



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:06 am BST

PDB ID : 2JCM  
Title : Crystal structure of Human Cytosolic 5'-Nucleotidase II in complex with beryllium trifluoride  
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Deposited on : 2006-12-27  
Resolution : 2.15 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

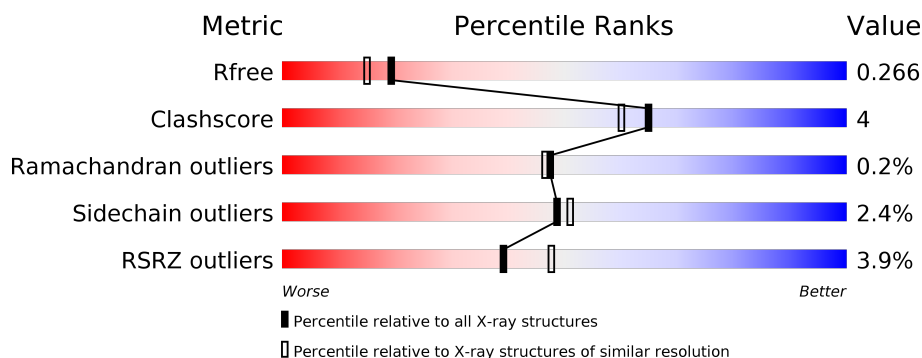
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	555	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4109 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 CYTOSOLIC PURINE 5'-NUCLEOTIDASE.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	467	Total	Be	C	F	N	O	S	0	3	0
			3837	1	2476	3	639	697	21			

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	X	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

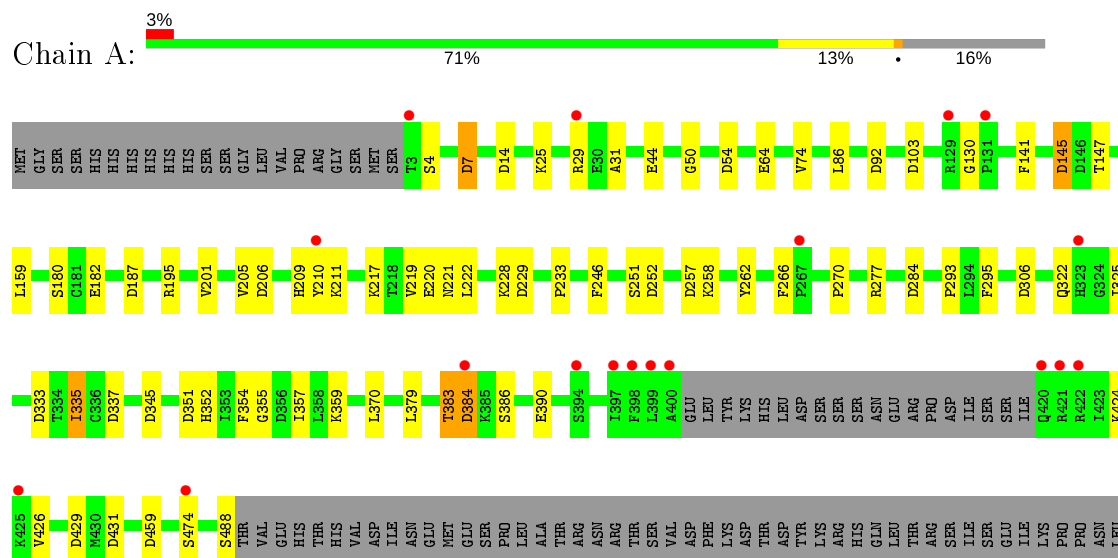
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	260	Total	O	0	0
			260	260		

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

These plots are drawn for all protein, RNA and DNA 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: CYTOSOLIC PURINE 5'-NUCLEOTIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.48 Å 128.26 Å 131.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.67 – 2.15 18.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.67-2.15) 98.2 (18.98-2.15)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.15 Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, $R_{free}$	0.210 , 0.266 0.217 , 0.266	Depositor DCC
$R_{free}$ test set	2089 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: UNX, MG, SO4, BFD

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	1.02	19/3923 (0.5%)	0.92	10/5294 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	ASP	CG-OD1	6.56	1.40	1.25
1	A	429	ASP	CG-OD1	6.54	1.40	1.25
1	A	337	ASP	CG-OD1	6.13	1.39	1.25
1	A	345	ASP	CG-OD1	5.91	1.39	1.25
1	A	64	GLU	CB-CG	5.90	1.63	1.52
1	A	187	ASP	CG-OD1	5.90	1.39	1.25
1	A	306	ASP	CG-OD1	5.85	1.38	1.25
1	A	431	ASP	CG-OD1	5.66	1.38	1.25
1	A	145[A]	ASP	CG-OD1	5.58	1.38	1.25
1	A	145[B]	ASP	CG-OD1	5.58	1.38	1.25
1	A	103	ASP	CG-OD1	5.38	1.37	1.25
1	A	384	ASP	CG-OD1	5.29	1.37	1.25
1	A	252	ASP	CG-OD1	5.28	1.37	1.25
1	A	54	ASP	CG-OD1	5.13	1.37	1.25
1	A	333	ASP	CG-OD1	5.12	1.37	1.25
1	A	14	ASP	CG-OD1	5.11	1.37	1.25
1	A	284	ASP	CG-OD1	5.09	1.37	1.25
1	A	229	ASP	CG-OD1	5.02	1.36	1.25
1	A	257	ASP	CG-OD1	5.02	1.36	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	337	ASP	CB-CG-OD1	7.24	124.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	257	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	195	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	92	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	333	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	351	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	459	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	431	ASP	CB-CG-OD1	5.03	122.83	118.30

