



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 10:25 AM JST

PDB ID : 9KI3 / pdb\_00009ki3  
Title : apo- Carbonic Anhydrase II pH 7.8 2.5 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

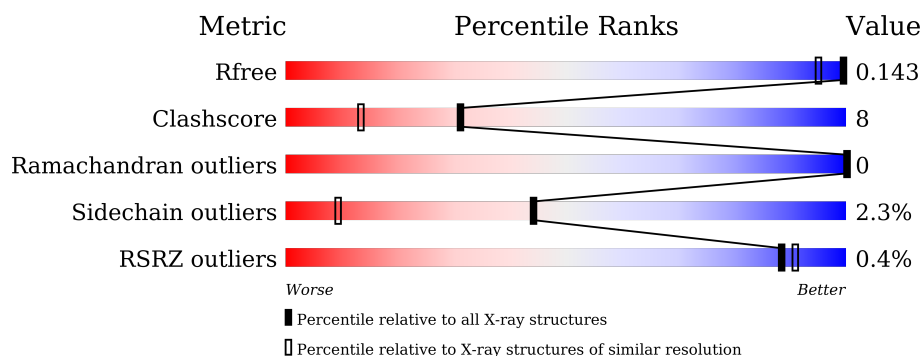
# 1 Overall quality at a glance

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	

## 2 Entry composition [i](#)

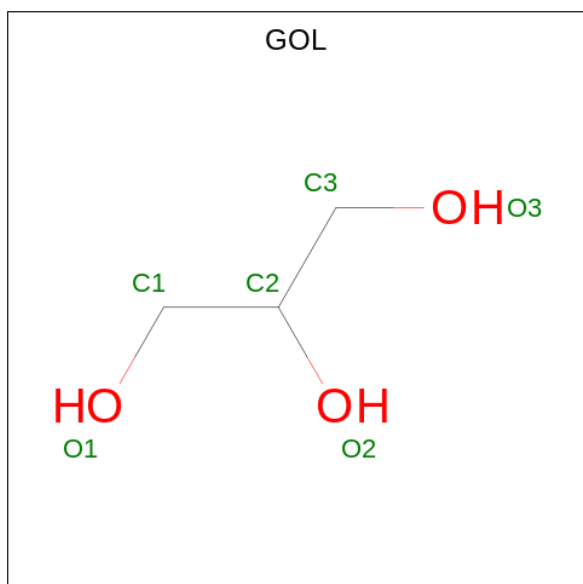
There are 3 unique types of molecules in this entry. The entry contains 2575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	257	2162	1380	373	407	2	0	13	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	407	407	407	0	0



- Molecule 1: Carbonic anhydrase 2

A134	Q137	G140	K154	K159	V160	V161	V163	L164	D175	K213	E214	S217	S220	L224	N230	E236	E239	P250	N253	K257	P260	K261	MET	SER	HIS	H4	G8	K9	H10	D19	E26	R27	D34	T35	H36	T37	A38	K39	L44	K45	P46	L47	D52	T55	L60	V68	E69	Q74	D75	K76	K80	G81	G82	D85	G86	T87	Y88	R89	Q92	S99	L100	T125	K127	Y128	G129	D130
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.16Å 41.49Å 72.47Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	30.00 – 1.20 30.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.20) 99.8 (30.00-1.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.119 , 0.140 0.126 , 0.143	Depositor DCC
$R_{free}$ test set	3780 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2575	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 6.74% 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

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	1.89	49/2224 (2.2%)	1.47	24/3015 (0.8%)

