



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:23 AM UTC

PDB ID : 1YDA / pdb_00001yda
Title : STRUCTURAL BASIS OF INHIBITOR AFFINITY TO VARIANTS OF HUMAN CARBONIC ANHYDRASE II
Authors : Nair, S.K.; Christianson, D.W.
Deposited on : 1994-12-22
Resolution : 2.10 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
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

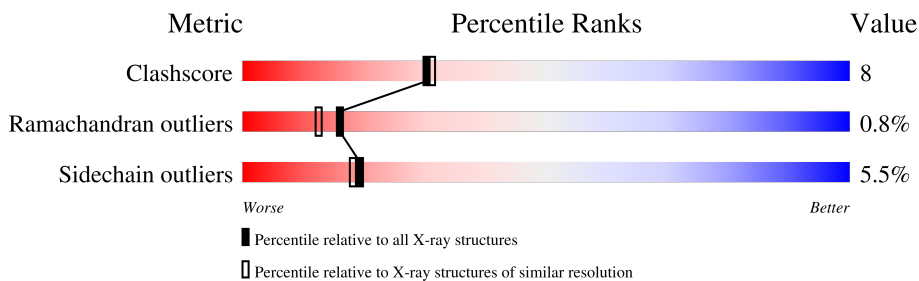
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	259	 63% 31% . . .

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
4	AZM	A	264	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2123 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 CARBONIC ANHYDRASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2029	1302	347	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLU	LEU	conflict	UNP P00918

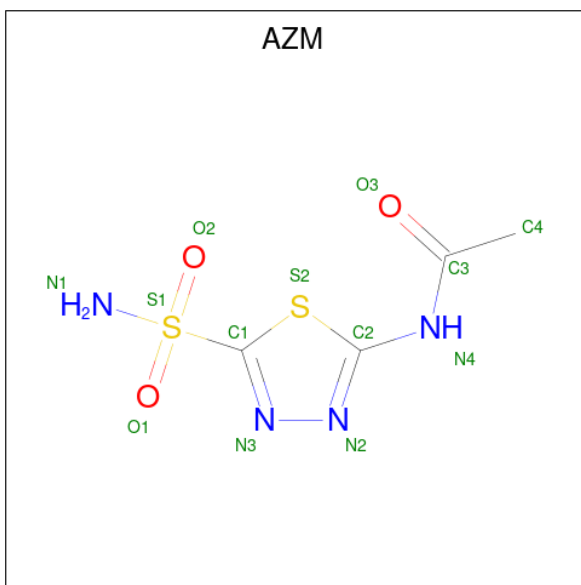
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is 5-ACETAMIDO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (CCD ID: AZM) (formula: C₄H₆N₄O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	13	4	4	3	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		

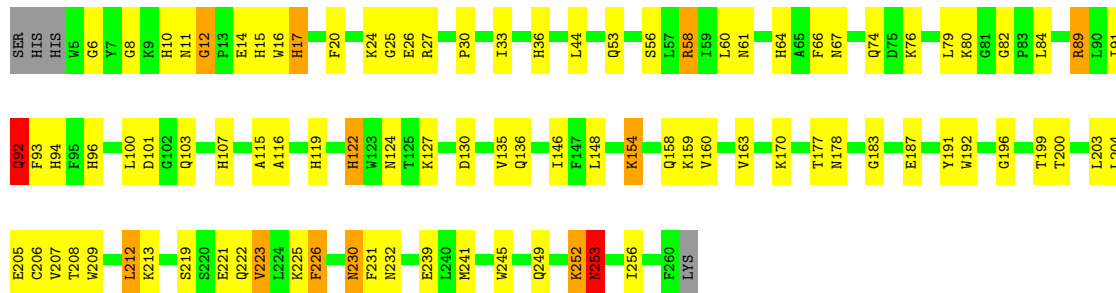
3 Residue-property plots

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: CARBONIC ANHYDRASE II

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.50-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2123	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: ZN, AZM, HG

