



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 10:05 AM EDT

PDB ID : 9DI4 / pdb\_00009di4  
Title : RMI1-RMI2 bound to cyclic peptide L4  
Authors : Bythell-Douglas, R.; Lau, Y.H.; Alcock, L.J.; Gao, T.; Deshpande, C.; Patel, K.  
Deposited on : 2024-09-05  
Resolution : 2.70 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

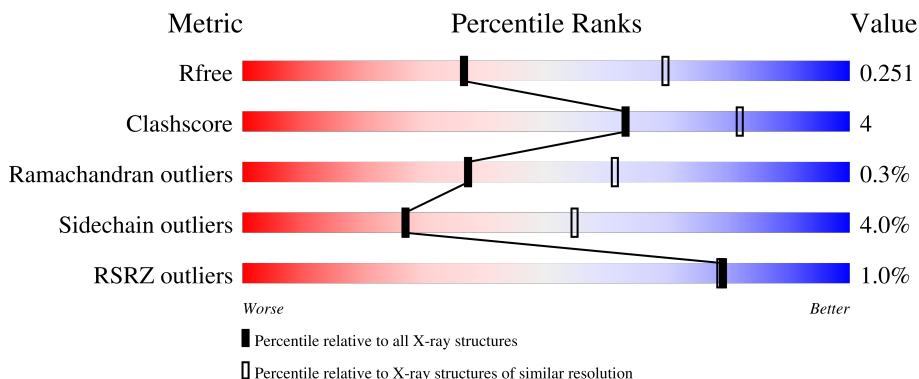
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


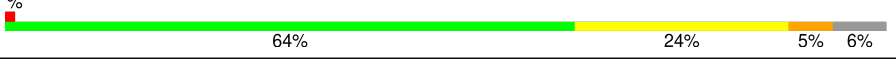
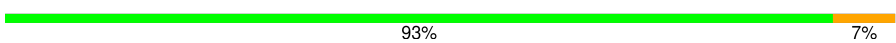
The reported resolution of this entry is 2.70 Å.

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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	152	
2	B	147	
3	C	15	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4655 atoms, of which 2334 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 RecQ-mediated genome instability protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	143	Total	C	H	N	O	S	31	0	0
			2275	717	1161	177	211	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	MET	-	initiating methionine	UNP Q9H9A7

- Molecule 2 is a protein called RecQ-mediated genome instability protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	138	Total	C	H	N	O	S	16	0	0
			2112	651	1062	202	188	9			

- Molecule 3 is a protein called L4 cyclic peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	15	Total	C	H	N	O	S	5	0	1
			228	80	111	15	21	1			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

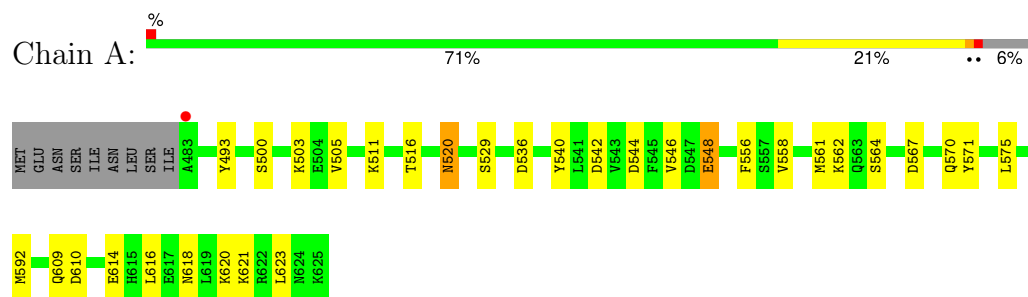
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	19	Total 19	O 19	0	0
5	C	4	Total 4	O 4	0	0

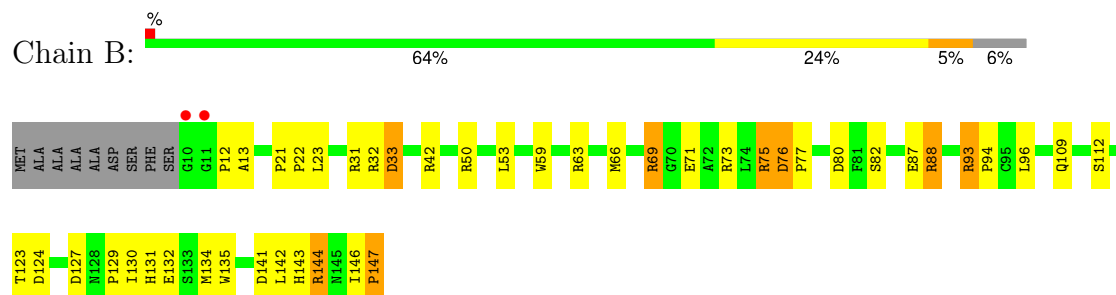
### 3 Residue-property plots [i](#)

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.

