Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 04:22 AM EDT

PDB ID	:	3KC2
Title	:	Crystal structure of mitochondrial HAD-like phosphatase from Saccharomyces cerevisiae
Authors	:	Nocek, B.; Evdokimova, E.; Kuznetsova, K.; Iakunine, A.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-10-20
Resolution	:	1.55 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

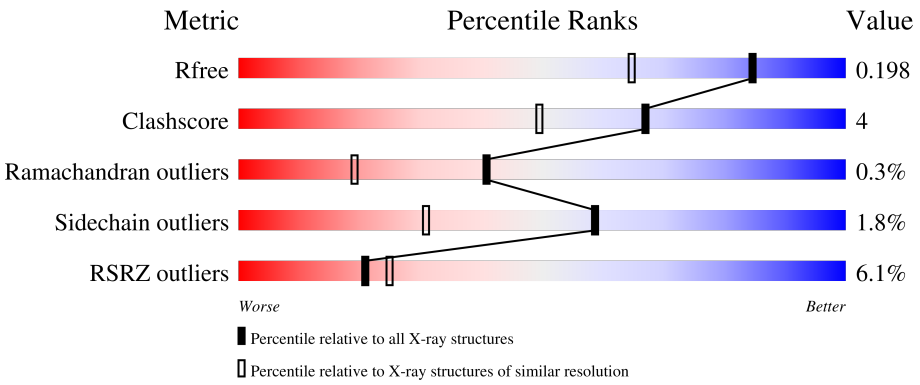
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (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 of 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
1	A	352	5% 85% 7% • 7%
1	B	352	6% 84% 6% • 9%

2 Entry composition (i)

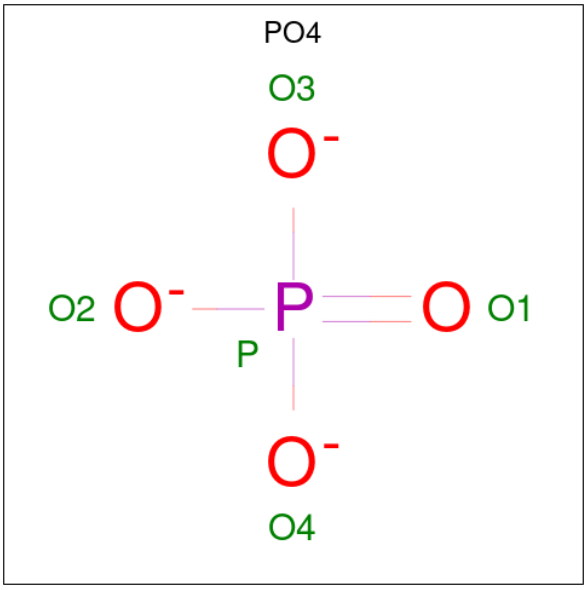
There are 4 unique types of molecules in this entry. The entry contains 6029 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein YKR070W.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	327	2581	1652	438	485	2	4	0	1	0
1	B	319	2545	1631	430	478	3	3	0	3	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

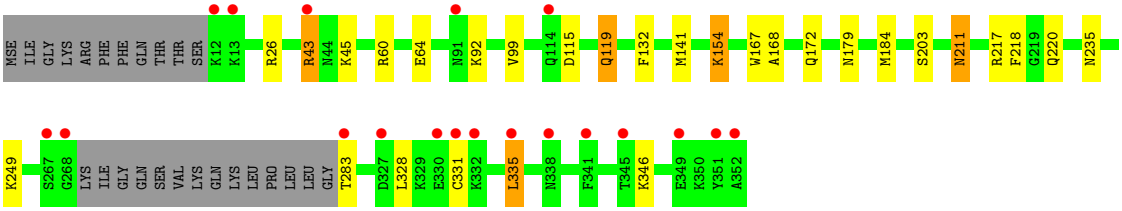
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	461	Total O 461 461	0	0
4	B	419	Total O 419 419	0	0

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.

