



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 10:28 AM JST

PDB ID : 9KI7 / pdb\_00009ki7  
Title : Zn- Carbonic Anhydrase II pH 7.8 1.5 atm CO2  
Authors : Kim, C.U.; Kim, J.K.  
Deposited on : 2024-11-11  
Resolution : 1.20 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

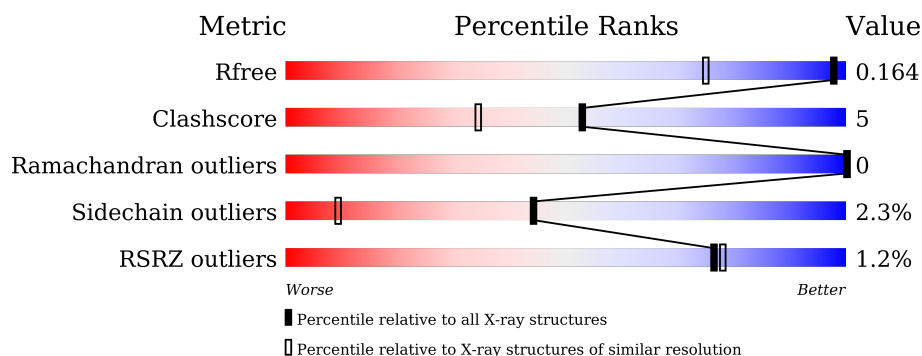
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.20 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))
$R_{free}$	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	260	

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
3	GOL	A	302	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2384 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.

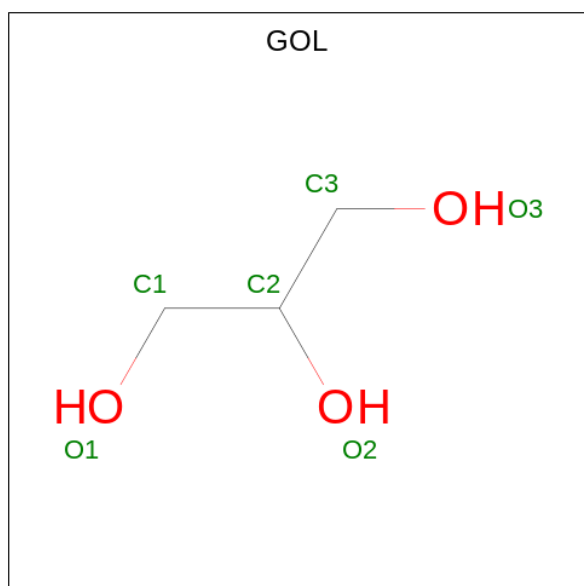
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	9	0
			2105	1352	359	392	2			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

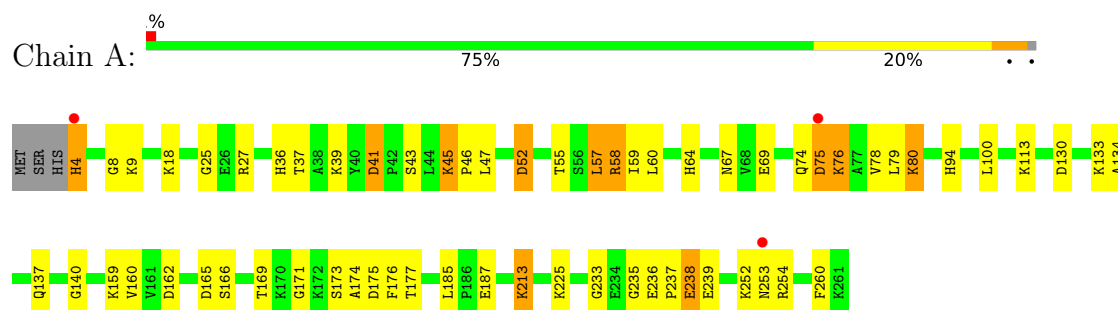
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	272	Total 272	O 272	0	0

### 3 Residue-property plots [i](#)

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 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.

