



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:43 PM UTC

PDB ID : 2FN7 / pdb_00002fn7
Title : Crystal structure of the lactate dehydrogenase from cryptosporidium parvum complexed with substrate (lactic acid) and cofactor (b-nicotinamide adenine dinucleotide)
Authors : Senkovich, O.A.; Chattopadhyay, D.
Deposited on : 2006-01-10
Resolution : 2.30 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

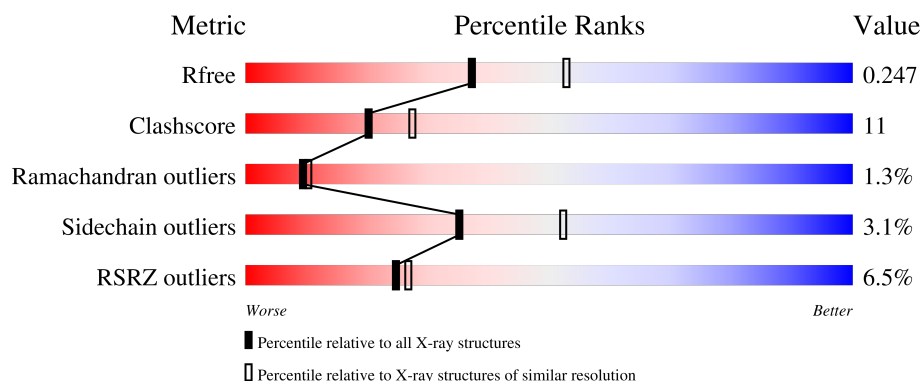
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	321	
1	B	321	

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
3	LAC	A	364	X	-	-	-
4	GOL	A	600	-	X	-	-
4	GOL	A	601	-	X	-	-
4	GOL	B	603	-	X	-	-

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.

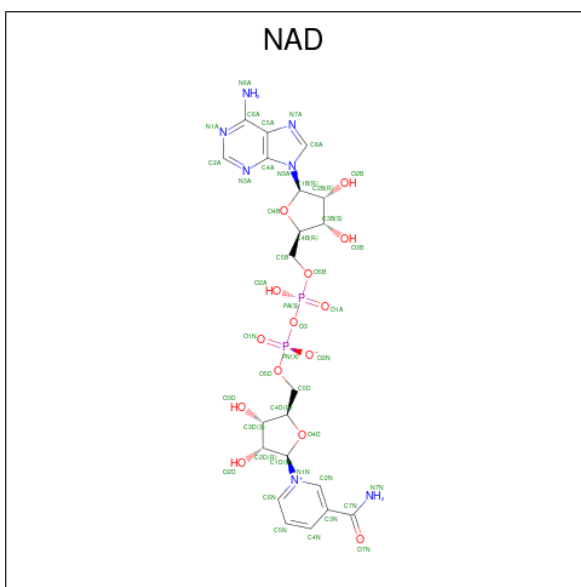
- Molecule 1 is a protein called Lactate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total 2356	C 1490	N 399	O 452	S 15	0	2	0
1	B	317	Total 2355	C 1490	N 399	O 451	S 15	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	VAL	SEE REMARK 999	GB 10444017
B	202	ALA	VAL	SEE REMARK 999	GB 10444017

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



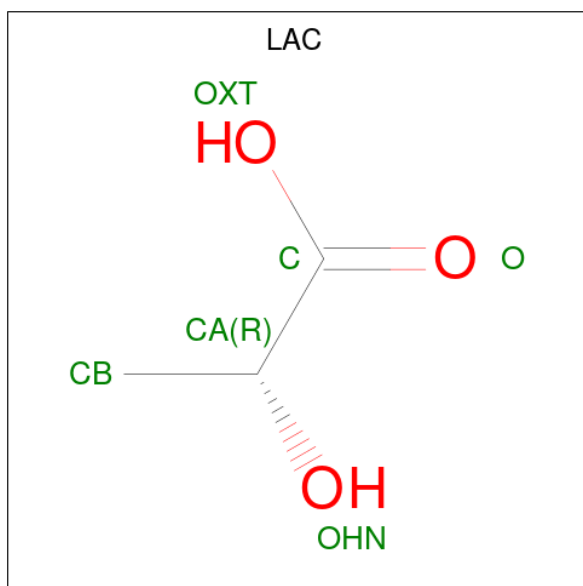
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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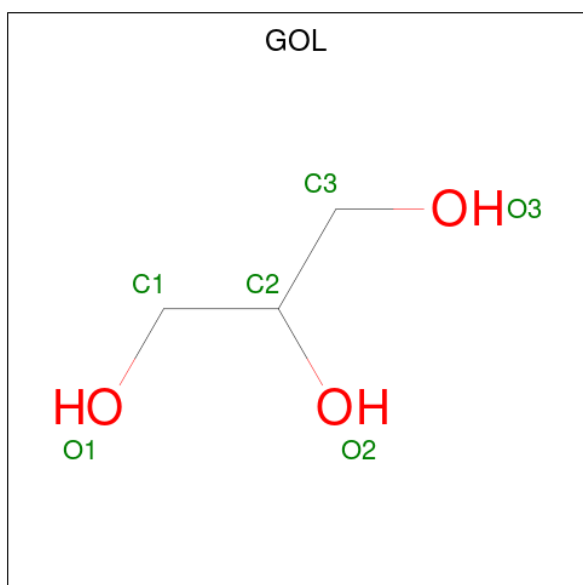
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is LACTIC ACID (CCD ID: LAC) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

