



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 05:18 am GMT

PDB ID : 4WEM  
Title : Co-complex structure of the F4 fimbrial adhesin FaeG variant ac with llama single domain antibody V1  
Authors : Moonens, K.; Van den Broeck, I.; Pardon, E.; De Kerpel, M.; Remaut, H.; De Greve, H.  
Deposited on : 2014-09-10  
Resolution : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

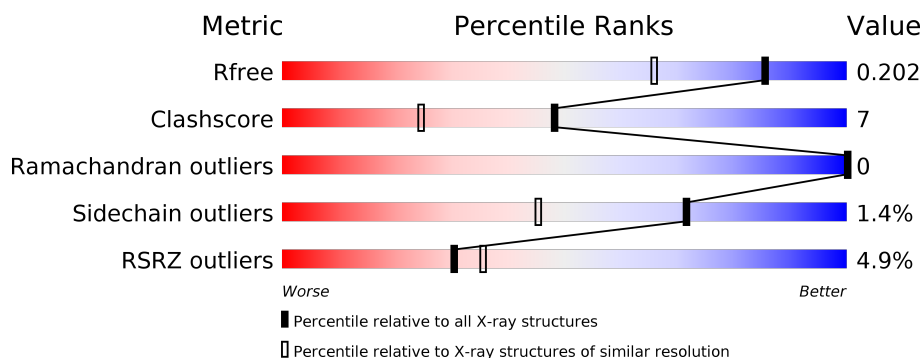
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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))
$R_{free}$	100719	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

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. 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	272	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>••</div> <div>9%</div> </div> </div>
2	B	127	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>•</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	301	-	-	X	X
3	PO4	B	1001	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3102 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 K88 fimbrial protein AC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	3	0
			1837	1156	313	366	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	TRP	-	expression tag	UNP L7XD53
A	10	MET	-	expression tag	UNP L7XD53
A	11	THR	-	expression tag	UNP L7XD53
A	12	GLY	-	expression tag	UNP L7XD53
A	13	HIS	-	expression tag	UNP L7XD53
A	14	HIS	-	expression tag	UNP L7XD53
A	15	HIS	-	expression tag	UNP L7XD53
A	16	HIS	-	expression tag	UNP L7XD53
A	17	HIS	-	expression tag	UNP L7XD53
A	18	HIS	-	expression tag	UNP L7XD53
A	263	ASP	-	expression tag	UNP L7XD53
A	264	ASN	-	expression tag	UNP L7XD53
A	275	LYS	-	expression tag	UNP L7XD53
A	276	GLN	-	expression tag	UNP L7XD53
A	277	ASP	-	expression tag	UNP L7XD53
A	278	PHE	-	expression tag	UNP L7XD53
A	279	ASN	-	expression tag	UNP L7XD53
A	280	GLY	-	expression tag	UNP L7XD53
A	281	SER	-	expression tag	UNP L7XD53
A	282	VAL	-	expression tag	UNP L7XD53
A	283	ASP	-	expression tag	UNP L7XD53
A	284	ILE	-	expression tag	UNP L7XD53
A	285	GLY	-	expression tag	UNP L7XD53
A	286	GLY	-	expression tag	UNP L7XD53
A	287	SER	-	expression tag	UNP L7XD53
A	288	ILE	-	expression tag	UNP L7XD53
A	289	THR	-	expression tag	UNP L7XD53

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Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	-	expression tag	UNP L7XD53

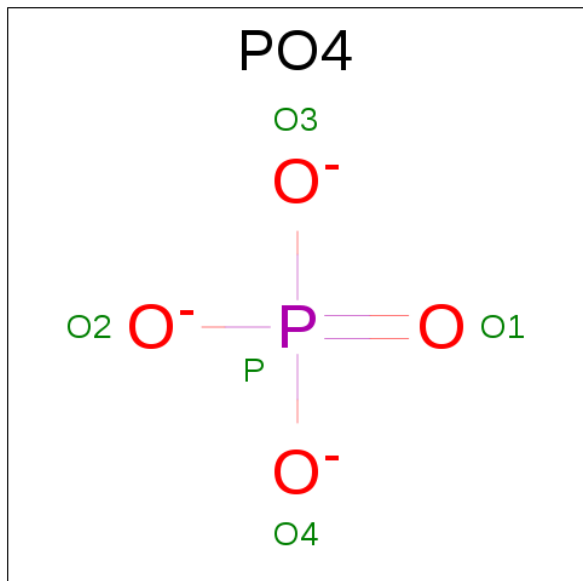
- Molecule 2 is a protein called Anti-F4+ETEC bacteria VHH variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	3	0
			941	591	168	178	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	922	HIS	-	expression tag	UNP R9W2R6
B	923	HIS	-	expression tag	UNP R9W2R6
B	924	HIS	-	expression tag	UNP R9W2R6
B	925	HIS	-	expression tag	UNP R9W2R6
B	926	HIS	-	expression tag	UNP R9W2R6
B	927	HIS	-	expression tag	UNP R9W2R6

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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

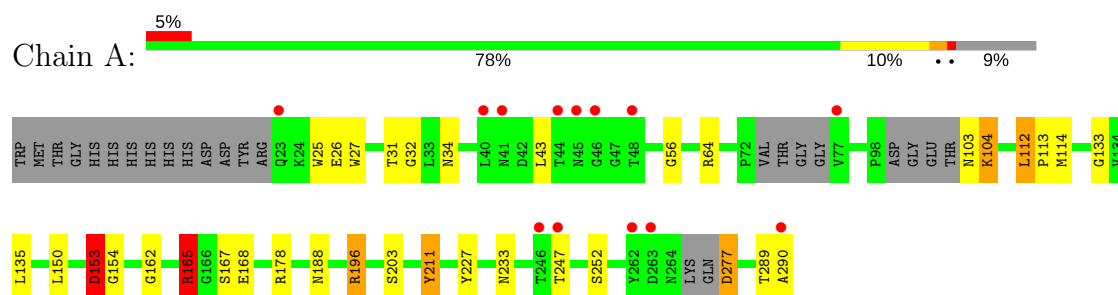
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	77	Total	O	0	0
			77	77		

