



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:18 AM EDT

PDB ID : 1I3L  
Title : MOLECULAR BASIS FOR SEVERE EPIMERASE-DEFICIENCY GALACTOSEMIA: X-RAY STRUCTURE OF THE HUMAN V94M-SUBSTITUTED UDP-GALACTOSE 4-EPIMERASE  
Authors : Thoden, J.B.; Wohlers, T.M.; Fridovich-Keil, J.L.; Holden, H.M.  
Deposited on : 2001-02-15  
Resolution : 1.50 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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

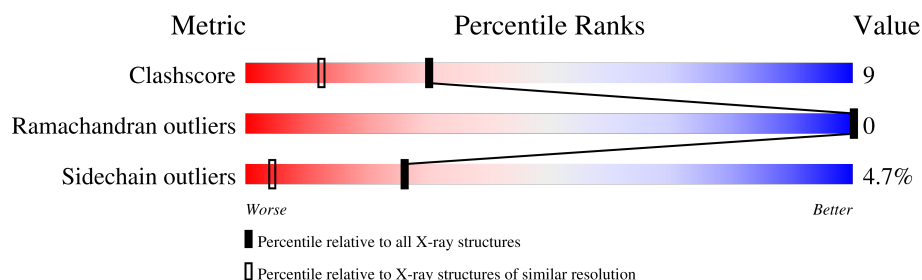
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	 74%      22%      •
1	B	348	 73%      22%      • •

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6522 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.

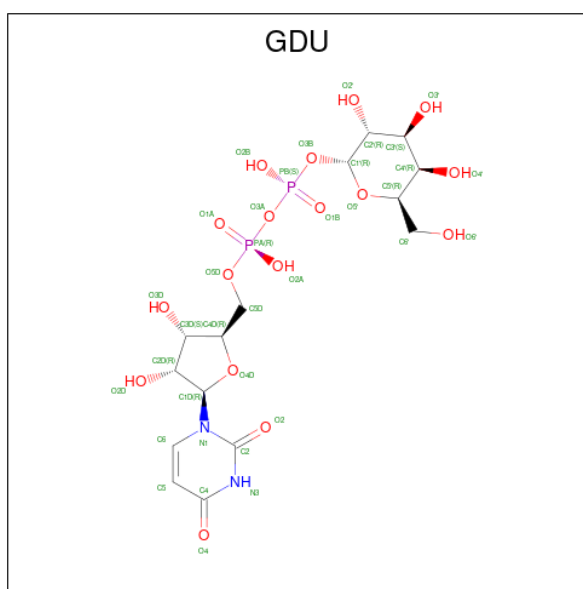
- Molecule 1 is a protein called UDP-GLUCOSE 4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	5	0
			2704	1710	468	510	16			
1	B	345	Total	C	N	O	S	0	9	0
			2711	1719	467	509	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	VAL	engineered mutation	UNP Q14376
B	94	MET	VAL	engineered mutation	UNP Q14376

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

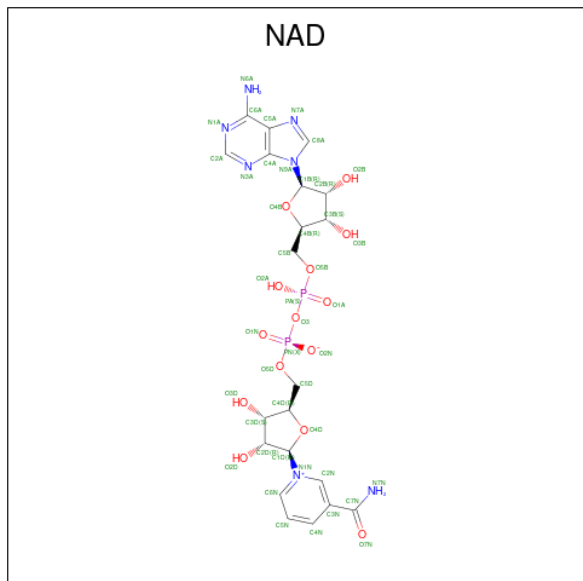
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

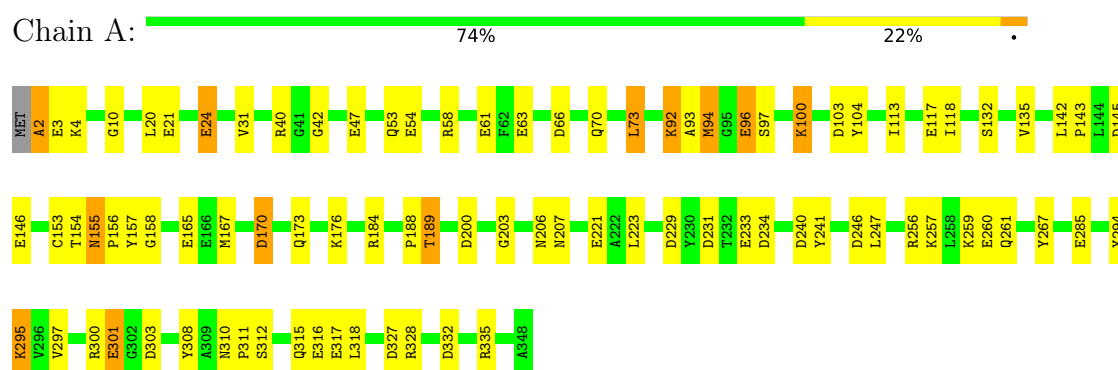
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	467	Total	O	0	0
			467	467		
7	B	468	Total	O	0	0
			468	468		

