



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QQX  
Title : Crystal structure of T. fusca Cas3-ATP  
Authors : Ke, A.; Huo, Y.; Nam, K.H.  
Deposited on : 2014-06-30  
Resolution : 3.34 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

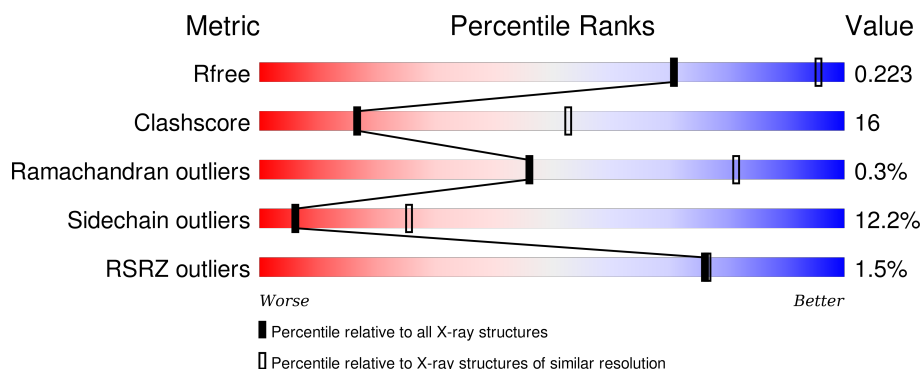
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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))
$R_{free}$	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	964	<div> <div>2%</div> <div>60% 28% 5% 6%</div> </div>
1	C	964	<div> <div>%</div> <div>58% 31% 5% 7%</div> </div>
1	E	964	<div> <div>%</div> <div>65% 25% • 7%</div> </div>
1	G	964	<div> <div>%</div> <div>54% 33% 5% 8%</div> </div>
2	B	12	<div> <div>8%</div> <div>25% 42% 25% 8%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	12	<div><div></div><div>33%</div><div>42%</div><div>17%</div><div>8%</div></div>
2	F	12	<div><div>17%</div><div>25%</div><div>42%</div><div>25%</div><div>8%</div></div>
2	H	12	<div><div>8%</div><div>25%</div><div>42%</div><div>25%</div><div>8%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28826 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 CRISPR-associated helicase, Cas3 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7028	4463	1251	1287	27			
1	C	899	Total	C	N	O	S	0	0	0
			6977	4428	1237	1285	27			
1	E	901	Total	C	N	O	S	0	0	0
			6995	4438	1242	1288	27			
1	G	887	Total	C	N	O	S	0	0	0
			6906	4390	1224	1266	26			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q47PJ0
A	-18	GLY	-	EXPRESSION TAG	UNP Q47PJ0
A	-17	SER	-	EXPRESSION TAG	UNP Q47PJ0
A	-16	SER	-	EXPRESSION TAG	UNP Q47PJ0
A	-15	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-14	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-13	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-12	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-11	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-10	HIS	-	EXPRESSION TAG	UNP Q47PJ0
A	-9	SER	-	EXPRESSION TAG	UNP Q47PJ0
A	-8	SER	-	EXPRESSION TAG	UNP Q47PJ0
A	-7	GLY	-	EXPRESSION TAG	UNP Q47PJ0
A	-6	LEU	-	EXPRESSION TAG	UNP Q47PJ0
A	-5	VAL	-	EXPRESSION TAG	UNP Q47PJ0
A	-4	PRO	-	EXPRESSION TAG	UNP Q47PJ0
A	-3	ARG	-	EXPRESSION TAG	UNP Q47PJ0
A	-2	GLY	-	EXPRESSION TAG	UNP Q47PJ0
A	-1	SER	-	EXPRESSION TAG	UNP Q47PJ0
A	0	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-19	MET	-	INITIATING METHIONINE	UNP Q47PJ0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	EXPRESSION TAG	UNP Q47PJ0
C	-17	SER	-	EXPRESSION TAG	UNP Q47PJ0
C	-16	SER	-	EXPRESSION TAG	UNP Q47PJ0
C	-15	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-14	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-13	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-12	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-11	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-10	HIS	-	EXPRESSION TAG	UNP Q47PJ0
C	-9	SER	-	EXPRESSION TAG	UNP Q47PJ0
C	-8	SER	-	EXPRESSION TAG	UNP Q47PJ0
C	-7	GLY	-	EXPRESSION TAG	UNP Q47PJ0
C	-6	LEU	-	EXPRESSION TAG	UNP Q47PJ0
C	-5	VAL	-	EXPRESSION TAG	UNP Q47PJ0
C	-4	PRO	-	EXPRESSION TAG	UNP Q47PJ0
C	-3	ARG	-	EXPRESSION TAG	UNP Q47PJ0
C	-2	GLY	-	EXPRESSION TAG	UNP Q47PJ0
C	-1	SER	-	EXPRESSION TAG	UNP Q47PJ0
C	0	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-19	MET	-	INITIATING METHIONINE	UNP Q47PJ0
E	-18	GLY	-	EXPRESSION TAG	UNP Q47PJ0
E	-17	SER	-	EXPRESSION TAG	UNP Q47PJ0
E	-16	SER	-	EXPRESSION TAG	UNP Q47PJ0
E	-15	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-14	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-13	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-12	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-11	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-10	HIS	-	EXPRESSION TAG	UNP Q47PJ0
E	-9	SER	-	EXPRESSION TAG	UNP Q47PJ0
E	-8	SER	-	EXPRESSION TAG	UNP Q47PJ0
E	-7	GLY	-	EXPRESSION TAG	UNP Q47PJ0
E	-6	LEU	-	EXPRESSION TAG	UNP Q47PJ0
E	-5	VAL	-	EXPRESSION TAG	UNP Q47PJ0
E	-4	PRO	-	EXPRESSION TAG	UNP Q47PJ0
E	-3	ARG	-	EXPRESSION TAG	UNP Q47PJ0
E	-2	GLY	-	EXPRESSION TAG	UNP Q47PJ0
E	-1	SER	-	EXPRESSION TAG	UNP Q47PJ0
E	0	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-19	MET	-	INITIATING METHIONINE	UNP Q47PJ0
G	-18	GLY	-	EXPRESSION TAG	UNP Q47PJ0
G	-17	SER	-	EXPRESSION TAG	UNP Q47PJ0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	EXPRESSION TAG	UNP Q47PJ0
G	-15	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-14	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-13	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-12	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-11	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-10	HIS	-	EXPRESSION TAG	UNP Q47PJ0
G	-9	SER	-	EXPRESSION TAG	UNP Q47PJ0
G	-8	SER	-	EXPRESSION TAG	UNP Q47PJ0
G	-7	GLY	-	EXPRESSION TAG	UNP Q47PJ0
G	-6	LEU	-	EXPRESSION TAG	UNP Q47PJ0
G	-5	VAL	-	EXPRESSION TAG	UNP Q47PJ0
G	-4	PRO	-	EXPRESSION TAG	UNP Q47PJ0
G	-3	ARG	-	EXPRESSION TAG	UNP Q47PJ0
G	-2	GLY	-	EXPRESSION TAG	UNP Q47PJ0
G	-1	SER	-	EXPRESSION TAG	UNP Q47PJ0
G	0	HIS	-	EXPRESSION TAG	UNP Q47PJ0

