wwPDB EM Validation Summary Report

Feb 6, 2024 – 04:11 AM EST

PDB ID	:	1ZKU
EMDB ID	:	EMD-1126
Title	:	Fitting of the gp9 structure in the EM density of bacteriophage T4 extended tail
Authors	:	Kostyuchenko, V.A.
Deposited on	:	2005-05-04
Resolution	:	15.00 Å(reported)
Based on initial model	:	1S2E

This is a wwPDB EM 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/EMValidationReportHelp
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:

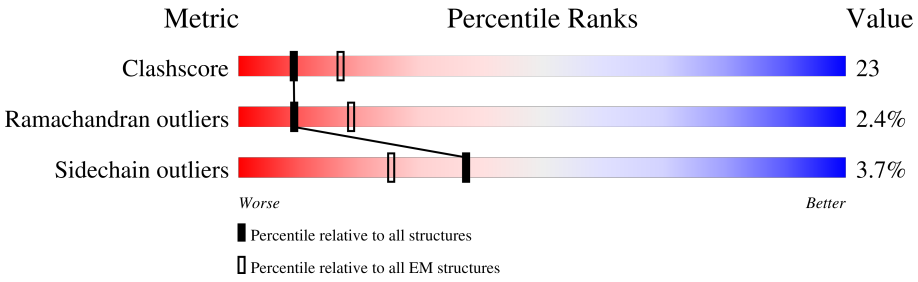
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	100% 70% 25% 5%
1	B	288	100% 70% 25% 5%
1	C	288	100% 72% 24% 5%
1	D	288	100% 70% 25% 5%
1	E	288	100% 70% 25% 5%
1	F	288	100% 71% 24% 5%
1	G	288	100% 71% 24% 5%
1	H	288	100% 70% 25% 5%

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Mol	Chain	Length	Quality of chain
1	I	288	100% 70% 25% 5%
1	J	288	100% 70% 25% 5%
1	K	288	100% 70% 25% 5%
1	L	288	100% 71% 24% 5%
1	M	288	100% 70% 25% 5%
1	N	288	100% 70% 25% 5%
1	O	288	100% 70% 25% 5%
1	P	288	100% 70% 25% 5%
1	Q	288	100% 70% 25% 5%
1	R	288	100% 71% 24% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39420 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 Baseplate structural protein Gp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	B	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	C	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	D	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	E	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	F	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	G	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	H	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	I	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	J	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	K	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	L	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	M	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	N	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	O	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	P	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	Q	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

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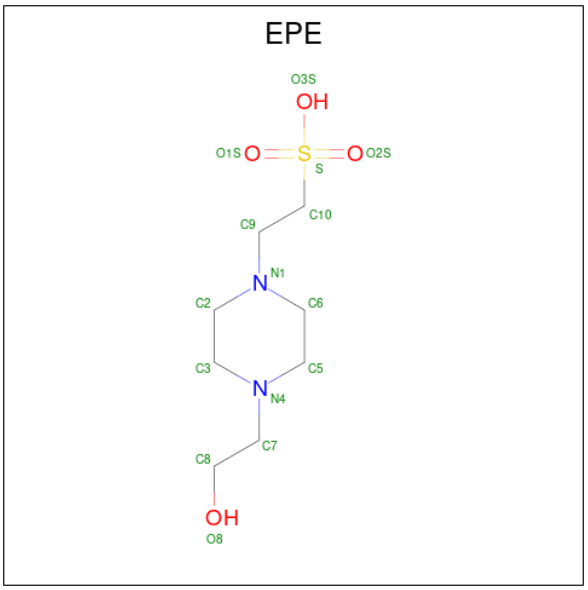
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	B	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	C	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	D	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	E	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	F	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	G	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	H	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	I	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	J	1	Total	C	N	O	S	0
			15	8	2	4	1	

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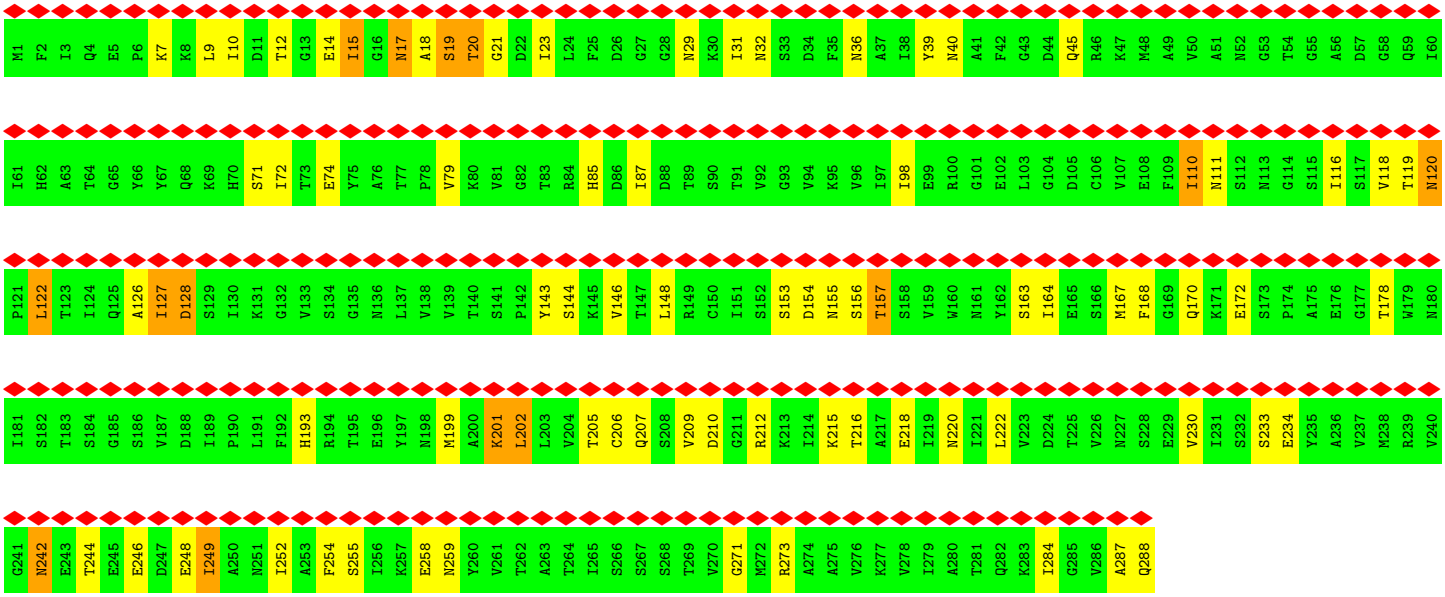
Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	L	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	M	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	N	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	O	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	P	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	Q	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	R	1	Total	C	N	O	S	0
			15	8	2	4	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

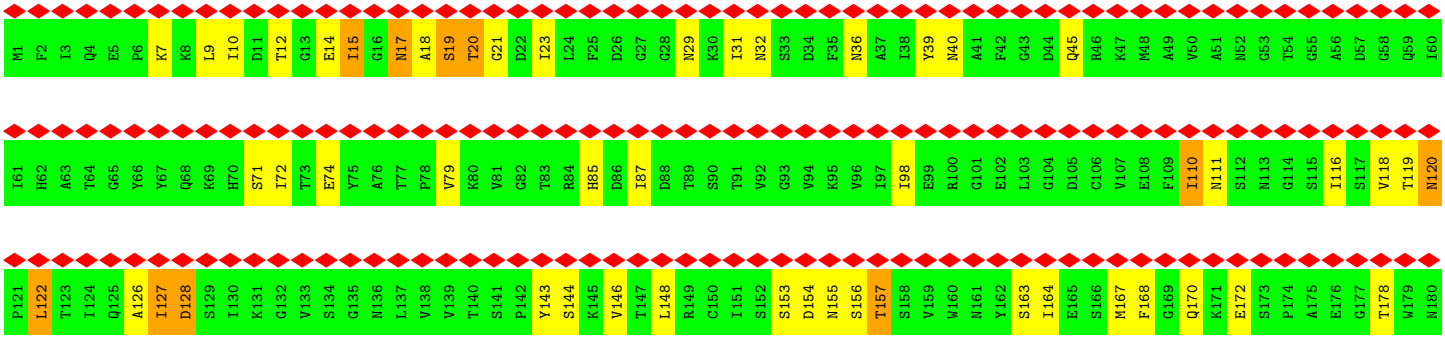
• Molecule 1: Baseplate structural protein Gp9

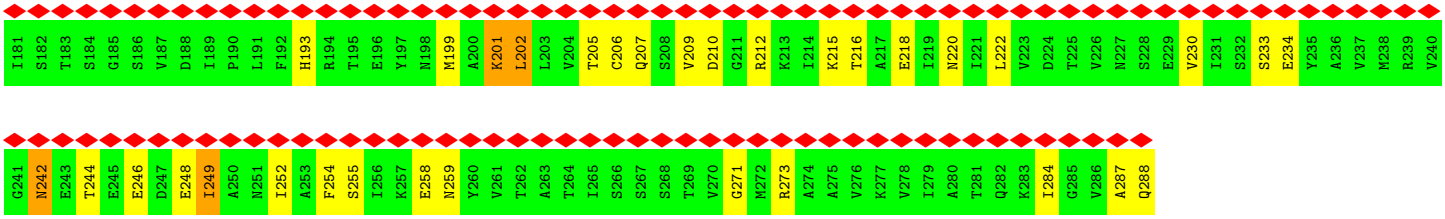
Chain A:



• Molecule 1: Baseplate structural protein Gp9

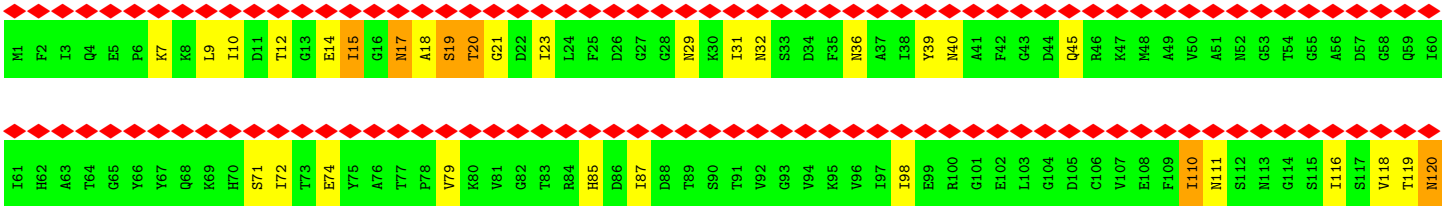
Chain B:





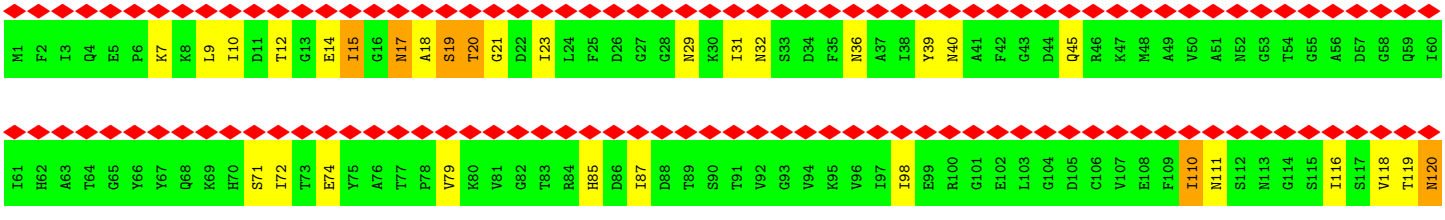
• Molecule 1: Baseplate structural protein Gp9

Chain C:



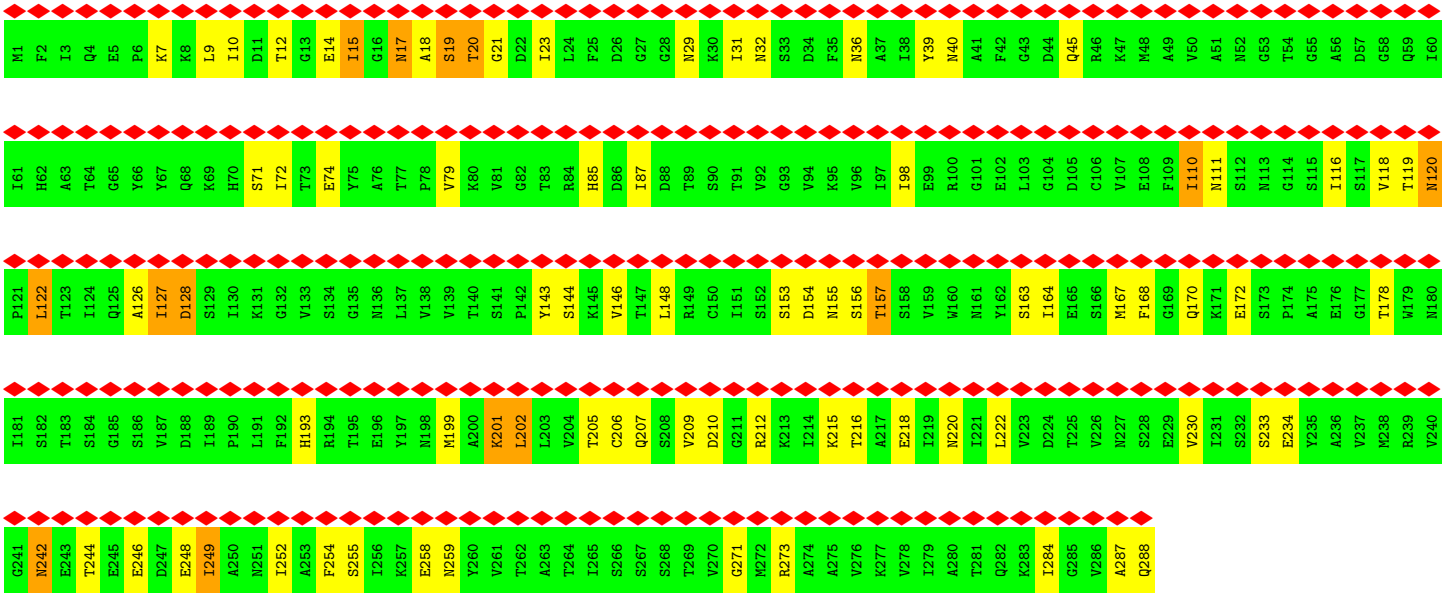
• Molecule 1: Baseplate structural protein Gp9

Chain D:



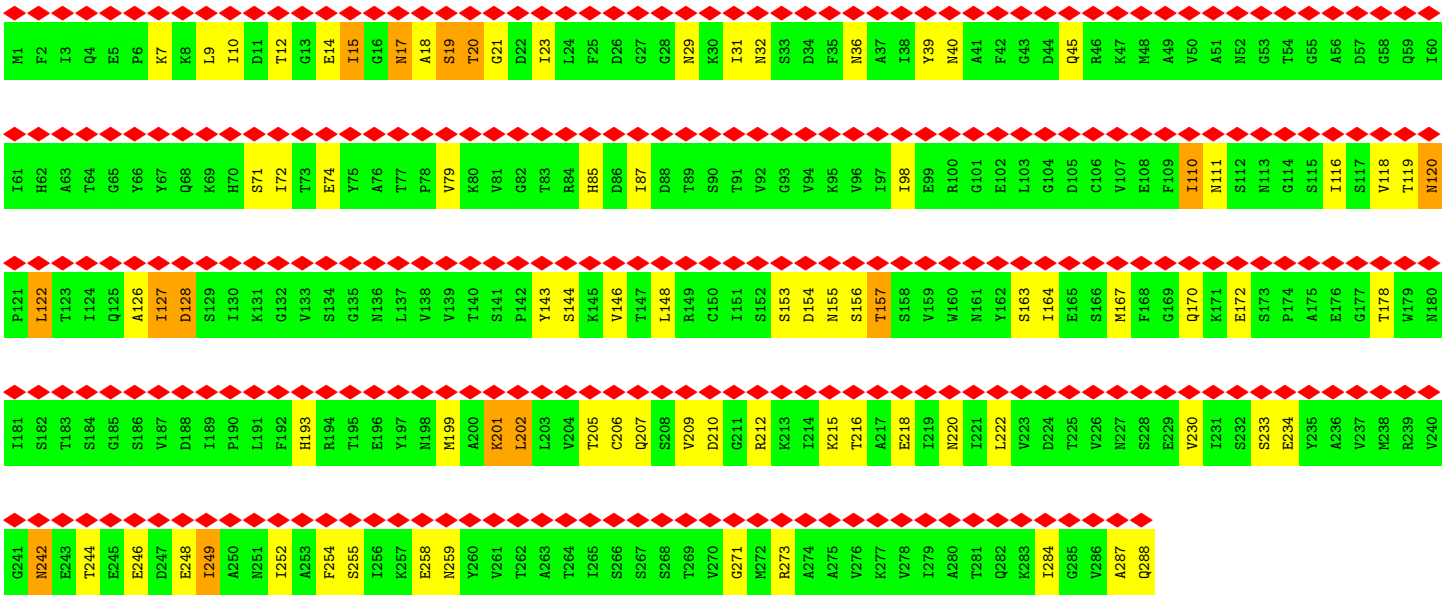
• Molecule 1: Baseplate structural protein Gp9

Chain E:



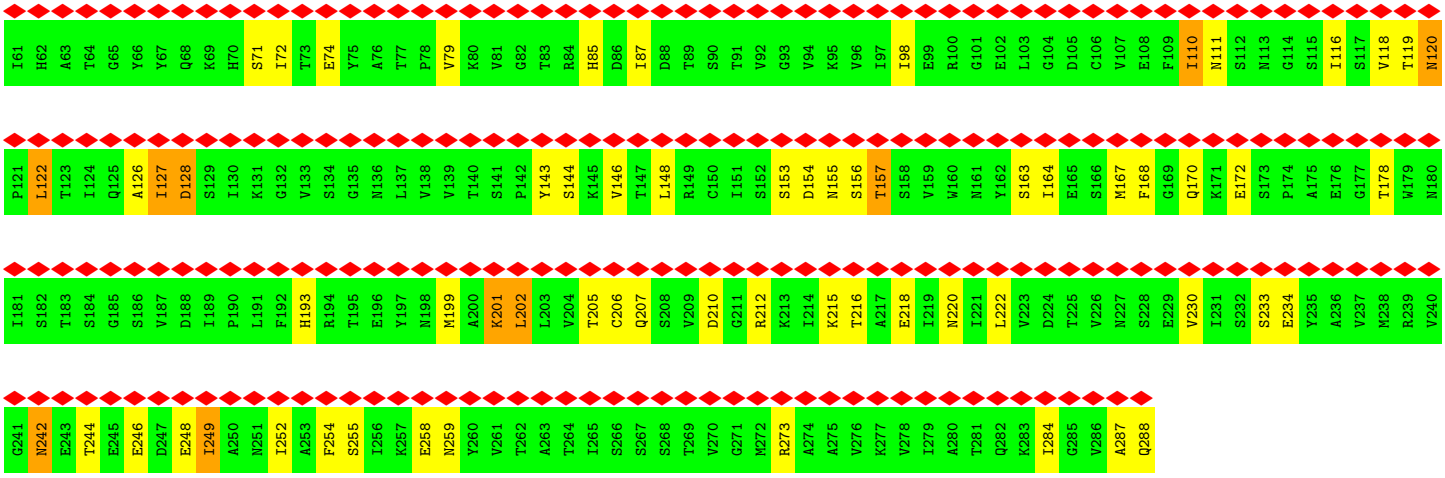
• Molecule 1: Baseplate structural protein Gp9

