D-C4D	-7.97	1.32	1.53
2	A	301	NAD	C2B-C1B	-7.88	1.28	1.53
2	D	301	NAD	C2B-C1B	-7.81	1.29	1.53
2	B	301	NAD	C2B-C1B	-7.74	1.29	1.53
2	C	301	NAD	C2B-C1B	-7.72	1.29	1.53
2	A	301	NAD	C3D-C4D	-7.51	1.33	1.53
2	C	301	NAD	C7N-N7N	7.37	1.46	1.33
2	D	301	NAD	C7N-N7N	7.09	1.46	1.33
2	B	301	NAD	PA-O3	7.07	1.67	1.59
2	C	301	NAD	PA-O3	6.97	1.67	1.59
2	A	301	NAD	C7N-N7N	6.84	1.45	1.33
2	B	301	NAD	C7N-N7N	6.68	1.45	1.33
2	D	301	NAD	O4B-C1B	6.13	1.56	1.42
2	D	301	NAD	PA-O3	6.13	1.66	1.59
2	B	301	NAD	O4B-C1B	5.88	1.55	1.42
2	C	301	NAD	O4B-C1B	5.72	1.55	1.42
2	A	301	NAD	O4B-C1B	5.69	1.55	1.42
2	B	301	NAD	O4D-C4D	5.39	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAD	C2B-C3B	5.08	1.67	1.53
2	D	301	NAD	O4B-C4B	5.01	1.56	1.45
2	C	301	NAD	O4B-C4B	4.99	1.56	1.45
2	D	301	NAD	O4D-C4D	4.62	1.55	1.45
2	C	301	NAD	O4D-C4D	4.61	1.55	1.45
2	C	301	NAD	C2D-C3D	4.60	1.65	1.53
2	C	301	NAD	C2B-C3B	4.60	1.65	1.53
2	A	301	NAD	C2B-C3B	4.59	1.65	1.53
2	B	301	NAD	O4B-C4B	4.55	1.55	1.45
2	A	301	NAD	O4B-C4B	4.55	1.55	1.45
2	A	301	NAD	C2D-C3D	4.50	1.65	1.53
2	A	301	NAD	C6A-N6A	4.40	1.45	1.34
2	B	301	NAD	C2B-C3B	4.35	1.65	1.53
2	D	301	NAD	C2D-C3D	4.34	1.65	1.53
2	B	301	NAD	C2D-C3D	4.26	1.64	1.53
2	D	301	NAD	C6A-N6A	4.18	1.44	1.34
2	A	301	NAD	O4D-C4D	4.08	1.54	1.45
2	C	301	NAD	C6A-N6A	4.08	1.44	1.34
2	B	301	NAD	C6A-N6A	3.98	1.44	1.34
2	B	301	NAD	C8A-N9A	-3.12	1.32	1.37
2	A	301	NAD	C8A-N9A	-3.08	1.32	1.37
2	B	301	NAD	C5A-N7A	-2.98	1.33	1.39
2	C	301	NAD	C8A-N9A	-2.96	1.32	1.37
3	D	302	A1LXB	O2-C2	2.88	1.43	1.39
2	C	301	NAD	C8A-N7A	2.78	1.37	1.31
2	A	301	NAD	C5A-N7A	-2.66	1.34	1.39
2	A	301	NAD	C5A-C4A	-2.61	1.34	1.39
2	B	301	NAD	C5A-C4A	-2.58	1.34	1.39
2	C	301	NAD	C5A-C4A	-2.44	1.34	1.39
2	A	301	NAD	C8A-N7A	2.41	1.36	1.31
2	D	301	NAD	C5A-N7A	-2.40	1.34	1.39
2	D	301	NAD	C5A-C4A	-2.40	1.34	1.39
2	D	301	NAD	C8A-N7A	2.36	1.36	1.31
2	D	301	NAD	C8A-N9A	-2.32	1.33	1.37
2	C	301	NAD	C5A-N7A	-2.22	1.35	1.39
2	D	301	NAD	C2A-N3A	2.18	1.37	1.33
3	D	302	A1LXB	C2-C1	-2.14	1.50	1.53
2	B	301	NAD	O2B-C2B	2.04	1.48	1.43

