Full wwPDB EM Validation 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 Full wwPDB EM Validation 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:

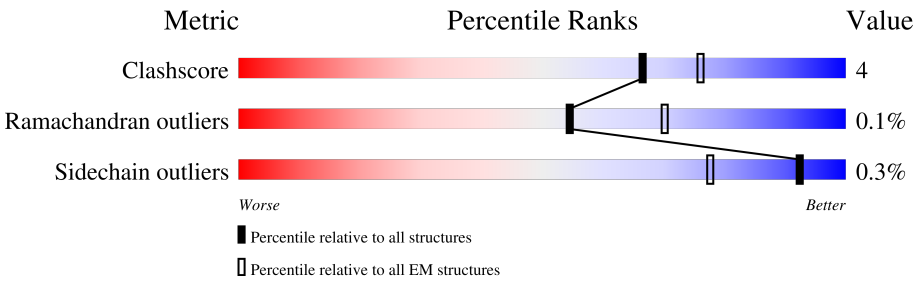
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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% •

Continued on next page...

Continued from previous page...

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.

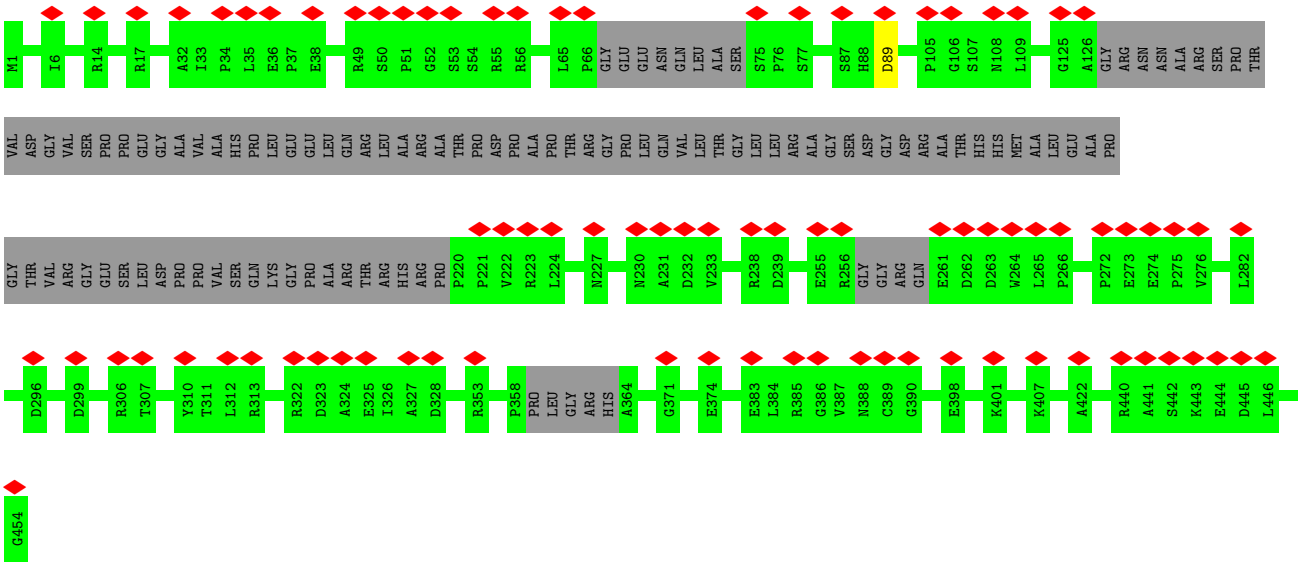
Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

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.

