



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:22 AM GMT

PDB ID : 3MTA  
Title : Glycogen phosphorylase complexed with 3-bromobenzaldehyde-4-(beta-D-glucopyranosyl)-thiosemicarbazone  
Authors : Alexacou, K.-M.  
Deposited on : 2010-04-30  
Resolution : 2.23 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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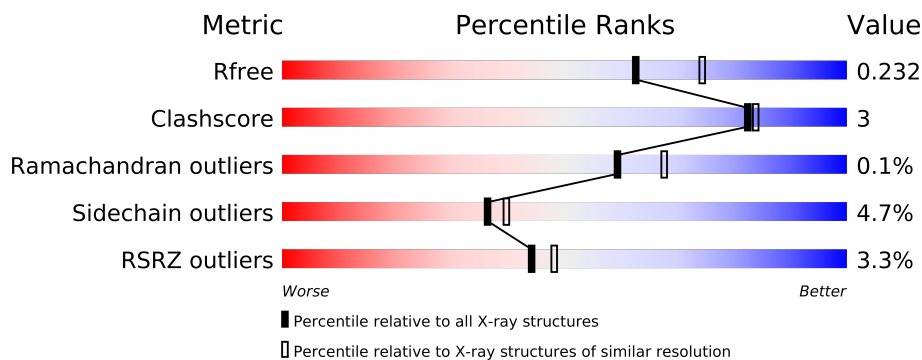
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.23 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	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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	842	

## 2 Entry composition i

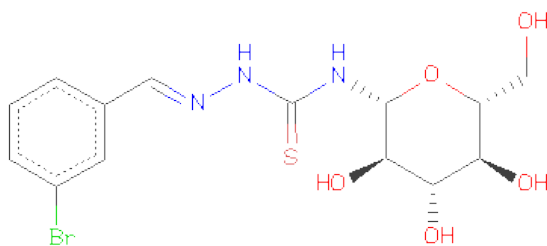
There are 3 unique types of molecules in this entry. The entry contains 6842 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	1	0
			6611	4214	1163	1204	1	29			

- Molecule 2 is N-({(2E)-2-[(3-BROMOPHENYL)METHYLIDENE]HYDRAZINO}CARBONOTHIOYL)-BETA-D-GLUCOPYRANOSYLAMINE (three-letter code: 22O) (formula: C<sub>14</sub>H<sub>18</sub>BrN<sub>3</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	1
			48	2	28	6	10	2		
2	A	1	Total	Br	C	N	O	S	0	0
			24	1	14	3	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total 159	O 159	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.92Å 128.92Å 116.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.23 29.60 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.23) 98.2 (29.60-2.23)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.233 0.198 , 0.232	Depositor DCC
$R_{free}$ test set	2413 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47632 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: 22O, LLP

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	0.42	0/6737	0.55	0/9117

There are no bond length outliers.

There are no bond angle outliers.

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	6611	0	6548	41	0
2	A	72	0	54	4	0
3	A	159	0	0	1	0
All	All	6842	0	6602	41	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 3.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:VAL:H	1:A:459:HIS:HD2	1.29	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:285:PHE:O	2:A:998:22O:BR1	2.58	0.77
1:A:138:ARG:O	1:A:138:ARG:HD3	1.84	0.76
1:A:730:GLU:O	1:A:734:ARG:HG3	1.93	0.69
1:A:270:ASN:OD1	1:A:271:LEU:HD13	1.97	0.63
1:A:235:ASN:H	1:A:235:ASN:HD22	1.45	0.63
1:A:549:LEU:HB3	1:A:555:VAL:HG23	1.81	0.62
1:A:678:ASN:HD22	1:A:679:MET:H	1.49	0.60
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.84	0.59
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.86	0.58
1:A:283:ASP:OD2	1:A:571[B]:HIS:HE1	1.88	0.57
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.89	0.55
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.90	0.55
1:A:450:HIS:HE1	3:A:944:HOH:O	1.89	0.54
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.08	0.54
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.91	0.53
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.74	0.52
1:A:678:ASN:HD22	1:A:678:ASN:N	2.06	0.52
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.94	0.50
1:A:568:LYS:HG3	1:A:574:LYS:HD3	1.94	0.49
1:A:64:VAL:HG12	2:A:920[A]:22O:H11	1.94	0.49
1:A:678:ASN:ND2	1:A:679:MET:H	2.10	0.48
1:A:229:PRO:HD3	2:A:920[A]:22O:BR1	2.71	0.46
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.80	0.46
1:A:325:ASN:ND2	1:A:327:ASP:OD1	2.49	0.46
1:A:64:VAL:HG12	2:A:920[B]:22O:BR1	2.72	0.45
1:A:144:LEU:HD23	1:A:147:MET:CE	2.48	0.44
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.98	0.44
1:A:72:GLN:O	1:A:76:GLU:HG2	2.17	0.44
1:A:270:ASN:OD1	1:A:271:LEU:N	2.50	0.44
1:A:65:GLY:O	1:A:69:ARG:HG2	2.18	0.44
1:A:680:LLP:NZ	1:A:680:LLP:O3	2.51	0.43
1:A:283:ASP:OD2	1:A:571[B]:HIS:CE1	2.70	0.42
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.01	0.42
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.56	0.41
1:A:506:ARG:NH1	1:A:533:ASP:OD2	2.54	0.41
1:A:678:ASN:ND2	1:A:678:ASN:N	2.67	0.41
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.93	0.41
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.85	0.40
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.98	0.40
1:A:15:VAL:HA	1:A:509:GLU:OE1	2.22	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	804/842 (96%)	782 (97%)	21 (3%)	1 (0%)	59 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	LYS

