



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 1HLP / pdb_00001hlp
Title : STRUCTURAL FEATURES STABILIZING HALOPHILIC MALATE DE-HYDROGENASE FROM AN ARCHAEABACTERIUM
Authors : Dym, O.; Mevarech, M.; Sussman, J.L.
Deposited on : 1994-10-04
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

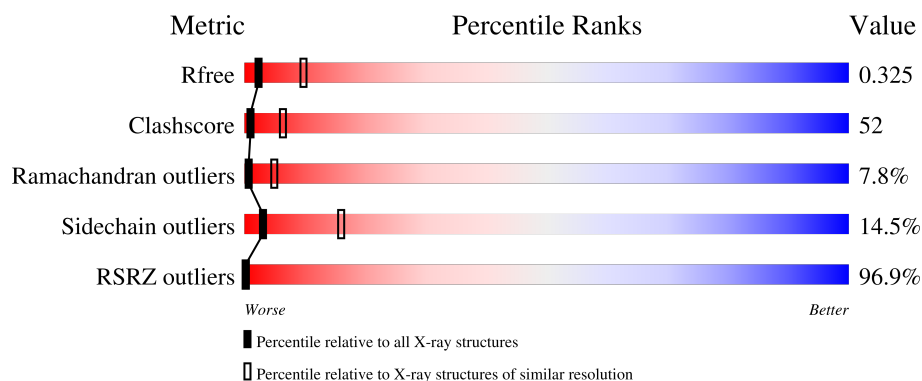
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	303	96% 33% 48% 17% .
1	B	303	98% 32% 50% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	330	-	-	-	X

2 Entry composition [i](#)

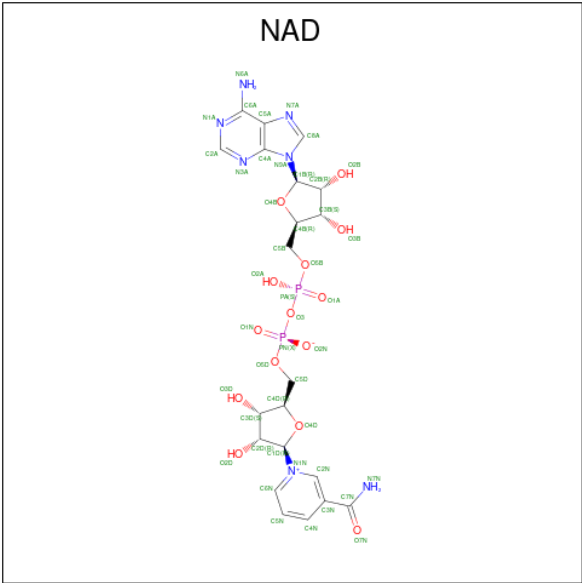
There are 2 unique types of molecules in this entry. The entry contains 4690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			
1	B	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			

