



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:07 am BST

PDB ID : 2UDP
Title : UDP-GALACTOSE 4-EPIMERASE COMPLEXED WITH UDP-PHENOL
Authors : Thoden, J.B.; Gulick, A.M.; Holden, H.M.
Deposited on : 1997-03-08
Resolution : 1.80 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 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) : 2.11

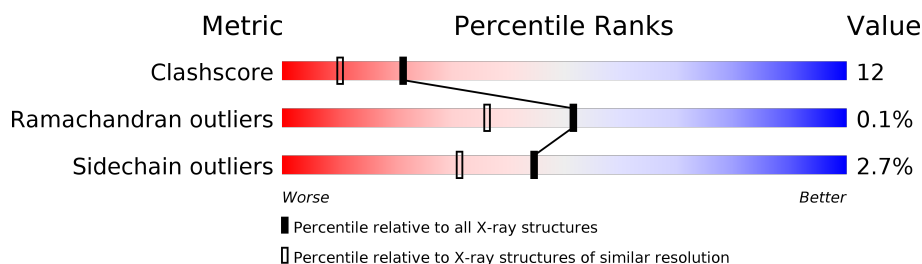
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 on 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	338	
1	B	338	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6294 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-GALACTOSE 4-EPIMERASE.

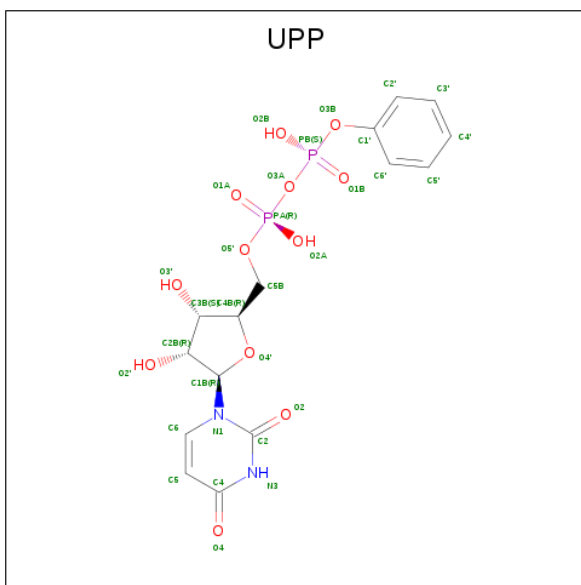
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2626	1656	463	495	12			
1	B	338	Total	C	N	O	S	0	0	0
			2626	1656	463	495	12			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is PHENYL-URIDINE-5'-DIPHOSPHATE (three-letter code: UPP) (formula: $C_{15}H_{18}N_2O_{12}P_2$).

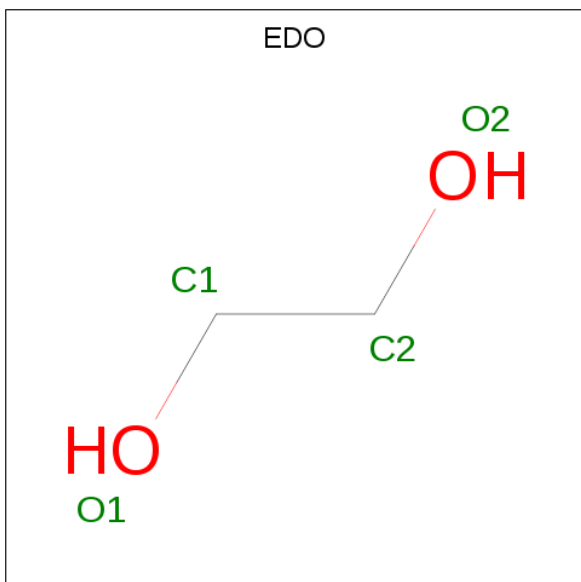


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 15	N 2	O 12	P 2	0	0
3	B	1	Total 31	C 15	N 2	O 12	P 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 6 is water.

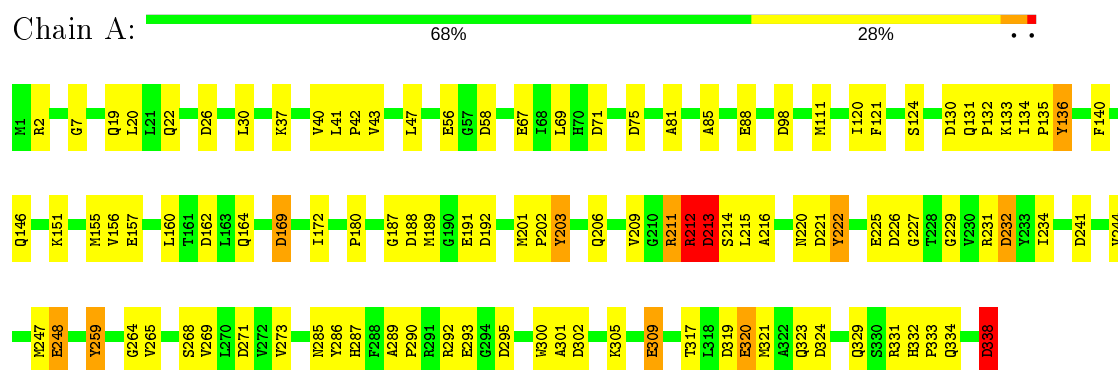
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	461	Total	O	0	0
			461	461		
6	B	426	Total	O	0	0
			426	426		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-GALACTOSE 4-EPIMERASE



