wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2023 – 06:17 AM EDT

PDB ID	:	1I3K
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 ⓘ 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	:	4.02b-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 ⓘ

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.
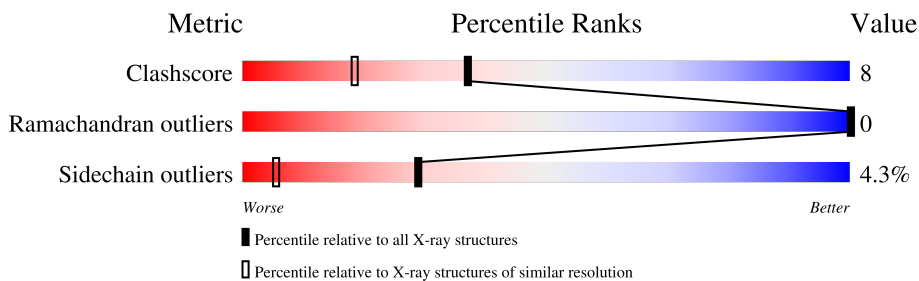
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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	78% 19% •
1	B	348	77% 18% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	B	972	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6568 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 2697	C 1706	N 467	O 508	S 16	0	3	0
1	B	345	Total 2716	C 1723	N 465	O 511	S 17	0	12	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
2	A	1	Total 1	Cl 1	0	0
2	B	3	Total 3	Cl 3	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			37	15	2	18	2		

Continued on next page...

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

- 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 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	494	Total 494	O 494	0	0
7	B	483	Total 483	O 483	0	0

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

Chain A:

• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain B:
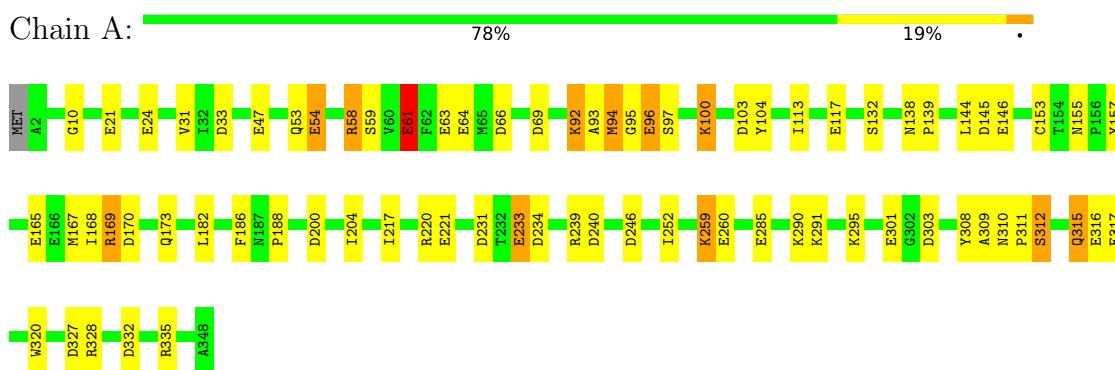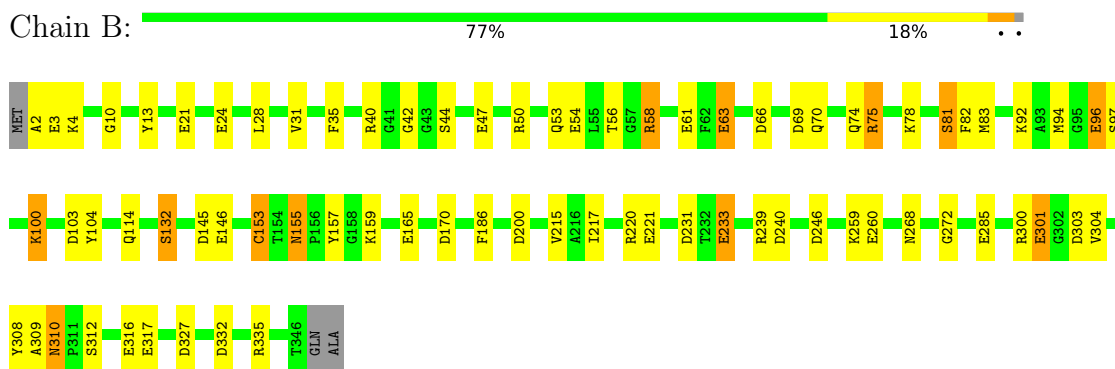
4 Data and refinement statistics ⓘ