Chain F:



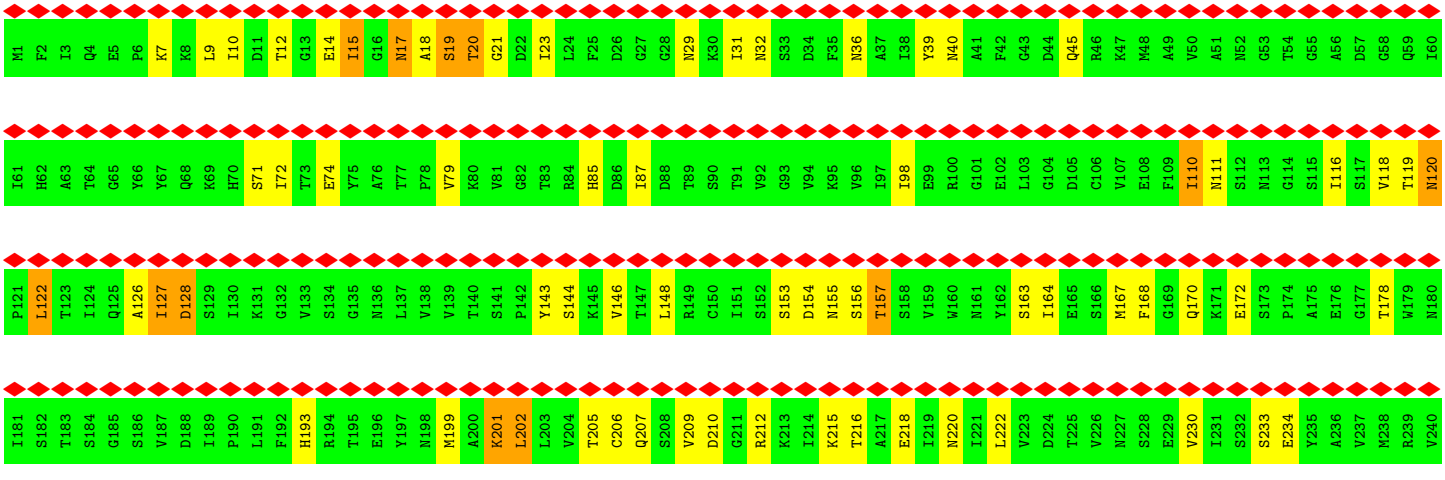
• Molecule 1: Baseplate structural protein Gp9

Chain G:



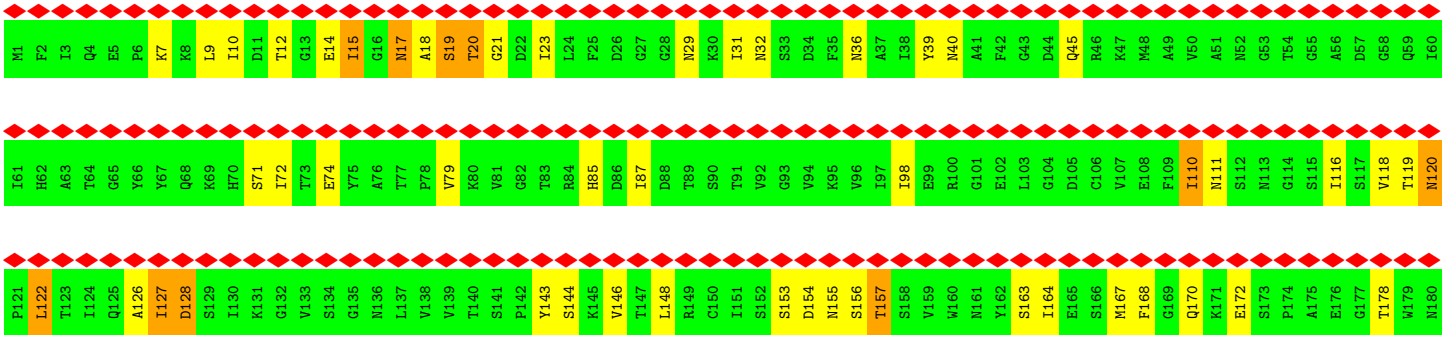
• Molecule 1: Baseplate structural protein Gp9

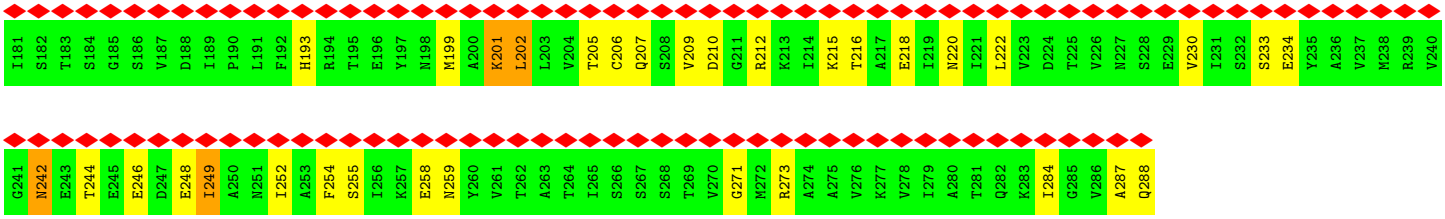
Chain H:



• Molecule 1: Baseplate structural protein Gp9

Chain I:



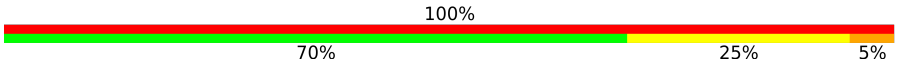


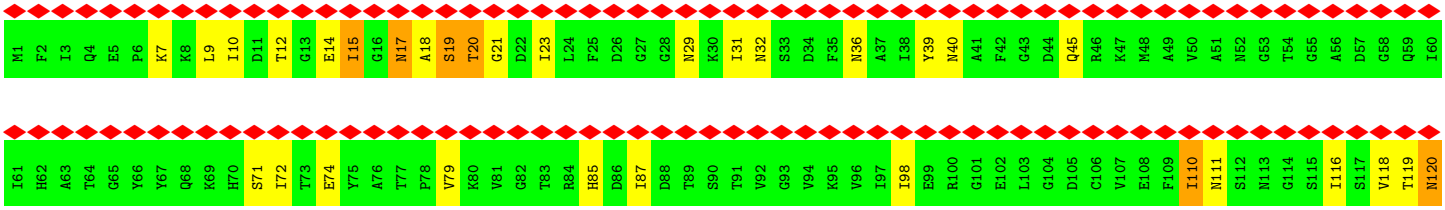
• Molecule 1: Baseplate structural protein Gp9

Chain J:

• Molecule 1: Baseplate structural protein Gp9

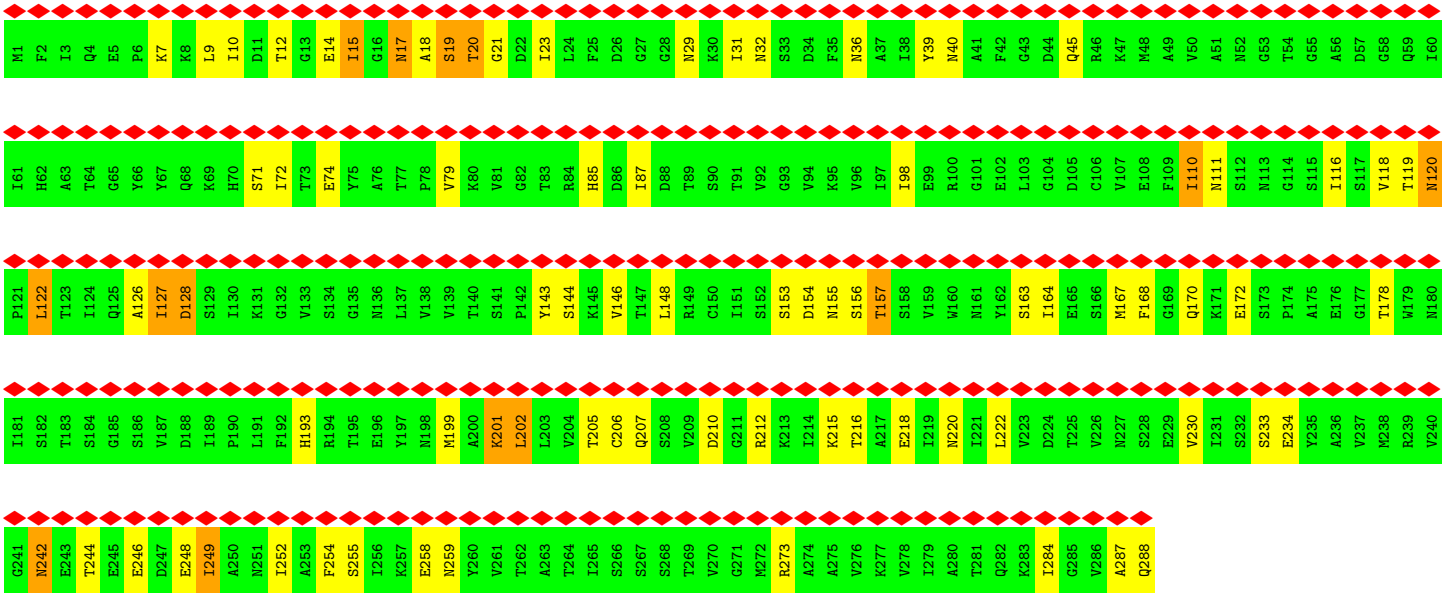
Chain K:





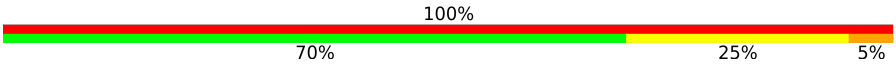
• Molecule 1: Baseplate structural protein Gp9

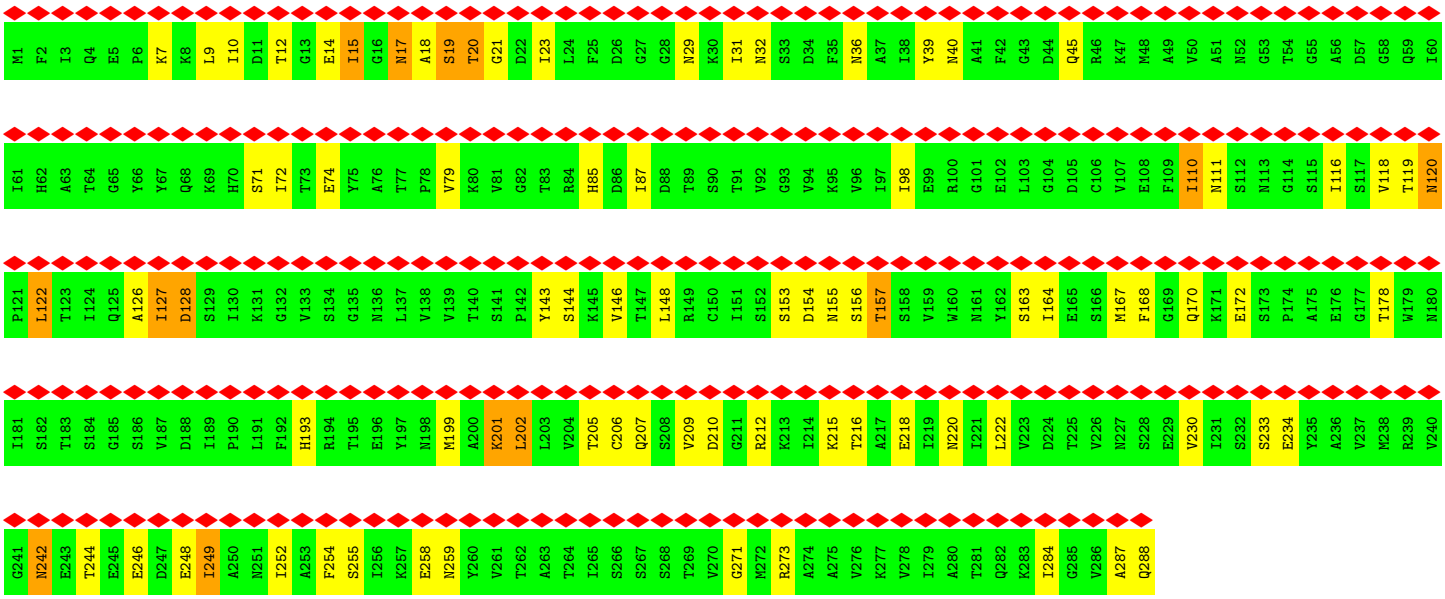
Chain L:



• Molecule 1: Baseplate structural protein Gp9

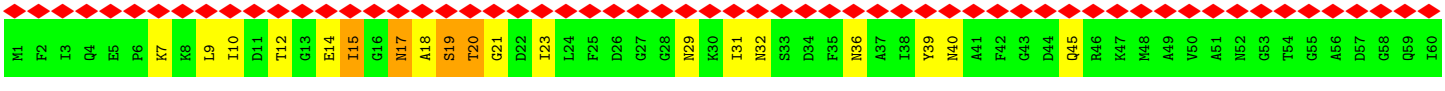
Chain M:

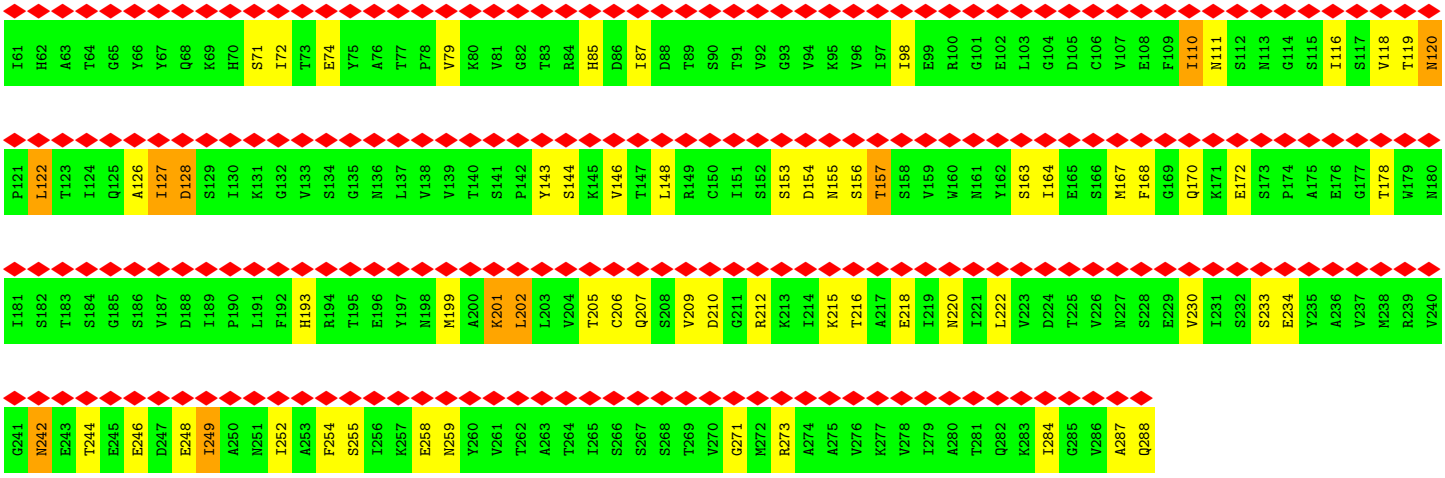




• Molecule 1: Baseplate structural protein Gp9

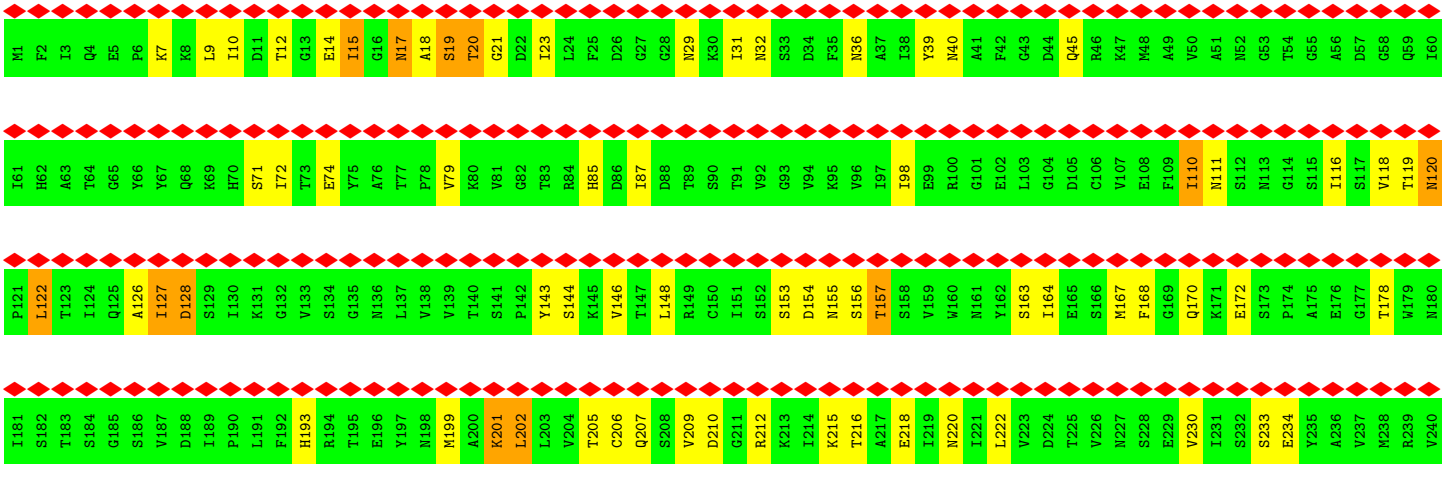
Chain N:





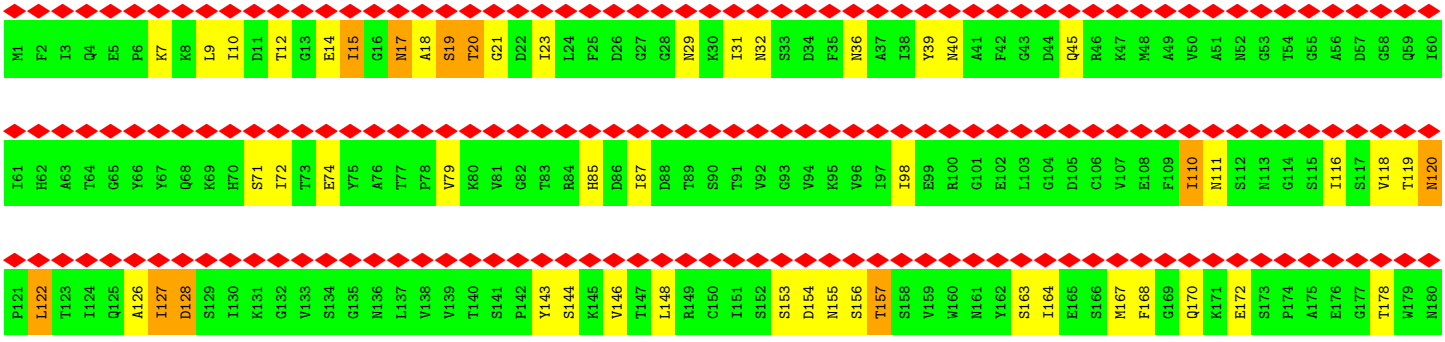
• Molecule 1: Baseplate structural protein Gp9

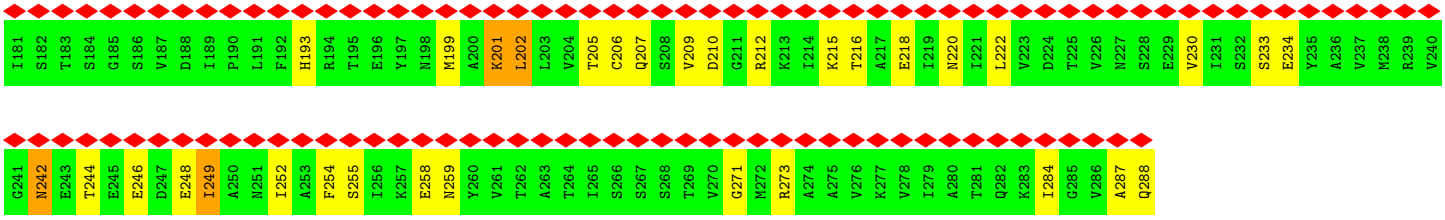
Chain O:



• Molecule 1: Baseplate structural protein Gp9

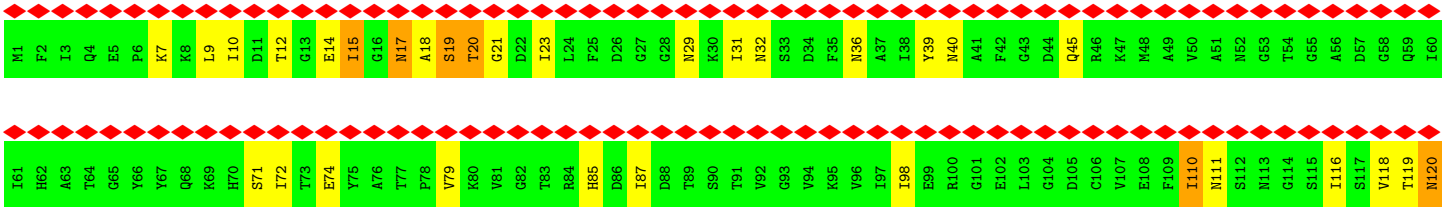
Chain P:





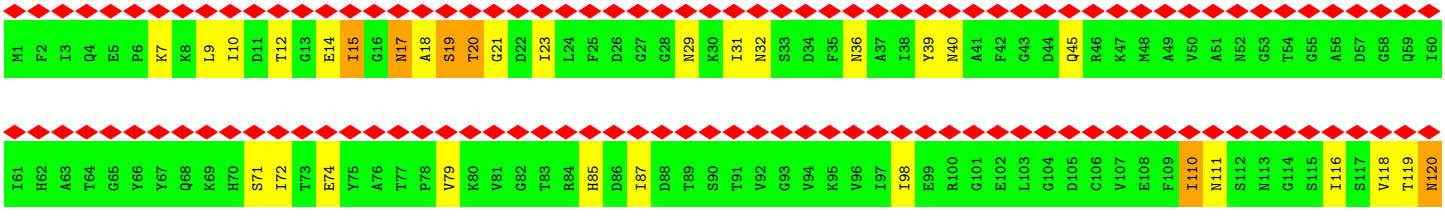
• Molecule 1: Baseplate structural protein Gp9

Chain Q:



• Molecule 1: Baseplate structural protein Gp9

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	3029	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	3.2	Depositor
Magnification	47000	Depositor
Image detector	GENERIC FILM	Depositor
Maximum map value	7.953	Depositor
Minimum map value	-2.953	Depositor
Average map value	0.059	Depositor
Map value standard deviation	0.533	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	714.6, 714.6, 1508.6	wwPDB
Map dimensions	180, 180, 380	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	3.97, 3.97, 3.97	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE

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	0.37	0/2205	0.67	1/2988 (0.0%)
1	B	0.37	0/2205	0.67	1/2988 (0.0%)
1	C	0.37	0/2205	0.67	1/2988 (0.0%)
1	D	0.37	0/2205	0.67	1/2988 (0.0%)
1	E	0.37	0/2205	0.67	1/2988 (0.0%)
1	F	0.37	0/2205	0.67	1/2988 (0.0%)
1	G	0.37	0/2205	0.67	1/2988 (0.0%)
1	H	0.37	0/2205	0.67	1/2988 (0.0%)
1	I	0.37	0/2205	0.67	1/2988 (0.0%)
1	J	0.37	0/2205	0.67	1/2988 (0.0%)
1	K	0.37	0/2205	0.67	1/2988 (0.0%)
1	L	0.37	0/2205	0.67	1/2988 (0.0%)
1	M	0.37	0/2205	0.67	1/2988 (0.0%)
1	N	0.37	0/2205	0.67	1/2988 (0.0%)
1	O	0.37	0/2205	0.67	1/2988 (0.0%)
1	P	0.37	0/2205	0.67	1/2988 (0.0%)
1	Q	0.37	0/2205	0.67	1/2988 (0.0%)
1	R	0.37	0/2205	0.67	1/2988 (0.0%)
All	All	0.37	0/39690	0.67	18/53784 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	19	SER	CA-C-N	-7.11	101.56	117.20
1	M	19	SER	CA-C-N	-7.11	101.56	117.20
1	A	19	SER	CA-C-N	-7.11	101.57	117.20
1	C	19	SER	CA-C-N	-7.11	101.57	117.20
1	I	19	SER	CA-C-N	-7.11	101.57	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2157	123	0
1	B	2175	0	2157	121	0
1	C	2175	0	2157	119	0
1	D	2175	0	2157	125	0
1	E	2175	0	2157	123	0
1	F	2175	0	2157	122	0
1	G	2175	0	2157	120	0
1	H	2175	0	2157	123	0
1	I	2175	0	2157	120	0
1	J	2175	0	2157	121	0
1	K	2175	0	2157	124	0
1	L	2175	0	2157	121	0
1	M	2175	0	2157	121	0
1	N	2175	0	2157	124	0
1	O	2175	0	2157	123	0
1	P	2175	0	2157	123	0
1	Q	2175	0	2157	122	0
1	R	2175	0	2157	121	0
2	A	15	0	18	3	0
2	B	15	0	18	3	0
2	C	15	0	18	3	0
2	D	15	0	18	4	0
2	E	15	0	18	3	0
2	F	15	0	18	3	0
2	G	15	0	18	3	0
2	H	15	0	18	3	0
2	I	15	0	18	3	0
2	J	15	0	18	3	0
2	K	15	0	18	3	0
2	L	15	0	18	3	0
2	M	15	0	18	3	0
2	N	15	0	18	3	0
2	O	15	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	15	0	18	3	0
2	Q	15	0	18	3	0
2	R	15	0	18	3	0
All	All	39420	0	39150	1808	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 23.

