



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:13 AM UTC

PDB ID : 1ADG / pdb_00001adg
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

<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

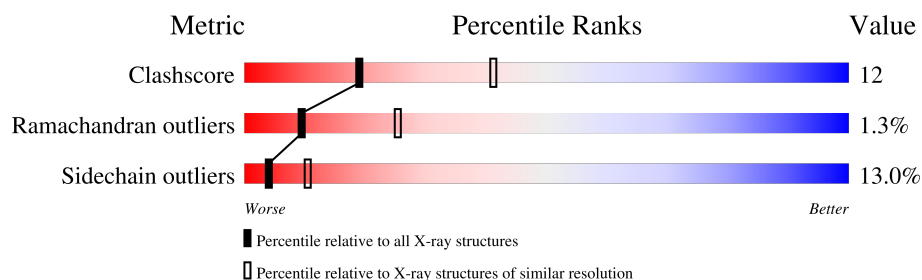
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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 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.

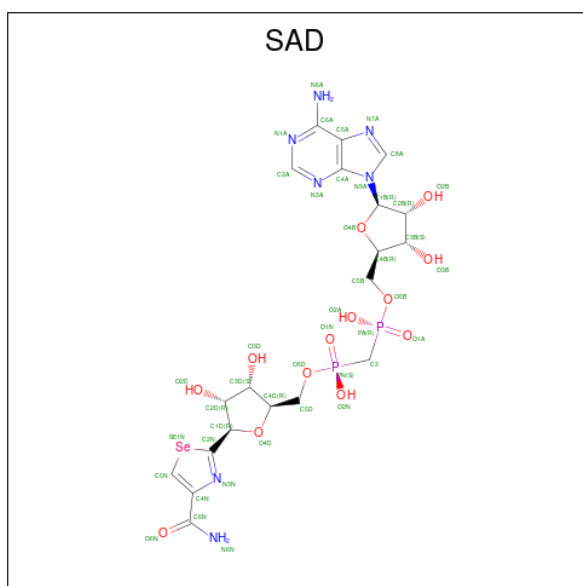
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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 (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-SELENAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (CCD ID: SAD) (formula: C₂₀H₂₇N₇O₁₃P₂Se).



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		

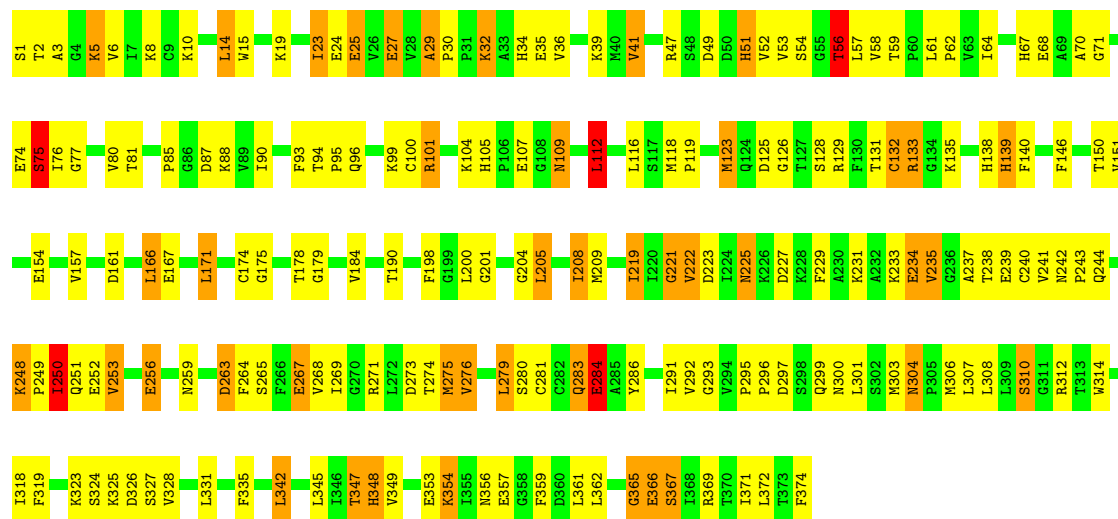
3 Residue-property plots

These plots are drawn for all protein, RNA, 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

Chain A: 



