



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:56 AM EST

PDB ID : 2AE8  
Title : Crystal Structure of Imidazoleglycerol-phosphate Dehydratase from *Staphylococcus aureus* subsp. *aureus* N315  
Authors : Kim, Y.; Quartey, P.; Holzle, D.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2005-07-21  
Resolution : 2.01 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

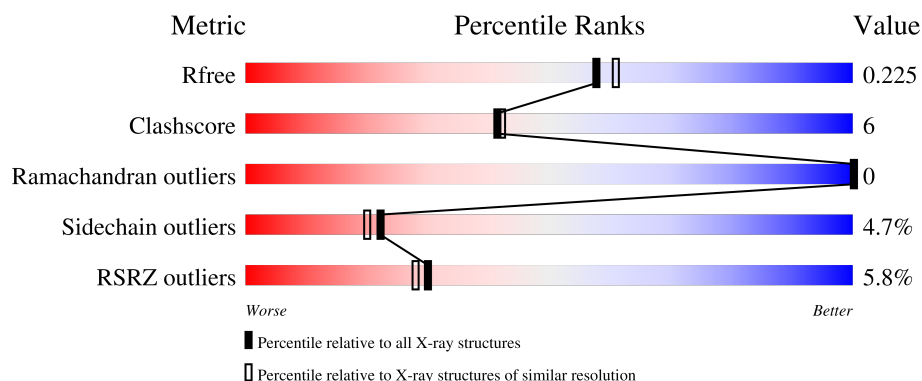
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 of 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	221	<div> <div>4%</div> <div>69%</div> <div>7%</div> <div>23%</div> </div>
1	B	221	<div> <div>5%</div> <div>69%</div> <div>7%</div> <div>22%</div> </div>
1	C	221	<div> <div>6%</div> <div>66%</div> <div>10%</div> <div>23%</div> </div>
1	D	221	<div> <div>4%</div> <div>67%</div> <div>10%</div> <div>23%</div> </div>
1	E	221	<div> <div>4%</div> <div>62%</div> <div>12%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	221	<div><div></div><div>4%</div><div>68%</div><div>9%</div><div>23%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9237 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 Imidazoleglycerol-phosphate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	Se	0	4	0
			1387	883	243	256	5			
1	B	172	Total	C	N	O	Se	0	2	0
			1378	875	242	256	5			
1	C	171	Total	C	N	O	Se	0	2	0
			1372	872	240	255	5			
1	D	171	Total	C	N	O	Se	0	3	0
			1382	878	243	256	5			
1	E	171	Total	C	N	O	Se	0	3	0
			1383	879	243	256	5			
1	F	170	Total	C	N	O	Se	0	3	0
			1373	874	241	253	5			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	HIS	-	expression tag	UNP P64373
A	-27	HIS	-	expression tag	UNP P64373
A	-26	HIS	-	expression tag	UNP P64373
A	-25	HIS	-	expression tag	UNP P64373
A	-24	HIS	-	expression tag	UNP P64373
A	-23	HIS	-	expression tag	UNP P64373
A	-22	SER	-	cloning artifact	UNP P64373
A	-21	SER	-	cloning artifact	UNP P64373
A	-20	GLY	-	cloning artifact	UNP P64373
A	-19	VAL	-	cloning artifact	UNP P64373
A	-18	ASP	-	cloning artifact	UNP P64373
A	-17	LEU	-	cloning artifact	UNP P64373
A	-16	GLY	-	cloning artifact	UNP P64373
A	-15	THR	-	cloning artifact	UNP P64373
A	-14	GLU	-	cloning artifact	UNP P64373
A	-13	ASN	-	cloning artifact	UNP P64373
A	-12	LEU	-	cloning artifact	UNP P64373

