



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:37 am BST

PDB ID : 2FN7  
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](mailto: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 : 2.11  
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) : 2.11

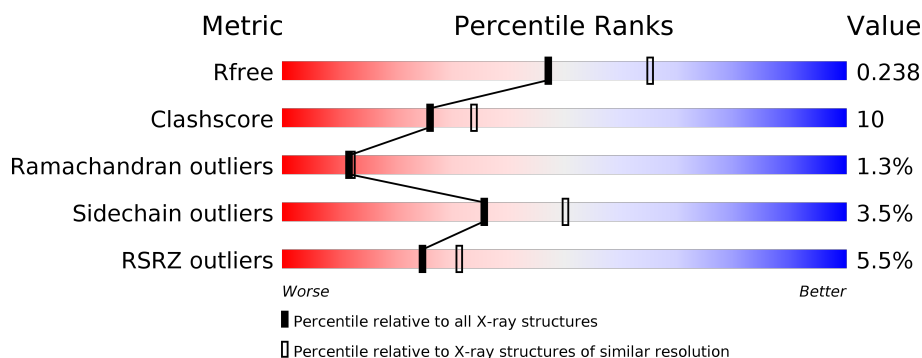
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

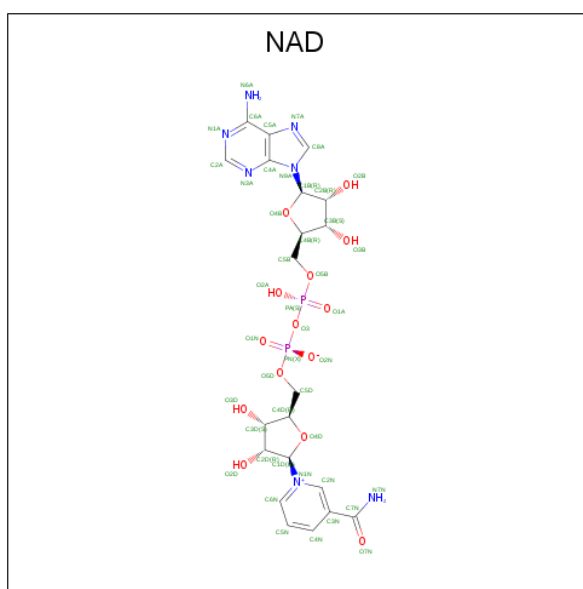
- Molecule 1 is a protein called Lactate Dehydrogenase.

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 (three-letter code: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ).



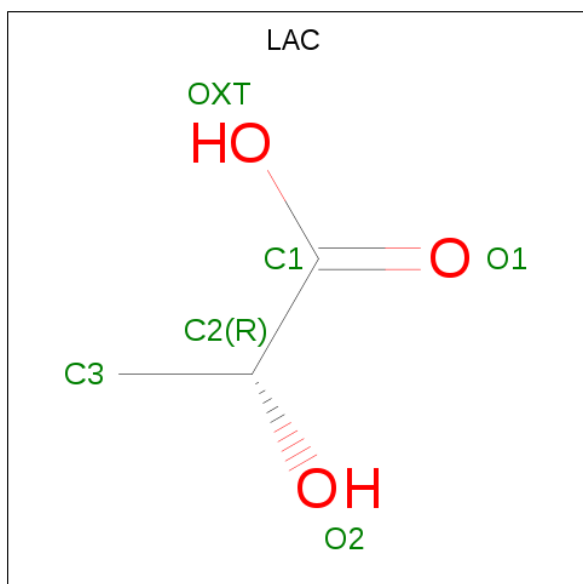
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

*Continued on next page...*

Continued from previous page...

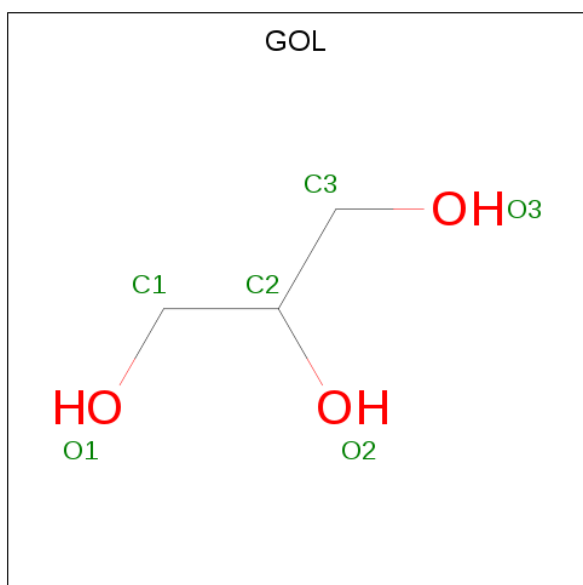
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	
			44	21	7	14	2	
								0
								0

