



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:07 AM UTC

PDB ID : 4Q8G / pdb_00004q8g
Title : Structure of the *Saccharomyces cerevisiae* PAN2 pseudoubiquitin-hydrolase
Authors : Schaefer, I.B.; Conti, E.
Deposited on : 2014-04-27
Resolution : 2.10 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
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

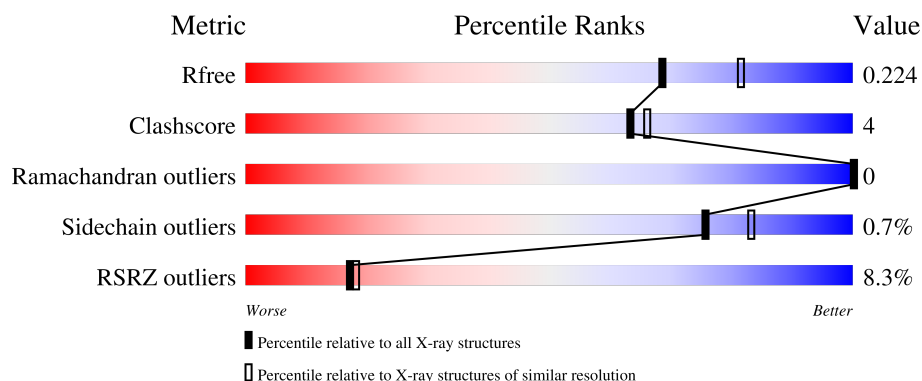
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	461	 7% 66% 8% 25%
1	B	461	 6% 71% 5% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11146 atoms, of which 5395 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 PAB-dependent poly(A)-specific ribonuclease subunit PAN2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	3	0
			5405	1744	2672	440	531	18			
1	B	353	Total	C	H	N	O	S	0	1	0
			5526	1787	2723	451	547	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	GLY	-	expression tag	UNP P53010
A	411	PRO	-	expression tag	UNP P53010
A	412	ASP	-	expression tag	UNP P53010
A	413	SER	-	expression tag	UNP P53010
A	414	MET	-	expression tag	UNP P53010
A	415	MET	-	expression tag	UNP P53010
B	410	GLY	-	expression tag	UNP P53010
B	411	PRO	-	expression tag	UNP P53010
B	412	ASP	-	expression tag	UNP P53010
B	413	SER	-	expression tag	UNP P53010
B	414	MET	-	expression tag	UNP P53010
B	415	MET	-	expression tag	UNP P53010

- 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		

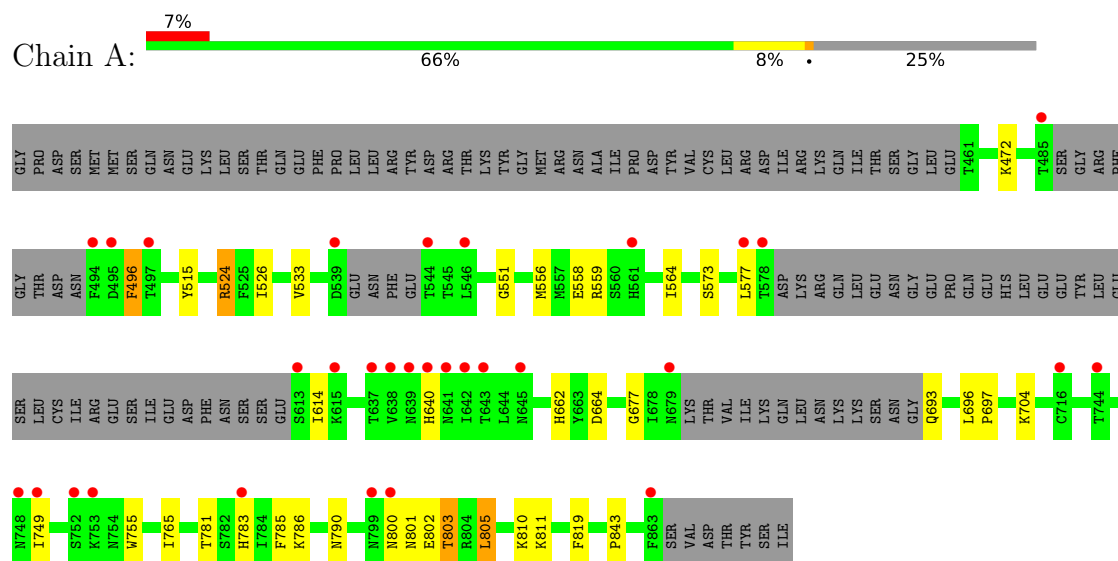
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	101	Total 101	O 101	0	0