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　　89.90Å　　96.90Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　1.50	Depositor
% Data completeness (in resolution range)	99.1 (50.00-1.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.174　,　0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6568	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: EDO, NAD, MG, CL, UPG

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	20/2766 (0.7%)	1.21	26/3740 (0.7%)
1	B	0.89	19/2825 (0.7%)	1.23	30/3821 (0.8%)
All	All	0.89	39/5591 (0.7%)	1.22	56/7561 (0.7%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[A]	GLU	CD-OE2	6.67	1.32	1.25
1	A	63[B]	GLU	CD-OE2	6.67	1.32	1.25
1	B	317	GLU	CD-OE2	6.57	1.32	1.25
1	A	233	GLU	CD-OE2	6.57	1.32	1.25
1	B	63	GLU	CD-OE2	6.49	1.32	1.25

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	145	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	303	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	B	170	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	66	ASP	CB-CG-OD2	-7.41	111.63	118.30

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	2697	0	2648	41	0
1	B	2716	0	2677	43	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	26	3	0
4	B	44	0	26	1	0
5	A	37	0	6	1	0
5	B	36	0	22	2	0
6	A	4	0	6	0	0
6	B	8	0	12	4	0
7	A	494	0	0	10	0
7	B	483	0	0	8	0
All	All	6568	0	5423	86	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 8.

The worst 5 of 86 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	1.44	0.97
1:B:58:ARG:HG3	1:B:58:ARG:HH11	1.38	0.89
1:B:94:MET:HB2	1:B:96:GLU:HG3	1.61	0.82
1:A:94:MET:HB3	1:A:96:GLU:CG	2.09	0.81
1:B:63:GLU:HG3	7:B:3032:HOH:O	1.83	0.78

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	348/348 (100%)	340 (98%)	8 (2%)	0	100	100
1	B	356/348 (102%)	349 (98%)	7 (2%)	0	100	100
All	All	704/696 (101%)	689 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/282 (100%)	271 (96%)	12 (4%)	30	6
1	B	292/282 (104%)	277 (95%)	15 (5%)	24	4
All	All	575/564 (102%)	548 (95%)	27 (5%)	29	4

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81[A]	SER
1	B	153	CYS
1	B	301	GLU
1	B	100	LYS
1	B	155	ASN

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	114	GLN
1	B	138	ASN
1	B	310	ASN
1	B	206	ASN
1	A	337	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	#$|Z| > 2$
5	UPG	B	901	-	35,38,38	0.70	0	53,58,58	0.97	4 (7%)
5	UPG	A	401[B]	-	35,38,38	1.42	1 (2%)	53,58,58	1.30	4 (7%)
4	NAD	B	900	-	42,48,48	1.20	5 (11%)	50,73,73	1.76	12 (24%)
5	UPG	A	401[A]	-	35,38,38	1.42	1 (2%)	53,58,58	1.30	4 (7%)
6	EDO	B	972	-	3,3,3	0.34	0	2,2,2	0.25	0
6	EDO	A	971	-	3,3,3	0.40	0	2,2,2	0.23	0
6	EDO	B	970	-	3,3,3	0.33	0	2,2,2	0.43	0
4	NAD	A	400	-	42,48,48	1.06	3 (7%)	50,73,73	1.79	6 (12%)

