



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2017 – 05:10 PM EST

PDB ID : 3K4W
Title : CRYSTAL STRUCTURE OF Uncharacterized Tim-Barrel Protein Bb4693
From Bordetella Bronchiseptica
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New
York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 1.92 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

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

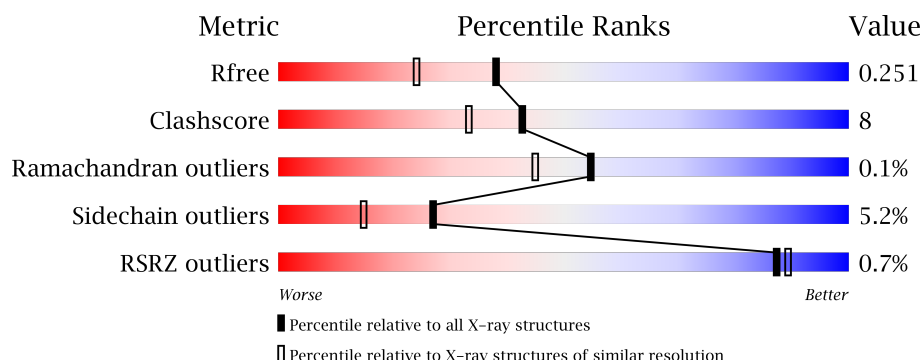
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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 ≥ 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	291	<div> <div>0.1%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>...</div> </div> </div>
1	B	291	<div> <div>0.1%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>...</div> </div> </div>
1	C	291	<div> <div></div> <div> <div></div> <div>79%</div> <div>15%</div> <div>...</div> </div> </div>
1	D	291	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>...</div> </div> </div>
1	E	291	<div> <div></div> <div> <div></div> <div>76%</div> <div>17%</div> <div>...</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	291	<div><div></div><div>79%16%<div><div></div><div></div><div></div></div></div></div>
1	G	291	<div><div>2%</div><div></div><div>72%21%<div><div></div><div></div><div></div></div></div></div>
1	H	291	<div><div></div><div>80%14%<div><div></div><div></div><div></div></div></div></div>
1	I	291	<div><div>%</div><div></div><div>79%17%<div><div></div><div></div><div></div></div></div></div>
1	J	291	<div><div></div><div>81%14%<div><div></div><div></div><div></div></div></div></div>
1	K	291	<div><div></div><div>85%11%<div><div></div><div></div><div></div></div></div></div>
1	L	291	<div><div></div><div>71%22%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28586 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 uncharacterized protein Bb4693.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			2215	1417	381	402	15			
1	B	281	Total	C	N	O	S	0	6	0
			2236	1430	382	408	16			
1	C	281	Total	C	N	O	S	0	2	0
			2220	1420	382	403	15			
1	D	281	Total	C	N	O	S	0	2	0
			2220	1421	381	402	16			
1	E	281	Total	C	N	O	S	0	5	0
			2231	1427	382	406	16			
1	F	281	Total	C	N	O	S	0	3	0
			2230	1428	384	401	17			
1	G	281	Total	C	N	O	S	0	2	0
