



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:04 pm BST

PDB ID : 6NIP  
Title : Crystal structure of a human anti-ZIKV-DENV neutralizing antibody MZ1 in complex with ZIKV E glycoprotein  
Authors : Sankhala, R.S.; Dussupt, V.; Donofrio, G.; Choe, M.; Modjarrad, K.; Michael, N.L.; Krebs, S.J.; Joyce, M.G.  
Deposited on : 2018-12-31  
Resolution : 4.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

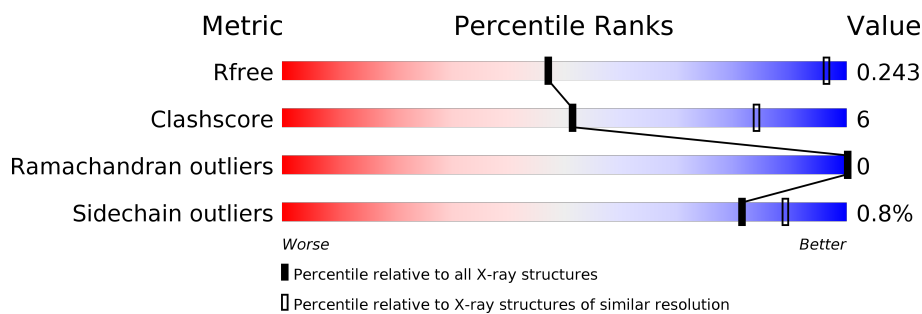
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.16 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	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	225	83% 15% .
1	H	225	85% 13% .
2	B	216	83% 16% .
2	L	216	89% 10% .
3	E	447	75% 14% 11%
3	Z	447	75% 14% 11%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12632 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 MZ1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	2	0
			1663	1049	273	332	9			
1	H	221	Total	C	N	O	S	0	2	0
			1663	1049	273	332	9			

- Molecule 2 is a protein called MZ1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1600	997	274	325	4			
2	L	214	Total	C	N	O	S	0	0	0
			1600	997	274	325	4			

- Molecule 3 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			
3	E	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	406	GLY	-	expression tag	UNP A0A024B7W1
Z	407	PRO	-	expression tag	UNP A0A024B7W1
Z	408	LEU	-	expression tag	UNP A0A024B7W1
Z	409	GLU	-	expression tag	UNP A0A024B7W1
Z	410	VAL	-	expression tag	UNP A0A024B7W1
Z	411	LEU	-	expression tag	UNP A0A024B7W1
Z	412	PHE	-	expression tag	UNP A0A024B7W1
Z	413	GLN	-	expression tag	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	414	GLY	-	expression tag	UNP A0A024B7W1
Z	415	PRO	-	expression tag	UNP A0A024B7W1
Z	416	GLY	-	expression tag	UNP A0A024B7W1
Z	417	SER	-	expression tag	UNP A0A024B7W1
Z	418	ALA	-	expression tag	UNP A0A024B7W1
Z	419	TRP	-	expression tag	UNP A0A024B7W1
Z	420	SER	-	expression tag	UNP A0A024B7W1
Z	421	HIS	-	expression tag	UNP A0A024B7W1
Z	422	PRO	-	expression tag	UNP A0A024B7W1
Z	423	GLN	-	expression tag	UNP A0A024B7W1
Z	424	PHE	-	expression tag	UNP A0A024B7W1
Z	425	GLU	-	expression tag	UNP A0A024B7W1
Z	426	LYS	-	expression tag	UNP A0A024B7W1
Z	427	GLY	-	expression tag	UNP A0A024B7W1
Z	428	GLY	-	expression tag	UNP A0A024B7W1
Z	429	GLY	-	expression tag	UNP A0A024B7W1
Z	430	SER	-	expression tag	UNP A0A024B7W1
Z	431	GLY	-	expression tag	UNP A0A024B7W1
Z	432	GLY	-	expression tag	UNP A0A024B7W1
Z	433	GLY	-	expression tag	UNP A0A024B7W1
Z	434	SER	-	expression tag	UNP A0A024B7W1
Z	435	GLY	-	expression tag	UNP A0A024B7W1
Z	436	GLY	-	expression tag	UNP A0A024B7W1
Z	437	GLY	-	expression tag	UNP A0A024B7W1
Z	438	SER	-	expression tag	UNP A0A024B7W1
Z	439	ALA	-	expression tag	UNP A0A024B7W1
Z	440	TRP	-	expression tag	UNP A0A024B7W1
Z	441	SER	-	expression tag	UNP A0A024B7W1
Z	442	HIS	-	expression tag	UNP A0A024B7W1
Z	443	PRO	-	expression tag	UNP A0A024B7W1
Z	444	GLN	-	expression tag	UNP A0A024B7W1
Z	445	PHE	-	expression tag	UNP A0A024B7W1
Z	446	GLU	-	expression tag	UNP A0A024B7W1
Z	447	LYS	-	expression tag	UNP A0A024B7W1
E	406	GLY	-	expression tag	UNP A0A024B7W1
E	407	PRO	-	expression tag	UNP A0A024B7W1
E	408	LEU	-	expression tag	UNP A0A024B7W1
E	409	GLU	-	expression tag	UNP A0A024B7W1
E	410	VAL	-	expression tag	UNP A0A024B7W1
E	411	LEU	-	expression tag	UNP A0A024B7W1
E	412	PHE	-	expression tag	UNP A0A024B7W1
E	413	GLN	-	expression tag	UNP A0A024B7W1