• Molecule 1: UDP-GALACTOSE 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	76.00Å 78.70Å 128.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6294	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: NA, NAD, UPP, EDO

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	0.77	10/2692 (0.4%)	1.39	40/3663 (1.1%)
1	B	0.77	8/2692 (0.3%)	1.42	47/3663 (1.3%)
All	All	0.77	18/5384 (0.3%)	1.40	87/7326 (1.2%)

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	0	1
1	B	1	1
All	All	1	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLU	CD-OE1	6.75	1.33	1.25
1	B	225	GLU	CD-OE1	6.63	1.32	1.25
1	A	56	GLU	CD-OE2	6.46	1.32	1.25
1	B	88	GLU	CD-OE1	6.45	1.32	1.25
1	A	88	GLU	CD-OE1	6.22	1.32	1.25
1	A	191	GLU	CD-OE1	6.08	1.32	1.25
1	A	309	GLU	CD-OE1	6.08	1.32	1.25
1	A	320	GLU	CD-OE1	5.88	1.32	1.25
1	B	56	GLU	CD-OE2	5.84	1.32	1.25
1	A	225	GLU	CD-OE2	5.84	1.32	1.25
1	B	248	GLU	CD-OE1	5.59	1.31	1.25
1	B	293	GLU	CD-OE1	5.49	1.31	1.25
1	B	95	GLU	CD-OE1	5.41	1.31	1.25
1	B	191	GLU	CD-OE1	5.41	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLU	CD-OE2	5.39	1.31	1.25
1	B	67	GLU	CD-OE2	5.35	1.31	1.25
1	A	67	GLU	CD-OE1	5.17	1.31	1.25
1	A	248	GLU	CD-OE2	5.08	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	26	ASP	CB-CG-OD1	-10.82	108.57	118.30
1	A	226	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	B	313	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	A	319	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	A	232	ASP	CB-CG-OD1	-9.07	110.14	118.30
1	B	106	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	B	226	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	B	324	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	B	295	ASP	CB-CG-OD1	8.54	125.99	118.30
1	B	338	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	A	124	SER	N-CA-CB	-8.53	97.71	110.50
1	A	162	ASP	CB-CG-OD1	-8.38	110.75	118.30
1	A	213	ASP	CB-CG-OD2	-8.29	110.83	118.30
1	A	192	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	B	212	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	B	212	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	B	295	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	31	ASP	CB-CG-OD2	7.71	125.23	118.30
1	B	162	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	71	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	324	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	302	ASP	CB-CG-OD2	7.55	125.09	118.30
1	B	238	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	26	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	130	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	130	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	188	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	B	241	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	169	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	222	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	A	71	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	58	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	226	ASP	CB-CG-OD1	6.80	124.42	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	A	58	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	169	ASP	CB-CG-OD1	-6.76	112.21	118.30
1	B	319	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	271	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	B	2	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	203	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	B	308	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	271	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	A	162	ASP	CB-CG-OD2	6.41	124.06	118.30
1	B	188	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	226	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	192	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	324	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	232	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	22	GLN	CA-CB-CG	-6.23	99.69	113.40
1	B	71	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	31	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	B	130	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	A	259	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	B	282	LYS	N-CA-CB	6.09	121.56	110.60
1	A	319	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	238	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	338	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	169	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	2	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	222	TYR	N-CA-CB	5.87	121.17	110.60
1	B	146	GLN	N-CA-CB	5.83	121.09	110.60
1	A	192	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	213	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	241	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	B	2	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	271	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	98	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	301	ALA	CB-CA-C	-5.57	101.75	110.10
1	B	278	LYS	CB-CA-C	5.55	121.51	110.40
1	A	188	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	295	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	162	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	212	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	241	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	338	ASP	CB-CG-OD1	5.41	123.17	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ASP	CB-CA-C	5.36	121.13	110.40
1	B	98	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	A	231	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	75	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	271	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	75	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	292	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	98	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	176	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	106	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	85	ALA	CB-CA-C	5.01	117.62	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	146	GLN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	TYR	Sidechain
1	B	299	TYR	Sidechain

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	2626	0	2557	65	0
1	B	2626	0	2557	62	0
2	A	44	0	26	0	0
2	B	44	0	26	3	0
3	A	31	0	16	1	0
3	B	31	0	16	0	0
4	B	1	0	0	0	0
5	B	4	0	6	0	0
6	A	461	0	0	5	0
6	B	426	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6294	0	5204	127	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 12.

