



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2020 – 12:23 PM EDT

PDB ID : 7K3U  
Title : X-ray crystallographic structure model of Lactococcus lactis prolidase mutant R293S  
Authors : Xu, S.; Grochulski, P.; Tanaka, T.  
Deposited on : 2020-09-13  
Resolution : 2.70 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](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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4
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)	:	2.14.4

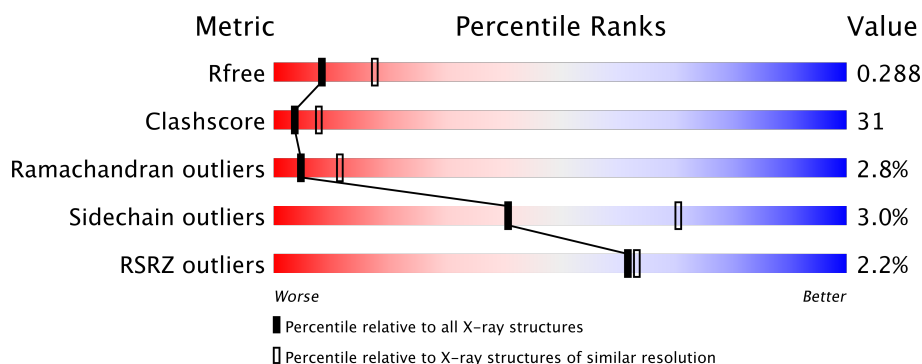
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	362	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>60%</span> <span>37%</span> </div> </div>
1	B	362	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>73%</span> <span>25%</span> </div> </div>
1	C	362	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>60%</span> <span>37%</span> </div> </div>
1	D	362	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>51%</span> <span>47%</span> </div> </div>
1	E	362	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>49%</span> <span>48%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	362	<div><div></div><div>2%</div><div>50%</div><div>46%</div><div></div></div>
1	G	362	<div><div></div><div>2%</div><div>55%</div><div>41%</div><div></div></div>
1	H	362	<div><div></div><div>2%</div><div>48%</div><div>47%</div><div></div></div>
1	I	362	<div><div></div><div>6%</div><div>35%</div><div>58%</div><div>7%</div></div>
1	J	362	<div><div></div><div>5%</div><div>40%</div><div>55%</div><div>5%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28480 atoms, of which 40 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 Aminopeptidase P family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	B	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	C	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	D	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	E	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	F	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	G	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	H	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	I	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	J	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	SER	ARG	engineered mutation	UNP A8WBX8
B	293	SER	ARG	engineered mutation	UNP A8WBX8
C	293	SER	ARG	engineered mutation	UNP A8WBX8
D	293	SER	ARG	engineered mutation	UNP A8WBX8
E	293	SER	ARG	engineered mutation	UNP A8WBX8
F	293	SER	ARG	engineered mutation	UNP A8WBX8
G	293	SER	ARG	engineered mutation	UNP A8WBX8
H	293	SER	ARG	engineered mutation	UNP A8WBX8
I	293	SER	ARG	engineered mutation	UNP A8WBX8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	293	SER	ARG	engineered mutation	UNP A8WBX8

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	H	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	88	Total	O	0	0
			88	88		
4	C	77	Total	O	0	0
			77	77		
4	D	38	Total	O	0	0
			38	38		
4	E	16	Total	O	0	0
			16	16		
4	F	35	Total	O	0	0
			35	35		
4	G	33	Total	O	0	0
			33	33		

