



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:54 AM UTC

PDB ID : 2R9G / pdb_00002r9g
Title : Crystal structure of the C-terminal fragment of AAA ATPase from *Enterococcus faecium*
Authors : Ramagopal, U.A.; Patskovsky, Y.; Bonanno, J.B.; Shi, W.; Toro, R.; Meyer, A.J.; Rutter, M.; Wu, B.; Groshong, C.; Gheyi, T.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-09-12
Resolution : 2.09 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 types of validation reports are described at

<https://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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

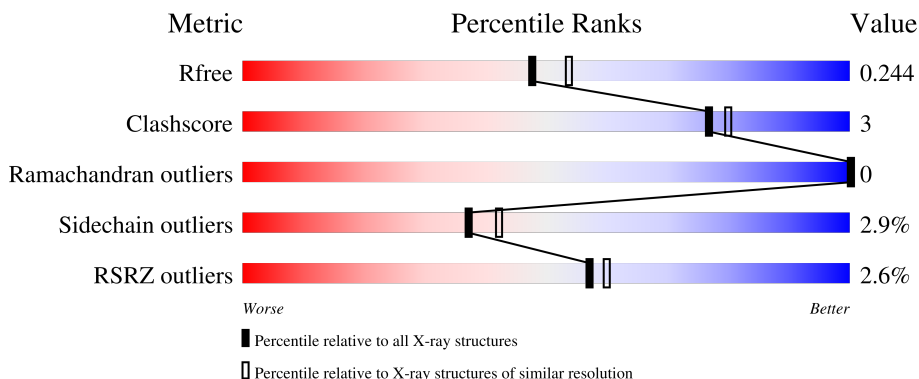
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	204	
1	B	204	
1	C	204	
1	D	204	

Continued on next page...

Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	204	
1	F	204	
1	G	204	
1	H	204	
1	I	204	
1	J	204	
1	K	204	
1	L	204	
1	M	204	
1	N	204	
1	O	204	
1	P	204	

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
2	ACT	F	703	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24661 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 AAA ATPase, central region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	3	0
			1433	908	253	267	5			
1	B	180	Total	C	N	O	S	0	9	0
			1472	930	263	274	5			
1	C	183	Total	C	N	O	S	0	6	0
			1469	930	260	274	5			
1	D	180	Total	C	N	O	S	0	8	0
			1466	925	263	274	4			
1	E	179	Total	C	N	O	S	0	9	0
			1463	926	262	270	5			
1	F	180	Total	C	N	O	S	0	5	0
			1441	913	255	269	4			
1	G	179	Total	C	N	O	S	0	9	0
			1465	930	259	271	5			
1	H	179	Total	C	N	O	S	0	4	0
			1433	905	255	269	4			
1	I	178	Total	C	N	O	S	0	4	0
			1430	908	252	266	4			
1	J	181	Total	C	N	O	S	0	3	0
			1438	909	255	270	4			
1	K	180	Total	C	N	O	S	0	4	0
			1440	911	255	269	5			
1	L	188	Total	C	N	O	S	0	5	0
			1503	951	268	280	4			
1	M	179	Total	C	N	O	S	0	6	0
			1443	915	254	270	4			
1	N	180	Total	C	N	O	S	0	2	0
			1429	904	254	267	4			
1	O	180	Total	C	N	O	S	0	4	0
			1437	910	256	267	4			
1	P	187	Total	C	N	O	S	0	3	0
			1489	940	266	279	4			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	expression tag	UNP Q3XY27
A	228	SER	-	expression tag	UNP Q3XY27
A	229	LEU	-	expression tag	UNP Q3XY27
A	423	GLU	-	expression tag	UNP Q3XY27
A	424	GLY	-	expression tag	UNP Q3XY27
A	425	HIS	-	expression tag	UNP Q3XY27
A	426	HIS	-	expression tag	UNP Q3XY27
A	427	HIS	-	expression tag	UNP Q3XY27
A	428	HIS	-	expression tag	UNP Q3XY27
A	429	HIS	-	expression tag	UNP Q3XY27
A	430	HIS	-	expression tag	UNP Q3XY27
B	227	MET	-	expression tag	UNP Q3XY27
B	228	SER	-	expression tag	UNP Q3XY27
B	229	LEU	-	expression tag	UNP Q3XY27
B	423	GLU	-	expression tag	UNP Q3XY27
B	424	GLY	-	expression tag	UNP Q3XY27
B	425	HIS	-	expression tag	UNP Q3XY27
B	426	HIS	-	expression tag	UNP Q3XY27
B	427	HIS	-	expression tag	UNP Q3XY27
B	428	HIS	-	expression tag	UNP Q3XY27
B	429	HIS	-	expression tag	UNP Q3XY27
B	430	HIS	-	expression tag	UNP Q3XY27
C	227	MET	-	expression tag	UNP Q3XY27
C	228	SER	-	expression tag	UNP Q3XY27
C	229	LEU	-	expression tag	UNP Q3XY27
C	423	GLU	-	expression tag	UNP Q3XY27
C	424	GLY	-	expression tag	UNP Q3XY27
C	425	HIS	-	expression tag	UNP Q3XY27
C	426	HIS	-	expression tag	UNP Q3XY27
C	427	HIS	-	expression tag	UNP Q3XY27
C	428	HIS	-	expression tag	UNP Q3XY27
C	429	HIS	-	expression tag	UNP Q3XY27
C	430	HIS	-	expression tag	UNP Q3XY27
D	227	MET	-	expression tag	UNP Q3XY27
D	228	SER	-	expression tag	UNP Q3XY27
D	229	LEU	-	expression tag	UNP Q3XY27
D	423	GLU	-	expression tag	UNP Q3XY27
D	424	GLY	-	expression tag	UNP Q3XY27
D	425	HIS	-	expression tag	UNP Q3XY27
D	426	HIS	-	expression tag	UNP Q3XY27
D	427	HIS	-	expression tag	UNP Q3XY27
D	428	HIS	-	expression tag	UNP Q3XY27

