



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2024 – 12:19 PM EST

PDB ID : 6UWI  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

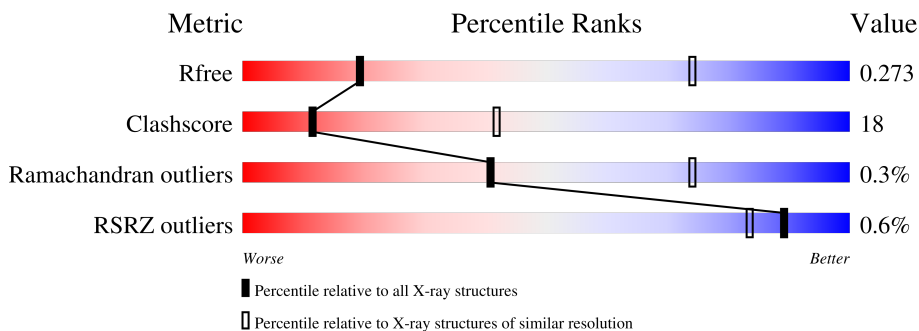
# 1 Overall quality at a glance

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.











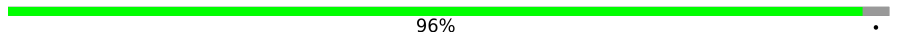
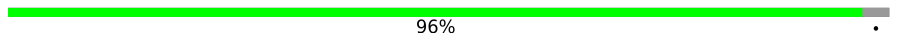
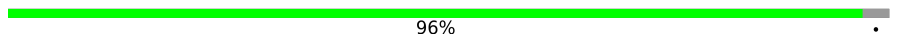
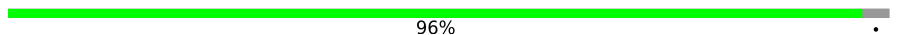
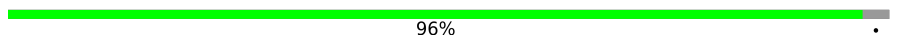
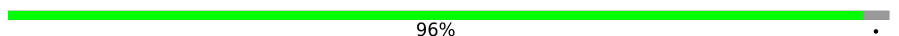
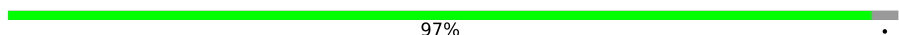
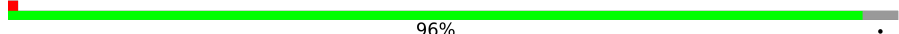
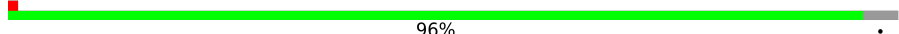
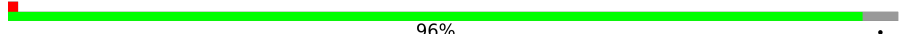
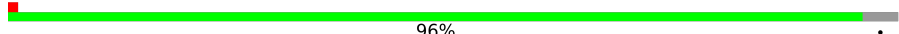
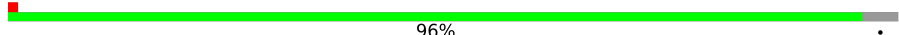
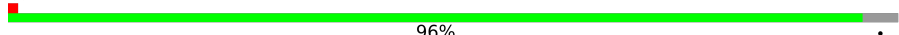
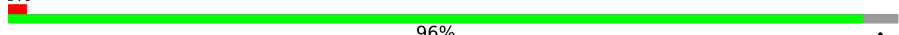
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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  $\geq 3$ , 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	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
1	G	667	 63% 34% .
1	H	667	 % 60% 36% ..
1	I	667	 % 61% 34% .
1	J	667	 % 61% 35% .
1	K	667	 % 61% 35% .
1	L	667	 % 60% 36% .
1	M	667	 % 61% 35% .
1	N	667	 61% 35% .
1	a	667	 96% .
1	b	667	 96% .
1	c	667	 96% .
1	d	667	 96% .
1	e	667	 96% .
1	f	667	 96% .
1	g	667	 97% .
1	h	667	 % 96% .
1	i	667	 % 96% .
1	j	667	 % 96% .
1	k	667	 % 96% .
1	l	667	 % 96% .
1	m	667	 % 96% .
1	n	667	 2% 96% .

## 2 Entry composition [i](#)

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

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

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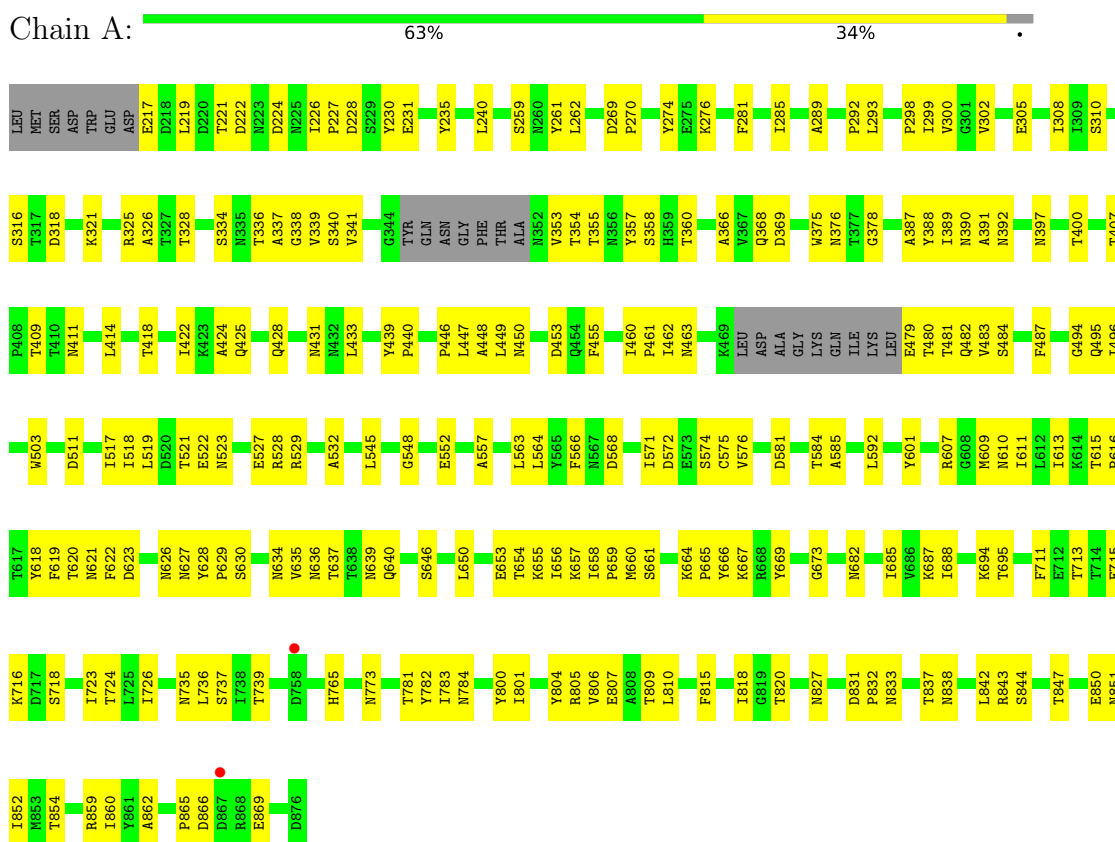
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	3	Total 3 Ca 3	0	3
2	I	3	Total 3 Ca 3	0	3
2	J	3	Total 3 Ca 3	0	3
2	K	3	Total 3 Ca 3	0	3
2	L	3	Total 3 Ca 3	0	3
2	M	3	Total 3 Ca 3	0	3
2	N	3	Total 3 Ca 3	0	3
2	a	3	Total 3 Ca 3	0	3
2	g	3	Total 3 Ca 3	0	3
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

