wwPDB EM Validation Summary Report (i)

Nov 12, 2022 – 12:13 PM EST

PDB ID	:	6PPB
EMDB ID	:	EMD-20432
Title	:	Kaposi's sarcoma-associated herpesvirus (KSHV), C5 portal vertex structure
Authors	:	Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on	:	2019-07-06
Resolution	:	4.30 Å(reported)

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:

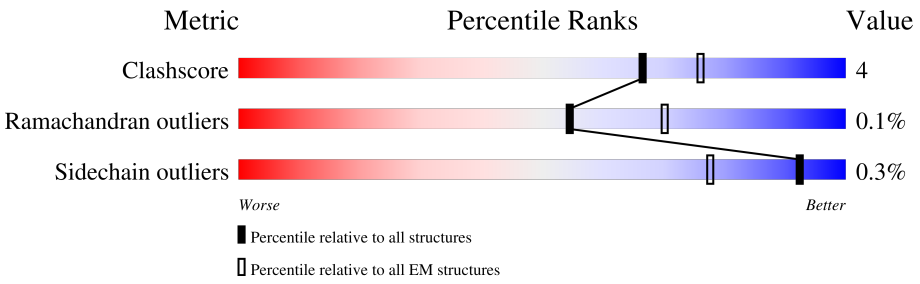
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 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	k	454	19% 76% 24%
2	l	549	8% 15% 85%
2	m	549	9% 15% 85%
3	n	2635	• • 98%
3	o	2635	• • 98%
4	S	1376	16% 82% 11% 7%
4	T	1376	22% 87% 12% •
4	W	1376	29% 85% 14% •

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Mol	Chain	Length	Quality of chain
4	X	1376	15% 82% 11% 6%
5	5	331	29% 70% 11% 19%
5	b	331	28% 96%
6	6	305	26% 88% 9%
6	7	305	28% 88% 8%
6	c	305	42% 96%
6	d	305	47% 98%
7	0	170	40% 43% 54%
7	1	170	34% 45% 54%
7	2	170	32% 44% 54%
7	3	170	30% 45% 54%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 62671 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 Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	k	344	2680	1722	467	477	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	165	PRO	LEU	conflict	UNP Q76RH8
k	281	SER	GLY	conflict	UNP Q76RH8

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	l	83	686	429	135	119	3	0	0
2	m	80	645	406	121	115	3	0	0

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	n	40	323	209	56	58	0	0
3	o	40	323	209	56	58	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	2220	THR	PRO	conflict	UNP Q2HR64
o	2220	THR	PRO	conflict	UNP Q2HR64

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	1281	10061	6401	1739	1852	69	0	0
4	T	1360	10667	6776	1851	1967	73	0	0
4	W	1354	10622	6748	1842	1960	72	0	0
4	X	1288	10108	6421	1755	1861	71	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1146	PRO	SER	conflict	UNP Q2HRA7
S	1157	ALA	THR	conflict	UNP Q2HRA7
T	1146	PRO	SER	conflict	UNP Q2HRA7
T	1157	ALA	THR	conflict	UNP Q2HRA7
W	1146	PRO	SER	conflict	UNP Q2HRA7
W	1157	ALA	THR	conflict	UNP Q2HRA7
X	1146	PRO	SER	conflict	UNP Q2HRA7
X	1157	ALA	THR	conflict	UNP Q2HRA7

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	b	321	2478	1586	424	453	15	0	0
5	5	268	2074	1336	344	381	13	0	0

- Molecule 6 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	c	294	2330	1485	397	434	14	0	0
6	d	300	2365	1505	401	444	15	0	0
6	6	294	2330	1485	397	434	14	0	0
6	7	294	2315	1478	391	431	15	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	11	LEU	PHE	conflict	UNP Q98832
c	117	LEU	PHE	conflict	UNP Q98832
c	134	ILE	PRO	conflict	UNP Q98832
c	167	GLY	ASP	conflict	UNP Q98832
d	11	LEU	PHE	conflict	UNP Q98832
d	117	LEU	PHE	conflict	UNP Q98832
d	134	ILE	PRO	conflict	UNP Q98832
d	167	GLY	ASP	conflict	UNP Q98832
6	11	LEU	PHE	conflict	UNP Q98832
6	117	LEU	PHE	conflict	UNP Q98832
6	134	ILE	PRO	conflict	UNP Q98832
6	167	GLY	ASP	conflict	UNP Q98832
7	11	LEU	PHE	conflict	UNP Q98832
7	117	LEU	PHE	conflict	UNP Q98832
7	134	ILE	PRO	conflict	UNP Q98832
7	167	GLY	ASP	conflict	UNP Q98832

- Molecule 7 is a protein called Small capsomere-interacting protein.

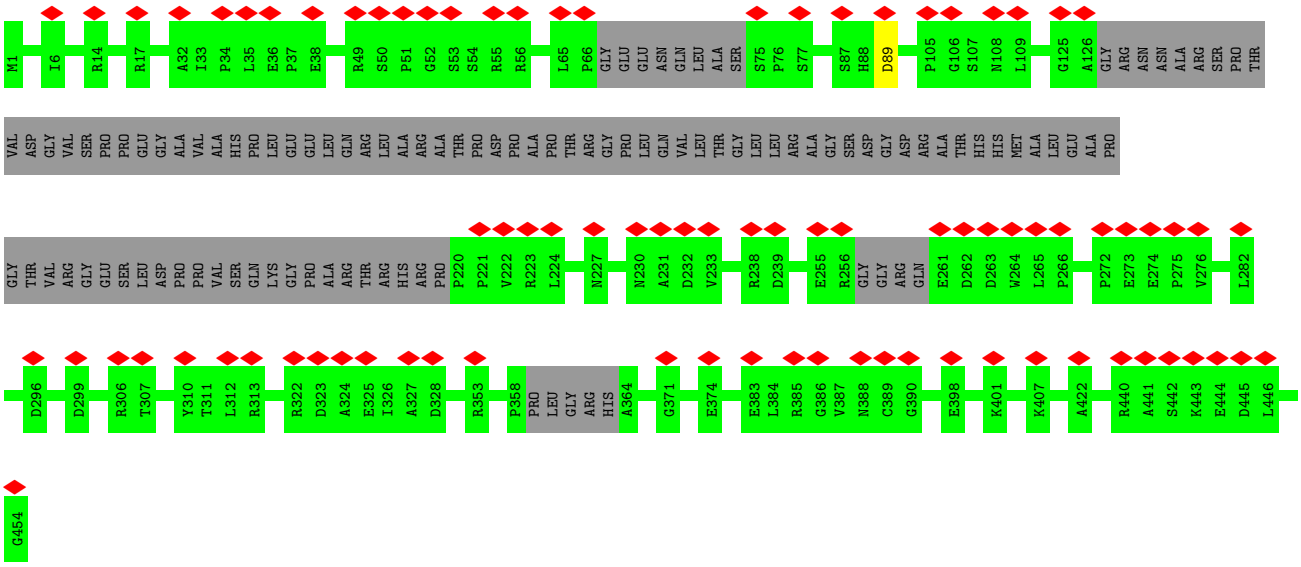
Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

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.

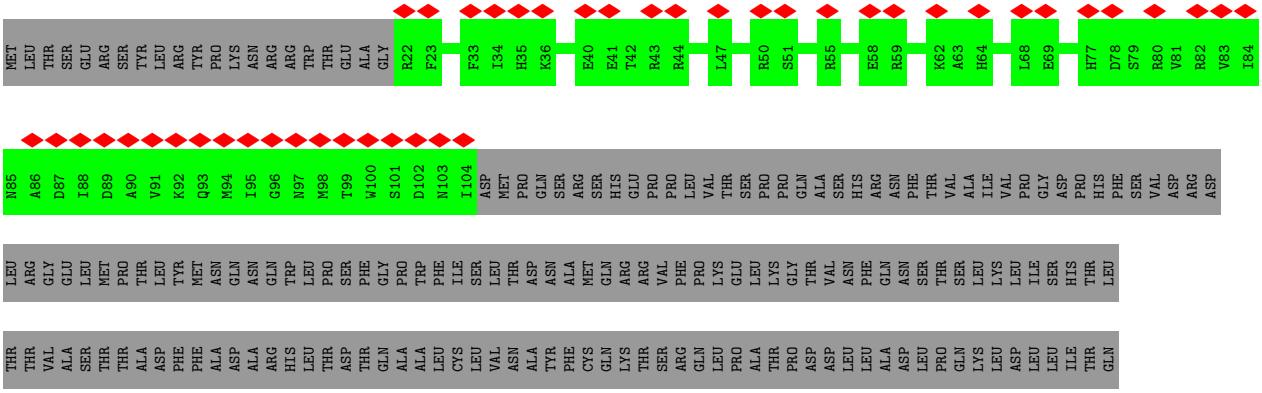
- Molecule 1: Capsid vertex component 1

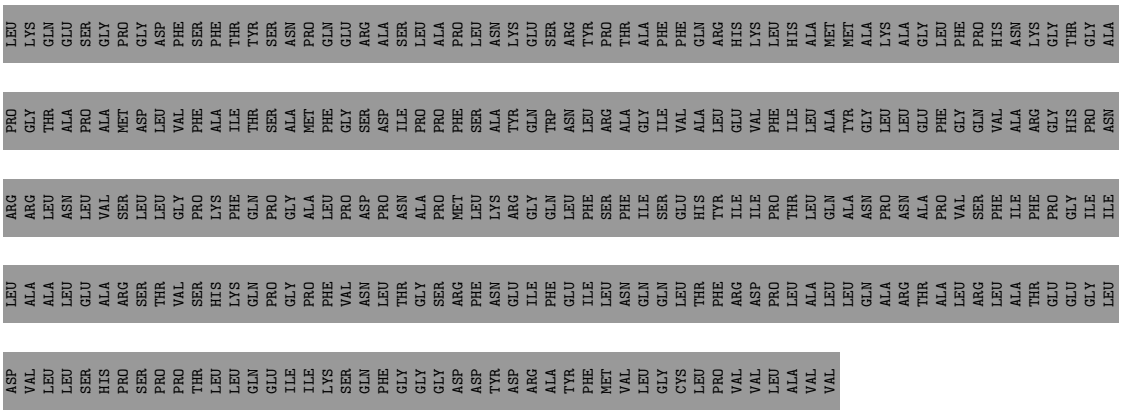
Chain k:



- Molecule 2: Capsid vertex component 2

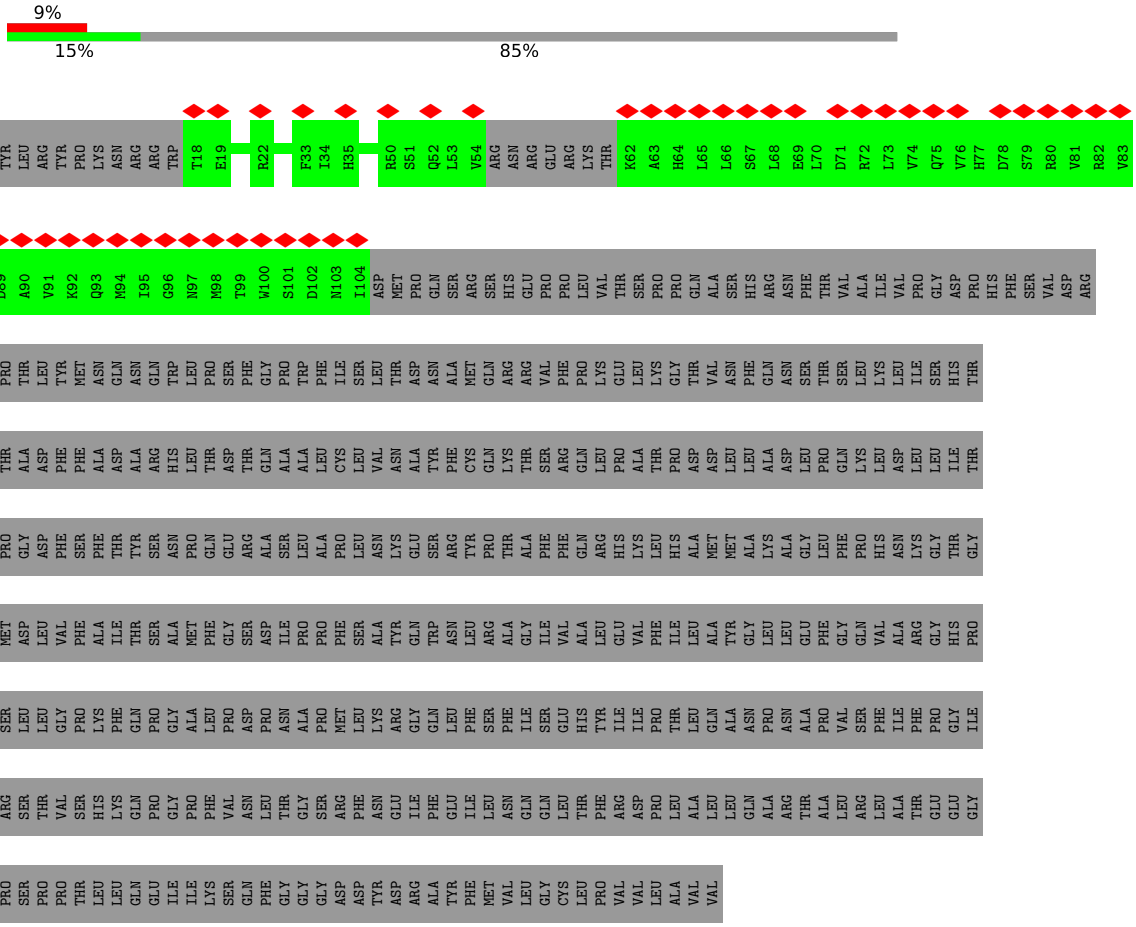
Chain l:





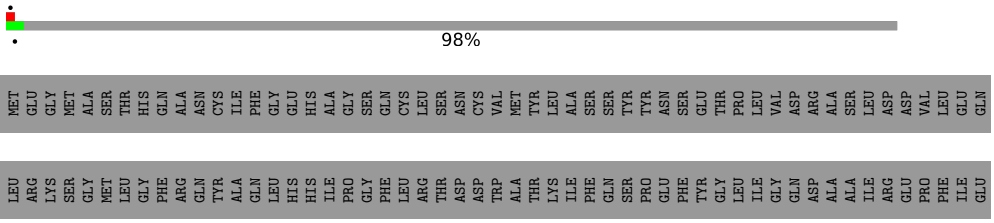
- Molecule 2: Capsid vertex component 2

Chain m:



- Molecule 3: Large tegument protein deneddylase

Chain n:



SER LEU ARG SER VAL LEU SER ARG ASN TYR ALA GLY THR VAL GLN TYR LEU ILE ILE ILE CYS GLN SER LYS ALA GLY ALA ILE VAL VAL LYS ASP LYS THR TYR TYR MET PHE ASP PRO HIS CYS ILE PRO ASN ILE PRO ASN SER PRO ALA HIS VAL ILE LYS THR ASN ASP VAL GLY

VAL LEU LEU PRO TYR ILE ALA THR HIS ASP THR GLU TYR THR GLY CYS PHE LEU TYR PHE ILE PRO HIS ASP TYR ILE SER PRO GLU HIS TYR ILE ALA ASN HIS TYR ARG THR ILE VAL PHE GLU GLU LEU HIS GLY PRO ARG MET ASP ILE SER ARG GLY VAL GLU SER CYS SER ILE

THR GLU ILE THR SER PRO SER VAL SER PRO ALA PRO SER GLU ALA PRO LEU ARG ARG ASP SER THR GLN SER GLN ASP GLU THR ARG PRO ARG ARG PRO ARG VAL VAL ILE PRO PRO TYR ASP PRO THR ASP ARG PRO ARG PRO PRO HIS GLN ASP ARG PRO PRO GLU GLN ALA ALA GLY