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 75.20Å 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	1.31	15/2837 (0.5%)	2.16	128/3834 (3.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	VAL	CA-CB	9.75	1.67	1.54
1	A	90	ILE	CA-CB	9.11	1.61	1.54
1	A	30	PRO	CA-C	7.77	1.56	1.51
1	A	138	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	51	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	105	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	219	ILE	CA-CB	6.19	1.62	1.53
1	A	157	VAL	CA-CB	6.11	1.63	1.54
1	A	328	VAL	CA-CB	-6.08	1.51	1.54
1	A	348	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	34	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	139	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	241	VAL	CA-CB	5.53	1.61	1.54
1	A	64	ILE	CA-CB	5.20	1.59	1.53
1	A	354	LYS	CA-CB	-5.16	1.46	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASN	OD1-CG-ND2	-10.21	112.39	122.60
1	A	99	LYS	N-CA-C	9.13	125.14	112.45
1	A	109	ASN	CA-CB-CG	8.95	121.55	112.60
1	A	356	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	A	365	GLY	CA-C-N	-8.51	109.90	122.41
1	A	365	GLY	C-N-CA	-8.51	109.90	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	N-CA-C	8.42	119.22	110.72
1	A	56	THR	CA-CB-OG1	-8.19	97.32	109.60
1	A	250	ILE	CA-C-O	-8.17	111.65	120.47
1	A	284	GLU	CA-CB-CG	7.95	129.99	114.10
1	A	359	PHE	CA-CB-CG	-7.71	106.09	113.80
1	A	225	ASN	CB-CG-ND2	7.67	127.91	116.40
1	A	125	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	234	GLU	CA-CB-CG	7.40	128.90	114.10
1	A	279	LEU	N-CA-C	-7.37	103.19	111.14
1	A	283	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	A	201	GLY	N-CA-C	-7.25	101.54	112.41
1	A	276	VAL	N-CA-C	-7.23	103.62	110.42
1	A	323	LYS	N-CA-C	-7.23	98.96	109.59
1	A	347	THR	N-CA-CB	-7.03	100.21	110.47
1	A	300	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	A	327	SER	N-CA-C	7.00	120.30	111.69
1	A	242	ASN	CA-CB-CG	6.95	119.55	112.60
1	A	250	ILE	CB-CA-C	-6.93	101.04	112.26
1	A	259	ASN	CB-CG-ND2	6.73	126.49	116.40
1	A	132	CYS	N-CA-C	-6.67	96.35	108.02
1	A	366	GLU	CB-CG-CD	6.62	123.86	112.60
1	A	105	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	A	256	GLU	N-CA-C	-6.49	103.83	111.03
1	A	248	LYS	CA-CB-CG	6.43	126.97	114.10
1	A	34	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	342	LEU	CA-C-O	6.39	126.82	119.35
1	A	304	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	56	THR	CA-CB-CG2	6.34	121.28	110.50
1	A	178	THR	CA-C-O	-6.31	114.19	120.82
1	A	2	THR	N-CA-C	6.27	120.19	112.54
1	A	275	MET	CA-C-N	6.26	128.35	120.72
1	A	275	MET	C-N-CA	6.26	128.35	120.72
1	A	138	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	276	VAL	CA-C-O	-6.22	113.96	121.18
1	A	374	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	356	ASN	CB-CG-ND2	6.17	125.66	116.40
1	A	324	SER	N-CA-C	6.15	117.65	111.07
1	A	244	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	A	23	ILE	N-CA-C	-6.14	99.46	108.54
1	A	161	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	5	LYS	N-CA-C	6.12	118.27	109.14
1	A	123	MET	N-CA-C	-6.09	101.75	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	HIS	CA-CB-CG	6.01	119.81	113.80
1	A	303	MET	N-CA-CB	-5.98	100.40	111.53
1	A	175	GLY	CA-C-O	-5.98	114.89	121.05
1	A	367	SER	N-CA-C	-5.96	98.10	110.80
