



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 AM UTC

PDB ID : 1ADF / pdb_00001adf
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 : 1993-10-18
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

<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

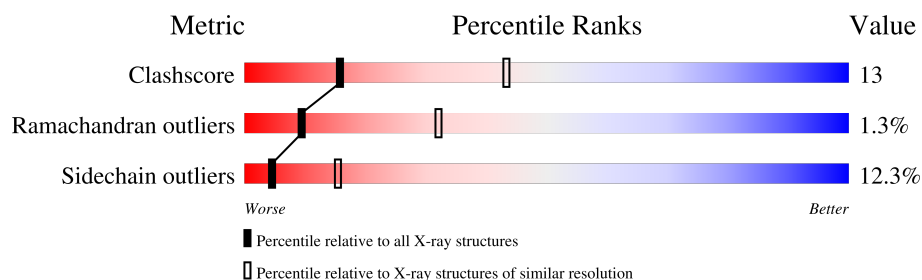
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	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.

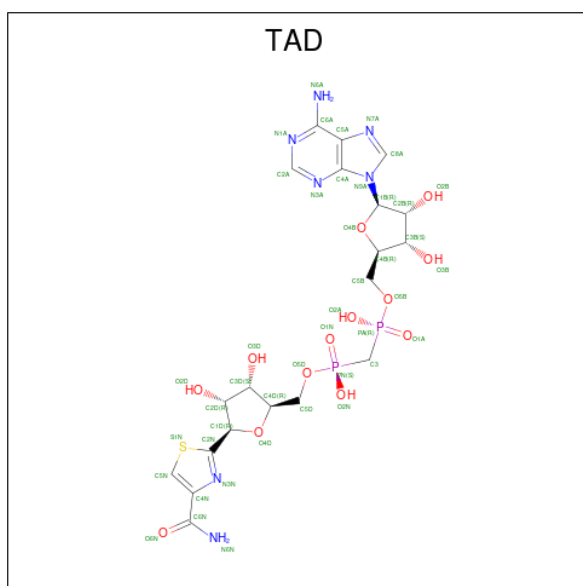
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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 (CCD ID: 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 (CCD ID: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			51	20	8	7	13	2	1		

- Molecule 4 is water.

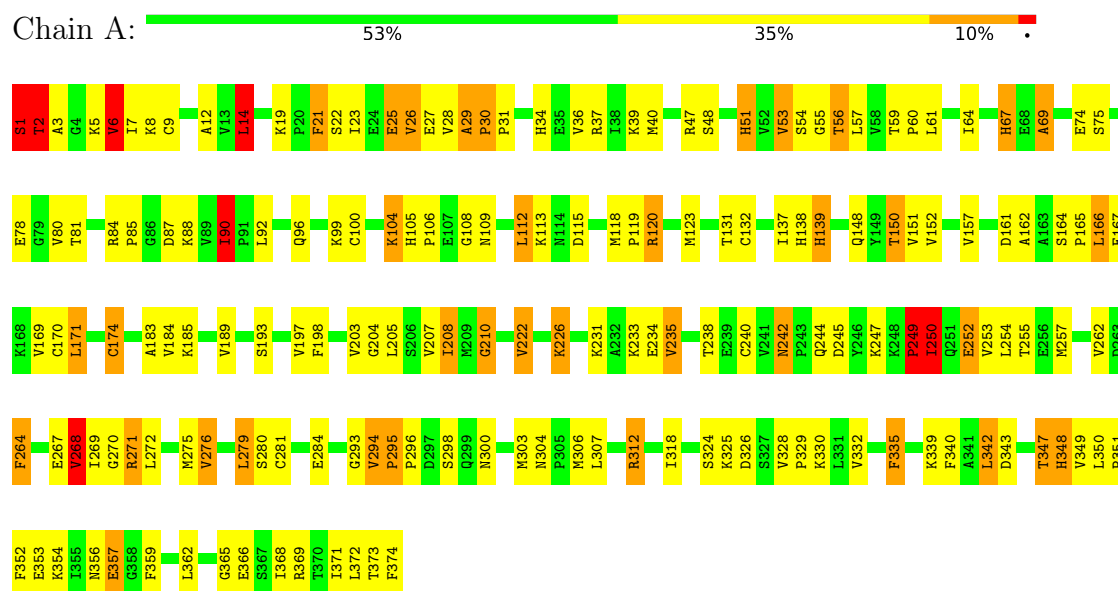
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	34	Total	H	O	0	0
			102	68	34		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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

