wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 11:23 PM EST

PDB ID	:	1GAV
Title	:	BACTERIOPHAGE GA PROTEIN CAPSID
Authors	:	Tars, K.; Bundule, M.; Liljas, L.
Deposited on	:	1997-01-28
Resolution	:	3.40 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
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.

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

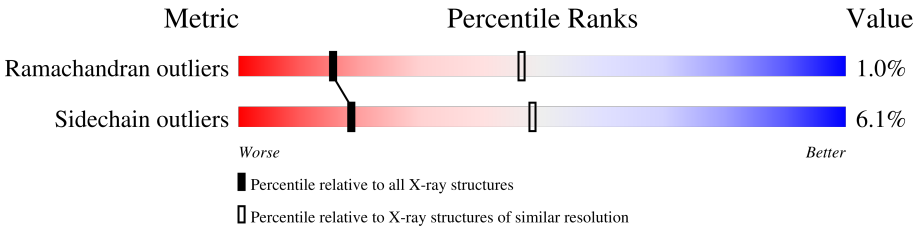
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	0	129	94% 5% ·
1	1	129	94% 5% ·
1	2	129	96% ·
1	3	129	92% 8%
1	4	129	94% 5% ·
1	5	129	96% ·
1	6	129	92% 8%
1	7	129	94% 5% ·
1	8	129	96% ·
1	9	129	92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	A	129	96%
1	B	129	92% 8%
1	C	129	94% 5%
1	D	129	95% 5%
1	E	129	92% 8%
1	F	129	94% 5%
1	G	129	96%
1	H	129	92% 8%
1	I	129	94% 5%
1	J	129	96%
1	K	129	92% 8%
1	L	129	94% 5%
1	M	129	96%
1	N	129	92% 8%
1	O	129	94% 5%
1	P	129	96%
1	Q	129	92% 8%
1	R	129	94% 5%
1	S	129	96%
1	T	129	92% 8%
1	U	129	94% 5%
1	V	129	95% 5%
1	W	129	92% 8%
1	X	129	94% 5%
1	Y	129	96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Z	129	92% 8%
1	a	129	96%
1	b	129	92% 8%
1	c	129	94% 5%
1	d	129	96%
1	e	129	92% 8%
1	f	129	94% 5%
1	g	129	96%
1	h	129	92% 8%
1	i	129	94% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 43335 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 BACTERIOPHAGE GA PROTEIN CAPSID.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	129	Total 963	C 612	N 164	O 187	0	0	0
1	B	129	Total 963	C 612	N 164	O 187	0	0	0
1	C	129	Total 963	C 612	N 164	O 187	0	0	0
1	D	129	Total 963	C 612	N 164	O 187	0	0	0
1	E	129	Total 963	C 612	N 164	O 187	0	0	0
1	F	129	Total 963	C 612	N 164	O 187	0	0	0
1	G	129	Total 963	C 612	N 164	O 187	0	0	0
1	H	129	Total 963	C 612	N 164	O 187	0	0	0
1	I	129	Total 963	C 612	N 164	O 187	0	0	0
1	J	129	Total 963	C 612	N 164	O 187	0	0	0
1	K	129	Total 963	C 612	N 164	O 187	0	0	0
1	L	129	Total 963	C 612	N 164	O 187	0	0	0
1	M	129	Total 963	C 612	N 164	O 187	0	0	0
1	N	129	Total 963	C 612	N 164	O 187	0	0	0
1	O	129	Total 963	C 612	N 164	O 187	0	0	0
1	P	129	Total 963	C 612	N 164	O 187	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	129	Total 963	C 612	N 164	O 187	0	0	0
1	R	129	Total 963	C 612	N 164	O 187	0	0	0
1	S	129	Total 963	C 612	N 164	O 187	0	0	0
1	T	129	Total 963	C 612	N 164	O 187	0	0	0
1	U	129	Total 963	C 612	N 164	O 187	0	0	0
1	V	129	Total 963	C 612	N 164	O 187	0	0	0
1	W	129	Total 963	C 612	N 164	O 187	0	0	0
1	X	129	Total 963	C 612	N 164	O 187	0	0	0
1	Y	129	Total 963	C 612	N 164	O 187	0	0	0
1	Z	129	Total 963	C 612	N 164	O 187	0	0	0
1	1	129	Total 963	C 612	N 164	O 187	0	0	0
1	2	129	Total 963	C 612	N 164	O 187	0	0	0
1	3	129	Total 963	C 612	N 164	O 187	0	0	0
1	4	129	Total 963	C 612	N 164	O 187	0	0	0
1	5	129	Total 963	C 612	N 164	O 187	0	0	0
1	6	129	Total 963	C 612	N 164	O 187	0	0	0
1	7	129	Total 963	C 612	N 164	O 187	0	0	0
1	8	129	Total 963	C 612	N 164	O 187	0	0	0
1	9	129	Total 963	C 612	N 164	O 187	0	0	0
1	0	129	Total 963	C 612	N 164	O 187	0	0	0
1	a	129	Total 963	C 612	N 164	O 187	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	b	129	Total 963	C 612	N 164	O 187	0	0	0
1	c	129	Total 963	C 612	N 164	O 187	0	0	0
1	d	129	Total 963	C 612	N 164	O 187	0	0	0
1	e	129	Total 963	C 612	N 164	O 187	0	0	0
1	f	129	Total 963	C 612	N 164	O 187	0	0	0
1	g	129	Total 963	C 612	N 164	O 187	0	0	0
1	h	129	Total 963	C 612	N 164	O 187	0	0	0
1	i	129	Total 963	C 612	N 164	O 187	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	THR	ALA	variant	UNP P07234
A	79	VAL	GLY	variant	UNP P07234
B	59	THR	ALA	variant	UNP P07234
B	79	VAL	GLY	variant	UNP P07234
C	59	THR	ALA	variant	UNP P07234
C	79	VAL	GLY	variant	UNP P07234
D	59	THR	ALA	variant	UNP P07234
D	79	VAL	GLY	variant	UNP P07234
E	59	THR	ALA	variant	UNP P07234
E	79	VAL	GLY	variant	UNP P07234
F	59	THR	ALA	variant	UNP P07234
F	79	VAL	GLY	variant	UNP P07234
G	59	THR	ALA	variant	UNP P07234
G	79	VAL	GLY	variant	UNP P07234
H	59	THR	ALA	variant	UNP P07234
H	79	VAL	GLY	variant	UNP P07234
I	59	THR	ALA	variant	UNP P07234
I	79	VAL	GLY	variant	UNP P07234
J	59	THR	ALA	variant	UNP P07234
J	79	VAL	GLY	variant	UNP P07234
K	59	THR	ALA	variant	UNP P07234
K	79	VAL	GLY	variant	UNP P07234
L	59	THR	ALA	variant	UNP P07234

