



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2023 – 11:31 AM EDT

PDB ID : 3Q9C
Title : Crystal Structure of H159A APAH complexed with N8-acetylspermidine
Authors : Lombardi, P.M.; Christianson, D.W.
Deposited on : 2011-01-07
Resolution : 2.30 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

<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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

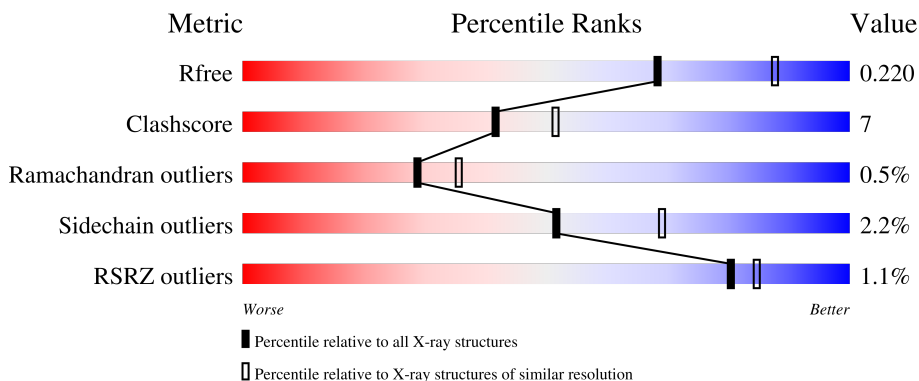
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



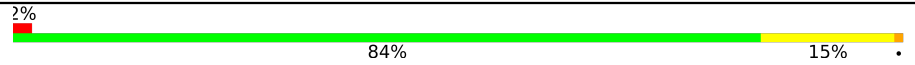
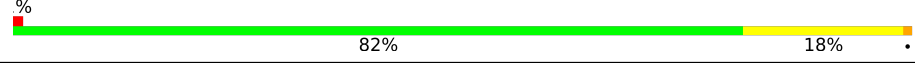
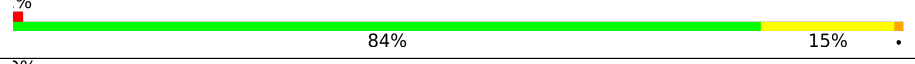

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	341	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 84%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 84% 15% . </div>
1	B	341	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, orange 2%, yellow 16%, green 83%);"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 83% 16% . </div>
1	C	341	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, yellow 13%, green 86%);"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 86% 13% . </div>
1	D	341	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 2%, orange 2%, yellow 17%, green 83%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 83% 17% . </div>
1	E	341	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 2%, orange 2%, yellow 18%, green 82%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 82% 18% . </div>

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Mol	Chain	Length	Quality of chain
1	F	341	 2% 84% 15%
1	G	341	 % 84% 16%
1	H	341	 % 82% 18%
1	I	341	 % 84% 15%
1	J	341	 2% 79% 20%
1	K	341	 % 84% 16%
1	L	341	 3% 82% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32700 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 Acetylpolyamine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2563	1641	433	480	9	0	0	0
1	B	341	2563	1641	433	480	9	0	0	0
1	C	341	2563	1641	433	480	9	0	0	0
1	D	341	2563	1641	433	480	9	0	0	0
1	E	341	2563	1641	433	480	9	0	0	0
1	F	341	2563	1641	433	480	9	0	0	0
1	G	341	2563	1641	433	480	9	0	0	0
1	H	341	2563	1641	433	480	9	0	0	0
1	I	341	2563	1641	433	480	9	0	0	0
1	J	341	2563	1641	433	480	9	0	0	0
1	K	341	2563	1641	433	480	9	0	0	0
1	L	341	2563	1641	433	480	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