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	429	HIS	-	expression tag	UNP Q3XY27
D	430	HIS	-	expression tag	UNP Q3XY27
E	227	MET	-	expression tag	UNP Q3XY27
E	228	SER	-	expression tag	UNP Q3XY27
E	229	LEU	-	expression tag	UNP Q3XY27
E	423	GLU	-	expression tag	UNP Q3XY27
E	424	GLY	-	expression tag	UNP Q3XY27
E	425	HIS	-	expression tag	UNP Q3XY27
E	426	HIS	-	expression tag	UNP Q3XY27
E	427	HIS	-	expression tag	UNP Q3XY27
E	428	HIS	-	expression tag	UNP Q3XY27
E	429	HIS	-	expression tag	UNP Q3XY27
E	430	HIS	-	expression tag	UNP Q3XY27
F	227	MET	-	expression tag	UNP Q3XY27
F	228	SER	-	expression tag	UNP Q3XY27
F	229	LEU	-	expression tag	UNP Q3XY27
F	423	GLU	-	expression tag	UNP Q3XY27
F	424	GLY	-	expression tag	UNP Q3XY27
F	425	HIS	-	expression tag	UNP Q3XY27
F	426	HIS	-	expression tag	UNP Q3XY27
F	427	HIS	-	expression tag	UNP Q3XY27
F	428	HIS	-	expression tag	UNP Q3XY27
F	429	HIS	-	expression tag	UNP Q3XY27
F	430	HIS	-	expression tag	UNP Q3XY27
G	227	MET	-	expression tag	UNP Q3XY27
G	228	SER	-	expression tag	UNP Q3XY27
G	229	LEU	-	expression tag	UNP Q3XY27
G	423	GLU	-	expression tag	UNP Q3XY27
G	424	GLY	-	expression tag	UNP Q3XY27
G	425	HIS	-	expression tag	UNP Q3XY27
G	426	HIS	-	expression tag	UNP Q3XY27
G	427	HIS	-	expression tag	UNP Q3XY27
G	428	HIS	-	expression tag	UNP Q3XY27
G	429	HIS	-	expression tag	UNP Q3XY27
G	430	HIS	-	expression tag	UNP Q3XY27
H	227	MET	-	expression tag	UNP Q3XY27
H	228	SER	-	expression tag	UNP Q3XY27
H	229	LEU	-	expression tag	UNP Q3XY27
H	423	GLU	-	expression tag	UNP Q3XY27
H	424	GLY	-	expression tag	UNP Q3XY27
H	425	HIS	-	expression tag	UNP Q3XY27
H	426	HIS	-	expression tag	UNP Q3XY27

