



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:34 AM UTC

PDB ID : 1I3L / pdb_00001i3l
Title : MOLECULAR BASIS FOR SEVERE EPIMERASE-DEFICIENCY GALACTOSEMIA: X-RAY STRUCTURE OF THE HUMAN V94M-SUBSTITUTED UDP-GALACTOSE 4-EPIMERASE
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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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

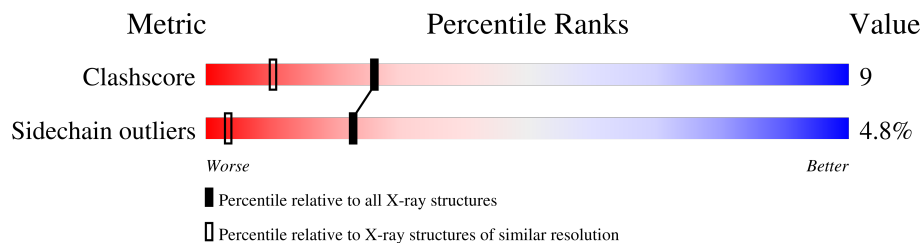
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4235 (1.50-1.50)
Sidechain outliers	187428	4150 (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 ≥ 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	
1	B	348	

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.

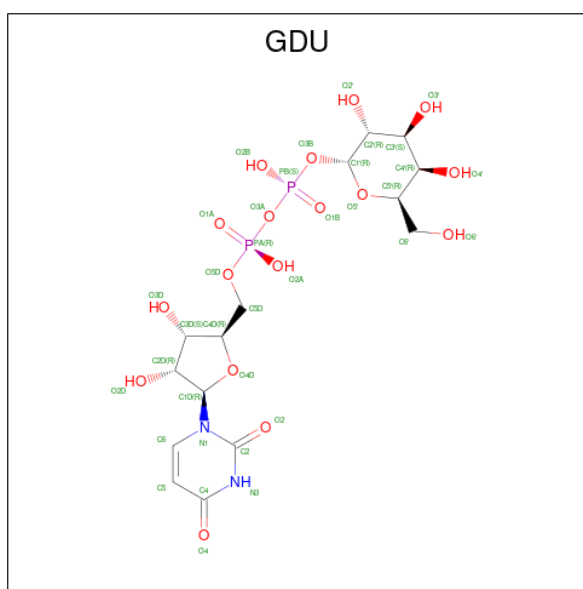
- Molecule 1 is a protein called UDP-GLUCOSE 4-EPIMERASE.

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 (CCD ID: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



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

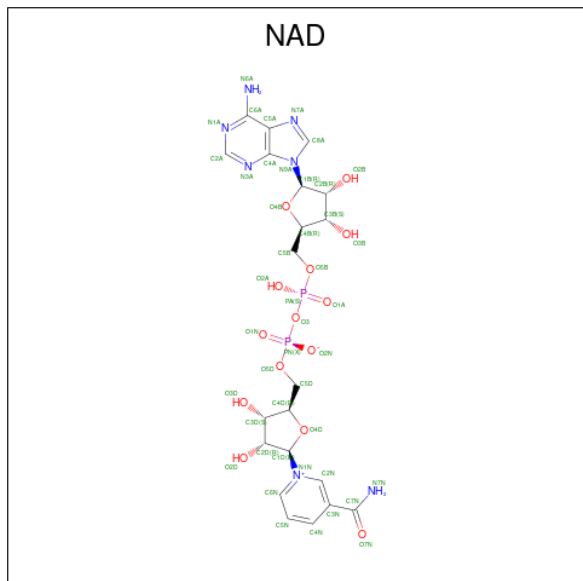
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 (CCD ID: 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.