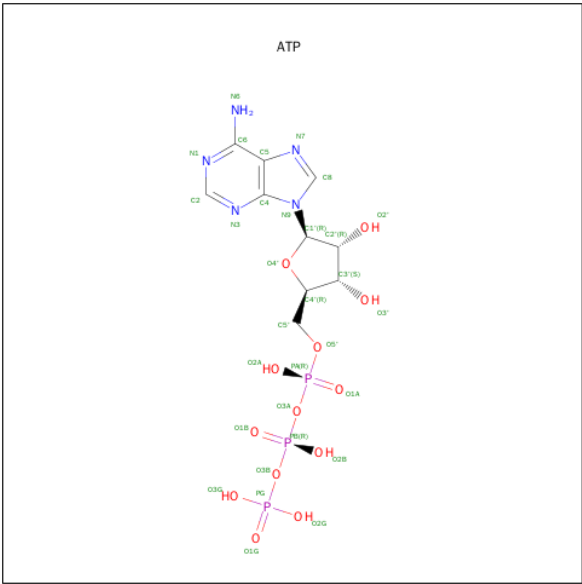
- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	D	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	F	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	H	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Fe	0	0
			2	2		
3	A	2	Total	Fe	0	0
			2	2		
3	C	2	Total	Fe	0	0
			2	2		
3	E	2	Total	Fe	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

