wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 11:47 PM EDT

PDB ID	:	1I3N
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 wwPDB X-ray Structure Validation Summary 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:

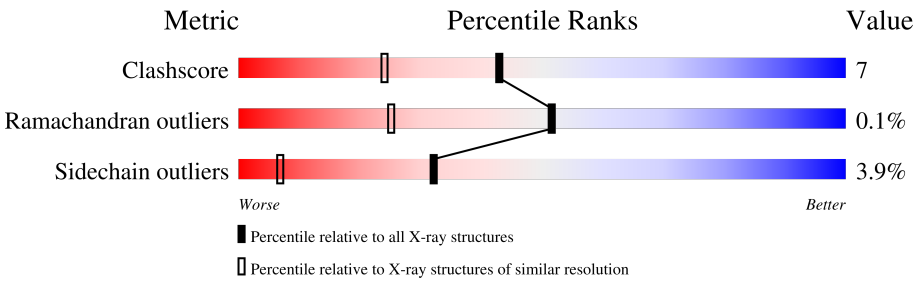
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.50 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 >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	80% 18% •
1	B	348	76% 21% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6500 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
			Total	C	N	O	S			
1	A	347	2697	1707	471	503	16	0	2	0
1	B	345	2706	1714	467	509	16	0	8	0

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

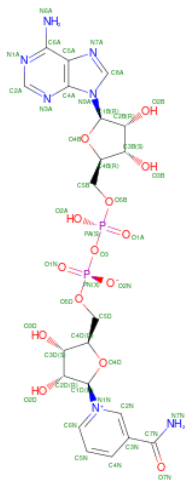
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

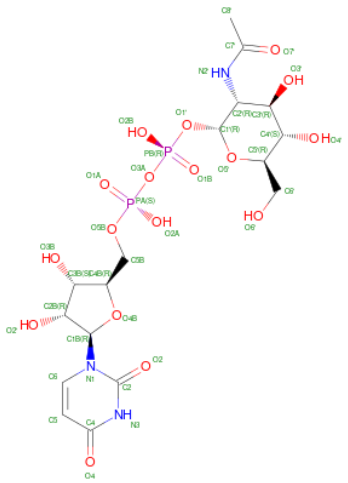
NAD



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

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).

UD1



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	40	17	3	18	2	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	39	17	3	17	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	498	498	498	0	0
			Total	O		
6	B	427	427	427	0	0

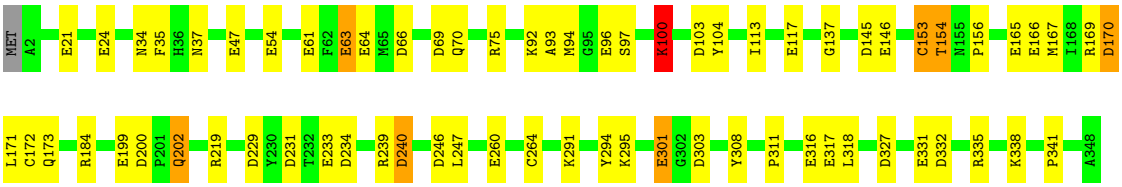
3 Residue-property plots (i)

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. 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.

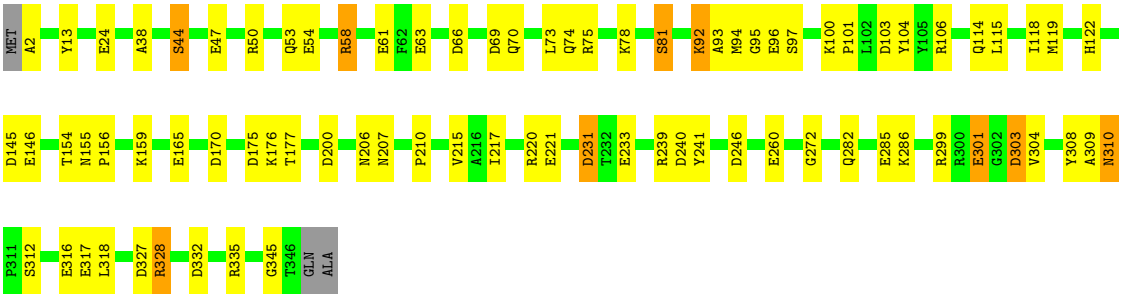
• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain A:



• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain B:



4 Data and refinement statistics (i)

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 90.00Å 96.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50	Depositor
% Data completeness (in resolution range)	97.3 (50.00-1.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.180 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6500	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

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: MG, CL, UD1, 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	0.89	18/2762 (0.7%)	1.23	31/3733 (0.8%)
1	B	0.90	13/2799 (0.5%)	1.28	34/3787 (0.9%)
All	All	0.90	31/5561 (0.6%)	1.25	65/7520 (0.9%)

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	1	0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLU	CD-OE2	8.47	1.34	1.25
1	A	117	GLU	CD-OE2	8.28	1.34	1.25
1	B	285	GLU	CD-OE2	6.89	1.33	1.25
1	B	146	GLU	CD-OE2	6.89	1.33	1.25
1	B	317	GLU	CD-OE2	6.89	1.33	1.25

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	ARG	NE-CZ-NH1	13.31	126.96	120.30
1	B	328	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	B	69	ASP	CB-CG-OD2	-9.35	109.88	118.30
1	B	145	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	B	200	ASP	CB-CG-OD1	8.86	126.27	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	154	THR	CA

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	2697	0	2661	24	0
1	B	2706	0	2655	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
5	A	40	0	6	0	0
5	B	39	0	25	3	0
6	A	498	0	0	4	0
6	B	427	0	0	12	0
All	All	6500	0	5399	75	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 7.

The worst 5 of 75 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:73:LEU:HD13	1:B:118[A]:ILE:HD13	1.40	1.03
5:B:901:UD1:H5'	6:B:1985:HOH:O	1.84	0.78
1:B:70:GLN:HG3	6:B:1270:HOH:O	1.83	0.77
1:B:155:ASN:HB3	1:B:156:PRO:HD2	1.66	0.76
1:A:63:GLU:HG3	6:A:1961:HOH:O	1.84	0.76

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	347/348 (100%)	340 (98%)	6 (2%)	1 (0%)	41	18
1	B	352/348 (101%)	341 (97%)	11 (3%)	0	100	100
All	All	699/696 (100%)	681 (97%)	17 (2%)	1 (0%)	51	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	THR

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	282/282 (100%)	272 (96%)	10 (4%)	36	9
1	B	287/282 (102%)	274 (96%)	13 (4%)	27	5
All	All	569/564 (101%)	546 (96%)	23 (4%)	32	6

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	176	LYS
1	B	231[B]	ASP
1	B	231[A]	ASP
1	B	233	GLU
1	A	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	B	206	ASN
1	B	339	GLN
1	B	224	ASN
1	A	202	GLN

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)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	NAD	A	400	-	42,48,48	1.12	4 (9%)	50,73,73	1.74	7 (14%)
5	UD1	A	401[A]	-	38,41,41	0.79	0	57,62,62	1.08	4 (7%)
5	UD1	B	901	-	38,41,41	0.85	1 (2%)	57,62,62	1.10	5 (8%)
4	NAD	B	900	-	42,48,48	1.01	2 (4%)	50,73,73	1.85	9 (18%)
5	UD1	A	401[B]	-	38,41,41	0.79	0	57,62,62	1.08	4 (7%)

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
4	NAD	A	400	-	-	9/26/62/62	0/5/5/5
5	UD1	A	401[A]	-	-	2/26/63/63	0/3/3/3
5	UD1	B	901	-	-	4/26/63/63	0/3/3/3
4	NAD	B	900	-	-	12/26/62/62	0/5/5/5
5	UD1	A	401[B]	-	-	2/26/63/63	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	NAD	C2N-N1N	3.67	1.39	1.35
4	B	900	NAD	C4N-C3N	2.81	1.44	1.39
5	B	901	UD1	C2'-N2'	2.67	1.50	1.45
4	B	900	NAD	PA-O2A	-2.41	1.44	1.55
4	A	400	NAD	C2A-N1A	2.34	1.38	1.33