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	79	VAL	GLY	variant	UNP P07234
M	59	THR	ALA	variant	UNP P07234
M	79	VAL	GLY	variant	UNP P07234
N	59	THR	ALA	variant	UNP P07234
N	79	VAL	GLY	variant	UNP P07234
O	59	THR	ALA	variant	UNP P07234
O	79	VAL	GLY	variant	UNP P07234
P	59	THR	ALA	variant	UNP P07234
P	79	VAL	GLY	variant	UNP P07234
Q	59	THR	ALA	variant	UNP P07234
Q	79	VAL	GLY	variant	UNP P07234
R	59	THR	ALA	variant	UNP P07234
R	79	VAL	GLY	variant	UNP P07234
S	59	THR	ALA	variant	UNP P07234
S	79	VAL	GLY	variant	UNP P07234
T	59	THR	ALA	variant	UNP P07234
T	79	VAL	GLY	variant	UNP P07234
U	59	THR	ALA	variant	UNP P07234
U	79	VAL	GLY	variant	UNP P07234
V	59	THR	ALA	variant	UNP P07234
V	79	VAL	GLY	variant	UNP P07234
W	59	THR	ALA	variant	UNP P07234
W	79	VAL	GLY	variant	UNP P07234
X	59	THR	ALA	variant	UNP P07234
X	79	VAL	GLY	variant	UNP P07234
Y	59	THR	ALA	variant	UNP P07234
Y	79	VAL	GLY	variant	UNP P07234
Z	59	THR	ALA	variant	UNP P07234
Z	79	VAL	GLY	variant	UNP P07234
1	59	THR	ALA	variant	UNP P07234
1	79	VAL	GLY	variant	UNP P07234
2	59	THR	ALA	variant	UNP P07234
2	79	VAL	GLY	variant	UNP P07234
3	59	THR	ALA	variant	UNP P07234
3	79	VAL	GLY	variant	UNP P07234
4	59	THR	ALA	variant	UNP P07234
4	79	VAL	GLY	variant	UNP P07234
5	59	THR	ALA	variant	UNP P07234
5	79	VAL	GLY	variant	UNP P07234
6	59	THR	ALA	variant	UNP P07234
6	79	VAL	GLY	variant	UNP P07234
7	59	THR	ALA	variant	UNP P07234