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	TYR	-	cloning artifact	UNP P64373
A	-10	PHE	-	cloning artifact	UNP P64373
A	-9	GLN	-	cloning artifact	UNP P64373
A	-8	SER	-	cloning artifact	UNP P64373
A	-7	ASN	-	cloning artifact	UNP P64373
A	-6	ILE	-	cloning artifact	UNP P64373
A	-5	GLY	-	cloning artifact	UNP P64373
A	-4	SER	-	cloning artifact	UNP P64373
A	-3	GLY	-	cloning artifact	UNP P64373
A	-2	SER	-	cloning artifact	UNP P64373
A	-1	ASN	-	cloning artifact	UNP P64373
A	0	ALA	-	cloning artifact	UNP P64373
B	-28	HIS	-	expression tag	UNP P64373
B	-27	HIS	-	expression tag	UNP P64373
B	-26	HIS	-	expression tag	UNP P64373
B	-25	HIS	-	expression tag	UNP P64373
B	-24	HIS	-	expression tag	UNP P64373
B	-23	HIS	-	expression tag	UNP P64373
B	-22	SER	-	cloning artifact	UNP P64373
B	-21	SER	-	cloning artifact	UNP P64373
B	-20	GLY	-	cloning artifact	UNP P64373
B	-19	VAL	-	cloning artifact	UNP P64373
B	-18	ASP	-	cloning artifact	UNP P64373
B	-17	LEU	-	cloning artifact	UNP P64373
B	-16	GLY	-	cloning artifact	UNP P64373
B	-15	THR	-	cloning artifact	UNP P64373
B	-14	GLU	-	cloning artifact	UNP P64373
B	-13	ASN	-	cloning artifact	UNP P64373
B	-12	LEU	-	cloning artifact	UNP P64373
B	-11	TYR	-	cloning artifact	UNP P64373
B	-10	PHE	-	cloning artifact	UNP P64373
B	-9	GLN	-	cloning artifact	UNP P64373
B	-8	SER	-	cloning artifact	UNP P64373
B	-7	ASN	-	cloning artifact	UNP P64373
B	-6	ILE	-	cloning artifact	UNP P64373
B	-5	GLY	-	cloning artifact	UNP P64373
B	-4	SER	-	cloning artifact	UNP P64373
B	-3	GLY	-	cloning artifact	UNP P64373
B	-2	SER	-	cloning artifact	UNP P64373
B	-1	ASN	-	cloning artifact	UNP P64373
B	0	ALA	-	cloning artifact	UNP P64373
C	-28	HIS	-	expression tag	UNP P64373

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-27	HIS	-	expression tag	UNP P64373
C	-26	HIS	-	expression tag	UNP P64373
C	-25	HIS	-	expression tag	UNP P64373
C	-24	HIS	-	expression tag	UNP P64373
C	-23	HIS	-	expression tag	UNP P64373
C	-22	SER	-	cloning artifact	UNP P64373
C	-21	SER	-	cloning artifact	UNP P64373
C	-20	GLY	-	cloning artifact	UNP P64373
C	-19	VAL	-	cloning artifact	UNP P64373
C	-18	ASP	-	cloning artifact	UNP P64373
C	-17	LEU	-	cloning artifact	UNP P64373
C	-16	GLY	-	cloning artifact	UNP P64373
C	-15	THR	-	cloning artifact	UNP P64373
C	-14	GLU	-	cloning artifact	UNP P64373
C	-13	ASN	-	cloning artifact	UNP P64373
C	-12	LEU	-	cloning artifact	UNP P64373
C	-11	TYR	-	cloning artifact	UNP P64373
C	-10	PHE	-	cloning artifact	UNP P64373
C	-9	GLN	-	cloning artifact	UNP P64373
C	-8	SER	-	cloning artifact	UNP P64373
C	-7	ASN	-	cloning artifact	UNP P64373
C	-6	ILE	-	cloning artifact	UNP P64373
C	-5	GLY	-	cloning artifact	UNP P64373
C	-4	SER	-	cloning artifact	UNP P64373
C	-3	GLY	-	cloning artifact	UNP P64373
C	-2	SER	-	cloning artifact	UNP P64373
C	-1	ASN	-	cloning artifact	UNP P64373
C	0	ALA	-	cloning artifact	UNP P64373
D	-28	HIS	-	expression tag	UNP P64373
D	-27	HIS	-	expression tag	UNP P64373
D	-26	HIS	-	expression tag	UNP P64373
D	-25	HIS	-	expression tag	UNP P64373
D	-24	HIS	-	expression tag	UNP P64373
D	-23	HIS	-	expression tag	UNP P64373
D	-22	SER	-	cloning artifact	UNP P64373
D	-21	SER	-	cloning artifact	UNP P64373
D	-20	GLY	-	cloning artifact	UNP P64373
D	-19	VAL	-	cloning artifact	UNP P64373
D	-18	ASP	-	cloning artifact	UNP P64373
D	-17	LEU	-	cloning artifact	UNP P64373
D	-16	GLY	-	cloning artifact	UNP P64373
D	-15	THR	-	cloning artifact	UNP P64373