### 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	701/730 (96%)	668 (95%)	33 (5%)	36 40

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	60	ARG
1	A	90	TYR
1	A	102	LEU
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	138	ARG
1	A	198	LEU
1	A	234	ARG
1	A	235	ASN
1	A	271	LEU
1	A	400	LEU

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Mol	Chain	Res	Type
1	A	444	LEU
1	A	510	GLU
1	A	522	LEU
1	A	552	GLU
1	A	565	VAL
1	A	568	LYS
1	A	579	ASN
1	A	596	LYS
1	A	613	TYR
1	A	622	LEU
1	A	662	LEU
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	721	LEU
1	A	765	LEU
1	A	782	LYS
1	A	790	LEU
1	A	831	ARG
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	235	ASN
1	A	264	GLN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	767	HIS
1	A	832	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z  > 2$
1	LLP	A	680	1	24,24,25	4.03	5 (20%)	30,32,34	1.34	4 (13%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O-C	18.13	1.23	1.11
1	A	680	LLP	O3-C3	-5.05	1.24	1.37
1	A	680	LLP	CA-C	2.79	1.53	1.48
1	A	680	LLP	C2-N1	2.61	1.38	1.33
1	A	680	LLP	C4'-NZ	-2.38	1.33	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C6-C5-C4	3.62	120.85	118.10
1	A	680	LLP	C5-C6-N1	-2.46	119.42	123.86
1	A	680	LLP	C-CA-N	-2.38	111.45	113.83
1	A	680	LLP	OP4-C5'-C5	2.04	113.42	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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$
2	22O	A	920[A]	-	25,25,25	3.35	6 (24%)	34,34,34	1.05	4 (11%)
2	22O	A	920[B]	-	25,25,25	3.24	6 (24%)	34,34,34	1.15	4 (11%)
2	22O	A	998	-	25,25,25	3.41	5 (20%)	34,34,34	1.38	4 (11%)

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
2	22O	A	920[A]	-	-	0/12/32/32	0/2/2/2
2	22O	A	920[B]	-	-	0/12/32/32	0/2/2/2
2	22O	A	998	-	-	0/12/32/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	22O	N2-N3	-15.04	1.22	1.38
2	A	920[B]	22O	N2-N3	-14.00	1.23	1.38
2	A	920[A]	22O	N2-N3	-13.92	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	920[A]	22O	C1-N1	5.38	1.49	1.43
2	A	998	22O	C9-C8	-4.61	1.38	1.46
2	A	920[B]	22O	C1-N1	4.33	1.48	1.43
2	A	998	22O	C7-S1	4.31	1.78	1.68
2	A	920[A]	22O	C9-C8	-3.99	1.39	1.46
2	A	920[B]	22O	C9-C8	-3.97	1.39	1.46
2	A	920[A]	22O	C8-N3	3.90	1.32	1.28
2	A	920[B]	22O	C8-N3	3.47	1.31	1.28
2	A	920[A]	22O	C7-S1	3.39	1.76	1.68
2	A	920[B]	22O	C7-S1	3.12	1.75	1.68
2	A	998	22O	C7-N2	-2.89	1.32	1.36
2	A	998	22O	C8-N3	2.84	1.31	1.28
2	A	920[A]	22O	C2-C1	2.44	1.55	1.52
2	A	920[B]	22O	C7-N2	-2.10	1.33	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	22O	O5-C1-N1	-3.88	101.67	108.07
2	A	998	22O	C2-C1-N1	-3.42	106.82	111.44
2	A	920[B]	22O	C8-N3-N2	2.91	120.59	115.87
2	A	998	22O	O5-C1-C2	2.89	112.29	109.70
2	A	920[B]	22O	O5-C1-C2	2.53	111.97	109.70
2	A	920[B]	22O	C5-O5-C1	2.39	115.82	112.50
2	A	920[A]	22O	N2-C7-N1	2.32	120.22	115.95
2	A	920[B]	22O	O5-C1-N1	-2.26	104.34	108.07
2	A	920[A]	22O	C8-N3-N2	2.25	119.53	115.87
2	A	920[A]	22O	O5-C5-C6	2.19	111.71	106.34
2	A	920[A]	22O	C2-C1-N1	2.16	114.35	111.44
2	A	998	22O	C14-C9-C8	-2.06	116.75	120.44

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	810/842 (96%)	-0.04	27 (3%)	44 48	27, 41, 60, 80	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	PHE	8.5
1	A	253	ASN	7.9
1	A	324	THR	4.5
1	A	435	ALA	3.3
1	A	555	VAL	3.3
1	A	254	LEU	3.2
1	A	250	ASN	3.2
1	A	556	HIS	3.1
1	A	314	SER	3.1
1	A	69	ARG	3.1
1	A	835	PRO	3.1
1	A	211	GLN	3.0
1	A	75	TYR	3.0
1	A	13	ILE	2.7
1	A	532	ARG	2.6
1	A	12	GLN	2.4
1	A	345	ALA	2.4
1	A	113	TYR	2.4
1	A	337	LEU	2.4
1	A	210	SER	2.4
1	A	20	GLY	2.3
1	A	344	LEU	2.3
1	A	832	GLN	2.2
1	A	22	GLU	2.2
1	A	553	TYR	2.2
1	A	358	ARG	2.1
1	A	285	PHE	2.1

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

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
1	LLP	A	680	24/25	0.12	-0.44	30,32,33,34	0

## 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
2	22O	A	998	24/24	0.17	0.89	39,56,66,71	0
2	22O	A	920[A]	24/24	0.11	-0.58	38,39,39,40	24
2	22O	A	920[B]	24/24	0.11	-0.62	43,45,45,46	24

## 6.5 Other polymers ⓘ

There are no such residues in this entry.