wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:31 AM GMT

PDB ID	:	3EUK
Title	:	Crystal structure of MukE-MukF(residues 292-443)-MukB(head domain)-ATPgammaS complex, asymmetric dimer
Authors	:	Woo, J.S.; Lim, J.H.; Shin, H.C.; Oh, B.H.
Deposited on	:	2008-10-10
Resolution	:	4.00 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
http://wwpdb.org/validation/2016/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:

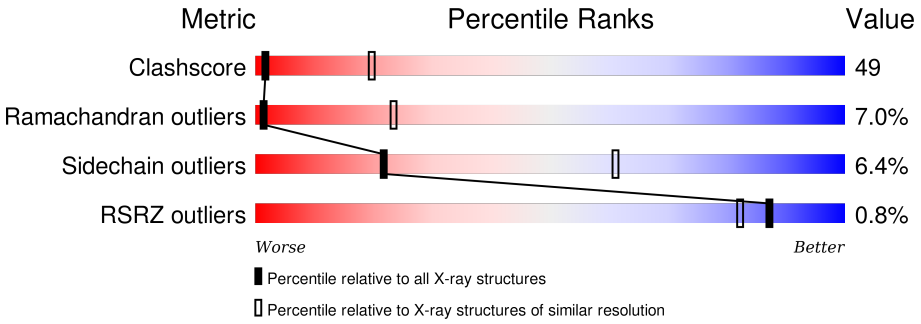
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.00 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))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 >=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 <=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	483	31% 54% 5% • 8%
1	C	483	33% 53% 8% 6%
1	F	483	31% 53% 7% 7%
1	H	483	32% 55% 8% • 5%
2	E	152	27% 33% 6% • 34%
2	J	152	25% 45% 11% 18%
3	L	238	3% 21% 47% 5% 27%

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Mol	Chain	Length	Quality of chain
3	M	238	3% 16% 24% 55%

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
5	MG	A	2012	-	-	-	X
5	MG	H	2014	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18401 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 Chromosome partition protein mukB, Linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3502	2212	616	659	15			
1	C	455	Total	C	N	O	S	0	0	0
			3594	2268	636	676	14			
1	F	447	Total	C	N	O	S	0	0	0
			3524	2226	622	662	14			
1	H	459	Total	C	N	O	S	0	0	0
			3620	2284	641	679	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP Q7VL96
A	31	HIS	-	EXPRESSION TAG	UNP Q7VL96
A	32	MET	-	EXPRESSION TAG	UNP Q7VL96
A	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
A	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
A	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
A	1435	GLN	GLU	ENGINEERED	UNP Q7VL96
A	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
C	30	GLY	-	EXPRESSION TAG	UNP Q7VL96
C	31	HIS	-	EXPRESSION TAG	UNP Q7VL96
C	32	MET	-	EXPRESSION TAG	UNP Q7VL96
C	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
C	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
C	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
C	1435	GLN	GLU	ENGINEERED	UNP Q7VL96
C	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
F	30	GLY	-	EXPRESSION TAG	UNP Q7VL96
F	31	HIS	-	EXPRESSION TAG	UNP Q7VL96
F	32	MET	-	EXPRESSION TAG	UNP Q7VL96
F	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
F	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
F	1435	GLN	GLU	ENGINEERED	UNP Q7VL96
F	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
H	30	GLY	-	EXPRESSION TAG	UNP Q7VL96
H	31	HIS	-	EXPRESSION TAG	UNP Q7VL96
H	32	MET	-	EXPRESSION TAG	UNP Q7VL96
H	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
H	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
H	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
H	1435	GLN	GLU	ENGINEERED	UNP Q7VL96
H	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96

- Molecule 2 is a protein called Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	101	Total	C	N	O	S	0	0	0
			803	509	139	153	2			
2	J	124	Total	C	N	O	S	0	0	0
			978	618	166	192	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	372	ASN	ASP	SEE REMARK 999	UNP Q7VL94
E	384	GLN	ARG	SEE REMARK 999	UNP Q7VL94
J	372	ASN	ASP	SEE REMARK 999	UNP Q7VL94
J	384	GLN	ARG	SEE REMARK 999	UNP Q7VL94