All (127) 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:221:ASP:HB2	6:A:523:HOH:O	1.63	0.95
1:B:327:HIS:O	1:B:331:ARG:HG3	1.78	0.84
1:A:232:ASP:HB2	1:A:300:TRP:HB2	1.65	0.79
1:A:264:GLY:HA2	1:A:301:ALA:O	1.86	0.76
1:B:133:LYS:O	1:B:134:ILE:HD12	1.84	0.75
1:B:117:LYS:HE2	1:B:169:ASP:OD2	1.87	0.74
1:B:203:TYR:CZ	1:B:212:ARG:HG2	2.23	0.74
1:B:131:GLN:OE1	1:B:132:PRO:HD2	1.90	0.72
1:A:131:GLN:OE1	1:A:132:PRO:HD2	1.89	0.71
1:A:269:VAL:O	1:A:273:VAL:HG23	1.90	0.71
1:A:20:LEU:HD23	1:A:244:VAL:HG22	1.73	0.71
1:A:43:VAL:HG11	1:A:189:MET:HG3	1.73	0.70
1:A:19:GLN:HB3	6:A:597:HOH:O	1.92	0.69
1:A:37:LYS:O	1:A:40:VAL:HG12	1.93	0.69
1:B:264:GLY:HA2	1:B:301:ALA:O	1.92	0.69
1:A:215:LEU:N	1:A:285:ASN:O	2.21	0.69
1:B:133:LYS:C	1:B:134:ILE:HD12	2.12	0.69
1:B:131:GLN:OE1	1:B:133:LYS:HB2	1.94	0.68
1:A:43:VAL:CG1	1:A:189:MET:HG3	2.24	0.68
1:A:289:ALA:HB1	1:A:290:PRO:HD2	1.75	0.68
1:B:307:ASP:OD1	1:B:313:ARG:NH1	2.20	0.67
1:A:232:ASP:HB2	1:A:300:TRP:CB	2.24	0.67
1:B:18:VAL:O	1:B:22:GLN:HG3	1.97	0.65
1:B:196:ILE:HG12	1:B:212:ARG:NH2	2.12	0.64
1:A:292:ARG:NH2	3:A:341:UPP:H2B	2.13	0.64
1:A:131:GLN:OE1	1:A:133:LYS:HD3	1.98	0.64
1:A:20:LEU:CD2	1:A:244:VAL:HG22	2.28	0.64
1:A:244:VAL:O	1:A:248:GLU:HG3	1.97	0.64
1:A:323:GLN:NE2	6:A:703:HOH:O	2.27	0.63
1:B:222:TYR:O	1:B:227:GLY:HA2	1.98	0.63
1:A:151:LYS:O	1:A:155:MET:HG3	1.98	0.62
1:B:22:GLN:OE1	6:B:796:HOH:O	2.16	0.61
1:B:244:VAL:O	1:B:248:GLU:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASP:HB2	6:A:630:HOH:O	2.01	0.60
1:A:317:THR:OG1	1:A:320:GLU:HG3	2.00	0.60
1:A:215:LEU:O	1:A:286:TYR:HA	2.02	0.59
1:A:215:LEU:HB3	1:A:286:TYR:HB3	1.84	0.59
1:B:289:ALA:HB1	1:B:290:PRO:HD2	1.84	0.59
1:A:41:LEU:HB2	1:A:42:PRO:HD3	1.85	0.59
1:B:222:TYR:C	1:B:224:THR:H	2.07	0.58
1:B:175:LEU:HD13	1:B:261:LEU:HD11	1.85	0.58
1:B:269:VAL:O	1:B:273:VAL:HG23	2.04	0.57
1:A:331:ARG:HB2	1:A:332:HIS:CD2	2.39	0.57
1:B:15:HIS:HA	1:B:189:MET:HE1	1.85	0.57
1:B:232:ASP:HB2	1:B:300:TRP:HB2	1.88	0.56
1:B:307:ASP:OD1	1:B:313:ARG:HD3	2.06	0.56
1:B:131:GLN:HG2	6:B:527:HOH:O	2.05	0.55
1:B:282:LYS:HD3	6:B:701:HOH:O	2.05	0.55
1:B:131:GLN:HB3	1:B:136:TYR:CE1	2.43	0.54
1:A:206:GLN:HB3	1:A:211:ARG:HB3	1.90	0.53
1:B:317:THR:OG1	1:B:320:GLU:HB2	2.09	0.53
1:A:187:GLY:O	1:A:331:ARG:HD3	2.08	0.53
1:B:282:LYS:HB3	6:B:704:HOH:O	2.08	0.53
1:B:232:ASP:HB2	1:B:300:TRP:CB	2.39	0.52
1:A:331:ARG:HB2	1:A:332:HIS:HD2	1.75	0.52
1:A:305:LYS:HE2	1:A:309:GLU:OE2	2.09	0.52
1:B:319:ASP:O	1:B:323:GLN:HG3	2.10	0.52
1:B:39:SER:OG	1:B:336:TYR:HB3	2.10	0.51
1:B:278:LYS:HB2	6:B:696:HOH:O	2.10	0.51
1:A:259:TYR:CD1	1:A:305:LYS:HG2	2.46	0.51
1:B:27:VAL:C	1:B:28:ILE:HD12	2.31	0.51
1:B:37:LYS:O	1:B:40:VAL:HG12	2.11	0.51
1:B:222:TYR:O	1:B:224:THR:N	2.43	0.50
1:B:217:ILE:HD13	1:B:269:VAL:HG12	1.94	0.50
1:A:22:GLN:NE2	1:A:47:LEU:O	2.43	0.50
1:B:203:TYR:OH	1:B:212:ARG:HG2	2.12	0.49
