Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 11:50 PM EDT

PDB ID	:	4LE5
Title	:	Structure of an Unusual S-adenosylmethionine synthetase from Campylobacter jejuni
Authors	:	Zano, S.P.; Pavlovsky, A.G.; Viola, R.E.
Deposited on	:	2013-06-25
Resolution	:	1.70 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 ⓘ 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 ⓘ) were used in the production of this report:

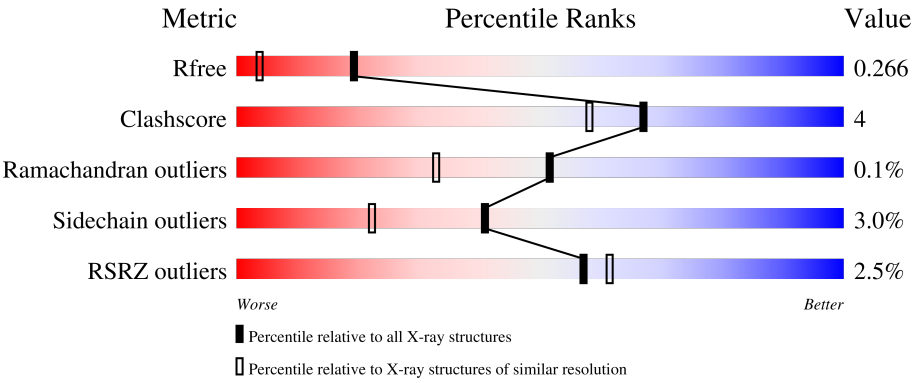
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	430	2% 83% 7% 10%
1	B	430	3% 78% 11% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6166 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 S-adenosylmethionine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2985	1889	502	577	17			
1	B	386	Total	C	N	O	S	0	1	0
			2990	1893	503	577	17			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	LYS	-	expression tag	UNP Q5HU08
A	400	GLY	-	expression tag	UNP Q5HU08
A	401	GLU	-	expression tag	UNP Q5HU08
A	402	LEU	-	expression tag	UNP Q5HU08
A	403	ASN	-	expression tag	UNP Q5HU08
A	404	SER	-	expression tag	UNP Q5HU08
A	405	LYS	-	expression tag	UNP Q5HU08
A	406	LEU	-	expression tag	UNP Q5HU08
A	407	GLU	-	expression tag	UNP Q5HU08
A	408	GLY	-	expression tag	UNP Q5HU08
A	409	LYS	-	expression tag	UNP Q5HU08
A	410	PRO	-	expression tag	UNP Q5HU08
A	411	ILE	-	expression tag	UNP Q5HU08
A	412	PRO	-	expression tag	UNP Q5HU08
A	413	ASN	-	expression tag	UNP Q5HU08
A	414	PRO	-	expression tag	UNP Q5HU08
A	415	LEU	-	expression tag	UNP Q5HU08
A	416	LEU	-	expression tag	UNP Q5HU08
A	417	GLY	-	expression tag	UNP Q5HU08
A	418	LEU	-	expression tag	UNP Q5HU08
A	419	ASP	-	expression tag	UNP Q5HU08
A	420	SER	-	expression tag	UNP Q5HU08
A	421	THR	-	expression tag	UNP Q5HU08
A	422	ARG	-	expression tag	UNP Q5HU08
A	423	THR	-	expression tag	UNP Q5HU08

