



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 10:07 AM JST

PDB ID : 6JTZ
Title : Crystal Structure of hRecQ1_D2-Zn-WH containing mutation on beta-hairpin
Authors : Das, T.; Mukhopadhyay, S.; Bose, M.; Das, A.K.; Ganguly, A.
Deposited on : 2019-04-12
Resolution : 2.80 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 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	:	2.23.2
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)	:	2.23.2

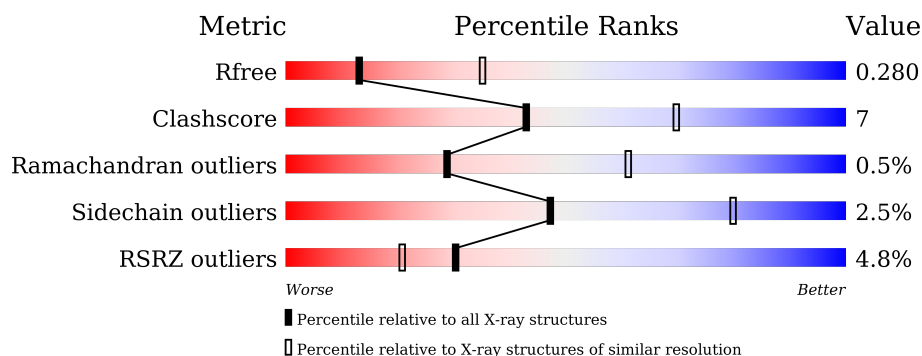
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	352	<div> <div>4%</div> <div>70%</div> <div>15%</div> <div>•</div> <div>14%</div> </div>
1	B	352	<div> <div>4%</div> <div>68%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4927 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 ATP-dependent DNA helicase Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2405	1519	418	448	20			
1	B	301	Total	C	N	O	S	0	0	0
			2381	1502	413	446	20			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	MET	-	initiating methionine	UNP P46063
A	262	GLY	-	expression tag	UNP P46063
A	263	SER	-	expression tag	UNP P46063
A	264	SER	-	expression tag	UNP P46063
A	265	HIS	-	expression tag	UNP P46063
A	266	HIS	-	expression tag	UNP P46063
A	267	HIS	-	expression tag	UNP P46063
A	268	HIS	-	expression tag	UNP P46063
A	269	HIS	-	expression tag	UNP P46063
A	270	HIS	-	expression tag	UNP P46063
A	271	SER	-	expression tag	UNP P46063
A	272	SER	-	expression tag	UNP P46063
A	273	GLY	-	expression tag	UNP P46063
A	274	LEU	-	expression tag	UNP P46063
A	275	VAL	-	expression tag	UNP P46063
A	276	PRO	-	expression tag	UNP P46063
A	277	ARG	-	expression tag	UNP P46063
A	278	GLY	-	expression tag	UNP P46063
A	279	SER	-	expression tag	UNP P46063
A	280	HIS	-	expression tag	UNP P46063
A	281	MET	-	expression tag	UNP P46063
A	?	-	PHE	deletion	UNP P46063
A	?	-	THR	deletion	UNP P46063
A	564	ALA	TYR	engineered mutation	UNP P46063
A	?	-	ALA	deletion	UNP P46063

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P46063
B	261	MET	-	initiating methionine	UNP P46063
B	262	GLY	-	expression tag	UNP P46063
B	263	SER	-	expression tag	UNP P46063
B	264	SER	-	expression tag	UNP P46063
B	265	HIS	-	expression tag	UNP P46063
B	266	HIS	-	expression tag	UNP P46063
B	267	HIS	-	expression tag	UNP P46063
B	268	HIS	-	expression tag	UNP P46063
B	269	HIS	-	expression tag	UNP P46063
B	270	HIS	-	expression tag	UNP P46063
B	271	SER	-	expression tag	UNP P46063
B	272	SER	-	expression tag	UNP P46063
B	273	GLY	-	expression tag	UNP P46063
B	274	LEU	-	expression tag	UNP P46063
B	275	VAL	-	expression tag	UNP P46063
B	276	PRO	-	expression tag	UNP P46063
B	277	ARG	-	expression tag	UNP P46063
B	278	GLY	-	expression tag	UNP P46063
B	279	SER	-	expression tag	UNP P46063
B	280	HIS	-	expression tag	UNP P46063
B	281	MET	-	expression tag	UNP P46063
B	?	-	PHE	deletion	UNP P46063
B	?	-	THR	deletion	UNP P46063
B	564	ALA	TYR	engineered mutation	UNP P46063
B	?	-	ALA	deletion	UNP P46063
B	?	-	THR	deletion	UNP P46063

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

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

- Molecule 3 is water.

