



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:45 PM BST

PDB ID : 6RMO
Title : Structure of Plasmodium falciparum IMP-nucleotidase
Authors : Carrique, L.; Ballut, L.; Violot, S.; Aghajari, N.
Deposited on : 2019-05-07
Resolution : 2.60 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 ⓘ symbol.

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

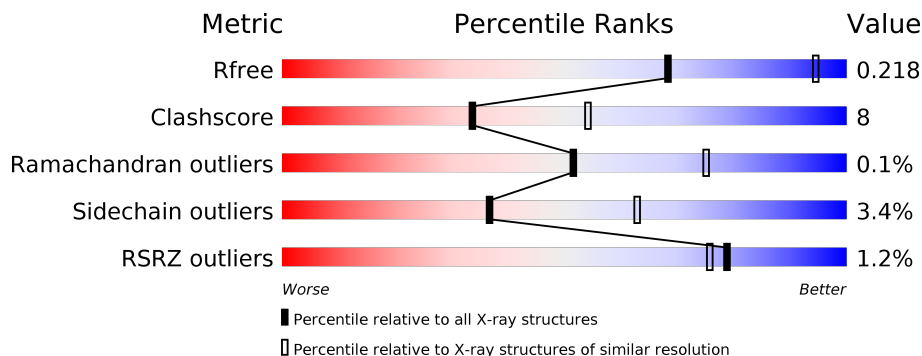
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.60 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.






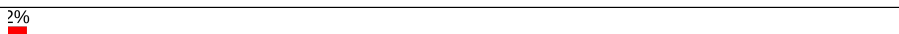
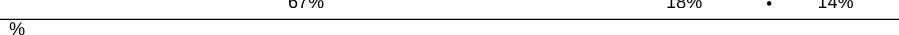




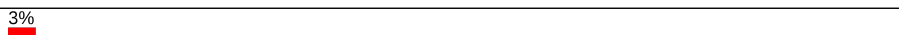
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	444	 73% 18% • 8%
1	H	444	 64% 18% 19%
1	I	444	 75% 20% • •
1	J	444	 67% 18% • 14%
1	K	444	 73% 22% 5%
1	L	444	 64% 21% • 14%
1	M	444	 78% 18% • •
1	N	444	 66% 20% • 14%
1	O	444	 77% 17% • 5%
1	P	444	 69% 16% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 52441 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 IMP-specific 5'-nucleotidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	Total 3323	C 2149	N 544	O 613	S 17	0	0	0
1	B	368	Total 2932	C 1909	N 475	O 532	S 16	0	0	0
1	C	410	Total 3328	C 2154	N 544	O 613	S 17	0	0	0
1	D	370	Total 2965	C 1927	N 480	O 542	S 16	0	0	0
1	E	408	Total 3279	C 2118	N 534	O 611	S 16	0	0	0
1	F	364	Total 2950	C 1910	N 481	O 543	S 16	0	0	0
1	G	407	Total 3264	C 2109	N 536	O 602	S 17	0	0	0
1	H	361	Total 2863	C 1855	N 466	O 526	S 16	0	0	0
1	I	432	Total 3486	C 2242	N 574	O 652	S 18	0	0	0
1	J	381	Total 3085	C 1999	N 506	O 564	S 16	0	0	0
1	K	423	Total 3447	C 2226	N 566	O 637	S 18	0	0	0
1	L	382	Total 3106	C 2010	N 508	O 572	S 16	0	0	0
1	M	431	Total 3512	C 2263	N 575	O 656	S 18	0	0	0
1	N	381	Total 3080	C 1999	N 506	O 559	S 16	0	0	0
1	O	423	Total 3433	C 2216	N 565	O 634	S 18	0	0	0
1	P	381	Total 3083	C 1995	N 505	O 567	S 16	0	0	0

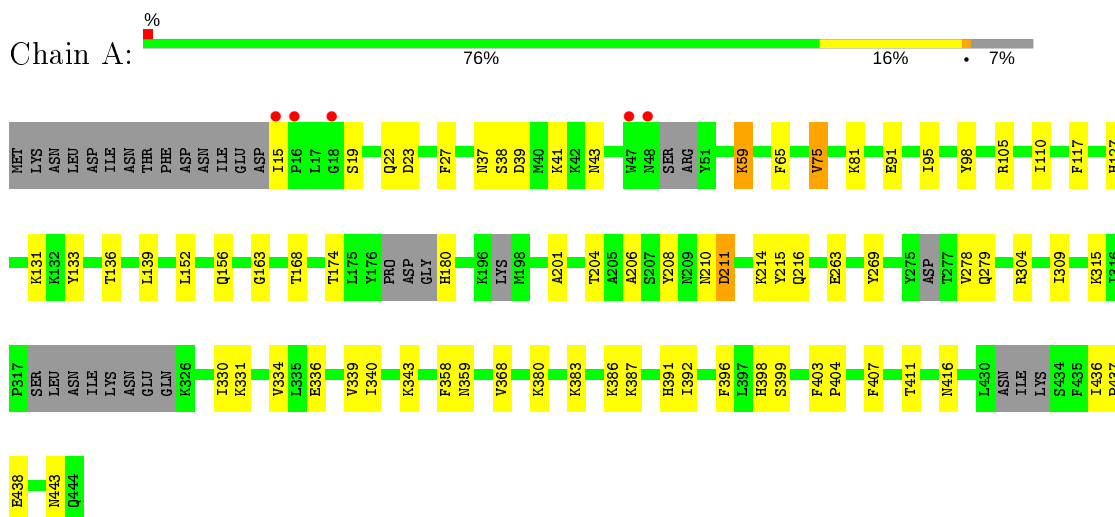
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	59	Total O 59 59	0	0
2	C	103	Total O 103 103	0	0
2	D	65	Total O 65 65	0	0
2	E	105	Total O 105 105	0	0
2	F	57	Total O 57 57	0	0
2	G	95	Total O 95 95	0	0
2	H	75	Total O 75 75	0	0
2	I	97	Total O 97 97	0	0
2	J	53	Total O 53 53	0	0
2	K	112	Total O 112 112	0	0
2	L	74	Total O 74 74	0	0
2	M	95	Total O 95 95	0	0
2	N	60	Total O 60 60	0	0
2	O	99	Total O 99 99	0	0
2	P	63	Total O 63 63	0	0