1:B:124:SER:CB	2:B:340:NAD:O7N	2.61	0.49
1:A:201:MET:N	1:A:202:PRO:HD2	2.27	0.48
1:A:203:TYR:CE1	1:A:215:LEU:HA	2.48	0.48
1:A:317:THR:O	1:A:321:MET:HG3	2.12	0.48
1:B:131:GLN:HB3	1:B:136:TYR:HE1	1.78	0.48
1:B:164:GLN:HB2	1:B:172:ILE:HD12	1.94	0.48
1:B:319:ASP:HB3	1:B:323:GLN:OE1	2.14	0.48
1:A:287:HIS:HE1	6:A:631:HOH:O	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PRO:O	1:B:254:PRO:HB3	2.15	0.47
1:A:289:ALA:HB1	1:A:290:PRO:CD	2.41	0.47
1:A:209:VAL:HG21	1:A:329:GLN:HE21	1.80	0.47
1:A:206:GLN:OE1	1:A:212:ARG:NE	2.47	0.47
1:A:214:SER:HA	1:A:285:ASN:O	2.16	0.46
1:A:222:TYR:HB2	1:A:227:GLY:O	2.16	0.46
1:B:7:GLY:HA2	1:B:31:ASP:OD2	2.15	0.46
1:B:134:ILE:HD11	1:B:136:TYR:CE1	2.50	0.46
1:B:217:ILE:HD13	1:B:269:VAL:CG1	2.45	0.46
1:A:120:ILE:HD11	1:A:247:MET:HA	1.96	0.46
1:A:133:LYS:H	1:A:133:LYS:HG3	1.58	0.46
1:A:156:VAL:O	1:A:160:LEU:HG	2.16	0.46
1:A:211:ARG:NH1	1:A:333:PRO:O	2.45	0.46
1:A:216:ALA:HB2	1:A:287:HIS:CE1	2.51	0.45
1:B:319:ASP:O	1:B:323:GLN:CG	2.65	0.45
1:A:169:ASP:N	1:A:169:ASP:OD1	2.49	0.45
1:A:30:LEU:HD13	1:A:30:LEU:C	2.37	0.45
1:A:229:GLY:O	1:A:268:SER:HA	2.17	0.45
1:B:21:LEU:HD22	1:B:50:LYS:HB3	1.99	0.45
1:B:183:ALA:HB1	1:B:189:MET:O	2.17	0.45
1:A:220:ASN:N	1:A:220:ASN:OD1	2.49	0.45
1:A:134:ILE:HA	1:A:135:PRO:C	2.37	0.44
1:B:124:SER:OG	2:B:340:NAD:O7N	2.28	0.44
1:B:222:TYR:C	1:B:224:THR:N	2.71	0.44
1:B:217:ILE:HG23	1:B:269:VAL:HG11	2.00	0.44
1:A:164:GLN:HB2	1:A:172:ILE:HD12	2.00	0.44
1:B:124:SER:HB2	2:B:340:NAD:O7N	2.18	0.44
1:B:41:LEU:N	1:B:42:PRO:CD	2.81	0.44
1:A:259:TYR:CE1	1:A:305:LYS:HG2	2.52	0.44
1:A:338:ASP:OD1	1:A:338:ASP:N	2.51	0.44
1:B:232:ASP:OD2	1:B:301:ALA:HB3	2.18	0.44
1:A:69:LEU:HD13	1:A:111:MET:HA	1.99	0.43
1:A:221:ASP:OD1	1:A:221:ASP:N	2.50	0.43
1:A:121:PHE:CZ	1:A:156:VAL:HG11	2.54	0.42
1:B:151:LYS:HD2	6:B:419:HOH:O	2.18	0.42
1:B:289:ALA:HB1	1:B:290:PRO:CD	2.47	0.42
1:B:28:ILE:HD12	1:B:28:ILE:N	2.34	0.42
1:A:136:TYR:HA	1:A:140:PHE:CE2	2.55	0.42
1:A:7:GLY:N	1:A:81:ALA:HB2	2.35	0.42
1:A:232:ASP:HA	1:A:265:VAL:O	2.20	0.41
1:B:265:VAL:HG13	1:B:265:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD11	1:A:247:MET:CA	2.50	0.41
1:A:211:ARG:NH1	1:A:334:GLN:HA	2.35	0.41
1:A:131:GLN:HG2	1:A:140:PHE:CD2	2.55	0.41
1:B:277:SER:HB2	1:B:283:PRO:HA	2.01	0.41
1:B:41:LEU:N	1:B:42:PRO:HD2	2.36	0.41
1:B:28:ILE:HG13	1:B:53:THR:HB	2.03	0.41
1:A:43:VAL:HG12	1:A:189:MET:HG3	2.01	0.41
1:B:89:SER:O	1:B:148:PRO:HG2	2.21	0.41
1:A:133:LYS:HB2	1:A:140:PHE:CZ	2.56	0.40
1:B:283:PRO:HG2	6:B:791:HOH:O	2.21	0.40
1:B:30:LEU:HD13	1:B:30:LEU:C	2.42	0.40
1:A:180:PRO:HA	1:A:234:ILE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	336/338 (99%)	325 (97%)	11 (3%)	0	100	100
1	B	336/338 (99%)	326 (97%)	9 (3%)	1 (0%)	41	27
All	All	672/676 (99%)	651 (97%)	20 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	PRO