- Molecule 3 is LACTIC ACID (three-letter code: LAC) (formula:  $C_3H_6O_3$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: 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

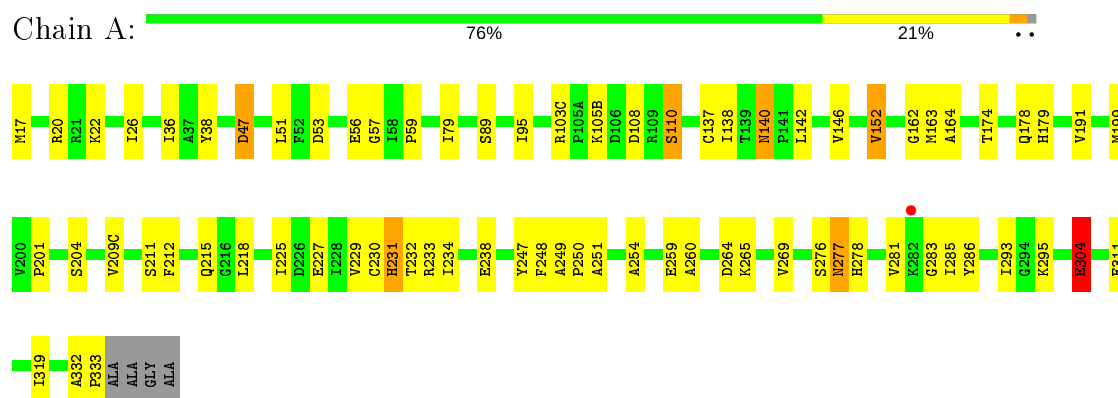
- Molecule 5 is water.

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

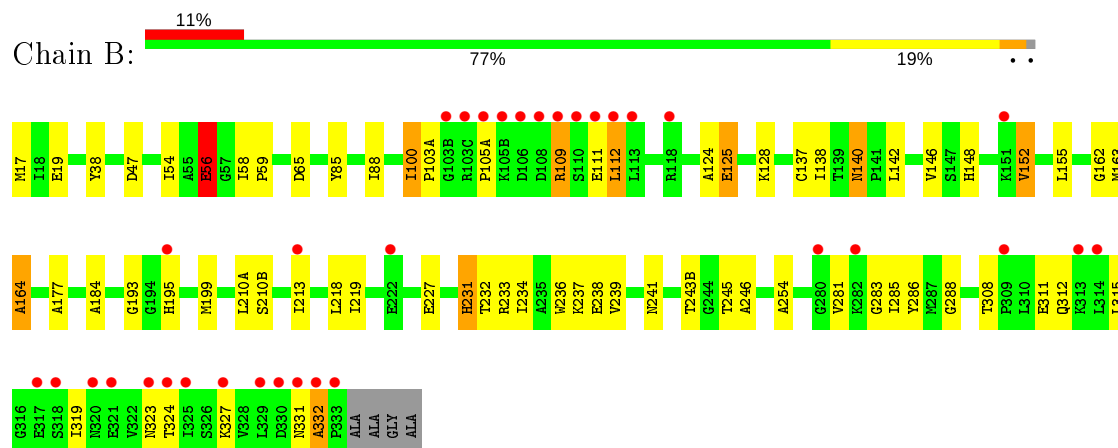
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	95.47Å 95.47Å 186.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 46.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.30) 100.0 (46.24-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.246 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	4465 reflections (8.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, NAD, LAC