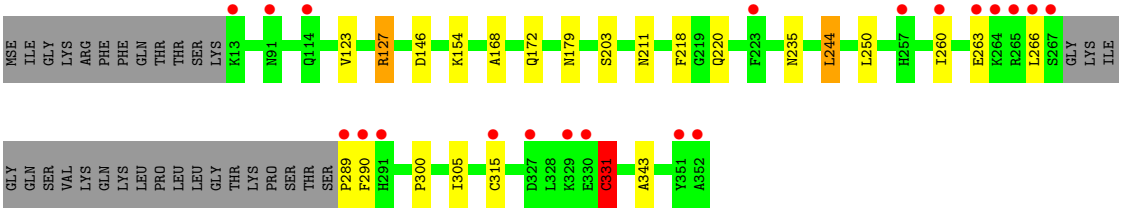
- Molecule 1: Uncharacterized protein YKR070W

Chain A:



- Molecule 1: Uncharacterized protein YKR070W

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.73Å 67.09Å 76.90Å 90.00° 110.45° 90.00°	Depositor
Resolution (Å)	40.00 – 1.55 36.03 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.55) 99.5 (36.03-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.144 , 0.169 0.175 , 0.198	Depositor DCC
R_{free} test set	4956 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6029	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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, 0.333 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, 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	0.71	0/2640	0.74	2/3578 (0.1%)
1	B	0.75	2/2609 (0.1%)	0.75	1/3533 (0.0%)
All	All	0.73	2/5249 (0.0%)	0.74	3/7111 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	CYS	CB-SG	-10.52	1.64	1.82
1	B	146	ASP	CB-CG	5.73	1.63	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	335	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	115	ASP	CB-CG-OD1	5.21	122.99	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	2581	0	2554	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2545	0	2528	22	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	461	0	0	6	0
4	B	419	0	0	1	0
All	All	6029	0	5082	40	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 4.

All (40) 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:A:172:GLN:HE22	1:B:218:PHE:H	1.28	0.80
1:A:179:ASN:HD21	1:A:235:ASN:HD21	1.30	0.79
1:B:263:GLU:HG3	1:B:290:PHE:CZ	2.17	0.79
1:A:218:PHE:H	1:B:172:GLN:HE22	1.32	0.78
1:B:179:ASN:HD21	1:B:235:ASN:HD21	1.34	0.76
1:B:260:ILE:HD12	1:B:289:PRO:HG3	1.71	0.71
1:A:203:SER:H	1:A:220:GLN:HE22	1.44	0.64
1:B:127:ARG:HH11	1:B:127:ARG:HG3	1.62	0.64
1:B:203:SER:H	1:B:220:GLN:HE22	1.44	0.64
1:B:127:ARG:HH11	1:B:127:ARG:CG	2.15	0.60
1:B:305:ILE:HD11	1:B:331:CYS:HB3	1.83	0.60
1:A:26:ARG:HD3	1:A:211:ASN:O	2.02	0.59
1:A:328:LEU:HD22	1:A:331:CYS:SG	2.45	0.56
1:B:266:LEU:HD13	4:B:749:HOH:O	2.05	0.56
1:A:283:THR:N	4:A:674:HOH:O	2.39	0.54
1:B:263:GLU:HG3	1:B:290:PHE:HZ	1.68	0.54
1:B:305:ILE:CD1	1:B:331:CYS:HB3	2.38	0.54
1:B:250:LEU:C	1:B:250:LEU:HD23	2.28	0.53
1:A:283:THR:N	4:A:376:HOH:O	2.42	0.52
1:A:167:TRP:CD2	1:B:168:ALA:HB2	2.48	0.48
1:A:43:ARG:HG2	4:A:461:HOH:O	2.13	0.48
1:B:127:ARG:CG	1:B:127:ARG:NH1	2.75	0.47
1:A:45:LYS:HD2	1:A:45:LYS:N	2.30	0.47
1:A:119:GLN:NE2	1:A:119:GLN:H	2.12	0.47
1:A:172:GLN:NE2	1:B:218:PHE:H	2.07	0.45
1:A:119:GLN:H	1:A:119:GLN:HE21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141[B]:MSE:HG2	4:A:629:HOH:O	2.17	0.44
1:A:154:LYS:HB3	1:A:184:MSE:SE	2.68	0.44
1:A:249:LYS:NZ	4:A:733:HOH:O	2.48	0.44
1:A:328:LEU:HB3	1:A:331:CYS:SG	2.58	0.43
1:B:300:PRO:O	1:B:305:ILE:HG12	2.19	0.43
1:B:179:ASN:ND2	1:B:235:ASN:HD21	2.10	0.43
1:B:315[B]:CYS:SG	1:B:343:ALA:CB	3.08	0.42
1:A:132:PHE:HB2	1:A:168:ALA:HB1	2.01	0.41
1:A:346:LYS:NZ	4:A:441:HOH:O	2.49	0.41
1:B:260:ILE:HD12	1:B:289:PRO:CG	2.43	0.41
1:A:218:PHE:H	1:B:172:GLN:NE2	2.08	0.40
1:A:60:ARG:O	1:A:64:GLU:HG3	2.22	0.40
1:A:99:VAL:HA	1:A:119:GLN:NE2	2.36	0.40
1:B:123:VAL:O	1:B:127:ARG:HD2	2.22	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	324/352 (92%)	314 (97%)	9 (3%)	1 (0%)	41	19
1	B	318/352 (90%)	312 (98%)	5 (2%)	1 (0%)	41	19
All	All	642/704 (91%)	626 (98%)	14 (2%)	2 (0%)	41	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	B	211	ASN