			2223	1423	381	403	16			
1	H	281	Total	C	N	O	S	0	4	0
			2226	1424	382	404	16			
1	I	281	Total	C	N	O	S	0	2	0
			2224	1423	384	402	15			
1	J	281	Total	C	N	O	S	0	2	0
			2220	1420	382	403	15			
1	K	281	Total	C	N	O	S	0	3	0
			2223	1422	381	404	16			
1	L	281	Total	C	N	O	S	0	1	0
			2215	1417	381	402	15			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	INSERTION	UNP Q7WEE2
A	1	LEU	-	INSERTION	UNP Q7WEE2
A	282	GLU	-	INSERTION	UNP Q7WEE2
A	283	GLY	-	INSERTION	UNP Q7WEE2
A	284	HIS	-	INSERTION	UNP Q7WEE2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	HIS	-	INSERTION	UNP Q7WEE2
A	286	HIS	-	INSERTION	UNP Q7WEE2
A	287	HIS	-	INSERTION	UNP Q7WEE2
A	288	HIS	-	INSERTION	UNP Q7WEE2
A	289	HIS	-	INSERTION	UNP Q7WEE2
B	0	SER	-	INSERTION	UNP Q7WEE2
B	1	LEU	-	INSERTION	UNP Q7WEE2
B	282	GLU	-	INSERTION	UNP Q7WEE2
B	283	GLY	-	INSERTION	UNP Q7WEE2
B	284	HIS	-	INSERTION	UNP Q7WEE2
B	285	HIS	-	INSERTION	UNP Q7WEE2
B	286	HIS	-	INSERTION	UNP Q7WEE2
B	287	HIS	-	INSERTION	UNP Q7WEE2
B	288	HIS	-	INSERTION	UNP Q7WEE2
B	289	HIS	-	INSERTION	UNP Q7WEE2
C	0	SER	-	INSERTION	UNP Q7WEE2
C	1	LEU	-	INSERTION	UNP Q7WEE2
C	282	GLU	-	INSERTION	UNP Q7WEE2
C	283	GLY	-	INSERTION	UNP Q7WEE2
C	284	HIS	-	INSERTION	UNP Q7WEE2
C	285	HIS	-	INSERTION	UNP Q7WEE2
C	286	HIS	-	INSERTION	UNP Q7WEE2
C	287	HIS	-	INSERTION	UNP Q7WEE2
C	288	HIS	-	INSERTION	UNP Q7WEE2
C	289	HIS	-	INSERTION	UNP Q7WEE2
D	0	SER	-	INSERTION	UNP Q7WEE2
D	1	LEU	-	INSERTION	UNP Q7WEE2
D	282	GLU	-	INSERTION	UNP Q7WEE2
D	283	GLY	-	INSERTION	UNP Q7WEE2
D	284	HIS	-	INSERTION	UNP Q7WEE2
D	285	HIS	-	INSERTION	UNP Q7WEE2
D	286	HIS	-	INSERTION	UNP Q7WEE2
D	287	HIS	-	INSERTION	UNP Q7WEE2
D	288	HIS	-	INSERTION	UNP Q7WEE2
D	289	HIS	-	INSERTION	UNP Q7WEE2
E	0	SER	-	INSERTION	UNP Q7WEE2
E	1	LEU	-	INSERTION	UNP Q7WEE2
E	282	GLU	-	INSERTION	UNP Q7WEE2
E	283	GLY	-	INSERTION	UNP Q7WEE2
E	284	HIS	-	INSERTION	UNP Q7WEE2
E	285	HIS	-	INSERTION	UNP Q7WEE2
E	286	HIS	-	INSERTION	UNP Q7WEE2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	287	HIS	-	INSERTION	UNP Q7WEE2
E	288	HIS	-	INSERTION	UNP Q7WEE2
E	289	HIS	-	INSERTION	UNP Q7WEE2
F	0	SER	-	INSERTION	UNP Q7WEE2
F	1	LEU	-	INSERTION	UNP Q7WEE2
F	282	GLU	-	INSERTION	UNP Q7WEE2
F	283	GLY	-	INSERTION	UNP Q7WEE2
F	284	HIS	-	INSERTION	UNP Q7WEE2
F	285	HIS	-	INSERTION	UNP Q7WEE2