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	427	HIS	-	expression tag	UNP Q3XY27
H	428	HIS	-	expression tag	UNP Q3XY27
H	429	HIS	-	expression tag	UNP Q3XY27
H	430	HIS	-	expression tag	UNP Q3XY27
I	227	MET	-	expression tag	UNP Q3XY27
I	228	SER	-	expression tag	UNP Q3XY27
I	229	LEU	-	expression tag	UNP Q3XY27
I	423	GLU	-	expression tag	UNP Q3XY27
I	424	GLY	-	expression tag	UNP Q3XY27
I	425	HIS	-	expression tag	UNP Q3XY27
I	426	HIS	-	expression tag	UNP Q3XY27
I	427	HIS	-	expression tag	UNP Q3XY27
I	428	HIS	-	expression tag	UNP Q3XY27
I	429	HIS	-	expression tag	UNP Q3XY27
I	430	HIS	-	expression tag	UNP Q3XY27
J	227	MET	-	expression tag	UNP Q3XY27
J	228	SER	-	expression tag	UNP Q3XY27
J	229	LEU	-	expression tag	UNP Q3XY27
J	423	GLU	-	expression tag	UNP Q3XY27
J	424	GLY	-	expression tag	UNP Q3XY27
J	425	HIS	-	expression tag	UNP Q3XY27
J	426	HIS	-	expression tag	UNP Q3XY27
J	427	HIS	-	expression tag	UNP Q3XY27
J	428	HIS	-	expression tag	UNP Q3XY27
J	429	HIS	-	expression tag	UNP Q3XY27
J	430	HIS	-	expression tag	UNP Q3XY27
K	227	MET	-	expression tag	UNP Q3XY27
K	228	SER	-	expression tag	UNP Q3XY27
K	229	LEU	-	expression tag	UNP Q3XY27
K	423	GLU	-	expression tag	UNP Q3XY27
K	424	GLY	-	expression tag	UNP Q3XY27
K	425	HIS	-	expression tag	UNP Q3XY27
K	426	HIS	-	expression tag	UNP Q3XY27
K	427	HIS	-	expression tag	UNP Q3XY27
K	428	HIS	-	expression tag	UNP Q3XY27
K	429	HIS	-	expression tag	UNP Q3XY27
K	430	HIS	-	expression tag	UNP Q3XY27
L	227	MET	-	expression tag	UNP Q3XY27
L	228	SER	-	expression tag	UNP Q3XY27
L	229	LEU	-	expression tag	UNP Q3XY27
L	423	GLU	-	expression tag	UNP Q3XY27
L	424	GLY	-	expression tag	UNP Q3XY27

Continued on next page...

Continued from previous page...

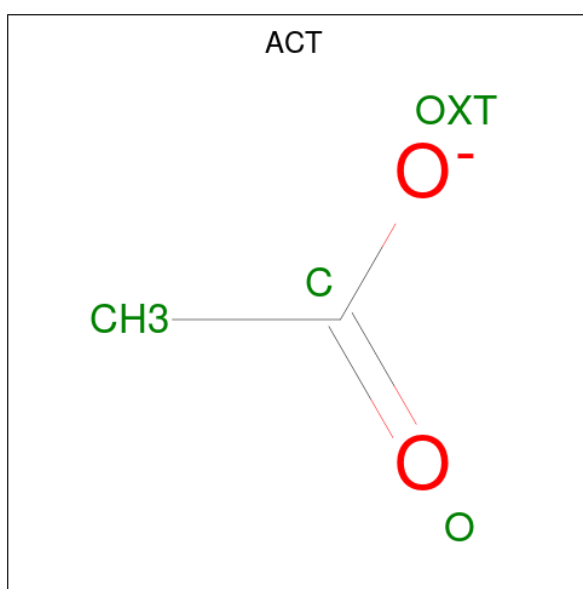
Chain	Residue	Modelled	Actual	Comment	Reference
L	425	HIS	-	expression tag	UNP Q3XY27
L	426	HIS	-	expression tag	UNP Q3XY27
L	427	HIS	-	expression tag	UNP Q3XY27
L	428	HIS	-	expression tag	UNP Q3XY27
L	429	HIS	-	expression tag	UNP Q3XY27
L	430	HIS	-	expression tag	UNP Q3XY27
M	227	MET	-	expression tag	UNP Q3XY27
M	228	SER	-	expression tag	UNP Q3XY27
M	229	LEU	-	expression tag	UNP Q3XY27
M	423	GLU	-	expression tag	UNP Q3XY27
M	424	GLY	-	expression tag	UNP Q3XY27
M	425	HIS	-	expression tag	UNP Q3XY27
M	426	HIS	-	expression tag	UNP Q3XY27
M	427	HIS	-	expression tag	UNP Q3XY27
M	428	HIS	-	expression tag	UNP Q3XY27
M	429	HIS	-	expression tag	UNP Q3XY27
M	430	HIS	-	expression tag	UNP Q3XY27
N	227	MET	-	expression tag	UNP Q3XY27
N	228	SER	-	expression tag	UNP Q3XY27
N	229	LEU	-	expression tag	UNP Q3XY27
N	423	GLU	-	expression tag	UNP Q3XY27
N	424	GLY	-	expression tag	UNP Q3XY27
N	425	HIS	-	expression tag	UNP Q3XY27
N	426	HIS	-	expression tag	UNP Q3XY27
N	427	HIS	-	expression tag	UNP Q3XY27
N	428	HIS	-	expression tag	UNP Q3XY27
N	429	HIS	-	expression tag	UNP Q3XY27
N	430	HIS	-	expression tag	UNP Q3XY27
O	227	MET	-	expression tag	UNP Q3XY27
O	228	SER	-	expression tag	UNP Q3XY27
O	229	LEU	-	expression tag	UNP Q3XY27
O	423	GLU	-	expression tag	UNP Q3XY27
O	424	GLY	-	expression tag	UNP Q3XY27
O	425	HIS	-	expression tag	UNP Q3XY27
O	426	HIS	-	expression tag	UNP Q3XY27
O	427	HIS	-	expression tag	UNP Q3XY27
O	428	HIS	-	expression tag	UNP Q3XY27
O	429	HIS	-	expression tag	UNP Q3XY27
O	430	HIS	-	expression tag	UNP Q3XY27
P	227	MET	-	expression tag	UNP Q3XY27
P	228	SER	-	expression tag	UNP Q3XY27
P	229	LEU	-	expression tag	UNP Q3XY27

