



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 3, 2025 – 12:49 PM EDT

PDB ID : 3E20 / pdb\_00003e20  
Title : Crystal structure of S.pombe eRF1/eRF3 complex  
Authors : Cheng, Z.; Lim, M.; Kong, C.; Song, H.  
Deposited on : 2008-08-05  
Resolution : 3.50 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 : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

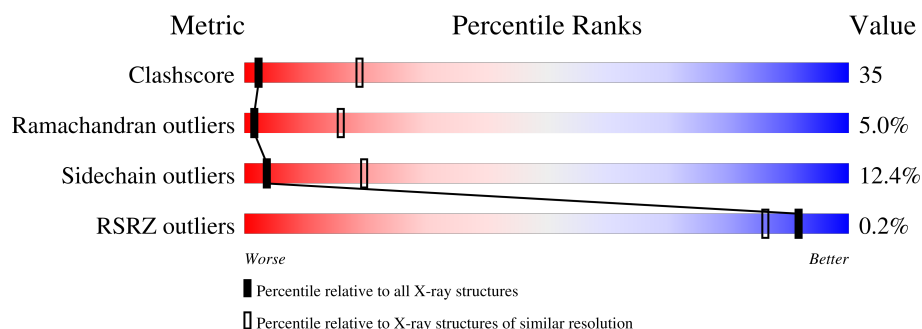
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	201	52% 37% 7% ..
1	D	201	50% 39% 7% ..
1	E	201	40% 43% 13% .
1	J	201	41% 46% 10% .
2	B	441	30% 22% 6% . 41%
2	C	441	32% 21% 6% . 41%
2	H	441	21% 15% . 60%

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Mol	Chain	Length	Quality of chain
2	K	441	<div><div><div><div><div></div><div>%</div></div><div><div></div><div>22%</div></div><div><div></div><div>14%</div></div><div><div></div><div>• •</div></div><div><div></div><div>60%</div></div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13096 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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	D	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	E	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	J	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	GLY	-	expression tag	UNP O74718
A	463	PRO	-	expression tag	UNP O74718
A	464	LEU	-	expression tag	UNP O74718
A	465	GLY	-	expression tag	UNP O74718
A	466	SER	-	expression tag	UNP O74718
D	462	GLY	-	expression tag	UNP O74718
D	463	PRO	-	expression tag	UNP O74718
D	464	LEU	-	expression tag	UNP O74718
D	465	GLY	-	expression tag	UNP O74718
D	466	SER	-	expression tag	UNP O74718
E	462	GLY	-	expression tag	UNP O74718
E	463	PRO	-	expression tag	UNP O74718
E	464	LEU	-	expression tag	UNP O74718
E	465	GLY	-	expression tag	UNP O74718
E	466	SER	-	expression tag	UNP O74718
J	462	GLY	-	expression tag	UNP O74718
J	463	PRO	-	expression tag	UNP O74718
J	464	LEU	-	expression tag	UNP O74718
J	465	GLY	-	expression tag	UNP O74718
J	466	SER	-	expression tag	UNP O74718

- Molecule 2 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	261	Total 2088	C 1321	N 347	O 405	S 15	0	0	0
2	B	261	Total 2088	C 1321	N 347	O 405	S 15	0	0	0
2	H	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0
2	K	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	expression tag	UNP P79063
C	-6	HIS	-	expression tag	UNP P79063
C	-5	HIS	-	expression tag	UNP P79063
C	-4	HIS	-	expression tag	UNP P79063
C	-3	HIS	-	expression tag	UNP P79063
C	-2	HIS	-	expression tag	UNP P79063
C	-1	HIS	-	expression tag	UNP P79063
C	0	MET	-	expression tag	UNP P79063
B	-7	MET	-	expression tag	UNP P79063
B	-6	HIS	-	expression tag	UNP P79063
B	-5	HIS	-	expression tag	UNP P79063
B	-4	HIS	-	expression tag	UNP P79063
B	-3	HIS	-	expression tag	UNP P79063
B	-2	HIS	-	expression tag	UNP P79063
B	-1	HIS	-	expression tag	UNP P79063
B	0	MET	-	expression tag	UNP P79063
H	-7	MET	-	expression tag	UNP P79063
H	-6	HIS	-	expression tag	UNP P79063
H	-5	HIS	-	expression tag	UNP P79063
H	-4	HIS	-	expression tag	UNP P79063
H	-3	HIS	-	expression tag	UNP P79063
H	-2	HIS	-	expression tag	UNP P79063
H	-1	HIS	-	expression tag	UNP P79063
H	0	MET	-	expression tag	UNP P79063
K	-7	MET	-	expression tag	UNP P79063
K	-6	HIS	-	expression tag	UNP P79063
K	-5	HIS	-	expression tag	UNP P79063
K	-4	HIS	-	expression tag	UNP P79063
K	-3	HIS	-	expression tag	UNP P79063
K	-2	HIS	-	expression tag	UNP P79063