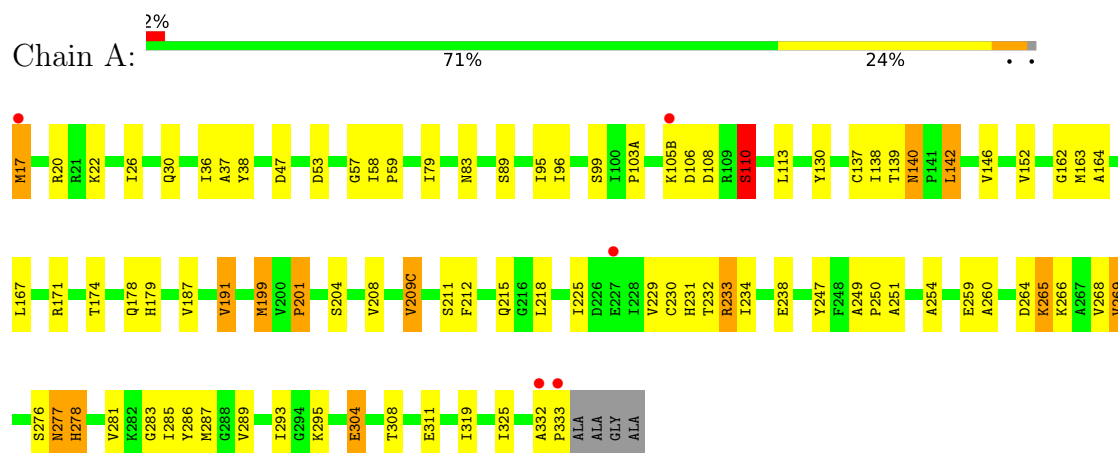
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total 93	O 93	0	0
5	B	49	Total 49	O 49	0	0

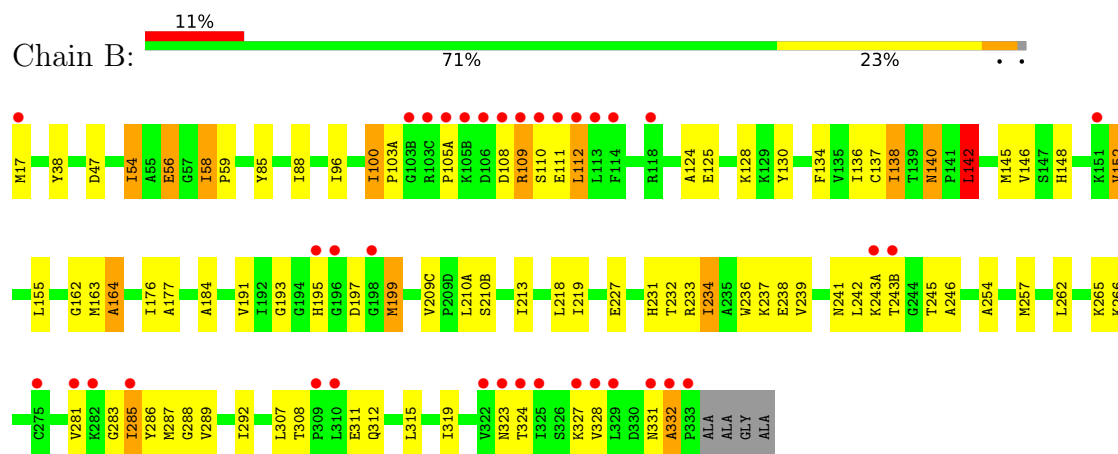
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactate Dehydrogenase



• Molecule 1: Lactate Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.47Å 95.47Å 186.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.30) 100.0 (50.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.246 0.206 , 0.247	Depositor DCC
R_{free} test set	4465 reflections (8.83%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4965	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: LAC, NAD, GOL

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	1.47	14/2405 (0.6%)	1.37	21/3259 (0.6%)
1	B	1.33	7/2399 (0.3%)	1.32	17/3251 (0.5%)
All	All	1.40	21/4804 (0.4%)	1.34	38/6510 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	MET	SD-CE	-8.47	1.58	1.79
1	A	251	ALA	CA-CB	6.93	1.64	1.53
1	B	17	MET	CG-SD	6.37	1.96	1.80
1	A	254	ALA	CA-CB	6.23	1.63	1.53
1	A	201	PRO	CA-C	6.22	1.61	1.52
1	A	37	ALA	CA-CB	5.91	1.62	1.53
1	B	136	ILE	CA-CB	5.70	1.61	1.54
1	A	187	VAL	CA-CB	-5.59	1.47	1.54
1	A	30	GLN	C-O	-5.57	1.17	1.24
1	A	268	VAL	CA-CB	5.53	1.60	1.54
1	A	308	THR	CA-CB	-5.45	1.45	1.53
1	B	289	VAL	CA-C	5.42	1.58	1.52
1	A	139	THR	CA-CB	5.38	1.61	1.53
1	B	285	ILE	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	CA-C	5.36	1.59	1.52
1	B	257	MET	SD-CE	5.33	1.92	1.79
1	A	17	MET	CG-SD	5.22	1.93	1.80
1	A	99	SER	CA-C	5.21	1.58	1.52
1	A	199	MET	SD-CE	-5.19	1.66	1.79
1	B	176	ILE	CA-CB	-5.18	1.48	1.54
1	A	167	LEU	CA-C	5.07	1.59	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	LYS	N-CA-C	7.78	120.85	111.82
1	B	138	ILE	N-CA-C	-7.70	106.40	113.71
1	B	130	TYR	N-CA-C	7.55	122.60	113.23
1	A	142	LEU	N-CA-C	7.50	123.68	111.37
1	A	265	LYS	N-CA-C	7.24	121.37	112.54
1	B	142	LEU	N-CA-C	7.14	123.08	111.37
1	A	278	HIS	N-CA-C	-6.93	98.64	108.96
1	B	266	LYS	N-CA-C	-6.86	101.92	111.52
1	A	113	LEU	N-CA-C	6.80	119.28	111.11
1	B	209(C)	VAL	N-CA-C	6.70	114.53	107.76
1	A	209(C)	VAL	CB-CA-C	-6.62	103.62	110.71
1	A	233	ARG	N-CA-C	6.60	118.47	111.28
1	B	134	PHE	N-CA-C	-6.51	98.11	108.73
1	B	197	ASP	N-CA-C	-6.46	104.89	112.89
1	B	191	VAL	N-CA-C	-6.26	98.50	107.77
1	B	54	ILE	N-CA-C	-6.20	103.92	113.16
1	A	58	ILE	CA-C-N	-6.18	112.19	119.05
1	A	58	ILE	C-N-CA	-6.18	112.19	119.05
1	A	266	LYS	N-CA-C	-6.15	103.44	111.74
1	A	201	PRO	N-CA-C	-6.02	100.06	112.47
1	B	96	ILE	N-CA-C	6.02	116.47	107.51
1	A	130	TYR	N-CA-C	5.98	120.85	113.50
1	B	47	ASP	N-CA-C	-5.85	101.86	110.52
1	B	234	ILE	CB-CA-C	-5.74	104.56	111.85
1	A	103(A)	PRO	N-CA-C	5.59	120.08	111.57
1	A	191	VAL	N-CA-C	-5.54	100.36	108.11
1	A	209(C)	VAL	N-CA-C	5.51	113.33	107.76
1	B	58	ILE	CB-CA-C	-5.38	106.95	114.00
1	B	262	LEU	N-CA-C	5.37	117.88	111.71
1	A	289	VAL	CB-CA-C	-5.33	104.13	109.89
1	B	307	LEU	N-CA-C	5.28	117.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ILE	N-CA-C	-5.22	100.13	107.75
1	A	269	VAL	CA-C-N	-5.19	114.45	119.90
1	A	269	VAL	C-N-CA	-5.19	114.45	119.90
1	A	110	SER	N-CA-C	5.16	117.81	111.82
1	A	96	ILE	N-CA-C	5.15	115.18	107.51
1	A	325	ILE	N-CA-C	-5.05	105.62	110.72
1	A	208	VAL	CB-CA-C	-5.03	105.51	111.09