F	286	HIS	-	INSERTION	UNP Q7WEE2
F	287	HIS	-	INSERTION	UNP Q7WEE2
F	288	HIS	-	INSERTION	UNP Q7WEE2
F	289	HIS	-	INSERTION	UNP Q7WEE2
G	0	SER	-	INSERTION	UNP Q7WEE2
G	1	LEU	-	INSERTION	UNP Q7WEE2
G	282	GLU	-	INSERTION	UNP Q7WEE2
G	283	GLY	-	INSERTION	UNP Q7WEE2
G	284	HIS	-	INSERTION	UNP Q7WEE2
G	285	HIS	-	INSERTION	UNP Q7WEE2
G	286	HIS	-	INSERTION	UNP Q7WEE2
G	287	HIS	-	INSERTION	UNP Q7WEE2
G	288	HIS	-	INSERTION	UNP Q7WEE2
G	289	HIS	-	INSERTION	UNP Q7WEE2
H	0	SER	-	INSERTION	UNP Q7WEE2
H	1	LEU	-	INSERTION	UNP Q7WEE2
H	282	GLU	-	INSERTION	UNP Q7WEE2
H	283	GLY	-	INSERTION	UNP Q7WEE2
H	284	HIS	-	INSERTION	UNP Q7WEE2
H	285	HIS	-	INSERTION	UNP Q7WEE2
H	286	HIS	-	INSERTION	UNP Q7WEE2
H	287	HIS	-	INSERTION	UNP Q7WEE2
H	288	HIS	-	INSERTION	UNP Q7WEE2
H	289	HIS	-	INSERTION	UNP Q7WEE2
I	0	SER	-	INSERTION	UNP Q7WEE2
I	1	LEU	-	INSERTION	UNP Q7WEE2
I	282	GLU	-	INSERTION	UNP Q7WEE2
I	283	GLY	-	INSERTION	UNP Q7WEE2
I	284	HIS	-	INSERTION	UNP Q7WEE2
I	285	HIS	-	INSERTION	UNP Q7WEE2
I	286	HIS	-	INSERTION	UNP Q7WEE2
I	287	HIS	-	INSERTION	UNP Q7WEE2
I	288	HIS	-	INSERTION	UNP Q7WEE2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	289	HIS	-	INSERTION	UNP Q7WEE2
J	0	SER	-	INSERTION	UNP Q7WEE2
J	1	LEU	-	INSERTION	UNP Q7WEE2
J	282	GLU	-	INSERTION	UNP Q7WEE2
J	283	GLY	-	INSERTION	UNP Q7WEE2
J	284	HIS	-	INSERTION	UNP Q7WEE2
J	285	HIS	-	INSERTION	UNP Q7WEE2
J	286	HIS	-	INSERTION	UNP Q7WEE2
J	287	HIS	-	INSERTION	UNP Q7WEE2
J	288	HIS	-	INSERTION	UNP Q7WEE2
J	289	HIS	-	INSERTION	UNP Q7WEE2
K	0	SER	-	INSERTION	UNP Q7WEE2
K	1	LEU	-	INSERTION	UNP Q7WEE2
K	282	GLU	-	INSERTION	UNP Q7WEE2
K	283	GLY	-	INSERTION	UNP Q7WEE2
K	284	HIS	-	INSERTION	UNP Q7WEE2
K	285	HIS	-	INSERTION	UNP Q7WEE2
K	286	HIS	-	INSERTION	UNP Q7WEE2
K	287	HIS	-	INSERTION	UNP Q7WEE2
K	288	HIS	-	INSERTION	UNP Q7WEE2
K	289	HIS	-	INSERTION	UNP Q7WEE2
L	0	SER	-	INSERTION	UNP Q7WEE2
L	1	LEU	-	INSERTION	UNP Q7WEE2
L	282	GLU	-	INSERTION	UNP Q7WEE2
L	283	GLY	-	INSERTION	UNP Q7WEE2
L	284	HIS	-	INSERTION	UNP Q7WEE2
L	285	HIS	-	INSERTION	UNP Q7WEE2
L	286	HIS	-	INSERTION	UNP Q7WEE2
L	287	HIS	-	INSERTION	UNP Q7WEE2
L	288	HIS	-	INSERTION	UNP Q7WEE2
L	289	HIS	-	INSERTION	UNP Q7WEE2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	159	Total O 159 159	0	0
2	B	147	Total O 147 147	0	0
2	C	195	Total O 195 195	0	0
2	D	142	Total O 142 142	0	0