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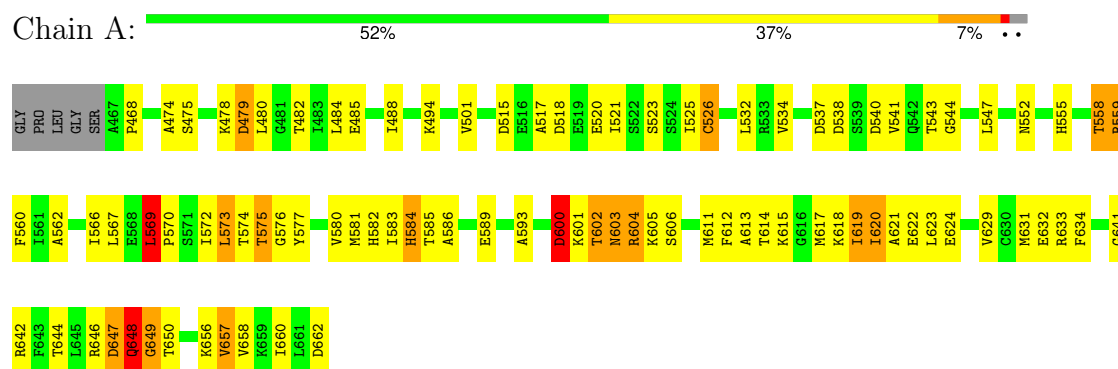
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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P79063
K	0	MET	-	expression tag	UNP P79063

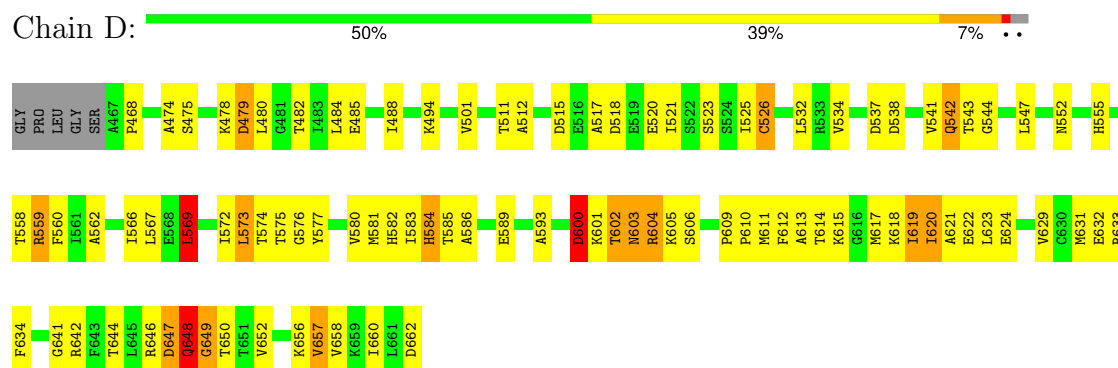
### 3 Residue-property plots

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.

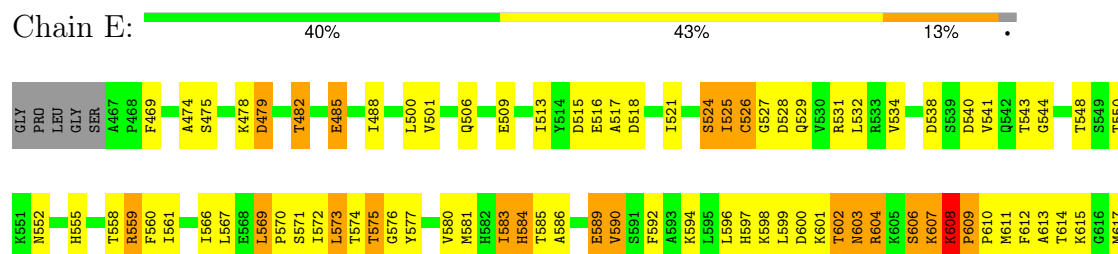
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

