



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 6UWI / pdb_00006uwi
Title : Crystal structure of the Clostridium difficile translocase CDTb
Authors : Pozharski, E.
Deposited on : 2019-11-05
Resolution : 3.70 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 : 4-5-2 with Phenix2.0
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)
Validation Pipeline (wwPDB-VP) : 2.49

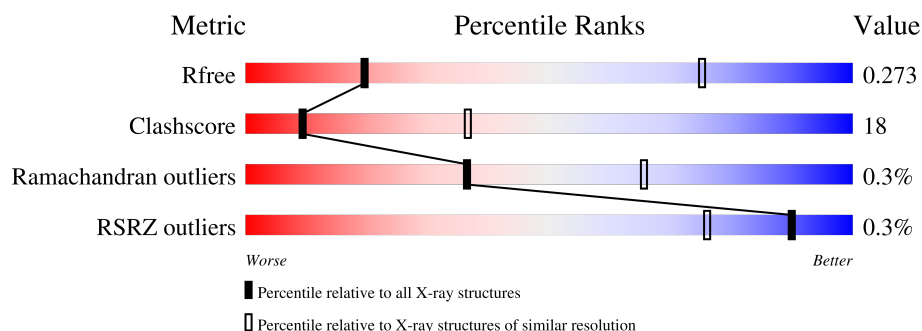
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



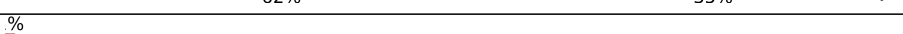
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 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	667	
1	B	667	
1	C	667	
1	D	667	
1	E	667	
1	F	667	

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Mol	Chain	Length	Quality of chain
1	G	667	 63%35%. .
1	H	667	 60%36%..
1	I	667	 61%35%.
1	J	667	 61%35%.
1	K	667	 %61%36%.
1	L	667	 60%36%.
1	M	667	 61%35%.
1	N	667	 %61%35%.
1	a	667	 62%34%.
1	b	667	 62%35%.
1	c	667	 62%35%.
1	d	667	 61%35%.
1	e	667	 62%34%.
1	f	667	 61%35%.
1	g	667	 62%35%.
1	h	667	 %61%35%.
1	i	667	 %60%36%.
1	j	667	 61%35%.
1	k	667	 61%35%.
1	l	667	 60%36%.
1	m	667	 %61%35%.
1	n	667	 %60%36%.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 141662 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 ADP-ribosyltransferase binding component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	644	0
			5067	3169	823	1065	10			
1	G	649	Total	C	N	O	S	0	649	0
			5105	3196	829	1070	10			
1	F	644	Total	C	N	O	S	0	644	0
			5070	3172	823	1065	10			
1	E	646	Total	C	N	O	S	0	646	0
			5087	3184	826	1067	10			
1	D	645	Total	C	N	O	S	0	645	0
			5078	3178	824	1066	10			
1	C	644	Total	C	N	O	S	0	644	0
			5067	3169	823	1065	10			
1	B	644	Total	C	N	O	S	0	644	0
			5070	3172	823	1065	10			
1	H	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	I	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	J	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	K	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	L	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	M	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	N	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	a	644	Total	C	N	O	S	0	644	0
			5067	3169	823	1065	10			
1	g	649	Total	C	N	O	S	0	649	0
			5105	3196	829	1070	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	f	644	Total	C	N	O	S	0	644	0
			5070	3172	823	1065	10			
1	e	646	Total	C	N	O	S	0	646	0
			5087	3184	826	1067	10			
1	d	645	Total	C	N	O	S	0	645	0
			5078	3178	824	1066	10			
1	c	644	Total	C	N	O	S	0	644	0
			5067	3169	823	1065	10			
1	b	644	Total	C	N	O	S	0	644	0
			5070	3172	823	1065	10			
1	h	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	i	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	j	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	k	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	l	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	m	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			
1	n	643	Total	C	N	O	S	0	643	0
			5035	3155	816	1054	10			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	3
			3	3		
2	G	3	Total	Ca	0	3
			3	3		
2	F	3	Total	Ca	0	3
			3	3		
2	E	3	Total	Ca	0	3
			3	3		
2	D	3	Total	Ca	0	3
			3	3		
2	C	3	Total	Ca	0	3
			3	3		
2	B	3	Total	Ca	0	3
			3	3		

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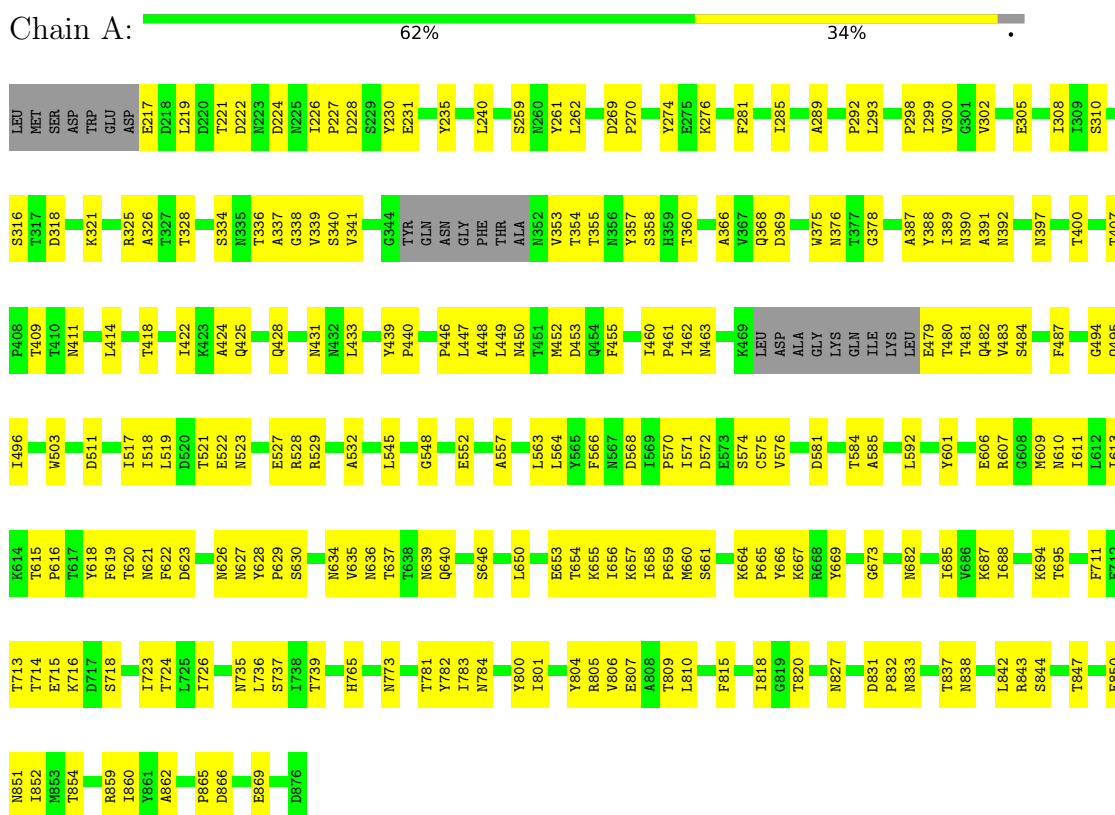
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total 3	Ca 3	0	3
2	I	3	Total 3	Ca 3	0	3
2	J	3	Total 3	Ca 3	0	3
2	K	3	Total 3	Ca 3	0	3
2	L	3	Total 3	Ca 3	0	3
2	M	3	Total 3	Ca 3	0	3
2	N	3	Total 3	Ca 3	0	3
2	a	3	Total 3	Ca 3	0	3
2	g	3	Total 3	Ca 3	0	3
2	f	3	Total 3	Ca 3	0	3
2	e	3	Total 3	Ca 3	0	3
2	d	3	Total 3	Ca 3	0	3
2	c	3	Total 3	Ca 3	0	3
2	b	3	Total 3	Ca 3	0	3
2	h	3	Total 3	Ca 3	0	3
2	i	3	Total 3	Ca 3	0	3
2	j	3	Total 3	Ca 3	0	3
2	k	3	Total 3	Ca 3	0	3
2	l	3	Total 3	Ca 3	0	3
2	m	3	Total 3	Ca 3	0	3
2	n	3	Total 3	Ca 3	0	3

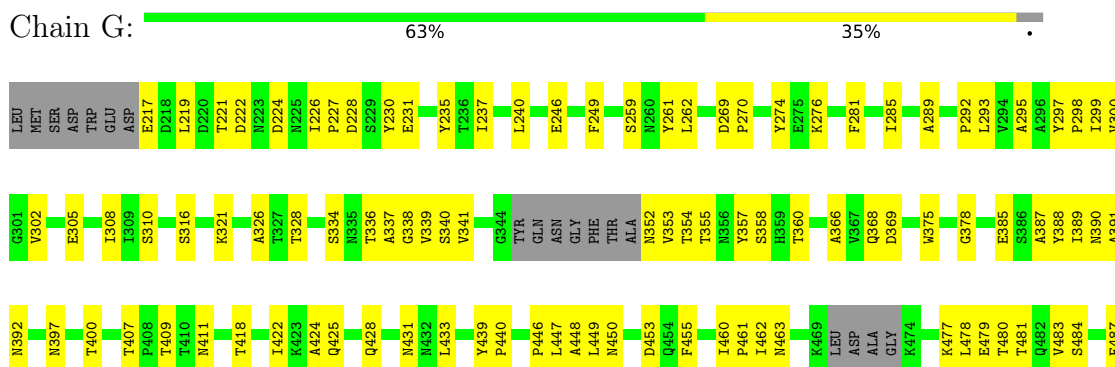
3 Residue-property plots

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: ADP-ribosyltransferase binding component