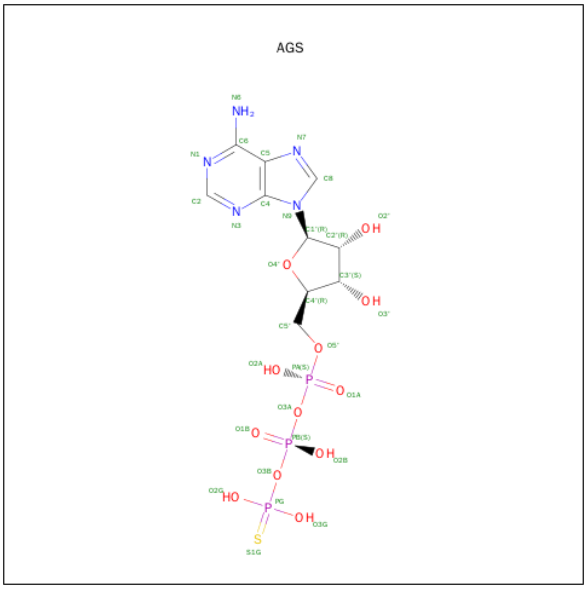
- Molecule 3 is a protein called Chromosome partition protein mukE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	173	Total	C	N	O	S	0	0	0
			1392	892	248	246	6			
3	M	107	Total	C	N	O	S	0	0	0
			860	554	143	157	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	219	ALA	GLU	SEE REMARK 999	UNP Q7VL95
M	219	ALA	GLU	SEE REMARK 999	UNP Q7VL95

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

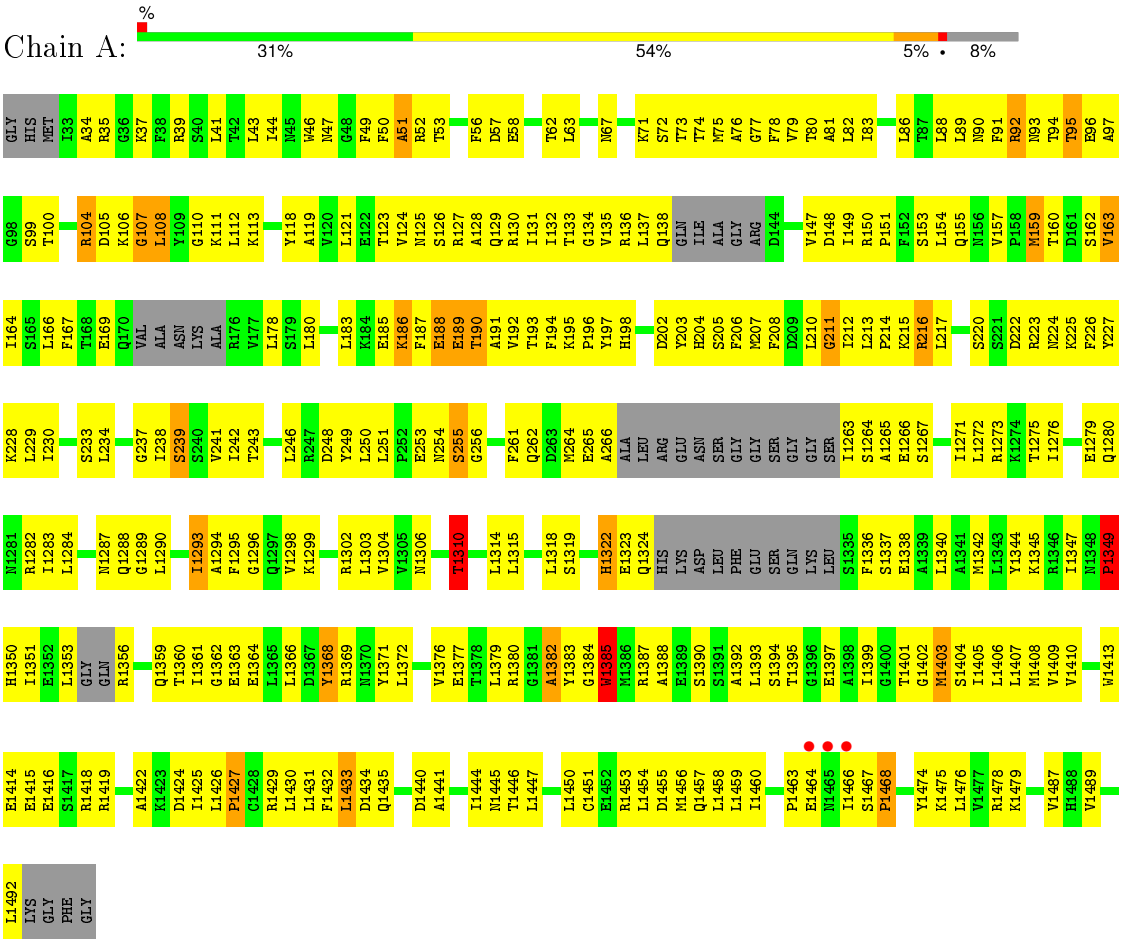
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Mg	0	0
			1	1		
5	A	2	Total	Mg	0	0
			2	2		
5	F	1	Total	Mg	0	0
			1	1		

