



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:13 pm BST

PDB ID : 5F9F  
Title : Crystal structure of RIG-I helicase-RD in complex with 24-mer blunt-end hairpin RNA  
Authors : Wang, C.; Marcotrigiano, J.; Miller, M.T.; Jiang, F.  
Deposited on : 2015-12-09  
Resolution : 2.60 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.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

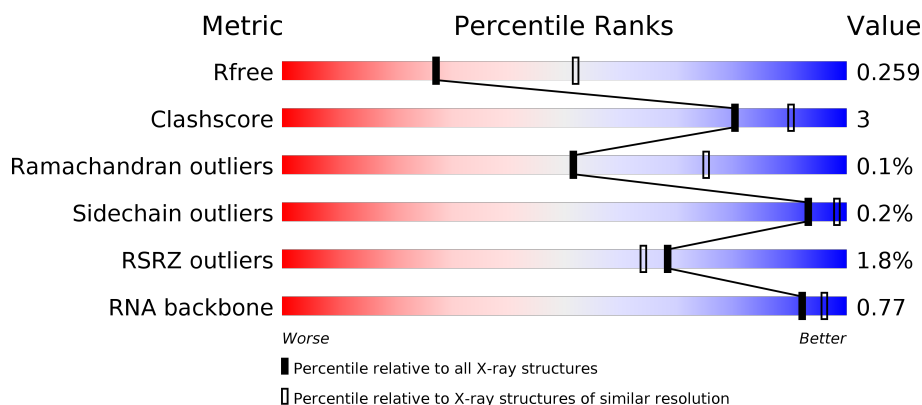
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 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	695	<div> <div></div> <div>91% 6% .</div> </div>
1	C	695	<div> <div></div> <div>90% 6% .</div> </div>
1	E	695	<div> <div>3%</div> <div>90% 7% .</div> </div>
1	G	695	<div> <div></div> <div>88% 8% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	695	 2% 91% 6%
1	K	695	 2% 89% 7%
2	B	24	 13% 96%
2	D	24	 8% 79% 21%
2	F	24	 8% 96%
2	H	24	 8% 100%
2	J	24	 13% 92% 8%
2	L	24	 4% 96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	G	1001	-	-	-	X
6	BU3	C	1005	-	-	-	X
6	BU3	G	1004	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34918 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5310	3393	902	982	33			
1	C	668	Total	C	N	O	S	0	0	0
			5266	3368	894	971	33			
1	E	672	Total	C	N	O	S	0	0	0
			5222	3338	882	969	33			
1	G	669	Total	C	N	O	S	0	0	0
			5282	3375	902	972	33			
1	I	674	Total	C	N	O	S	0	0	0
			5306	3395	899	979	33			
1	K	672	Total	C	N	O	S	0	0	0
			5256	3362	889	971	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	SER	-	expression tag	UNP O95786
C	231	SER	-	expression tag	UNP O95786
E	231	SER	-	expression tag	UNP O95786
G	231	SER	-	expression tag	UNP O95786
I	231	SER	-	expression tag	UNP O95786
K	231	SER	-	expression tag	UNP O95786

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			
2	D	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			
2	F	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			
2	J	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			
2	L	24	Total	C	N	O	P	0	0	0
			506	229	88	166	23			

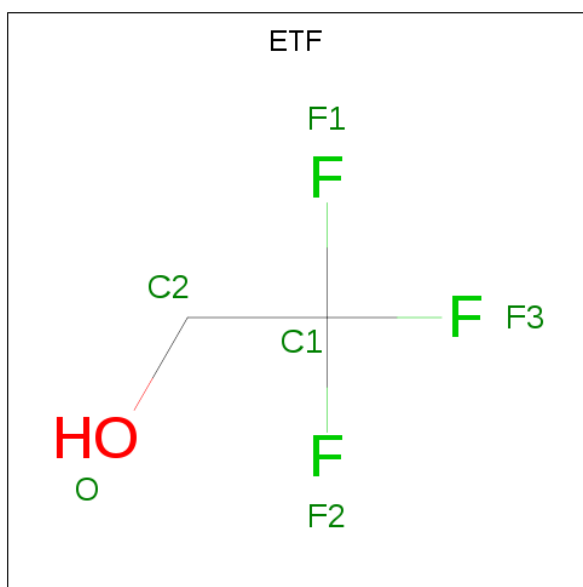
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