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	NAD	C6N-C5N-C4N	5.88	127.99	119.44
4	B	900	NAD	C5N-C6N-N1N	-5.67	112.26	120.40
4	A	400	NAD	C5N-C4N-C3N	-5.40	113.96	120.34
4	B	900	NAD	C5N-C4N-C3N	-5.05	114.36	120.34
4	A	400	NAD	C5N-C6N-N1N	-4.53	113.90	120.40

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	NAD	O4D-C1D-N1N-C2N
4	B	900	NAD	C5D-O5D-PN-O2N
4	B	900	NAD	O4D-C1D-N1N-C2N
4	B	900	NAD	O4D-C1D-N1N-C6N
5	A	401[A]	UD1	C1'-O1'-PB-O3A

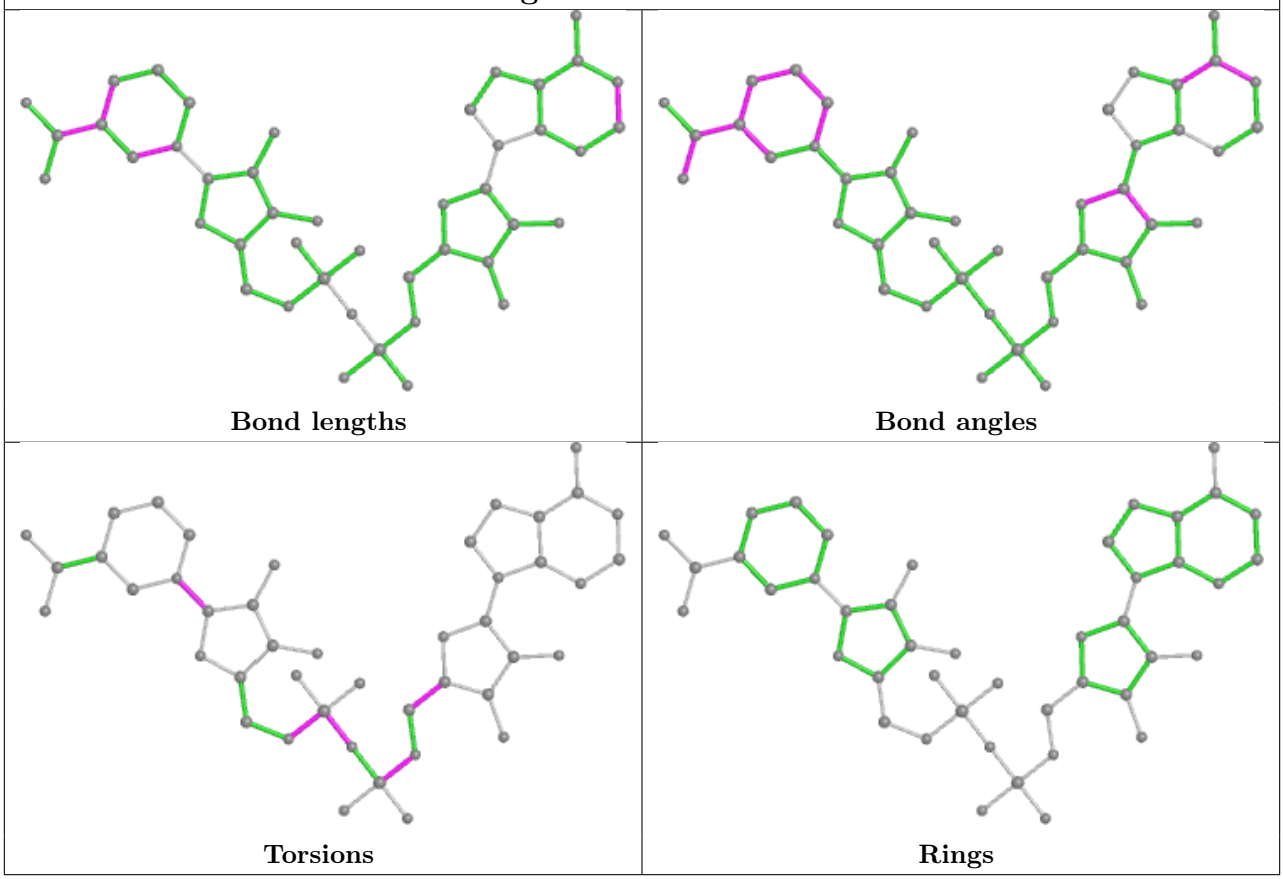
There are no ring outliers.

