wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 09:38 pm GMT

PDB ID	:	6R21
EMDB ID	:	EMD-4706
Title	:	Cryo-EM structure of T7 bacteriophage fiberless tail complex
Authors	:	Cuervo, A.; Fabrega-Ferrer, M.; Machon, C.; Conesa, J.J.; Perez-Ruiz, M.; Coll, M.; Carrascosa, J.L.
Deposited on	:	2019-03-15
Resolution	:	3.33 Å(reported)
Based on initial models	:	6QWP, 5MU4, ?

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:

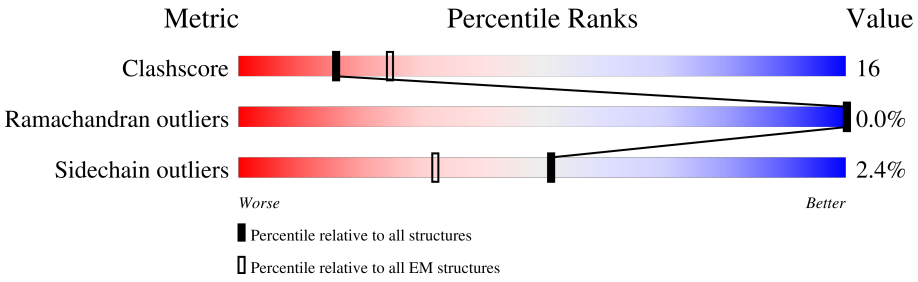
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.33 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	536	62% 25% • 10%
1	B	536	62% 26% • 10%
1	C	536	62% 24% • 10%
1	D	536	62% 25% • 10%
1	E	536	62% 24% • 10%
1	F	536	62% 26% • 10%
1	G	536	62% 25% • 10%
1	H	536	62% 26% • 10%

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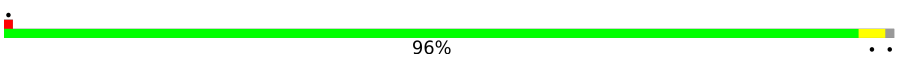
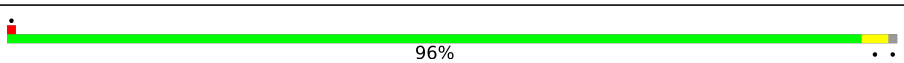
Mol	Chain	Length	Quality of chain
1	I	536	
1	J	536	
1	K	536	
1	L	536	
2	M	231	
2	N	231	
2	O	231	
2	P	231	
2	Q	231	
2	R	231	
2	S	231	
2	T	231	
2	U	231	
2	V	231	
2	W	231	
2	X	231	
3	a	794	
3	b	794	
3	c	794	
3	d	794	
3	e	794	
3	f	794	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 101064 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	B	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	C	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	D	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	E	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	F	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	G	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	H	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	I	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	J	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	K	483	Total 3780	C 2379	N 638	O 746	S 17	0	0
1	L	483	Total 3780	C 2379	N 638	O 746	S 17	0	0

- Molecule 2 is a protein called Tail tubular protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	190	Total 1512	C 939	N 258	O 308	S 7	0	0
2	N	191	Total 1520	C 944	N 259	O 309	S 8	0	0
2	O	190	Total 1512	C 939	N 258	O 308	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	191	Total	C	N	O	S	0	0
			1520	944	259	309	8		
2	Q	190	Total	C	N	O	S	0	0
			1512	939	258	308	7		
2	R	191	Total	C	N	O	S	0	0
			1520	944	259	309	8		
2	S	190	Total	C	N	O	S	0	0
			1512	939	258	308	7		
2	T	191	Total	C	N	O	S	0	0
			1520	944	259	309	8		
2	U	190	Total	C	N	O	S	0	0
			1512	939	258	308	7		
2	V	191	Total	C	N	O	S	0	0
			1520	944	259	309	8		
2	W	190	Total	C	N	O	S	0	0
			1512	939	258	308	7		
2	X	191	Total	C	N	O	S	0	0
			1520	944	259	309	8		

