

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 8, 2020 – 01:25 PM BST

PDB ID : 5O2X

Title: Extended catalytic domain of H. jecorina LPMO9A a.k.a EG4

Authors: Hansson, H.; Karkehabadi, S.; Mikkelsen, N.E.; Sandgren, M.; Kelemen, B.;

Kaper, T.

Deposited on : 2017-05-23

Resolution : 0.95 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.13.1

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)

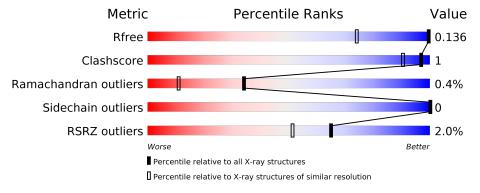
Validation Pipeline (wwPDB-VP) : 2.13.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 0.95 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1243 (1.06-0.86)
Clashscore	141614	1321 (1.06-0.86)
Ramachandran outliers	138981	1233 (1.06-0.86)
Sidechain outliers	138945	1235 (1.06-0.86)
RSRZ outliers	127900	1209 (1.06-0.86)

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 >=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 <=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	
			2%	
1	A	248	95%	5%



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2655 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.

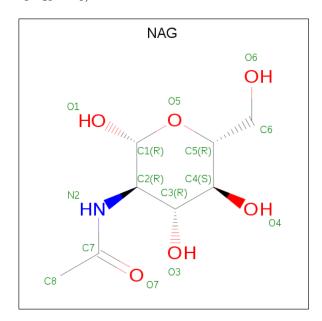
• Molecule 1 is a protein called Glycoside hydrolase family 61.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace			
1	Λ	248	Total	С	N	О	S	0	28	0
	A	240	1994	1279	324	387	4	U	20	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIC	_	expression tag	UNP G0R6T8

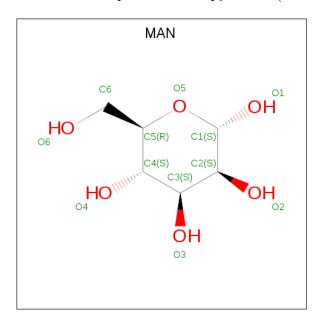
• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15			O 6	0	1
2	A	1	Total 14	C 8		O 5	0	0



• Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 22 12 10	0	1
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 22 12 10	0	1
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 22 12 10	0	1
3	A	1	Total C O 22 12 10	0	1
3	A	1	Total C O 11 6 5	0	0
			$C_{\alpha}$	ntinued on	ant maga

Continued on next page...



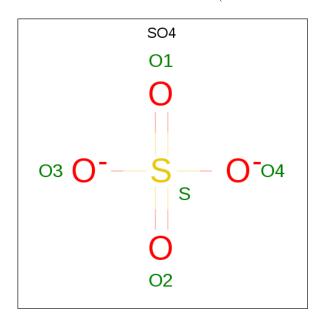
 $Continued\ from\ previous\ page...$ 

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

• Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

 $\bullet$  Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



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

• Molecule 6 is water.

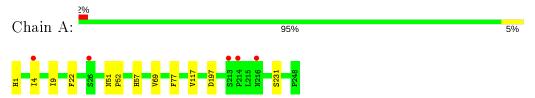
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	372	Total O 407 407	0	46



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Glycoside hydrolase family 61





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	42.82Å 61.55Å 47.78Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 112.03° 90.00°	Depositor
Resolution (Å)	44.29 - 0.95	Depositor
resolution (A)	23.75 - 0.95	EDS
% Data completeness	89.0 (44.29-0.95)	Depositor
(in resolution range)	89.0 (23.75-0.95)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.85 (at 0.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
P. P.	0.115 , $0.127$	Depositor
$R, R_{free}$	0.125 , $0.136$	DCC
$R_{free}$ test set	6451  reflections  (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	5.6	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2655	wwPDB-VP
Average B, all atoms $(Å^2)$	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.67% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MAN, HIC, NAG, CU, 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).