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	TYR	Sidechain
1	B	38	TYR	Sidechain

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	2356	0	2389	52	0
1	B	2355	0	2388	56	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
3	A	6	0	0	0	0
4	A	12	0	8	1	0
4	B	6	0	5	1	0
5	A	93	0	0	4	0
5	B	49	0	0	2	0
All	All	4965	0	4842	109	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 11.

All (109) 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:199:MET:HE2	1:A:233:ARG:HA	1.21	1.16
1:B:109:ARG:HH22	1:B:236:TRP:CG	1.84	0.95
1:A:174:THR:O	1:A:178:GLN:HG3	1.77	0.84
1:A:230:CYS:SG	5:A:691:HOH:O	2.36	0.83
1:A:79:ILE:C	1:A:79:ILE:HD12	2.06	0.80
1:B:199:MET:CE	1:B:232:THR:HG22	2.13	0.78
1:B:315:LEU:O	1:B:319:ILE:HG13	1.85	0.76
1:B:199:MET:HE1	1:B:232:THR:HG22	1.65	0.75
2:A:401:NAD:H6N	5:A:602:HOH:O	1.86	0.74
1:A:231:HIS:HE1	1:A:238:GLU:OE2	1.70	0.72
1:A:140:ASN:HD22	1:A:142:LEU:H	1.39	0.71
1:B:199:MET:HE2	1:B:233:ARG:HA	1.72	0.69
1:B:56:GLU:H	1:B:56:GLU:CD	2.02	0.68
1:B:210(B):SER:O	1:B:213:ILE:HB	1.95	0.67
1:B:281:VAL:HG21	1:B:287:MET:HE2	1.81	0.63
1:A:199:MET:HE3	1:A:232:THR:HG22	1.82	0.62
1:A:108:ASP:OD1	1:A:110:SER:HB2	2.00	0.61
1:A:138:ILE:O	2:A:401:NAD:H2N	2.01	0.61
1:B:109:ARG:HH22	1:B:236:TRP:CD1	2.18	0.60
1:B:199:MET:CE	1:B:233:ARG:HA	2.32	0.60
1:B:199:MET:HE2	1:B:233:ARG:CA	2.31	0.59
1:B:140:ASN:HD22	1:B:142:LEU:H	1.51	0.59
1:B:109:ARG:NH1	1:B:109:ARG:HG2	2.18	0.59
1:B:100:ILE:HB	1:B:103(A):PRO:HD2	1.84	0.58
1:B:199:MET:HE2	1:B:233:ARG:HG3	1.86	0.58
1:A:199:MET:HE2	1:A:233:ARG:CA	2.14	0.57
1:A:247:TYR:C	1:A:250:PRO:HD2	2.29	0.57
1:A:137[A]:CYS:HB2	1:A:146:VAL:HG22	1.85	0.57
1:A:276:SER:O	1:A:277:ASN:CG	2.47	0.57
1:B:109:ARG:CG	1:B:109:ARG:HH11	2.18	0.57
1:B:164:ALA:HB1	1:B:195:HIS:HB2	1.86	0.57
1:A:276:SER:HB3	1:A:283:GLY:HA2	1.87	0.56
1:A:285:ILE:HG12	1:A:286:TYR:N	2.21	0.56
1:A:146:VAL:HG21	1:A:162:GLY:HA3	1.88	0.55
1:A:260:ALA:HA	1:A:265:LYS:HD3	1.89	0.55
1:A:142:LEU:C	1:A:142:LEU:HD13	2.32	0.55
1:A:278:HIS:ND1	1:A:304:GLU:OE2	2.38	0.55
1:B:199:MET:HE3	1:B:232:THR:HG22	1.89	0.55
1:A:137[B]:CYS:HB3	1:A:146:VAL:HG22	1.88	0.54
1:B:239:VAL:HG11	1:B:246:ALA:HB2	1.90	0.53
1:B:308:THR:O	1:B:312:GLN:HG3	2.09	0.53
1:B:112:LEU:HA	5:B:615:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:OE2	4:B:603:GOL:O1	2.22	0.53
1:B:85:TYR:O	1:B:88:ILE:HG12	2.11	0.51
1:B:138:ILE:HD11	1:B:254:ALA:HB2	1.93	0.51
1:B:177:ALA:HB2	1:B:184:ALA:HA	1.93	0.51
1:A:249:ALA:N	1:A:250:PRO:CD	2.74	0.51
1:B:236:TRP:CZ2	1:B:237:LYS:HG2	2.46	0.51
1:A:20:ARG:HD3	1:A:47:ASP:OD2	2.11	0.50
1:B:58:ILE:N	1:B:59:PRO:HD2	2.27	0.50
1:B:155:LEU:HD12	1:B:155:LEU:N	2.27	0.50
1:B:231:HIS:HE1	1:B:238:GLU:OE2	1.94	0.49
1:A:311:GLU:OE2	4:A:600:GOL:O3	2.21	0.49
1:B:163:MET:C	1:B:163:MET:SD	2.96	0.49
1:B:213:ILE:HD13	1:B:219:ILE:O	2.13	0.48
1:B:148:HIS:O	1:B:152:VAL:HG13	2.13	0.48
1:A:211[B]:SER:OG	1:A:215:GLN:NE2	2.45	0.48
1:A:332:ALA:HB1	1:A:333:PRO:HD2	1.96	0.47
1:A:36:ILE:HD13	1:A:95:ILE:HG21	1.96	0.47
1:A:259:GLU:CD	5:A:692:HOH:O	2.58	0.47
1:A:234:ILE:HD12	1:A:234:ILE:O	2.13	0.47
1:A:26:ILE:HD13	1:A:26:ILE:N	2.29	0.47
1:A:57:GLY:HA2	1:B:241:ASN:HD22	1.80	0.47
1:B:109:ARG:NH2	1:B:236:TRP:CG	2.67	0.47
1:B:142:LEU:O	1:B:146:VAL:HG23	2.15	0.46
1:B:210(A):LEU:O	1:B:213:ILE:HG12	2.15	0.46
1:A:163:MET:C	1:A:163:MET:SD	2.98	0.46
1:A:264:ASP:CG	1:A:295:LYS:HD3	2.41	0.46
2:B:402:NAD:H6N	5:B:609:HOH:O	2.16	0.46
1:B:145:MET:HA	1:B:145:MET:HE2	1.98	0.45
1:A:79:ILE:C	1:A:79:ILE:CD1	2.81	0.45
1:A:233:ARG:NH1	5:A:660:HOH:O	2.47	0.45
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.81	0.45
1:A:83:ASN:OD1	1:A:83:ASN:C	2.60	0.45
1:B:105(A):PRO:HD2	1:B:245:THR:HG21	1.99	0.45
1:B:109:ARG:HG2	1:B:109:ARG:HH11	1.75	0.44
1:A:204:SER:HB3	1:A:311:GLU:OE2	2.18	0.44
1:A:22:LYS:NZ	1:A:89:SER:O	2.42	0.43
1:A:281:VAL:HG21	1:A:287:MET:HE2	2.00	0.43
1:A:225:ILE:O	1:A:229:VAL:HG23	2.19	0.43
1:B:108:ASP:C	1:B:110:SER:H	2.26	0.43
1:A:140:ASN:HA	1:A:142:LEU:N	2.34	0.43
1:A:281:VAL:CG1	1:A:319:ILE:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:HE1	1:A:218:LEU:O	2.02	0.42
1:A:199:MET:O	1:A:201:PRO:HD3	2.19	0.42
1:A:209(C):VAL:CG1	1:A:212:PHE:CE1	3.02	0.42
1:B:281:VAL:HG11	1:B:319:ILE:HD13	2.01	0.42
1:B:327:LYS:O	1:B:328:VAL:C	2.61	0.42
1:A:276:SER:O	1:A:277:ASN:CB	2.67	0.42
1:B:124:ALA:O	1:B:128:LYS:HB2	2.20	0.42
1:B:193:GLY:O	1:B:288:GLY:HA3	2.19	0.42
1:B:323:ASN:O	1:B:327:LYS:HG3	2.18	0.42
1:A:53:ASP:HB3	1:A:59:PRO:HD3	2.02	0.42
1:B:146:VAL:HG21	1:B:162:GLY:HA3	2.01	0.42
1:B:242:LEU:O	1:B:243(A):LYS:C	2.61	0.42
1:B:285:ILE:HD12	1:B:286:TYR:H	1.83	0.42
1:B:58:ILE:HB	1:B:59:PRO:HD3	2.00	0.42
1:A:191:VAL:HG22	1:A:201:PRO:HA	2.02	0.41
1:B:138:ILE:HD11	1:B:254:ALA:CB	2.50	0.41
1:A:199:MET:CE	1:A:232:THR:HG22	2.50	0.41
1:A:269:VAL:HB	1:A:293:ILE:HD12	2.01	0.41
1:B:155:LEU:N	1:B:155:LEU:CD1	2.84	0.41
1:A:79:ILE:HD12	1:A:79:ILE:O	2.20	0.41
1:B:331:ASN:O	1:B:332:ALA:HB3	2.20	0.41
1:B:58:ILE:HB	1:B:59:PRO:CD	2.51	0.41
1:B:137[A]:CYS:HB2	1:B:146:VAL:HG22	2.03	0.41
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.91	0.40
1:A:105(B):LYS:HD2	1:A:106:ASP:CG	2.46	0.40

