

wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 10:14 AM JST

PDB ID : 6LL7

Title: Type II inorganic pyrophosphatase (PPase) from the psychrophilic bacterium

Shewanella sp. AS-11, Mn-activated form

Authors: Horitani, M.; Kusubayashi, K.; Oshima, K.; Yato, A.; Sugimoto, H.; Watan-

abe, K.

Deposited on : 2019-12-21

Resolution : 2.20 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
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 (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$

EDS : 2.36

buster-report : 1.1.7 (2018)

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)

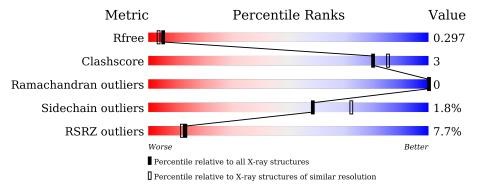
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	309	94%	5% •
1	В	309	93%	6% •
1	С	309	93%	6% •
1	D	309	7% 93%	6% •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9646 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	306	Total	С	N	О	S	0	0	0
1	A	300	2340	1488	380	455	17	0	0	U
1	В	306	Total	С	N	О	S	0	0	0
1	Ъ	300	2340	1488	380	455	17	0	0	
1	С	306	Total	С	N	О	S	0	0	0
1		300	2340	1488	380	455	17	0	0	
1	D	306	Total	С	N	О	S	0	0	0
1	ש	300	2340	1488	380	455	17	U	U	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP L8AXY8
A	1	GLY	-	cloning artifact	UNP L8AXY8
A	116	SER	ARG	conflict	UNP L8AXY8
В	0	MET	-	cloning artifact	UNP L8AXY8
В	1	GLY	_	cloning artifact	UNP L8AXY8
В	116	SER	ARG	conflict	UNP L8AXY8
С	0	MET	_	cloning artifact	UNP L8AXY8
С	1	GLY	-	cloning artifact	UNP L8AXY8
С	116	SER	ARG	conflict	UNP L8AXY8
D	0	MET	-	cloning artifact	UNP L8AXY8
D	1	GLY	-	cloning artifact	UNP L8AXY8
D	116	SER	ARG	conflict	UNP L8AXY8

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Mn 2 2	0	0
2	С	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	С	1	Total Ca 1 1	0	0

• Molecule 4 is water.

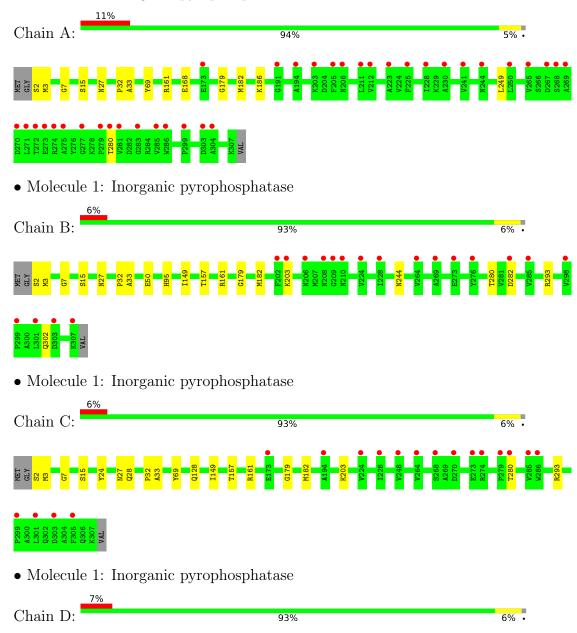
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	В	78	Total O 78 78	0	0
4	С	72	Total O 72 72	0	0
4	D	63	Total O 63 63	0	0



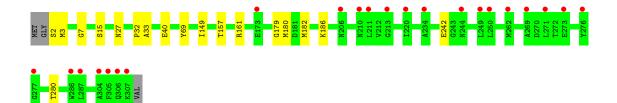
3 Residue-property plots (i)

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: Inorganic pyrophosphatase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	52.53Å 75.57Å 85.67Å	Donositon
a, b, c, α , β , γ	107.40° 90.06° 92.17°	Depositor
Resolution (Å)	47.51 - 2.20	Depositor
Resolution (A)	47.47 - 2.20	EDS
% Data completeness	95.0 (47.51-2.20)	Depositor
(in resolution range)	$95.0 \ (47.47 - 2.20)$	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.94 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D.D.	0.256 , 0.297	Depositor
R, R_{free}	0.259 , 0.297	DCC
R_{free} test set	2985 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 32.6	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9646	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.12% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MN, CA