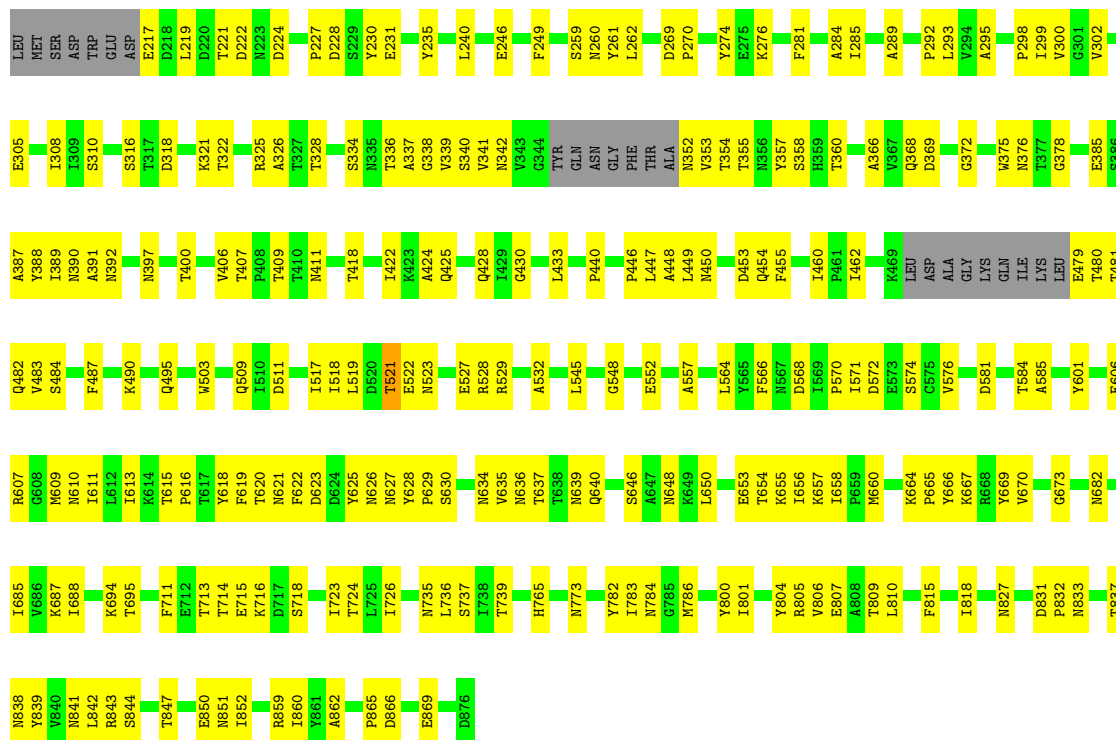
• Molecule 1: ADP-ribosyltransferase binding component





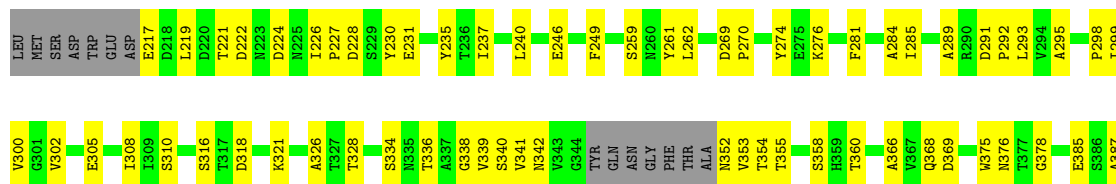
• Molecule 1: ADP-ribosyltransferase binding component

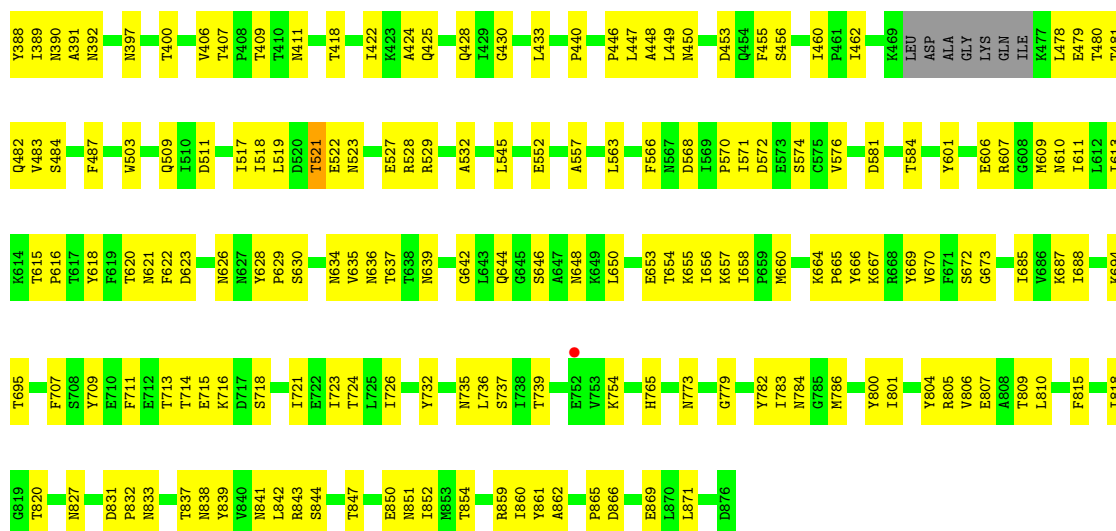
Chain F: 62% 35%



• Molecule 1: ADP-ribosyltransferase binding component

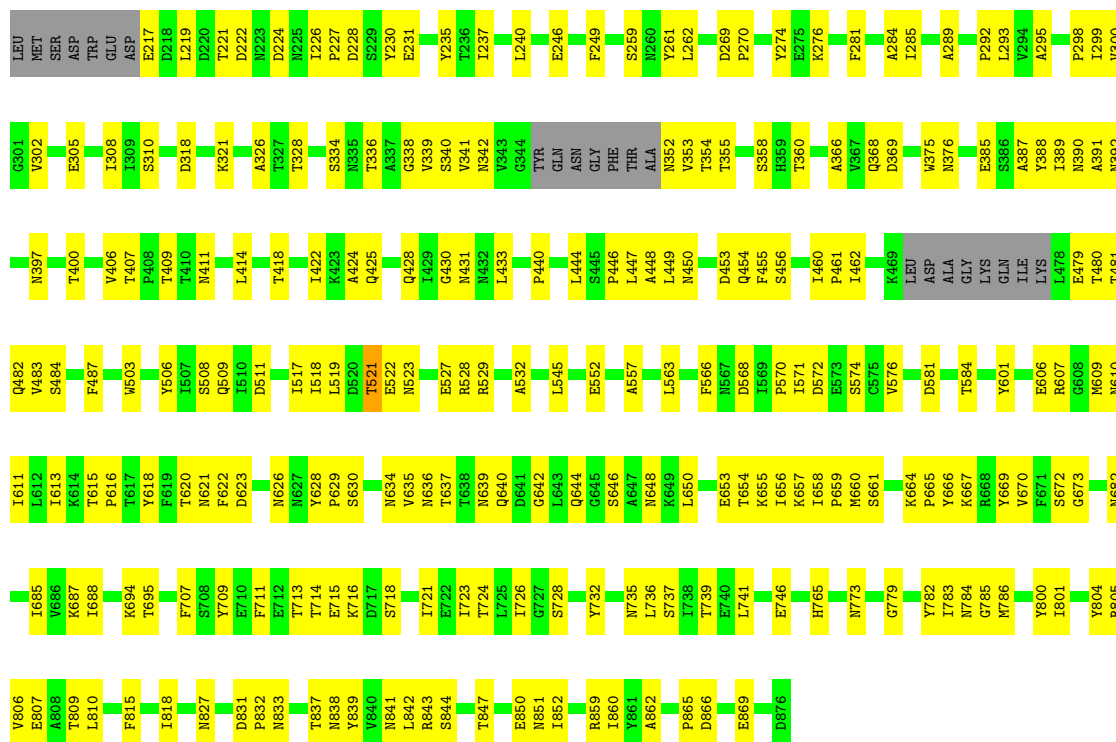
Chain E: 62% 35%





• Molecule 1: ADP-ribosyltransferase binding component

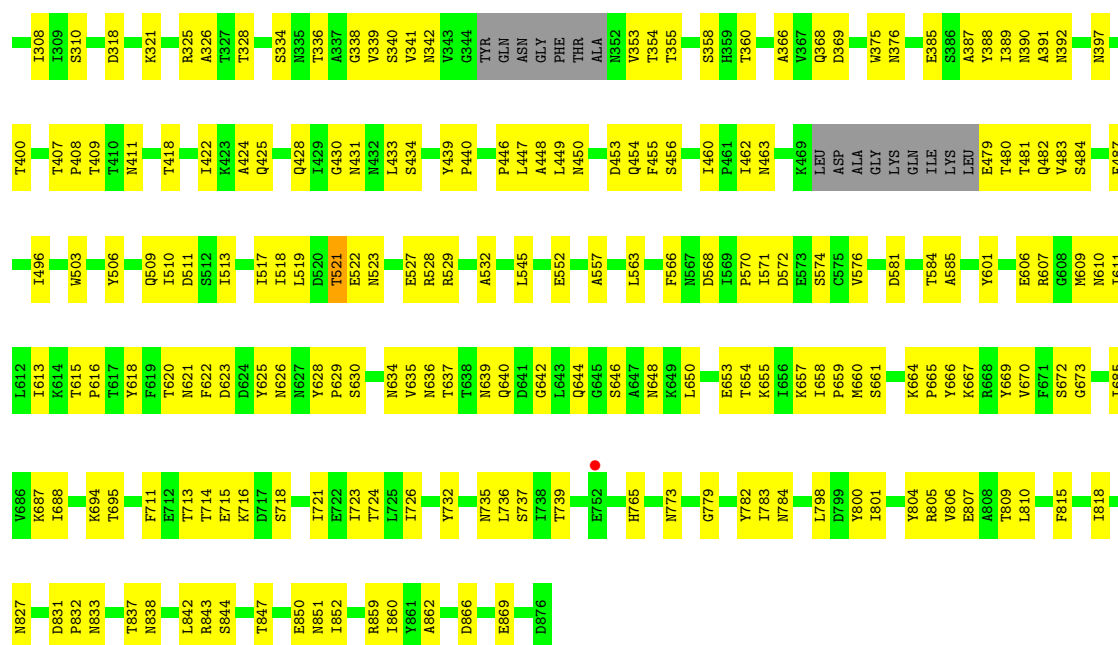
Chain D: 61% 36%



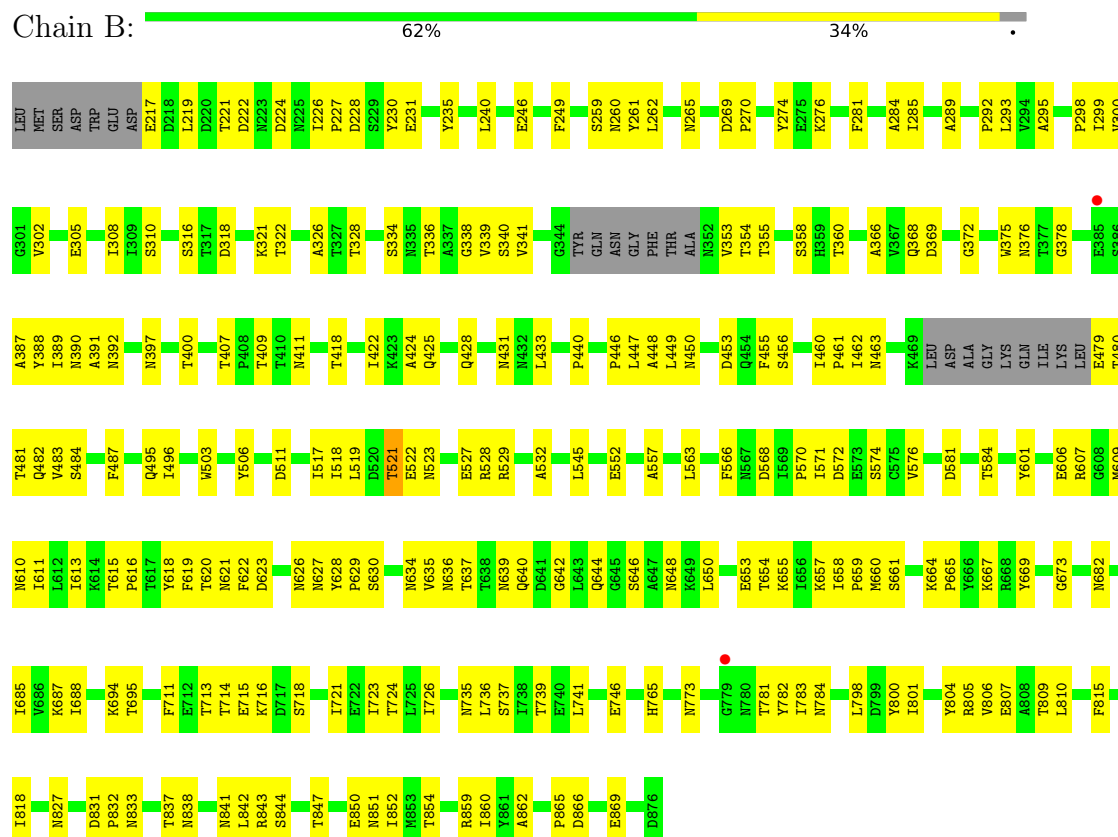
• Molecule 1: ADP-ribosyltransferase binding component