There are no symmetry-related clashes.

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	317/321 (99%)	307 (97%)	8 (2%)	2 (1%)	21 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	316/321 (98%)	289 (92%)	21 (7%)	6 (2%)	6	5
All	All	633/642 (99%)	596 (94%)	29 (5%)	8 (1%)	9	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	B	283	GLY
1	B	111	GLU
1	B	243(B)	THR
1	B	332	ALA
1	A	164	ALA
1	B	164	ALA
1	B	324	THR

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	260/258 (101%)	255 (98%)	5 (2%)	50	69
1	B	259/258 (100%)	248 (96%)	11 (4%)	26	40
All	All	519/516 (101%)	503 (97%)	16 (3%)	35	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	110	SER
1	A	140	ASN
1	A	152	VAL
1	A	304	GLU
1	B	54	ILE
1	B	56	GLU
1	B	100	ILE

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Mol	Chain	Res	Type
1	B	109	ARG
1	B	112	LEU
1	B	125	GLU
1	B	140	ASN
1	B	142	LEU
1	B	152	VAL
1	B	227	GLU
1	B	234	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	140	ASN
1	A	179	HIS
1	A	190	ASN
1	A	221	GLN
1	A	231	HIS
1	A	312	GLN
1	B	132(B)	ASN
1	B	140	ASN
1	B	178	GLN
1	B	179	HIS
1	B	221	GLN
1	B	231	HIS
1	B	241	ASN
1	B	277	ASN
1	B	312	GLN
1	B	323	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	402	-	46,48,48	2.28	14 (30%)	64,73,73	3.13	17 (26%)
2	NAD	A	401	-	46,48,48	2.90	19 (41%)	64,73,73	3.01	18 (28%)
4	GOL	B	603	-	5,5,5	4.81	5 (100%)	5,5,5	6.05	3 (60%)
4	GOL	A	600	-	5,5,5	4.99	4 (80%)	5,5,5	6.06	3 (60%)
4	GOL	A	601	-	5,5,5	5.15	5 (100%)	5,5,5	6.06	3 (60%)
3	LAC	A	364	-	4,5,5	2.99	3 (75%)	2,6,6	2.07	1 (50%)