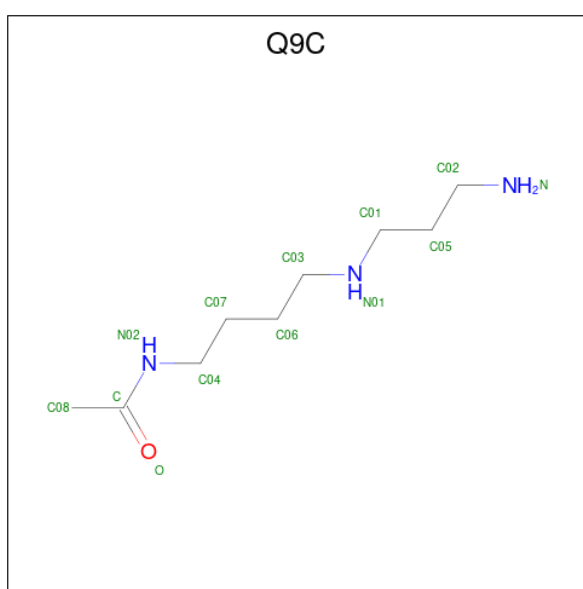
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ALA	HIS	engineered mutation	UNP Q48935
B	159	ALA	HIS	engineered mutation	UNP Q48935
C	159	ALA	HIS	engineered mutation	UNP Q48935
D	159	ALA	HIS	engineered mutation	UNP Q48935
E	159	ALA	HIS	engineered mutation	UNP Q48935

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Chain	Residue	Modelled	Actual	Comment	Reference
F	159	ALA	HIS	engineered mutation	UNP Q48935
G	159	ALA	HIS	engineered mutation	UNP Q48935
H	159	ALA	HIS	engineered mutation	UNP Q48935
I	159	ALA	HIS	engineered mutation	UNP Q48935
J	159	ALA	HIS	engineered mutation	UNP Q48935
K	159	ALA	HIS	engineered mutation	UNP Q48935
L	159	ALA	HIS	engineered mutation	UNP Q48935

- Molecule 2 is N-{4-[(3-aminopropyl)amino]butyl}acetamide (three-letter code: Q9C) (formula: C₉H₂₁N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 13	C 9	N 3	O 1	0	0
2	B	1	Total 13	C 9	N 3	O 1	0	0
2	C	1	Total 13	C 9	N 3	O 1	0	0
2	D	1	Total 13	C 9	N 3	O 1	0	0
2	E	1	Total 13	C 9	N 3	O 1	0	0
2	F	1	Total 13	C 9	N 3	O 1	0	0
2	G	1	Total 13	C 9	N 3	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			13	9	3	1		
2	I	1	Total	C	N	O	0	0
			13	9	3	1		
2	J	1	Total	C	N	O	0	0
			13	9	3	1		
2	K	1	Total	C	N	O	0	0
			13	9	3	1		
2	L	1	Total	C	N	O	0	0
			13	9	3	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	G	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	I	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	L	1	Total	K	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Na 1	0	0
5	J	1	Total 1	Na 1	0	0
5	K	1	Total 1	Na 1	0	0
5	L	1	Total 1	Na 1	0	0

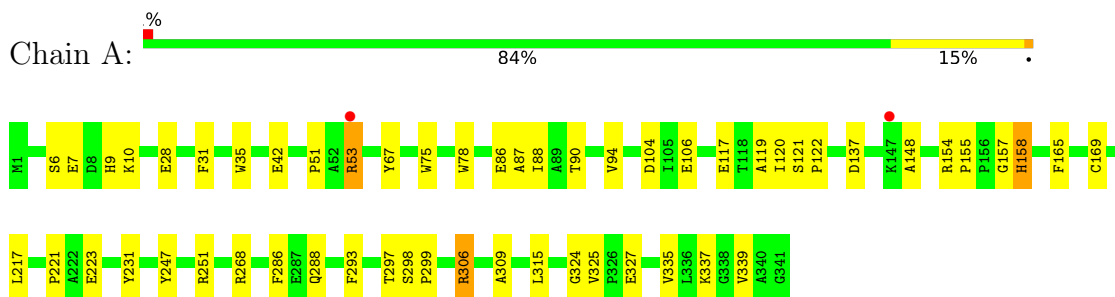
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	149	Total 149	O 149	0	0
6	B	127	Total 127	O 127	0	0
6	C	176	Total 176	O 176	0	0
6	D	149	Total 149	O 149	0	0
6	E	141	Total 141	O 141	0	0
6	F	142	Total 142	O 142	0	0
6	G	149	Total 149	O 149	0	0
6	H	148	Total 148	O 148	0	0
6	I	157	Total 157	O 157	0	0
6	J	109	Total 109	O 109	0	0
6	K	180	Total 180	O 180	0	0
6	L	125	Total 125	O 125	0	0