Continued on next page...

Continued from previous page...

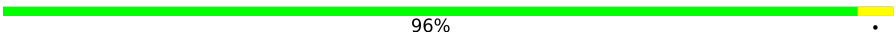
Chain	Residue	Modelled	Actual	Comment	Reference
7	79	VAL	GLY	variant	UNP P07234
8	59	THR	ALA	variant	UNP P07234
8	79	VAL	GLY	variant	UNP P07234
9	59	THR	ALA	variant	UNP P07234
9	79	VAL	GLY	variant	UNP P07234
0	59	THR	ALA	variant	UNP P07234
0	79	VAL	GLY	variant	UNP P07234
a	59	THR	ALA	variant	UNP P07234
a	79	VAL	GLY	variant	UNP P07234
b	59	THR	ALA	variant	UNP P07234
b	79	VAL	GLY	variant	UNP P07234
c	59	THR	ALA	variant	UNP P07234
c	79	VAL	GLY	variant	UNP P07234
d	59	THR	ALA	variant	UNP P07234
d	79	VAL	GLY	variant	UNP P07234
e	59	THR	ALA	variant	UNP P07234
e	79	VAL	GLY	variant	UNP P07234
f	59	THR	ALA	variant	UNP P07234
f	79	VAL	GLY	variant	UNP P07234
g	59	THR	ALA	variant	UNP P07234
g	79	VAL	GLY	variant	UNP P07234
h	59	THR	ALA	variant	UNP P07234
h	79	VAL	GLY	variant	UNP P07234
i	59	THR	ALA	variant	UNP P07234
i	79	VAL	GLY	variant	UNP P07234

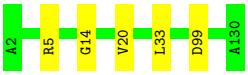
3 Residue-property plots (i)

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. 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. 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: BACTERIOPHAGE GA PROTEIN CAPSID

Chain A:



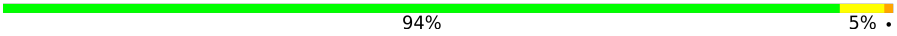


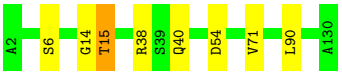
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain B:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

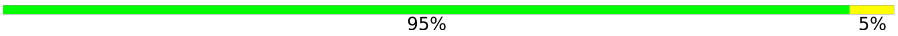
Chain C:

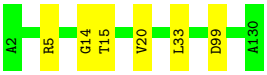




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

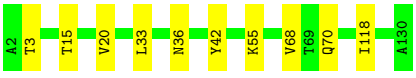
Chain D:





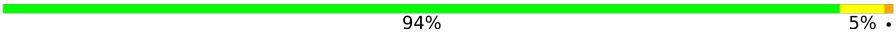
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

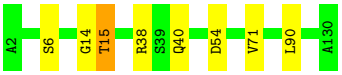
Chain E:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

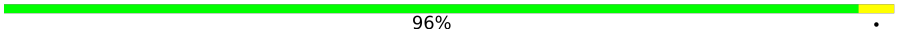
Chain F:

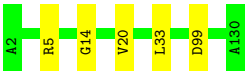




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain G:



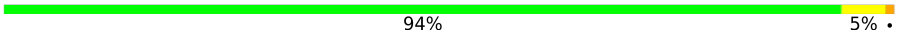


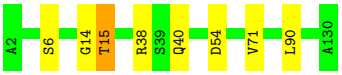
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain H:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

