



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 11:16 PM GMT

PDB ID : 4AB4  
Title : Structure of Xenobiotic Reductase B from *Pseudomonas putida* in complex with TNT  
Authors : Carvalho, A.L.; Mukhopadhyay, A.; Romao, M.J.; Bursakov, S.; Kladova, A.; Ramos, J.L.; Van Dillewijn, P.  
Deposited on : 2011-12-06  
Resolution : 1.50 Å(reported)

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A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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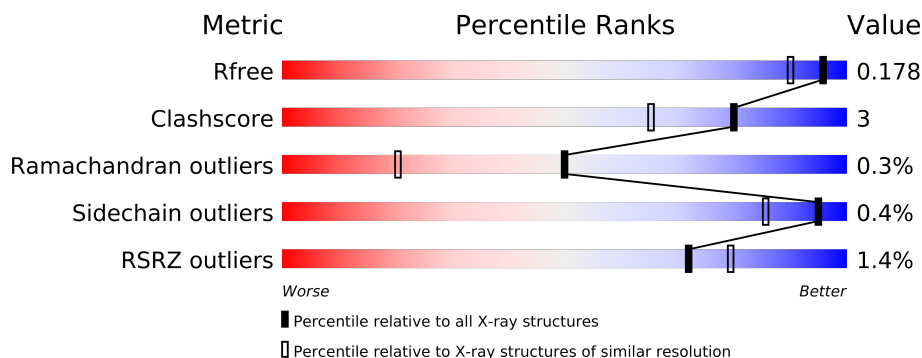
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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	362	
1	B	362	

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	SO4	A	1352	-	X
3	SO4	A	1353	-	X
3	SO4	B	1352	-	X
4	GOL	A	1356	-	X
5	TNL	A	1357	-	X
5	TNL	B	1354	-	X
6	EDO	B	1353	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6318 atoms, of which 32 are hydrogens 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 XENOBIOTIC REDUCTASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	4	0
			2662	1676	472	508	6			
1	B	349	Total	C	N	O	S	0	4	0
			2669	1679	473	511	6			

There are 26 discrepancies between the modelled and reference sequences:

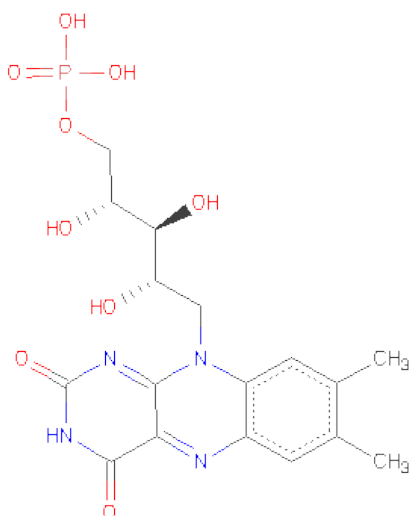
Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LYS	-	EXPRESSION TAG	UNP Q88PD0
A	351	LEU	-	EXPRESSION TAG	UNP Q88PD0
A	352	ALA	-	EXPRESSION TAG	UNP Q88PD0
A	353	ALA	-	EXPRESSION TAG	UNP Q88PD0
A	354	ALA	-	EXPRESSION TAG	UNP Q88PD0
A	355	LEU	-	EXPRESSION TAG	UNP Q88PD0
A	356	GLU	-	EXPRESSION TAG	UNP Q88PD0
A	357	HIS	-	EXPRESSION TAG	UNP Q88PD0
A	358	HIS	-	EXPRESSION TAG	UNP Q88PD0
A	359	HIS	-	EXPRESSION TAG	UNP Q88PD0
A	360	HIS	-	EXPRESSION TAG	UNP Q88PD0
A	361	HIS	-	EXPRESSION TAG	UNP Q88PD0
A	362	HIS	-	EXPRESSION TAG	UNP Q88PD0
B	350	LYS	-	EXPRESSION TAG	UNP Q88PD0
B	351	LEU	-	EXPRESSION TAG	UNP Q88PD0
B	352	ALA	-	EXPRESSION TAG	UNP Q88PD0
B	353	ALA	-	EXPRESSION TAG	UNP Q88PD0
B	354	ALA	-	EXPRESSION TAG	UNP Q88PD0
B	355	LEU	-	EXPRESSION TAG	UNP Q88PD0
B	356	GLU	-	EXPRESSION TAG	UNP Q88PD0
B	357	HIS	-	EXPRESSION TAG	UNP Q88PD0
B	358	HIS	-	EXPRESSION TAG	UNP Q88PD0
B	359	HIS	-	EXPRESSION TAG	UNP Q88PD0
B	360	HIS	-	EXPRESSION TAG	UNP Q88PD0
B	361	HIS	-	EXPRESSION TAG	UNP Q88PD0

