



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

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PDB ID : 6IBC
EMDB ID: : EMD-4447
Title : Thermophage P23-45 procapsid
Authors : Bayfield, O.W.; Klimuk, E.; Winkler, D.C.; Hesketh, E.L.; Chechik, M.;
Cheng, N.; Dykeman, E.C.; Minakhin, L.; Ranson, N.A.; Severinov, K.;
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Deposited on : 2018-11-29
Resolution : 4.39 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

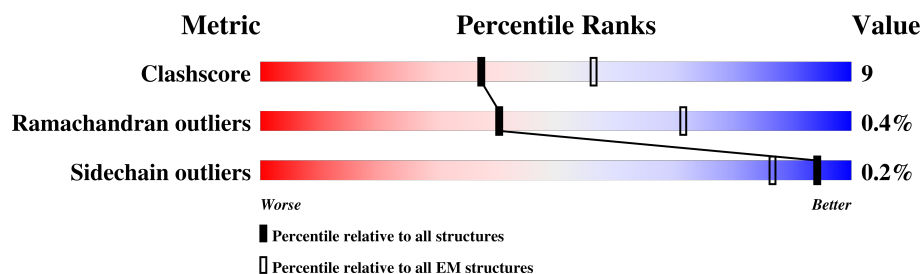
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.39 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	409	
1	B	409	
1	C	409	
1	D	409	
1	E	409	
1	F	409	
1	G	409	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19758 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

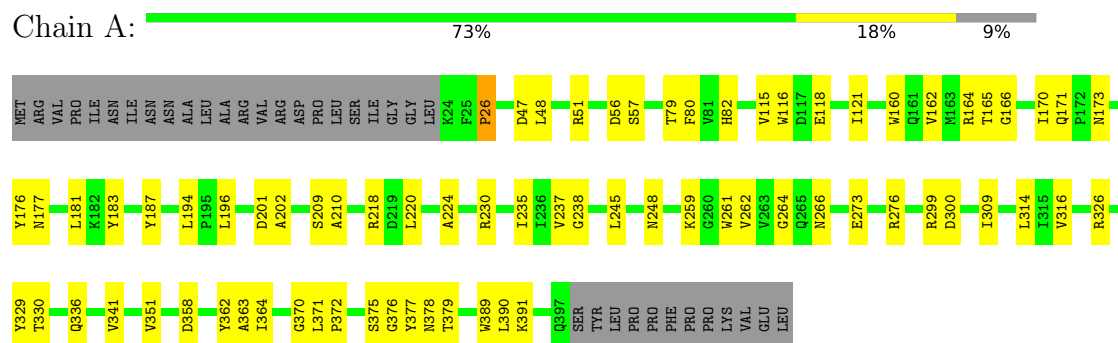
- Molecule 1 is a protein called Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2848	1822	494	528	4		
1	B	374	Total	C	N	O	S	0	0
			2848	1822	494	528	4		
1	C	374	Total	C	N	O	S	0	0
			2848	1822	494	528	4		
1	D	374	Total	C	N	O	S	0	0
			2848	1822	494	528	4		
1	E	374	Total	C	N	O	S	0	0
			2848	1822	494	528	4		
1	F	373	Total	C	N	O	S	0	0
			2839	1817	492	526	4		
1	G	345	Total	C	N	O	S	0	0
			2679	1720	463	492	4		

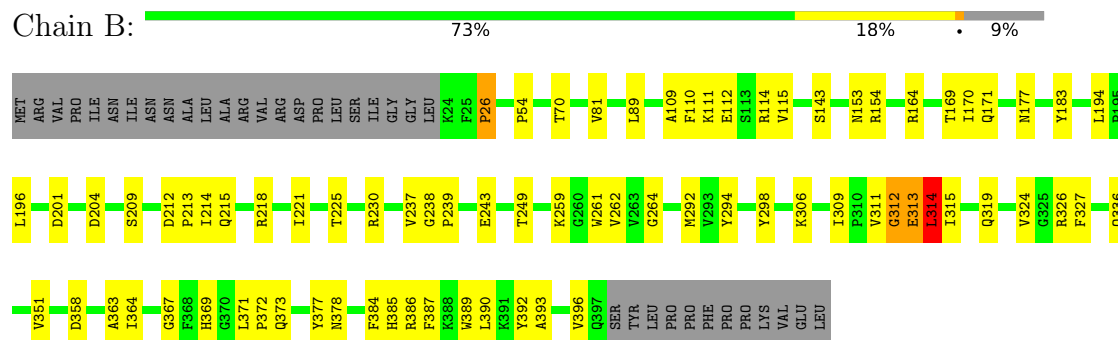
3 Residue-property plots

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. 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.