- Molecule 1: Carbonic anhydrase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.84Å 41.05Å 71.56Å 90.00° 104.11° 90.00°	Depositor
Resolution (Å)	30.00 – 1.20 30.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-1.20) 96.4 (30.00-1.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.133 , 0.156 0.141 , 0.164	Depositor DCC
$R_{free}$ test set	3508 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	2.07	63/2179 (2.9%)	1.72	41/2956 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	SER	C-O	12.41	1.39	1.23
1	A	58	ARG	CB-CG	-12.39	1.15	1.52
1	A	45	LYS	C-N	11.64	1.48	1.33
1	A	175	ASP	CB-CG	-11.47	1.23	1.52
1	A	75	ASP	CG-OD1	10.78	1.45	1.25
1	A	27	ARG	CZ-NH2	-10.39	1.20	1.33
1	A	237	PRO	N-CA	9.64	1.58	1.47
1	A	57	LEU	CA-C	-9.55	1.43	1.52
1	A	100	LEU	CA-CB	9.46	1.72	1.54
1	A	253	ASN	C-O	9.27	1.38	1.23
1	A	238	GLU	C-O	-9.01	1.13	1.24
1	A	58	ARG	N-CA	-8.91	1.34	1.46
1	A	76	LYS	C-N	-8.43	1.21	1.33
1	A	169	THR	CA-C	8.33	1.62	1.52
1	A	69	GLU	CA-CB	-8.18	1.40	1.53
1	A	236	GLU	CA-C	8.06	1.64	1.52
1	A	60	LEU	N-CA	-7.98	1.36	1.46
1	A	60	LEU	CA-C	7.95	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ALA	N-CA	-7.88	1.35	1.45
1	A	176	PHE	CA-C	-7.71	1.44	1.53
1	A	60	LEU	CB-CG	-7.46	1.38	1.53
1	A	27	ARG	CZ-NH1	7.30	1.43	1.32
1	A	175	ASP	CA-CB	7.17	1.65	1.53
1	A	137	GLN	CD-OE1	6.71	1.36	1.23
1	A	9	LYS	N-CA	6.62	1.54	1.46
1	A	52	ASP	CG-OD1	6.57	1.37	1.25
1	A	8	GLY	C-O	6.55	1.29	1.23
1	A	213	LYS	CD-CE	6.52	1.72	1.52
1	A	43	SER	CA-C	6.34	1.61	1.52
1	A	45	LYS	N-CA	6.30	1.54	1.45
1	A	113	LYS	CE-NZ	-6.30	1.30	1.49
1	A	171	GLY	C-O	6.28	1.33	1.24
1	A	237	PRO	CA-CB	-6.14	1.45	1.53
1	A	160	VAL	N-CA	-6.11	1.39	1.46
1	A	60	LEU	CA-CB	6.02	1.64	1.53
1	A	239	GLU	CD-OE1	6.01	1.36	1.25
1	A	237	PRO	CA-C	5.99	1.60	1.52
1	A	253	ASN	C-N	5.99	1.41	1.33
1	A	58	ARG	CZ-NH1	-5.94	1.24	1.32
1	A	166	SER	CA-CB	-5.93	1.43	1.53
1	A	78	VAL	CA-CB	-5.80	1.46	1.55
1	A	233	GLY	N-CA	5.72	1.52	1.45
1	A	69	GLU	CG-CD	-5.69	1.37	1.52
1	A	254	ARG	C-O	-5.62	1.17	1.23
1	A	78	VAL	CB-CG2	-5.61	1.34	1.52
1	A	252	LYS	C-O	-5.58	1.18	1.24
1	A	25	GLY	C-O	5.54	1.28	1.23
1	A	69	GLU	CA-C	-5.51	1.45	1.52
1	A	100	LEU	CA-C	-5.47	1.45	1.52
1	A	76	LYS	N-CA	5.41	1.53	1.46
1	A	239	GLU	CD-OE2	5.38	1.35	1.25
1	A	45	LYS	CA-CB	-5.37	1.44	1.53
1	A	173	SER	C-N	-5.36	1.26	1.33
1	A	18	LYS	N-CA	5.34	1.52	1.46
1	A	41	ASP	N-CA	-5.30	1.41	1.46
1	A	254	ARG	N-CA	-5.28	1.39	1.45
1	A	260	PHE	N-CA	5.28	1.52	1.45
1	A	162	ASP	CG-OD1	5.18	1.35	1.25
1	A	185	LEU	CA-C	5.14	1.59	1.52
1	A	37	THR	CB-OG1	-5.12	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	VAL	C-N	-5.10	1.27	1.33
1	A	176	PHE	C-N	-5.08	1.26	1.33
1	A	46	PRO	N-CA	5.07	1.53	1.47