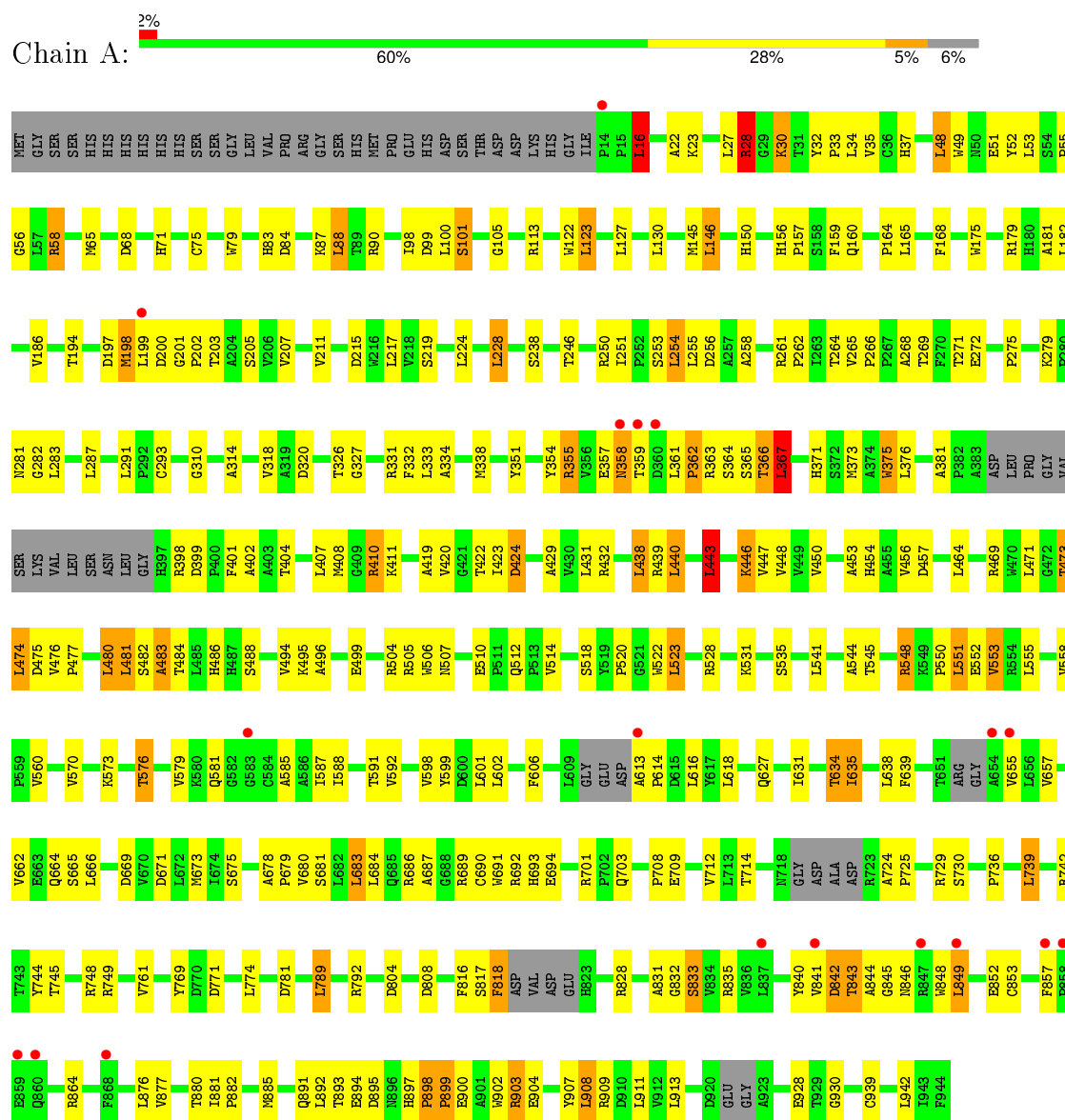


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CRISPR-associated helicase, Cas3 family

