



# wwPDB X-ray Structure Validation Summary Report

Aug 27, 2023 – 10:48 PM EDT

PDB ID : 3KWV  
Title : Structural basis for the unfolding of anthrax lethal factor by protective antigen oligomers  
Authors : Feld, G.K.; Kintzer, A.F.; Krantz, B.A.  
Deposited on : 2009-12-01  
Resolution : 3.10 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 : 2.35  
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

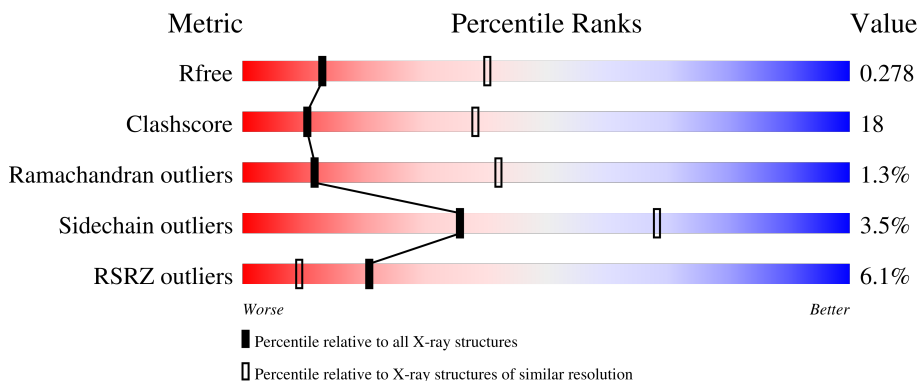
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	548	
1	B	548	
1	D	548	
1	E	548	
2	C	263	

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Mol	Chain	Length	Quality of chain
2	F	263	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '8%', a green segment labeled '49%', a yellow segment labeled '33%', and a grey segment on the right labeled '16%'. A small black dot is visible on the yellow segment.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20349 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4178	2617	718	837	6	0	0	0
1	B	526	4169	2612	717	834	6	0	0	0
1	D	526	4171	2613	717	835	6	0	0	0
1	E	528	4187	2622	720	839	6	0	0	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	PRO	VAL	engineered mutation	UNP P13423
A	304	GLY	HIS	engineered mutation	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	ASN	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	GLU	deletion	UNP P13423
A	?	-	VAL	deletion	UNP P13423
A	?	-	HIS	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	PHE	deletion	UNP P13423
A	?	-	PHE	deletion	UNP P13423
A	?	-	ASP	deletion	UNP P13423
A	?	-	ILE	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	VAL	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P13423
B	303	PRO	VAL	engineered mutation	UNP P13423
B	304	GLY	HIS	engineered mutation	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	ASN	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	GLU	deletion	UNP P13423
B	?	-	VAL	deletion	UNP P13423
B	?	-	HIS	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
B	?	-	ASP	deletion	UNP P13423
B	?	-	ILE	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	VAL	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
D	303	PRO	VAL	engineered mutation	UNP P13423
D	304	GLY	HIS	engineered mutation	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	ASN	deletion	UNP P13423
D	?	-	ALA	deletion	UNP P13423
D	?	-	GLU	deletion	UNP P13423
D	?	-	VAL	deletion	UNP P13423
D	?	-	HIS	deletion	UNP P13423
D	?	-	ALA	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423
D	?	-	PHE	deletion	UNP P13423
D	?	-	PHE	deletion	UNP P13423
D	?	-	ASP	deletion	UNP P13423
D	?	-	ILE	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423
D	?	-	VAL	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
E	303	PRO	VAL	engineered mutation	UNP P13423
E	304	GLY	HIS	engineered mutation	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	ASN	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	GLU	deletion	UNP P13423
E	?	-	VAL	deletion	UNP P13423
E	?	-	HIS	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423
E	?	-	ASP	deletion	UNP P13423
E	?	-	ILE	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	VAL	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423

- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1816	1164	290	359	3			
2	F	222	Total	C	N	O	S	0	0	0
			1816	1164	290	359	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total 2	Ca 2	0	0