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	1.20	9/2405 (0.4%)	1.03	3/3259 (0.1%)
1	B	1.09	5/2399 (0.2%)	0.97	2/3251 (0.1%)
All	All	1.14	14/4804 (0.3%)	1.00	5/6510 (0.1%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	GLU	CG-CD	7.84	1.63	1.51
1	B	56	GLU	CB-CG	6.63	1.64	1.52
1	A	227	GLU	CD-OE1	6.47	1.32	1.25
1	A	304	GLU	CG-CD	6.37	1.61	1.51
1	A	56	GLU	CG-CD	6.30	1.61	1.51
1	A	227	GLU	CD-OE2	6.01	1.32	1.25
1	B	17	MET	CG-SD	5.97	1.96	1.81
1	A	227	GLU	CG-CD	5.75	1.60	1.51
1	A	251	ALA	CA-CB	5.64	1.64	1.52
1	A	152	VAL	CB-CG2	-5.33	1.41	1.52
1	B	125	GLU	CB-CG	5.31	1.62	1.52
1	A	248	PHE	CE2-CZ	5.16	1.47	1.37
1	B	19	GLU	CG-CD	5.05	1.59	1.51
1	A	254	ALA	CA-CB	5.03	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LEU	CA-CB-CG	7.37	132.25	115.30
1	B	65	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	47	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	103(C)	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	47	ASP	CB-CG-OD1	5.37	123.13	118.30

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 ⓘ

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	48	0
1	B	2355	0	2388	51	0
2	A	44	0	26	3	0
2	B	44	0	26	1	0
3	A	6	0	5	1	0
4	A	12	0	8	0	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	4847	101	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 10.

All (101) 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:174:THR:O	1:A:178:GLN:HG3	1.77	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:CYS:SG	5:A:691:HOH:O	2.36	0.83
1:B:199:MET:CE	1:B:232:THR:HG22	2.13	0.78
1:A:199:MET:HE2	1:A:233:ARG:HA	1.67	0.76
1:A:79:ILE:HD12	1:A:79:ILE:C	2.06	0.76
1:B:315:LEU:O	1:B:319:ILE:HG13	1.85	0.76
1:A:199:MET:CE	1:A:233:ARG:HA	2.16	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:HE3	1:B:232:THR:HG22	1.72	0.69
1:B:210(B):SER:O	1:B:213:ILE:HB	1.95	0.67
1:B:199:MET:HE2	1:B:233:ARG:HG3	1.79	0.63
1:B:56:GLU:H	1:B:56:GLU:CD	2.02	0.63
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:199:MET:HE1	1:B:232:THR:HG22	1.82	0.61
1:B:199:MET:CE	1:B:233:ARG:HA	2.32	0.60
2:A:401:NAD:C5N	3:A:364:LAC:H2	2.33	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:A:137[A]:CYS:HB2	1:A:146:VAL:HG22	1.85	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:278:HIS:ND1	1:A:304:GLU:OE2	2.38	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
1:B:311:GLU:OE2	4:B:603:GOL:O1	2.22	0.53
1:A:247:TYR:C	1:A:250:PRO:HD2	2.29	0.52
1:A:276:SER:O	1:A:277:ASN:CG	2.47	0.52
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:C	1:A:142:LEU:HD13	2.32	0.50
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:N	1:B:155:LEU:HD12	2.27	0.50
1:A:199:MET:HE1	1:A:232:THR:HG22	1.92	0.49
1:B:231:HIS:HE1	1:B:238:GLU:OE2	1.94	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:199:MET:HE3	1:A:233:ARG:HA	1.93	0.48
1:B:199:MET:HE2	1:B:233:ARG:HA	1.94	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:234:ILE:O	1:A:234:ILE:HD12	2.13	0.47
1:A:26:ILE:N	1:A:26:ILE:HD13	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:B:199:MET:HE1	1:B:232:THR:C	2.36	0.46
2:B:402:NAD:H6N	5:B:609:HOH:O	2.16	0.46
1:A:233:ARG:NH1	5:A:660:HOH:O	2.47	0.45
1:A:22:LYS:NZ	1:A:89:SER:O	2.42	0.45
1:B:218:LEU:HA	1:B:218:LEU:HD23	1.81	0.45
1:B:105(A):PRO:HD2	1:B:245:THR:HG21	1.99	0.45
1:B:163:MET:C	1:B:163:MET:SD	2.96	0.44
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.75	0.44
1:A:204:SER:HB3	1:A:311:GLU:OE2	2.18	0.44
1:B:199:MET:HE1	1:B:232:THR:O	2.18	0.44
1:A:225:ILE:O	1:A:229:VAL:HG23	2.19	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
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:A:259:GLU:CD	5:A:692:HOH:O	2.58	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:199:MET:CE	1:A:232:THR:HG22	2.50	0.42
1:A:163:MET:SD	1:A:163:MET:C	2.98	0.41
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: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:B:199:MET:HE2	1:B:233:ARG:CA	2.51	0.41
1:A:264:ASP:CG	1:A:295:LYS:HD3	2.41	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:137[A]:CYS:HB2	1:B:146:VAL:HG22	2.03	0.41
1:B:58:ILE:HB	1:B:59:PRO:CD	2.51	0.41
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.91	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%)	25	31
1	B	316/321 (98%)	289 (92%)	21 (7%)	6 (2%)	8	7
All	All	633/642 (99%)	596 (94%)	29 (5%)	8 (1%)	12	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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%)	253 (97%)	7 (3%)	44	61
1	B	259/258 (100%)	248 (96%)	11 (4%)	30	42
All	All	519/516 (101%)	501 (96%)	18 (4%)	36	50