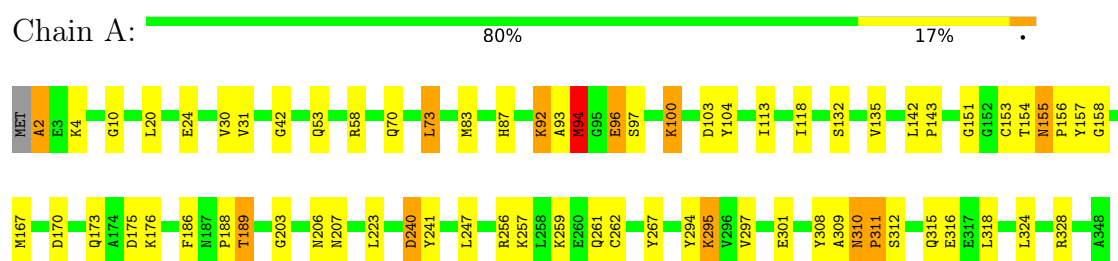
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	467	Total	O	0	0
			467	467		
7	B	468	Total	O	0	0
			468	468		

3 Residue-property plots

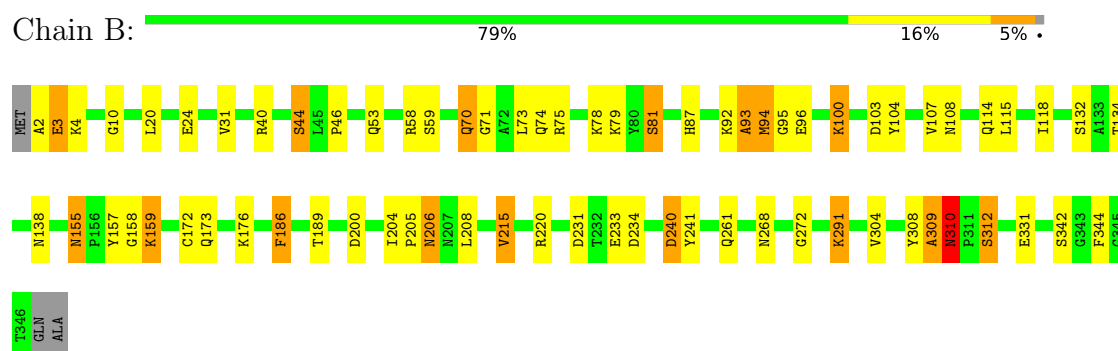
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, α , β , γ	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 ²)	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: CL, MG, GDU, EDO, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	0/2781	1.44	19/3761 (0.5%)
1	B	0.98	0/2808	1.45	30/3799 (0.8%)
All	All	0.97	0/5589	1.44	49/7560 (0.6%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	LYS	CA-C-N	-12.33	103.45	122.81
1	A	92	LYS	C-N-CA	-12.33	103.45	122.81
1	A	186	PHE	CA-CB-CG	-7.29	106.51	113.80
1	A	311	PRO	CB-CA-C	-7.22	101.91	110.00
1	A	94	MET	N-CA-C	-7.11	102.59	112.25
1	A	92	LYS	N-CA-CB	6.91	121.30	110.87
1	B	93	ALA	N-CA-CB	6.74	120.08	109.71
1	A	2	ALA	CB-CA-C	6.67	120.50	110.50
1	A	240	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	309	ALA	N-CA-C	6.42	120.03	110.52
1	B	94	MET	N-CA-C	-6.42	104.60	112.88
1	B	231	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	309	ALA	N-CA-C	6.31	119.85	110.52
1	B	95	GLY	N-CA-C	-6.26	106.68	115.32
1	B	107	VAL	N-CA-C	6.16	116.33	110.42
1	B	4	LYS	N-CA-C	6.15	118.72	110.35
1	B	92	LYS	N-CA-CB	6.08	120.58	110.85
1	B	92	LYS	CA-C-N	-6.06	112.51	121.24
1	B	92	LYS	C-N-CA	-6.06	112.51	121.24
1	A	30	VAL	N-CA-C	-6.01	98.88	107.77
1	B	155	ASN	N-CA-C	5.93	119.42	109.09
1	B	234	ASP	CA-CB-CG	5.86	118.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	GLU	N-CA-C	5.84	117.45	111.14
1	B	208	LEU	N-CA-C	5.84	117.33	110.97
1	B	344	PHE	CA-C-N	-5.78	112.93	120.91
1	B	344	PHE	C-N-CA	-5.78	112.93	120.91
1	B	312	SER	N-CA-C	5.74	117.22	111.07
1	A	262	CYS	N-CA-C	5.71	120.09	113.18
1	B	241	TYR	CB-CA-C	5.66	119.07	109.84
1	B	240	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	151	GLY	N-CA-C	-5.54	105.63	112.33
1	B	46	PRO	N-CA-C	-5.53	102.59	111.38
1	A	87	HIS	N-CA-C	5.51	117.99	107.75
1	B	215	VAL	N-CA-C	-5.48	105.19	110.72
1	A	175	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	310	ASN	N-CA-C	-5.45	98.69	109.10
1	B	205	PRO	N-CA-CB	5.45	108.16	103.31
1	A	324	LEU	N-CA-C	5.39	118.33	109.76
1	B	268	ASN	CB-CA-C	-5.38	100.43	109.53
1	B	186	PHE	CA-CB-CG	-5.38	108.42	113.80
1	B	200	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	87	HIS	N-CA-C	5.30	117.86	107.57
1	A	94	MET	N-CA-CB	-5.20	103.10	110.79
1	B	95	GLY	CA-C-N	5.09	127.52	120.29
1	B	95	GLY	C-N-CA	5.09	127.52	120.29
1	B	40	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	79	LYS	N-CA-C	5.07	116.81	111.28
1	A	96	GLU	N-CA-C	5.03	117.88	111.69
1	B	310	ASN	N-CA-C	-5.02	99.65	108.69