5.1 Standard geometry

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	1.27	16/2837 (0.6%)	2.11	110/3834 (2.9%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ILE	CA-CB	9.53	1.61	1.54
1	A	294	VAL	CA-CB	8.06	1.64	1.54
1	A	105	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	139	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	222	VAL	CA-CB	6.48	1.62	1.54
1	A	332	VAL	CA-CB	6.42	1.62	1.54
1	A	268	VAL	CA-CB	6.39	1.62	1.54
1	A	34	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	67	HIS	CG-ND1	-6.04	1.31	1.38
1	A	348	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	51	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	138	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	21	PHE	CA-CB	-5.26	1.45	1.53
1	A	329	PRO	CA-CB	-5.12	1.45	1.53
1	A	348	HIS	CG-ND1	-5.05	1.32	1.38
1	A	28	VAL	CA-CB	5.01	1.60	1.53

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	VAL	CA-C-O	9.49	129.85	120.27
1	A	87	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	115	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	270	GLY	O-C-N	-7.59	112.91	122.32
1	A	78	GLU	CA-CB-CG	7.57	129.23	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLY	O-C-N	7.48	130.02	123.36
1	A	242	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	347	THR	N-CA-CB	-7.31	101.18	110.90
1	A	276	VAL	CA-C-O	-7.22	113.19	120.85
1	A	300	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	A	109	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	A	34	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	2	THR	N-CA-C	6.98	125.68	110.80
1	A	51	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	23	ILE	N-CA-C	-6.96	99.70	108.89
1	A	245	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	56	THR	CA-CB-OG1	-6.83	99.35	109.60
1	A	284	GLU	N-CA-C	6.80	119.27	111.11
1	A	118	MET	CA-C-O	-6.76	113.38	121.22
1	A	272	LEU	N-CA-C	6.68	118.36	111.14
1	A	51	HIS	CB-CG-ND1	6.64	132.65	122.70
1	A	113	LYS	N-CA-C	-6.54	103.90	112.41
1	A	304	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	99	LYS	N-CA-C	6.53	121.40	113.17
1	A	250	ILE	N-CA-C	-6.52	104.67	111.58
1	A	374	PHE	CA-CB-CG	-6.50	107.30	113.80
1	A	1	SER	N-CA-C	-6.47	92.87	111.00
1	A	184	VAL	N-CA-C	6.39	117.02	110.82
1	A	161	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	306	MET	CA-CB-CG	-6.35	101.40	114.10
1	A	75	SER	CA-CB-OG	6.32	123.73	111.10
1	A	109	ASN	CB-CG-ND2	6.28	125.82	116.40
1	A	99	LYS	CA-C-N	-6.24	111.73	123.27
1	A	99	LYS	C-N-CA	-6.24	111.73	123.27
1	A	69	ALA	N-CA-C	6.20	118.27	108.79
1	A	235	VAL	N-CA-CB	-6.18	97.53	111.87
1	A	30	PRO	CA-C-N	6.17	126.49	119.83
1	A	30	PRO	C-N-CA	6.17	126.49	119.83
1	A	252	GLU	N-CA-C	-5.98	104.39	111.03
1	A	69	ALA	CA-C-O	-5.88	114.94	121.23
1	A	193	SER	N-CA-C	5.85	117.88	110.33
1	A	166	LEU	N-CA-C	5.84	119.88	112.87
1	A	55	GLY	N-CA-C	-5.84	107.74	114.69
1	A	105	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	A	108	GLY	CA-C-O	-5.82	116.06	121.18
