



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:02 pm BST

PDB ID : 6FL0  
Title : Crystal structure of the membrane attack complex assembly inhibitor BGA71 from Lyme disease agent *Borrelia burgdorferi*  
Authors : Brangulis, K.; Akopjana, I.; Petrovskis, I.; Kazaks, A.; Tars, K.  
Deposited on : 2018-01-25  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

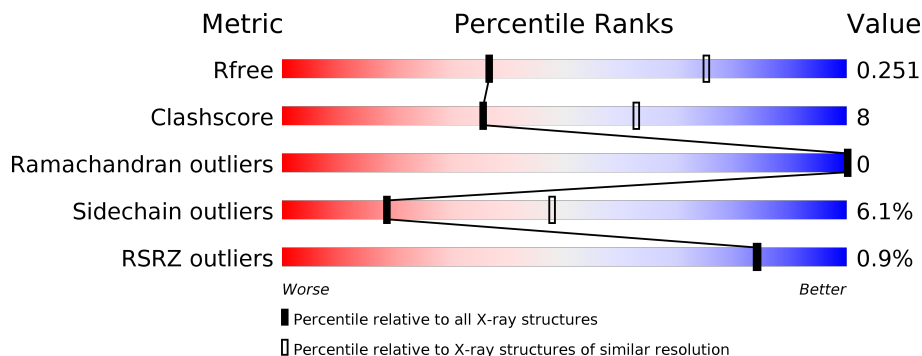
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	194	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 72%; height: 100%; background-color: green;"></div> <div style="width: 22%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>72%      22%      • 6%</p> </div> </div>
1	B	194	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 6%; height: 100%; background-color: red;"></div> <div style="width: 74%; height: 100%; background-color: green;"></div> <div style="width: 13%; height: 100%; background-color: yellow;"></div> <div style="width: 12%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>6%      74%      13%      • 12%</p> </div> </div>
1	C	194	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 3%; height: 100%; background-color: red;"></div> <div style="width: 74%; height: 100%; background-color: green;"></div> <div style="width: 18%; height: 100%; background-color: yellow;"></div> <div style="width: 7%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>3%      74%      18%      • 7%</p> </div> </div>
1	D	194	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 76%; height: 100%; background-color: green;"></div> <div style="width: 15%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>76%      15%      • 6%</p> </div> </div>
1	E	194	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 70%; height: 100%; background-color: green;"></div> <div style="width: 23%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>70%      23%      •• 6%</p> </div> </div>
1	F	194	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 65%; height: 100%; background-color: green;"></div> <div style="width: 20%; height: 100%; background-color: yellow;"></div> <div style="width: 11%; height: 100%; background-color: orange;"></div> <div style="width: 100%; height: 100%; background-color: grey; opacity: 0.5;"></div> </div> <div style="margin-left: 10px;"> <p>65%      20%      • 11%</p> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	194	 73% 14% • 12%
1	H	194	 68% 21% • 11% 3%
1	I	194	 73% 17% • 7%
1	J	194	 75% 17% • 7%
1	K	194	 68% 12% • 19% 3%
1	L	194	 72% 20% • 7%
1	M	194	 70% 17% • 12% 3%
1	N	194	 59% 26% • 11%
1	O	194	 70% 22% • 6%
1	P	194	 68% 20% • 8%
1	Q	194	 64% 24% • 10%
1	R	194	 61% 22% • 14%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 26099 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 membrane attack complex assembly inhibitor BGA71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1517	956	253	304	4	0	0	0
1	B	170	1332	837	224	268	3	0	0	0
1	C	181	1503	947	251	301	4	0	0	0
1	D	183	1517	956	253	304	4	0	0	0
1	E	183	1514	953	253	304	4	0	0	0
1	F	173	1434	908	237	285	4	0	0	0
1	G	170	1411	895	232	280	4	0	0	0
1	H	173	1433	906	236	287	4	0	0	0
1	I	181	1502	947	250	301	4	0	0	0
1	J	181	1503	947	251	301	4	0	0	0
1	K	158	1268	795	215	254	4	0	0	0
1	L	181	1503	947	251	301	4	0	0	0
1	M	171	1418	897	233	284	4	0	0	0
1	N	172	1425	901	234	286	4	0	0	0
1	O	183	1514	953	253	304	4	0	0	0
1	P	178	1475	931	244	296	4	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	175	1450	918	239	289	4	0	0	0
1	R	166	1380	874	228	274	4	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP Q6ASF4
A	3	ALA	-	expression tag	UNP Q6ASF4
A	4	MET	-	expression tag	UNP Q6ASF4
A	5	GLY	-	expression tag	UNP Q6ASF4
B	2	GLY	-	expression tag	UNP Q6ASF4
B	3	ALA	-	expression tag	UNP Q6ASF4
B	4	MET	-	expression tag	UNP Q6ASF4
B	5	GLY	-	expression tag	UNP Q6ASF4
C	2	GLY	-	expression tag	UNP Q6ASF4
C	3	ALA	-	expression tag	UNP Q6ASF4
C	4	MET	-	expression tag	UNP Q6ASF4
C	5	GLY	-	expression tag	UNP Q6ASF4
D	2	GLY	-	expression tag	UNP Q6ASF4
D	3	ALA	-	expression tag	UNP Q6ASF4
D	4	MET	-	expression tag	UNP Q6ASF4
D	5	GLY	-	expression tag	UNP Q6ASF4
E	2	GLY	-	expression tag	UNP Q6ASF4
E	3	ALA	-	expression tag	UNP Q6ASF4
E	4	MET	-	expression tag	UNP Q6ASF4
E	5	GLY	-	expression tag	UNP Q6ASF4
F	2	GLY	-	expression tag	UNP Q6ASF4
F	3	ALA	-	expression tag	UNP Q6ASF4
F	4	MET	-	expression tag	UNP Q6ASF4
F	5	GLY	-	expression tag	UNP Q6ASF4
G	2	GLY	-	expression tag	UNP Q6ASF4
G	3	ALA	-	expression tag	UNP Q6ASF4
G	4	MET	-	expression tag	UNP Q6ASF4
G	5	GLY	-	expression tag	UNP Q6ASF4
H	2	GLY	-	expression tag	UNP Q6ASF4
H	3	ALA	-	expression tag	UNP Q6ASF4
H	4	MET	-	expression tag	UNP Q6ASF4
H	5	GLY	-	expression tag	UNP Q6ASF4
I	2	GLY	-	expression tag	UNP Q6ASF4
I	3	ALA	-	expression tag	UNP Q6ASF4