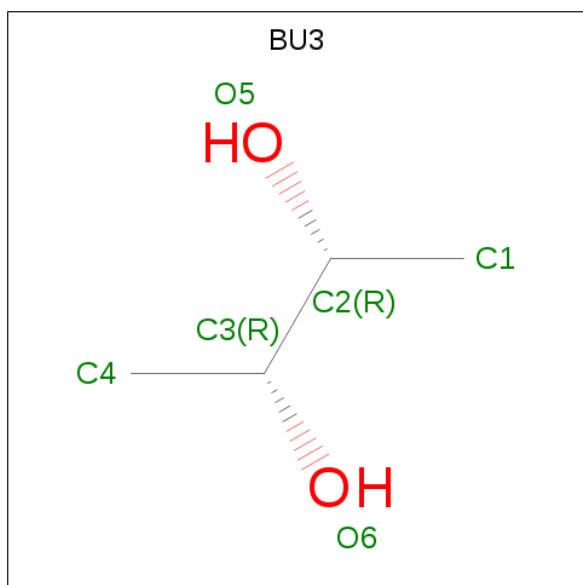
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Mg	0	0
			1	1		
4	I	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		

- Molecule 5 is TRIFLUOROETHANOL (three-letter code: ETF) (formula: C<sub>2</sub>H<sub>3</sub>F<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			6	2	3	1		
5	E	1	Total	C	F	O	0	0
			6	2	3	1		
5	G	1	Total	C	F	O	0	0
			6	2	3	1		
5	K	1	Total	C	F	O	0	0
			6	2	3	1		

- Molecule 6 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 4 2	0	0
6	A	1	Total C O 6 4 2	0	0
6	C	1	Total C O 6 4 2	0	0
6	C	1	Total C O 6 4 2	0	0
6	C	1	Total C O 6 4 2	0	0
6	C	1	Total C O 6 4 2	0	0
6	E	1	Total C O 6 4 2	0	0
6	E	1	Total C O 6 4 2	0	0
6	G	1	Total C O 6 4 2	0	0
6	G	1	Total C O 6 4 2	0	0
6	G	1	Total C O 6 4 2	0	0
6	I	1	Total C O 6 4 2	0	0
6	K	1	Total C O 6 4 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	2	Total O 2 2	0	0
7	C	14	Total O 14 14	0	0
7	D	4	Total O 4 4	0	0
7	E	16	Total O 16 16	0	0
7	F	3	Total O 3 3	0	0
7	G	21	Total O 21 21	0	0

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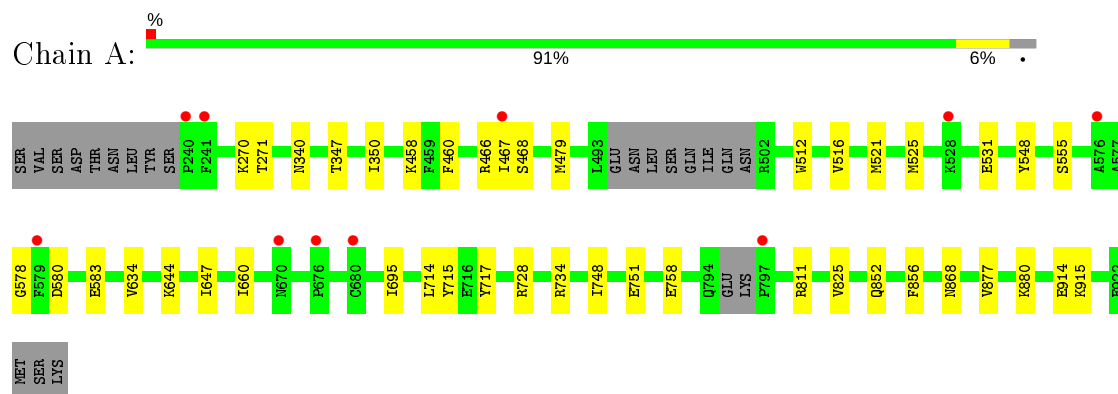
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	3	Total 3	O 3	0	0
7	I	7	Total 7	O 7	0	0
7	J	1	Total 1	O 1	0	0
7	K	20	Total 20	O 20	0	0
7	L	1	Total 1	O 1	0	0