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 (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	LYS	C-N	15.69	1.53	1.33
1	A	37	THR	CA-CB	-13.89	1.34	1.54
1	A	45	LYS	CA-CB	-13.57	1.31	1.53
1	A	45	LYS	CA-C	-13.15	1.35	1.52
1	A	47	LEU	CB-CG	-11.82	1.29	1.53
1	A	47	LEU	N-CA	-11.56	1.30	1.45
1	A	76	LYS	C-N	-10.49	1.18	1.33
1	A	36	HIS	CB-CG	-9.21	1.37	1.50
1	A	36	HIS	CG-ND1	-9.05	1.28	1.38
1	A	161	VAL	CA-CB	8.87	1.65	1.54
1	A	8	GLY	N-CA	8.25	1.55	1.45
1	A	19	ASP	CG-OD2	-8.20	1.09	1.25
1	A	34	ASP	CG-OD2	-7.92	1.10	1.25
1	A	213	LYS	CE-NZ	7.82	1.72	1.49
1	A	236	GLU	CA-C	7.80	1.61	1.52
1	A	37	THR	CB-OG1	-7.76	1.31	1.43
1	A	137	GLN	CD-NE2	-7.56	1.17	1.33
1	A	239	GLU	CD-OE1	7.13	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	LYS	CA-C	6.93	1.60	1.52
1	A	213	LYS	CD-CE	6.77	1.72	1.52
1	A	19	ASP	CG-OD1	-6.75	1.12	1.25
1	A	38	ALA	C-N	-6.75	1.24	1.33
1	A	80	LYS	CA-CB	6.38	1.64	1.53
1	A	85	ASP	CA-C	6.37	1.60	1.52
1	A	39	LYS	CA-CB	-6.27	1.42	1.53
1	A	9	LYS	CA-CB	-6.15	1.43	1.53
1	A	39	LYS	N-CA	6.09	1.53	1.46
1	A	10	HIS	N-CA	-6.05	1.38	1.46
1	A	86	GLY	N-CA	-5.93	1.35	1.45
1	A	253	ASN	C-N	5.79	1.42	1.33
1	A	4	HIS	N-CA	5.77	1.57	1.46
1	A	47	LEU	CG-CD2	5.73	1.71	1.52
1	A	250	PRO	CA-CB	5.62	1.61	1.53
1	A	86	GLY	CA-C	5.61	1.59	1.52
1	A	175	ASP	CB-CG	5.59	1.66	1.52
1	A	230	ASN	N-CA	-5.54	1.39	1.46
1	A	36	HIS	CA-CB	-5.52	1.43	1.53
1	A	8	GLY	C-O	5.48	1.29	1.23
1	A	60	LEU	N-CA	-5.47	1.39	1.46
1	A	89	ARG	CB-CG	-5.38	1.36	1.52
1	A	36	HIS	C-O	5.35	1.31	1.24
1	A	164	LEU	CA-C	5.35	1.59	1.52
1	A	100	LEU	CG-CD2	-5.31	1.35	1.52
1	A	55	THR	CA-CB	5.21	1.62	1.53
1	A	87	THR	N-CA	-5.15	1.39	1.46
1	A	164	LEU	N-CA	-5.09	1.40	1.46
1	A	100	LEU	CA-C	-5.05	1.46	1.52
1	A	27[A]	ARG	CZ-NH1	5.04	1.39	1.32
1	A	27[B]	ARG	CZ-NH1	5.04	1.39	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LYS	N-CA-C	10.92	125.00	110.36
1	A	36	HIS	CB-CG-CD2	9.19	143.14	131.20
1	A	36	HIS	CB-CG-ND1	-9.04	109.13	122.70
1	A	213	LYS	CD-CE-NZ	9.01	140.72	111.90
1	A	47	LEU	CA-CB-CG	8.59	146.35	116.30
1	A	239	GLU	CA-CB-CG	-8.54	97.02	114.10
1	A	47	LEU	CB-CG-CD1	8.22	135.37	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LEU	CD1-CG-CD2	-7.88	93.46	110.80
1	A	239	GLU	CB-CG-CD	7.61	125.54	112.60
1	A	37	THR	OG1-CB-CG2	-7.17	94.96	109.30
1	A	45	LYS	CA-C-N	-7.08	112.34	119.92
1	A	45	LYS	C-N-CA	-7.08	112.34	119.92
1	A	89	ARG	CG-CD-NE	-6.80	97.05	112.00
1	A	75	ASP	N-CA-CB	6.75	120.29	110.58
1	A	9	LYS	CB-CA-C	-6.26	100.40	110.79
1	A	230	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	74	GLN	CA-C-O	-6.06	114.96	121.38
1	A	239	GLU	CG-CD-OE1	6.01	132.23	118.40
1	A	36	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	213	LYS	CG-CD-CE	-5.74	98.11	111.30
1	A	130	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	68	VAL	CB-CA-C	5.49	117.60	110.96
1	A	69	GLU	O-C-N	5.35	129.45	123.19
1	A	52	ASP	CB-CA-C	5.21	119.55	110.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	76	LYS	Mainchain
1	A	8	GLY	Mainchain

## 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	2162	0	2093	34	2
2	A	6	0	8	1	0
3	A	407	0	0	25	8
All	All	2575	0	2101	35	8

