



# wwPDB X-ray Structure Validation Summary Report i

Nov 19, 2023 – 05:14 PM JST

PDB ID : 6LQO  
Title : EBV tegument protein BBRF2/BSRF1 complex  
Authors : He, H.P.; Luo, M.; Cao, Y.L.; Gao, S.  
Deposited on : 2020-01-14  
Resolution : 3.09 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 i 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](#) ①) 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 : 2.36  
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

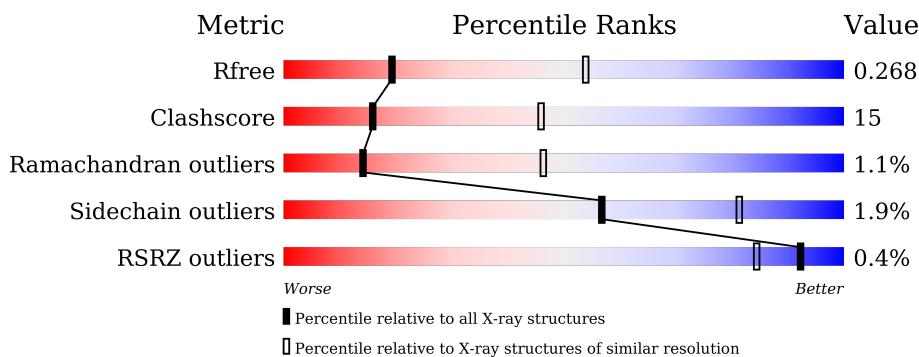
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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.



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Mol	Chain	Length	Quality of chain			
2	H	131	50%	18%	.	31%
2	I	131	46%	21%	.	33%
2	J	131	47%	22%	.	29%
2	K	131	44%	18%		38%
2	L	131	47%	24%	.	28%
2	M	131	50%	14%	.	34%

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16191 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 Cytoplasmic envelopment protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total 2052	C 1295	N 364	O 377	S 16	0	1	0
1	B	254	Total 2020	C 1275	N 357	O 372	S 16	0	0	0
1	C	242	Total 1927	C 1219	N 343	O 349	S 16	0	0	0
1	D	254	Total 2011	C 1271	N 356	O 368	S 16	0	0	0
1	E	257	Total 2033	C 1283	N 359	O 375	S 16	0	0	0
1	F	255	Total 2027	C 1280	N 358	O 373	S 16	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP K9US56
A	11	PRO	-	expression tag	UNP K9US56
A	12	HIS	-	expression tag	UNP K9US56
A	13	MET	-	expression tag	UNP K9US56
A	14	GLY	-	expression tag	UNP K9US56
A	15	GLY	-	expression tag	UNP K9US56
A	16	SER	-	expression tag	UNP K9US56
B	10	GLY	-	expression tag	UNP K9US56
B	11	PRO	-	expression tag	UNP K9US56
B	12	HIS	-	expression tag	UNP K9US56
B	13	MET	-	expression tag	UNP K9US56
B	14	GLY	-	expression tag	UNP K9US56
B	15	GLY	-	expression tag	UNP K9US56
B	16	SER	-	expression tag	UNP K9US56
C	10	GLY	-	expression tag	UNP K9US56
C	11	PRO	-	expression tag	UNP K9US56
C	12	HIS	-	expression tag	UNP K9US56

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	MET	-	expression tag	UNP K9US56
C	14	GLY	-	expression tag	UNP K9US56
C	15	GLY	-	expression tag	UNP K9US56
C	16	SER	-	expression tag	UNP K9US56
D	10	GLY	-	expression tag	UNP K9US56
D	11	PRO	-	expression tag	UNP K9US56
D	12	HIS	-	expression tag	UNP K9US56
D	13	MET	-	expression tag	UNP K9US56
D	14	GLY	-	expression tag	UNP K9US56
D	15	GLY	-	expression tag	UNP K9US56
D	16	SER	-	expression tag	UNP K9US56
E	10	GLY	-	expression tag	UNP K9US56
E	11	PRO	-	expression tag	UNP K9US56
E	12	HIS	-	expression tag	UNP K9US56
E	13	MET	-	expression tag	UNP K9US56
E	14	GLY	-	expression tag	UNP K9US56
E	15	GLY	-	expression tag	UNP K9US56
E	16	SER	-	expression tag	UNP K9US56
F	10	GLY	-	expression tag	UNP K9US56
F	11	PRO	-	expression tag	UNP K9US56
F	12	HIS	-	expression tag	UNP K9US56
F	13	MET	-	expression tag	UNP K9US56
F	14	GLY	-	expression tag	UNP K9US56
F	15	GLY	-	expression tag	UNP K9US56
F	16	SER	-	expression tag	UNP K9US56

