

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 10:12 AM JST

PDB ID : 7YS9

Title: Crystal Structure of UDP-glucose 4-epimerase (Rv3634c) in complex with both

UDP-Glucose and UDP-Galactose in chainA from Mycobacterium tuberculosis

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Deposited on : 2022-08-11

Resolution : 1.65 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 (i) 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 (1)) 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 : 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

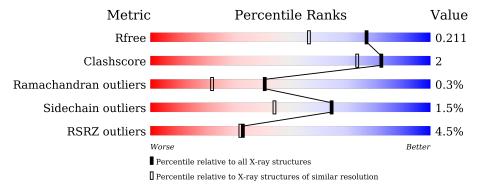
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.65 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$		
R_{free}	130704	1827 (1.66-1.66)		
Clashscore	141614	1931 (1.66-1.66)		
Ramachandran outliers	138981	1891 (1.66-1.66)		
Sidechain outliers	138945	1891 (1.66-1.66)		
RSRZ outliers	127900	1791 (1.66-1.66)		

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 <=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	320	92%						
1	В	320	92%	5% •					



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5889 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 UDP-glucose 4-epimerase.

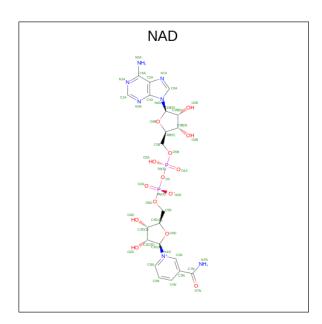
\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	310	Total	С	N	О	S	0	5	0
1	11	310	2370	1489	429	449	3	U	0	
1	D	311	Total	С	N	Ο	S	0	11	0
1	Б	311	2416	1515	440	458	3	0	11	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	HIS	-	expression tag	UNP P9WN67
A	316	HIS	-	expression tag	UNP P9WN67
A	317	HIS	-	expression tag	UNP P9WN67
A	318	HIS	-	expression tag	UNP P9WN67
A	319	HIS	-	expression tag	UNP P9WN67
A	320	HIS	-	expression tag	UNP P9WN67
В	315	HIS	-	expression tag	UNP P9WN67
В	316	HIS	-	expression tag	UNP P9WN67
В	317	HIS	-	expression tag	UNP P9WN67
В	318	HIS	-	expression tag	UNP P9WN67
В	319	HIS	-	expression tag	UNP P9WN67
В	320	HIS	-	expression tag	UNP P9WN67

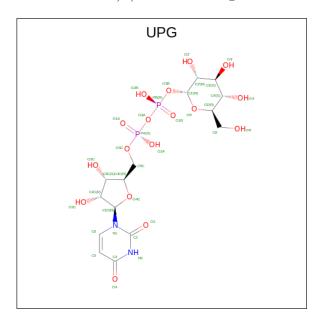
• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	Λ	1	Total	С	N	О	Р	0	0	
$\begin{array}{ c c c c c } & Z & A & A & A & A & A & A & A & A & A$	A	1	44	21	7	14	2	U		
2	D	1	Total	С	N	О	Р	0	0	
2	Б	1	44	21	7	14	2	U		

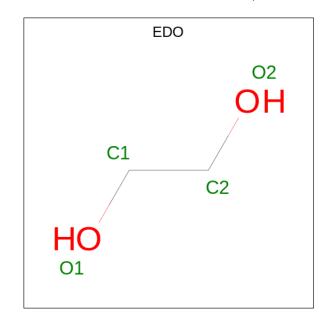
• Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36		N 2		P 2	0	1

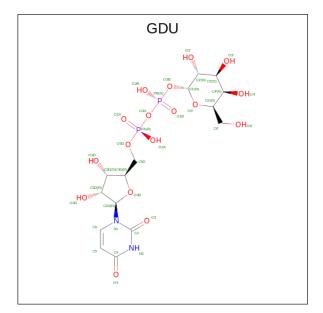


• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



M	lol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	4	A	1	Total C O 4 2 2	0	0
4	4	В	1	Total C O 4 2 2	0	0

• Molecule 5 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).