1	A	247	LYS	N-CA-C	-5.82	106.31	113.41
1	A	51	HIS	CA-C-N	5.79	128.39	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	HIS	C-N-CA	5.79	128.39	120.46
1	A	132	CYS	N-CA-C	-5.78	97.90	108.02
1	A	138	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	30	PRO	O-C-N	5.76	123.86	121.15
1	A	356	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	328	VAL	CA-C-N	5.73	125.20	119.24
1	A	328	VAL	C-N-CA	5.73	125.20	119.24
1	A	109	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	365	GLY	CA-C-N	-5.71	113.21	122.34
1	A	365	GLY	C-N-CA	-5.71	113.21	122.34
1	A	347	THR	CB-CA-C	5.66	118.53	109.02
1	A	264	PHE	O-C-N	-5.66	116.03	123.21
1	A	294	VAL	CA-C-O	5.65	127.53	119.95
1	A	120	ARG	N-CA-C	-5.65	106.51	113.41
1	A	303	MET	CG-SD-CE	-5.62	88.53	100.90
1	A	295	PRO	CA-C-N	5.58	125.20	119.56
1	A	295	PRO	C-N-CA	5.58	125.20	119.56
1	A	304	ASN	CA-C-N	5.58	125.94	119.47
1	A	304	ASN	C-N-CA	5.58	125.94	119.47
1	A	119	PRO	O-C-N	-5.53	116.65	123.01
1	A	235	VAL	O-C-N	-5.51	115.73	122.12
1	A	164	SER	CA-CB-OG	5.47	122.05	111.10
1	A	56	THR	CA-CB-CG2	5.45	119.76	110.50
1	A	343	ASP	N-CA-C	5.45	121.02	113.45
1	A	357	GLU	N-CA-C	-5.43	105.44	111.36
1	A	365	GLY	CA-C-O	-5.39	113.86	119.20
1	A	29	ALA	CA-C-N	5.37	123.53	119.66
1	A	29	ALA	C-N-CA	5.37	123.53	119.66
1	A	203	VAL	CB-CA-C	-5.37	103.41	112.16
1	A	339	LYS	CG-CD-CE	-5.34	99.01	111.30
1	A	14	LEU	N-CA-C	-5.32	99.10	108.20
1	A	324	SER	N-CA-C	5.32	116.76	111.07
1	A	335	PHE	N-CA-C	-5.32	105.49	111.28
1	A	2	THR	N-CA-CB	-5.30	101.54	110.49
1	A	255	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	300	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	342	LEU	CD1-CG-CD2	-5.29	99.16	110.80
1	A	249	PRO	CA-N-CD	-5.28	104.61	112.00
1	A	108	GLY	N-CA-C	-5.24	102.34	111.62
1	A	208	ILE	O-C-N	5.23	127.02	121.89
1	A	47	ARG	O-C-N	-5.20	116.13	122.22
1	A	347	THR	N-CA-C	-5.20	107.61	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	CYS	CA-C-O	-5.18	113.91	120.28
1	A	303	MET	N-CA-CB	-5.15	101.95	111.53
1	A	233	LYS	O-C-N	5.15	127.37	122.07
1	A	207	VAL	N-CA-C	-5.12	105.50	110.42
1	A	150	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	210	GLY	N-CA-C	-5.11	106.57	112.50
1	A	6	VAL	CA-C-O	-5.11	116.47	121.58
1	A	203	VAL	CA-C-N	5.10	125.61	120.00
1	A	203	VAL	C-N-CA	5.10	125.61	120.00
1	A	312	ARG	N-CA-C	5.10	117.63	110.23
1	A	184	VAL	N-CA-CB	-5.10	103.17	110.52
1	A	295	PRO	CB-CA-C	5.08	117.12	110.92
1	A	25	GLU	N-CA-C	-5.07	101.70	109.76
1	A	59	THR	N-CA-C	-5.07	102.37	108.25
1	A	255	THR	CA-CB-CG2	5.05	119.09	110.50
1	A	332	VAL	N-CA-C	-5.05	105.78	110.53
1	A	53	VAL	CA-C-O	-5.04	115.51	120.85
1	A	36	VAL	N-CA-C	-5.03	100.66	108.81
1	A	174	CYS	CA-C-N	5.03	125.42	119.94
1	A	174	CYS	C-N-CA	5.03	125.42	119.94
1	A	284	GLU	N-CA-CB	-5.01	102.47	109.94

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	73	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	76	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 13.