*Continued on next page...*

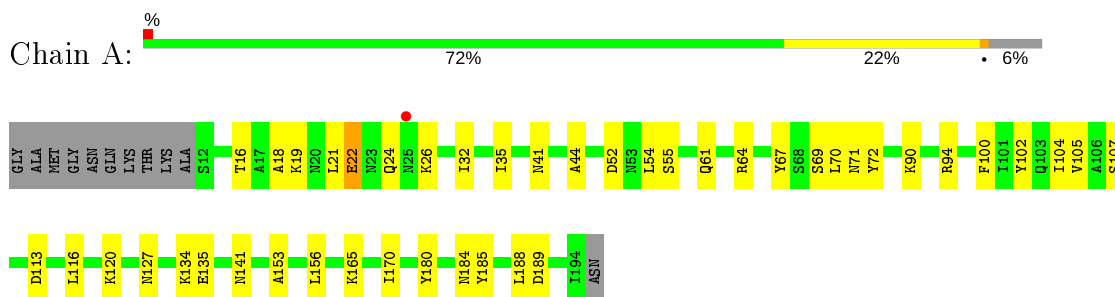
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	4	MET	-	expression tag	UNP Q6ASF4
I	5	GLY	-	expression tag	UNP Q6ASF4
J	2	GLY	-	expression tag	UNP Q6ASF4
J	3	ALA	-	expression tag	UNP Q6ASF4
J	4	MET	-	expression tag	UNP Q6ASF4
J	5	GLY	-	expression tag	UNP Q6ASF4
K	2	GLY	-	expression tag	UNP Q6ASF4
K	3	ALA	-	expression tag	UNP Q6ASF4
K	4	MET	-	expression tag	UNP Q6ASF4
K	5	GLY	-	expression tag	UNP Q6ASF4
L	2	GLY	-	expression tag	UNP Q6ASF4
L	3	ALA	-	expression tag	UNP Q6ASF4
L	4	MET	-	expression tag	UNP Q6ASF4
L	5	GLY	-	expression tag	UNP Q6ASF4
M	2	GLY	-	expression tag	UNP Q6ASF4
M	3	ALA	-	expression tag	UNP Q6ASF4
M	4	MET	-	expression tag	UNP Q6ASF4
M	5	GLY	-	expression tag	UNP Q6ASF4
N	2	GLY	-	expression tag	UNP Q6ASF4
N	3	ALA	-	expression tag	UNP Q6ASF4
N	4	MET	-	expression tag	UNP Q6ASF4
N	5	GLY	-	expression tag	UNP Q6ASF4
O	2	GLY	-	expression tag	UNP Q6ASF4
O	3	ALA	-	expression tag	UNP Q6ASF4
O	4	MET	-	expression tag	UNP Q6ASF4
O	5	GLY	-	expression tag	UNP Q6ASF4
P	2	GLY	-	expression tag	UNP Q6ASF4
P	3	ALA	-	expression tag	UNP Q6ASF4
P	4	MET	-	expression tag	UNP Q6ASF4
P	5	GLY	-	expression tag	UNP Q6ASF4
Q	2	GLY	-	expression tag	UNP Q6ASF4
Q	3	ALA	-	expression tag	UNP Q6ASF4
Q	4	MET	-	expression tag	UNP Q6ASF4
Q	5	GLY	-	expression tag	UNP Q6ASF4
R	2	GLY	-	expression tag	UNP Q6ASF4
R	3	ALA	-	expression tag	UNP Q6ASF4
R	4	MET	-	expression tag	UNP Q6ASF4
R	5	GLY	-	expression tag	UNP Q6ASF4