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-34	MET	-	initiating methionine	UNP P03746
M	-33	ARG	-	expression tag	UNP P03746
M	-32	GLY	-	expression tag	UNP P03746
M	-31	SER	-	expression tag	UNP P03746
M	-30	HIS	-	expression tag	UNP P03746
M	-29	HIS	-	expression tag	UNP P03746
M	-28	HIS	-	expression tag	UNP P03746
M	-27	HIS	-	expression tag	UNP P03746
M	-26	HIS	-	expression tag	UNP P03746
M	-25	HIS	-	expression tag	UNP P03746
M	-24	GLY	-	expression tag	UNP P03746
M	-23	MET	-	expression tag	UNP P03746
M	-22	ALA	-	expression tag	UNP P03746
M	-21	SER	-	expression tag	UNP P03746
M	-20	MET	-	expression tag	UNP P03746
M	-19	THR	-	expression tag	UNP P03746
M	-18	GLY	-	expression tag	UNP P03746
M	-17	GLY	-	expression tag	UNP P03746
M	-16	ASN	-	expression tag	UNP P03746
M	-15	ASN	-	expression tag	UNP P03746
M	-14	MET	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-13	GLY	-	expression tag	UNP P03746
M	-12	ARG	-	expression tag	UNP P03746
M	-11	ASP	-	expression tag	UNP P03746
M	-10	LEU	-	expression tag	UNP P03746
M	-9	TYR	-	expression tag	UNP P03746
M	-8	ASP	-	expression tag	UNP P03746
M	-7	ASP	-	expression tag	UNP P03746
M	-6	ASP	-	expression tag	UNP P03746
M	-5	ASP	-	expression tag	UNP P03746
M	-4	LYS	-	expression tag	UNP P03746
M	-3	ASP	-	expression tag	UNP P03746
M	-2	PRO	-	expression tag	UNP P03746
M	-1	SER	-	expression tag	UNP P03746
M	0	SER	-	expression tag	UNP P03746
N	-34	MET	-	initiating methionine	UNP P03746
N	-33	ARG	-	expression tag	UNP P03746
N	-32	GLY	-	expression tag	UNP P03746
N	-31	SER	-	expression tag	UNP P03746
N	-30	HIS	-	expression tag	UNP P03746
N	-29	HIS	-	expression tag	UNP P03746
N	-28	HIS	-	expression tag	UNP P03746
N	-27	HIS	-	expression tag	UNP P03746
N	-26	HIS	-	expression tag	UNP P03746
N	-25	HIS	-	expression tag	UNP P03746
N	-24	GLY	-	expression tag	UNP P03746
N	-23	MET	-	expression tag	UNP P03746
N	-22	ALA	-	expression tag	UNP P03746
N	-21	SER	-	expression tag	UNP P03746
N	-20	MET	-	expression tag	UNP P03746
N	-19	THR	-	expression tag	UNP P03746
N	-18	GLY	-	expression tag	UNP P03746
N	-17	GLY	-	expression tag	UNP P03746
N	-16	ASN	-	expression tag	UNP P03746
N	-15	ASN	-	expression tag	UNP P03746
N	-14	MET	-	expression tag	UNP P03746
N	-13	GLY	-	expression tag	UNP P03746
N	-12	ARG	-	expression tag	UNP P03746
N	-11	ASP	-	expression tag	UNP P03746
N	-10	LEU	-	expression tag	UNP P03746
N	-9	TYR	-	expression tag	UNP P03746
N	-8	ASP	-	expression tag	UNP P03746
N	-7	ASP	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-6	ASP	-	expression tag	UNP P03746
N	-5	ASP	-	expression tag	UNP P03746
N	-4	LYS	-	expression tag	UNP P03746
N	-3	ASP	-	expression tag	UNP P03746
N	-2	PRO	-	expression tag	UNP P03746
N	-1	SER	-	expression tag	UNP P03746
N	0	SER	-	expression tag	UNP P03746
O	-34	MET	-	initiating methionine	UNP P03746
O	-33	ARG	-	expression tag	UNP P03746
O	-32	GLY	-	expression tag	UNP P03746
O	-31	SER	-	expression tag	UNP P03746
O	-30	HIS	-	expression tag	UNP P03746
O	-29	HIS	-	expression tag	UNP P03746
O	-28	HIS	-	expression tag	UNP P03746
O	-27	HIS	-	expression tag	UNP P03746
O	-26	HIS	-	expression tag	UNP P03746
O	-25	HIS	-	expression tag	UNP P03746
O	-24	GLY	-	expression tag	UNP P03746
O	-23	MET	-	expression tag	UNP P03746
O	-22	ALA	-	expression tag	UNP P03746
O	-21	SER	-	expression tag	UNP P03746
O	-20	MET	-	expression tag	UNP P03746
O	-19	THR	-	expression tag	UNP P03746
O	-18	GLY	-	expression tag	UNP P03746
O	-17	GLY	-	expression tag	UNP P03746
O	-16	ASN	-	expression tag	UNP P03746
O	-15	ASN	-	expression tag	UNP P03746
O	-14	MET	-	expression tag	UNP P03746
O	-13	GLY	-	expression tag	UNP P03746
O	-12	ARG	-	expression tag	UNP P03746
O	-11	ASP	-	expression tag	UNP P03746
O	-10	LEU	-	expression tag	UNP P03746
O	-9	TYR	-	expression tag	UNP P03746
O	-8	ASP	-	expression tag	UNP P03746
O	-7	ASP	-	expression tag	UNP P03746
O	-6	ASP	-	expression tag	UNP P03746
O	-5	ASP	-	expression tag	UNP P03746
O	-4	LYS	-	expression tag	UNP P03746
O	-3	ASP	-	expression tag	UNP P03746
O	-2	PRO	-	expression tag	UNP P03746
O	-1	SER	-	expression tag	UNP P03746
O	0	SER	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-34	MET	-	initiating methionine	UNP P03746
P	-33	ARG	-	expression tag	UNP P03746
P	-32	GLY	-	expression tag	UNP P03746
P	-31	SER	-	expression tag	UNP P03746
P	-30	HIS	-	expression tag	UNP P03746
P	-29	HIS	-	expression tag	UNP P03746
P	-28	HIS	-	expression tag	UNP P03746
P	-27	HIS	-	expression tag	UNP P03746
P	-26	HIS	-	expression tag	UNP P03746
P	-25	HIS	-	expression tag	UNP P03746
P	-24	GLY	-	expression tag	UNP P03746
P	-23	MET	-	expression tag	UNP P03746
P	-22	ALA	-	expression tag	UNP P03746
P	-21	SER	-	expression tag	UNP P03746
P	-20	MET	-	expression tag	UNP P03746
P	-19	THR	-	expression tag	UNP P03746
P	-18	GLY	-	expression tag	UNP P03746
P	-17	GLY	-	expression tag	UNP P03746
P	-16	ASN	-	expression tag	UNP P03746
P	-15	ASN	-	expression tag	UNP P03746
P	-14	MET	-	expression tag	UNP P03746
P	-13	GLY	-	expression tag	UNP P03746
P	-12	ARG	-	expression tag	UNP P03746
P	-11	ASP	-	expression tag	UNP P03746
P	-10	LEU	-	expression tag	UNP P03746
P	-9	TYR	-	expression tag	UNP P03746
P	-8	ASP	-	expression tag	UNP P03746
P	-7	ASP	-	expression tag	UNP P03746
P	-6	ASP	-	expression tag	UNP P03746
P	-5	ASP	-	expression tag	UNP P03746
P	-4	LYS	-	expression tag	UNP P03746
P	-3	ASP	-	expression tag	UNP P03746
P	-2	PRO	-	expression tag	UNP P03746
P	-1	SER	-	expression tag	UNP P03746
P	0	SER	-	expression tag	UNP P03746
Q	-34	MET	-	initiating methionine	UNP P03746
Q	-33	ARG	-	expression tag	UNP P03746
Q	-32	GLY	-	expression tag	UNP P03746
Q	-31	SER	-	expression tag	UNP P03746
Q	-30	HIS	-	expression tag	UNP P03746
Q	-29	HIS	-	expression tag	UNP P03746
Q	-28	HIS	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-27	HIS	-	expression tag	UNP P03746
Q	-26	HIS	-	expression tag	UNP P03746
Q	-25	HIS	-	expression tag	UNP P03746
Q	-24	GLY	-	expression tag	UNP P03746
Q	-23	MET	-	expression tag	UNP P03746
Q	-22	ALA	-	expression tag	UNP P03746
Q	-21	SER	-	expression tag	UNP P03746
Q	-20	MET	-	expression tag	UNP P03746
Q	-19	THR	-	expression tag	UNP P03746
Q	-18	GLY	-	expression tag	UNP P03746
Q	-17	GLY	-	expression tag	UNP P03746
Q	-16	ASN	-	expression tag	UNP P03746
Q	-15	ASN	-	expression tag	UNP P03746
Q	-14	MET	-	expression tag	UNP P03746
Q	-13	GLY	-	expression tag	UNP P03746
Q	-12	ARG	-	expression tag	UNP P03746
Q	-11	ASP	-	expression tag	UNP P03746
Q	-10	LEU	-	expression tag	UNP P03746
Q	-9	TYR	-	expression tag	UNP P03746
Q	-8	ASP	-	expression tag	UNP P03746
Q	-7	ASP	-	expression tag	UNP P03746
Q	-6	ASP	-	expression tag	UNP P03746
Q	-5	ASP	-	expression tag	UNP P03746
Q	-4	LYS	-	expression tag	UNP P03746
Q	-3	ASP	-	expression tag	UNP P03746
Q	-2	PRO	-	expression tag	UNP P03746
Q	-1	SER	-	expression tag	UNP P03746
Q	0	SER	-	expression tag	UNP P03746
R	-34	MET	-	initiating methionine	UNP P03746
R	-33	ARG	-	expression tag	UNP P03746
R	-32	GLY	-	expression tag	UNP P03746
R	-31	SER	-	expression tag	UNP P03746
R	-30	HIS	-	expression tag	UNP P03746
R	-29	HIS	-	expression tag	UNP P03746
R	-28	HIS	-	expression tag	UNP P03746
R	-27	HIS	-	expression tag	UNP P03746
R	-26	HIS	-	expression tag	UNP P03746
R	-25	HIS	-	expression tag	UNP P03746
R	-24	GLY	-	expression tag	UNP P03746
R	-23	MET	-	expression tag	UNP P03746
R	-22	ALA	-	expression tag	UNP P03746
R	-21	SER	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-20	MET	-	expression tag	UNP P03746
R	-19	THR	-	expression tag	UNP P03746
R	-18	GLY	-	expression tag	UNP P03746
R	-17	GLY	-	expression tag	UNP P03746
R	-16	ASN	-	expression tag	UNP P03746
R	-15	ASN	-	expression tag	UNP P03746
R	-14	MET	-	expression tag	UNP P03746
R	-13	GLY	-	expression tag	UNP P03746
R	-12	ARG	-	expression tag	UNP P03746
R	-11	ASP	-	expression tag	UNP P03746
R	-10	LEU	-	expression tag	UNP P03746
R	-9	TYR	-	expression tag	UNP P03746
R	-8	ASP	-	expression tag	UNP P03746
R	-7	ASP	-	expression tag	UNP P03746
R	-6	ASP	-	expression tag	UNP P03746
R	-5	ASP	-	expression tag	UNP P03746
R	-4	LYS	-	expression tag	UNP P03746
R	-3	ASP	-	expression tag	UNP P03746
R	-2	PRO	-	expression tag	UNP P03746
R	-1	SER	-	expression tag	UNP P03746
R	0	SER	-	expression tag	UNP P03746
S	-34	MET	-	initiating methionine	UNP P03746
S	-33	ARG	-	expression tag	UNP P03746
S	-32	GLY	-	expression tag	UNP P03746
S	-31	SER	-	expression tag	UNP P03746
S	-30	HIS	-	expression tag	UNP P03746
S	-29	HIS	-	expression tag	UNP P03746
S	-28	HIS	-	expression tag	UNP P03746
S	-27	HIS	-	expression tag	UNP P03746
S	-26	HIS	-	expression tag	UNP P03746
S	-25	HIS	-	expression tag	UNP P03746
S	-24	GLY	-	expression tag	UNP P03746
S	-23	MET	-	expression tag	UNP P03746
S	-22	ALA	-	expression tag	UNP P03746
S	-21	SER	-	expression tag	UNP P03746
S	-20	MET	-	expression tag	UNP P03746
S	-19	THR	-	expression tag	UNP P03746
S	-18	GLY	-	expression tag	UNP P03746
S	-17	GLY	-	expression tag	UNP P03746
S	-16	ASN	-	expression tag	UNP P03746
S	-15	ASN	-	expression tag	UNP P03746
S	-14	MET	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-13	GLY	-	expression tag	UNP P03746
S	-12	ARG	-	expression tag	UNP P03746
S	-11	ASP	-	expression tag	UNP P03746
S	-10	LEU	-	expression tag	UNP P03746
S	-9	TYR	-	expression tag	UNP P03746
S	-8	ASP	-	expression tag	UNP P03746
S	-7	ASP	-	expression tag	UNP P03746
S	-6	ASP	-	expression tag	UNP P03746
S	-5	ASP	-	expression tag	UNP P03746
S	-4	LYS	-	expression tag	UNP P03746
S	-3	ASP	-	expression tag	UNP P03746
S	-2	PRO	-	expression tag	UNP P03746
S	-1	SER	-	expression tag	UNP P03746
S	0	SER	-	expression tag	UNP P03746
T	-34	MET	-	initiating methionine	UNP P03746
T	-33	ARG	-	expression tag	UNP P03746
T	-32	GLY	-	expression tag	UNP P03746
T	-31	SER	-	expression tag	UNP P03746
T	-30	HIS	-	expression tag	UNP P03746
T	-29	HIS	-	expression tag	UNP P03746
T	-28	HIS	-	expression tag	UNP P03746
T	-27	HIS	-	expression tag	UNP P03746
T	-26	HIS	-	expression tag	UNP P03746
T	-25	HIS	-	expression tag	UNP P03746
T	-24	GLY	-	expression tag	UNP P03746
T	-23	MET	-	expression tag	UNP P03746
T	-22	ALA	-	expression tag	UNP P03746
T	-21	SER	-	expression tag	UNP P03746
T	-20	MET	-	expression tag	UNP P03746
T	-19	THR	-	expression tag	UNP P03746
T	-18	GLY	-	expression tag	UNP P03746
T	-17	GLY	-	expression tag	UNP P03746
T	-16	ASN	-	expression tag	UNP P03746
T	-15	ASN	-	expression tag	UNP P03746
T	-14	MET	-	expression tag	UNP P03746
T	-13	GLY	-	expression tag	UNP P03746
T	-12	ARG	-	expression tag	UNP P03746
T	-11	ASP	-	expression tag	UNP P03746
T	-10	LEU	-	expression tag	UNP P03746
T	-9	TYR	-	expression tag	UNP P03746
T	-8	ASP	-	expression tag	UNP P03746
T	-7	ASP	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-6	ASP	-	expression tag	UNP P03746
T	-5	ASP	-	expression tag	UNP P03746
T	-4	LYS	-	expression tag	UNP P03746
T	-3	ASP	-	expression tag	UNP P03746
T	-2	PRO	-	expression tag	UNP P03746
T	-1	SER	-	expression tag	UNP P03746
T	0	SER	-	expression tag	UNP P03746
U	-34	MET	-	initiating methionine	UNP P03746
U	-33	ARG	-	expression tag	UNP P03746
U	-32	GLY	-	expression tag	UNP P03746
U	-31	SER	-	expression tag	UNP P03746
U	-30	HIS	-	expression tag	UNP P03746
U	-29	HIS	-	expression tag	UNP P03746
U	-28	HIS	-	expression tag	UNP P03746
U	-27	HIS	-	expression tag	UNP P03746
U	-26	HIS	-	expression tag	UNP P03746
U	-25	HIS	-	expression tag	UNP P03746
U	-24	GLY	-	expression tag	UNP P03746
U	-23	MET	-	expression tag	UNP P03746
U	-22	ALA	-	expression tag	UNP P03746
U	-21	SER	-	expression tag	UNP P03746
U	-20	MET	-	expression tag	UNP P03746
U	-19	THR	-	expression tag	UNP P03746
U	-18	GLY	-	expression tag	UNP P03746
U	-17	GLY	-	expression tag	UNP P03746
U	-16	ASN	-	expression tag	UNP P03746
U	-15	ASN	-	expression tag	UNP P03746
U	-14	MET	-	expression tag	UNP P03746
U	-13	GLY	-	expression tag	UNP P03746
U	-12	ARG	-	expression tag	UNP P03746
U	-11	ASP	-	expression tag	UNP P03746
U	-10	LEU	-	expression tag	UNP P03746
U	-9	TYR	-	expression tag	UNP P03746
U	-8	ASP	-	expression tag	UNP P03746
U	-7	ASP	-	expression tag	UNP P03746
U	-6	ASP	-	expression tag	UNP P03746
U	-5	ASP	-	expression tag	UNP P03746
U	-4	LYS	-	expression tag	UNP P03746
U	-3	ASP	-	expression tag	UNP P03746
U	-2	PRO	-	expression tag	UNP P03746
U	-1	SER	-	expression tag	UNP P03746
U	0	SER	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-34	MET	-	initiating methionine	UNP P03746
V	-33	ARG	-	expression tag	UNP P03746
V	-32	GLY	-	expression tag	UNP P03746
V	-31	SER	-	expression tag	UNP P03746
V	-30	HIS	-	expression tag	UNP P03746
V	-29	HIS	-	expression tag	UNP P03746
V	-28	HIS	-	expression tag	UNP P03746
V	-27	HIS	-	expression tag	UNP P03746
V	-26	HIS	-	expression tag	UNP P03746
V	-25	HIS	-	expression tag	UNP P03746
V	-24	GLY	-	expression tag	UNP P03746
V	-23	MET	-	expression tag	UNP P03746
V	-22	ALA	-	expression tag	UNP P03746
V	-21	SER	-	expression tag	UNP P03746
V	-20	MET	-	expression tag	UNP P03746
V	-19	THR	-	expression tag	UNP P03746
V	-18	GLY	-	expression tag	UNP P03746
V	-17	GLY	-	expression tag	UNP P03746
V	-16	ASN	-	expression tag	UNP P03746
V	-15	ASN	-	expression tag	UNP P03746
V	-14	MET	-	expression tag	UNP P03746
V	-13	GLY	-	expression tag	UNP P03746
V	-12	ARG	-	expression tag	UNP P03746
V	-11	ASP	-	expression tag	UNP P03746
V	-10	LEU	-	expression tag	UNP P03746
V	-9	TYR	-	expression tag	UNP P03746
V	-8	ASP	-	expression tag	UNP P03746
V	-7	ASP	-	expression tag	UNP P03746
V	-6	ASP	-	expression tag	UNP P03746
V	-5	ASP	-	expression tag	UNP P03746
V	-4	LYS	-	expression tag	UNP P03746
V	-3	ASP	-	expression tag	UNP P03746
V	-2	PRO	-	expression tag	UNP P03746
V	-1	SER	-	expression tag	UNP P03746
V	0	SER	-	expression tag	UNP P03746
W	-34	MET	-	initiating methionine	UNP P03746
W	-33	ARG	-	expression tag	UNP P03746
W	-32	GLY	-	expression tag	UNP P03746
W	-31	SER	-	expression tag	UNP P03746
W	-30	HIS	-	expression tag	UNP P03746
W	-29	HIS	-	expression tag	UNP P03746
W	-28	HIS	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-27	HIS	-	expression tag	UNP P03746
W	-26	HIS	-	expression tag	UNP P03746
W	-25	HIS	-	expression tag	UNP P03746
W	-24	GLY	-	expression tag	UNP P03746
W	-23	MET	-	expression tag	UNP P03746
W	-22	ALA	-	expression tag	UNP P03746
W	-21	SER	-	expression tag	UNP P03746
W	-20	MET	-	expression tag	UNP P03746
W	-19	THR	-	expression tag	UNP P03746
W	-18	GLY	-	expression tag	UNP P03746
W	-17	GLY	-	expression tag	UNP P03746
W	-16	ASN	-	expression tag	UNP P03746
W	-15	ASN	-	expression tag	UNP P03746
W	-14	MET	-	expression tag	UNP P03746
W	-13	GLY	-	expression tag	UNP P03746
W	-12	ARG	-	expression tag	UNP P03746
W	-11	ASP	-	expression tag	UNP P03746
W	-10	LEU	-	expression tag	UNP P03746
W	-9	TYR	-	expression tag	UNP P03746
W	-8	ASP	-	expression tag	UNP P03746
W	-7	ASP	-	expression tag	UNP P03746
W	-6	ASP	-	expression tag	UNP P03746
W	-5	ASP	-	expression tag	UNP P03746
W	-4	LYS	-	expression tag	UNP P03746
W	-3	ASP	-	expression tag	UNP P03746
W	-2	PRO	-	expression tag	UNP P03746
W	-1	SER	-	expression tag	UNP P03746
W	0	SER	-	expression tag	UNP P03746
X	-34	MET	-	initiating methionine	UNP P03746
X	-33	ARG	-	expression tag	UNP P03746
X	-32	GLY	-	expression tag	UNP P03746
X	-31	SER	-	expression tag	UNP P03746
X	-30	HIS	-	expression tag	UNP P03746
X	-29	HIS	-	expression tag	UNP P03746
X	-28	HIS	-	expression tag	UNP P03746
X	-27	HIS	-	expression tag	UNP P03746
X	-26	HIS	-	expression tag	UNP P03746
X	-25	HIS	-	expression tag	UNP P03746
X	-24	GLY	-	expression tag	UNP P03746
X	-23	MET	-	expression tag	UNP P03746
X	-22	ALA	-	expression tag	UNP P03746
X	-21	SER	-	expression tag	UNP P03746

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-20	MET	-	expression tag	UNP P03746
X	-19	THR	-	expression tag	UNP P03746
X	-18	GLY	-	expression tag	UNP P03746
X	-17	GLY	-	expression tag	UNP P03746
X	-16	ASN	-	expression tag	UNP P03746
X	-15	ASN	-	expression tag	UNP P03746
X	-14	MET	-	expression tag	UNP P03746
X	-13	GLY	-	expression tag	UNP P03746
X	-12	ARG	-	expression tag	UNP P03746
X	-11	ASP	-	expression tag	UNP P03746
X	-10	LEU	-	expression tag	UNP P03746
X	-9	TYR	-	expression tag	UNP P03746
X	-8	ASP	-	expression tag	UNP P03746
X	-7	ASP	-	expression tag	UNP P03746
X	-6	ASP	-	expression tag	UNP P03746
X	-5	ASP	-	expression tag	UNP P03746
X	-4	LYS	-	expression tag	UNP P03746
X	-3	ASP	-	expression tag	UNP P03746
X	-2	PRO	-	expression tag	UNP P03746
X	-1	SER	-	expression tag	UNP P03746
X	0	SER	-	expression tag	UNP P03746

- Molecule 3 is a protein called Tail tubular protein gp12.