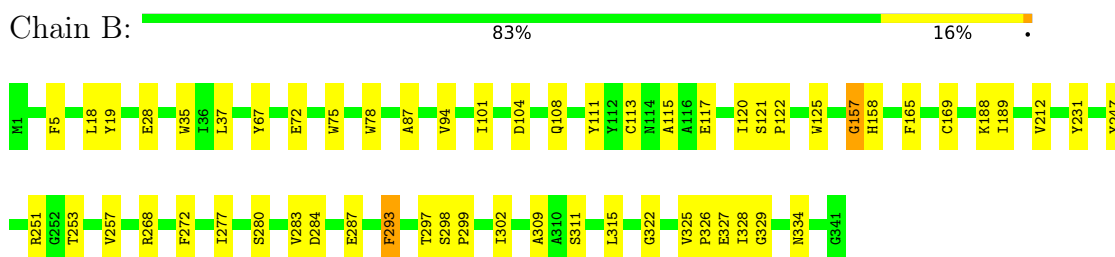
3 Residue-property plots [i](#)

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.

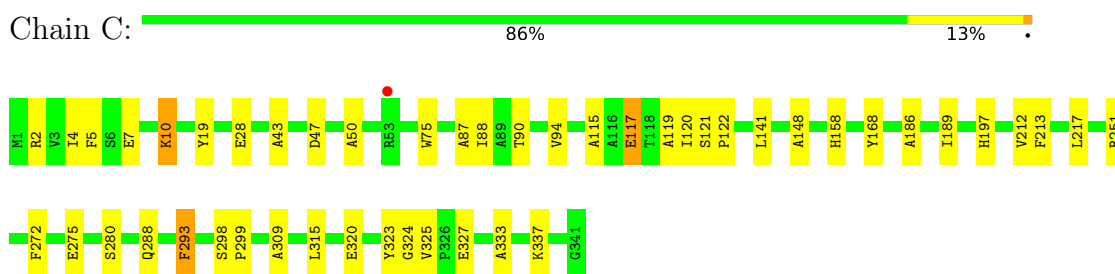
- Molecule 1: Acetylpolyamine amidohydrolase



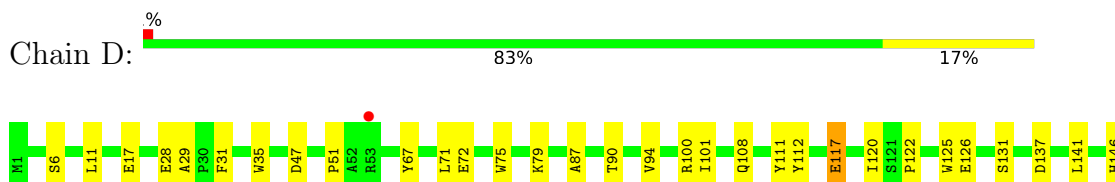
- Molecule 1: Acetylpolyamine amidohydrolase

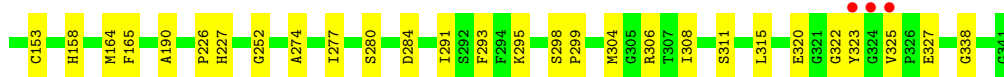


- Molecule 1: Acetylpolyamine amidohydrolase

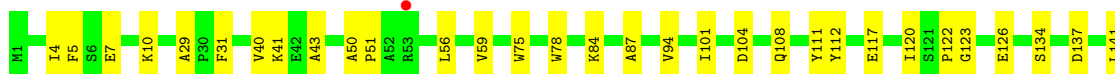
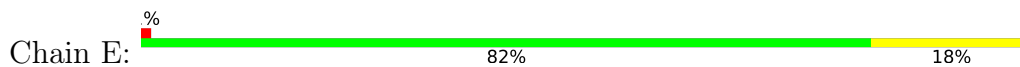