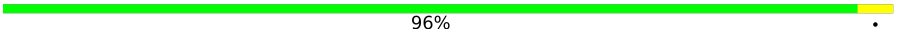
Chain I:

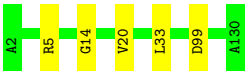




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain J:



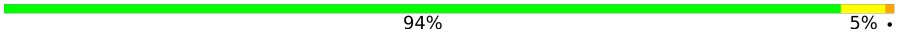


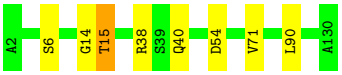
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain K:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

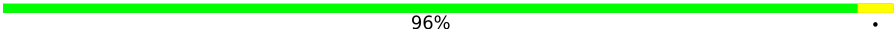
Chain L:

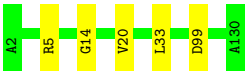




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain M:



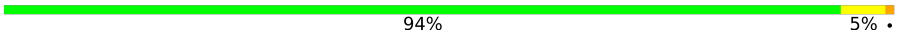


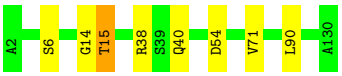
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain N:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

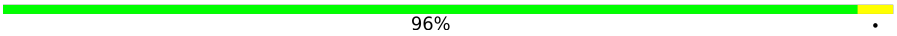
Chain O:

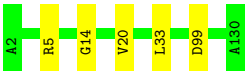




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain P:



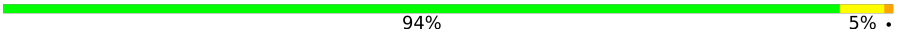


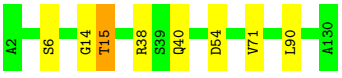
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Q:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

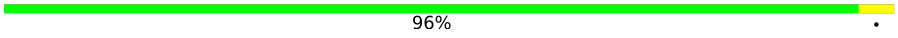
Chain R:

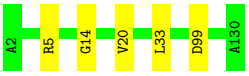




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain S:



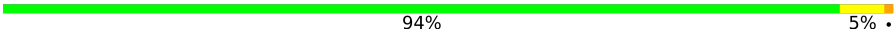


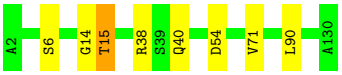
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain T:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

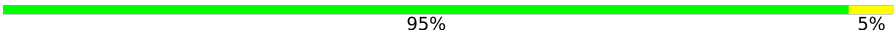
Chain U:

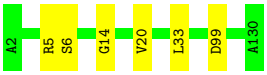




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain V:



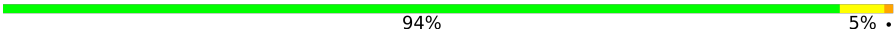


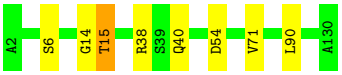
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain W:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

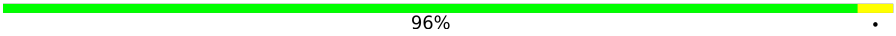
Chain X:

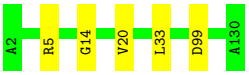




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Y:



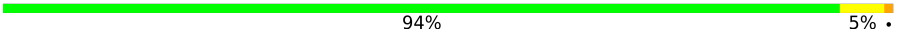


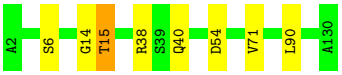
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Z:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

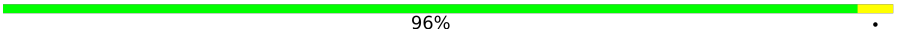
Chain 1:

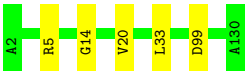




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 2:



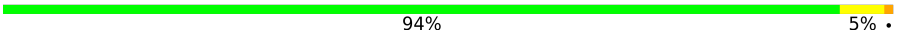


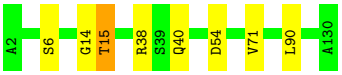
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 3:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