1 monomer is involved in 3 short contacts:

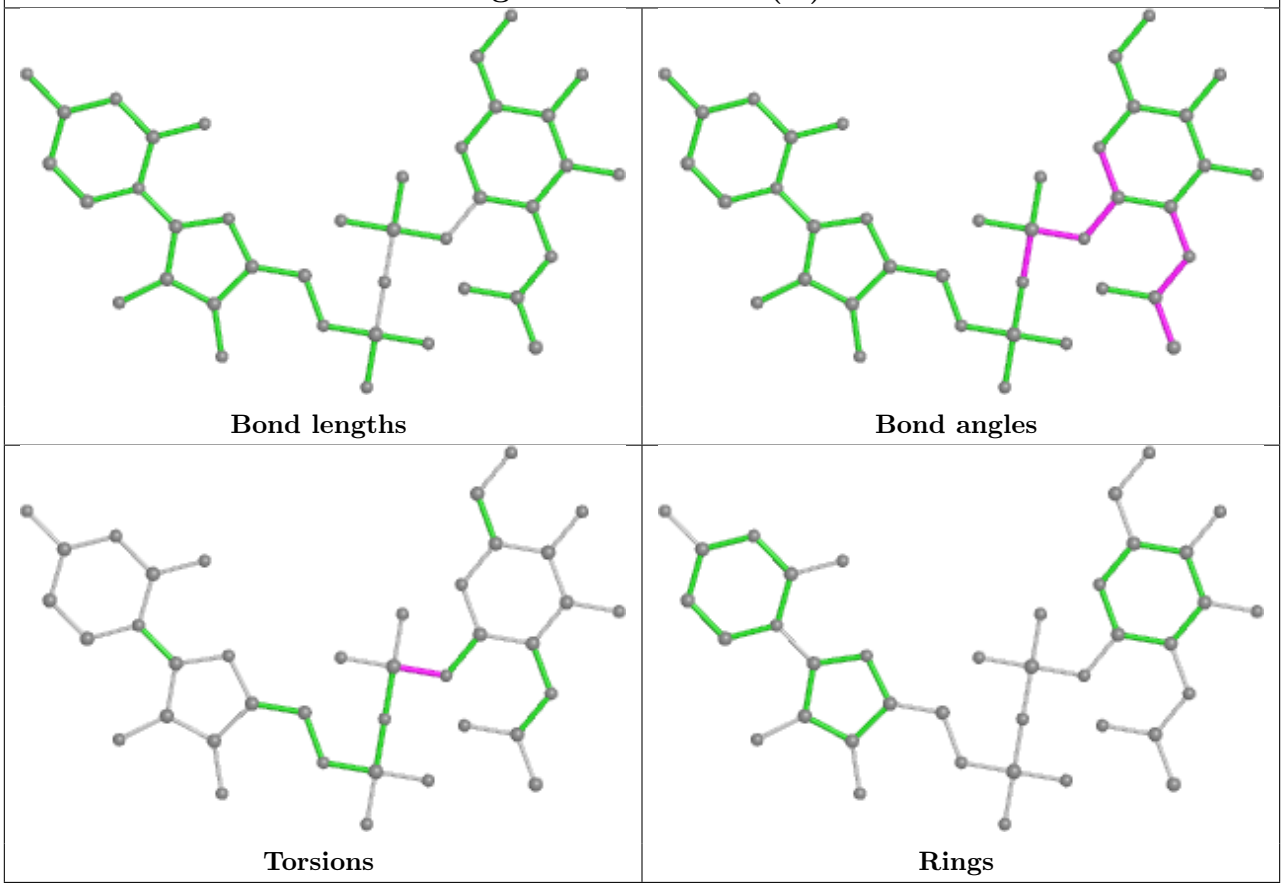
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	UD1	3	0