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	56	0
1	B	2711	0	2673	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	22	0	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	10	0
7	B	468	0	0	8	1
All	All	6522	0	5434	104	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 (104) 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: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:113:ILE:HG12	1:A:167:MET:HE1	1.74	0.70
1:A:203:GLY:HA2	7:A:1667:HOH:O	1.92	0.69
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:HD22	1:B:310:ASN:C	2.08	0.61
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: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:A:94:MET:CB	1:A:96:GLU:HG3	2.29	0.56
1:A:83:MET:HE1	1:A:259:LYS:HZ1	1.71	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
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:A:83:MET:HE1	1:A:259:LYS:NZ	2.27	0.48
1:B:100:LYS:NZ	7:B:1840:HOH:O	2.46	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HA	1:A:153:CYS:SG	2.56	0.46
1:A:142:LEU:HA	1:A:143:PRO:C	2.41	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: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:A:100:LYS:NZ	7:A:1616:HOH:O	2.52	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:A:73:LEU:HB3	1:A:118:ILE:HD13	2.01	0.43
1:A:294:TYR:CD2	1:A:294:TYR:C	2.97	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:20:LEU:C	1:A:20:LEU:HD23	2.45	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
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](#)

There are no protein backbone outliers to report in this entry.

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%)	24	4
1	B	289/282 (102%)	272 (94%)	17 (6%)	18	2
All	All	574/564 (102%)	544 (95%)	30 (5%)	23	3

All (30) 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	256	ARG
1	A	295	LYS
1	A	301	GLU

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Mol	Chain	Res	Type
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	304	VAL
1	B	310	ASN
1	B	342	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	74	GLN
1	A	155	ASN
1	A	224	ASN
1	A	315	GLN
1	B	36	HIS
1	B	74	GLN
1	B	310	ASN
1	B	337	GLN
1	B	339	GLN

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](#)