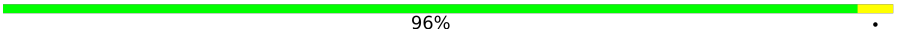
Chain 4:

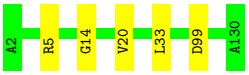




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 5:



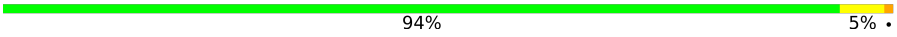


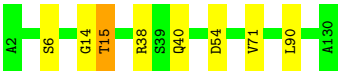
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 6:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

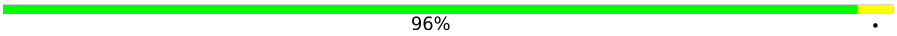
Chain 7:

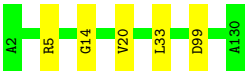




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 8:



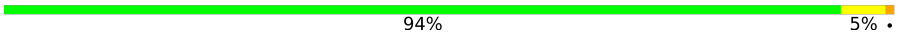


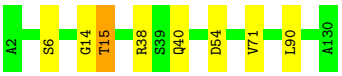
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 9:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

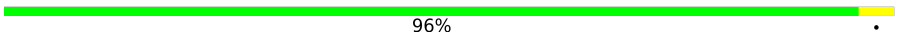
Chain 0:

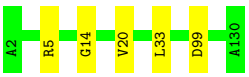




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain a:



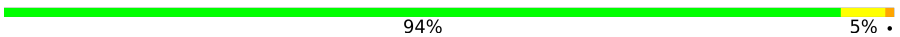


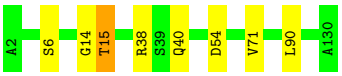
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain b:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

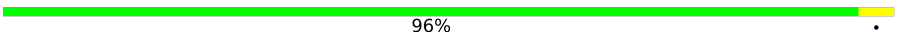
Chain c:

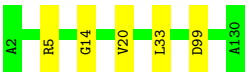




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain d:



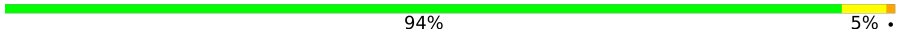


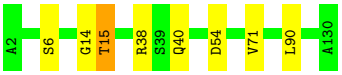
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain e:

• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

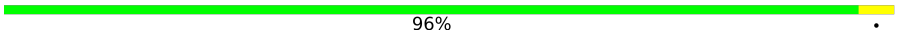
Chain f:

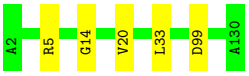




• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

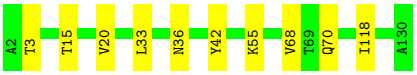
Chain g:





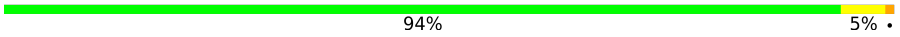
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

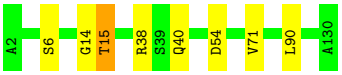
Chain h:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain i:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	272.70Å 293.50Å 339.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 49.31 – 3.39	Depositor EDS
% Data completeness (in resolution range)	66.0 (30.00-3.40) 65.4 (49.31-3.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.02 (at 3.40Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.279 , (Not available) 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	43335	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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)