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	GLY	-	expression tag	UNP Q5HU08
A	425	HIS	-	expression tag	UNP Q5HU08
A	426	HIS	-	expression tag	UNP Q5HU08
A	427	HIS	-	expression tag	UNP Q5HU08
A	428	HIS	-	expression tag	UNP Q5HU08
A	429	HIS	-	expression tag	UNP Q5HU08
A	430	HIS	-	expression tag	UNP Q5HU08
B	399	LYS	-	expression tag	UNP Q5HU08
B	400	GLY	-	expression tag	UNP Q5HU08
B	401	GLU	-	expression tag	UNP Q5HU08
B	402	LEU	-	expression tag	UNP Q5HU08
B	403	ASN	-	expression tag	UNP Q5HU08
B	404	SER	-	expression tag	UNP Q5HU08
B	405	LYS	-	expression tag	UNP Q5HU08
B	406	LEU	-	expression tag	UNP Q5HU08
B	407	GLU	-	expression tag	UNP Q5HU08
B	408	GLY	-	expression tag	UNP Q5HU08
B	409	LYS	-	expression tag	UNP Q5HU08
B	410	PRO	-	expression tag	UNP Q5HU08
B	411	ILE	-	expression tag	UNP Q5HU08
B	412	PRO	-	expression tag	UNP Q5HU08
B	413	ASN	-	expression tag	UNP Q5HU08
B	414	PRO	-	expression tag	UNP Q5HU08
B	415	LEU	-	expression tag	UNP Q5HU08
B	416	LEU	-	expression tag	UNP Q5HU08
B	417	GLY	-	expression tag	UNP Q5HU08
B	418	LEU	-	expression tag	UNP Q5HU08
B	419	ASP	-	expression tag	UNP Q5HU08
B	420	SER	-	expression tag	UNP Q5HU08
B	421	THR	-	expression tag	UNP Q5HU08
B	422	ARG	-	expression tag	UNP Q5HU08
B	423	THR	-	expression tag	UNP Q5HU08
B	424	GLY	-	expression tag	UNP Q5HU08
B	425	HIS	-	expression tag	UNP Q5HU08
B	426	HIS	-	expression tag	UNP Q5HU08
B	427	HIS	-	expression tag	UNP Q5HU08
B	428	HIS	-	expression tag	UNP Q5HU08
B	429	HIS	-	expression tag	UNP Q5HU08
B	430	HIS	-	expression tag	UNP Q5HU08

- Molecule 2 is water.

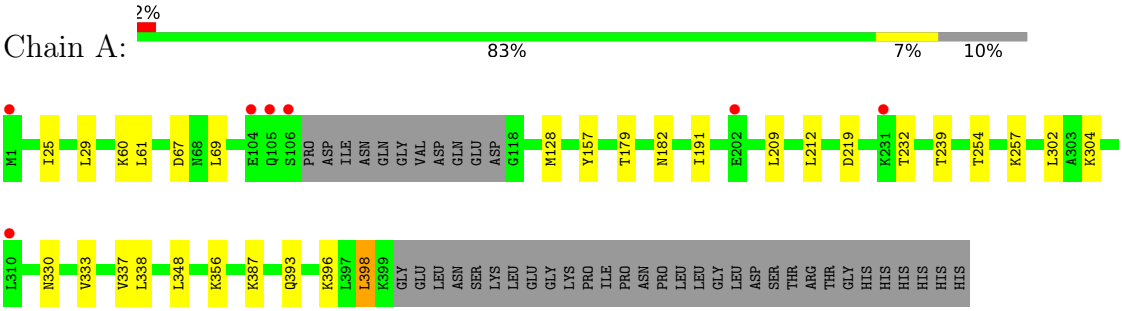
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	95	Total O 95 95	0	0
2	B	96	Total O 96 96	0	0

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.

