



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 1P77 / pdb_00001p77
Title : CRYSTAL STRUCTURE OF SHIKIMATE DEHYDROGENASE (AROE)
FROM HAEMOPHILUS INFLUENZAE
Authors : Ye, S.; von Delft, F.; Brooun, A.; Knuth, M.W.; Swanson, R.V.; McRee, D.E.
Deposited on : 2003-04-30
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

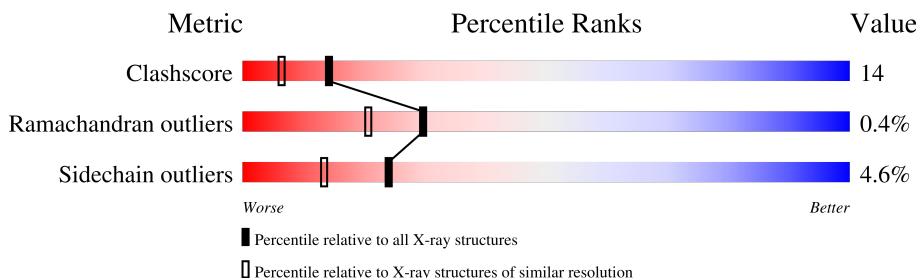
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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	272	

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
3	ATR	A	300	X	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2347 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 Shikimate 5-dehydrogenase.

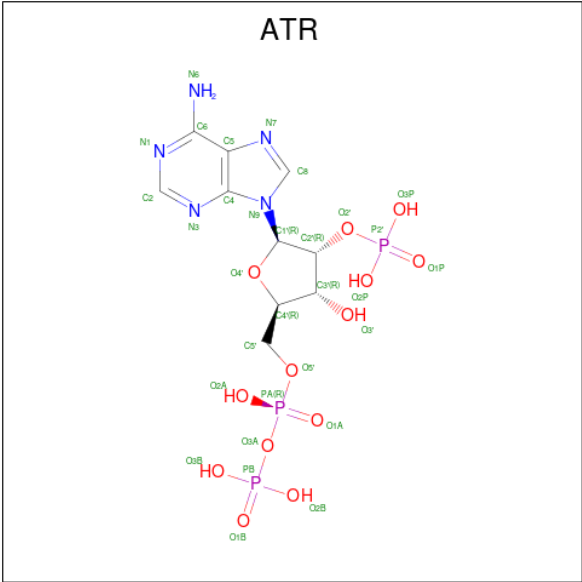
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2055	1312	345	388	10	0	0	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (CCD ID: ATR) (formula: C₁₀H₁₆N₅O₁₃P₃).



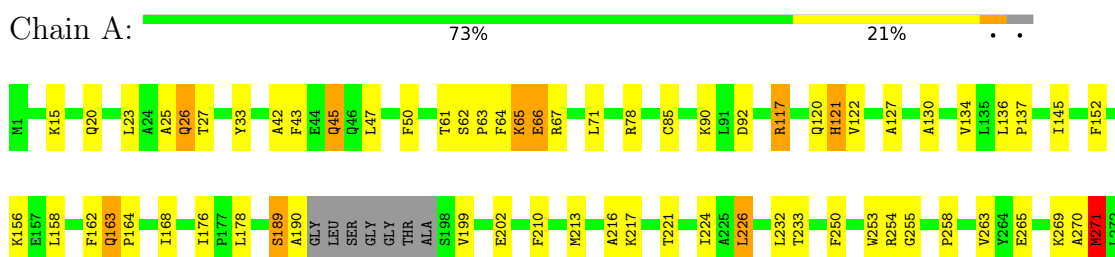
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	257	Total	O	0	0
			257	257		

Note EDS was not executed.

- Molecule 1: Shikimate 5-dehydrogenase



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.05Å 82.73Å 82.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	100.0 (20.00-1.95)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.203 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2347	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: ATR, ACT