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	GLU	-	cloning artifact	UNP P64373
D	-13	ASN	-	cloning artifact	UNP P64373
D	-12	LEU	-	cloning artifact	UNP P64373
D	-11	TYR	-	cloning artifact	UNP P64373
D	-10	PHE	-	cloning artifact	UNP P64373
D	-9	GLN	-	cloning artifact	UNP P64373
D	-8	SER	-	cloning artifact	UNP P64373
D	-7	ASN	-	cloning artifact	UNP P64373
D	-6	ILE	-	cloning artifact	UNP P64373
D	-5	GLY	-	cloning artifact	UNP P64373
D	-4	SER	-	cloning artifact	UNP P64373
D	-3	GLY	-	cloning artifact	UNP P64373
D	-2	SER	-	cloning artifact	UNP P64373
D	-1	ASN	-	cloning artifact	UNP P64373
D	0	ALA	-	cloning artifact	UNP P64373
E	-28	HIS	-	expression tag	UNP P64373
E	-27	HIS	-	expression tag	UNP P64373
E	-26	HIS	-	expression tag	UNP P64373
E	-25	HIS	-	expression tag	UNP P64373
E	-24	HIS	-	expression tag	UNP P64373
E	-23	HIS	-	expression tag	UNP P64373
E	-22	SER	-	cloning artifact	UNP P64373
E	-21	SER	-	cloning artifact	UNP P64373
E	-20	GLY	-	cloning artifact	UNP P64373
E	-19	VAL	-	cloning artifact	UNP P64373
E	-18	ASP	-	cloning artifact	UNP P64373
E	-17	LEU	-	cloning artifact	UNP P64373
E	-16	GLY	-	cloning artifact	UNP P64373
E	-15	THR	-	cloning artifact	UNP P64373
E	-14	GLU	-	cloning artifact	UNP P64373
E	-13	ASN	-	cloning artifact	UNP P64373
E	-12	LEU	-	cloning artifact	UNP P64373
E	-11	TYR	-	cloning artifact	UNP P64373
E	-10	PHE	-	cloning artifact	UNP P64373
E	-9	GLN	-	cloning artifact	UNP P64373
E	-8	SER	-	cloning artifact	UNP P64373
E	-7	ASN	-	cloning artifact	UNP P64373
E	-6	ILE	-	cloning artifact	UNP P64373
E	-5	GLY	-	cloning artifact	UNP P64373
E	-4	SER	-	cloning artifact	UNP P64373
E	-3	GLY	-	cloning artifact	UNP P64373
E	-2	SER	-	cloning artifact	UNP P64373

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	cloning artifact	UNP P64373
E	0	ALA	-	cloning artifact	UNP P64373
F	-28	HIS	-	expression tag	UNP P64373
F	-27	HIS	-	expression tag	UNP P64373
F	-26	HIS	-	expression tag	UNP P64373
F	-25	HIS	-	expression tag	UNP P64373
F	-24	HIS	-	expression tag	UNP P64373
F	-23	HIS	-	expression tag	UNP P64373
F	-22	SER	-	cloning artifact	UNP P64373
F	-21	SER	-	cloning artifact	UNP P64373
F	-20	GLY	-	cloning artifact	UNP P64373
F	-19	VAL	-	cloning artifact	UNP P64373
F	-18	ASP	-	cloning artifact	UNP P64373
F	-17	LEU	-	cloning artifact	UNP P64373
F	-16	GLY	-	cloning artifact	UNP P64373
F	-15	THR	-	cloning artifact	UNP P64373
F	-14	GLU	-	cloning artifact	UNP P64373
F	-13	ASN	-	cloning artifact	UNP P64373
F	-12	LEU	-	cloning artifact	UNP P64373
F	-11	TYR	-	cloning artifact	UNP P64373
F	-10	PHE	-	cloning artifact	UNP P64373
F	-9	GLN	-	cloning artifact	UNP P64373
F	-8	SER	-	cloning artifact	UNP P64373
F	-7	ASN	-	cloning artifact	UNP P64373
F	-6	ILE	-	cloning artifact	UNP P64373
F	-5	GLY	-	cloning artifact	UNP P64373
F	-4	SER	-	cloning artifact	UNP P64373
F	-3	GLY	-	cloning artifact	UNP P64373
F	-2	SER	-	cloning artifact	UNP P64373
F	-1	ASN	-	cloning artifact	UNP P64373
F	0	ALA	-	cloning artifact	UNP P64373

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0
2	D	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	3	Total 3	Mg 3	0	0
2	F	3	Total 3	Mg 3	0	0