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	423	GLU	-	expression tag	UNP Q3XY27
P	424	GLY	-	expression tag	UNP Q3XY27
P	425	HIS	-	expression tag	UNP Q3XY27
P	426	HIS	-	expression tag	UNP Q3XY27
P	427	HIS	-	expression tag	UNP Q3XY27
P	428	HIS	-	expression tag	UNP Q3XY27
P	429	HIS	-	expression tag	UNP Q3XY27
P	430	HIS	-	expression tag	UNP Q3XY27

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



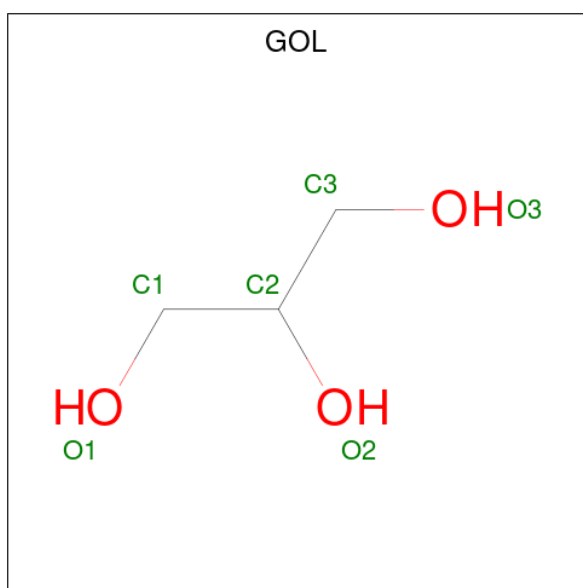
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	O	1	Total	C	O	0	0
			4	2	2		
2	O	1	Total	C	O	0	0
			4	2	2		
2	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

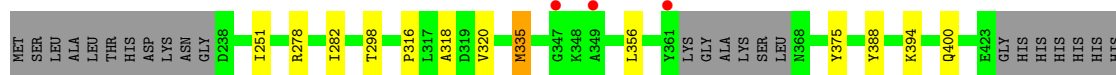
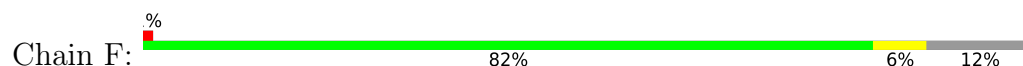
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total 90	O 90	0	0
4	B	99	Total 99	O 99	0	0
4	C	82	Total 82	O 82	0	0
4	D	83	Total 83	O 83	0	0
4	E	103	Total 103	O 103	0	0
4	F	89	Total 89	O 89	0	0
4	G	85	Total 85	O 85	0	0
4	H	79	Total 79	O 79	0	0
4	I	76	Total 76	O 76	0	0
4	J	78	Total 78	O 78	0	0
4	K	94	Total 94	O 94	0	0
4	L	80	Total 80	O 80	0	0
4	M	66	Total 66	O 66	0	0
4	N	69	Total 69	O 69	0	0
4	O	85	Total 85	O 85	0	0
4	P	80	Total 80	O 80	0	0

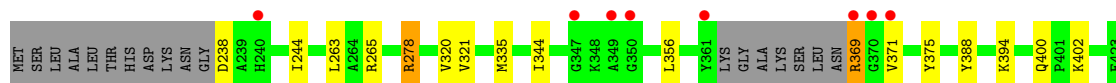
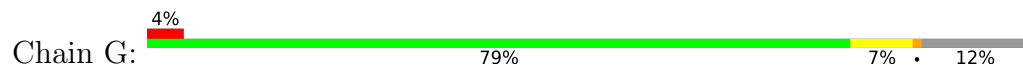
- Molecule 1: AAA ATPase, central region



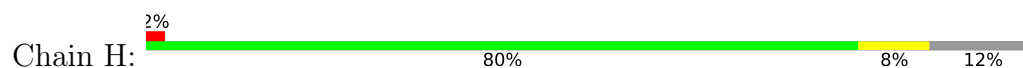
- Molecule 1: AAA ATPase, central region