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 (35) 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:213:LYS:CE	1:A:213:LYS:NZ	1.72	1.49
1:A:46:PRO:HD2	3:A:617:HOH:O	1.21	1.34
1:A:27[A]:ARG:NH2	3:A:402:HOH:O	1.73	1.18
1:A:214[B]:GLU:OE1	3:A:403:HOH:O	1.76	0.99
1:A:27[A]:ARG:CZ	3:A:402:HOH:O	2.12	0.88
1:A:27[B]:ARG:NH1	3:A:404:HOH:O	2.02	0.87
1:A:175:ASP:HB3	3:A:517:HOH:O	1.77	0.85
1:A:27[A]:ARG:NH1	3:A:402:HOH:O	2.07	0.82
1:A:175:ASP:HB3	3:A:501:HOH:O	1.84	0.78
1:A:45:LYS:HB3	3:A:617:HOH:O	1.91	0.71
1:A:99:SER:C	1:A:100:LEU:HD12	2.17	0.69
1:A:26:GLU:OE2	3:A:405:HOH:O	2.14	0.65
1:A:162[A]:ASP:OD2	3:A:406:HOH:O	2.15	0.64
1:A:224:LEU:HD23	3:A:538:HOH:O	1.97	0.64
1:A:224:LEU:CD2	3:A:538:HOH:O	2.44	0.64
1:A:159:LYS:HE3	3:A:716:HOH:O	2.03	0.58
1:A:175:ASP:CB	3:A:501:HOH:O	2.49	0.56
1:A:100:LEU:HD12	1:A:100:LEU:N	2.20	0.55
1:A:127:LYS:NZ	3:A:416:HOH:O	2.43	0.52
1:A:127:LYS:HE2	1:A:128:TYR:CZ	2.48	0.49
1:A:257:LYS:HE3	3:A:459:HOH:O	2.14	0.46
1:A:45:LYS:O	1:A:82:GLY:HA2	2.16	0.46
1:A:46:PRO:CD	3:A:617:HOH:O	2.08	0.45
1:A:4:HIS:N	3:A:423:HOH:O	2.50	0.45
1:A:175:ASP:CG	3:A:501:HOH:O	2.58	0.45
1:A:36:HIS:ND1	3:A:407:HOH:O	2.16	0.44
1:A:134:ALA:O	1:A:140:GLY:HA3	2.18	0.42
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.54	0.42
1:A:154:LYS:HB2	1:A:217[C]:SER:O	2.20	0.42
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.50	0.41
1:A:44:LEU:HA	3:A:415:HOH:O	2.19	0.41
2:A:301:GOL:H11	3:A:422:HOH:O	2.18	0.41
1:A:213:LYS:HE2	3:A:737:HOH:O	2.19	0.41
1:A:10:HIS:ND1	3:A:412:HOH:O	2.36	0.41
1:A:80:LYS:HE3	1:A:80:LYS:HB2	1.94	0.40

All (8) 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)
3:A:411:HOH:O	3:A:495:HOH:O[1_545]	1.98	0.22
1:A:4:HIS:CE1	3:A:698:HOH:O[1_655]	2.05	0.15
3:A:673:HOH:O	3:A:676:HOH:O[2_645]	2.06	0.14
3:A:423:HOH:O	3:A:723:HOH:O[1_655]	2.09	0.11
3:A:514:HOH:O	3:A:706:HOH:O[2_655]	2.16	0.04
3:A:437:HOH:O	3:A:515:HOH:O[2_545]	2.17	0.03
1:A:4:HIS:ND1	3:A:698:HOH:O[1_655]	2.18	0.02
3:A:651:HOH:O	3:A:660:HOH:O[1_655]	2.19	0.01

## 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	269/260 (104%)	259 (96%)	10 (4%)	0	100	100

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	236/225 (105%)	230 (98%)	6 (2%)	42	8

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS

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Mol	Chain	Res	Type
1	A	47	LEU
1	A	80	LYS
1	A	92	GLN
1	A	220[A]	SER
1	A	220[B]	SER

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	249	GLN
1	A	253	ASN

### 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](#)

1 ligand is modelled in this entry.

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	$\# Z  > 2$
2	GOL	A	301	-	5,5,5	3.35	2 (40%)	5,5,5	1.71	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
2	GOL	A	301	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GOL	O2-C2	6.53	1.62	1.43
2	A	301	GOL	C1-C2	-3.13	1.38	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GOL	O1-C1-C2	-2.49	98.24	110.20
2	A	301	GOL	O2-C2-C3	-2.19	99.50	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	76:LYS	C	77:ALA	N	1.18

## 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%)	-0.33	1 (0%) 88 91	4, 13, 31, 56	14 (5%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	HIS	3.0

### 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
2	GOL	A	301	6/6	0.94	0.09	15,22,24,32	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.