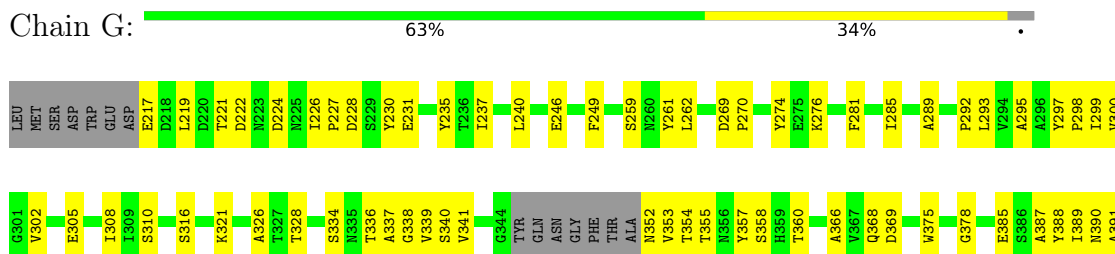
### 3 Residue-property plots i

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: ADP-ribosyltransferase binding component

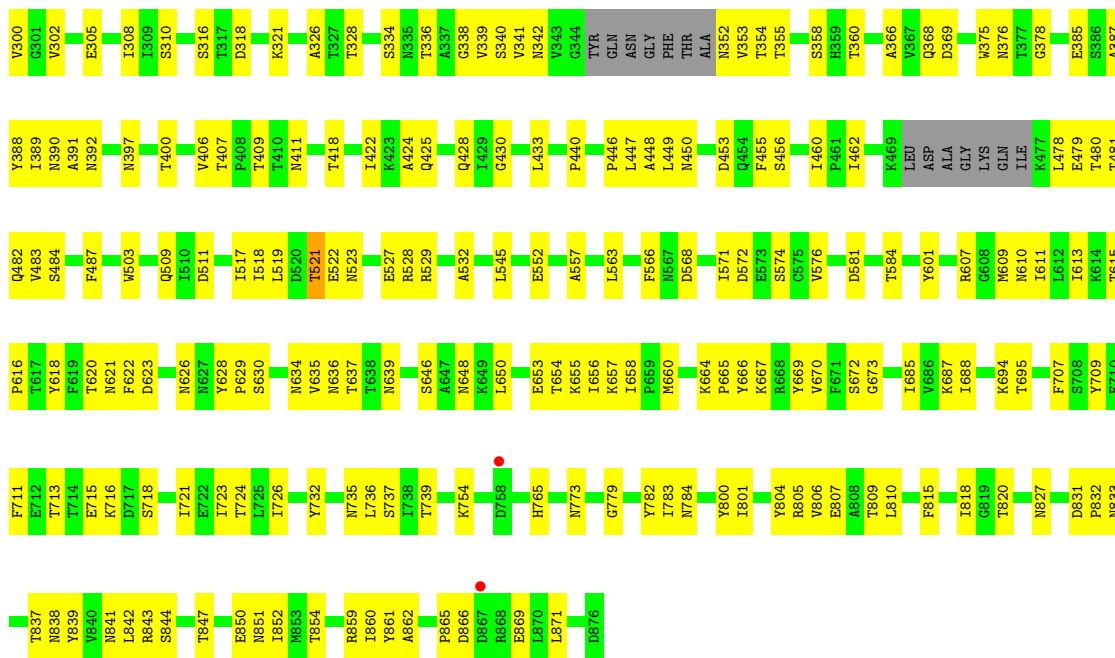


- Molecule 1: ADP-ribosyltransferase binding component