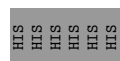
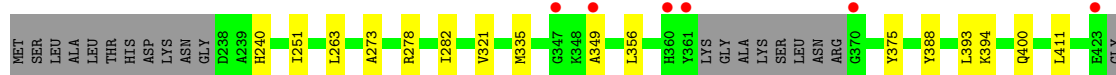
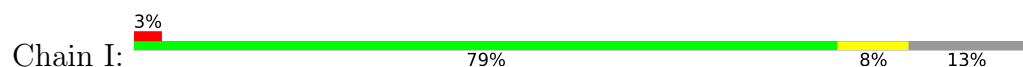
- Molecule 1: AAA ATPase, central region



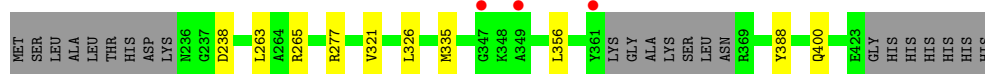
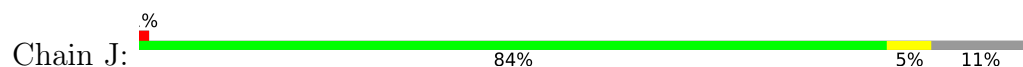
- Molecule 1: AAA ATPase, central region



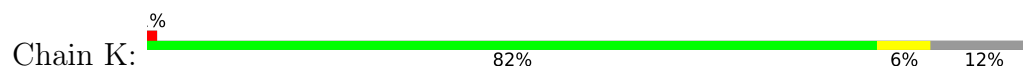
- Molecule 1: AAA ATPase, central region

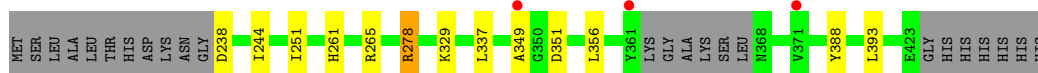


- Molecule 1: AAA ATPase, central region

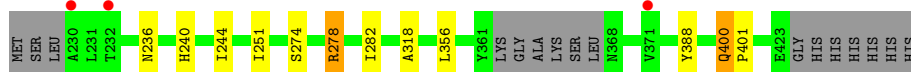
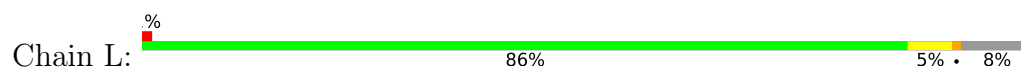


- Molecule 1: AAA ATPase, central region

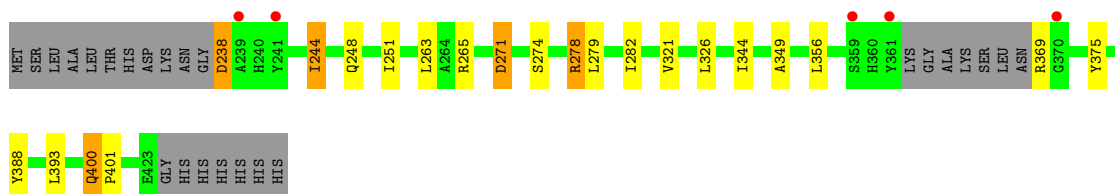
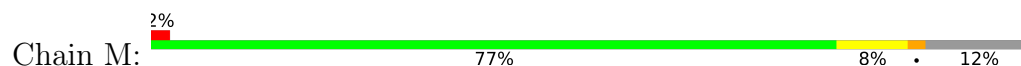




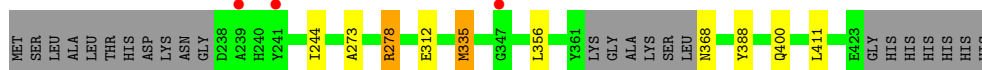
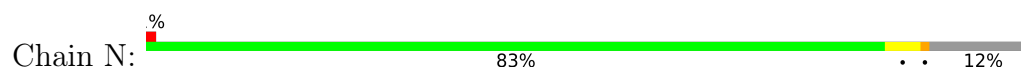
- Molecule 1: AAA ATPase, central region



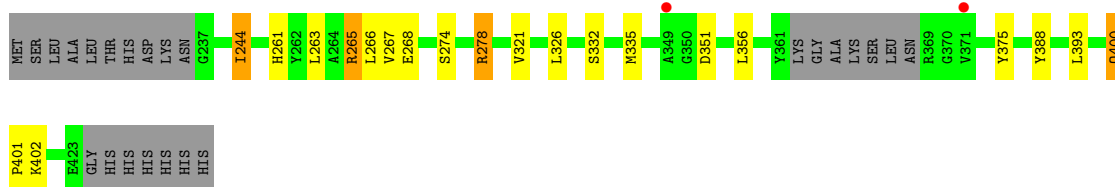
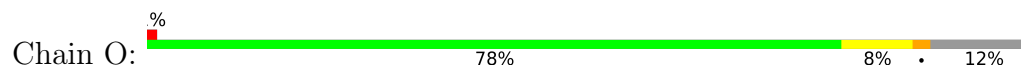
- Molecule 1: AAA ATPase, central region