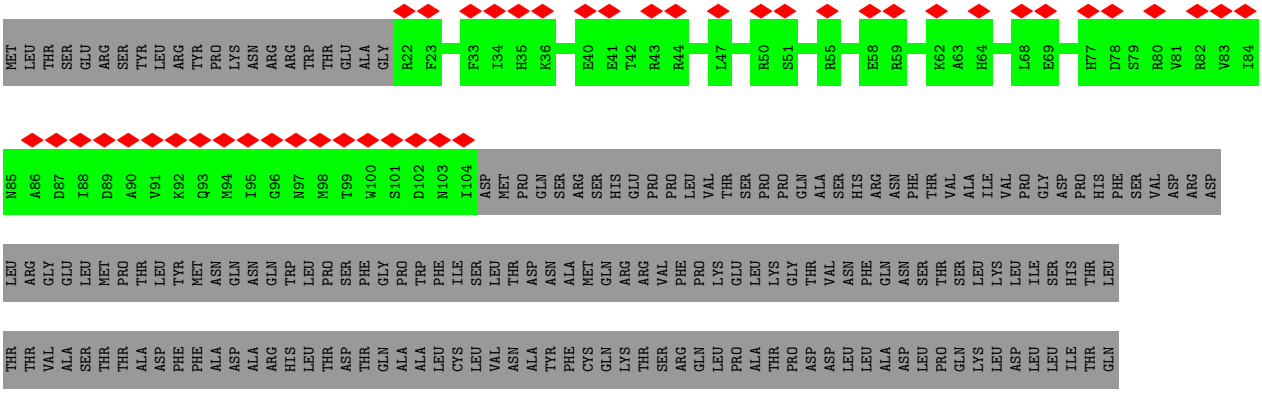
- Molecule 1: Capsid vertex component 1

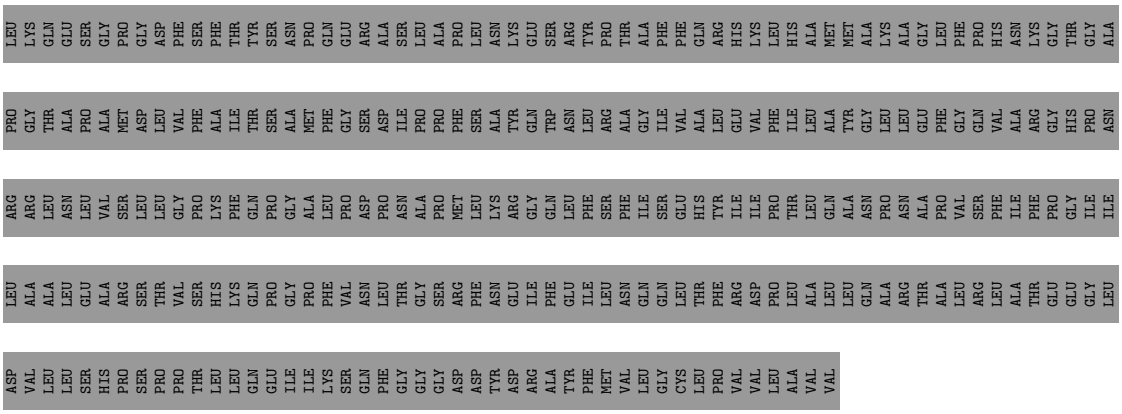
Chain k:



- Molecule 2: Capsid vertex component 2

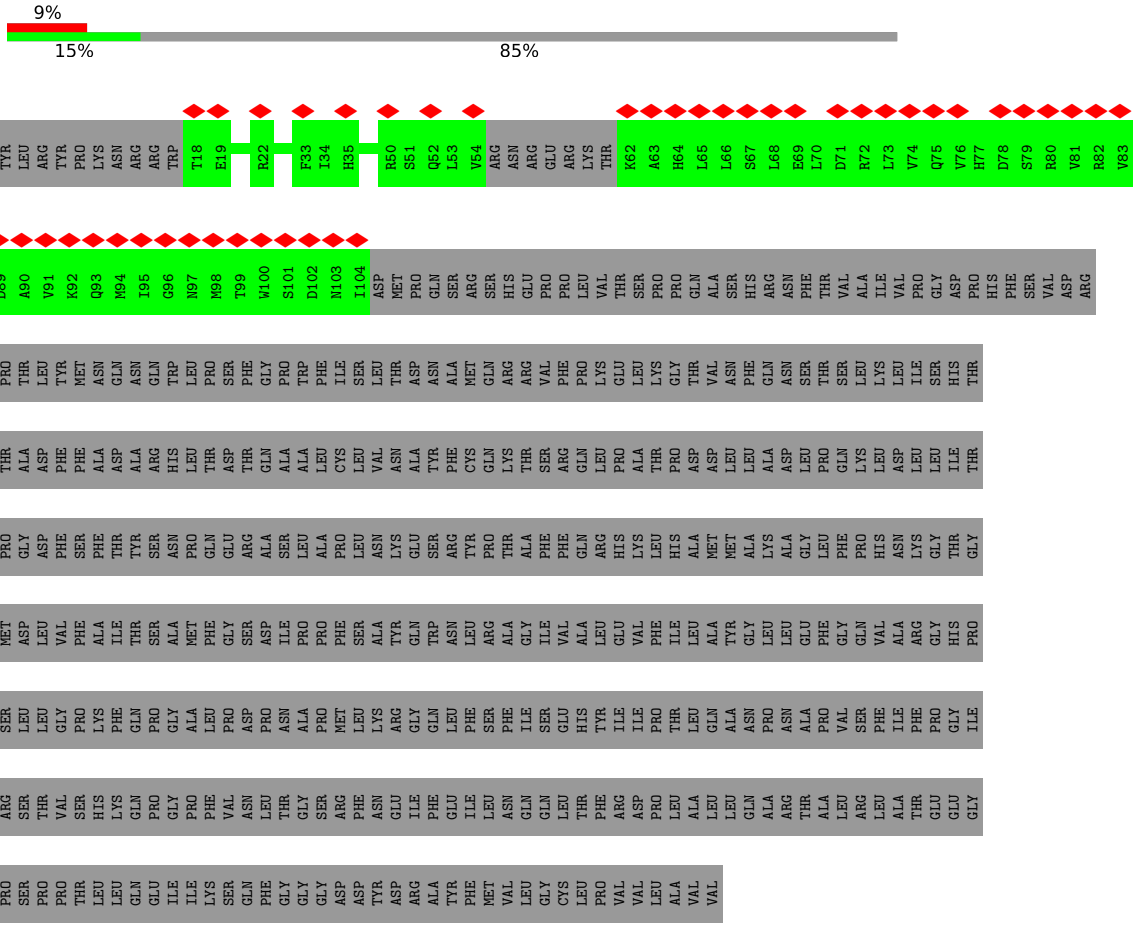
Chain l:





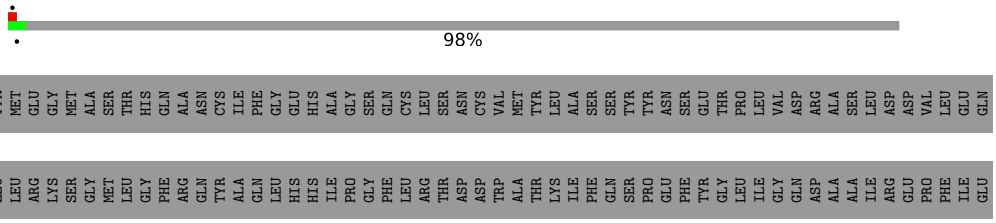
- Molecule 2: Capsid vertex component 2

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 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 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