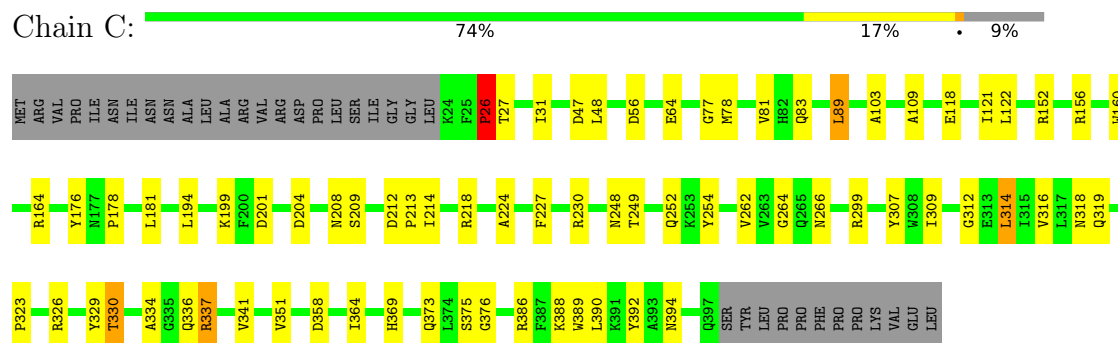
- Molecule 1: Major head protein




- Molecule 1: Major head protein

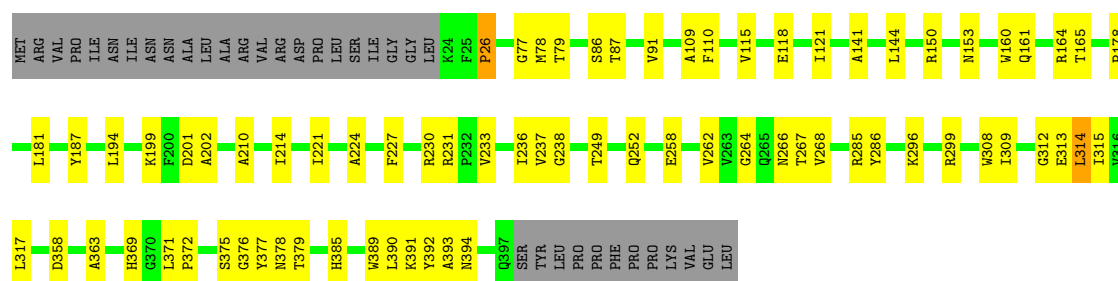


- Molecule 1: Major head protein



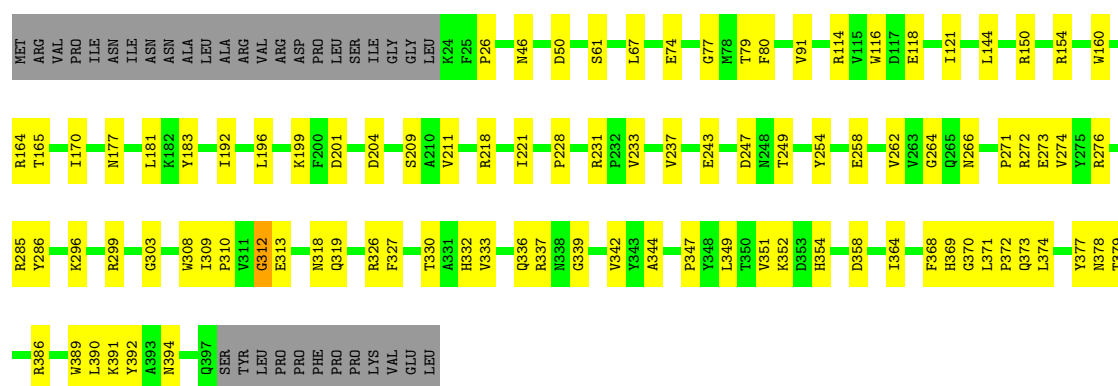
- Molecule 1: Major head protein

Chain D: 



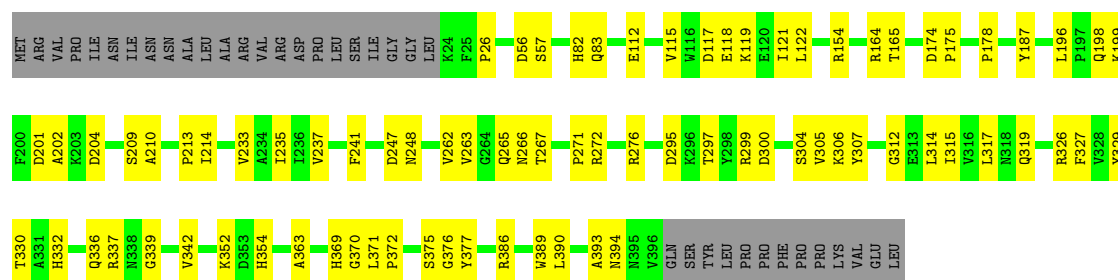
- Molecule 1: Major head protein

Chain E: 