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.

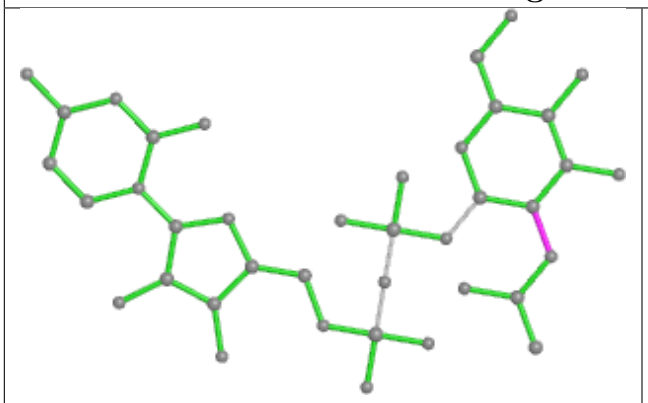
Ligand NAD A 400



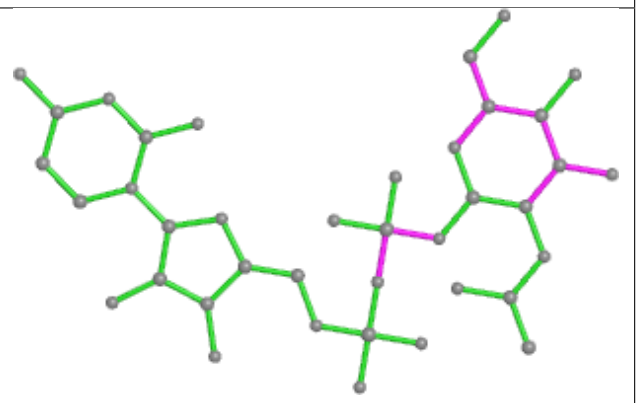
Ligand UD1 A 401 (A)