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

ALA ALA TYR PHE GLU ASN ILE ILE THR ALA LEU SER THR PHE GLN 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

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

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

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

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

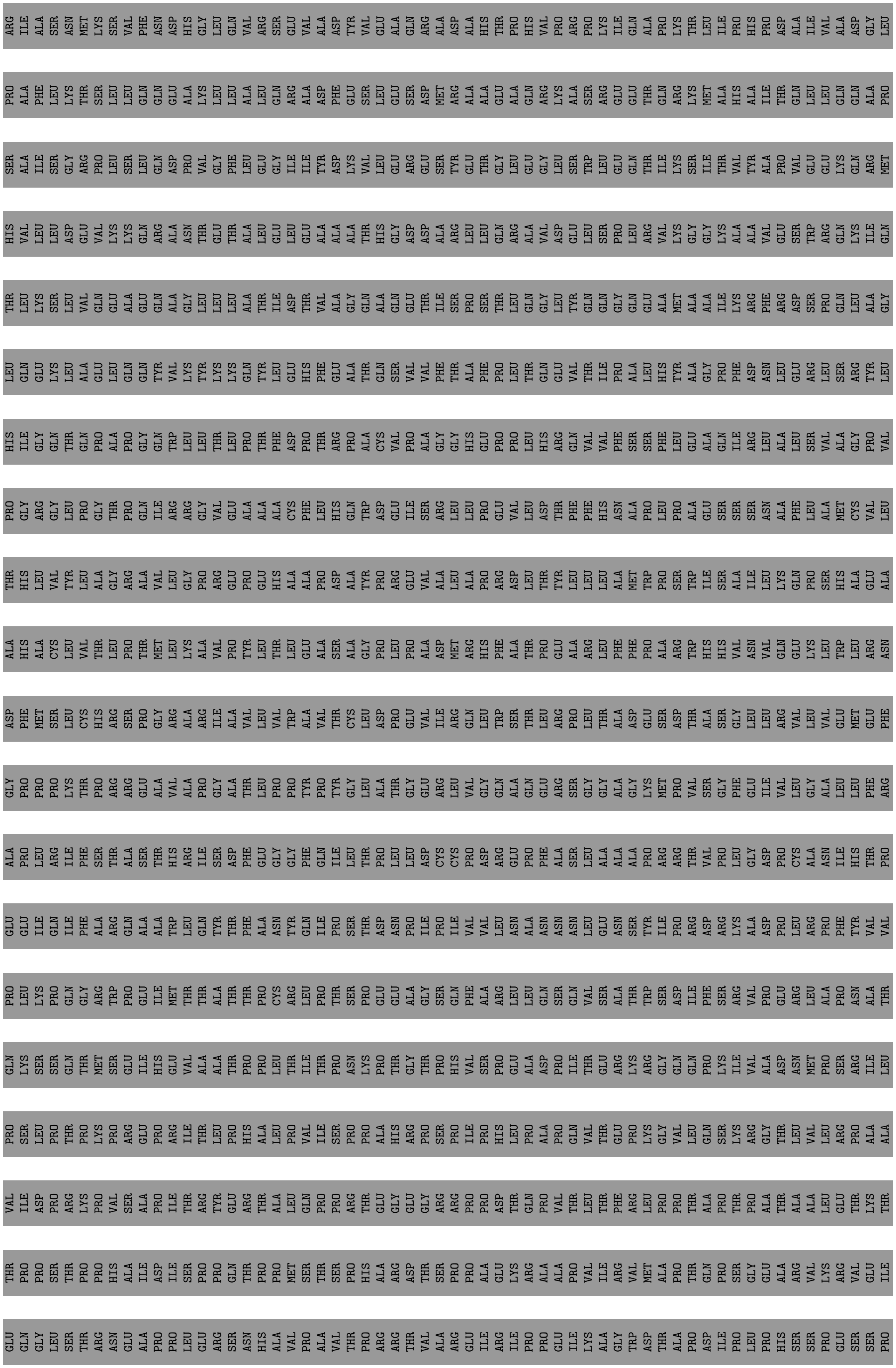
GLY TYR GLY SER VAL GLN ASP TYR LYS GLU THR VAL GLN ILE ILE SER SER LEU VAL GLY ILE GLN LYS LEU VAL ARG ASP GLN GLY ALA ASP LYS TRP ALA THR ALA VAL THR ARG LEU THR ASP LEU LYS SER THR LEU ALA THR THR ALA ILE GLU THR ALA THR LYS ARG LYS LEU