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	1.12	14/2089 (0.7%)	1.94	58/2836 (2.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	122	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	17	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	96	HIS	CG-ND1	-6.34	1.31	1.38
1	A	119	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	10	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	94	HIS	CG-ND1	-5.88	1.31	1.38
1	A	207	VAL	CA-CB	5.85	1.61	1.54
1	A	64	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	15	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	36	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	253	ASN	CA-CB	5.18	1.62	1.53
1	A	17	HIS	CG-ND1	-5.16	1.32	1.38
1	A	223	VAL	CA-CB	5.06	1.61	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASN	OD1-CG-ND2	-14.65	107.94	122.60
1	A	93	PHE	CA-CB-CG	10.00	123.80	113.80
1	A	253	ASN	CA-CB-CG	9.52	122.12	112.60
1	A	178	ASN	OD1-CG-ND2	-9.05	113.55	122.60
1	A	230	ASN	CB-CG-ND2	9.02	129.94	116.40
1	A	230	ASN	OD1-CG-ND2	-8.53	114.07	122.60
1	A	92	GLN	OE1-CD-NE2	-8.45	114.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASN	CA-CB-CG	8.42	121.02	112.60
1	A	253	ASN	CB-CG-ND2	7.67	127.91	116.40
1	A	115	ALA	N-CA-C	7.34	120.15	111.71
1	A	24	LYS	CB-CG-CD	-7.16	94.84	111.30
1	A	122	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	A	119	HIS	CB-CG-CD2	-7.03	122.06	131.20
1	A	67	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	A	249	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	15	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	226	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	130	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	92	GLN	CG-CD-NE2	6.43	126.04	116.40
1	A	89	ARG	N-CA-C	6.13	119.16	109.96
1	A	136	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	A	158	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	A	14	GLU	CA-CB-CG	6.00	126.10	114.10
1	A	159	LYS	CA-CB-CG	5.95	126.01	114.10
1	A	25	GLY	CA-C-O	5.89	128.83	122.47
1	A	36	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	96	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	107	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	A	82	GLY	CA-C-N	5.73	126.48	120.12
1	A	82	GLY	C-N-CA	5.73	126.48	120.12
1	A	36	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	101	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	158	GLN	N-CA-C	5.64	117.43	111.28
1	A	245	TRP	CB-CG-CD1	-5.60	118.50	126.90
1	A	64	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	209	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	A	66	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	191	TYR	N-CA-C	5.42	118.41	109.85
1	A	208	THR	N-CA-C	-5.41	98.95	108.20
1	A	61	ASN	N-CA-C	-5.36	100.00	108.73
1	A	12	GLY	CA-C-N	5.34	125.41	119.32
1	A	12	GLY	C-N-CA	5.34	125.41	119.32
1	A	103	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	A	225	LYS	CA-CB-CG	-5.26	103.57	114.10
1	A	11	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	192	TRP	N-CA-C	-5.22	101.37	109.72
1	A	17	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	10	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	154	LYS	CA-C-N	5.13	124.58	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LYS	C-N-CA	5.13	124.58	119.24
1	A	119	HIS	CB-CG-ND1	5.13	130.39	122.70
1	A	187	GLU	N-CA-CB	-5.08	102.64	110.16
1	A	253	ASN	N-CA-CB	5.05	119.03	110.49
1	A	209	TRP	CD1-CG-CD2	5.04	114.37	106.30
1	A	84	LEU	CA-C-N	-5.04	116.00	123.05
1	A	84	LEU	C-N-CA	-5.04	116.00	123.05
1	A	200	THR	N-CA-C	-5.03	102.55	110.14
1	A	209	TRP	CG-CD1-NE1	-5.00	103.69	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2029	0	1977	32	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	13	0	6	2	0
5	A	79	0	0	1	0
All	All	2123	0	1983	33	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 8.