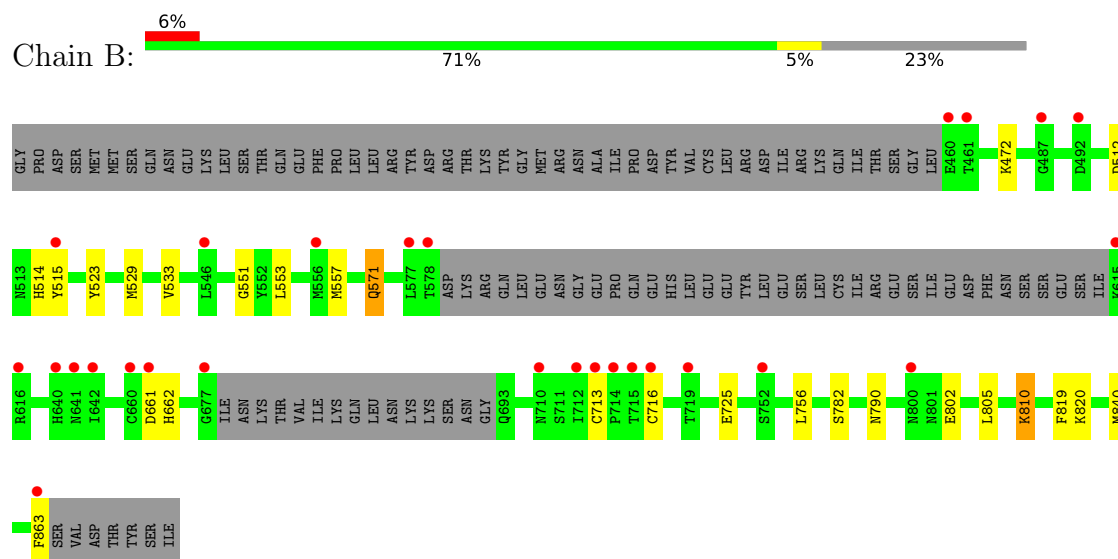
3 Residue-property plots

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: PAB-dependent poly(A)-specific ribonuclease subunit PAN2



- Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.51Å 74.03Å 175.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.10 48.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.33-2.10) 99.7 (48.33-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1631)	Depositor
R, R_{free}	0.184 , 0.221 0.192 , 0.224	Depositor DCC
R_{free} test set	2688 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11146	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	1/2787 (0.0%)	0.87	2/3785 (0.1%)
1	B	0.81	1/2862 (0.0%)	0.89	1/3886 (0.0%)
All	All	0.81	2/5649 (0.0%)	0.88	3/7671 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	PHE	CA-CB	-6.52	1.43	1.53
1	B	790	ASN	CG-OD1	5.93	1.34	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	810	LYS	N-CA-C	-5.12	100.55	108.90
1	A	640	HIS	CA-C-N	5.11	130.89	121.70
1	A	640	HIS	C-N-CA	5.11	130.89	121.70