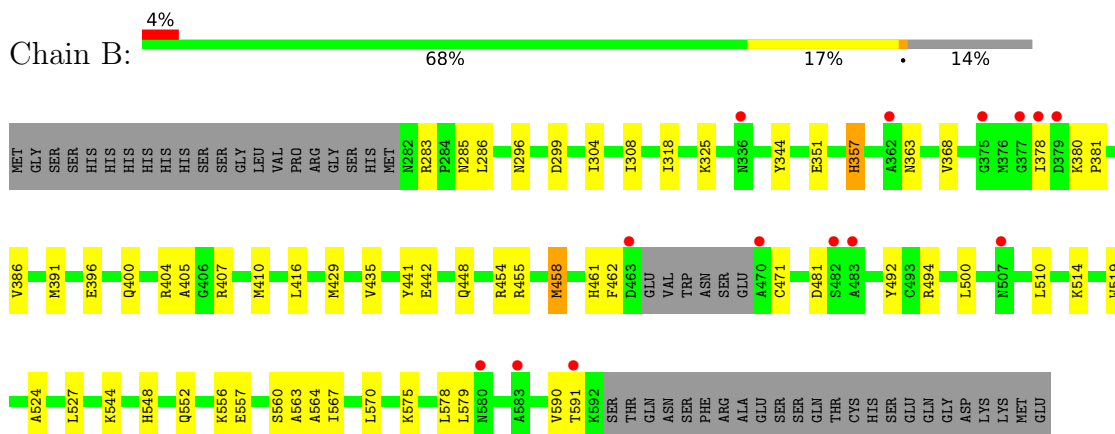
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	72	Total O 72 72	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	67	Total	O	0	0
			67	67		

- Molecule 1: ATP-dependent DNA helicase Q1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.95Å 101.83Å 73.43Å 90.00° 99.07° 90.00°	Depositor
Resolution (Å)	19.69 – 2.80 19.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.69-2.80) 99.3 (19.69-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.227 , 0.282 0.227 , 0.280	Depositor DCC
R_{free} test set	950 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	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	0.91	EDS
Total number of atoms	4927	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.67% 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

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	0/2447	0.45	0/3294
1	B	0.30	0/2423	0.44	0/3265
All	All	0.31	0/4870	0.45	0/6559

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

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	2405	0	2393	34	0
1	B	2381	0	2355	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	72	0	0	8	0
3	B	67	0	0	1	0
All	All	4927	0	4748	65	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 7.

All (65) 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:353:LYS:NZ	1:B:564:ALA:O	1.93	1.01
1:A:388:HIS:O	3:A:801:HOH:O	1.99	0.80
1:A:378:ILE:HG21	1:A:404:ARG:HD3	1.71	0.72
1:A:560:SER:O	1:B:357:HIS:NE2	2.23	0.71
1:A:417:TYR:N	3:A:801:HOH:O	2.14	0.66
1:A:563:ALA:O	1:B:344:TYR:OH	2.08	0.65
1:B:442:GLU:HB3	1:B:461:HIS:HE1	1.62	0.65
1:A:325:LYS:NZ	3:A:806:HOH:O	2.33	0.61
3:A:806:HOH:O	1:B:325:LYS:NZ	2.33	0.60
1:B:442:GLU:HB3	1:B:461:HIS:CE1	2.35	0.60
1:B:455:ARG:HD2	1:B:471:CYS:HB2	1.83	0.59
1:A:315:GLN:HG3	1:A:384:ARG:HG3	1.86	0.57
1:A:296:ASN:HB3	1:A:299:ASP:HB2	1.87	0.56
1:B:286:LEU:O	1:B:455:ARG:NH2	2.36	0.56
1:B:378:ILE:HG21	1:B:404:ARG:HD3	1.88	0.55
1:B:441:TYR:OH	1:B:557:GLU:OE2	2.12	0.55
1:B:590:VAL:HG22	1:B:591:THR:H	1.73	0.53
1:A:381:PRO:HA	1:A:407:ARG:HB2	1.90	0.53
1:A:494:ARG:HG2	1:A:579:LEU:HD13	1.90	0.52
1:A:514:LYS:NZ	3:A:814:HOH:O	2.41	0.52
1:B:448:GLN:O	1:B:544:LYS:NZ	2.41	0.52
1:A:378:ILE:HG23	1:A:378:ILE:O	2.10	0.52
1:A:501:LYS:O	1:A:505:GLU:HG3	2.10	0.52
1:B:283:ARG:NH2	1:B:405:ALA:O	2.43	0.51
1:B:381:PRO:HA	1:B:407:ARG:HB2	1.93	0.51
1:B:285:ASN:ND2	1:B:410:MET:O	2.43	0.51
1:B:492:TYR:HD1	1:B:519:TRP:HZ2	1.58	0.50
1:B:304:ILE:O	1:B:308:ILE:HG12	2.12	0.50
1:A:431:VAL:HG11	1:A:559:TYR:CZ	2.47	0.49
1:B:494:ARG:NH1	1:B:579:LEU:O	2.46	0.49
1:B:391:MET:HA	1:B:416:LEU:HD11	1.95	0.48
1:B:548:HIS:O	1:B:552:GLN:HG3	2.13	0.48
1:A:386:VAL:HG23	1:A:405:ALA:HB2	1.95	0.47
1:B:575:LYS:HD3	1:B:578:LEU:HD11	1.96	0.47
1:A:319:ILE:HA	1:A:387:ILE:O	2.15	0.47
1:A:292:GLN:NE2	1:A:540:GLU:HG2	2.30	0.47
1:A:357:HIS:CE1	1:B:567:ILE:HD12	2.50	0.47
1:A:500:LEU:HD23	1:A:510:LEU:HD12	1.97	0.47
1:B:363:ASN:OD1	1:B:380:LYS:NZ	2.47	0.47
1:A:344:TYR:HA	1:A:348:LEU:HD11	1.97	0.46
1:A:289:GLU:OE2	1:A:291:ARG:NE	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG13	1:B:429:MET:HG3	1.98	0.46
1:B:318:ILE:HG23	1:B:368:VAL:HG23	1.96	0.46
1:A:485:GLU:HG3	1:A:592:LYS:HB2	1.97	0.45
1:A:456:VAL:O	1:A:460:GLN:HG3	2.17	0.45
1:A:416:LEU:HD12	3:A:801:HOH:O	2.16	0.45
1:A:446:TYR:O	1:A:454:ARG:NH1	2.49	0.45
1:A:465:VAL:O	3:A:802:HOH:O	2.21	0.45
1:B:378:ILE:HG21	1:B:404:ARG:HH11	1.80	0.45
1:B:481:ASP:OD1	1:B:481:ASP:N	2.49	0.43
1:A:512:PRO:O	1:A:516:ILE:HG13	2.18	0.43
1:A:383:VAL:HB	1:A:405:ALA:HA	2.00	0.43
1:B:524:ALA:HB3	1:B:527:LEU:HD23	1.99	0.43
1:B:454:ARG:O	1:B:458:MET:HG3	2.18	0.43
1:B:510:LEU:HA	1:B:514:LYS:HE2	2.01	0.42
1:A:577:ASN:OD1	3:A:803:HOH:O	2.21	0.42
1:B:396:GLU:O	1:B:400:GLN:HG2	2.19	0.42
1:A:302:GLU:O	1:A:306:LYS:HG3	2.20	0.41
1:A:378:ILE:HD12	1:A:378:ILE:HA	1.92	0.41
1:A:292:GLN:NE2	1:A:293:LYS:O	2.54	0.41
1:B:296:ASN:HB3	1:B:299:ASP:HB2	2.02	0.41
1:B:570:LEU:O	3:B:801:HOH:O	2.22	0.41
1:B:575:LYS:O	1:B:578:LEU:HD12	2.21	0.41
1:B:386:VAL:HG23	1:B:405:ALA:HB2	2.03	0.41
1:B:500:LEU:HD23	1:B:510:LEU:HD12	2.02	0.41