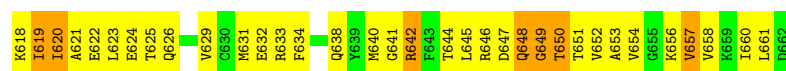


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit



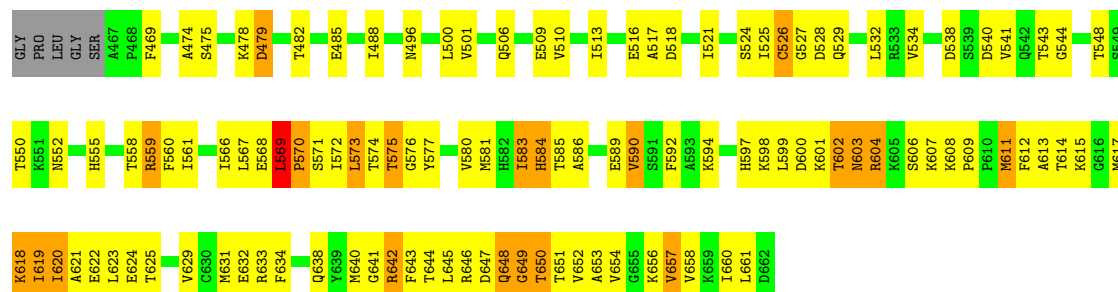
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit





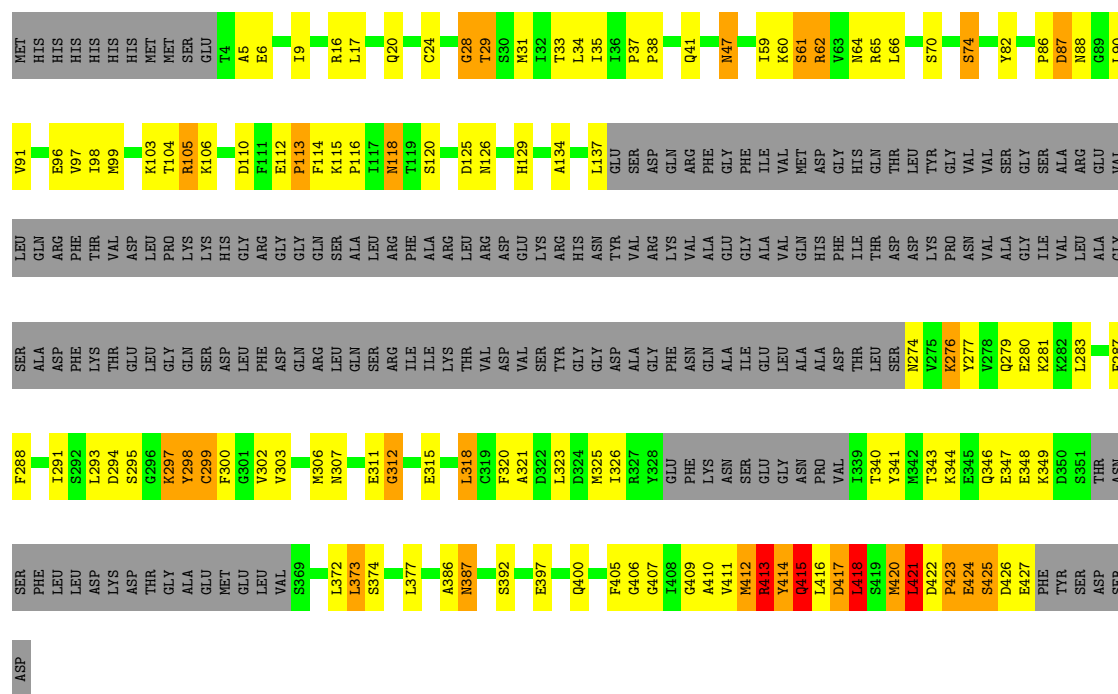
• Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