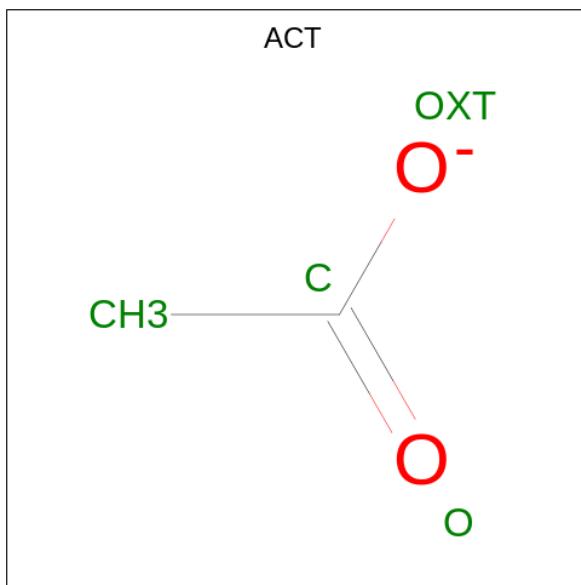
- Molecule 2 is a protein called Tegument protein UL51 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	91	Total	C	N	O	S	0	0	0
			691	430	123	134	4			
2	I	88	Total	C	N	O	S	0	0	0
			671	419	121	127	4			
2	J	93	Total	C	N	O	S	0	0	0
			707	443	126	134	4			
2	K	81	Total	C	N	O	S	0	0	0
			620	389	112	115	4			
2	L	94	Total	C	N	O	S	0	0	0
			717	448	129	136	4			
2	M	86	Total	C	N	O	S	0	0	0
			657	410	118	125	4			

There are 30 discrepancies between the modelled and reference sequences:

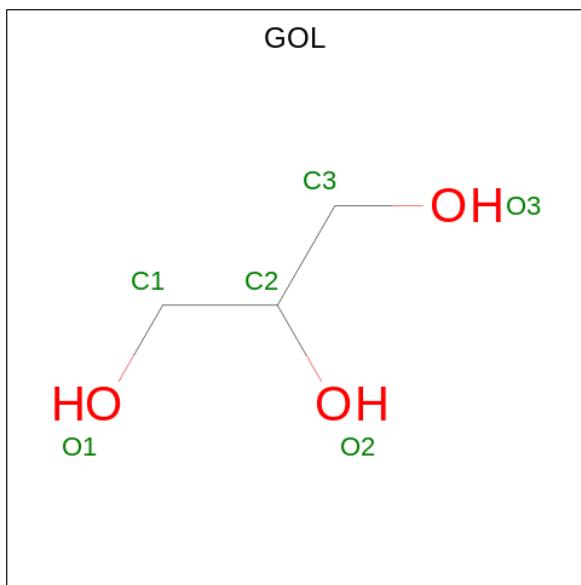
Chain	Residue	Modelled	Actual	Comment	Reference
H	29	GLY	-	expression tag	UNP P0CK62
H	30	PRO	-	expression tag	UNP P0CK62
H	31	LEU	-	expression tag	UNP P0CK62
H	32	GLY	-	expression tag	UNP P0CK62
H	33	SER	-	expression tag	UNP P0CK62
I	29	GLY	-	expression tag	UNP P0CK62
I	30	PRO	-	expression tag	UNP P0CK62
I	31	LEU	-	expression tag	UNP P0CK62
I	32	GLY	-	expression tag	UNP P0CK62
I	33	SER	-	expression tag	UNP P0CK62
J	29	GLY	-	expression tag	UNP P0CK62
J	30	PRO	-	expression tag	UNP P0CK62
J	31	LEU	-	expression tag	UNP P0CK62
J	32	GLY	-	expression tag	UNP P0CK62
J	33	SER	-	expression tag	UNP P0CK62
K	29	GLY	-	expression tag	UNP P0CK62
K	30	PRO	-	expression tag	UNP P0CK62
K	31	LEU	-	expression tag	UNP P0CK62
K	32	GLY	-	expression tag	UNP P0CK62
K	33	SER	-	expression tag	UNP P0CK62
L	29	GLY	-	expression tag	UNP P0CK62
L	30	PRO	-	expression tag	UNP P0CK62
L	31	LEU	-	expression tag	UNP P0CK62
L	32	GLY	-	expression tag	UNP P0CK62
L	33	SER	-	expression tag	UNP P0CK62
M	29	GLY	-	expression tag	UNP P0CK62
M	30	PRO	-	expression tag	UNP P0CK62
M	31	LEU	-	expression tag	UNP P0CK62
M	32	GLY	-	expression tag	UNP P0CK62
M	33	SER	-	expression tag	UNP P0CK62