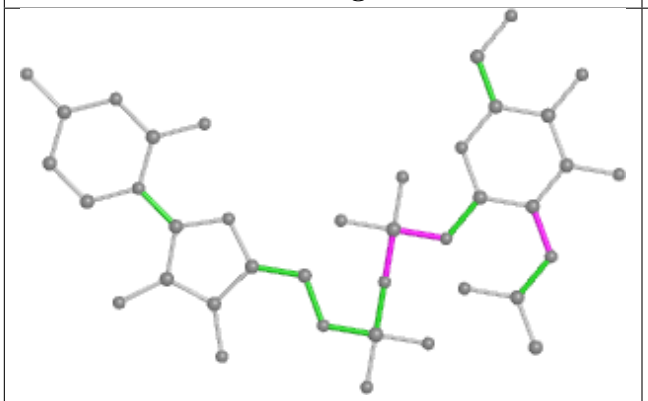
Ligand UD1 B 901



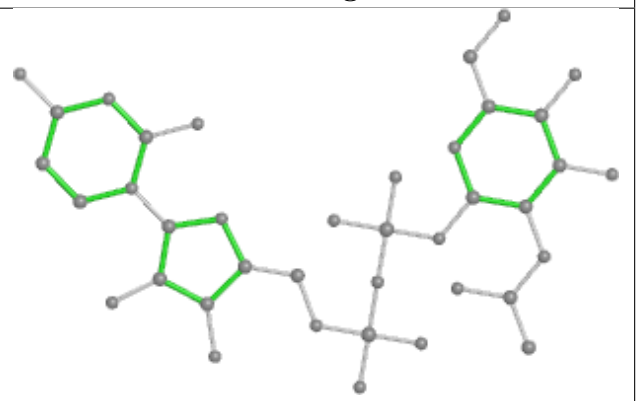
Bond lengths



Bond angles

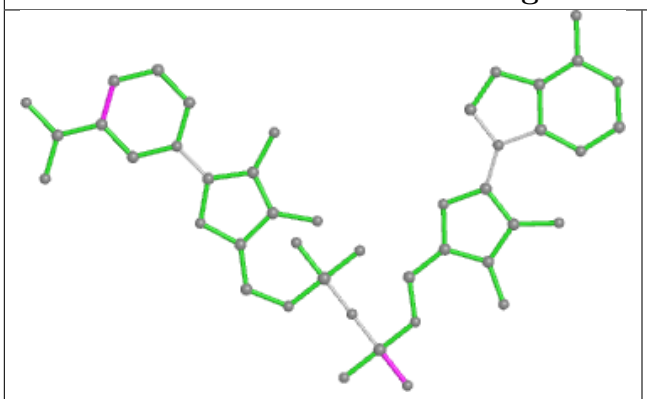


Torsions

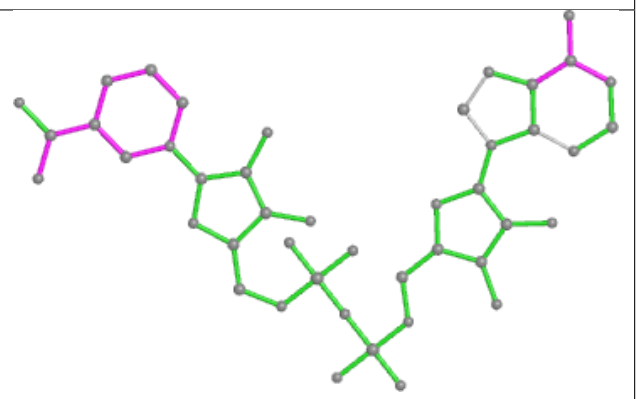


Rings

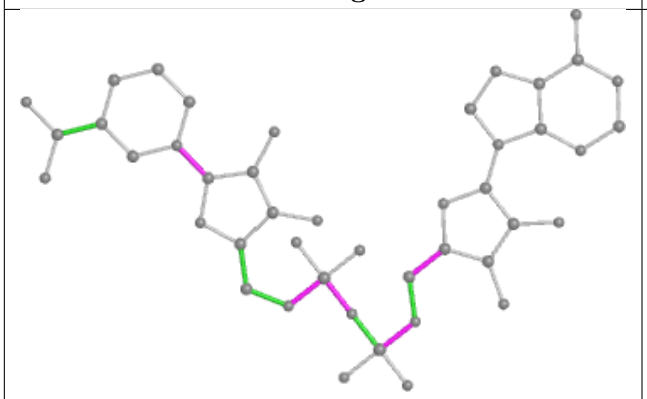