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	LYS	N-CA-C	18.08	136.46	114.04
1	A	236	GLU	O-C-N	-11.05	110.49	120.99
1	A	45	LYS	CA-C-N	-10.84	108.32	119.92
1	A	45	LYS	C-N-CA	-10.84	108.32	119.92
1	A	58	ARG	CA-CB-CG	10.64	135.39	114.10
1	A	55	THR	CA-CB-CG2	-8.95	95.28	110.50
1	A	37	THR	OG1-CB-CG2	-8.86	91.59	109.30
1	A	4	HIS	CA-CB-CG	8.71	122.51	113.80
1	A	39	LYS	CA-CB-CG	8.46	131.02	114.10
1	A	74	GLN	CB-CG-CD	-8.11	98.82	112.60
1	A	236	GLU	CA-C-O	8.11	129.70	121.27
1	A	58	ARG	CB-CA-C	-7.86	97.23	110.43
1	A	75	ASP	N-CA-CB	7.85	122.05	110.35
1	A	75	ASP	CB-CG-OD1	7.55	135.77	118.40
1	A	27	ARG	NE-CZ-NH2	-7.55	112.41	119.20
1	A	237	PRO	CB-CA-C	-7.39	101.38	111.21
1	A	4	HIS	N-CA-CB	7.26	122.84	110.50
1	A	130	ASP	CB-CG-OD1	7.24	135.06	118.40
1	A	76	LYS	CA-C-N	7.18	135.01	121.87
1	A	76	LYS	C-N-CA	7.18	135.01	121.87
1	A	159	LYS	CD-CE-NZ	6.98	134.23	111.90
1	A	27	ARG	NE-CZ-NH1	6.58	128.09	121.50
1	A	76	LYS	CG-CD-CE	6.54	126.34	111.30
1	A	169	THR	O-C-N	6.28	131.53	123.11
1	A	175	ASP	CB-CA-C	-6.21	99.42	109.72
1	A	76	LYS	CA-C-O	6.16	126.76	119.06
1	A	159	LYS	CG-CD-CE	6.09	125.31	111.30
1	A	78	VAL	CA-CB-CG1	6.03	120.65	110.40
1	A	171	GLY	N-CA-C	5.96	122.96	115.21
1	A	58	ARG	CG-CD-NE	-5.95	98.91	112.00
1	A	43	SER	CA-CB-OG	-5.70	99.69	111.10
1	A	76	LYS	CB-CA-C	-5.64	99.11	109.15
1	A	59	ILE	O-C-N	-5.33	117.39	123.10
1	A	177	THR	N-CA-C	5.17	118.53	110.32
1	A	175	ASP	OD1-CG-OD2	5.17	135.30	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	OD1-CG-OD2	-5.13	110.58	122.90
1	A	225	LYS	CB-CG-CD	5.13	123.10	111.30
1	A	253	ASN	CA-C-O	-5.11	115.66	122.51
1	A	235	GLY	N-CA-C	-5.08	108.30	115.32
1	A	37	THR	N-CA-CB	5.03	118.36	110.46
1	A	9	LYS	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	LYS	Mainchain
1	A	58	ARG	Sidechain

## 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	2105	0	2059	18	0
2	A	1	0	0	0	0
3	A	6	0	8	3	0
4	A	272	0	0	12	5
All	All	2384	0	2067	21	5

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 5.