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	2733	2672	2629	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2803	2723	2692	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	112	0	0	5	0
3	B	101	0	0	6	0
All	All	5751	5395	5321	43	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 (43) 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:693:GLN:N	3:A:1100:HOH:O	1.94	0.98
1:A:811:LYS:NZ	3:A:1095:HOH:O	2.04	0.89
1:A:677:GLY:O	3:A:1108:HOH:O	2.07	0.73
1:A:704:LYS:NZ	3:A:1067:HOH:O	2.26	0.68
1:A:802:GLU:OE2	3:A:1087:HOH:O	2.11	0.67
1:B:514:HIS:N	3:B:1057:HOH:O	2.31	0.64
1:A:496:PHE:CB	1:A:564:ILE:HD11	2.33	0.59
1:B:553:LEU:HG	1:B:557:MET:CE	2.33	0.57
1:A:533:VAL:HG12	1:A:551:GLY:HA2	1.85	0.57
1:A:556:MET:SD	1:A:559:ARG:NH2	2.78	0.56
1:B:820:LYS:NZ	3:B:1077:HOH:O	2.39	0.53
1:B:472:LYS:NZ	3:B:1045:HOH:O	2.39	0.52
1:B:533:VAL:HG12	1:B:551:GLY:HA2	1.92	0.52
1:B:725:GLU:OE1	3:B:1061:HOH:O	2.19	0.51
1:A:524:ARG:NH2	1:A:558:GLU:OE1	2.44	0.50
1:A:662:HIS:O	1:A:664:ASP:N	2.44	0.50
1:B:713:CYS:SG	1:B:716:CYS:N	2.77	0.50
1:B:661:ASP:C	1:B:662:HIS:CG	2.91	0.49
1:B:713:CYS:HB3	1:B:716:CYS:HB3	1.95	0.48
1:A:515:TYR:HB2	1:A:805:LEU:HD22	1.95	0.48
1:B:802:GLU:OE1	3:B:1049:HOH:O	2.20	0.47
1:B:523:TYR:HB3	1:B:529:MET:HE3	1.96	0.46
1:A:810:LYS:HG2	1:A:819:PHE:CD1	2.51	0.46
1:B:810:LYS:HG2	1:B:819:PHE:CD1	2.51	0.46
1:A:696:LEU:N	1:A:697:PRO:HD2	2.32	0.45
1:B:515:TYR:CD1	1:B:515:TYR:C	2.95	0.45
1:B:662:HIS:HB2	1:B:713:CYS:SG	2.57	0.45
1:B:713:CYS:CB	1:B:716:CYS:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HA	1:A:790:ASN:HD21	1.81	0.44
1:A:749:ILE:HG23	1:A:755:TRP:CD2	2.52	0.44
1:A:800:ASN:O	1:A:801:ASN:HB2	2.16	0.44
1:B:863:PHE:O	3:B:1071:HOH:O	2.21	0.43
1:B:756:LEU:HD22	1:B:840:MET:HE3	1.99	0.43
1:B:515:TYR:HB2	1:B:805:LEU:HD12	2.01	0.43
1:A:765:ILE:HG12	1:A:781:THR:HB	2.00	0.43
1:A:573:SER:O	1:A:577:LEU:HD13	2.19	0.43
1:A:614:ILE:HG12	1:A:803:THR:HG22	2.00	0.42
1:A:472:LYS:HE2	1:A:843:PRO:HD3	2.00	0.42
1:B:512:ASP:OD1	1:B:571:GLN:HG3	2.19	0.42
1:A:783[A]:HIS:CD2	1:A:785:PHE:CZ	3.09	0.41
1:A:786:LYS:HB3	1:B:782:SER:HA	2.03	0.41
1:B:553:LEU:HG	1:B:557:MET:HE3	2.03	0.40
1:A:577:LEU:HD12	1:A:577:LEU:N	2.36	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	337/461 (73%)	324 (96%)	13 (4%)	0	100	100
1	B	348/461 (76%)	335 (96%)	13 (4%)	0	100	100
All	All	685/922 (74%)	659 (96%)	26 (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	305/433 (70%)	302 (99%)	3 (1%)	68	76
1	B	314/433 (72%)	313 (100%)	1 (0%)	86	91
All	All	619/866 (72%)	615 (99%)	4 (1%)	76	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	ARG
1	A	803	THR
1	A	805	LEU
1	B	571	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	GLN
1	A	501	ASN
1	A	623	ASN
1	A	662	HIS
1	A	790	ASN
1	B	493	ASN
1	B	501	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

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	344/461 (74%)	0.32	31 (9%) 15 16	20, 53, 91, 105	3 (0%)
1	B	353/461 (76%)	0.28	27 (7%) 20 21	21, 53, 94, 161	1 (0%)
All	All	697/922 (75%)	0.30	58 (8%) 17 18	20, 53, 92, 161	4 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	863	PHE	5.8
1	A	539	ASP	5.3
1	A	716	CYS	5.1
1	B	460	GLU	5.0
1	A	863	PHE	5.0
1	A	639	ASN	4.6
1	B	641	ASN	4.6
1	A	638	VAL	4.6
1	A	494	PHE	4.6
1	A	783[A]	HIS	4.5
1	A	544	THR	4.3
1	A	637	THR	4.0
1	B	642	ILE	3.5
1	A	640	HIS	3.5
1	A	546	LEU	3.5
1	A	613	SER	3.3
1	B	713	CYS	3.2
1	A	641	ASN	3.1
1	B	677	GLY	3.0
1	A	485	THR	3.0
1	A	495	ASP	3.0
1	B	640	HIS	3.0
1	B	716	CYS	2.9
1	B	492	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	661	ASP	2.9
1	B	616	ARG	2.9
1	A	578	THR	2.9
1	B	712	ILE	2.8
1	A	753	LYS	2.8
1	B	615	LYS	2.8
1	A	561	HIS	2.7
1	B	461	THR	2.7
1	A	642	ILE	2.7
1	B	578	THR	2.7
1	A	643	THR	2.6
1	B	710	ASN	2.6
1	B	719	THR	2.6
1	B	715	THR	2.6
1	A	748	ASN	2.6
1	B	660	CYS	2.5
1	A	749	ILE	2.5
1	A	752	SER	2.5
1	A	645	ASN	2.5
1	A	799	ASN	2.5
1	A	679	ASN	2.4
1	A	744	THR	2.4
1	B	714	PRO	2.2
1	A	577	LEU	2.2
1	B	577	LEU	2.2
1	B	546	LEU	2.2
1	B	515	TYR	2.2
1	B	752	SER	2.2
1	A	615	LYS	2.2
1	A	800	ASN	2.1
1	B	800	ASN	2.1
1	B	556	MET	2.0
1	A	497	THR	2.0
1	B	487	GLY	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 [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, 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
2	ZN	B	901	1/1	0.69	0.23	491,491,491,491	0
2	ZN	A	901	1/1	0.98	0.03	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.