1	A	59	THR	CB-CA-C	5.94	118.11	109.20
1	A	29	ALA	CA-C-N	5.94	124.00	119.66
1	A	29	ALA	C-N-CA	5.94	124.00	119.66
1	A	259	ASN	CA-CB-CG	-5.91	106.69	112.60
1	A	39	LYS	CA-CB-CG	-5.88	102.33	114.10
1	A	354	LYS	CB-CG-CD	-5.85	97.84	111.30
1	A	128	SER	O-C-N	-5.84	116.38	123.10
1	A	2	THR	N-CA-CB	-5.79	100.78	110.39
1	A	87	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	101	ARG	CA-C-O	-5.78	113.57	120.10
1	A	32	LYS	CB-CG-CD	-5.77	98.04	111.30
1	A	283	GLN	CG-CD-NE2	5.74	125.01	116.40
1	A	140	PHE	O-C-N	5.74	129.92	123.27
1	A	238	THR	N-CA-C	-5.73	106.42	113.41
1	A	80	VAL	CA-C-O	5.72	127.78	120.97
1	A	75	SER	CA-C-O	-5.72	114.46	120.80
1	A	250	ILE	N-CA-CB	5.68	121.06	110.77
1	A	112	LEU	N-CA-C	5.68	122.89	110.80
1	A	275	MET	CB-CG-SD	-5.67	95.69	112.70
1	A	112	LEU	O-C-N	-5.67	115.05	122.59
1	A	303	MET	CG-SD-CE	-5.61	88.56	100.90
1	A	27	GLU	CA-CB-CG	-5.61	102.89	114.10
1	A	348	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	52	VAL	O-C-N	5.59	127.39	121.91
1	A	154	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	354	LYS	N-CA-C	5.58	118.88	112.57
1	A	326	ASP	N-CA-C	5.57	117.43	111.36
1	A	319	PHE	N-CA-CB	-5.55	103.75	112.13
1	A	314	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	A	314	TRP	N-CA-C	-5.51	99.91	108.90
1	A	2	THR	CA-C-O	5.51	126.16	119.38
1	A	242	ASN	CA-C-N	5.49	125.58	119.32
1	A	242	ASN	C-N-CA	5.49	125.58	119.32
1	A	221	GLY	CA-C-O	-5.49	116.14	120.91
1	A	61	LEU	CA-C-O	-5.47	114.99	120.63
1	A	259	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	140	PHE	CA-C-N	5.46	130.11	122.08
1	A	140	PHE	C-N-CA	5.46	130.11	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	N-CA-C	5.41	117.62	111.02
1	A	229	PHE	N-CA-C	5.35	117.86	111.71
1	A	93	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	179	GLY	O-C-N	-5.34	117.06	122.19
1	A	133	ARG	CG-CD-NE	-5.34	100.26	112.00
1	A	166	LEU	N-CA-C	5.31	119.38	113.01
1	A	263	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	67	HIS	CA-CB-CG	5.29	119.09	113.80
1	A	57	LEU	N-CA-C	-5.28	100.56	108.96
1	A	41	VAL	CG1-CB-CG2	-5.26	99.22	110.80
1	A	105	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	293	GLY	O-C-N	5.25	129.52	122.70
1	A	139	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	208	ILE	O-C-N	5.18	126.96	121.89
1	A	248	LYS	N-CA-C	5.17	117.78	110.24
1	A	308	LEU	CA-C-N	5.17	127.20	120.28
1	A	308	LEU	C-N-CA	5.17	127.20	120.28
1	A	354	LYS	CA-C-N	5.17	127.54	120.77
1	A	354	LYS	C-N-CA	5.17	127.54	120.77
1	A	366	GLU	CA-C-O	5.14	126.26	120.92
1	A	349	VAL	N-CA-C	-5.13	100.13	107.78
1	A	267	GLU	CA-C-O	5.12	126.38	120.84
1	A	314	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	150	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	126	GLY	O-C-N	-5.09	116.17	122.23
1	A	366	GLU	N-CA-CB	5.09	117.93	110.35
1	A	3	ALA	O-C-N	-5.08	116.26	122.11
1	A	335	PHE	N-CA-C	-5.08	105.75	111.28
1	A	76	ILE	O-C-N	-5.07	117.71	122.98
1	A	30	PRO	N-CA-C	5.05	115.32	110.47
1	A	25	GLU	N-CA-C	-5.04	101.47	109.59
1	A	291	ILE	N-CA-C	-5.04	101.08	108.54
1	A	146	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	35	GLU	CA-CB-CG	-5.04	104.03	114.10
1	A	359	PHE	N-CA-C	-5.03	105.26	111.40
1	A	51	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	A	105	HIS	CB-CG-ND1	5.00	130.20	122.70
1	A	107	GLU	CB-CG-CD	5.00	121.10	112.60