Chain J: 41% 46% 10%



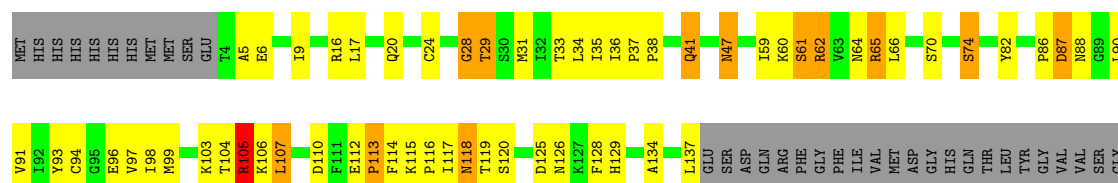
• Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain C: 32% 21% 6% 41%

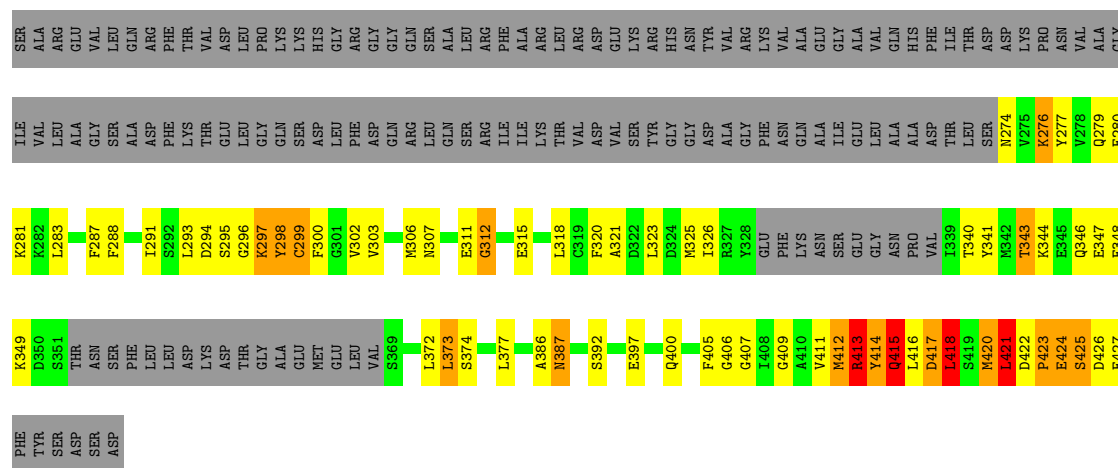


• Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain B: 30% 22% 6% 41%

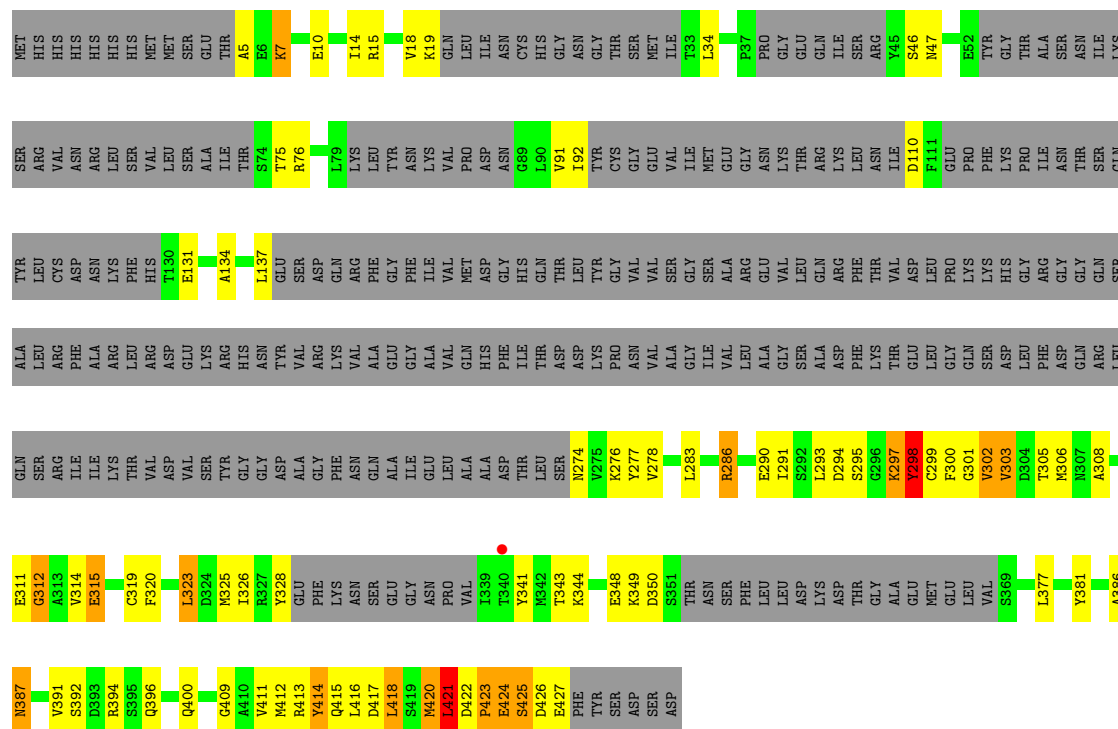






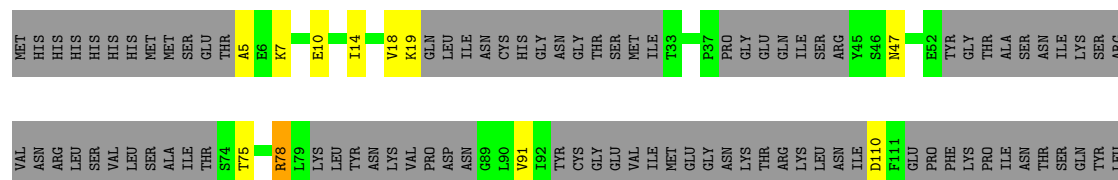
• Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain H: 21% 15% 60%



• Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain K: 22% 14% 60%



V391	S392	D393	R394	S395	Q396	Q400	F405	G406	G407	I408	G409	A410	V411	M412	R413	Y414	Q415	L416	D417	L418	S419	M420	L421	D422	P423	E424	S425	D426	E427	PHE	TYR	SER	ASP	SER	ASP																			
A313	V314	D315	C319	F320	L323	D324	N325	I326	R327	Y328	GLU	PHE	LYS	ASN	GLN	ASN	ILE	GLU	LEU	ALA	PRO	VAL	I339	T340	Y341	M342	T343	K344	E348	K349	D350	S351	THR	ASN	SER	PHE	LEU	LEU	ASP	LYS	ASP	THR	GLY	ALA	GLU	MET	GLU	LEU	VAL	S369	L377	Y381	A386	N387