- Molecule 1: Acetylpolyamine amidohydrolase

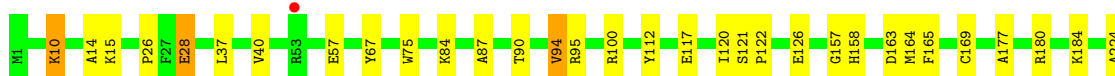
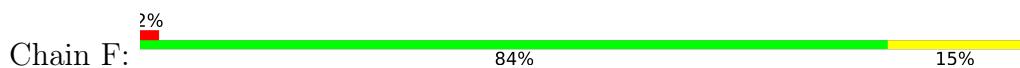




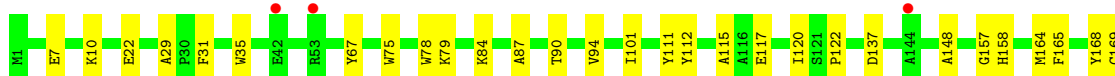
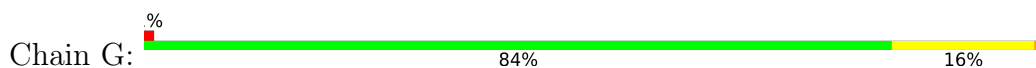
- Molecule 1: Acetylpolyamine amidohydrolase



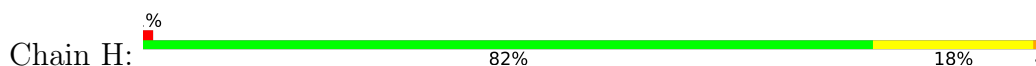
- Molecule 1: Acetylpolyamine amidohydrolase



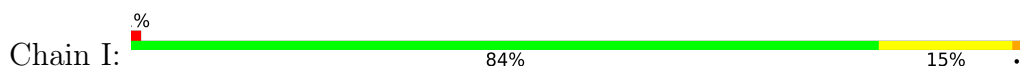
- Molecule 1: Acetylpolyamine amidohydrolase

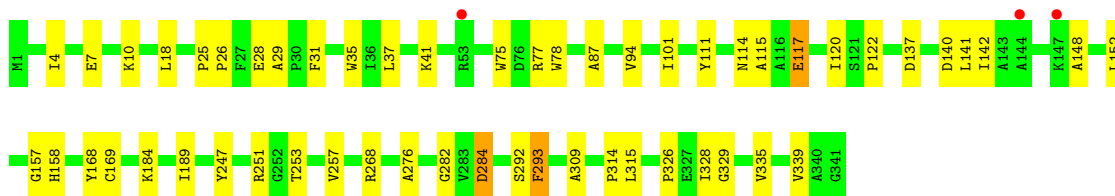


- Molecule 1: Acetylpolyamine amidohydrolase

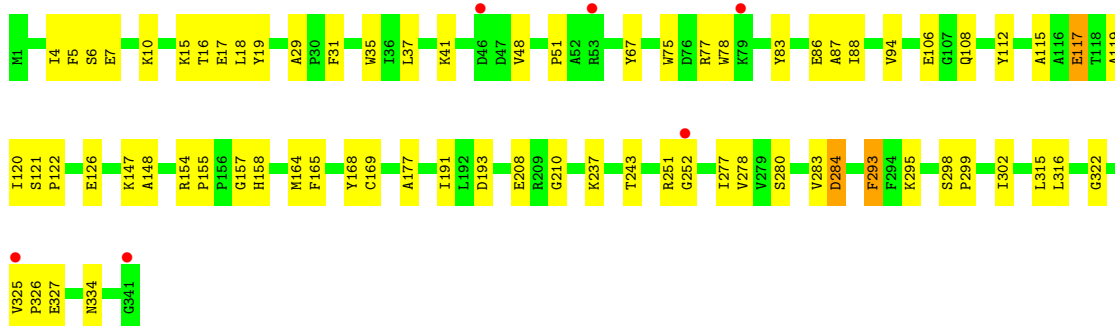
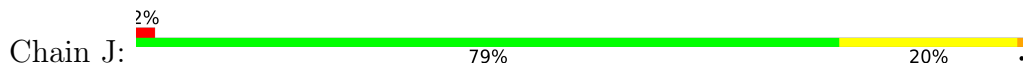