TYR GLY GLY ASN LYS GLY ARG GLY GLY ASN LYS GLY ARG GLY GLY LYS THR GLY ARG GLY GLY ASN GLU GLY ARG GLY GLY HIS GLN PRO PRO ASP GLU HIS GLN PRO PRO HIS ILE THR ALA GLU HIS MET ASP GLN SER ASP GLY GLN GLY ALA ASP GLY ASP MET ASP SER THR PRO

ALA ASN GLY GLU THR SER VAL THR GLU THR PRO GLY PRO GLU PRO ASN PRO PRO ALA ARG PRO ASP ARG GLU PRO PRO PRO THR PRO ALA THR PRO GLY ALA THR ALA LEU LEU SER ASP LEU THR ALA THR ARG GLY GLN LYS ARG LYS PHE SER SER LEU LYS GLU SER TYR PRO

ILE ASP SER PRO PRO SER ASP ASP ASP VAL SER GLN PRO SER GLN GLN THR ALA PRO ASP THR GLU ASP ILE TRP ILE ASP ASP PRO LEU THR PRO LEU TYR PRO LEU THR ASP THR PRO SER PHE ASP ILE THR ALA ASP VAL THR PRO ASP ASN THR HIS PRO GLU LYS ALA ALA

ASP GLY ASP PHE THR ASN LYS THR THR SER THR ASP ALA ASP ARG TYR ALA SER ALA SER GLN GLU SER LEU GLY THR LEU VAL SER PRO TYR ASP PHE THR ASN LEU ASP THR LEU LEU ALA GLU LEU GLY ARG LEU GLY THR ALA GLN PRO ILE PRO VAL ILE VAL ASP ARG LEU THR

SER ARG PRO PHE ARG GLU ALA SER ALA LEU GLN ALA MET ASP ARG ILE LEU THR HIS VAL VAL LEU GLU TYR GLY LEU VAL SER GLY TYR SER THR ALA ALA PRO SER LYS CYS THR HIS VAL LEU GLN PHE PHE ILE LEU TRP GLY GLU LYS LEU GLY ILE PRO THR GLU ASP ALA LYS

THR LEU LEU GLU SER ALA LEU GLU ILE PRO ALA MET CYS GLU ILE VAL GLN GLN GLY ARG LEU LYS GLU PRO THR PHE SER ARG HIS ILE ILE SER LYS LEU ASN PRO CYS LEU GLU SER LEU HIS ALA THR SER ARG GLN ASP PHE LYS SER LEU ILE GLN ALA PHE ASN ALA GLU GLY

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ALA ALA TYR PHE GLU ASN ILE ILE THR ALA LEU SER THR PHE GLN PRO PRO PRO GLN SER GLN GLN THR PHE GLU VAL LEU PRO ASP LEU LYS LEU ARG THR LEU VAL GLU HIS LEU THR LEU VAL GLU ALA GLN VAL THR THR GLN THR VAL GLU SER LEU GLN ALA TYR LEU GLN SER

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SER LEU ASP TRP PRO HIS ALA PRO ALA GLU ALA VAL GLU PRO LEU PRO VAL LEU THR SER LEU ARG GLY LYS ILE ALA GLU ALA LEU THR ARG GLN GLU ASN LYS ASN ALA ALA VAL ASP GLN ILE LEU THR ASP ALA GLU GLY LEU LEU LYS ASN ILE THR ASP PRO ASN GLY ALA HIS PHE

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ASN VAL PRO LYS LEU GLY GLU ALA PHE THR GLY GLY PRO HIS LEU LEU THR SER PRO SER VAL ARG GLN SER LEU SER THR LEU CYS THR THR LEU LEU ARG ASP ALA LEU ASP ALA LEU GLU LYS LYS ASP PRO ALA LEU LEU GLY GLU GLY THR THR LEU ALA LEU GLU THR LEU LEU

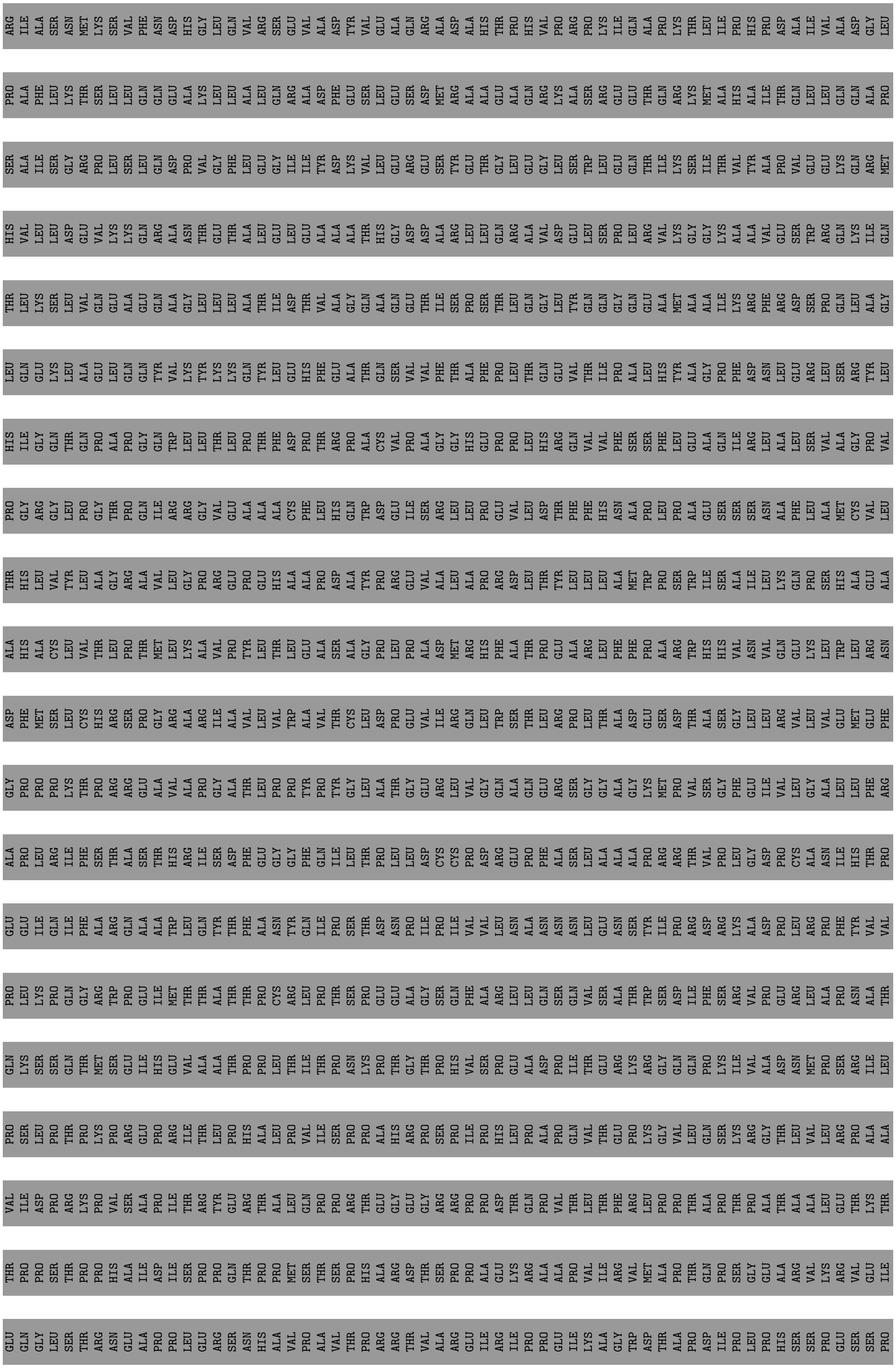
GLY TYR GLY SER VAL GLN ASP TYR LYS GLU THR VAL GLN ILE ILE SER SER LEU VAL GLY ILE GLN LYS LEU VAL ARG ASP GLN GLY ALA ASP LYS TRP ALA THR ALA VAL THR ARG LEU THR ASP LEU LYS SER THR LEU ALA THR THR ALA ILE GLU THR ALA THR LYS ARG LYS LEU

TYR ARG LEU ILE GLN ARG ASP LEU LYS GLU ALA GLN LYS HIS GLU THR ASN ARG ALA MET GLU GLU TRP LYS GLN LYS VAL LEU ALA LEU ASP ASN ALA SER PRO GLU ARG VAL ALA ALA THR LEU LEU GLN GLN ALA PRO THR ALA LYS ALA ARG GLU PHE ALA GLU LYS HIS PHE LYS ILE

LEU LEU PRO VAL PRO ALA ASP ALA PRO VAL GLN ALA SER PRO THR PRO MET GLU TYR SER ALA SER PRO LEU PRO ASP PRO LYS ASP ILE ASP ARG ALA THR SER ILE HIS GLY GLU GLN ALA TRP LYS LYS ILE GLN GLN ALA PHE LYS ASP PHE ASN PHE ALA VAL LEU ARG PRO ALA

ASP TRP ASP ALA LEU ALA ALA GLU TYR GLN ARG ARG GLY SER PRO LEU PRO ALA ALA VAL GLY PRO ALA LEU SER GLY PHE LEU GLU THR ILE LEU GLY THR LEU ASN ASP ILE TYR MET ASP LYS LEU ARG SER PHE LEU PRO ASP ALA GLN PRO PHE GLN ALA PRO PRO PHE ASP TRP

LEU THR PRO TYR GLN ASP GLN VAL SER PHE PHE LEU ARG THR ILE GLY LEU PRO LEU VAL ARG ALA LEU ALA ASP LYS ILE SER VAL GLN ALA LEU ARG LEU SER HIS ALA LEU GLN SER GLY ASP LEU GLN GLN ALA THR VAL GLY THR PRO LEU GLU LEU PRO ALA THR GLU TYR ALA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PRO ALA PHE LEU LYS THR SER LEU LEU GLN GLN GLU ALA LYS LEU LEU ALA LEU GLN ARG ALA ASP PHE GLU SER LEU GLU SER ASP MET ARG ALA ALA GLU ALA GLN ARG LYS ALA SER ARG GLU GLU THR GLN ARG LYS MET ALA HIS ALA ILE THR GLN LEU LEU GLN GLN ALA PRO
SER ALA ILE SER GLY ARG PRO LEU SER LEU GLN GLN ASP PRO VAL GLY PHE LEU GLU GLY ILE ILE TYR ASP LYS VAL LEU GLU ARG GLU SER TYR GLU THR GLY LEU GLU GLY LEU SER TRP LEU GLU GLN THR ILE LYS SER ILE THR VAL TYR ALA PRO VAL GLU GLU LYS GLN ARG MET
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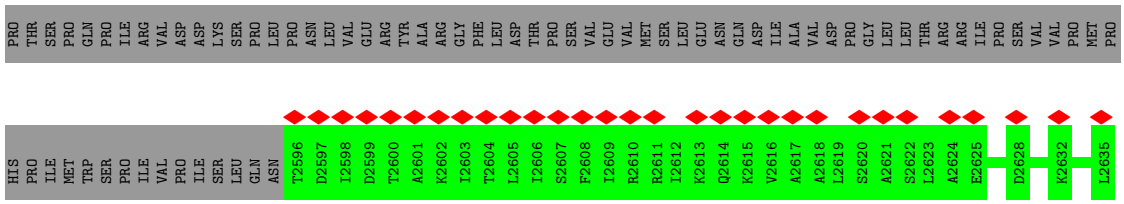
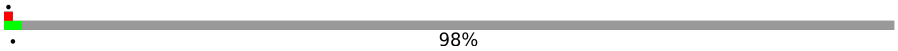
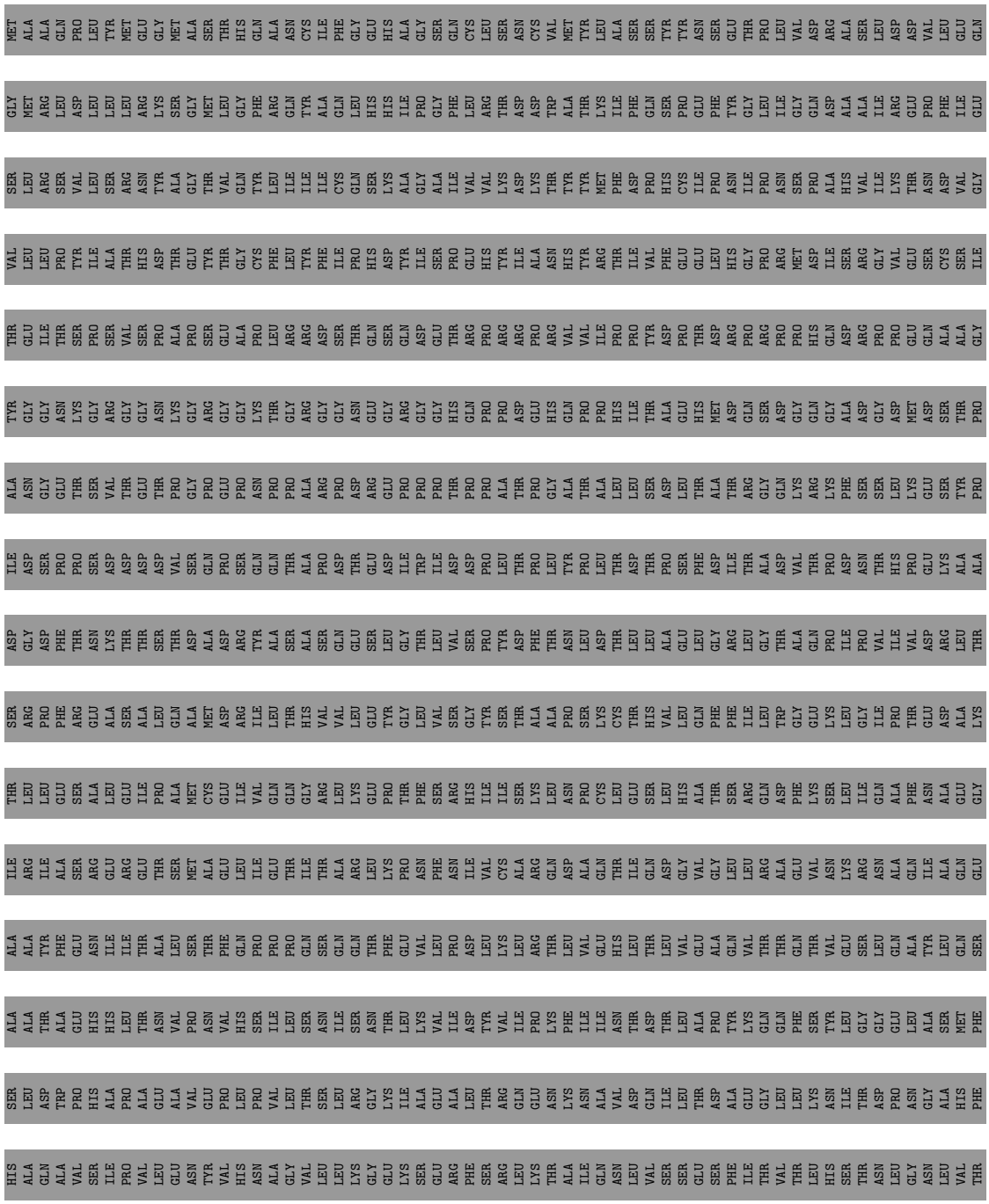


- Molecule 3: Large tegument protein deneddylase

Chain o:





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GLY TYR GLY SER VAL GLN ASP TYR LYS GLU THR VAL GLN ILE ILE SER SER LEU VAL GLY ILE GLN LYS LEU VAL ARG ASP GLN GLY ALA ASP LYS TRP ALA THR ALA VAL THR ARG LEU THR ASP LEU LYS SER THR LEU ALA THR THR ALA ILE GLU THR ALA THR LYS ARG LYS LEU