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

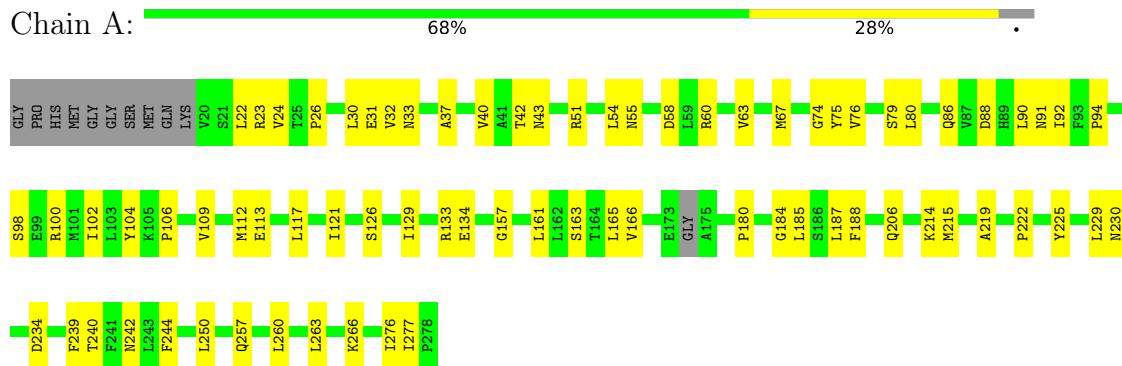
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	5	Total O 5 5	0	0
5	F	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0
5	J	1	Total O 1 1	0	0
5	K	4	Total O 4 4	0	0
5	L	2	Total O 2 2	0	0
5	M	3	Total O 3 3	0	0

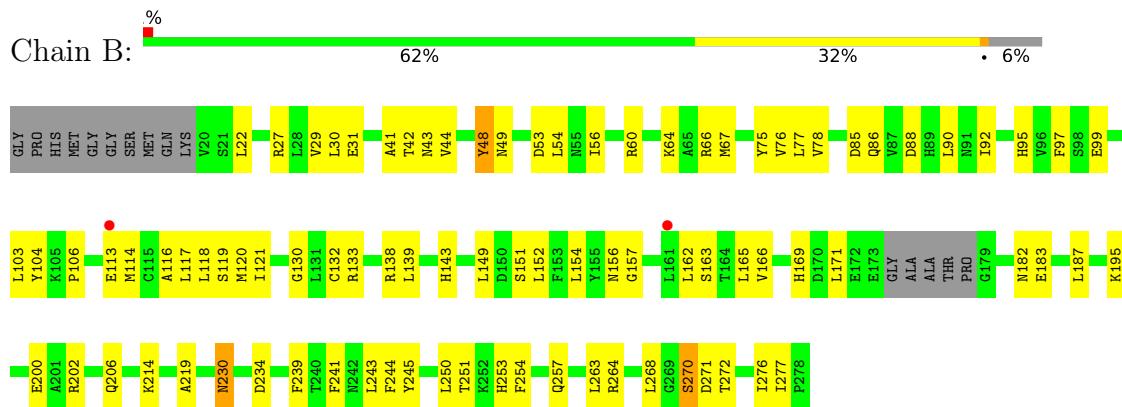
### 3 Residue-property plots [\(i\)](#)

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.