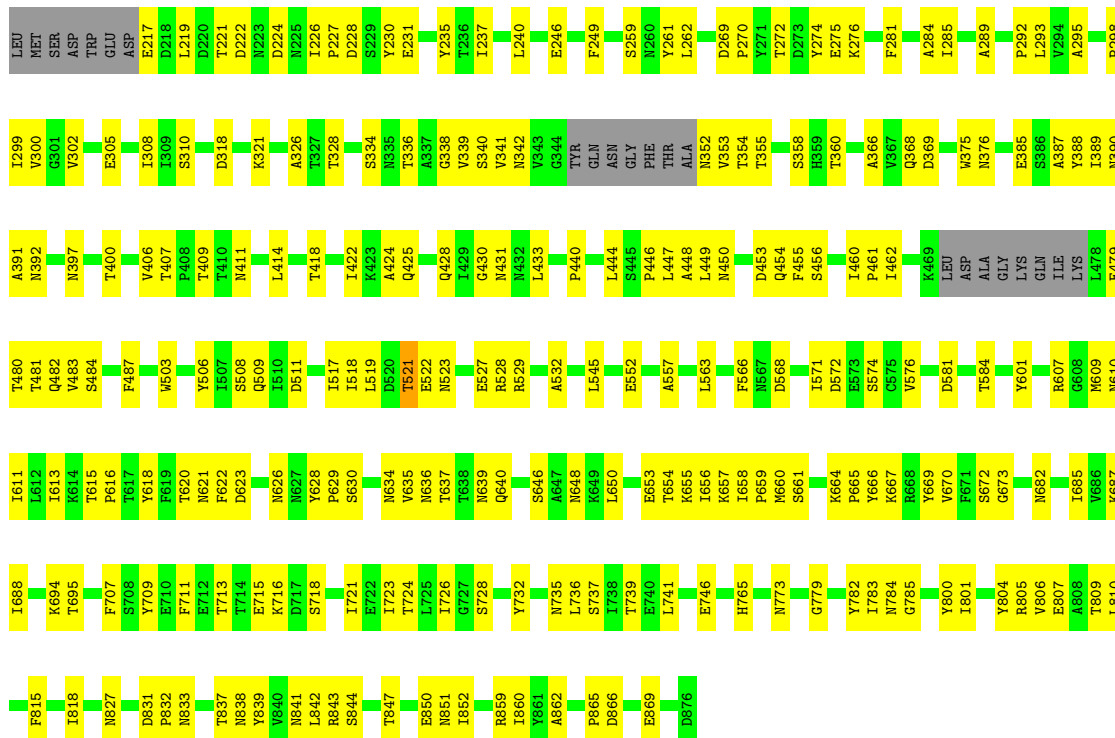






- Molecule 1: ADP-ribosyltransferase binding component

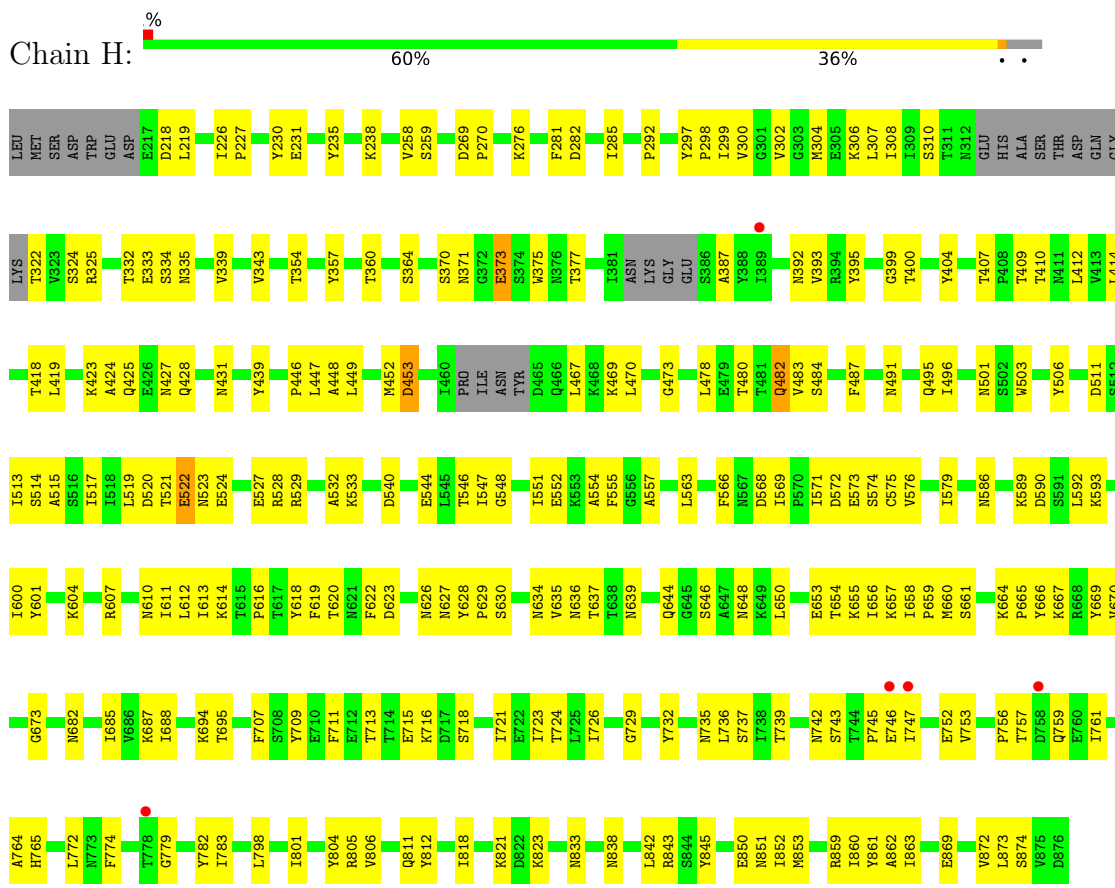
Chain D: 61% 35%



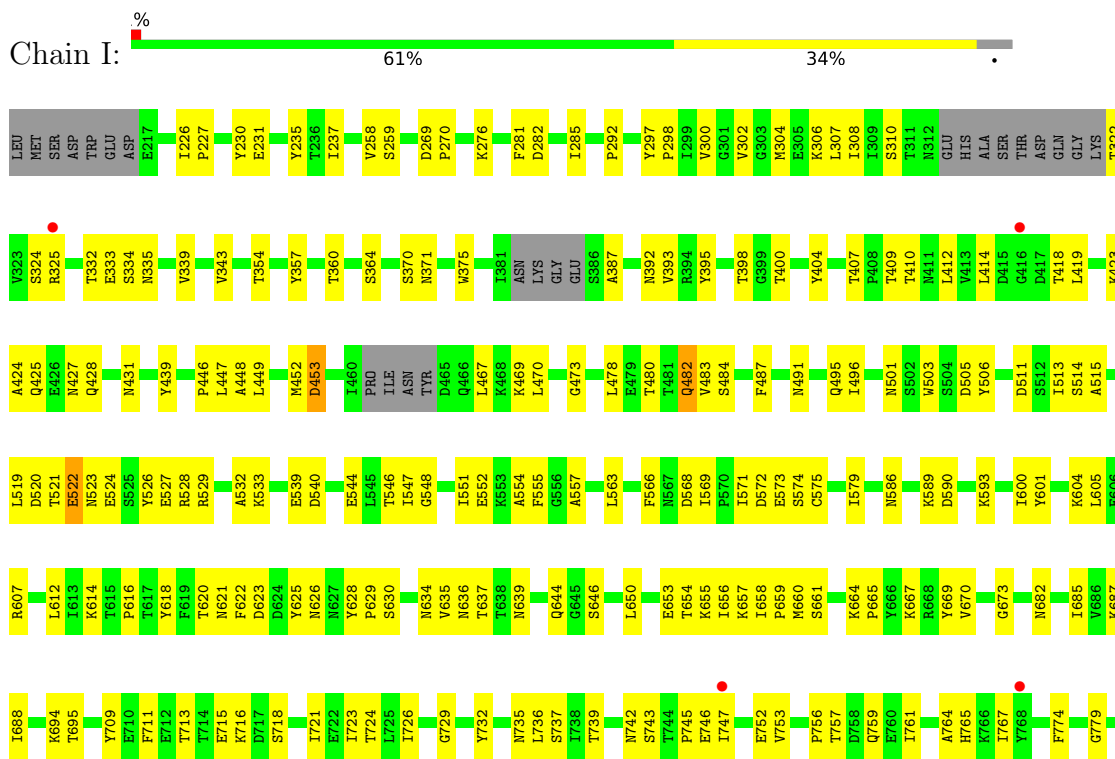
- Molecule 1: ADP-ribosyltransferase binding component