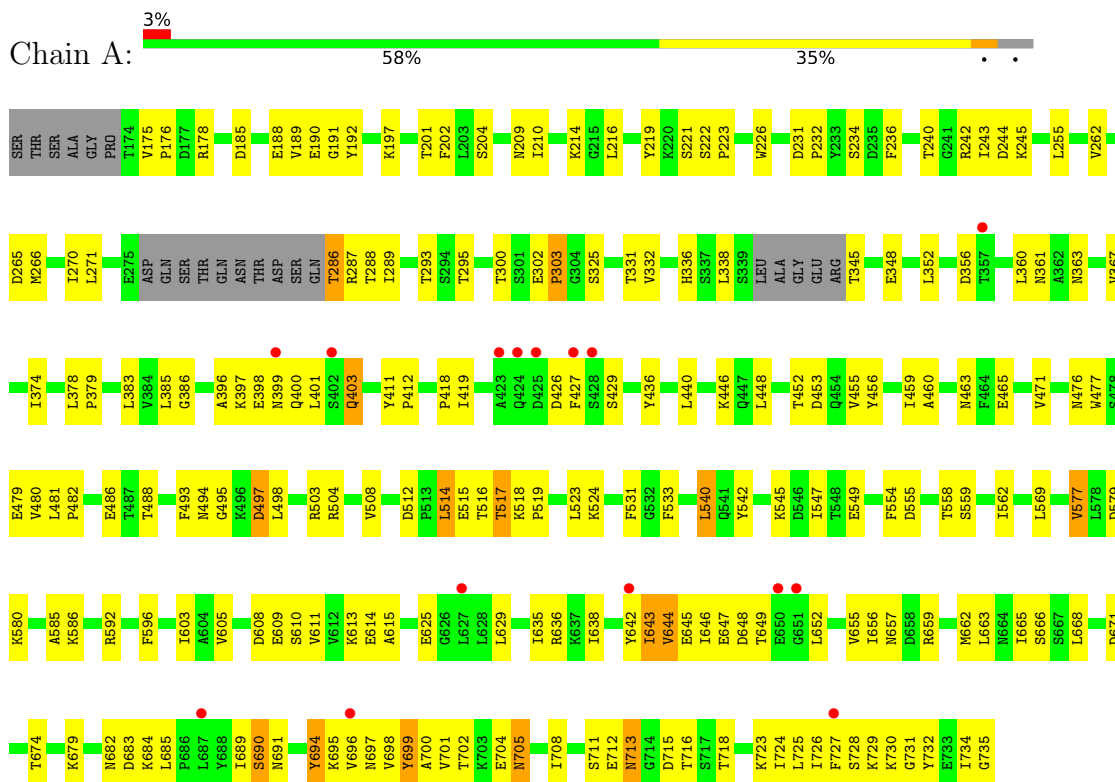
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	E	1	Total 1	O 1	0	0

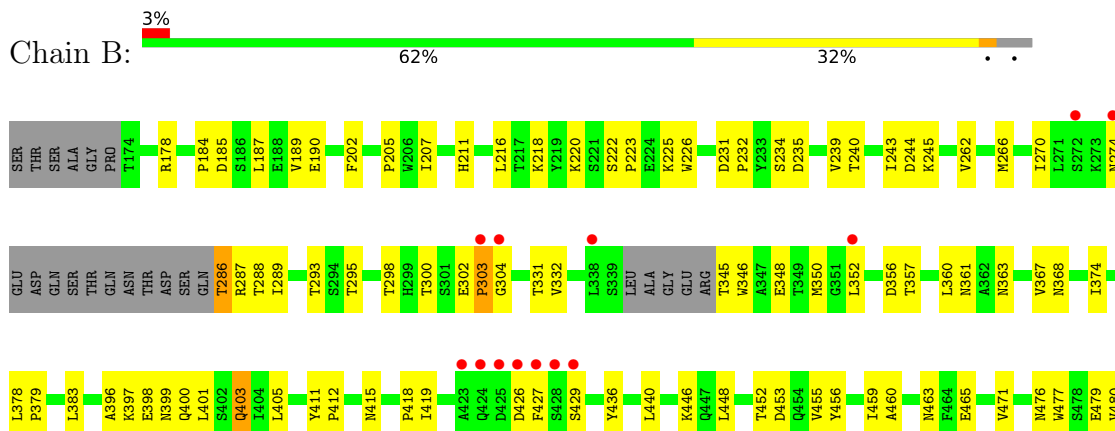
### 3 Residue-property plots [i](#)

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.