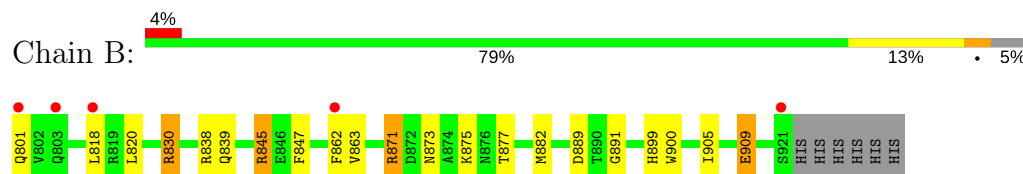
### 3 Residue-property plots [i](#)

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: K88 fimbrial protein AC



- Molecule 2: Anti-F4+ETEC bacteria VHH variable region



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.48Å 145.48Å 38.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.62 – 1.55 47.62 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.62-1.55) 99.9 (47.62-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.169 , 0.193 0.179 , 0.202	Depositor DCC
$R_{free}$ test set	3461 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1.34	10/1874 (0.5%)	1.36	14/2543 (0.6%)
2	B	1.35	4/967 (0.4%)	1.70	11/1301 (0.8%)
All	All	1.34	14/2841 (0.5%)	1.49	25/3844 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	CB-CG	-9.54	1.34	1.52
2	B	900	TRP	CG-CD1	8.21	1.48	1.36
1	A	203	SER	CB-OG	-7.69	1.32	1.42
1	A	32	GLY	N-CA	7.33	1.57	1.46
2	B	900	TRP	CD1-NE1	-6.42	1.27	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	871	ARG	NE-CZ-NH1	25.09	132.84	120.30
2	B	871	ARG	NE-CZ-NH2	-23.34	108.63	120.30
1	A	165	ARG	NE-CZ-NH1	17.88	129.24	120.30
1	A	165	ARG	NE-CZ-NH2	-16.62	111.99	120.30
2	B	871	ARG	CD-NE-CZ	11.57	139.79	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ASP	Mainchain
1	A	165	ARG	Sidechain

## 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	1837	0	1818	21	0
2	B	941	0	926	17	0
3	A	15	0	0	3	0
3	B	5	0	0	0	0
4	A	227	0	0	7	0
4	B	77	0	0	8	0
All	All	3102	0	2744	38	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.

The worst 5 of 38 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)
2:B:909:GLU:CD	4:B:1155:HOH:O	1.67	1.34
1:A:277:ASP:N	4:A:575:HOH:O	1.75	1.15
1:A:104:LYS:HE3	1:A:168:GLU:O	1.61	0.98
2:B:871:ARG:HD2	2:B:873:ASN:OD1	1.73	0.87
1:A:56:GLY:H	1:A:233:ASN:HD22	1.25	0.84

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	243/272 (89%)	239 (98%)	4 (2%)	0	100	100
2	B	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
All	All	365/399 (92%)	358 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	193/210 (92%)	191 (99%)	2 (1%)	80	61
2	B	99/102 (97%)	96 (97%)	3 (3%)	46	14
All	All	292/312 (94%)	287 (98%)	5 (2%)	71	36

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	112	LEU
2	B	830	ARG
2	B	845[A]	ARG
2	B	845[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
2	B	884	ASN
2	B	801	GLN
1	A	188	ASN
1	A	233	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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$
3	PO4	A	301	-	4,4,4	1.51	1 (25%)	6,6,6	1.94	1 (16%)
3	PO4	A	302	-	4,4,4	0.73	0	6,6,6	1.76	1 (16%)
3	PO4	A	303	-	4,4,4	1.40	0	6,6,6	2.90	3 (50%)
3	PO4	B	1001	-	4,4,4	2.52	1 (25%)	6,6,6	2.34	4 (66%)

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
3	PO4	A	301	-	-	0/0/0/0	0/0/0/0
3	PO4	A	302	-	-	0/0/0/0	0/0/0/0
3	PO4	A	303	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1001	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	PO4	P-O4	-2.10	1.47	1.54
3	B	1001	PO4	P-O1	5.03	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	PO4	O2-P-O1	-5.59	87.17	110.97
3	A	301	PO4	O3-P-O2	-3.99	93.25	107.90
3	A	302	PO4	O4-P-O1	-3.54	95.88	110.97
3	B	1001	PO4	O4-P-O2	-3.14	96.34	107.90
3	B	1001	PO4	O3-P-O1	-2.33	101.04	110.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	PO4	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	248/272 (91%)	0.05	13 (5%) 28 32	16, 29, 58, 79	0
2	B	121/127 (95%)	0.07	5 (4%) 38 43	19, 35, 56, 82	0
All	All	369/399 (92%)	0.06	18 (4%) 30 35	16, 31, 58, 82	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	7.6
1	A	263	ASP	4.5
1	A	40	LEU	4.3
2	B	801	GLN	3.9
1	A	246	THR	3.8

### 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 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	301	5/5	0.98	0.21	5.03	35,36,38,42	0
3	PO4	B	1001	5/5	0.96	0.14	1.93	41,42,45,47	0
3	PO4	A	302	5/5	0.99	0.06	-1.56	28,30,33,39	0
3	PO4	A	303	5/5	0.91	0.22	-	33,36,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.