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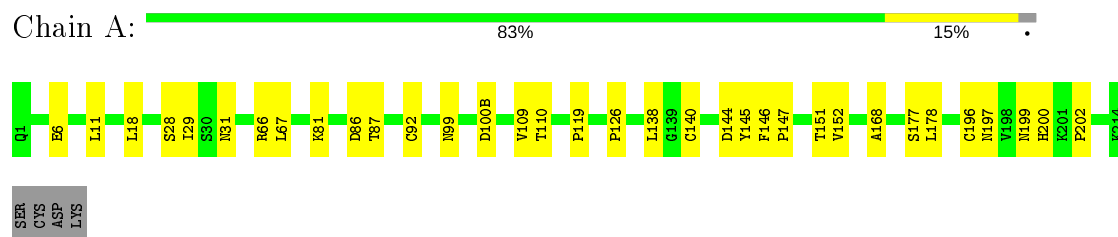
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Chain	Residue	Modelled	Actual	Comment	Reference
E	414	GLY	-	expression tag	UNP A0A024B7W1
E	415	PRO	-	expression tag	UNP A0A024B7W1
E	416	GLY	-	expression tag	UNP A0A024B7W1
E	417	SER	-	expression tag	UNP A0A024B7W1
E	418	ALA	-	expression tag	UNP A0A024B7W1
E	419	TRP	-	expression tag	UNP A0A024B7W1
E	420	SER	-	expression tag	UNP A0A024B7W1
E	421	HIS	-	expression tag	UNP A0A024B7W1
E	422	PRO	-	expression tag	UNP A0A024B7W1
E	423	GLN	-	expression tag	UNP A0A024B7W1
E	424	PHE	-	expression tag	UNP A0A024B7W1
E	425	GLU	-	expression tag	UNP A0A024B7W1
E	426	LYS	-	expression tag	UNP A0A024B7W1
E	427	GLY	-	expression tag	UNP A0A024B7W1
E	428	GLY	-	expression tag	UNP A0A024B7W1
E	429	GLY	-	expression tag	UNP A0A024B7W1
E	430	SER	-	expression tag	UNP A0A024B7W1
E	431	GLY	-	expression tag	UNP A0A024B7W1
E	432	GLY	-	expression tag	UNP A0A024B7W1
E	433	GLY	-	expression tag	UNP A0A024B7W1
E	434	SER	-	expression tag	UNP A0A024B7W1
E	435	GLY	-	expression tag	UNP A0A024B7W1
E	436	GLY	-	expression tag	UNP A0A024B7W1
E	437	GLY	-	expression tag	UNP A0A024B7W1
E	438	SER	-	expression tag	UNP A0A024B7W1
E	439	ALA	-	expression tag	UNP A0A024B7W1
E	440	TRP	-	expression tag	UNP A0A024B7W1
E	441	SER	-	expression tag	UNP A0A024B7W1
E	442	HIS	-	expression tag	UNP A0A024B7W1
E	443	PRO	-	expression tag	UNP A0A024B7W1
E	444	GLN	-	expression tag	UNP A0A024B7W1
E	445	PHE	-	expression tag	UNP A0A024B7W1
E	446	GLU	-	expression tag	UNP A0A024B7W1
E	447	LYS	-	expression tag	UNP A0A024B7W1