All (74) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	C4D-O4D-C1D	-8.67	101.98	109.92
2	B	301	NAD	C4D-O4D-C1D	-7.81	102.77	109.92
2	A	301	NAD	C4D-O4D-C1D	-7.25	103.28	109.92
2	C	301	NAD	N6A-C6A-N1A	-7.25	102.24	118.38
2	C	301	NAD	C4A-N9A-C1B	-6.75	110.85	126.63
2	D	301	NAD	N6A-C6A-N1A	-6.57	103.74	118.38
2	A	301	NAD	N6A-C6A-N1A	-6.13	104.72	118.38
2	A	301	NAD	N3A-C2A-N1A	-6.02	119.47	128.58
2	C	301	NAD	C1B-N9A-C8A	5.99	140.38	127.09
2	B	301	NAD	N3A-C2A-N1A	-5.82	119.77	128.58
2	C	301	NAD	C5A-C6A-N6A	5.75	137.52	123.29
2	B	301	NAD	N6A-C6A-N1A	-5.73	105.61	118.38
2	B	301	NAD	C4A-N9A-C1B	-5.73	113.24	126.63
2	C	301	NAD	N3A-C2A-N1A	-5.71	119.95	128.58
2	C	301	NAD	C4D-O4D-C1D	-5.56	104.84	109.92
2	D	301	NAD	C5A-C4A-N3A	-5.49	119.16	126.72
2	A	301	NAD	C5A-C4A-N3A	-5.43	119.24	126.72
2	D	301	NAD	C4A-N9A-C1B	-5.35	114.12	126.63
2	D	301	NAD	C5A-C6A-N6A	5.33	136.48	123.29
2	A	301	NAD	C4A-N9A-C1B	-5.15	114.58	126.63
2	B	301	NAD	C5A-C6A-N6A	4.97	135.59	123.29
2	C	301	NAD	C5A-C4A-N3A	-4.97	119.88	126.72
2	D	301	NAD	N3A-C2A-N1A	-4.92	121.13	128.58
2	D	301	NAD	C1B-N9A-C8A	4.91	137.99	127.09
2	B	301	NAD	C1B-N9A-C8A	4.83	137.82	127.09
2	A	301	NAD	C5A-C6A-N6A	4.72	134.97	123.29
2	B	301	NAD	C5A-C4A-N3A	-4.65	120.31	126.72
2	C	301	NAD	N9A-C8A-N7A	-4.57	107.45	113.94
2	A	301	NAD	N9A-C8A-N7A	-4.44	107.64	113.94
2	B	301	NAD	N9A-C8A-N7A	-4.42	107.67	113.94
2	A	301	NAD	N3A-C4A-N9A	4.22	134.35	127.17
2	A	301	NAD	C1B-N9A-C8A	4.13	136.25	127.09
2	D	301	NAD	N9A-C8A-N7A	-4.09	108.14	113.94
2	B	301	NAD	N3A-C4A-N9A	3.67	133.41	127.17
2	A	301	NAD	C2A-N3A-C4A	3.66	120.78	111.83
2	D	301	NAD	N3A-C4A-N9A	3.62	133.32	127.17
2	C	301	NAD	C2A-N3A-C4A	3.53	120.45	111.83
2	B	301	NAD	C3B-C2B-C1B	3.40	107.89	101.46
2	A	301	NAD	C4A-N9A-C8A	3.27	109.17	105.74
2	D	301	NAD	C3B-C2B-C1B	3.26	107.62	101.46
2	B	301	NAD	C5A-N7A-C8A	3.18	108.44	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	C2A-N3A-C4A	3.16	119.55	111.83
2	C	301	NAD	C5A-N7A-C8A	3.12	108.35	103.45
3	D	302	A1LXB	C3-C4-C5	3.11	112.39	107.37
2	B	301	NAD	C2A-N3A-C4A	3.08	119.36	111.83
2	D	301	NAD	C5A-N7A-C8A	3.05	108.25	103.45
2	B	301	NAD	C4A-N9A-C8A	3.04	108.93	105.74
2	C	301	NAD	C3N-C7N-N7N	3.01	121.45	117.74
3	D	302	A1LXB	O5-C2-C3	2.94	108.71	104.91
2	C	301	NAD	N3A-C4A-N9A	2.94	132.16	127.17
2	D	301	NAD	C6A-C5A-C4A	2.89	121.13	117.18
2	C	301	NAD	C4A-N9A-C8A	2.88	108.76	105.74
2	A	301	NAD	C5A-N7A-C8A	2.78	107.82	103.45
2	A	301	NAD	C2B-C1B-N9A	-2.77	106.42	113.30
2	B	301	NAD	C4B-O4B-C1B	-2.73	103.44	109.47
2	C	301	NAD	C4A-C5A-N7A	-2.72	107.47	110.58
2	B	301	NAD	C6A-C5A-C4A	2.67	120.82	117.18
3	D	302	A1LXB	O1A-C1-C2	-2.48	119.72	123.85
2	B	301	NAD	O4B-C4B-C3B	2.42	109.95	105.15
2	C	301	NAD	C4B-O4B-C1B	-2.42	104.13	109.47
2	A	301	NAD	C4B-O4B-C1B	-2.41	104.14	109.47
2	C	301	NAD	C2D-C3D-C4D	2.38	107.21	102.61
2	A	301	NAD	C6A-C5A-C4A	2.28	120.30	117.18
2	C	301	NAD	C6N-N1N-C2N	-2.27	119.95	121.88
2	D	301	NAD	O3-PN-O1N	-2.27	103.88	110.70
2	B	301	NAD	O3D-C3D-C2D	-2.26	104.56	111.82
2	A	301	NAD	C2D-C3D-C4D	2.24	106.93	102.61
2	C	301	NAD	O2A-PA-O3	2.18	113.18	107.27
2	C	301	NAD	C2B-C3B-C4B	2.11	106.69	102.61
2	A	301	NAD	O4B-C1B-C2B	-2.09	102.14	106.62
2	D	301	NAD	C2B-C3B-C4B	2.09	106.65	102.61
2	A	301	NAD	C3B-C2B-C1B	2.08	105.40	101.46
2	D	301	NAD	C4A-C5A-N7A	-2.06	108.23	110.58
2	D	301	NAD	C4A-N9A-C8A	2.03	107.87	105.74