All (21) 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)
3:A:302:GOL:C2	3:A:302:GOL:O2	1.63	1.46
1:A:76:LYS:O	4:A:401:HOH:O	1.98	0.81
1:A:57:LEU:HB2	4:A:504:HOH:O	1.90	0.70
1:A:4:HIS:HB2	4:A:649:HOH:O	1.96	0.65
1:A:238:GLU:HG2	4:A:501:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:GOL:O2	3:A:302:GOL:C3	2.46	0.61
1:A:36:HIS:ND1	4:A:402:HOH:O	2.08	0.60
3:A:302:GOL:C2	3:A:302:GOL:HO2	2.07	0.59
1:A:64[B]:HIS:HD2	4:A:579:HOH:O	1.87	0.57
1:A:47[B]:LEU:HD11	1:A:79:LEU:HD11	1.86	0.56
1:A:165:ASP:HB2	4:A:605:HOH:O	2.10	0.52
1:A:64[B]:HIS:CD2	4:A:579:HOH:O	2.62	0.51
1:A:4:HIS:CB	4:A:649:HOH:O	2.55	0.51
1:A:134:ALA:O	1:A:140:GLY:HA3	2.15	0.47
1:A:238:GLU:OE1	4:A:404:HOH:O	2.21	0.45
1:A:57:LEU:HD12	4:A:411:HOH:O	2.18	0.43
1:A:80:LYS:HB3	1:A:80:LYS:HE2	1.47	0.43
1:A:41:ASP:OD1	1:A:41:ASP:C	2.61	0.42
1:A:133:LYS:HZ2	1:A:133:LYS:HG2	1.69	0.42
1:A:67:ASN:HD22	1:A:94:HIS:HB3	1.85	0.41
1:A:57:LEU:CB	4:A:504:HOH:O	2.60	0.41

All (5) 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)
4:A:403:HOH:O	4:A:445:HOH:O[1_565]	1.79	0.41
4:A:442:HOH:O	4:A:650:HOH:O[2_646]	1.85	0.35
4:A:403:HOH:O	4:A:486:HOH:O[1_565]	1.89	0.31
4:A:519:HOH:O	4:A:643:HOH:O[2_645]	2.11	0.09
4:A:447:HOH:O	4:A:596:HOH:O[1_545]	2.17	0.03

## 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	264/260 (102%)	253 (96%)	11 (4%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	231/225 (103%)	226 (98%)	5 (2%)	45 10

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	75	ASP
1	A	80	LYS
1	A	187	GLU
1	A	213	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	137	GLN
1	A	249	GLN
1	A	255	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 2 ligands modelled in this entry, 1 is 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	GOL	A	302	-	5,5,5	3.68	4 (80%)	5,5,5	2.13	2 (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	GOL	A	302	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	GOL	O2-C2	6.86	1.63	1.43
3	A	302	GOL	C1-C2	-3.28	1.38	1.51
3	A	302	GOL	O3-C3	2.27	1.52	1.42
3	A	302	GOL	C3-C2	2.19	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	GOL	O1-C1-C2	-3.30	94.38	110.20
3	A	302	GOL	O2-C2-C3	-2.26	99.15	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	GOL	3	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	257/260 (98%)	-0.24	3 (1%) 76 78	6, 14, 30, 54	9 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	HIS	3.0
1	A	253	ASN	2.7
1	A	75	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