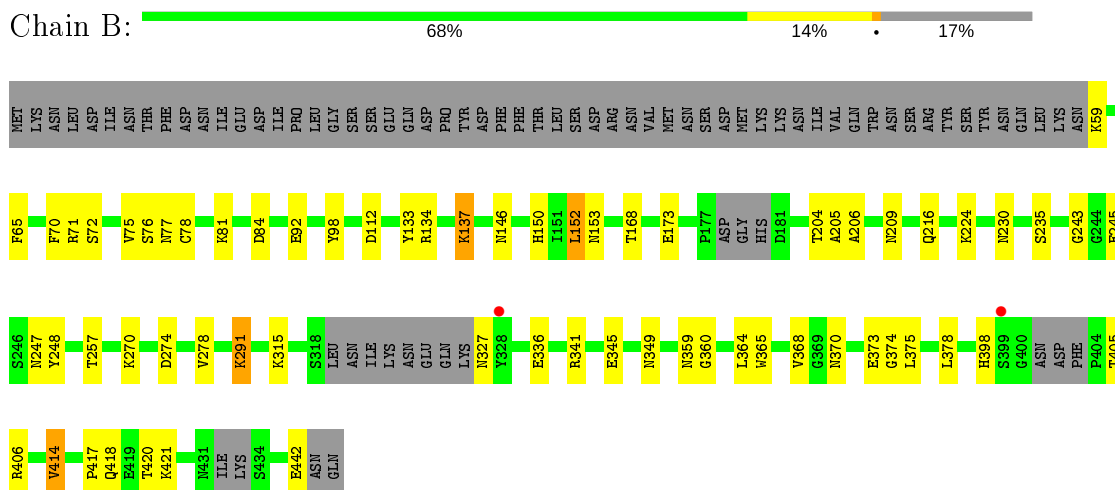
3 Residue-property plots [i](#)

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: IMP-specific 5'-nucleotidase, putative