	\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	
	5	Λ	Λ 1		С	N	О	Р	0	1	
	\mathcal{A}	1	36	15	2	17	2	U			
ĺ	E	5 B	B 1	Total	С	N	О	Р	0	0	
	6			36	15	2	17	2	U		

$\bullet\,$ Molecule 6 is water.

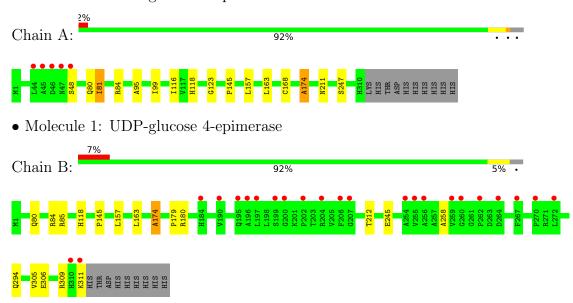
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	479	Total O 479 479	0	0
6	В	420	Total O 420 420	0	0



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: UDP-glucose 4-epimerase





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	51.35Å 76.85Å 80.16Å	Donositon	
a, b, c, α , β , γ	90.00° 91.81° 90.00°	Depositor	
Resolution (Å)	24.62 - 1.65	Depositor	
rtesolution (A)	24.62 - 1.65	EDS	
% Data completeness	89.3 (24.62-1.65)	Depositor	
(in resolution range)	89.3 (24.62-1.65)	EDS	
R_{merge}	0.04	Depositor	
R_{sum}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	6.51 (at 1.65Å)	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
R, R_{free}	0.186 , 0.212	Depositor	
it, it free	0.186 , 0.211	DCC	
R_{free} test set	3406 reflections $(5.09%)$	wwPDB-VP	
Wilson B-factor (Å ²)	16.4	Xtriage	
Anisotropy	0.212	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28, 37.9	EDS	
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.34$	Xtriage	
	0.001 for -h,l,k		
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage	
	0.023 for h,-k,-l		
F_o, F_c correlation	0.96	EDS	
Total number of atoms	5889	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	19.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.47% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: UPG, EDO, GDU, 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		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.27	0/2432	0.55	0/3318	
1	В	0.26	0/2488	0.52	0/3396	
All	All	0.26	0/4920	0.53	0/6714	

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	2370	0	2323	11	0
1	В	2416	0	2360	13	0
2	A	44	0	26	2	0
2	В	44	0	26	1	0
3	A	36	0	22	1	0
4	A	4	0	6	1	0
4	В	4	0	6	1	0
5	A	36	0	22	1	0
5	В	36	0	22	0	0
6	A	479	0	0	4	0
6	В	420	0	0	3	0
All	All	5889	0	4813	24	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 2.