Continued on next page...

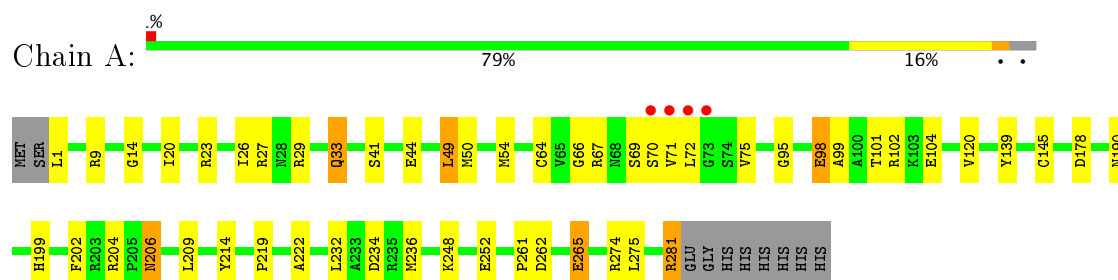
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	168	Total 168	O 168	0	0
2	F	171	Total 171	O 171	0	0
2	G	114	Total 114	O 114	0	0
2	H	155	Total 155	O 155	0	0
2	I	159	Total 159	O 159	0	0
2	J	161	Total 161	O 161	0	0
2	K	175	Total 175	O 175	0	0
2	L	157	Total 157	O 157	0	0

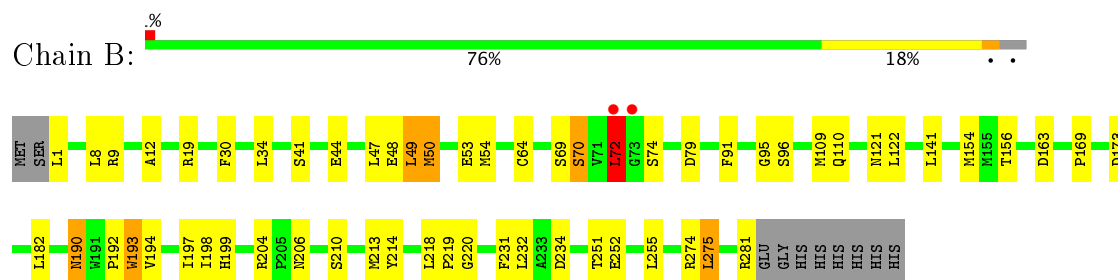
3 Residue-property plots [i](#)

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.

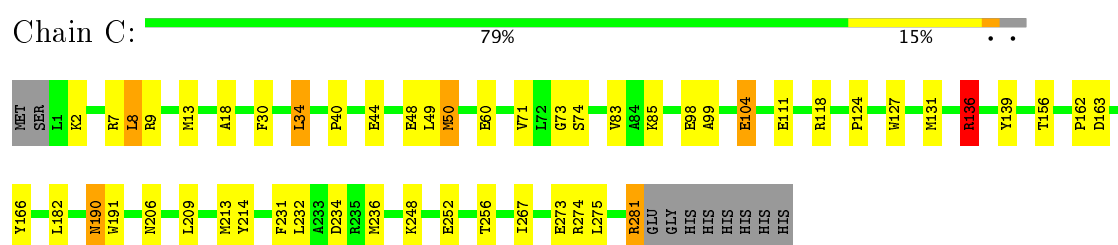
- Molecule 1: uncharacterized protein Bb4693



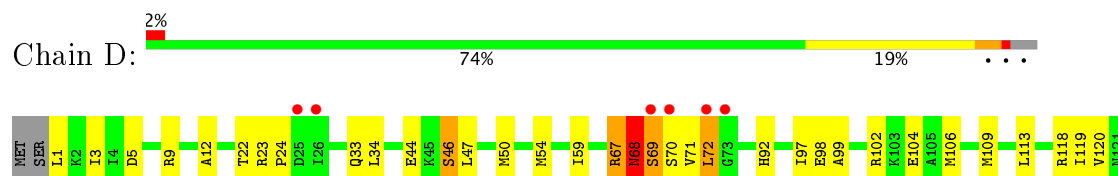
- Molecule 1: uncharacterized protein Bb4693