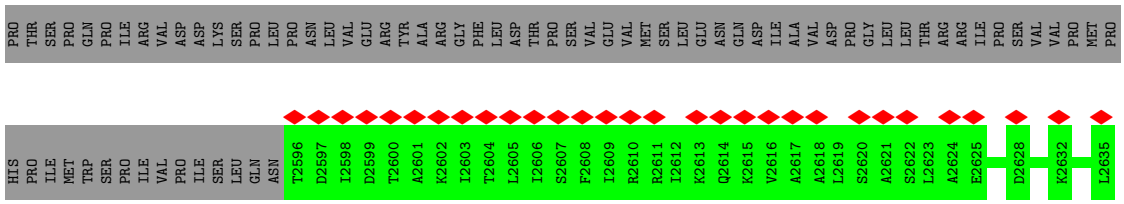
TYR ARG LEU ILE GLN ARG ASP LEU LYS GLU ALA GLN LYS HIS GLU THR ASN ARG ALA MET GLU GLU TRP LYS GLN LYS VAL LEU ALA LEU ASP ASN ALA SER PRO GLU ARG VAL ALA THR LEU LEU GLN GLN ALA PRO THR ALA LYS ALA ARG GLU PHE ALA GLU LYS HIS PHE LYS ILE

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

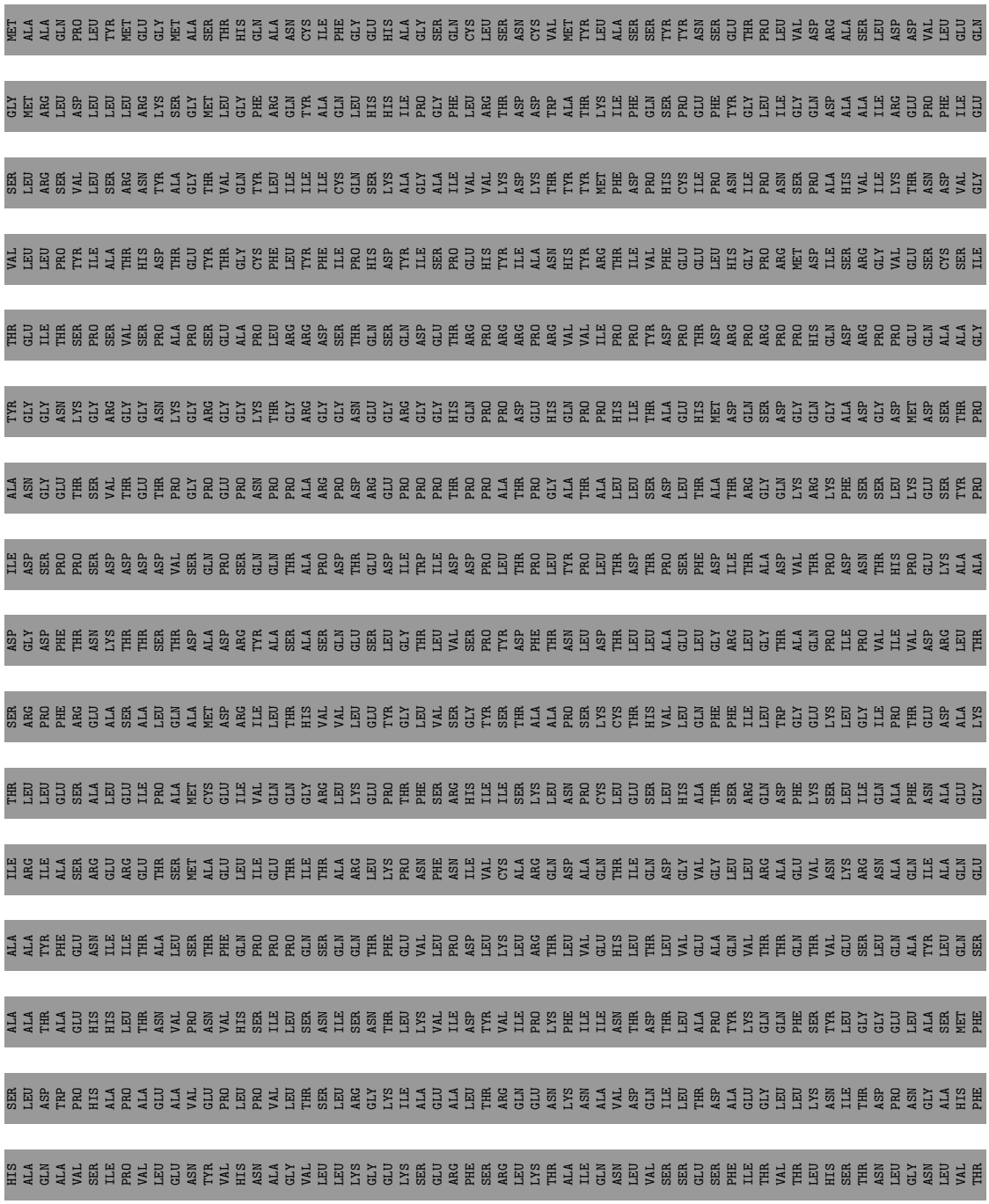
LEU THR PRO TYR GLN ASP GLN VAL SER PHE PHE LEU ARG THR ILE GLY LEU PRO LEU VAL ARG ALA LEU ALA ASP LYS ILE SER VAL GLN ALA LEU ARG LEU SER HIS ALA LEU GLN SER GLY ASP LEU GLN GLN ALA THR VAL GLY THR PRO LEU GLU LEU PRO ALA THR GLU TYR ALA