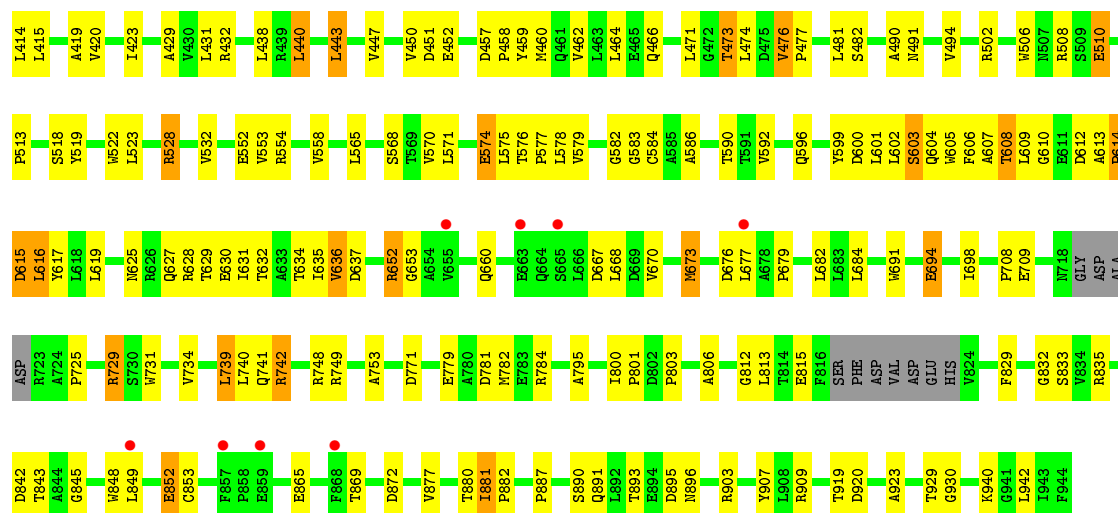


- Molecule 1: CRISPR-associated helicase, Cas3 family

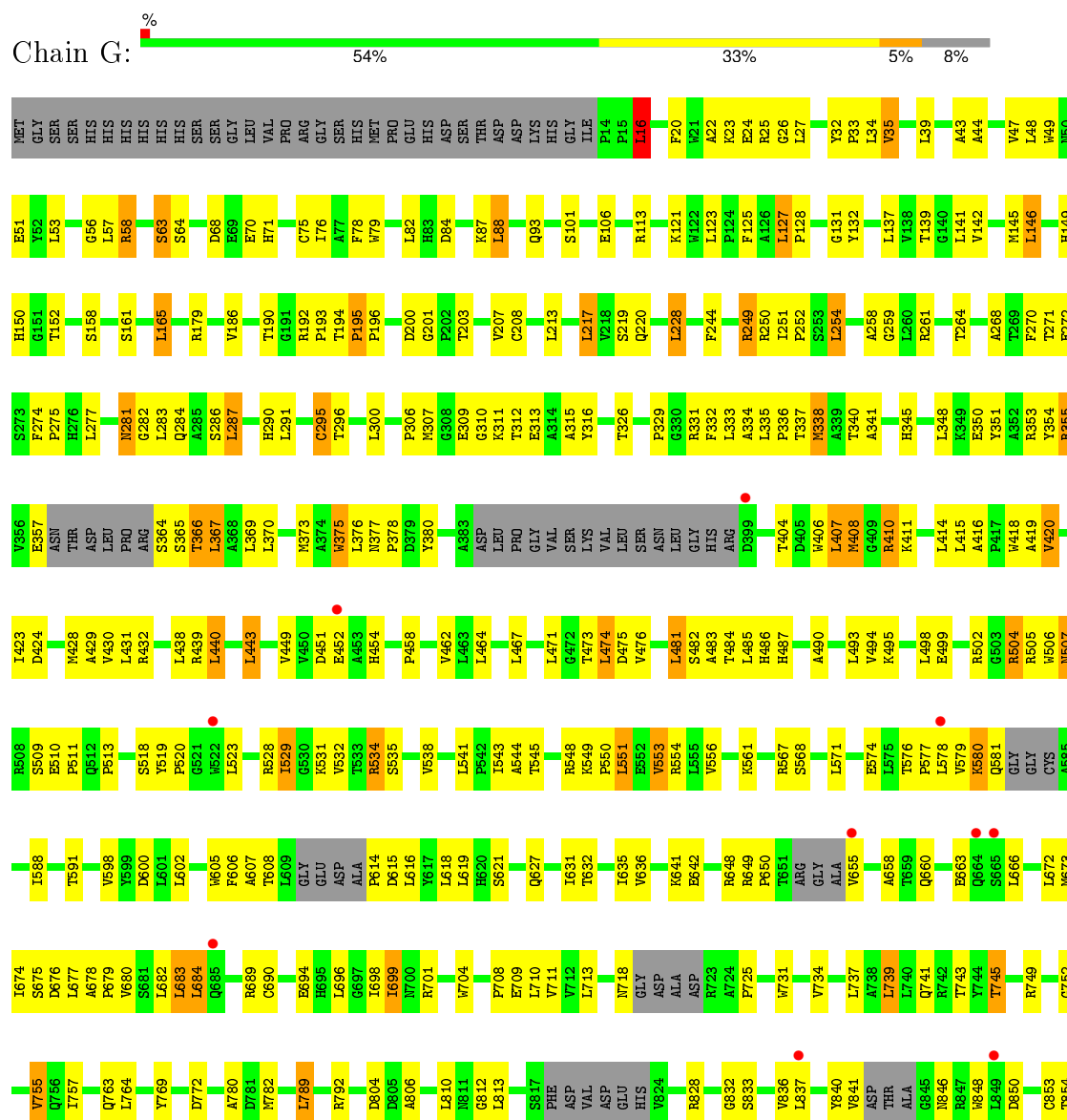


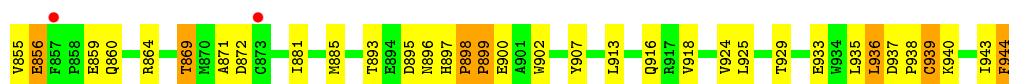






- Molecule 1: CRISPR-associated helicase, Cas3 family

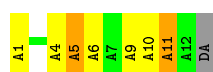




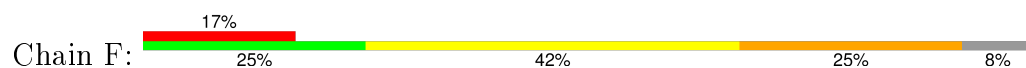
- Molecule 2: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.25Å 222.81Å 125.09Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	46.98 – 3.34 46.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.98-3.34) 91.0 (46.98-3.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.172 , 0.227 0.170 , 0.223	Depositor DCC
$R_{free}$ test set	1533 reflections (2.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.3	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82162 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FE, ATP

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	0.49	2/7205 (0.0%)	0.70	10/9828 (0.1%)
1	C	0.49	1/7151 (0.0%)	0.70	6/9754 (0.1%)
1	E	0.52	1/7170 (0.0%)	0.73	7/9782 (0.1%)
1	G	0.49	4/7077 (0.1%)	0.68	6/9649 (0.1%)
2	B	1.00	0/222	1.96	13/339 (3.8%)
2	D	1.06	0/222	1.98	11/339 (3.2%)
2	F	1.01	0/222	2.09	15/339 (4.4%)
2	H	0.93	0/222	1.71	5/339 (1.5%)
All	All	0.52	8/29491 (0.0%)	0.78	73/40369 (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	1
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	899	PRO	N-CD	5.46	1.55	1.47
1	G	898	PRO	N-CD	5.34	1.55	1.47
1	A	898	PRO	N-CD	5.25	1.55	1.47
1	C	275	PRO	N-CD	5.17	1.55	1.47