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 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.

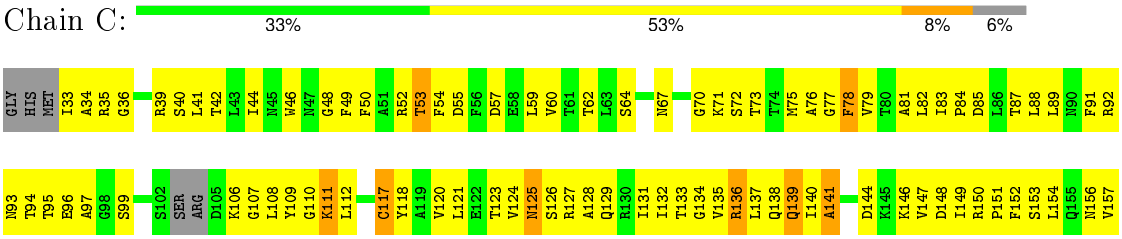
- Molecule 1: Chromosome partition protein mukB, Linker

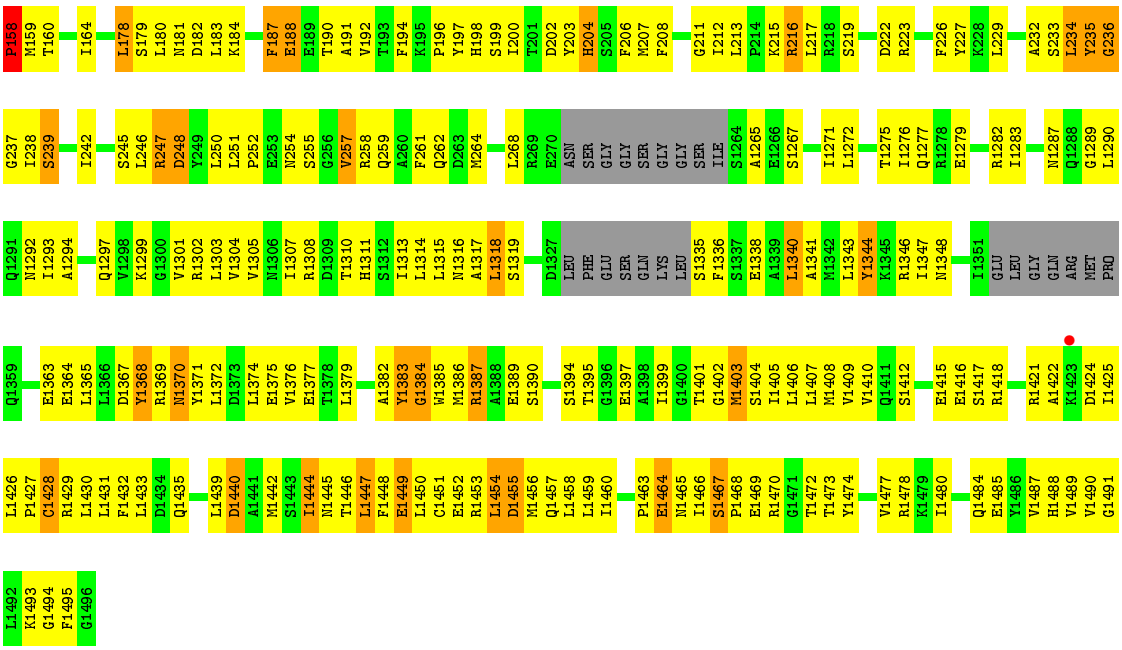
Chain A:



- Molecule 1: Chromosome partition protein mukB, Linker

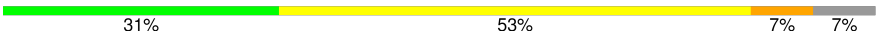
Chain C:

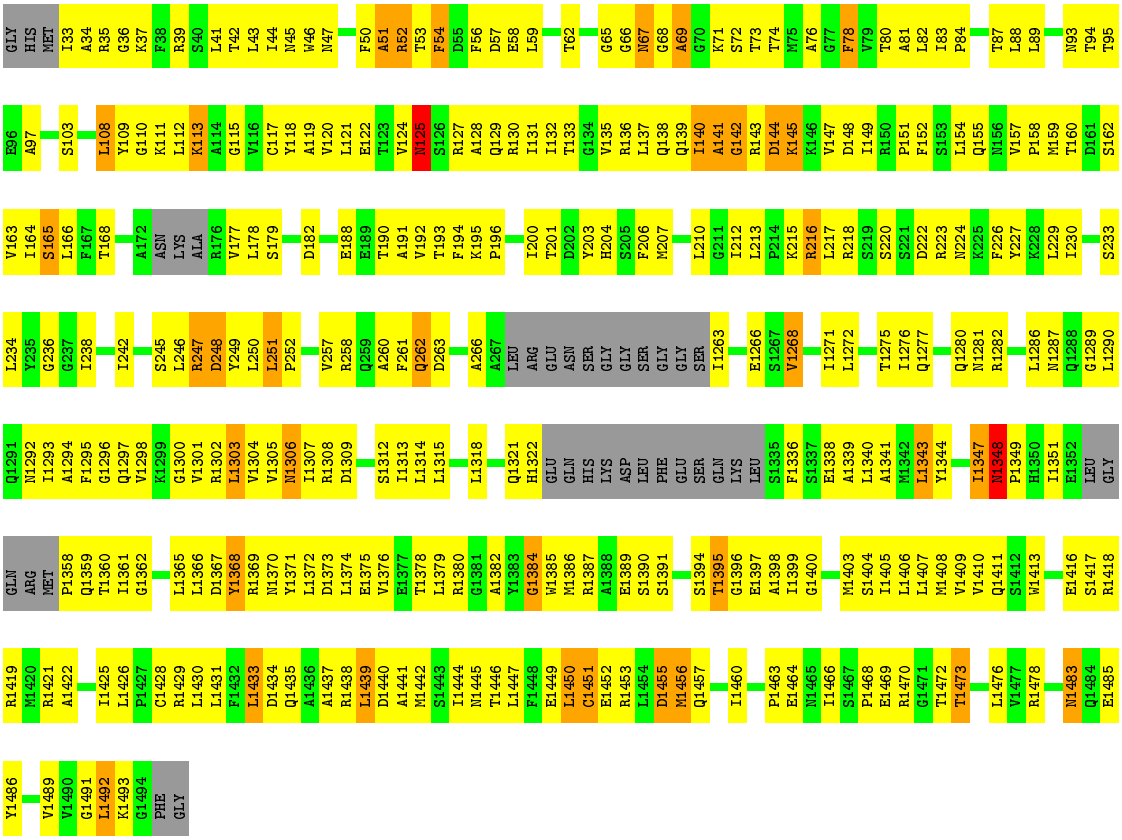




• Molecule 1: Chromosome partition protein mukB, Linker