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	105(B)	LYS
1	A	110	SER
1	A	140	ASN
1	A	152	VAL
1	A	231	HIS
1	A	304	GLU
1	B	54	ILE
1	B	56	GLU
1	B	100	ILE
1	B	109	ARG
1	B	112	LEU
1	B	125	GLU
1	B	140	ASN
1	B	152	VAL
1	B	227	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	231	HIS
1	B	234	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	179	HIS
1	A	221	GLN
1	A	231	HIS
1	A	241	ASN
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	312	GLN
1	B	323	ASN

### 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 carbohydrates 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	A	401	-	42,48,48	2.80	19 (45%)	50,73,73	1.98	11 (22%)
4	GOL	A	601	-	5,5,5	4.87	5 (100%)	5,5,5	5.71	3 (60%)
2	NAD	B	402	-	42,48,48	2.25	13 (30%)	50,73,73	1.93	12 (24%)
4	GOL	A	600	-	5,5,5	4.69	4 (80%)	5,5,5	5.72	3 (60%)
3	LAC	A	364	-	2,5,5	1.95	1 (50%)	3,6,6	1.56	1 (33%)
4	GOL	B	603	-	5,5,5	4.52	5 (100%)	5,5,5	5.70	3 (60%)

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	401	-	-	5/26/62/62	0/5/5/5
4	GOL	A	601	-	-	2/4/4/4	-
2	NAD	B	402	-	-	5/26/62/62	0/5/5/5
4	GOL	A	600	-	-	2/4/4/4	-
3	LAC	A	364	-	1/1/2/2	0/0/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GOL	C3-C2	-8.53	1.16	1.51
4	A	601	GOL	C3-C2	-8.32	1.17	1.51
4	B	603	GOL	C3-C2	-7.96	1.18	1.51
2	A	401	NAD	C8A-N7A	-6.74	1.22	1.34
2	A	401	NAD	C2N-N1N	6.59	1.43	1.35
2	B	402	NAD	C4N-C3N	6.15	1.49	1.39
2	A	401	NAD	C2B-C1B	-5.56	1.45	1.53
2	A	401	NAD	C5N-C4N	5.42	1.50	1.38
2	B	402	NAD	C8A-N7A	-5.37	1.25	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C6N-N1N	5.23	1.48	1.35
2	B	402	NAD	C2N-N1N	5.21	1.41	1.35
4	A	601	GOL	O1-C1	4.50	1.61	1.42
2	B	402	NAD	C6N-N1N	4.26	1.45	1.35
2	B	402	NAD	C2B-C1B	-4.23	1.47	1.53
4	A	600	GOL	O1-C1	4.07	1.59	1.42
2	A	401	NAD	O4B-C1B	3.95	1.46	1.41
2	A	401	NAD	C2D-C1D	-3.92	1.47	1.53
2	A	401	NAD	C3N-C7N	3.83	1.56	1.50
2	A	401	NAD	C3B-C4B	3.70	1.62	1.53
2	A	401	NAD	O4D-C1D	3.69	1.46	1.41
4	B	603	GOL	C1-C2	-3.55	1.37	1.51
4	B	603	GOL	O1-C1	3.52	1.57	1.42
4	A	601	GOL	O2-C2	-3.47	1.33	1.43
2	B	402	NAD	C2A-N1A	3.26	1.40	1.33
4	A	601	GOL	C1-C2	-3.26	1.38	1.51
4	A	600	GOL	O2-C2	-3.18	1.33	1.43
4	B	603	GOL	O3-C3	3.08	1.55	1.42
2	A	401	NAD	PA-O1A	-2.89	1.40	1.50
3	A	364	LAC	C3-C2	2.76	1.62	1.51
2	A	401	NAD	C4N-C3N	2.71	1.43	1.39
2	B	402	NAD	C2D-C1D	-2.69	1.49	1.53
2	A	401	NAD	O4B-C4B	-2.64	1.39	1.45
4	A	600	GOL	C1-C2	-2.63	1.40	1.51
2	B	402	NAD	C3B-C4B	2.61	1.59	1.53
2	A	401	NAD	PN-O1N	-2.50	1.42	1.50
4	A	601	GOL	O3-C3	2.49	1.52	1.42
2	A	401	NAD	PA-O2A	-2.48	1.43	1.55
2	B	402	NAD	C7N-N7N	2.44	1.37	1.33
2	B	402	NAD	C3N-C7N	2.35	1.54	1.50
2	A	401	NAD	C2A-N1A	2.34	1.38	1.33
2	B	402	NAD	C5N-C4N	2.30	1.43	1.38
2	A	401	NAD	C5B-C4B	2.23	1.58	1.51
2	B	402	NAD	PN-O1N	-2.22	1.43	1.50
2	A	401	NAD	C7N-N7N	2.16	1.37	1.33
2	A	401	NAD	PA-O5B	-2.09	1.50	1.59
4	B	603	GOL	O2-C2	-2.07	1.37	1.43
2	B	402	NAD	O4D-C4D	2.03	1.49	1.45