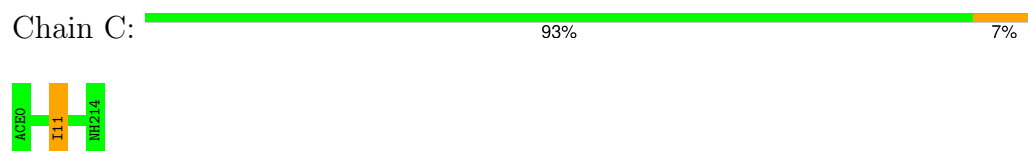
- Molecule 1: RecQ-mediated genome instability protein 1



- Molecule 2: RecQ-mediated genome instability protein 2



- Molecule 3: L4 cyclic peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.30Å 136.30Å 88.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 2.70 49.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.17-2.70) 99.8 (49.17-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.169 , 0.248 0.172 , 0.251	Depositor DCC
$R_{free}$ test set	674 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 27.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: NH2, ZN, ACE

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	1.04	0/1132	1.86	30/1527 (2.0%)
2	B	1.03	1/1073 (0.1%)	1.91	34/1453 (2.3%)
3	C	1.02	0/118	1.91	1/160 (0.6%)
All	All	1.03	1/2323 (0.0%)	1.89	65/3140 (2.1%)

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	1
2	B	0	6
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	HIS	CG-CD2	-5.08	1.30	1.35

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	MET	CG-SD-CE	10.78	124.62	100.90
1	A	579	GLN	N-CA-C	-7.63	102.91	111.07
2	B	87	GLU	CB-CG-CD	7.07	124.61	112.60
1	A	520	ASN	CB-CA-C	-7.04	97.46	109.51
2	B	76	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	592	MET	CG-SD-CE	-6.86	85.81	100.90
2	B	12	PRO	N-CA-CB	6.83	109.69	103.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ARG	N-CA-CB	6.57	121.59	110.49
1	A	570	GLN	CB-CA-C	6.54	121.98	110.85
1	A	621	LYS	CB-CG-CD	6.54	126.34	111.30
2	B	94	PRO	CB-CA-C	6.48	119.99	110.85
1	A	610	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	544	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	88	ARG	NE-CZ-NH1	-6.43	115.07	121.50
2	B	93	ARG	N-CA-CB	6.38	119.99	109.98
1	A	610	ASP	CB-CA-C	6.36	120.39	109.51
1	A	584	ASP	CB-CA-C	6.34	121.32	110.79
2	B	80	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	503	LYS	N-CA-CB	6.26	119.59	110.26
1	A	584	ASP	N-CA-C	-6.25	104.47	111.28
2	B	13	ALA	CA-C-N	-6.24	112.71	122.51
2	B	13	ALA	C-N-CA	-6.24	112.71	122.51
2	B	80	ASP	CB-CA-C	6.22	120.15	109.51
2	B	69	ARG	CA-CB-CG	6.15	126.40	114.10
2	B	144	ARG	N-CA-CB	6.12	119.76	110.28
2	B	93	ARG	N-CA-C	-6.06	101.94	109.64
1	A	583	ARG	NE-CZ-NH1	-5.99	115.52	121.50
1	A	516	THR	OG1-CB-CG2	-5.97	97.37	109.30
2	B	73	ARG	NE-CZ-NH2	5.94	124.55	119.20
2	B	23	LEU	N-CA-CB	-5.91	101.05	109.85
2	B	112	SER	O-C-N	-5.84	117.73	121.88
2	B	147	PRO	N-CA-CB	-5.83	96.58	103.00
1	A	609	GLN	N-CA-CB	-5.82	100.70	111.52
1	A	623	LEU	N-CA-CB	-5.78	101.06	110.42
1	A	511	LYS	CB-CG-CD	5.71	124.44	111.30
1	A	616	LEU	N-CA-CB	-5.66	101.81	110.01
1	A	620	LYS	CB-CG-CD	5.64	124.26	111.30
1	A	542	ASP	CB-CA-C	5.57	119.18	109.65
1	A	620	LYS	CB-CA-C	5.57	119.77	110.92
3	C	11	ILE	CA-C-O	5.52	122.94	119.51
2	B	94	PRO	N-CA-CB	-5.50	97.96	103.19
1	A	540	TYR	CA-CB-CG	5.46	123.72	113.90
2	B	71	GLU	CB-CG-CD	5.44	121.86	112.60
2	B	96	LEU	N-CA-CB	-5.44	101.90	110.49
1	A	567	ASP	CA-CB-CG	5.39	117.99	112.60
2	B	33	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	143	HIS	CB-CG-ND1	-5.33	114.71	122.70
2	B	132	GLU	N-CA-C	5.27	116.70	111.07
2	B	75	ARG	NE-CZ-NH1	-5.25	116.25	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	HIS	CB-CG-CD2	5.24	138.01	131.20
2	B	127	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	546	VAL	O-C-N	5.22	128.16	122.57
1	A	579	GLN	N-CA-CB	5.22	117.57	110.01
2	B	31	ARG	NE-CZ-NH1	-5.22	116.28	121.50
2	B	87	GLU	CG-CD-OE1	5.21	130.37	118.40
2	B	143	HIS	CA-CB-CG	-5.21	108.59	113.80
2	B	129	PRO	N-CD-CG	-5.18	95.44	103.20
1	A	505	VAL	O-C-N	5.12	127.90	122.67
1	A	614	GLU	CB-CA-C	5.12	119.39	110.68
1	A	562	LYS	N-CA-CB	5.12	117.60	109.82
1	A	558	VAL	N-CA-CB	5.10	114.43	110.45
2	B	13	ALA	N-CA-C	-5.08	102.87	110.23
2	B	124	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	556	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	548	GLU	CB-CG-CD	5.02	121.13	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	ARG	Sidechain
2	B	144	ARG	Sidechain
2	B	32	ARG	Sidechain
2	B	42	ARG	Sidechain
2	B	63	ARG	Sidechain
2	B	88	ARG	Sidechain
2	B	93	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	1114	1161	1159	8	0
2	B	1050	1062	1059	12	0
3	C	117	111	110	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	15	0	0	2	0
5	B	19	0	0	0	0
5	C	4	0	0	0	0
All	All	2321	2334	2328	18	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 4.