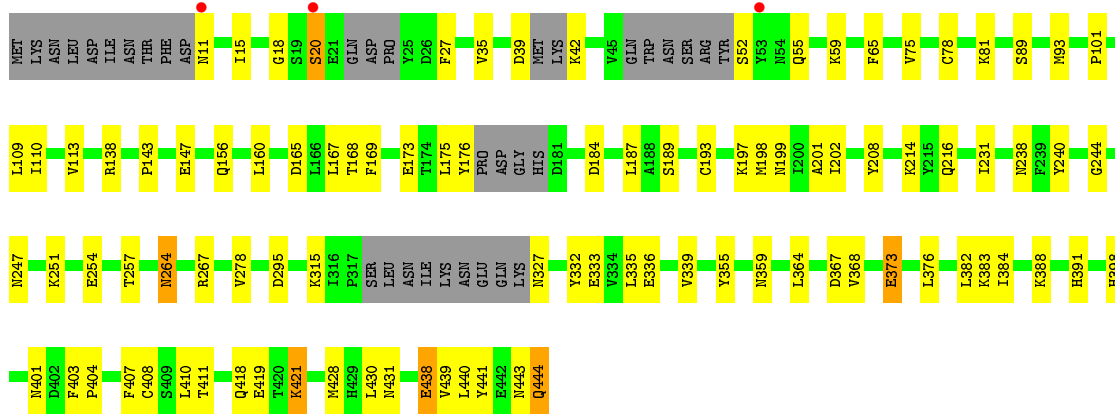


- Molecule 1: IMP-specific 5'-nucleotidase, putative

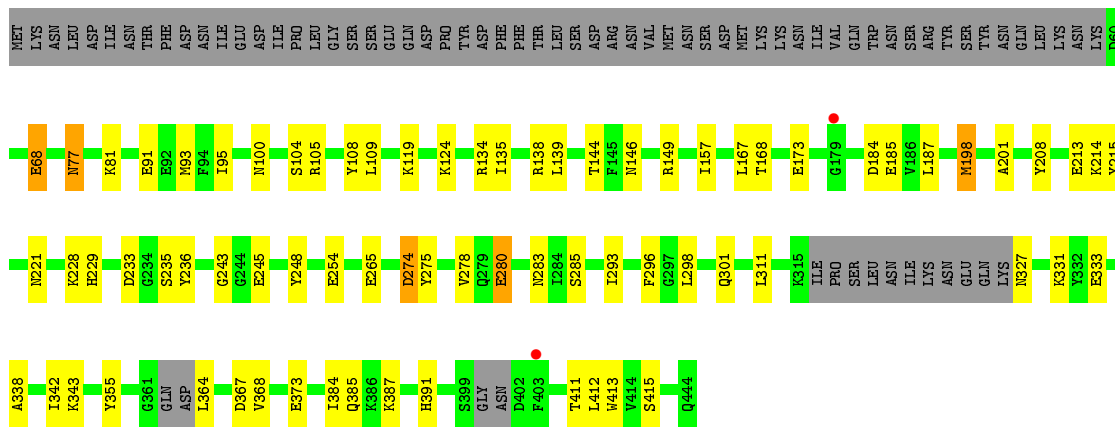


- Molecule 1: IMP-specific 5'-nucleotidase, putative

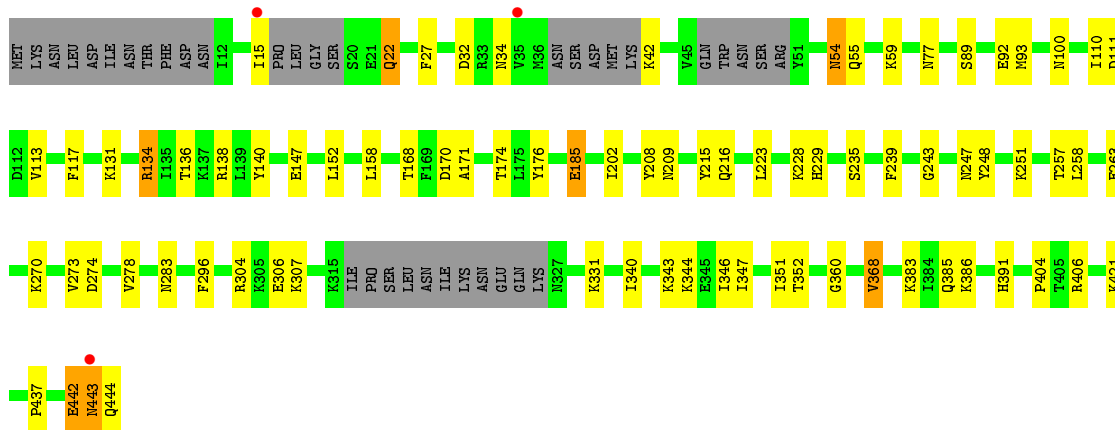
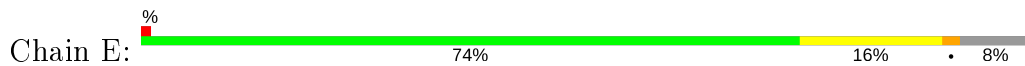