All (24) 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:306:GLU:HB2	6:B:501:HOH:O	1.76	0.83
1:B:212[A]:THR:HG21	1:B:245:GLU:HB3	1.66	0.77
1:A:163:LEU:HD11	1:B:145:PRO:HD3	1.76	0.67
1:A:123:GLY:HA3	3:A:402[A]:UPG:O6'	2.01	0.61
1:B:306:GLU:CD	6:B:501:HOH:O	2.41	0.59
1:A:145:PRO:HD3	1:B:163:LEU:HD11	1.86	0.56
1:A:48:SER:HA	6:A:503:HOH:O	2.07	0.54
1:A:81[A]:ILE:HD13	6:A:714:HOH:O	2.11	0.51
1:B:118:HIS:HB2	1:B:157:LEU:CD1	2.42	0.50
1:B:212[A]:THR:CG2	1:B:245:GLU:HB3	2.38	0.50
1:B:306:GLU:CB	6:B:501:HOH:O	2.47	0.48
1:B:179:PRO:O	1:B:180:ARG:HB2	2.15	0.47
1:A:48:SER:CA	6:A:503:HOH:O	2.64	0.46
1:A:118:HIS:HB2	1:A:157:LEU:CD1	2.46	0.46
1:A:211:ASN:O	1:A:247:SER:HA	2.15	0.45
2:A:401:NAD:C4N	5:A:404[B]:GDU:H4'	2.47	0.44
1:B:258:ALA:HB1	1:B:305:VAL:HG21	2.00	0.44
1:A:95:ALA:O	1:A:99:ILE:HB	2.19	0.42
1:A:116:ILE:O	1:A:168:CYS:HA	2.20	0.42
1:B:294:GLN:HG2	4:B:403:EDO:H22	2.02	0.42
1:B:306:GLU:HA	1:B:309:ARG:HG2	2.01	0.42
4:A:403:EDO:H11	6:A:560:HOH:O	2.20	0.41
1:A:174:ALA:O	2:A:401:NAD:H4N	2.21	0.41
1:B:174:ALA:O	2:B:401:NAD:H4N	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/320~(98%)	307 (98%)	5 (2%)	1 (0%)	41 22
1	В	320/320 (100%)	313 (98%)	6 (2%)	1 (0%)	41 22
All	All	633/640 (99%)	620 (98%)	11 (2%)	2 (0%)	41 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	174	ALA
1	A	174	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	246/251 (98%)	242 (98%)	4 (2%)	62 41		
1	В	251/251 (100%)	247 (98%)	4 (2%)	62 41		
All	All	497/502 (99%)	489 (98%)	8 (2%)	65 41		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	81[A]	ILE
1	A	81[B]	ILE
1	A	84	ARG
1	В	80	GLN
1	В	84	ARG
1	В	85	ARG
1	В	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	Trunc	Chain	Dag	Res Link		ond leng	$\overline{ ext{gths}}$	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	В	401	_	42,48,48	0.77	1 (2%)	50,73,73	0.82	2 (4%)
4	EDO	A	403	_	3,3,3	0.07	0	2,2,2	0.25	0
4	EDO	В	403	-	3,3,3	0.06	0	2,2,2	0.26	0
5	GDU	A	404[B]	-	35,38,38	0.39	0	53,58,58	0.51	1 (1%)
2	NAD	A	401	_	42,48,48	0.72	1 (2%)	50,73,73	0.85	4 (8%)
5	GDU	В	402	_	35,38,38	0.37	0	53,58,58	0.43	0
3	UPG	A	402[A]	_	35,38,38	0.43	0	53,58,58	0.47	0

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	В	401	-	-	7/26/62/62	0/5/5/5
4	EDO	A	403	_	-	1/1/1/1	_

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	В	403	-	-	1/1/1/1	-
5	GDU	A	404[B]	-	-	5/23/59/59	0/3/3/3
2	NAD	A	401	-	-	9/26/62/62	0/5/5/5
5	GDU	В	402	-	-	4/23/59/59	0/3/3/3
3	UPG	A	402[A]	-	-	3/23/59/59	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
2	В	401	NAD	C2N-N1N	3.22	1.38	1.35
2	A	401	NAD	C2N-N1N	2.72	1.38	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	В	401	NAD	C6N-N1N-C2N	-2.82	119.40	121.97
2	A	401	NAD	O4D-C1D-C2D	-2.57	103.17	106.93
2	A	401	NAD	C5A-C6A-N6A	2.25	123.76	120.35
2	В	401	NAD	C5A-C6A-N6A	2.12	123.58	120.35
5	A	404[B]	GDU	O3A-PB-O3B	2.08	106.68	102.48
2	A	401	NAD	O4B-C1B-C2B	-2.06	103.92	106.93
2	A	401	NAD	C6N-N1N-C2N	-2.03	120.13	121.97