Chain C: 62% 34%



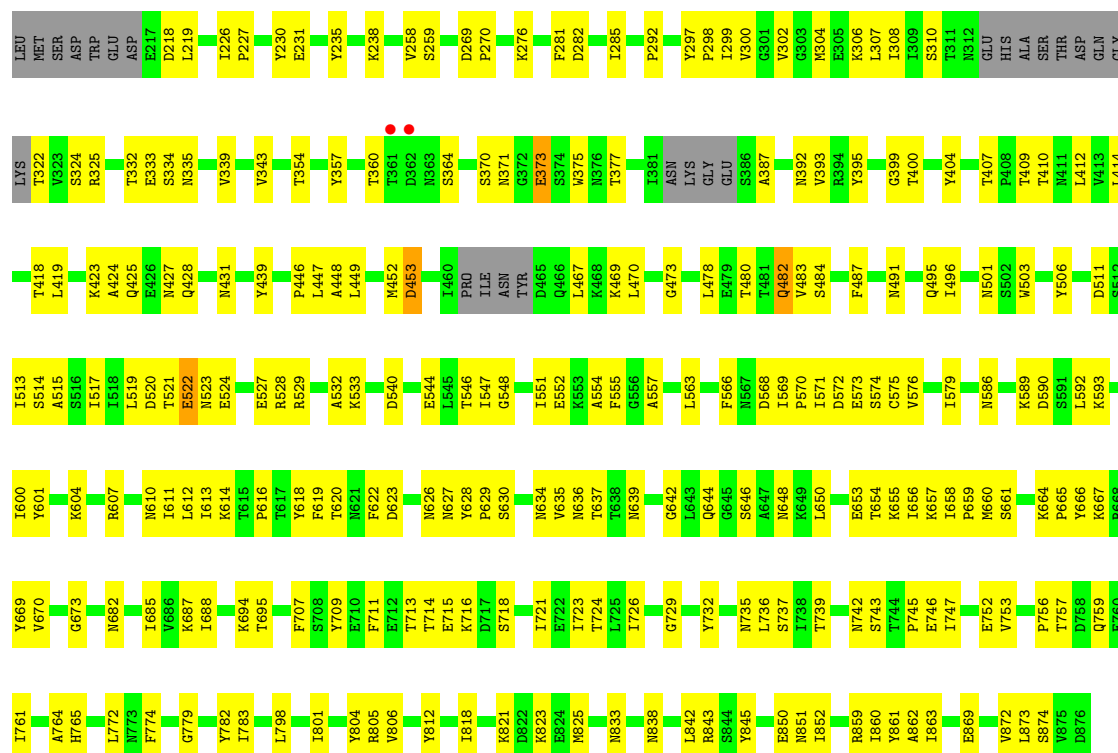


• Molecule 1: ADP-ribosyltransferase binding component



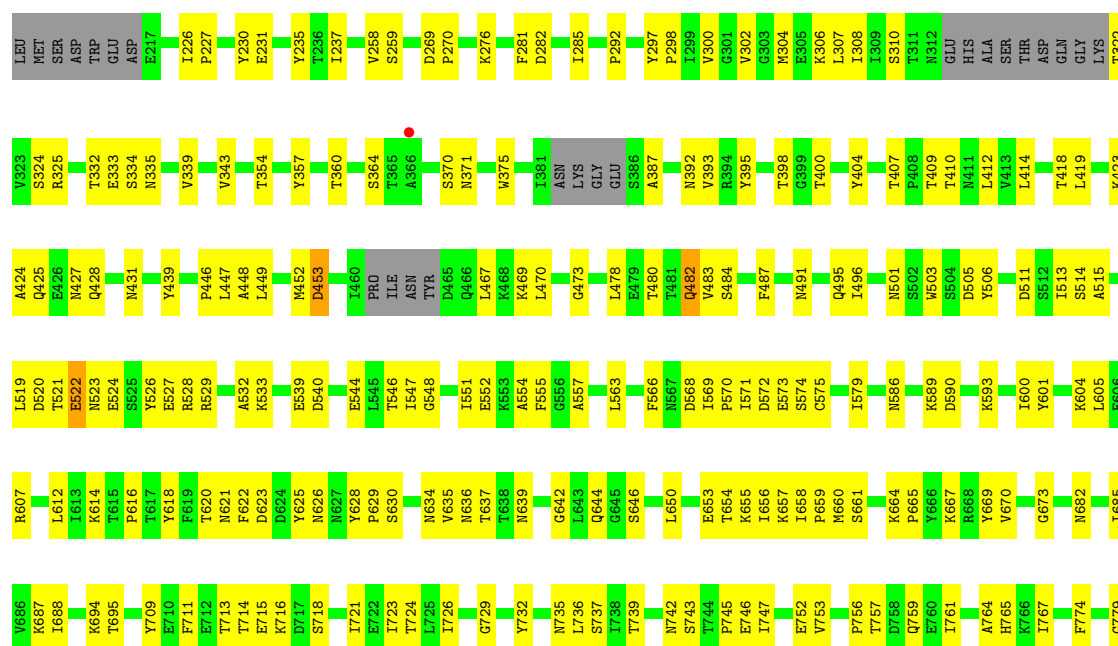
• Molecule 1: ADP-ribosyltransferase binding component





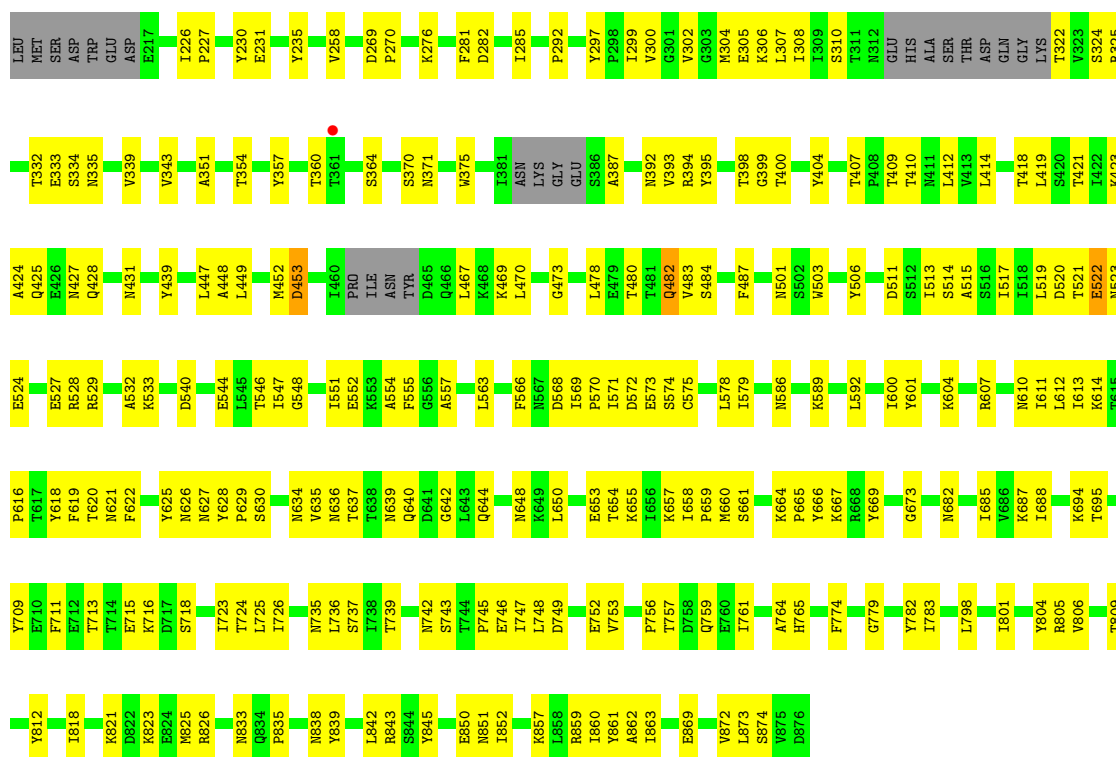
• Molecule 1: ADP-ribosyltransferase binding component

Chain I: 61% 35%



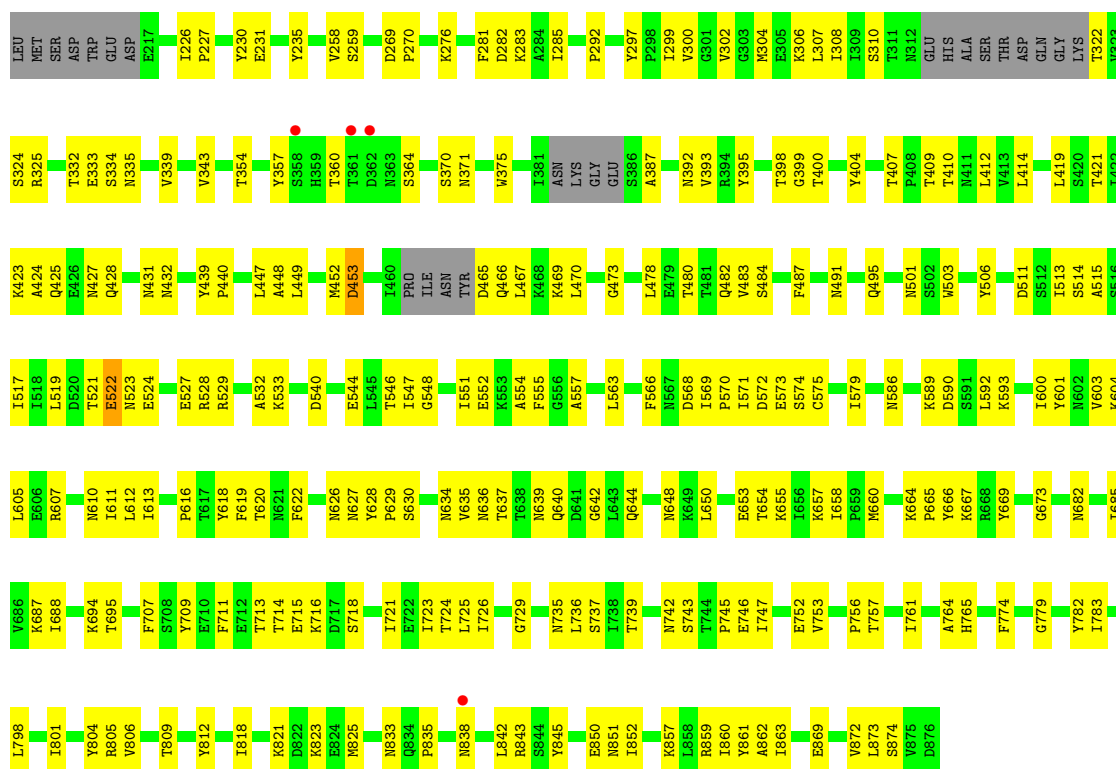
• Molecule 1: ADP-ribosyltransferase binding component

Chain J:  61% 35% .