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	402	-	-	5/30/62/62	0/5/5/5
2	NAD	A	401	-	-	6/30/62/62	0/5/5/5
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	A	600	-	-	2/4/4/4	-
4	GOL	A	601	-	-	2/4/4/4	-
3	LAC	A	364	-	1/1/2/2	1/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GOL	C3-C2	-9.22	1.16	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	GOL	C3-C2	-8.99	1.17	1.51
2	A	401	NAD	PA-O3	8.79	1.69	1.59
4	B	603	GOL	C3-C2	-8.61	1.18	1.51
2	A	401	NAD	C2N-N1N	7.29	1.43	1.35
2	B	402	NAD	C4N-C3N	6.87	1.49	1.39
2	A	401	NAD	C5N-C4N	6.68	1.50	1.38
2	B	402	NAD	C2N-N1N	5.75	1.41	1.35
2	A	401	NAD	C6N-N1N	5.63	1.48	1.35
2	B	402	NAD	PA-O3	5.42	1.65	1.59
2	A	401	NAD	C8A-N7A	-4.69	1.22	1.31
2	B	402	NAD	C6N-N1N	4.60	1.45	1.35
4	A	601	GOL	O1-C1	4.52	1.61	1.42
4	A	600	GOL	O1-C1	4.09	1.59	1.42
2	A	401	NAD	O4D-C1D	4.07	1.46	1.40
3	A	364	LAC	O-C	4.02	1.34	1.22
4	B	603	GOL	C1-C2	-3.85	1.37	1.51
2	A	401	NAD	C3N-C7N	3.85	1.56	1.50
2	A	401	NAD	C3B-C4B	3.73	1.62	1.53
3	A	364	LAC	OXT-C	-3.56	1.19	1.30
4	A	601	GOL	O2-C2	-3.56	1.33	1.43
4	A	601	GOL	C1-C2	-3.54	1.38	1.51
4	B	603	GOL	O1-C1	3.54	1.57	1.42
2	B	402	NAD	C8A-N7A	-3.41	1.25	1.31
2	B	402	NAD	C2A-N1A	3.40	1.40	1.33
4	A	600	GOL	O2-C2	-3.26	1.33	1.43
4	B	603	GOL	O3-C3	3.09	1.55	1.42
2	A	401	NAD	C4N-C3N	2.99	1.43	1.39
2	A	401	NAD	PA-O1A	-2.93	1.40	1.50
2	A	401	NAD	C5A-N7A	-2.85	1.33	1.39
4	A	600	GOL	C1-C2	-2.85	1.40	1.51
2	B	402	NAD	C5N-C4N	2.84	1.43	1.38
2	A	401	NAD	O4B-C4B	-2.65	1.39	1.45
2	B	402	NAD	C3B-C4B	2.63	1.59	1.53
2	B	402	NAD	C5A-N7A	-2.61	1.34	1.39
3	A	364	LAC	CB-CA	2.61	1.62	1.50
2	A	401	NAD	C2B-C1B	-2.60	1.45	1.53
2	B	402	NAD	C7N-N7N	2.53	1.37	1.33
2	A	401	NAD	PN-O1N	-2.53	1.42	1.50
2	A	401	NAD	PA-O2A	-2.52	1.43	1.55
4	A	601	GOL	O3-C3	2.50	1.52	1.42
2	A	401	NAD	C2A-N1A	2.44	1.38	1.33
2	B	402	NAD	C3N-C7N	2.35	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C5B-C4B	2.32	1.58	1.51
2	A	401	NAD	C7N-N7N	2.25	1.37	1.33
2	B	402	NAD	PN-O1N	-2.25	1.43	1.50
2	A	401	NAD	PA-O5B	-2.18	1.50	1.59
4	B	603	GOL	O2-C2	-2.11	1.37	1.43
2	B	402	NAD	C6N-C5N	2.10	1.43	1.38
2	B	402	NAD	O4D-C4D	2.04	1.49	1.45

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAD	N9A-C8A-N7A	13.16	132.61	113.94
2	A	401	NAD	N9A-C8A-N7A	13.00	132.38	113.94
2	B	402	NAD	C4A-N9A-C8A	-12.74	92.36	105.74
2	A	401	NAD	C4A-N9A-C8A	-12.10	93.04	105.74
4	A	601	GOL	O3-C3-C2	11.33	161.37	110.38
4	A	600	GOL	O3-C3-C2	11.22	160.88	110.38
4	B	603	GOL	O3-C3-C2	10.56	157.90	110.38
4	B	603	GOL	O2-C2-C3	7.73	141.20	109.18
4	A	601	GOL	O2-C2-C3	7.06	138.40	109.18
4	A	600	GOL	O2-C2-C3	6.70	136.93	109.18
2	B	402	NAD	C5N-C4N-C3N	-6.44	114.04	120.36
2	B	402	NAD	C5A-N7A-C8A	-6.28	93.57	103.45
2	A	401	NAD	C5A-N7A-C8A	-6.28	93.57	103.45
2	B	402	NAD	C1B-N9A-C8A	6.17	140.79	127.09
2	A	401	NAD	C5N-C6N-N1N	-5.40	113.02	120.38
2	A	401	NAD	C5N-C4N-C3N	-5.26	115.19	120.36
2	A	401	NAD	C2N-N1N-C1D	-4.52	109.15	119.13
2	A	401	NAD	C6N-C5N-C4N	4.48	125.91	119.45
2	B	402	NAD	C5N-C6N-N1N	-4.43	114.34	120.38
2	B	402	NAD	C2N-N1N-C1D	-4.39	109.45	119.13
2	B	402	NAD	C6N-C5N-C4N	4.36	125.73	119.45
2	B	402	NAD	C2N-C3N-C4N	4.21	123.15	118.26
2	A	401	NAD	C1B-N9A-C8A	3.99	135.96	127.09
2	A	401	NAD	C6N-N1N-C1D	3.79	127.17	119.73
4	A	600	GOL	O1-C1-C2	3.50	126.14	110.38
2	B	402	NAD	C6N-N1N-C1D	3.45	126.50	119.73
2	A	401	NAD	C2N-C3N-C4N	3.41	122.22	118.26
2	B	402	NAD	C4N-C3N-C7N	-3.09	112.65	121.06
2	A	401	NAD	C4A-C5A-N7A	3.07	114.09	110.58
4	B	603	GOL	O1-C1-C2	3.06	124.17	110.38
2	A	401	NAD	C4N-C3N-C7N	-3.01	112.87	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	364	LAC	OXT-C-O	2.84	130.53	124.08
2	A	401	NAD	O2B-C2B-C3B	2.82	120.86	111.82
2	B	402	NAD	C4A-C5A-N7A	2.67	113.64	110.58
2	B	402	NAD	C4B-O4B-C1B	-2.63	103.66	109.47
2	B	402	NAD	C6N-N1N-C2N	2.56	124.05	121.88
2	B	402	NAD	O2B-C2B-C3B	2.35	119.35	111.82
4	A	601	GOL	O1-C1-C2	2.34	120.89	110.38
2	B	402	NAD	O7N-C7N-N7N	2.33	125.98	122.62
2	A	401	NAD	O4B-C1B-C2B	-2.21	101.89	106.62
2	A	401	NAD	C6N-N1N-C2N	2.10	123.67	121.88
2	A	401	NAD	C4B-O4B-C1B	-2.10	104.84	109.47
2	B	402	NAD	C3N-C7N-N7N	-2.04	115.22	117.74
2	A	401	NAD	O5B-C5B-C4B	-2.03	102.07	108.99
2	A	401	NAD	O3D-C3D-C4D	-2.02	105.27	111.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	364	LAC	CA