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	282/282 (100%)	277 (98%)	5 (2%)	59	48
1	B	282/282 (100%)	272 (96%)	10 (4%)	36	21
All	All	564/564 (100%)	549 (97%)	15 (3%)	44	31

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	211	ARG
1	A	212	ARG
1	A	213	ASP
1	A	338	ASP
1	B	131	GLN
1	B	177	TYR
1	B	212	ARG
1	B	220	ASN
1	B	221	ASP
1	B	277	SER
1	B	278	LYS
1	B	282	LYS
1	B	313	ARG
1	B	320	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	158	GLN
1	A	198	ASN
1	A	199	ASN
1	A	267	ASN
1	A	329	GLN
1	B	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	220	ASN
1	B	329	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	UPP	A	341	-	27,33,33	1.85	6 (22%)	31,49,49	1.17	1 (3%)
2	NAD	B	340	-	42,48,48	1.09	2 (4%)	50,73,73	1.49	9 (18%)
2	NAD	A	340	-	42,48,48	1.28	7 (16%)	50,73,73	1.67	10 (20%)
3	UPP	B	341	-	27,33,33	2.04	6 (22%)	31,49,49	0.95	1 (3%)
5	EDO	B	410	-	3,3,3	0.26	0	2,2,2	0.29	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
3	UPP	A	341	-	-	3/19/37/37	0/3/3/3
2	NAD	B	340	-	-	4/26/62/62	0/5/5/5
2	NAD	A	340	-	-	8/26/62/62	0/5/5/5
3	UPP	B	341	-	-	3/19/37/37	0/3/3/3
5	EDO	B	410	-	-	1/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	341	UPP	PB-O3B	-6.33	1.48	1.60
3	A	341	UPP	PB-O3B	-4.43	1.51	1.60
3	A	341	UPP	O3B-C1'	4.06	1.49	1.40
3	A	341	UPP	C4-N3	3.77	1.39	1.33
3	B	341	UPP	C4-N3	3.71	1.39	1.33
3	B	341	UPP	O3B-C1'	3.55	1.48	1.40
2	A	340	NAD	C2N-C3N	3.01	1.43	1.39
3	B	341	UPP	C6-C5	-2.98	1.31	1.38
2	A	340	NAD	C6N-N1N	2.94	1.42	1.35
3	A	341	UPP	C6-C5	-2.81	1.31	1.38
2	A	340	NAD	C2D-C1D	-2.63	1.49	1.53
3	A	341	UPP	PB-O1B	2.59	1.60	1.50
2	B	340	NAD	C6N-N1N	2.55	1.41	1.35
2	A	340	NAD	C2A-N1A	2.44	1.38	1.33
2	B	340	NAD	C2N-C3N	2.37	1.42	1.39
3	B	341	UPP	C6-N1	2.36	1.38	1.35
2	A	340	NAD	C4N-C3N	2.34	1.43	1.39
3	A	341	UPP	C6-N1	2.13	1.38	1.35
2	A	340	NAD	C7N-N7N	2.09	1.37	1.33
2	A	340	NAD	O4B-C1B	-2.08	1.38	1.41
3	B	341	UPP	PB-O1B	2.00	1.58	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	340	NAD	C4N-C3N-C7N	-6.24	104.35	121.04
2	A	340	NAD	C5A-C6A-N6A	5.47	128.66	120.35
3	A	341	UPP	C5-C4-N3	-5.01	112.29	123.31
2	B	340	NAD	C4N-C3N-C7N	-4.08	110.13	121.04
2	B	340	NAD	O4D-C1D-C2D	-4.03	101.03	106.93
3	B	341	UPP	C5-C4-N3	-3.65	115.28	123.31
2	B	340	NAD	C5A-C6A-N6A	3.62	125.86	120.35
2	B	340	NAD	C2N-C3N-C4N	3.25	121.95	118.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	NAD	C3N-C2N-N1N	-2.99	117.50	120.43
2	A	340	NAD	N6A-C6A-N1A	-2.98	112.38	118.57
2	A	340	NAD	C3N-C2N-N1N	-2.94	117.55	120.43
2	A	340	NAD	C3N-C7N-N7N	-2.55	114.69	117.75
2	A	340	NAD	C2N-C3N-C7N	2.42	126.50	119.46
2	A	340	NAD	O7N-C7N-C3N	2.36	122.46	119.63
2	A	340	NAD	O4B-C4B-C5B	-2.28	101.87	109.37
2	B	340	NAD	C2N-N1N-C1D	-2.25	114.12	119.14
2	B	340	NAD	C5A-C6A-N1A	-2.17	115.42	120.35
2	A	340	NAD	O4B-C1B-C2B	-2.13	103.81	106.93
2	B	340	NAD	C2N-C3N-C7N	2.02	125.32	119.46
2	A	340	NAD	C6N-N1N-C2N	2.00	123.80	121.97
2	B	340	NAD	C3D-C2D-C1D	2.00	103.99	100.98

There are no chirality outliers.