- Molecule 1: Acetylpolyamine amidohydrolase

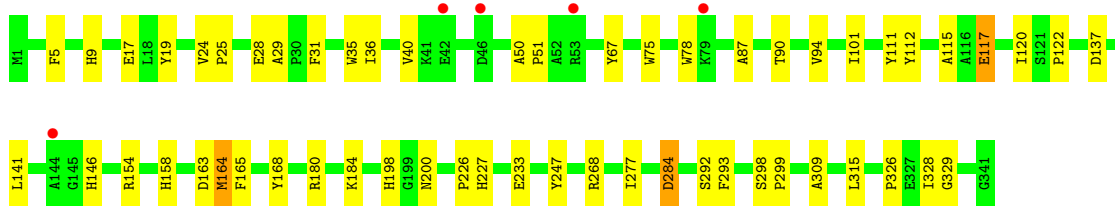
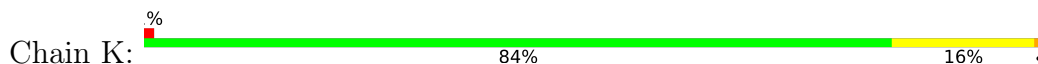




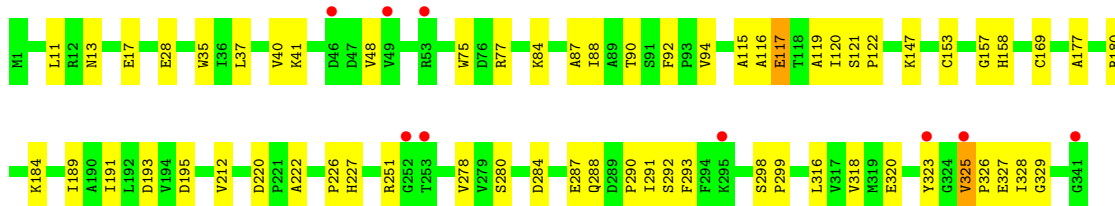
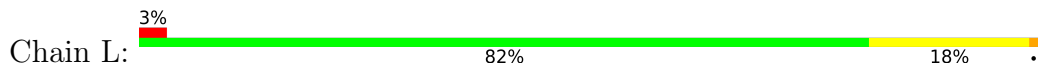
- Molecule 1: Acetylpolyamine amidohydrolase



- Molecule 1: Acetylpolyamine amidohydrolase



- Molecule 1: Acetylpolyamine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.46Å 120.15Å 118.45Å 98.47° 94.41° 115.89°	Depositor
Resolution (Å)	50.00 – 2.30 38.86 – 2.31	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.30) 88.0 (38.86-2.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.31Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.227 0.180 , 0.220	Depositor DCC
R_{free} test set	24038 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtrriage
Anisotropy	0.368	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32700	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZN, NA, K, Q9C

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	0.40	0/2630	0.60	0/3574
1	B	0.37	0/2630	0.57	0/3574
1	C	0.41	0/2630	0.61	0/3574
1	D	0.39	0/2630	0.57	0/3574
1	E	0.37	0/2630	0.58	0/3574
1	F	0.37	0/2630	0.57	0/3574
1	G	0.39	0/2630	0.58	0/3574
1	H	0.39	0/2630	0.59	0/3574
1	I	0.39	0/2630	0.59	1/3574 (0.0%)
1	J	0.36	0/2630	0.56	0/3574
1	K	0.39	0/2630	0.60	0/3574
1	L	0.38	0/2630	0.57	0/3574
All	All	0.38	0/31560	0.58	1/42888 (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	I	282	GLY	N-CA-C	-5.05	100.47	113.10