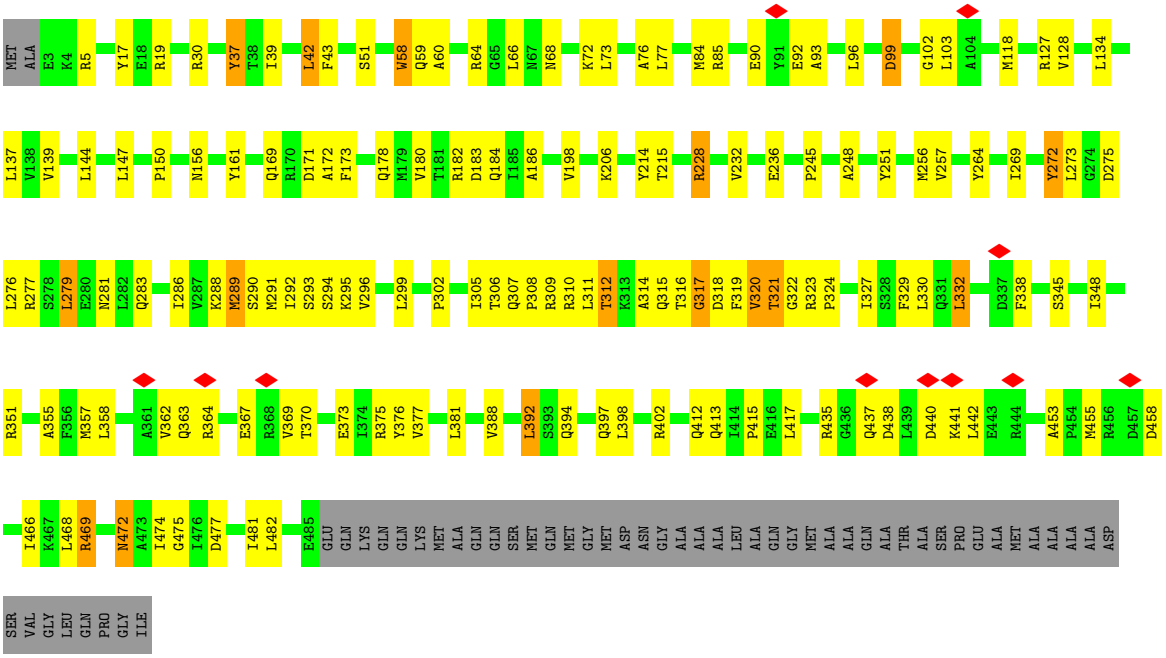
Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		
3	b	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		
3	c	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		
3	d	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		
3	e	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		
3	f	784	Total	C	N	O	S	0	0
			6252	3967	1074	1196	15		

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.

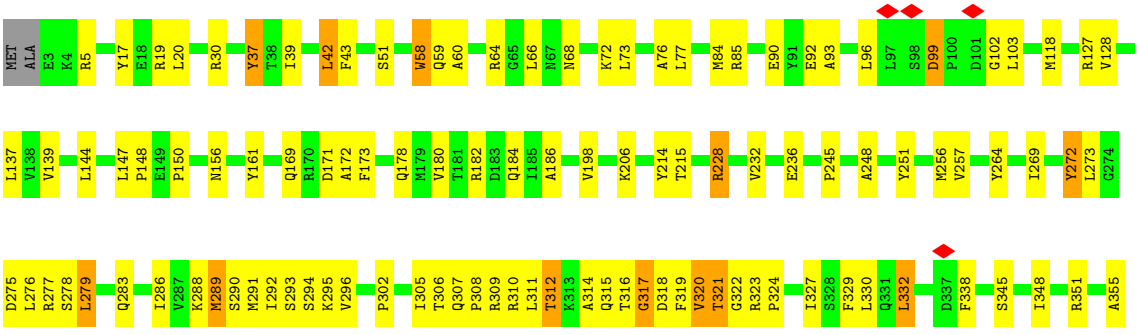
• Molecule 1: Portal protein

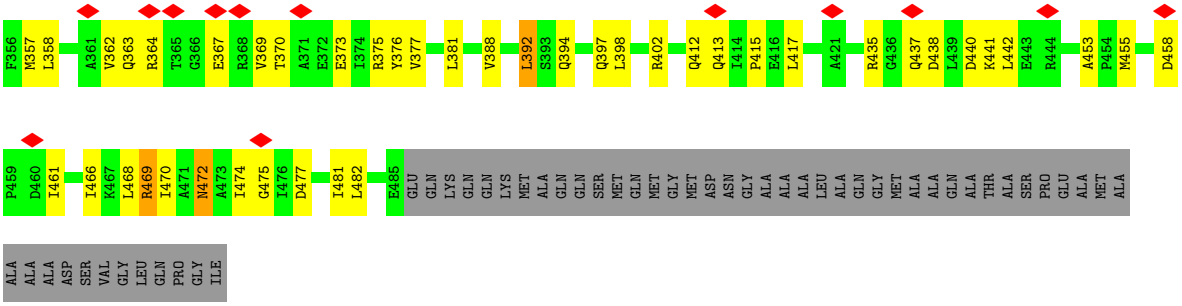
Chain A:



• Molecule 1: Portal protein

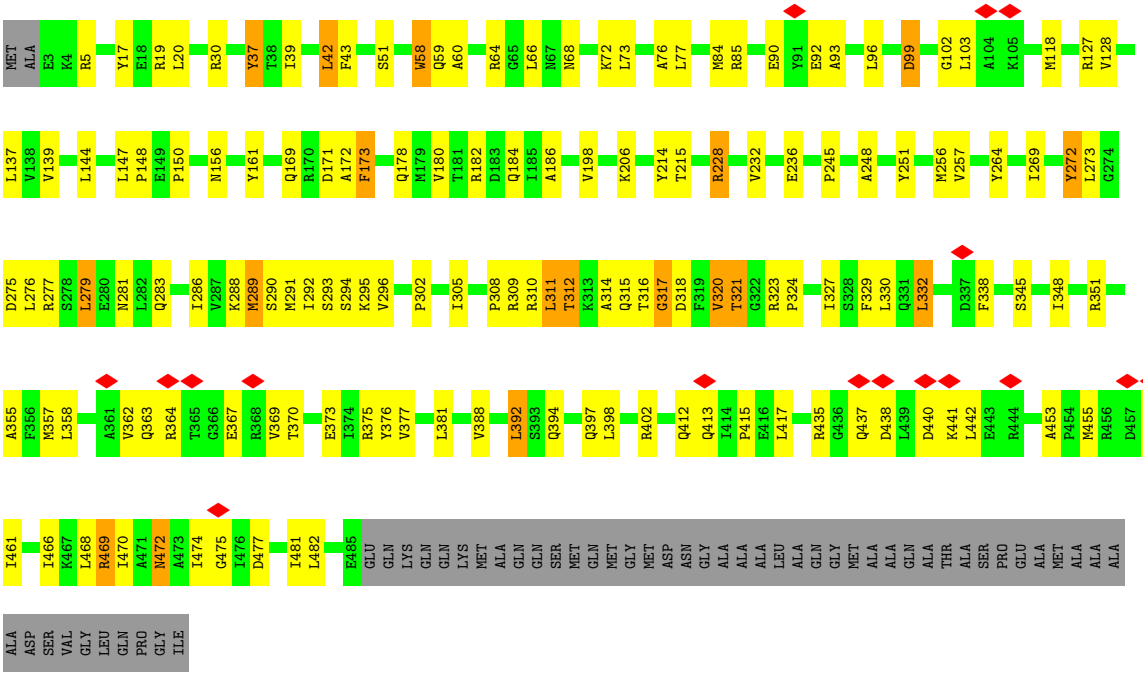
Chain B:





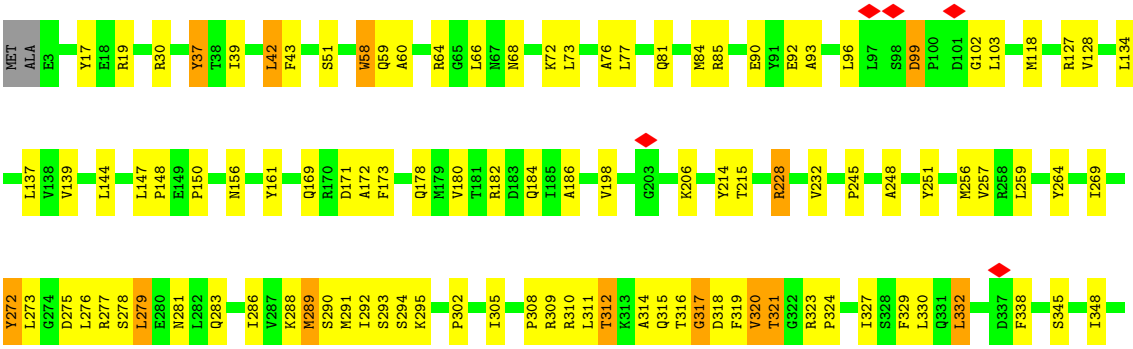
• Molecule 1: Portal protein

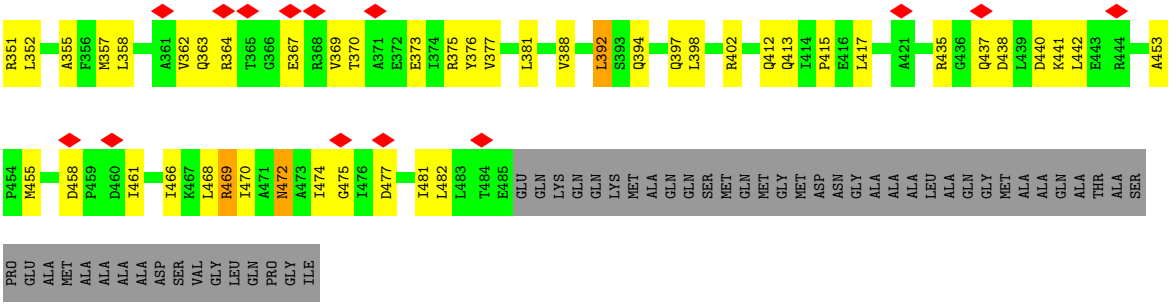
Chain C:



• Molecule 1: Portal protein

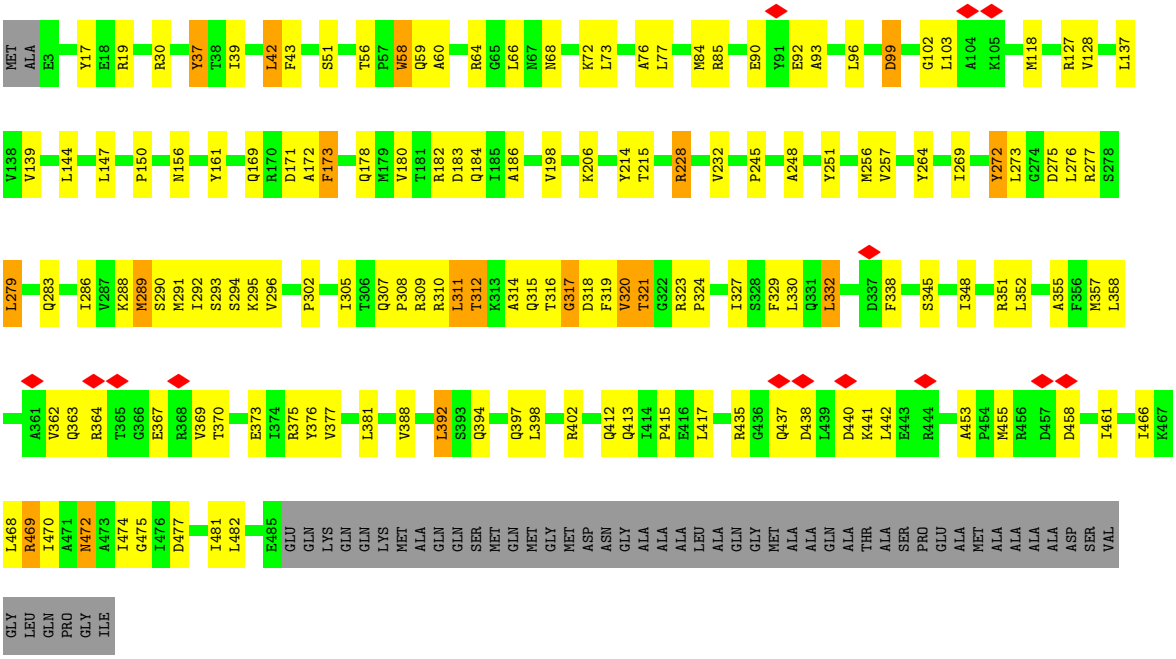
Chain D:





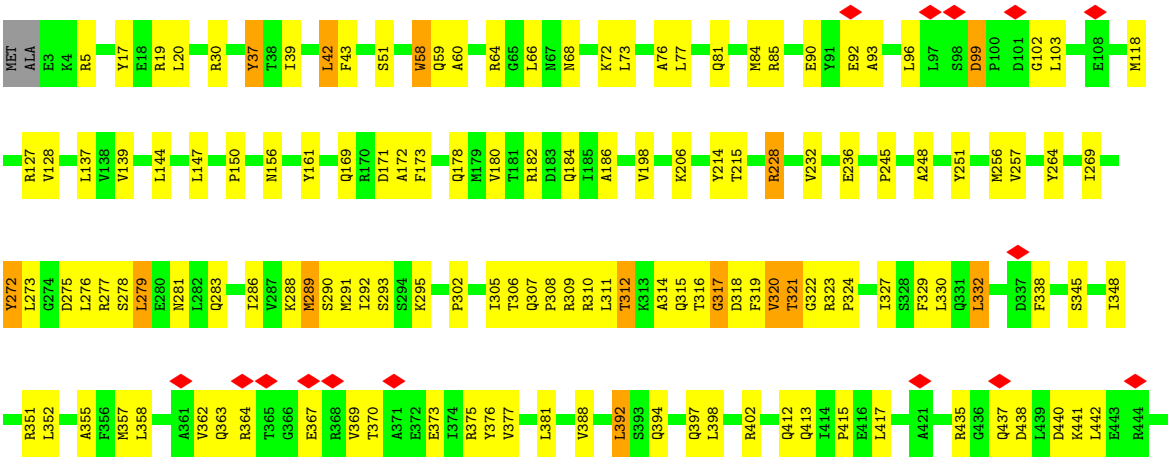
• Molecule 1: Portal protein

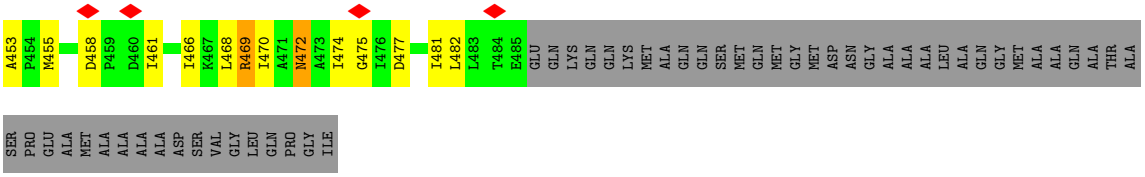
Chain E:



• Molecule 1: Portal protein

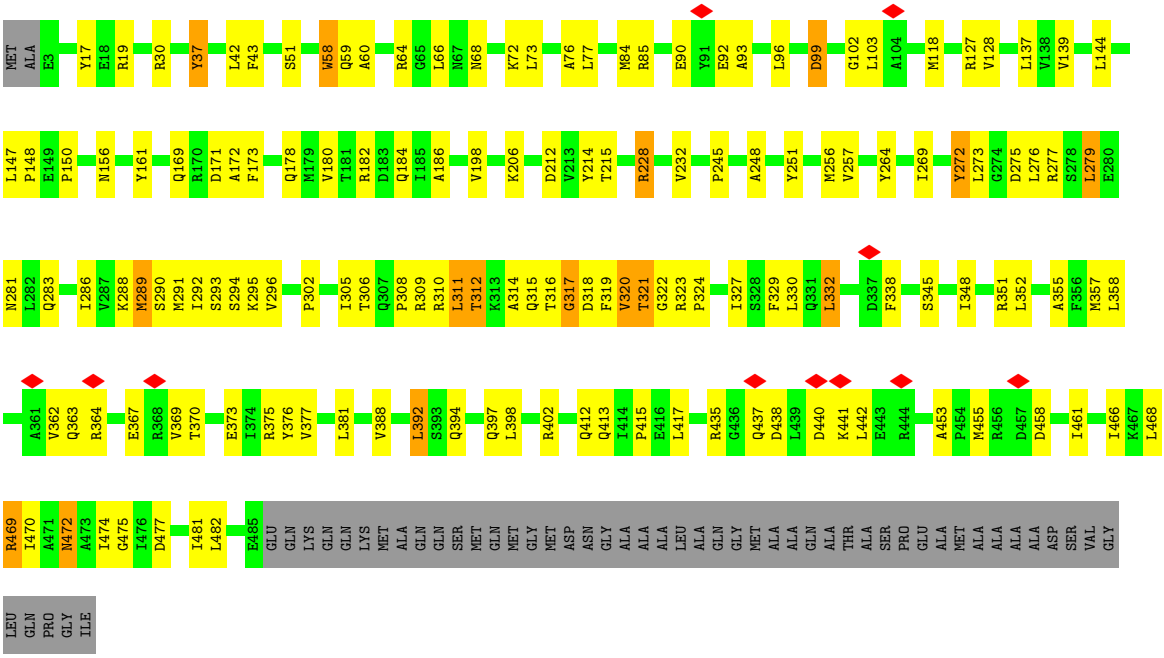
Chain F:





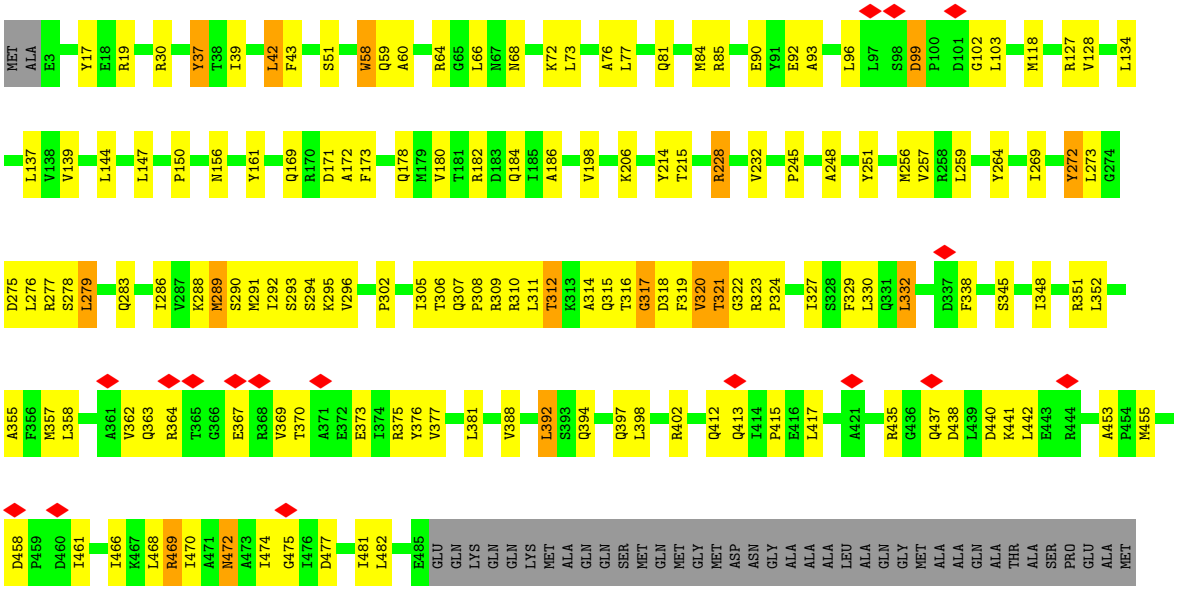
• Molecule 1: Portal protein

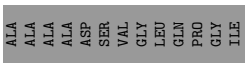
Chain G:



• Molecule 1: Portal protein

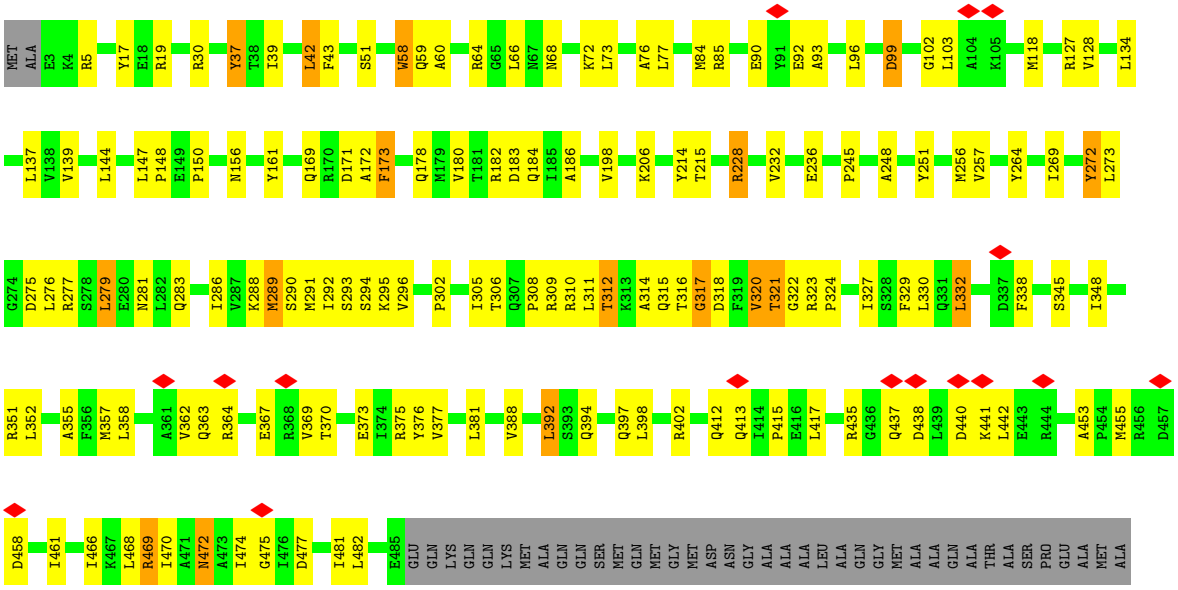
Chain H:

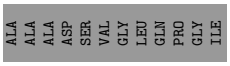




• Molecule 1: Portal protein

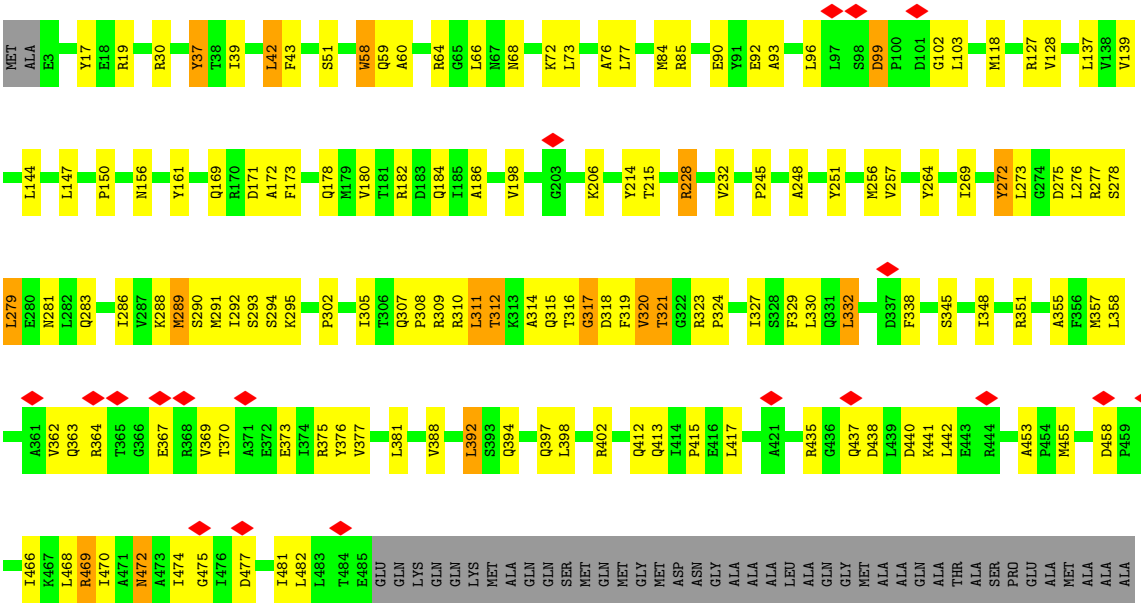
Chain I:





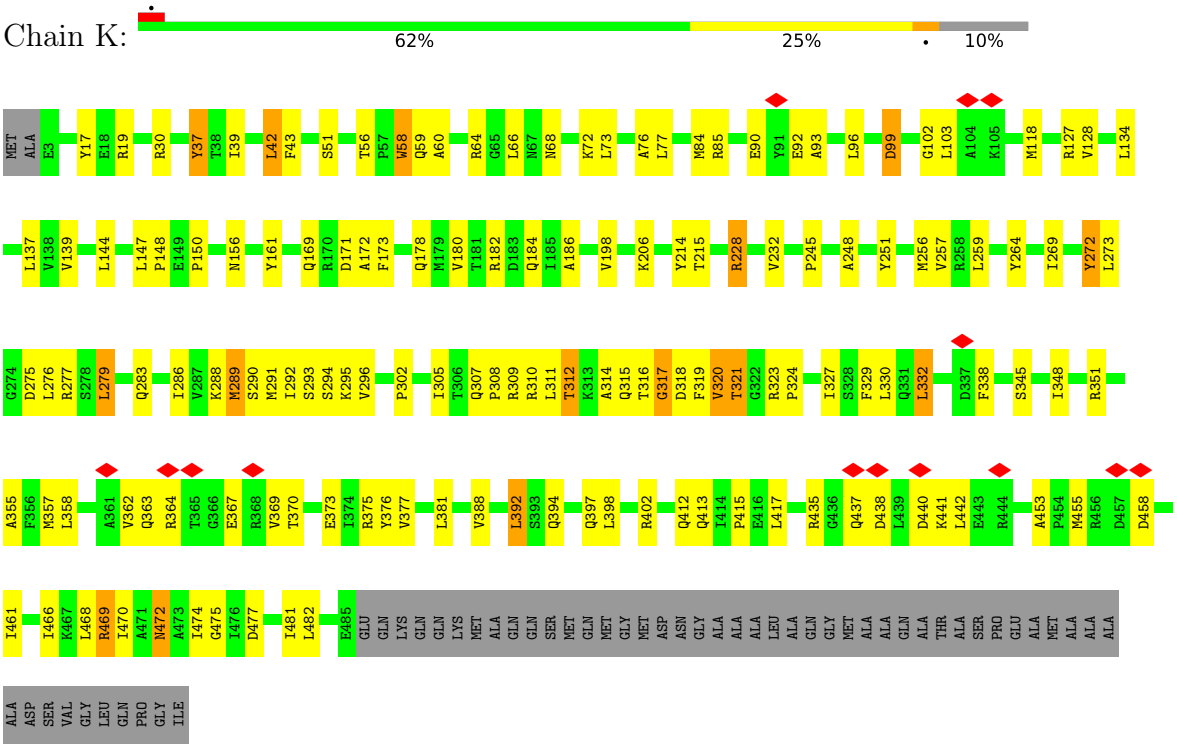
• Molecule 1: Portal protein

Chain J:



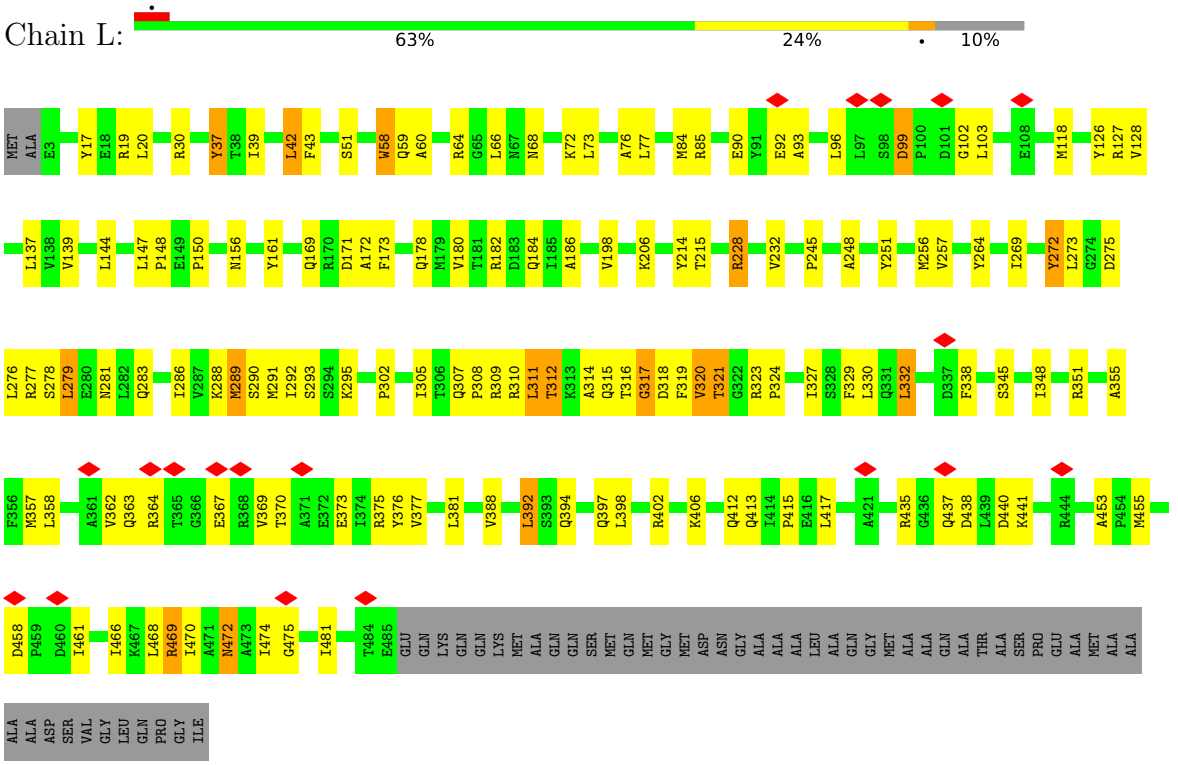
• Molecule 1: Portal protein

Chain K:



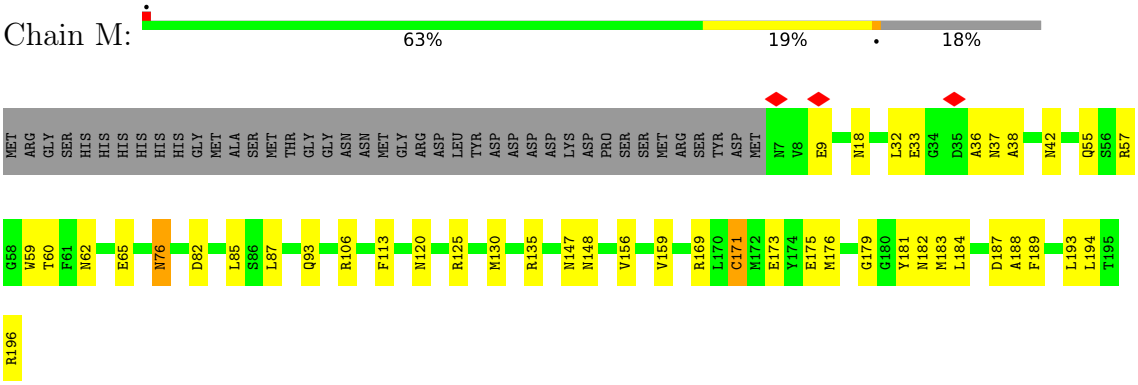
• Molecule 1: Portal protein

Chain L:



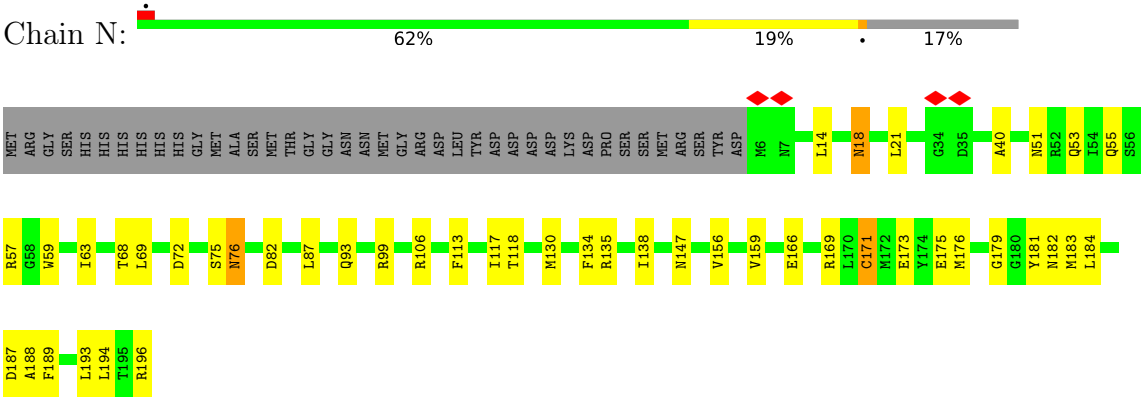
• Molecule 2: Tail tubular protein gp11

Chain M:



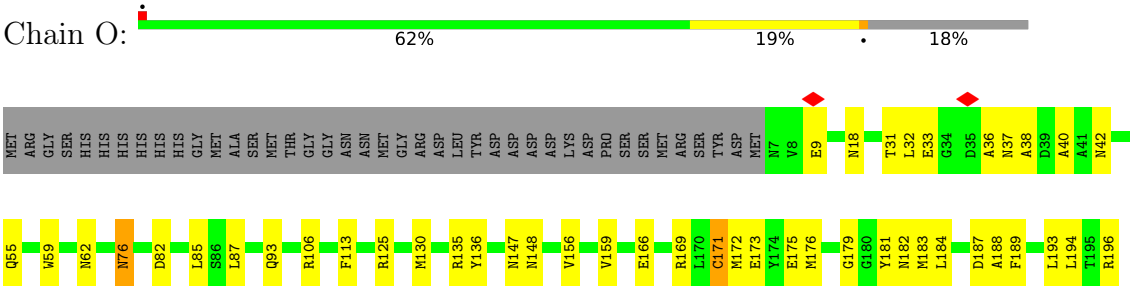
• Molecule 2: Tail tubular protein gp11

Chain N:



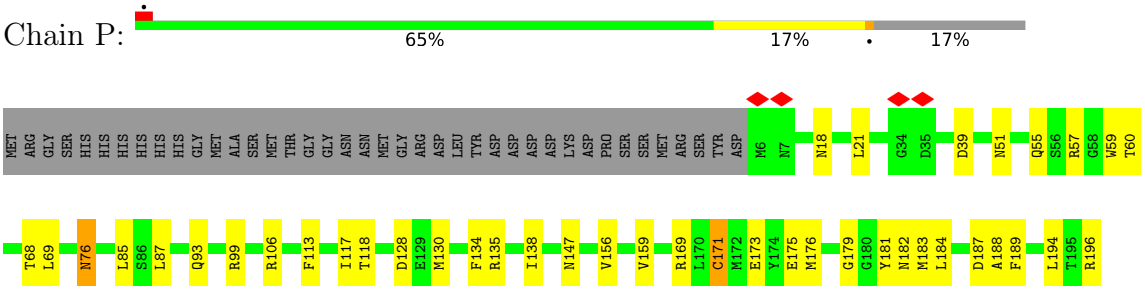
• Molecule 2: Tail tubular protein gp11

Chain O:



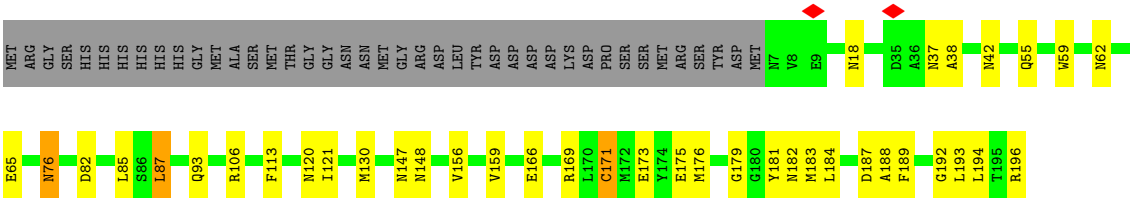
• Molecule 2: Tail tubular protein gp11

Chain P:

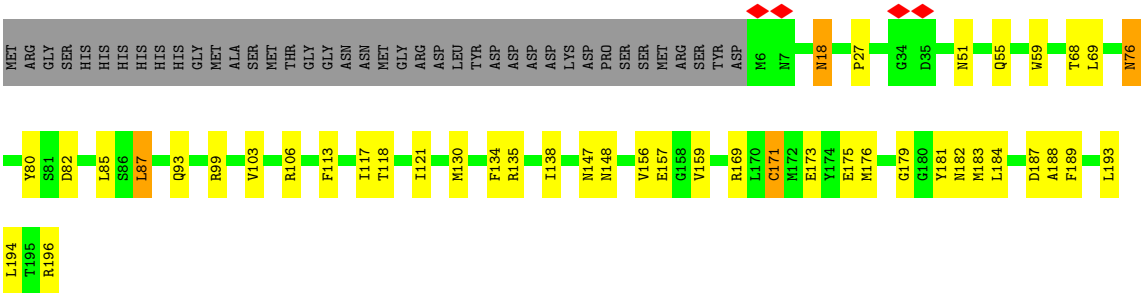


• Molecule 2: Tail tubular protein gp11

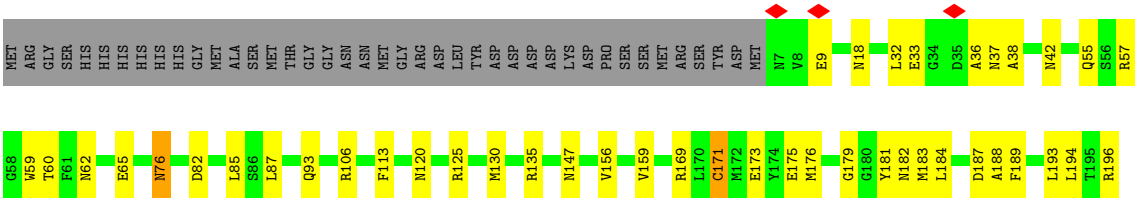
Chain Q:



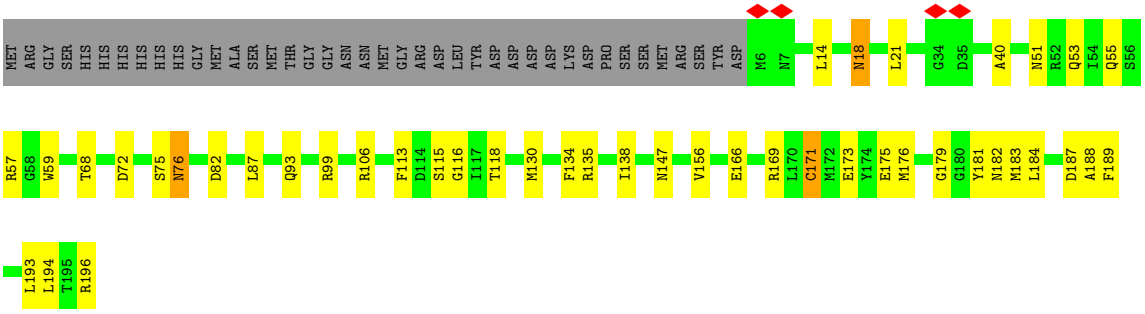
• Molecule 2: Tail tubular protein gp11



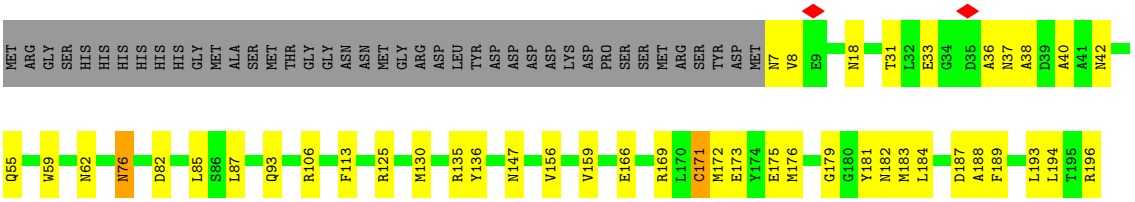
• Molecule 2: Tail tubular protein gp11



• Molecule 2: Tail tubular protein gp11

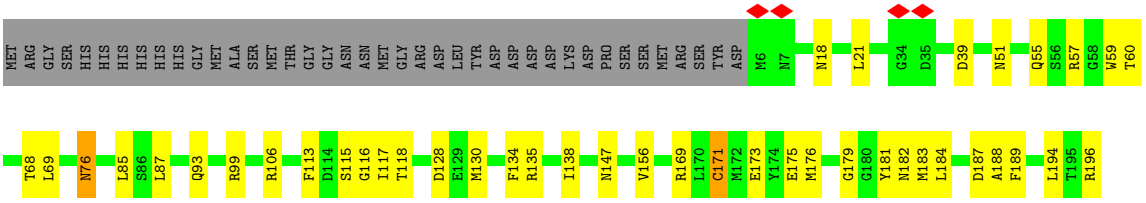


• Molecule 2: Tail tubular protein gp11



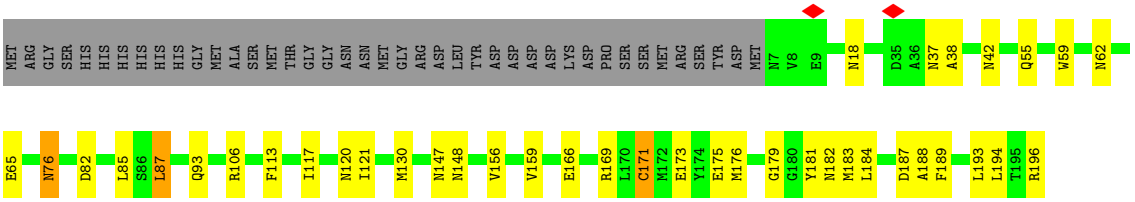
• Molecule 2: Tail tubular protein gp11

Chain V:



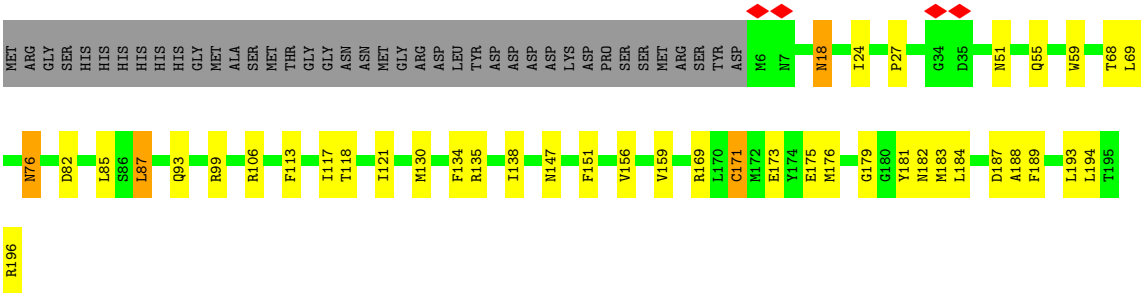
• Molecule 2: Tail tubular protein gp11

Chain W:



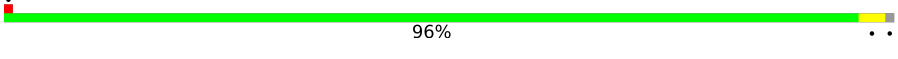
• Molecule 2: Tail tubular protein gp11

Chain X:



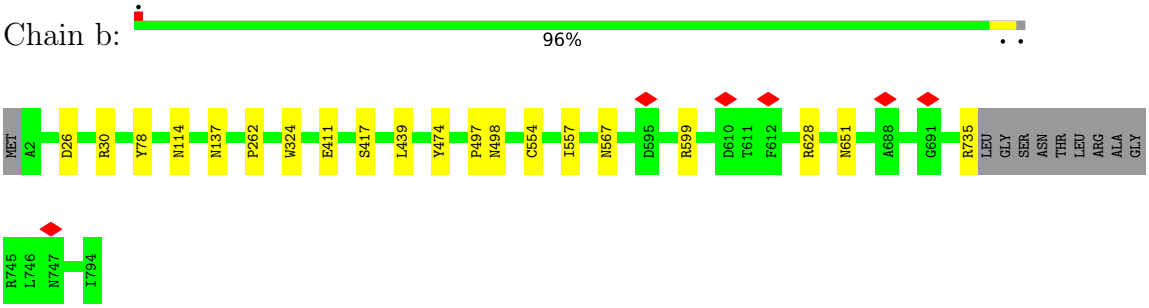
• Molecule 3: Tail tubular protein gp12

Chain a:



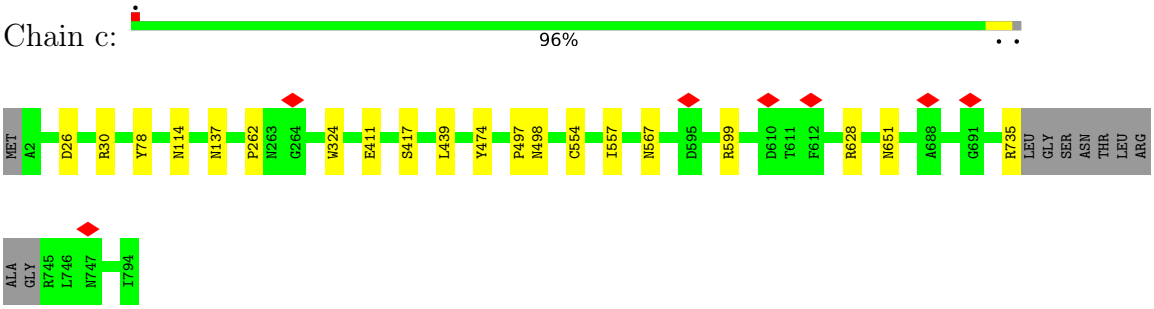
• Molecule 3: Tail tubular protein gp12

Chain b:



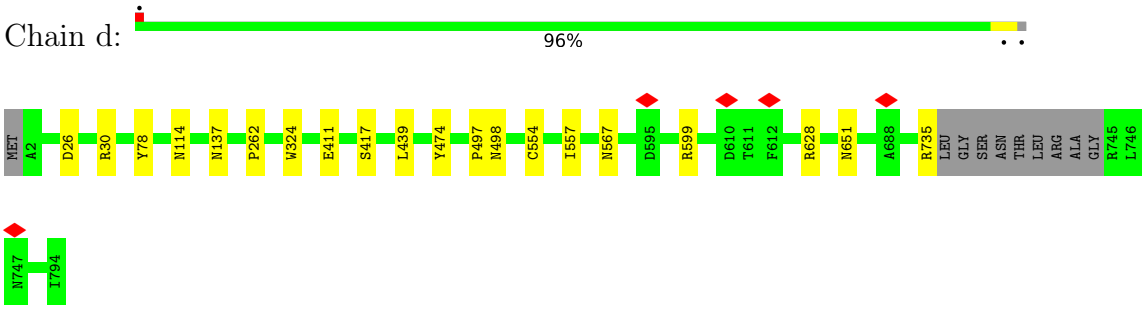
• Molecule 3: Tail tubular protein gp12

Chain c:



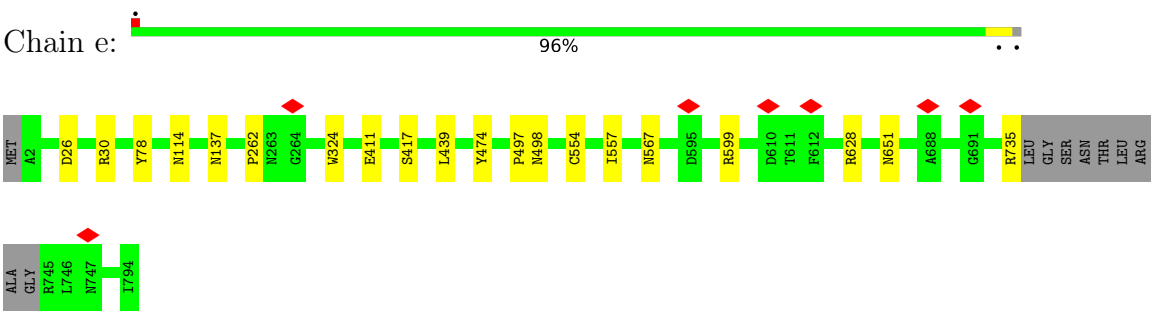
• Molecule 3: Tail tubular protein gp12

Chain d:



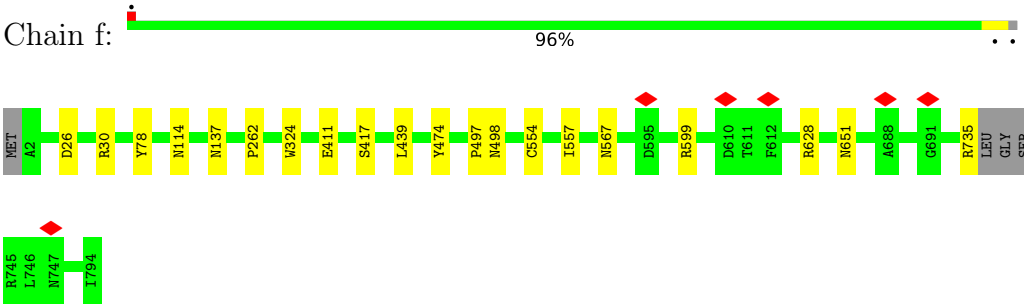
• Molecule 3: Tail tubular protein gp12

Chain e:



• Molecule 3: Tail tubular protein gp12

Chain f:


96%
MET
A2
D26
R30
Y78
N114
N137
P262
W324
E411
S417
L439
Y474
P497
N498
C554
I557
N567
D595
R599
D610
T611
F612
R628
N651
A688
G691
R735
LEU
GLY
SER
ASN
THR
LEU
ARG
ALA
GLY
R745
L746
N747
I794

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	92382	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 ($e^-/Å^2$)	0.84	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0113	Depositor
Map size (Å)	366.8, 366.8, 366.8	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	B	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	C	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	D	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	E	1.08	12/3840 (0.3%)	0.98	12/5201 (0.2%)
1	F	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	G	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	H	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	I	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	J	1.08	11/3840 (0.3%)	0.98	12/5201 (0.2%)
1	K	1.08	12/3840 (0.3%)	0.98	12/5201 (0.2%)
1	L	1.08	12/3840 (0.3%)	0.98	12/5201 (0.2%)
2	M	0.44	0/1538	0.64	2/2082 (0.1%)
2	N	0.42	0/1546	0.63	2/2092 (0.1%)
2	O	0.43	0/1538	0.63	2/2082 (0.1%)
2	P	0.44	0/1546	0.63	2/2092 (0.1%)
2	Q	0.45	1/1538 (0.1%)	0.63	2/2082 (0.1%)
2	R	0.41	0/1546	0.62	2/2092 (0.1%)
2	S	0.44	0/1538	0.64	2/2082 (0.1%)
2	T	0.42	0/1546	0.63	2/2092 (0.1%)
2	U	0.43	0/1538	0.63	2/2082 (0.1%)
2	V	0.44	0/1546	0.63	2/2092 (0.1%)
2	W	0.45	0/1538	0.63	2/2082 (0.1%)
2	X	0.42	0/1546	0.62	2/2092 (0.1%)
3	a	0.53	0/6411	0.66	2/8719 (0.0%)
3	b	0.53	0/6411	0.66	2/8719 (0.0%)
3	c	0.53	0/6411	0.66	2/8719 (0.0%)
3	d	0.53	0/6411	0.66	2/8719 (0.0%)
3	e	0.53	0/6411	0.66	2/8719 (0.0%)
3	f	0.53	0/6411	0.66	2/8719 (0.0%)
All	All	0.81	136/103050 (0.1%)	0.82	180/139770 (0.1%)

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	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
3	a	0	5
3	b	0	5
3	c	0	5
3	d	0	5
3	e	0	5
3	f	0	5
All	All	0	42

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	TYR	CG-CD1	-8.30	1.28	1.39
1	K	37	TYR	CG-CD1	-8.30	1.28	1.39
1	J	37	TYR	CG-CD1	-8.28	1.28	1.39
1	F	272	TYR	CG-CD1	-8.27	1.28	1.39
1	F	37	TYR	CG-CD1	-8.24	1.28	1.39

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	d	26	ASP	CB-CG-OD1	9.27	126.64	118.30
3	c	26	ASP	CB-CG-OD1	9.26	126.63	118.30
1	H	127	ARG	NE-CZ-NH1	9.24	124.92	120.30
3	b	26	ASP	CB-CG-OD1	9.23	126.61	118.30
1	B	127	ARG	NE-CZ-NH1	9.23	124.91	120.30

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	ALA	Peptide
1	B	453	ALA	Peptide
1	C	453	ALA	Peptide
1	D	453	ALA	Peptide
1	E	453	ALA	Peptide

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	3780	0	3781	229	0
1	B	3780	0	3782	227	0
1	C	3780	0	3781	242	0
1	D	3780	0	3782	228	0
1	E	3780	0	3781	238	0
1	F	3780	0	3782	237	0
1	G	3780	0	3781	226	0
1	H	3780	0	3782	226	0
1	I	3780	0	3781	236	0
1	J	3780	0	3782	223	0
1	K	3780	0	3781	230	0
1	L	3780	0	3782	232	0
2	M	1512	0	1431	90	0
2	N	1520	0	1438	96	0
2	O	1512	0	1431	96	0
2	P	1520	0	1438	93	0
2	Q	1512	0	1431	87	0
2	R	1520	0	1438	98	0
2	S	1512	0	1431	92	0
2	T	1520	0	1438	93	0
2	U	1512	0	1431	95	0
2	V	1520	0	1438	94	0
2	W	1512	0	1431	86	0
2	X	1520	0	1438	94	0
3	a	6252	0	6008	0	0
3	b	6252	0	6008	0	0
3	c	6252	0	6008	0	0
3	d	6252	0	6008	0	0
3	e	6252	0	6008	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	6252	0	6008	0	0
All	All	101064	0	98640	2554	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 16.

The worst 5 of 2554 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:D:370:THR:HG21	1:E:441:LYS:CG	1.28	1.64
1:E:370:THR:HG21	1:F:441:LYS:CG	1.26	1.64
1:F:370:THR:HG21	1:G:441:LYS:CG	1.27	1.64
1:H:370:THR:HG21	1:I:441:LYS:CG	1.26	1.63
1:B:370:THR:HG21	1:C:441:LYS:CG	1.26	1.61

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	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	B	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	C	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	D	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	E	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	F	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	G	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	H	481/536 (90%)	443 (92%)	38 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	J	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	K	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
1	L	481/536 (90%)	443 (92%)	38 (8%)	0	100	100
2	M	188/231 (81%)	169 (90%)	19 (10%)	0	100	100
2	N	189/231 (82%)	172 (91%)	17 (9%)	0	100	100
2	O	188/231 (81%)	168 (89%)	20 (11%)	0	100	100
2	P	189/231 (82%)	172 (91%)	17 (9%)	0	100	100
2	Q	188/231 (81%)	168 (89%)	20 (11%)	0	100	100
2	R	189/231 (82%)	170 (90%)	19 (10%)	0	100	100
2	S	188/231 (81%)	170 (90%)	18 (10%)	0	100	100
2	T	189/231 (82%)	172 (91%)	17 (9%)	0	100	100
2	U	188/231 (81%)	169 (90%)	19 (10%)	0	100	100
2	V	189/231 (82%)	170 (90%)	19 (10%)	0	100	100
2	W	188/231 (81%)	167 (89%)	21 (11%)	0	100	100
2	X	189/231 (82%)	170 (90%)	19 (10%)	0	100	100
3	a	780/794 (98%)	640 (82%)	139 (18%)	1 (0%)	51	82
3	b	780/794 (98%)	639 (82%)	140 (18%)	1 (0%)	51	82
3	c	780/794 (98%)	640 (82%)	139 (18%)	1 (0%)	51	82
3	d	780/794 (98%)	640 (82%)	139 (18%)	1 (0%)	51	82
3	e	780/794 (98%)	639 (82%)	140 (18%)	1 (0%)	51	82
3	f	780/794 (98%)	640 (82%)	139 (18%)	1 (0%)	51	82
All	All	12714/13968 (91%)	11191 (88%)	1517 (12%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	a	497	PRO
3	b	497	PRO
3	c	497	PRO
3	d	497	PRO
3	e	497	PRO