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
5	UPG	B	901	-	-	1/23/59/59	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UPG	A	401[B]	-	-	4/23/59/59	0/3/3/3
4	NAD	B	900	-	-	9/26/62/62	0/5/5/5
5	UPG	A	401[A]	-	-	2/23/59/59	0/3/3/3
6	EDO	B	972	-	-	1/1/1/1	-
6	EDO	A	971	-	-	1/1/1/1	-
6	EDO	B	970	-	-	1/1/1/1	-
4	NAD	A	400	-	-	10/26/62/62	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401[A]	UPG	PB-O3B	7.14	1.79	1.60
5	A	401[B]	UPG	PB-O3B	7.14	1.79	1.60
4	B	900	NAD	C4N-C3N	3.61	1.45	1.39
4	A	400	NAD	C2N-N1N	3.23	1.38	1.35
4	B	900	NAD	C2N-N1N	2.69	1.38	1.35

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	NAD	C5N-C4N-C3N	-6.96	112.11	120.34
4	A	400	NAD	C5N-C6N-N1N	-5.48	112.55	120.40
5	A	401[A]	UPG	O5'-C1'-O3B	-5.25	104.50	111.36
5	A	401[B]	UPG	O5'-C1'-O3B	-5.25	104.50	111.36
4	B	900	NAD	C5N-C6N-N1N	-5.15	113.02	120.40

There are no chirality outliers.
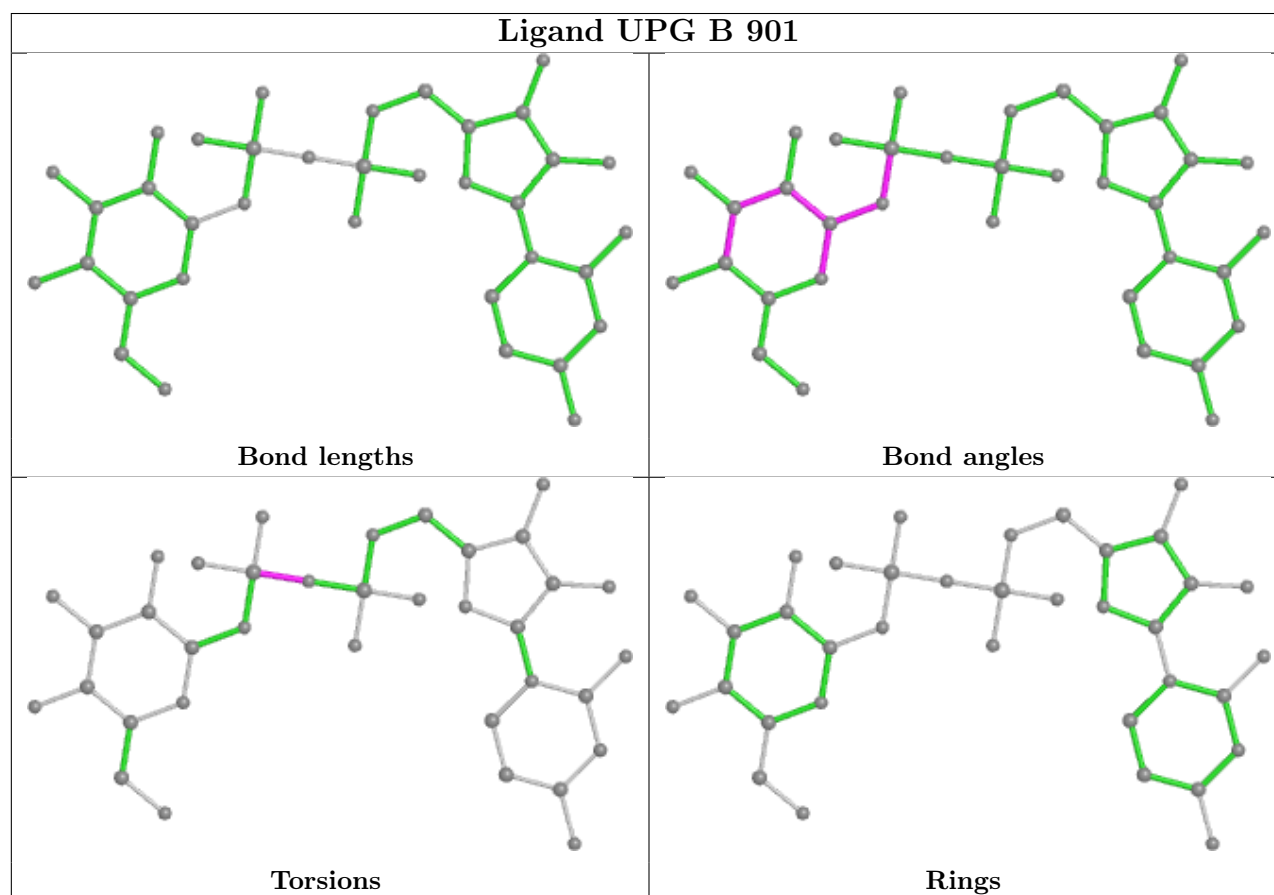
5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	NAD	C5B-O5B-PA-O2A
4	A	400	NAD	C5D-O5D-PN-O2N
4	A	400	NAD	O4D-C1D-N1N-C2N
4	B	900	NAD	O4D-C1D-N1N-C2N
5	A	401[A]	UPG	C1'-O3B-PB-O3A