Mal	Chain	Bond	Bond lengths		nd angles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.65	0/2093	0.80	$2/2882 \ (0.1\%)$

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	22	PHE	CB-CG-CD1	5.66	124.76	120.80
1	A	197	ASP	CB-CG-OD1	5.38	123.14	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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	1994	0	1937	4	0
2	A	29	0	19	0	0
3	A	209	0	190	0	0
4	A	1	0	0	0	0
5	A	15	0	0	0	0
6	A	407	0	0	0	0
All	All	2655	0	2146	4	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 1.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	Clash overlap (Å)	
1:A:4[B]:ILE:HD12	1:A:77:PHE:HB3	1.98	0.44	
1:A:51[A]:ASN:CG	1:A:52[A]:PRO:HD2	2.40	0.41	
1:A:9:ILE:HG21	1:A:69[A]:VAL:HG12	2.03	0.41	
1:A:117:VAL:CG2	1:A:231:SER:HB3	2.51	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	273/248 (110%)	266 (97%)	6 (2%)	1 (0%)	34 11	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Α	57	HIS

#### 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	$226/200 \ (113\%)$	226 (100%)	0	100 100		



There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Ros	Ros	Res	Ros	Res	Res Link	B	Bond lengths			Bond angles		
				LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2						
1	HIC	A	1	1,4	8,11,12	1.23	1 (12%)	6,14,16	0.60	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
1	HIC	A	1	1,4	-	0/5/6/8	0/1/1/1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	A	1	HIC	CD2-NE2	-3.05	1.33	1.38

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.



### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	T	Chain	Res	Link	Во	ond leng	$\operatorname{sths}$	В	ond ang	gles
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	301[A]	_	14,14,15	0.63	0	17,19,21	0.74	0
2	NAG	A	301[B]	_	14,14,15	0.63	0	17,19,21	0.93	1 (5%)
3	MAN	A	304	1	11,11,12	0.91	1 (9%)	15,15,17	0.80	0
5	SO4	A	319	-	4,4,4	0.41	0	6,6,6	0.65	0
3	MAN	A	306	1	11,11,12	0.70	0	15, 15, 17	0.93	1 (6%)
3	MAN	A	316	1	11,11,12	0.51	0	15,15,17	1.62	1 (6%)
2	NAG	A	302	1	14,14,15	0.72	0	17,19,21	0.70	1 (5%)
5	SO4	A	321	-	4,4,4	0.57	0	6,6,6	0.74	0
3	MAN	A	303	1	11,11,12	0.54	0	15,15,17	0.93	0
5	SO4	A	320	-	4,4,4	0.40	0	$6,\!6,\!6$	0.69	0
3	MAN	A	317	1	11,11,12	0.50	0	15,15,17	0.81	0
3	MAN	A	310[A]	1	11,11,12	0.71	0	15, 15, 17	1.33	2 (13%)
3	MAN	A	310[B]	1	11,11,12	0.66	0	15,15,17	1.98	3 (20%)
3	MAN	A	313[B]	1	11,11,12	0.34	0	15,15,17	1.38	1 (6%)
3	MAN	A	313[A]	1	11,11,12	0.76	0	15,15,17	0.87	1 (6%)
3	MAN	A	308[B]	1	11,11,12	0.87	0	15,15,17	1.54	2 (13%)
3	MAN	A	315	1	11,11,12	0.77	0	15,15,17	1.70	3 (20%)
3	MAN	A	308[A]	1	11,11,12	0.70	0	15,15,17	1.35	2 (13%)
3	MAN	A	309	1	11,11,12	0.64	0	15,15,17	1.18	2 (13%)
3	MAN	A	311	1	11,11,12	0.37	0	15,15,17	0.94	1 (6%)
3	MAN	A	305	1	11,11,12	0.59	0	15,15,17	1.08	0
3	MAN	A	312	1	11,11,12	0.60	0	15,15,17	0.75	1 (6%)
3	MAN	A	314[A]	1	11,11,12	0.91	1 (9%)	15,15,17	1.58	3 (20%)



Mol	Т	Chain	Res	Link	В	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	MAN	A	314[B]	1	11,11,12	0.51	0	15,15,17	1.16	1 (6%)
3	MAN	A	307	1	11,11,12	0.70	0	15,15,17	1.31	1 (6%)