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	PN-O3-PA-O5B
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C5D-O5D-PN-O2N
2	В	401	NAD	C5D-O5D-PN-O1N
2	В	401	NAD	C5D-O5D-PN-O2N
3	A	402[A]	UPG	C1'-O3B-PB-O3A
5	A	404[B]	GDU	PB-O3A-PA-O5D
5	В	402	GDU	PB-O3A-PA-O5D
5	В	402	GDU	O5'-C5'-C6'-O6'
5	В	402	GDU	C4'-C5'-C6'-O6'
5	A	404[B]	GDU	C1'-O3B-PB-O3A
5	A	404[B]	GDU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
5	A	404[B]	GDU	O5'-C5'-C6'-O6'
2	A	401	NAD	PA-O3-PN-O1N
2	В	401	NAD	PA-O3-PN-O1N
5	A	404[B]	GDU	C1'-O3B-PB-O2B
5	В	402	GDU	C1'-O3B-PB-O3A
2	В	401	NAD	PN-O3-PA-O5B
3	A	402[A]	UPG	PB-O3A-PA-O5C
2	A	401	NAD	C5B-O5B-PA-O3
3	A	402[A]	UPG	C1'-O3B-PB-O1B
2	A	401	NAD	PA-O3-PN-O2N
2	В	401	NAD	PA-O3-PN-O2N
4	A	403	EDO	O1-C1-C2-O2
4	В	403	EDO	O1-C1-C2-O2
2	A	401	NAD	C5D-O5D-PN-O3
2	В	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	O4B-C4B-C5B-O5B
2	В	401	NAD	O4B-C4B-C5B-O5B

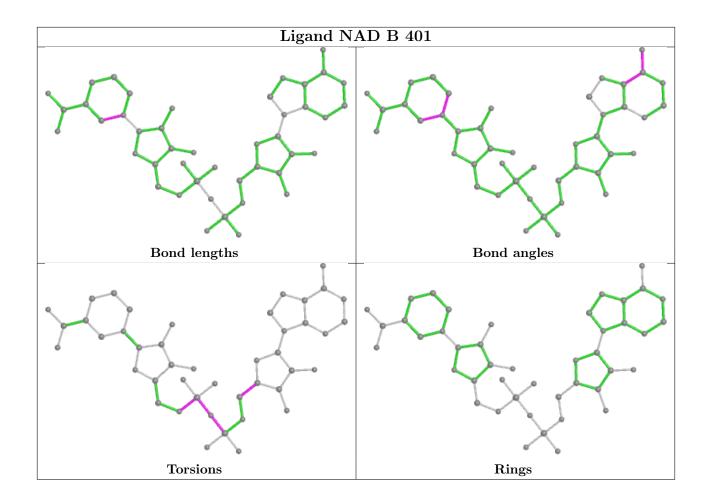
There are no ring outliers.

6 monomers are involved in 6 short contacts:

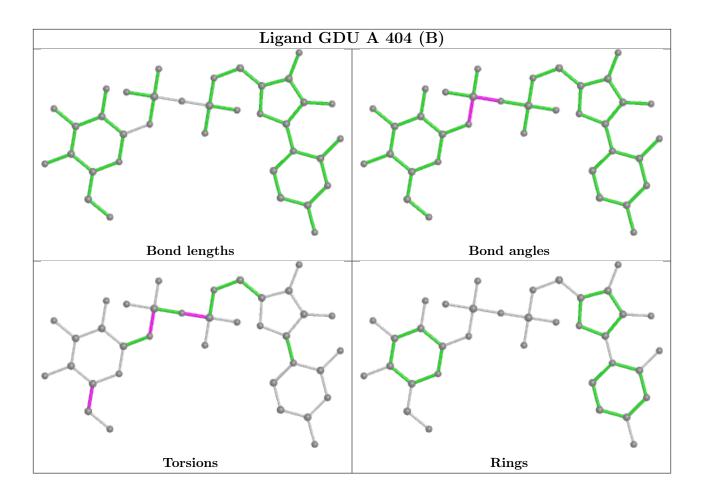
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	NAD	1	0
4	A	403	EDO	1	0
4	В	403	EDO	1	0
5	A	404[B]	GDU	1	0
2	A	401	NAD	2	0
3	A	402[A]	UPG	1	0

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 then 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.