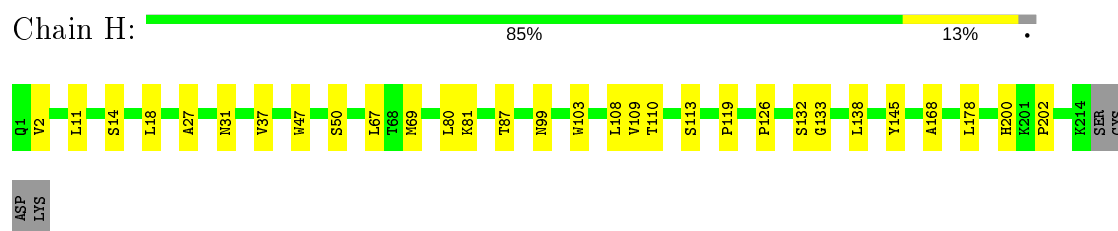
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

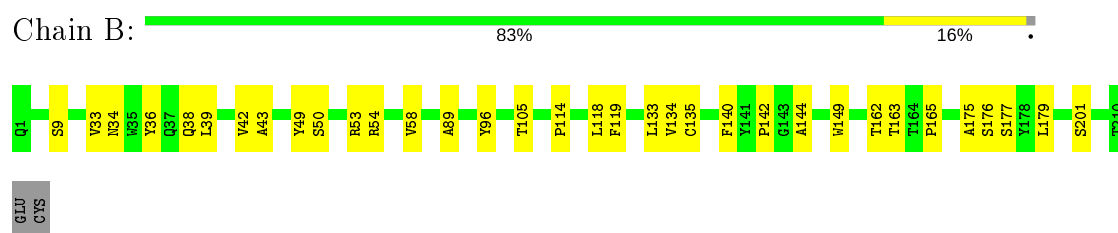
- Molecule 1: MZ1 Heavy chain



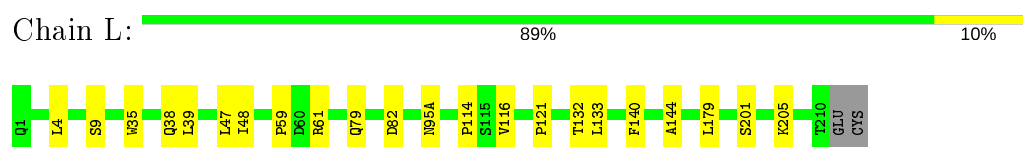
- Molecule 1: MZ1 Heavy chain



- Molecule 2: MZ1 Light Chain

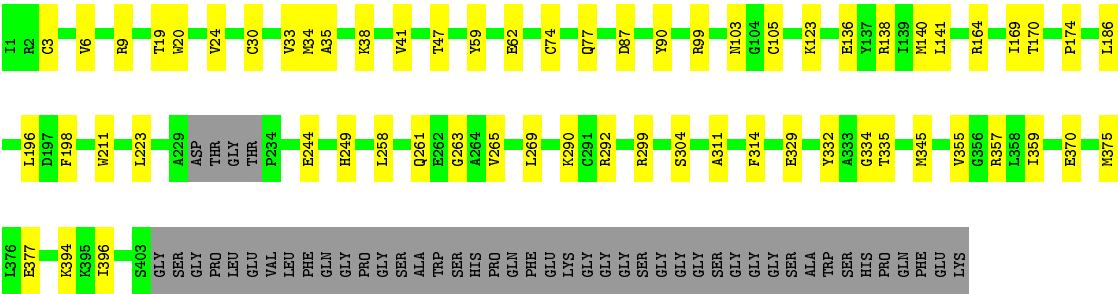


- Molecule 2: MZ1 Light Chain

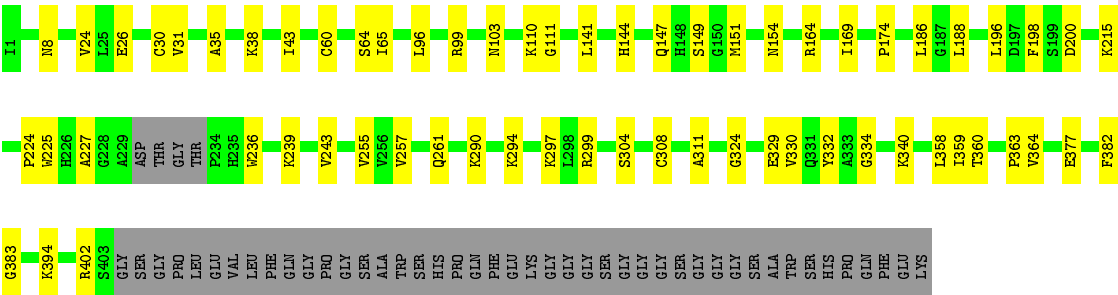


- Molecule 3: Envelope protein E





● Molecule 3: Envelope protein E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	417.33Å 69.30Å 212.58Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	14.99 – 4.16 49.34 – 4.21	Depositor EDS
% Data completeness (in resolution range)	70.1 (14.99-4.16) 70.1 (49.34-4.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.188 , 0.237 0.195 , 0.243	Depositor DCC
$R_{free}$ test set	1456 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	12632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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](#)

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	0.31	0/1704	0.51	0/2326
1	H	0.30	0/1704	0.53	0/2326
2	B	0.31	0/1638	0.52	0/2238
2	L	0.31	0/1638	0.50	0/2238
3	E	0.28	0/3117	0.48	0/4220
3	Z	0.29	0/3117	0.49	0/4220
All	All	0.30	0/12918	0.50	0/17568

There are no bond length outliers.

There are no bond angle outliers.

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	1663	0	1624	20	0