All (18) torsion outliers are listed below:

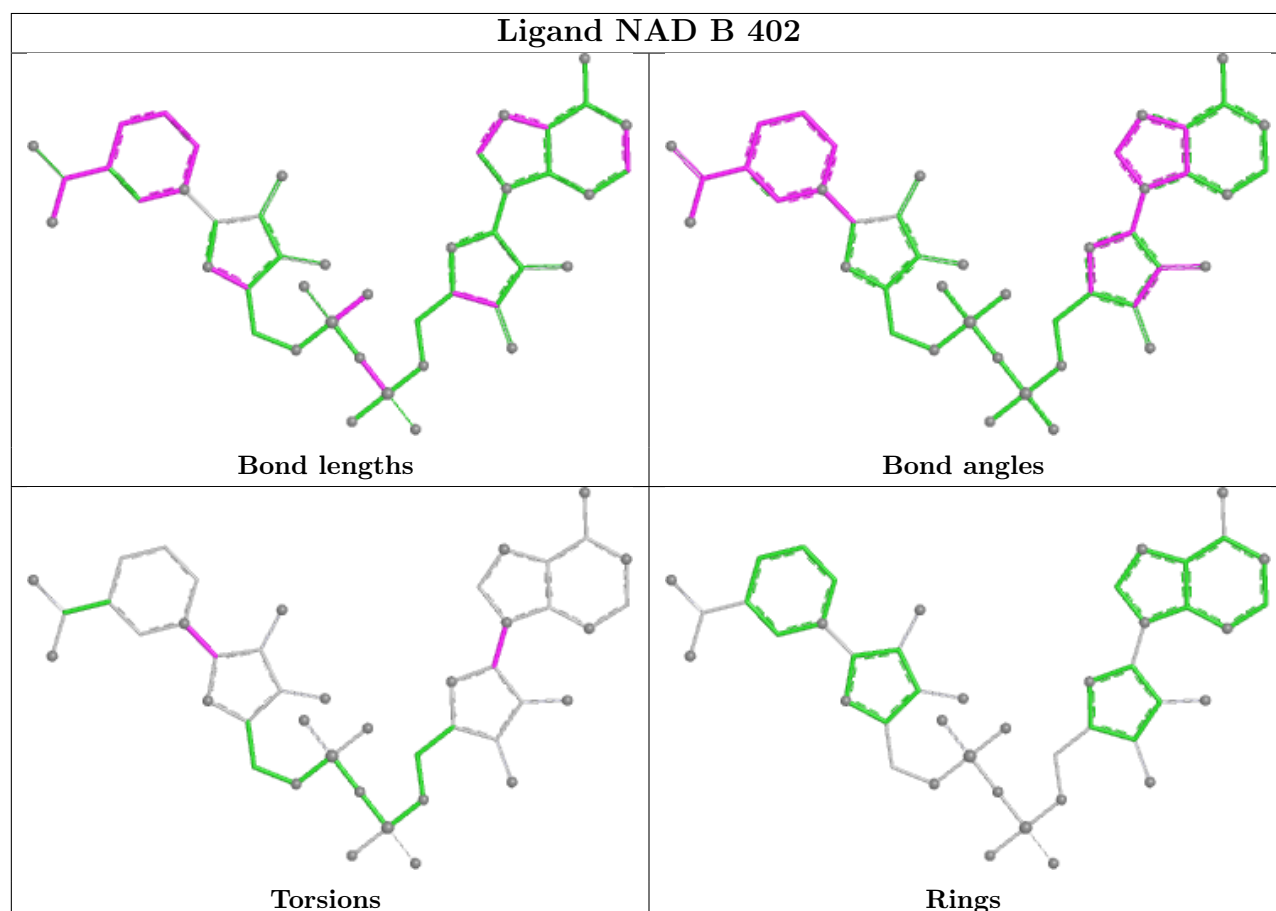
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	402	NAD	O4D-C1D-N1N-C2N
2	B	402	NAD	O4D-C1D-N1N-C6N
2	B	402	NAD	C2D-C1D-N1N-C2N
2	B	402	NAD	C2D-C1D-N1N-C6N
4	A	600	GOL	O1-C1-C2-C3
4	A	600	GOL	C1-C2-C3-O3
4	A	601	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-C3
4	B	603	GOL	C1-C2-C3-O3
4	A	601	GOL	O1-C1-C2-O2
3	A	364	LAC	O-C-CA-CB
2	A	401	NAD	C2B-C1B-N9A-C8A
2	B	402	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	O4B-C4B-C5B-O5B