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	C5B-O5B-PA-O1A
2	B	301	NAD	C5B-O5B-PA-O3
2	B	301	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	C2D-C1D-N1N-C2N
2	B	301	NAD	C2D-C1D-N1N-C6N
2	C	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	O4D-C1D-N1N-C6N
2	C	301	NAD	C2D-C1D-N1N-C6N
2	D	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	C5B-O5B-PA-O2A
2	A	301	NAD	C5B-O5B-PA-O3
2	B	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C2B-C1B-N9A-C8A
2	A	301	NAD	C2D-C1D-N1N-C6N
2	C	301	NAD	C2D-C1D-N1N-C2N
2	D	301	NAD	C2D-C1D-N1N-C6N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	D	301	NAD	O4D-C1D-N1N-C6N
2	C	301	NAD	C2B-C1B-N9A-C8A
2	B	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	C2B-C1B-N9A-C8A
2	D	301	NAD	O4B-C4B-C5B-O5B
3	D	302	A1LXB	O1B-C1-C2-O5

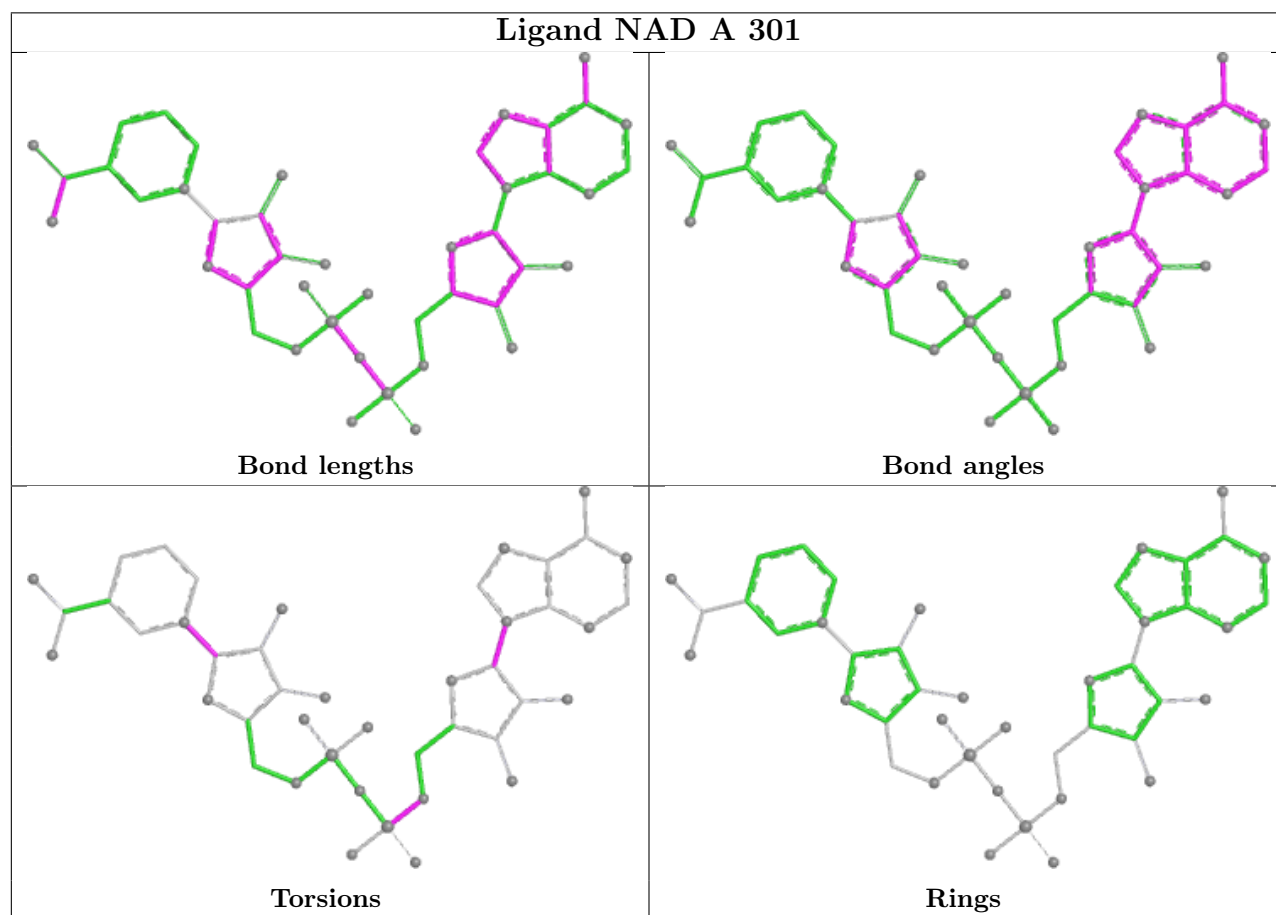
There are no ring outliers.