ILE	LYS	THR	VAL	ASP	VAL	SER	TYR	GLY	ASP	ALA	GLY	PHE	ASN	VAL	ALA	GLN	ASN	ILE	GLU	LEU	ALA	ALA	THR	SER	N274	V275	K276	Y277	V278	K281	K282	L283	R286	E290	I291	S292	L293	D294	S295	G296	K297	Y298	C299	F300	G301	V302	V303	D304	T305	M306	M307	A308	E311	G312
CYS	ASP	ASN	LYS	PHE	HIS	T130	E131	L137	GLU	SER	GLN	ASP	GLN	PHE	GLY	PHE	ILE	VAL	VAL	MET	ASP	GLY	HIS	THR	LEU	TYR	GLY	VAL	VAL	SER	GLY	SER	ALA	ARG	GLU	VAL	LEU	GLN	ARG	PRO	LYS	LYS	HIS	GLY	ARG	GLY	GLN	SER	ALA	LEU	ARG	PHE		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.85Å 129.85Å 332.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.50) 99.7 (30.00-3.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.258 , 0.280 0.277 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 178.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/1547	0.85	4/2089 (0.2%)
1	D	0.46	0/1547	0.84	3/2089 (0.1%)
1	E	0.61	2/1547 (0.1%)	0.98	6/2089 (0.3%)
1	J	0.58	0/1547	0.97	7/2089 (0.3%)
2	B	0.40	0/2119	0.87	6/2848 (0.2%)
2	C	0.41	0/2119	0.85	6/2848 (0.2%)
2	H	0.40	0/1425	0.76	0/1901
2	K	0.40	0/1425	0.78	2/1901 (0.1%)
All	All	0.47	2/13276 (0.0%)	0.87	34/17854 (0.2%)