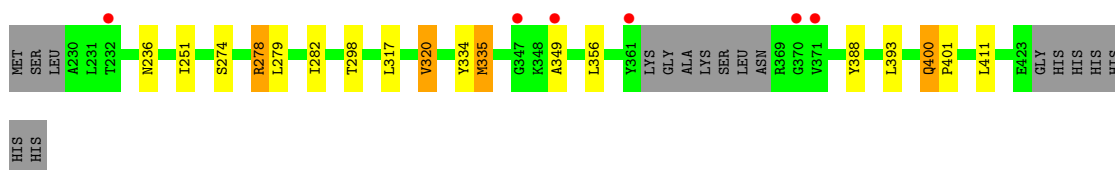
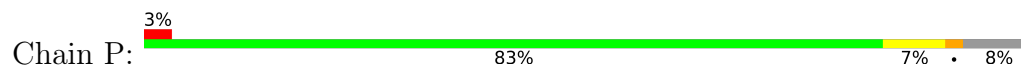
- Molecule 1: AAA ATPase, central region



- Molecule 1: AAA ATPase, central region



- Molecule 1: AAA ATPase, central region



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.78Å 103.39Å 103.37Å 90.01° 88.69° 86.05°	Depositor
Resolution (Å)	20.00 – 2.09 20.00 – 2.09	Depositor EDS
% Data completeness (in resolution range)	87.1 (20.00-2.09) 87.0 (20.00-2.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.197 , 0.248 0.198 , 0.244	Depositor DCC
R_{free} test set	5308 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24661	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 46.70 % 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 1.1029e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACT, GOL

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	0.51	0/1473	0.92	0/1996
1	B	0.52	0/1515	0.91	0/2051
1	C	0.51	0/1518	0.91	0/2053
1	D	0.50	0/1506	0.94	2/2039 (0.1%)
1	E	0.50	0/1509	0.92	0/2041
1	F	0.52	0/1488	0.92	2/2018 (0.1%)
1	G	0.52	0/1512	0.92	2/2047 (0.1%)
1	H	0.59	1/1464 (0.1%)	0.96	0/1984
1	I	0.50	0/1471	0.92	2/1993 (0.1%)
1	J	0.51	0/1478	0.91	0/2002
1	K	0.54	0/1480	0.94	0/2004
1	L	0.51	0/1551	0.91	0/2101
1	M	0.51	0/1493	0.91	2/2023 (0.1%)
1	N	0.52	0/1466	0.92	0/1986
1	O	0.67	5/1480 (0.3%)	0.96	2/2004 (0.1%)
1	P	0.53	0/1533	0.92	0/2077
All	All	0.53	6/23937 (0.0%)	0.92	12/32419 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	268	GLU	C-O	-6.19	1.16	1.24
1	O	266	LEU	C-O	-5.59	1.17	1.24
1	O	265[A]	ARG	C-O	-5.09	1.18	1.24
1	O	265[B]	ARG	C-O	-5.09	1.18	1.24
1	H	308	LEU	C-O	-5.05	1.17	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	TYR	CA-C-N	6.49	126.72	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	TYR	C-N-CA	6.49	126.72	119.32
1	G	375	TYR	CA-C-N	6.02	125.70	119.56
1	G	375	TYR	C-N-CA	6.02	125.70	119.56
1	F	375	TYR	CA-C-N	5.51	125.86	119.47