TYR ARG LEU ILE GLN ARG ASP LEU LYS GLU ALA GLN LYS HIS GLU THR ASN ARG ALA MET GLU GLU TRP LYS GLN LYS VAL LEU ALA LEU ASP ASN ALA SER PRO GLU ARG VAL ALA THR LEU LEU GLN GLN ALA PRO THR ALA LYS ALA ARG GLU PHE ALA GLU LYS HIS PHE LYS ILE

LEU LEU PRO VAL PRO ALA ASP ALA PRO VAL GLN ALA SER PRO THR PRO MET GLU TYR SER ALA SER PRO LEU PRO ASP PRO LYS ASP ILE ASP ARG ALA THR SER ILE HIS GLY GLU GLN ALA TRP LYS LYS ILE GLN GLN ALA PHE LYS ASP PHE ASN PHE ALA VAL LEU ARG PRO ALA

ASP TRP ASP ALA LEU ALA ALA GLU TYR GLN ARG ARG GLY SER PRO LEU PRO ALA ALA VAL GLY PRO ALA LEU SER GLY PHE LEU GLU THR ILE LEU GLY THR LEU ASN ASP ILE TYR MET ASP LYS LEU ARG SER PHE LEU PRO ASP ALA GLN PRO PHE GLN ALA PRO PRO PHE ASP TRP

LEU THR PRO TYR GLN ASP GLN VAL SER PHE PHE LEU ARG THR ILE GLY LEU PRO LEU VAL ARG ALA LEU ALA ASP LYS ILE SER VAL GLN ALA LEU ARG LEU SER HIS ALA LEU GLN SER GLY ASP LEU GLN GLN ALA THR VAL GLY THR PRO LEU GLU LEU PRO ALA THR GLU TYR ALA

ARG ILE ALA SER ASN MET LYS SER VAL PHE ASN ASP HIS GLY LEU GLN VAL ARG SER GLU VAL ALA ASP TYR VAL GLU ALA GLN ARG ALA ASP ALA HIS THR PRO HIS VAL PRO ARG PRO LYS ILE GLN ALA PRO LYS THR LEU ILE PRO HIS PRO ASP ALA ILE VAL ALA ASP GLY LEU

PRO ALA PHE LEU LYS THR SER LEU LEU GLN GLN GLU ALA LYS LEU LEU ALA LEU GLN ARG ALA ASP PHE GLU SER LEU GLU SER ASP MET ARG ALA ALA GLU ALA GLN ARG LYS ALA SER ARG GLU GLU THR GLN ARG LYS MET ALA HIS ALA ILE THR GLN LEU LEU GLN GLN ALA PRO

SER ALA ILE SER GLY ARG PRO LEU SER LEU GLN ASP PRO VAL GLY PHE LEU GLU GLY ILE ILE TYR ASP LYS VAL LEU GLU ARG GLU SER TYR GLU THR GLY LEU GLU GLY LEU SER TRP LEU GLU GLN THR ILE LYS SER ILE THR VAL TYR ALA PRO VAL GLU GLU LYS GLN ARG MET

HIS VAL LEU LEU ASP GLU VAL LYS LYS GLN ARG ALA ASN THR GLU THR ALA LEU GLU LEU GLU ALA ALA ALA THR HIS GLY ASP ASP ALA ARG LEU LEU GLN ARG ALA ALA VAL ASP GLU LEU SER PRO LEU ARG VAL LYS GLY GLY LYS ALA ALA VAL GLU SER TRP ARG GLN LYS ILE GLN

THR LEU LYS SER LEU VAL GLN GLU ALA GLU GLN ALA GLY LEU LEU LEU ALA THR ILE ASP THR VAL ALA GLY GLN ALA GLN GLU THR ILE SER PRO SER THR LEU GLN GLY LEU TYR GLN GLN GLY GLN GLU ALA MET ALA ALA ILE LYS ARG PHE ARG ASP SER PRO GLN LEU ALA GLY

LEU GLN GLU LYS LEU ALA GLU LEU GLN GLN TYR VAL LYS TYR LYS LYS GLN TYR LEU GLU HIS PHE GLU ALA THR GLN SER VAL VAL PHE THR ALA PHE PRO LEU THR GLN GLU VAL THR ILE PRO ALA LEU HIS TYR ALA GLY PRO PHE ASP ASN LEU GLU ARG LEU SER ARG TYR LEU

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THR HIS LEU VAL TYR LEU ALA GLY ARG ALA VAL LEU GLY PRO ARG GLU PRO GLU HIS ALA ALA PRO ASP ALA TYR PRO ARG GLU VAL ALA LEU ALA PRO ARG ASP LEU THR TYR LEU LEU LEU ALA MET TRP PRO SER TRP ILE SER ALA ILE LEU LYS GLN PRO SER HIS ALA GLU ALA

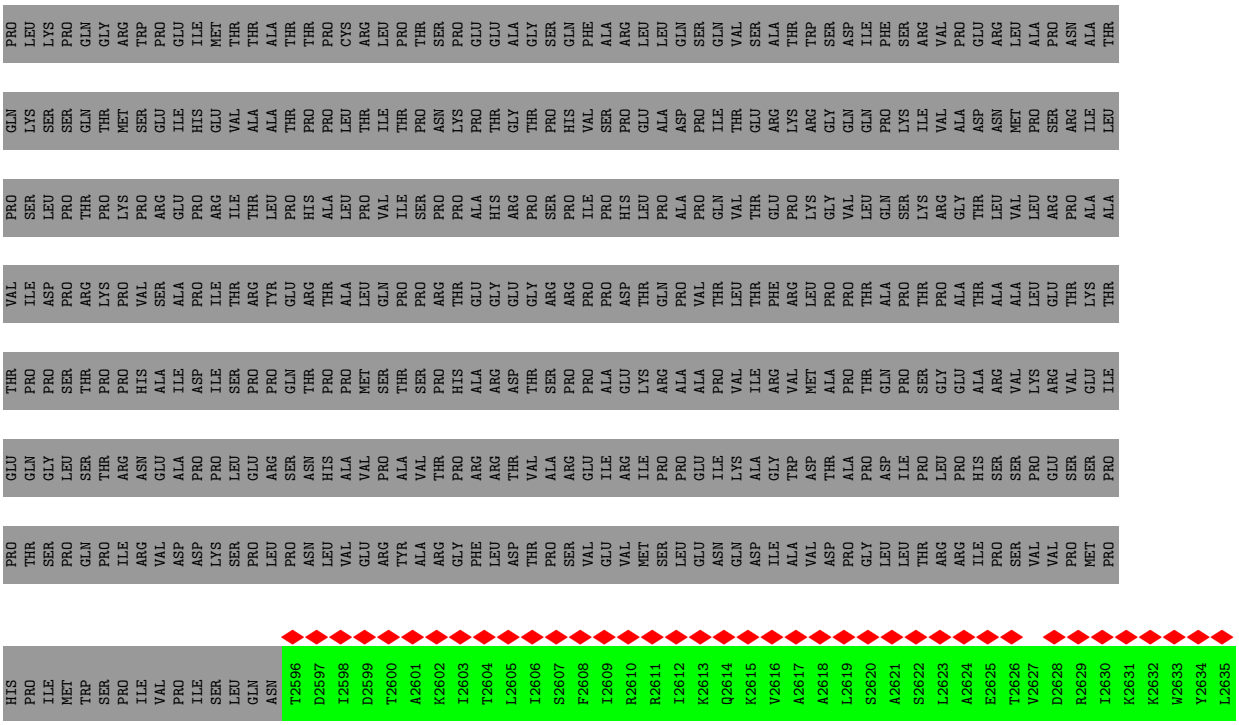
ALA HIS ALA CYS LEU VAL THR LEU PRO THR MET LEU LYS ALA VAL PRO TYR LEU THR LEU GLU ALA SER ALA GLY PRO LEU PRO ALA ASP MET ARG HIS PHE ALA THR PRO GLU ALA ARG LEU PHE PHE PRO ALA ARG TRP HIS HIS VAL ASN VAL GLN GLU LYS LEU TRP LEU ARG ASN

ASP PHE MET SER LEU CYS HIS ARG SER PRO GLY ARG ALA ARG ILE ALA VAL LEU VAL TRP ALA VAL THR CYS LEU ASP PRO GLU VAL ILE ARG GLN LEU TRP SER THR LEU ARG PRO LEU THR ALA ASP GLU SER ASP THR ALA SER GLY LEU LEU ARG VAL LEU VAL GLU MET GLU PHE

GLY PRO PRO LYS THR PRO ARG ARG GLU ALA VAL ALA PRO GLY ALA THR LEU PRO PRO TYR PRO TYR GLY LEU ALA THR GLY GLU ARG LEU VAL GLY GLN ALA GLN GLU ARG SER GLY GLY ALA GLY LYS MET PRO VAL SER GLY PHE GLU ILE VAL LEU GLY ALA LEU LEU PHE ARG

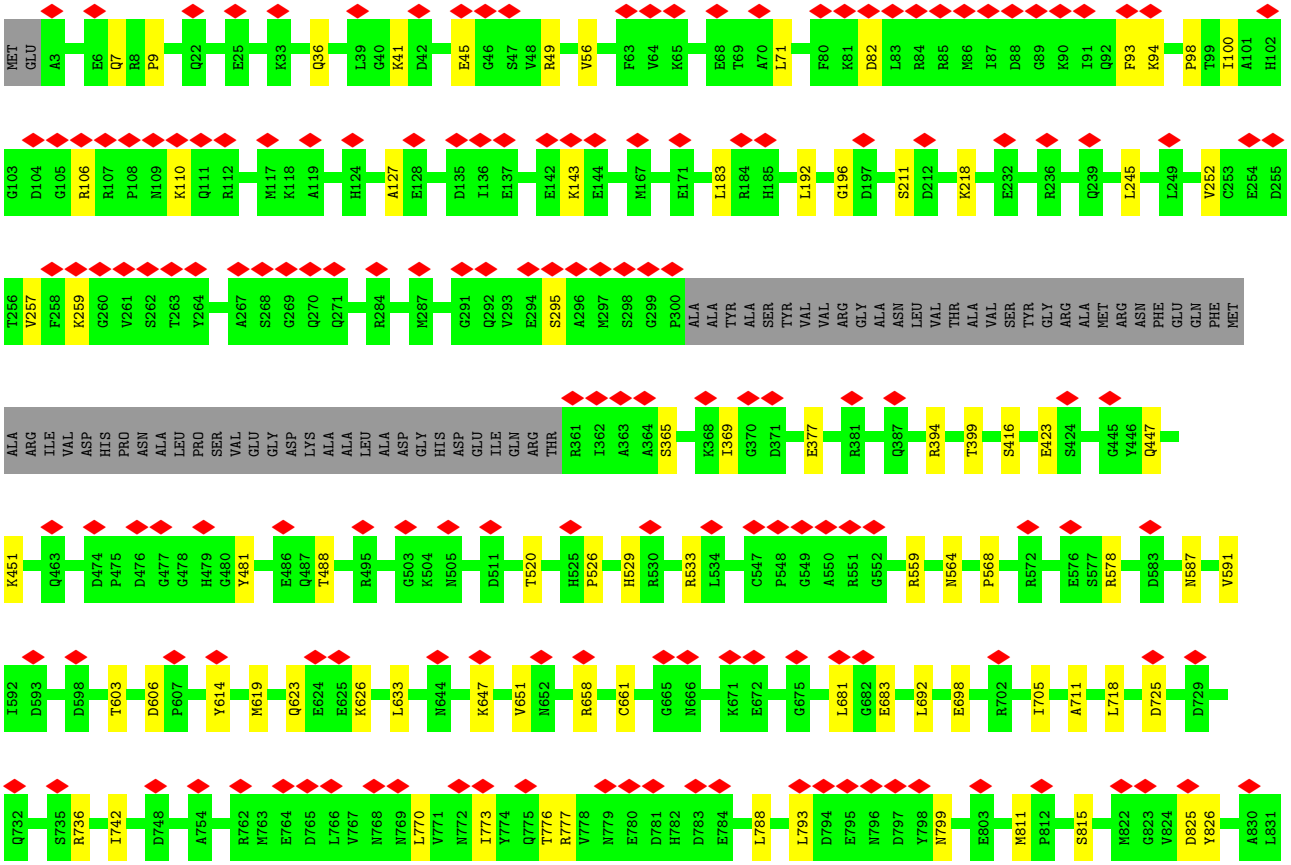
ALA PRO LEU ARG ILE PHE SER THR ALA SER THR HIS ARG ILE SER ASP PHE GLU GLY GLY PHE GLN ILE LEU THR PRO LEU LEU ASP CYS CYS PRO ASP ARG GLU PRO PHE ALA SER LEU ALA ALA ALA PRO ARG ARG THR VAL PRO LEU GLY ASP PRO CYS ALA ASN ILE HIS THR PRO

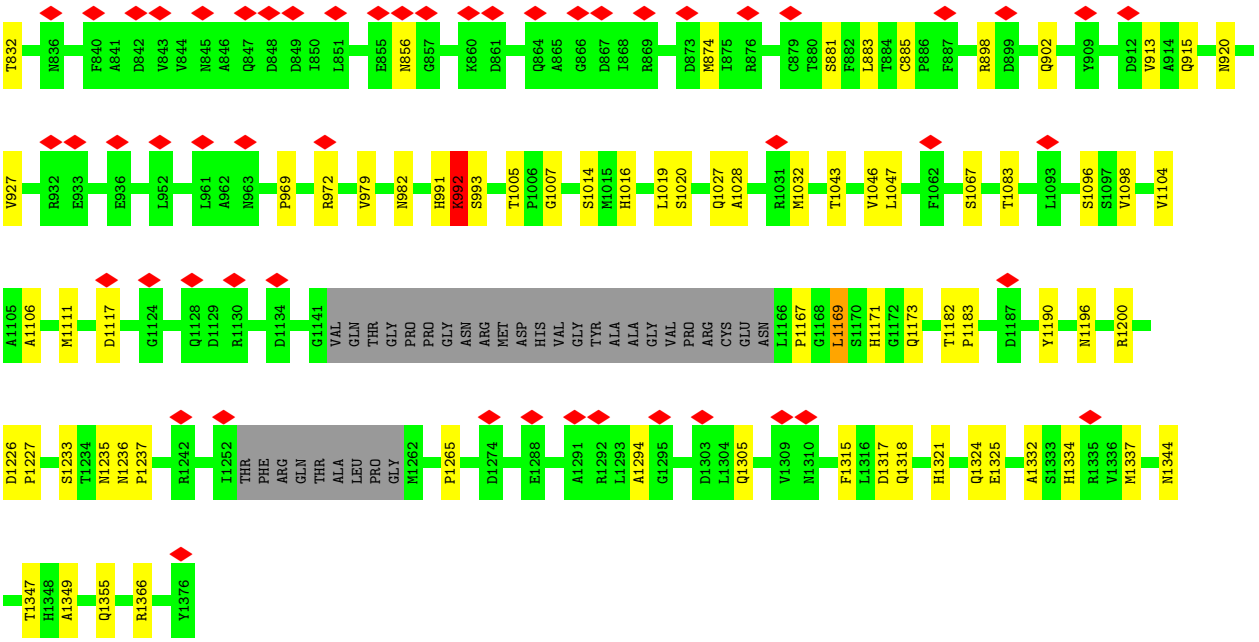
GLU GLU ILE GLN ILE PHE ALA ARG GLN ALA ALA TRP LEU GLN TYR THR PHE ALA ASN TYR GLN ILE PRO SER THR ASP ASN PRO ILE PRO ILE VAL VAL LEU ASN ALA ASN ASN ASN LEU GLU ASN SER TYR ILE PRO ARG ASP ARG LYS ALA ASP PRO LEU ARG PRO PHE TYR VAL VAL