All (33) bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	GOL	O3-C3-C2	10.67	161.37	110.20
4	A	600	GOL	O3-C3-C2	10.57	160.88	110.20
4	B	603	GOL	O3-C3-C2	9.95	157.90	110.20
4	B	603	GOL	O2-C2-C3	7.28	141.20	109.12
4	A	601	GOL	O2-C2-C3	6.65	138.40	109.12
4	A	600	GOL	O2-C2-C3	6.31	136.93	109.12
2	B	402	NAD	C5N-C4N-C3N	-5.33	114.04	120.34
2	A	401	NAD	C5N-C6N-N1N	-5.15	113.02	120.40
2	A	401	NAD	C4A-C5A-N7A	4.50	114.09	109.40
2	A	401	NAD	C2N-N1N-C1D	-4.48	109.15	119.14
2	A	401	NAD	C6N-C5N-C4N	4.45	125.91	119.44
2	A	401	NAD	C5N-C4N-C3N	-4.35	115.19	120.34
2	B	402	NAD	C2N-N1N-C1D	-4.35	109.45	119.14
2	B	402	NAD	C6N-C5N-C4N	4.33	125.73	119.44
2	B	402	NAD	C2N-C3N-C4N	4.32	123.15	118.26
2	B	402	NAD	C5N-C6N-N1N	-4.23	114.34	120.40
2	B	402	NAD	C4A-C5A-N7A	4.06	113.64	109.40
2	A	401	NAD	C2N-C3N-C4N	3.49	122.22	118.26
2	A	401	NAD	O4B-C1B-C2B	-3.44	101.89	106.93
4	A	600	GOL	O1-C1-C2	3.32	126.14	110.20
2	B	402	NAD	C4N-C3N-C7N	-3.13	112.65	121.04
2	A	401	NAD	C4N-C3N-C7N	-3.05	112.87	121.04
4	B	603	GOL	O1-C1-C2	2.91	124.17	110.20
2	A	401	NAD	O2B-C2B-C3B	2.79	120.86	111.82
2	B	402	NAD	O4B-C1B-C2B	-2.49	103.29	106.93
2	A	401	NAD	C1B-N9A-C4A	2.48	131.00	126.64
2	B	402	NAD	O7N-C7N-N7N	2.40	125.98	122.58
3	A	364	LAC	C3-C2-C1	2.33	118.86	110.44
2	B	402	NAD	O2B-C2B-C3B	2.33	119.35	111.82
2	B	402	NAD	C6N-N1N-C2N	2.28	124.05	121.97
4	A	601	GOL	O1-C1-C2	2.23	120.89	110.20
2	B	402	NAD	C3N-C7N-N7N	-2.10	115.22	117.75
2	A	401	NAD	O5B-C5B-C4B	-2.01	102.07	108.99

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	364	LAC	C2

All (16) torsion outliers are listed below:

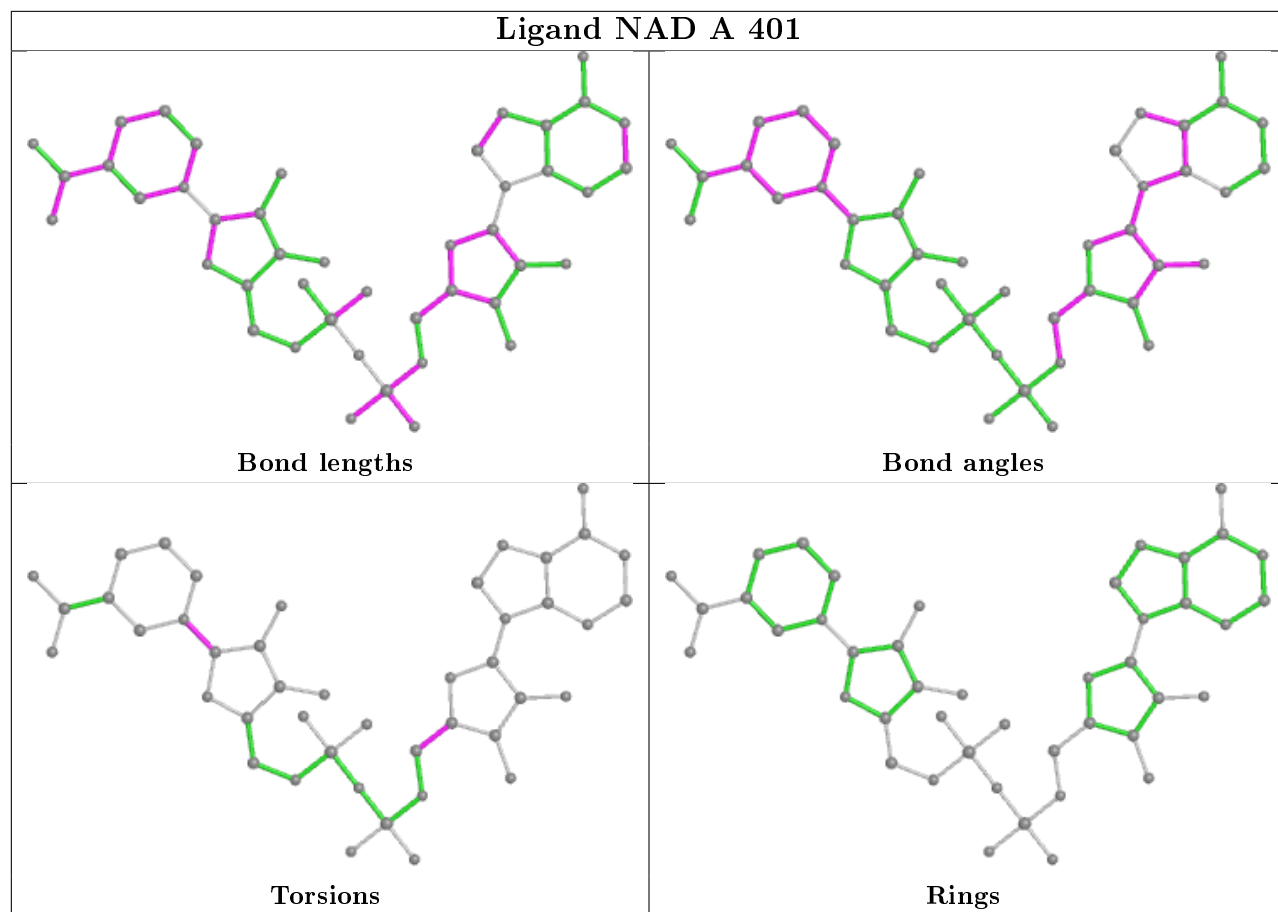
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
4	A	601	GOL	C1-C2-C3-O3
2	B	402	NAD	O4D-C1D-N1N-C2N
2	B	402	NAD	O4D-C1D-N1N-C6N
2	B	402	NAD	C2D-C1D-N1N-C2N
2	B	402	NAD	C2D-C1D-N1N-C6N
4	A	600	GOL	O1-C1-C2-C3
4	A	600	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-C3
4	B	603	GOL	C1-C2-C3-O3
4	A	601	GOL	O1-C1-C2-O2
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	402	NAD	O4B-C4B-C5B-O5B