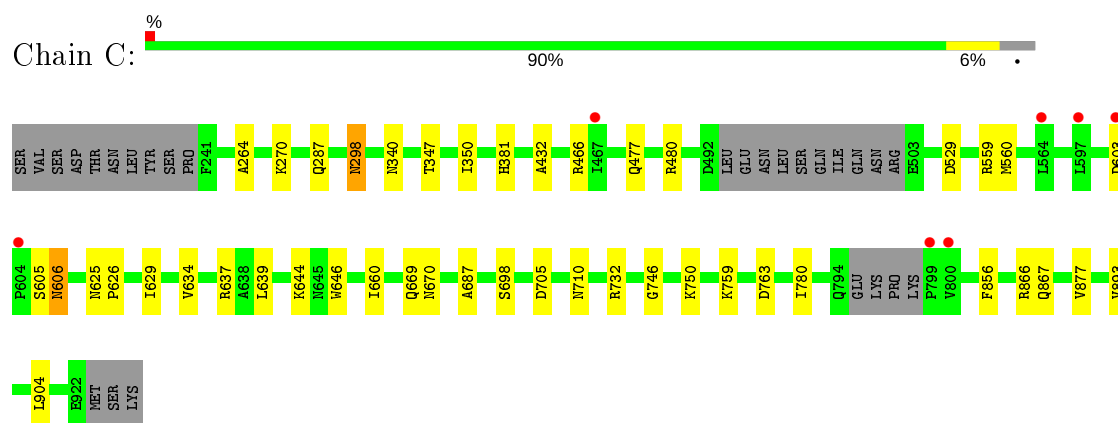
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

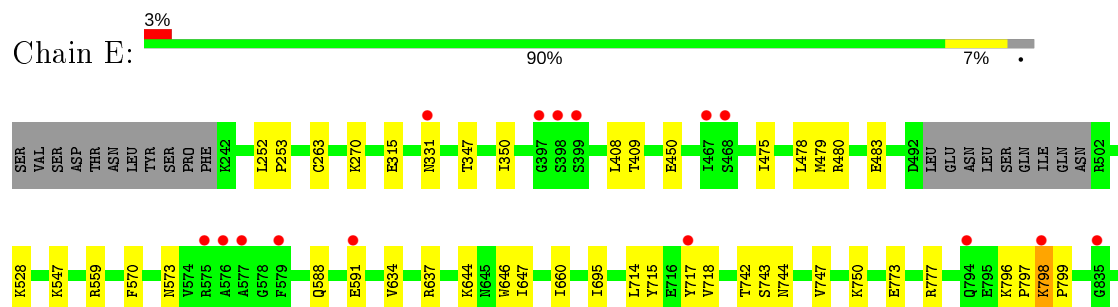
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



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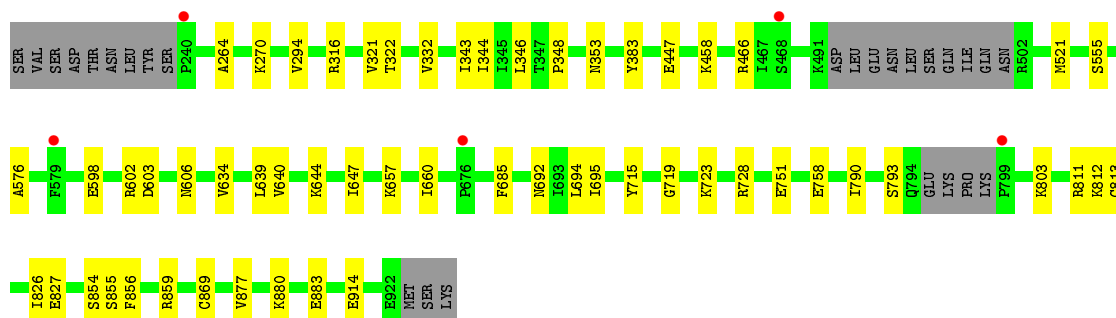
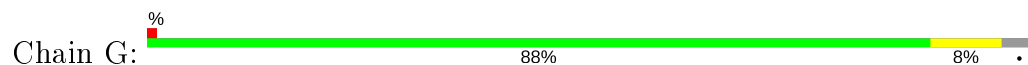