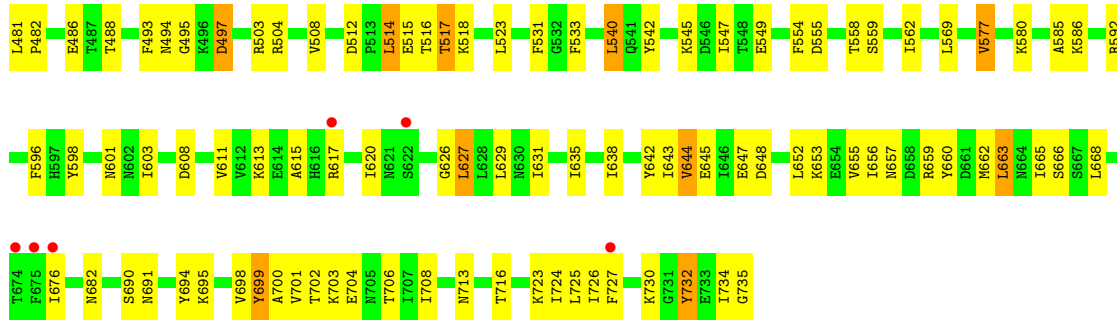
- Molecule 1: Protective antigen PA-63



- Molecule 1: Protective antigen PA-63



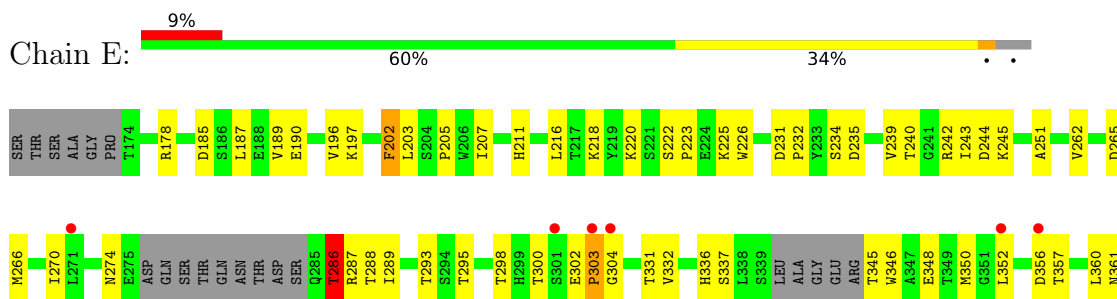


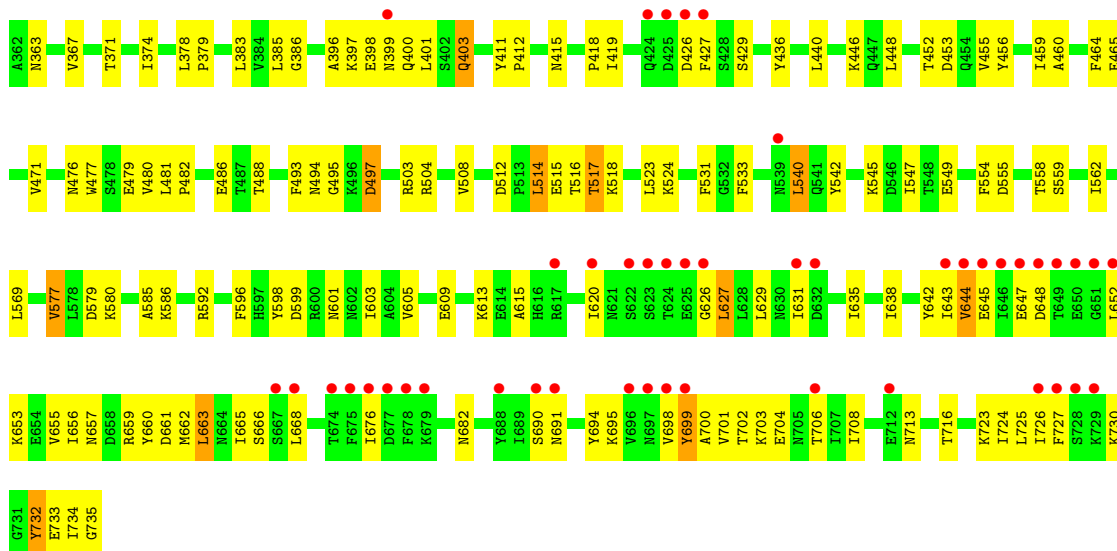


● Molecule 1: Protective antigen PA-63

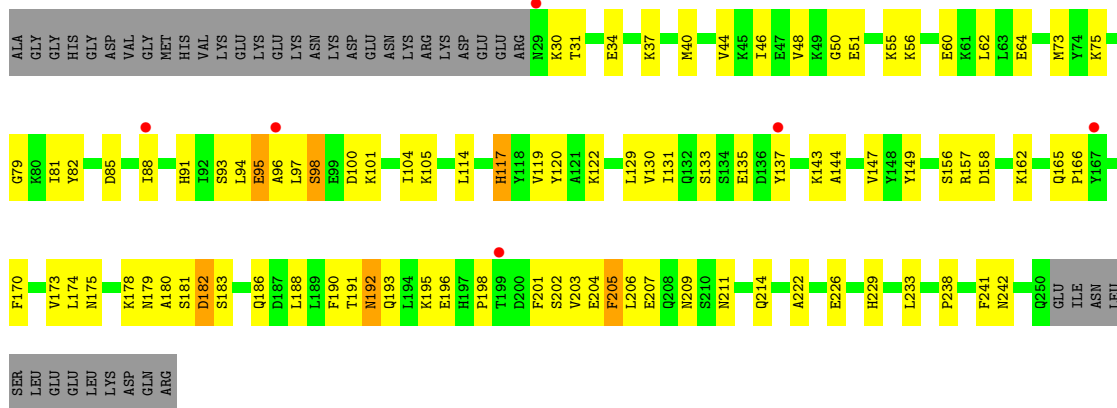


● Molecule 1: Protective antigen PA-63

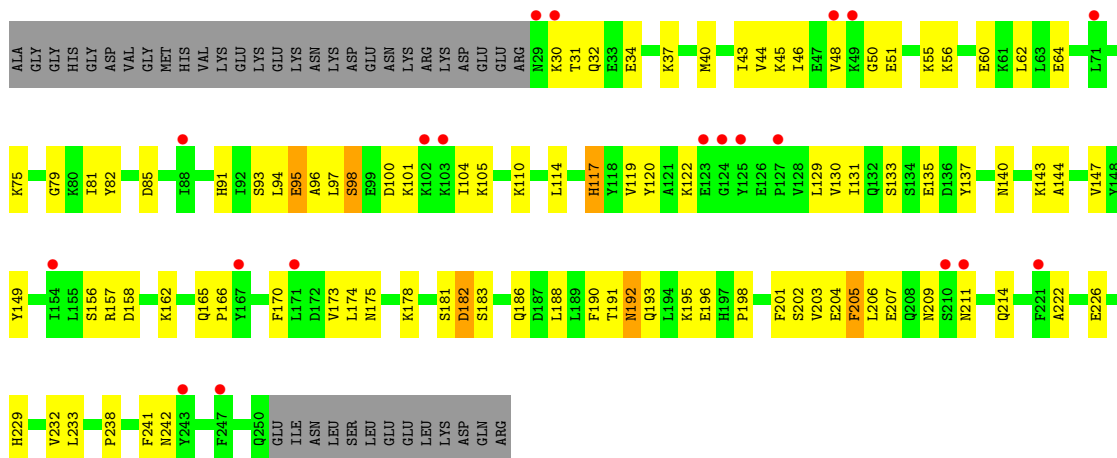




• Molecule 2: Lethal factor



• Molecule 2: Lethal factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.38Å 178.38Å 240.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.10 49.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.1 (49.84-3.10) 92.1 (49.84-3.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.249 , 0.281 0.245 , 0.278	Depositor DCC
$R_{free}$ test set	2000 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	20349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/4249	0.41	0/5764
1	B	0.23	0/4240	0.41	0/5752
1	D	0.26	0/4242	0.41	0/5754
1	E	0.25	0/4258	0.41	0/5776
2	C	0.23	0/1850	0.39	1/2493 (0.0%)
2	F	0.23	0/1850	0.39	1/2493 (0.0%)
All	All	0.25	0/20689	0.40	2/28032 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	182	ASP	CB-CG-OD2	5.21	122.98	118.30
2	F	182	ASP	CB-CG-OD2	5.19	122.97	118.30