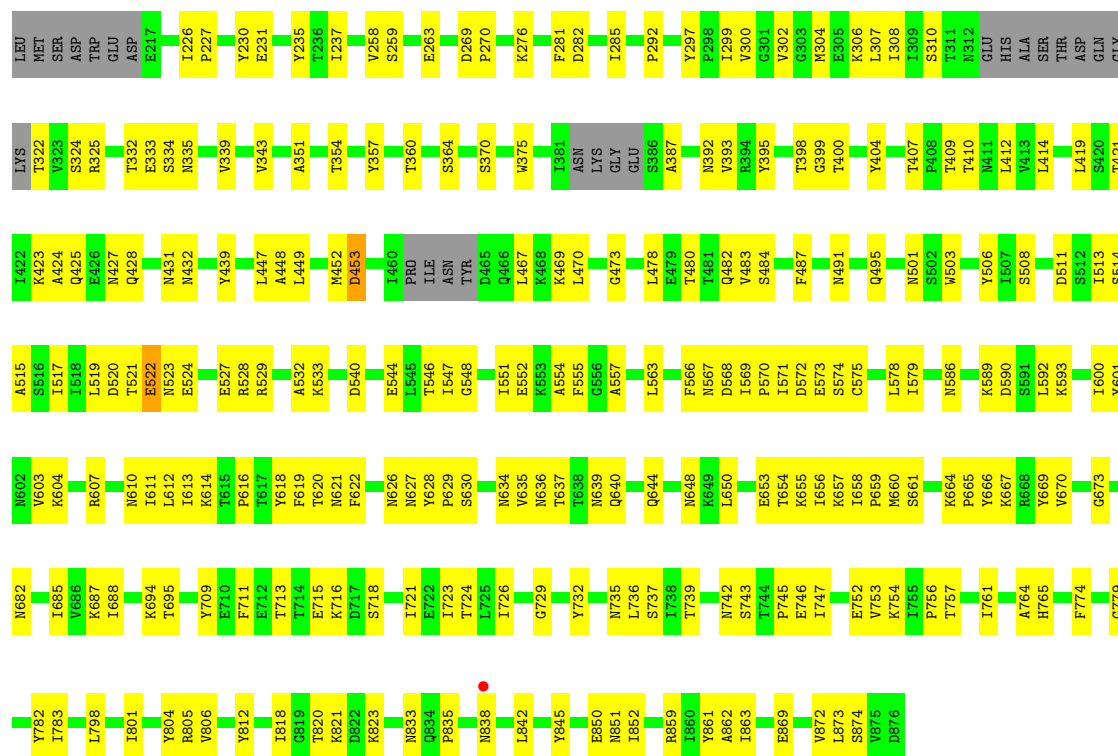
• Molecule 1: ADP-ribosyltransferase binding component

Chain K:  61% 36% .



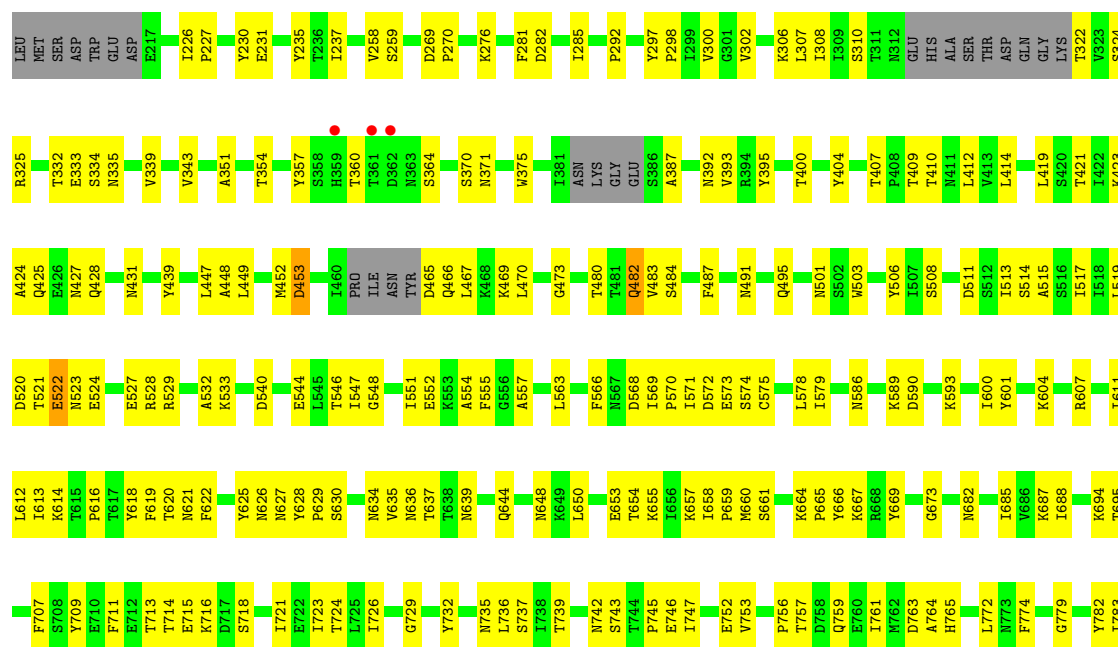
• Molecule 1: ADP-ribosyltransferase binding component

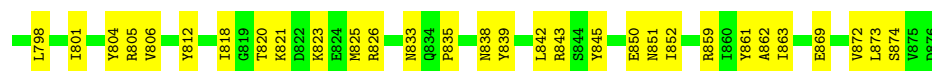
Chain L:  60% 36%



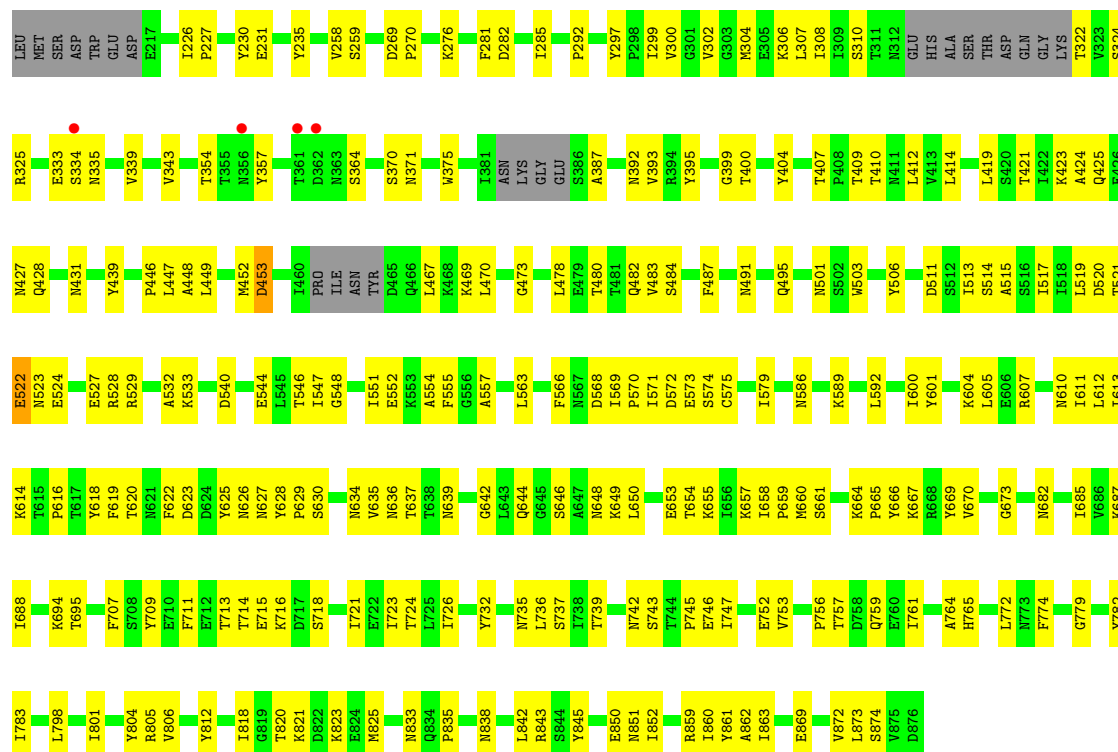
• Molecule 1: ADP-ribosyltransferase binding component