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	0.95	4/2093 (0.2%)	1.30	24/2833 (0.8%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	C-O	-11.34	1.10	1.24
1	A	122	VAL	C-O	-10.57	1.12	1.24
1	A	27	THR	C-O	-5.88	1.15	1.23
1	A	26	GLN	N-CA	-5.45	1.39	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	HIS	ND1-CE1-NE2	-10.23	98.17	108.40
1	A	189	SER	CA-C-N	10.01	139.71	121.70
1	A	189	SER	C-N-CA	10.01	139.71	121.70
1	A	121	HIS	CE1-NE2-CD2	-9.27	99.73	109.00
1	A	65	LYS	CA-C-N	9.24	132.45	120.44
1	A	65	LYS	C-N-CA	9.24	132.45	120.44
1	A	270	ALA	CA-C-N	8.32	137.43	121.54
1	A	270	ALA	C-N-CA	8.32	137.43	121.54
1	A	152	PHE	N-CA-C	8.05	120.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	HIS	ND1-CG-CD2	-7.00	99.10	106.10
1	A	253	TRP	CA-C-N	6.66	133.45	121.92
1	A	253	TRP	C-N-CA	6.66	133.45	121.92
1	A	254	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	271	MET	N-CA-CB	6.31	121.16	110.49
1	A	199	VAL	N-CA-C	6.27	117.51	109.30
1	A	25	ALA	CA-C-N	6.22	128.91	120.38
1	A	25	ALA	C-N-CA	6.22	128.91	120.38
1	A	255	GLY	O-C-N	-6.19	114.78	122.34
1	A	121	HIS	CG-ND1-CE1	-6.14	98.87	109.30
1	A	254	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	65	LYS	N-CA-C	5.60	117.06	111.07
1	A	145	ILE	N-CA-C	5.59	116.00	108.17
1	A	176	ILE	N-CA-C	-5.13	103.92	108.95
1	A	66	GLU	N-CA-CB	5.10	117.41	110.01

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	271	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	HIS	Sidechain
1	A	189	SER	Mainchain

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	2055	0	2061	59	0
2	A	4	0	3	0	0
3	A	31	0	11	9	0
4	A	257	0	0	10	1
All	All	2347	0	2075	59	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 14.

All (59) 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:163:GLN:HE22	1:A:168:ILE:HG23	1.27	0.99
1:A:190:ALA:HA	3:A:300:ATR:C5	1.95	0.96
1:A:190:ALA:HB2	3:A:300:ATR:C4	1.96	0.96
1:A:92:ASP:O	4:A:369:HOH:O	1.91	0.87
1:A:163:GLN:NE2	1:A:168:ILE:HG23	1.92	0.83
1:A:226:LEU:C	1:A:226:LEU:HD23	2.06	0.81
1:A:66:GLU:HG3	4:A:558:HOH:O	1.82	0.79
1:A:163:GLN:HE21	1:A:163:GLN:HA	1.49	0.76
1:A:163:GLN:NE2	1:A:168:ILE:CG2	2.51	0.74
1:A:190:ALA:CA	3:A:300:ATR:C5	2.66	0.73
1:A:130:ALA:HB1	1:A:213:MET:HE1	1.70	0.73
1:A:265:GLU:OE2	4:A:325:HOH:O	2.08	0.72
1:A:190:ALA:HA	3:A:300:ATR:N7	2.05	0.71
1:A:130:ALA:HB1	1:A:213:MET:CE	2.21	0.70
1:A:190:ALA:CB	3:A:300:ATR:C5	2.69	0.70
1:A:156:LYS:O	1:A:156:LYS:HD3	1.92	0.70
1:A:163:GLN:HE22	1:A:168:ILE:CG2	2.02	0.70
1:A:23:LEU:HD23	1:A:263:VAL:HG21	1.77	0.66
1:A:190:ALA:C	4:A:456:HOH:O	2.38	0.66
1:A:117:ARG:HD3	1:A:117:ARG:H	1.60	0.65
1:A:210:PHE:CZ	1:A:232:LEU:HD13	2.32	0.64
1:A:117:ARG:O	1:A:120:GLN:HG3	1.98	0.63
1:A:26:GLN:NE2	1:A:263:VAL:HG23	2.12	0.63
1:A:226:LEU:C	1:A:226:LEU:CD2	2.74	0.60
1:A:163:GLN:NE2	4:A:309:HOH:O	2.35	0.59
1:A:190:ALA:HB2	3:A:300:ATR:C5	2.32	0.58
1:A:90:LYS:NZ	4:A:556:HOH:O	2.38	0.56
1:A:190:ALA:HB2	3:A:300:ATR:N3	2.21	0.56
1:A:20:GLN:HG3	1:A:33:TYR:CE1	2.42	0.55
1:A:190:ALA:CB	3:A:300:ATR:C4	2.76	0.54
1:A:226:LEU:HD23	1:A:226:LEU:O	2.08	0.54
1:A:190:ALA:O	4:A:456:HOH:O	2.19	0.53
1:A:217:LYS:C	1:A:217:LYS:HD2	2.34	0.53
1:A:163:GLN:N	1:A:164:PRO:CD	2.73	0.52
1:A:45:GLN:HE21	1:A:45:GLN:H	1.57	0.52
1:A:47:LEU:O	1:A:50:PHE:HB3	2.11	0.51
1:A:45:GLN:H	1:A:45:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:HB1	1:A:158:LEU:HD12	1.92	0.51
1:A:163:GLN:NE2	1:A:163:GLN:HA	2.24	0.49
1:A:47:LEU:HD23	1:A:71:LEU:HD12	1.95	0.49
1:A:26:GLN:NE2	1:A:263:VAL:CG2	2.76	0.49
1:A:26:GLN:HE22	1:A:263:VAL:HG23	1.77	0.48
1:A:221:THR:OG1	1:A:224:ILE:HG12	2.14	0.48
1:A:78:ARG:HD3	4:A:464:HOH:O	2.14	0.46
1:A:117:ARG:HD3	1:A:117:ARG:N	2.30	0.46
1:A:202:GLU:OE2	4:A:357:HOH:O	2.21	0.45
1:A:61:THR:HA	1:A:65:LYS:HE3	1.98	0.44
1:A:216:ALA:HA	4:A:548:HOH:O	2.19	0.43
1:A:190:ALA:HA	3:A:300:ATR:C6	2.48	0.43
1:A:15:LYS:HA	1:A:15:LYS:HE2	2.01	0.42
1:A:63:PRO:HD2	1:A:64:PHE:CE1	2.55	0.42
1:A:162:PHE:C	1:A:164:PRO:CD	2.92	0.42
1:A:162:PHE:C	1:A:164:PRO:HD2	2.45	0.42
1:A:42:ALA:O	1:A:43:PHE:C	2.61	0.42
1:A:163:GLN:NE2	1:A:168:ILE:HG22	2.31	0.41
1:A:134:VAL:O	1:A:137:PRO:HD2	2.19	0.41
1:A:210:PHE:CD2	1:A:210:PHE:N	2.88	0.41
1:A:136:LEU:HB3	1:A:137:PRO:HD3	2.03	0.41
1:A:250:PHE:CD1	1:A:258:PRO:HG3	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)
4:A:411:HOH:O	4:A:416:HOH:O[4_555]	2.12	0.08