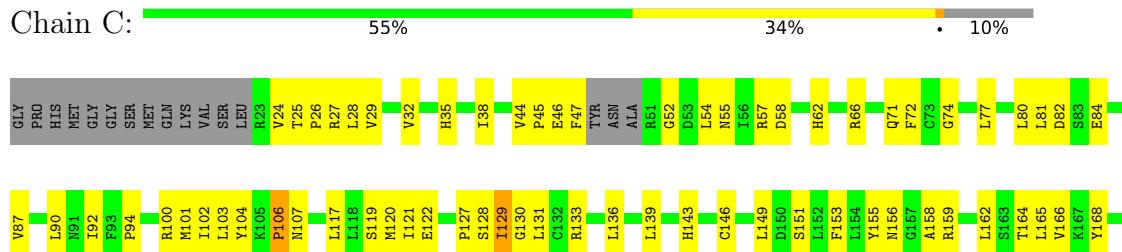
- Molecule 1: Cytoplasmic envelopment protein 1



- Molecule 1: Cytoplasmic envelopment protein 1



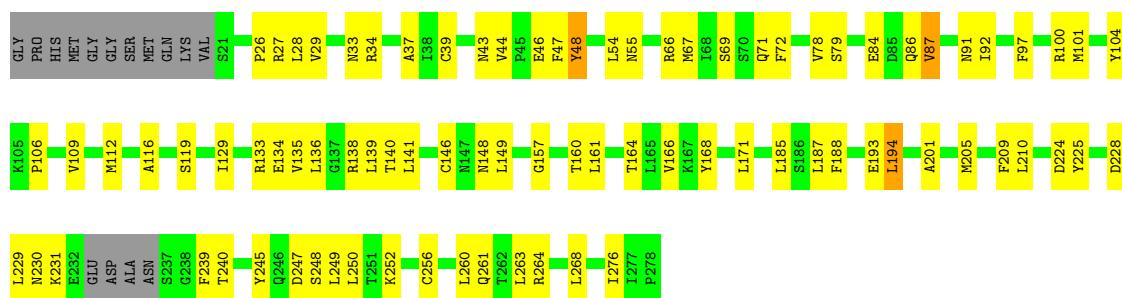
- Molecule 1: Cytoplasmic envelopment protein 1





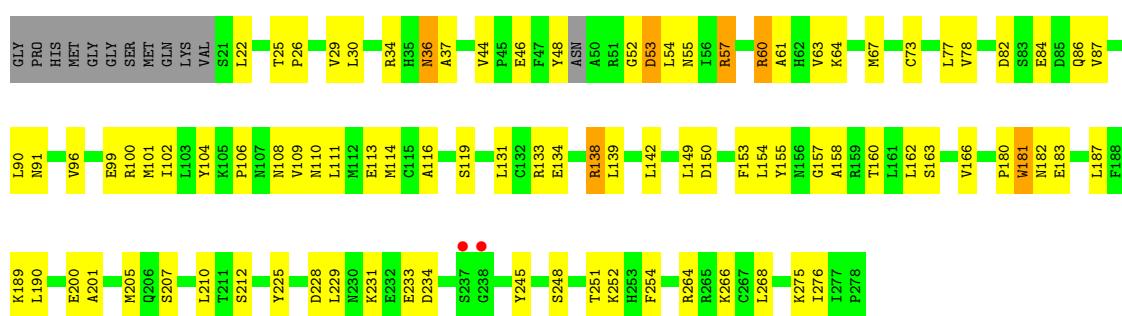
- Molecule 1: Cytoplasmic envelopment protein 1