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	2563	0	2489	39	0
1	B	2563	0	2489	35	0
1	C	2563	0	2489	33	0
1	D	2563	0	2489	39	0
1	E	2563	0	2489	37	0
1	F	2563	0	2489	34	0
1	G	2563	0	2490	35	0
1	H	2563	0	2490	37	0
1	I	2563	0	2489	29	0
1	J	2563	0	2489	52	0
1	K	2563	0	2489	32	0
1	L	2563	0	2489	36	0
2	A	13	0	21	1	0
2	B	13	0	21	2	0
2	C	13	0	21	5	0
2	D	13	0	21	1	0
2	E	13	0	21	0	0
2	F	13	0	21	0	0
2	G	13	0	21	1	0
2	H	13	0	21	1	0
2	I	13	0	21	2	0
2	J	13	0	21	1	0
2	K	13	0	21	0	0
2	L	13	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	149	0	0	3	0
6	B	127	0	0	2	0
6	C	176	0	0	3	0
6	D	149	0	0	3	0
6	E	141	0	0	0	0
6	F	142	0	0	2	0
6	G	149	0	0	1	0
6	H	148	0	0	2	0
6	I	157	0	0	3	0
6	J	109	0	0	1	0
6	K	180	0	0	3	0
6	L	125	0	0	2	0
All	All	32700	0	30122	425	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 7.

The worst 5 of 425 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:D:31:PHE:HD2	1:D:35:TRP:HE1	1.22	0.82
1:D:31:PHE:HD2	1:D:35:TRP:NE1	1.85	0.73
1:A:31:PHE:HD2	1:A:35:TRP:NE1	1.87	0.72
1:D:29:ALA:HB3	1:D:31:PHE:CE1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:GLY:HA2	1:H:169:CYS:HB3	1.73	0.70

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	339/341 (99%)	324 (96%)	13 (4%)	2 (1%)	25	31
1	B	339/341 (99%)	323 (95%)	14 (4%)	2 (1%)	25	31
1	C	339/341 (99%)	324 (96%)	13 (4%)	2 (1%)	25	31
1	D	339/341 (99%)	320 (94%)	18 (5%)	1 (0%)	41	50
1	E	339/341 (99%)	324 (96%)	13 (4%)	2 (1%)	25	31
1	F	339/341 (99%)	324 (96%)	11 (3%)	4 (1%)	13	14
1	G	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	41	50
1	H	339/341 (99%)	323 (95%)	14 (4%)	2 (1%)	25	31
1	I	339/341 (99%)	324 (96%)	14 (4%)	1 (0%)	41	50
1	J	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	41	50
1	K	339/341 (99%)	324 (96%)	14 (4%)	1 (0%)	41	50
1	L	339/341 (99%)	322 (95%)	14 (4%)	3 (1%)	17	20
All	All	4068/4092 (99%)	3878 (95%)	168 (4%)	22 (0%)	29	35

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	GLY
1	C	324	GLY
1	D	94	VAL
1	H	94	VAL

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Mol	Chain	Res	Type
1	K	94	VAL

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	252/252 (100%)	244 (97%)	8 (3%)	39	54
1	B	252/252 (100%)	246 (98%)	6 (2%)	49	66
1	C	252/252 (100%)	247 (98%)	5 (2%)	55	72
1	D	252/252 (100%)	246 (98%)	6 (2%)	49	66
1	E	252/252 (100%)	247 (98%)	5 (2%)	55	72
1	F	252/252 (100%)	247 (98%)	5 (2%)	55	72
1	G	252/252 (100%)	246 (98%)	6 (2%)	49	66
1	H	252/252 (100%)	247 (98%)	5 (2%)	55	72
1	I	252/252 (100%)	245 (97%)	7 (3%)	43	60
1	J	252/252 (100%)	248 (98%)	4 (2%)	62	78
1	K	252/252 (100%)	245 (97%)	7 (3%)	43	60
1	L	252/252 (100%)	249 (99%)	3 (1%)	71	84
All	All	3024/3024 (100%)	2957 (98%)	67 (2%)	52	69