All (19) torsion outliers are listed below:

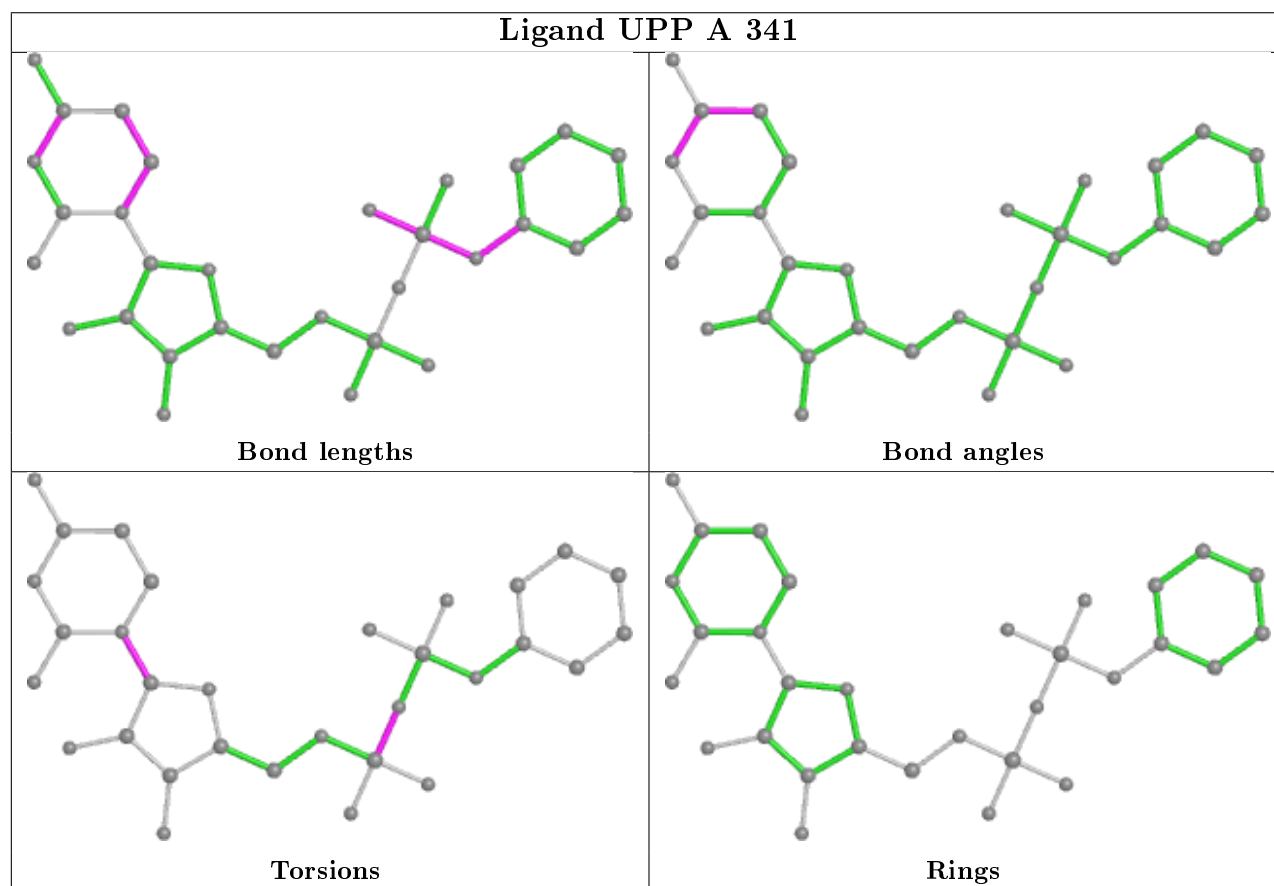
Mol	Chain	Res	Type	Atoms
3	B	341	UPP	O4'-C1B-N1-C6
3	B	341	UPP	PB-O3A-PA-O5'
3	A	341	UPP	C2B-C1B-N1-C6
3	A	341	UPP	O4'-C1B-N1-C6
3	A	341	UPP	PB-O3A-PA-O5'
2	A	340	NAD	C5B-O5B-PA-O1A
2	A	340	NAD	C4N-C3N-C7N-N7N
2	A	340	NAD	C4N-C3N-C7N-O7N
2	A	340	NAD	C5B-O5B-PA-O3
2	A	340	NAD	C5B-O5B-PA-O2A
2	B	340	NAD	C5D-O5D-PN-O3
2	A	340	NAD	C4B-C5B-O5B-PA
2	A	340	NAD	O4B-C4B-C5B-O5B
2	B	340	NAD	PA-O3-PN-O1N
2	B	340	NAD	PA-O3-PN-O2N
2	A	340	NAD	PA-O3-PN-O2N
3	B	341	UPP	C1'-O3B-PB-O1B
2	B	340	NAD	O4B-C4B-C5B-O5B
5	B	410	EDO	O1-C1-C2-O2