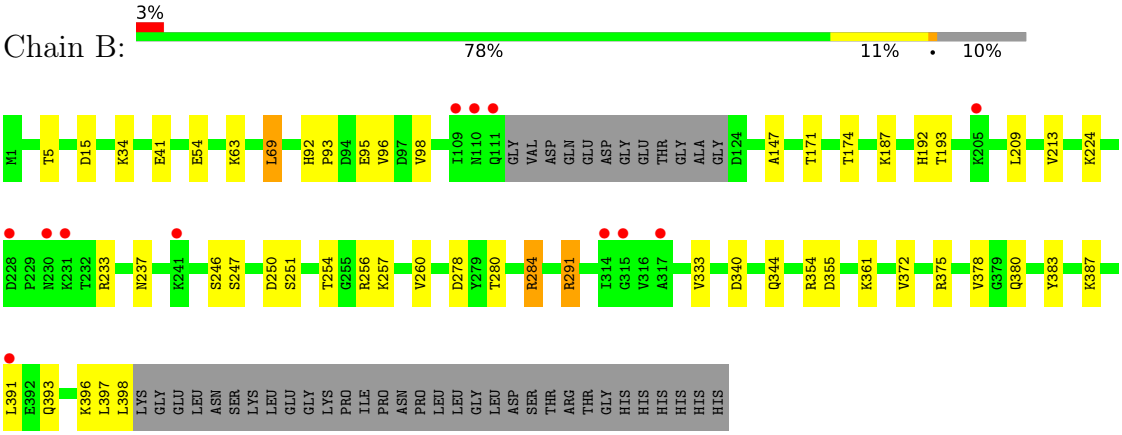
• Molecule 1: S-adenosylmethionine synthetase

Chain A:



• Molecule 1: S-adenosylmethionine synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.66Å 113.08Å 62.18Å 90.00° 116.49° 90.00°	Depositor
Resolution (Å)	29.94 – 1.70 29.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	80.3 (29.94-1.70) 80.3 (29.92-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.263 0.226 , 0.266	Depositor DCC
R_{free} test set	3345 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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

5.1 Standard geometry

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	0.42	0/3041	0.62	0/4111
1	B	0.41	0/3050	0.66	3/4125 (0.1%)
All	All	0.42	0/6091	0.64	3/8236 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	LEU	CA-CB-CG	6.76	130.85	115.30
1	B	291	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	284	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

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	A	2985	0	2968	21	0
1	B	2990	0	2974	26	0
2	A	95	0	0	4	0
2	B	96	0	0	0	0
All	All	6166	0	5942	47	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 (47) 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:67:ASP:HB2	2:A:547:HOH:O	1.83	0.79
1:A:333:VAL:CG2	1:A:337:VAL:HB	2.12	0.79
1:B:192:HIS:CD2	1:B:193:THR:HG23	2.18	0.79
1:B:192:HIS:HD2	1:B:193:THR:HG23	1.51	0.76
2:A:560:HOH:O	1:B:193:THR:HG21	1.88	0.74
1:B:93:PRO:O	1:B:96:VAL:HG22	1.89	0.72
1:B:5:THR:OG1	1:B:174:THR:HG22	1.90	0.71
1:A:356:LYS:NZ	2:A:567:HOH:O	2.26	0.67
1:A:191:ILE:O	1:A:232:THR:HG22	1.95	0.66
1:B:278:ASP:OD1	1:B:280:THR:HG22	1.97	0.64
1:B:147:ALA:O	1:B:171:THR:HG21	1.97	0.63
1:B:257:LYS:HB3	1:B:260:VAL:HG22	1.82	0.62
1:A:179:THR:HG23	1:A:182:ASN:H	1.66	0.60
1:B:63:LYS:NZ	1:B:98:VAL:O	2.40	0.55
1:B:397:LEU:O	1:B:398:LEU:HB2	2.07	0.54
1:A:333:VAL:HG22	1:A:337:VAL:HB	1.89	0.54
1:A:209:LEU:C	1:A:209:LEU:HD23	2.29	0.53
1:A:393:GLN:HA	1:A:396:LYS:HE2	1.92	0.52
1:B:41:GLU:HA	1:B:254:THR:HG21	1.92	0.52
1:B:361:LYS:HG3	1:B:361:LYS:O	2.10	0.52
1:B:361:LYS:O	1:B:361:LYS:CG	2.58	0.52
1:A:333:VAL:CG2	1:A:337:VAL:CB	2.88	0.51
1:A:157:TYR:CZ	1:A:212:LEU:HD11	2.46	0.50
1:B:209:LEU:HD21	1:B:237:ASN:ND2	2.25	0.50
1:B:193:THR:HG22	1:B:233:ARG:HB3	1.94	0.50
1:A:25:ILE:HD13	1:A:69:LEU:HD13	1.95	0.48
1:A:333:VAL:HG23	1:A:337:VAL:HB	1.95	0.48
1:A:330:ASN:H	1:A:330:ASN:HD22	1.62	0.48
1:A:333:VAL:HG21	1:A:337:VAL:CG1	2.43	0.47
1:B:256:ARG:O	1:B:257:LYS:HD2	2.14	0.47
1:B:393[A]:GLN:HE22	1:B:396:LYS:HD2	1.81	0.46
1:B:354:ARG:HD2	1:B:355:ASP:OD1	2.16	0.46
1:A:330:ASN:H	1:A:330:ASN:ND2	2.14	0.45
1:B:247:SER:HA	1:B:250:ASP:O	2.16	0.45
1:A:333:VAL:CG2	1:A:337:VAL:CG1	2.95	0.45
1:A:219:ASP:HB2	2:A:516:HOH:O	2.16	0.45
1:A:25:ILE:HD13	1:A:69:LEU:CD1	2.47	0.44
1:B:375:ARG:HH21	1:B:380:GLN:HE21	1.66	0.44
1:A:25:ILE:HD11	1:A:69:LEU:HD22	1.99	0.43
1:B:372:VAL:HG12	1:B:383:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASP:O	1:B:344:GLN:HG2	2.19	0.42
1:B:34:LYS:HD2	1:B:34:LYS:HA	1.84	0.42
1:B:15:ASP:HB2	1:B:257:LYS:HD3	2.02	0.42
1:A:302:LEU:HD23	1:A:398:LEU:HD13	2.01	0.42
1:A:29:LEU:HD11	1:A:61:LEU:HD22	2.03	0.41
1:B:291:ARG:NE	1:B:378:VAL:HG13	2.36	0.41
1:B:92:HIS:O	1:B:95:GLU:HG2	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	384/430 (89%)	373 (97%)	11 (3%)	0	100 100
1	B	383/430 (89%)	374 (98%)	8 (2%)	1 (0%)	41 24
All	All	767/860 (89%)	747 (97%)	19 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	246	SER