Ligand NAD B 900



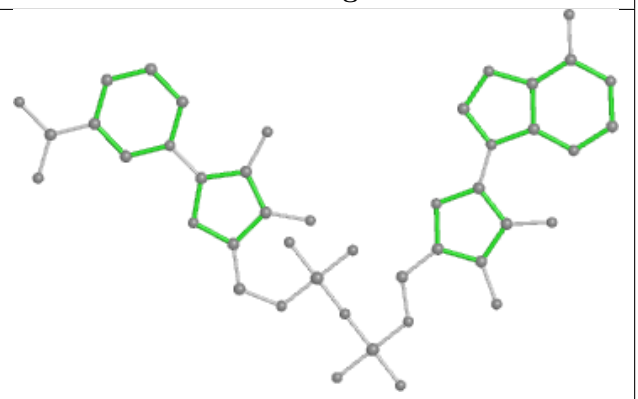
Bond lengths



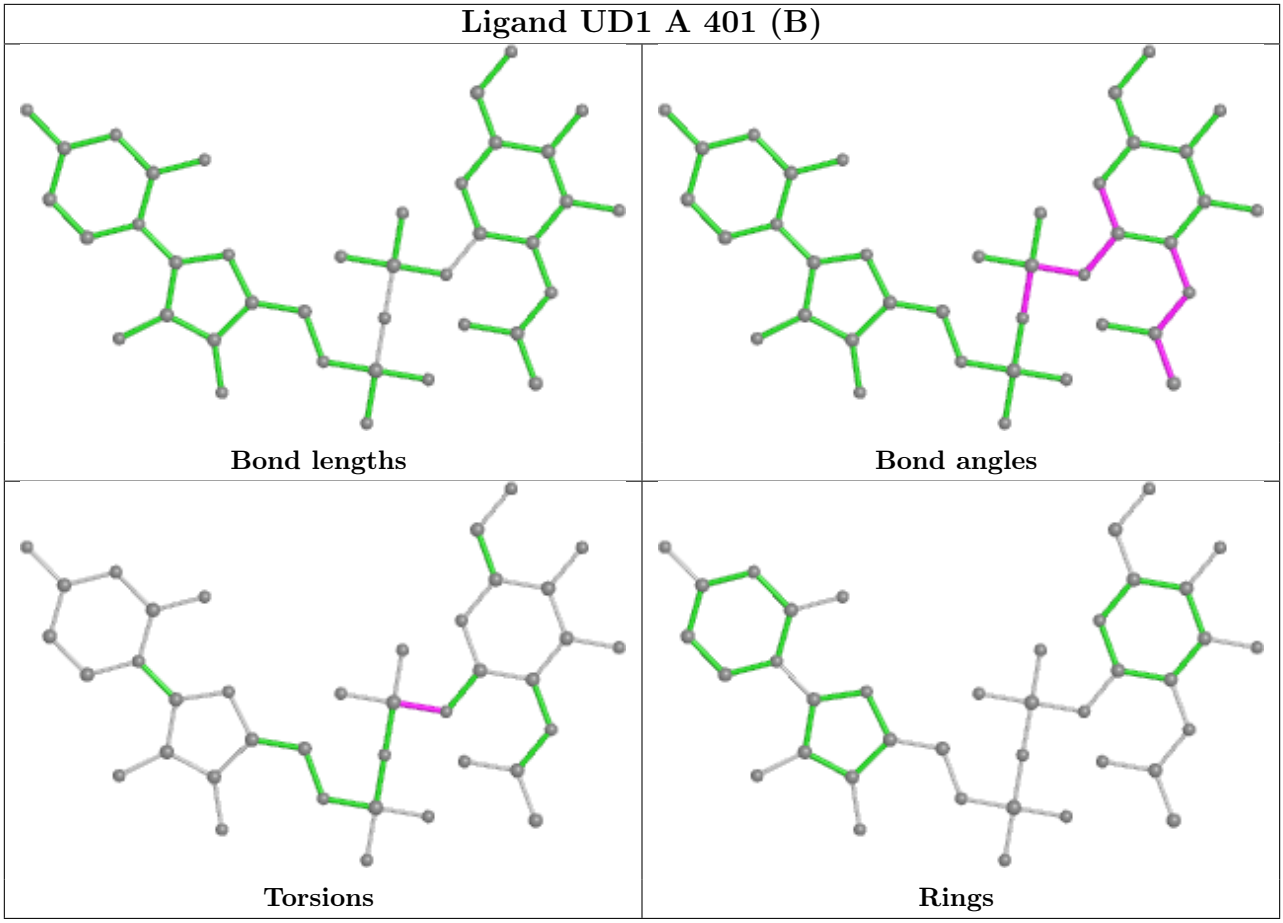
Bond angles



Torsions



Rings



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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.