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	299/352 (85%)	285 (95%)	13 (4%)	1 (0%)	41 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	297/352 (84%)	278 (94%)	17 (6%)	2 (1%)	22	53
All	All	596/704 (85%)	563 (94%)	30 (5%)	3 (0%)	29	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	B	563	ALA
1	B	435	VAL

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	261/309 (84%)	254 (97%)	7 (3%)	44	78
1	B	258/309 (84%)	252 (98%)	6 (2%)	50	82
All	All	519/618 (84%)	506 (98%)	13 (2%)	47	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ARG
1	A	315	GLN
1	A	374	PHE
1	A	376	MET
1	A	448	GLN
1	A	560	SER
1	A	577	ASN
1	B	351	GLU
1	B	357	HIS
1	B	458	MET
1	B	462	PHE
1	B	556	LYS
1	B	560	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	292	GLN
1	A	461	HIS

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 monosaccharides 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	303/352 (86%)	0.20	15 (4%) 28 19	18, 38, 70, 93	0
1	B	301/352 (85%)	0.17	14 (4%) 31 22	21, 36, 63, 78	0
All	All	604/704 (85%)	0.19	29 (4%) 30 21	18, 37, 66, 93	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	VAL	4.5
1	A	379	ASP	4.3
1	A	483	ALA	3.7
1	A	362	ALA	3.5
1	A	463	ASP	3.5
1	B	591	THR	3.4
1	A	481	ASP	3.0
1	B	470	ALA	2.9
1	B	583	ALA	2.8
1	A	591	THR	2.8
1	A	484	PHE	2.7
1	B	483	ALA	2.7
1	B	580	ASN	2.7
1	A	538	PRO	2.6
1	B	336	ASN	2.6
1	A	482	SER	2.5
1	A	592	LYS	2.5
1	B	463	ASP	2.4
1	B	379	ASP	2.3
1	A	536	THR	2.3
1	B	507	ASN	2.3
1	B	362	ALA	2.3
1	A	470	ALA	2.2
1	A	358	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	ILE	2.1
1	A	460	GLN	2.0
1	B	375	GLY	2.0
1	B	377	GLY	2.0
1	B	482	SER	2.0

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, 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(\AA^2)	Q<0.9
2	ZN	A	701	1/1	0.97	0.11	54,54,54,54	0
2	ZN	B	701	1/1	0.99	0.10	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.