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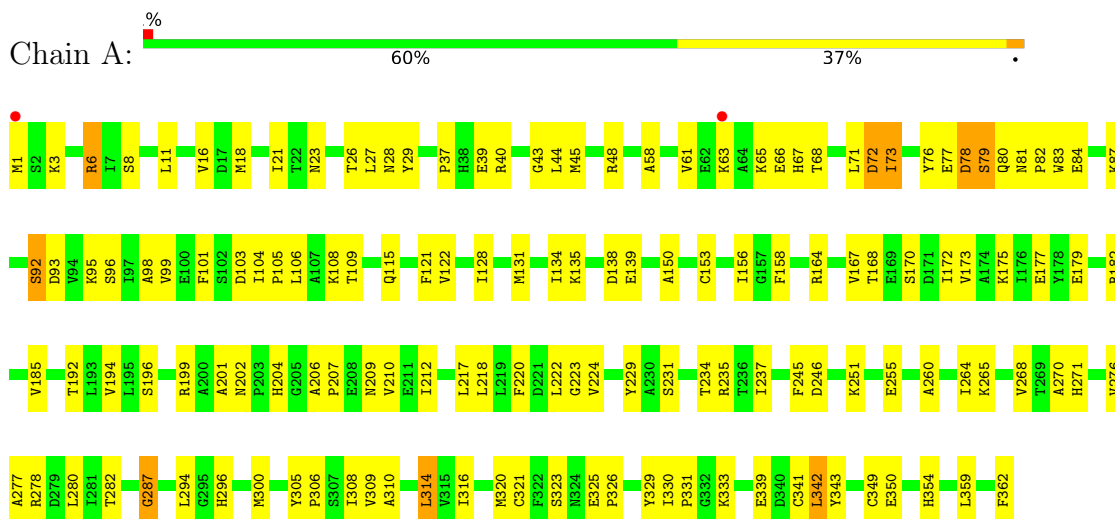
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	14	Total 14	O 14	0	0
4	I	15	Total 15	O 15	0	0
4	J	26	Total 26	O 26	0	0

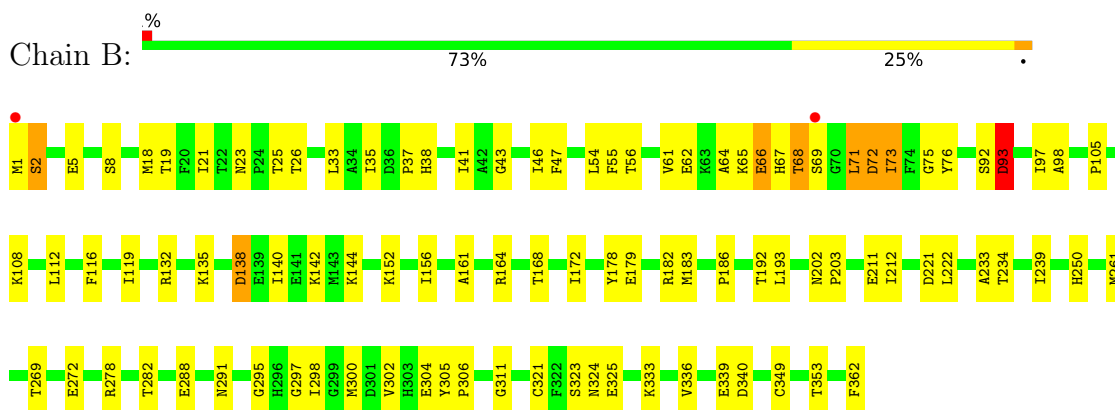
### 3 Residue-property plots

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.

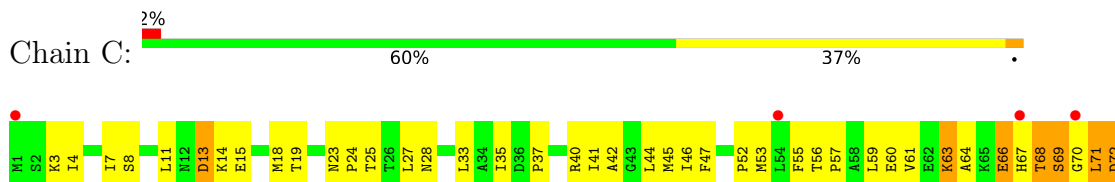
#### • Molecule 1: Aminopeptidase P family protein