## Chain D



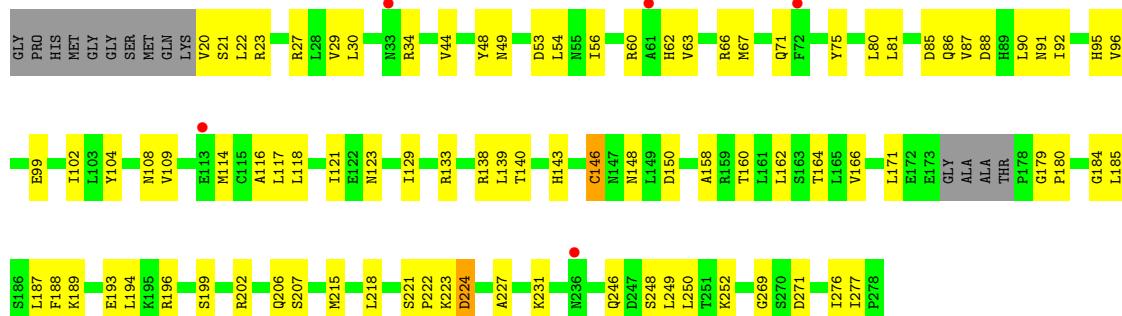
- Molecule 1: Cytoplasmic envelopment protein 1

Chain E



- Molecule 1: Cytoplasmic envelopment protein 1

### Chain F:



- Molecule 2: Tegument protein UL51 homolog

## Chain H





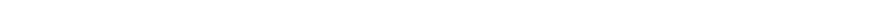
- Molecule 2: Tegument protein UL51 homolog

Chain I:



GLY	PRO	LEU	SER	GLU	CYS	ASP	ARG	TRP	ARG	ALA	GLU	TLE	ASP	L445	L447	P448	G54	D556	D557	R558	M63	G64	S65	L66	R67	Q68	V69	Y70	A73	V74	Q75	A76	H82	R85	F86	D87	A88	V89	V98	Q102	L106	I113	M117	V122
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

M130	GLY	LEU	K133	
A134	LEU	LEU	ASP	LYS
	GLN	ALA	GLY	ASP
	SER	LEU	ALA	LEU
	GLU	LEU	VAL	ALA
	MET	THR	VAL	LYS
		ALA	LEU	LYS
			ALA	MET

Chain J:  47% 22% • 29%

M130	G131	L132	K133	A134	L135	L136
	ASP					
		LYS				
		GLN				
		ALA				
		GLY				
	ASP					
	SER					
		LEU				
		ALA				
		LEU				
		MET				
		GLU				
		MET				
		GLU				
		LYS				
		LYS				
		VAL				
		ALA				
		THR				
		ALA				
		LEU				
		MET				
		ASP				

- Molecule 2: Tegument protein UL51 homolog

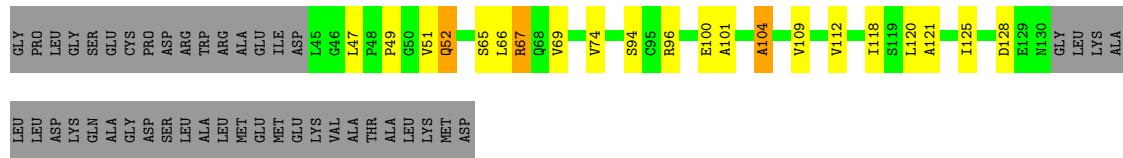
Chain K:  44% 18% 38%

- Molecule 2: Tegument protein UL51 homolog

Term	Percentage
Chronic disease	47%
Healthcare system	24%
Medical treatment	23%
Healthcare worker	20%
Healthcare facility	18%
Healthcare service	15%
Healthcare provider	12%
Healthcare professional	10%
Healthcare institution	8%
Healthcare organization	5%

- Molecule 2: Tegument protein UL51 homolog

Chain M:  50% 14% : 34%



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.78 Å    161.85 Å    97.86 Å 90.00°    100.78°    90.00°	Depositor
Resolution (Å)	44.34 – 3.09 48.07 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.34-3.09) 99.5 (48.07-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.34 (at 3.07 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155, REFMAC 5.8.0258	Depositor
$R$ , $R_{free}$	0.217 , 0.269 0.217 , 0.268	Depositor DCC
$R_{free}$ test set	2000 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.8	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16191	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 3.18% 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  $< |L| >$ ,  $< L^2 >$  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: GOL, ACT