The worst 5 of 1808 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:B:18:ALA:HB3	1:B:23:ILE:HD11	1.41	1.03
1:E:18:ALA:HB3	1:E:23:ILE:HD11	1.41	1.02
1:Q:18:ALA:HB3	1:Q:23:ILE:HD11	1.41	1.02
1:F:18:ALA:HB3	1:F:23:ILE:HD11	1.41	1.02
1:I:18:ALA:HB3	1:I:23:ILE:HD11	1.41	1.02

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33
1	B	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33
1	C	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33
1	D	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33
1	E	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33
1	F	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	6 33
1	G	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	6	33
1	I	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	J	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	K	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	L	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	M	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	N	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	O	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	6	33
1	P	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
1	Q	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	6	33
1	R	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	6	33
All	All	5148/5184 (99%)	4766 (93%)	256 (5%)	126 (2%)	9	33

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	128	ASP
1	B	20	THR
1	B	128	ASP
1	C	20	THR

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 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	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	B	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	C	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	D	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	E	244/244 (100%)	235 (96%)	9 (4%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	G	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	H	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	I	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	J	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	K	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	L	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	M	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	N	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	O	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	P	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	Q	244/244 (100%)	235 (96%)	9 (4%)	34	58
1	R	244/244 (100%)	235 (96%)	9 (4%)	34	58
All	All	4392/4392 (100%)	4230 (96%)	162 (4%)	37	58

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	202	LEU
1	P	242	ASN
1	N	120	ASN
1	O	148	LEU
1	Q	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	111	ASN
1	N	17	ASN
1	K	227	ASN
1	L	227	ASN
1	N	125	GLN

5.3.3 RNA

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)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EPE	G	307	-	15,15,15	1.79	2 (13%)	18,20,20	3.59	12 (66%)
2	EPE	P	316	-	15,15,15	1.79	2 (13%)	18,20,20	3.59	12 (66%)
2	EPE	R	318	-	15,15,15	1.78	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	A	301	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	N	314	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	C	303	-	15,15,15	1.78	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	D	304	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	B	302	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	H	308	-	15,15,15	1.79	2 (13%)	18,20,20	3.61	12 (66%)
2	EPE	K	311	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	O	315	-	15,15,15	1.77	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	Q	317	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	L	312	-	15,15,15	1.78	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	M	313	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	F	306	-	15,15,15	1.77	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	I	309	-	15,15,15	1.78	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	J	310	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)
2	EPE	E	305	-	15,15,15	1.79	2 (13%)	18,20,20	3.60	12 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	G	307	-	-	6/9/19/19	0/1/1/1
2	EPE	P	316	-	-	6/9/19/19	0/1/1/1
2	EPE	R	318	-	-	6/9/19/19	0/1/1/1
2	EPE	A	301	-	-	6/9/19/19	0/1/1/1
2	EPE	N	314	-	-	6/9/19/19	0/1/1/1
2	EPE	C	303	-	-	6/9/19/19	0/1/1/1
2	EPE	D	304	-	-	6/9/19/19	0/1/1/1
2	EPE	B	302	-	-	6/9/19/19	0/1/1/1
2	EPE	H	308	-	-	6/9/19/19	0/1/1/1
2	EPE	K	311	-	-	6/9/19/19	0/1/1/1
2	EPE	O	315	-	-	6/9/19/19	0/1/1/1
2	EPE	Q	317	-	-	6/9/19/19	0/1/1/1
2	EPE	L	312	-	-	6/9/19/19	0/1/1/1
2	EPE	M	313	-	-	6/9/19/19	0/1/1/1
2	EPE	F	306	-	-	6/9/19/19	0/1/1/1
2	EPE	I	309	-	-	6/9/19/19	0/1/1/1
2	EPE	J	310	-	-	6/9/19/19	0/1/1/1
2	EPE	E	305	-	-	6/9/19/19	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	EPE	O3S-S	4.81	1.64	1.47
2	K	311	EPE	O3S-S	4.81	1.64	1.47
2	H	308	EPE	O3S-S	4.81	1.64	1.47
2	Q	317	EPE	O3S-S	4.81	1.64	1.47
2	E	305	EPE	O3S-S	4.81	1.64	1.47

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	306	EPE	O2S-S-C10	7.02	115.37	106.92
2	O	315	EPE	O2S-S-C10	7.02	115.37	106.92
2	C	303	EPE	O2S-S-C10	7.01	115.36	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	312	EPE	O2S-S-C10	7.01	115.36	106.92
2	E	305	EPE	O2S-S-C10	7.00	115.35	106.92

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EPE	C9-C10-S-O1S
2	B	302	EPE	C9-C10-S-O1S
2	C	303	EPE	C9-C10-S-O1S
2	D	304	EPE	C9-C10-S-O1S
2	E	305	EPE	C9-C10-S-O1S

There are no ring outliers.

18 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	307	EPE	3	0
2	P	316	EPE	3	0
2	R	318	EPE	3	0
2	A	301	EPE	3	0
2	N	314	EPE	3	0
2	C	303	EPE	3	0
2	D	304	EPE	4	0
2	B	302	EPE	3	0
2	H	308	EPE	3	0
2	K	311	EPE	3	0
2	O	315	EPE	3	0
2	Q	317	EPE	3	0
2	L	312	EPE	3	0
2	M	313	EPE	3	0
2	F	306	EPE	3	0
2	I	309	EPE	3	0
2	J	310	EPE	3	0
2	E	305	EPE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

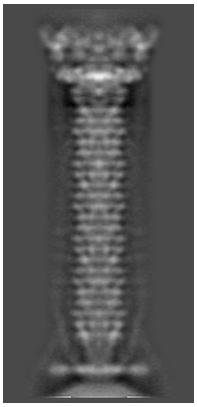
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1126. These allow visual inspection of the internal detail of the map and identification of artifacts.

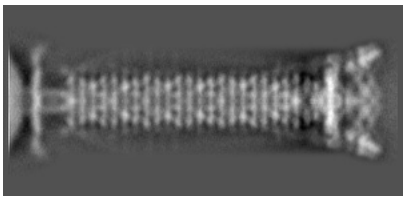
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

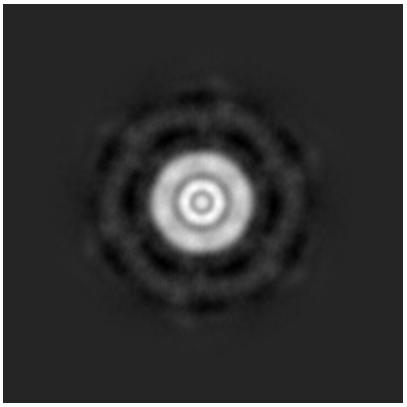
6.1.1 Primary map



X



Y

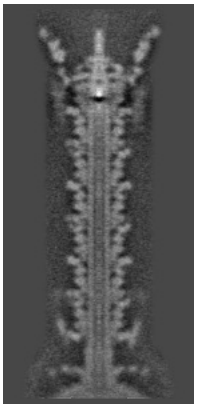


Z

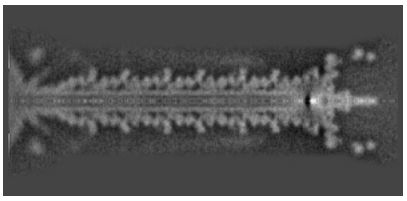
The images above show the map projected in three orthogonal directions.

6.2 Central slices

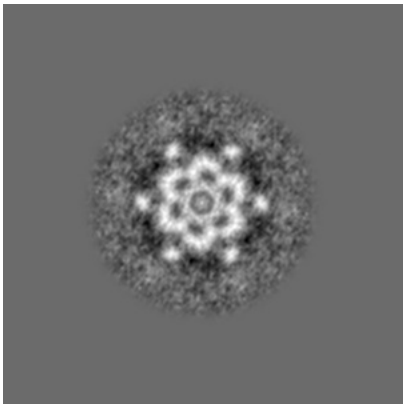
6.2.1 Primary map



X Index: 90



Y Index: 90

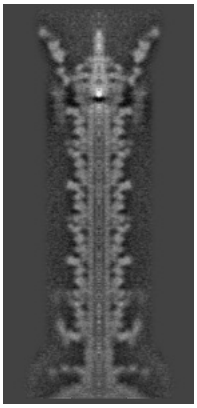


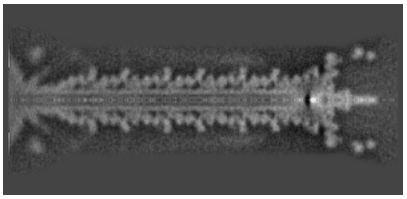
Z Index: 190

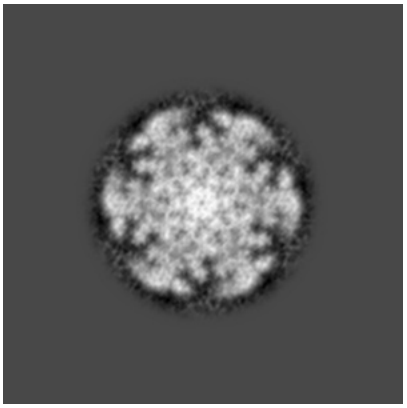
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 89

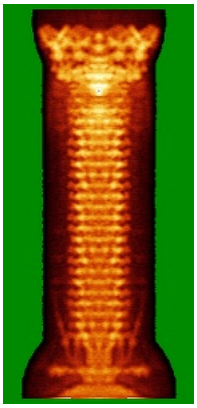

Y Index: 90

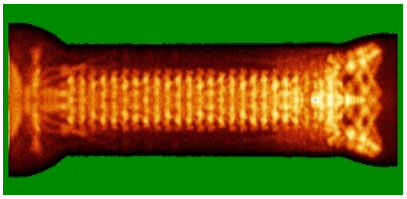

Z Index: 310

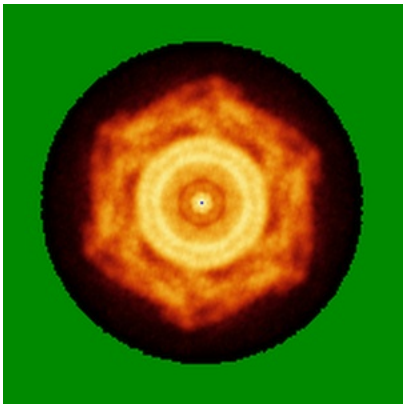
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