- Molecule 1: uncharacterized protein Bb4693

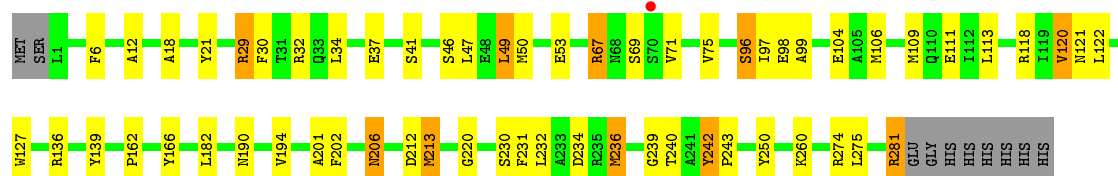


- Molecule 1: uncharacterized protein Bb4693



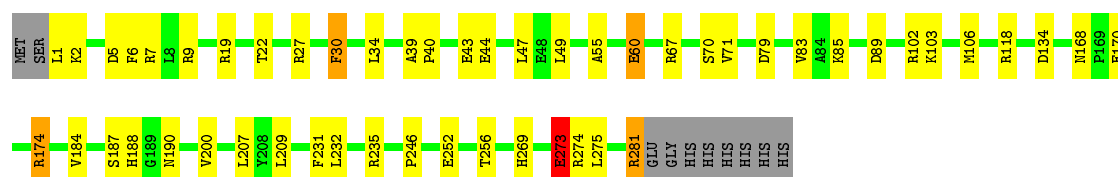
- Molecule 1: uncharacterized protein Bb4693

Chain E: 76% 17% . .

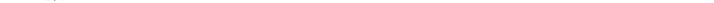


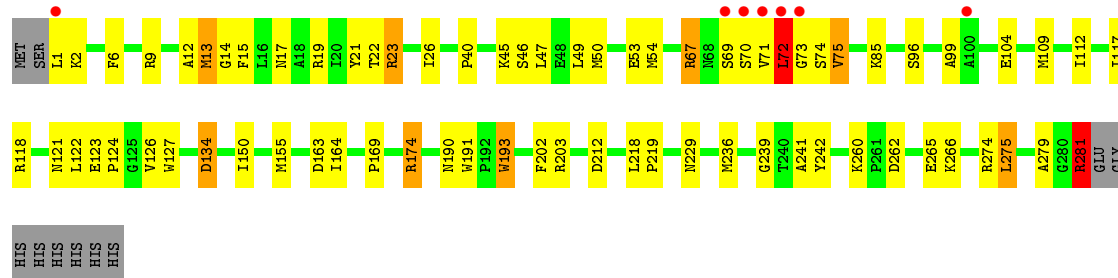
- Molecule 1: uncharacterized protein Bb4693

Chain F: 79% 16% ..

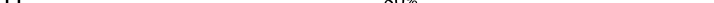


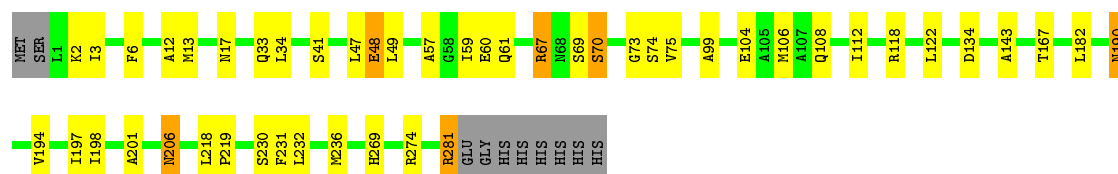
- Molecule 1: uncharacterized protein Bb4693