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

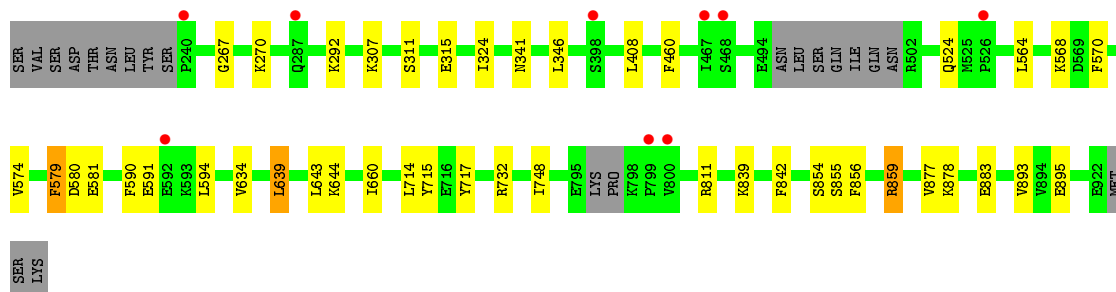
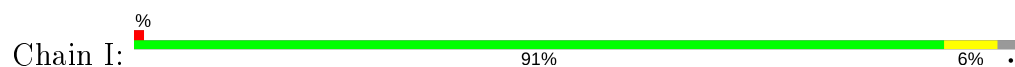




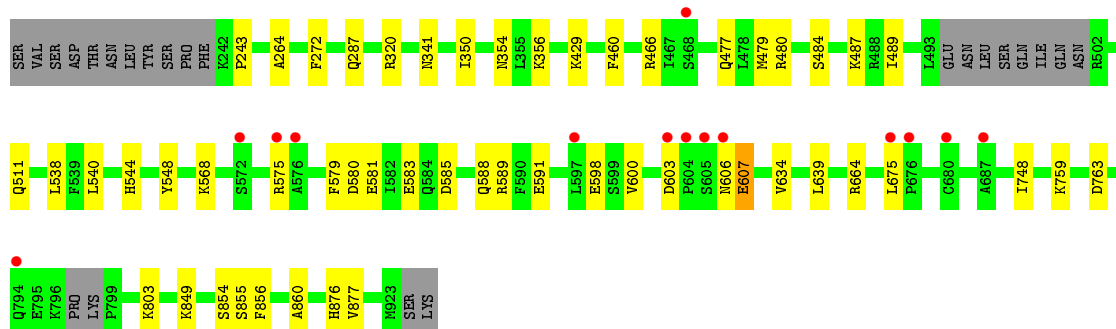
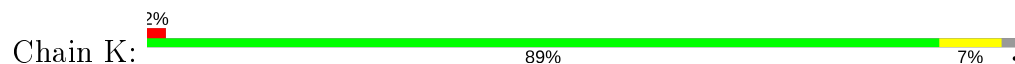
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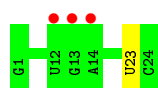


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

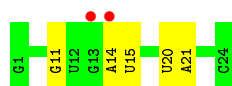
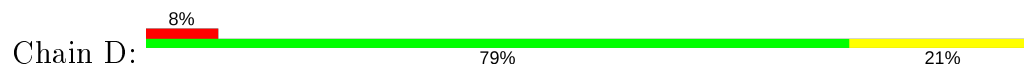


- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')





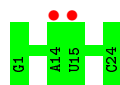
- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')



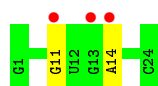
- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')



- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')



- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')



- Molecule 2: RNA (5'-R(\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*AP\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.52Å 174.25Å 308.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.60 29.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.99-2.60) 87.3 (29.99-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, $R_{free}$	0.203 , 0.259 0.205 , 0.259	Depositor DCC
$R_{free}$ test set	8318 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	34918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% 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: BU3, ZN, ETF, MG

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	0.23	0/5419	0.38	0/7325
1	C	0.22	0/5373	0.38	0/7260
1	E	0.23	0/5330	0.40	0/7222
1	G	0.22	0/5390	0.38	0/7284
1	I	0.23	0/5414	0.39	1/7315 (0.0%)
1	K	0.23	0/5362	0.39	0/7251
2	B	0.13	0/566	0.67	0/879
2	D	0.14	0/566	0.67	0/879
2	F	0.13	0/566	0.66	0/879
2	H	0.13	0/566	0.67	0/879
2	J	0.13	0/566	0.67	0/879
2	L	0.13	0/566	0.66	0/879
All	All	0.22	0/35684	0.42	1/48931 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	859	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	5310	0	5266	25	0
1	C	5266	0	5231	32	0
1	E	5222	0	5107	31	0
1	G	5282	0	5242	34	0
1	I	5306	0	5267	31	0
1	K	5256	0	5183	36	0
2	B	506	0	256	1	0
2	D	506	0	256	3	0
2	F	506	0	256	1	0
2	H	506	0	256	0	0
2	J	506	0	256	1	0
2	L	506	0	256	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	I	2	0	0	0	0
4	K	1	0	0	0	0
5	A	6	0	3	1	0
5	E	6	0	3	0	0
5	G	6	0	3	1	0
5	K	6	0	3	0	0
6	A	12	0	20	1	0
6	C	24	0	40	4	0
6	E	12	0	20	4	0
6	G	18	0	30	5	0
6	I	6	0	10	3	0
6	K	6	0	10	1	0
7	A	34	0	0	0	0
7	B	2	0	0	0	0
7	C	14	0	0	0	0
7	D	4	0	0	0	0
7	E	16	0	0	0	0
7	F	3	0	0	0	0
7	G	21	0	0	0	0
7	H	3	0	0	0	0
7	I	7	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	20	0	0	0	0
7	L	1	0	0	0	0
All	All	34918	0	32974	185	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 3.

The worst 5 of 185 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:K:600:VAL:O	1:K:606:ASN:ND2	2.03	0.92
1:G:826:ILE:HG22	1:G:827:GLU:HG3	1.67	0.76
1:E:480:ARG:HA	1:E:483:GLU:HG2	1.73	0.70
1:G:880:LYS:O	1:K:287:GLN:NE2	2.19	0.69
1:I:570:PHE:O	1:I:574:VAL:HG23	1.93	0.68

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	667/695 (96%)	642 (96%)	24 (4%)	1 (0%)	51	75
1	C	662/695 (95%)	633 (96%)	29 (4%)	0	100	100
1	E	668/695 (96%)	628 (94%)	39 (6%)	1 (0%)	51	75
1	G	663/695 (95%)	635 (96%)	28 (4%)	0	100	100
1	I	668/695 (96%)	635 (95%)	33 (5%)	0	100	100
1	K	666/695 (96%)	635 (95%)	31 (5%)	0	100	100
All	All	3994/4170 (96%)	3808 (95%)	184 (5%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	798	LYS
1	A	914	GLU

### 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	578/623 (93%)	578 (100%)	0	100	100
1	C	572/623 (92%)	570 (100%)	2 (0%)	92	98
1	E	558/623 (90%)	557 (100%)	1 (0%)	93	98
1	G	573/623 (92%)	571 (100%)	2 (0%)	92	98
1	I	575/623 (92%)	573 (100%)	2 (0%)	92	98
1	K	565/623 (91%)	564 (100%)	1 (0%)	93	98
All	All	3421/3738 (92%)	3413 (100%)	8 (0%)	93	98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	316	ARG
1	K	607	GLU
1	I	579	PHE
1	E	331	ASN
1	G	813	CYS

