



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 10:24 AM EST

PDB ID : 1ADF
Title : CRYSTALLOGRAPHIC STUDIES OF TWO ALCOHOL DEHYDROGENASE-BOUND ANALOGS OF THIAZOLE-4-CARBOXAMIDE ADENINE DINUCLEOTIDE (TAD), THE ACTIVE ANABOLITE OF THE ANTITUMOR AGENT TIAZOFURIN
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Deposited on : unknown
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

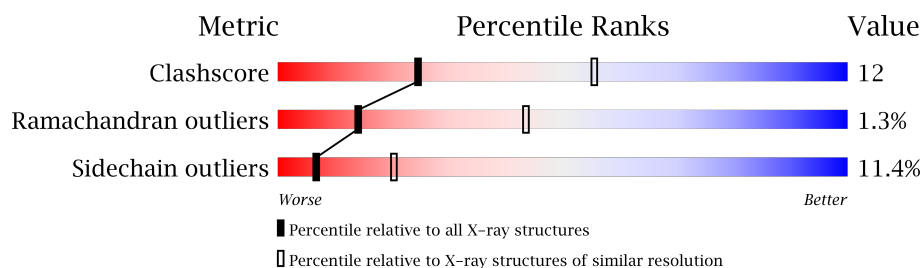
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3547 atoms, of which 683 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.

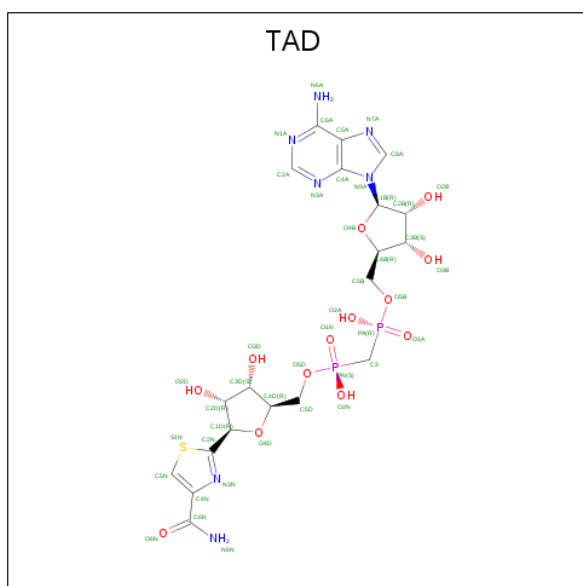
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	H	N	O	S	0	0	0
			3392	1769	607	472	521	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).



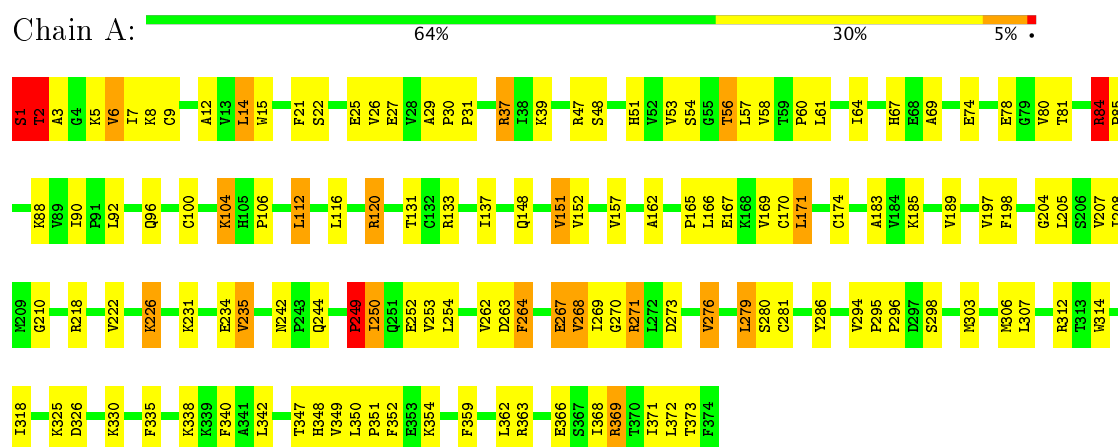
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	34	Total	H	O	0	0
			102	68	34		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ALCOHOL 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	56.30Å 75.40Å 181.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3547	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: TAD, ZN