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	A	980	-	3,3,3	0.43	0	2,2,2	0.06	0
2	GDU	A	401	-	37,38,38	1.40	1 (2%)	55,58,58	1.47	6 (10%)
2	GDU	B	901	-	37,38,38	1.01	1 (2%)	55,58,58	1.04	2 (3%)
5	NAD	B	900	-	46,48,48	1.16	7 (15%)	64,73,73	1.51	6 (9%)
5	NAD	A	400	-	46,48,48	1.24	6 (13%)	64,73,73	1.70	7 (10%)
6	EDO	B	981	-	3,3,3	0.41	0	2,2,2	0.06	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
6	EDO	A	980	-	-	1/1/1/1	-
2	GDU	A	401	-	-	3/23/59/59	0/3/3/3
2	GDU	B	901	-	-	4/23/59/59	0/3/3/3
5	NAD	B	900	-	-	4/30/62/62	0/5/5/5
5	NAD	A	400	-	-	8/30/62/62	0/5/5/5
6	EDO	B	981	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDU	PA-O3A	7.11	1.67	1.59
2	B	901	GDU	PA-O3A	4.72	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	400	NAD	C2N-N1N	3.56	1.38	1.35
5	B	900	NAD	C4N-C3N	3.23	1.44	1.39
5	A	400	NAD	PN-O3	2.80	1.62	1.59
5	A	400	NAD	C4N-C3N	2.75	1.43	1.39
5	B	900	NAD	PA-O2A	-2.28	1.44	1.55
5	A	400	NAD	C8A-N7A	2.21	1.35	1.31
5	B	900	NAD	C6N-N1N	2.16	1.40	1.35
5	A	400	NAD	PA-O2A	-2.12	1.45	1.55
5	B	900	NAD	C2N-N1N	2.12	1.37	1.35
5	B	900	NAD	O4D-C1D	-2.11	1.38	1.40
5	A	400	NAD	PN-O2N	-2.08	1.45	1.55
5	B	900	NAD	PN-O2N	-2.08	1.45	1.55
5	B	900	NAD	C2A-N1A	2.02	1.37	1.33

All (21) 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
5	A	400	NAD	C5N-C4N-C3N	-6.01	114.46	120.36
5	A	400	NAD	C6N-C5N-C4N	5.97	128.06	119.45
5	A	400	NAD	C5N-C6N-N1N	-5.65	112.68	120.38
5	B	900	NAD	C5N-C4N-C3N	-5.48	114.98	120.36
5	B	900	NAD	C5N-C6N-N1N	-4.92	113.68	120.38
5	A	400	NAD	C6N-N1N-C2N	4.88	126.03	121.88
5	B	900	NAD	C6N-N1N-C2N	4.78	125.94	121.88
5	B	900	NAD	C6N-C5N-C4N	4.71	126.24	119.45
2	B	901	GDU	O5'-C1'-O3B	-3.61	106.65	111.36
2	A	401	GDU	C1'-O5'-C5'	-3.56	106.77	113.72
5	A	400	NAD	C3N-C7N-N7N	3.24	121.73	117.74
2	A	401	GDU	O5'-C5'-C4'	-3.13	104.06	109.70
2	A	401	GDU	O2-C2-N1	2.94	126.63	122.80
5	B	900	NAD	C2N-C3N-C4N	2.69	121.38	118.26
2	A	401	GDU	O2B-PB-O3A	-2.39	100.80	107.27
5	A	400	NAD	C2N-C3N-C4N	2.38	121.03	118.26
5	A	400	NAD	O7N-C7N-N7N	-2.25	119.36	122.62
5	B	900	NAD	C3N-C7N-N7N	2.23	120.49	117.74
2	A	401	GDU	O3'-C3'-C4'	-2.05	105.55	110.38
2	B	901	GDU	O3A-PA-O1A	-2.04	104.56	110.70

There are no chirality outliers.

