



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:31 PM UTC

PDB ID : 5V8O / pdb_00005v8o
Title : Discovery of a high affinity inhibitor of cGAS
Authors : Hall, J.
Deposited on : 2017-03-22
Resolution : 3.10 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) : 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

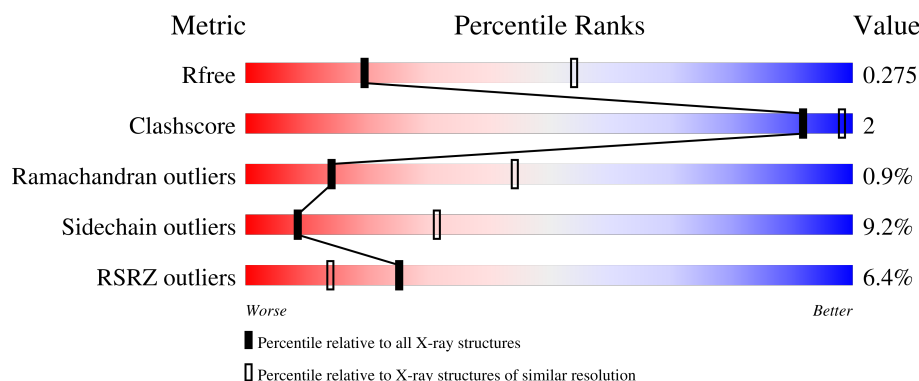
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	362	6% 84% 11% ..
1	B	362	7% 86% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10489 atoms, of which 5049 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.

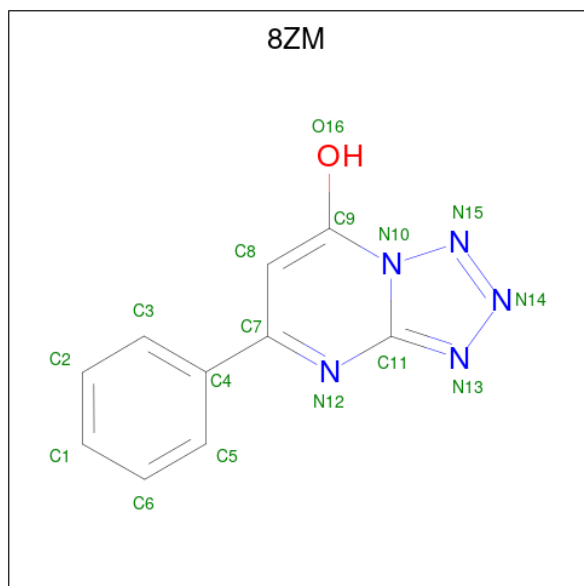
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	351	Total	C	H	N	O	S	0	0	0
			5298	1742	2576	469	497	14			
1	B	349	Total	C	H	N	O	S	0	0	0
			5109	1692	2466	449	489	13			

- 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		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5-phenyltetrazolo[1,5-a]pyrimidin-7-ol (CCD ID: 8ZM) (formula: C₁₀H₇N₅O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 23 10 7 5 1	0	0
3	B	1	Total C N O 16 10 5 1	0	0
3	B	1	Total C N O 16 10 5 1	0	0

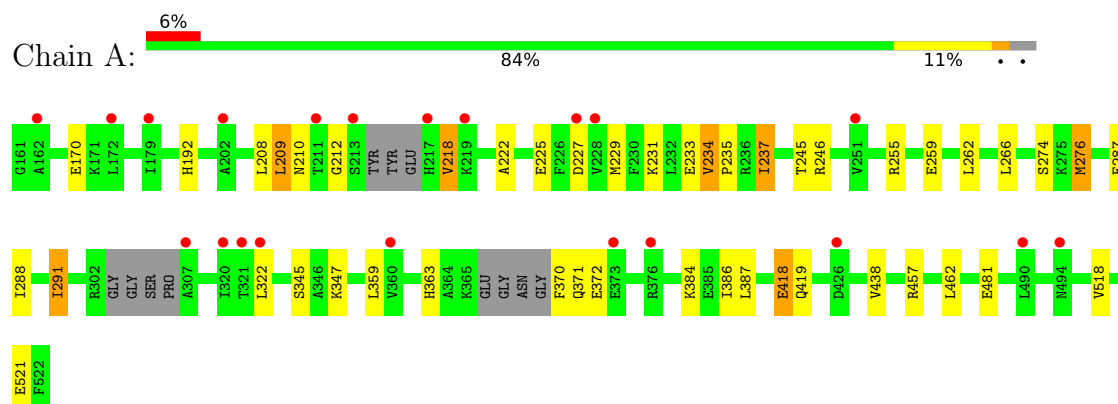
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	11	Total O 11 11	0	0