All (76) 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:H4D	3:A:378:TAD:O1A	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:H	1:A:250:ILE:HD12	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:226:LYS:HZ3	1:A:242:ASN:HD22	1.60	0.49
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:123:MET:HE3	1:A:139:HIS:ND1	2.29	0.48
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:40:MET:HE3	1:A:150:THR:HG22	1.96	0.47
1:A:8:LYS:HG2	1:A:25:GLU:HG3	1.97	0.47
1:A:271:ARG:O	1:A:275:MET:HE3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:37:ARG:HG3	1:A:151:VAL:HG22	1.99	0.44
1:A:359:PHE:O	1:A:362:LEU:HB3	2.18	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:271:ARG:C	1:A:275:MET:HE3	2.43	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:257:MET:HB3	1:A:257:MET:HE2	1.85	0.42
1:A:40:MET:HE3	1:A:150:THR:CG2	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:12:ALA:HB1	1:A:21:PHE:HB3	2.02	0.41
1:A:60:PRO:HG2	1:A:120:ARG:O	2.19	0.41
1:A:307:LEU:O	1:A:312:ARG:HD2	2.21	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: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: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%)	9	32

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%)	270 (88%)	38 (12%)	4	15

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	6	VAL
1	A	14	LEU
1	A	19	LYS
1	A	26	VAL

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Mol	Chain	Res	Type
1	A	39	LYS
1	A	54	SER
1	A	81	THR
1	A	90	ILE
1	A	104	LYS
1	A	131	THR
1	A	167	GLU
1	A	171	LEU
1	A	185	LYS
1	A	205	LEU
1	A	222	VAL
1	A	226	LYS
1	A	235	VAL
1	A	238	THR
1	A	249	PRO
1	A	250	ILE
1	A	254	LEU
1	A	268	VAL
1	A	271	ARG
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	353	GLU
1	A	357	GLU
1	A	366	GLU
1	A	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	242	ASN
1	A	244	GLN
1	A	259	ASN
1	A	299	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 oligosaccharides 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	-	42,47,47	1.10	5 (11%)	62,72,72	2.59	25 (40%)

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	-	-	11/30/62/62	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	C5A-N7A	-3.26	1.33	1.39
3	A	378	TAD	PA-O2A	-2.62	1.50	1.56
3	A	378	TAD	C4N-N3N	-2.24	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	378	TAD	PN-O2N	-2.15	1.51	1.56
3	A	378	TAD	C2N-S1N	2.07	1.78	1.73

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	378	TAD	C5A-C4A-N3A	-6.81	117.35	126.72
3	A	378	TAD	N3A-C4A-N9A	6.62	138.43	127.17
3	A	378	TAD	O6N-C6N-C4N	5.43	125.46	120.25
3	A	378	TAD	C6A-C5A-C4A	5.31	124.42	117.18
3	A	378	TAD	C5N-S1N-C2N	-5.22	83.35	89.52
3	A	378	TAD	C6A-C5A-N7A	-4.88	122.68	132.09
3	A	378	TAD	C4N-C6N-N6N	-4.40	111.80	116.28
3	A	378	TAD	C4N-N3N-C2N	-4.30	106.21	110.65
3	A	378	TAD	C1D-C2N-N3N	-4.27	118.72	124.48
3	A	378	TAD	S1N-C2N-N3N	4.22	119.69	114.19
3	A	378	TAD	O1A-PA-C3	4.15	119.98	109.05
3	A	378	TAD	N3A-C2A-N1A	-3.64	123.07	128.58
3	A	378	TAD	C6N-C4N-N3N	-3.04	114.67	121.42
3	A	378	TAD	C2A-N3A-C4A	2.81	118.69	111.83
3	A	378	TAD	N6A-C6A-N1A	2.74	124.47	118.38
3	A	378	TAD	O3D-C3D-C2D	-2.46	103.93	111.82
3	A	378	TAD	O4D-C1D-C2D	2.40	108.47	105.15
3	A	378	TAD	O2A-PA-C3	-2.34	97.05	106.73
3	A	378	TAD	C4A-N9A-C8A	2.25	108.10	105.74
3	A	378	TAD	C2D-C1D-C2N	-2.23	110.72	114.94
3	A	378	TAD	O2A-PA-O1A	2.22	117.18	109.95
3	A	378	TAD	C2A-N1A-C6A	2.16	122.28	118.73
3	A	378	TAD	O4D-C4D-C3D	2.15	109.42	105.15
3	A	378	TAD	C4N-C5N-S1N	2.14	112.72	110.24
3	A	378	TAD	C5N-C4N-C6N	2.13	127.37	123.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	378	TAD	PN-C3-PA-O1A
3	A	378	TAD	PN-C3-PA-O2A
3	A	378	TAD	PN-C3-PA-O5B
3	A	378	TAD	C5D-O5D-PN-C3
3	A	378	TAD	C5D-O5D-PN-O1N
3	A	378	TAD	C4D-C5D-O5D-PN