4 monomers are involved in 13 short contacts:

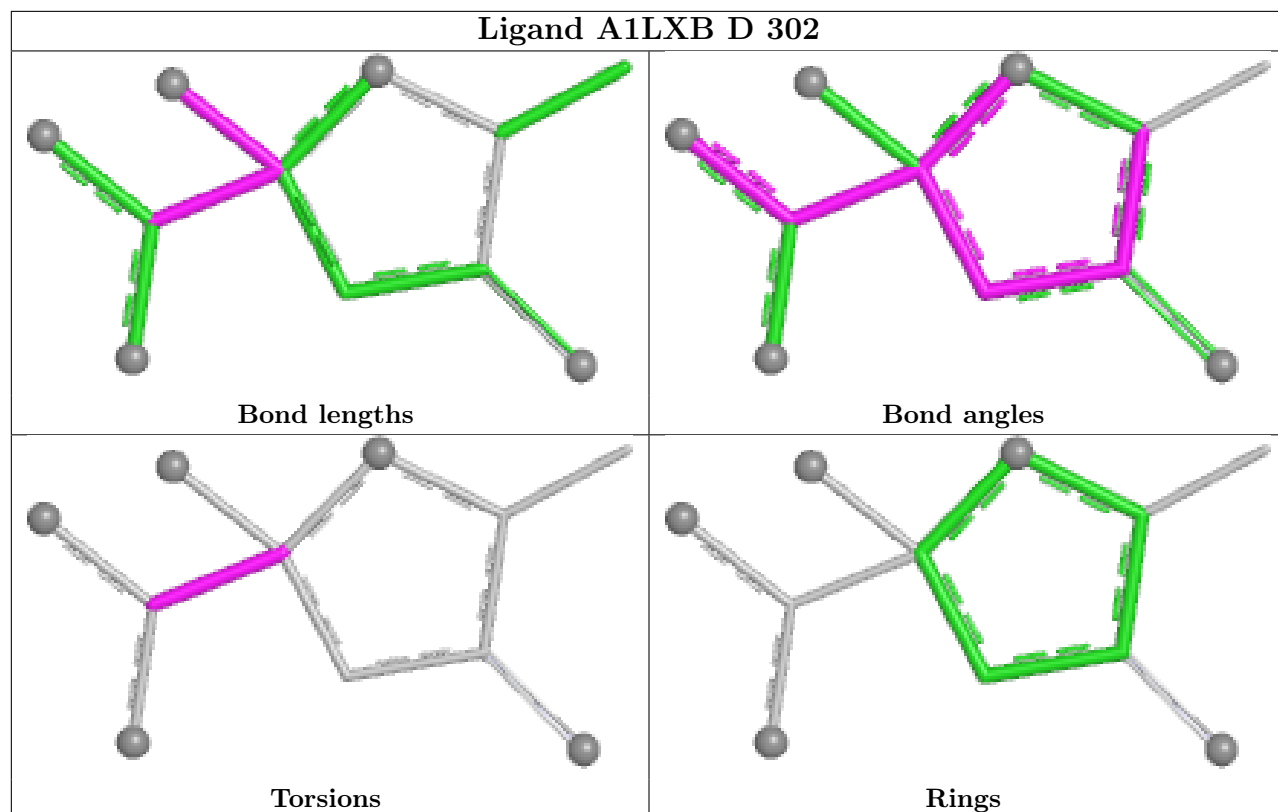
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	2	0
2	C	301	NAD	4	0
2	B	301	NAD	5	0
2	D	301	NAD	2	0

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

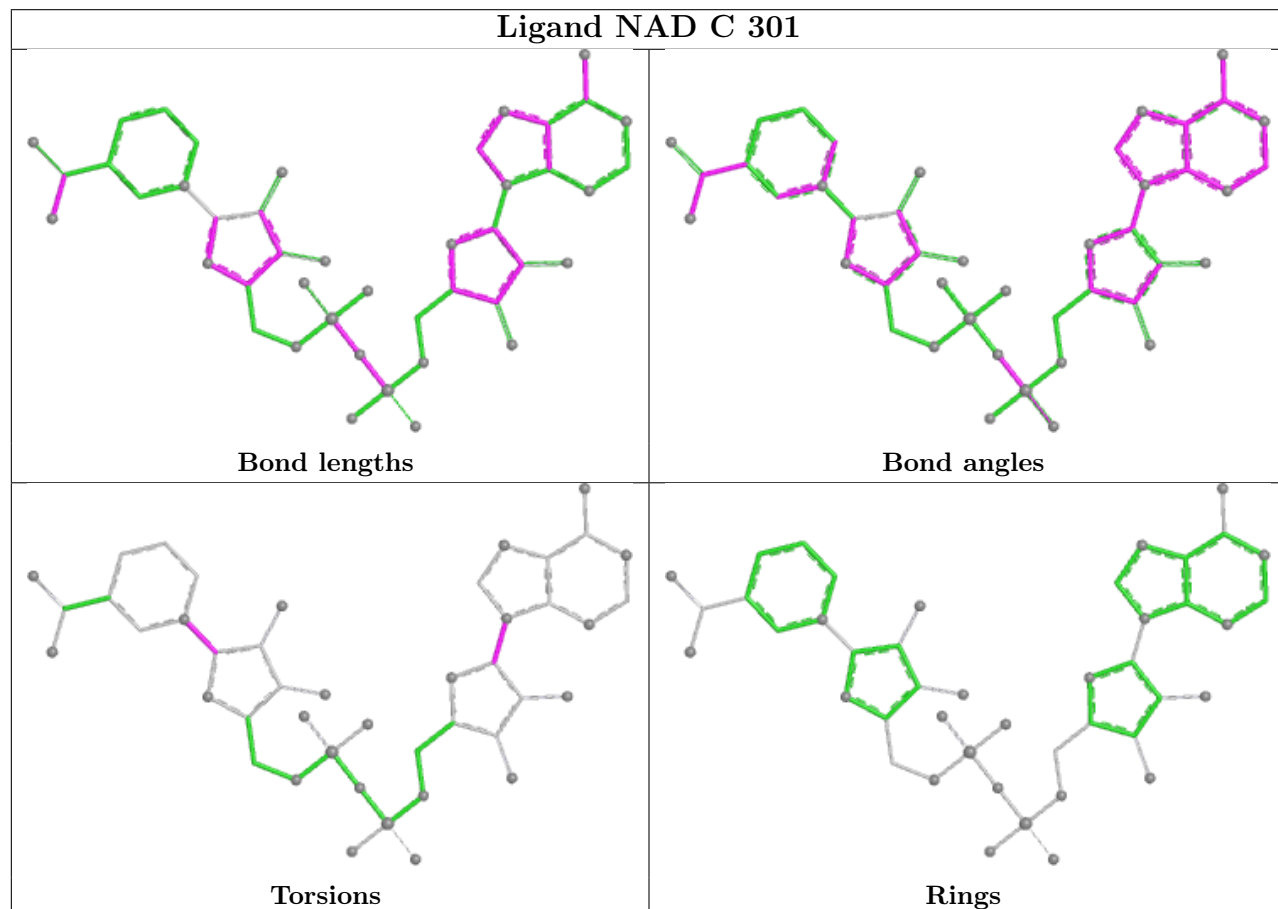
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