• Molecule 1: IMP-specific 5'-nucleotidase, putative

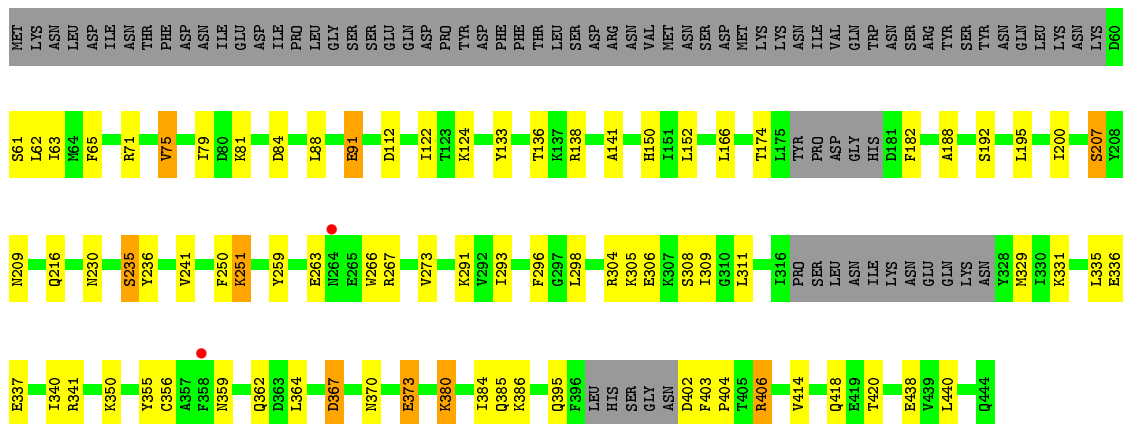


• Molecule 1: IMP-specific 5'-nucleotidase, putative

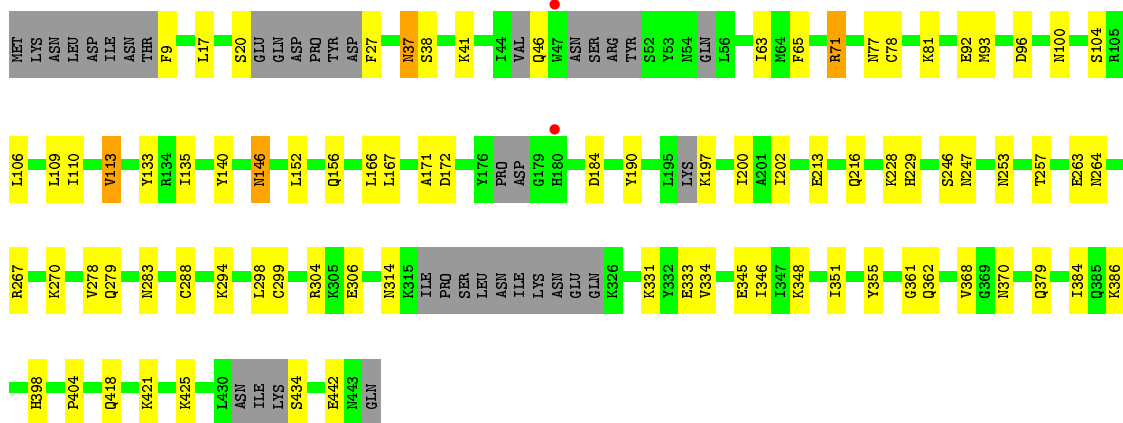


• Molecule 1: IMP-specific 5'-nucleotidase, putative

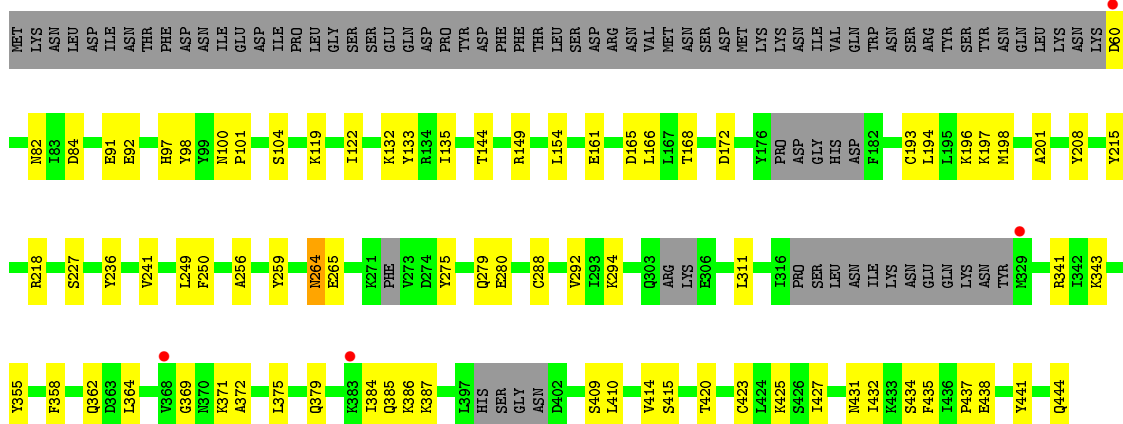




• Molecule 1: IMP-specific 5'-nucleotidase, putative