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	64	1
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	67	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 12.

All (67) 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:32:LYS:O	1:A:77:GLY:HA3	2.12	0.50
1:A:345:LEU:O	1:A:369:ARG:HB2	2.11	0.50
1:A:252:GLU:O	1:A:256:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD12	1:A:301:LEU:O	2.15	0.46
1:A:204:GLY:O	1:A:208:ILE:HG13	2.15	0.46
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.77	0.45
1:A:251:GLN:HB2	1:A:281:CYS:HB3	1.98	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:HE3	1:A:8:LYS:HB2	1.67	0.45
1:A:221:GLY:O	1:A:240:CYS:HA	2.17	0.45
1:A:231:LYS:O	1:A:234:GLU:HB2	2.17	0.45
1:A:100:CYS:O	1:A:104:LYS:HG2	2.16	0.45
1:A:123:MET:HA	1:A:123:MET:HE2	2.00	0.44
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:HD13	1:A:250:ILE:N	2.28	0.43
1:A:269:ILE:CG2	1:A:271:ARG:HG3	2.49	0.43
1:A:68:GLU:CD	1:A:369:ARG:HH21	2.27	0.42
1:A:267:GLU:HG3	1:A:275:MET:HA	2.02	0.42
1:A:41:VAL:HG23	1:A:71:GLY:HA2	2.02	0.42
1:A:205:LEU:HD21	1:A:231:LYS:HG2	2.01	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:123:MET:HE3	1:A:139:HIS:ND1	2.35	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:HD23	1:A:116:LEU:HA	1.91	0.41
1:A:354:LYS:O	1:A:357:GLU:HB2	2.21	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
3:A:378:SAD:PA	3:A:378:SAD:H4D	2.61	0.41
1:A:209:MET:HG3	1:A:235:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	9 25

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%)	268 (87%)	40 (13%)	4 10

All (40) 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	25	GLU
1	A	49	ASP
1	A	54	SER
1	A	56	THR
1	A	75	SER
1	A	81	THR
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	292	VAL
1	A	299	GLN
1	A	310	SER
1	A	331	LEU
1	A	347	THR

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Mol	Chain	Res	Type
1	A	362	LEU
1	A	366	GLU
1	A	371	ILE
1	A	372	LEU

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	42,47,47	1.53	5 (11%)	59,72,72	2.46	22 (37%)

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	-	-	12/28/62/62	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	SAD	SE1N-C2N	-5.41	1.77	1.88
3	A	378	SAD	SE1N-C5N	-5.27	1.71	1.86
3	A	378	SAD	C5A-N7A	-2.71	1.34	1.39
3	A	378	SAD	C4N-N3N	-2.21	1.33	1.38
3	A	378	SAD	PA-O2A	-2.10	1.51	1.56

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	378	SAD	C4N-N3N-C2N	-8.43	105.14	113.49
3	A	378	SAD	C5A-C4A-N3A	-5.87	118.64	126.72
3	A	378	SAD	N3A-C4A-N9A	5.19	136.00	127.17
3	A	378	SAD	C4N-C6N-N6N	-4.56	111.64	116.28
3	A	378	SAD	N3A-C2A-N1A	-4.39	121.94	128.58
3	A	378	SAD	C6A-C5A-C4A	3.96	122.59	117.18
3	A	378	SAD	C6A-C5A-N7A	-3.85	124.67	132.09
3	A	378	SAD	C2D-C1D-C2N	3.79	122.11	114.94
3	A	378	SAD	O2A-PA-O1A	3.27	120.59	109.95
3	A	378	SAD	C5D-C4D-C3D	-3.22	103.62	115.21
3	A	378	SAD	O6N-C6N-C4N	3.17	123.29	120.25
3	A	378	SAD	C2A-N3A-C4A	3.07	119.33	111.83
3	A	378	SAD	SE1N-C2N-N3N	2.92	120.17	113.38
3	A	378	SAD	O3B-C3B-C2B	2.78	120.74	111.82
3	A	378	SAD	C2B-C1B-N9A	2.71	120.03	113.30
3	A	378	SAD	C2A-N1A-C6A	2.70	123.16	118.73
3	A	378	SAD	C4A-N9A-C8A	2.49	108.36	105.74
3	A	378	SAD	SE1N-C5N-C4N	2.35	114.44	111.07
3	A	378	SAD	N9A-C8A-N7A	-2.33	110.63	113.94
3	A	378	SAD	O2N-PN-C3	2.30	116.24	106.73
3	A	378	SAD	O4D-C4D-C3D	2.27	109.67	105.15
3	A	378	SAD	O2N-PN-O1N	2.08	116.72	109.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