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

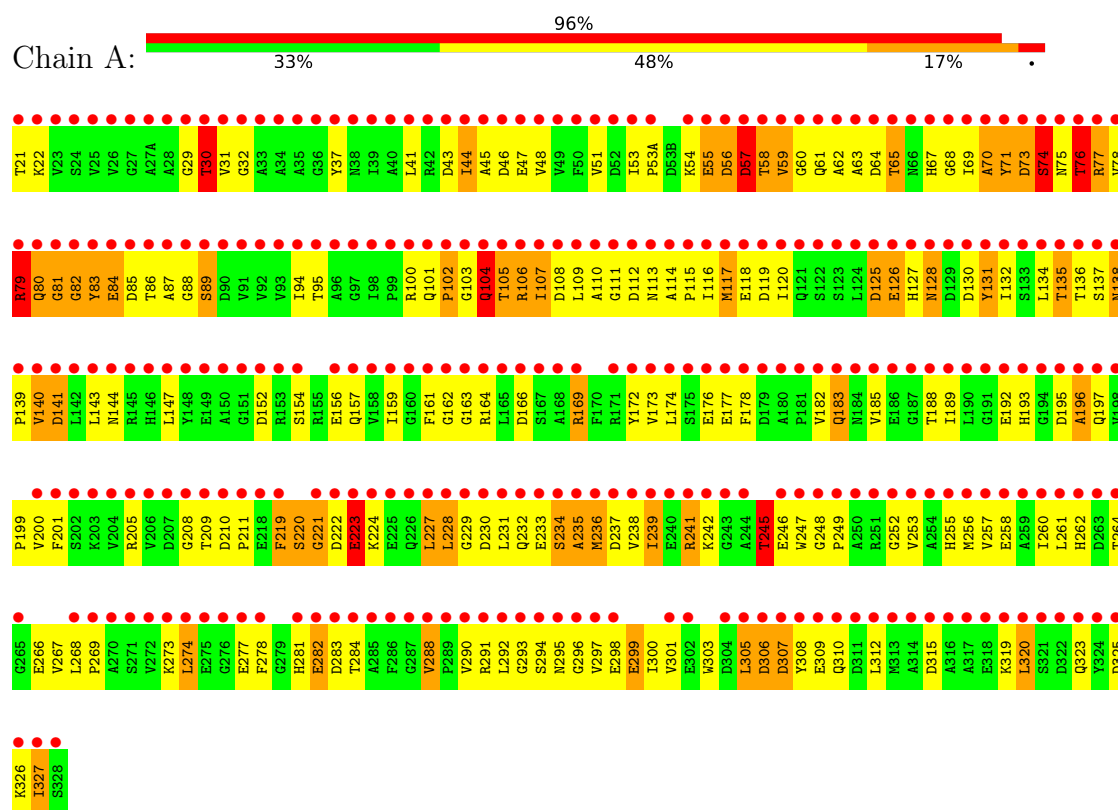


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

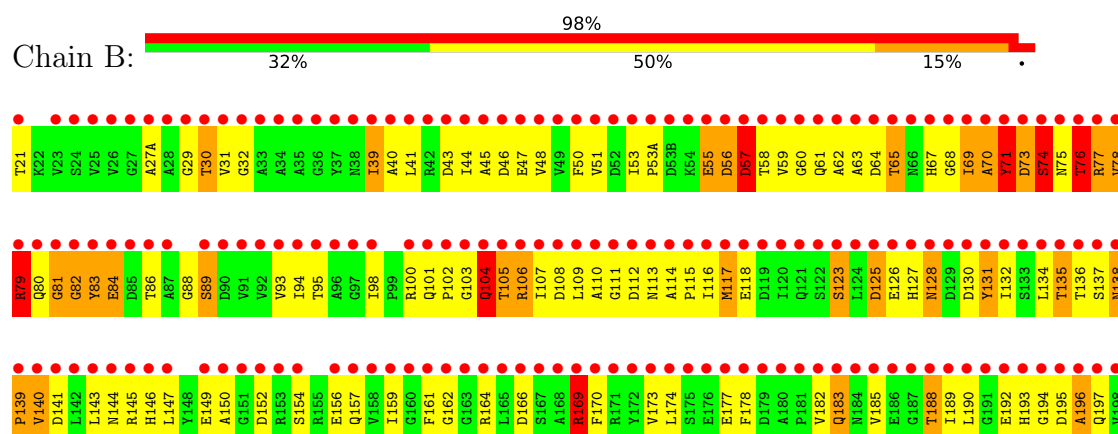
3 Residue-property plots

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: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