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	A	0	2
1	D	0	2
1	E	0	3
1	J	0	1
2	B	0	1
2	C	0	1
2	H	0	1
2	K	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	609	PRO	CA-C	6.40	1.58	1.52
1	E	608	LYS	N-CA	-5.98	1.37	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	608	LYS	CA-C-N	10.89	131.60	120.38
1	E	608	LYS	C-N-CA	10.89	131.60	120.38
2	B	105	ARG	CG-CD-NE	8.02	129.65	112.00
1	E	609	PRO	N-CA-C	-7.90	101.06	110.70
1	D	600	ASP	N-CA-C	7.70	115.09	108.78

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	569	LEU	Peptide
1	A	647	ASP	Peptide
2	C	413	ARG	Peptide
1	D	569	LEU	Peptide
1	D	647	ASP	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1524	0	1569	91	0
1	D	1524	0	1569	93	0
1	E	1524	0	1569	123	0
1	J	1524	0	1569	106	0
2	B	2088	0	2077	155	0
2	C	2088	0	2077	143	0
2	H	1412	0	1388	121	0
2	K	1412	0	1388	92	0
All	All	13096	0	13206	920	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 35.

The worst 5 of 920 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)
2:B:425:SER:CB	2:B:426:ASP:HA	1.52	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:414:TYR:CE2	2:H:416:LEU:HD11	1.60	1.36
2:C:425:SER:CB	2:C:426:ASP:HA	1.52	1.34
2:H:425:SER:CB	2:H:426:ASP:HA	1.51	1.29
2:K:425:SER:CB	2:K:426:ASP:HA	1.52	1.23

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	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	5	32
1	D	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	5	32
1	E	194/201 (96%)	164 (84%)	23 (12%)	7 (4%)	3	22
1	J	194/201 (96%)	166 (86%)	23 (12%)	5 (3%)	4	28
2	B	253/441 (57%)	201 (79%)	33 (13%)	19 (8%)	1	9
2	C	253/441 (57%)	203 (80%)	31 (12%)	19 (8%)	1	9
2	H	155/441 (35%)	113 (73%)	30 (19%)	12 (8%)	1	9
2	K	155/441 (35%)	114 (74%)	31 (20%)	10 (6%)	1	12
All	All	1592/2568 (62%)	1301 (82%)	211 (13%)	80 (5%)	1	16

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	575	THR
1	A	648	GLN
2	C	87	ASP
2	C	299	CYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/175 (98%)	150 (87%)	22 (13%)	3	18
1	D	172/175 (98%)	149 (87%)	23 (13%)	3	18
1	E	172/175 (98%)	142 (83%)	30 (17%)	1	9
1	J	172/175 (98%)	144 (84%)	28 (16%)	2	11
2	B	232/383 (61%)	206 (89%)	26 (11%)	5	22
2	C	232/383 (61%)	208 (90%)	24 (10%)	6	26
2	H	154/383 (40%)	141 (92%)	13 (8%)	9	32
2	K	154/383 (40%)	139 (90%)	15 (10%)	6	27
All	All	1460/2232 (65%)	1279 (88%)	181 (12%)	4	20

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	618	LYS
1	J	552	ASN
1	E	629	VAL
2	H	303	VAL
1	J	590	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	118	ASN
2	B	415	GLN
1	J	584	HIS
2	B	121	GLN
2	B	346	GLN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 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(Å²)	Q<0.9	
1	A	196/201 (97%)	-1.09	0	100	100	69, 77, 80, 82	0
1	D	196/201 (97%)	-1.12	0	100	100	69, 77, 80, 82	0
1	E	196/201 (97%)	-1.25	0	100	100	49, 58, 67, 72	0
1	J	196/201 (97%)	-1.23	0	100	100	49, 58, 67, 72	0
2	B	261/441 (59%)	-0.86	0	100	100	66, 79, 83, 83	0
2	C	261/441 (59%)	-0.87	0	100	100	66, 79, 83, 83	0
2	H	175/441 (39%)	-0.52	1 (0%)	85	72	66, 83, 116, 122	0
2	K	175/441 (39%)	-0.42	3 (1%)	69	49	66, 83, 118, 138	0
All	All	1656/2568 (64%)	-0.93	4 (0%)	92	86	49, 77, 98, 138	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	340	THR	5.0
2	K	130	THR	3.1
2	K	276	LYS	3.0
2	H	340	THR	2.2

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.