



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:50 AM BST

PDB ID : 5V8O  
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](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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

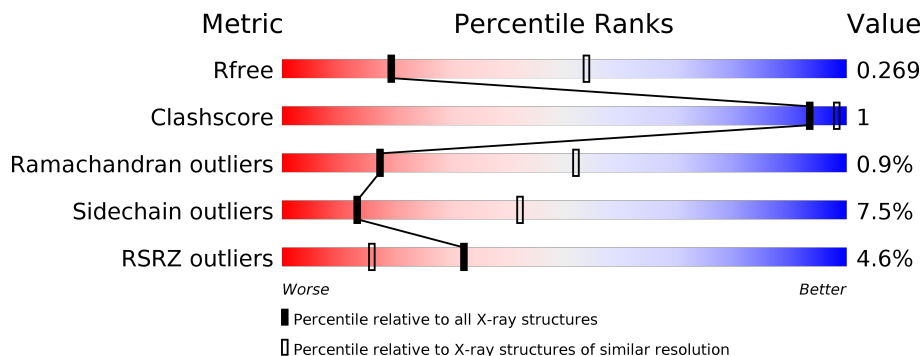
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 on 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	362	 2% 86% 10% ..
1	B	362	 6% 89% 7% ..

## 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.

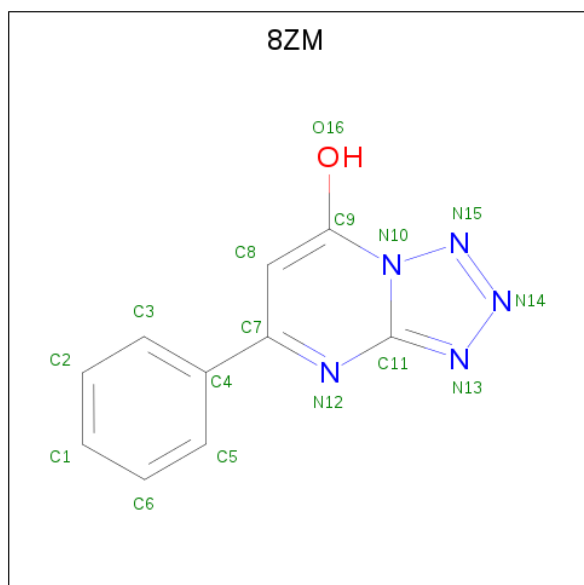
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 5-phenyltetrazolo[1,5-a]pyrimidin-7-ol (three-letter code: 8ZM) (formula: C<sub>10</sub>H<sub>7</sub>N<sub>5</sub>O).



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

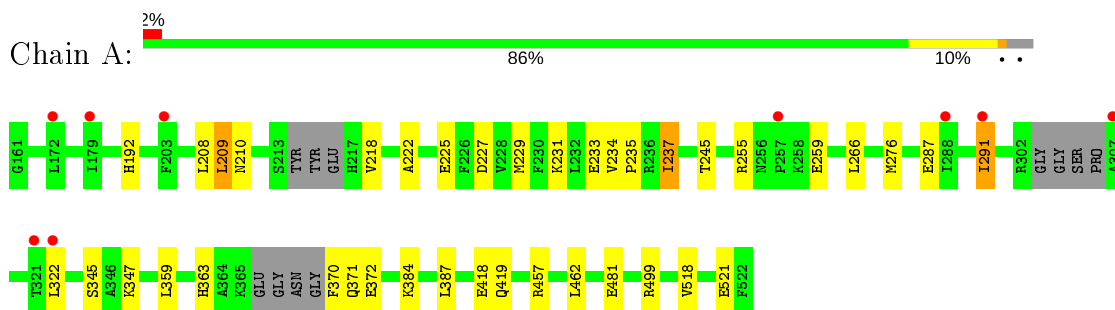
- Molecule 4 is water.

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

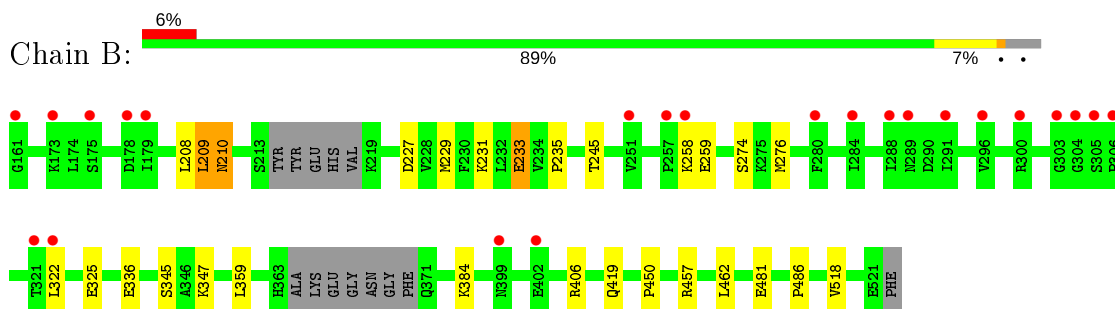
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.13Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.224 , 0.252 0.233 , 0.269	Depositor DCC
$R_{free}$ test set	731 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.5	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtrriage'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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8ZM, 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	0.50	0/2774	0.69	2/3746 (0.1%)
1	B	0.49	0/2694	0.67	3/3649 (0.1%)
All	All	0.50	0/5468	0.68	5/7395 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	LEU	CB-CA-C	-8.68	93.71	110.20
1	B	210	ASN	N-CA-C	6.53	128.63	111.00
1	A	210	ASN	N-CA-C	5.37	125.49	111.00
1	B	245	THR	N-CA-C	-5.09	97.26	111.00
1	A	245	THR	N-CA-C	-5.07	97.30	111.00

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	2722	2576	2592	10	0
1	B	2643	2466	2473	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15	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 1.