Chain M:  61% 35%

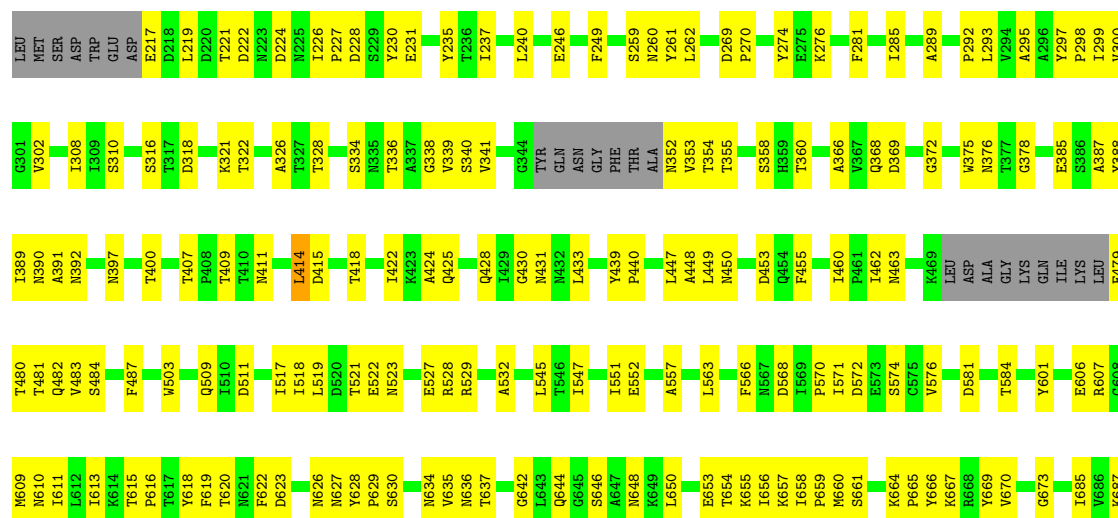


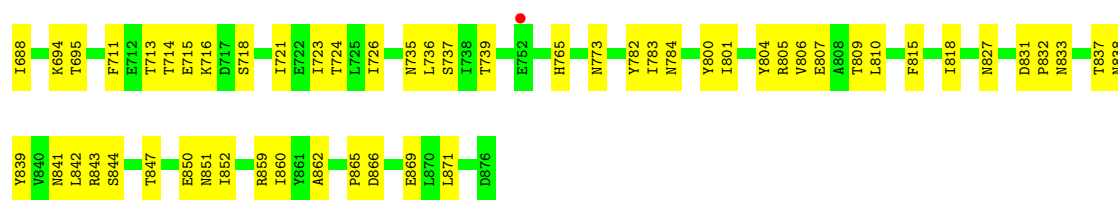


• Molecule 1: ADP-ribosyltransferase binding component



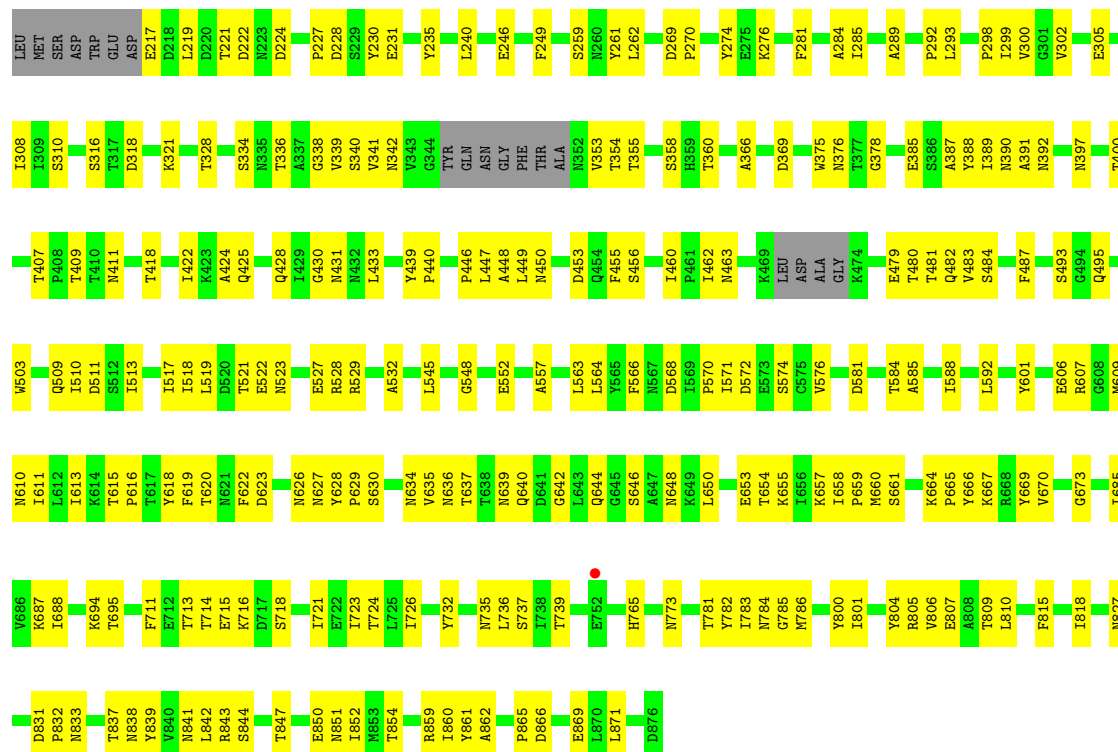
• Molecule 1: ADP-ribosyltransferase binding component





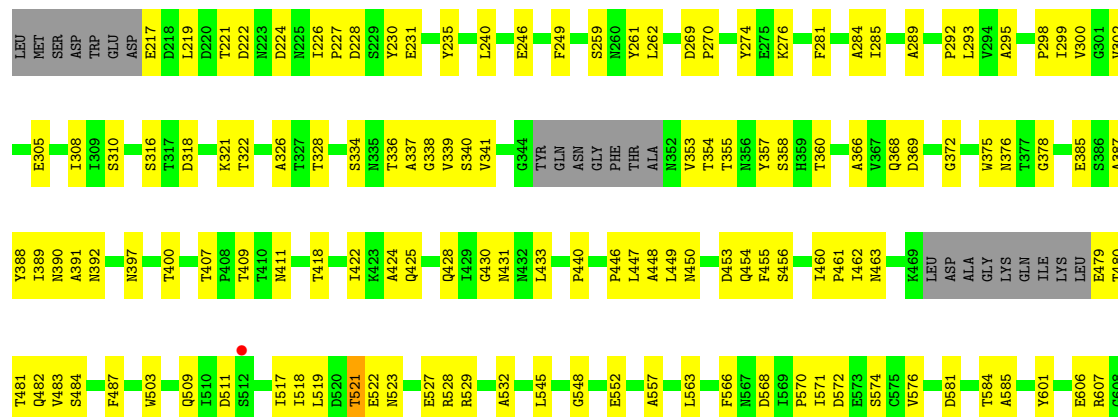
• Molecule 1: ADP-ribosyltransferase binding component

Chain g: 62% 35%

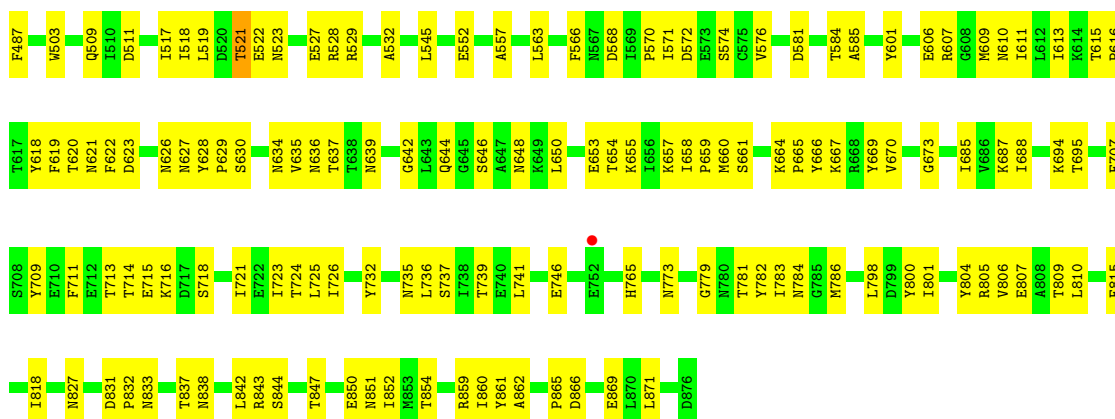


• Molecule 1: ADP-ribosyltransferase binding component

Chain f: 61% 35%

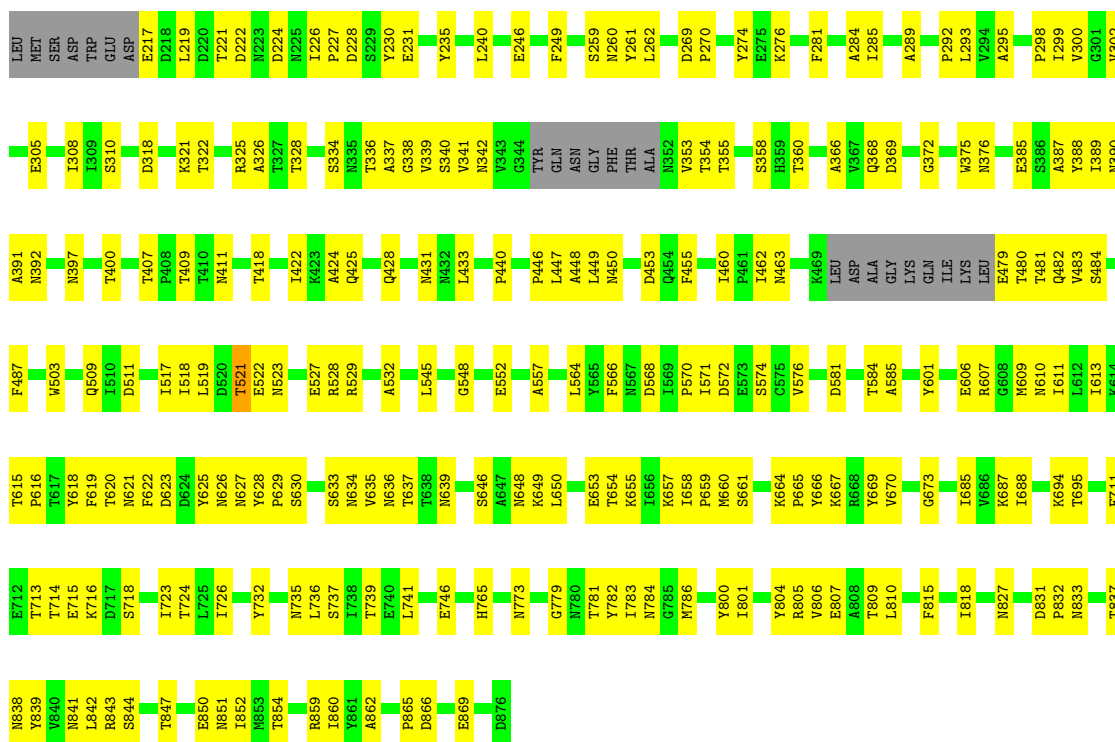






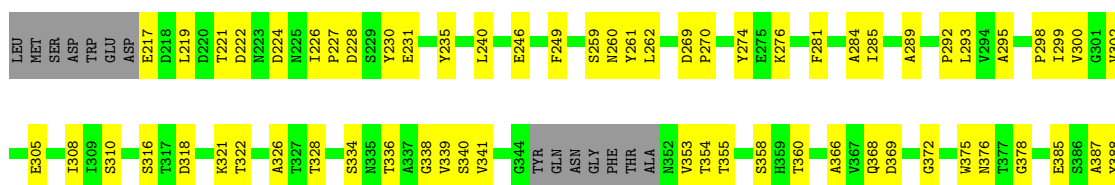
• Molecule 1: ADP-ribosyltransferase binding component