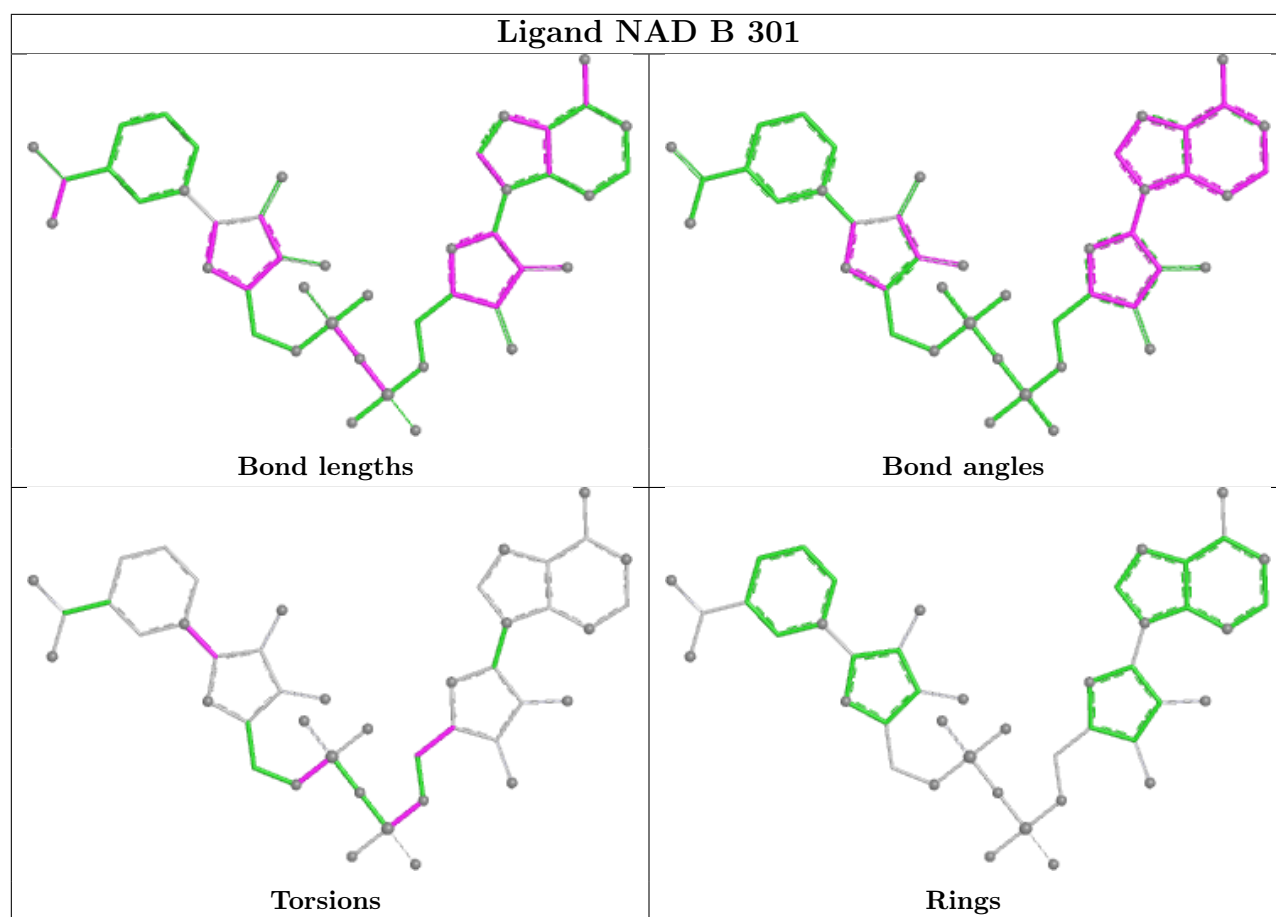


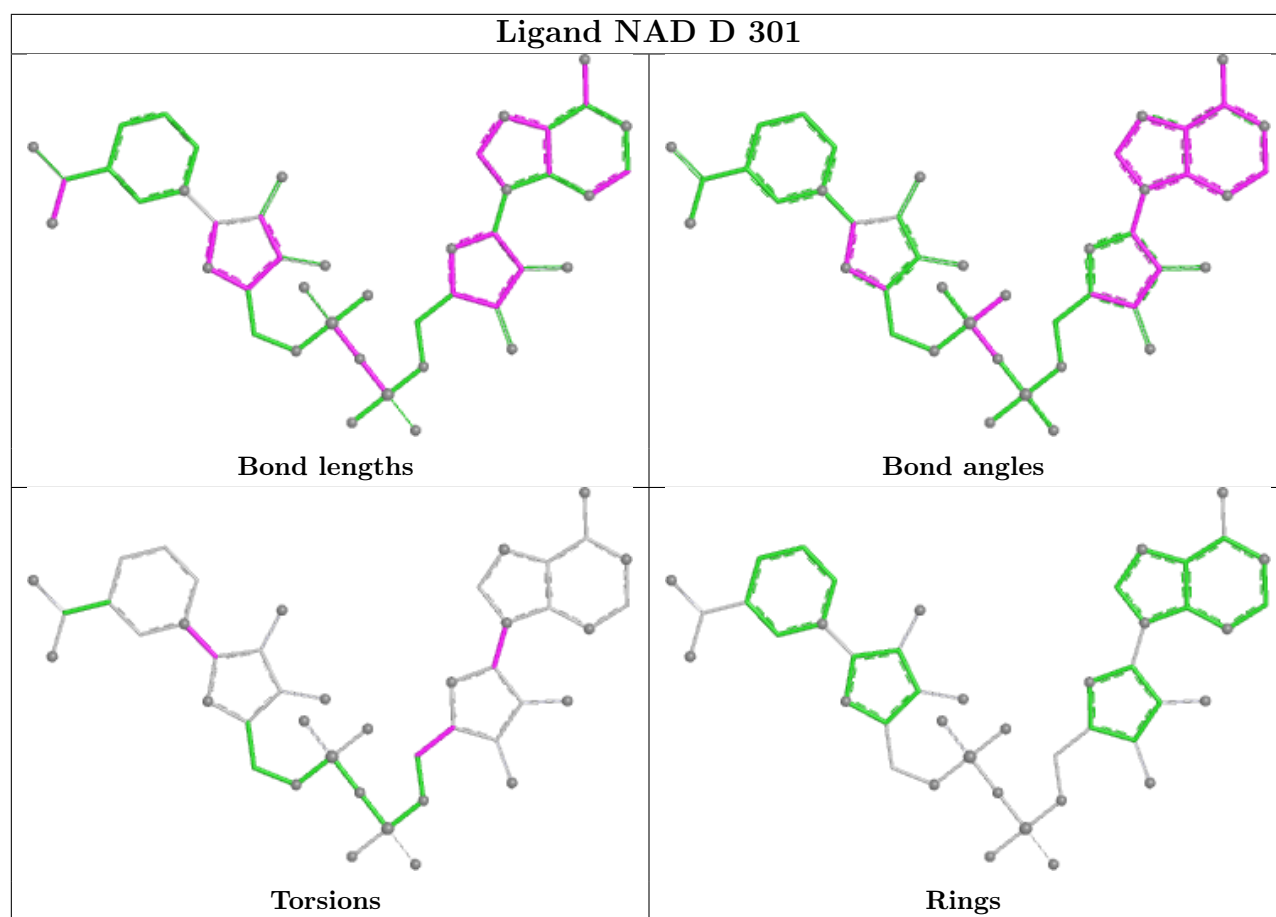
Ligand A1LXB D 302



Ligand NAD C 301







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(Å²)	Q<0.9	
1	A	248/264 (93%)	0.74	10 (4%)	42	50	10, 20, 31, 38	0
1	B	249/264 (94%)	0.87	21 (8%)	17	21	11, 20, 34, 50	0
1	C	250/264 (94%)	1.02	30 (12%)	9	11	13, 22, 35, 42	1 (0%)
1	D	247/264 (93%)	0.95	26 (10%)	11	14	12, 22, 34, 39	0
All	All	994/1056 (94%)	0.89	87 (8%)	15	19	10, 21, 34, 50	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	42[A]	ILE	4.7
1	C	51	ALA	4.0
1	B	252	TRP	3.8
1	B	210	ALA	3.7
1	C	45	THR	3.6
1	A	201	GLY	3.5
1	B	209	ALA	3.5
1	C	71	ALA	3.5
1	D	76	VAL	3.3
1	A	47	LEU	3.2
1	C	43	SER	3.2
1	D	203	SER	3.1
1	D	72	LEU	3.0
1	B	212	VAL	2.9
1	B	204	GLU	2.9
1	D	13	VAL	2.9
1	C	52	SER	2.9
1	B	51	ALA	2.9
1	B	201	GLY	2.9
1	C	54	ALA	2.8
1	A	95	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	35	ALA	2.8
1	D	73	VAL	2.7
1	B	203	SER	2.7
1	C	53	ILE	2.7
1	D	170	VAL	2.6
1	D	71	ALA	2.6
1	C	5	THR	2.6
