



# Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 03:11 PM GMT

PDB ID : 3QPY  
Title : Crystal structure of a mutant (K57A) of 3-deoxy-D-manno-octulosonate 8-phosphate synthase (KDO8PS) from *Neisseria meningitidis*  
Authors : Allison, T.M.; Jameson, G.B.; Parker, E.J.  
Deposited on : 2011-02-14  
Resolution : 1.95 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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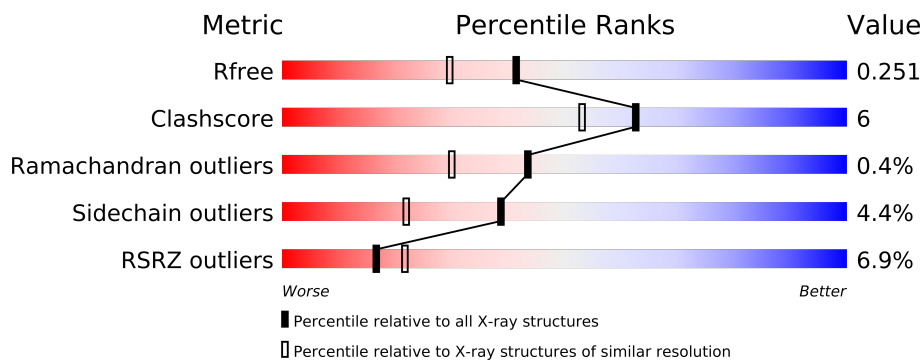
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
1	C	280	
1	D	280	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NA	B	281	-	X
4	GOL	C	281	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8574 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-dehydro-3-deoxyphosphooctonatealdolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	3	0
			1939	1242	331	355	11			
1	B	250	Total	C	N	O	S	0	6	0
			1956	1261	327	357	11			
1	C	251	Total	C	N	O	S	0	7	0
			1982	1277	335	359	11			
1	D	249	Total	C	N	O	S	0	7	0
			1950	1252	325	362	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
B	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
C	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
D	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	243	Total	O	0	0
			243	243		
5	C	188	Total	O	0	0
			188	188		
5	D	143	Total	O	0	0
			143	143		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.43Å 86.18Å 163.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.84 – 1.95 31.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (33.84-1.95) 97.9 (31.26-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.205 , 0.252 0.203 , 0.251	Depositor DCC
$R_{free}$ test set	4210 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.6	EDS
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 83643 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, NA