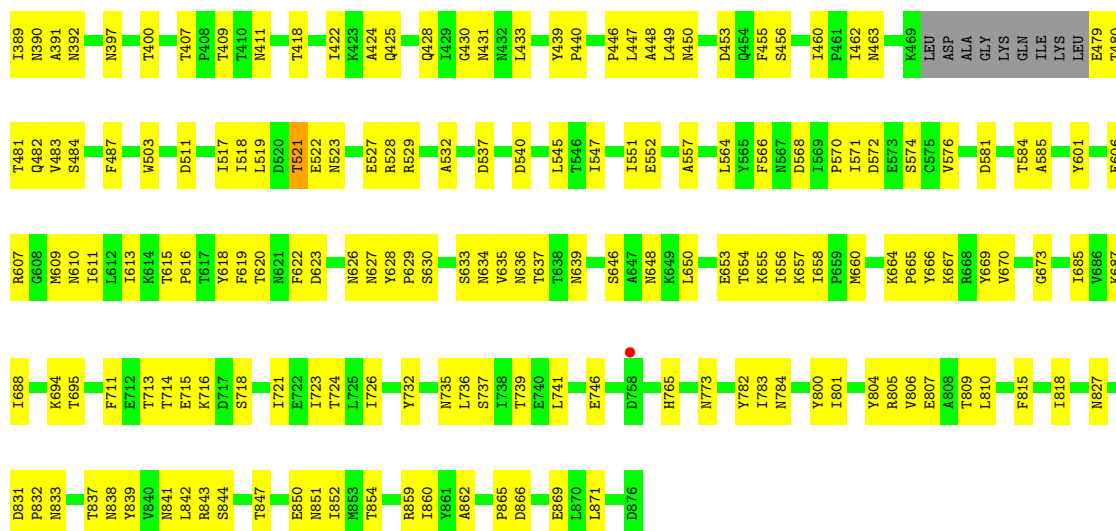
Chain c: 62% 35%



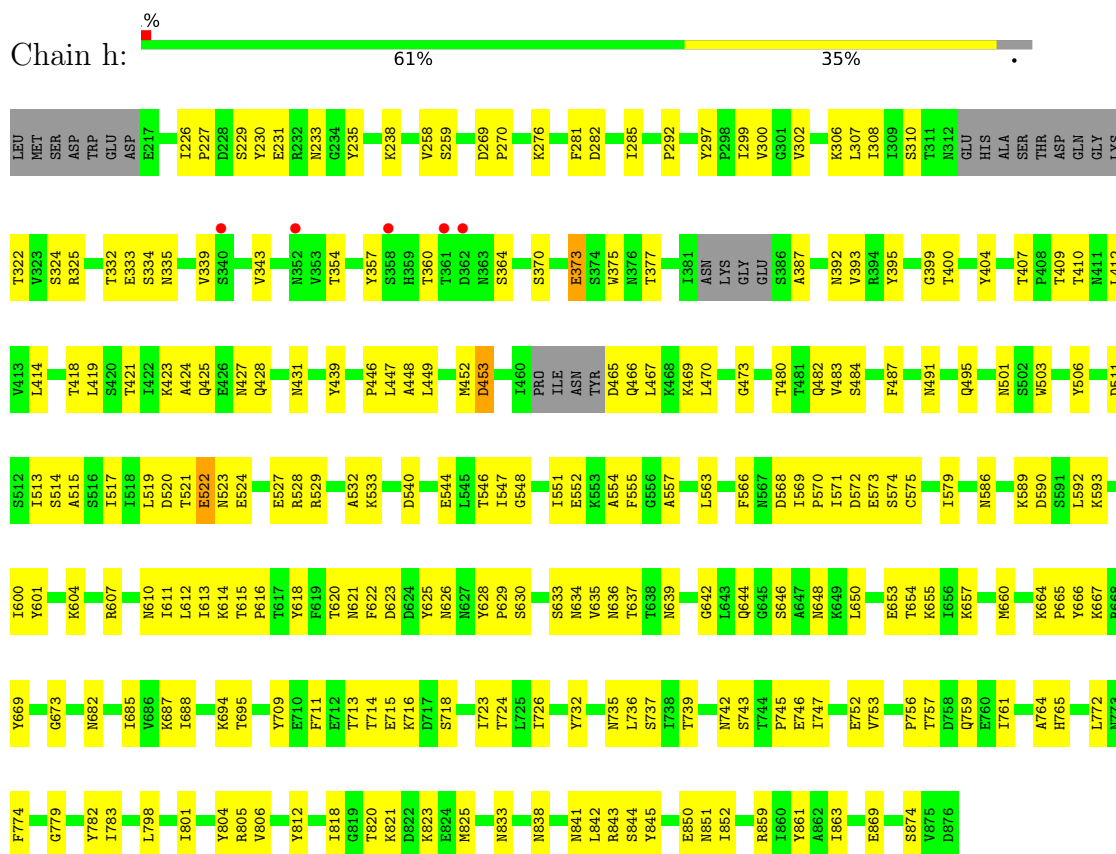
• Molecule 1: ADP-ribosyltransferase binding component

Chain b: 62% 35%

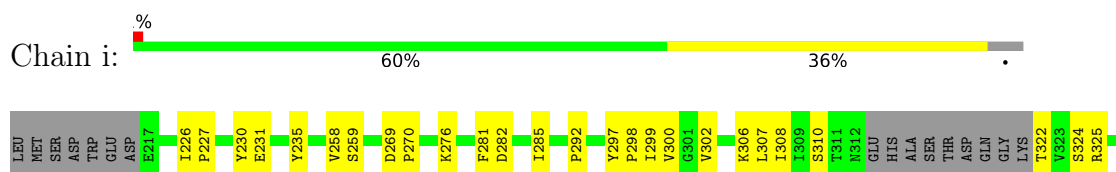


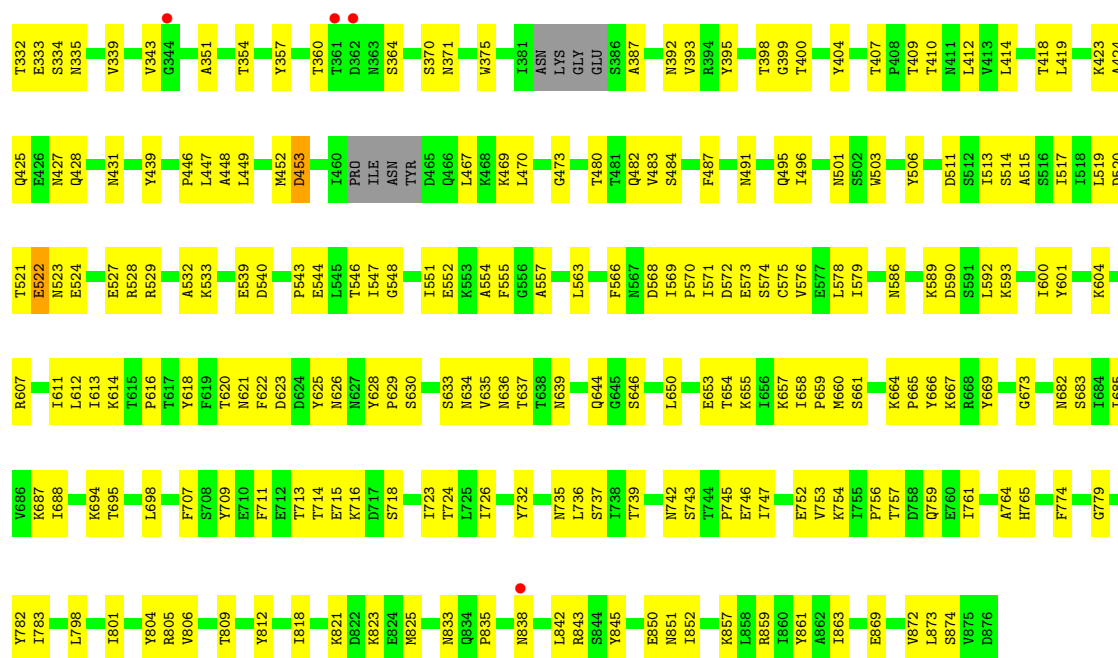


• Molecule 1: ADP-ribosyltransferase binding component



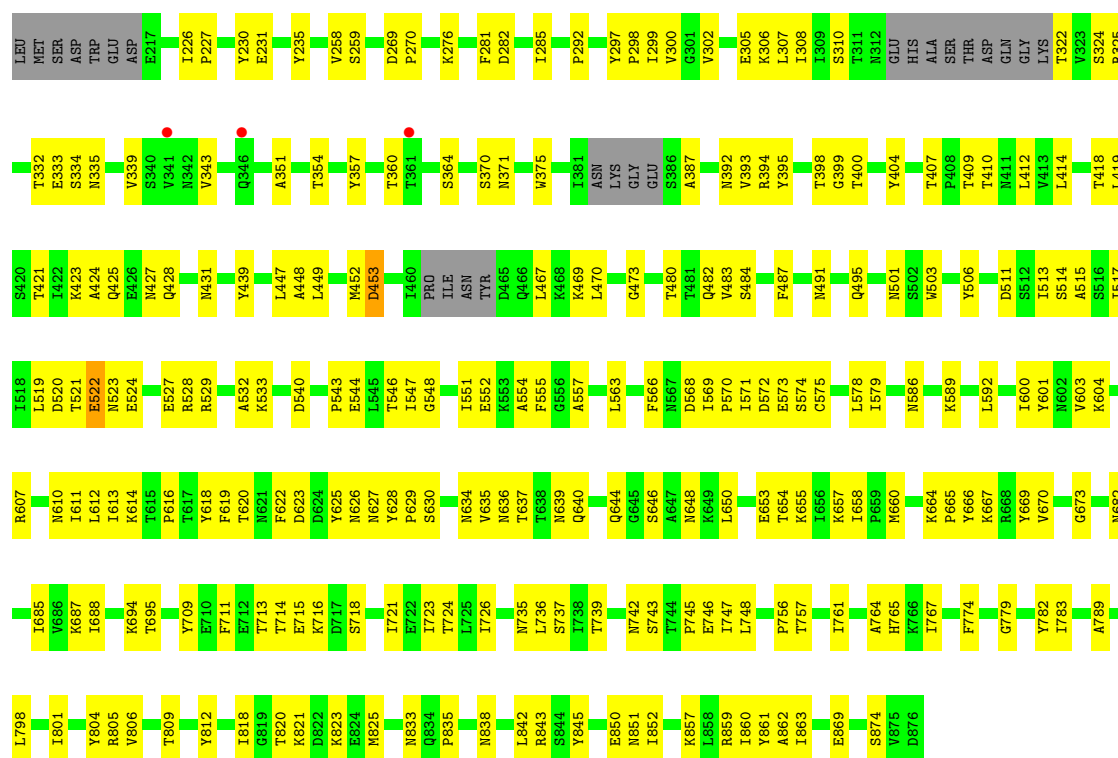
• Molecule 1: ADP-ribosyltransferase binding component