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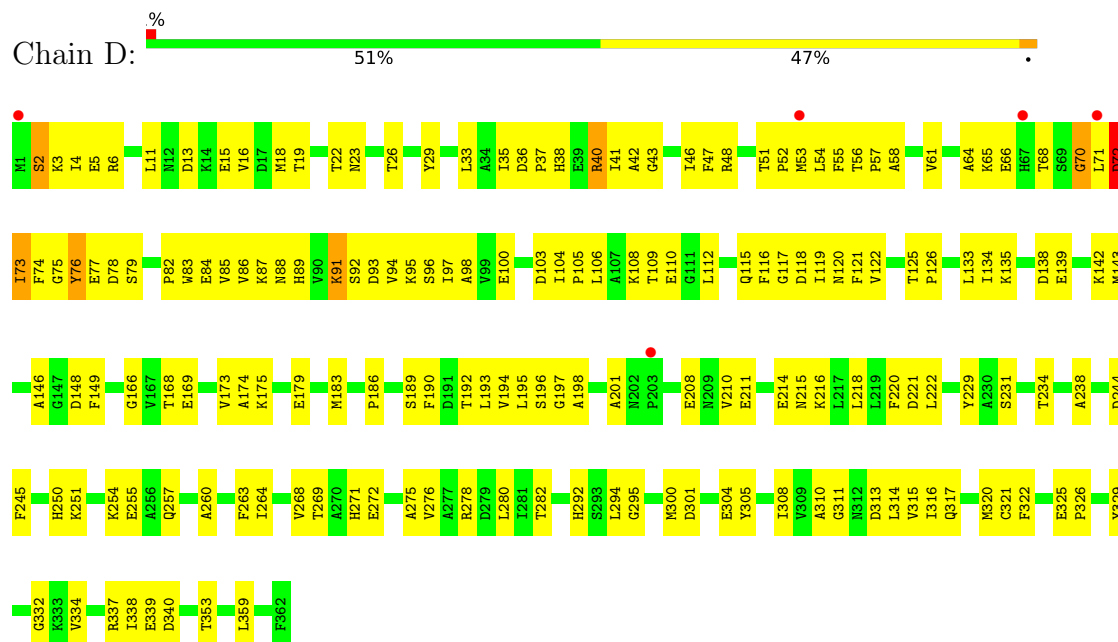
#### • Molecule 1: Aminopeptidase P family protein