All (33) 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:160:VAL:O	1:A:163:VAL:HG12	2.02	0.60
1:A:58:ARG:HH12	1:A:60:LEU:HD13	1.69	0.57
1:A:74:GLN:HB2	1:A:76:LYS:HE3	1.87	0.56
4:A:264:AZM:S2	4:A:264:AZM:O3	2.64	0.55
1:A:58:ARG:HH11	1:A:60:LEU:HD22	1.71	0.55
1:A:146:ILE:HG12	1:A:212:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:THR:OG1	4:A:264:AZM:N1	2.42	0.52
1:A:56:SER:O	1:A:177:THR:HA	2.10	0.52
1:A:219:SER:OG	1:A:222:GLN:HG3	2.09	0.52
1:A:253:ASN:C	1:A:253:ASN:HD22	2.19	0.51
1:A:89:ARG:O	1:A:122:HIS:HA	2.11	0.51
1:A:33:ILE:HG12	1:A:256:ILE:HD13	1.94	0.49
1:A:91:ILE:HG23	1:A:92:GLN:HG3	1.94	0.48
1:A:58:ARG:NH1	1:A:60:LEU:HD13	2.29	0.48
1:A:253:ASN:C	1:A:253:ASN:ND2	2.73	0.46
1:A:116:ALA:HB3	1:A:148:LEU:HD22	1.97	0.45
1:A:124:ASN:OD1	1:A:127:LYS:HB3	2.16	0.45
1:A:17:HIS:HA	1:A:20:PHE:O	2.16	0.44
1:A:154:LYS:HE3	1:A:183:GLY:O	2.16	0.44
1:A:27:ARG:HH21	1:A:196:GLY:H	1.65	0.43
1:A:6:GLY:O	1:A:12:GLY:HA2	2.18	0.43
1:A:205:GLU:C	1:A:206:CYS:SG	3.01	0.43
1:A:213:LYS:HB3	1:A:213:LYS:HE2	1.73	0.42
1:A:135:VAL:HB	1:A:204:LEU:HD13	2.01	0.42
1:A:252:LYS:O	1:A:253:ASN:HB3	2.19	0.42
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.20	0.42
1:A:231:PHE:CE2	1:A:241:MET:HA	2.54	0.41
1:A:170:LYS:HB2	1:A:231:PHE:O	2.20	0.41
1:A:80:LYS:HB2	5:A:285:HOH:O	2.20	0.41
1:A:16:TRP:HE3	1:A:203:LEU:HD11	1.85	0.41
1:A:223:VAL:O	1:A:226:PHE:HB2	2.20	0.41
1:A:8:GLY:O	1:A:12:GLY:N	2.54	0.40
1:A:204:LEU:HB3	1:A:206:CYS:SG	2.61	0.40

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	253/259 (98%)	235 (93%)	16 (6%)	2 (1%)	16 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	252	LYS

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	220/224 (98%)	208 (94%)	12 (6%)	19 18

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	30	PRO
1	A	44	LEU
1	A	53	GLN
1	A	58	ARG
1	A	79	LEU
1	A	92	GLN
1	A	100	LEU
1	A	212	LEU
1	A	221	GLU
1	A	239	GLU
1	A	253	ASN

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	253	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 ⓘ

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	$\# Z > 2$
4	AZM	A	264	2	13,13,13	2.22	4 (30%)	19,19,19	5.90	14 (73%)

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
4	AZM	A	264	2	-	2/10/10/10	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	264	AZM	C2-N4	-4.65	1.31	1.38
4	A	264	AZM	O2-S1	4.00	1.49	1.43
4	A	264	AZM	C1-S2	-3.43	1.69	1.73
4	A	264	AZM	O1-S1	2.18	1.46	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	264	AZM	O2-S1-O1	-17.27	95.57	120.27
4	A	264	AZM	O2-S1-C1	12.42	124.16	105.65
4	A	264	AZM	O2-S1-N1	8.03	119.57	108.39
4	A	264	AZM	N4-C2-N2	-7.03	114.53	120.81
4	A	264	AZM	O1-S1-C1	-3.96	99.75	105.65
4	A	264	AZM	C1-S2-C2	-3.43	83.84	85.47
4	A	264	AZM	S2-C2-N2	3.43	118.35	114.52
4	A	264	AZM	S1-C1-N3	-3.19	118.27	121.95
4	A	264	AZM	O1-S1-N1	-3.06	104.13	108.39
4	A	264	AZM	S2-C2-N4	2.42	126.96	123.72
4	A	264	AZM	C3-N4-C2	-2.39	120.11	124.05
4	A	264	AZM	O3-C3-C4	-2.38	117.81	122.05
4	A	264	AZM	S2-C1-S1	2.34	124.73	121.62
4	A	264	AZM	C2-N2-N3	-2.26	109.14	112.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	264	AZM	S2-C1-S1-O1
4	A	264	AZM	N3-C1-S1-O1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	264	AZM	2	0

5.7 Other polymers [i](#)

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

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.