There are no ring outliers.
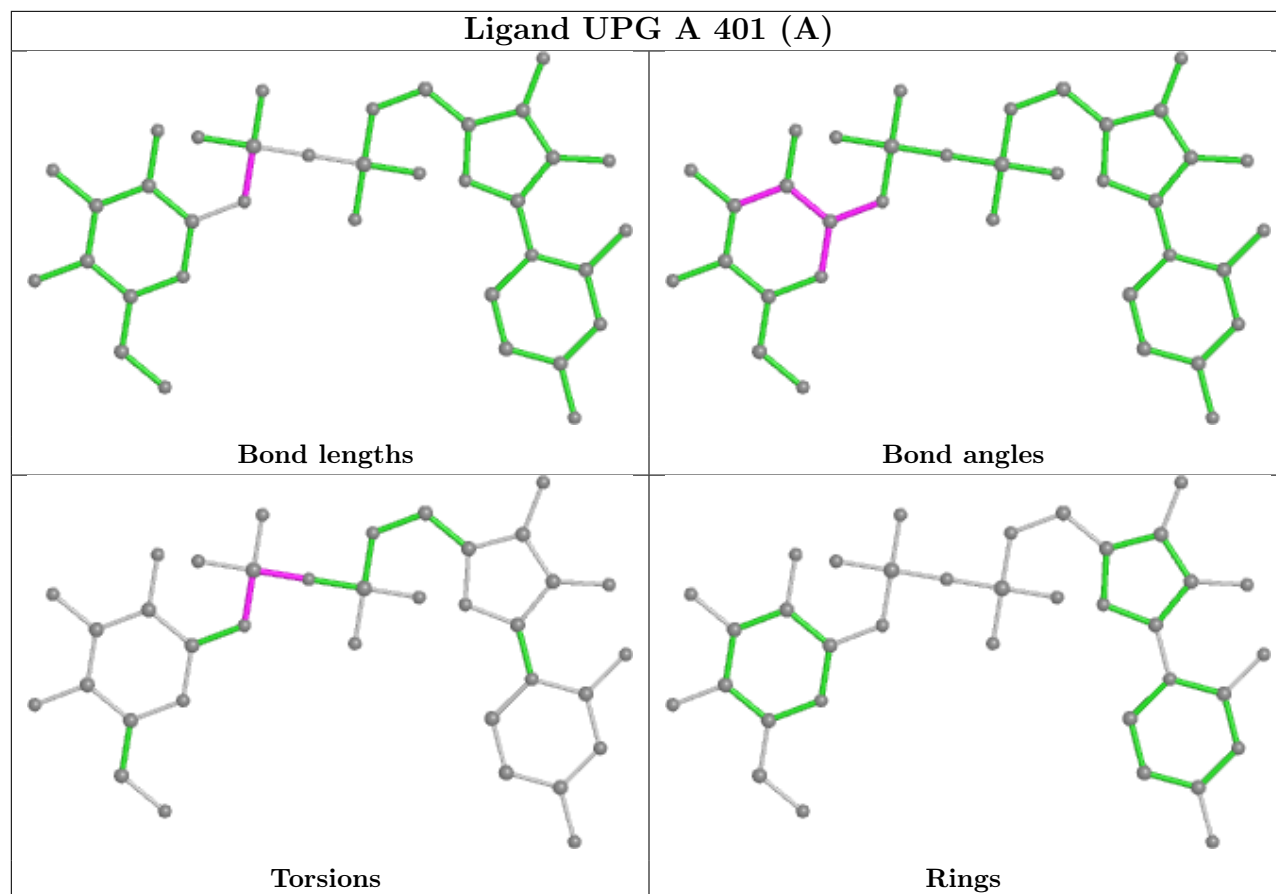
5 monomers are involved in 10 short contacts:

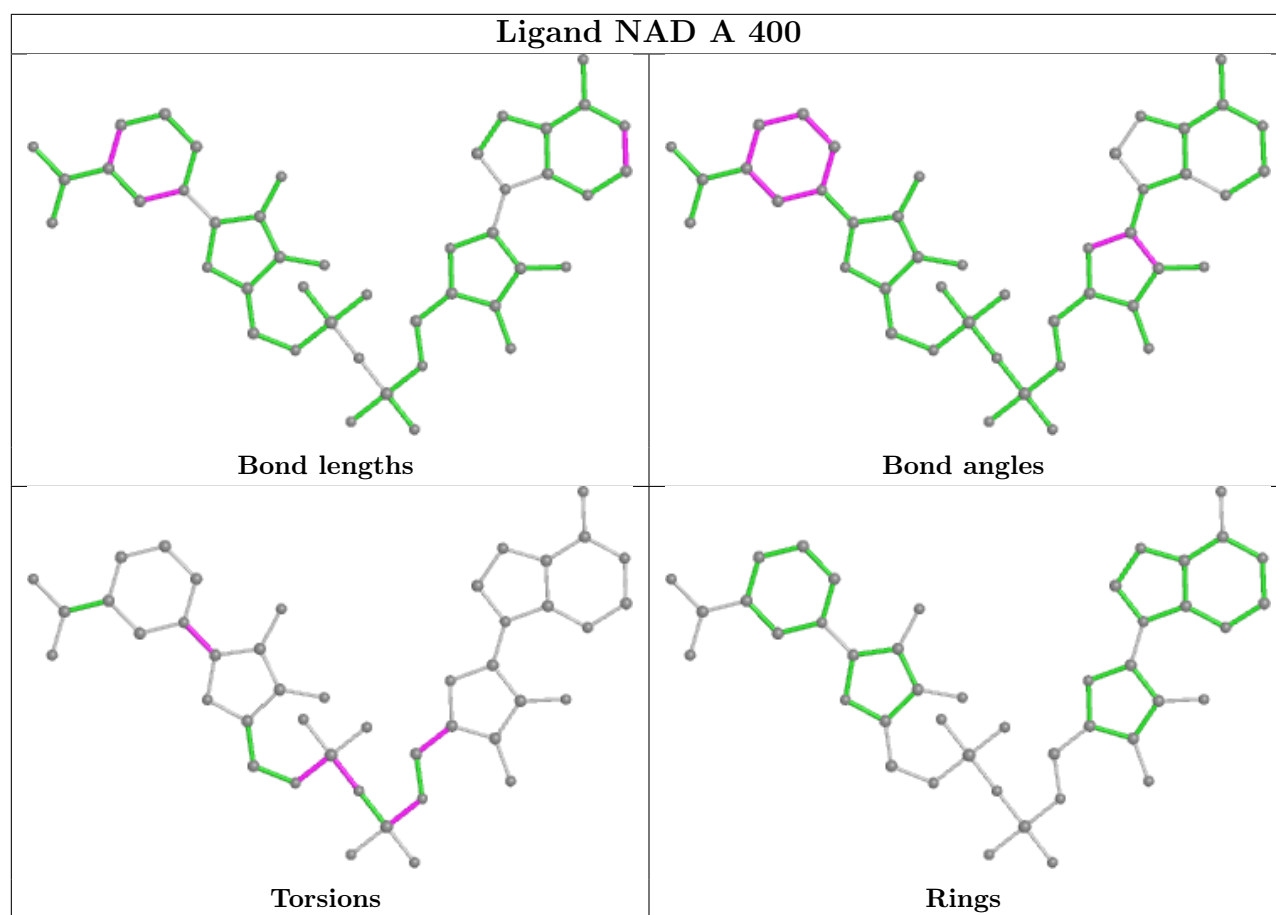| Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	UPG	2	0
4	B	900	NAD	1	0
5	A	401[A]	UPG	1	0
6	B	972	EDO	4	0
4	A	400	NAD	3	0