P199	G265	K326
V200	E266	I327
F201	V267	S328
S202	L268	
F203	P269	
V204	A270	
R205	S271	
V206	V272	
D207	K273	
G208	L274	
T209	E275	
D210	G276	
P211	E277	
E218	F278	
F219	G279	
S220	H281	
G221	E282	
D222	D283	
F223	T284	
K224	A285	
E225	F286	
Q226	G287	
L227	V288	
L228	P289	
G229	V290	
D230	R291	
L231	L292	
Q232	G293	
E233	S294	
S234	N295	
A235	G296	
M236	V297	
D237	E298	
V238	E299	
T239	I300	
E240	V301	
R241	E302	
K242	V303	
G243	D304	
A244	L305	
T245	D306	
E246	D307	
W247	Y308	
G248	E309	
F249	Q310	
A250	D311	
R251	L312	
G252	M313	
V253	A314	
A254	D315	
H255	A316	
M256	A317	
V257	E318	
E258	K319	
A259	L320	
I260	S321	
L261	D322	
H262	Q323	
D263	Y324	
T264	D325	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.60Å 130.60Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 10.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.0 (10.00-3.20) 73.2 (10.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.83Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.280 0.315 , 0.325	Depositor DCC
R_{free} test set	3012 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	1/2338 (0.0%)	1.32	24/3175 (0.8%)
1	B	0.89	0/2338	1.32	23/3175 (0.7%)
All	All	0.90	1/4676 (0.0%)	1.32	47/6350 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	THR	CA-CB	6.01	1.61	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PHE	N-CA-C	-14.13	95.88	111.28
1	B	219	PHE	N-CA-C	-13.77	96.28	111.28
1	A	138	ASN	N-CA-C	12.40	130.15	113.77
1	A	57	ASP	N-CA-C	-12.04	96.71	111.40
1	B	57	ASP	N-CA-C	-11.38	98.85	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2301	0	2165	233	0
1	B	2301	0	2165	261	0
2	A	44	0	26	10	0
2	B	44	0	26	12	0
All	All	4690	0	4382	474	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 52.

The worst 5 of 474 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:48:VAL:HB	1:B:77:ARG:HB2	1.50	0.94
1:B:291:ARG:HG2	1:B:298:GLU:HB2	1.51	0.92
1:A:249:PRO:O	1:A:253:VAL:HG23	1.70	0.92
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.32	0.90
1:A:62:ALA:H	1:A:79:ARG:HH12	1.19	0.90

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	301/303 (99%)	230 (76%)	46 (15%)	25 (8%)	0	4
1	B	301/303 (99%)	232 (77%)	47 (16%)	22 (7%)	1	6
All	All	602/606 (99%)	462 (77%)	93 (15%)	47 (8%)	1	5

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	THR

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Mol	Chain	Res	Type
1	A	55	GLU
1	A	70	ALA
1	A	71	TYR
1	A	106	ARG

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	244/244 (100%)	207 (85%)	37 (15%)	3	14
1	B	244/244 (100%)	210 (86%)	34 (14%)	3	17
All	All	488/488 (100%)	417 (86%)	71 (14%)	3	16

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	219	PHE
1	B	227	LEU
1	B	274	LEU
1	A	227	LEU
1	A	223	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	GLN
1	B	197	GLN
1	B	281	HIS
1	B	193	HIS
1	A	281	HIS

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	330	-	46,48,48	1.29	5 (10%)	64,73,73	2.29	15 (23%)
2	NAD	B	330	-	46,48,48	2.13	7 (15%)	64,73,73	2.40	22 (34%)

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	330	-	-	7/30/62/62	0/5/5/5
2	NAD	B	330	-	-	8/30/62/62	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	NAD	PN-O3	8.20	1.68	1.59
2	B	330	NAD	PA-O3	7.27	1.67	1.59
2	B	330	NAD	C2N-N1N	5.94	1.41	1.35
2	A	330	NAD	C2N-N1N	4.94	1.40	1.35
2	A	330	NAD	C6N-N1N	2.56	1.41	1.35

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	NAD	C4D-O4D-C1D	-9.94	100.83	109.92
2	B	330	NAD	C4D-O4D-C1D	-9.17	101.53	109.92
2	B	330	NAD	C5A-C4A-N3A	-6.92	117.19	126.72
2	A	330	NAD	C5A-C4A-N3A	-5.86	118.65	126.72
2	A	330	NAD	C6A-C5A-N7A	-5.72	121.07	132.09