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	0.55	1/1974 (0.1%)	0.57	0/2665
1	B	0.53	0/2003	0.58	1/2707 (0.0%)
1	C	0.51	0/2023	0.58	0/2733
1	D	0.49	0/1993	0.59	2/2695 (0.1%)
All	All	0.52	1/7993 (0.0%)	0.58	3/10800 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLU	CD-OE2	-5.04	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7[A]	ASP	CB-CG-OD1	6.00	123.69	118.30
1	D	7[B]	ASP	CB-CG-OD1	6.00	123.69	118.30
1	B	172	ASP	CB-CG-OD2	5.61	123.35	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	0	15	0
1	B	1956	0	0	11	0
1	C	1982	0	0	16	0
1	D	1950	0	0	7	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	1	0	0	0	0
4	C	6	0	8	0	0
5	A	163	0	0	4	0
5	B	243	0	0	4	0
5	C	188	0	0	6	0
5	D	143	0	0	1	0
All	All	8574	0	8	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:GLU:CG	5:B:382:HOH:O	2.31	0.79
1:D:6:ASN:CB	1:D:7[A]:ASP:OD2	2.38	0.72
1:B:190:ASN:ND2	5:B:824:HOH:O	2.25	0.69
1:A:214[B]:ARG:NH1	1:A:214[B]:ARG:CG	2.56	0.66
1:A:120:ASP:OD2	1:C:67:ARG:NH2	2.30	0.65
1:D:7[A]:ASP:N	1:D:7[A]:ASP:OD2	2.30	0.65
1:C:100:GLN:NE2	5:C:395:HOH:O	2.29	0.64
1:C:215:ARG:N	1:C:215:ARG:CD	2.61	0.63
1:C:165[B]:ARG:NH1	5:C:883:HOH:O	2.33	0.61
1:D:129:GLY:O	1:D:159:LYS:NZ	2.33	0.61
1:A:196:ASP:OD2	1:A:199:HIS:ND1	2.35	0.58
1:C:52:LYS:CD	1:C:234:PHE:CZ	2.87	0.57
1:A:201:LEU:O	1:A:202:GLN:CB	2.53	0.57
1:A:215:ARG:O	1:A:260:PHE:CZ	2.60	0.55
1:C:140:LEU:CD2	1:C:144:GLN:CB	2.86	0.54
1:B:136:LYS:CE	1:B:164:GLU:OE1	2.55	0.53
1:C:159:LYS:NZ	5:C:700:HOH:O	2.41	0.53
1:A:263:ARG:NE	5:A:618:HOH:O	2.41	0.53
1:A:29:ASP:O	1:A:33:GLN:CG	2.56	0.53
1:D:135:LYS:NZ	1:D:196:ASP:OD2	2.42	0.52
1:C:267[A]:LEU:CD1	1:D:267[A]:LEU:CD1	2.89	0.51
1:C:37:HIS:CE1	1:C:254:LEU:O	2.63	0.51
1:A:217:GLN:NE2	5:A:772:HOH:O	2.44	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165[B]:ARG:CD	5:C:625:HOH:O	2.61	0.48
1:B:136:LYS:NZ	5:B:345:HOH:O	2.47	0.47
1:C:196:ASP:OD2	1:C:199:HIS:ND1	2.47	0.47
1:A:44:LYS:NZ	1:A:258:GLU:OE2	2.47	0.47
1:C:60[B]:ARG:CG	5:C:404:HOH:O	2.64	0.46
1:B:190:ASN:CG	5:B:824:HOH:O	2.54	0.46
1:B:92:ASP:OD1	1:B:94:HIS:CE1	2.68	0.46
1:C:228:THR:O	1:C:229:ARG:CB	2.65	0.45
1:B:229:ARG:NH2	1:B:274:GLN:O	2.50	0.45
1:A:276:ILE:C	5:A:297:HOH:O	2.54	0.45
1:A:267:LEU:CD1	1:B:267[B]:LEU:CD2	2.94	0.44
1:A:265:LYS:NZ	5:A:310:HOH:O	2.50	0.44
1:B:277:LEU:CD2	1:B:278:THR:N	2.81	0.44
1:D:165:ARG:CG	5:D:689:HOH:O	2.67	0.43
1:C:201[B]:LEU:C	5:C:370:HOH:O	2.56	0.43
1:A:60:ARG:NH1	1:C:120:ASP:OD1	2.52	0.42
1:A:229:ARG:NH2	1:A:274:GLN:O	2.53	0.41
1:B:120:ASP:OD1	1:D:60:ARG:NH1	2.54	0.41
1:C:52:LYS:CE	1:C:234:PHE:CZ	3.04	0.41
1:A:228:THR:O	1:A:229:ARG:CB	2.68	0.41
1:B:26:GLU:O	1:B:69:VAL:CG1	2.69	0.41

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	247/280 (88%)	242 (98%)	4 (2%)	1 (0%)	43	30
1	B	250/280 (89%)	245 (98%)	4 (2%)	1 (0%)	43	30
1	C	251/280 (90%)	247 (98%)	3 (1%)	1 (0%)	43	30
1	D	249/280 (89%)	246 (99%)	2 (1%)	1 (0%)	43	30
All	All	997/1120 (89%)	980 (98%)	13 (1%)	4 (0%)	43	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	ARG
1	A	229	ARG
1	D	229	ARG
1	B	229	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	213/235 (91%)	204 (96%)	9 (4%)	40	24
1	B	219/235 (93%)	208 (95%)	11 (5%)	34	16
1	C	221/235 (94%)	213 (96%)	8 (4%)	47	31
1	D	218/235 (93%)	204 (94%)	14 (6%)	25	10
All	All	871/940 (93%)	829 (95%)	42 (5%)	39	17

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	52	LYS
1	A	56	ASP
1	A	67	ARG
1	A	84	GLU
1	A	141	SER
1	A	165	ARG
1	A	173	ASN
1	A	234	PHE
1	B	24[A]	VAL
1	B	24[B]	VAL
1	B	76	LYS
1	B	84	GLU
1	B	95	GLU
1	B	150	GLU
1	B	190	ASN
1	B	200[A]	SER