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.71	0/2379	0.79	0/3223	
1	В	0.71	0/2379	0.82	$2/3223 \ (0.1\%)$	
1	С	0.71	0/2379	0.80	$1/3223 \ (0.0\%)$	
1	D	0.71	0/2379	0.79	0/3223	
All	All	0.71	0/9516	0.80	$3/12892 \ (0.0\%)$	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	293	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	С	293	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	В	244	ASN	CB-CA-C	5.33	121.05	110.40

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	2340	0	2353	10	0
1	В	2340	0	2353	14	0
1	С	2340	0	2353	13	0
1	D	2340	0	2353	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	С	1	0	0	0	0
4	A	63	0	0	3	0
4	В	78	0	0	4	0
4	С	72	0	0	4	0
4	D	63	0	0	5	0
All	All	9646	0	9412	50	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 3.

The worst 5 of 50 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:282:ASP:OD1	1:D:242:GLU:HA	1.73	0.89
1:B:179:GLY:HA2	1:B:182:MET:CE	2.28	0.64
1:C:179:GLY:HA2	1:C:182:MET:CE	2.28	0.63
1:A:179:GLY:HA2	1:A:182:MET:CE	2.30	0.62
1:C:27:ASN:HD21	1:C:33:ALA:H	1.48	0.62

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	304/309~(98%)	297 (98%)	7 (2%)	0	100	100
1	В	304/309 (98%)	296 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
1	C	304/309 (98%)	295 (97%)	9 (3%)	0	100	100
1	D	304/309 (98%)	298 (98%)	6 (2%)	0	100	100
All	All	1216/1236 (98%)	1186 (98%)	30 (2%)	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	$256/258 \ (99\%)$	251 (98%)	5 (2%)	55 69		
1	В	256/258~(99%)	251 (98%)	5 (2%)	55 69		
1	С	$256/258 \ (99\%)$	252 (98%)	4 (2%)	62 76		
1	D	256/258~(99%)	252 (98%)	4 (2%)	62 76		
All	All	$1024/1032 \ (99\%)$	1006 (98%)	18 (2%)	59 72		

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	SER
1	D	280	THR
1	D	149	ILE
1	В	280	THR
1	С	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	27	ASN
1	D	306	GLN
1	В	306	GLN
1	С	27	ASN
1	С	128	GLN



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 10 ligands modelled in this entry, 10 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 (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^{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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	306/309 (99%)	0.70	35 (11%) 5 4	23, 39, 86, 105	0
1	В	306/309 (99%)	0.53	19 (6%) 20 19	23, 36, 67, 100	0
1	С	306/309 (99%)	0.47	18 (5%) 22 21	24, 36, 73, 85	0
1	D	306/309 (99%)	0.62	22 (7%) 15 14	24, 39, 70, 103	0
All	All	1224/1236 (99%)	0.58	94 (7%) 13 12	23, 38, 73, 105	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	303	ASP	5.9
1	A	228	ILE	5.3
1	D	277	GLY	5.2
1	D	211	LEU	5.0
1	A	271	LEU	5.0

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^{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.



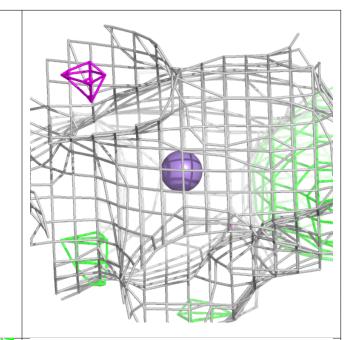
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	MN	A	401	1/1	0.97	0.08	31,31,31,31	0
2	MN	В	401	1/1	0.98	0.08	27,27,27,27	0
2	MN	С	401	1/1	0.98	0.08	29,29,29,29	0
2	MN	С	402	1/1	0.98	0.08	27,27,27,27	0
2	MN	D	402	1/1	0.98	0.11	31,31,31,31	0
3	CA	A	403	1/1	0.98	0.10	33,33,33,33	0
3	CA	С	403	1/1	0.98	0.10	30,30,30,30	0
2	MN	A	402	1/1	0.99	0.13	27,27,27,27	0
2	MN	В	402	1/1	0.99	0.12	24,24,24,24	0
2	MN	D	401	1/1	0.99	0.06	32,32,32,32	0

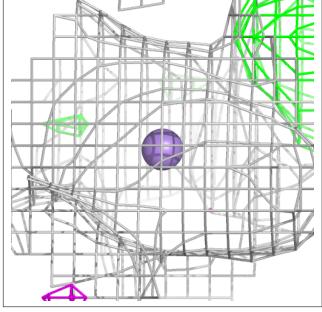
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