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

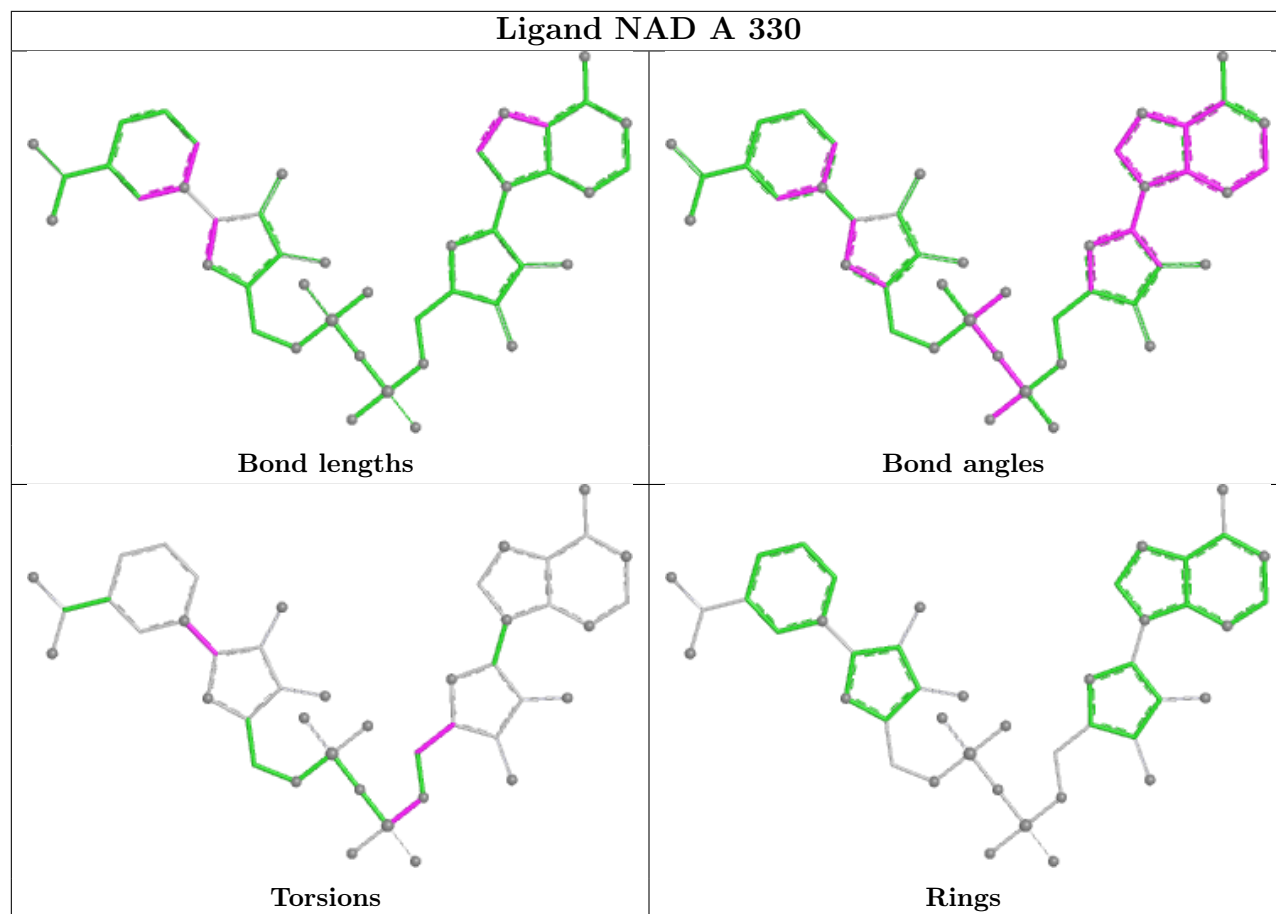
Mol	Chain	Res	Type	Atoms
2	A	330	NAD	O4D-C1D-N1N-C2N
2	A	330	NAD	O4D-C1D-N1N-C6N
2	A	330	NAD	C2D-C1D-N1N-C2N
2	A	330	NAD	C2D-C1D-N1N-C6N
2	B	330	NAD	O4D-C1D-N1N-C2N