All (20) torsion outliers are listed below:

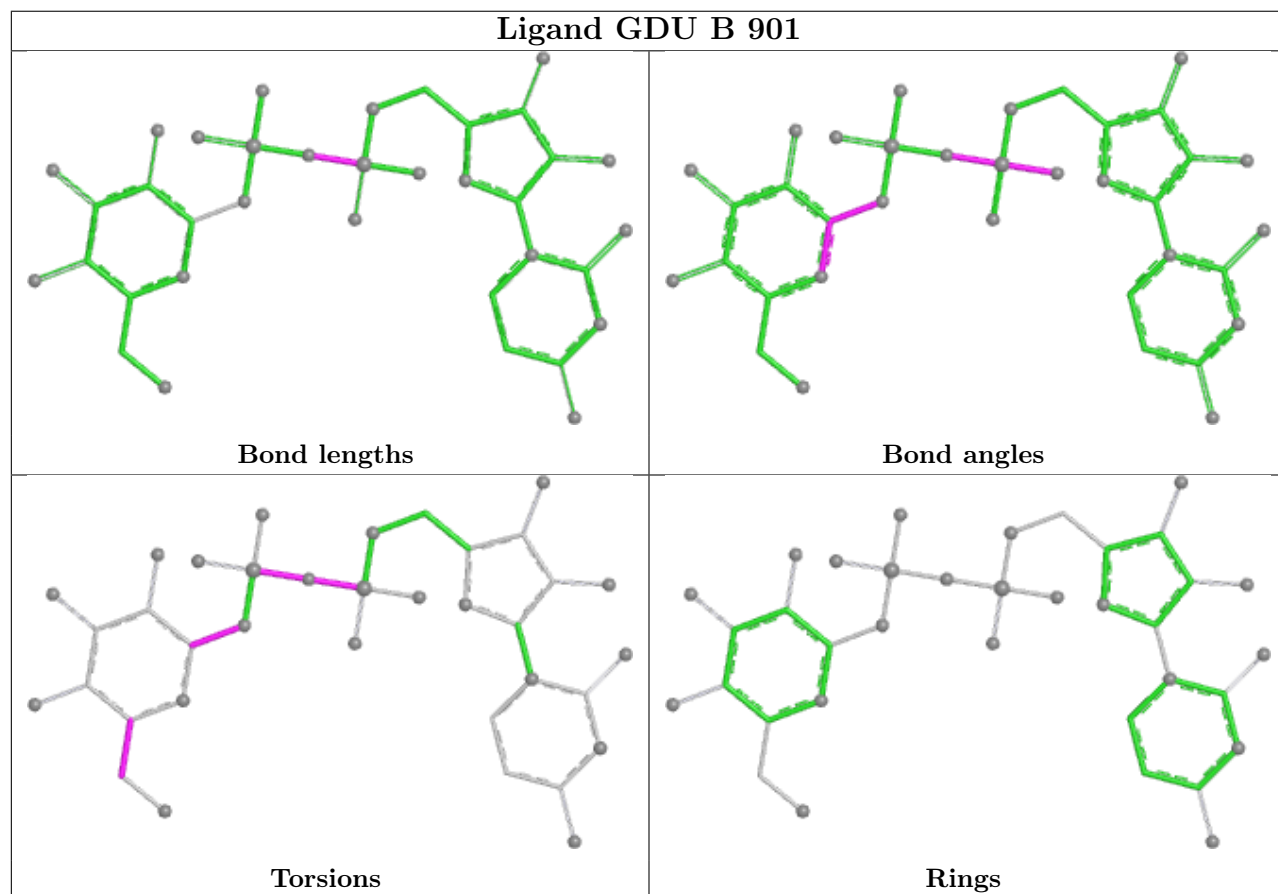
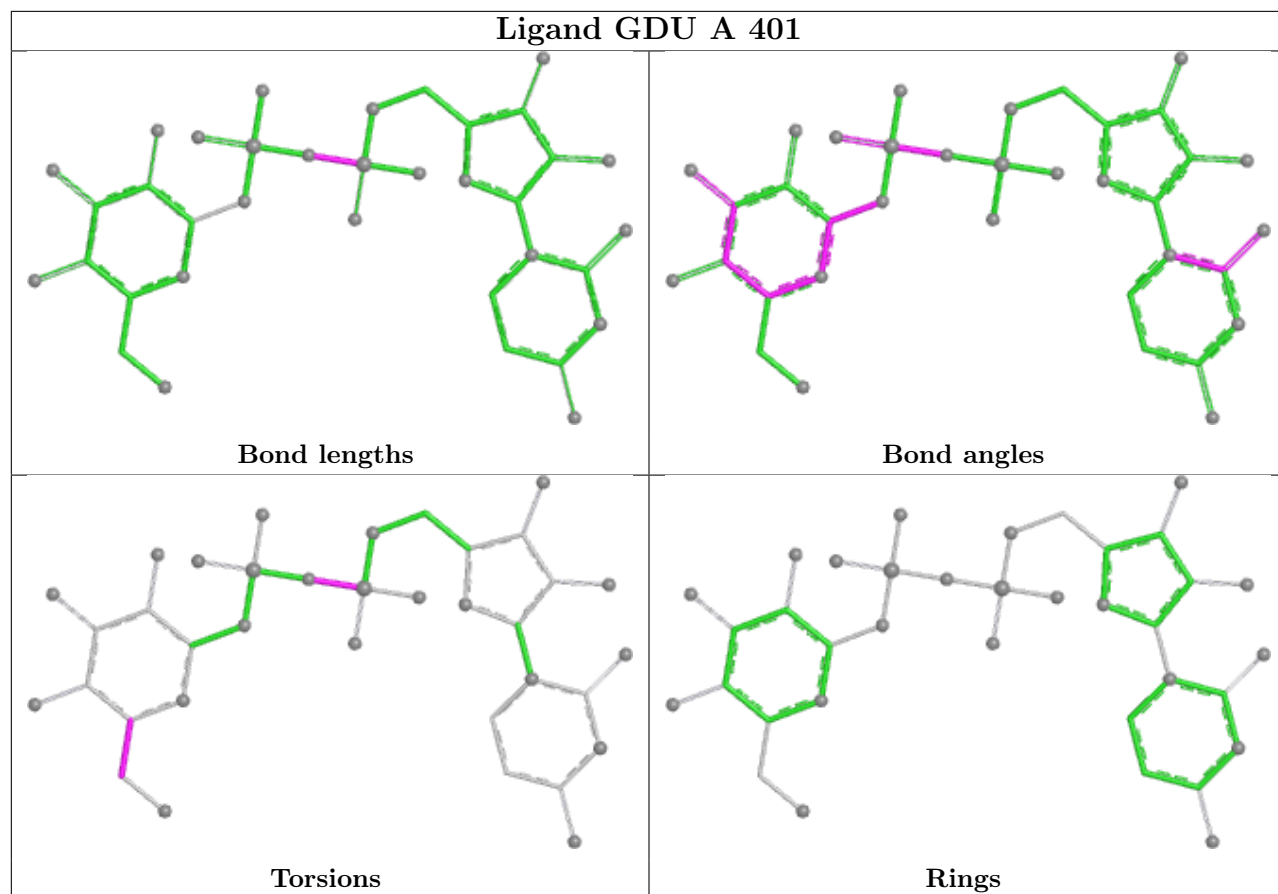
Mol	Chain	Res	Type	Atoms
2	A	401	GDU	PB-O3A-PA-O5D
5	A	400	NAD	C5B-O5B-PA-O2A
5	A	400	NAD	C5D-O5D-PN-O2N
5	A	400	NAD	O4D-C1D-N1N-C2N
5	B	900	NAD	O4D-C1D-N1N-C2N
2	A	401	GDU	O5'-C5'-C6'-O6'
2	A	401	GDU	C4'-C5'-C6'-O6'
2	B	901	GDU	PB-O3A-PA-O5D
5	A	400	NAD	C5D-O5D-PN-O3
5	B	900	NAD	PA-O3-PN-O2N
6	A	980	EDO	O1-C1-C2-O2
5	A	400	NAD	O4D-C1D-N1N-C6N
5	B	900	NAD	O4D-C1D-N1N-C6N
5	A	400	NAD	PA-O3-PN-O2N
2	B	901	GDU	C2'-C1'-O3B-PB
2	B	901	GDU	O5'-C5'-C6'-O6'
2	B	901	GDU	PA-O3A-PB-O2B
5	A	400	NAD	PA-O3-PN-O1N
5	A	400	NAD	C4B-C5B-O5B-PA
5	B	900	NAD	O4B-C4B-C5B-O5B