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	4178	0	4149	171	0
1	B	4169	0	4143	145	0
1	D	4171	0	4142	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4187	0	4157	154	0
2	C	1816	0	1797	59	0
2	F	1816	0	1797	65	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	20349	0	20185	746	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 746 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:A:266:MET:H	1:A:295:THR:HG21	1.36	0.90
1:D:699:TYR:HA	1:D:726:ILE:HG12	1.58	0.86
1:A:699:TYR:HA	1:A:726:ILE:HG12	1.58	0.85
1:D:210:ILE:HD11	2:F:188:LEU:HB2	1.59	0.84
1:D:625:GLU:HB3	1:D:679:LYS:HE3	1.57	0.84

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	521/548 (95%)	471 (90%)	45 (9%)	5 (1%)	<b>15</b> 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	520/548 (95%)	462 (89%)	54 (10%)	4 (1%)	19	54
1	D	520/548 (95%)	468 (90%)	47 (9%)	5 (1%)	15	49
1	E	522/548 (95%)	469 (90%)	47 (9%)	6 (1%)	14	46
2	C	220/263 (84%)	183 (83%)	30 (14%)	7 (3%)	4	22
2	F	220/263 (84%)	183 (83%)	30 (14%)	7 (3%)	4	22
All	All	2523/2718 (93%)	2236 (89%)	253 (10%)	34 (1%)	12	42

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	732	TYR
2	C	162	LYS
1	D	732	TYR
2	F	162	LYS
1	A	303	PRO

### 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	474/491 (96%)	455 (96%)	19 (4%)	31	65
1	B	473/491 (96%)	456 (96%)	17 (4%)	35	67
1	D	473/491 (96%)	455 (96%)	18 (4%)	33	66
1	E	475/491 (97%)	457 (96%)	18 (4%)	33	66
2	C	200/236 (85%)	196 (98%)	4 (2%)	55	80
2	F	200/236 (85%)	196 (98%)	4 (2%)	55	80
All	All	2295/2436 (94%)	2215 (96%)	80 (4%)	36	68

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	713	ASN

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Mol	Chain	Res	Type
1	E	644	VAL
1	E	240	THR
1	E	514	LEU
1	E	713	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 8 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

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	527/548 (96%)	0.04	15 (2%) 53 30	46, 82, 173, 206	0
1	B	526/548 (95%)	0.02	19 (3%) 42 22	45, 83, 158, 206	0
1	D	526/548 (95%)	0.20	44 (8%) 11 4	47, 82, 171, 206	0
1	E	528/548 (96%)	0.28	52 (9%) 7 2	46, 84, 160, 205	0
2	C	222/263 (84%)	0.06	6 (2%) 54 31	69, 126, 169, 201	0
2	F	222/263 (84%)	0.36	20 (9%) 9 3	68, 126, 170, 198	0
All	All	2551/2718 (93%)	0.15	156 (6%) 21 9	45, 92, 169, 206	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	674	THR	9.5
1	E	425	ASP	8.8
1	A	427	PHE	7.8
1	A	425	ASP	7.8
1	E	624	THR	6.8

### 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
3	CA	A	736	1/1	0.98	0.22	52,52,52,52	0
3	CA	D	737	1/1	0.98	0.19	55,55,55,55	0
3	CA	B	736	1/1	0.99	0.22	57,57,57,57	0
3	CA	B	737	1/1	0.99	0.17	48,48,48,48	0
3	CA	D	736	1/1	0.99	0.20	65,65,65,65	0
3	CA	A	737	1/1	0.99	0.15	45,45,45,45	0
3	CA	E	736	1/1	0.99	0.17	52,52,52,52	0
3	CA	E	737	1/1	0.99	0.20	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.