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	261/272 (96%)	253 (97%)	7 (3%)	1 (0%)	30	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	MET

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	217/220 (99%)	207 (95%)	10 (5%)	24	13

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	62	SER
1	A	85	CYS
1	A	117	ARG
1	A	163	GLN
1	A	178	LEU
1	A	226	LEU
1	A	233	THR
1	A	269	LYS
1	A	271	MET

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	45	GLN
1	A	70	GLN
1	A	77	GLN
1	A	114	ASN
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	163	GLN
1	A	186	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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$
2	ACT	A	301	-	3,3,3	0.27	0	3,3,3	2.11	1 (33%)
3	ATR	A	300	-	32,33,33	2.05	9 (28%)	50,52,52	2.40	16 (32%)

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	ATR	A	300	-	1/1/7/7	4/21/37/37	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	ATR	PB-O1B	6.11	1.69	1.50
3	A	300	ATR	P2'-O3P	3.97	1.69	1.54
3	A	300	ATR	P2'-O2P	3.57	1.68	1.54
3	A	300	ATR	PA-O2A	3.49	1.71	1.55
3	A	300	ATR	C5-C4	3.44	1.45	1.39
3	A	300	ATR	C5-N7	-2.94	1.33	1.39
3	A	300	ATR	C5-C6	2.87	1.49	1.41
3	A	300	ATR	C4-N9	-2.57	1.32	1.37
3	A	300	ATR	PA-O3A	2.46	1.62	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	ATR	O3'-C3'-C2'	-5.83	94.87	111.19
3	A	300	ATR	C2'-C1'-N9	5.61	122.98	113.75
3	A	300	ATR	C5-C4-N3	-4.72	120.22	126.72
3	A	300	ATR	N3-C4-N9	4.67	135.10	127.17
3	A	300	ATR	C4-N9-C1'	-4.58	115.93	126.63
3	A	300	ATR	O4'-C1'-N9	4.53	116.80	108.09
3	A	300	ATR	O2'-C2'-C3'	4.47	127.70	111.68
3	A	300	ATR	C4-N9-C8	4.03	109.97	105.74
3	A	300	ATR	C2-N3-C4	3.49	120.35	111.83
3	A	300	ATR	N3-C2-N1	-3.42	123.40	128.58
3	A	300	ATR	C1'-N9-C8	3.06	133.88	127.09
2	A	301	ACT	OXT-C-CH3	2.90	127.20	115.05
3	A	300	ATR	N9-C8-N7	-2.86	109.87	113.94
3	A	300	ATR	P2'-O2'-C2'	2.41	129.87	123.43
3	A	300	ATR	C3'-C2'-C1'	2.09	106.80	102.81
3	A	300	ATR	C2-N1-C6	2.03	122.07	118.73
3	A	300	ATR	O2B-PB-O1B	-2.03	102.94	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	300	ATR	C2'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	ATR	C5'-O5'-PA-O2A
3	A	300	ATR	C5'-O5'-PA-O3A