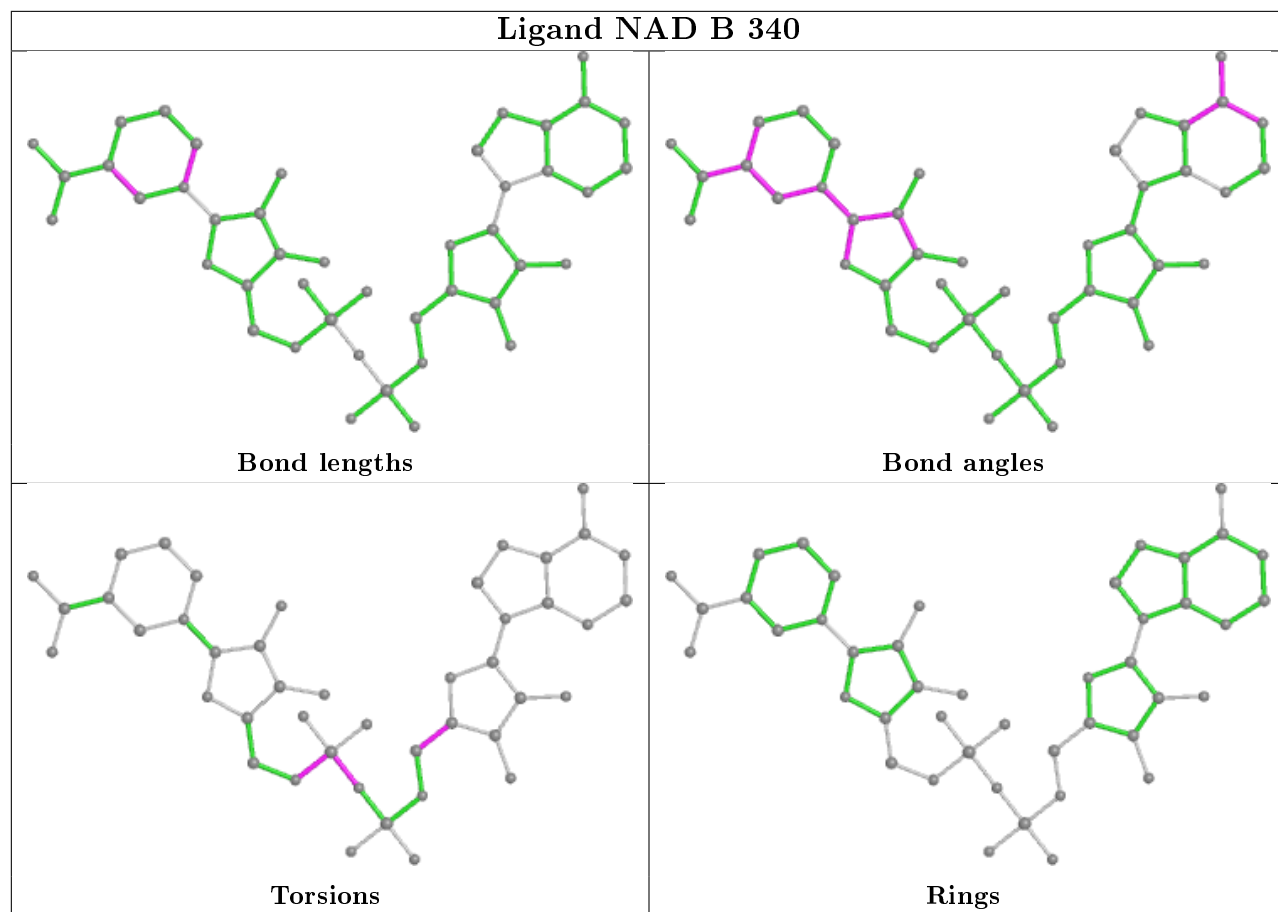
There are no ring outliers.