- Molecule 4: Major capsid protein

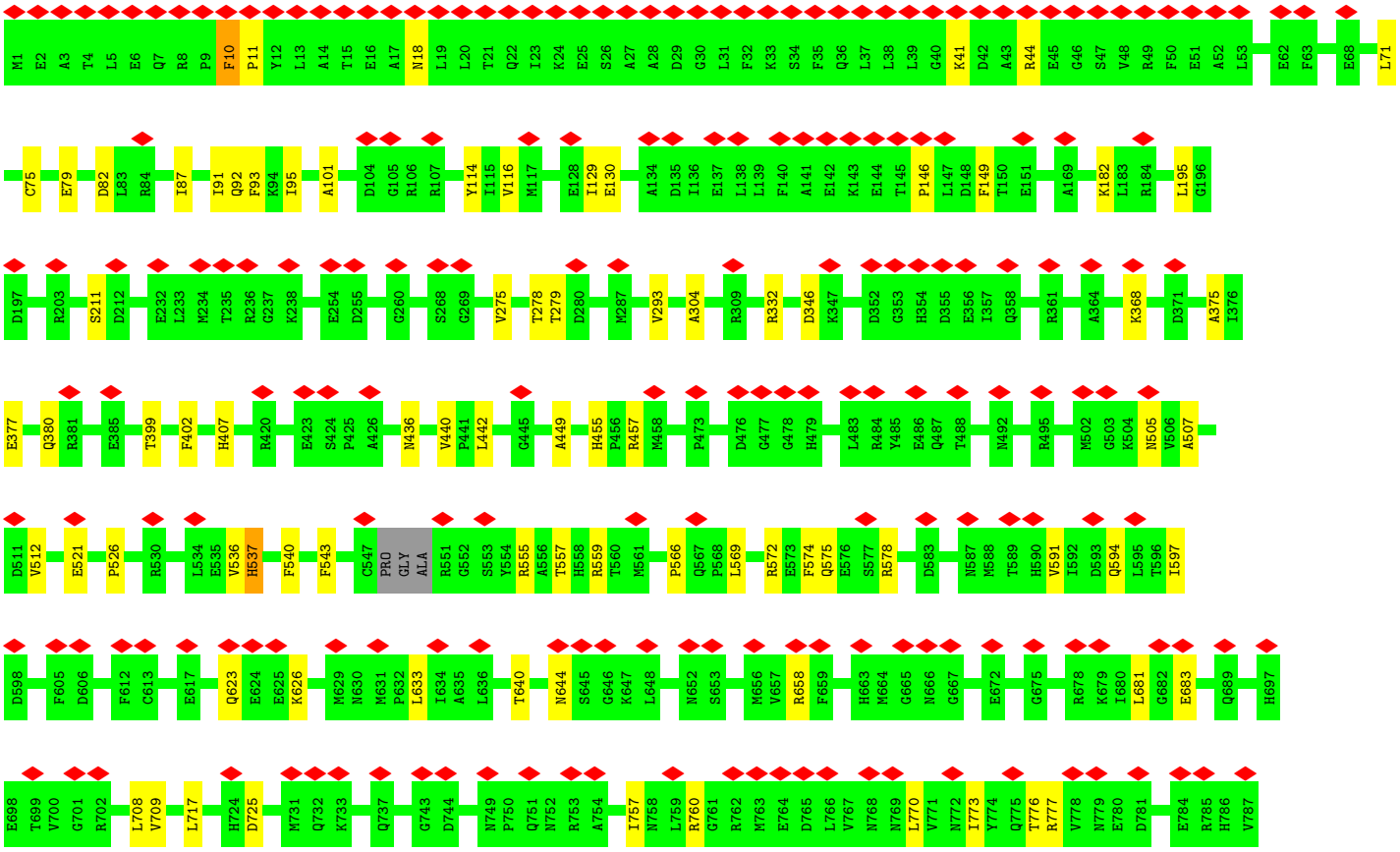
Chain S:

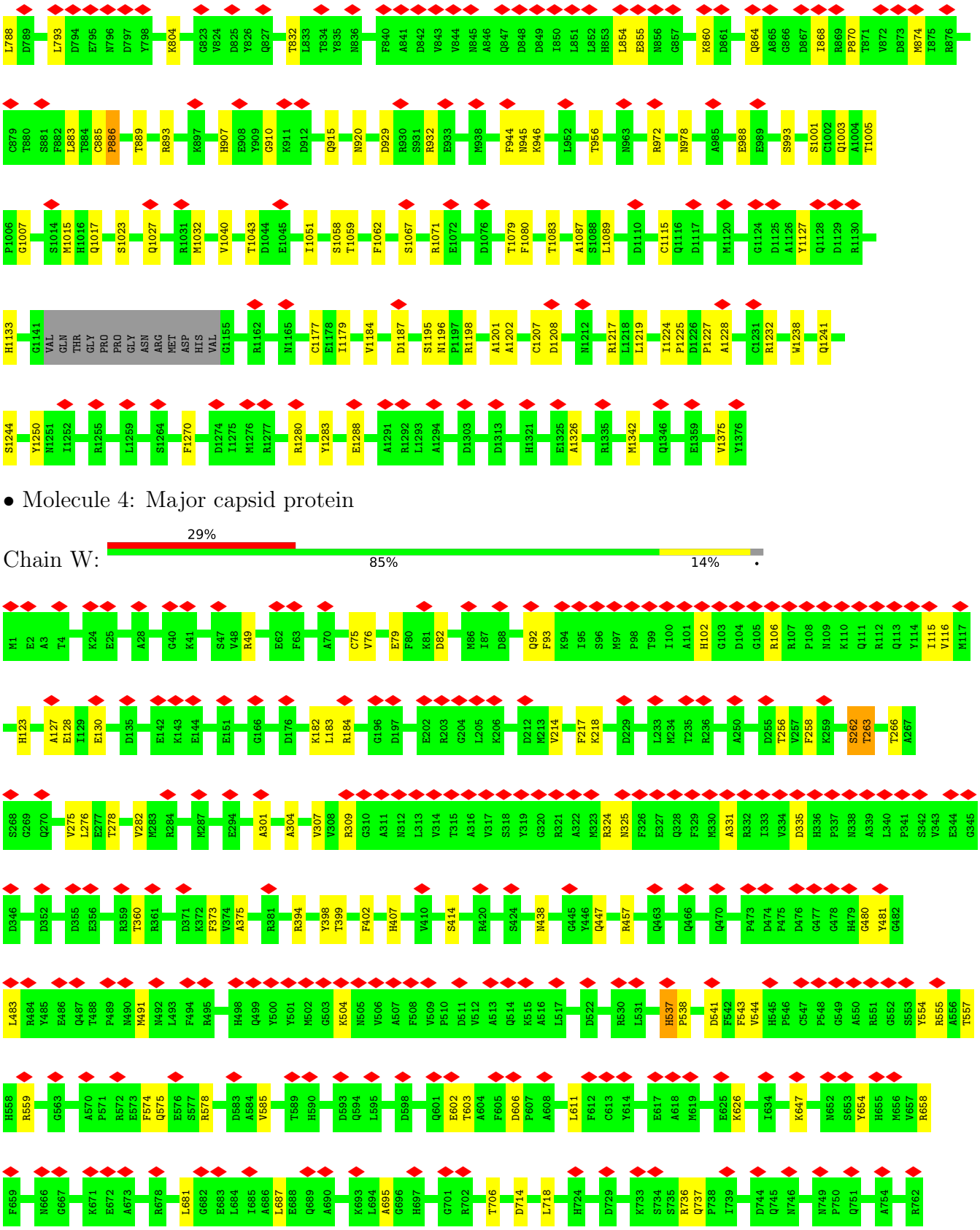




- Molecule 4: Major capsid protein

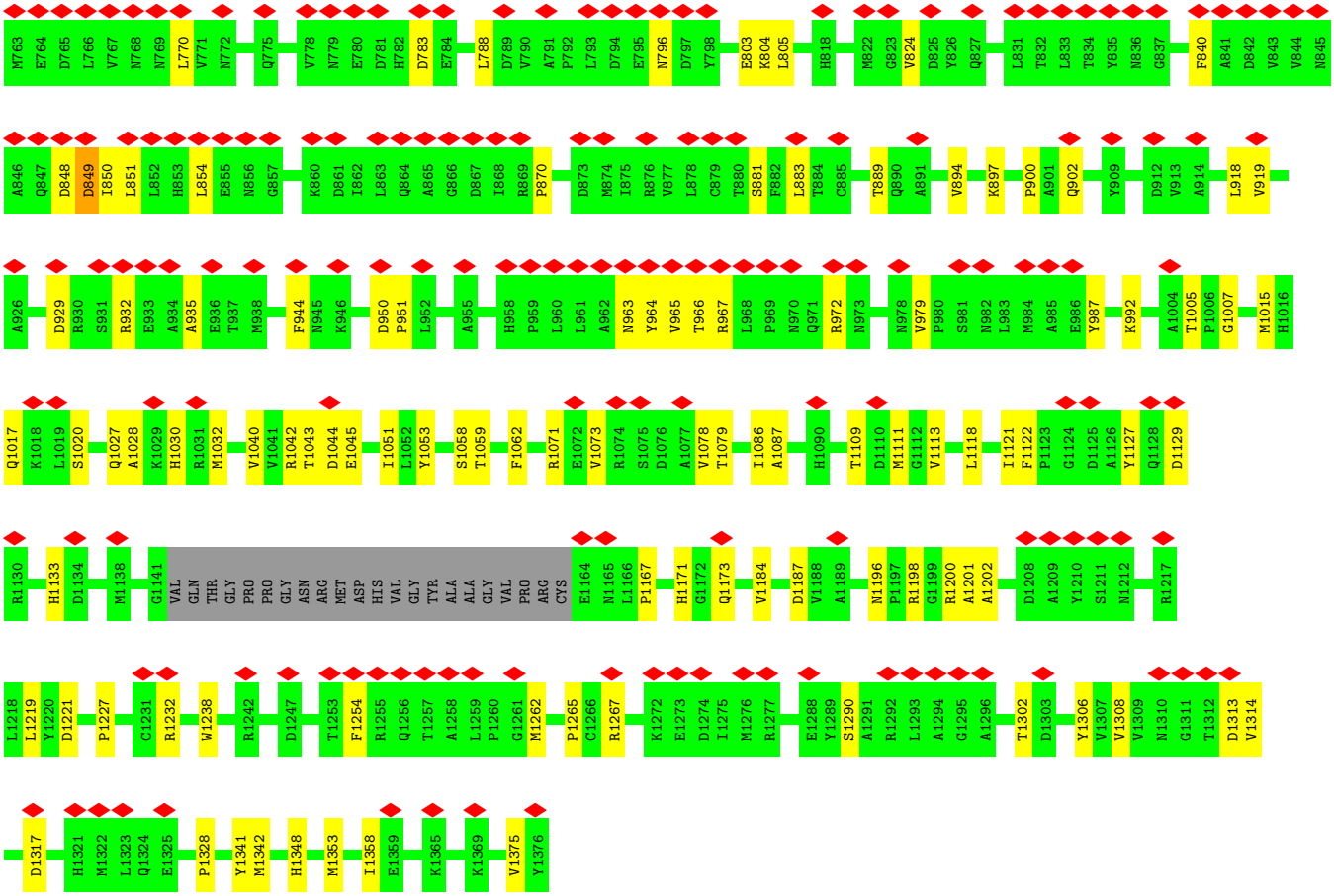
Chain T:





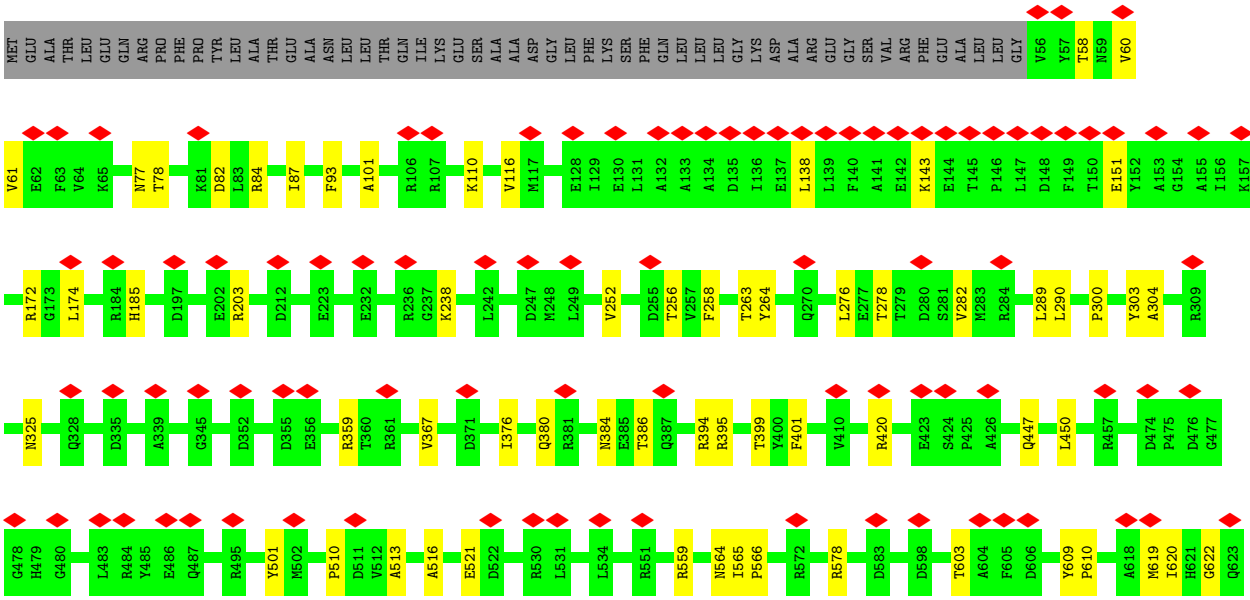
- Molecule 4: Major capsid protein

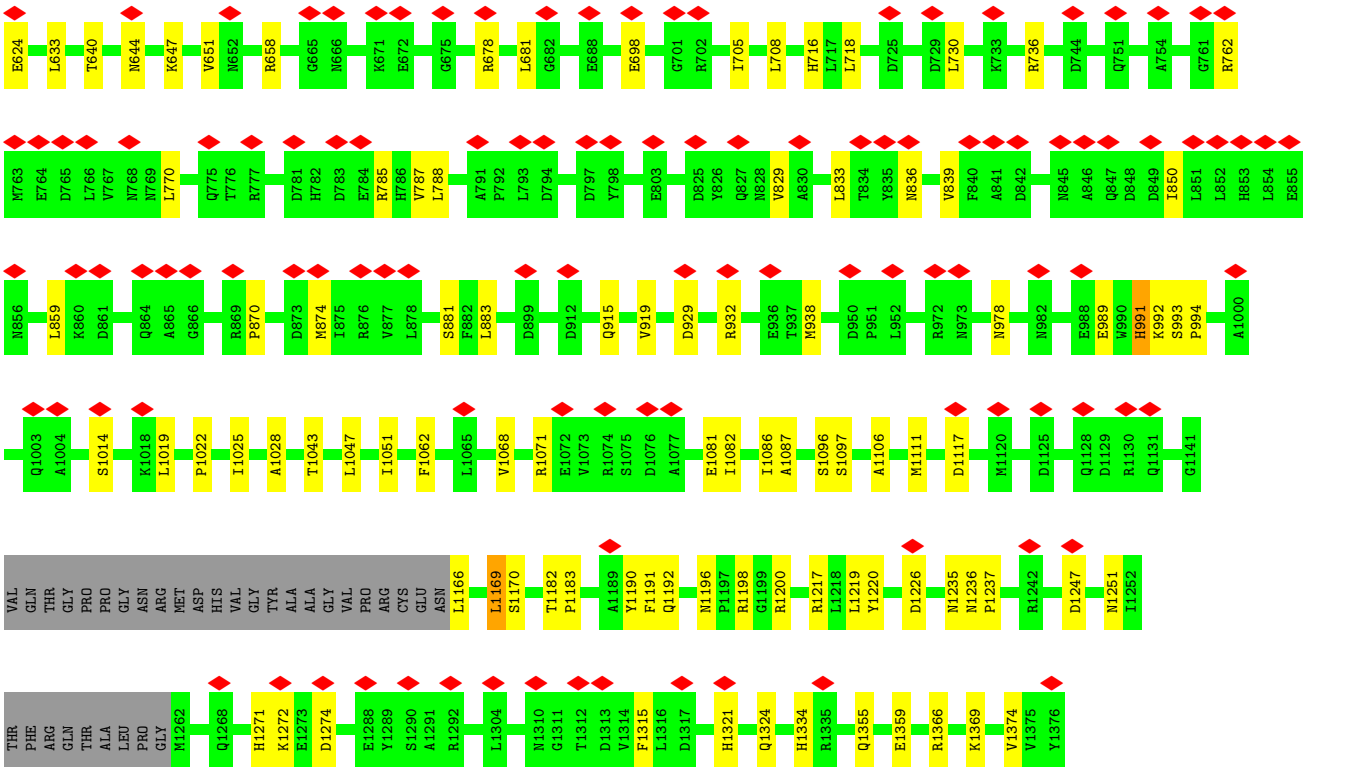
Chain W:



- Molecule 4: Major capsid protein

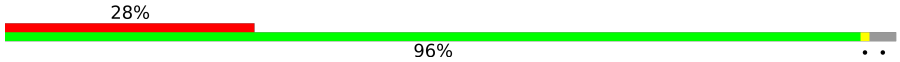
Chain X:

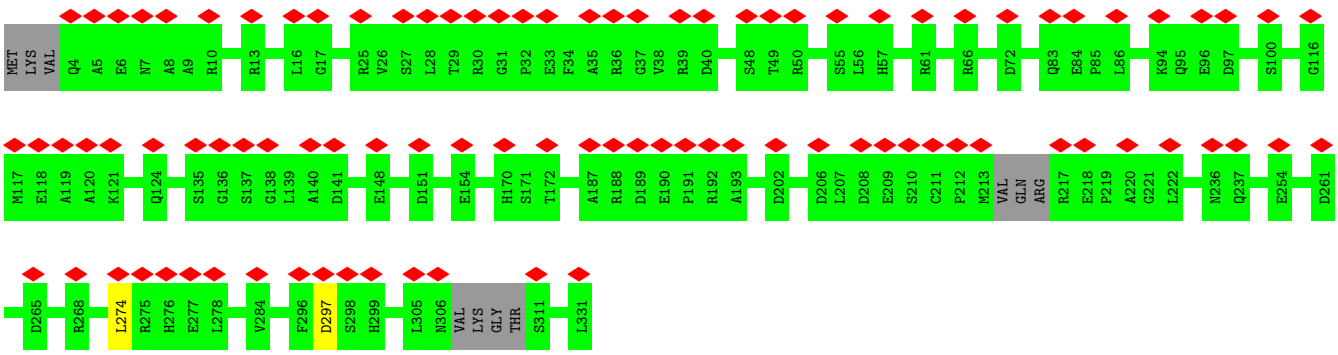




- Molecule 5: Triplex capsid protein 1

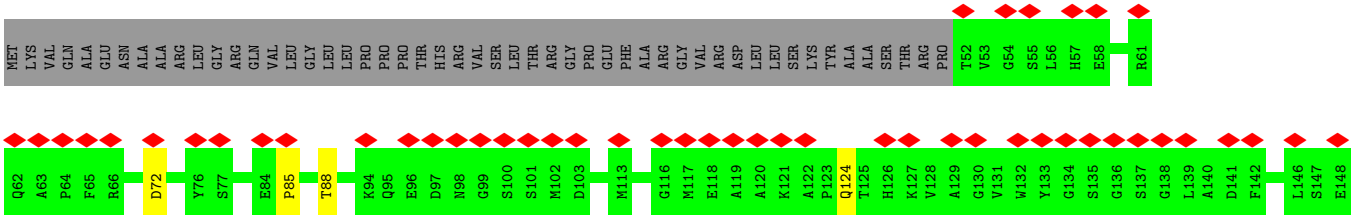
Chain b:

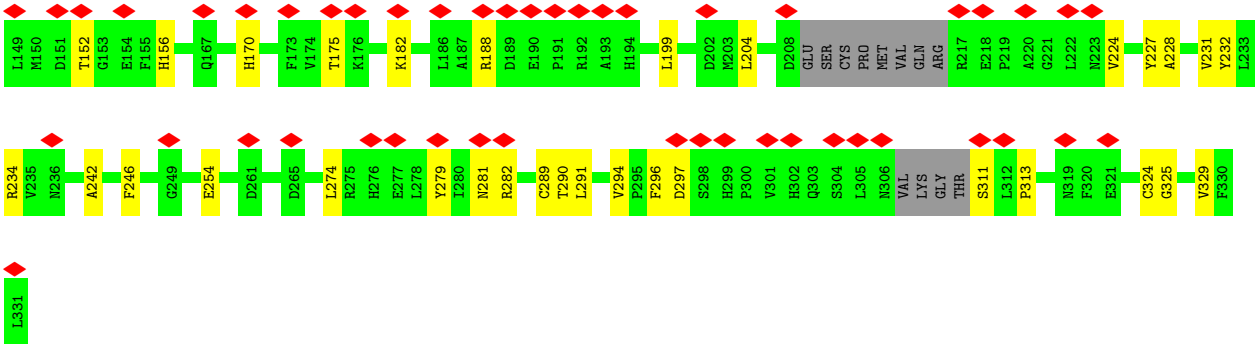




- Molecule 5: Triplex capsid protein 1

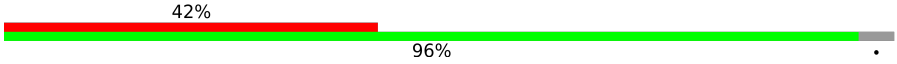
Chain 5:

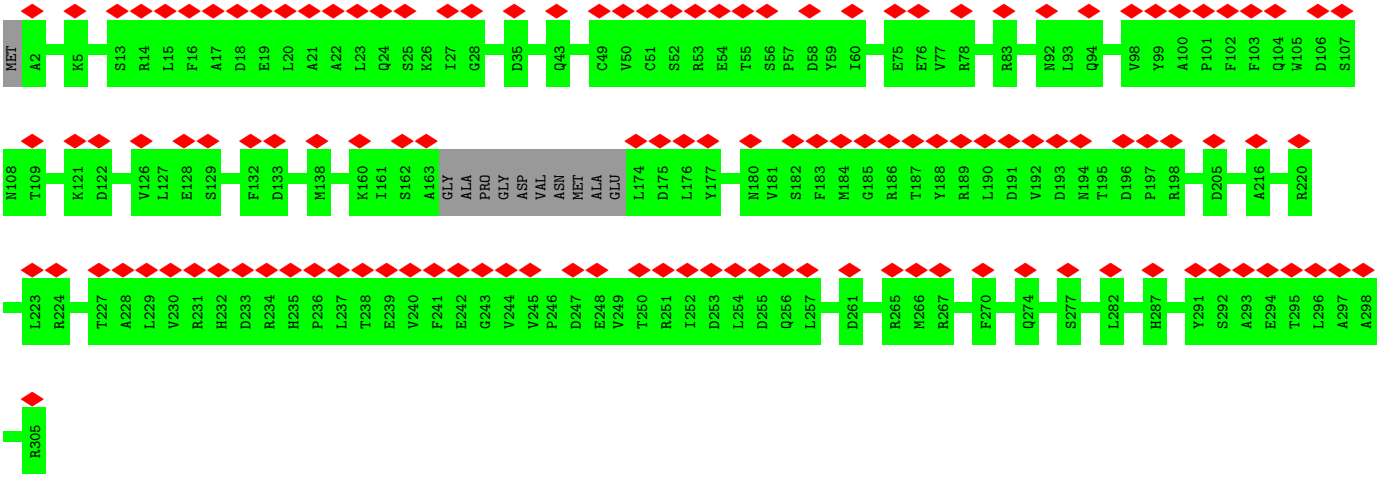




• Molecule 6: Triplex capsid protein 2

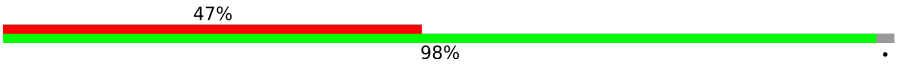
Chain c:

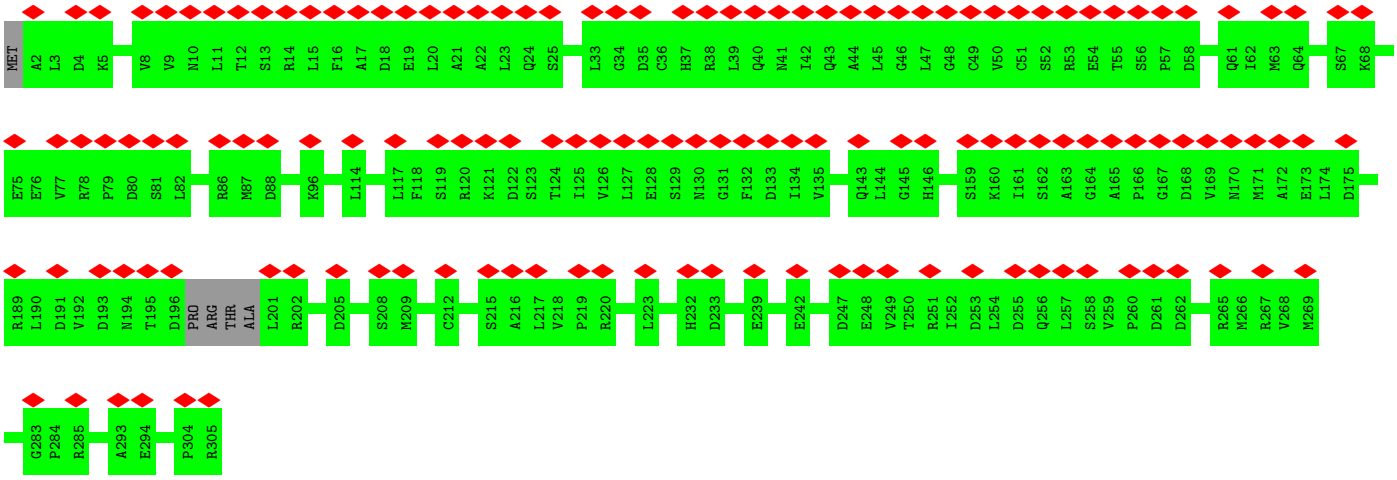




• Molecule 6: Triplex capsid protein 2

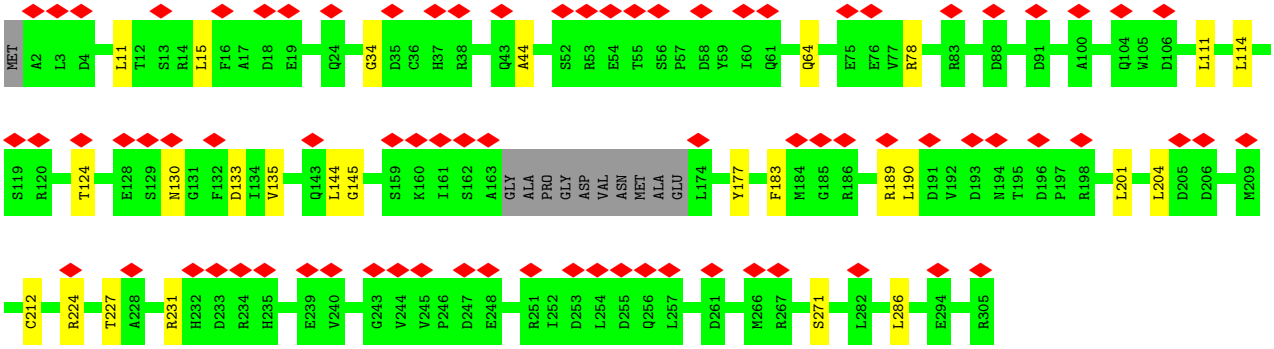
Chain d:





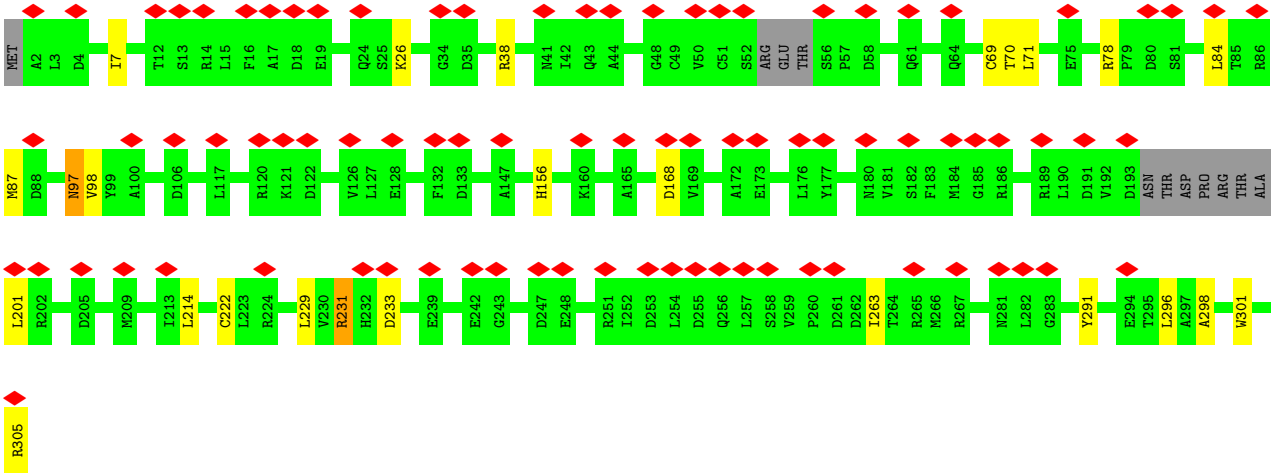
• Molecule 6: Triplex capsid protein 2

Chain 6: 26% 88% 9%



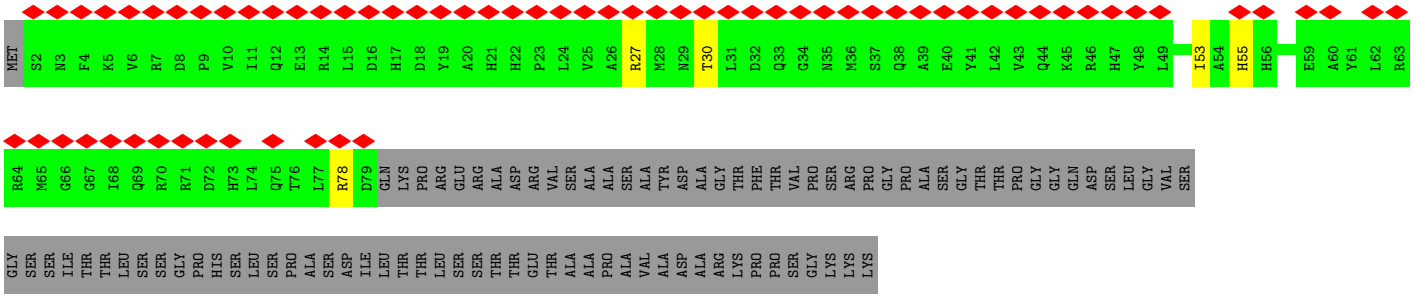
- Molecule 6: Triplex capsid protein 2

Chain 7: 28% 88% 8%



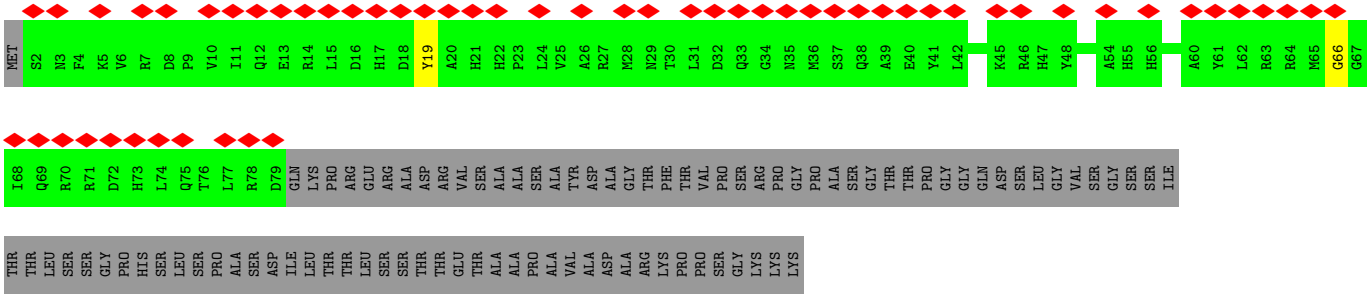
- Molecule 7: Small capsomere-interacting protein