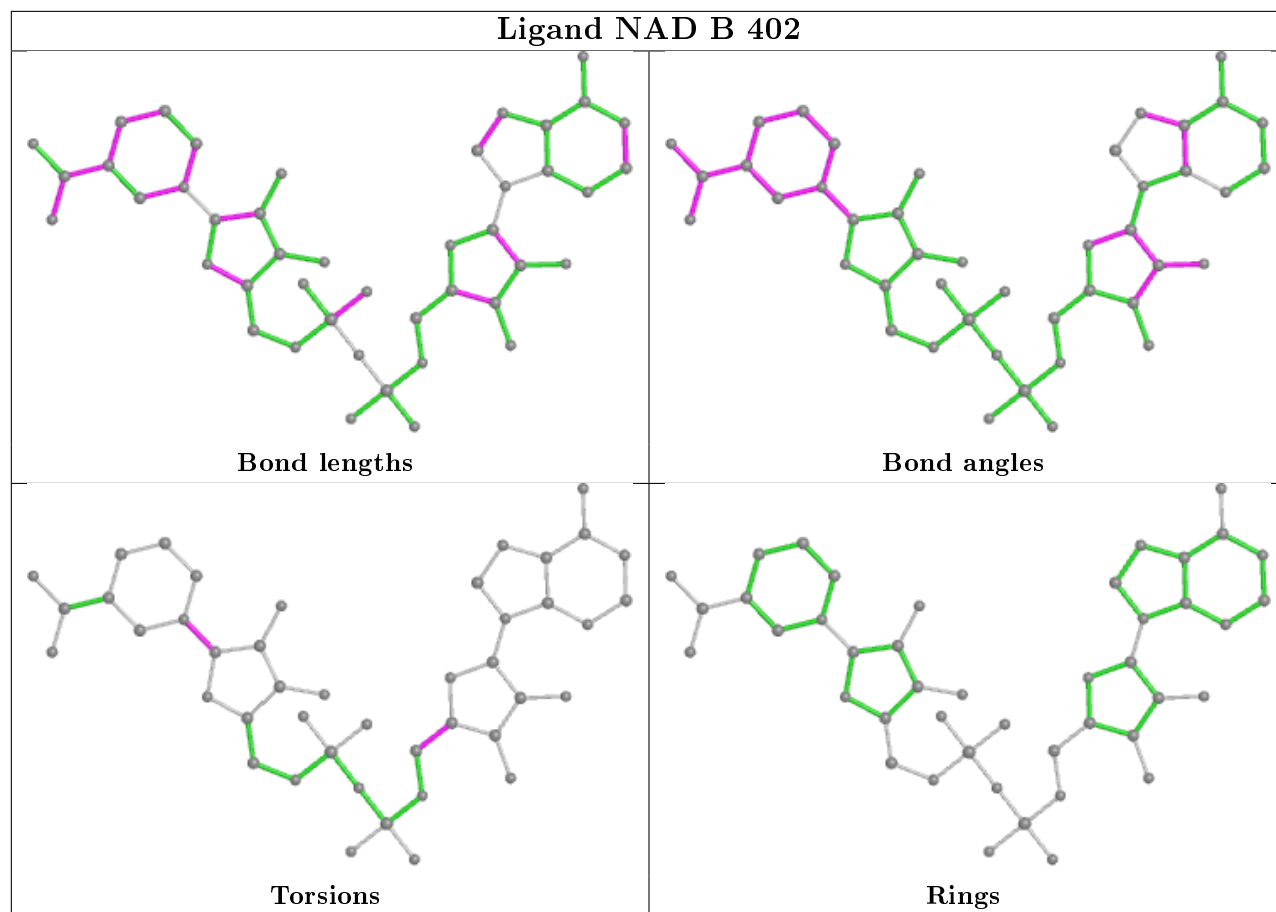
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	3	0
2	B	402	NAD	1	0
3	A	364	LAC	1	0
4	B	603	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/321 (98%)	-0.16	1 (0%) 94 96	18, 33, 50, 74	0
1	B	317/321 (98%)	0.36	34 (10%) 6 8	20, 43, 76, 101	0
All	All	634/642 (98%)	0.10	35 (5%) 25 31	18, 37, 66, 101	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	SER	8.8
1	B	333	PRO	8.3
1	B	105(B)	LYS	7.1
1	B	106	ASP	6.2
1	B	332	ALA	5.2
1	B	331	ASN	4.9
1	B	109	ARG	4.8
1	B	325	ILE	4.8
1	B	324	THR	4.7
1	B	108	ASP	4.6
1	B	111	GLU	3.9
1	B	330	ASP	3.6
1	B	105(A)	PRO	3.6
1	B	321	GLU	3.1
1	B	195	HIS	3.0
1	B	323	ASN	2.9
1	A	282	LYS	2.8
1	B	282	LYS	2.8
1	B	309	PRO	2.7
1	B	327	LYS	2.7
1	B	112	LEU	2.6
1	B	222	GLU	2.6
1	B	329	LEU	2.5
1	B	320	ASN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	280	GLY	2.4
1	B	103(B)	GLY	2.4
1	B	151	LYS	2.2
1	B	118	ARG	2.2
1	B	317	GLU	2.2
1	B	213	ILE	2.1
1	B	313	LYS	2.1
1	B	314	LEU	2.1
1	B	113	LEU	2.0
1	B	103(C)	ARG	2.0
1	B	318	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