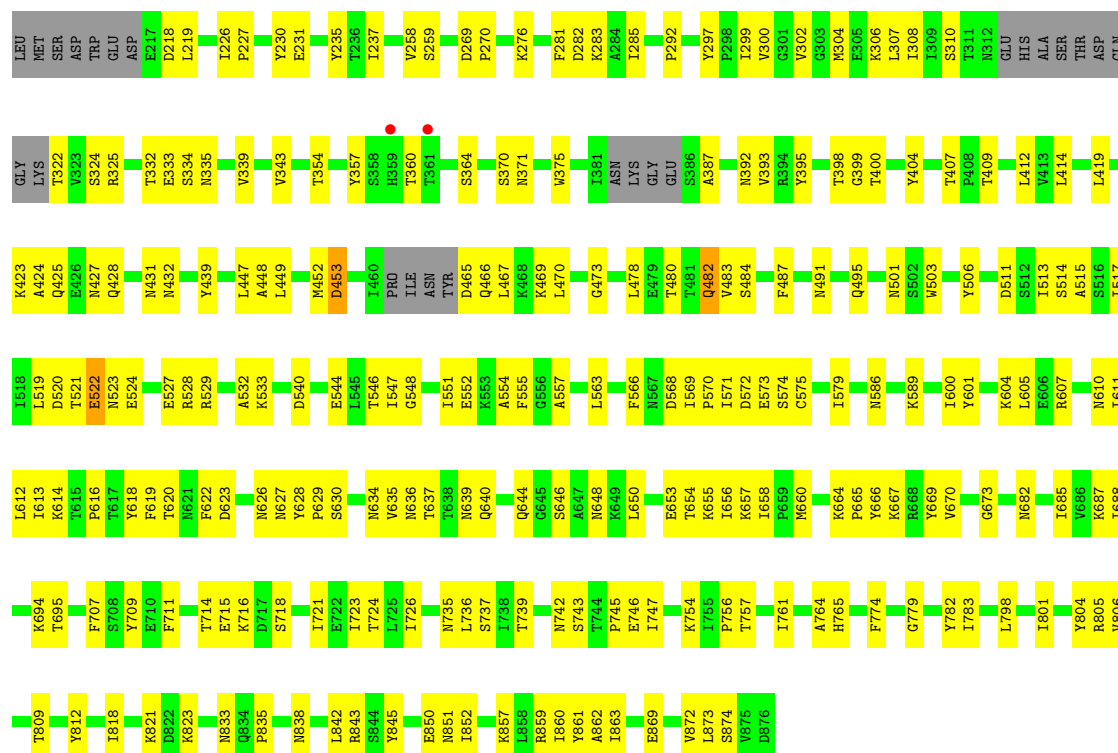
• Molecule 1: ADP-ribosyltransferase binding component

Chain j: 61% 35% .



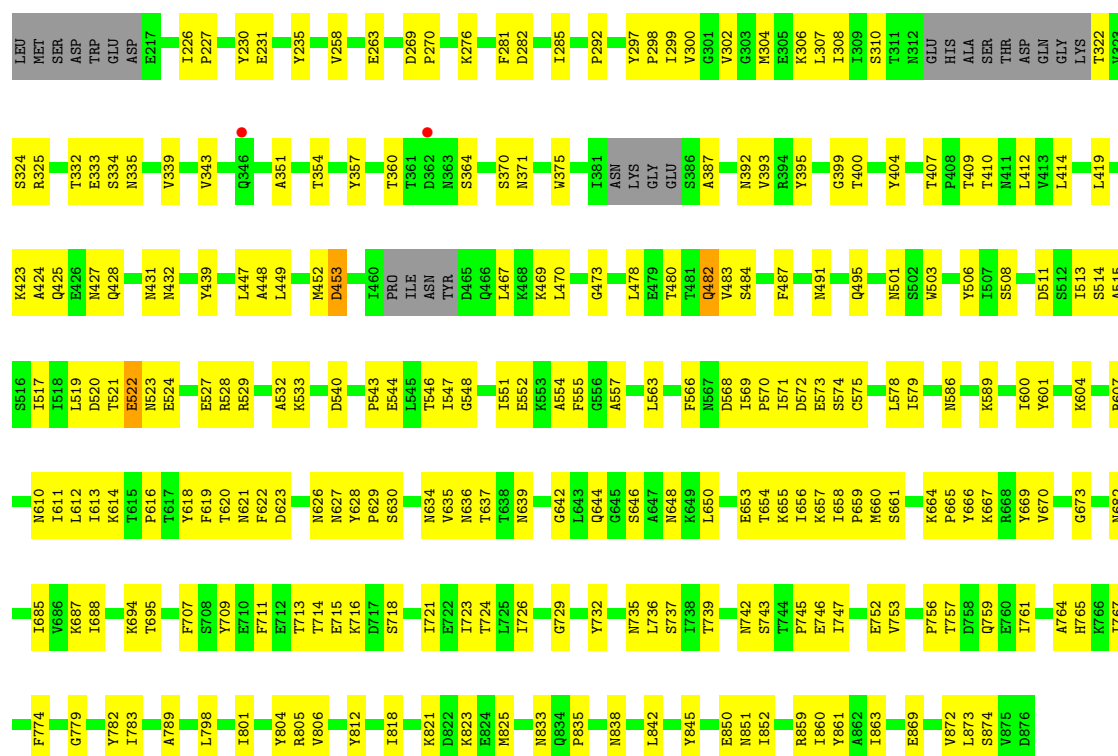
• Molecule 1: ADP-ribosyltransferase binding component

Chain k: 61% 35% .

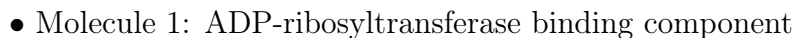


• Molecule 1: ADP-ribosyltransferase binding component

Chain 1: 60% 36%



• Molecule 1: ADP-ribosyltransferase binding component



F774
G779
Y782 I783
L798
I801
Y804 R805 V806
Y812
I818
G819
T820
K821
S822
K823
E824 S825
N833
Q834 P835
N838
L842
R843
S844
Y845
E850
N851
I852
R859
I860
Y861
A862
I863
E869
V872
L873
S874
V875 S876

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	190.49Å 190.96Å 192.25Å 108.74° 94.47° 108.03°	Depositor
Resolution (Å)	39.75 – 3.70 39.75 – 3.70	Depositor EDS
% Data completeness (in resolution range)	91.8 (39.75-3.70) 88.8 (39.75-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.248 , 0.273 0.248 , 0.273	Depositor DCC
R_{free} test set	11604 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	135.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 434.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.219 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	141662	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	h	0	2
1	i	0	2
1	j	0	3
1	k	0	2
1	l	0	2
1	m	0	2
1	n	0	2
All	All	0	39

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	521[1]	THR	Peptide
1	C	521[1]	THR	Peptide
1	D	521[1]	THR	Peptide
1	E	521[1]	THR	Peptide
1	F	521[1]	THR	Peptide

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	5067	0	4427	178	0
1	B	5070	0	4424	183	0
1	C	5067	0	4411	186	0
1	D	5078	0	4441	190	0
1	E	5087	0	4488	186	0
1	F	5070	0	4457	179	0
1	G	5105	0	4476	185	0
1	H	5035	0	4486	187	0
1	I	5035	0	4428	184	0
1	J	5035	0	4438	180	0
1	K	5035	0	4448	180	0
1	L	5035	0	4449	179	0
1	M	5035	0	4469	181	0
1	N	5035	0	4490	181	0
1	a	5067	0	4506	182	0
1	b	5070	0	4468	181	0
1	c	5067	0	4466	182	0
1	d	5078	0	4497	184	0
1	e	5087	0	4490	180	0
1	f	5070	0	4500	179	0
1	g	5105	0	4571	184	0
1	h	5035	0	4424	173	0
1	i	5035	0	4444	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	5035	0	4443	182	0
1	k	5035	0	4422	176	0
1	l	5035	0	4456	180	0
1	m	5035	0	4440	176	0
1	n	5035	0	4410	181	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
2	M	3	0	0	0	0
2	N	3	0	0	0	0
2	a	3	0	0	0	0
2	b	3	0	0	0	0
2	c	3	0	0	0	0
2	d	3	0	0	0	0
2	e	3	0	0	0	0
2	f	3	0	0	0	0
2	g	3	0	0	0	0
2	h	3	0	0	0	0
2	i	3	0	0	0	0
2	j	3	0	0	0	0
2	k	3	0	0	0	0
2	l	3	0	0	0	0
2	m	3	0	0	0	0
2	n	3	0	0	0	0
All	All	141662	0	124869	4784	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 18.

The worst 5 of 4784 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:765[2]:HIS:HE2	1:g:804[2]:TYR:HH	1.07	1.02
1:F:634[1]:ASN:HB2	1:F:654[1]:THR:HG22	1.42	1.00
1:A:765[1]:HIS:HE2	1:A:804[1]:TYR:HH	1.06	0.98
1:E:765[1]:HIS:HE2	1:E:804[1]:TYR:HH	1.08	0.98
1:B:765[1]:HIS:HE2	1:B:804[1]:TYR:HH	1.09	0.94

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	638/667 (96%)	555 (87%)	81 (13%)	2 (0%)	36	65
1	B	638/667 (96%)	555 (87%)	82 (13%)	1 (0%)	43	72
1	C	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	43	72
1	D	639/667 (96%)	558 (87%)	79 (12%)	2 (0%)	36	65
1	E	640/667 (96%)	553 (86%)	85 (13%)	2 (0%)	36	65
1	F	638/667 (96%)	554 (87%)	83 (13%)	1 (0%)	43	72
1	G	643/667 (96%)	560 (87%)	82 (13%)	1 (0%)	43	72
1	H	635/667 (95%)	542 (85%)	89 (14%)	4 (1%)	21	52
1	I	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	24	56
1	J	635/667 (95%)	540 (85%)	92 (14%)	3 (0%)	24	56
1	K	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	36	65
1	L	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	36	65
1	M	635/667 (95%)	544 (86%)	88 (14%)	3 (0%)	24	56
1	N	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	36	65
1	a	638/667 (96%)	554 (87%)	82 (13%)	2 (0%)	36	65
1	b	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	43	72
1	d	639/667 (96%)	556 (87%)	81 (13%)	2 (0%)	36	65
1	e	640/667 (96%)	553 (86%)	85 (13%)	2 (0%)	36	65
1	f	638/667 (96%)	554 (87%)	83 (13%)	1 (0%)	43	72
1	g	643/667 (96%)	562 (87%)	80 (12%)	1 (0%)	43	72
1	h	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	24	56
1	i	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	36	65
1	j	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	36	65
1	k	635/667 (95%)	541 (85%)	91 (14%)	3 (0%)	24	56
1	l	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	24	56
1	m	635/667 (95%)	543 (86%)	90 (14%)	2 (0%)	36	65
1	n	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	36	65
All	All	17838/18676 (96%)	15358 (86%)	2424 (14%)	56 (0%)	36	65