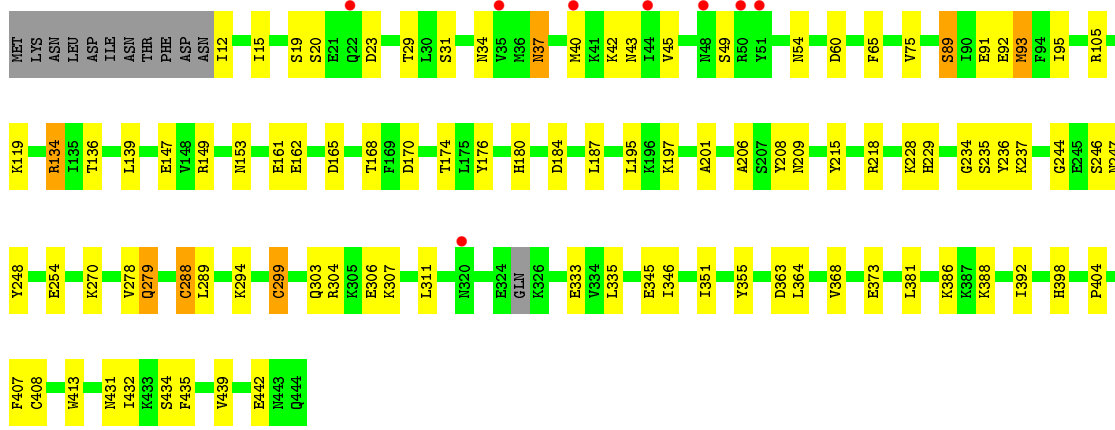


• Molecule 1: IMP-specific 5'-nucleotidase, putative

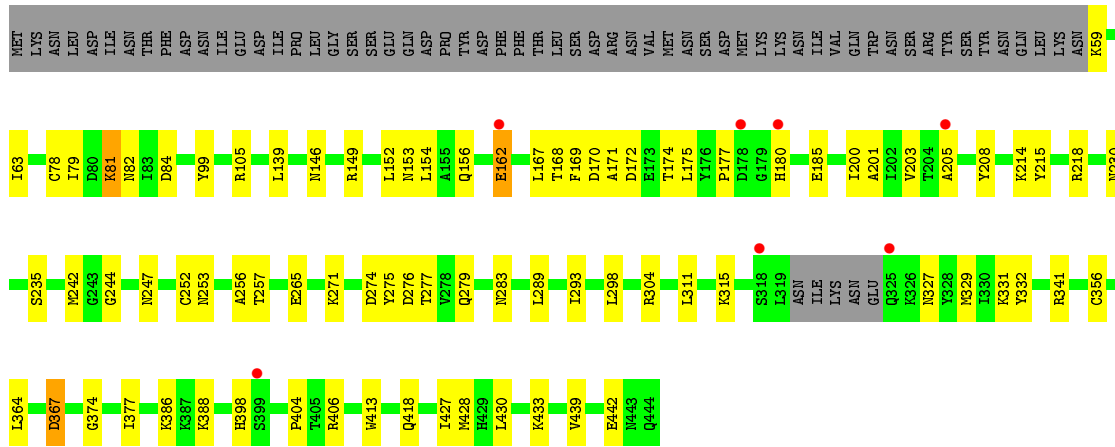


• Molecule 1: IMP-specific 5'-nucleotidase, putative

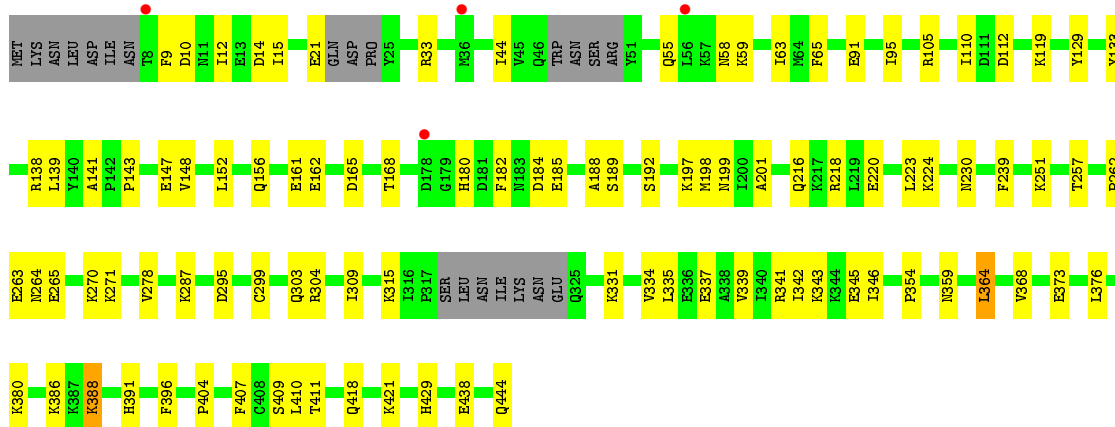
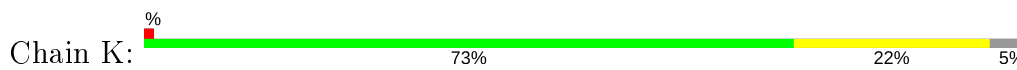




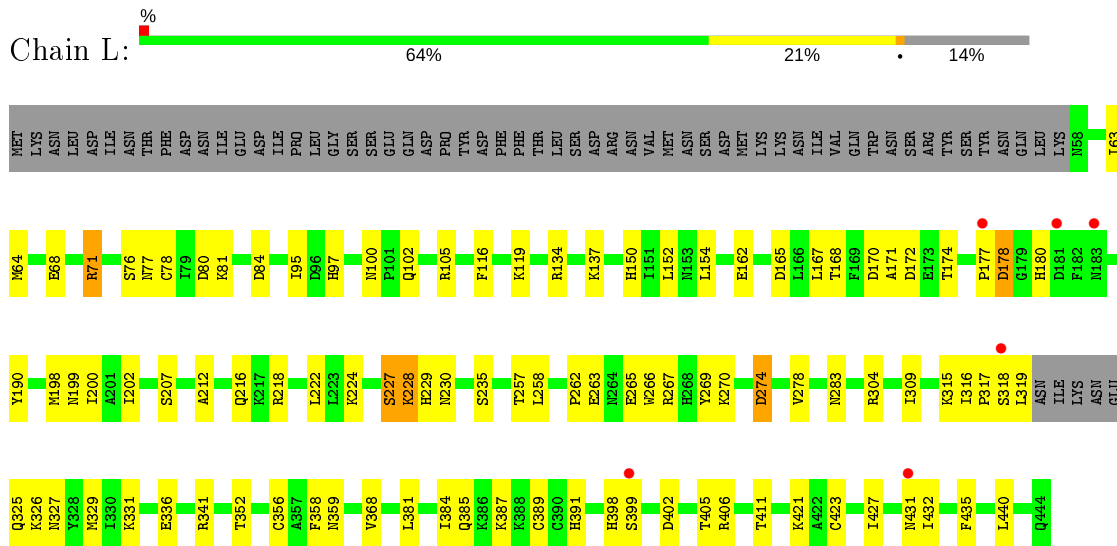
- Molecule 1: IMP-specific 5'-nucleotidase, putative