### 3 Residue-property plots

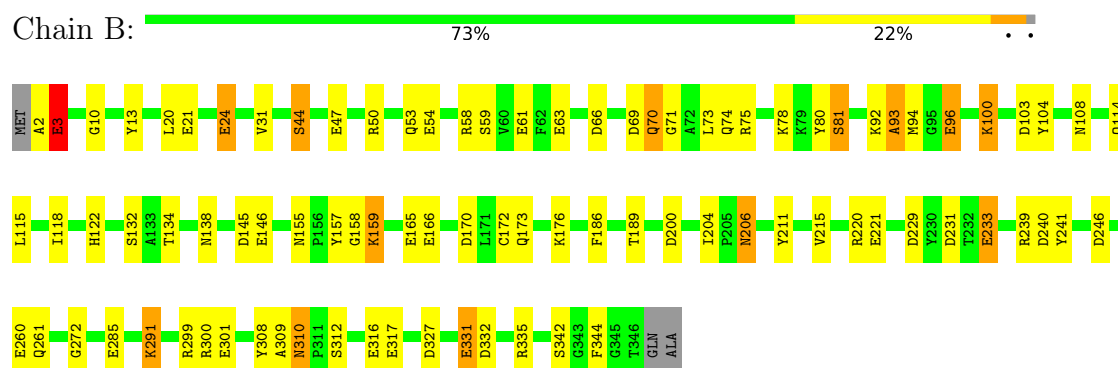
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: UDP-GLUCOSE 4-EPIMERASE



#### • Molecule 1: UDP-GLUCOSE 4-EPIMERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.10Å 89.80Å 97.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50	Depositor
% Data completeness (in resolution range)	97.4 (50.00-1.50)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.181 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAD, CL, GDU, MG

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	0.89	20/2781 (0.7%)	1.26	26/3761 (0.7%)
1	B	0.91	21/2808 (0.7%)	1.29	33/3799 (0.9%)
All	All	0.90	41/5589 (0.7%)	1.28	59/7560 (0.8%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	GLU	CD-OE2	7.96	1.34	1.25
1	B	146	GLU	CD-OE2	7.40	1.33	1.25
1	A	146	GLU	CD-OE2	6.58	1.32	1.25
1	B	165	GLU	CD-OE2	6.50	1.32	1.25
1	B	301	GLU	CD-OE2	6.38	1.32	1.25
1	B	260	GLU	CD-OE2	6.36	1.32	1.25
1	A	301	GLU	CD-OE2	6.18	1.32	1.25
1	B	166	GLU	CD-OE2	6.04	1.32	1.25
1	A	316	GLU	CD-OE2	6.01	1.32	1.25
1	A	260	GLU	CD-OE2	5.99	1.32	1.25
1	A	117	GLU	CD-OE2	5.97	1.32	1.25
1	A	285	GLU	CD-OE2	5.96	1.32	1.25
1	A	54	GLU	CD-OE2	5.96	1.32	1.25
1	A	61	GLU	CD-OE2	5.95	1.32	1.25
1	B	233	GLU	CD-OE2	5.92	1.32	1.25
1	A	233	GLU	CD-OE2	5.89	1.32	1.25
1	B	96	GLU	CD-OE2	5.79	1.32	1.25
1	B	54	GLU	CD-OE2	5.79	1.32	1.25
1	A	63[A]	GLU	CD-OE2	5.74	1.31	1.25
1	A	63[B]	GLU	CD-OE2	5.74	1.31	1.25
1	A	221	GLU	CD-OE2	5.70	1.31	1.25
1	B	24[A]	GLU	CD-OE2	5.69	1.31	1.25
1	B	24[B]	GLU	CD-OE2	5.69	1.31	1.25
1	B	21	GLU	CD-OE2	5.69	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CD-OE2	5.68	1.31	1.25
1	A	317	GLU	CD-OE2	5.61	1.31	1.25
1	B	285	GLU	CD-OE2	5.57	1.31	1.25
1	B	3	GLU	CD-OE2	5.55	1.31	1.25
1	A	3	GLU	CD-OE2	5.53	1.31	1.25
1	B	316	GLU	CD-OE2	5.37	1.31	1.25
1	A	21	GLU	CD-OE2	5.22	1.31	1.25
1	A	165	GLU	CD-OE2	5.18	1.31	1.25
1	B	221	GLU	CD-OE2	5.15	1.31	1.25
1	A	24[A]	GLU	CD-OE2	5.15	1.31	1.25
1	A	24[B]	GLU	CD-OE2	5.15	1.31	1.25
1	B	331	GLU	CD-OE2	5.12	1.31	1.25
1	B	47	GLU	CD-OE2	5.05	1.31	1.25
1	A	96	GLU	CD-OE2	5.04	1.31	1.25
1	B	63[A]	GLU	CD-OE2	5.04	1.31	1.25
1	B	63[B]	GLU	CD-OE2	5.04	1.31	1.25
1	B	61	GLU	CD-OE2	5.01	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	A	303	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	A	66	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	145	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	66	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	327	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	246	ASP	CB-CG-OD1	7.48	125.04	118.30
1	B	145	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	92	LYS	C-N-CA	-7.30	103.45	121.70
1	A	332	ASP	CB-CG-OD1	7.25	124.83	118.30
1	B	300	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	93	ALA	N-CA-CB	7.13	120.08	110.10
1	B	200	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	246	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	327	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	2	ALA	CB-CA-C	6.93	120.50	110.10
1	A	184	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	335	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	50	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	327	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	246	ASP	CB-CG-OD2	-6.58	112.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	B	231	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	234	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	69	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	69	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	335	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	66	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	170	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	92	LYS	N-CA-CB	5.95	121.30	110.60
1	B	241	TYR	CB-CG-CD2	5.93	124.56	121.00
1	A	145	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	299	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	231	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	300	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	256	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	246	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	92	LYS	N-CA-CB	5.54	120.58	110.60
1	A	170	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	229	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	40	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	239	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	170	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	332	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	B	231	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	229	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	303	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	2	ALA	N-CA-CB	5.30	117.53	110.10
1	B	50	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	344	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	66	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	200	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	332	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	200	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	332	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	335	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	211	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	A	300	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	13	TYR	CB-CG-CD2	-5.03	117.98	121.00