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	1433	0	1409	8	0
1	B	1472	0	1450	5	0
1	C	1469	0	1449	6	0
1	D	1466	0	1439	9	0
1	E	1463	0	1449	6	0
1	F	1441	0	1417	8	0
1	G	1465	0	1447	14	0
1	H	1433	0	1396	9	0
1	I	1430	0	1404	6	0
1	J	1438	0	1409	5	0
1	K	1440	0	1415	8	0
1	L	1503	0	1481	22	0
1	M	1443	0	1419	13	0
1	N	1429	0	1402	5	0
1	O	1437	0	1419	10	0
1	P	1489	0	1464	11	0
2	B	4	0	3	1	0
2	C	8	0	6	0	0
2	E	8	0	6	0	0
2	F	4	0	3	2	0
2	K	4	0	3	0	0
2	L	8	0	6	1	0
2	O	8	0	6	0	0
2	P	4	0	3	1	0
3	E	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	6	0	8	0	0
3	J	6	0	8	1	0
3	P	6	0	8	0	0
4	A	90	0	0	0	0
4	B	99	0	0	0	0
4	C	82	0	0	1	0
4	D	83	0	0	0	0
4	E	103	0	0	0	0
4	F	89	0	0	0	0
4	G	85	0	0	1	0
4	H	79	0	0	0	0
4	I	76	0	0	0	0
4	J	78	0	0	0	0
4	K	94	0	0	0	0
4	L	80	0	0	0	0
4	M	66	0	0	0	0
4	N	69	0	0	0	0
4	O	85	0	0	1	0
4	P	80	0	0	0	0
All	All	24661	0	22937	133	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 133 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:G:369[B]:ARG:HH11	1:G:369[B]:ARG:HG3	1.05	1.15
1:G:369[B]:ARG:HG3	1:G:369[B]:ARG:NH1	1.75	0.93
1:L:240[B]:HIS:NE2	1:L:244[B]:ILE:HD11	1.85	0.92
1:G:369[B]:ARG:HH11	1:G:369[B]:ARG:CG	1.90	0.85
1:G:371[A]:VAL:HG22	1:G:371[A]:VAL:O	1.79	0.82

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	A	179/204 (88%)	179 (100%)	0	0	100	100
1	B	184/204 (90%)	182 (99%)	2 (1%)	0	100	100
1	C	184/204 (90%)	183 (100%)	1 (0%)	0	100	100
1	D	183/204 (90%)	182 (100%)	1 (0%)	0	100	100
1	E	183/204 (90%)	183 (100%)	0	0	100	100
1	F	181/204 (89%)	181 (100%)	0	0	100	100
1	G	183/204 (90%)	182 (100%)	1 (0%)	0	100	100
1	H	178/204 (87%)	178 (100%)	0	0	100	100
1	I	178/204 (87%)	177 (99%)	1 (1%)	0	100	100
1	J	180/204 (88%)	180 (100%)	0	0	100	100
1	K	180/204 (88%)	178 (99%)	2 (1%)	0	100	100
1	L	189/204 (93%)	189 (100%)	0	0	100	100
1	M	181/204 (89%)	179 (99%)	2 (1%)	0	100	100
1	N	178/204 (87%)	178 (100%)	0	0	100	100
1	O	180/204 (88%)	179 (99%)	1 (1%)	0	100	100
1	P	187/204 (92%)	187 (100%)	0	0	100	100
All	All	2908/3264 (89%)	2897 (100%)	11 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	A	146/162 (90%)	141 (97%)	5 (3%)	32	35
1	B	150/162 (93%)	145 (97%)	5 (3%)	33	37
1	C	151/162 (93%)	144 (95%)	7 (5%)	24	25
1	D	149/162 (92%)	145 (97%)	4 (3%)	39	45
1	E	149/162 (92%)	143 (96%)	6 (4%)	28	29
1	F	148/162 (91%)	145 (98%)	3 (2%)	48	56
1	G	149/162 (92%)	140 (94%)	9 (6%)	17	15
1	H	144/162 (89%)	142 (99%)	2 (1%)	59	67
1	I	145/162 (90%)	139 (96%)	6 (4%)	27	29
1	J	146/162 (90%)	144 (99%)	2 (1%)	59	67
1	K	147/162 (91%)	146 (99%)	1 (1%)	76	83
1	L	154/162 (95%)	149 (97%)	5 (3%)	34	38
1	M	148/162 (91%)	138 (93%)	10 (7%)	14	12
1	N	145/162 (90%)	140 (97%)	5 (3%)	32	35
1	O	146/162 (90%)	140 (96%)	6 (4%)	27	29
1	P	152/162 (94%)	146 (96%)	6 (4%)	28	31
All	All	2369/2592 (91%)	2287 (96%)	82 (4%)	37	35

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	271[A]	ASP
1	O	278[A]	ARG
1	M	278[A]	ARG
1	N	278	ARG
1	O	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	378	HIS
1	P	397	GLN
1	J	400	GLN
1	N	368	ASN
1	D	400	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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	$\# Z > 2$
2	ACT	C	707	-	3,3,3	0.95	0	3,3,3	0.95	0
2	ACT	L	706	-	3,3,3	0.91	0	3,3,3	0.91	0
3	GOL	J	1	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	H	1	-	5,5,5	0.39	0	5,5,5	0.47	0
2	ACT	O	704	-	3,3,3	0.78	0	3,3,3	1.30	0
2	ACT	F	703	-	3,3,3	0.89	0	3,3,3	1.53	0
2	ACT	B	1	-	3,3,3	0.77	0	3,3,3	1.57	0
2	ACT	E	1	-	3,3,3	0.82	0	3,3,3	1.37	0
2	ACT	C	1	-	3,3,3	0.90	0	3,3,3	1.43	0
2	ACT	P	702	-	3,3,3	0.75	0	3,3,3	1.70	2 (66%)
2	ACT	L	1	-	3,3,3	0.81	0	3,3,3	1.56	0
2	ACT	K	1	-	3,3,3	0.84	0	3,3,3	1.37	0
2	ACT	E	705	-	3,3,3	0.84	0	3,3,3	1.21	0
3	GOL	P	1	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	E	706	-	5,5,5	0.36	0	5,5,5	0.66	0
2	ACT	O	701	-	3,3,3	0.81	0	3,3,3	1.45	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
3	GOL	H	1	-	-	4/4/4/4	-
3	GOL	P	1	-	-	1/4/4/4	-
3	GOL	J	1	-	-	2/4/4/4	-
3	GOL	E	706	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	702	ACT	OXT-C-O	-2.11	114.18	122.03
2	P	702	ACT	OXT-C-CH3	2.05	123.66	115.05