1	D	12	THR	2.6
1	A	213	ALA	2.6
1	B	68	ALA	2.6
1	C	205	ASP	2.5
1	B	54	ALA	2.5
1	B	207	VAL	2.5
1	D	51	ALA	2.5
1	D	81	VAL	2.5
1	C	49	GLU	2.5
1	A	203	SER	2.5
1	C	47	LEU	2.4
1	B	197	ALA	2.4
1	D	46	HIS	2.4
1	B	200	THR	2.4
1	D	79	VAL	2.4
1	D	78	THR	2.4
1	B	178	ALA	2.3
1	C	125	LEU	2.3
1	C	197	ALA	2.3
1	D	45	THR	2.3
1	C	46	HIS	2.3
1	B	193	ILE	2.3
1	C	50	LEU	2.3
1	C	171	SER	2.3
1	C	73	VAL	2.3
1	C	144	GLY	2.3
1	B	205	ASP	2.3
1	D	30	PHE	2.3
1	A	53	ILE	2.3
1	A	252	TRP	2.2
1	D	252	TRP	2.2
1	B	199	GLU	2.2
1	A	209	ALA	2.2
1	D	74	ALA	2.2
1	C	77	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	76	VAL	2.2
1	C	126	ALA	2.2
1	D	201	GLY	2.2
1	B	53	ILE	2.2
1	D	17	ALA	2.2
1	D	129	ALA	2.2
1	D	254	ASN	2.2
1	C	220	ILE	2.2
1	B	73	VAL	2.1
1	C	201	GLY	2.1
1	C	72	LEU	2.1
1	B	71	ALA	2.1
1	B	126	ALA	2.1
1	C	254	ASN	2.1
1	A	39	ALA	2.1
1	D	210	ALA	2.1
1	D	243	GLY	2.1
1	A	56	VAL	2.1
1	C	37	VAL	2.1
1	D	47	LEU	2.1
1	D	50	LEU	2.1
1	C	147	ASN	2.0
1	D	120	VAL	2.0
1	C	143	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