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	0.97	1/2837 (0.0%)	1.72	41/3834 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	LYS	CD-CE	5.43	1.64	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	A	363	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	15	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	218	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	47	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	369	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	314	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	A	37	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	15	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	303	MET	CG-SD-CE	-7.29	88.53	100.20
1	A	120	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	78	GLU	CA-CB-CG	7.20	129.23	113.40
1	A	306	MET	CA-CB-CG	-7.00	101.40	113.30
1	A	80	VAL	CA-C-N	-6.96	101.89	117.20
1	A	1	SER	N-CA-C	-6.71	92.87	111.00
1	A	314	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	363	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	37	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	369	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	235	VAL	N-CA-CB	-6.35	97.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	263	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	306	MET	CG-SD-CE	-6.16	90.35	100.20
1	A	270	GLY	O-C-N	-6.12	112.91	122.70
1	A	120	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	133	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	276	VAL	CA-CB-CG2	-5.94	101.99	110.90
1	A	207	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	A	235	VAL	CB-CA-C	5.79	122.39	111.40
1	A	58	VAL	CG1-CB-CG2	-5.77	101.66	110.90
1	A	286	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	6	VAL	CA-CB-CG2	-5.64	102.44	110.90
1	A	235	VAL	CA-CB-CG2	-5.51	102.64	110.90
1	A	270	GLY	CA-C-N	5.46	129.21	117.20
1	A	2	THR	N-CA-C	5.43	125.68	111.00
1	A	15	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	A	84	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	151	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	A	56	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	314	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	264	PHE	CA-C-N	5.00	128.21	117.20

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	2785	607	2848	67	0
2	A	2	0	0	0	0
3	A	43	8	25	5	0
4	A	34	68	0	2	0
All	All	2864	683	2873	70	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 (70) 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:352:PHE:HA	1:A:372:LEU:HG	1.66	0.76
1:A:249:PRO:HB2	1:A:252:GLU:HG3	1.68	0.75
1:A:6:VAL:HG22	1:A:29:ALA:HA	1.69	0.74
1:A:347:THR:HG21	1:A:368:ILE:H	1.50	0.73
1:A:347:THR:HG21	1:A:368:ILE:N	2.05	0.70
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.73	0.70
1:A:171:LEU:HD11	1:A:369:ARG:HG2	1.75	0.68
3:A:378:TAD:O1A	3:A:378:TAD:H4D	1.98	0.64
3:A:378:TAD:H4D	3:A:378:TAD:PA	2.39	0.62
1:A:88:LYS:HD3	1:A:166:LEU:HD21	1.83	0.61
1:A:31:PRO:HG3	1:A:37:ARG:HB2	1.83	0.59
1:A:347:THR:HG23	1:A:348:HIS:ND1	2.17	0.59
1:A:165:PRO:HG2	1:A:335:PHE:HE2	1.67	0.59
1:A:269:ILE:HG21	1:A:271:ARG:HD3	1.83	0.58
1:A:250:ILE:HD12	1:A:250:ILE:H	1.69	0.58
1:A:84:ARG:HD3	1:A:85:PRO:HD2	1.87	0.56
1:A:269:ILE:O	3:A:378:TAD:H1D	2.05	0.56
1:A:88:LYS:HE3	1:A:162:ALA:O	2.05	0.56
1:A:171:LEU:HD23	1:A:342:LEU:HB3	1.87	0.56
1:A:198:PHE:HB2	1:A:267:GLU:HA	1.89	0.54
1:A:250:ILE:HA	1:A:253:VAL:HG22	1.90	0.53
1:A:8:LYS:HA	1:A:26:VAL:O	2.09	0.53
1:A:351:PRO:HG2	1:A:354:LYS:HG2	1.91	0.52
1:A:14:LEU:HD21	1:A:53:VAL:HG13	1.92	0.51
1:A:170:CYS:SG	1:A:371:ILE:HD12	2.51	0.50
1:A:231:LYS:O	1:A:234:GLU:HB3	2.12	0.49
1:A:226:LYS:NZ	1:A:242:ASN:ND2	2.61	0.49
1:A:226:LYS:NZ	1:A:242:ASN:HD22	2.11	0.48
3:A:378:TAD:H51N	3:A:378:TAD:H31	1.70	0.48
1:A:14:LEU:HD11	1:A:53:VAL:HG22	1.96	0.48
1:A:326:ASP:O	1:A:330:LYS:HE2	2.13	0.47
1:A:8:LYS:HG2	1:A:25:GLU:HG3	1.97	0.47
1:A:96:GLN:HB3	1:A:325:LYS:HG3	1.97	0.47
1:A:204:GLY:CA	1:A:268:VAL:HG21	2.45	0.46
1:A:51:HIS:HB3	1:A:57:LEU:HB2	1.98	0.46
1:A:12:ALA:HA	1:A:22:SER:O	2.16	0.46
1:A:262:VAL:HG22	1:A:281:CYS:O	2.16	0.45
1:A:347:THR:HG22	1:A:369:ARG:O	2.17	0.45
1:A:189:VAL:HA	1:A:264:PHE:CE2	2.52	0.45
1:A:269:ILE:HA	3:A:378:TAD:H52A	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:HZ3	1:A:242:ASN:HD22	1.65	0.44
1:A:359:PHE:O	1:A:362:LEU:HB3	2.18	0.44
1:A:37:ARG:HG3	1:A:151:VAL:HG22	1.99	0.44
1:A:88:LYS:CD	1:A:166:LEU:HD21	2.46	0.44
1:A:1:SER:O	1:A:3:ALA:N	2.50	0.44
1:A:48:SER:HB2	1:A:67:HIS:HE1	1.83	0.43
1:A:279:LEU:HD22	1:A:312:ARG:HD3	2.00	0.43
1:A:61:LEU:HD12	4:A:390:HOH:O	2.18	0.43
1:A:335:PHE:CE1	1:A:342:LEU:HD12	2.53	0.43
1:A:30:PRO:HA	1:A:31:PRO:HD3	1.83	0.42
1:A:350:LEU:HD13	1:A:354:LYS:HB2	2.01	0.42
1:A:197:VAL:HG21	1:A:208:ILE:HG12	2.02	0.42
1:A:7:ILE:O	1:A:27:GLU:HA	2.19	0.42
1:A:92:LEU:HD11	1:A:325:LYS:HG2	2.00	0.42
1:A:56:THR:CG2	1:A:296:PRO:HD2	2.50	0.42
1:A:269:ILE:CG2	1:A:271:ARG:HD3	2.50	0.42
1:A:9:CYS:HB2	1:A:148:GLN:HB2	2.02	0.42
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.71	0.42
1:A:64:ILE:HG13	1:A:137:ILE:HG21	2.02	0.41
1:A:60:PRO:HG2	1:A:120:ARG:O	2.19	0.41
1:A:12:ALA:HB1	1:A:21:PHE:HB3	2.02	0.41
1:A:307:LEU:O	1:A:312:ARG:HD2	2.21	0.41
1:A:100:CYS:O	1:A:104:LYS:HG2	2.21	0.41
1:A:166:LEU:HA	1:A:169:VAL:HG22	2.03	0.41
1:A:37:ARG:HD2	1:A:74:GLU:OE1	2.21	0.41
1:A:69:ALA:O	1:A:90:ILE:HG23	2.20	0.41
1:A:1:SER:HB2	1:A:2:THR:H	1.71	0.41
1:A:51:HIS:HD2	4:A:384:HOH:O	2.02	0.41
1:A:152:VAL:HG21	1:A:157:VAL:HB	2.01	0.41
1:A:183:ALA:HB3	1:A:210:GLY:HA3	2.02	0.41