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	2704	0	2653	53	0
1	B	2711	0	2673	50	0
2	A	36	0	22	1	0
2	B	36	0	22	2	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
5	A	44	0	26	2	0
5	B	44	0	26	0	0
6	A	4	0	6	1	0
6	B	4	0	6	1	0
7	A	467	0	0	9	0
7	B	468	0	0	10	1
All	All	6522	0	5434	103	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (103) 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:94:MET:HB3	1:A:96:GLU:HG3	1.43	1.00
1:B:173:GLN:HA	1:B:176:LYS:HE2	1.55	0.88
1:A:155:ASN:ND2	1:A:158:GLY:H	1.75	0.85
1:B:94:MET:HB2	1:B:96:GLU:HG3	1.59	0.83
1:A:100:LYS:HD3	1:A:103:ASP:HB2	1.68	0.74
1:B:132:SER:OG	1:B:134[A]:THR:HG22	1.89	0.73
1:B:70:GLN:HG2	7:B:1299:HOH:O	1.87	0.73
1:A:113:ILE:HG12	1:A:167:MET:HE1	1.72	0.72
1:B:94:MET:CB	1:B:96:GLU:HG3	2.19	0.72
1:B:132:SER:OG	1:B:134[B]:THR:HG23	1.90	0.72
1:A:315:GLN:HG3	7:A:1345:HOH:O	1.89	0.71
1:A:94:MET:HB3	1:A:96:GLU:CG	2.18	0.71
1:B:176:LYS:HD2	7:B:1750:HOH:O	1.90	0.71
1:A:203:GLY:HA2	7:A:1667:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HE3	7:B:1895:HOH:O	1.92	0.68
1:B:74:GLN:O	1:B:78:LYS:HG3	1.97	0.65
1:B:122:HIS:ND1	7:B:1734:HOH:O	2.30	0.65
1:B:173:GLN:CA	1:B:176:LYS:HE2	2.27	0.65
1:B:206:ASN:ND2	2:B:901:GDU:O6'	2.30	0.64
1:A:2:ALA:HB1	7:A:1801:HOH:O	1.96	0.62
1:A:42:GLY:O	6:A:980:EDO:H22	2.00	0.62
1:B:70:GLN:O	1:B:74:GLN:HG3	1.99	0.62
1:B:70:GLN:OE1	1:B:114[B]:GLN:NE2	2.31	0.62
1:B:100:LYS:HD3	1:B:103:ASP:HB2	1.83	0.61
1:A:173:GLN:O	1:A:176:LYS:NZ	2.30	0.59
1:A:207[B]:ASN:OD1	2:A:401:GDU:H6'2	2.03	0.59
1:A:97:SER:HA	1:A:104:TYR:CE1	2.39	0.57
1:B:44:SER:HB3	7:B:1722:HOH:O	2.03	0.57
1:B:58:ARG:HG2	7:B:1886:HOH:O	2.04	0.57
1:B:310:ASN:HD22	1:B:310:ASN:C	2.08	0.57
1:A:94:MET:CB	1:A:96:GLU:HG3	2.29	0.56
1:A:155:ASN:ND2	1:A:157:TYR:HB3	2.22	0.55
1:B:310:ASN:HD22	1:B:312:SER:H	1.54	0.55
1:A:155:ASN:HD22	1:A:157:TYR:N	2.05	0.55
1:B:173:GLN:HA	1:B:173:GLN:OE1	2.07	0.54
1:A:155:ASN:HD21	1:A:158:GLY:H	1.56	0.54
1:B:310:ASN:ND2	1:B:312:SER:H	2.06	0.54
1:B:138:ASN:HB2	7:B:1915:HOH:O	2.08	0.53
1:A:100:LYS:HD3	1:A:103:ASP:CB	2.37	0.53
1:B:132:SER:CB	1:B:134[A]:THR:HG22	2.38	0.53
1:A:100:LYS:HD2	1:A:104:TYR:CE1	2.44	0.52
1:B:100:LYS:HE2	1:B:103:ASP:OD1	2.09	0.52
1:A:261:GLN:NE2	7:A:1659:HOH:O	2.35	0.52
1:B:155:ASN:OD1	1:B:158:GLY:N	2.30	0.52
2:B:901:GDU:H6'2	2:B:901:GDU:O2A	2.10	0.52
1:B:73:LEU:HD12	1:B:114[B]:GLN:HG3	1.92	0.52
1:A:240:ASP:HB2	1:A:308:TYR:HA	1.92	0.51
1:B:215:VAL:HG22	1:B:220:ARG:HB2	1.91	0.51