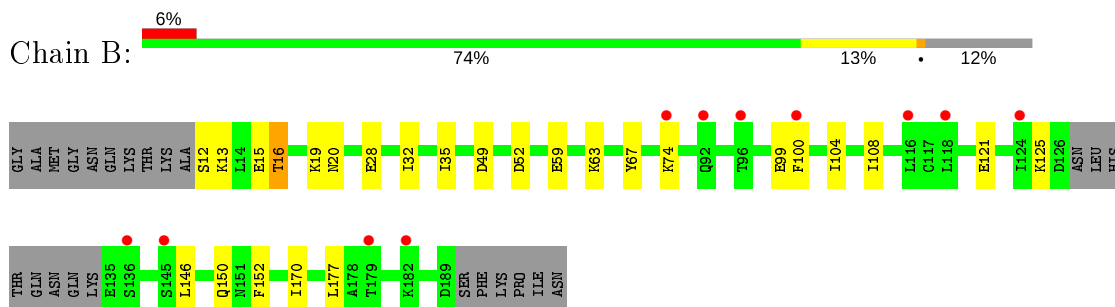
### 3 Residue-property plots [i](#)

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.

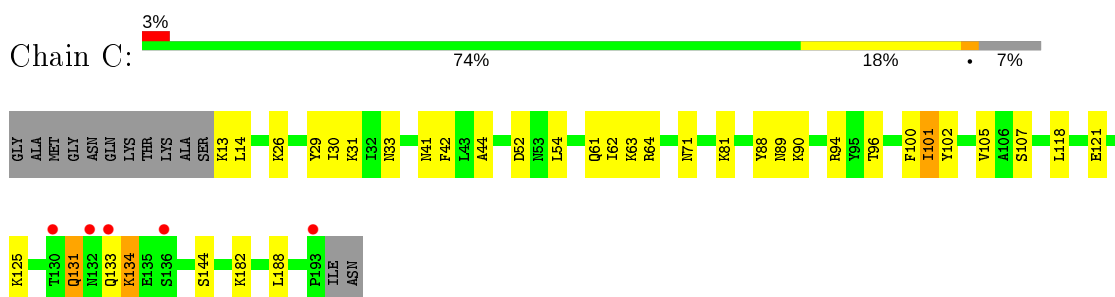
- Molecule 1: membrane attack complex assembly inhibitor BGA71



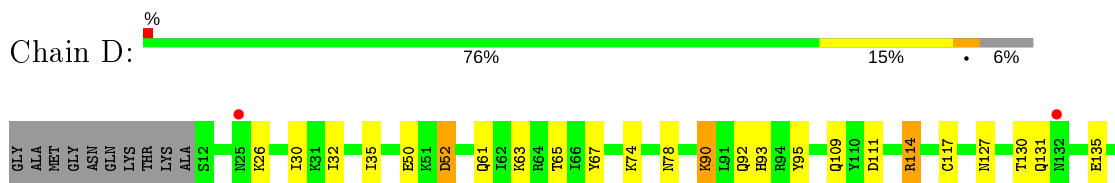
- Molecule 1: membrane attack complex assembly inhibitor BGA71