Chain G:  2% 72% 21%

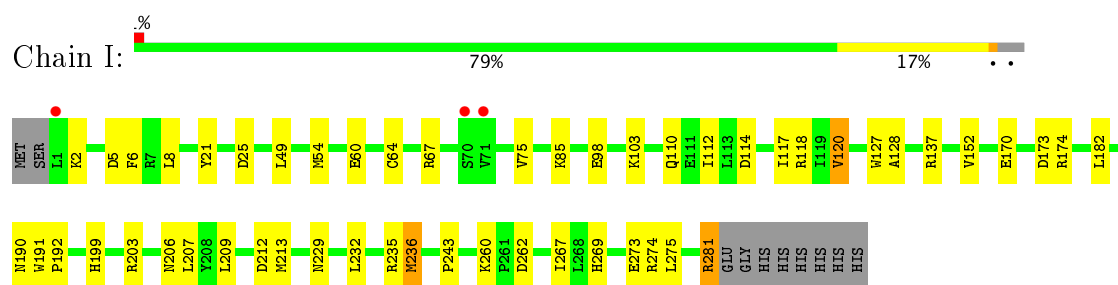


- Molecule 1: uncharacterized protein Bb4693

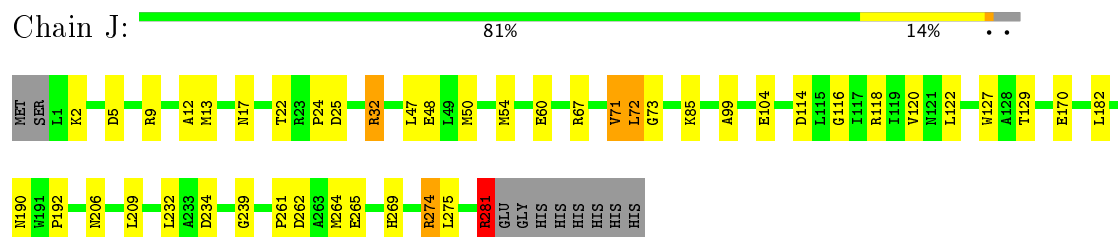
Chain H:  80% 14% . .



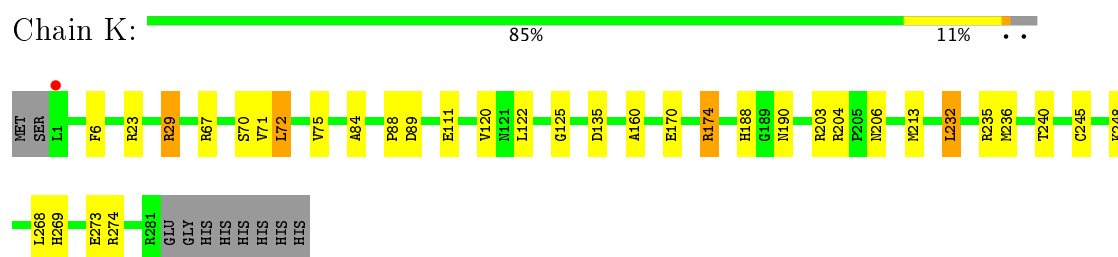
- Molecule 1: uncharacterized protein Bb4693



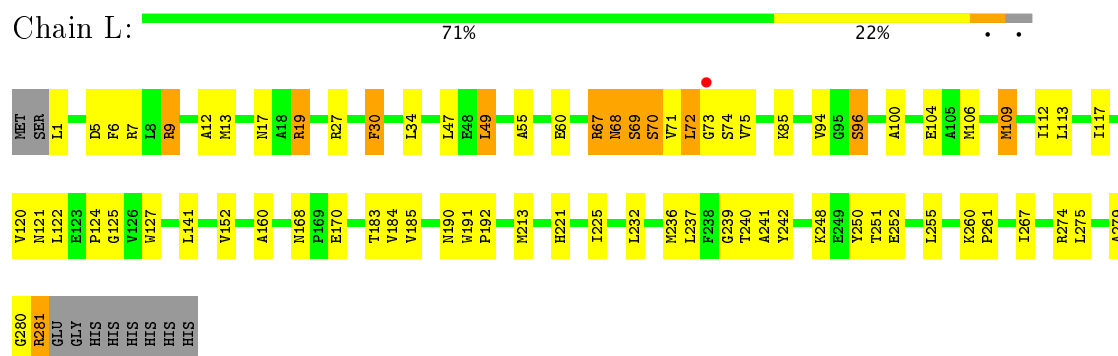
- Molecule 1: uncharacterized protein Bb4693