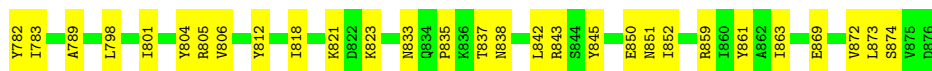
Chain C: 63% 34%



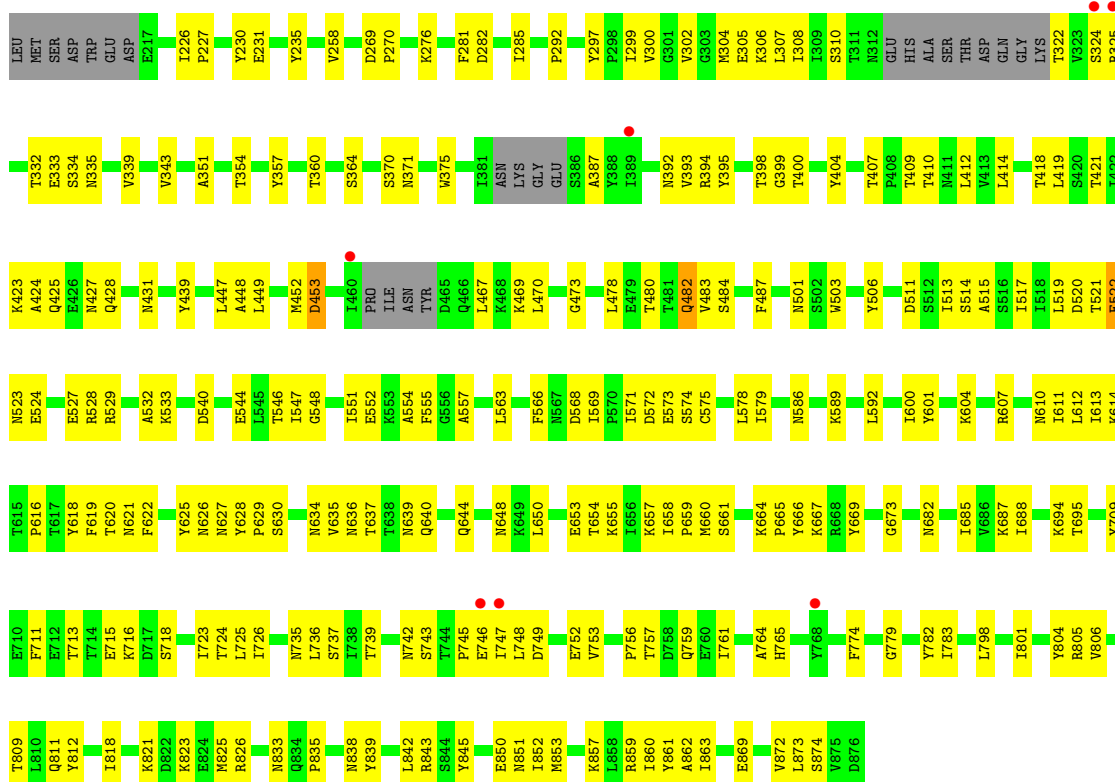


• Molecule 1: ADP-ribosyltransferase binding component

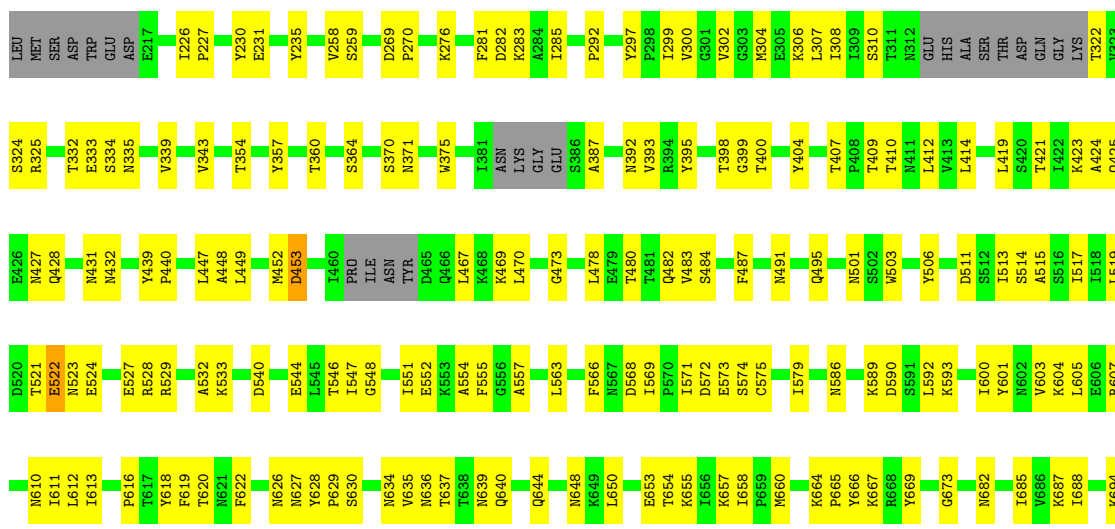




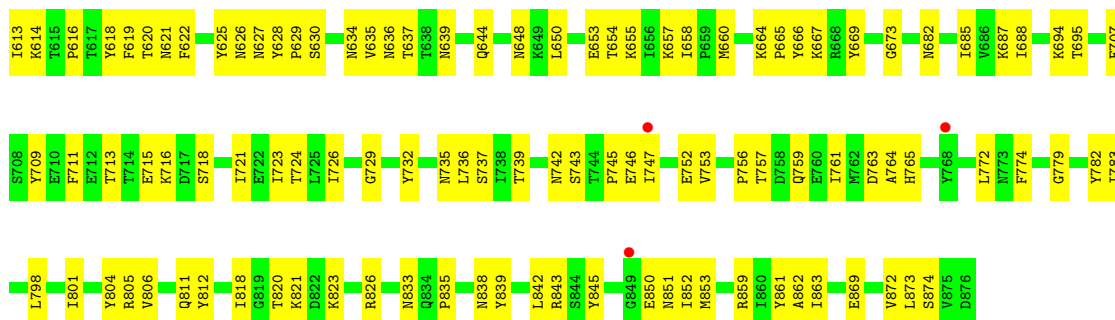
● Molecule 1: ADP-ribosyltransferase binding component



● Molecule 1: ADP-ribosyltransferase binding component

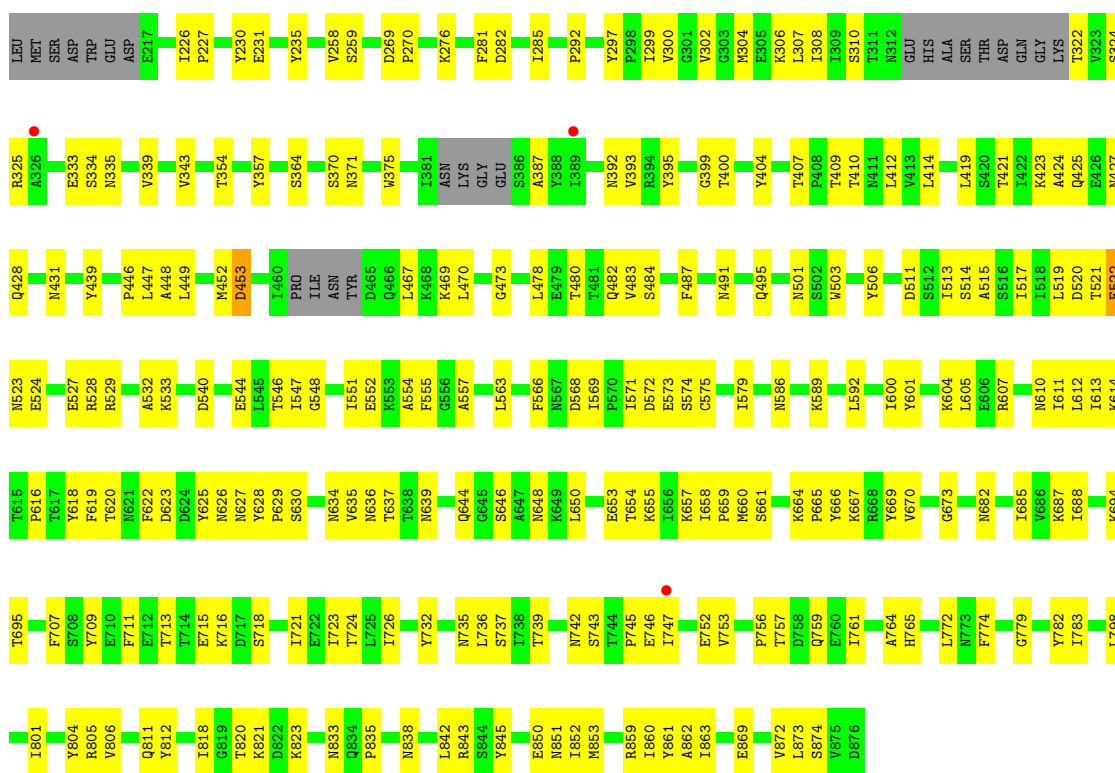






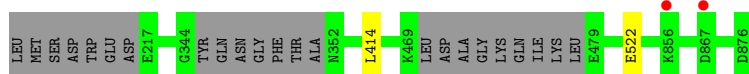
- Molecule 1: ADP-ribosyltransferase binding component

Chain N: 61% 35%



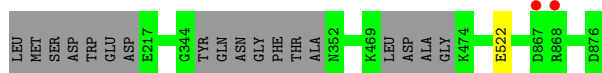