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	28	GLU
1	K	158	HIS
1	L	117	GLU
1	D	293	PHE
1	D	158	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	227	HIS
1	L	13	ASN
1	L	69	ASN
1	H	69	ASN
1	I	288	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 48 ligands modelled in this entry, 36 are monoatomic - leaving 12 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
2	Q9C	C	403	4	12,12,12	1.06	2 (16%)	12,12,12	2.62	3 (25%)
2	Q9C	G	407	4	12,12,12	1.09	1 (8%)	12,12,12	2.64	3 (25%)
2	Q9C	D	404	4	12,12,12	1.06	1 (8%)	12,12,12	2.66	3 (25%)
2	Q9C	K	411	4	12,12,12	1.05	2 (16%)	12,12,12	2.64	3 (25%)
2	Q9C	L	412	4	12,12,12	1.11	2 (16%)	12,12,12	2.68	3 (25%)
2	Q9C	B	402	4	12,12,12	1.01	2 (16%)	12,12,12	2.71	3 (25%)
2	Q9C	I	409	4	12,12,12	1.05	2 (16%)	12,12,12	2.55	3 (25%)
2	Q9C	E	405	4	12,12,12	1.10	2 (16%)	12,12,12	2.60	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Q9C	F	406	4	12,12,12	1.03	1 (8%)	12,12,12	2.72	3 (25%)
2	Q9C	A	401	4	12,12,12	1.02	1 (8%)	12,12,12	2.73	3 (25%)
2	Q9C	H	408	4	12,12,12	1.07	2 (16%)	12,12,12	2.65	3 (25%)
2	Q9C	J	410	4	12,12,12	1.06	1 (8%)	12,12,12	2.71	3 (25%)

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
2	Q9C	C	403	4	-	6/10/10/10	-
2	Q9C	G	407	4	-	7/10/10/10	-
2	Q9C	D	404	4	-	6/10/10/10	-
2	Q9C	K	411	4	-	7/10/10/10	-
2	Q9C	L	412	4	-	7/10/10/10	-
2	Q9C	B	402	4	-	6/10/10/10	-
2	Q9C	I	409	4	-	5/10/10/10	-
2	Q9C	E	405	4	-	5/10/10/10	-
2	Q9C	F	406	4	-	5/10/10/10	-
2	Q9C	A	401	4	-	6/10/10/10	-
2	Q9C	H	408	4	-	4/10/10/10	-
2	Q9C	J	410	4	-	7/10/10/10	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	408	Q9C	C08-C	-2.63	1.45	1.50
2	G	407	Q9C	C08-C	-2.62	1.45	1.50
2	J	410	Q9C	C08-C	-2.49	1.45	1.50
2	E	405	Q9C	C08-C	-2.48	1.45	1.50
2	A	401	Q9C	C08-C	-2.46	1.45	1.50

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	409	Q9C	C08-C-N02	6.43	127.48	116.09
2	K	411	Q9C	C08-C-N02	6.35	127.34	116.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	Q9C	C08-C-N02	6.30	127.25	116.09
2	D	404	Q9C	C08-C-N02	6.28	127.22	116.09
2	F	406	Q9C	C08-C-N02	6.26	127.17	116.09

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Q9C	N02-C04-C07-C06
2	E	405	Q9C	N01-C03-C06-C07
2	B	402	Q9C	N01-C01-C05-C02
2	D	404	Q9C	N01-C01-C05-C02
2	G	407	Q9C	N02-C04-C07-C06

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	Q9C	5	0
2	G	407	Q9C	1	0
2	D	404	Q9C	1	0
2	B	402	Q9C	2	0
2	I	409	Q9C	2	0
2	A	401	Q9C	1	0
2	H	408	Q9C	1	0
2	J	410	Q9C	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, 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	341/341 (100%)	-0.36	2 (0%) 89 92	11, 22, 35, 50	0
1	B	341/341 (100%)	-0.30	0 100 100	13, 26, 38, 50	0
1	C	341/341 (100%)	-0.45	1 (0%) 94 96	9, 21, 32, 52	0
1	D	341/341 (100%)	-0.39	4 (1%) 79 83	14, 24, 37, 52	0
1	E	341/341 (100%)	-0.26	2 (0%) 89 92	13, 25, 38, 56	0
1	F	341/341 (100%)	-0.35	6 (1%) 68 74	15, 25, 41, 58	0
1	G	341/341 (100%)	-0.33	3 (0%) 84 88	13, 23, 35, 50	0
1	H	341/341 (100%)	-0.36	2 (0%) 89 92	15, 25, 36, 52	0
1	I	341/341 (100%)	-0.38	3 (0%) 84 88	14, 23, 35, 56	0
1	J	341/341 (100%)	-0.15	6 (1%) 68 74	14, 30, 44, 59	0
1	K	341/341 (100%)	-0.41	5 (1%) 73 79	12, 22, 33, 53	0
1	L	341/341 (100%)	-0.16	9 (2%) 56 63	13, 25, 39, 56	0
All	All	4092/4092 (100%)	-0.33	43 (1%) 80 85	9, 24, 38, 59	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	53	ARG	5.3
1	J	341	GLY	5.0
1	G	53	ARG	4.3
1	K	53	ARG	4.2
1	G	144	ALA	3.8

