



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1MRE
Title : PREPARATION, CHARACTERIZATION AND CRYSTALLIZATION OF AN ANTIBODY FAB FRAGMENT THAT RECOGNIZES RNA. CRYSTAL STRUCTURES OF NATIVE FAB AND THREE FAB-MONONUCLEOTIDE COMPLEXES
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Deposited on : 1994-06-13
Resolution : 2.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

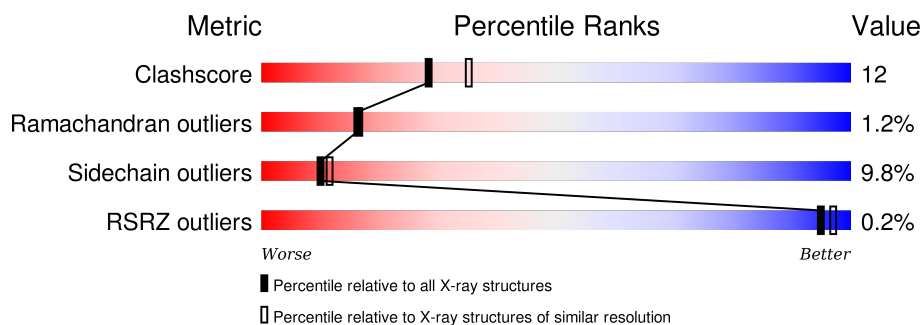
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	L	219	<div> <div style="width: 75%;"></div> <div style="width: 21%;"></div> <div style="width: 4%;"></div> </div> <div>75% 21% .</div>
2	H	215	<div> <div style="width: 66%;"></div> <div style="width: 26%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>66% 26% 5% .</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
4	IMD	L	902	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3316 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 IGG2B-KAPPA JEL103 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	0	0
			1672	1043	290	333	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	LEU	CONFLICT	PIR PC4203
L	27B	LEU	ILE	CONFLICT	PIR PC4203
L	27A	SER	THR	CONFLICT	PIR PC4203
L	34	HIS	GLU	CONFLICT	PIR PC4203
L	87	PHE	TYR	CONFLICT	PIR PC4203
L	89	SER	PHE	CONFLICT	PIR PC4203
L	91	SER	GLY	CONFLICT	PIR PC4203
L	92	THR	SER	CONFLICT	PIR PC4203
L	153	LYS	SER	CONFLICT	PIR PC4203
L	167	ASN	ASP	CONFLICT	PIR PC4203

- Molecule 2 is a protein called IGG2B-KAPPA JEL103 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1535	976	244	308	7			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	LYS	ARG	CONFLICT	GB 387221
H	16	ALA	THR	CONFLICT	GB 387221
H	20	LEU	MET	CONFLICT	GB 387221
H	25	SER	ALA	CONFLICT	GB 387221
H	31	SER	ASN	CONFLICT	GB 387221
H	34	MET	ILE	CONFLICT	GB 387221

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Chain	Residue	Modelled	Actual	Comment	Reference
H	35	GLN	GLY	CONFLICT	GB 387221
H	39	GLN	GLU	CONFLICT	GB 387221
H	43	GLN	HIS	CONFLICT	GB 387221
H	50	GLU	ASP	CONFLICT	GB 387221
H	52	ASP	TYR	CONFLICT	GB 387221
H	53	SER	GLY	CONFLICT	GB 387221
H	54	ASP	GLY	CONFLICT	GB 387221
H	55	SER	GLY	CONFLICT	GB 387221
H	56	TYR	PHE	CONFLICT	GB 387221
H	61	GLN	GLU	CONFLICT	GB 387221
H	62	LYS	ASN	CONFLICT	GB 387221
H	71	VAL	ALA	CONFLICT	GB 387221
H	89	VAL	ILE	CONFLICT	GB 387221
H	91	TYR	HIS	CONFLICT	GB 387221
H	?	-	ARG	DELETION	GB 387221
H	?	-	GLY	DELETION	GB 387221
H	?	-	ILE	DELETION	GB 387221
H	?	-	TYR	DELETION	GB 387221
H	?	-	TYR	DELETION	GB 387221
H	95	LEU	SER	CONFLICT	GB 387221
H	96	ARG	SER	CONFLICT	GB 387221
H	97	GLY	PRO	CONFLICT	GB 387221
H	102	TYR	SER	CONFLICT	GB 387221
H	140	LEU	SER	CONFLICT	GB 387221
H	151	SER	PRO	CONFLICT	GB 387221

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

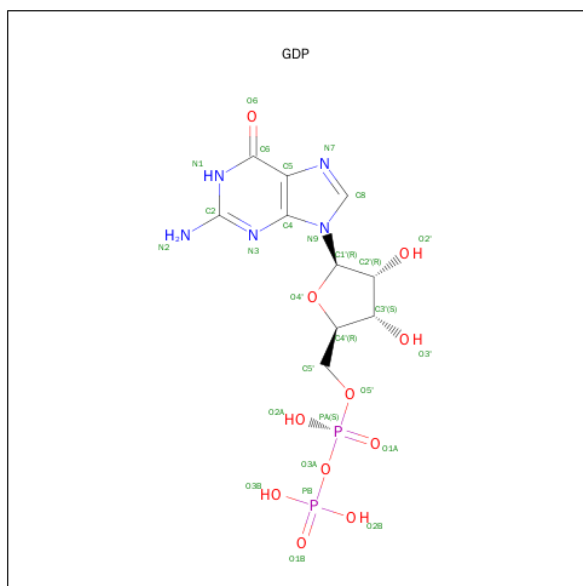
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Zn 1 1	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N		0	0
			5	3	2			