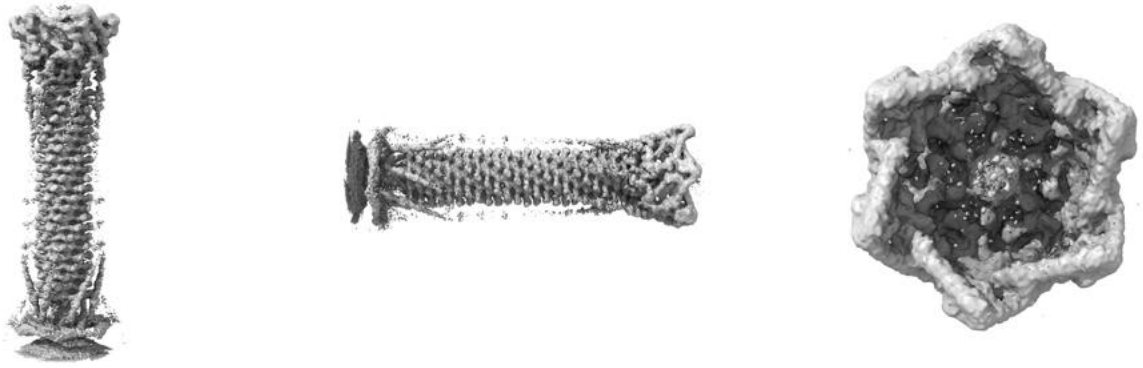

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

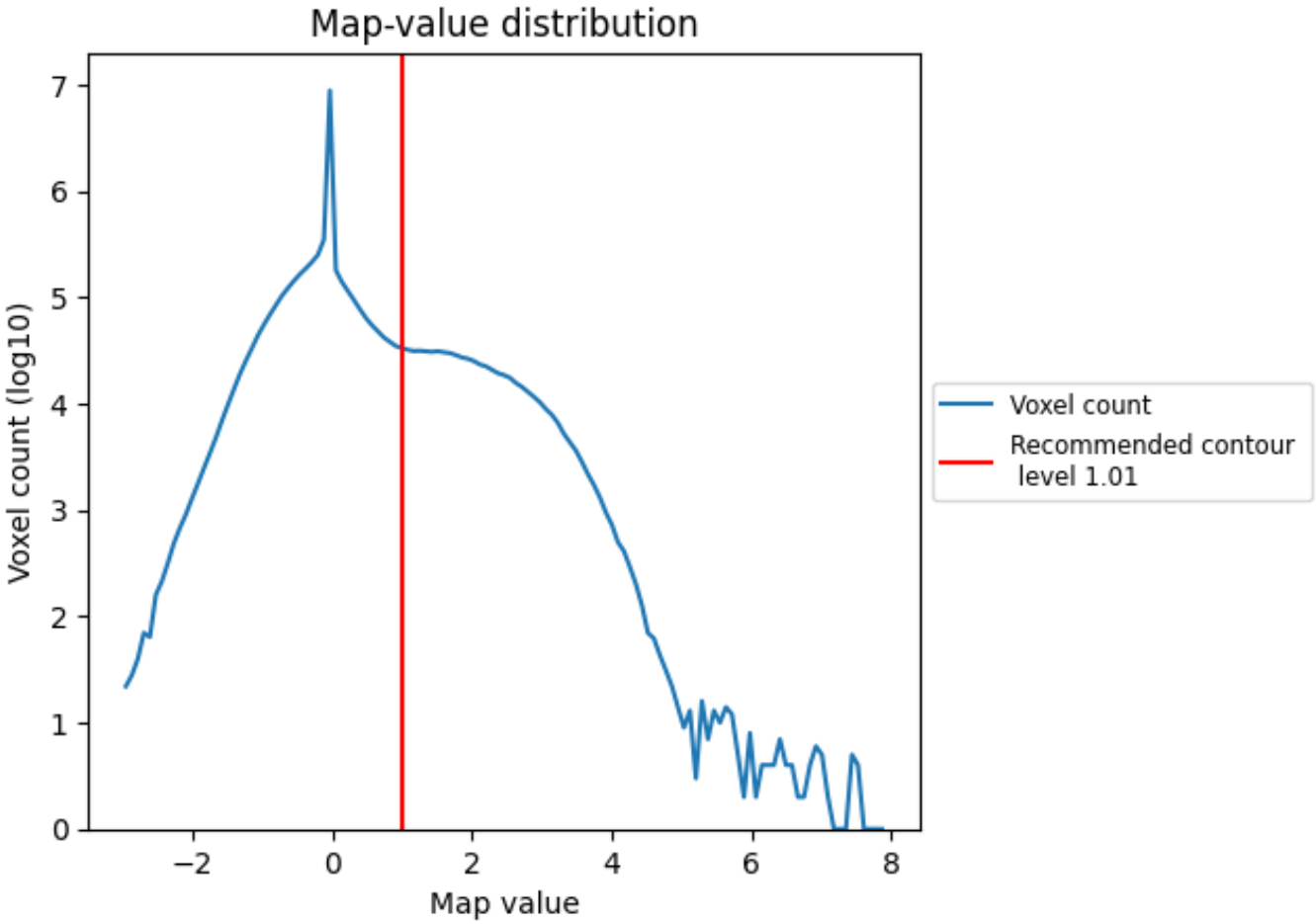
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

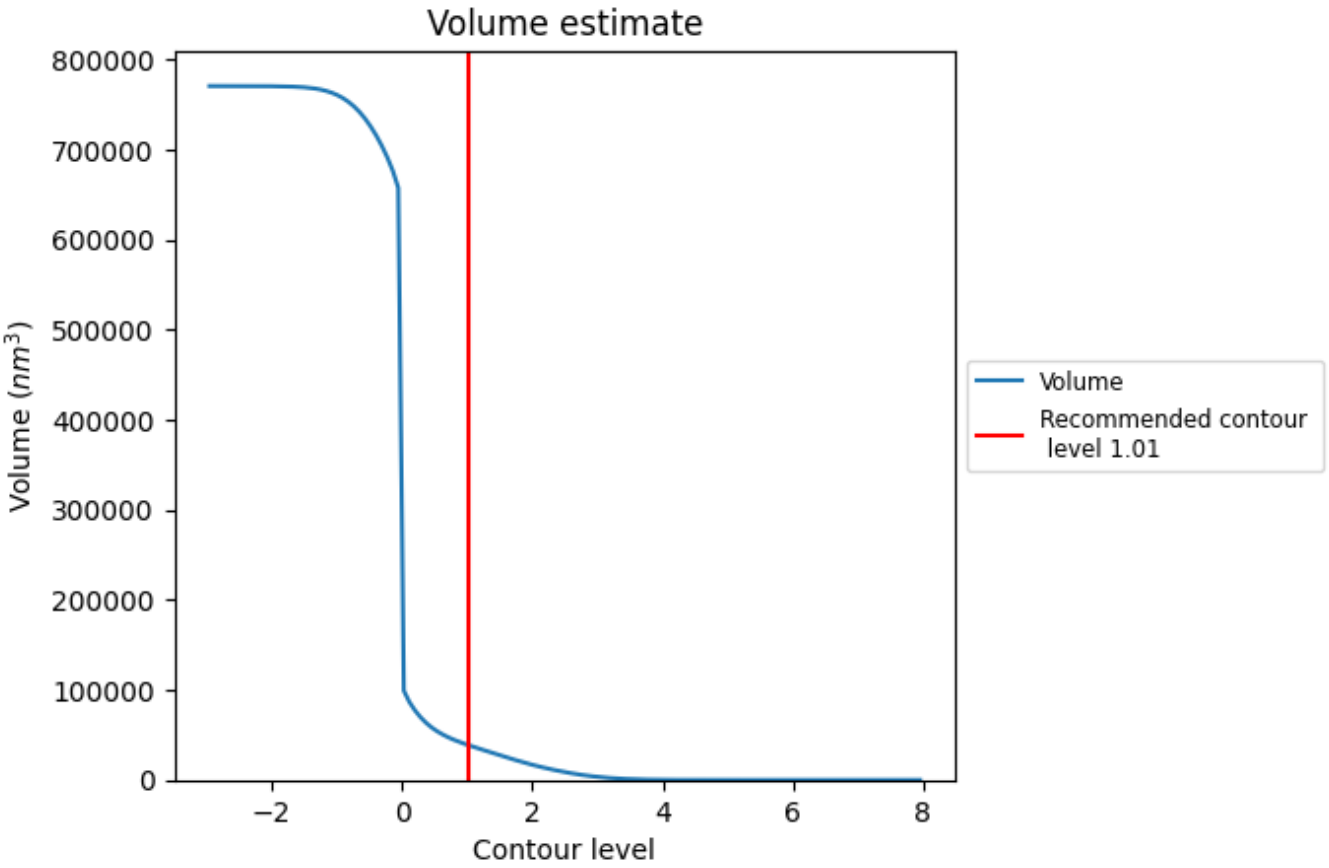
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 38892 nm^3; this corresponds to an approximate mass of 35132 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

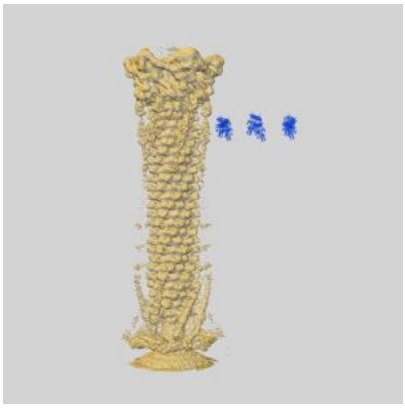
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

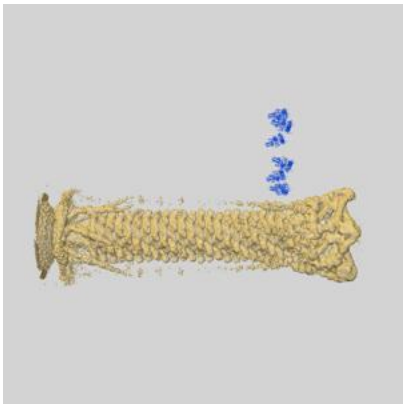
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1126 and PDB model 1ZKU. Per-residue inclusion information can be found in section 3 on page 7.