1	G	195	PRO	N-CD	5.16	1.55	1.47

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	F	11	DA	O4'-C4'-C3'	10.51	112.31	106.00
2	B	5	DA	O4'-C1'-N9	-10.19	100.87	108.00
2	H	10	DA	C1'-O4'-C4'	-9.94	100.16	110.10
2	D	10	DA	C1'-O4'-C4'	-9.85	100.25	110.10
2	F	11	DA	O4'-C1'-N9	9.33	114.53	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	C	355	ARG	Sidechain
1	E	852	GLU	Peptide
1	G	355	ARG	Sidechain

## 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	7028	0	6975	227	0
1	C	6977	0	6922	233	0
1	E	6995	0	6939	184	0
1	G	6906	0	6862	297	0
2	B	197	0	99	12	0
2	D	197	0	99	8	0
2	F	197	0	99	7	0
2	H	197	0	99	15	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	31	0	12	1	0
4	C	31	0	12	6	0
4	E	31	0	12	2	0
4	G	31	0	12	7	0
All	All	28826	0	28142	939	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 16.

The worst 5 of 939 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:28:ARG:O	1:A:28:ARG:CD	1.95	1.14
1:A:28:ARG:HD2	1:A:30:LYS:HZ1	1.08	1.14
1:C:452:GLU:HG3	1:C:454:HIS:NE2	1.66	1.10
1:G:268:ALA:HB2	1:G:355:ARG:HH12	1.10	1.07
1:A:28:ARG:O	1:A:28:ARG:HD3	1.50	1.07

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	889/964 (92%)	825 (93%)	60 (7%)	4 (0%)	39	77
1	C	887/964 (92%)	803 (90%)	79 (9%)	5 (1%)	30	69
1	E	891/964 (92%)	844 (95%)	46 (5%)	1 (0%)	56	89
1	G	869/964 (90%)	792 (91%)	75 (9%)	2 (0%)	52	86
All	All	3536/3856 (92%)	3264 (92%)	260 (7%)	12 (0%)	46	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	GLN
1	A	749	ARG
1	C	374	ALA
1	C	660	GLN
1	G	752	GLY