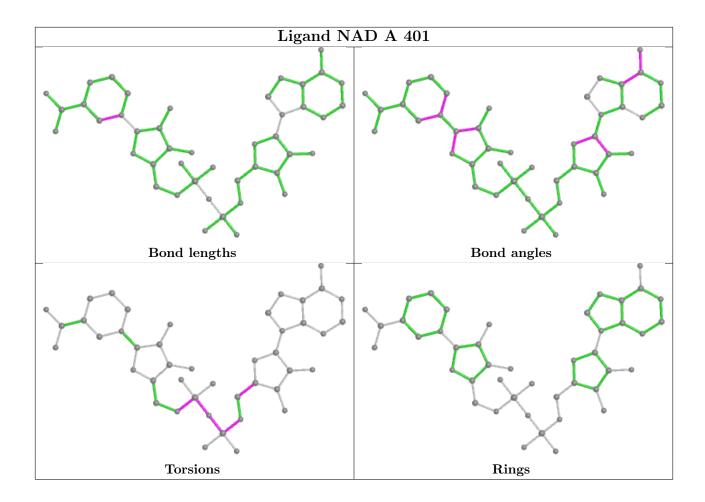




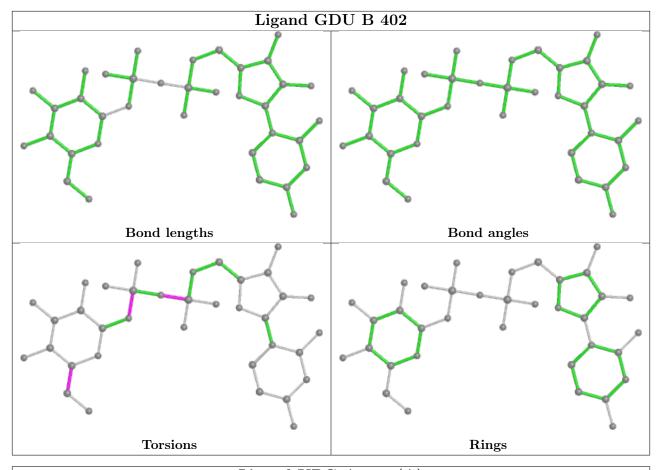


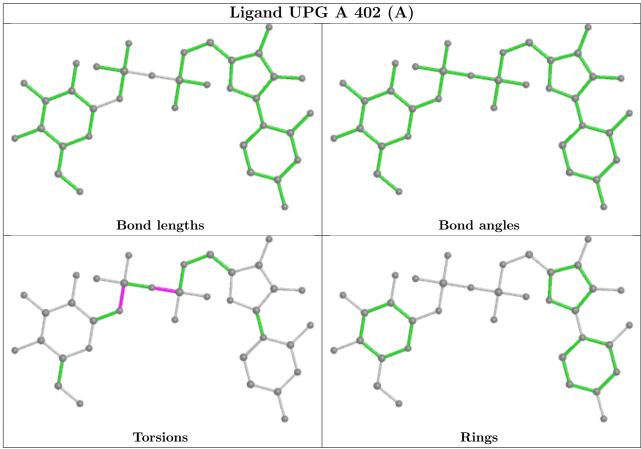














5.7 Other polymers (i)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	310/320 (96%)	-0.06	5 (1%) 72	75	9, 13, 24, 34	5 (1%)
1	В	311/320 (97%)	0.29	23 (7%) 14	14	10, 16, 39, 48	4 (1%)
All	All	621/640 (97%)	0.12	28 (4%) 33	32	9, 14, 34, 48	9 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	5.0
1	В	259	VAL	4.6
1	В	256	ALA	4.5
1	В	207	GLY	4.2
1	В	199	SER	4.2
1	В	262	PRO	4.1
1	В	310	HIS	3.9
1	A	48	SER	3.6
1	A	47	ASN	3.4
1	В	197	LEU	3.4
1	В	200	GLY	3.3
1	В	195	GLN	3.2
1	В	196	ALA	3.0
1	В	202	PRO	2.8
1	A	46	ASP	2.6
1	В	255[A]	VAL	2.6
1	В	206	PHE	2.5
1	В	267	PHE	2.5
1	В	272	LEU	2.4
1	В	311	LYS	2.4
1	В	184	HIS	2.2
1	В	270	PRO	2.2
1	В	254	ALA	2.2
1	A	44	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	В	260	GLY	2.1
1	В	264	ASP	2.1
1	В	204	ARG	2.0
1	В	190	VAL	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 monosaccharides 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^{th} 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.