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Mol	Chain	Res	Type
1	B	200[B]	SER
1	B	202	GLN
1	B	214	ARG
1	C	40	GLU
1	C	60[A]	ARG
1	C	60[B]	ARG
1	C	140	LEU
1	C	165[A]	ARG
1	C	165[B]	ARG
1	C	215	ARG
1	C	277	LEU
1	D	7[A]	ASP
1	D	7[B]	ASP
1	D	29	ASP
1	D	33	GLN
1	D	43	ARG
1	D	67	ARG
1	D	95	GLU
1	D	165	ARG
1	D	173	ASN
1	D	186	GLN
1	D	215	ARG
1	D	235	LEU
1	D	254	LEU
1	D	256	LEU

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 chains 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 ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z  > 2$
4	GOL	C	281	-	5,5,5	0.58	0	5,5,5	0.74	0

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
4	GOL	C	281	-	-	0/4/4/4	0/0/0/0

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.

## 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, 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	250/280 (89%)	0.42	17 (6%) 17 22	19, 36, 54, 75	1 (0%)
1	B	250/280 (89%)	0.24	8 (3%) 45 52	20, 30, 46, 67	1 (0%)
1	C	251/280 (89%)	0.29	14 (5%) 24 30	21, 32, 48, 63	0
1	D	249/280 (88%)	0.58	30 (12%) 5 6	21, 40, 63, 72	0
All	All	1000/1120 (89%)	0.38	69 (6%) 17 22	19, 34, 58, 75	2 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	7.5
1	D	254	LEU	6.2
1	D	66	TYR	5.3
1	C	253	PRO	5.2
1	A	237	SER	5.2
1	B	278	THR	4.9
1	C	277	LEU	4.9
1	A	214[A]	ARG	4.7
1	C	255	HIS	4.6
1	A	215	ARG	4.3
1	A	66	TYR	4.2
1	A	275	PRO	4.1
1	A	67	ARG	3.9
1	D	26	GLU	3.8
1	A	276	ILE	3.8
1	D	276	ILE	3.6
1	D	30[A]	SER	3.5
1	A	213	GLY	3.2
1	B	255	HIS	3.2
1	B	277	LEU	3.2
1	C	256	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	3.1
1	D	237[A]	SER	3.0
1	B	237	SER	3.0
1	D	202	GLN	3.0
1	D	203	THR	3.0
1	A	202	GLN	3.0
1	D	255	HIS	3.0
1	D	62	SER	3.0
1	D	172	ASP	2.9
1	A	33	GLN	2.9
1	C	233	LEU	2.7
1	A	254	LEU	2.7
1	D	33	GLN	2.7
1	C	254	LEU	2.7
1	D	67	ARG	2.7
1	A	64	HIS	2.6
1	C	237	SER	2.6
1	D	97	HIS	2.6
1	D	22	ILE	2.6
1	D	27	SER	2.6
1	C	215	ARG	2.5
1	A	104	GLU	2.5
1	B	214	ARG	2.4
1	D	101	PRO	2.4
1	A	65	SER	2.4
1	B	256	LEU	2.3
1	A	29	ASP	2.3
1	D	104	GLU	2.3
1	D	72	GLU	2.3
1	D	100	GLN	2.2
1	A	234	PHE	2.2
1	D	64	HIS	2.2
1	C	276	ILE	2.2
1	D	186	GLN	2.2
1	C	235	LEU	2.2
1	C	195	PHE	2.1
1	D	61	SER	2.1
1	D	78	PHE	2.1
1	A	216	ALA	2.1
1	D	83	ALA	2.1
1	B	194	ILE	2.1
1	D	60	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	LEU	2.1
1	D	256	LEU	2.1
1	C	33	GLN	2.1
1	D	105	VAL	2.0
1	D	25	LEU	2.0
1	D	71	LEU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	B	281	1/1	0.27	9.23	26,26,26,26	0
4	GOL	C	281	6/6	0.30	6.38	17,25,29,30	0
2	CL	A	281	1/1	0.15	1.83	29,29,29,29	0
2	CL	C	282	1/1	0.15	0.66	19,19,19,19	1
2	CL	D	281	1/1	0.12	0.41	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.