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	3837	0	3771	31	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	0	0	0
5	A	260	0	0	5	0
All	All	4109	0	3771	31	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 (31) 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:219:VAL:HG11	1:A:258:LYS:HD2	1.54	0.89
1:A:386:SER:O	1:A:390:GLU:HG3	1.89	0.72
1:A:210:TYR:CD2	1:A:211:LYS:HG3	2.31	0.65
1:A:352:HIS:CD2	1:A:355:GLY:H	2.16	0.62
1:A:322:GLN:O	1:A:325:ILE:HG22	2.02	0.59
1:A:182:GLU:HG3	5:A:2089:HOH:O	2.02	0.58
1:A:25:LYS:O	1:A:29:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:HIS:HD2	1:A:354:PHE:H	1.53	0.55
1:A:233:PRO:HB2	1:A:270:PRO:HA	1.89	0.55
1:A:180:SER:HB3	5:A:2123:HOH:O	2.10	0.52
1:A:357:ILE:HG13	1:A:370:LEU:HD13	1.92	0.52
1:A:209:HIS:HD2	5:A:2137:HOH:O	1.94	0.50
1:A:31:ALA:HB1	1:A:379:LEU:HD22	1.95	0.49
1:A:74:VAL:HG13	1:A:86:LEU:HB3	1.93	0.49
1:A:217:LYS:HA	1:A:220:GLU:HG2	1.96	0.48
1:A:293:PRO:CB	1:A:359:LYS:HG3	2.45	0.47
1:A:383:THR:CG2	1:A:384:ASP:N	2.78	0.47
1:A:293:PRO:HB3	1:A:359:LYS:HG3	1.99	0.45
1:A:222:LEU:HD13	1:A:262:TYR:HB2	1.98	0.45
1:A:209:HIS:HE1	5:A:2107:HOH:O	1.99	0.45
1:A:295:PHE:HZ	1:A:335:ILE:HD13	1.80	0.45
1:A:145[A]:ASP:O	1:A:147:THR:HG23	2.16	0.44
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.44
1:A:4:SER:O	1:A:7:ASP:HB2	2.19	0.43
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.91	0.43
1:A:424:LYS:HB3	1:A:424:LYS:NZ	2.33	0.43
1:A:219:VAL:CG1	1:A:258:LYS:HD2	2.36	0.42
1:A:228:LYS:HG2	1:A:266:PHE:CZ	2.54	0.42
1:A:295:PHE:HZ	1:A:335:ILE:CD1	2.32	0.42
1:A:210:TYR:HB2	5:A:2132:HOH:O	2.20	0.41
1:A:50:GLY:HA3	1:A:246:PHE:CZ	2.56	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	465/555 (84%)	453 (97%)	11 (2%)	1 (0%)	47 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLY

### 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	415/496 (84%)	404 (97%)	11 (3%)	44	46

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	141	PHE
1	A	221	ASN
1	A	251[A]	SER
1	A	251[B]	SER
1	A	277	ARG
1	A	335	ILE
1	A	383	THR
1	A	426	VAL
1	A	474	SER
1	A	488	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	209	HIS
1	A	221	ASN
1	A	352	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules 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	BFD	A	52	1,3	8,11,12	3.25	3 (37%)	3,15,17	1.47	1 (33%)

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	BFD	A	52	1,3	-	0/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	BFD	F1-BE	-6.48	1.38	1.54
1	A	52	BFD	F3-BE	-4.63	1.42	1.54
1	A	52	BFD	F2-BE	-4.31	1.43	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	BFD	OD2-CG-CB	-2.36	119.52	124.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 2 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	SO4	A	1492	-	4,4,4	0.17	0	6,6,6	0.20	0
4	SO4	A	1491	-	4,4,4	0.37	0	6,6,6	0.79	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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	466/555 (83%)	-0.07	18 (3%)	39 48	2, 10, 34, 56	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	PHE	7.2
1	A	399	LEU	6.4
1	A	210	TYR	4.8
1	A	3	THR	4.5
1	A	421	ARG	4.3
1	A	323	HIS	4.2
1	A	400	ALA	3.4
1	A	129	ARG	3.3
1	A	420	GLN	3.3
1	A	397	ILE	3.1
1	A	422	ARG	2.7
1	A	131	PRO	2.6
1	A	29	ARG	2.6
1	A	384	ASP	2.4
1	A	267	PRO	2.3
1	A	394	SER	2.2
1	A	474	SER	2.1
1	A	425	LYS	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. 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( $\text{\AA}^2$ )	Q<0.9
1	BFD	A	52	12/13	0.97	0.06	2,4,5,6	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
2	UNX	A	1489	1/1	0.90	0.26	42,42,42,42	0
4	SO4	A	1492	5/5	0.91	0.18	64,64,65,66	0
4	SO4	A	1491	5/5	0.97	0.09	24,29,33,33	0
3	MG	A	1490	1/1	0.98	0.05	10,10,10,10	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.