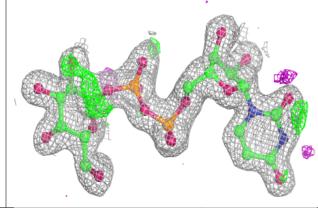
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	EDO	В	403	4/4	0.77	0.30	42,43,44,44	0
4	EDO	A	403	4/4	0.90	0.36	32,33,33,34	0
5	GDU	В	402	36/36	0.95	0.09	21,23,24,25	2
2	NAD	A	401	44/44	0.97	0.07	9,10,11,11	0
2	NAD	В	401	44/44	0.97	0.07	9,10,12,12	0
5	GDU	A	404[B]	36/36	0.97	0.09	16,16,17,17	36
3	UPG	A	402[A]	36/36	0.97	0.08	8,9,11,11	36

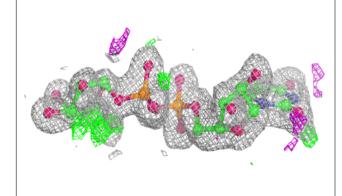
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

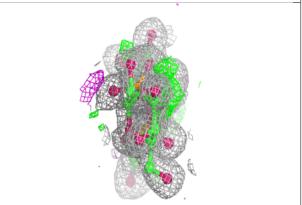


Electron density around GDU B 402:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

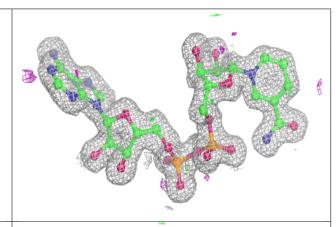


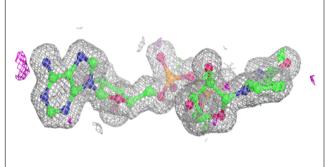


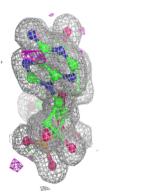


Electron density around NAD A 401:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



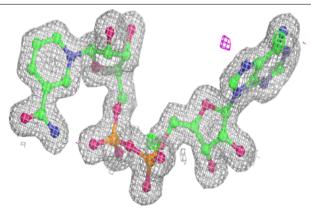


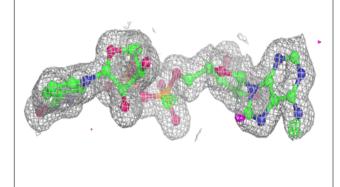


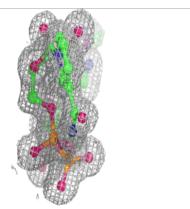


Electron density around NAD B 401:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

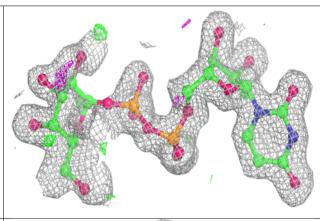


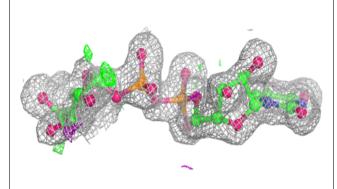


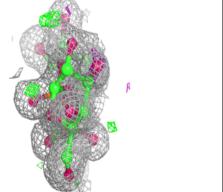


Electron density around GDU A 404 (B):

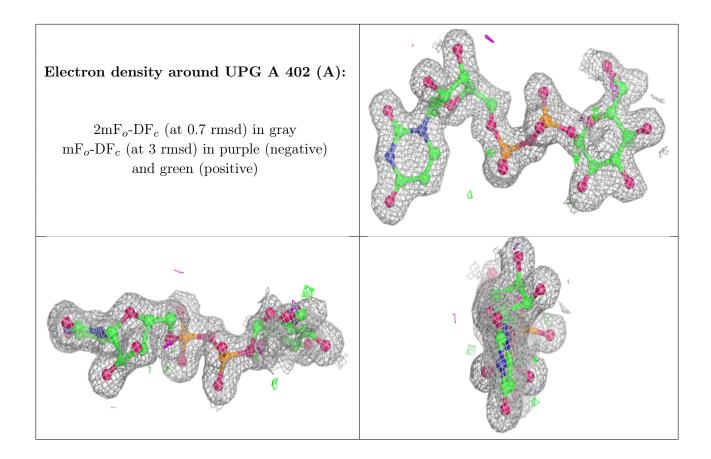
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