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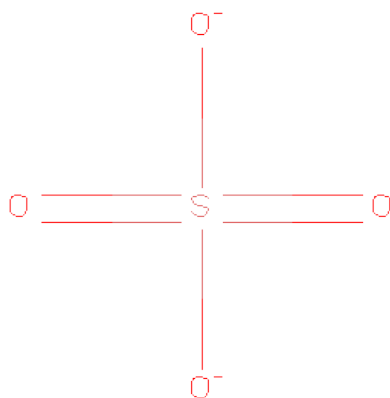
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	HIS	-	EXPRESSION TAG	UNP Q88PD0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



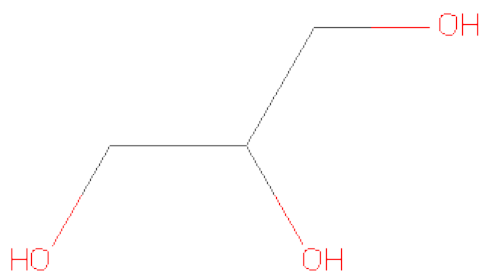
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	39	17	8	4	9	1	0	0
2	B	1	39	17	8	4	9	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



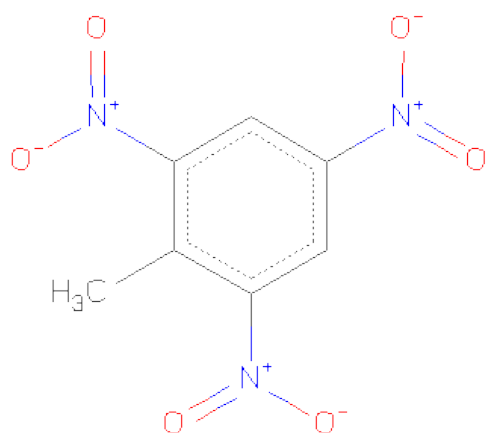
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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



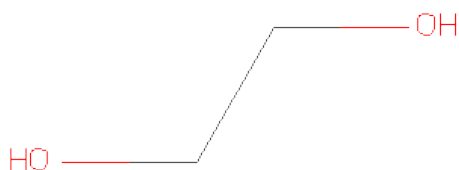
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2,4,6-TRINITROTOLUENE (three-letter code: TNL) (formula:  $C_7H_5N_3O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	2	0
			21	7	5	3	6		
5	B	1	Total	C	H	N	O	2	0
			21	7	5	3	6		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	448	Total 448	O 448	0	0
7	B	376	Total 376	O 376	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: XENOBIOTIC REDUCTASE B

Chain A: 



- Molecule 1: XENOBIOTIC REDUCTASE B

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.01Å 104.87Å 106.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.17 – 1.50 19.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.3 (21.17-1.50) 92.3 (19.99-1.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.34 (at 1.50Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.160 , 0.184 0.155 , 0.178	Depositor DCC
$R_{free}$ test set	5550 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 38.2	EDS
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 111018 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2820e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: FMN, GOL, TNL, EDO, SO4

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	0.41	0/2737	0.61	0/3731
1	B	0.39	0/2744	0.60	0/3739
All	All	0.40	0/5481	0.60	0/7470

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	2662	0	0	9	0
1	B	2669	0	0	6	0
2	A	31	8	11	2	0
2	B	31	8	11	2	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	24	4	0
5	A	16	5	0	2	0
5	B	16	5	0	4	0
6	B	4	6	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	448	0	0	2	0
7	B	376	0	0	1	0
All	All	6286	32	46	19	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.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:ARG:NE	4:A:1356:GOL:H2	1.99	0.76
1:B:75[B]:ASP:OD2	1:B:79:ARG:NH1	2.26	0.68
1:A:198:SER:N	4:A:1356:GOL:O2	2.29	0.66
1:B:233:HIS:CE1	5:B:1354:TNL:H5	2.33	0.63
1:A:265[A]:GLU:OE1	4:A:1354:GOL:H2	1.99	0.62