- Molecule 1: uncharacterized protein Bb4693



- Molecule 1: uncharacterized protein Bb4693



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.92Å 248.77Å 90.62Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	25.97 – 1.92 25.97 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.5 (25.97-1.92) 95.5 (25.97-1.92)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.251 0.192 , 0.251	Depositor DCC
R_{free} test set	13295 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 20.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28586	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	5/2277 (0.2%)	0.97	5/3097 (0.2%)
1	B	1.10	2/2313 (0.1%)	0.99	7/3146 (0.2%)
1	C	1.11	1/2285 (0.0%)	0.97	5/3108 (0.2%)
1	D	1.14	2/2285 (0.1%)	1.00	8/3107 (0.3%)
1	E	1.10	6/2305 (0.3%)	0.96	4/3135 (0.1%)
1	F	1.10	3/2298 (0.1%)	0.99	8/3123 (0.3%)
1	G	1.07	1/2288 (0.0%)	1.03	11/3111 (0.4%)
1	H	1.11	4/2297 (0.2%)	0.96	5/3124 (0.2%)
1	I	1.09	0/2290	0.96	6/3115 (0.2%)
1	J	1.12	4/2285 (0.2%)	1.04	9/3108 (0.3%)
1	K	1.04	1/2291 (0.0%)	0.98	10/3116 (0.3%)
1	L	1.07	1/2277 (0.0%)	0.98	9/3097 (0.3%)
All	All	1.10	30/27491 (0.1%)	0.99	87/37387 (0.2%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	CYS	CB-SG	-9.82	1.65	1.82
1	C	104	GLU	CG-CD	7.85	1.63	1.51
1	E	96	SER	CB-OG	-6.33	1.34	1.42
1	E	206[A]	ASN	CB-CG	5.92	1.64	1.51
1	E	206[B]	ASN	CB-CG	5.92	1.64	1.51

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	274	ARG	NE-CZ-NH2	-16.16	112.22	120.30
1	J	274	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	G	275	LEU	CB-CG-CD1	-9.03	95.65	111.00
1	H	274	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	G	274	ARG	NE-CZ-NH2	-8.38	116.11	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2215	0	2186	38	0
1	B	2236	0	2210	35	0
1	C	2220	0	2192	31	0
1	D	2220	0	2195	46	0
1	E	2231	0	2206	42	0
1	F	2230	0	2212	25	0
1	G	2223	0	2196	56	0
1	H	2226	0	2202	26	0
1	I	2224	0	2194	29	0
1	J	2220	0	2192	28	0
1	K	2223	0	2195	13	0
1	L	2215	0	2186	62	0
2	A	159	0	0	5	0
2	B	147	0	0	1	0
2	C	195	0	0	6	0
2	D	142	0	0	3	0
2	E	168	0	0	4	0
2	F	171	0	0	4	0
2	G	114	0	0	3	0
2	H	155	0	0	1	0
2	I	159	0	0	3	0
2	J	161	0	0	4	0
2	K	175	0	0	1	0
2	L	157	0	0	4	0
All	All	28586	0	26366	412	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 8.