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	G	317	HIS
1	K	606	ASN
1	I	619	GLN
1	C	507	GLN
1	G	606	ASN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	23/24 (95%)	0	0
2	D	23/24 (95%)	1 (4%)	0
2	F	23/24 (95%)	0	0
2	H	23/24 (95%)	0	0
2	J	23/24 (95%)	0	0
2	L	23/24 (95%)	0	0
All	All	138/144 (95%)	1 (0%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	15	U

There are no RNA pucker outliers to report.

## 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 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	$\# Z  > 2$
6	BU3	G	1005	-	4,5,5	0.49	0	6,6,6	0.47	0
6	BU3	C	1005	-	4,5,5	0.50	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BU3	G	1003	-	4,5,5	0.52	0	6,6,6	0.34	0
6	BU3	G	1004	-	4,5,5	0.50	0	6,6,6	0.39	0
6	BU3	A	1005	-	4,5,5	0.49	0	6,6,6	0.35	0
6	BU3	C	1006	-	4,5,5	0.47	0	6,6,6	0.36	0
6	BU3	K	1004	-	4,5,5	0.50	0	6,6,6	0.37	0
6	BU3	C	1003	-	4,5,5	0.49	0	6,6,6	0.37	0
5	ETF	A	1003	-	5,5,5	0.40	0	7,7,7	0.63	0
6	BU3	E	1003	-	4,5,5	0.53	0	6,6,6	0.37	0
5	ETF	K	1003	-	5,5,5	0.40	0	7,7,7	0.63	0
5	ETF	E	1002	-	5,5,5	0.39	0	7,7,7	0.63	0
6	BU3	E	1004	-	4,5,5	0.54	0	6,6,6	0.40	0
5	ETF	G	1002	-	5,5,5	0.39	0	7,7,7	0.66	0
6	BU3	C	1004	-	4,5,5	0.54	0	6,6,6	0.36	0
6	BU3	I	1004	-	4,5,5	0.52	0	6,6,6	0.33	0
6	BU3	A	1004	-	4,5,5	0.49	0	6,6,6	0.39	0

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
6	BU3	G	1005	-	-	4/4/4/4	-
6	BU3	C	1005	-	-	0/4/4/4	-
6	BU3	G	1003	-	-	0/4/4/4	-
6	BU3	G	1004	-	-	4/4/4/4	-
6	BU3	A	1005	-	-	4/4/4/4	-
6	BU3	C	1006	-	-	4/4/4/4	-
6	BU3	K	1004	-	-	4/4/4/4	-
6	BU3	C	1003	-	-	0/4/4/4	-
5	ETF	A	1003	-	-	0/3/3/3	-
6	BU3	E	1003	-	-	2/4/4/4	-
5	ETF	K	1003	-	-	0/3/3/3	-
5	ETF	E	1002	-	-	1/3/3/3	-
6	BU3	E	1004	-	-	4/4/4/4	-
5	ETF	G	1002	-	-	3/3/3/3	-
6	BU3	C	1004	-	-	4/4/4/4	-
6	BU3	I	1004	-	-	0/4/4/4	-
6	BU3	A	1004	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1005	BU3	O5-C2-C3-O6
6	G	1005	BU3	C1-C2-C3-O6
6	G	1005	BU3	O5-C2-C3-C4
6	K	1004	BU3	C1-C2-C3-O6
6	K	1004	BU3	O5-C2-C3-C4