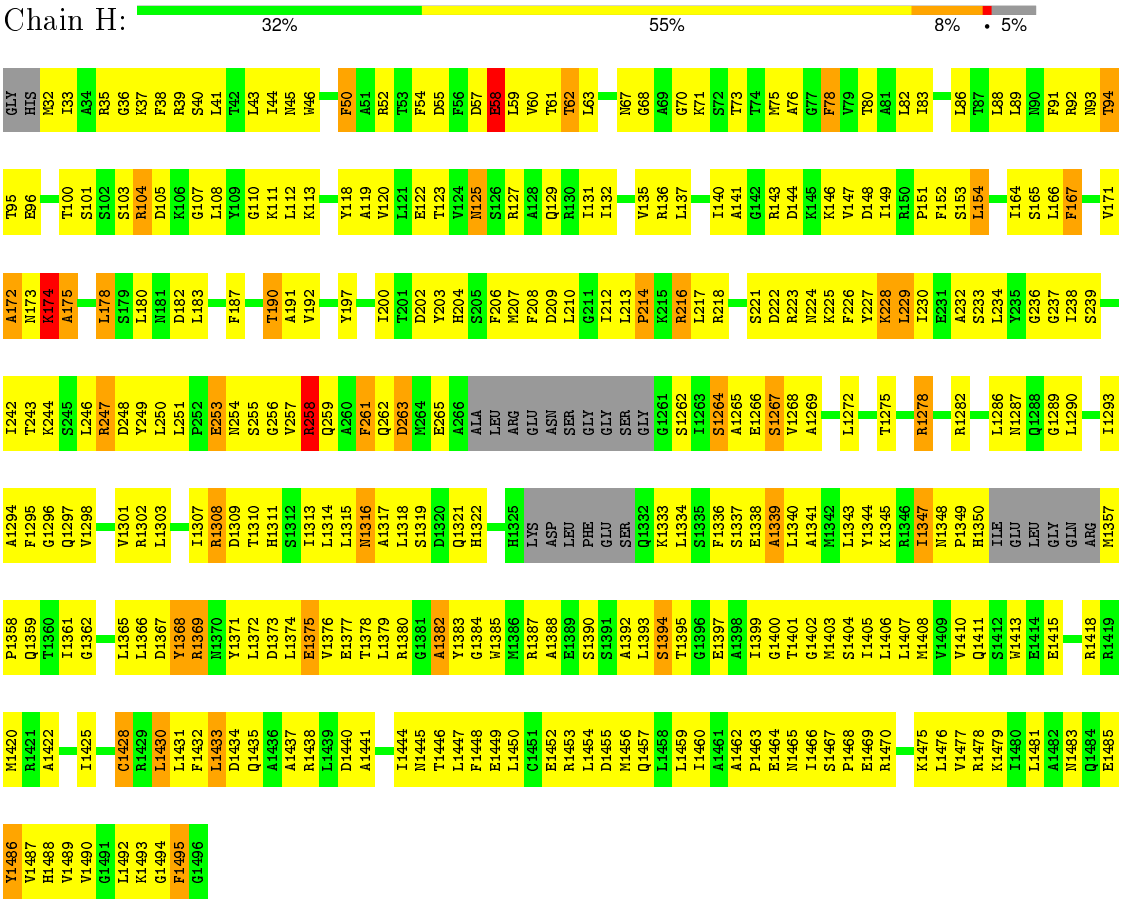
Chain F:





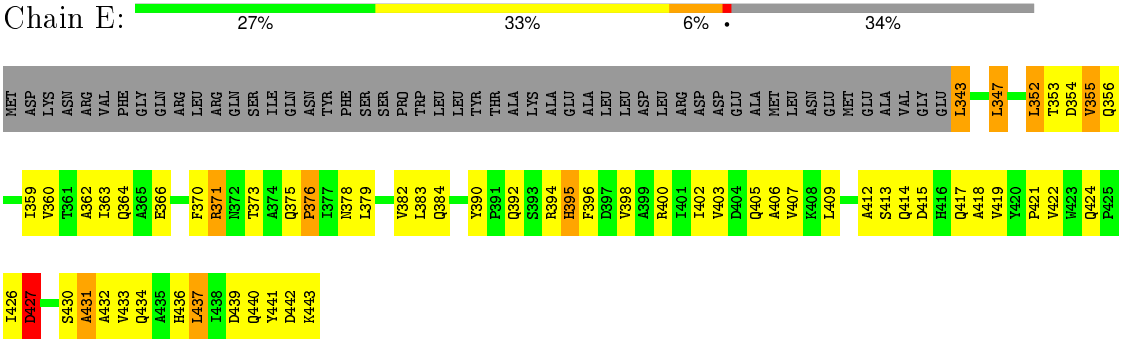
• Molecule 1: Chromosome partition protein mukB, Linker

Chain H:



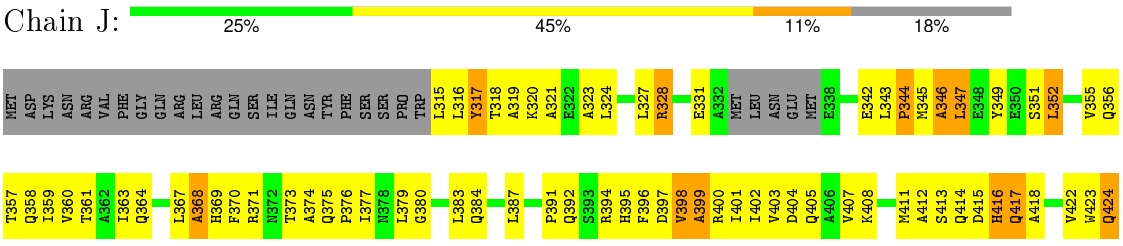
• Molecule 2: Chromosome partition protein mukF

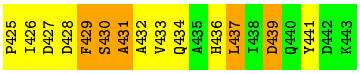
Chain E:



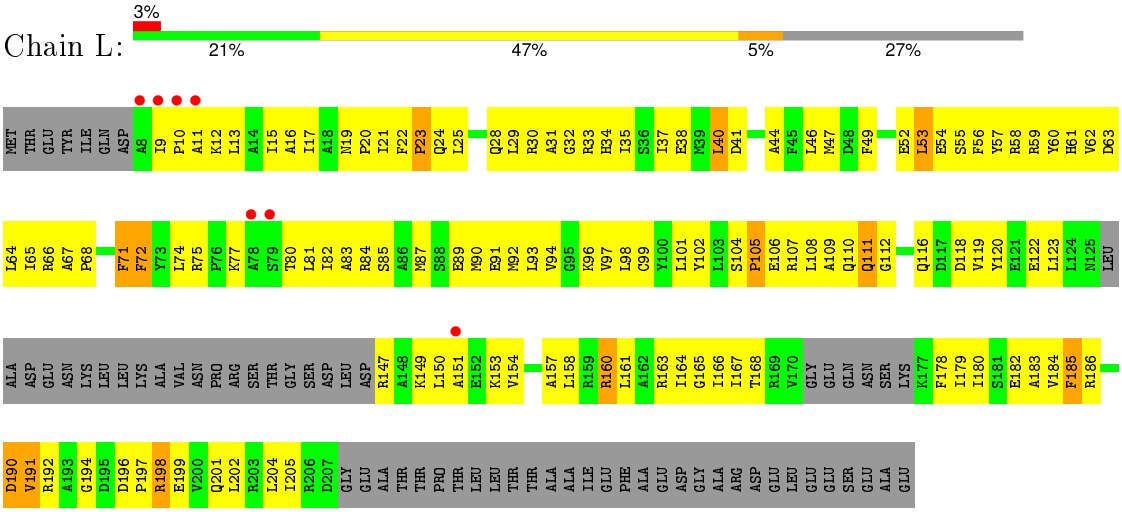
• Molecule 2: Chromosome partition protein mukF

Chain J:

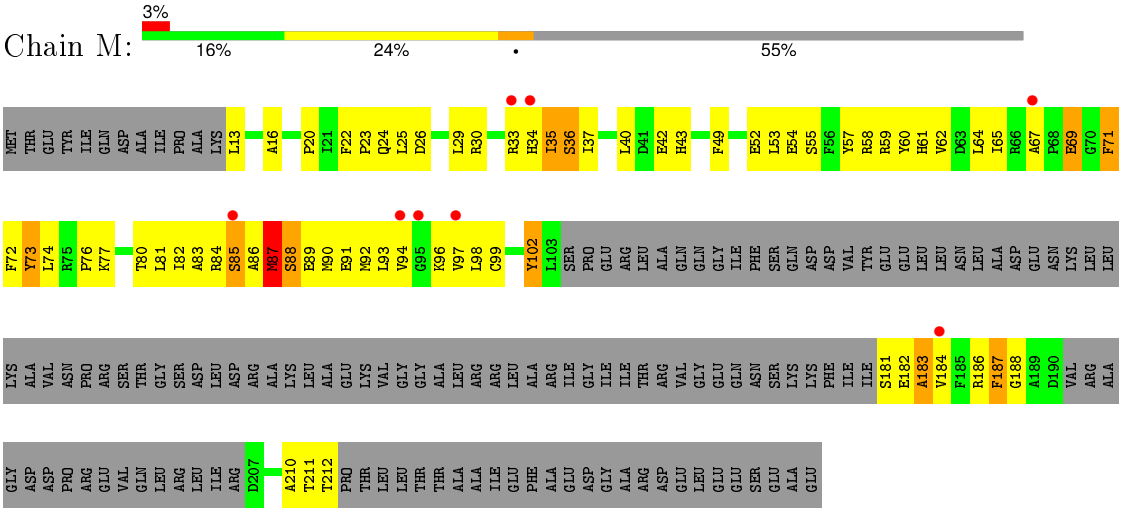




• Molecule 3: Chromosome partition protein mukE



• Molecule 3: Chromosome partition protein mukE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	172.41Å 172.41Å 491.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.92 – 3.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-4.00) 92.7 (29.92-3.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.324 0.278 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	108.7	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Outliers	0 of 34948 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18401	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, AGS

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	0.35	1/3551 (0.0%)	0.59	0/4784
1	C	0.35	0/3645	0.59	0/4908
1	F	0.36	0/3574	0.60	1/4816 (0.0%)
1	H	0.38	0/3673	0.61	1/4946 (0.0%)
2	E	0.34	0/820	0.58	0/1118
2	J	0.43	0/995	0.60	0/1354
3	L	0.36	1/1415 (0.1%)	0.55	0/1902
3	M	0.41	0/877	0.61	0/1180
All	All	0.36	2/18550 (0.0%)	0.60	2/25008 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	11	ALA	CA-CB	5.20	1.63	1.52
1	A	189	GLU	CD-OE1	5.17	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1348	ASN	N-CA-C	5.71	126.42	111.00
1	H	58	GLU	N-CA-C	-5.63	95.79	111.00

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	3502	0	3557	343	0
1	C	3594	0	3648	371	0
1	F	3524	0	3587	366	0
1	H	3620	0	3680	369	0
2	E	803	0	784	68	0
2	J	978	0	953	149	0
3	L	1392	0	1424	147	0
3	M	860	0	845	130	0
4	A	31	0	12	6	0
4	C	31	0	12	1	0
4	F	31	0	12	6	0
4	H	31	0	12	8	0
5	A	2	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
All	All	18401	0	18526	1821	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 49.

The worst 5 of 1821 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:J:321:ALA:HA	3:M:83:ALA:HB3	1.26	1.14
1:C:247:ARG:HD3	1:C:1369:ARG:HD3	1.12	1.11
1:A:190:THR:HG22	1:A:191:ALA:H	1.11	1.11
1:H:44:ILE:HB	1:H:118:TYR:HB2	1.29	1.06
1:C:1405:ILE:HA	1:C:1408:MET:HE2	1.38	1.06

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	430/483 (89%)	328 (76%)	75 (17%)	27 (6%)	2 27
1	C	445/483 (92%)	338 (76%)	82 (18%)	25 (6%)	2 29
1	F	437/483 (90%)	334 (76%)	73 (17%)	30 (7%)	1 24
1	H	451/483 (93%)	314 (70%)	102 (23%)	35 (8%)	1 20
2	E	99/152 (65%)	69 (70%)	23 (23%)	7 (7%)	1 23
2	J	120/152 (79%)	88 (73%)	20 (17%)	12 (10%)	1 13
3	L	167/238 (70%)	127 (76%)	27 (16%)	13 (8%)	1 20
3	M	101/238 (42%)	74 (73%)	18 (18%)	9 (9%)	1 17
All	All	2250/2712 (83%)	1672 (74%)	420 (19%)	158 (7%)	1 23

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	190	THR
1	A	1382	ALA
1	A	1468	PRO
1	C	111	LYS