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	328/366 (90%)	318 (97%)	10 (3%)	41 22
1	B	331/366 (90%)	321 (97%)	10 (3%)	41 22
All	All	659/732 (90%)	639 (97%)	20 (3%)	41 22

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	128	MET
1	A	239	THR
1	A	254	THR
1	A	257	LYS
1	A	304	LYS
1	A	338	LEU
1	A	348	LEU
1	A	387	LYS
1	A	398	LEU
1	B	54	GLU
1	B	69	LEU
1	B	187	LYS
1	B	213	VAL
1	B	224	LYS
1	B	251	SER
1	B	284	ARG
1	B	333	VAL
1	B	387	LYS
1	B	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	89	GLN
1	A	172	GLN
1	A	330	ASN
1	B	58	ASN
1	B	125	GLN
1	B	192	HIS
1	B	330	ASN
1	B	351	ASN
1	B	380	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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>2			OWAB(Å^2)	Q<0.9
1	A	388/430 (90%)	0.00	7 (1%)	68	72	26, 37, 54, 88	0
1	B	386/430 (89%)	0.05	12 (3%)	49	53	27, 39, 55, 78	0
All	All	774/860 (90%)	0.02	19 (2%)	57	61	26, 37, 55, 88	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	GLY	4.8
1	B	110	ASN	4.1
1	B	109	ILE	3.6
1	A	202	GLU	3.3
1	A	105	GLN	3.1
1	B	111	GLN	2.9
1	A	1	MET	2.8
1	A	310	LEU	2.7
1	B	231	LYS	2.7
1	A	104	GLU	2.7
1	B	241	LYS	2.5
1	A	106	SER	2.5
1	B	228	ASP	2.4
1	B	205	LYS	2.3
1	B	230	ASN	2.2
1	B	317	ALA	2.2
1	B	314	ILE	2.1
1	B	391	LEU	2.0
1	A	231	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.