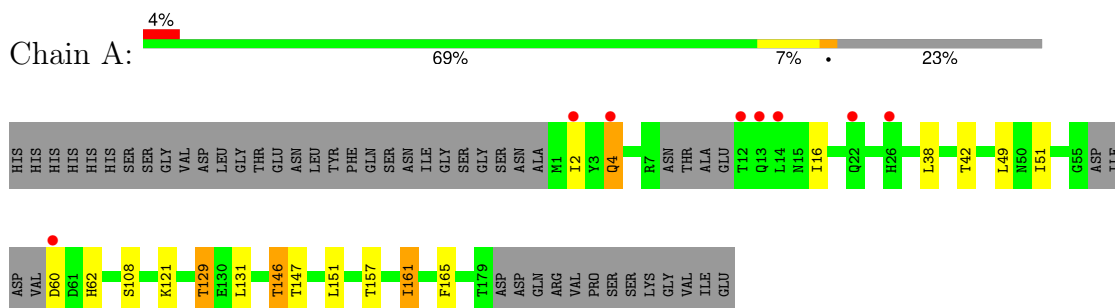
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total 160	O 160	0	0
3	B	153	Total 153	O 153	0	0
3	C	153	Total 153	O 153	0	0
3	D	138	Total 138	O 138	0	0
3	E	188	Total 188	O 188	0	0
3	F	154	Total 154	O 154	0	0

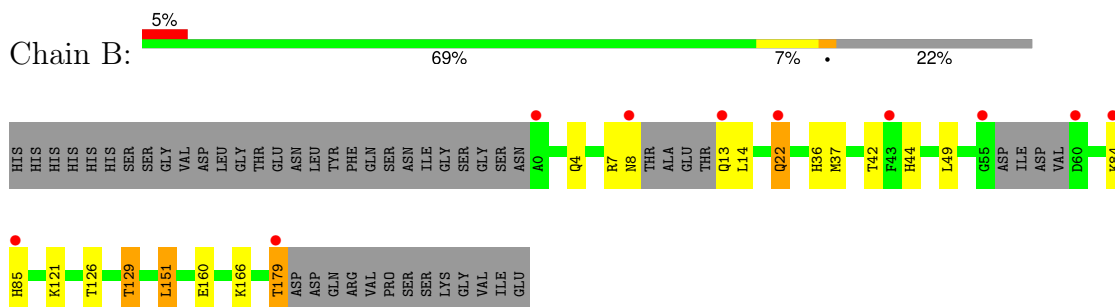
### 3 Residue-property plots [i](#)

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.

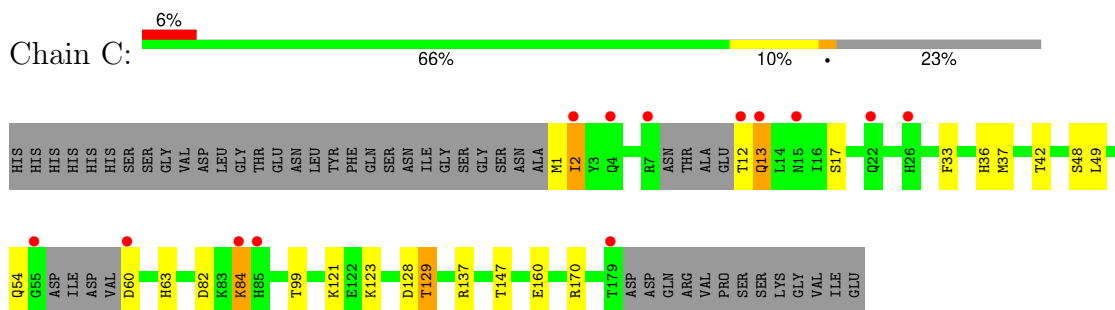
- Molecule 1: Imidazoglycerol-phosphate dehydratase