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



- Molecule 3: Large tegument protein deneddylase

Chain o: 98%



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 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 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 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

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

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

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

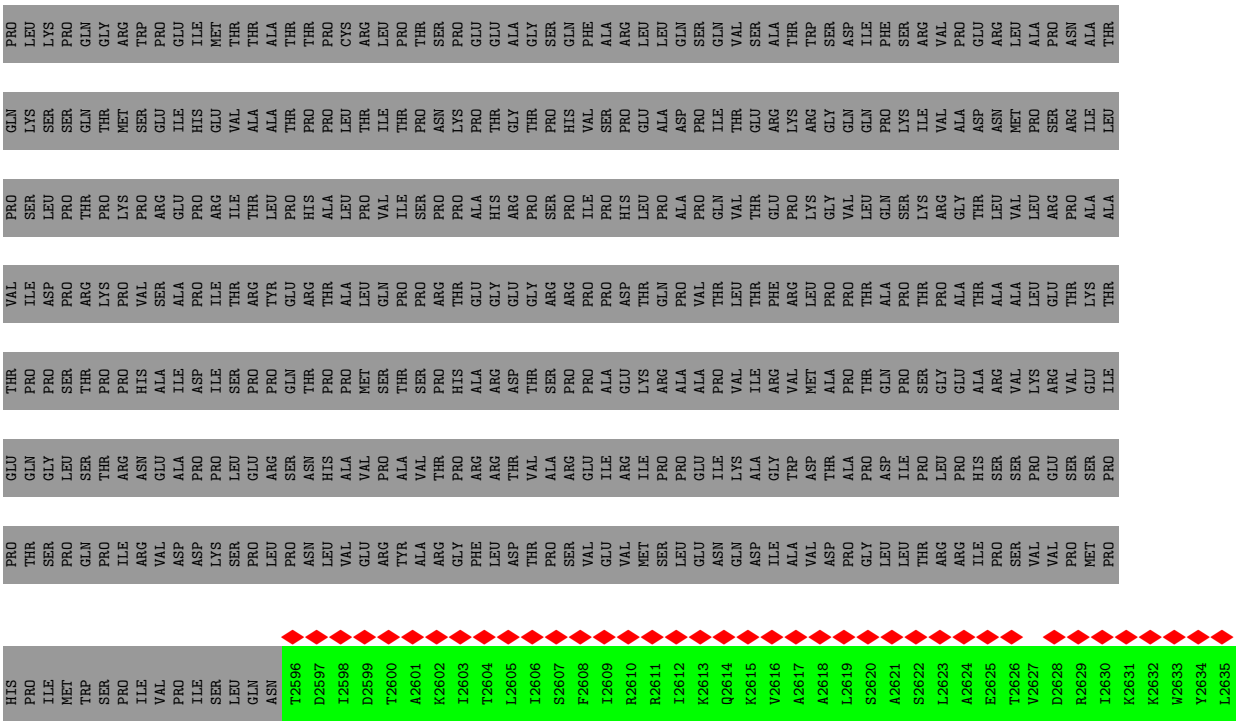
ALA HIS ALA CYS LEU VAL THR LEU PRO THR MET LEU LYS ALA VAL PRO TYR LEU THR LEU GLU ALA SER ALA GLY PRO LEU PRO ALA ASP MET ARG HIS PHE ALA THR PRO GLU ALA ARG LEU PHE PHE PRO ALA ARG TRP HIS HIS VAL ASN VAL GLN GLU LYS LEU TRP LEU ARG ASN