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, 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(Å ²)	Q<0.9
4	ZN	G	343	1/1	0.65	0.14	105,105,105,105	0
2	Q9C	D	404	13/13	0.78	0.27	41,46,55,55	0
2	Q9C	F	406	13/13	0.78	0.32	54,57,62,63	0
2	Q9C	A	401	13/13	0.78	0.31	60,61,68,68	0
2	Q9C	E	405	13/13	0.79	0.29	51,54,60,62	0
2	Q9C	L	412	13/13	0.84	0.32	59,62,67,67	0
2	Q9C	G	407	13/13	0.84	0.25	43,45,50,50	0
2	Q9C	J	410	13/13	0.86	0.23	50,51,53,53	0
2	Q9C	B	402	13/13	0.86	0.23	47,50,53,53	0
2	Q9C	H	408	13/13	0.86	0.25	37,44,48,50	0
4	ZN	B	343	1/1	0.89	0.11	100,100,100,100	0
2	Q9C	C	403	13/13	0.89	0.22	38,40,46,47	0
2	Q9C	I	409	13/13	0.90	0.18	31,33,42,42	0
2	Q9C	K	411	13/13	0.91	0.18	36,38,41,41	0
4	ZN	J	343	1/1	0.91	0.08	85,85,85,85	0
4	ZN	E	343	1/1	0.94	0.08	89,89,89,89	0
4	ZN	I	343	1/1	0.96	0.10	88,88,88,88	0
5	NA	A	344	1/1	0.96	0.08	19,19,19,19	0
5	NA	D	344	1/1	0.96	0.04	19,19,19,19	0
4	ZN	C	343	1/1	0.97	0.04	59,59,59,59	0
5	NA	C	344	1/1	0.97	0.04	19,19,19,19	0
4	ZN	H	343	1/1	0.97	0.04	58,58,58,58	0
5	NA	E	344	1/1	0.97	0.04	17,17,17,17	0
5	NA	G	344	1/1	0.97	0.06	18,18,18,18	0
5	NA	I	344	1/1	0.97	0.04	22,22,22,22	0
4	ZN	F	343	1/1	0.98	0.05	58,58,58,58	0
5	NA	H	344	1/1	0.98	0.04	27,27,27,27	0
4	ZN	K	343	1/1	0.98	0.06	89,89,89,89	0
5	NA	J	344	1/1	0.98	0.05	14,14,14,14	0
5	NA	L	344	1/1	0.98	0.07	26,26,26,26	0
5	NA	B	344	1/1	0.99	0.04	24,24,24,24	0
3	K	H	342	1/1	0.99	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	I	342	1/1	0.99	0.10	28,28,28,28	0
4	ZN	A	343	1/1	0.99	0.04	52,52,52,52	0
5	NA	F	344	1/1	0.99	0.07	27,27,27,27	0
3	K	B	342	1/1	0.99	0.08	25,25,25,25	0
3	K	C	342	1/1	0.99	0.09	18,18,18,18	0
4	ZN	D	343	1/1	0.99	0.03	55,55,55,55	0
4	ZN	L	343	1/1	0.99	0.04	54,54,54,54	0
5	NA	K	344	1/1	0.99	0.06	18,18,18,18	0
3	K	G	342	1/1	0.99	0.10	21,21,21,21	0
3	K	E	342	1/1	1.00	0.10	20,20,20,20	0
3	K	J	342	1/1	1.00	0.11	26,26,26,26	0
3	K	K	342	1/1	1.00	0.12	21,21,21,21	0
3	K	L	342	1/1	1.00	0.09	24,24,24,24	0
3	K	F	342	1/1	1.00	0.06	20,20,20,20	0
3	K	A	342	1/1	1.00	0.08	19,19,19,19	0
3	K	D	342	1/1	1.00	0.07	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.