



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1ADG
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 : 2.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

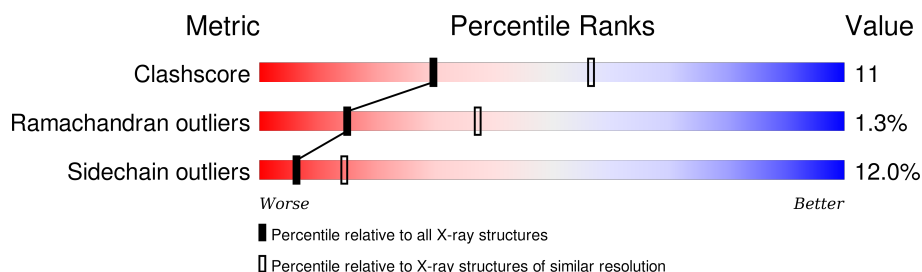
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	 62% 31% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3601 atoms, of which 719 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.

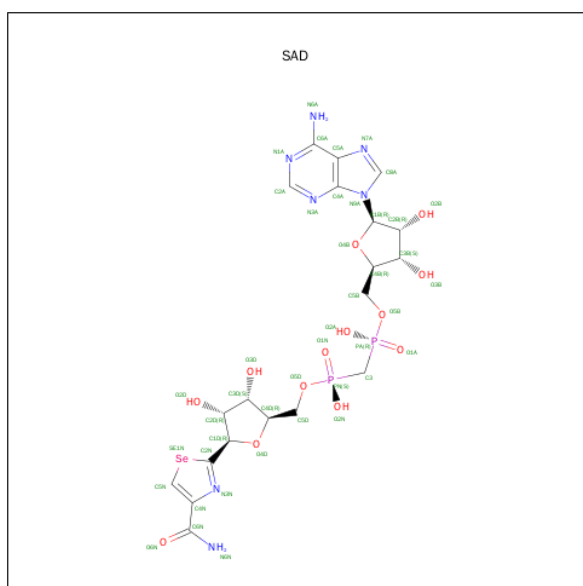
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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 2 2	0	0

- Molecule 3 is BETA-METHYLENE-SELENAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: SAD) (formula: $C_{20}H_{27}N_7O_{13}P_2Se$).



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

- Molecule 4 is water.

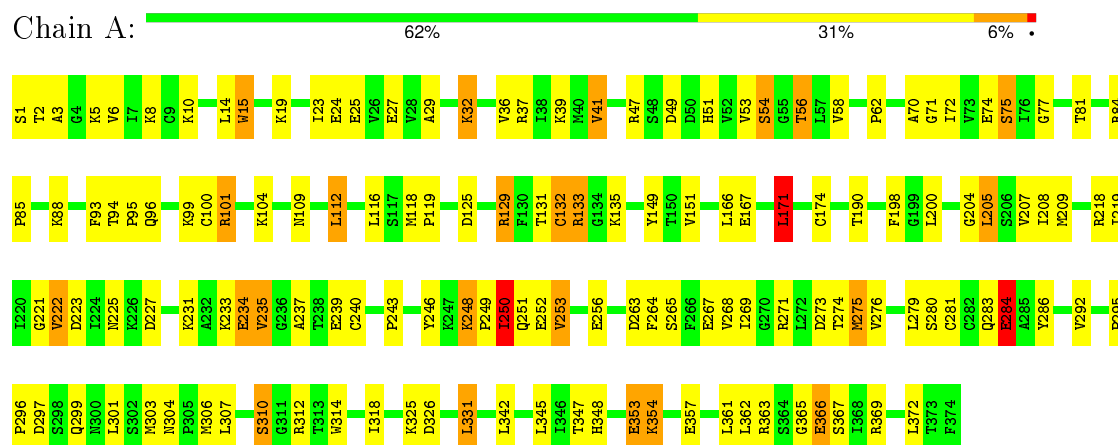
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	52	Total	H	O	0	0
			156	104	52		

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 errors 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 will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	56.30Å 75.20Å 182.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3601	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: ZN, SAD