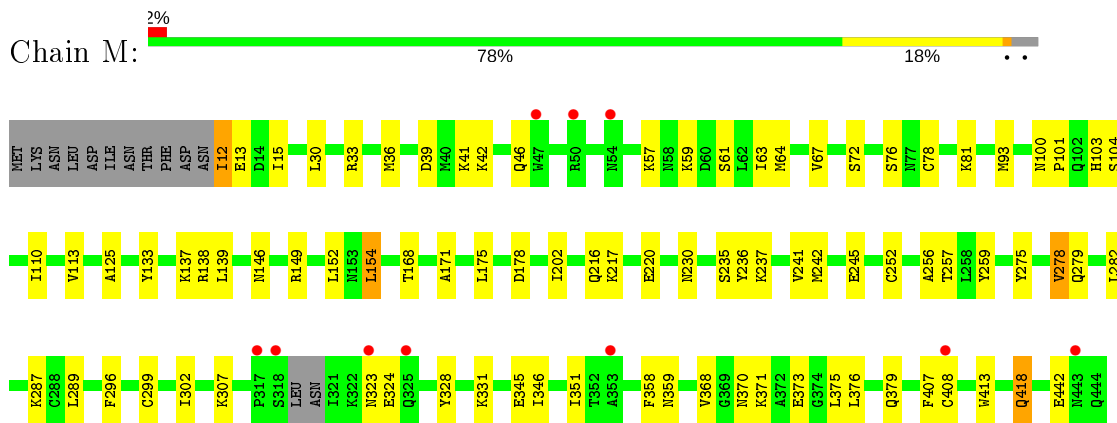
- Molecule 1: IMP-specific 5'-nucleotidase, putative



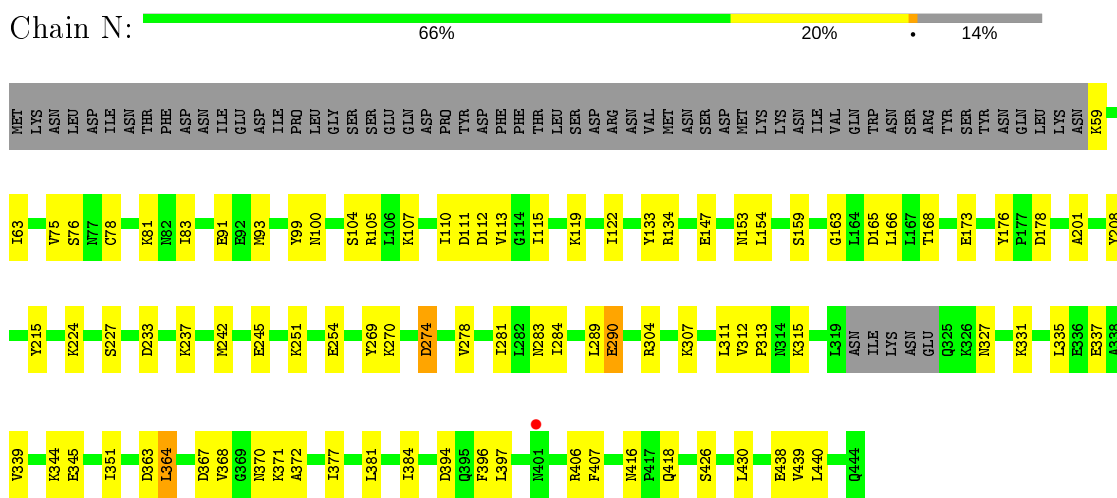
- Molecule 1: IMP-specific 5'-nucleotidase, putative