Chain 0: 40% 43% 54%



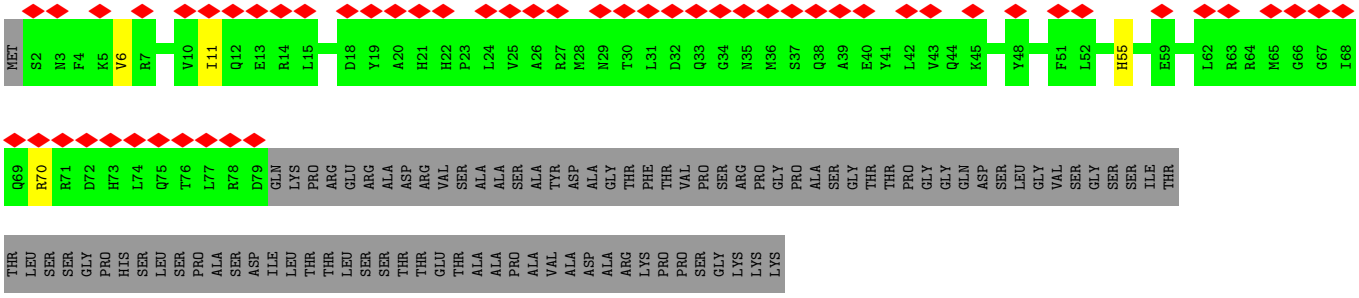
- Molecule 7: Small capsomere-interacting protein

Chain 1: 34% 45% 54%



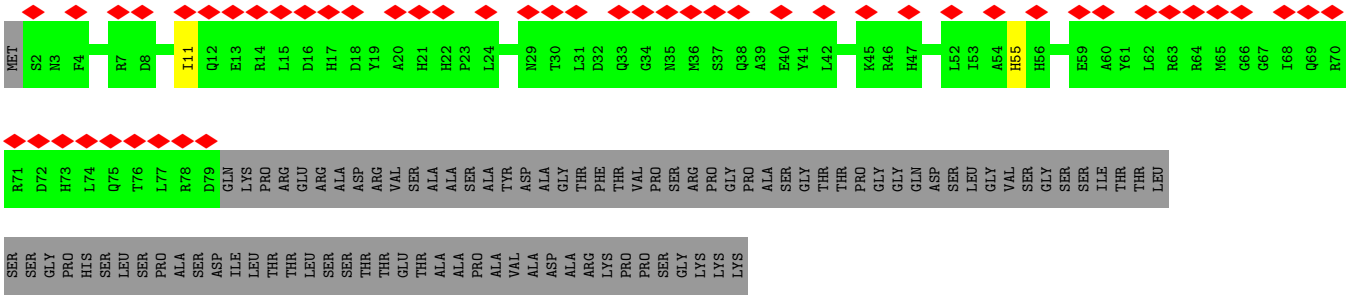
- Molecule 7: Small capsomere-interacting protein

Chain 2:



- Molecule 7: Small capsomere-interacting protein

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	39773	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	k	0.31	0/2753	0.52	1/3755 (0.0%)
2	l	0.27	0/698	0.48	0/942
2	m	0.25	0/656	0.45	0/887
3	n	0.32	0/326	0.45	0/437
3	o	0.32	0/326	0.45	0/437
4	S	0.32	0/10300	0.56	3/13998 (0.0%)
4	T	0.34	0/10919	0.58	1/14839 (0.0%)
4	W	0.32	0/10874	0.57	1/14780 (0.0%)
4	X	0.33	0/10350	0.56	1/14071 (0.0%)
5	5	0.30	0/2127	0.58	2/2891 (0.1%)
5	b	0.32	0/2540	0.60	2/3452 (0.1%)
6	6	0.30	0/2376	0.59	0/3234
6	7	0.29	0/2360	0.58	1/3210 (0.0%)
6	c	0.30	0/2376	0.56	0/3234
6	d	0.30	0/2411	0.55	0/3281
7	0	0.27	0/682	0.47	0/919
7	1	0.27	0/682	0.47	0/919
7	2	0.27	0/682	0.47	0/919
7	3	0.27	0/682	0.47	0/919
All	All	0.32	0/64120	0.56	12/87124 (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
4	S	0	2
4	T	0	5
4	W	0	5
4	X	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	297	ASP	CB-CG-OD1	8.70	126.13	118.30
5	b	297	ASP	CB-CG-OD1	8.55	126.00	118.30
5	b	274	LEU	CA-CB-CG	5.95	128.99	115.30
4	T	708	LEU	CA-CB-CG	5.68	128.37	115.30
5	5	296	PHE	C-N-CA	5.67	135.87	121.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	S	991	HIS	Peptide
4	S	992	LYS	Peptide
4	T	10	PHE	Peptide
4	T	505	ASN	Peptide
4	T	537	HIS	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	k	2680	0	2675	0	0
2	l	686	0	704	0	0
2	m	645	0	653	0	0
3	n	323	0	353	0	0
3	o	323	0	353	0	0
4	S	10061	0	9954	92	0
4	T	10667	0	10542	96	0
4	W	10622	0	10500	107	0
4	X	10108	0	9980	92	0
5	5	2074	0	2050	19	0
5	b	2478	0	2466	0	0
6	6	2330	0	2354	18	0
6	7	2315	0	2335	14	0
6	c	2330	0	2354	0	0
6	d	2365	0	2379	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	0	666	0	647	4	0
7	1	666	0	647	2	0
7	2	666	0	647	4	0
7	3	666	0	647	2	0
All	All	62671	0	62240	404	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 4.

The worst 5 of 404 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)
4:S:777:ARG:NH2	4:S:885:CYS:O	2.27	0.67
4:T:536:VAL:HG13	4:T:1244:SER:HA	1.77	0.66
4:S:770:LEU:HD21	4:S:883:LEU:HD22	1.76	0.66
4:W:770:LEU:HD21	4:W:883:LEU:HD22	1.76	0.66
4:W:929:ASP:OD1	4:W:932:ARG:NH2	2.29	0.66

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	k	334/454 (74%)	322 (96%)	12 (4%)	0	100	100
2	l	81/549 (15%)	81 (100%)	0	0	100	100
2	m	76/549 (14%)	75 (99%)	1 (1%)	0	100	100
3	n	38/2635 (1%)	38 (100%)	0	0	100	100
3	o	38/2635 (1%)	38 (100%)	0	0	100	100
4	S	1273/1376 (92%)	1179 (93%)	92 (7%)	2 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	T	1354/1376 (98%)	1273 (94%)	78 (6%)	3 (0%)	47	81
4	W	1350/1376 (98%)	1287 (95%)	61 (4%)	2 (0%)	51	85
4	X	1282/1376 (93%)	1201 (94%)	79 (6%)	2 (0%)	47	81
5	5	262/331 (79%)	250 (95%)	12 (5%)	0	100	100
5	b	315/331 (95%)	307 (98%)	8 (2%)	0	100	100
6	6	290/305 (95%)	275 (95%)	15 (5%)	0	100	100
6	7	288/305 (94%)	275 (96%)	13 (4%)	0	100	100
6	c	290/305 (95%)	282 (97%)	8 (3%)	0	100	100
6	d	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
7	0	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	1	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	2	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	3	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
All	All	7871/14888 (53%)	7475 (95%)	387 (5%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	W	263	THR
4	T	10	PHE
4	X	992	LYS
4	S	992	LYS
4	S	993	SER

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	k	293/377 (78%)	293 (100%)	0	100	100
2	l	76/473 (16%)	76 (100%)	0	100	100
2	m	71/473 (15%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	35/2239 (2%)	35 (100%)	0	100	100
3	o	35/2239 (2%)	35 (100%)	0	100	100
4	S	1094/1166 (94%)	1086 (99%)	8 (1%)	84	90
4	T	1154/1166 (99%)	1154 (100%)	0	100	100
4	W	1150/1166 (99%)	1149 (100%)	1 (0%)	93	97
4	X	1097/1166 (94%)	1092 (100%)	5 (0%)	88	93
5	5	229/281 (82%)	229 (100%)	0	100	100
5	b	272/281 (97%)	272 (100%)	0	100	100
6	6	267/274 (97%)	266 (100%)	1 (0%)	91	94
6	7	264/274 (96%)	259 (98%)	5 (2%)	57	75
6	c	267/274 (97%)	267 (100%)	0	100	100
6	d	270/274 (98%)	270 (100%)	0	100	100
7	0	70/141 (50%)	70 (100%)	0	100	100
7	1	70/141 (50%)	70 (100%)	0	100	100
7	2	70/141 (50%)	70 (100%)	0	100	100
7	3	70/141 (50%)	70 (100%)	0	100	100
All	All	6854/12687 (54%)	6834 (100%)	20 (0%)	92	95

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	130	ASN
6	7	97	ASN
6	7	305	ARG
6	7	231	ARG
4	S	1169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
5	b	124	GLN
6	6	110	GLN
6	c	40	GLN
6	d	146	HIS
6	6	281	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

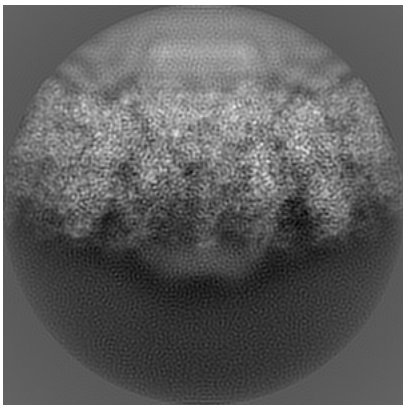
6 Map visualisation (i)

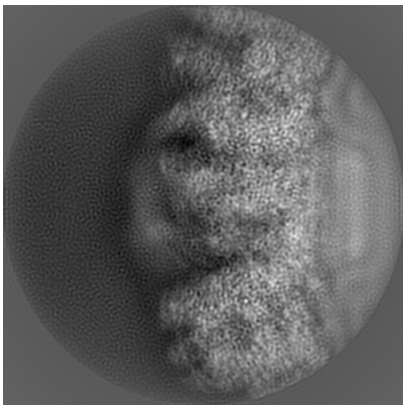
This section contains visualisations of the EMDB entry EMD-20432. These allow visual inspection of the internal detail of the map and identification of artifacts.

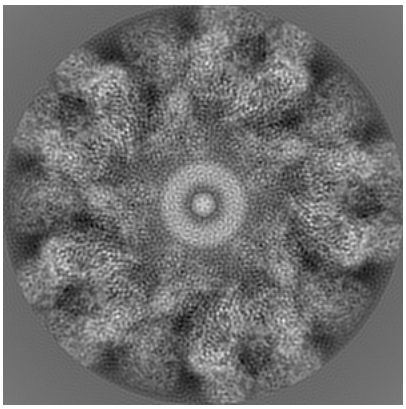
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

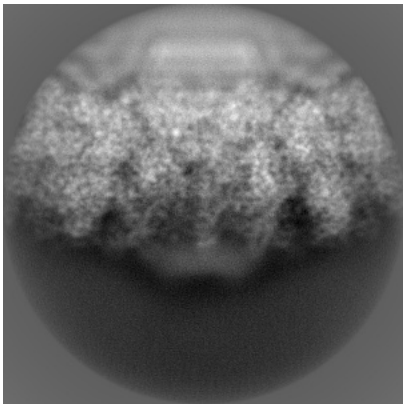
6.1.1 Primary map

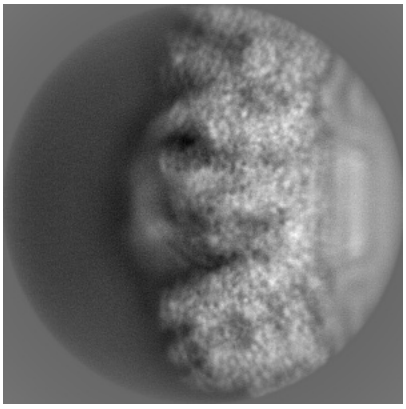

X

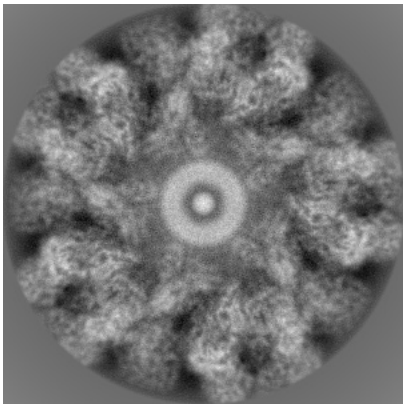

Y


Z

6.1.2 Raw map


X

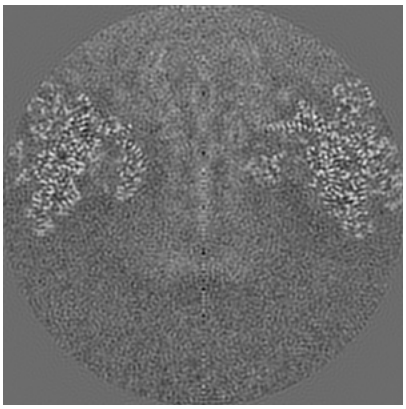

Y

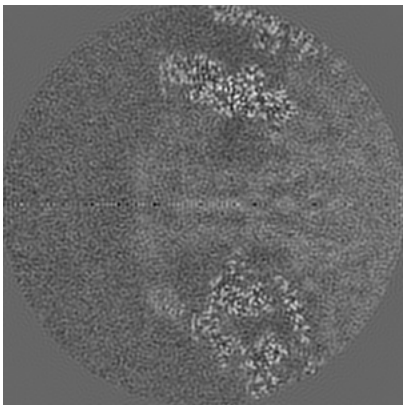

Z

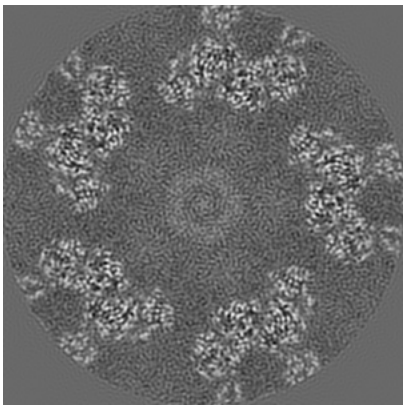
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