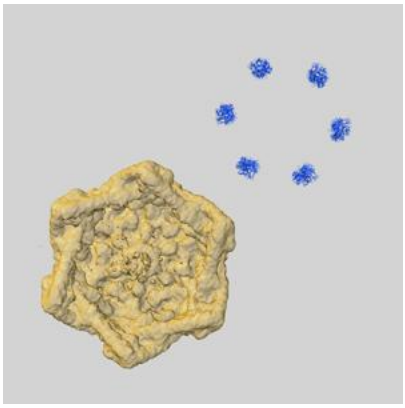
9.1 Map-model overlay



X



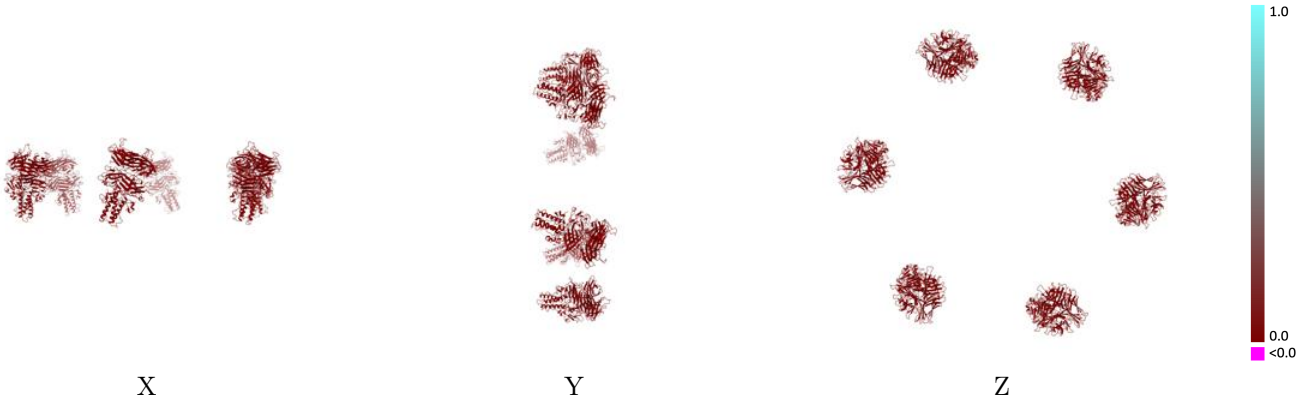
Y



Z

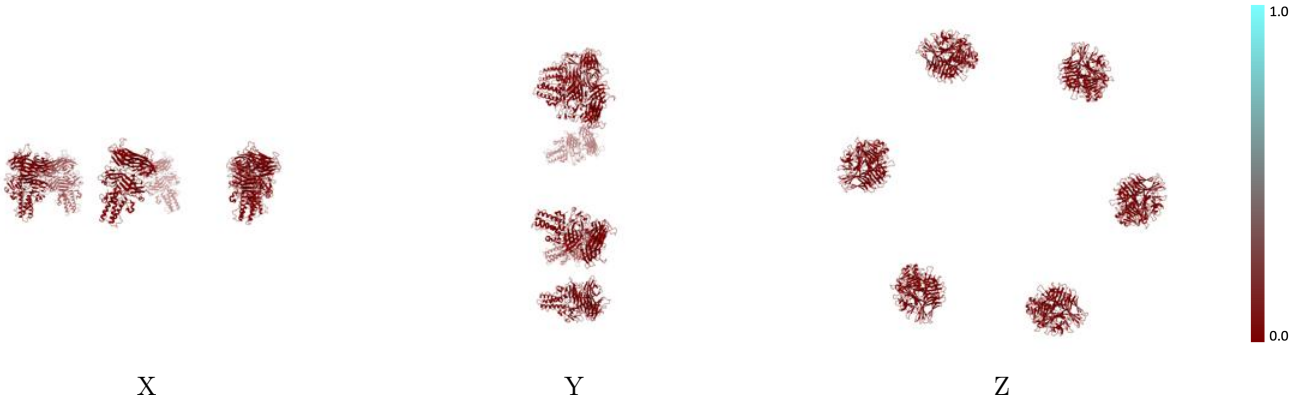
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



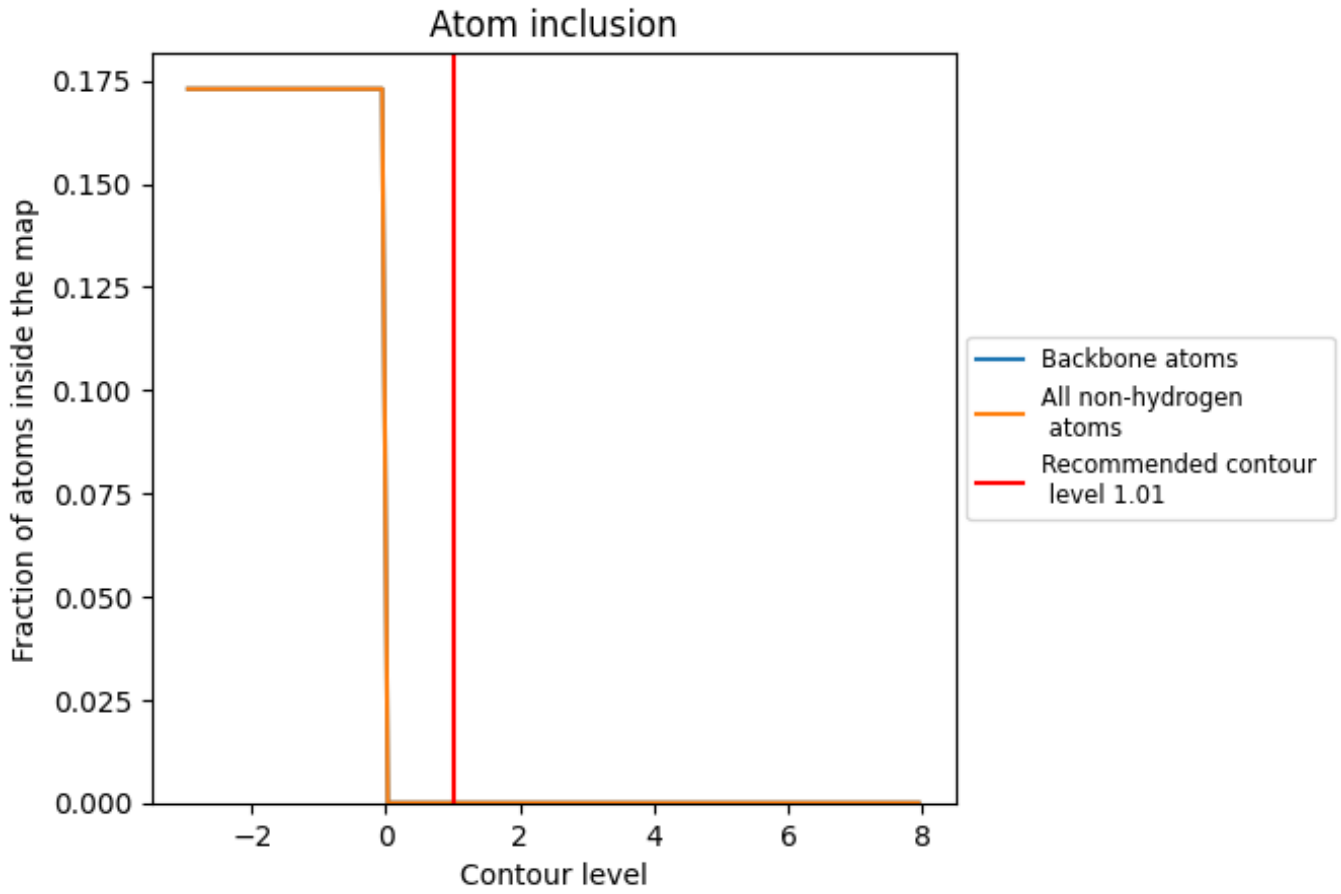
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.01).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.0000	0.0000
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0000
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0000	0.0000
K	0.0000	0.0000
L	0.0000	0.0000
M	0.0000	0.0000
N	0.0000	0.0000
O	0.0000	0.0000
P	0.0000	0.0000
Q	0.0000	0.0000
R	0.0000	0.0000