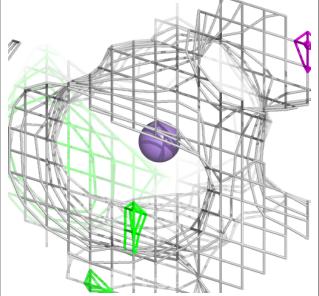


Electron density around MN A 401:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



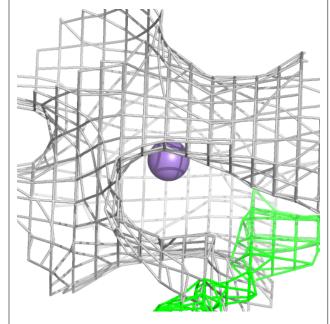


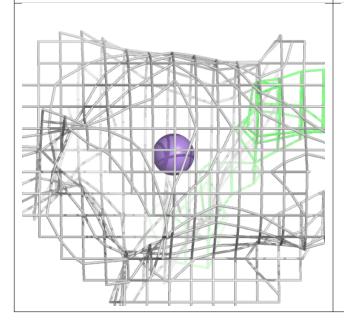


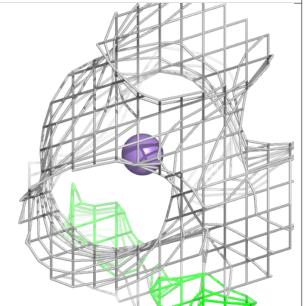


Electron density around MN B 401:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









Electron density around MN C 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN C 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN D 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

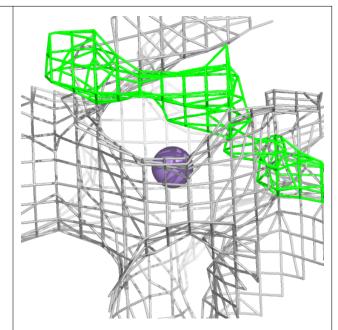


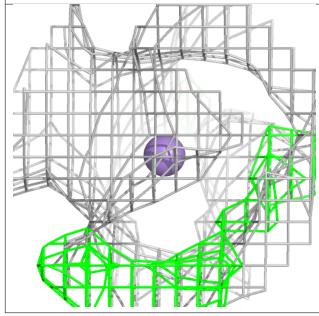
Electron density around MN A 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

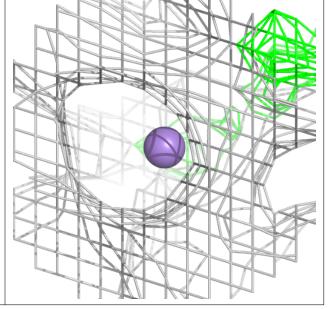


Electron density around MN B 402:

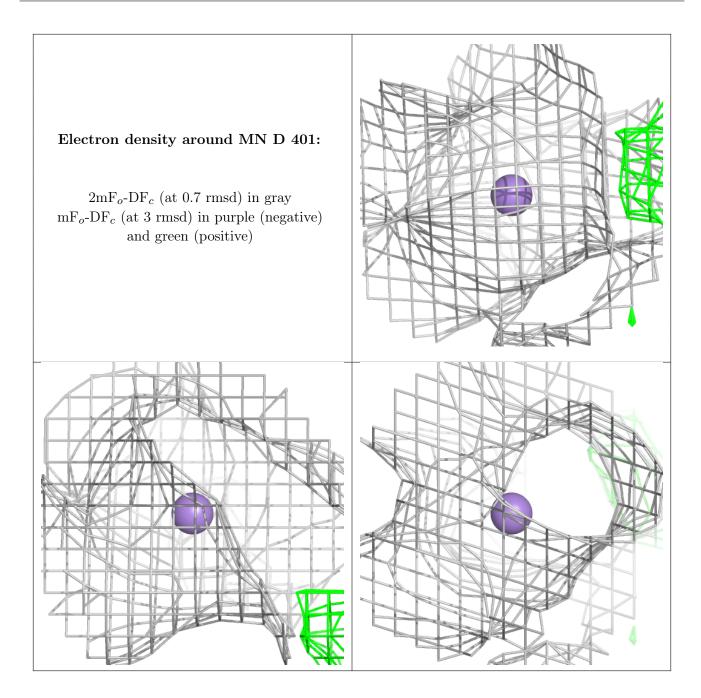
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