- Molecule 1: ADP-ribosyltransferase binding component

Chain a: 96%



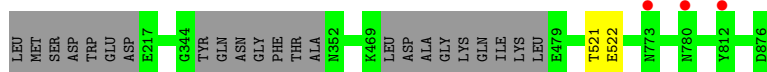
- Molecule 1: ADP-ribosyltransferase binding component

Chain g: 97%



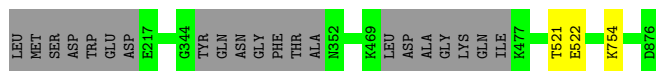
- Molecule 1: ADP-ribosyltransferase binding component

Chain f: 96%



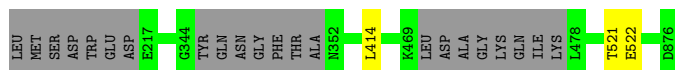
- Molecule 1: ADP-ribosyltransferase binding component

Chain e: 96%



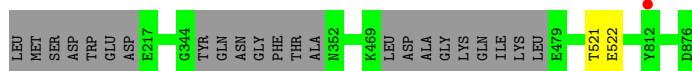
- Molecule 1: ADP-ribosyltransferase binding component

Chain d: 96%



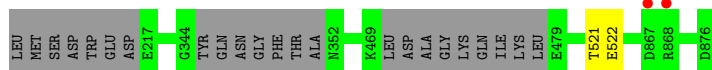
- Molecule 1: ADP-ribosyltransferase binding component