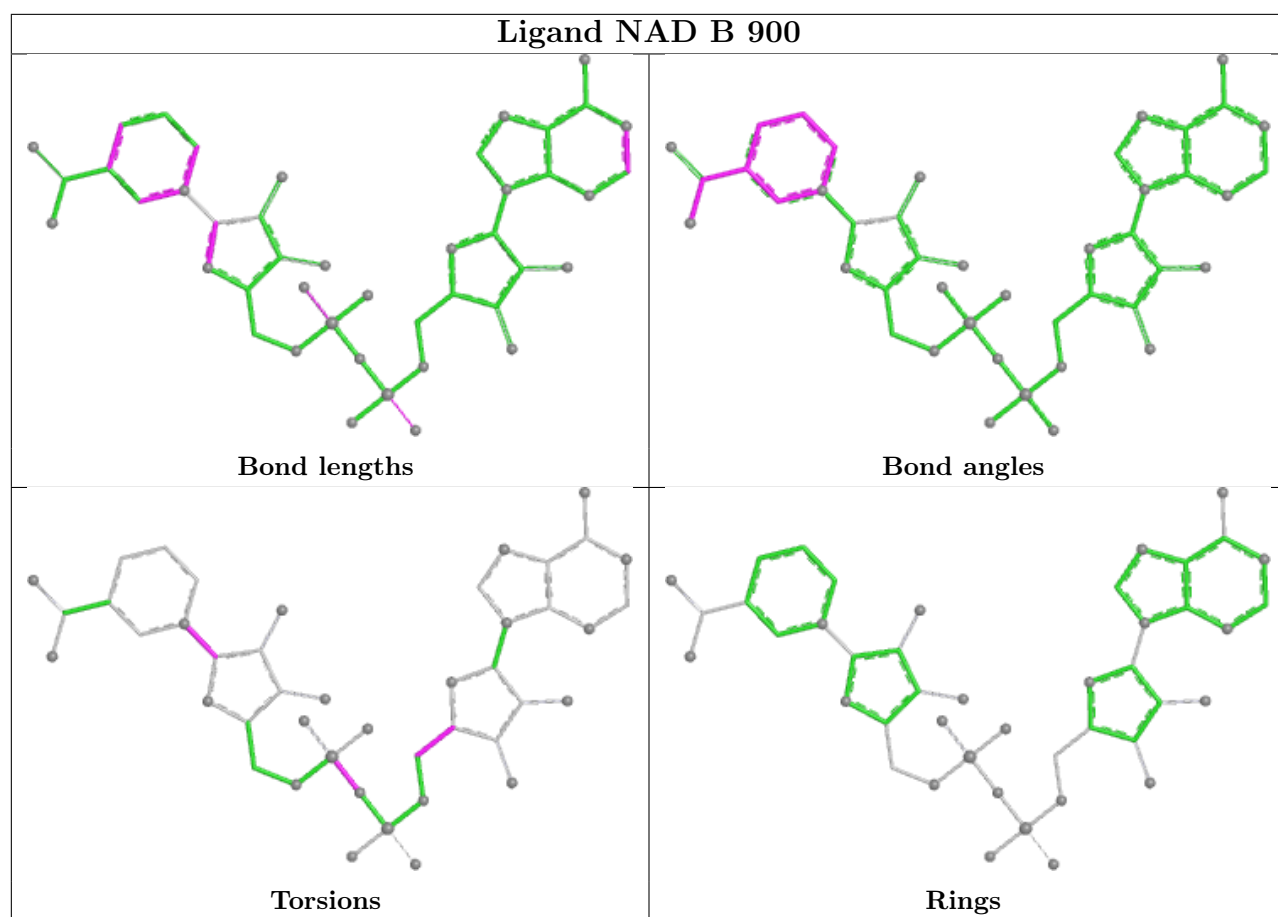
There are no ring outliers.