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	0.44	0/2091	0.60	0/2822
1	B	0.45	0/2055	0.65	0/2772
1	C	0.44	0/1958	0.65	0/2636
1	D	0.43	0/2047	0.61	1/2762 (0.0%)
1	E	0.49	2/2069 (0.1%)	0.69	0/2792
1	F	0.41	0/2063	0.59	0/2783
2	H	0.41	0/698	0.61	0/946
2	I	0.46	0/677	0.57	0/915
2	J	0.40	0/713	0.59	0/964
2	K	0.46	1/627 (0.2%)	0.62	0/850
2	L	0.44	0/724	0.59	0/979
2	M	0.49	0/664	0.61	0/900
All	All	0.44	3/16386 (0.0%)	0.62	1/22121 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	46	GLU	CD-OE1	-6.35	1.18	1.25
1	E	46	GLU	CD-OE2	-5.80	1.19	1.25
2	K	95	CYS	CB-SG	-5.23	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	ILE	C-N-CA	-6.07	106.53	121.70

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	2052	0	2080	51	0
1	B	2020	0	2043	63	0
1	C	1927	0	1962	74	0
1	D	2011	0	2040	60	0
1	E	2033	0	2055	74	0
1	F	2027	0	2051	73	0
2	H	691	0	701	23	0
2	I	671	0	689	19	0
2	J	707	0	729	23	0
2	K	620	0	642	21	0
2	L	717	0	740	27	0
2	M	657	0	672	19	0
3	C	4	0	3	0	0
3	E	4	0	3	0	0
3	H	4	0	3	0	0
4	C	6	0	8	1	0
4	E	6	0	8	0	0
4	M	6	0	8	0	0
5	B	6	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	5	0	0	0	0
5	F	3	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	0	0
5	K	4	0	0	0	0
5	L	2	0	0	0	0
5	M	3	0	0	0	0
All	All	16191	0	16437	476	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 15.

The worst 5 of 476 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:E:134:GLU:HG2	1:E:138:ARG:HH22	1.24	1.01
1:D:54:LEU:HD22	1:D:134:GLU:HB3	1.48	0.94
1:E:133:ARG:HH21	1:E:180:PRO:HD2	1.32	0.93
1:B:187:LEU:HD11	2:I:66:LEU:HD23	1.52	0.91
1:E:187:LEU:HD21	2:K:66:LEU:HD13	1.53	0.91

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	255/269 (95%)	234 (92%)	21 (8%)	0	100 100
1	B	250/269 (93%)	231 (92%)	17 (7%)	2 (1%)	19 54
1	C	234/269 (87%)	209 (89%)	22 (9%)	3 (1%)	12 42
1	D	250/269 (93%)	236 (94%)	13 (5%)	1 (0%)	34 69
1	E	253/269 (94%)	224 (88%)	23 (9%)	6 (2%)	6 27
1	F	251/269 (93%)	238 (95%)	12 (5%)	1 (0%)	34 69
2	H	89/131 (68%)	82 (92%)	5 (6%)	2 (2%)	6 29
2	I	84/131 (64%)	80 (95%)	4 (5%)	0	100 100
2	J	89/131 (68%)	83 (93%)	4 (4%)	2 (2%)	6 29
2	K	79/131 (60%)	78 (99%)	1 (1%)	0	100 100
2	L	92/131 (70%)	85 (92%)	5 (5%)	2 (2%)	6 29
2	M	84/131 (64%)	78 (93%)	3 (4%)	3 (4%)	3 20
All	All	2010/2400 (84%)	1858 (92%)	130 (6%)	22 (1%)	14 46

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	PRO

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Mol	Chain	Res	Type
1	B	270	SER
2	J	134	ALA
2	M	52	GLN
1	E	36	ASN