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 UPG B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG A 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 900

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG A 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 400

Bond lengths

Bond angles

Torsions

Rings
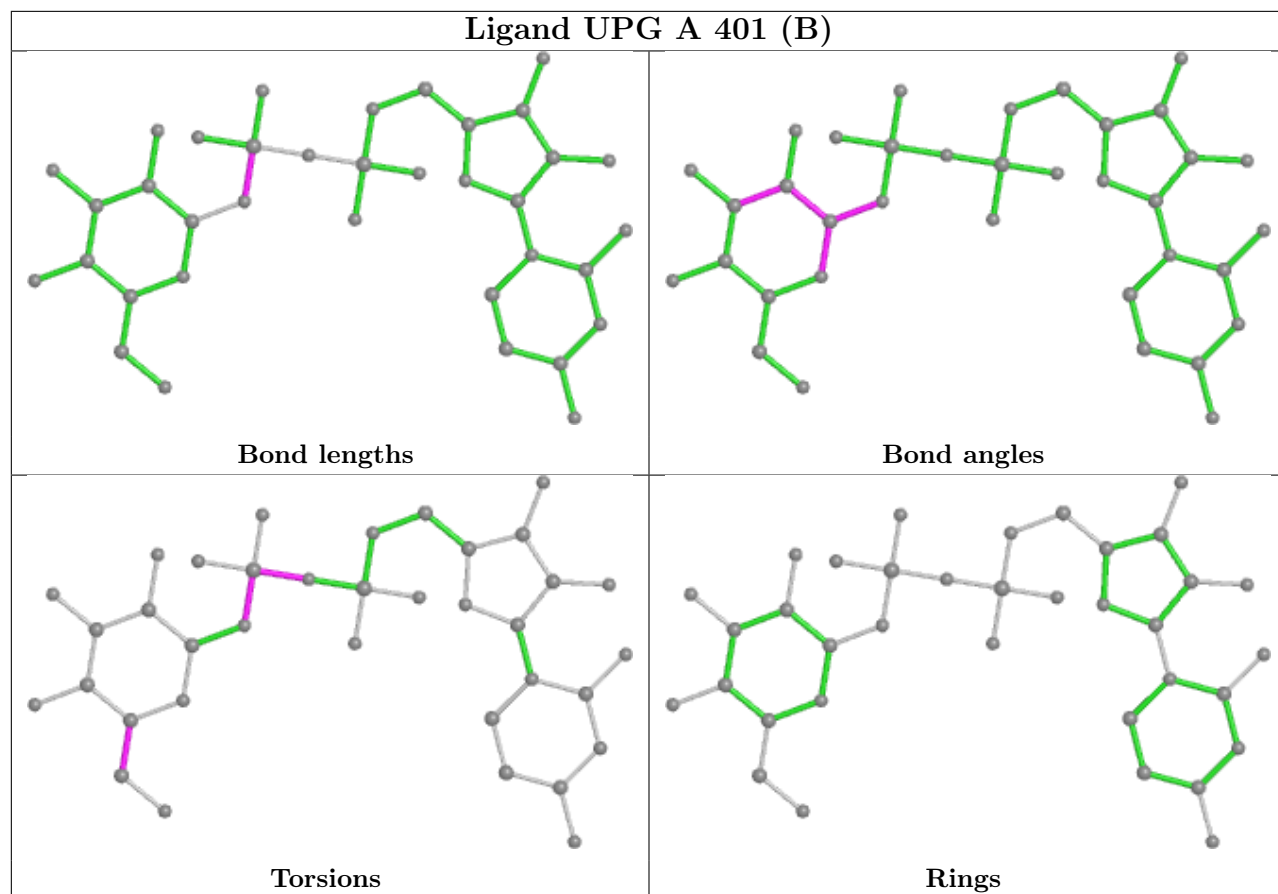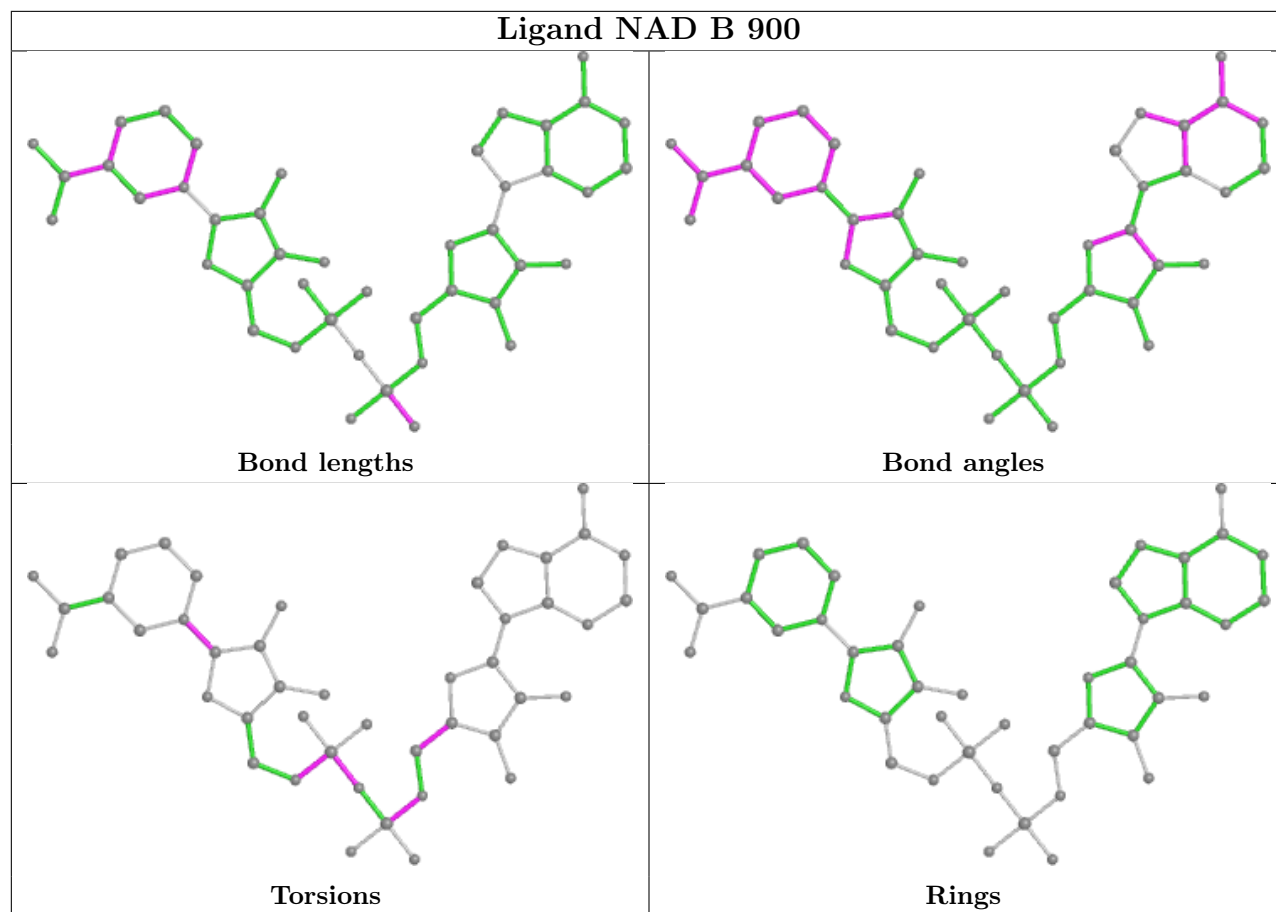
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.