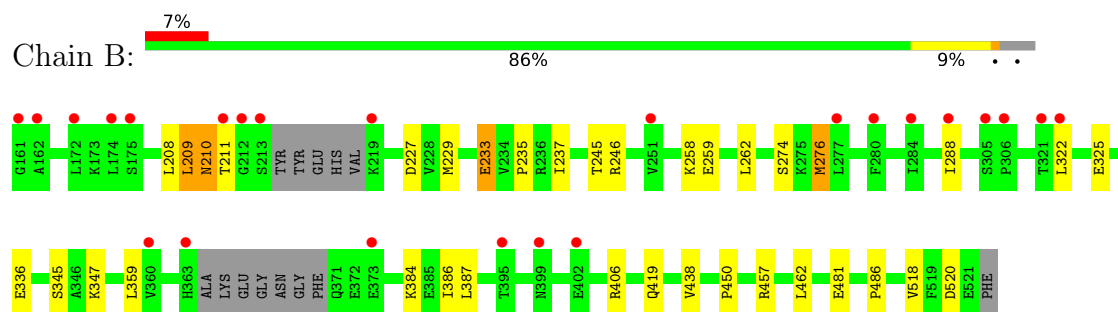
3 Residue-property plots

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 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: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.73Å 48.06Å 89.49Å 90.00° 110.65° 90.00°	Depositor
Resolution (Å)	52.31 – 3.10 52.31 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (52.31-3.10) 96.9 (52.31-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.224 , 0.252 0.239 , 0.275	Depositor DCC
R_{free} test set	731 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	90.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10489	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, 8ZM

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	0.88	0/2774	1.23	8/3746 (0.2%)
1	B	0.87	0/2694	1.22	7/3649 (0.2%)
All	All	0.88	0/5468	1.23	15/7395 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASN	N-CA-C	12.22	128.63	111.52
1	A	210	ASN	N-CA-C	10.12	125.49	111.92
1	B	209	LEU	CB-CA-C	-9.36	93.71	110.37
1	B	209	LEU	CA-C-N	8.08	133.57	122.34
1	B	209	LEU	C-N-CA	8.08	133.57	122.34
1	B	245	THR	N-CA-C	-7.36	97.26	108.96
1	A	245	THR	N-CA-C	-7.32	97.30	109.46
1	A	212	GLY	CA-C-N	6.48	133.37	121.70
1	A	212	GLY	C-N-CA	6.48	133.37	121.70
1	A	234	VAL	CB-CA-C	6.38	116.32	110.13
1	A	418	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	218	VAL	CB-CA-C	-5.55	102.19	111.29
1	B	520	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	211	THR	N-CA-C	5.22	119.65	113.28
1	A	170	GLU	CB-CG-CD	5.12	121.31	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	2722	2576	2592	11	0
1	B	2643	2466	2473	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	7	0	0	0
3	B	32	0	0	0	0
4	A	14	0	0	0	0
4	B	11	0	0	2	0
All	All	5440	5049	5065	17	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 2.

All (17) 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:B:406:ARG:NH2	4:B:701:HOH:O	2.34	0.60
1:A:209:LEU:CD2	1:A:209:LEU:O	2.50	0.59
1:A:209:LEU:O	1:A:209:LEU:HD22	2.08	0.54
1:B:450:PRO:C	4:B:701:HOH:O	2.52	0.52
1:A:370:PHE:CG	1:A:370:PHE:O	2.63	0.51
1:A:234:VAL:HG23	1:A:237:ILE:HG21	1.92	0.50
1:A:287:GLU:O	1:A:291:ILE:HG23	2.11	0.50
1:A:222:ALA:HB1	1:A:225:GLU:HB2	1.95	0.48
1:B:419:GLN:HB3	1:B:518:VAL:HG22	1.95	0.48
1:A:234:VAL:CG2	1:A:237:ILE:HG21	2.44	0.47
1:A:262:LEU:HD23	1:A:276:MET:HE2	1.95	0.47
1:B:262:LEU:HD23	1:B:276:MET:HE2	1.95	0.47
1:B:336:GLU:HG2	1:B:486:PRO:HG2	1.98	0.46
1:A:192:HIS:CE1	1:A:291:ILE:HG22	2.52	0.45
1:B:233:GLU:HA	1:B:325:GLU:HB3	2.03	0.41
1:A:419:GLN:HB3	1:A:518:VAL:HG22	2.02	0.41
1:A:363:HIS:CG	1:A:372:GLU:HA	2.56	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	343/362 (95%)	325 (95%)	14 (4%)	4 (1%)	10	37
1	B	343/362 (95%)	322 (94%)	19 (6%)	2 (1%)	21	52
All	All	686/724 (95%)	647 (94%)	33 (5%)	6 (1%)	14	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	VAL
1	A	235	PRO
1	A	345	SER
1	B	345	SER
1	A	521	GLU
1	B	235	PRO