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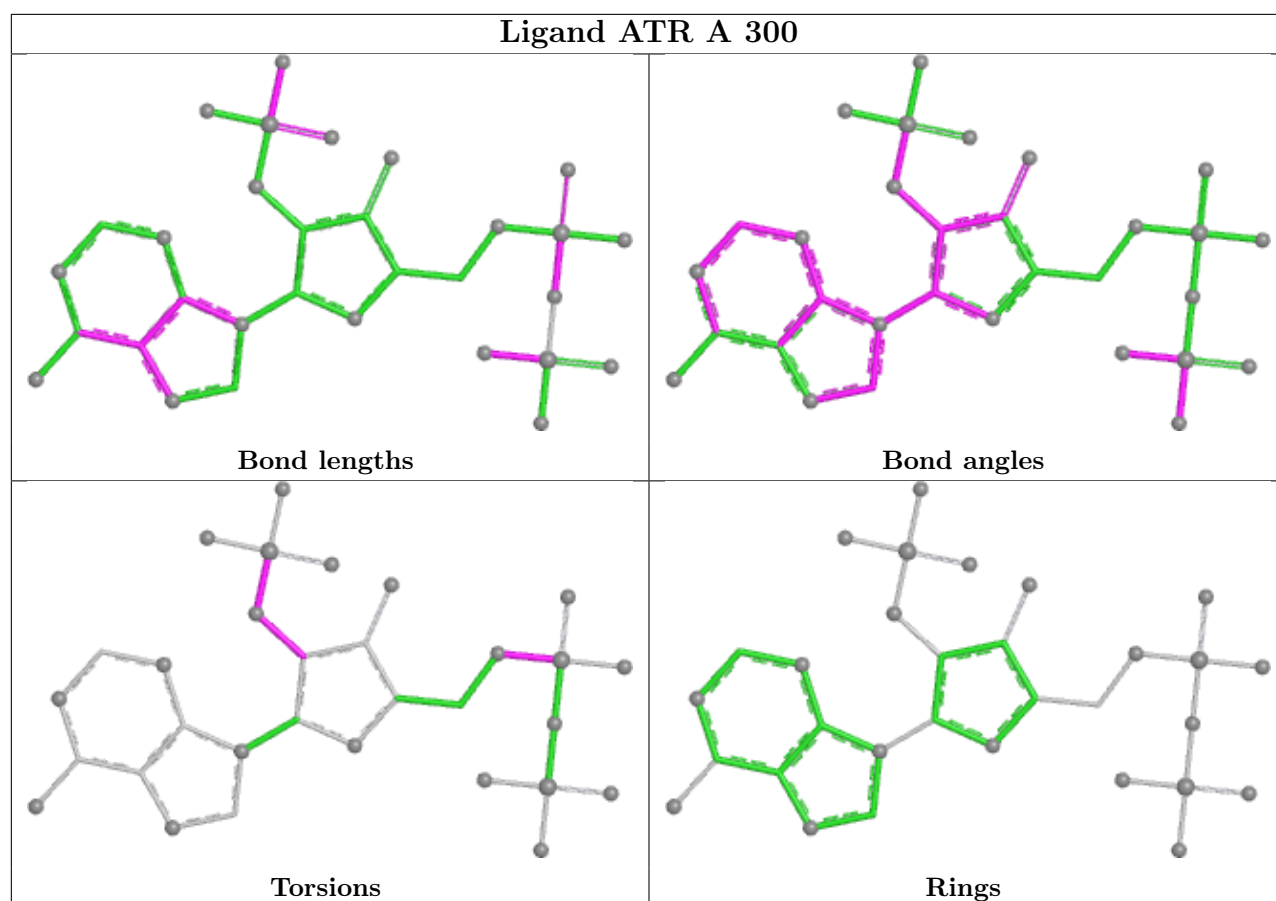
Mol	Chain	Res	Type	Atoms
3	A	300	ATR	C3'-C2'-O2'-P2'
3	A	300	ATR	C2'-O2'-P2'-O1P

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	ATR	9	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.