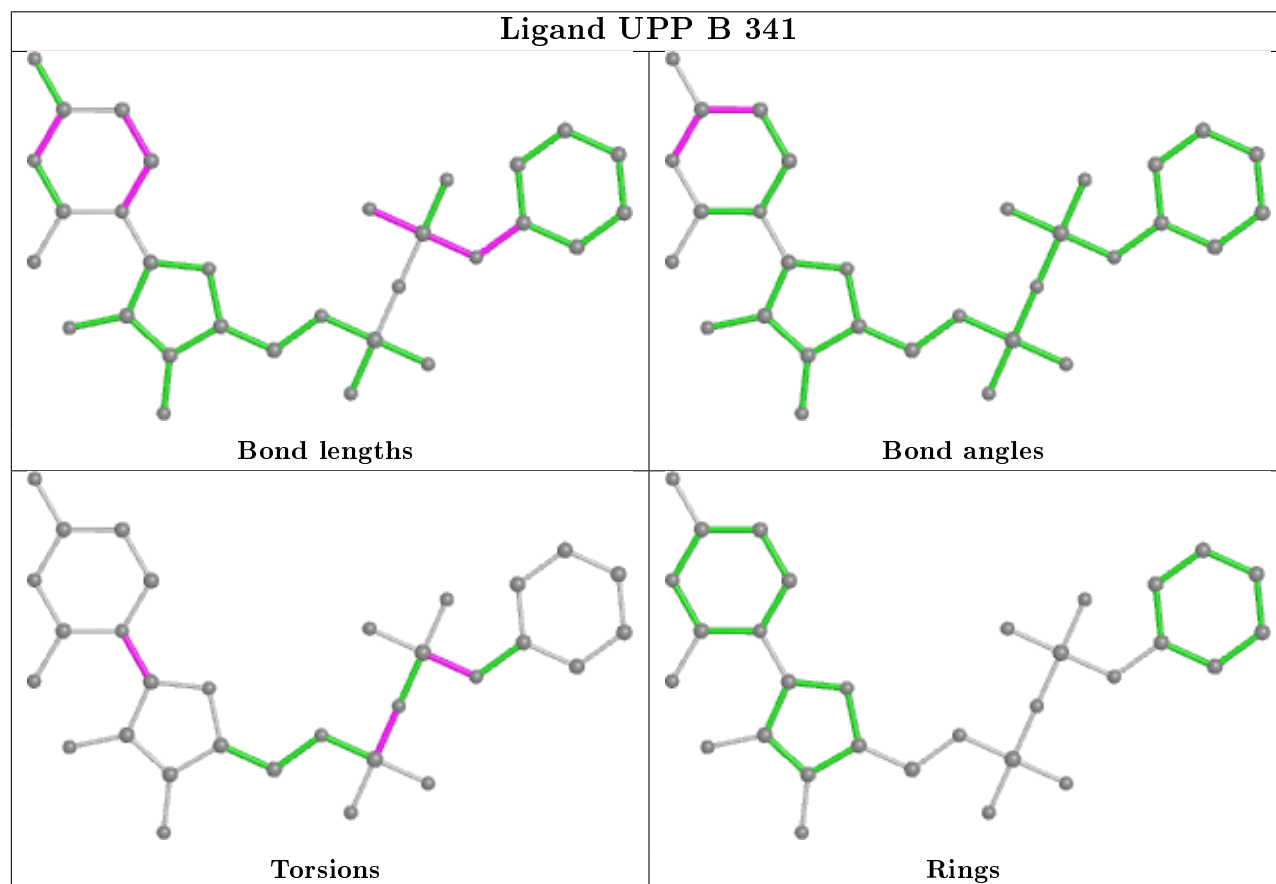
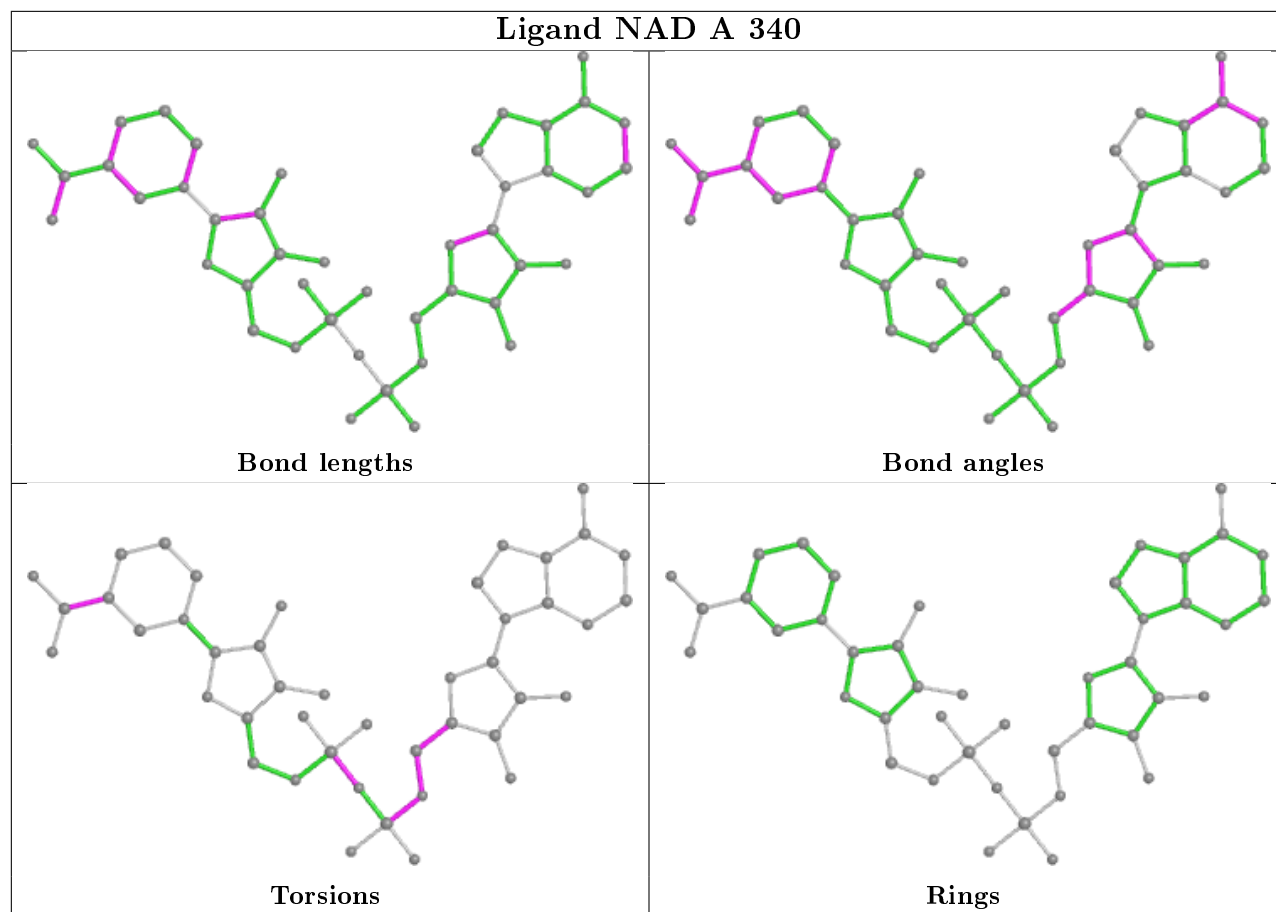
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	341	UPP	1	0
2	B	340	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 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

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.