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

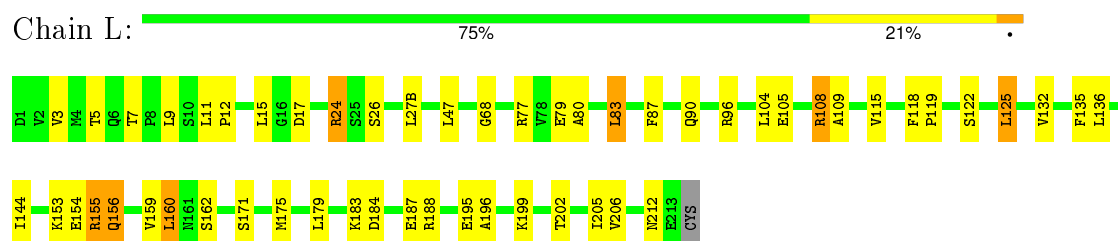


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	33	Total 33	O 33	0	0
6	L	42	Total 42	O 42	0	0

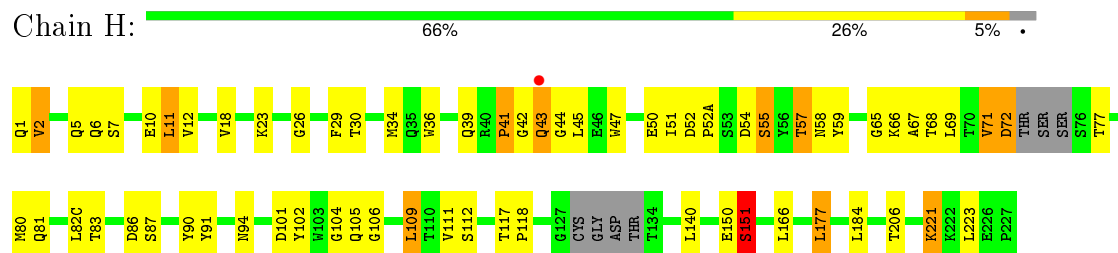
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: IGG2B-KAPPA JEL103 FAB (LIGHT CHAIN)



- Molecule 2: IGG2B-KAPPA JEL103 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.20Å 75.50Å 104.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30 55.95 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 75.1 (55.95-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.05Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25253 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3316	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GDP, ZN, IMD

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	L	0.48	0/1710	0.79	0/2323
2	H	1.82	1/1576 (0.1%)	0.86	2/2158 (0.1%)
All	All	1.31	1/3286 (0.0%)	0.82	2/4481 (0.0%)

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	L	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	151	SER	CB-OG	69.66	2.32	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	SER	CA-CB-OG	-13.74	74.11	111.20
2	H	151	SER	N-CA-CB	-5.17	102.74	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	205	ILE	CB

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	L	1672	0	1605	28	0
2	H	1535	0	1441	47	0
3	L	1	0	0	0	0
4	L	5	0	4	0	0
5	L	28	0	11	0	0
6	H	33	0	0	0	0
6	L	42	0	0	0	0
All	All	3316	0	3061	73	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 12.

The worst 5 of 73 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:H:5:GLN:HB2	2:H:23:LYS:HE3	1.68	0.74
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.73	0.71
2:H:29:PHE:HZ	2:H:71:VAL:HG22	1.60	0.67
1:L:160:LEU:HG	2:H:177:LEU:HD23	1.80	0.62
1:L:155:ARG:HG2	1:L:179:LEU:HD11	1.81	0.62

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	L	216/219 (99%)	210 (97%)	4 (2%)	2 (1%)	21	24
2	H	202/215 (94%)	190 (94%)	9 (4%)	3 (2%)	13	12
All	All	418/434 (96%)	400 (96%)	13 (3%)	5 (1%)	16	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	7	SER
2	H	43	GLN
1	L	212	ASN
2	H	41	PRO
1	L	68	GLY

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	L	190/197 (96%)	169 (89%)	21 (11%)	8	8
2	H	168/186 (90%)	154 (92%)	14 (8%)	14	17
All	All	358/383 (94%)	323 (90%)	35 (10%)	10	11

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	156	GLN
1	L	199	LYS
2	H	177	LEU
1	L	159	VAL
1	L	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	43	GLN

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Mol	Chain	Res	Type
2	H	203	GLN
2	H	105	GLN
2	H	6	GLN
2	H	172	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	GDP	L	901	-	23,30,30	1.63	3 (13%)	30,47,47	2.80	8 (26%)
4	IMD	L	902	3	3,5,5	0.17	0	4,5,5	0.50	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
5	GDP	L	901	-	-	0/12/32/32	0/3/3/3
4	IMD	L	902	3	-	0/0/0/0	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	C2-N1	2.12	1.39	1.35
5	L	901	GDP	C6-N1	2.40	1.37	1.33
5	L	901	GDP	C6-C5	6.04	1.53	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	901	GDP	C5-C6-N1	-10.00	109.92	123.59
5	L	901	GDP	C4'-O4'-C1'	-4.18	105.12	109.72
5	L	901	GDP	C1'-N9-C4	-2.80	122.71	126.94
5	L	901	GDP	N3-C2-N1	-2.54	123.57	127.44
5	L	901	GDP	O4'-C4'-C5'	2.01	116.52	109.32

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	L	218/219 (99%)	-0.54	0 100 100	11, 27, 45, 80	0
2	H	208/215 (96%)	-0.32	1 (0%) 91 94	11, 35, 62, 79	0
All	All	426/434 (98%)	-0.43	1 (0%) 95 97	11, 29, 58, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	43	GLN	5.5

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	IMD	L	902	5/5	0.96	0.18	2.54	66,66,68,69	0
5	GDP	L	901	28/28	0.93	0.11	-0.64	21,48,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	L	600	1/1	0.96	0.06	-1.51	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.