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	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	B	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	C	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	D	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	E	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	F	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	G	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	H	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	I	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	J	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	K	409/442 (92%)	399 (98%)	10 (2%)	49 75
1	L	409/442 (92%)	399 (98%)	10 (2%)	49 75
2	M	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	N	164/198 (83%)	160 (98%)	4 (2%)	49 75
2	O	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	P	164/198 (83%)	159 (97%)	5 (3%)	41 70
2	Q	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	R	164/198 (83%)	159 (97%)	5 (3%)	41 70
2	S	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	T	164/198 (83%)	160 (98%)	4 (2%)	49 75
2	U	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	V	164/198 (83%)	159 (97%)	5 (3%)	41 70
2	W	163/198 (82%)	156 (96%)	7 (4%)	29 62
2	X	164/198 (83%)	159 (97%)	5 (3%)	41 70
3	a	681/688 (99%)	669 (98%)	12 (2%)	59 79
3	b	681/688 (99%)	669 (98%)	12 (2%)	59 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	c	681/688 (99%)	669 (98%)	12 (2%)	59 79
3	d	681/688 (99%)	669 (98%)	12 (2%)	59 79
3	e	681/688 (99%)	669 (98%)	12 (2%)	59 79
3	f	681/688 (99%)	669 (98%)	12 (2%)	59 79
All	All	10956/11808 (93%)	10694 (98%)	262 (2%)	51 75

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	498	ASN
3	e	30	ARG
3	f	651	ASN
1	J	364	ARG
1	J	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 242 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	109	GLN
3	e	617	HIS
2	U	120	ASN
3	e	567	ASN
3	f	617	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 Map visualisation

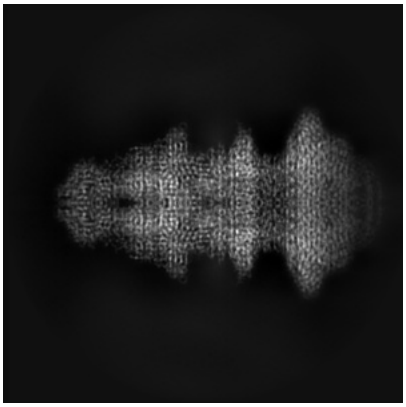
This section contains visualisations of the EMDB entry EMD-4706. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

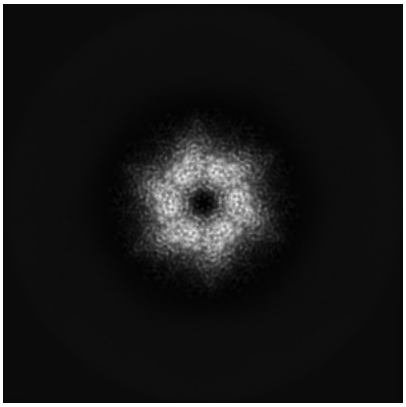
6.1 Orthogonal projections

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: 175

Y Index: 175

Z Index: 175

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: 189

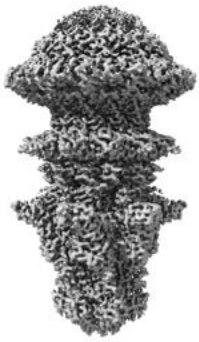
Y Index: 199

Z Index: 204

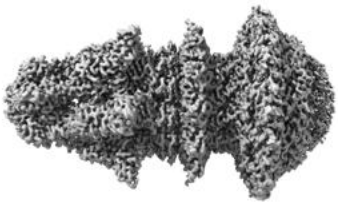
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

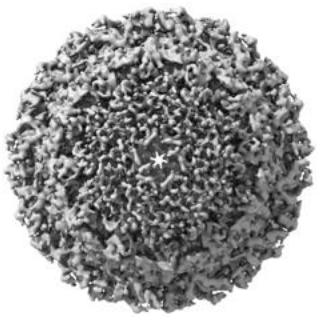
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0113. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

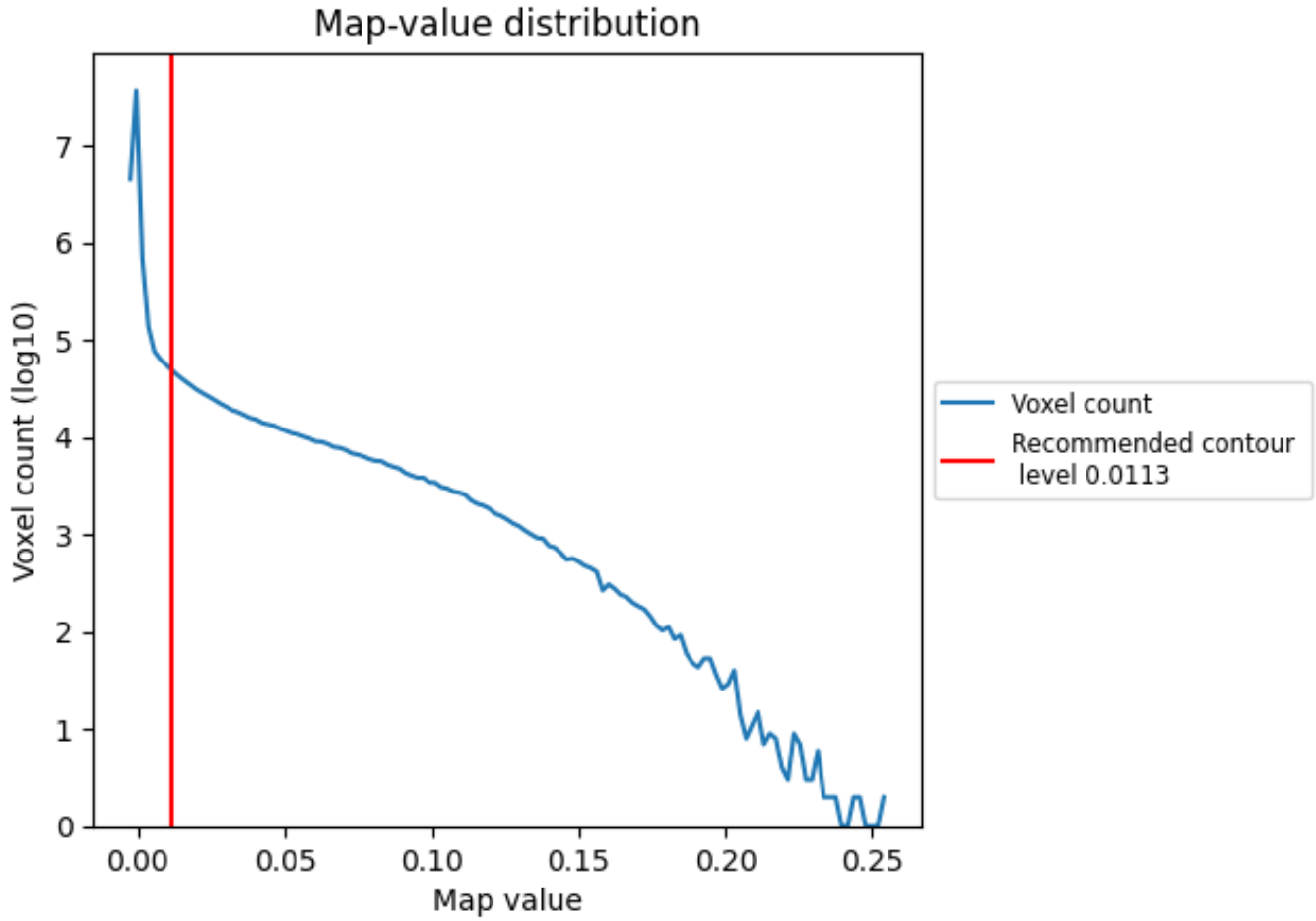
6.5 Mask visualisation (i)

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

7 Map analysis

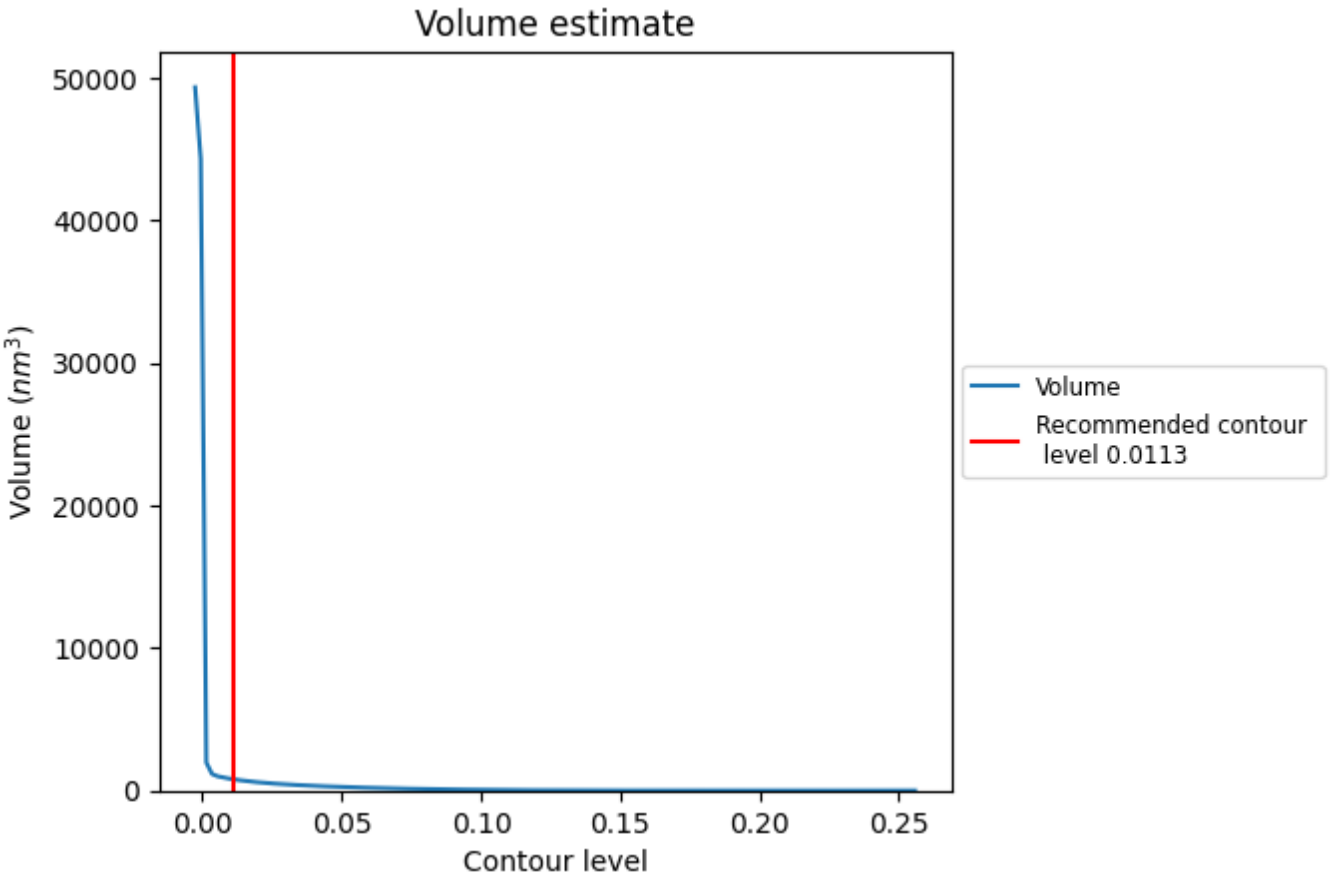
This section contains the results of statistical analysis of the map.

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.

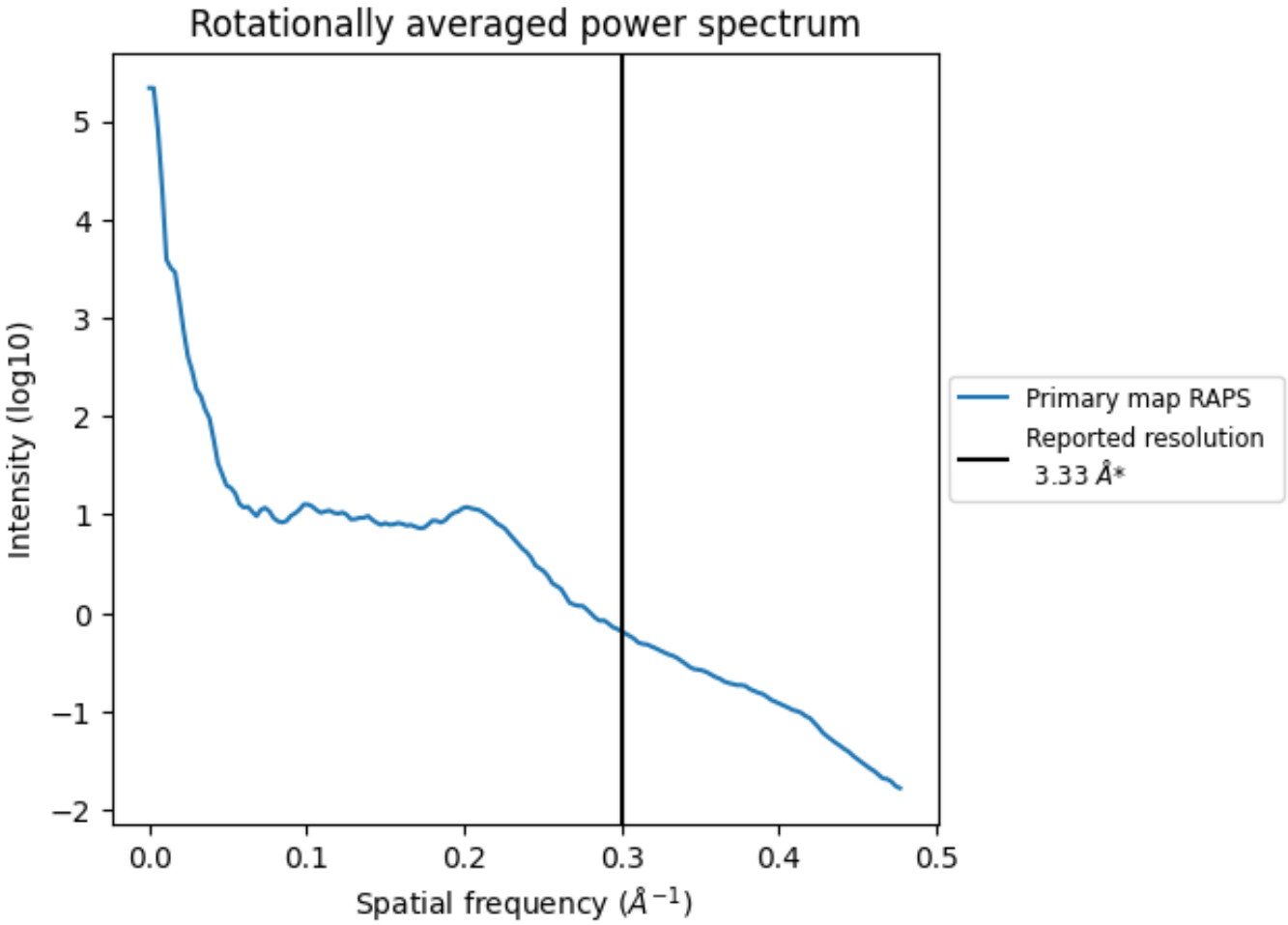
7.2 Volume estimate (i)