1:B:73:LEU:CD1	1:B:114[B]:GLN:HG3	2.41	0.51
1:A:170:ASP:OD1	1:B:159:LYS:HE2	2.10	0.51
1:A:223:LEU:HB3	1:A:294:TYR:HB3	1.92	0.51
1:A:310:ASN:OD1	1:A:312:SER:OG	2.30	0.50
1:B:10:GLY:HA3	1:B:31:VAL:HG13	1.93	0.49
1:A:93:ALA:HB2	1:A:104:TYR:OH	2.13	0.49
1:A:207[B]:ASN:ND2	7:A:1478:HOH:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TYR:CE1	1:A:318:LEU:HD13	2.48	0.49
1:A:188:PRO:HD2	5:A:400:NAD:O7N	2.13	0.49
1:B:70:GLN:HB3	1:B:114[B]:GLN:NE2	2.29	0.47
1:B:240:ASP:HB2	1:B:308:TYR:HA	1.97	0.47
1:B:53:GLN:HG3	1:B:58:ARG:O	2.14	0.46
1:A:132:SER:HB2	5:A:400:NAD:H5N	1.98	0.46
1:A:100:LYS:HD3	1:A:103:ASP:OD1	2.14	0.46
1:A:135:VAL:HA	1:A:153:CYS:SG	2.56	0.46
1:A:93:ALA:HB3	7:A:1973:HOH:O	2.14	0.46
1:B:104:TYR:O	1:B:108:ASN:HB2	2.16	0.45
1:B:3:GLU:OE2	1:B:81:SER:O	2.34	0.45
1:A:155:ASN:HD22	1:A:157:TYR:H	1.65	0.45
1:B:331:GLU:HB2	7:B:1843:HOH:O	2.16	0.45
1:A:167:MET:HE3	1:A:167:MET:HB3	1.83	0.45
1:A:53:GLN:HG3	1:A:58:ARG:O	2.16	0.44
1:B:204:ILE:HD12	6:B:981:EDO:H22	1.98	0.44
1:A:311:PRO:HB3	7:A:1477:HOH:O	2.17	0.44
1:A:20:LEU:HD21	1:A:24[B]:GLU:OE2	2.17	0.44
1:A:94:MET:HB3	1:A:96:GLU:OE2	2.17	0.44
1:A:100:LYS:HD2	1:A:104:TYR:HE1	1.83	0.44
1:A:189[A]:THR:HG21	1:A:241:TYR:HD1	1.83	0.44
1:A:173:GLN:NE2	1:A:173:GLN:HA	2.32	0.43
1:A:176:LYS:HB2	7:A:1658:HOH:O	2.19	0.43
1:B:70:GLN:HG2	1:B:70:GLN:H	1.65	0.43
1:A:10:GLY:HA3	1:A:31:VAL:HG13	2.00	0.43
1:A:94:MET:O	1:A:94:MET:HG3	2.18	0.43
1:B:100:LYS:NZ	7:B:1840:HOH:O	2.46	0.43
1:B:272:GLY:HA2	1:B:309:ALA:O	2.19	0.43
1:A:70:GLN:HG3	1:A:118:ILE:HD11	2.00	0.43
1:A:155:ASN:HD22	1:A:158:GLY:H	1.61	0.43
1:B:291:LYS:NZ	7:B:1897:HOH:O	2.47	0.43
1:A:73:LEU:HB3	1:A:118:ILE:HD13	2.01	0.43
1:B:93:ALA:HB2	1:B:157:TYR:CB	2.50	0.42
1:B:115:LEU:O	1:B:118:ILE:HG22	2.20	0.42
1:A:97:SER:O	1:A:156:PRO:HG2	2.20	0.42
1:A:189[A]:THR:HG21	1:A:241:TYR:CD1	2.54	0.42
1:B:71:GLY:O	1:B:75:ARG:HG3	2.20	0.42
1:B:20:LEU:O	1:B:24[B]:GLU:HG3	2.20	0.41
1:A:142:LEU:HA	1:A:143:PRO:C	2.41	0.41
1:A:295:LYS:HD3	1:A:297:VAL:HG13	2.03	0.41
1:A:94:MET:SD	1:A:206:ASN:ND2	2.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HE3	7:A:1706:HOH:O	2.19	0.41
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.89	0.41
1:B:172:CYS:O	1:B:176:LYS:HD3	2.21	0.41
1:B:94:MET:HB3	1:B:96:GLU:HG3	2.01	0.40
1:B:132:SER:HB3	1:B:134[A]:THR:HG22	2.02	0.40
1:B:2:ALA:HB3	1:B:81:SER:HB3	2.02	0.40
1:B:186:PHE:CE2	1:B:309:ALA:HB2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1213:HOH:O	7:B:1885:HOH:O[4_555]	2.08	0.12