### 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	746/796 (94%)	655 (88%)	91 (12%)	6	25
1	C	740/796 (93%)	641 (87%)	99 (13%)	5	21
1	E	741/796 (93%)	669 (90%)	72 (10%)	10	37
1	G	734/796 (92%)	635 (86%)	99 (14%)	5	21
All	All	2961/3184 (93%)	2600 (88%)	361 (12%)	6	25

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	662	VAL
1	E	172	SER
1	G	684	LEU
1	C	703	GLN
1	C	920	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	645	GLN
1	E	896	ASN
1	E	290	HIS
1	C	358	ASN
1	E	94	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ATP	A	1003	-	24,33,33	1.04	1 (4%)	31,52,52	1.87	6 (19%)
4	ATP	C	1003	-	24,33,33	0.99	1 (4%)	31,52,52	2.26	7 (22%)
4	ATP	E	1003	-	24,33,33	1.04	1 (4%)	31,52,52	2.05	7 (22%)
4	ATP	G	1003	-	24,33,33	1.00	1 (4%)	31,52,52	1.94	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1003	-	-	0/18/38/38	0/3/3/3
4	ATP	C	1003	-	-	0/18/38/38	0/3/3/3
4	ATP	E	1003	-	-	0/18/38/38	0/3/3/3
4	ATP	G	1003	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1003	ATP	C5-C4	2.28	1.45	1.40
4	A	1003	ATP	C5-C4	2.46	1.46	1.40
4	G	1003	ATP	C5-C4	2.58	1.46	1.40
4	C	1003	ATP	C5-C4	2.66	1.46	1.40

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	1003	ATP	N3-C2-N1	-8.37	122.49	128.89
4	E	1003	ATP	N3-C2-N1	-7.41	123.22	128.89
4	G	1003	ATP	N3-C2-N1	-6.43	123.97	128.89
4	A	1003	ATP	N3-C2-N1	-6.20	124.15	128.89
4	G	1003	ATP	PA-O3A-PB	-5.26	117.95	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ATP	1	0
4	C	1003	ATP	6	0
4	E	1003	ATP	2	0
4	G	1003	ATP	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	903/964 (93%)	-0.18	18 (1%) 68 67	61, 100, 153, 226	0
1	C	899/964 (93%)	-0.17	11 (1%) 81 81	65, 105, 153, 202	0
1	E	901/964 (93%)	-0.24	9 (0%) 84 85	57, 91, 141, 181	0
1	G	887/964 (92%)	-0.09	12 (1%) 78 79	66, 114, 170, 234	0
2	B	11/12 (91%)	0.80	1 (9%) 11 11	95, 98, 170, 217	0
2	D	11/12 (91%)	0.50	0 100 100	91, 106, 184, 194	0
2	F	11/12 (91%)	1.01	2 (18%) 2 2	80, 95, 175, 217	0
2	H	11/12 (91%)	0.30	1 (9%) 11 11	94, 113, 199, 208	0
All	All	3634/3904 (93%)	-0.16	54 (1%) 76 76	57, 103, 157, 234	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	849	LEU	4.5
1	A	654	ALA	3.8
1	G	857	PHE	3.6
1	A	359	THR	3.4
1	E	857	PHE	3.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FE	A	1001	1/1	0.95	0.20	1.68	79,79,79,79	0
3	FE	E	1001	1/1	0.95	0.18	0.81	80,80,80,80	0
3	FE	G	1001	1/1	0.99	0.15	0.38	77,77,77,77	0
4	ATP	E	1003	31/31	0.93	0.21	0.35	91,111,120,128	0
4	ATP	A	1003	31/31	0.86	0.23	0.23	97,119,131,132	0
3	FE	C	1001	1/1	0.99	0.17	0.22	77,77,77,77	0
4	ATP	G	1003	31/31	0.86	0.26	0.12	128,151,159,161	0
3	FE	A	1002	1/1	0.99	0.17	0.04	73,73,73,73	0
3	FE	G	1002	1/1	0.98	0.16	-0.13	79,79,79,79	0
3	FE	C	1002	1/1	0.96	0.17	-0.17	82,82,82,82	0
4	ATP	C	1003	31/31	0.86	0.22	-0.38	124,143,160,164	0
3	FE	E	1002	1/1	0.99	0.15	-0.47	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.