Chain c: 96%



- Molecule 1: ADP-ribosyltransferase binding component

Chain b: 96%

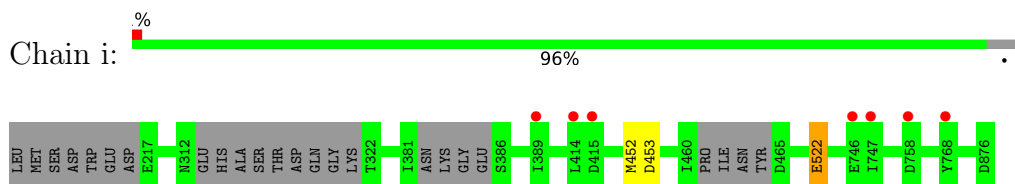


- Molecule 1: ADP-ribosyltransferase binding component

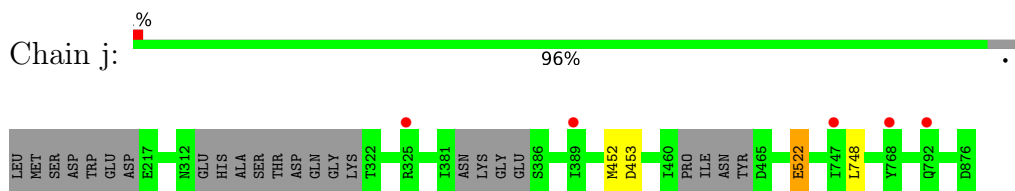
Chain h: 96%



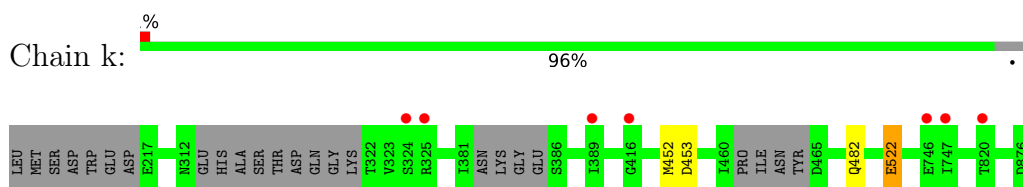
- Molecule 1: ADP-ribosyltransferase binding component



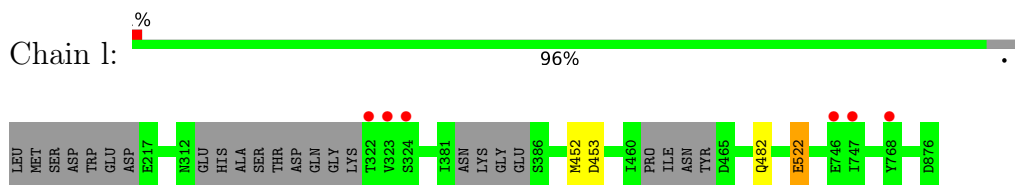
- Molecule 1: ADP-ribosyltransferase binding component



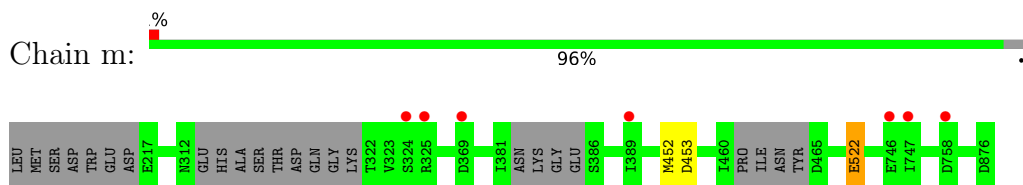
- Molecule 1: ADP-ribosyltransferase binding component



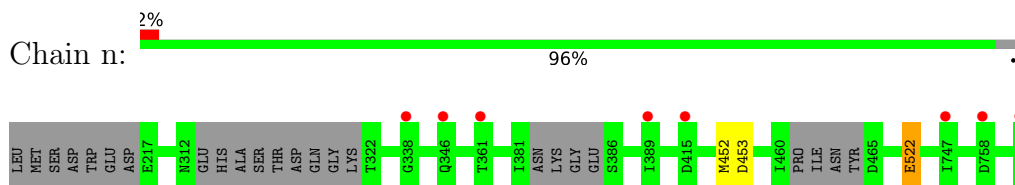
- Molecule 1: ADP-ribosyltransferase binding component



- Molecule 1: ADP-ribosyltransferase binding component



- Molecule 1: ADP-ribosyltransferase binding component



D876



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 3.66Å)	Xtrriage
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	11423 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.0	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , -4.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.219 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	141662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	173	0
1	B	5070	0	4424	181	0
1	C	5067	0	4411	183	0
1	D	5078	0	4441	186	0
1	E	5087	0	4488	182	0
1	F	5070	0	4457	175	0
1	G	5105	0	4476	182	0
1	H	5035	0	4486	185	0
1	I	5035	0	4428	180	0
1	J	5035	0	4438	177	0
1	K	5035	0	4448	177	0
1	L	5035	0	4449	181	0
1	M	5035	0	4469	177	0
1	N	5035	0	4490	178	0
1	a	5067	0	4477	0	0
1	b	5070	0	4440	0	0
1	c	5067	0	4449	0	0
1	d	5078	0	4472	0	0
1	e	5087	0	4456	0	0
1	f	5070	0	4474	0	0
1	g	5105	0	4548	0	0
1	h	5035	0	4409	0	0
1	i	5035	0	4434	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	5035	0	4424	0	0
1	k	5035	0	4410	0	0
1	l	5035	0	4437	0	0
1	m	5035	0	4415	0	0
1	n	5035	0	4395	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
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	124572	2368	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 2368 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: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
1:G:765[1]:HIS:HE2	1:G:804[1]:TYR:HH	1.08	0.92