The volume at the recommended contour level is 785 nm^3; this corresponds to an approximate mass of 709 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)

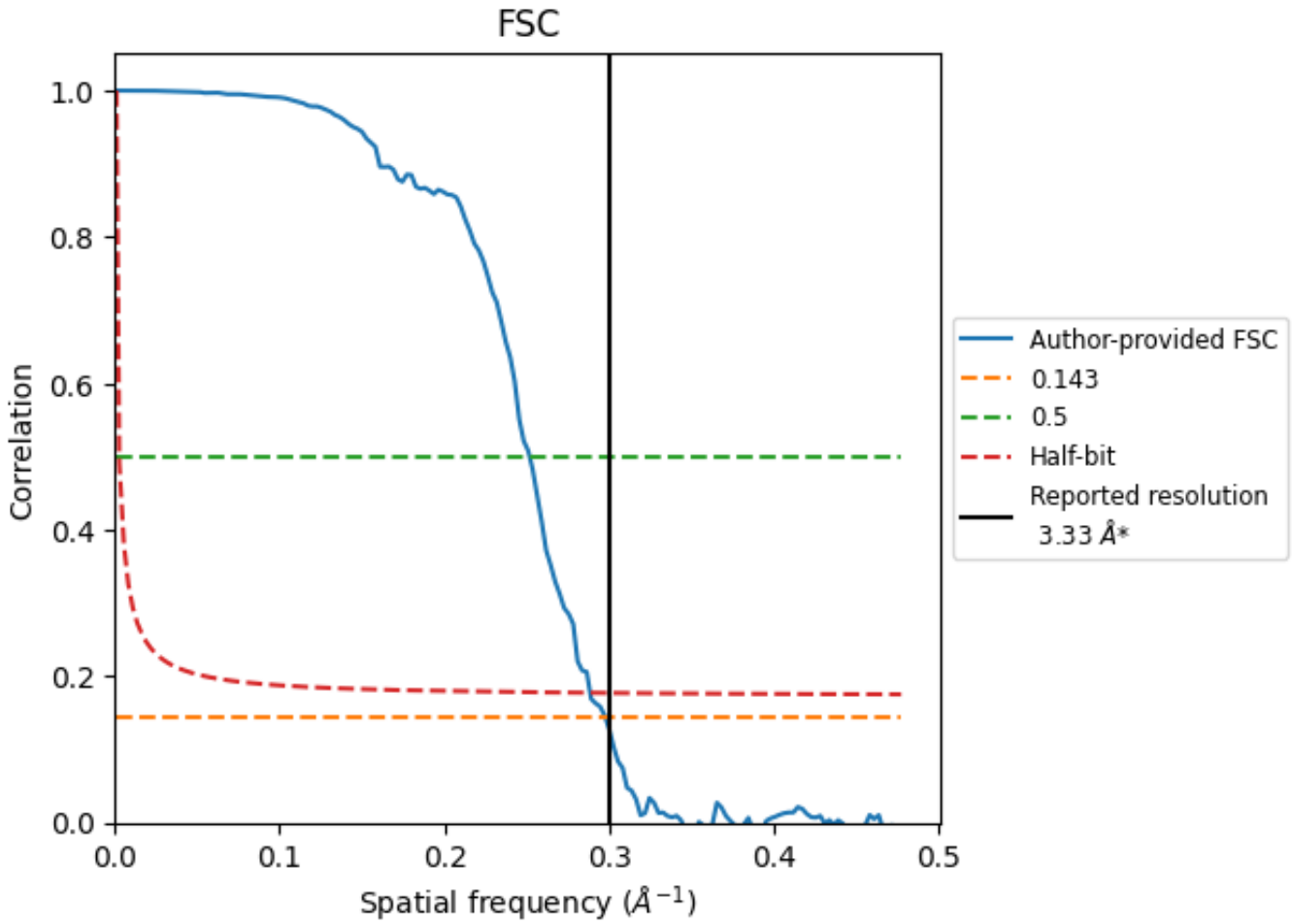


*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

8.2 Resolution estimates (i)

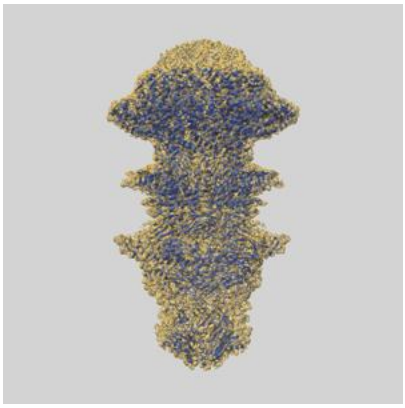
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.36	3.97	3.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

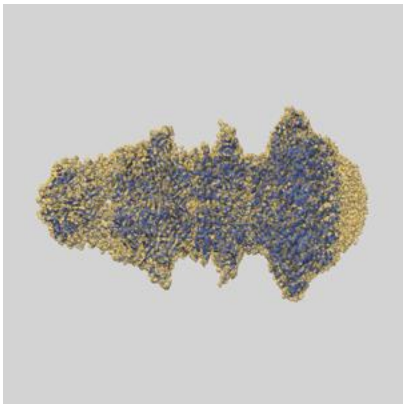
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4706 and PDB model 6R21. Per-residue inclusion information can be found in section 3 on page 16.

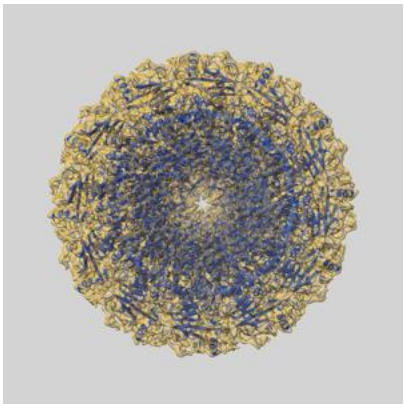
9.1 Map-model overlay



X



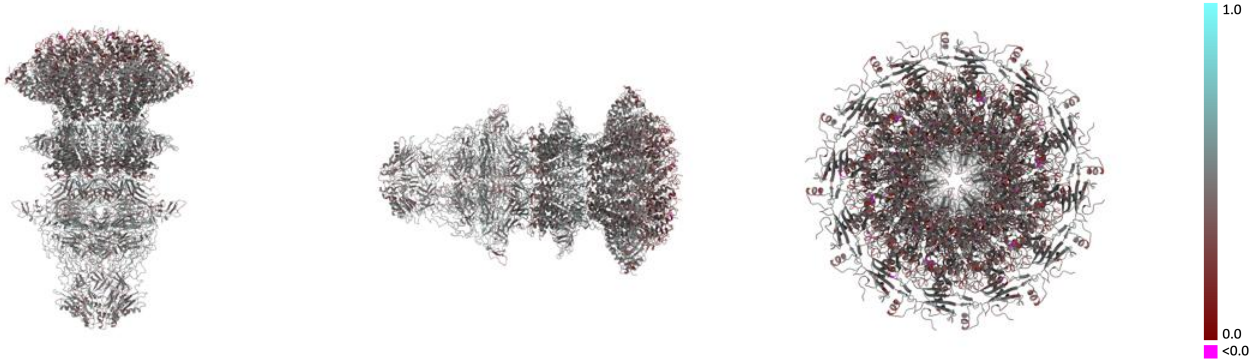
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0113 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.

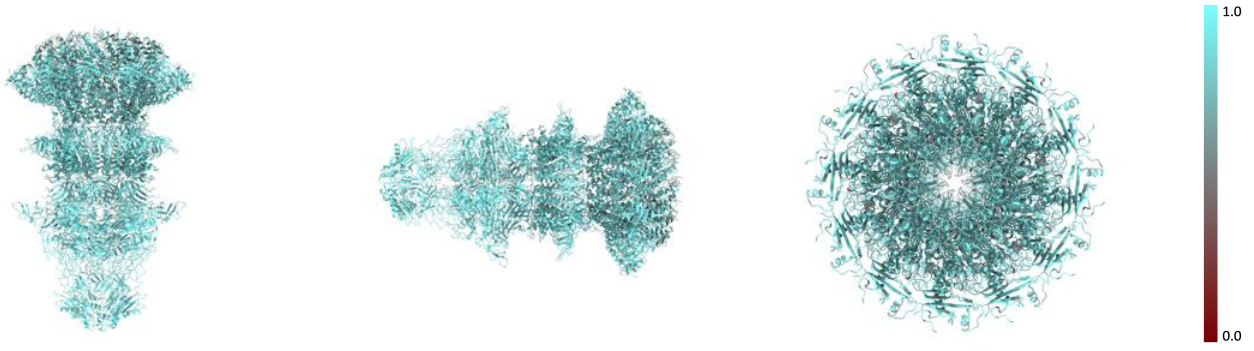
9.2 Q-score mapped to coordinate model



X Y Z

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.

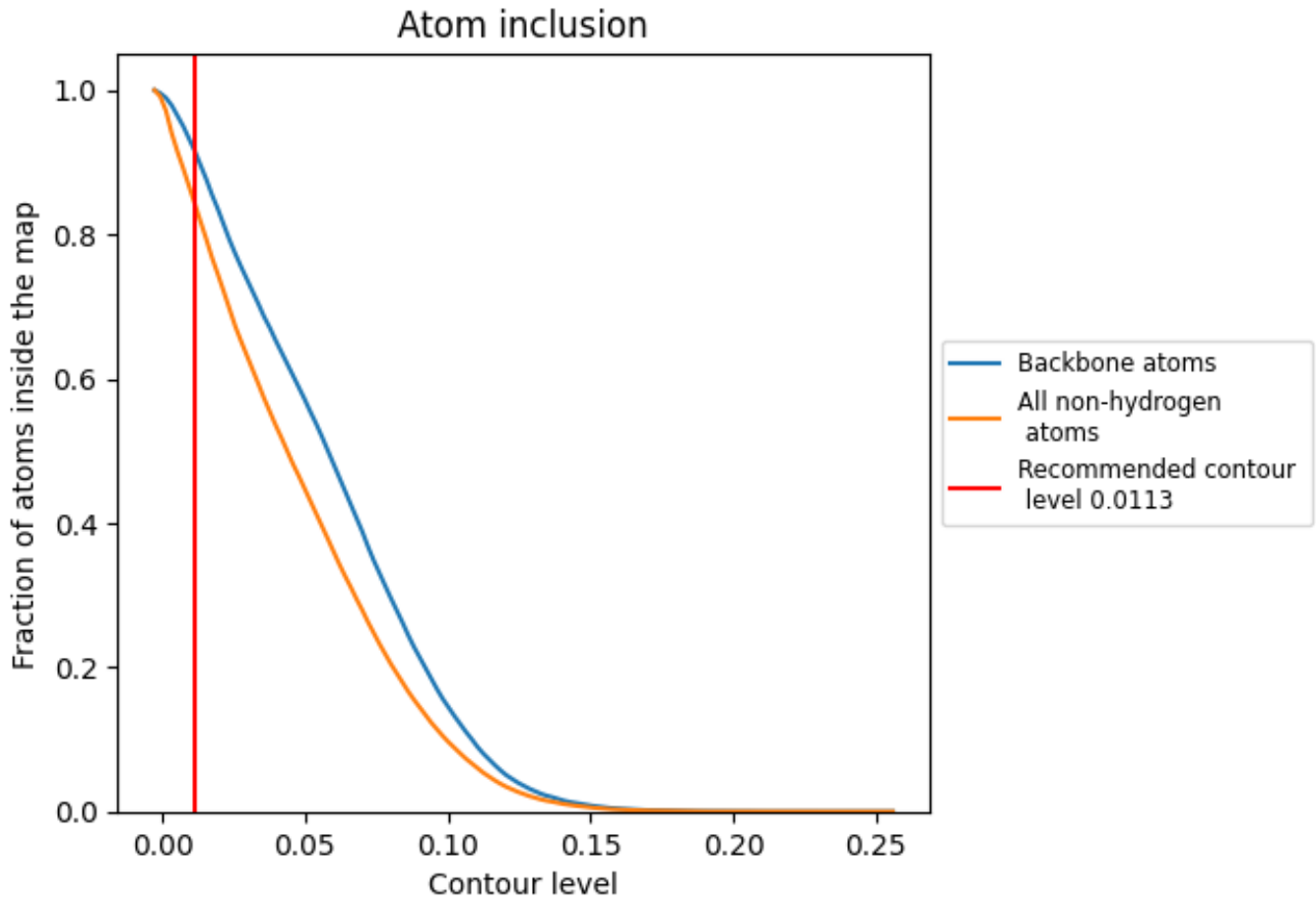
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0113).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.0113) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8444	0.4330
A	0.8131	0.4200
B	0.8012	0.3930
C	0.8131	0.4170
D	0.8009	0.3940
E	0.8144	0.4180
F	0.7988	0.3930
G	0.8158	0.4200
H	0.8017	0.3930
I	0.8126	0.4160
J	0.8006	0.3940
K	0.8147	0.4170
L	0.7985	0.3920
M	0.8604	0.4520
N	0.8585	0.4450
O	0.8604	0.4540
P	0.8477	0.4480
Q	0.8604	0.4530
R	0.8592	0.4480
S	0.8611	0.4510
T	0.8571	0.4470
U	0.8591	0.4520
V	0.8483	0.4480
W	0.8584	0.4510
X	0.8585	0.4450
a	0.8854	0.4610
b	0.8834	0.4590
c	0.8805	0.4580
d	0.8846	0.4600
e	0.8812	0.4600
f	0.8836	0.4600