- Molecule 1: Imidazoglycerol-phosphate dehydratase

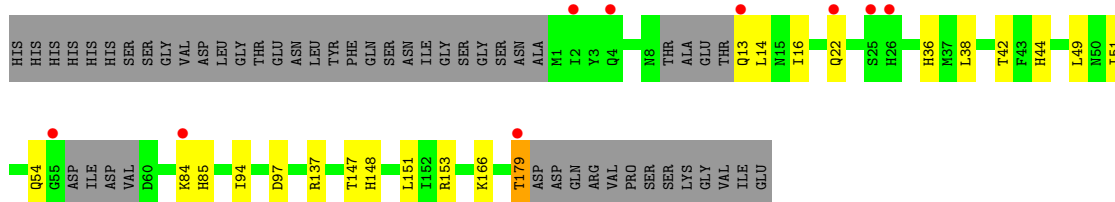


- Molecule 1: Imidazoglycerol-phosphate dehydratase

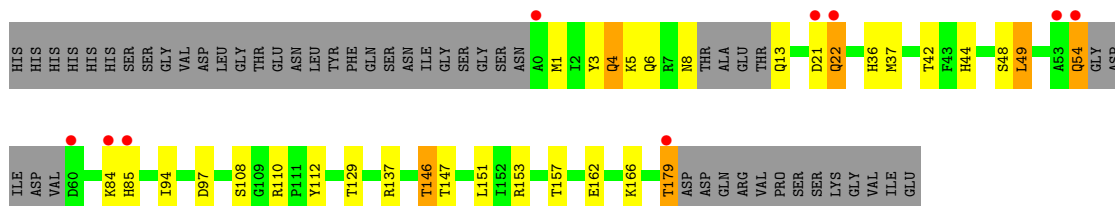


- Molecule 1: Imidazoglycerol-phosphate dehydratase

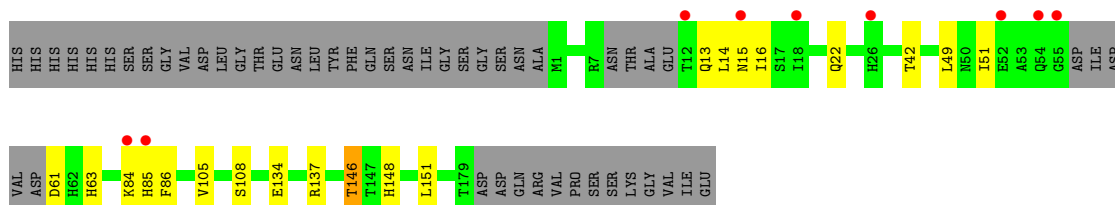




• Molecule 1: Imidazoglycerol-phosphate dehydratase



• Molecule 1: Imidazoglycerol-phosphate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.25Å 129.25Å 180.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 2.01 40.80 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.80-2.01) 99.6 (40.80-2.01)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.188 , 0.226 0.187 , 0.225	Depositor DCC
$R_{free}$ test set	9765 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.000 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.000 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.020 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: MG

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	0.54	0/1406	0.62	0/1887
1	B	0.54	0/1396	0.59	1/1873 (0.1%)
1	C	0.55	0/1391	0.61	0/1868
1	D	0.56	0/1401	0.61	0/1880
1	E	0.62	0/1401	0.68	0/1879
1	F	0.56	0/1392	0.60	0/1868
All	All	0.56	0/8387	0.62	1/11255 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	LEU	CA-CB-CG	5.12	127.09	115.30

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	1387	0	1387	13	0
1	B	1378	0	1374	17	0
1	C	1372	0	1370	16	0
1	D	1382	0	1381	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1383	0	1383	30	1
1	F	1373	0	1378	16	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	160	0	0	2	0
3	B	153	0	0	6	0
3	C	153	0	0	6	0
3	D	138	0	0	3	0
3	E	188	0	0	0	1
3	F	154	0	0	7	0
All	All	9237	0	8273	105	1

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 6.