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	706	GOL	C1-C2-C3-O3
3	H	1	GOL	C1-C2-C3-O3
3	J	1	GOL	C1-C2-C3-O3
3	H	1	GOL	O1-C1-C2-C3
3	P	1	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	GOL	1	0
2	F	703	ACT	2	0
2	B	1	ACT	1	0
2	P	702	ACT	1	0
2	L	1	ACT	1	0

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, 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	180/204 (88%)	-0.12	1 (0%) 85 87	16, 31, 60, 84	3 (1%)
1	B	180/204 (88%)	-0.11	7 (3%) 43 45	13, 29, 61, 86	9 (5%)
1	C	183/204 (89%)	0.02	7 (3%) 44 46	16, 32, 70, 100	6 (3%)
1	D	180/204 (88%)	0.07	7 (3%) 43 45	17, 33, 64, 97	8 (4%)
1	E	179/204 (87%)	-0.12	5 (2%) 55 57	14, 29, 60, 93	9 (5%)
1	F	180/204 (88%)	-0.12	3 (1%) 69 71	15, 32, 67, 97	5 (2%)
1	G	179/204 (87%)	0.04	8 (4%) 38 40	17, 33, 63, 96	9 (5%)
1	H	179/204 (87%)	-0.12	5 (2%) 55 57	13, 31, 57, 86	4 (2%)
1	I	178/204 (87%)	-0.02	6 (3%) 48 50	18, 34, 64, 97	4 (2%)
1	J	181/204 (88%)	-0.08	3 (1%) 69 71	17, 32, 60, 87	3 (1%)
1	K	180/204 (88%)	-0.18	3 (1%) 69 71	12, 31, 63, 90	4 (2%)
1	L	188/204 (92%)	0.02	3 (1%) 70 73	14, 33, 69, 105	5 (2%)
1	M	179/204 (87%)	0.04	5 (2%) 55 57	15, 34, 68, 99	6 (3%)
1	N	180/204 (88%)	-0.07	3 (1%) 69 71	18, 33, 63, 88	2 (1%)
1	O	180/204 (88%)	-0.14	2 (1%) 78 80	16, 30, 65, 87	4 (2%)
1	P	187/204 (91%)	-0.02	6 (3%) 50 53	11, 32, 64, 99	3 (1%)
All	All	2893/3264 (88%)	-0.05	74 (2%) 57 60	11, 32, 64, 105	84 (2%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	369[A]	ARG	7.0
1	G	370[A]	GLY	7.0
1	E	371[A]	VAL	6.1
1	E	370[A]	GLY	6.0
1	D	371[A]	VAL	5.4

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	706	6/6	0.79	0.16	49,57,62,65	0
2	ACT	P	702	4/4	0.80	0.16	44,50,51,54	0
3	GOL	J	1	6/6	0.81	0.14	63,76,79,79	0
2	ACT	E	1	4/4	0.82	0.14	44,48,48,49	0
3	GOL	H	1	6/6	0.83	0.14	59,65,67,69	0
3	GOL	P	1	6/6	0.84	0.11	46,56,58,62	0
2	ACT	O	701	4/4	0.85	0.16	47,48,50,51	0
2	ACT	C	707	4/4	0.85	0.15	28,31,37,43	0
2	ACT	L	1	4/4	0.85	0.13	47,47,49,53	0
2	ACT	C	1	4/4	0.86	0.14	44,48,50,50	0
2	ACT	E	705	4/4	0.90	0.12	40,42,43,48	0
2	ACT	F	703	4/4	0.92	0.10	40,43,45,48	0
2	ACT	B	1	4/4	0.92	0.09	47,47,47,51	0
2	ACT	L	706	4/4	0.92	0.10	25,31,32,35	0
2	ACT	O	704	4/4	0.94	0.08	33,34,36,40	0
2	ACT	K	1	4/4	0.94	0.11	36,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.