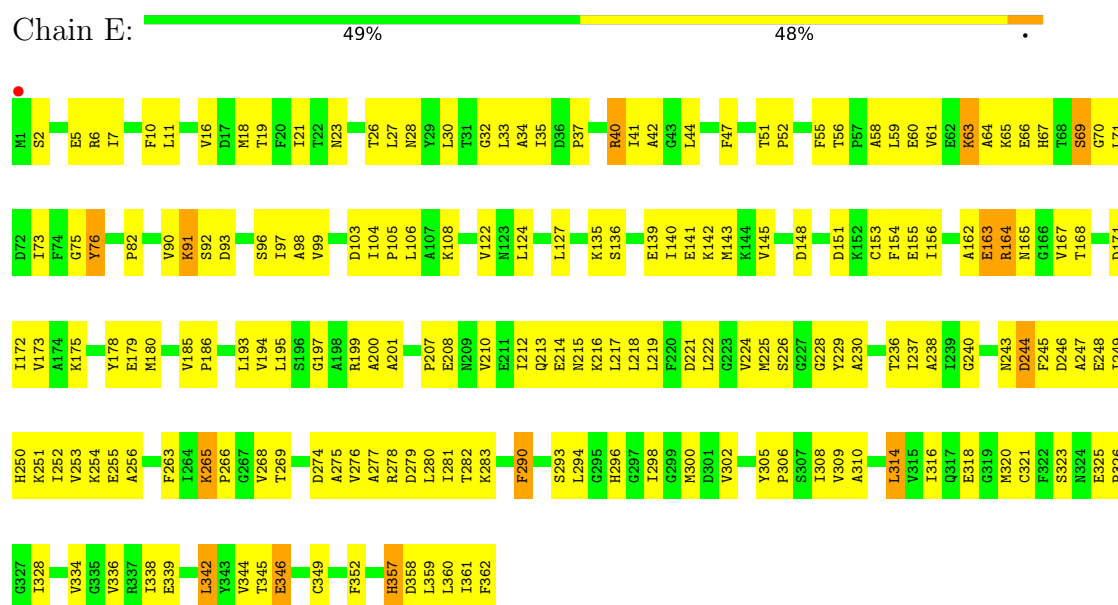




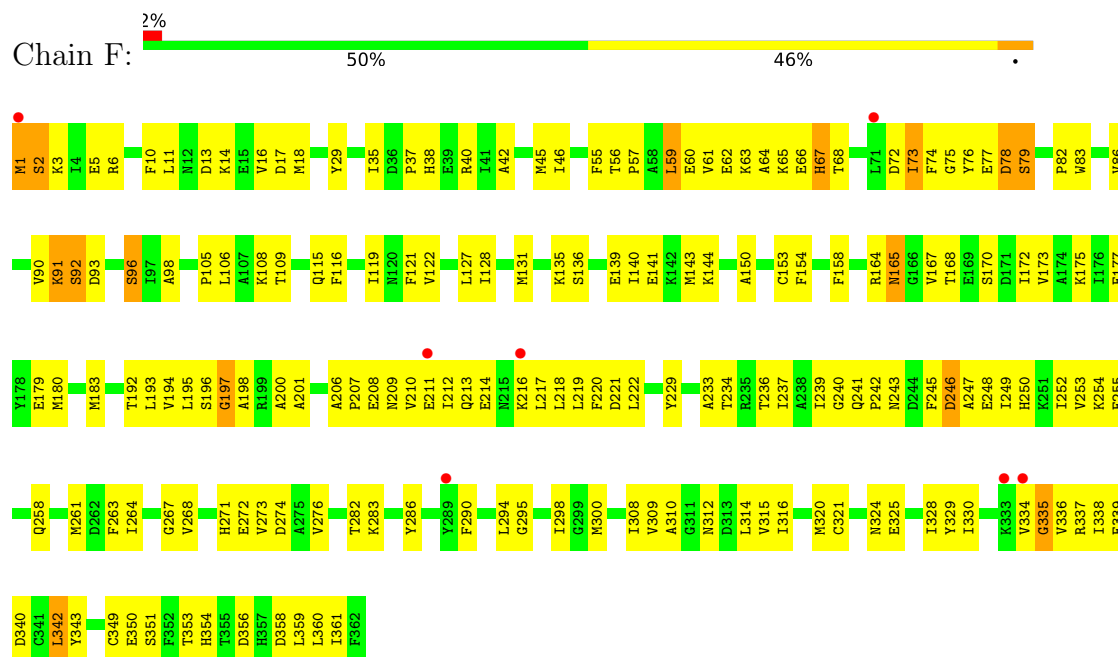
● Molecule 1: Aminopeptidase P family protein



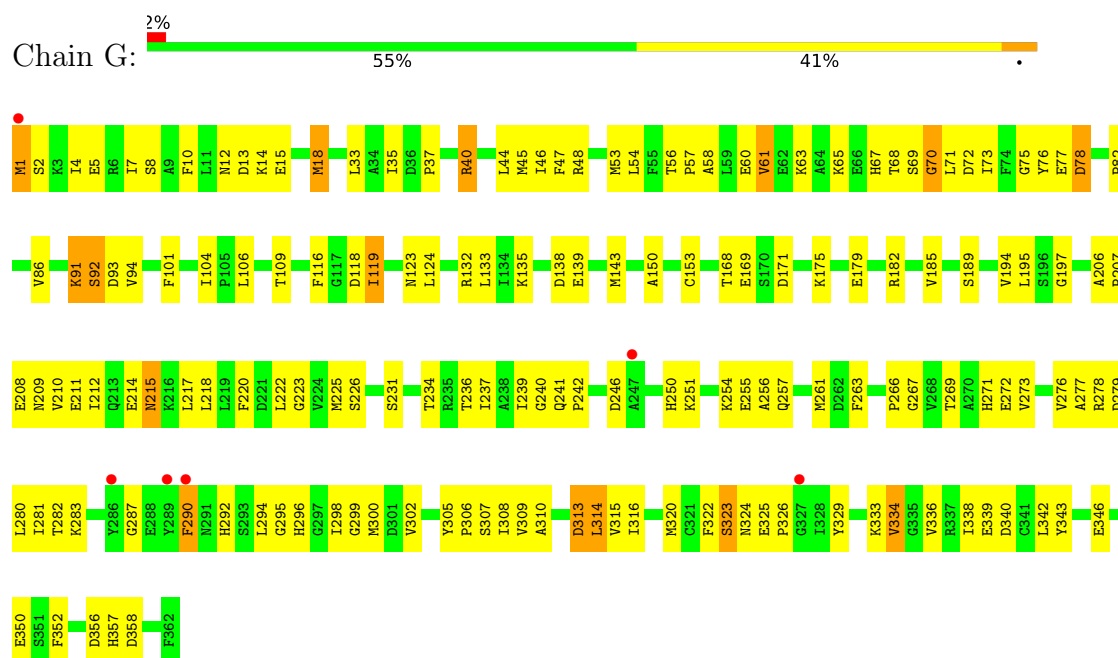
● Molecule 1: Aminopeptidase P family protein