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	1.01	3/2837 (0.1%)	1.75	46/3834 (1.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	VAL	CA-CB	5.86	1.67	1.54
1	A	366	GLU	CB-CG	5.43	1.62	1.52
1	A	366	GLU	CG-CD	5.36	1.59	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	129	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	363	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	218	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	314	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	A	314	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	15	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	284	GLU	CA-CB-CG	7.54	129.99	113.40
1	A	101	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	41	VAL	CG1-CB-CG2	-7.30	99.22	110.90
1	A	303	MET	CG-SD-CE	-7.28	88.56	100.20
1	A	84	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	37	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	234	GLU	CA-CB-CG	7.05	128.90	113.40
1	A	149	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	A	15	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	56	THR	CA-CB-CG2	6.34	121.28	112.40
1	A	125	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LYS	CA-CB-CG	6.17	126.97	113.40
1	A	314	TRP	CG-CD2-CE3	6.16	139.44	133.90
1	A	246	TYR	CB-CG-CD1	-6.06	117.36	121.00
1	A	129	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	37	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	133	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	171	LEU	CA-CB-CG	5.89	128.86	115.30
1	A	303	MET	N-CA-CB	-5.67	100.40	110.60
1	A	275	MET	CB-CG-SD	-5.57	95.69	112.40
1	A	56	THR	CA-CB-OG1	-5.56	97.32	109.00
1	A	133	ARG	CG-CD-NE	-5.49	100.26	111.80
1	A	54	SER	CA-C-N	5.44	127.08	116.20
1	A	132	CYS	N-CA-C	-5.43	96.35	111.00
1	A	326	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	15	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	347	THR	N-CA-CB	-5.31	100.21	110.30
1	A	354	LYS	CB-CG-CD	-5.29	97.84	111.60
1	A	72	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	A	250	ILE	CB-CA-C	-5.28	101.04	111.60
1	A	314	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	99	LYS	N-CA-C	5.24	125.14	111.00
1	A	32	LYS	CB-CG-CD	-5.22	98.04	111.60
1	A	207	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	292	VAL	CA-CB-CG2	-5.20	103.09	110.90
1	A	3	ALA	CA-C-N	5.07	126.33	116.20
1	A	331	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	39	LYS	CA-CB-CG	-5.03	102.33	113.40
1	A	2	THR	N-CA-CB	-5.01	100.78	110.30

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	2785	607	2848	61	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	43	8	25	6	0
4	A	52	104	0	3	0
All	All	2882	719	2873	64	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 11.

All (64) 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:248:LYS:HG3	1:A:253:VAL:HG12	1.70	0.73
1:A:10:LYS:HA	1:A:24:GLU:O	1.90	0.72
1:A:250:ILE:H	1:A:250:ILE:HD13	1.56	0.70
1:A:47:ARG:HG2	3:A:378:SAD:H3D	1.74	0.68
1:A:304:ASN:OD1	1:A:306:MET:HB2	1.93	0.68
1:A:200:LEU:HD12	1:A:223:ASP:HB2	1.81	0.63
1:A:6:VAL:HG22	1:A:29:ALA:HA	1.82	0.61
1:A:269:ILE:O	3:A:378:SAD:H1D	2.00	0.60
1:A:171:LEU:HD23	1:A:342:LEU:HD22	1.84	0.59
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.85	0.57
1:A:219:ILE:HB	1:A:237:ALA:HA	1.86	0.56
1:A:8:LYS:HG3	1:A:27:GLU:HG3	1.87	0.55
1:A:263:ASP:HB3	1:A:264:PHE:CD2	2.42	0.54
1:A:94:THR:HG21	1:A:318:ILE:HG21	1.90	0.54
1:A:231:LYS:HB3	4:A:395:HOH:O	2.08	0.53
1:A:243:PRO:HB3	1:A:250:ILE:HD12	1.91	0.53
3:A:378:SAD:H32	4:A:404:HOH:O	2.09	0.51
1:A:15:TRP:HA	1:A:62:PRO:HB3	1.93	0.50
1:A:74:GLU:OE1	1:A:75:SER:HB2	2.11	0.50
1:A:14:LEU:HD11	1:A:53:VAL:HG22	1.92	0.50
1:A:345:LEU:O	1:A:369:ARG:HB2	2.11	0.50
1:A:32:LYS:O	1:A:77:GLY:HA3	2.12	0.50
1:A:252:GLU:O	1:A:256:GLU:HB2	2.13	0.49
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.94	0.49
1:A:51:HIS:HB3	1:A:56:THR:HG22	1.95	0.48
1:A:284:GLU:O	1:A:310:SER:HB2	2.14	0.48
1:A:307:LEU:O	1:A:312:ARG:HD2	2.14	0.48
1:A:269:ILE:HA	3:A:378:SAD:H52A	1.95	0.48
3:A:378:SAD:H51N	3:A:378:SAD:H31	1.63	0.47
1:A:23:ILE:HG13	1:A:353:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:HB3	1:A:325:LYS:HB2	1.97	0.47
1:A:295:PRO:HA	1:A:296:PRO:HD2	1.79	0.47
1:A:301:LEU:O	1:A:301:LEU:HD12	2.15	0.46
1:A:204:GLY:O	1:A:208:ILE:HG13	2.15	0.46
1:A:251:GLN:HB2	1:A:281:CYS:HB3	1.98	0.45
1:A:19:LYS:HD3	1:A:19:LYS:HA	1.77	0.45
1:A:32:LYS:HD2	1:A:129:ARG:NH2	2.31	0.45
1:A:88:LYS:HD2	1:A:166:LEU:HD21	1.99	0.45
1:A:348:HIS:CD2	1:A:361:LEU:HD13	2.52	0.45
1:A:8:LYS:HB2	1:A:8:LYS:HE3	1.67	0.45
1:A:231:LYS:O	1:A:234:GLU:HB2	2.17	0.45
1:A:221:GLY:O	1:A:240:CYS:HA	2.17	0.45
1:A:100:CYS:O	1:A:104:LYS:HG2	2.16	0.45
1:A:269:ILE:HG22	1:A:271:ARG:HG3	2.00	0.43
1:A:198:PHE:O	1:A:268:VAL:HB	2.19	0.43
1:A:250:ILE:N	1:A:250:ILE:HD13	2.28	0.43
1:A:269:ILE:CG2	1:A:271:ARG:HG3	2.49	0.43
1:A:267:GLU:HG3	1:A:275:MET:HA	2.02	0.42
1:A:205:LEU:HD21	1:A:231:LYS:HG2	2.01	0.42
1:A:41:VAL:HG23	1:A:71:GLY:HA2	2.02	0.42
1:A:295:PRO:HB2	1:A:297:ASP:OD1	2.20	0.42
1:A:367:SER:HB3	4:A:387:HOH:O	2.19	0.42
1:A:36:VAL:O	1:A:151:VAL:HA	2.20	0.42
1:A:58:VAL:O	1:A:119:PRO:HG2	2.20	0.41
1:A:225:ASN:ND2	1:A:227:ASP:H	2.18	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.91	0.41
1:A:354:LYS:O	1:A:357:GLU:HB2	2.21	0.41
3:A:378:SAD:H4D	3:A:378:SAD:PA	2.61	0.41
1:A:94:THR:HA	1:A:95:PRO:HD3	1.67	0.41
1:A:204:GLY:CA	1:A:268:VAL:HG11	2.51	0.41
1:A:209:MET:HG3	1:A:235:VAL:HG13	2.03	0.41
1:A:248:LYS:HG3	1:A:253:VAL:CG1	2.46	0.40
1:A:74:GLU:O	1:A:85:PRO:HB3	2.22	0.40
1:A:24:GLU:OE1	1:A:132:CYS:SG	2.79	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)
1:A:101:ARG:HH21	1:A:283:GLN:HE22[3_555]	1.16	0.44