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522[1]	GLU
1	G	522[1]	GLU
1	F	522[1]	GLU
1	E	522[1]	GLU
1	D	522[1]	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 84 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	644/667 (96%)	-0.92	0 100 100	37, 63, 87, 99	644 (100%)
1	B	644/667 (96%)	-0.93	2 (0%) 90 76	37, 63, 86, 102	644 (100%)
1	C	644/667 (96%)	-0.95	1 (0%) 91 80	38, 63, 86, 98	644 (100%)
1	D	645/667 (96%)	-0.93	0 100 100	38, 64, 85, 99	645 (100%)
1	E	646/667 (96%)	-0.91	1 (0%) 91 80	37, 65, 88, 99	646 (100%)
1	F	644/667 (96%)	-0.93	0 100 100	38, 64, 87, 100	644 (100%)
1	G	649/667 (97%)	-0.96	1 (0%) 91 80	38, 63, 86, 100	649 (100%)
1	H	643/667 (96%)	-0.83	2 (0%) 90 76	40, 66, 88, 99	643 (100%)
1	I	643/667 (96%)	-0.82	1 (0%) 91 80	38, 67, 89, 100	643 (100%)
1	J	643/667 (96%)	-0.84	1 (0%) 91 80	38, 66, 89, 99	643 (100%)
1	K	643/667 (96%)	-0.89	4 (0%) 85 66	39, 65, 87, 98	643 (100%)
1	L	643/667 (96%)	-0.87	1 (0%) 91 80	40, 66, 88, 98	643 (100%)
1	M	643/667 (96%)	-0.86	3 (0%) 87 69	38, 65, 88, 100	643 (100%)
1	N	643/667 (96%)	-0.80	4 (0%) 85 66	39, 66, 87, 101	643 (100%)
1	a	644/667 (96%)	-0.92	1 (0%) 91 80	37, 60, 81, 94	644 (100%)
1	b	644/667 (96%)	-0.89	1 (0%) 91 80	36, 61, 83, 93	644 (100%)
1	c	644/667 (96%)	-0.90	0 100 100	34, 60, 82, 94	644 (100%)
1	d	645/667 (96%)	-0.94	1 (0%) 91 80	37, 59, 81, 93	645 (100%)
1	e	646/667 (96%)	-0.90	0 100 100	36, 60, 81, 93	646 (100%)
1	f	644/667 (96%)	-0.91	1 (0%) 91 80	35, 60, 81, 94	644 (100%)
1	g	649/667 (97%)	-0.88	1 (0%) 91 80	36, 59, 81, 96	649 (100%)
1	h	643/667 (96%)	-0.82	5 (0%) 82 60	37, 62, 83, 94	643 (100%)
1	i	643/667 (96%)	-0.82	4 (0%) 85 66	35, 62, 82, 96	643 (100%)
1	j	643/667 (96%)	-0.87	3 (0%) 87 69	36, 62, 82, 93	643 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	k	643/667 (96%)	-0.83	2 (0%) 90 76	36, 62, 83, 94	643 (100%)
1	l	643/667 (96%)	-0.83	2 (0%) 90 76	37, 63, 84, 94	643 (100%)
1	m	643/667 (96%)	-0.82	4 (0%) 85 66	38, 62, 83, 95	643 (100%)
1	n	643/667 (96%)	-0.87	4 (0%) 85 66	36, 62, 82, 94	643 (100%)
All	All	18034/18676 (96%)	-0.88	50 (0%) 90 76	34, 63, 85, 102	18034 (100%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	362[2]	ASP	5.8
1	g	752[2]	GLU	4.6
1	H	362[1]	ASP	4.3
1	i	361[2]	THR	4.1
1	n	362[2]	ASP	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	CA	J	902[1]	1/1	0.99	0.04	111,111,111,111	1
2	CA	J	903[1]	1/1	0.99	0.03	111,111,111,111	1
2	CA	N	902[1]	1/1	0.99	0.02	85,85,85,85	1
2	CA	c	903[2]	1/1	0.99	0.04	111,111,111,111	1
2	CA	j	902[2]	1/1	0.99	0.03	103,103,103,103	1
2	CA	G	903[1]	1/1	1.00	0.02	103,103,103,103	1
2	CA	F	901[1]	1/1	1.00	0.01	88,88,88,88	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	F	902[1]	1/1	1.00	0.02	100,100,100,100	1
2	CA	F	903[1]	1/1	1.00	0.01	114,114,114,114	1
2	CA	E	901[1]	1/1	1.00	0.01	105,105,105,105	1
2	CA	E	902[1]	1/1	1.00	0.01	87,87,87,87	1
2	CA	E	903[1]	1/1	1.00	0.02	124,124,124,124	1
2	CA	D	901[1]	1/1	1.00	0.01	99,99,99,99	1
2	CA	D	902[1]	1/1	1.00	0.02	93,93,93,93	1
2	CA	D	903[1]	1/1	1.00	0.03	126,126,126,126	1
2	CA	C	901[1]	1/1	1.00	0.01	105,105,105,105	1
2	CA	C	902[1]	1/1	1.00	0.02	89,89,89,89	1
2	CA	C	903[1]	1/1	1.00	0.01	98,98,98,98	1
2	CA	B	901[1]	1/1	1.00	0.02	116,116,116,116	1
2	CA	B	902[1]	1/1	1.00	0.01	102,102,102,102	1
2	CA	B	903[1]	1/1	1.00	0.02	115,115,115,115	1
2	CA	H	901[1]	1/1	1.00	0.01	106,106,106,106	1
2	CA	H	902[1]	1/1	1.00	0.01	92,92,92,92	1
2	CA	H	903[1]	1/1	1.00	0.01	122,122,122,122	1
2	CA	I	901[1]	1/1	1.00	0.01	115,115,115,115	1
2	CA	I	902[1]	1/1	1.00	0.01	97,97,97,97	1
2	CA	I	903[1]	1/1	1.00	0.02	132,132,132,132	1
2	CA	J	901[1]	1/1	1.00	0.02	87,87,87,87	1
2	CA	A	901[1]	1/1	1.00	0.01	82,82,82,82	1
2	CA	A	902[1]	1/1	1.00	0.02	89,89,89,89	1
2	CA	K	901[1]	1/1	1.00	0.01	116,116,116,116	1
2	CA	K	902[1]	1/1	1.00	0.01	93,93,93,93	1
2	CA	K	903[1]	1/1	1.00	0.02	100,100,100,100	1
2	CA	L	901[1]	1/1	1.00	0.01	87,87,87,87	1
2	CA	L	902[1]	1/1	1.00	0.01	82,82,82,82	1
2	CA	L	903[1]	1/1	1.00	0.03	104,104,104,104	1
2	CA	M	901[1]	1/1	1.00	0.01	105,105,105,105	1
2	CA	M	902[1]	1/1	1.00	0.01	106,106,106,106	1
2	CA	M	903[1]	1/1	1.00	0.03	112,112,112,112	1
2	CA	N	901[1]	1/1	1.00	0.01	93,93,93,93	1
2	CA	A	903[1]	1/1	1.00	0.01	117,117,117,117	1
2	CA	N	903[1]	1/1	1.00	0.02	83,83,83,83	1
2	CA	a	901[2]	1/1	1.00	0.00	103,103,103,103	1
2	CA	a	902[2]	1/1	1.00	0.01	93,93,93,93	1
2	CA	a	903[2]	1/1	1.00	0.01	121,121,121,121	1
2	CA	g	901[2]	1/1	1.00	0.01	96,96,96,96	1
2	CA	g	902[2]	1/1	1.00	0.01	85,85,85,85	1
2	CA	g	903[2]	1/1	1.00	0.02	87,87,87,87	1
2	CA	f	901[2]	1/1	1.00	0.01	105,105,105,105	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	f	902[2]	1/1	1.00	0.01	102,102,102,102	1
2	CA	f	903[2]	1/1	1.00	0.03	113,113,113,113	1
2	CA	e	901[2]	1/1	1.00	0.01	87,87,87,87	1
2	CA	e	902[2]	1/1	1.00	0.01	79,79,79,79	1
2	CA	e	903[2]	1/1	1.00	0.03	106,106,106,106	1
2	CA	d	901[2]	1/1	1.00	0.01	117,117,117,117	1
2	CA	d	902[2]	1/1	1.00	0.01	82,82,82,82	1
2	CA	d	903[2]	1/1	1.00	0.02	96,96,96,96	1
2	CA	c	901[2]	1/1	1.00	0.02	87,87,87,87	1
2	CA	c	902[2]	1/1	1.00	0.03	98,98,98,98	1
2	CA	G	901[1]	1/1	1.00	0.02	84,84,84,84	1
2	CA	b	901[2]	1/1	1.00	0.02	112,112,112,112	1
2	CA	b	902[2]	1/1	1.00	0.01	87,87,87,87	1
2	CA	b	903[2]	1/1	1.00	0.02	134,134,134,134	1
2	CA	h	901[2]	1/1	1.00	0.01	84,84,84,84	1
2	CA	h	902[2]	1/1	1.00	0.02	98,98,98,98	1
2	CA	h	903[2]	1/1	1.00	0.01	114,114,114,114	1
2	CA	i	901[2]	1/1	1.00	0.01	112,112,112,112	1
2	CA	i	902[2]	1/1	1.00	0.01	115,115,115,115	1
2	CA	i	903[2]	1/1	1.00	0.03	116,116,116,116	1
2	CA	j	901[2]	1/1	1.00	0.01	104,104,104,104	1
2	CA	G	902[1]	1/1	1.00	0.01	82,82,82,82	1
2	CA	j	903[2]	1/1	1.00	0.01	100,100,100,100	1
2	CA	k	901[2]	1/1	1.00	0.01	102,102,102,102	1
2	CA	k	902[2]	1/1	1.00	0.02	96,96,96,96	1
2	CA	k	903[2]	1/1	1.00	0.03	147,147,147,147	1
2	CA	l	901[2]	1/1	1.00	0.01	108,108,108,108	1
2	CA	l	902[2]	1/1	1.00	0.01	94,94,94,94	1
2	CA	l	903[2]	1/1	1.00	0.02	124,124,124,124	1
2	CA	m	901[2]	1/1	1.00	0.01	91,91,91,91	1
2	CA	m	902[2]	1/1	1.00	0.02	103,103,103,103	1
2	CA	m	903[2]	1/1	1.00	0.01	112,112,112,112	1
2	CA	n	901[2]	1/1	1.00	0.03	97,97,97,97	1
2	CA	n	902[2]	1/1	1.00	0.01	97,97,97,97	1
2	CA	n	903[2]	1/1	1.00	0.01	93,93,93,93	1

6.5 Other polymers

There are no such residues in this entry.