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1005	BU3	2	0
6	G	1003	BU3	2	0
6	G	1004	BU3	1	0
6	A	1005	BU3	1	0
6	C	1006	BU3	2	0
6	K	1004	BU3	1	0
5	A	1003	ETF	1	0
6	E	1003	BU3	2	0
6	E	1004	BU3	2	0
5	G	1002	ETF	1	0
6	C	1004	BU3	2	0
6	I	1004	BU3	3	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	673/695 (96%)	-0.37	10 (1%) 73 70	17, 43, 85, 138	0
1	C	668/695 (96%)	-0.23	7 (1%) 82 80	21, 50, 95, 151	0
1	E	672/695 (96%)	-0.12	18 (2%) 54 48	24, 55, 107, 152	0
1	G	669/695 (96%)	-0.26	5 (0%) 87 86	25, 50, 88, 124	0
1	I	674/695 (96%)	-0.15	9 (1%) 77 73	27, 55, 96, 136	0
1	K	672/695 (96%)	-0.16	14 (2%) 63 58	24, 55, 99, 146	0
2	B	24/24 (100%)	-0.07	3 (12%) 3 2	30, 38, 99, 142	0
2	D	24/24 (100%)	-0.26	2 (8%) 11 8	25, 39, 121, 124	0
2	F	24/24 (100%)	-0.44	0 100 100	34, 43, 100, 109	0
2	H	24/24 (100%)	-0.29	2 (8%) 11 8	31, 42, 109, 115	0
2	J	24/24 (100%)	-0.24	3 (12%) 3 2	34, 46, 107, 110	0
2	L	24/24 (100%)	-0.31	1 (4%) 36 29	34, 46, 111, 118	0
All	All	4172/4314 (96%)	-0.22	74 (1%) 68 64	17, 51, 98, 152	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	606	ASN	5.7
1	E	576	ALA	5.6
1	K	604	PRO	3.8
1	K	794	GLN	3.8
2	B	12	U	3.8

### 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 ⓘ

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( $\text{\AA}^2$ )	Q<0.9
6	BU3	G	1004	6/6	0.55	0.64	87,98,107,110	0
3	ZN	G	1001	1/1	0.66	0.52	210,210,210,210	0
5	ETF	K	1003	6/6	0.74	0.38	85,120,127,128	0
6	BU3	C	1005	6/6	0.77	0.44	86,100,104,112	0
6	BU3	A	1005	6/6	0.77	0.39	61,75,81,93	0
3	ZN	C	1001	1/1	0.84	0.32	99,99,99,99	0
6	BU3	G	1003	6/6	0.84	0.33	42,62,76,83	0
6	BU3	C	1003	6/6	0.85	0.38	48,70,78,87	0
6	BU3	E	1004	6/6	0.85	0.31	72,85,93,97	0
6	BU3	C	1006	6/6	0.86	0.32	57,65,67,75	0
5	ETF	E	1002	6/6	0.87	0.37	50,106,115,120	0
6	BU3	E	1003	6/6	0.87	0.28	69,71,75,88	0
6	BU3	A	1004	6/6	0.87	0.28	59,71,77,86	0
6	BU3	I	1004	6/6	0.88	0.34	39,61,73,82	0
4	MG	C	1002	1/1	0.88	0.42	56,56,56,56	0
4	MG	K	1002	1/1	0.89	0.30	62,62,62,62	0
6	BU3	G	1005	6/6	0.90	0.26	71,77,88,95	0
5	ETF	A	1003	6/6	0.90	0.24	37,69,80,82	0
3	ZN	A	1001	1/1	0.91	0.28	97,97,97,97	0
6	BU3	K	1004	6/6	0.91	0.28	51,52,61,68	0
5	ETF	G	1002	6/6	0.93	0.30	50,83,90,108	0
4	MG	I	1003	1/1	0.94	0.17	57,57,57,57	0
4	MG	I	1002	1/1	0.94	0.30	51,51,51,51	0
3	ZN	I	1001	1/1	0.94	0.32	102,102,102,102	0
3	ZN	E	1001	1/1	0.95	0.15	95,95,95,95	0
6	BU3	C	1004	6/6	0.95	0.37	17,56,70,73	0
4	MG	H	101	1/1	0.97	0.20	46,46,46,46	0
3	ZN	K	1001	1/1	0.97	0.24	94,94,94,94	0
4	MG	A	1002	1/1	0.98	0.30	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.