- Molecule 1: membrane attack complex assembly inhibitor BGA71



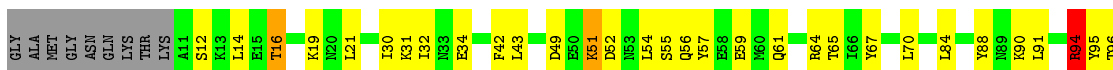
- Molecule 1: membrane attack complex assembly inhibitor BGA71





- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain E: 70% 23% 6%



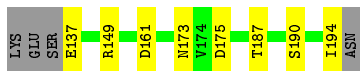
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain F: 65% 20% 11%



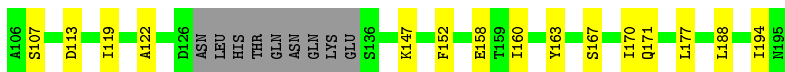
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain G: 73% 14% 12%



- Molecule 1: membrane attack complex assembly inhibitor BGA71

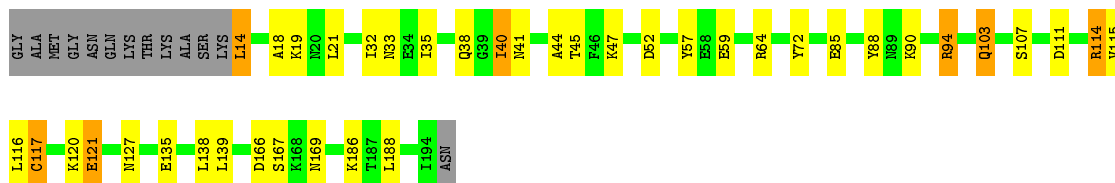
Chain H: 68% 21% 11%



- Molecule 1: membrane attack complex assembly inhibitor BGA71

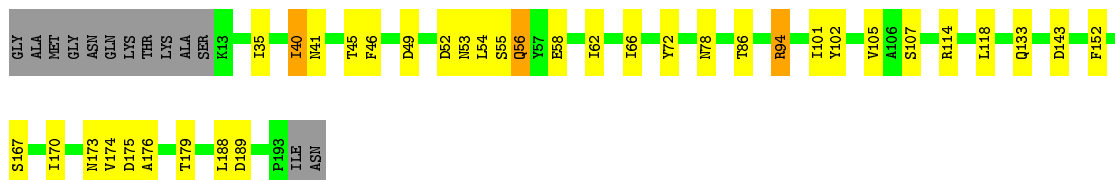
Chain I: 73% 17% 7%





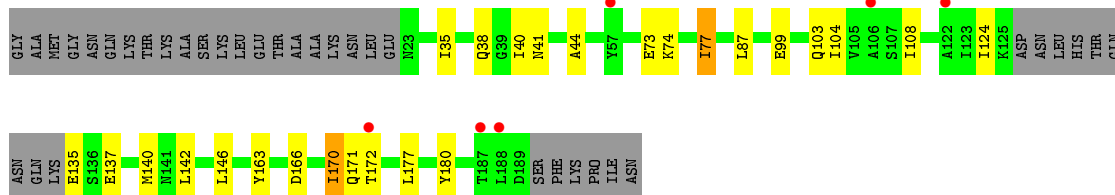
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain J: 75% 17% 7%



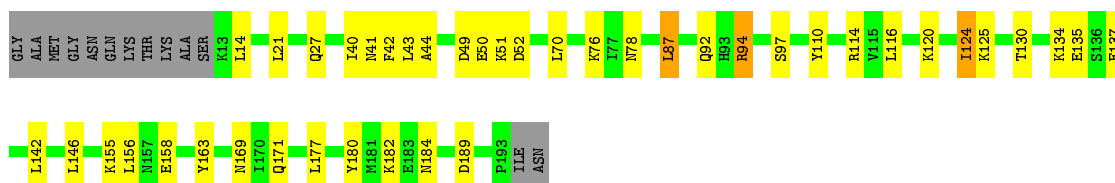
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain K: 3% 68% 12% 19%