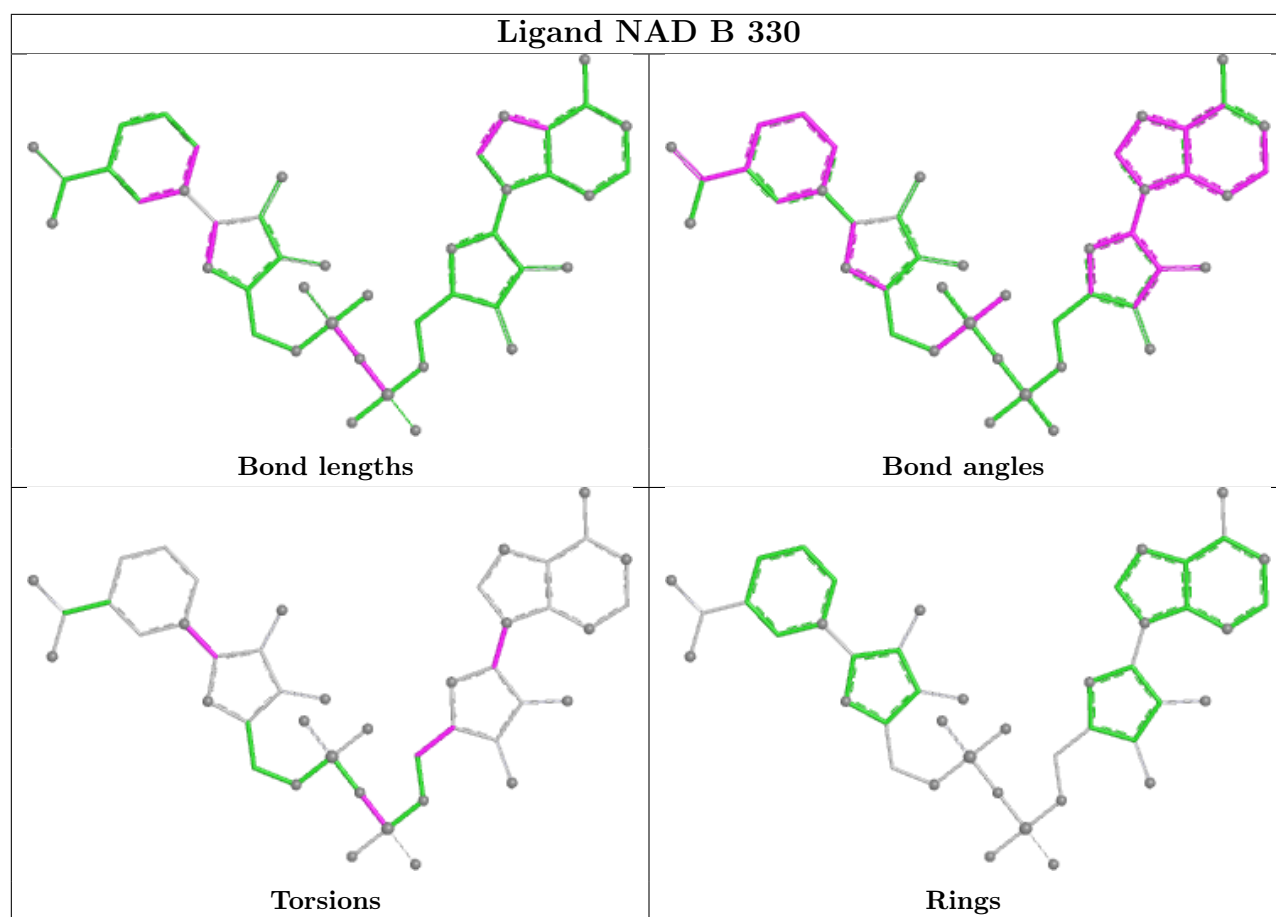
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	NAD	10	0
2	B	330	NAD	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	303/303 (100%)	5.99	291 (96%) 0 0	2, 16, 35, 46	0
1	B	303/303 (100%)	5.31	296 (97%) 0 0	2, 16, 35, 46	0
All	All	606/606 (100%)	5.65	587 (96%) 0 0	2, 16, 35, 46	0