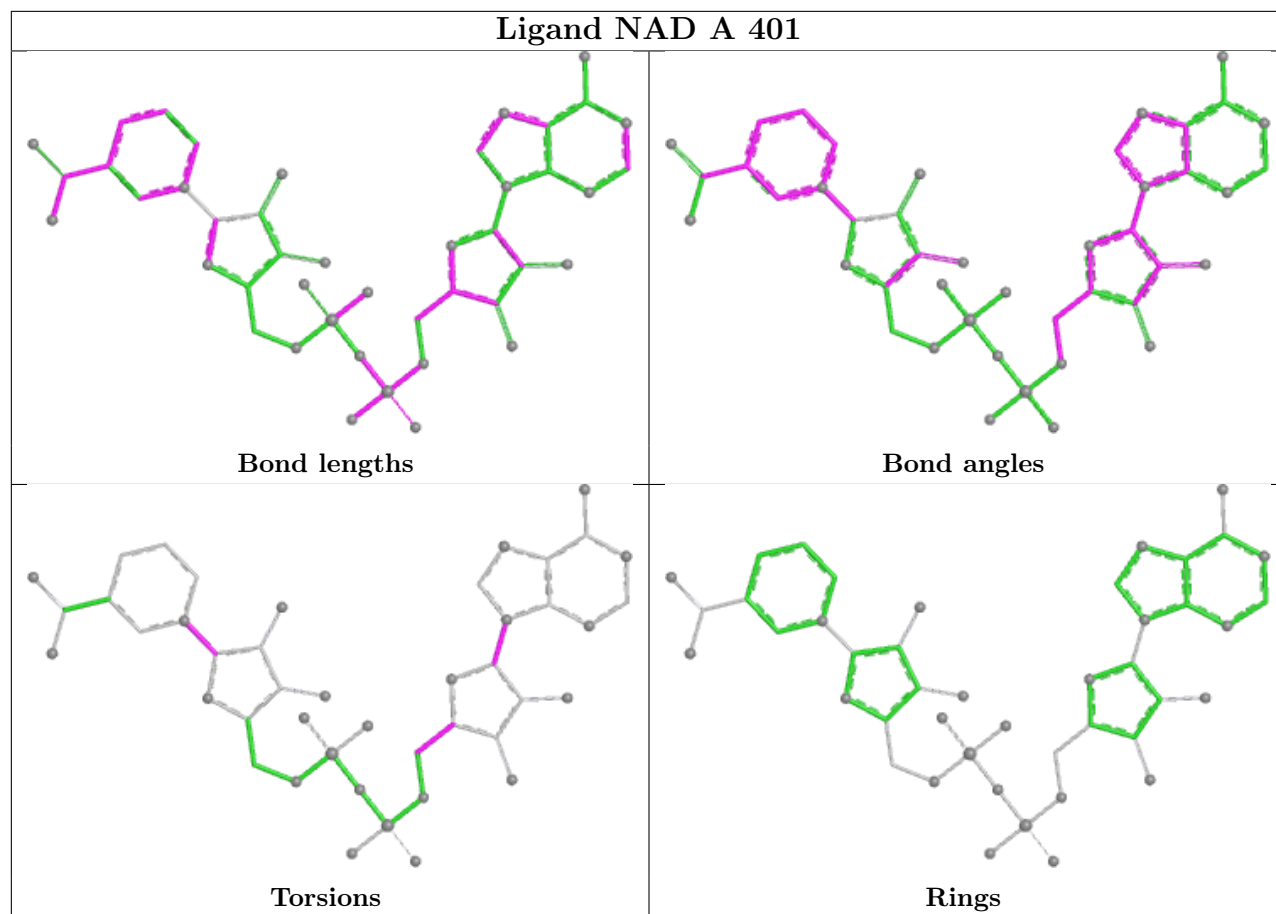
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	NAD	1	0
2	A	401	NAD	2	0
4	B	603	GOL	1	0
4	A	600	GOL	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 [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	317/321 (98%)	-0.06	5 (1%) 70 72	18, 33, 50, 74	2 (0%)
1	B	317/321 (98%)	0.56	36 (11%) 10 11	20, 43, 76, 101	1 (0%)
All	All	634/642 (98%)	0.25	41 (6%) 25 27	18, 37, 66, 101	3 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	PRO	7.2
1	B	110	SER	5.0
1	B	105(B)	LYS	5.0
1	B	195	HIS	4.9
1	B	112	LEU	4.8
1	A	333	PRO	4.6
1	B	332	ALA	4.5
1	B	105(A)	PRO	4.4
1	B	106	ASP	4.2
1	B	111	GLU	4.1
1	B	109	ARG	3.9
1	B	103(B)	GLY	3.8
1	B	17	MET	3.7
1	A	17	MET	3.7
1	B	243(B)	THR	3.6
1	B	108	ASP	3.2
1	B	325	ILE	3.2
1	B	114	PHE	3.2
1	B	329	LEU	3.2
1	A	332	ALA	3.0
1	B	243(A)	LYS	2.9
1	A	227	GLU	2.9
1	B	328	VAL	2.8
1	B	103(C)	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	285	ILE	2.7
1	B	309	PRO	2.6
1	B	281	VAL	2.6
1	B	323	ASN	2.5
1	B	324	THR	2.5
1	B	275	CYS	2.4
1	B	310	LEU	2.4
1	B	118	ARG	2.3
1	B	151	LYS	2.3
1	B	198	GLY	2.3
1	B	282	LYS	2.3
1	B	113	LEU	2.2
1	B	322	VAL	2.2
1	B	331	ASN	2.1
1	B	196	GLY	2.1
1	B	327	LYS	2.1
1	A	105(B)	LYS	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 ⓘ