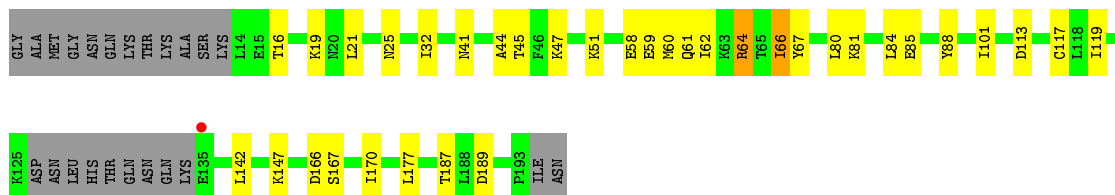
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain L: 72% 20% 7%



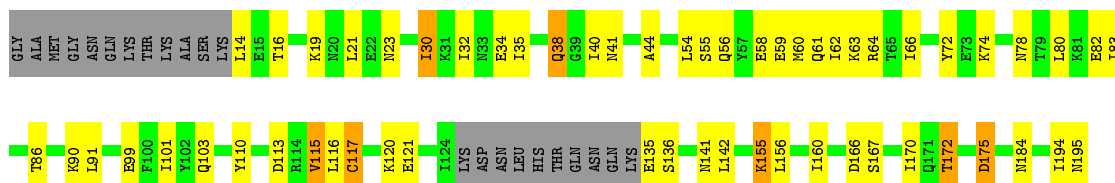
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain M: 70% 17% 12%



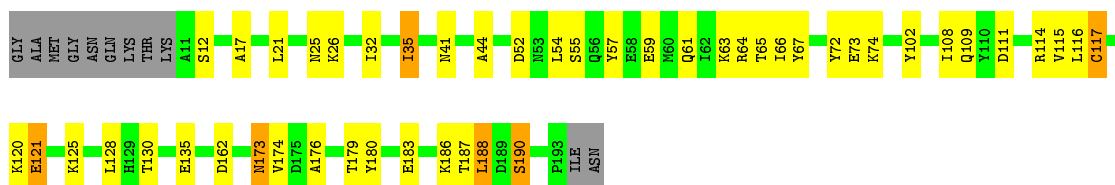
- Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain N: 



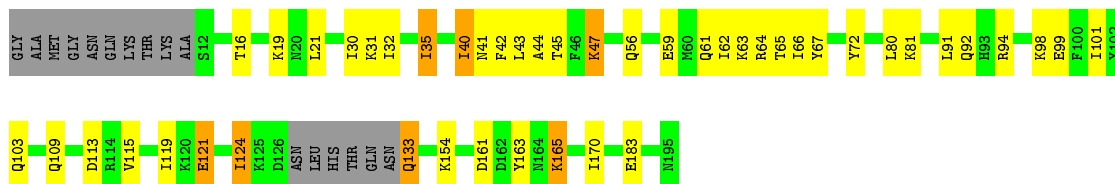
• Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain O: 



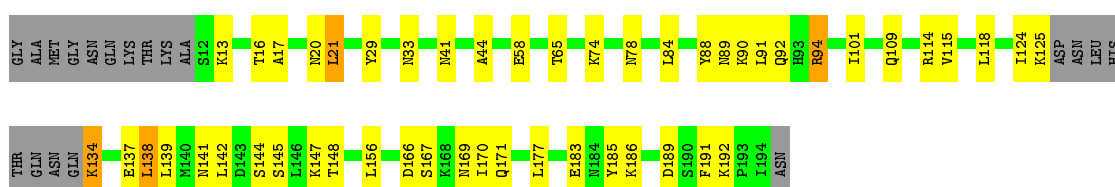
• Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain P: 



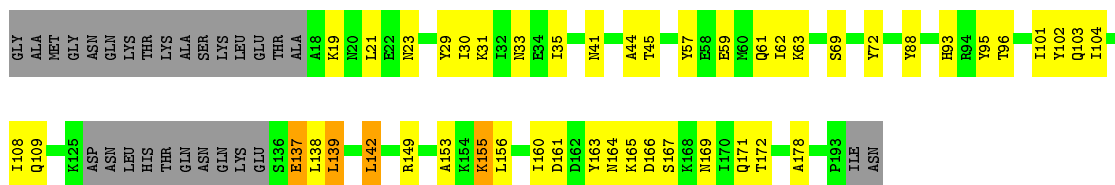
• Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain Q: 