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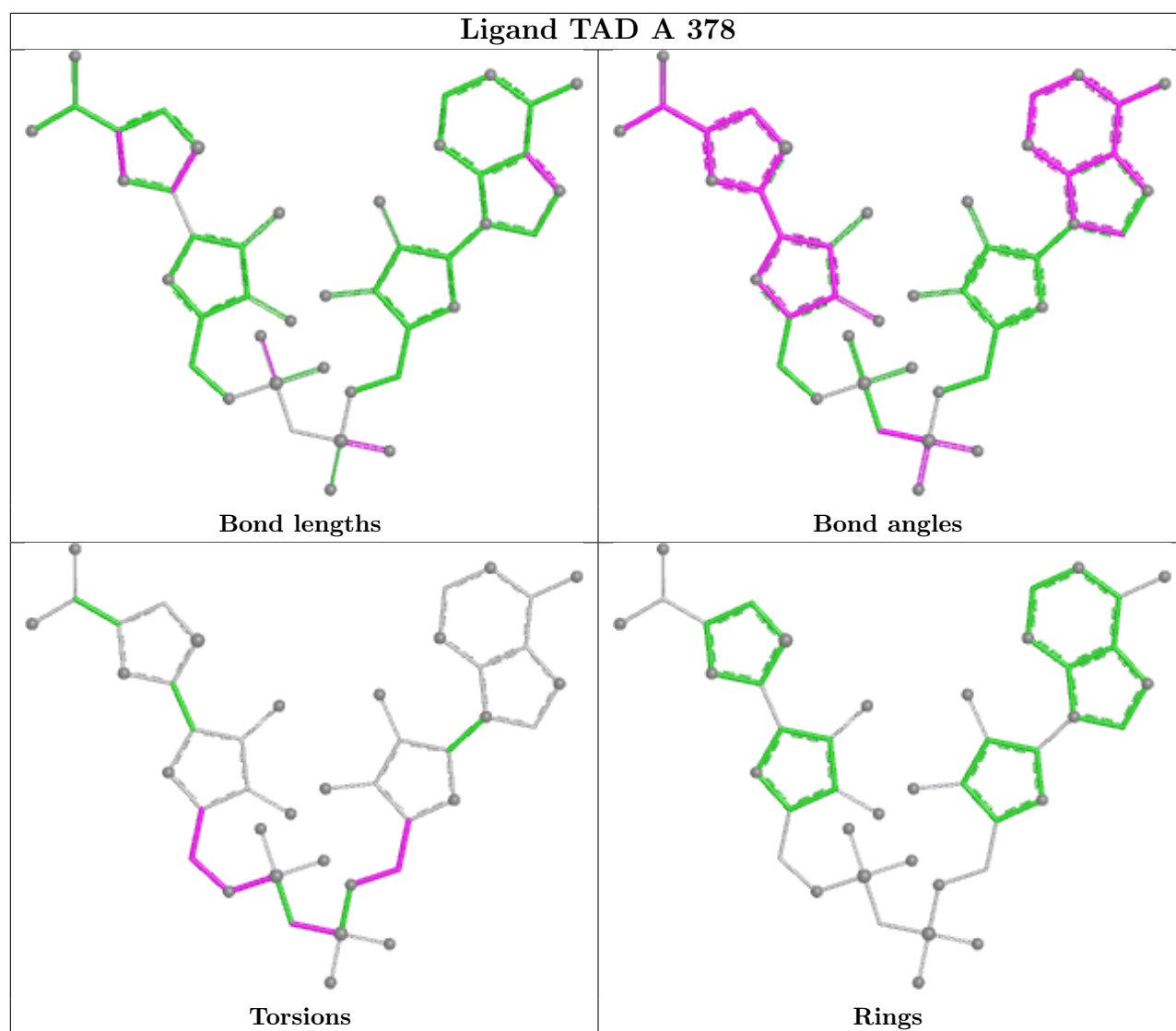
Mol	Chain	Res	Type	Atoms
3	A	378	TAD	O4B-C4B-C5B-O5B
3	A	378	TAD	C3B-C4B-C5B-O5B
3	A	378	TAD	C3D-C4D-C5D-O5D
3	A	378	TAD	C4B-C5B-O5B-PA
3	A	378	TAD	O4D-C4D-C5D-O5D

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

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.