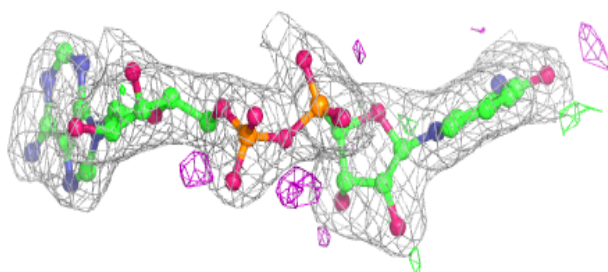
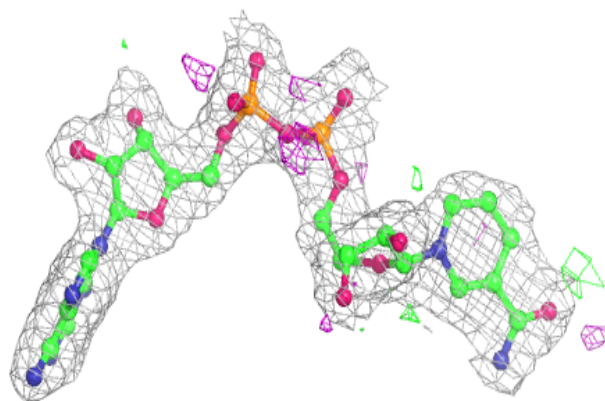
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	600	6/6	0.78	0.18	52,54,56,58	0
4	GOL	B	603	6/6	0.85	0.21	63,65,65,68	0
4	GOL	A	601	6/6	0.87	0.21	69,71,72,72	0
3	LAC	A	364	6/6	0.96	0.15	29,32,35,37	0
2	NAD	B	402	44/44	0.96	0.11	31,37,41,42	0
2	NAD	A	401	44/44	0.97	0.11	18,27,30,35	0

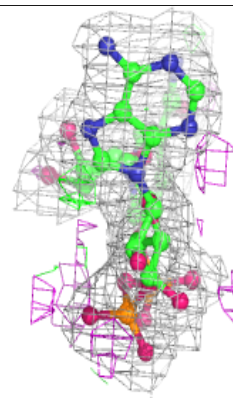
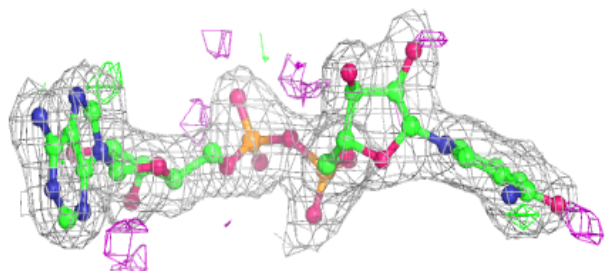
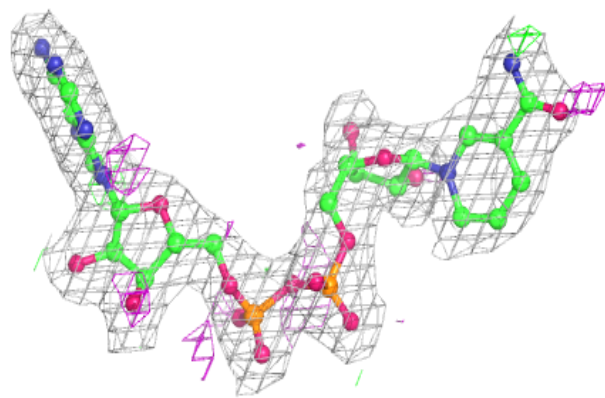
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAD B 402:**

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

**Electron density around NAD A 401:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.