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	638/667 (96%)	555 (87%)	81 (13%)	2 (0%)	41	74
1	B	638/667 (96%)	555 (87%)	82 (13%)	1 (0%)	47	78
1	C	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	47	78
1	D	639/667 (96%)	558 (87%)	79 (12%)	2 (0%)	41	74
1	E	640/667 (96%)	553 (86%)	85 (13%)	2 (0%)	41	74
1	F	638/667 (96%)	554 (87%)	83 (13%)	1 (0%)	47	78
1	G	643/667 (96%)	560 (87%)	82 (13%)	1 (0%)	47	78
1	H	635/667 (95%)	542 (85%)	89 (14%)	4 (1%)	25	62
1	I	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	29	66
1	J	635/667 (95%)	540 (85%)	92 (14%)	3 (0%)	29	66
1	K	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	41	74
1	L	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	41	74
1	M	635/667 (95%)	544 (86%)	88 (14%)	3 (0%)	29	66
1	N	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	41	74
1	a	638/667 (96%)	554 (87%)	82 (13%)	2 (0%)	41	74
1	b	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	638/667 (96%)	553 (87%)	84 (13%)	1 (0%)	47	78
1	d	639/667 (96%)	556 (87%)	81 (13%)	2 (0%)	41	74
1	e	640/667 (96%)	553 (86%)	85 (13%)	2 (0%)	41	74
1	f	638/667 (96%)	554 (87%)	83 (13%)	1 (0%)	47	78
1	g	643/667 (96%)	562 (87%)	80 (12%)	1 (0%)	47	78
1	h	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	29	66
1	i	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	41	74
1	j	635/667 (95%)	542 (85%)	91 (14%)	2 (0%)	41	74
1	k	635/667 (95%)	541 (85%)	91 (14%)	3 (0%)	29	66
1	l	635/667 (95%)	542 (85%)	90 (14%)	3 (0%)	29	66
1	m	635/667 (95%)	543 (86%)	90 (14%)	2 (0%)	41	74
1	n	635/667 (95%)	541 (85%)	92 (14%)	2 (0%)	41	74
All	All	17838/18676 (96%)	15358 (86%)	2424 (14%)	56 (0%)	41	74

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 monosaccharides 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	644/667 (96%)	-0.89	2 (0%) 94 90	72, 123, 168, 194	644 (100%)
1	B	644/667 (96%)	-0.88	1 (0%) 95 93	73, 123, 167, 198	644 (100%)
1	C	644/667 (96%)	-0.88	3 (0%) 91 85	74, 123, 167, 191	644 (100%)
1	D	645/667 (96%)	-0.84	0 100 100	74, 124, 166, 193	645 (100%)
1	E	646/667 (96%)	-0.87	2 (0%) 94 90	72, 126, 172, 193	646 (100%)
1	F	644/667 (96%)	-0.93	0 100 100	75, 124, 169, 195	644 (100%)
1	G	649/667 (97%)	-0.91	2 (0%) 94 90	74, 122, 167, 194	649 (100%)
1	H	643/667 (96%)	-0.81	5 (0%) 86 78	78, 128, 170, 193	643 (100%)
1	I	643/667 (96%)	-0.78	4 (0%) 89 83	73, 131, 174, 194	643 (100%)
1	J	643/667 (96%)	-0.79	7 (1%) 80 71	75, 129, 172, 193	643 (100%)
1	K	643/667 (96%)	-0.84	7 (1%) 80 71	76, 127, 169, 191	643 (100%)
1	L	643/667 (96%)	-0.85	4 (0%) 89 83	78, 128, 171, 191	643 (100%)
1	M	643/667 (96%)	-0.82	5 (0%) 86 78	73, 127, 171, 194	643 (100%)
1	N	643/667 (96%)	-0.84	3 (0%) 91 85	76, 128, 170, 197	643 (100%)
1	a	644/667 (96%)	-0.90	2 (0%) 94 90	76, 124, 166, 193	644 (100%)
1	b	644/667 (96%)	-0.88	2 (0%) 94 90	73, 126, 172, 192	644 (100%)
1	c	644/667 (96%)	-0.86	1 (0%) 95 93	69, 124, 169, 193	644 (100%)
1	d	645/667 (96%)	-0.94	0 100 100	77, 122, 167, 191	645 (100%)
1	e	646/667 (96%)	-0.91	0 100 100	75, 123, 167, 191	646 (100%)
1	f	644/667 (96%)	-0.88	3 (0%) 91 85	73, 123, 166, 194	644 (100%)
1	g	649/667 (97%)	-0.88	2 (0%) 94 90	73, 122, 168, 197	649 (100%)
1	h	643/667 (96%)	-0.80	4 (0%) 89 83	77, 129, 171, 193	643 (100%)
1	i	643/667 (96%)	-0.78	7 (1%) 80 71	73, 127, 169, 198	643 (100%)
1	j	643/667 (96%)	-0.79	5 (0%) 86 78	75, 127, 168, 191	643 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	k	643/667 (96%)	-0.72	7 (1%) 80 71	75, 128, 171, 193	643 (100%)
1	l	643/667 (96%)	-0.77	6 (0%) 84 76	76, 130, 173, 193	643 (100%)
1	m	643/667 (96%)	-0.80	7 (1%) 80 71	77, 128, 171, 196	643 (100%)
1	n	643/667 (96%)	-0.74	11 (1%) 70 59	75, 128, 169, 193	643 (100%)
All	All	18034/18676 (96%)	-0.84	102 (0%) 89 83	69, 126, 170, 198	18034 (100%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	747[1]	ILE	7.9
1	n	747[2]	ILE	7.7
1	l	747[2]	ILE	6.7
1	h	746[2]	GLU	6.7
1	m	747[2]	ILE	5.8