All (105) 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:B:85:HIS:HB3	1:B:179:THR:HG22	1.33	1.10
1:D:85:HIS:HB3	1:D:179:THR:HG22	1.19	1.09
1:D:85:HIS:CB	1:D:179:THR:HG22	2.05	0.82
1:B:85:HIS:HB3	1:B:179:THR:CG2	2.09	0.81
1:E:22:GLN:NE2	1:E:22:GLN:HA	1.96	0.79
1:E:85:HIS:HB3	1:E:179:THR:HG22	1.65	0.78
1:D:153:ARG:HH11	1:F:148:HIS:HD2	1.33	0.76
1:E:44:HIS:CE1	1:E:166[B]:LYS:HD3	2.21	0.76
1:B:121:LYS:O	1:B:129:THR:HG21	1.86	0.75
1:A:121:LYS:O	1:A:129:THR:HG21	1.89	0.72
1:C:121:LYS:O	1:C:129:THR:HG21	1.91	0.70
1:C:2:ILE:HD11	1:C:17:SER:HB2	1.75	0.69
1:E:6:GLN:HE21	1:E:8:ASN:HD21	1.40	0.67
1:D:148:HIS:HD2	1:E:153:ARG:HH11	1.42	0.67
1:D:85:HIS:HB3	1:D:179:THR:CG2	2.11	0.66
1:B:126:THR:HG23	3:B:1081:HOH:O	1.95	0.66
1:E:42:THR:HG22	1:E:49:LEU:HB2	1.77	0.66
1:C:82:ASP:O	1:C:84:LYS:HE2	1.96	0.66
1:F:84:LYS:HD2	1:F:85:HIS:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:HIS:CB	1:B:179:THR:HG22	2.22	0.62
1:B:129:THR:HG23	3:B:1023:HOH:O	2.00	0.61
1:D:94:ILE:HG13	1:D:166[B]:LYS:HG2	1.84	0.60
1:E:22:GLN:HA	1:E:22:GLN:HE21	1.66	0.59
1:A:108:SER:OG	1:A:146:THR:HG22	2.01	0.59
1:E:22:GLN:HE21	1:E:22:GLN:CA	2.16	0.59
1:B:8:ASN:HD22	1:B:13:GLN:HA	1.66	0.58
1:F:16:ILE:HG12	1:F:51:ILE:HG12	1.85	0.58
1:C:60:ASP:HB3	3:C:1054:HOH:O	2.03	0.58
1:C:123:LYS:HE3	1:C:128:ASP:OD2	2.03	0.58
1:F:15:ASN:HB2	3:F:1167:HOH:O	2.05	0.57
1:C:129:THR:CG2	3:C:1025:HOH:O	2.51	0.57
1:B:4:GLN:HG2	3:B:1158:HOH:O	2.04	0.57
1:E:22:GLN:NE2	1:E:22:GLN:CA	2.66	0.56
1:D:137[B]:ARG:NH2	3:D:1012:HOH:O	2.27	0.54
1:E:110:ARG:O	1:E:146:THR:HG22	2.08	0.54
1:E:36[A]:HIS:CD2	1:E:37:MSE:CE	2.91	0.53
1:D:16:ILE:HG12	1:D:51:ILE:HG12	1.90	0.52
1:C:129:THR:HG22	3:C:1025:HOH:O	2.10	0.52
1:E:146:THR:HG21	3:F:1070:HOH:O	2.11	0.51
1:E:94:ILE:CD1	1:E:166[B]:LYS:HG2	2.41	0.51
1:E:1:MSE:HE2	1:E:3:TYR:OH	2.12	0.50
1:E:108:SER:OG	1:E:146:THR:CG2	2.60	0.50
1:A:2:ILE:HG22	1:A:4:GLN:HG2	1.94	0.49
1:A:146:THR:HG21	3:C:1052:HOH:O	2.11	0.49
1:F:86:PHE:HB3	3:F:1165:HOH:O	2.11	0.49
1:E:44:HIS:NE2	1:E:166[B]:LYS:HD3	2.27	0.49
1:A:60:ASP:HB2	3:A:1158:HOH:O	2.12	0.49
1:C:36[A]:HIS:CD2	1:C:37:MSE:HE2	2.48	0.49
1:C:84:LYS:HB3	3:C:1147:HOH:O	2.13	0.49
1:E:108:SER:OG	1:E:146:THR:HG23	2.13	0.49
1:F:108:SER:OG	1:F:146:THR:HG22	2.12	0.49
1:A:161[A]:ILE:HD12	1:A:165:PHE:CD2	2.48	0.48
1:F:13:GLN:HG3	3:F:1067:HOH:O	2.14	0.48
1:C:33:PHE:CZ	1:C:37:MSE:HE3	2.49	0.48
1:E:42:THR:CG2	1:E:49:LEU:HB2	2.43	0.47
1:D:13:GLN:HB2	1:D:54:GLN:HB2	1.96	0.47
1:F:137[B]:ARG:NH2	3:F:1038:HOH:O	2.47	0.47
1:C:137[B]:ARG:NH2	3:C:1015:HOH:O	2.47	0.47
1:C:42:THR:HG22	1:C:49:LEU:HB2	1.96	0.47
1:F:134:GLU:OE1	1:F:137[A]:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:OG	1:A:146:THR:CG2	2.61	0.47
1:F:61:ASP:HB2	3:F:1118:HOH:O	2.15	0.47
1:D:148:HIS:HE1	1:E:97:ASP:O	1.98	0.46
1:E:4:GLN:HG2	1:E:5:LYS:N	2.31	0.46
1:E:85:HIS:CB	1:E:179:THR:HG22	2.39	0.46
1:A:38:LEU:O	1:A:42:THR:HG23	2.16	0.45
1:E:21:ASP:OD1	1:E:21:ASP:C	2.53	0.45
1:D:94:ILE:CD1	1:D:166[B]:LYS:HG2	2.47	0.45
1:B:36[A]:HIS:CD2	1:B:37:MSE:CE	3.00	0.45
1:C:63:HIS:HE1	1:D:36[A]:HIS:CD2	2.34	0.45
1:C:13:GLN:HG2	1:C:54:GLN:O	2.17	0.45
1:E:13:GLN:N	1:E:13:GLN:OE1	2.49	0.45
1:B:42:THR:CG2	1:B:49:LEU:HB2	2.47	0.44
1:E:94:ILE:HD12	1:E:166[B]:LYS:HG2	1.99	0.44
1:B:36[A]:HIS:CD2	1:B:37:MSE:HE2	2.53	0.44
1:A:16:ILE:HG12	1:A:51:ILE:HG12	2.01	0.43
1:B:22:GLN:NE2	1:B:22:GLN:HA	2.32	0.43
1:E:112:TYR:HB3	1:E:146:THR:HB	2.00	0.43
1:D:13:GLN:N	3:D:1090:HOH:O	2.51	0.43
1:E:129:THR:HG21	1:E:157:THR:HG21	2.00	0.43
1:A:42:THR:HG22	1:A:49:LEU:HB2	2.01	0.43
1:F:42:THR:HG22	1:F:49:LEU:HB2	2.01	0.43
1:D:44:HIS:CE1	1:D:166[B]:LYS:HD3	2.54	0.42
3:D:1135:HOH:O	1:F:146:THR:HG21	2.19	0.42
1:E:36[A]:HIS:CD2	1:E:37:MSE:HE2	2.53	0.42
1:B:126:THR:HG21	3:B:1139:HOH:O	2.19	0.42
1:E:162:GLU:OE2	1:E:166[A]:LYS:NZ	2.53	0.42
1:D:94:ILE:CG1	1:D:166[B]:LYS:HG2	2.48	0.42
1:A:62:HIS:HA	1:A:131:LEU:HD22	2.01	0.41
1:A:129:THR:HG22	3:A:1028:HOH:O	2.21	0.41
1:F:63:HIS:HD2	3:F:1104:HOH:O	2.02	0.41
1:F:108:SER:OG	1:F:146:THR:CG2	2.68	0.41
1:D:153:ARG:HD2	1:F:148:HIS:CD2	2.56	0.41
1:D:97:ASP:O	1:F:148:HIS:HE1	2.03	0.41
1:B:129:THR:CG2	3:B:1023:HOH:O	2.65	0.41
1:B:151:LEU:HD11	1:B:160:GLU:HG2	2.02	0.41
1:B:179:THR:HG23	3:B:1103:HOH:O	2.20	0.41
1:D:42:THR:HG22	1:D:49:LEU:HB2	2.03	0.41
1:E:54:GLN:HE21	1:E:54:GLN:HB3	1.70	0.41
1:E:94:ILE:HG13	1:E:166[B]:LYS:HG2	2.03	0.41
1:C:33:PHE:CE1	1:C:37:MSE:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:O	1:D:42:THR:HG23	2.21	0.41
1:C:99:THR:HG21	1:C:160:GLU:HA	2.04	0.40
1:B:44:HIS:CE1	1:B:166:LYS:HE3	2.56	0.40
1:A:157:THR:O	1:A:161[A]:ILE:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137[B]:ARG:NH2	3:E:1041:HOH:O[4_465]	2.14	0.06