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	372/374 (100%)	320 (86%)	47 (13%)	5 (1%)	15 37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	280	SER
1	A	365	GLY
1	A	174	CYS
1	A	286	TYR

5.3.2 Protein sidechains [i](#)

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%)	271 (88%)	37 (12%)	6 14

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	25	GLU
1	A	49	ASP
1	A	54	SER
1	A	75	SER

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Mol	Chain	Res	Type
1	A	81	THR
1	A	93	PHE
1	A	109	ASN
1	A	118	MET
1	A	131	THR
1	A	133	ARG
1	A	135	LYS
1	A	167	GLU
1	A	171	LEU
1	A	190	THR
1	A	205	LEU
1	A	222	VAL
1	A	233	LYS
1	A	235	VAL
1	A	239	GLU
1	A	249	PRO
1	A	250	ILE
1	A	253	VAL
1	A	265	SER
1	A	273	ASP
1	A	274	THR
1	A	276	VAL
1	A	279	LEU
1	A	284	GLU
1	A	299	GLN
1	A	310	SER
1	A	331	LEU
1	A	353	GLU
1	A	362	LEU
1	A	366	GLU
1	A	372	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	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 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	SAD	A	378	-	35,47,47	1.34	4 (11%)	41,72,72	2.44	15 (36%)

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	SAD	A	378	-	-	0/18/62/62	0/4/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	378	SAD	PA-O2A	-2.09	1.51	1.56
3	A	378	SAD	O4B-C1B	2.86	1.44	1.41
3	A	378	SAD	PN-O5D	3.23	1.61	1.57
3	A	378	SAD	PA-O5B	4.59	1.62	1.57

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	378	SAD	N3A-C2A-N1A	-9.09	121.94	128.89
3	A	378	SAD	C4N-C6N-N6N	-4.66	111.64	116.21
3	A	378	SAD	O5B-PA-O1A	-3.15	105.61	113.98
3	A	378	SAD	C1B-N9A-C4A	-3.04	122.35	126.94
3	A	378	SAD	C5D-C4D-C3D	-2.92	103.62	115.21
3	A	378	SAD	O5D-PN-O1N	-2.63	106.97	113.98
3	A	378	SAD	O2N-PN-O1N	2.10	116.72	110.12
3	A	378	SAD	O2N-PN-C3	2.15	116.24	106.88
3	A	378	SAD	O4D-C4D-C3D	2.24	109.67	105.15
3	A	378	SAD	C2A-N1A-C6A	2.46	123.16	118.77
3	A	378	SAD	O3B-C3B-C2B	2.74	120.74	111.83
3	A	378	SAD	C4A-C5A-N7A	2.92	112.17	109.48
3	A	378	SAD	O2A-PA-O1A	3.33	120.59	110.12
3	A	378	SAD	C2B-C1B-N9A	3.75	120.03	114.29
3	A	378	SAD	O6N-C6N-C4N	3.93	123.29	119.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	378	SAD	6	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.