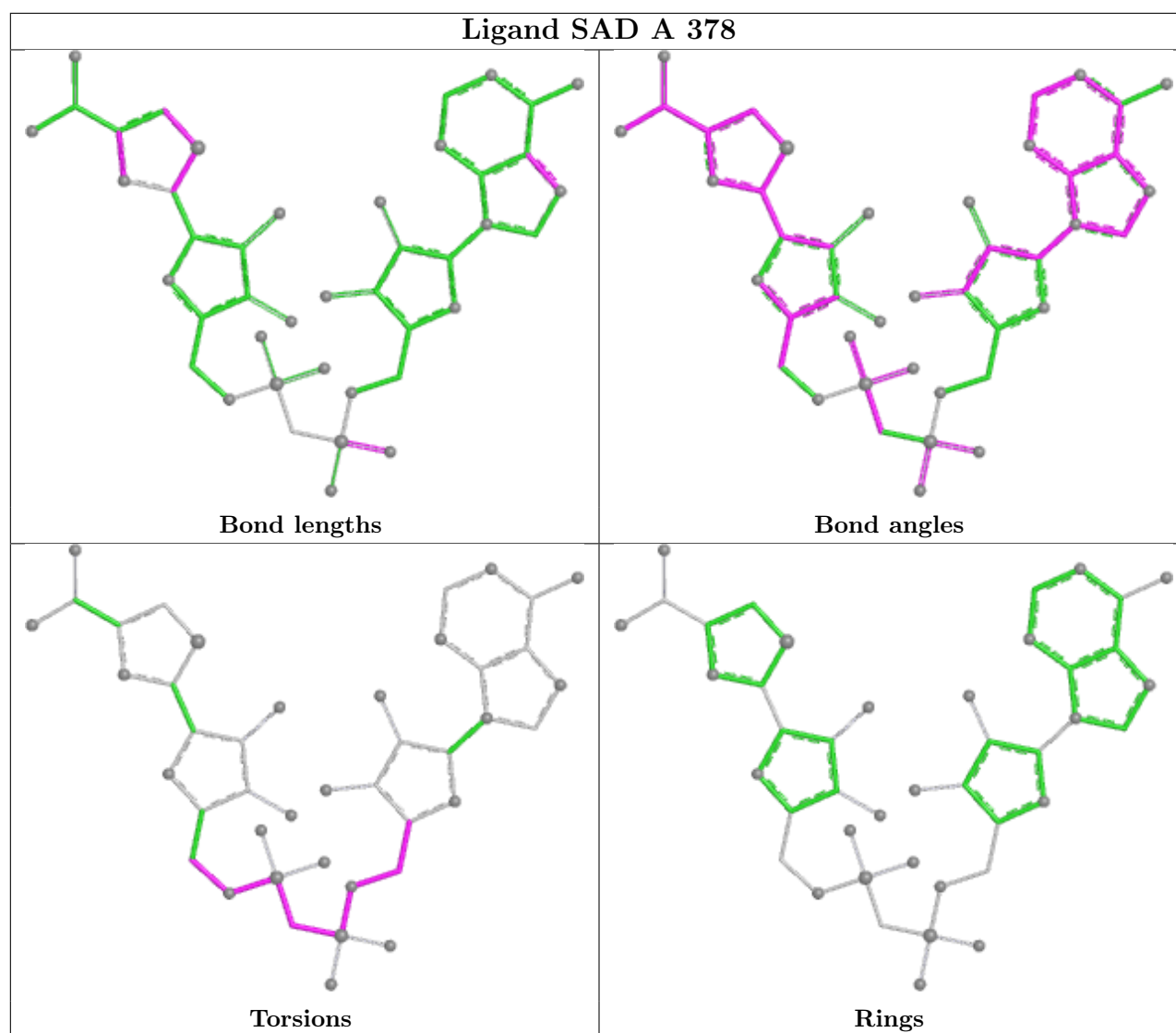
Mol	Chain	Res	Type	Atoms
3	A	378	SAD	PN-C3-PA-O1A
3	A	378	SAD	C5D-O5D-PN-C3
3	A	378	SAD	C4D-C5D-O5D-PN
3	A	378	SAD	C5D-O5D-PN-O1N
3	A	378	SAD	PN-C3-PA-O2A
3	A	378	SAD	PN-C3-PA-O5B
3	A	378	SAD	PA-C3-PN-O2N
3	A	378	SAD	C4B-C5B-O5B-PA
3	A	378	SAD	C5B-O5B-PA-O2A
3	A	378	SAD	PA-C3-PN-O1N
3	A	378	SAD	C5D-O5D-PN-O2N
3	A	378	SAD	O4B-C4B-C5B-O5B

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

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.