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/348 (101%)	341 (97%)	9 (3%)	0	100	100
1	B	353/348 (101%)	343 (97%)	10 (3%)	0	100	100
All	All	703/696 (101%)	684 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	285/282 (101%)	272 (95%)	13 (5%)	27 5
1	B	289/282 (102%)	273 (94%)	16 (6%)	21 3
All	All	574/564 (102%)	545 (95%)	29 (5%)	26 4

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	73	LEU
1	A	92	LYS
1	A	94	MET
1	A	100	LYS
1	A	154	THR
1	A	155	ASN
1	A	189[A]	THR
1	A	189[B]	THR
1	A	247	LEU
1	A	259	LYS
1	A	295	LYS
1	A	301	GLU
1	B	3	GLU
1	B	44	SER
1	B	59	SER
1	B	70	GLN
1	B	81	SER
1	B	100	LYS
1	B	159	LYS
1	B	189[A]	THR
1	B	189[B]	THR
1	B	206	ASN
1	B	233	GLU
1	B	261[A]	GLN
1	B	261[B]	GLN
1	B	291	LYS
1	B	310	ASN
1	B	342	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	155	ASN
1	A	224	ASN
1	A	339	GLN
1	B	36	HIS
1	B	224	ASN
1	B	310	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
6	EDO	B	981	-	3,3,3	0.45	0	2,2,2	0.04	0
6	EDO	A	980	-	3,3,3	0.47	0	2,2,2	0.01	0
2	GDU	A	401	-	31,38,38	1.21	3 (9%)	41,58,58	1.88	6 (14%)
5	NAD	A	400	-	42,48,48	1.09	4 (9%)	50,73,73	1.90	11 (22%)
5	NAD	B	900	-	42,48,48	1.10	4 (9%)	50,73,73	1.73	10 (20%)
2	GDU	B	901	-	31,38,38	1.23	3 (9%)	41,58,58	1.48	4 (9%)



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
6	EDO	B	981	-	-	0/1/1/1	-
6	EDO	A	980	-	-	1/1/1/1	-
2	GDU	A	401	-	-	4/21/59/59	0/3/3/3
5	NAD	A	400	-	-	11/26/62/62	0/5/5/5
5	NAD	B	900	-	-	7/26/62/62	0/5/5/5
2	GDU	B	901	-	-	5/21/59/59	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	GDU	C4-N3	4.11	1.40	1.33
2	A	401	GDU	C4-N3	3.70	1.39	1.33
2	B	901	GDU	C6-N1	3.57	1.40	1.35
5	A	400	NAD	C2N-N1N	3.23	1.38	1.35
5	B	900	NAD	C4N-C3N	2.93	1.44	1.39
2	A	401	GDU	C6-C5	-2.88	1.31	1.38
2	A	401	GDU	C6-N1	2.74	1.39	1.35
2	B	901	GDU	C6-C5	-2.69	1.32	1.38
5	A	400	NAD	C4N-C3N	2.50	1.43	1.39
5	B	900	NAD	PA-O2A	-2.25	1.44	1.55
5	B	900	NAD	O4D-C1D	-2.11	1.38	1.41
5	A	400	NAD	PA-O2A	-2.09	1.45	1.55
5	A	400	NAD	PN-O2N	-2.05	1.45	1.55
5	B	900	NAD	PN-O2N	-2.05	1.45	1.55

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GDU	O5'-C1'-O3B	-6.58	102.76	111.36
2	A	401	GDU	O3A-PB-O3B	6.30	115.18	102.48
5	A	400	NAD	C6N-C5N-C4N	5.93	128.06	119.44
5	A	400	NAD	C5N-C6N-N1N	-5.39	112.68	120.40
5	A	400	NAD	C5N-C4N-C3N	-4.97	114.46	120.34
2	B	901	GDU	O3A-PB-O3B	4.82	112.21	102.48
5	B	900	NAD	C5N-C6N-N1N	-4.69	113.68	120.40
5	B	900	NAD	C6N-C5N-C4N	4.68	126.24	119.44
5	B	900	NAD	C5N-C4N-C3N	-4.54	114.98	120.34
5	A	400	NAD	C6N-N1N-C2N	4.45	126.03	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	NAD	C6N-N1N-C2N	4.35	125.94	121.97
2	B	901	GDU	C5-C4-N3	-4.34	113.76	123.31
2	A	401	GDU	C5-C4-N3	-4.07	114.35	123.31
2	B	901	GDU	O5'-C1'-O3B	-3.61	106.65	111.36
2	A	401	GDU	C1'-O5'-C5'	-3.52	106.77	113.69
5	A	400	NAD	C3N-C7N-N7N	3.31	121.73	117.75
5	B	900	NAD	C3N-C2N-N1N	-3.13	117.36	120.43
2	A	401	GDU	O5'-C5'-C4'	-3.10	104.06	109.69
5	A	400	NAD	C3N-C2N-N1N	-2.83	117.66	120.43
5	B	900	NAD	C2N-C3N-C4N	2.76	121.38	118.26
5	A	400	NAD	C2N-C3N-C4N	2.45	121.03	118.26
5	A	400	NAD	C5A-C6A-N1A	-2.40	114.91	120.35
5	B	900	NAD	C3N-C7N-N7N	2.28	120.49	117.75
5	A	400	NAD	O7N-C7N-N7N	-2.26	119.36	122.58
5	B	900	NAD	O4B-C1B-C2B	-2.13	103.82	106.93
5	A	400	NAD	O4B-C1B-C2B	-2.11	103.84	106.93
2	A	401	GDU	O3'-C3'-C4'	-2.08	105.55	110.35
5	B	900	NAD	C4A-C5A-N7A	2.07	111.56	109.40
2	B	901	GDU	O4D-C1D-C2D	-2.05	103.93	106.93
5	A	400	NAD	N6A-C6A-N1A	2.03	122.79	118.57
5	B	900	NAD	C5A-C6A-N1A	-2.00	115.82	120.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GDU	PB-O3A-PA-O5D
5	A	400	NAD	C5B-O5B-PA-O2A
5	A	400	NAD	C5D-O5D-PN-O2N
5	A	400	NAD	O4D-C1D-N1N-C2N
5	B	900	NAD	O4D-C1D-N1N-C2N
2	A	401	GDU	O5'-C5'-C6'-O6'
2	A	401	GDU	C4'-C5'-C6'-O6'
2	B	901	GDU	C1'-O3B-PB-O3A
6	A	980	EDO	O1-C1-C2-O2
2	B	901	GDU	PB-O3A-PA-O5D
2	A	401	GDU	C1'-O3B-PB-O3A
5	A	400	NAD	C5B-O5B-PA-O3
5	A	400	NAD	C5D-O5D-PN-O3
5	B	900	NAD	C5B-O5B-PA-O3
5	B	900	NAD	PA-O3-PN-O2N
5	A	400	NAD	PA-O3-PN-O2N