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	NAG	A	301[A]	-	-	0/6/23/26	0/1/1/1
2	NAG	A	301[B]	-	-	0/6/23/26	0/1/1/1
3	MAN	A	304	1	-	0/2/19/22	0/1/1/1
3	MAN	A	306	1	-	2/2/19/22	0/1/1/1
3	MAN	A	316	1	-	0/2/19/22	0/1/1/1
2	NAG	A	302	1	-	0/6/23/26	0/1/1/1
3	MAN	A	303	1	-	0/2/19/22	0/1/1/1
3	MAN	A	317	1	-	0/2/19/22	0/1/1/1
3	MAN	A	310[A]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	310[B]	1	-	1/2/19/22	0/1/1/1
3	MAN	A	313[B]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	313[A]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	308[B]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	315	1	-	0/2/19/22	0/1/1/1
3	MAN	A	308[A]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	309	1	-	1/2/19/22	0/1/1/1
3	MAN	A	311	1	-	0/2/19/22	0/1/1/1
3	MAN	A	305	1	-	0/2/19/22	0/1/1/1
3	MAN	A	312	1	-	0/2/19/22	0/1/1/1
3	MAN	A	314[A]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	314[B]	1	-	0/2/19/22	0/1/1/1
3	MAN	A	307	1	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
3	A	314[A]	MAN	O5-C1	-2.51	1.39	1.43
3	A	304	MAN	C2-C3	2.13	1.55	1.52

The worst 5 of 27 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
3	Α	316	MAN	C1-O5-C5	4.76	118.64	112.19
3	A	310[B]	MAN	C2-C3-C4	-4.61	102.92	110.89
3	A	313[B]	MAN	C1-O5-C5	4.04	117.66	112.19
3	A	315	MAN	C1-C2-C3	-3.86	104.92	109.67
3	A	308[B]	MAN	C1-O5-C5	3.85	117.41	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	307	MAN	O5-C5-C6-O6
3	A	306	MAN	C4-C5-C6-O6
3	A	306	MAN	O5-C5-C6-O6
3	A	310[B]	MAN	C4-C5-C6-O6
3	A	309	MAN	C4-C5-C6-O6

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 (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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	247/248 (99%)	0.47	5 (2%) 65 5	51	4, 6, 13, 22	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	PRO	3.1
1	A	26	SER	2.6
1	A	216	ASN	2.1
1	A	4[A]	ILE	2.1
1	A	213	SER	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
1	HIC	A	1	11/12	0.99	0.07	5,6,7,9	0

### 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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	${f B-factors}({f \AA}^2)$	Q < 0.9
5	SO4	A	321	5/5	0.72	0.29	17,50,56,61	0
3	MAN	A	307	11/12	0.83	0.14	14,18,27,28	11
3	MAN	A	316	11/12	0.84	0.15	15,17,25,26	11
3	MAN	A	303	11/12	0.86	0.17	14,16,20,21	11
3	MAN	A	315	11/12	0.88	0.15	15,19,27,31	11
3	MAN	A	305	11/12	0.89	0.09	13,16,20,20	11
5	SO4	A	320	5/5	0.91	0.30	20,29,33,34	5
3	MAN	A	314[B]	11/12	0.92	0.13	9,11,16,20	11
3	MAN	A	314[A]	11/12	0.92	0.13	8,10,13,14	11
5	SO4	A	319	5/5	0.94	0.18	17,18,21,22	5
3	MAN	A	310[B]	11/12	0.95	0.11	7,9,12,13	11
3	MAN	A	306	11/12	0.95	0.09	6,8,12,14	11
3	MAN	A	310[A]	11/12	0.95	0.11	7,9,12,16	11
3	MAN	A	309	11/12	0.96	0.09	8,9,14,20	11
3	MAN	A	313[A]	11/12	0.96	0.14	5,6,8,10	11
3	MAN	A	308[B]	11/12	0.96	0.12	7,9,12,18	11
3	MAN	A	313[B]	11/12	0.96	0.14	7,8,9,11	11
3	MAN	A	308[A]	11/12	0.96	0.12	7,9,12,15	11
2	NAG	A	301[A]	14/15	0.97	0.15	8,9,11,12	1
2	NAG	A	301[B]	14/15	0.97	0.15	8,9,12,14	1
2	NAG	A	302	14/15	0.98	0.09	5,6,8,8	14
3	MAN	A	304	11/12	0.98	0.08	5,6,8,9	11
3	MAN	A	317	11/12	0.98	0.09	5,5,7,7	0
3	MAN	A	312	11/12	0.99	0.07	5,5,6,9	0
3	MAN	A	311	11/12	0.99	0.08	4,4,5,6	0
4	CU	A	318	1/1	1.00	0.07	5,5,5,5	1

# 6.5 Other polymers (i)

There are no such residues in this entry.