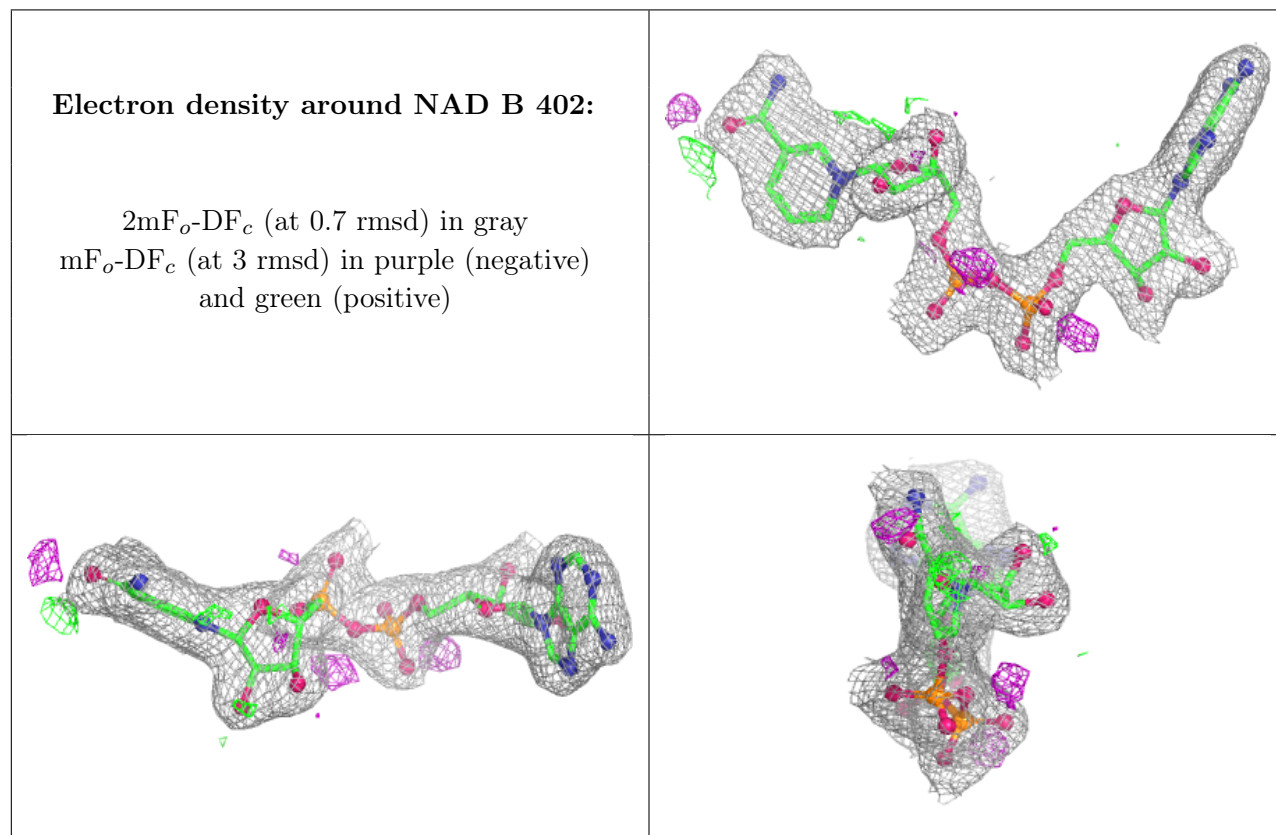
There are no oligosaccharides in this entry.

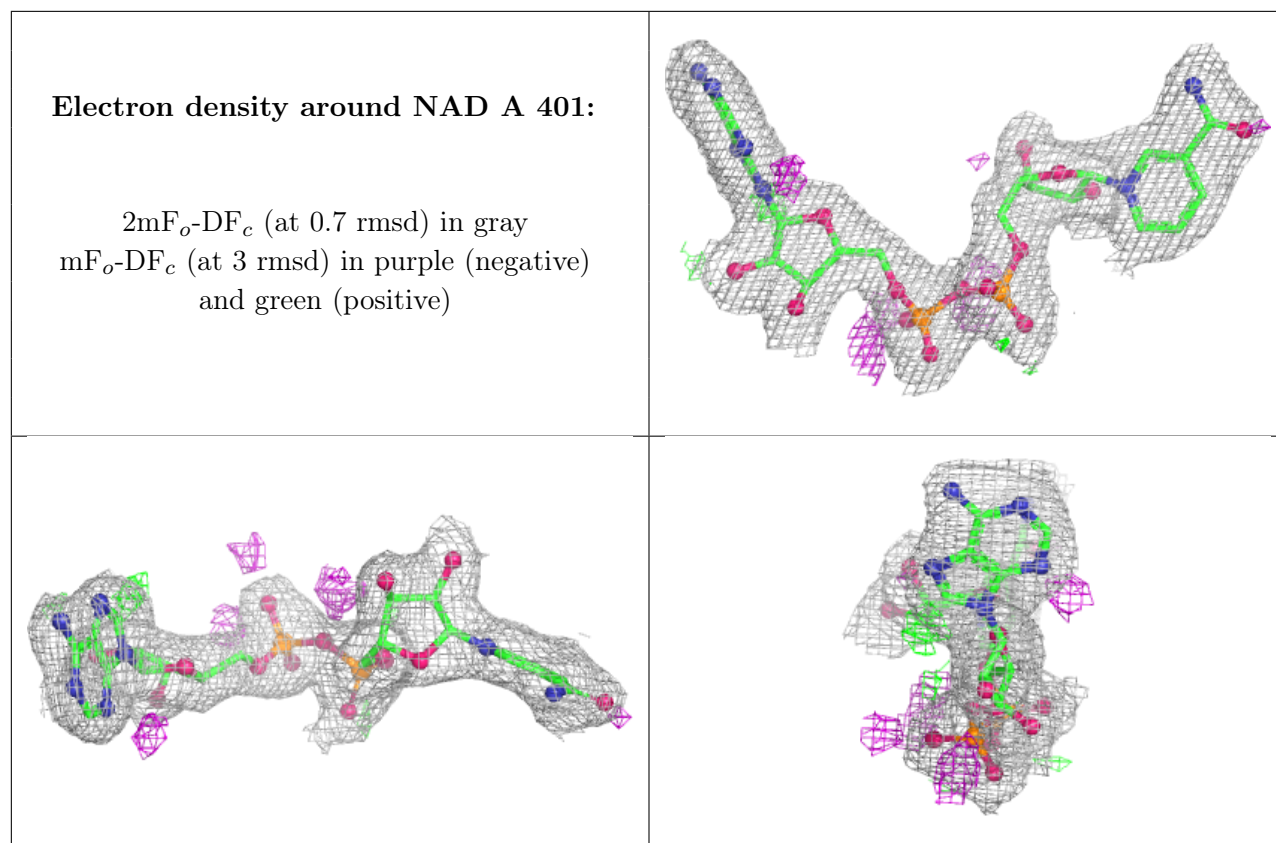
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	A	600	6/6	0.86	0.18	52,54,56,58	0
4	GOL	B	603	6/6	0.88	0.16	63,65,65,68	0
4	GOL	A	601	6/6	0.90	0.21	69,71,72,72	0
3	LAC	A	364	6/6	0.96	0.09	29,32,35,37	0
2	NAD	B	402	44/44	0.96	0.08	31,37,41,42	0
2	NAD	A	401	44/44	0.97	0.06	18,27,30,35	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.