• Molecule 1: membrane attack complex assembly inhibitor BGA71

Chain R: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.18Å 239.18Å 56.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.87 – 2.90 59.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.87-2.90) 99.9 (59.79-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15.71 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.192 , 0.248 0.201 , 0.251	Depositor DCC
$R_{free}$ test set	4045 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.005 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	26099	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.49% 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](#)

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	0.46	0/1535	0.61	0/2062
1	B	0.34	0/1343	0.49	0/1808
1	C	0.38	0/1521	0.58	0/2043
1	D	0.40	0/1535	0.57	0/2062
1	E	0.53	1/1532 (0.1%)	0.66	0/2058
1	F	0.55	0/1450	0.68	0/1946
1	G	0.39	0/1427	0.55	0/1916
1	H	0.54	1/1449 (0.1%)	0.63	0/1946
1	I	0.54	1/1520 (0.1%)	0.62	0/2043
1	J	0.44	0/1521	0.64	0/2043
1	K	0.37	0/1280	0.51	0/1719
1	L	0.39	0/1521	0.60	0/2043
1	M	0.46	0/1434	0.61	0/1925
1	N	0.48	0/1441	0.65	0/1936
1	O	0.59	1/1532 (0.1%)	0.67	0/2058
1	P	0.45	0/1491	0.63	1/2000 (0.1%)
1	Q	0.51	0/1466	0.67	0/1966
1	R	0.43	0/1396	0.58	0/1873
All	All	0.46	4/26394 (0.0%)	0.61	1/35447 (0.0%)

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	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	2
1	J	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	1
1	N	0	1
1	P	0	1
1	Q	0	1
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	121	GLU	CD-OE1	-5.19	1.20	1.25
1	O	121	GLU	CD-OE2	-5.16	1.20	1.25
1	H	158	GLU	CD-OE2	-5.04	1.20	1.25
1	E	59	GLU	CD-OE2	-5.00	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	40	ILE	N-CA-C	-6.36	93.83	111.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain
1	D	114	ARG	Sidechain
1	E	94	ARG	Sidechain
1	F	114	ARG	Sidechain
1	H	94	ARG	Sidechain

## 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	1517	0	1528	23	0
1	B	1332	0	1280	11	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1503	0	1513	22	0
1	D	1517	0	1529	25	2
1	E	1514	0	1523	28	1
1	F	1434	0	1453	43	0
1	G	1411	0	1428	20	0
1	H	1433	0	1444	29	0
1	I	1502	0	1511	30	1
1	J	1503	0	1512	20	0
1	K	1268	0	1230	16	0
1	L	1503	0	1513	23	0
1	M	1418	0	1429	16	2
1	N	1425	0	1433	44	0
1	O	1514	0	1523	33	0
1	P	1475	0	1488	24	0
1	Q	1450	0	1471	32	1
1	R	1380	0	1394	28	1
All	All	26099	0	26202	424	4

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 424 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:F:117:CYS:CB	1:O:117:CYS:SG	2.34	1.15
1:Q:84:LEU:HD13	1:Q:101:ILE:HD11	1.14	1.14
1:F:117:CYS:SG	1:O:117:CYS:CB	2.42	1.07
1:I:117:CYS:CB	1:N:117:CYS:SG	2.46	1.02
1:I:117:CYS:SG	1:N:117:CYS:CB	2.48	1.01

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:CYS:SG	1:M:117:CYS:SG[1_556]	1.65	0.55
1:E:127:ASN:OD1	1:Q:58:GLU:OE1[1_554]	2.06	0.14
1:I:90:LYS:NZ	1:R:164:ASN:OD1[1_556]	2.12	0.08
1:D:127:ASN:OD1	1:M:58:GLU:OE2[1_556]	2.18	0.02