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

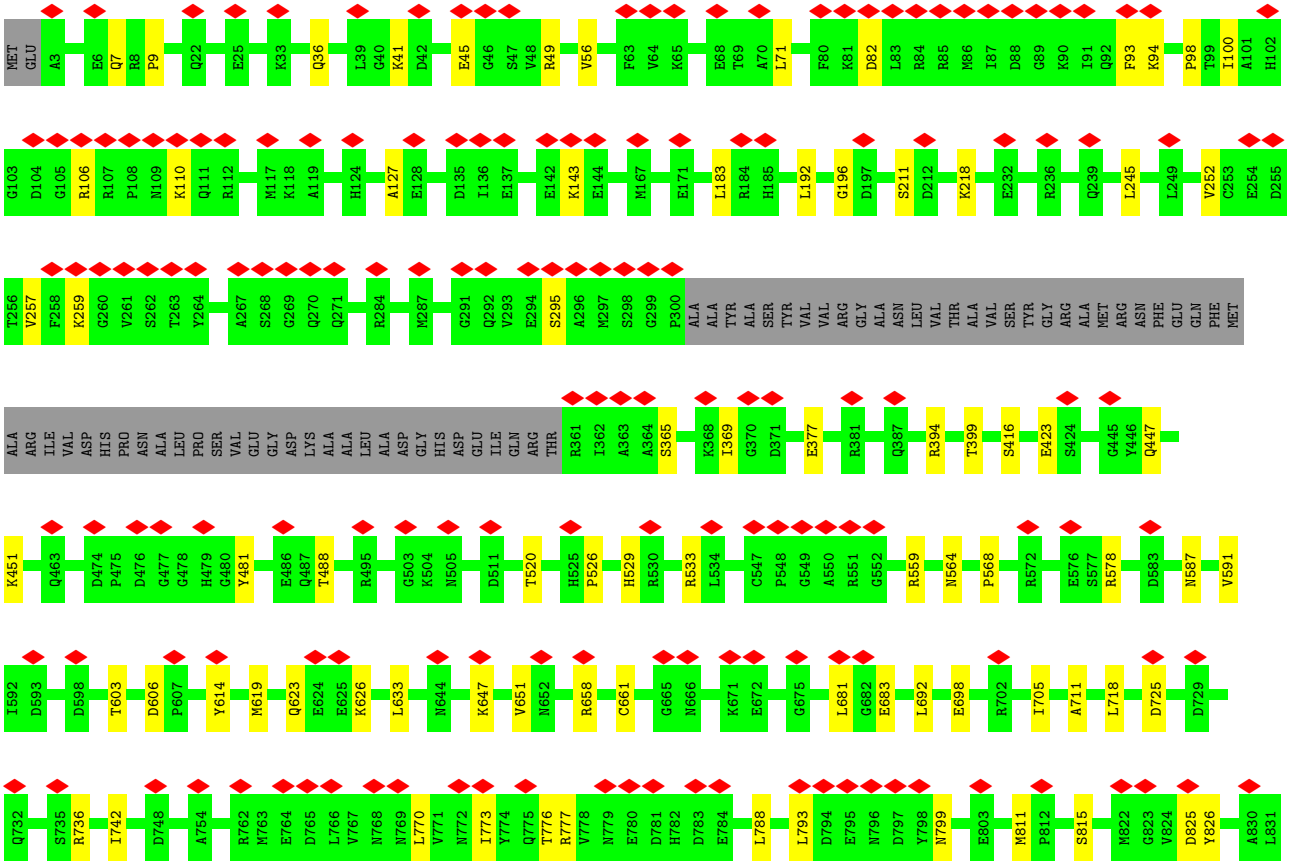
ALA PRO LEU ARG ILE PHE SER THR ALA SER THR HIS ARG ILE SER ASP PHE GLU GLY GLY PHE GLN ILE LEU THR PRO LEU LEU ASP CYS CYS PRO ASP ARG GLU PRO PHE ALA SER LEU ALA ALA ALA PRO ARG ARG THR VAL PRO LEU GLY ASP PRO CYS ALA ASN ILE HIS THR PRO