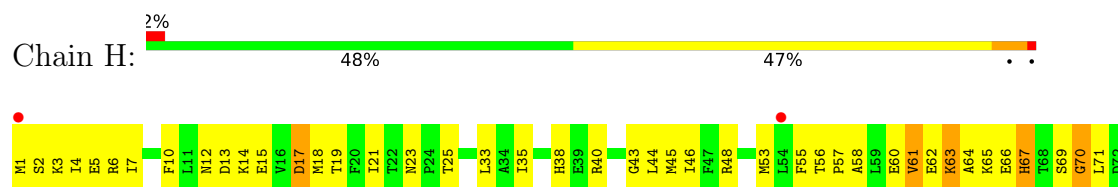
- Molecule 1: Aminopeptidase P family protein

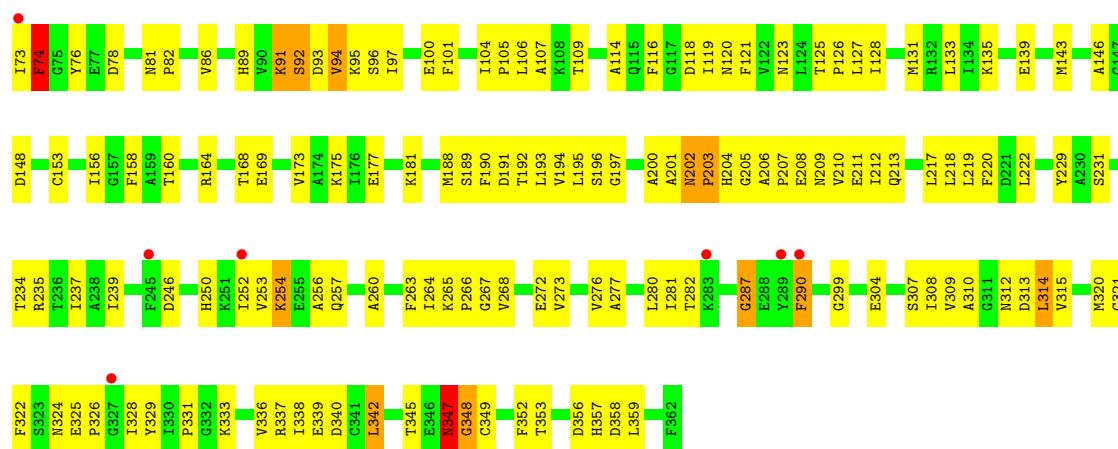


- Molecule 1: Aminopeptidase P family protein

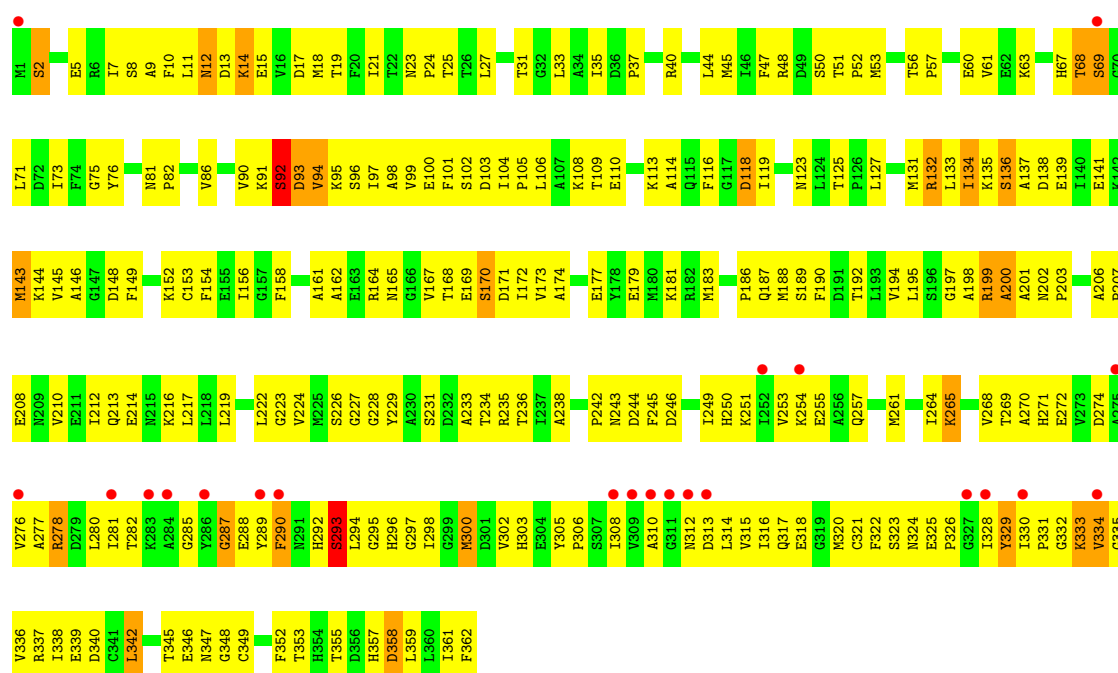


- Molecule 1: Aminopeptidase P family protein

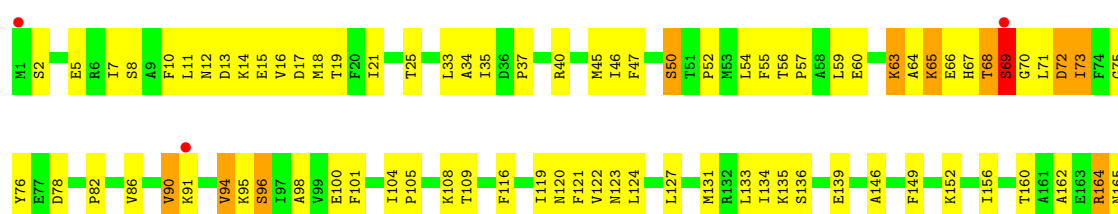


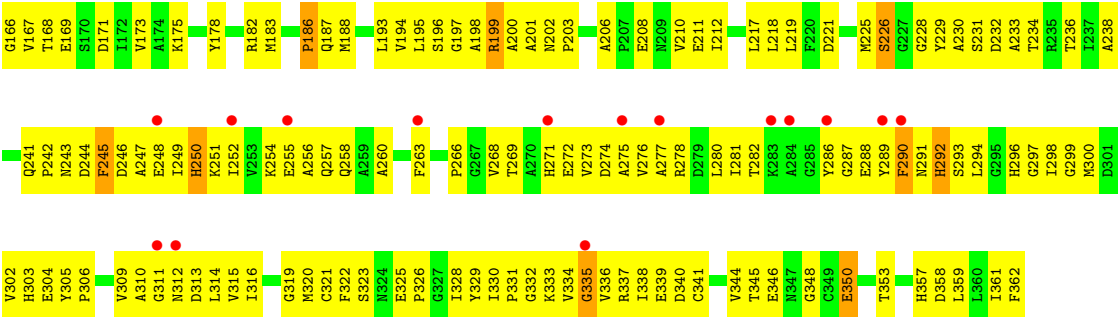


• Molecule 1: Aminopeptidase P family protein



• Molecule 1: Aminopeptidase P family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.30Å 80.00Å 187.15Å 90.00° 102.03° 90.00°	Depositor
Resolution (Å)	49.19 – 2.70 49.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.19-2.70) 94.7 (49.19-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.198 , 0.288 0.199 , 0.288	Depositor DCC
$R_{free}$ test set	5831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7153e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN

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	0.45	0/2856	0.63	1/3864 (0.0%)