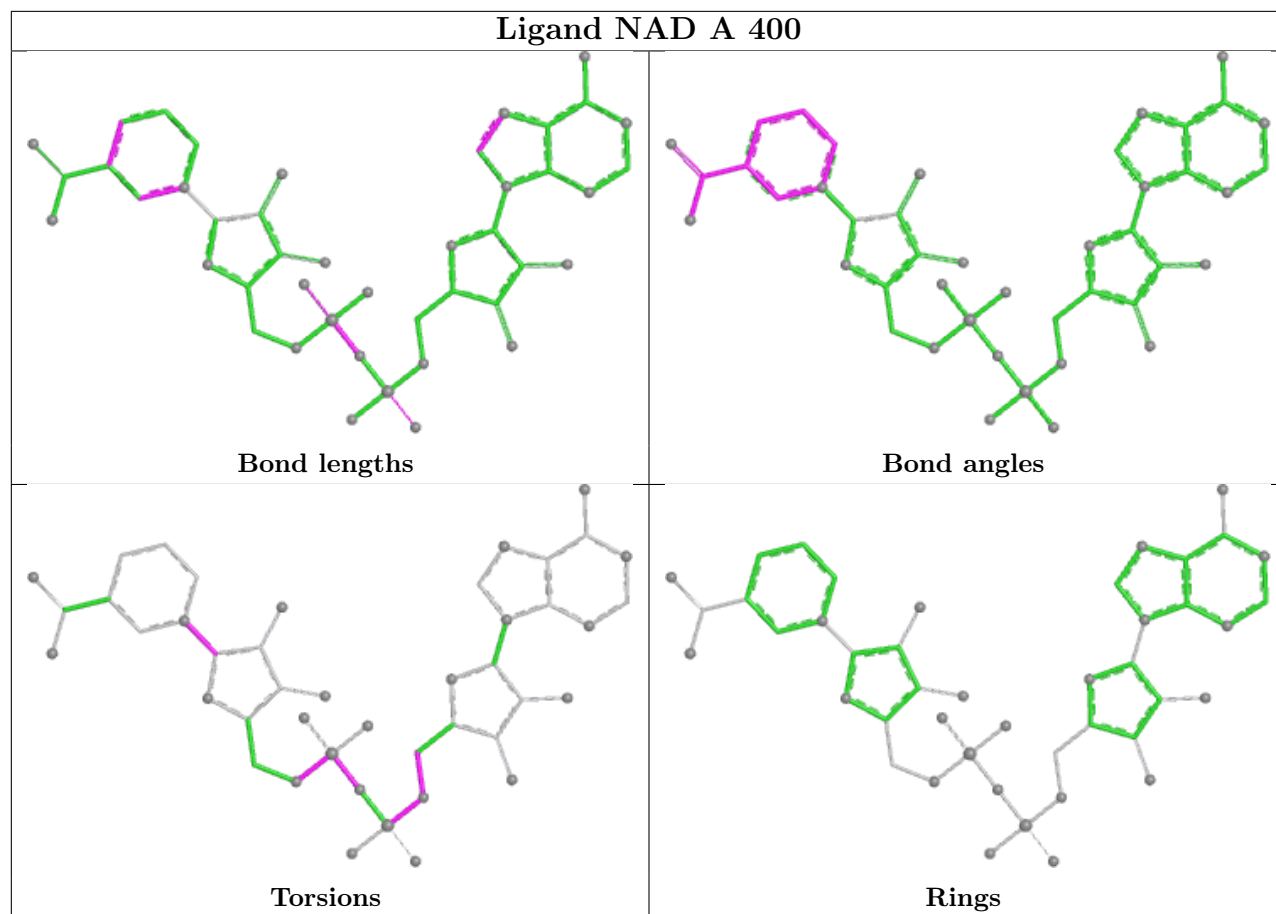
4 monomers are involved in 6 short contacts:

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

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.