• Molecule 1: IMP-specific 5'-nucleotidase, putative

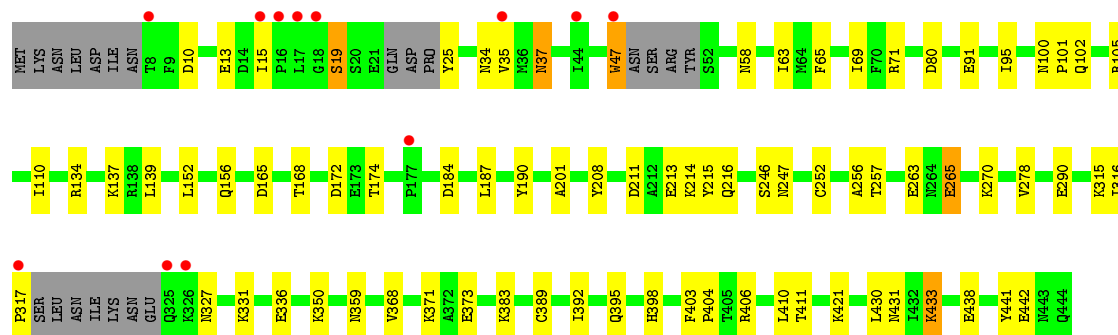


• Molecule 1: IMP-specific 5'-nucleotidase, putative

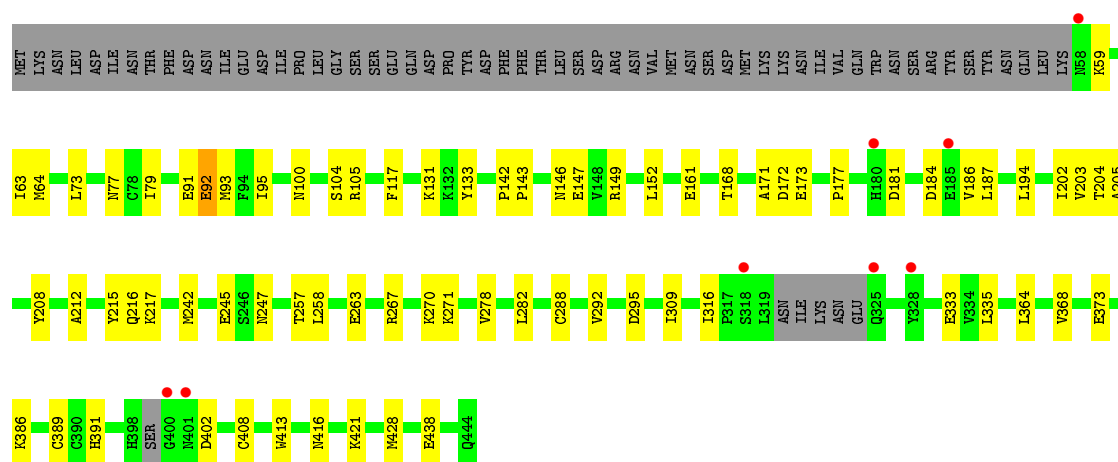


• Molecule 1: IMP-specific 5'-nucleotidase, putative





- Molecule 1: IMP-specific 5'-nucleotidase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	148.96Å 204.07Å 149.28Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	48.30 – 2.60 48.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.30-2.60) 91.2 (48.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.210 , 0.218	Depositor DCC
R_{free} test set	12515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 19.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.317 for l,k,-h 0.329 for h,-k,-l 0.399 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52441	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 20.60 % 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 8.3947e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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	0.25	0/3390	0.41	0/4577
1	B	0.24	0/2993	0.40	0/4050
1	C	0.25	0/3394	0.42	1/4579 (0.0%)
1	D	0.25	0/3027	0.40	0/4093
1	E	0.25	0/3345	0.42	0/4519
1	F	0.25	0/3007	0.41	0/4058
1	G	0.26	0/3326	0.41	0/4485
1	H	0.26	0/2918	0.42	0/3949
1	I	0.25	0/3558	0.40	0/4806
1	J	0.25	0/3151	0.41	0/4255
1	K	0.25	0/3518	0.41	0/4746
1	L	0.25	0/3173	0.42	0/4287
1	M	0.25	0/3587	0.41	0/4844
1	N	0.25	0/3146	0.41	0/4248
1	O	0.25	0/3504	0.42	0/4730
1	P	0.24	0/3148	0.40	0/4254
All	All	0.25	0/52185	0.41	1/70480 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	LEU	CB-CG-CD1	-5.94	100.89	111.00

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	3323	0	3278	46	0
1	B	2932	0	2884	48	0
1	C	3328	0	3309	71	0
1	D	2965	0	2911	52	0
1	E	3279	0	3217	54	1
1	F	2950	0	2951	54	0
1	G	3264	0	3194	58	0
1	H	2863	0	2802	58	0
1	I	3486	0	3438	65	0
1	J	3085	0	3078	51	0
1	K	3447	0	3427	66	0
1	L	3106	0	3086	73	1
1	M	3512	0	3479	59	0
1	N	3080	0	3081	58	0
1	O	3433	0	3405	57	0
1	P	3083	0	3054	51	0
2	A	93	0	0	14	0
2	B	59	0	0	9	0
2	C	103	0	0	15	0
2	D	65	0	0	19	0
2	E	105	0	0	23	1
2	F	57	0	0	10	0
2	G	95	0	0	24	0
2	H	75	0	0	23	0
2	I	97	0	0	20	1
2	J	53	0	0	11	0
2	K	112	0	0	19	0
2	L	74	0	0	26	0
2	M	95	0	0	21	0
2	N	60	0	0	18	0
2	O	99	0	0	21	0
2	P	63	0	0	13	0
All	All	52441	0	50594	864	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 8.