1	B	0.56	1/2856 (0.0%)	0.70	0/3864
1	C	0.53	1/2856 (0.0%)	0.66	1/3864 (0.0%)
1	D	0.43	0/2856	0.60	0/3864
1	E	0.39	0/2856	0.59	0/3864
1	F	0.47	0/2856	0.65	2/3864 (0.1%)
1	G	0.47	0/2856	0.63	0/3864
1	H	0.41	0/2856	0.59	0/3864
1	I	0.40	0/2856	0.59	2/3864 (0.1%)
1	J	0.47	1/2856 (0.0%)	0.61	1/3864 (0.0%)
All	All	0.46	3/28560 (0.0%)	0.62	7/38640 (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	B	0	2
1	E	0	2
1	G	0	1
1	J	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	CYS	CB-SG	-6.16	1.71	1.82
1	C	349	CYS	CB-SG	-5.57	1.72	1.81
1	J	91	LYS	CB-CG	5.52	1.67	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	MET	CB-CG-SD	-7.70	89.29	112.40
1	C	71	LEU	CA-CB-CG	-6.31	100.80	115.30
1	J	91	LYS	CD-CE-NZ	-6.22	97.40	111.70
1	I	69	SER	N-CA-C	-5.89	95.09	111.00
1	F	1	MET	CA-CB-CG	5.75	123.07	113.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	311	GLY	Peptide
1	B	93	ASP	Peptide
1	E	63	LYS	Peptide
1	E	65	LYS	Peptide
1	G	1	MET	Peptide