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	280/334 (84%)	253 (90%)	27 (10%)	8	30
1	B	266/334 (80%)	243 (91%)	23 (9%)	10	34
All	All	546/668 (82%)	496 (91%)	50 (9%)	8	31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	209	LEU
1	A	227	ASP
1	A	229	MET
1	A	231	LYS
1	A	233	GLU
1	A	237	ILE
1	A	246	ARG
1	A	255	ARG
1	A	259	GLU
1	A	266	LEU
1	A	274	SER
1	A	276	MET
1	A	288	ILE
1	A	291	ILE
1	A	322	LEU
1	A	347	LYS
1	A	359	LEU
1	A	371	GLN
1	A	384	LYS
1	A	386	ILE
1	A	387	LEU
1	A	418	GLU
1	A	438	VAL
1	A	457	ARG
1	A	462	LEU
1	A	481	GLU
1	B	208	LEU
1	B	209	LEU
1	B	210	ASN
1	B	227	ASP
1	B	229	MET
1	B	233	GLU
1	B	237	ILE
1	B	246	ARG
1	B	258	LYS
1	B	259	GLU
1	B	274	SER
1	B	276	MET
1	B	288	ILE
1	B	322	LEU
1	B	347	LYS
1	B	359	LEU

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Mol	Chain	Res	Type
1	B	384	LYS
1	B	386	ILE
1	B	387	LEU
1	B	438	VAL
1	B	457	ARG
1	B	462	LEU
1	B	481	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	260	ASN
1	A	351	GLN
1	A	448	GLN
1	A	451	GLN
1	A	466	ASN
1	B	210	ASN
1	B	260	ASN
1	B	351	GLN
1	B	448	GLN
1	B	451	GLN
1	B	466	ASN
1	B	507	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	8ZM	B	603	-	17,18,18	0.51	0	21,25,25	0.89	1 (4%)
3	8ZM	A	602	-	17,18,18	0.46	0	21,25,25	0.95	1 (4%)
3	8ZM	B	602	-	17,18,18	0.38	0	21,25,25	0.63	0

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	8ZM	B	603	-	-	0/4/4/4	0/3/3/3
3	8ZM	A	602	-	-	0/4/4/4	0/3/3/3
3	8ZM	B	602	-	-	0/4/4/4	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	8ZM	C7-N12-C11	3.08	120.55	117.06
3	B	603	8ZM	C7-N12-C11	2.88	120.32	117.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 95th 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 ²)	Q < 0.9
1	A	351/362 (96%)	0.45	21 (5%)	27 15	55, 97, 150, 219	0
1	B	349/362 (96%)	0.48	24 (6%)	23 12	54, 106, 214, 246	0
All	All	700/724 (96%)	0.46	45 (6%)	25 14	54, 101, 196, 246	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	THR	7.4
1	B	305	SER	6.3
1	B	213	SER	5.6
1	B	280	PHE	4.5
1	A	217	HIS	4.3
1	B	251	VAL	4.1
1	A	494	ASN	4.0
1	B	211	THR	4.0
1	A	322	LEU	3.9
1	B	284	ILE	3.3
1	B	322	LEU	3.3
1	A	213	SER	3.3
1	B	402	GLU	3.2
1	B	288	ILE	3.1
1	B	161	GLY	3.0
1	B	399	ASN	2.9
1	B	360	VAL	2.8
1	A	227	ASP	2.7
1	B	162	ALA	2.7
1	A	490	LEU	2.7
1	A	228	VAL	2.7
1	A	179	ILE	2.6
1	B	219	LYS	2.6
1	B	212	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	360	VAL	2.5
1	A	320	ILE	2.4
1	A	376	ARG	2.4
1	B	373	GLU	2.4
1	B	321	THR	2.4
1	B	174	LEU	2.3
1	B	306	PRO	2.3
1	A	162	ALA	2.3
1	A	172	LEU	2.3
1	A	202	ALA	2.2
1	A	426	ASP	2.2
1	B	363	HIS	2.2
1	A	211	THR	2.1
1	A	251	VAL	2.1
1	B	395	THR	2.1
1	A	373	GLU	2.1
1	B	175	SER	2.1
1	A	219	LYS	2.0
1	A	307	ALA	2.0
1	B	172	LEU	2.0
1	B	277	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	8ZM	A	602	16/16	0.75	0.16	122,125,126,126	0
3	8ZM	B	603	16/16	0.83	0.18	119,123,128,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	8ZM	B	602	16/16	0.86	0.14	99,103,106,107	0
2	ZN	B	601	1/1	0.99	0.06	76,76,76,76	0
2	ZN	A	601	1/1	0.99	0.07	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.