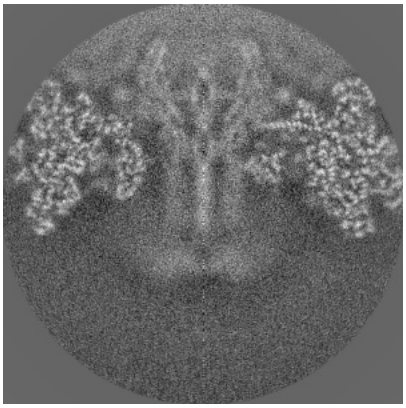
6.2.1 Primary map

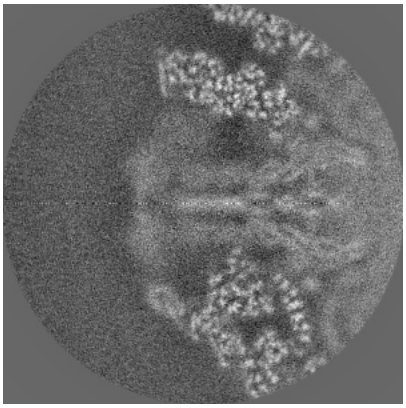

X Index: 192

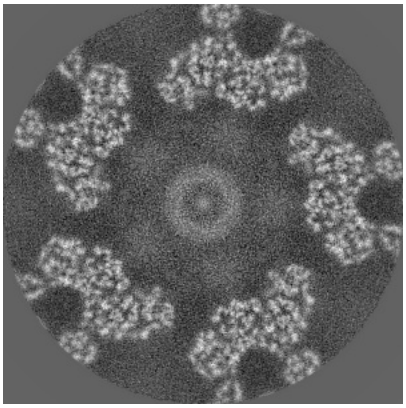

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

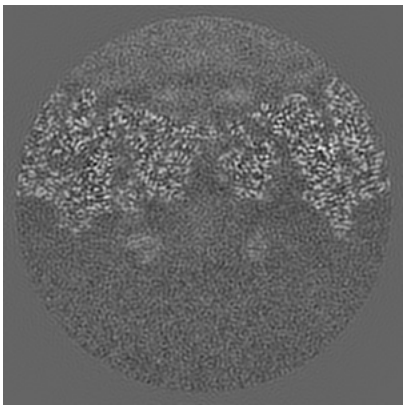

Y Index: 192


Z Index: 192

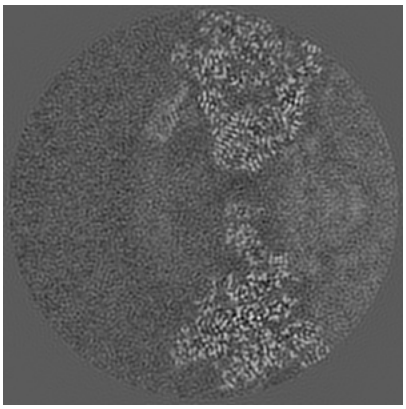
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

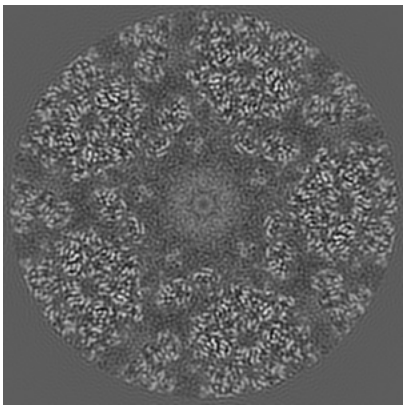
6.3.1 Primary map



X Index: 262

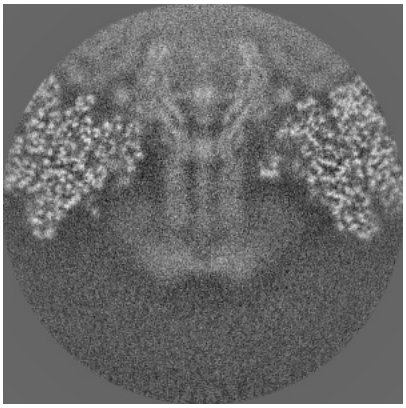


Y Index: 242

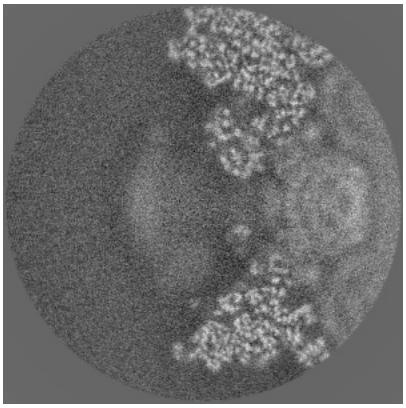


Z Index: 246

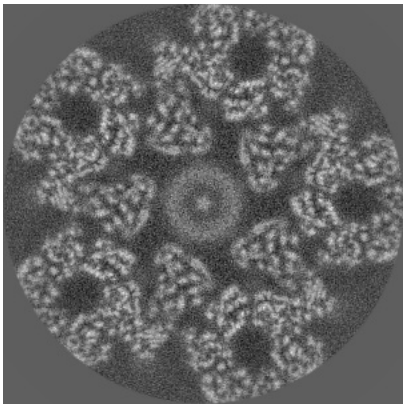
6.3.2 Raw map



X Index: 199



Y Index: 154

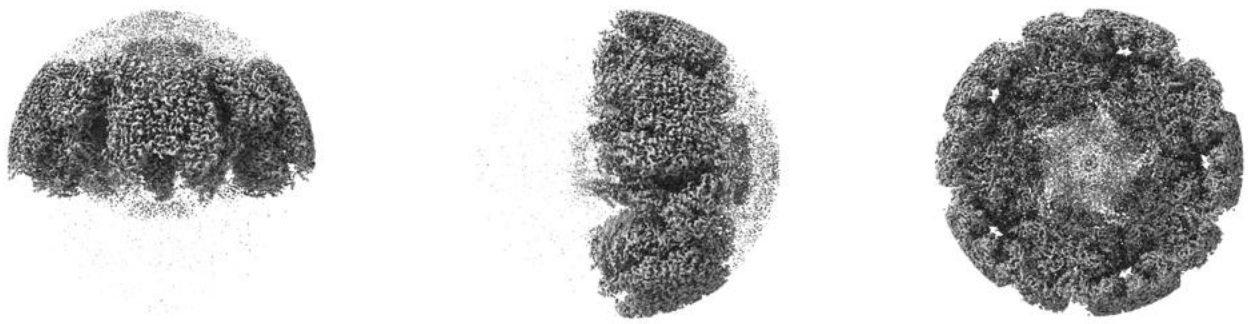


Z Index: 216

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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

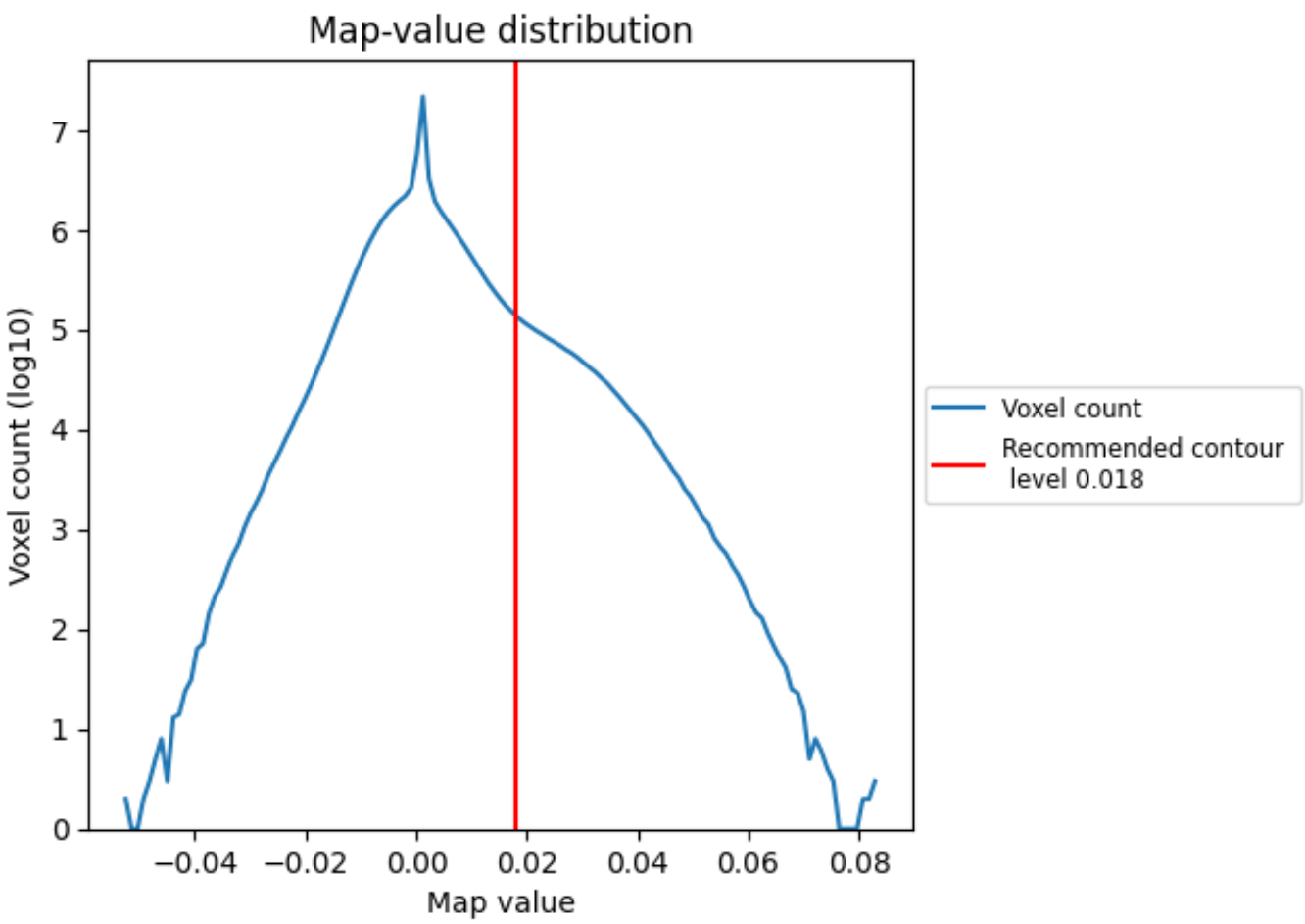
6.5 Mask visualisation (i)

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

7 Map analysis (i)

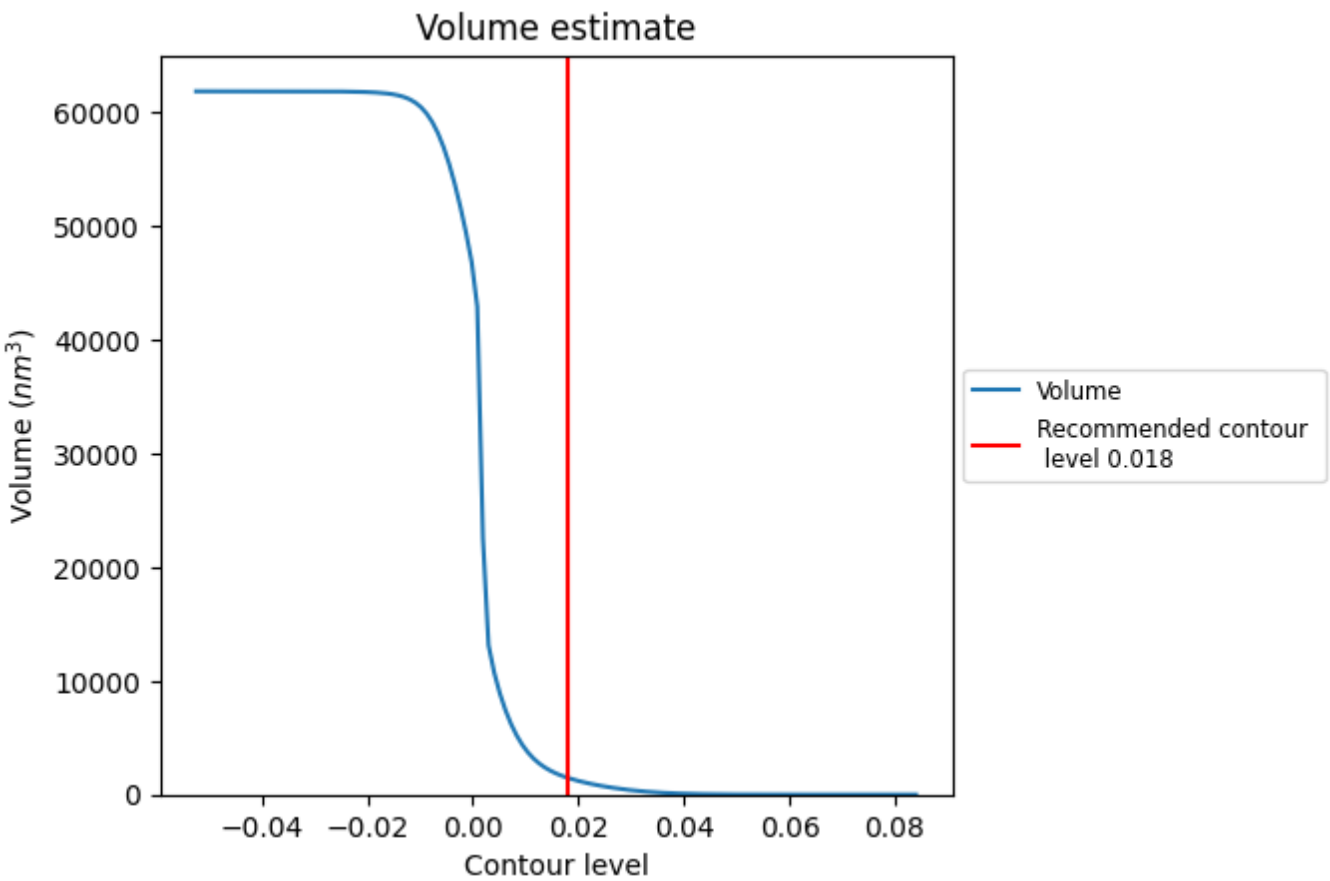
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