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	372/374 (100%)	336 (90%)	31 (8%)	5 (1%)	14	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	112	LEU
1	A	174	CYS
1	A	249	PRO
1	A	106	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	308/308 (100%)	273 (89%)	35 (11%)	7	20

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	14	LEU
1	A	39	LYS
1	A	54	SER
1	A	81	THR
1	A	84	ARG
1	A	104	LYS
1	A	116	LEU
1	A	131	THR
1	A	167	GLU
1	A	171	LEU
1	A	185	LYS
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	222	VAL
1	A	226	LYS
1	A	235	VAL
1	A	249	PRO
1	A	250	ILE
1	A	254	LEU
1	A	267	GLU
1	A	268	VAL
1	A	271	ARG
1	A	273	ASP
1	A	276	VAL
1	A	279	LEU
1	A	280	SER
1	A	294	VAL
1	A	295	PRO
1	A	298	SER
1	A	318	ILE
1	A	340	PHE
1	A	349	VAL
1	A	366	GLU
1	A	373	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	242	ASN
1	A	244	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	TAD	A	378	-	39,47,47	1.53	5 (12%)	39,72,72	2.32	13 (33%)

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	TAD	A	378	-	-	0/18/62/62	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	378	TAD	PA-O2A	-2.61	1.50	1.56
3	A	378	TAD	PN-O2N	-2.14	1.51	1.56
3	A	378	TAD	C5N-S1N	3.11	1.75	1.70
3	A	378	TAD	PA-O5B	3.89	1.61	1.57
3	A	378	TAD	PN-O5D	5.85	1.64	1.57

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	378	TAD	N3A-C2A-N1A	-6.64	123.07	128.86
3	A	378	TAD	C4N-C6N-N6N	-4.45	111.80	116.23
3	A	378	TAD	C4D-O4D-C1D	-2.68	106.38	109.48
3	A	378	TAD	O3D-C3D-C2D	-2.47	103.93	111.83
3	A	378	TAD	O2A-PA-C3	-2.23	97.05	106.54
3	A	378	TAD	C2A-N1A-C6A	2.01	122.28	118.77
3	A	378	TAD	O2A-PA-O1A	2.12	117.18	110.09
3	A	378	TAD	O4D-C4D-C3D	2.14	109.42	105.17
3	A	378	TAD	O4D-C1D-C2D	2.50	108.47	104.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	378	TAD	N6A-C6A-N1A	2.88	124.47	118.77
3	A	378	TAD	C4A-C5A-N7A	3.48	112.77	109.41
3	A	378	TAD	O1A-PA-C3	4.45	119.98	108.97
3	A	378	TAD	O6N-C6N-C4N	6.84	125.46	119.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	378	TAD	5	0

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.