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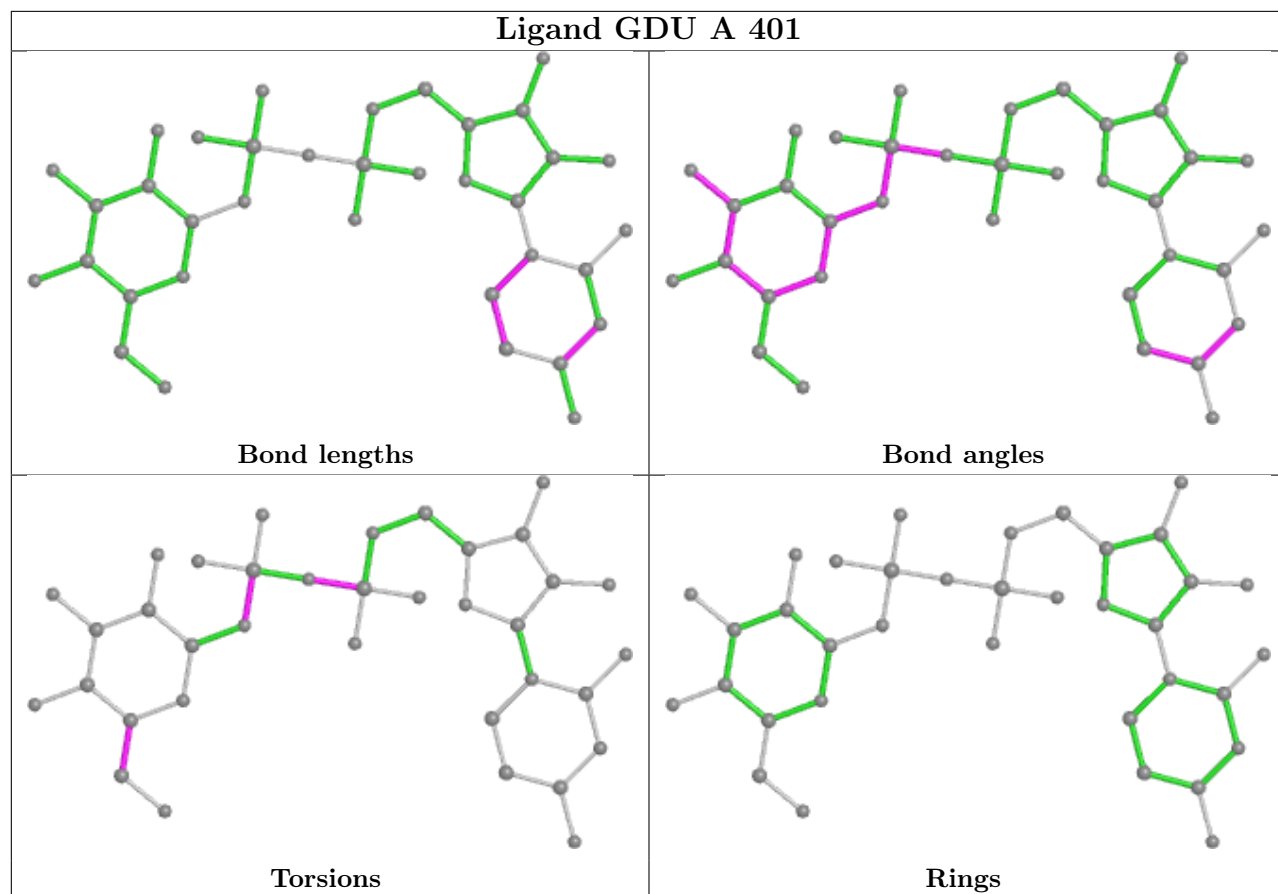
Mol	Chain	Res	Type	Atoms
2	B	901	GDU	O5'-C5'-C6'-O6'
5	B	900	NAD	O4B-C4B-C5B-O5B
5	B	900	NAD	C5D-O5D-PN-O3
5	A	400	NAD	O4B-C4B-C5B-O5B
2	B	901	GDU	PA-O3A-PB-O2B
5	A	400	NAD	PA-O3-PN-O1N
5	A	400	NAD	C4B-C5B-O5B-PA
2	B	901	GDU	C2'-C1'-O3B-PB
5	A	400	NAD	C5B-O5B-PA-O1A
5	A	400	NAD	C5D-O5D-PN-O1N
5	B	900	NAD	C5B-O5B-PA-O1A
5	B	900	NAD	C5B-O5B-PA-O2A