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	351/362 (97%)	338 (96%)	12 (3%)	1 (0%)	50	20
1	B	351/362 (97%)	338 (96%)	12 (3%)	1 (0%)	50	20
All	All	702/724 (97%)	676 (96%)	24 (3%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	GLU
1	B	286	GLU

### 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	270/281 (96%)	269 (100%)	1 (0%)	95	85
1	B	271/281 (96%)	270 (100%)	1 (0%)	95	85
All	All	541/562 (96%)	539 (100%)	2 (0%)	95	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	PHE
1	B	311	PHE

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 ⓘ

11 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	FMN	A	1351	-	33,33,33	0.89	1 (3%)	46,50,50	1.65	7 (15%)
3	SO4	A	1352	-	4,4,4	0.37	0	6,6,6	0.24	0
3	SO4	A	1353	-	4,4,4	0.20	0	6,6,6	0.11	0
4	GOL	A	1354	-	5,5,5	0.35	0	5,5,5	0.26	0
4	GOL	A	1355	-	5,5,5	0.47	0	5,5,5	0.22	0
4	GOL	A	1356	-	5,5,5	0.40	0	5,5,5	0.32	0
5	TNL	A	1357	-	16,16,16	2.25	5 (31%)	23,23,23	2.40	6 (26%)
2	FMN	B	1351	-	33,33,33	1.02	2 (6%)	46,50,50	1.43	5 (10%)
3	SO4	B	1352	-	4,4,4	0.14	0	6,6,6	0.11	0
6	EDO	B	1353	-	3,3,3	0.51	0	2,2,2	0.37	0
5	TNL	B	1354	-	16,16,16	2.24	3 (18%)	23,23,23	2.94	7 (30%)

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	FMN	A	1351	-	-	0/18/18/18	0/0/3/3
3	SO4	A	1352	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1353	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1354	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1355	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1356	-	-	0/4/4/4	0/0/0/0
5	TNL	A	1357	-	-	0/12/12/12	0/1/1/1
2	FMN	B	1351	-	-	0/18/18/18	0/0/3/3
3	SO4	B	1352	-	-	0/0/0/0	0/0/0/0
6	EDO	B	1353	-	-	0/1/1/1	0/0/0/0
5	TNL	B	1354	-	-	0/12/12/12	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1354	TNL	O41-N4	5.52	1.32	1.23
5	A	1357	TNL	O41-N4	5.39	1.32	1.23
5	A	1357	TNL	O21-N2	3.92	1.29	1.23
5	B	1354	TNL	O61-N6	3.90	1.29	1.23
5	B	1354	TNL	O21-N2	3.87	1.29	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1354	TNL	C6-C1-C2	8.96	119.58	113.15
5	A	1357	TNL	C6-C1-C2	8.81	119.47	113.15
5	B	1354	TNL	C3-C4-N4	5.64	123.17	118.71
2	A	1351	FMN	C2'-C1'-N10	-5.64	104.97	112.45
5	B	1354	TNL	C3-C2-N2	5.45	121.29	115.82

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	349/362 (96%)	-0.39	4 (1%) 77 84	2, 5, 14, 39	0
1	B	349/362 (96%)	-0.29	6 (1%) 67 74	2, 6, 19, 36	0
All	All	698/724 (96%)	-0.34	10 (1%) 72 79	2, 6, 17, 39	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	3.9
1	A	130	LEU	3.9
1	A	350	LYS	3.2
1	B	133	PRO	3.0
1	B	132	ARG	2.8

### 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( $\text{\AA}^2$ )	Q<0.9
5	TNL	A	1357	16/16	0.25	36.93	5,29,36,36	13
3	SO4	B	1352	5/5	0.24	24.32	35,36,37,37	0
5	TNL	B	1354	16/16	0.25	16.68	10,34,41,41	13
3	SO4	A	1352	5/5	0.13	5.86	26,27,30,31	0
6	EDO	B	1353	4/4	0.15	5.56	30,37,37,38	0
3	SO4	A	1353	5/5	0.17	5.34	23,26,27,28	0
4	GOL	A	1356	6/6	0.15	3.21	25,26,27,28	0
4	GOL	A	1354	6/6	0.12	1.87	10,25,27,28	0
2	FMN	B	1351	31/31	0.07	0.51	1,4,9,9	0
4	GOL	A	1355	6/6	0.07	0.45	6,7,8,8	0
2	FMN	A	1351	31/31	0.07	0.34	2,4,8,8	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.