## 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	2801	0	2748	126	0
1	B	2801	0	2748	76	0
1	C	2801	0	2748	135	0
1	D	2801	0	2748	169	0
1	E	2801	0	2748	181	0
1	F	2801	0	2748	204	0
1	G	2801	0	2748	161	0
1	H	2801	0	2748	192	1
1	I	2801	0	2748	269	1
1	J	2801	0	2748	258	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
3	C	6	8	7	0	0
3	D	6	8	8	0	0
3	G	6	8	8	1	0
4	A	38	0	0	6	1
4	B	88	0	0	0	0
4	C	77	0	0	5	0
4	D	38	0	0	5	0
4	E	16	0	0	4	1
4	F	35	0	0	1	0
4	G	33	0	0	3	0
4	H	14	0	0	2	0
4	I	15	0	0	10	0
4	J	26	0	0	6	0
All	All	28440	40	27519	1750	2

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 31.

The worst 5 of 1750 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:E:70:GLY:O	1:E:71:LEU:HD22	1.12	1.24
1:H:196:SER:HB2	1:H:218:LEU:CD1	1.71	1.19
1:I:282:THR:HG23	1:I:287:GLY:N	1.61	1.15
1:J:16:VAL:HG13	1:J:96:SER:HB3	1.27	1.13
1:H:196:SER:HB2	1:H:218:LEU:HD13	1.28	1.10

All (2) 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)
4:A:536:HOH:O	4:E:511:HOH:O[2_455]	0.49	1.71
1:H:358:ASP:OD1	1:I:68:THR:OG1[2_355]	2.02	0.18



## 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	360/362 (99%)	338 (94%)	16 (4%)	6 (2%)	9	23
1	B	360/362 (99%)	337 (94%)	15 (4%)	8 (2%)	6	17
1	C	360/362 (99%)	323 (90%)	29 (8%)	8 (2%)	6	17
1	D	360/362 (99%)	321 (89%)	32 (9%)	7 (2%)	8	20
1	E	360/362 (99%)	318 (88%)	38 (11%)	4 (1%)	14	34
1	F	360/362 (99%)	306 (85%)	43 (12%)	11 (3%)	4	9
1	G	360/362 (99%)	317 (88%)	33 (9%)	10 (3%)	5	11
1	H	360/362 (99%)	300 (83%)	47 (13%)	13 (4%)	3	7
1	I	360/362 (99%)	304 (84%)	38 (11%)	18 (5%)	2	4
1	J	360/362 (99%)	307 (85%)	36 (10%)	17 (5%)	2	4
All	All	3600/3620 (99%)	3171 (88%)	327 (9%)	102 (3%)	5	11

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	B	66	GLU
1	B	68	THR
1	B	72	ASP
1	B	93	ASP

### 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	303/303 (100%)	299 (99%)	4 (1%)	69	87
1	B	303/303 (100%)	300 (99%)	3 (1%)	76	91
1	C	303/303 (100%)	300 (99%)	3 (1%)	76	91
1	D	303/303 (100%)	296 (98%)	7 (2%)	50	78
1	E	303/303 (100%)	290 (96%)	13 (4%)	29	57
1	F	303/303 (100%)	290 (96%)	13 (4%)	29	57
1	G	303/303 (100%)	292 (96%)	11 (4%)	35	64
1	H	303/303 (100%)	293 (97%)	10 (3%)	38	67
1	I	303/303 (100%)	286 (94%)	17 (6%)	21	45
1	J	303/303 (100%)	294 (97%)	9 (3%)	41	70
All	All	3030/3030 (100%)	2940 (97%)	90 (3%)	41	70