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	385/413 (93%)	368 (96%)	17 (4%)	35 71
1	C	391/413 (95%)	367 (94%)	24 (6%)	23 63
1	F	385/413 (93%)	357 (93%)	28 (7%)	17 57
1	H	395/413 (96%)	366 (93%)	29 (7%)	17 57
2	E	85/129 (66%)	76 (89%)	9 (11%)	8 39
2	J	102/129 (79%)	93 (91%)	9 (9%)	12 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	145/198 (73%)	140 (97%)	5 (3%)	44 77
3	M	90/198 (46%)	85 (94%)	5 (6%)	26 65
All	All	1978/2306 (86%)	1852 (94%)	126 (6%)	22 61

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	222	ASP
1	F	1447	LEU
3	L	71	PHE
1	F	248	ASP
1	F	1306	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	405	GLN
1	F	1285	GLN
3	L	50	GLN
2	E	424	GLN
1	F	155	GLN

5.3.3 RNA

There are no RNA molecules 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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	AGS	A	2001	-	24,33,33	2.21	8 (33%)	28,52,52	1.73	4 (14%)
4	AGS	C	2002	-	24,33,33	2.19	9 (37%)	28,52,52	1.79	4 (14%)
4	AGS	F	2003	-	24,33,33	2.26	9 (37%)	28,52,52	1.78	6 (21%)
4	AGS	H	2004	-	24,33,33	2.28	8 (33%)	28,52,52	1.77	4 (14%)

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
4	AGS	A	2001	-	-	0/15/38/38	0/3/3/3
4	AGS	C	2002	-	-	0/15/38/38	0/3/3/3
4	AGS	F	2003	-	-	0/15/38/38	0/3/3/3
4	AGS	H	2004	-	-	0/15/38/38	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2004	AGS	PG-S1G	-5.93	1.79	1.90
4	F	2003	AGS	PG-S1G	-5.64	1.79	1.90
4	A	2001	AGS	PG-S1G	-5.31	1.80	1.90
4	C	2002	AGS	PG-S1G	-5.05	1.80	1.90
4	F	2003	AGS	PG-O3G	-2.54	1.46	1.55

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2004	AGS	N3-C2-N1	-5.00	125.07	128.89
4	F	2003	AGS	N3-C2-N1	-4.88	125.16	128.89
4	C	2002	AGS	N3-C2-N1	-4.80	125.22	128.89
4	A	2001	AGS	N3-C2-N1	-4.72	125.28	128.89
4	C	2002	AGS	O3A-PA-O5'	-3.28	94.23	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	AGS	6	0
4	C	2002	AGS	1	0
4	F	2003	AGS	6	0
4	H	2004	AGS	8	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

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^{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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	442/483 (91%)	-0.45	3 (0%) 89 84	66, 137, 179, 199	0
1	C	455/483 (94%)	-0.54	1 (0%) 95 94	75, 121, 160, 182	0
1	F	447/483 (92%)	-0.50	0 100 100	67, 120, 157, 176	0
1	H	459/483 (95%)	-0.65	0 100 100	51, 106, 143, 158	0
2	E	101/152 (66%)	-0.50	0 100 100	95, 130, 178, 193	0
2	J	124/152 (81%)	-0.49	0 100 100	88, 124, 188, 194	0
3	L	173/238 (72%)	-0.19	7 (4%) 42 31	93, 168, 195, 198	0
3	M	107/238 (44%)	0.47	8 (7%) 17 12	102, 199, 200, 200	0
All	All	2308/2712 (85%)	-0.46	19 (0%) 87 82	51, 126, 192, 200	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	79	SER	3.1
3	M	34	HIS	2.8
1	A	1465	ASN	2.7
3	M	33	ARG	2.7
3	L	151	ALA	2.7

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^{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	LLDF	B-factors(Å^2)	Q<0.9
5	MG	H	2014	1/1	0.98	0.42	3.21	107,107,107,107	0
5	MG	A	2012	1/1	0.99	0.42	2.75	77,77,77,77	0
4	AGS	H	2004	31/31	0.93	0.27	1.15	98,101,105,105	0
4	AGS	A	2001	31/31	0.92	0.32	0.45	115,144,156,157	0
4	AGS	C	2002	31/31	0.96	0.24	0.29	85,91,99,99	0
4	AGS	F	2003	31/31	0.96	0.17	-0.43	87,93,101,103	0
5	MG	A	2011	1/1	0.99	0.55	-	56,56,56,56	0
5	MG	F	2013	1/1	0.99	0.27	-	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.