All (18) 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:548:GLU:OE2	5:A:801:HOH:O	2.14	0.65
1:A:571:TYR:CE2	1:A:575:LEU:HD21	2.36	0.61
2:B:50:ARG:NH1	2:B:146:ILE:O	2.33	0.61
2:B:53:LEU:HD21	2:B:146:ILE:HG21	1.84	0.57
2:B:76:ASP:HB2	2:B:77:PRO:CD	2.37	0.55
2:B:142:LEU:HD23	2:B:142:LEU:C	2.37	0.50
2:B:76:ASP:HB2	2:B:77:PRO:HD2	1.96	0.48
1:A:493:TYR:CE2	2:B:141:ASP:OD2	2.67	0.48
1:A:493:TYR:HE2	2:B:141:ASP:OD2	1.96	0.47
2:B:134:MET:O	2:B:135:TRP:C	2.58	0.46
1:A:561:MET:SD	1:A:561:MET:C	3.00	0.45
1:A:618:ASN:ND2	5:A:802:HOH:O	2.50	0.44
2:B:130:ILE:O	2:B:131:HIS:C	2.62	0.43
2:B:21:PRO:CB	2:B:22:PRO:CD	2.98	0.41
2:B:109:GLN:NE2	2:B:109:GLN:HA	2.36	0.41
1:A:561:MET:O	1:A:564:SER:OG	2.33	0.41
2:B:59:TRP:C	2:B:59:TRP:CD1	2.99	0.41
1:A:536:ASP:OD1	1:A:536:ASP:C	2.65	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	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
2	B	136/147 (92%)	126 (93%)	9 (7%)	1 (1%)	19	42
3	C	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	290/314 (92%)	274 (94%)	15 (5%)	1 (0%)	37	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	69	ARG

### 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	130/139 (94%)	126 (97%)	4 (3%)	35	64
2	B	110/115 (96%)	105 (96%)	5 (4%)	23	50
3	C	13/13 (100%)	12 (92%)	1 (8%)	10	26
All	All	253/267 (95%)	243 (96%)	10 (4%)	27	55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	SER
1	A	520	ASN
1	A	529	SER
1	A	583	ARG
2	B	33	ASP
2	B	75	ARG
2	B	82	SER
2	B	123	THR
2	B	147	PRO
3	C	11	ILE

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	563	GLN
2	B	145	ASN

### 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	143/152 (94%)	-0.64	1 (0%) 84 83	35, 55, 84, 113	0
2	B	138/147 (93%)	-0.44	2 (1%) 73 73	37, 61, 100, 124	0
3	C	13/15 (86%)	-0.77	0 100 100	38, 50, 60, 64	0
All	All	294/314 (93%)	-0.55	3 (1%) 79 79	35, 57, 97, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	10	GLY	5.9
2	B	11	GLY	3.0
1	A	483	ALA	2.4

### 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
4	ZN	A	701	1/1	0.99	0.10	70,70,70,70	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	B	201	1/1	0.99	0.03	98,98,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.