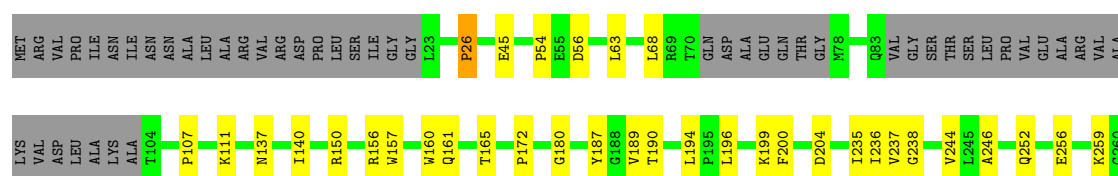
- Molecule 1: Major head protein

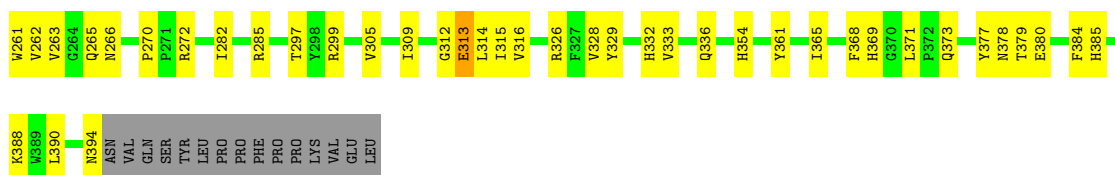
Chain F: 



- Molecule 1: Major head protein

Chain G: 





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	38044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	99	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.43	0/2922	0.62	1/3992 (0.0%)
1	B	0.42	0/2922	0.62	1/3992 (0.0%)
1	C	0.41	0/2922	0.62	2/3992 (0.1%)
1	D	0.40	0/2922	0.61	1/3992 (0.0%)
1	E	0.39	0/2922	0.59	1/3992 (0.0%)
1	F	0.37	0/2913	0.58	1/3980 (0.0%)
1	G	0.32	0/2750	0.55	1/3750 (0.0%)
All	All	0.39	0/20273	0.60	8/27690 (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	B	0	4
1	C	0	6
1	D	0	2
1	E	0	3
1	G	0	2
All	All	0	18

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	26	PRO	N-CA-CB	6.76	111.41	103.30
1	A	26	PRO	N-CA-CB	6.51	111.12	103.30
1	D	26	PRO	N-CA-CB	6.45	111.04	103.30
1	B	26	PRO	N-CA-CB	6.19	110.73	103.30
1	E	26	PRO	N-CA-CB	6.18	110.72	103.30

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	ASP	Peptide
1	B	312	GLY	Peptide
1	B	314	LEU	Peptide
1	B	336	GLN	Peptide
1	B	358	ASP	Peptide

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	2848	0	2616	47	0
1	B	2848	0	2616	47	0
1	C	2848	0	2616	52	0
1	D	2848	0	2616	49	0
1	E	2848	0	2616	70	0
1	F	2839	0	2608	55	0
1	G	2679	0	2479	47	0
All	All	19758	0	18167	336	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 9.

The worst 5 of 336 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:378:ASN:ND2	1:F:299:ARG:HH12	1.58	1.02
1:E:378:ASN:HD21	1:F:299:ARG:HH12	1.23	0.85
1:E:378:ASN:HD21	1:F:299:ARG:NH1	1.80	0.78
1:D:262:VAL:H	1:D:266:ASN:HB2	1.54	0.73
1:E:262:VAL:H	1:E:266:ASN:HB2	1.56	0.69

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 PDB entries followed by that with respect to all EM entries.

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	372/409 (91%)	342 (92%)	29 (8%)	1 (0%)	43	80
1	B	372/409 (91%)	332 (89%)	37 (10%)	3 (1%)	21	64
1	C	372/409 (91%)	333 (90%)	37 (10%)	2 (0%)	31	73
1	D	372/409 (91%)	332 (89%)	39 (10%)	1 (0%)	43	80
1	E	372/409 (91%)	344 (92%)	28 (8%)	0	100	100
1	F	371/409 (91%)	341 (92%)	29 (8%)	1 (0%)	43	80
1	G	339/409 (83%)	309 (91%)	28 (8%)	2 (1%)	27	69
All	All	2570/2863 (90%)	2333 (91%)	227 (9%)	10 (0%)	40	76

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	B	26	PRO
1	D	26	PRO
1	B	313	GLU
1	G	26	PRO

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 PDB entries followed by that with respect to all EM entries.

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	270/352 (77%)	270 (100%)	0	100	100
1	B	270/352 (77%)	269 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	270/352 (77%)	269 (100%)	1 (0%)	92	95
1	D	270/352 (77%)	270 (100%)	0	100	100
1	E	270/352 (77%)	270 (100%)	0	100	100
1	F	269/352 (76%)	269 (100%)	0	100	100
1	G	259/352 (74%)	258 (100%)	1 (0%)	92	95
All	All	1878/2464 (76%)	1875 (100%)	3 (0%)	94	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	ASN
1	C	218	ARG
1	G	237	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	248	ASN
1	E	369	HIS
1	G	332	HIS
1	E	265	GLN
1	E	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [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.