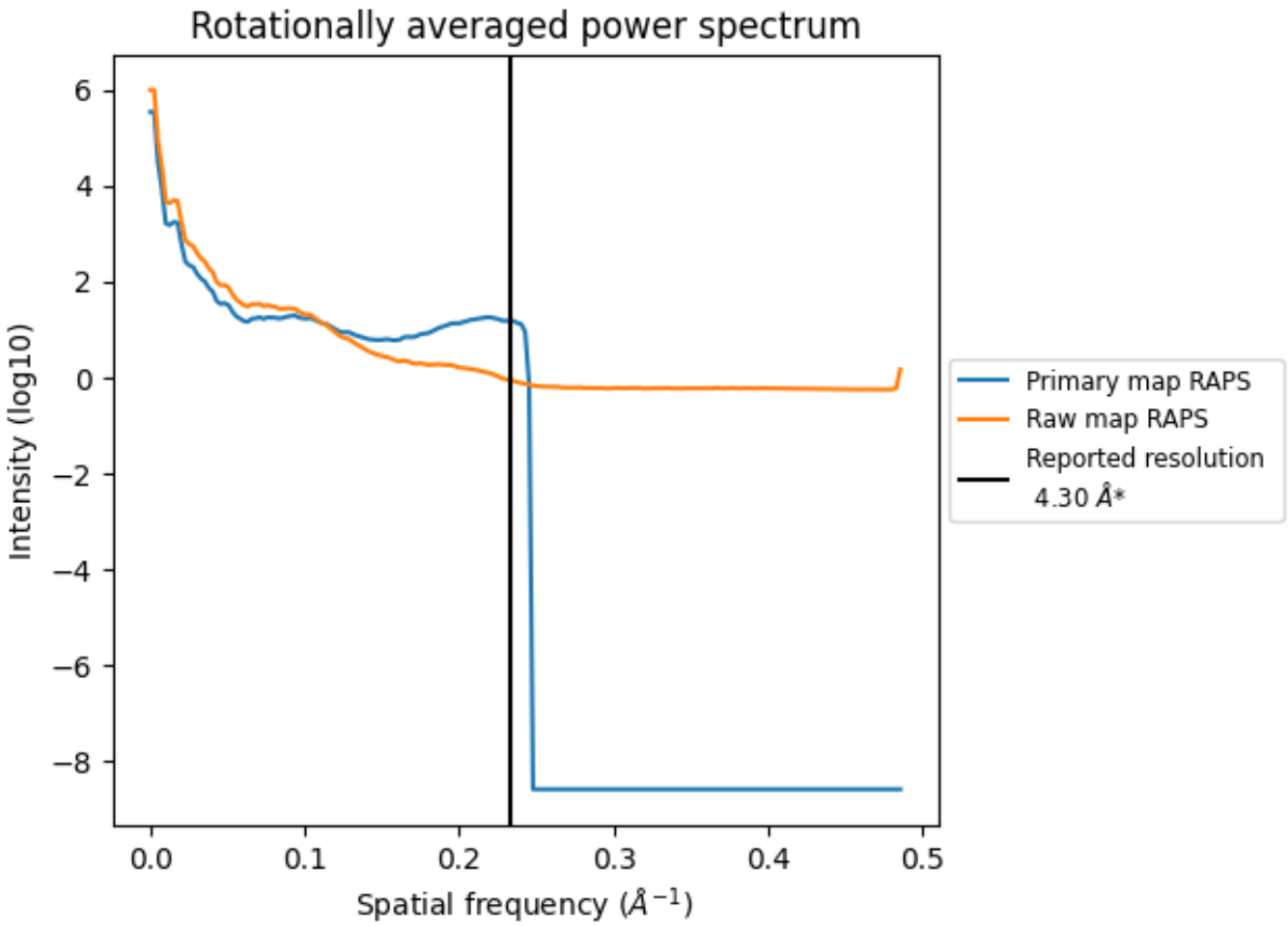
7.2 Volume estimate (i)



The volume at the recommended contour level is 1471 nm^3; this corresponds to an approximate mass of 1329 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)

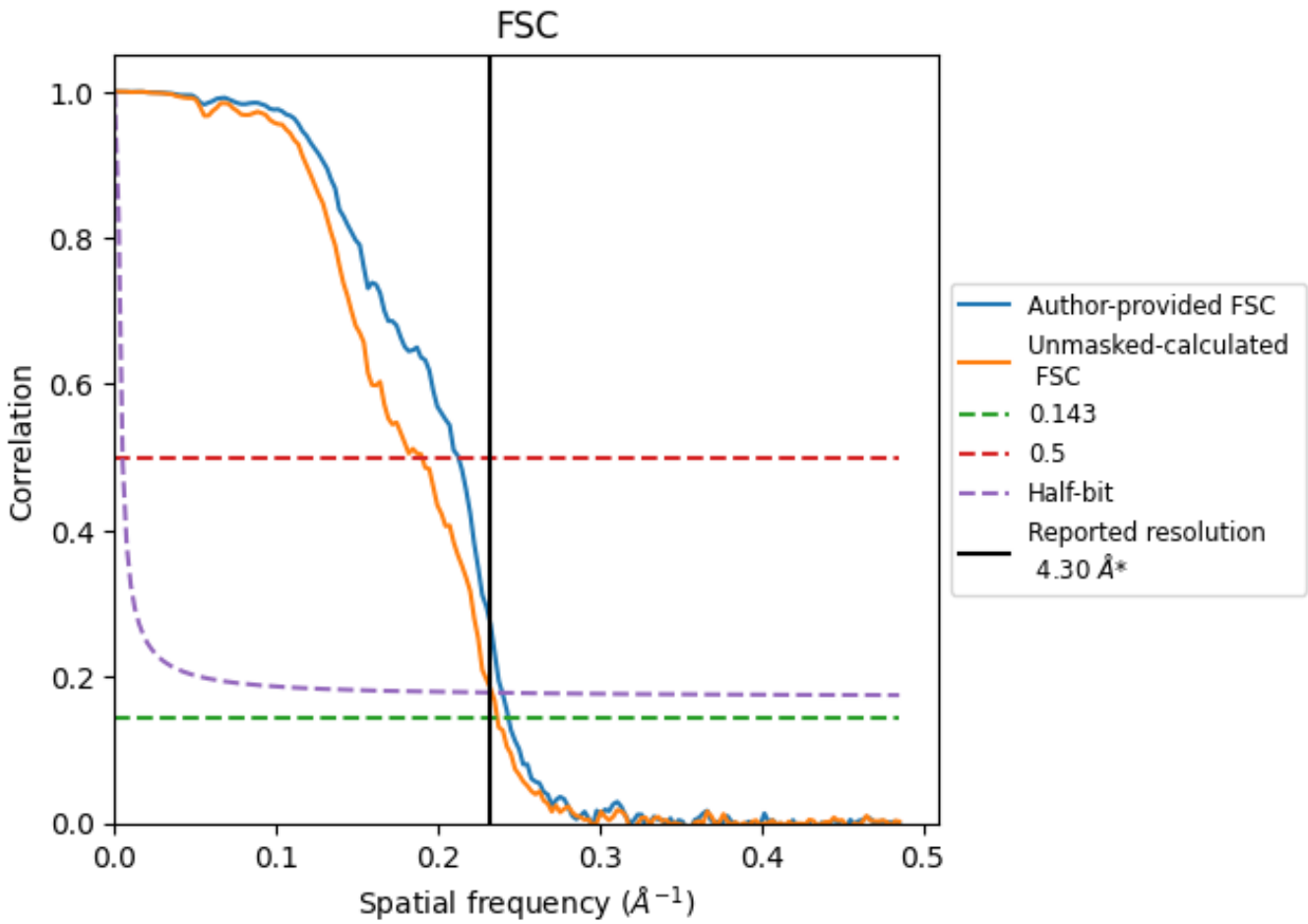


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

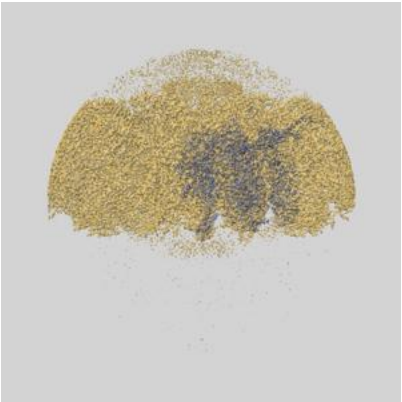
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.10	4.70	4.17
Unmasked-calculated*	4.22	5.26	4.28

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

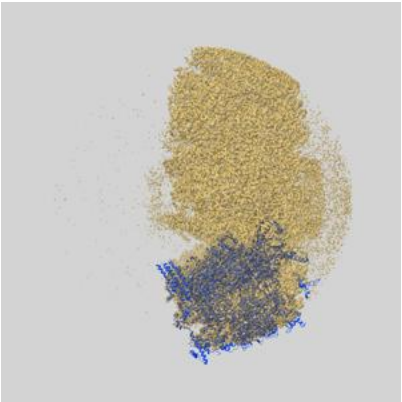
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20432 and PDB model 6PPB. Per-residue inclusion information can be found in section 3 on page 7.

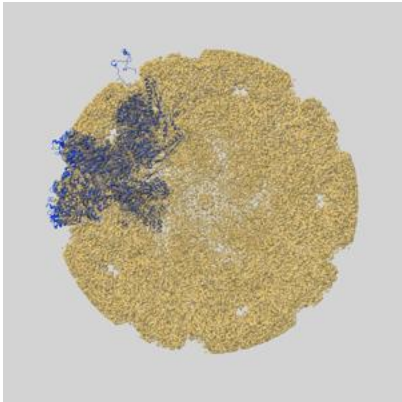
9.1 Map-model overlay (i)



X



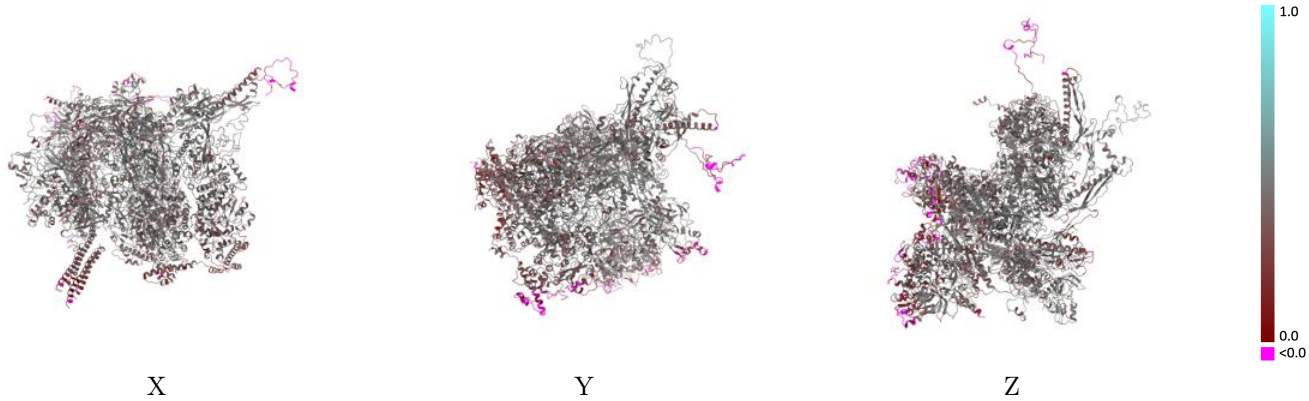
Y



Z

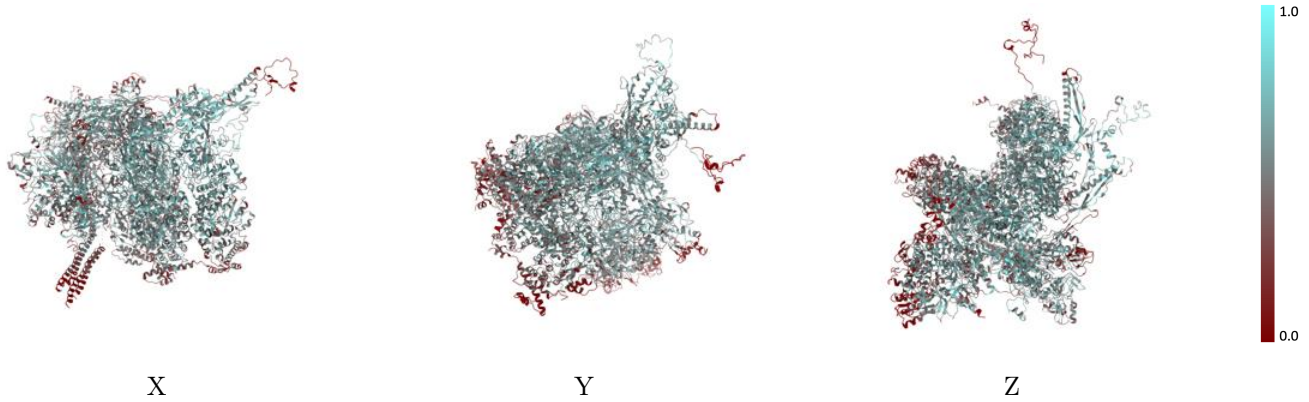
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



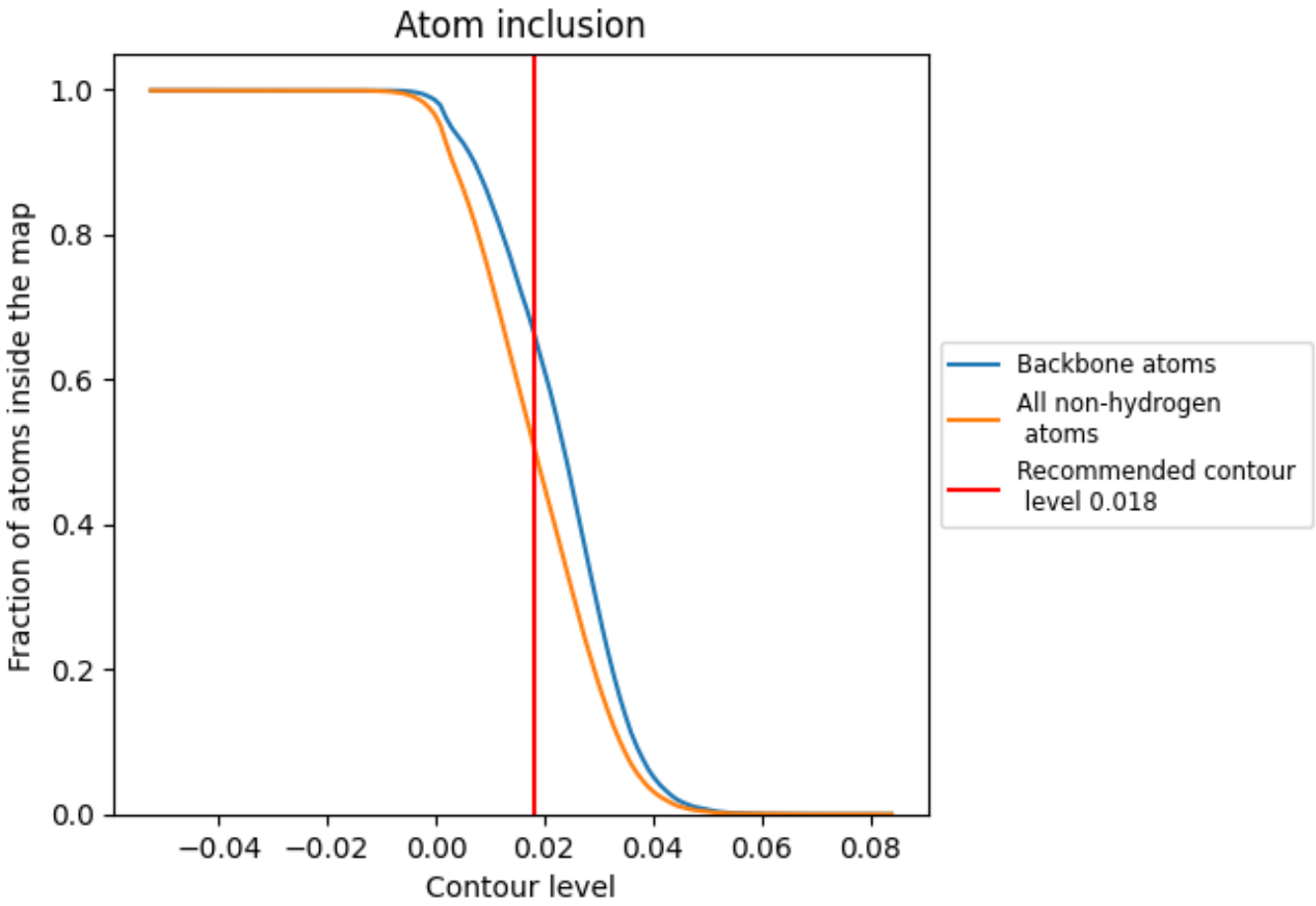
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5110	0.3950
0	0.1246	0.1290
1	0.3442	0.3100
2	0.3318	0.3150
3	0.3209	0.3080
5	0.4655	0.4070
6	0.5321	0.4240
7	0.5108	0.4190
S	0.5794	0.4360
T	0.5485	0.3970
W	0.4928	0.3780
X	0.5867	0.4410
b	0.5021	0.3890
c	0.3941	0.3340
d	0.3856	0.3190
k	0.5197	0.4070
l	0.3660	0.3370
m	0.2957	0.3030
n	0.2190	0.2400
o	0.1524	0.2560