The worst 5 of 587 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	GLY	19.2
1	A	254	ALA	15.2
1	A	208	GLY	13.2
1	A	314	ALA	12.7
1	A	105	THR	12.6

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](#)

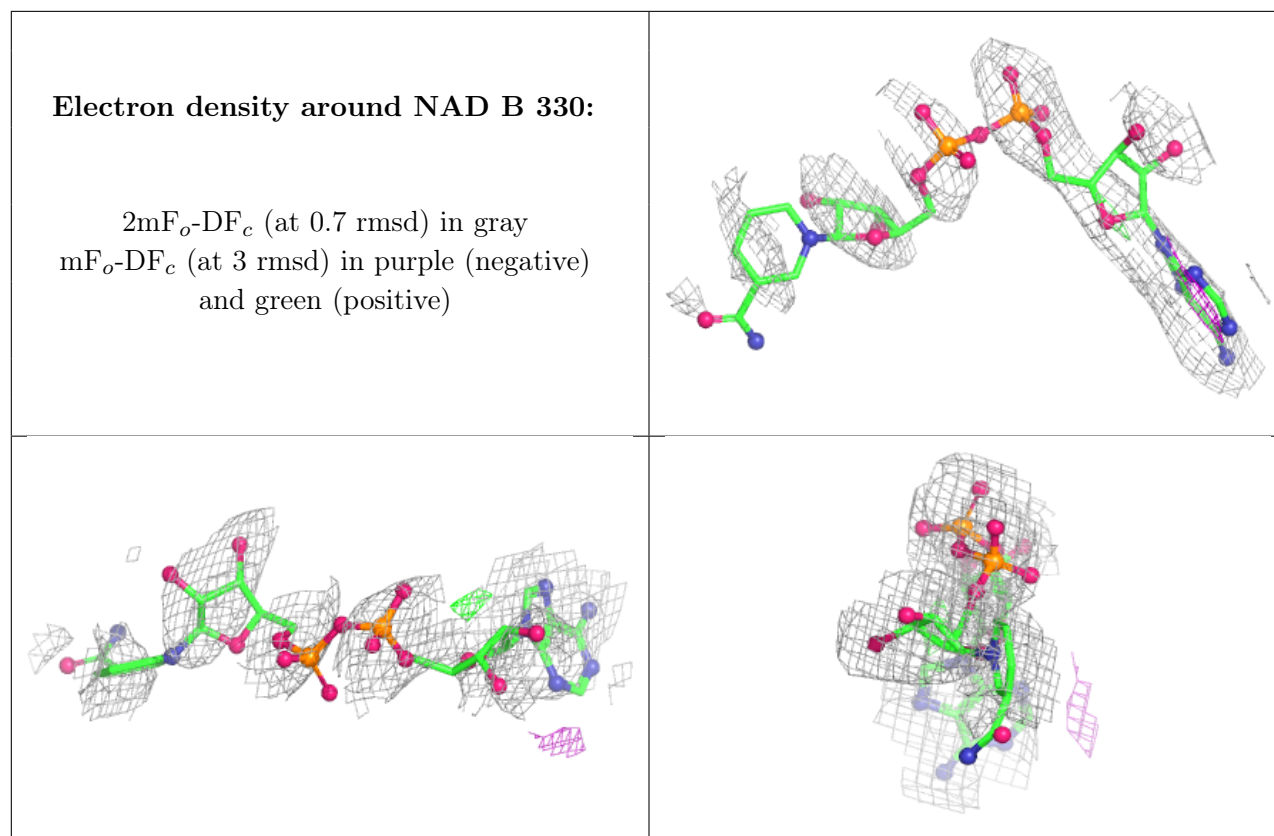
There are no oligosaccharides in this entry.