1	H	1663	0	1624	20	0
2	B	1600	0	1558	18	0
2	L	1600	0	1558	14	0
3	E	3053	0	2987	37	0
3	Z	3053	0	2987	37	0
All	All	12632	0	12338	139	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 6.

The worst 5 of 139 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:119:PRO:HB3	1:A:145:TYR:HB3	1.66	0.75
3:Z:311:ALA:HB2	3:Z:394:LYS:HB3	1.72	0.72
2:B:36:TYR:HH	2:B:96:TYR:HH	1.36	0.71
2:L:121:PRO:HB3	2:L:132:THR:H	1.56	0.70
1:A:18:LEU:HD11	1:A:109:VAL:HG11	1.72	0.70

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	221/225 (98%)	214 (97%)	7 (3%)	0	100	100
1	H	221/225 (98%)	211 (96%)	10 (4%)	0	100	100
2	B	212/216 (98%)	195 (92%)	17 (8%)	0	100	100
2	L	212/216 (98%)	195 (92%)	17 (8%)	0	100	100
3	E	395/447 (88%)	382 (97%)	13 (3%)	0	100	100
3	Z	395/447 (88%)	379 (96%)	16 (4%)	0	100	100
All	All	1656/1776 (93%)	1576 (95%)	80 (5%)	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	193/195 (99%)	189 (98%)	4 (2%)	53	71
1	H	193/195 (99%)	193 (100%)	0	100	100
2	B	181/183 (99%)	179 (99%)	2 (1%)	73	84
2	L	181/183 (99%)	178 (98%)	3 (2%)	60	78
3	E	334/366 (91%)	331 (99%)	3 (1%)	78	88
3	Z	334/366 (91%)	332 (99%)	2 (1%)	86	92
All	All	1416/1488 (95%)	1402 (99%)	14 (1%)	81	86

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Z	30	CYS
3	Z	249	HIS
2	L	4	LEU
2	B	201	SER
3	E	330	VAL

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.