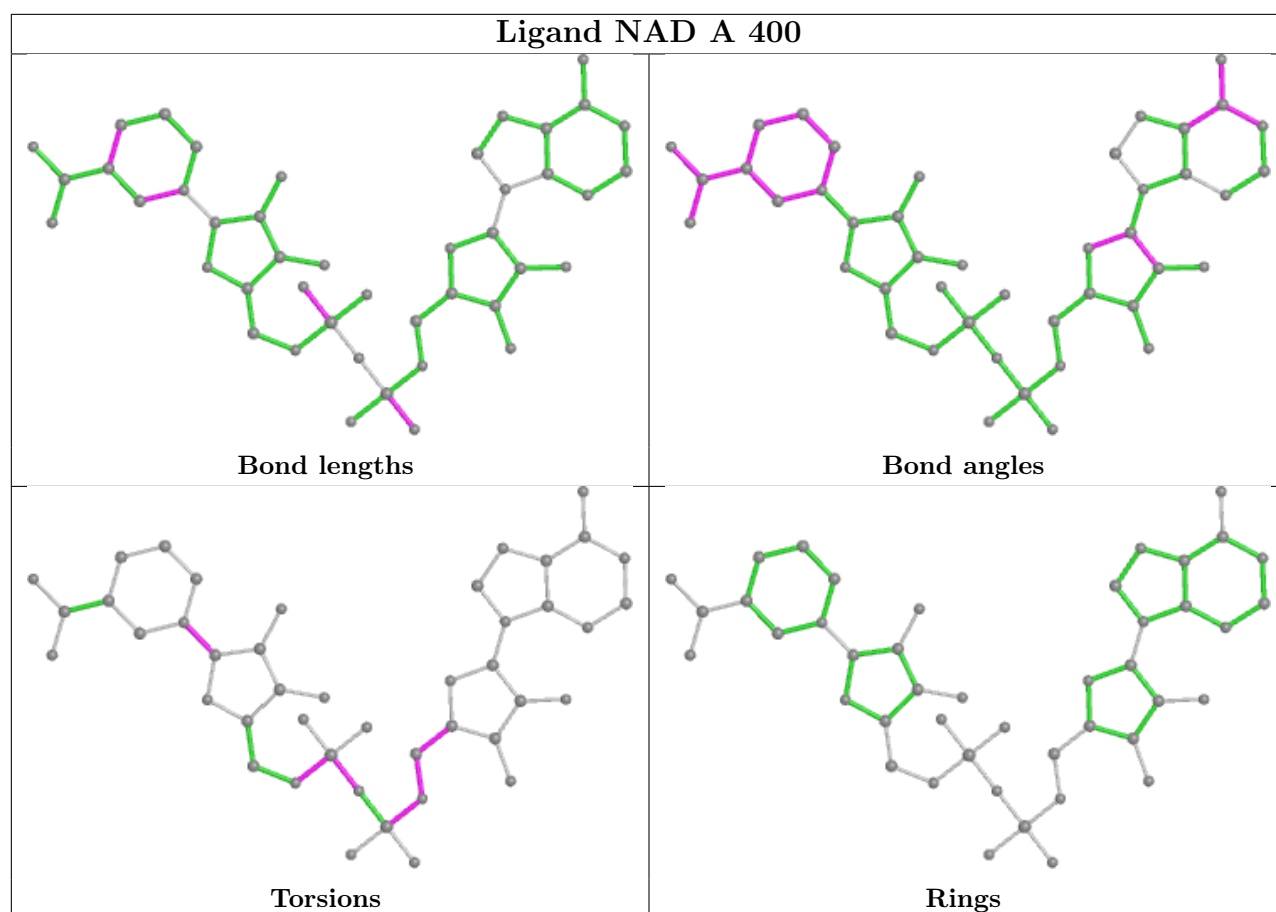
There are no ring outliers.

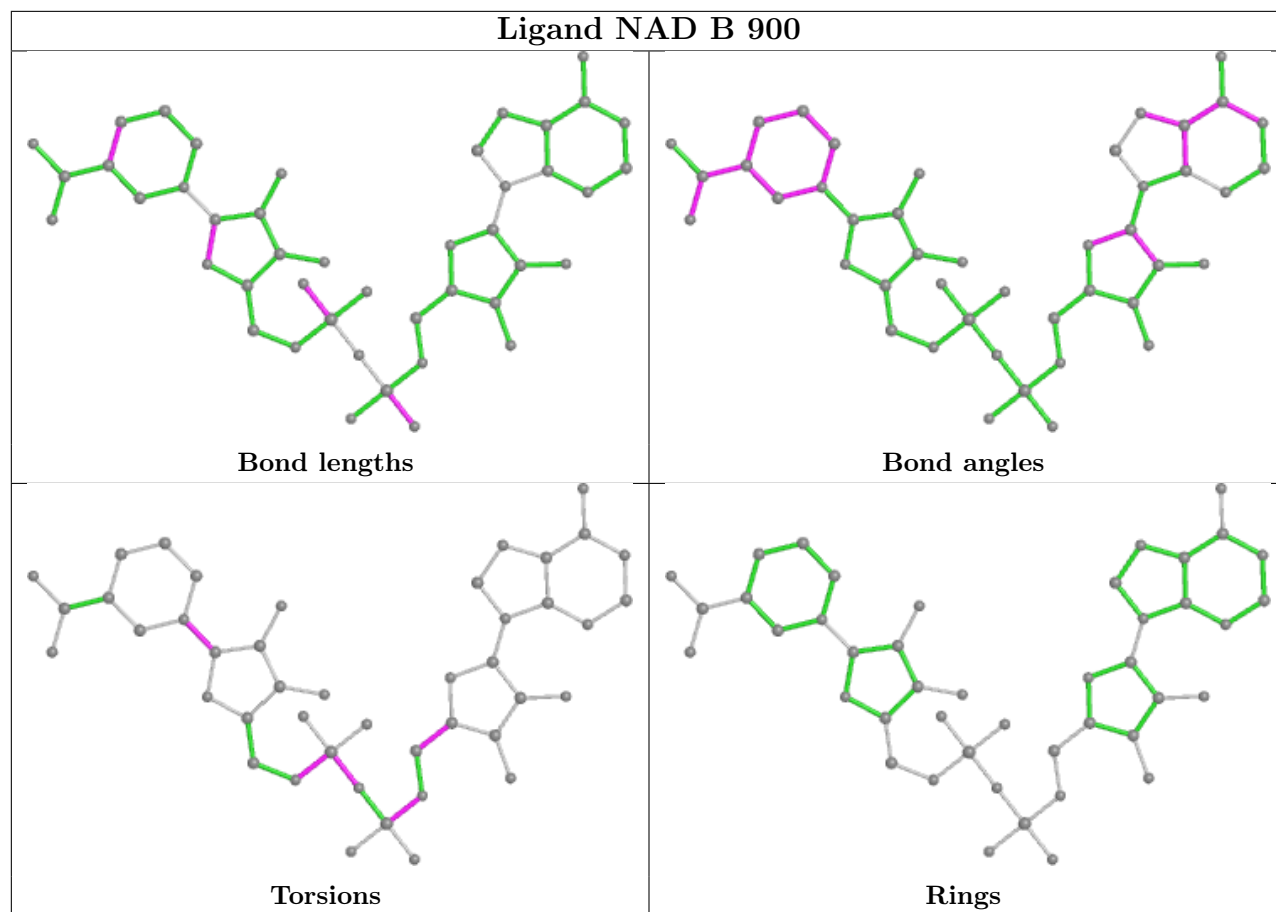
5 monomers are involved in 7 short contacts:

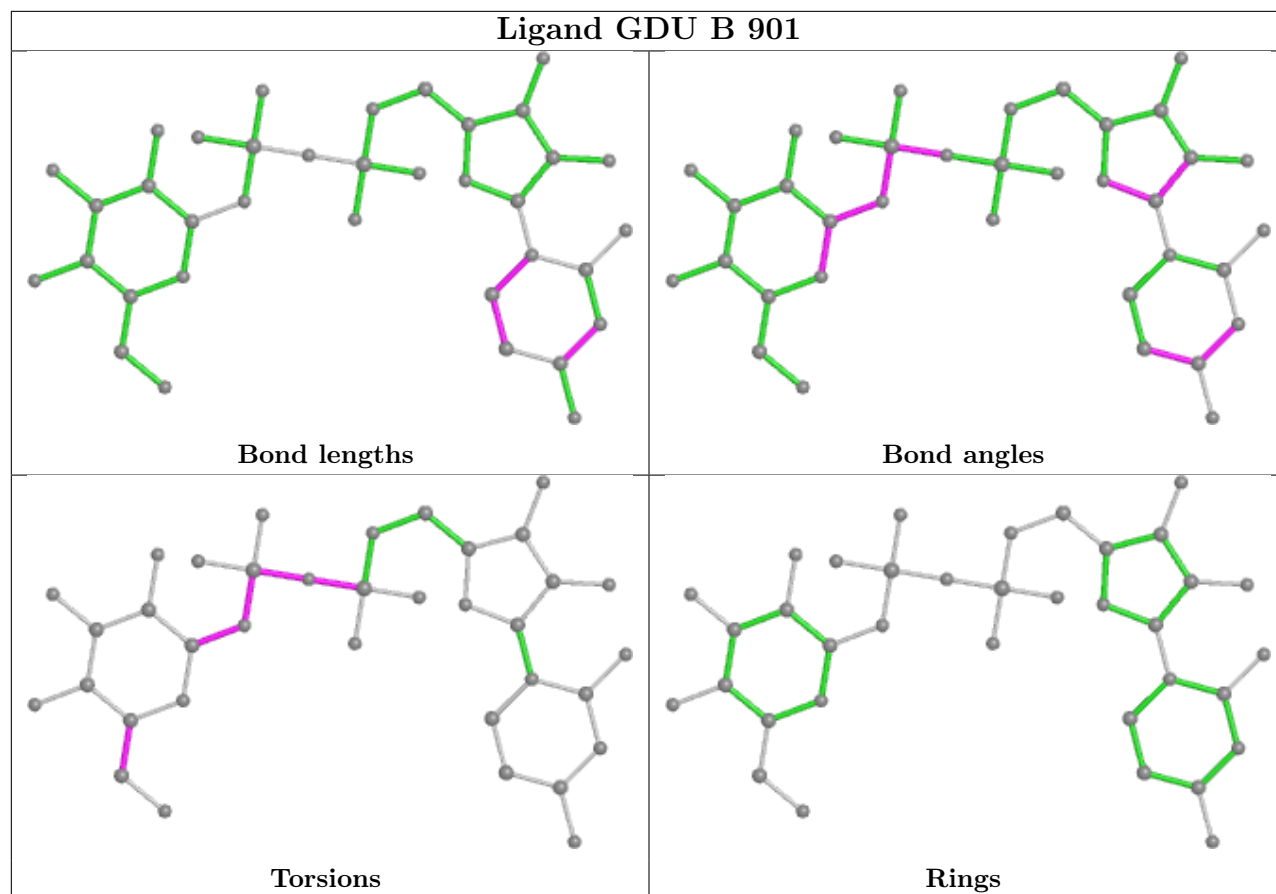
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	981	EDO	1	0
6	A	980	EDO	1	0
2	A	401	GDU	1	0
5	A	400	NAD	2	0
2	B	901	GDU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.