The worst 5 of 864 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:I:119:LYS:NZ	2:I:501:HOH:O	1.92	1.00
1:A:152:LEU:N	2:A:501:HOH:O	1.88	0.99
1:D:138:ARG:NH1	2:D:503:HOH:O	1.96	0.98
1:H:215:TYR:OH	2:H:501:HOH:O	1.81	0.98
1:K:112:ASP:OD2	2:K:501:HOH:O	1.83	0.97

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)
2:E:595:HOH:O	2:I:578:HOH:O[1_655]	1.92	0.28
1:E:216:GLN:OE1	1:L:228:LYS:NZ[2_655]	2.16	0.04

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	398/444 (90%)	383 (96%)	14 (4%)	1 (0%)	41	64
1	B	358/444 (81%)	344 (96%)	14 (4%)	0	100	100
1	C	398/444 (90%)	381 (96%)	17 (4%)	0	100	100
1	D	362/444 (82%)	348 (96%)	14 (4%)	0	100	100
1	E	398/444 (90%)	381 (96%)	13 (3%)	4 (1%)	15	32
1	F	356/444 (80%)	338 (95%)	17 (5%)	1 (0%)	41	64
1	G	389/444 (88%)	372 (96%)	17 (4%)	0	100	100
1	H	349/444 (79%)	338 (97%)	11 (3%)	0	100	100
1	I	428/444 (96%)	404 (94%)	24 (6%)	0	100	100
1	J	377/444 (85%)	356 (94%)	20 (5%)	1 (0%)	41	64
1	K	415/444 (94%)	395 (95%)	19 (5%)	1 (0%)	47	71
1	L	378/444 (85%)	363 (96%)	15 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	427/444 (96%)	406 (95%)	20 (5%)	1 (0%)	47	71
1	N	377/444 (85%)	362 (96%)	15 (4%)	0	100	100
1	O	415/444 (94%)	397 (96%)	18 (4%)	0	100	100
1	P	375/444 (84%)	359 (96%)	16 (4%)	0	100	100
All	All	6200/7104 (87%)	5927 (96%)	264 (4%)	9 (0%)	51	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	443	ASN
1	F	359	ASN
1	M	359	ASN
1	E	32	ASP
1	A	163	GLY

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	365/413 (88%)	353 (97%)	12 (3%)	38	64
1	B	314/413 (76%)	307 (98%)	7 (2%)	52	76
1	C	368/413 (89%)	357 (97%)	11 (3%)	41	67
1	D	318/413 (77%)	305 (96%)	13 (4%)	30	56
1	E	358/413 (87%)	346 (97%)	12 (3%)	37	63
1	F	325/413 (79%)	312 (96%)	13 (4%)	31	57
1	G	353/413 (86%)	343 (97%)	10 (3%)	43	69
1	H	307/413 (74%)	299 (97%)	8 (3%)	46	72
1	I	385/413 (93%)	369 (96%)	16 (4%)	30	55
1	J	338/413 (82%)	328 (97%)	10 (3%)	41	67
1	K	382/413 (92%)	369 (97%)	13 (3%)	37	63
1	L	342/413 (83%)	326 (95%)	16 (5%)	26	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	391/413 (95%)	378 (97%)	13 (3%)	38	64
1	N	337/413 (82%)	323 (96%)	14 (4%)	30	55
1	O	379/413 (92%)	366 (97%)	13 (3%)	37	63
1	P	337/413 (82%)	328 (97%)	9 (3%)	44	71
All	All	5599/6608 (85%)	5409 (97%)	190 (3%)	37	63

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	431	ASN
1	J	276	ASP
1	O	263	GLU
1	I	75	VAL
1	I	288	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	216	GLN
1	P	247	ASN
1	L	385	GLN
1	E	216	GLN
1	N	146	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](#)

There are no ligands in this entry.

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	412/444 (92%)	-0.01	5 (1%) 79 76	38, 52, 73, 96	0
1	B	368/444 (82%)	-0.07	2 (0%) 91 89	38, 59, 79, 112	0
1	C	410/444 (92%)	0.00	3 (0%) 87 86	37, 52, 76, 89	0
1	D	370/444 (83%)	0.00	2 (0%) 91 89	38, 58, 82, 113	0
1	E	408/444 (91%)	-0.04	3 (0%) 87 86	35, 51, 78, 96	0
1	F	364/444 (81%)	-0.02	2 (0%) 91 89	35, 58, 85, 112	0
1	G	407/444 (91%)	-0.01	2 (0%) 91 89	38, 52, 71, 88	0
1	H	361/444 (81%)	-0.04	4 (1%) 80 78	37, 59, 89, 108	0
1	I	432/444 (97%)	0.03	8 (1%) 66 62	33, 53, 100, 140	0
1	J	381/444 (85%)	0.09	7 (1%) 68 64	34, 60, 88, 137	0
1	K	423/444 (95%)	-0.01	4 (0%) 84 82	36, 51, 77, 141	0
1	L	382/444 (86%)	0.00	6 (1%) 72 68	34, 56, 83, 118	0
1	M	431/444 (97%)	0.07	10 (2%) 60 54	35, 52, 103, 165	0
1	N	381/444 (85%)	0.04	1 (0%) 94 93	38, 61, 90, 169	0
1	O	423/444 (95%)	0.09	12 (2%) 53 46	36, 53, 85, 120	0
1	P	381/444 (85%)	0.00	8 (2%) 63 58	37, 60, 86, 142	0
All	All	6334/7104 (89%)	0.01	79 (1%) 79 76	33, 55, 86, 169	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	325	GLN	5.8
1	O	8	THR	5.4
1	O	325	GLN	5.1
1	G	47	TRP	4.6
1	M	317	PRO	4.5

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.