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	D	903[1]	1/1	0.83	0.16	126,126,126,126	1
2	CA	A	903[1]	1/1	0.92	0.09	117,117,117,117	1
2	CA	G	902[1]	1/1	0.93	0.15	82,82,82,82	1
2	CA	J	901[1]	1/1	0.94	0.08	87,87,87,87	1
2	CA	C	903[1]	1/1	0.96	0.10	98,98,98,98	1
2	CA	H	903[1]	1/1	0.96	0.10	122,122,122,122	1
2	CA	G	903[1]	1/1	0.96	0.08	103,103,103,103	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	M	903[1]	1/1	0.96	0.07	112,112,112,112	1
2	CA	a	901[2]	1/1	0.96	0.09	103,103,103,103	1
2	CA	a	903[2]	1/1	0.96	0.10	121,121,121,121	1
2	CA	f	903[2]	1/1	0.96	0.07	113,113,113,113	1
2	CA	b	901[2]	1/1	0.96	0.17	112,112,112,112	1
2	CA	b	902[2]	1/1	0.96	0.12	87,87,87,87	1
2	CA	k	903[2]	1/1	0.96	0.10	147,147,147,147	1
2	CA	I	901[1]	1/1	0.97	0.12	115,115,115,115	1
2	CA	G	901[1]	1/1	0.97	0.15	84,84,84,84	1
2	CA	e	903[2]	1/1	0.97	0.09	106,106,106,106	1
2	CA	d	901[2]	1/1	0.97	0.14	117,117,117,117	1
2	CA	c	901[2]	1/1	0.97	0.12	87,87,87,87	1
2	CA	L	903[1]	1/1	0.97	0.10	104,104,104,104	1
2	CA	B	902[1]	1/1	0.97	0.13	102,102,102,102	1
2	CA	j	901[2]	1/1	0.97	0.19	104,104,104,104	1
2	CA	C	901[1]	1/1	0.97	0.14	105,105,105,105	1
2	CA	H	901[1]	1/1	0.98	0.09	106,106,106,106	1
2	CA	A	902[1]	1/1	0.98	0.12	89,89,89,89	1
2	CA	g	903[2]	1/1	0.98	0.07	87,87,87,87	1
2	CA	f	901[2]	1/1	0.98	0.13	105,105,105,105	1
2	CA	E	901[1]	1/1	0.98	0.12	105,105,105,105	1
2	CA	e	901[2]	1/1	0.98	0.11	87,87,87,87	1
2	CA	I	903[1]	1/1	0.98	0.11	132,132,132,132	1
2	CA	E	903[1]	1/1	0.98	0.11	124,124,124,124	1
2	CA	d	903[2]	1/1	0.98	0.08	96,96,96,96	1
2	CA	K	903[1]	1/1	0.98	0.08	100,100,100,100	1
2	CA	B	901[1]	1/1	0.98	0.16	116,116,116,116	1
2	CA	M	901[1]	1/1	0.98	0.13	105,105,105,105	1
2	CA	b	903[2]	1/1	0.98	0.11	134,134,134,134	1
2	CA	h	901[2]	1/1	0.98	0.12	84,84,84,84	1
2	CA	h	902[2]	1/1	0.98	0.12	98,98,98,98	1
2	CA	i	901[2]	1/1	0.98	0.16	112,112,112,112	1
2	CA	D	901[1]	1/1	0.98	0.15	99,99,99,99	1
2	CA	j	903[2]	1/1	0.98	0.09	100,100,100,100	1
2	CA	k	901[2]	1/1	0.98	0.15	102,102,102,102	1
2	CA	N	903[1]	1/1	0.98	0.07	83,83,83,83	1
2	CA	l	901[2]	1/1	0.98	0.12	108,108,108,108	1
2	CA	l	902[2]	1/1	0.98	0.14	94,94,94,94	1
2	CA	l	903[2]	1/1	0.98	0.11	124,124,124,124	1
2	CA	n	901[2]	1/1	0.98	0.14	97,97,97,97	1
2	CA	n	903[2]	1/1	0.98	0.09	93,93,93,93	1
2	CA	K	902[1]	1/1	0.99	0.14	93,93,93,93	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	F	902[1]	1/1	0.99	0.14	100,100,100,100	1
2	CA	L	901[1]	1/1	0.99	0.12	87,87,87,87	1
2	CA	c	902[2]	1/1	0.99	0.10	98,98,98,98	1
2	CA	c	903[2]	1/1	0.99	0.08	111,111,111,111	1
2	CA	B	903[1]	1/1	0.99	0.09	115,115,115,115	1
2	CA	F	903[1]	1/1	0.99	0.09	114,114,114,114	1
2	CA	M	902[1]	1/1	0.99	0.12	106,106,106,106	1
2	CA	H	902[1]	1/1	0.99	0.16	92,92,92,92	1
2	CA	N	901[1]	1/1	0.99	0.15	93,93,93,93	1
2	CA	h	903[2]	1/1	0.99	0.10	114,114,114,114	1
2	CA	A	901[1]	1/1	0.99	0.15	82,82,82,82	1
2	CA	i	902[2]	1/1	0.99	0.16	115,115,115,115	1
2	CA	i	903[2]	1/1	0.99	0.09	116,116,116,116	1
2	CA	C	902[1]	1/1	0.99	0.13	89,89,89,89	1
2	CA	j	902[2]	1/1	0.99	0.13	103,103,103,103	1
2	CA	a	902[2]	1/1	0.99	0.16	93,93,93,93	1
2	CA	I	902[1]	1/1	0.99	0.15	97,97,97,97	1
2	CA	k	902[2]	1/1	0.99	0.12	96,96,96,96	1
2	CA	g	901[2]	1/1	0.99	0.15	96,96,96,96	1
2	CA	E	902[1]	1/1	0.99	0.15	87,87,87,87	1
2	CA	F	901[1]	1/1	0.99	0.10	88,88,88,88	1
2	CA	J	902[1]	1/1	0.99	0.10	111,111,111,111	1
2	CA	m	901[2]	1/1	0.99	0.10	91,91,91,91	1
2	CA	m	902[2]	1/1	0.99	0.14	103,103,103,103	1
2	CA	m	903[2]	1/1	0.99	0.09	112,112,112,112	1
2	CA	J	903[1]	1/1	0.99	0.08	111,111,111,111	1
2	CA	K	901[1]	1/1	0.99	0.12	116,116,116,116	1
2	CA	d	902[2]	1/1	1.00	0.13	82,82,82,82	1
2	CA	f	902[2]	1/1	1.00	0.12	102,102,102,102	1
2	CA	D	902[1]	1/1	1.00	0.12	93,93,93,93	1
2	CA	g	902[2]	1/1	1.00	0.13	85,85,85,85	1
2	CA	e	902[2]	1/1	1.00	0.10	79,79,79,79	1
2	CA	N	902[1]	1/1	1.00	0.13	85,85,85,85	1
2	CA	n	902[2]	1/1	1.00	0.18	97,97,97,97	1
2	CA	L	902[1]	1/1	1.00	0.10	82,82,82,82	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.