## 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	169/221 (76%)	161 (95%)	8 (5%)	0	100	100
1	B	168/221 (76%)	160 (95%)	8 (5%)	0	100	100
1	C	167/221 (76%)	160 (96%)	7 (4%)	0	100	100
1	D	168/221 (76%)	159 (95%)	9 (5%)	0	100	100
1	E	168/221 (76%)	161 (96%)	7 (4%)	0	100	100
1	F	167/221 (76%)	160 (96%)	7 (4%)	0	100	100
All	All	1007/1326 (76%)	961 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	152/187 (81%)	145 (95%)	7 (5%)	23	21
1	B	151/187 (81%)	145 (96%)	6 (4%)	27	26
1	C	151/187 (81%)	142 (94%)	9 (6%)	16	13
1	D	152/187 (81%)	146 (96%)	6 (4%)	27	27
1	E	152/187 (81%)	142 (93%)	10 (7%)	14	10
1	F	151/187 (81%)	146 (97%)	5 (3%)	33	33
All	All	909/1122 (81%)	866 (95%)	43 (5%)	22	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	129	THR
1	A	146	THR
1	A	147	THR
1	A	151	LEU
1	A	161[A]	ILE
1	A	161[B]	ILE
1	B	7	ARG
1	B	22	GLN
1	B	84	LYS
1	B	129	THR
1	B	151	LEU
1	B	179	THR
1	C	1	MSE
1	C	2	ILE
1	C	12	THR
1	C	13	GLN
1	C	48	SER
1	C	84	LYS
1	C	129	THR
1	C	147	THR
1	C	170	ARG
1	D	14	LEU
1	D	22	GLN
1	D	84	LYS
1	D	147	THR
1	D	151	LEU