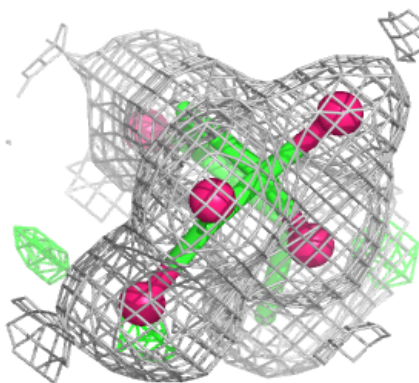
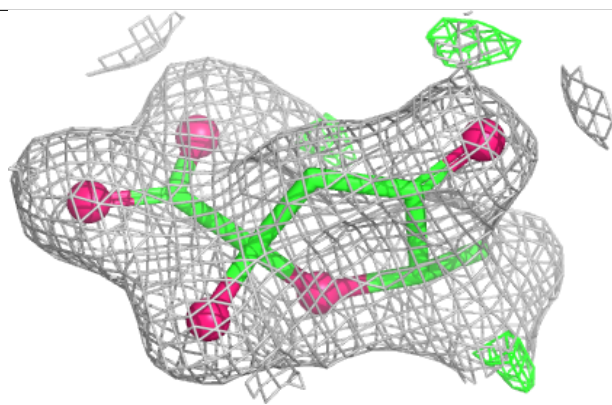
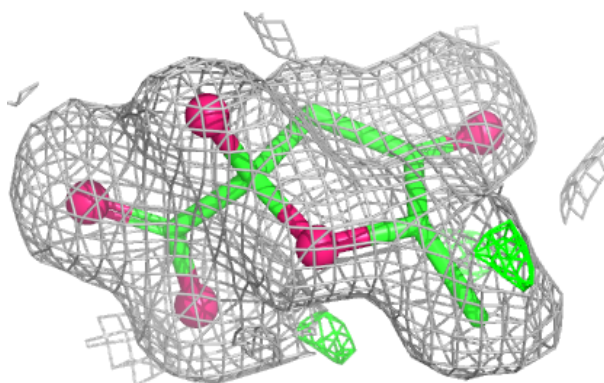
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1LXB	D	302	11/11	0.84	0.11	21,25,27,29	0
2	NAD	D	301	44/44	0.91	0.09	19,23,27,29	0
2	NAD	B	301	44/44	0.91	0.09	11,18,23,27	0
2	NAD	A	301	44/44	0.92	0.08	13,19,24,25	0
2	NAD	C	301	44/44	0.93	0.09	15,23,26,28	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.

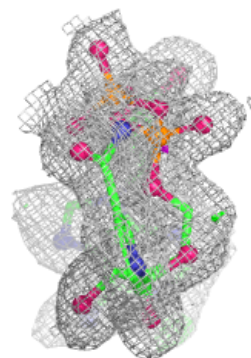
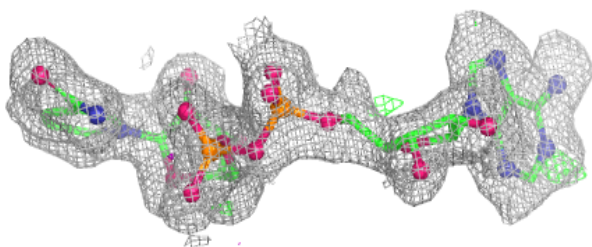
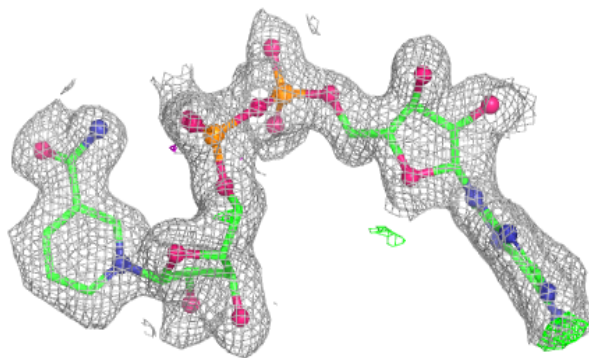
Electron density around A1LXB D 302:

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

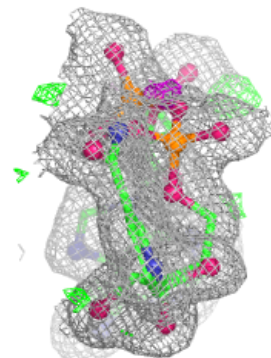
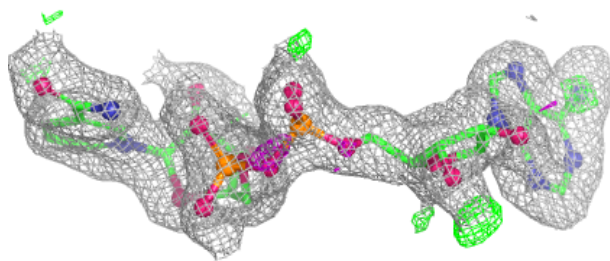
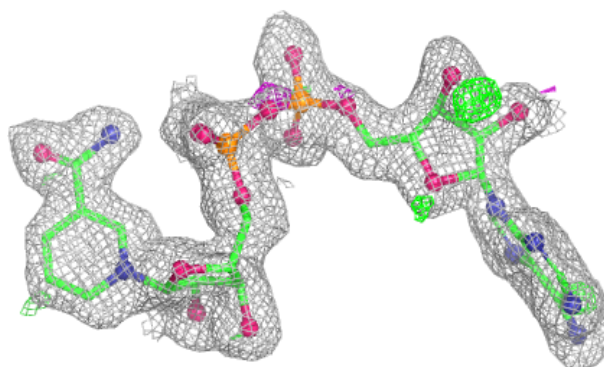


Electron density around NAD D 301:

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

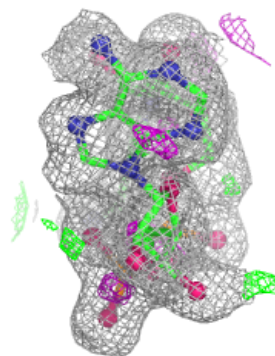
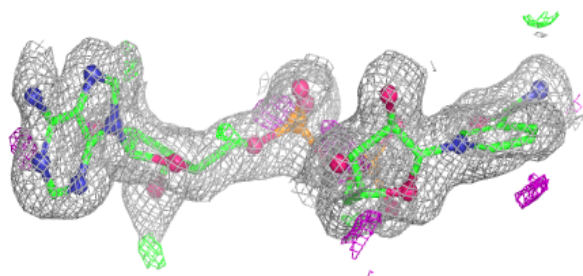
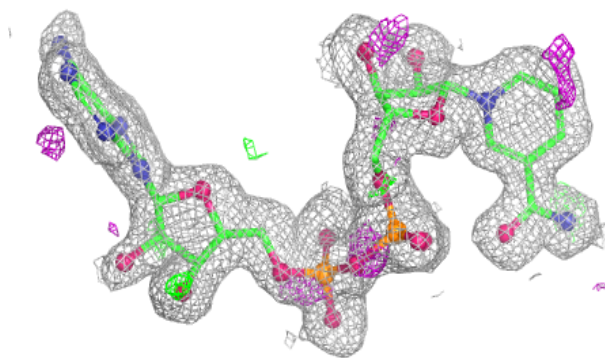
**Electron density around NAD B 301:**

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

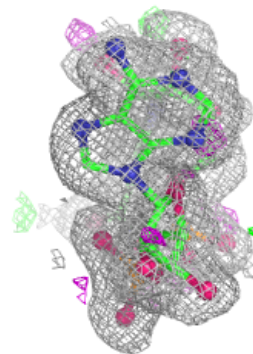
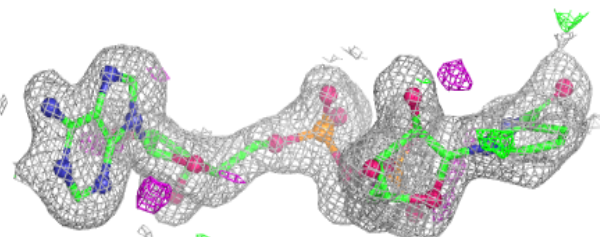
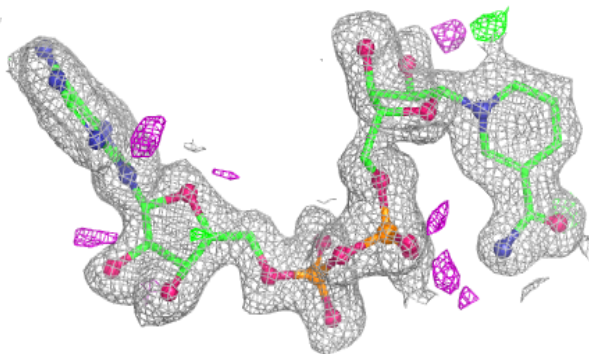


Electron density around NAD A 301:

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

**Electron density around NAD C 301:**

$2mF_o-DF_c$ (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.