### 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	233/239 (98%)	232 (100%)	1 (0%)	91 96
1	B	230/239 (96%)	226 (98%)	4 (2%)	60 83
1	C	220/239 (92%)	215 (98%)	5 (2%)	50 77
1	D	228/239 (95%)	224 (98%)	4 (2%)	59 82
1	E	230/239 (96%)	223 (97%)	7 (3%)	41 71
1	F	231/239 (97%)	229 (99%)	2 (1%)	78 91
2	H	76/108 (70%)	75 (99%)	1 (1%)	69 87
2	I	74/108 (68%)	72 (97%)	2 (3%)	44 74
2	J	78/108 (72%)	74 (95%)	4 (5%)	24 56
2	K	69/108 (64%)	69 (100%)	0	100 100
2	L	79/108 (73%)	75 (95%)	4 (5%)	24 56
2	M	73/108 (68%)	72 (99%)	1 (1%)	67 86
All	All	1821/2082 (88%)	1786 (98%)	35 (2%)	57 81

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	87	ASP
2	J	130	ASN
2	L	123	SER
1	D	224	ASP
1	D	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	148	ASN
1	F	148	ASN
2	H	75	GLN

### 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 [\(i\)](#)

6 ligands are modelled in this entry.

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	GOL	E	302	-	5,5,5	0.39	0	5,5,5	0.80	0
3	ACT	H	201	-	3,3,3	0.85	0	3,3,3	1.17	0
3	ACT	C	301	-	3,3,3	0.88	0	3,3,3	0.95	0
3	ACT	E	301	-	3,3,3	0.67	0	3,3,3	1.36	0
4	GOL	M	201	-	5,5,5	0.36	0	5,5,5	0.46	0
4	GOL	C	302	-	5,5,5	0.50	0	5,5,5	0.47	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
4	GOL	M	201	-	-	2/4/4/4	-
4	GOL	E	302	-	-	0/4/4/4	-
4	GOL	C	302	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	GOL	O1-C1-C2-C3
4	C	302	GOL	C1-C2-C3-O3
4	M	201	GOL	C1-C2-C3-O3
4	C	302	GOL	O1-C1-C2-O2
4	M	201	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	GOL	1	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 [\(i\)](#)

### 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	258/269 (95%)	-0.30	0   100   100	35, 61, 124, 151	0
1	B	254/269 (94%)	-0.08	2 (0%)   86   72	37, 79, 122, 152	0
1	C	242/269 (89%)	-0.16	0   100   100	36, 85, 117, 143	0
1	D	254/269 (94%)	-0.29	0   100   100	36, 64, 110, 128	0
1	E	257/269 (95%)	-0.15	2 (0%)   86   72	38, 74, 139, 188	0
1	F	255/269 (94%)	-0.04	5 (1%)   65   44	43, 91, 137, 168	0
2	H	91/131 (69%)	-0.18	0   100   100	39, 63, 118, 135	0
2	I	88/131 (67%)	-0.35	0   100   100	43, 69, 112, 141	0
2	J	93/131 (70%)	-0.30	0   100   100	39, 69, 124, 138	0
2	K	81/131 (61%)	-0.21	0   100   100	37, 66, 120, 141	0
2	L	94/131 (71%)	-0.20	0   100   100	38, 72, 114, 124	0
2	M	86/131 (65%)	-0.32	0   100   100	32, 61, 125, 139	0
All	All	2053/2400 (85%)	-0.19	9 (0%)   92   84	32, 71, 127, 188	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	236	ASN	3.4
1	B	113	GLU	3.2
1	B	161	LEU	2.7
1	F	72	PHE	2.7
1	E	237	SER	2.6

### 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
4	GOL	M	201	6/6	0.85	0.20	78,79,79,80	0
3	ACT	C	301	4/4	0.89	0.23	56,57,58,58	0
4	GOL	C	302	6/6	0.90	0.26	64,64,64,64	0
3	ACT	H	201	4/4	0.90	0.39	47,49,50,51	0
3	ACT	E	301	4/4	0.92	0.39	59,60,60,61	0
4	GOL	E	302	6/6	0.93	0.19	70,71,71,71	0

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.