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	290	PHE
1	G	292	HIS
1	J	69	SER
1	F	340	ASP
1	G	72	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	213	GLN
1	F	324	ASN
1	I	213	GLN
1	E	215	ASN
1	H	291	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 20 are monoatomic - leaving 5 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
3	GOL	D	403	-	5,5,5	0.89	0	5,5,5	0.66	0
3	GOL	G	403	-	5,5,5	0.94	0	5,5,5	0.87	0
3	GOL	B	403	-	5,5,5	0.97	0	5,5,5	1.31	1 (20%)
3	GOL	C	403	-	5,5,5	1.64	2 (40%)	5,5,5	2.01	1 (20%)
3	GOL	A	403	-	5,5,5	1.19	0	5,5,5	1.03	1 (20%)

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
3	GOL	D	403	-	-	0/4/4/4	-
3	GOL	G	403	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	A	403	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	GOL	O2-C2	-2.53	1.35	1.43
3	C	403	GOL	C1-C2	2.16	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	GOL	C3-C2-C1	-4.03	96.04	111.70
3	B	403	GOL	C3-C2-C1	-2.49	102.01	111.70
3	A	403	GOL	C3-C2-C1	-2.07	103.65	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	403	GOL	1	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 [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<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	362/362 (100%)	-0.24	2 (0%) 89 91	41, 58, 93, 137	0
1	B	362/362 (100%)	-0.34	2 (0%) 89 91	27, 35, 68, 115	0
1	C	362/362 (100%)	-0.37	6 (1%) 70 72	28, 45, 90, 180	0
1	D	362/362 (100%)	-0.28	5 (1%) 75 77	38, 60, 111, 158	0
1	E	362/362 (100%)	-0.16	1 (0%) 94 95	43, 73, 108, 145	0
1	F	362/362 (100%)	-0.09	7 (1%) 66 69	34, 65, 115, 160	0
1	G	362/362 (100%)	-0.25	6 (1%) 70 72	34, 56, 91, 169	0
1	H	362/362 (100%)	-0.08	9 (2%) 57 59	49, 72, 104, 143	0
1	I	362/362 (100%)	0.14	22 (6%) 21 20	52, 85, 123, 157	0
1	J	362/362 (100%)	-0.05	18 (4%) 28 27	38, 69, 119, 159	0
All	All	3620/3620 (100%)	-0.17	78 (2%) 62 63	27, 63, 109, 180	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	13.2
1	A	1	MET	13.1
1	G	1	MET	8.5
1	C	70	GLY	7.1
1	I	311	GLY	7.0

### 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
3	GOL	G	403	6/6	0.80	0.28	91,109,123,124	0
2	MN	A	402	1/1	0.89	0.25	58,58,58,58	0
3	GOL	C	403	6/6	0.90	0.17	49,66,87,105	0
3	GOL	D	403	6/6	0.91	0.15	56,74,89,89	0
3	GOL	B	403	6/6	0.91	0.20	44,57,80,96	0
3	GOL	A	403	6/6	0.91	0.20	45,68,87,87	0
2	MN	E	401	1/1	0.95	0.17	69,69,69,69	0
2	MN	I	401	1/1	0.96	0.12	79,79,79,79	0
2	MN	D	401	1/1	0.96	0.20	59,59,59,59	0
2	MN	J	402	1/1	0.96	0.17	64,64,64,64	0
2	MN	F	401	1/1	0.96	0.15	69,69,69,69	0
2	MN	H	401	1/1	0.97	0.24	71,71,71,71	0
2	MN	J	401	1/1	0.97	0.15	63,63,63,63	0
2	MN	F	402	1/1	0.98	0.21	62,62,62,62	0
2	MN	G	402	1/1	0.98	0.17	44,44,44,44	0
2	MN	C	402	1/1	0.98	0.17	35,35,35,35	0
2	MN	H	402	1/1	0.98	0.18	72,72,72,72	0
2	MN	C	401	1/1	0.98	0.17	42,42,42,42	0
2	MN	I	402	1/1	0.98	0.15	78,78,78,78	0
2	MN	G	401	1/1	0.98	0.16	40,40,40,40	0
2	MN	B	402	1/1	0.99	0.16	33,33,33,33	0
2	MN	B	401	1/1	0.99	0.20	30,30,30,30	0
2	MN	D	402	1/1	0.99	0.15	34,34,34,34	0
2	MN	E	402	1/1	0.99	0.19	67,67,67,67	0
2	MN	A	401	1/1	0.99	0.22	53,53,53,53	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.