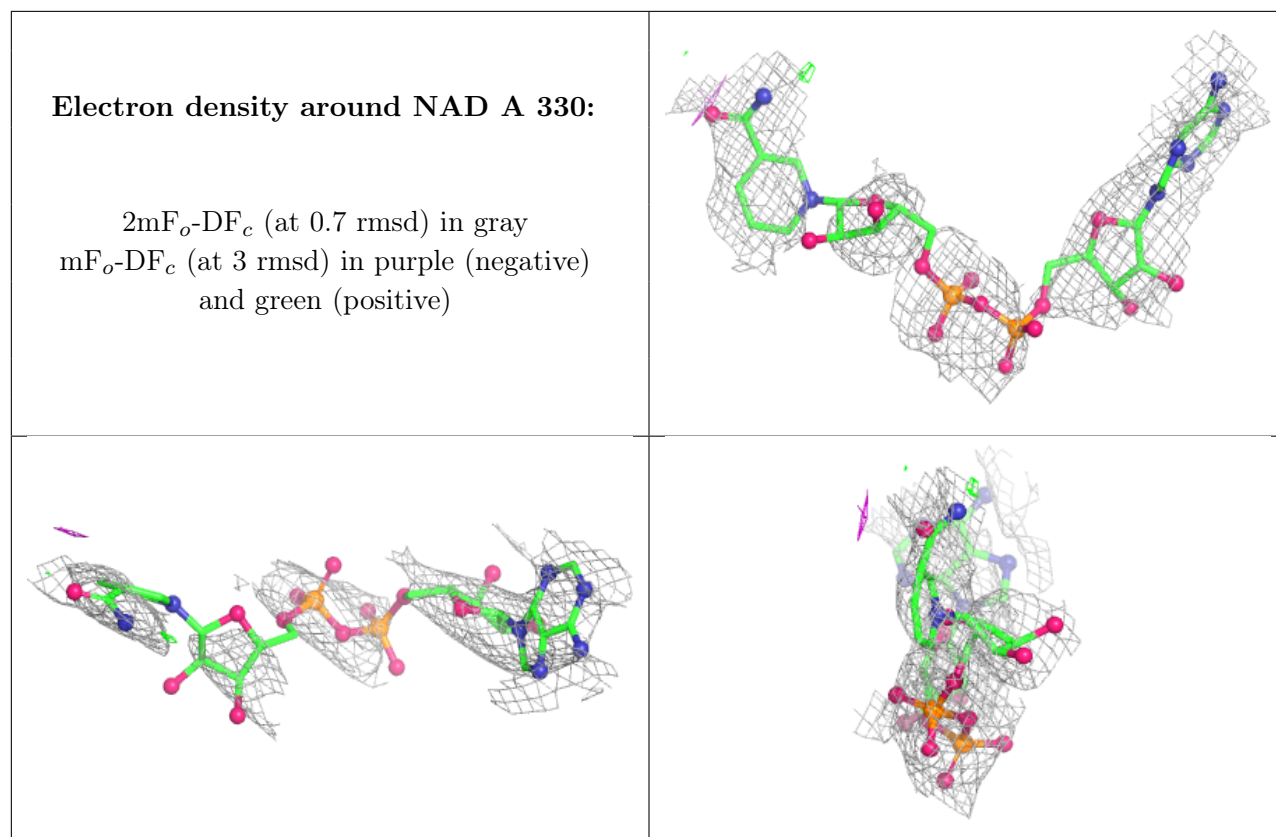
6.4 Ligands [i](#)

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
2	NAD	B	330	44/44	0.44	0.42	21,31,36,39	0
2	NAD	A	330	44/44	0.52	0.34	20,29,34,36	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.