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	281/301 (93%)	275 (98%)	6 (2%)	53	24
1	B	279/301 (93%)	275 (99%)	4 (1%)	67	41
All	All	560/602 (93%)	550 (98%)	10 (2%)	59	31

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	92	LYS
1	A	119	GLN
1	A	154	LYS
1	A	217	ARG
1	A	335	LEU
1	B	127	ARG
1	B	154	LYS
1	B	244	LEU
1	B	331	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	119	GLN
1	A	172	GLN
1	A	179	ASN
1	A	220	GLN
1	A	313	ASN
1	B	81	GLN
1	B	172	GLN
1	B	179	ASN
1	B	182	ASN
1	B	220	GLN
1	B	313	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
2	PO4	B	354	3	4,4,4	0.62	0	6,6,6	0.71	0
2	PO4	A	354	-	4,4,4	1.95	2 (50%)	6,6,6	1.31	1 (16%)
2	PO4	A	353	3	4,4,4	1.12	0	6,6,6	0.93	0
2	PO4	B	355	-	4,4,4	1.45	1 (25%)	6,6,6	0.54	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	354	PO4	P-O1	2.91	1.57	1.50
2	B	355	PO4	P-O3	-2.77	1.46	1.54
2	A	354	PO4	P-O3	-2.58	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	354	PO4	O4-P-O3	2.36	115.26	107.91

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 (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, 95th 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	324/352 (92%)	0.14	19 (5%)	22	26	5, 10, 21, 26	0
1	B	316/352 (89%)	0.19	20 (6%)	20	23	5, 9, 19, 27	0
All	All	640/704 (90%)	0.17	39 (6%)	21	25	5, 9, 20, 27	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	TYR	5.6
1	A	352	ALA	5.5
1	B	266	LEU	5.4
1	B	352	ALA	5.0
1	B	267	SER	5.0
1	B	289	PRO	4.9
1	A	331	CYS	4.9
1	A	330	GLU	4.5
1	A	327	ASP	4.4
1	B	290	PHE	4.2
1	B	291	HIS	4.0
1	A	13	LYS	4.0
1	A	349	GLU	3.8
1	B	265	ARG	3.7
1	A	283	THR	3.7
1	A	332	LYS	3.7
1	A	91	ASN	3.6
1	B	263	GLU	3.5
1	A	268	GLY	3.4
1	B	264	LYS	3.4
1	B	327	ASP	2.9
1	B	13	LYS	2.8
1	B	315[A]	CYS	2.7
1	B	351	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	330	GLU	2.6
1	B	257	HIS	2.6
1	B	114	GLN	2.6
1	A	267	SER	2.5
1	A	43	ARG	2.5
1	B	329	LYS	2.5
1	A	12	LYS	2.4
1	A	114	GLN	2.4
1	A	338	ASN	2.4
1	A	341	PHE	2.3
1	B	223	PHE	2.2
1	B	260	ILE	2.2
1	A	335	LEU	2.1
1	B	91	ASN	2.0
1	A	345	THR	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, 95th 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(Å^2)	Q<0.9
2	PO4	A	354	5/5	0.90	0.13	22,27,31,34	0
2	PO4	A	353	5/5	0.95	0.14	17,17,20,20	0
2	PO4	B	355	5/5	0.96	0.09	22,26,28,31	0
2	PO4	B	354	5/5	0.97	0.16	16,16,20,22	0
3	MG	B	353	1/1	0.99	0.15	12,12,12,12	0
3	MG	B	356	1/1	0.99	0.14	16,16,16,16	0
3	MG	A	355	1/1	1.00	0.14	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.