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	0	0.82	0/980	0.84	0/1336
1	1	0.82	0/980	0.84	0/1336
1	2	0.82	0/980	0.87	0/1336
1	3	0.88	0/980	0.90	1/1336 (0.1%)
1	4	0.82	0/980	0.84	0/1336
1	5	0.82	0/980	0.87	0/1336
1	6	0.88	0/980	0.90	1/1336 (0.1%)
1	7	0.82	0/980	0.84	0/1336
1	8	0.82	0/980	0.87	0/1336
1	9	0.88	0/980	0.90	1/1336 (0.1%)
1	A	0.82	0/980	0.87	0/1336
1	B	0.88	0/980	0.90	1/1336 (0.1%)
1	C	0.82	0/980	0.84	0/1336
1	D	0.82	0/980	0.87	0/1336
1	E	0.88	0/980	0.90	1/1336 (0.1%)
1	F	0.82	0/980	0.84	0/1336
1	G	0.82	0/980	0.87	0/1336
1	H	0.88	0/980	0.90	1/1336 (0.1%)
1	I	0.82	0/980	0.84	0/1336
1	J	0.82	0/980	0.87	0/1336
1	K	0.88	0/980	0.90	1/1336 (0.1%)
1	L	0.82	0/980	0.84	0/1336
1	M	0.82	0/980	0.87	0/1336
1	N	0.88	0/980	0.90	1/1336 (0.1%)
1	O	0.82	0/980	0.84	0/1336
1	P	0.82	0/980	0.87	0/1336
1	Q	0.88	0/980	0.90	1/1336 (0.1%)
1	R	0.82	0/980	0.84	0/1336
1	S	0.82	0/980	0.87	0/1336
1	T	0.88	0/980	0.90	1/1336 (0.1%)
1	U	0.82	0/980	0.84	0/1336
1	V	0.82	0/980	0.87	0/1336
1	W	0.88	0/980	0.90	1/1336 (0.1%)
1	X	0.82	0/980	0.84	0/1336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Y	0.82	0/980	0.87	0/1336
1	Z	0.88	0/980	0.90	1/1336 (0.1%)
1	a	0.82	0/980	0.87	0/1336
1	b	0.88	0/980	0.90	1/1336 (0.1%)
1	c	0.82	0/980	0.84	0/1336
1	d	0.82	0/980	0.87	0/1336
1	e	0.88	0/980	0.90	1/1336 (0.1%)
1	f	0.82	0/980	0.84	0/1336
1	g	0.82	0/980	0.87	0/1336
1	h	0.88	0/980	0.90	1/1336 (0.1%)
1	i	0.82	0/980	0.84	0/1336
All	All	0.84	0/44100	0.87	15/60120 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	42	TYR	N-CA-C	-5.65	95.74	111.00
1	T	42	TYR	N-CA-C	-5.65	95.74	111.00
1	Z	42	TYR	N-CA-C	-5.65	95.74	111.00
1	E	42	TYR	N-CA-C	-5.65	95.75	111.00
1	K	42	TYR	N-CA-C	-5.65	95.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	1	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	2	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	3	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	4	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	5	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	6	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	7	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9 34
1	8	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	9	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	A	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	B	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	C	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	D	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	E	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	F	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	G	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	H	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	I	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	J	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	K	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	L	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9 34
1	M	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	N	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	O	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	P	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	Q	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	R	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	S	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51
1	T	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19 51
1	U	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9 34
1	V	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
1	X	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	34
1	Y	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19	51
1	Z	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
1	a	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19	51
1	b	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
1	c	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9	34
1	d	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19	51
1	e	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
1	f	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	34
1	g	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19	51
1	h	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
1	i	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	34
All	All	5715/5805 (98%)	5172 (90%)	483 (8%)	60 (1%)	15	46

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	THR
1	C	14	GLY
1	C	15	THR
1	E	15	THR
1	F	14	GLY

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	0	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	1	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	2	104/104 (100%)	100 (96%)	4 (4%)	33	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	4	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	5	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	6	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	7	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	8	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	9	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	A	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	B	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	C	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	D	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	E	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	F	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	G	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	H	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	I	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	J	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	K	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	L	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	M	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	N	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	O	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	P	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	Q	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	R	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	S	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	T	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	U	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	V	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	W	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	X	104/104 (100%)	97 (93%)	7 (7%)	16	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	Z	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	a	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	b	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	c	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	d	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	e	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	f	104/104 (100%)	97 (93%)	7 (7%)	16	46
1	g	104/104 (100%)	100 (96%)	4 (4%)	33	61
1	h	104/104 (100%)	96 (92%)	8 (8%)	13	40
1	i	104/104 (100%)	97 (93%)	7 (7%)	16	46
All	All	4680/4680 (100%)	4395 (94%)	285 (6%)	18	48

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	99	ASP
1	b	70	GLN
1	f	15	THR
1	P	33	LEU
1	O	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	73	ASN
1	5	73	ASN
1	i	36	ASN
1	Z	70	GLN
1	3	36	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 monosaccharides 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.