All (15) 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:O	1:A:209:LEU:CD2	2.50	0.59
1:A:209:LEU:O	1:A:209:LEU:HD22	2.08	0.54
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:450:PRO:C	4:B:701:HOH:O	2.52	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: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 [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	343/362 (95%)	325 (95%)	14 (4%)	4 (1%)	13	44
1	B	343/362 (95%)	322 (94%)	19 (6%)	2 (1%)	25	59
All	All	686/724 (95%)	647 (94%)	33 (5%)	6 (1%)	17	52

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 [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	280/334 (84%)	257 (92%)	23 (8%)	11	38
1	B	266/334 (80%)	248 (93%)	18 (7%)	16	45
All	All	546/668 (82%)	505 (92%)	41 (8%)	13	42

All (41) 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	255	ARG
1	A	259	GLU
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	276	MET
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	387	LEU
1	A	418	GLU
1	A	457	ARG
1	A	462	LEU
1	A	481	GLU
1	A	499	ARG
1	B	208	LEU
1	B	209	LEU
1	B	210	ASN
1	B	227	ASP
1	B	229	MET
1	B	231	LYS
1	B	233	GLU
1	B	258	LYS
1	B	259	GLU
1	B	274	SER
1	B	276	MET
1	B	322	LEU
1	B	347	LYS
1	B	359	LEU
1	B	384	LYS
1	B	457	ARG
1	B	462	LEU
1	B	481	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	A	602	-	13,18,18	0.95	1 (7%)	16,25,25	1.66	3 (18%)
3	8ZM	B	603	-	13,18,18	0.91	1 (7%)	16,25,25	1.27	2 (12%)
3	8ZM	B	602	-	13,18,18	0.99	1 (7%)	16,25,25	1.42	3 (18%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	8ZM	C8-C7	3.05	1.44	1.39
3	B	602	8ZM	C8-C7	3.00	1.44	1.39
3	B	603	8ZM	C8-C7	3.00	1.44	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	8ZM	C7-C8-C9	5.41	120.45	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	8ZM	C7-C8-C9	4.65	119.94	116.80
3	B	603	8ZM	C7-C8-C9	3.22	118.97	116.80
3	B	603	8ZM	O16-C9-C8	2.47	128.56	121.91
3	B	602	8ZM	O16-C9-C8	2.23	127.91	121.91
3	A	602	8ZM	O16-C9-C8	2.04	127.40	121.91
3	A	602	8ZM	C8-C7-N12	-2.01	120.40	122.23
3	B	602	8ZM	N13-N14-N15	2.00	112.42	110.11

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, 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	351/362 (96%)	0.10	9 (2%) 56 33	56, 98, 150, 217	0
1	B	349/362 (96%)	0.27	23 (6%) 18 7	53, 105, 214, 247	0
All	All	700/724 (96%)	0.18	32 (4%) 32 16	53, 101, 195, 247	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	SER	11.3
1	B	288	ILE	5.7
1	A	321	THR	4.4
1	B	251	VAL	4.4
1	B	304	GLY	4.3
1	B	175	SER	4.2
1	B	179	ILE	3.5
1	A	179	ILE	3.3
1	B	284	ILE	3.1
1	A	322	LEU	3.1
1	A	257	PRO	3.0
1	A	307	ALA	3.0
1	A	172	LEU	2.9
1	B	296	VAL	2.9
1	A	288	ILE	2.9
1	B	399	ASN	2.8
1	B	258	LYS	2.6
1	B	280	PHE	2.6
1	B	402	GLU	2.5
1	B	306	PRO	2.5
1	B	321	THR	2.4
1	A	291	ILE	2.4
1	A	203	PHE	2.4
1	B	291	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	173	LYS	2.3
1	B	289	ASN	2.3
1	B	303	GLY	2.2
1	B	178	ASP	2.2
1	B	161	GLY	2.2
1	B	322	LEU	2.1
1	B	300	ARG	2.1
1	B	257	PRO	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 monosaccharides 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	8ZM	A	602	16/16	0.84	0.24	122,125,126,126	0
3	8ZM	B	603	16/16	0.86	0.37	119,123,128,129	0
3	8ZM	B	602	16/16	0.90	0.25	99,103,106,107	0
2	ZN	A	601	1/1	0.99	0.19	78,78,78,78	0
2	ZN	B	601	1/1	0.99	0.18	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.