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Mol	Chain	Res	Type
1	D	179	THR
1	E	4	GLN
1	E	22	GLN
1	E	48	SER
1	E	49	LEU
1	E	54	GLN
1	E	84	LYS
1	E	146	THR
1	E	147	THR
1	E	151	LEU
1	E	179	THR
1	F	14	LEU
1	F	22	GLN
1	F	105	VAL
1	F	146	THR
1	F	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	HIS
1	A	54	GLN
1	B	6	GLN
1	B	8	ASN
1	B	22	GLN
1	C	13	GLN
1	C	63	HIS
1	D	6	GLN
1	D	26	HIS
1	D	54	GLN
1	D	148	HIS
1	E	6	GLN
1	E	13	GLN
1	E	22	GLN
1	E	54	GLN
1	F	63	HIS
1	F	85	HIS
1	F	148	HIS

### 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 oligosaccharides in this entry.

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

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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	166/221 (75%)	0.21	8 (4%)	36 35	12, 32, 54, 59	4 (2%)
1	B	167/221 (75%)	0.19	10 (5%)	29 27	15, 31, 52, 63	2 (1%)
1	C	166/221 (75%)	0.27	13 (7%)	20 19	14, 31, 55, 62	2 (1%)
1	D	166/221 (75%)	0.13	9 (5%)	32 30	13, 29, 54, 61	3 (1%)
1	E	166/221 (75%)	0.01	9 (5%)	32 30	11, 27, 48, 57	3 (1%)
1	F	165/221 (74%)	0.21	9 (5%)	32 30	13, 31, 55, 61	3 (1%)
All	All	996/1326 (75%)	0.17	58 (5%)	30 28	11, 31, 54, 63	17 (1%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	GLN	5.9
1	C	12	THR	4.7
1	E	179	THR	4.3
1	C	2	ILE	4.0
1	F	26	HIS	3.4
1	B	22	GLN	3.3
1	C	26	HIS	3.2
1	A	4	GLN	3.1
1	F	12	THR	3.1
1	B	55	GLY	3.0
1	E	54	GLN	3.0
1	A	2	ILE	2.9
1	A	26	HIS	2.9
1	D	26	HIS	2.9
1	F	55	GLY	2.8
1	D	13	GLN	2.8
1	B	0	ALA	2.8
1	E	0	ALA	2.8
1	A	12	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	22	GLN	2.7
1	D	55	GLY	2.7
1	E	85	HIS	2.7
1	C	4	GLN	2.7
1	F	18	ILE	2.7
1	F	52	GLU	2.6
1	F	85	HIS	2.6
1	D	84	LYS	2.5
1	A	22	GLN	2.5
1	B	179	THR	2.5
1	C	15	ASN	2.5
1	D	25	SER	2.5
1	C	7	ARG	2.5
1	B	60	ASP	2.4
1	F	15	ASN	2.4
1	B	43	PHE	2.4
1	E	21	ASP	2.4
1	C	55	GLY	2.3
1	E	60	ASP	2.3
1	B	84	LYS	2.3
1	E	84	LYS	2.3
1	F	84	LYS	2.3
1	C	13	GLN	2.3
1	D	2	ILE	2.3
1	E	53	ALA	2.3
1	F	54	GLN	2.3
1	B	85	HIS	2.2
1	A	14	LEU	2.2
1	C	84	LYS	2.2
1	B	8	ASN	2.2
1	B	13	GLN	2.2
1	C	179	THR	2.1
1	C	22	GLN	2.1
1	C	60	ASP	2.1
1	A	13	GLN	2.1
1	D	179	THR	2.1
1	D	4	GLN	2.1
1	A	60	ASP	2.0
1	C	85	HIS	2.0

## 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 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<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	MG	A	1001	1/1	0.81	0.20	65,65,65,65	0
2	MG	F	1016	1/1	0.83	0.15	58,58,58,58	0
2	MG	D	1010	1/1	0.92	0.11	52,52,52,52	0
2	MG	A	1003	1/1	0.93	0.12	65,65,65,65	0
2	MG	E	1013	1/1	0.94	0.08	43,43,43,43	0
2	MG	B	1007	1/1	0.95	0.08	49,49,49,49	0
2	MG	E	1015	1/1	0.96	0.10	44,44,44,44	0
2	MG	B	1006	1/1	0.97	0.07	41,41,41,41	0
2	MG	F	1012	1/1	0.97	0.04	21,21,21,21	0
2	MG	C	1008	1/1	0.97	0.07	45,45,45,45	0
2	MG	C	1009	1/1	0.98	0.05	22,22,22,22	0
2	MG	F	1005	1/1	0.98	0.11	22,22,22,22	0
2	MG	C	1011	1/1	0.98	0.06	43,43,43,43	0
2	MG	E	1014	1/1	0.98	0.10	14,14,14,14	0
2	MG	A	1002	1/1	0.99	0.04	24,24,24,24	0
2	MG	B	1004	1/1	0.99	0.08	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.