The worst 5 of 412 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:G:281:ARG:HG2	2:G:1454:HOH:O	1.47	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:ASN:O	1:L:74:SER:HB2	1.53	1.06
1:G:67:ARG:HG3	1:G:67:ARG:HH21	1.16	1.05
1:C:136:ARG:HD2	2:E:292:HOH:O	1.60	1.00
1:D:71:VAL:HG12	1:D:72:LEU:O	1.62	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/291 (96%)	270 (96%)	10 (4%)	0	100	100
1	B	285/291 (98%)	278 (98%)	7 (2%)	0	100	100
1	C	281/291 (97%)	274 (98%)	7 (2%)	0	100	100
1	D	281/291 (97%)	270 (96%)	10 (4%)	1 (0%)	38	26
1	E	284/291 (98%)	274 (96%)	10 (4%)	0	100	100
1	F	282/291 (97%)	275 (98%)	7 (2%)	0	100	100
1	G	281/291 (97%)	270 (96%)	11 (4%)	0	100	100
1	H	283/291 (97%)	278 (98%)	5 (2%)	0	100	100
1	I	281/291 (97%)	272 (97%)	9 (3%)	0	100	100
1	J	281/291 (97%)	274 (98%)	6 (2%)	1 (0%)	38	26
1	K	282/291 (97%)	273 (97%)	9 (3%)	0	100	100
1	L	280/291 (96%)	272 (97%)	8 (3%)	0	100	100
All	All	3381/3492 (97%)	3280 (97%)	99 (3%)	2 (0%)	55	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ARG
1	J	269	HIS

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	234/242 (97%)	222 (95%)	12 (5%)	28	15
1	B	239/242 (99%)	226 (95%)	13 (5%)	26	14
1	C	235/242 (97%)	223 (95%)	12 (5%)	28	15
1	D	235/242 (97%)	223 (95%)	12 (5%)	28	15
1	E	238/242 (98%)	229 (96%)	9 (4%)	38	26
1	F	236/242 (98%)	221 (94%)	15 (6%)	20	9
1	G	235/242 (97%)	220 (94%)	15 (6%)	20	9
1	H	237/242 (98%)	229 (97%)	8 (3%)	42	30
1	I	235/242 (97%)	224 (95%)	11 (5%)	30	18
1	J	235/242 (97%)	220 (94%)	15 (6%)	20	9
1	K	236/242 (98%)	225 (95%)	11 (5%)	30	18
1	L	234/242 (97%)	221 (94%)	13 (6%)	25	12
All	All	2829/2904 (97%)	2683 (95%)	146 (5%)	27	15

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	71	VAL
1	G	72	LEU
1	L	9	ARG
1	F	85	LYS
1	G	6	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	269	HIS
1	F	278	GLN
1	J	278	GLN
1	E	68	ASN
1	J	269	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	281/291 (96%)	-0.44	4 (1%) 75 79	6, 15, 34, 60	0
1	B	281/291 (96%)	-0.48	2 (0%) 87 89	6, 17, 30, 42	0
1	C	281/291 (96%)	-0.58	0 100 100	6, 15, 25, 32	0
1	D	281/291 (96%)	-0.34	6 (2%) 64 68	6, 15, 36, 53	0
1	E	281/291 (96%)	-0.52	1 (0%) 92 93	6, 16, 29, 39	0
1	F	281/291 (96%)	-0.60	0 100 100	5, 15, 26, 36	0
1	G	281/291 (96%)	-0.44	7 (2%) 58 62	6, 17, 31, 58	0
1	H	281/291 (96%)	-0.51	0 100 100	5, 17, 27, 41	0
1	I	281/291 (96%)	-0.55	3 (1%) 80 83	7, 16, 29, 45	0
1	J	281/291 (96%)	-0.58	0 100 100	5, 15, 28, 39	0
1	K	281/291 (96%)	-0.58	1 (0%) 92 93	5, 16, 28, 43	0
1	L	281/291 (96%)	-0.59	1 (0%) 92 93	7, 16, 30, 46	0
All	All	3372/3492 (96%)	-0.52	25 (0%) 87 89	5, 16, 30, 60	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	SER	5.0
1	A	71	VAL	4.7
1	K	1	LEU	4.6
1	G	72	LEU	4.5
1	D	72	LEU	4.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.