## 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	181/194 (93%)	170 (94%)	11 (6%)	0	100	100
1	B	166/194 (86%)	161 (97%)	5 (3%)	0	100	100
1	C	179/194 (92%)	169 (94%)	10 (6%)	0	100	100
1	D	181/194 (93%)	173 (96%)	8 (4%)	0	100	100
1	E	181/194 (93%)	174 (96%)	7 (4%)	0	100	100
1	F	169/194 (87%)	163 (96%)	6 (4%)	0	100	100
1	G	166/194 (86%)	158 (95%)	8 (5%)	0	100	100
1	H	169/194 (87%)	164 (97%)	5 (3%)	0	100	100
1	I	179/194 (92%)	173 (97%)	6 (3%)	0	100	100
1	J	179/194 (92%)	168 (94%)	11 (6%)	0	100	100
1	K	154/194 (79%)	148 (96%)	6 (4%)	0	100	100
1	L	179/194 (92%)	176 (98%)	3 (2%)	0	100	100
1	M	167/194 (86%)	157 (94%)	10 (6%)	0	100	100
1	N	168/194 (87%)	157 (94%)	11 (6%)	0	100	100
1	O	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
1	P	174/194 (90%)	164 (94%)	10 (6%)	0	100	100
1	Q	171/194 (88%)	162 (95%)	9 (5%)	0	100	100
1	R	162/194 (84%)	157 (97%)	5 (3%)	0	100	100
All	All	3106/3492 (89%)	2965 (96%)	141 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	172/179 (96%)	162 (94%)	10 (6%)	20	50
1	B	136/179 (76%)	129 (95%)	7 (5%)	24	56
1	C	170/179 (95%)	160 (94%)	10 (6%)	19	49
1	D	172/179 (96%)	160 (93%)	12 (7%)	15	41
1	E	171/179 (96%)	159 (93%)	12 (7%)	15	41
1	F	162/179 (90%)	152 (94%)	10 (6%)	18	47
1	G	159/179 (89%)	156 (98%)	3 (2%)	57	84
1	H	162/179 (90%)	154 (95%)	8 (5%)	25	57
1	I	170/179 (95%)	160 (94%)	10 (6%)	19	49
1	J	170/179 (95%)	162 (95%)	8 (5%)	26	59
1	K	135/179 (75%)	130 (96%)	5 (4%)	34	68
1	L	170/179 (95%)	158 (93%)	12 (7%)	14	40
1	M	160/179 (89%)	152 (95%)	8 (5%)	24	57
1	N	161/179 (90%)	145 (90%)	16 (10%)	8	24
1	O	171/179 (96%)	157 (92%)	14 (8%)	11	32
1	P	167/179 (93%)	154 (92%)	13 (8%)	12	34
1	Q	164/179 (92%)	151 (92%)	13 (8%)	12	34
1	R	156/179 (87%)	148 (95%)	8 (5%)	24	56
All	All	2928/3222 (91%)	2749 (94%)	179 (6%)	18	48

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	167	SER
1	L	124	ILE
1	Q	139	LEU
1	J	41	ASN
1	K	77	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	89	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	K	33	ASN
1	P	103	GLN
1	I	127	ASN
1	J	78	ASN

### 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, 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	183/194 (94%)	-0.16	1 (0%) 91 91	13, 25, 48, 57	0
1	B	170/194 (87%)	0.97	11 (6%) 18 14	55, 75, 89, 102	0
1	C	181/194 (93%)	0.21	5 (2%) 53 49	19, 41, 65, 84	0
1	D	183/194 (94%)	-0.06	2 (1%) 80 80	14, 28, 52, 67	0
1	E	183/194 (94%)	-0.19	0 100 100	12, 25, 46, 55	0
1	F	173/194 (89%)	-0.19	0 100 100	13, 24, 46, 63	0
1	G	170/194 (87%)	-0.24	0 100 100	12, 22, 42, 66	0
1	H	173/194 (89%)	-0.10	2 (1%) 79 79	14, 28, 52, 87	0
1	I	181/194 (93%)	-0.16	0 100 100	11, 24, 49, 66	0
1	J	181/194 (93%)	-0.22	0 100 100	9, 22, 45, 58	0
1	K	158/194 (81%)	0.77	6 (3%) 40 36	48, 65, 87, 104	0
1	L	181/194 (93%)	-0.20	0 100 100	9, 22, 39, 52	0
1	M	171/194 (88%)	-0.08	1 (0%) 89 89	16, 27, 50, 71	0
1	N	172/194 (88%)	-0.11	0 100 100	14, 26, 51, 60	0
1	O	183/194 (94%)	-0.18	0 100 100	10, 27, 46, 63	0
1	P	178/194 (91%)	-0.23	0 100 100	11, 22, 46, 73	0
1	Q	175/194 (90%)	-0.24	0 100 100	12, 24, 42, 58	0
1	R	166/194 (85%)	-0.02	0 100 100	19, 32, 54, 67	0
All	All	3162/3492 (90%)	-0.03	28 (0%) 84 84	9, 28, 72, 104	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	SER	3.9
1	C	132	ASN	3.7
1	D	132	ASN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	133	GLN	3.0
1	M	135	GLU	2.9

## 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.