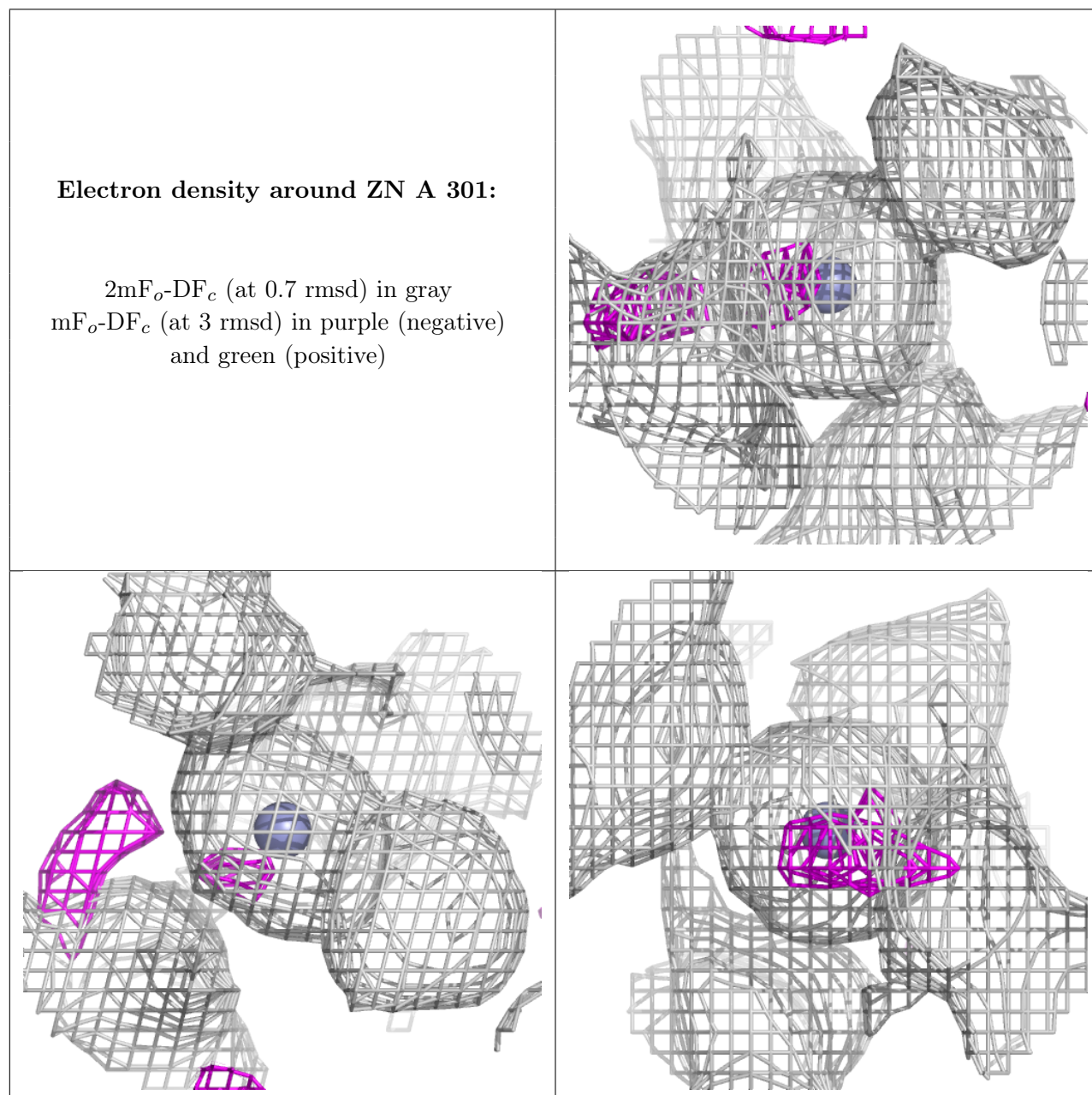
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	302	6/6	0.94	0.10	17,25,31,37	0
2	ZN	A	301	1/1	1.00	0.01	7,7,7,7	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.