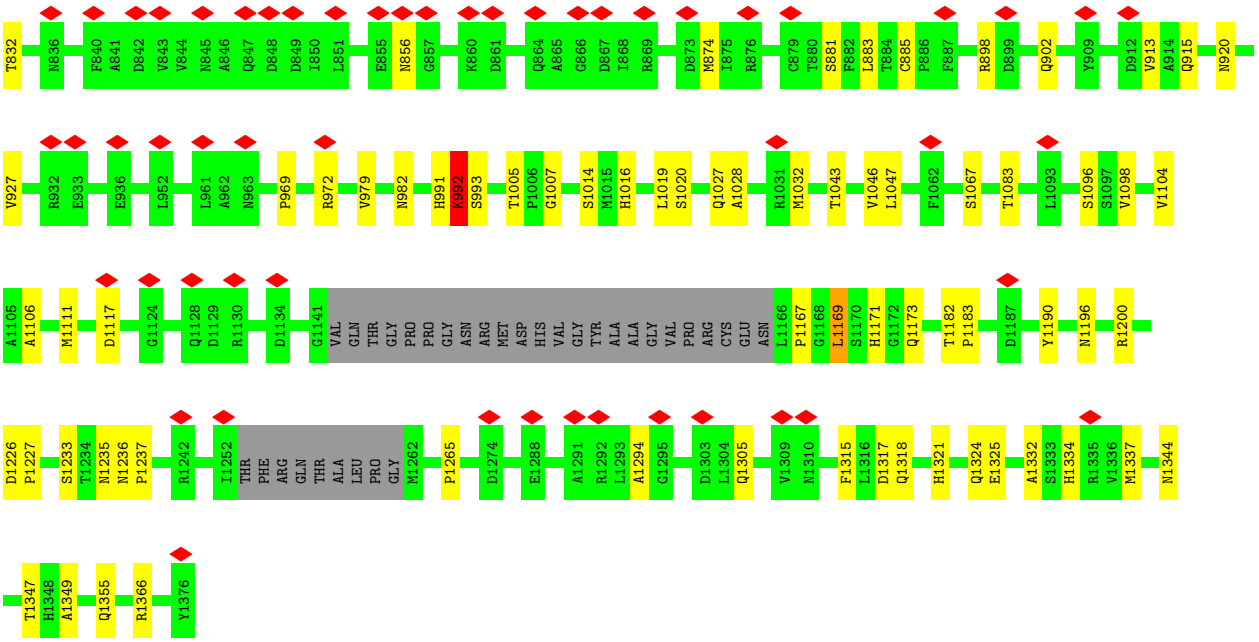
GLU GLU ILE GLN ILE PHE ALA ARG GLN ALA ALA TRP LEU GLN TYR THR PHE ALA ASN TYR GLN ILE PRO SER THR ASP ASN PRO ILE PRO ILE VAL VAL LEU ASN ALA ASN ASN ASN LEU GLU ASN SER TYR ILE PRO ARG ASP ARG LYS ALA ASP PRO LEU ARG PRO PHE TYR VAL VAL



- Molecule 4: Major capsid protein

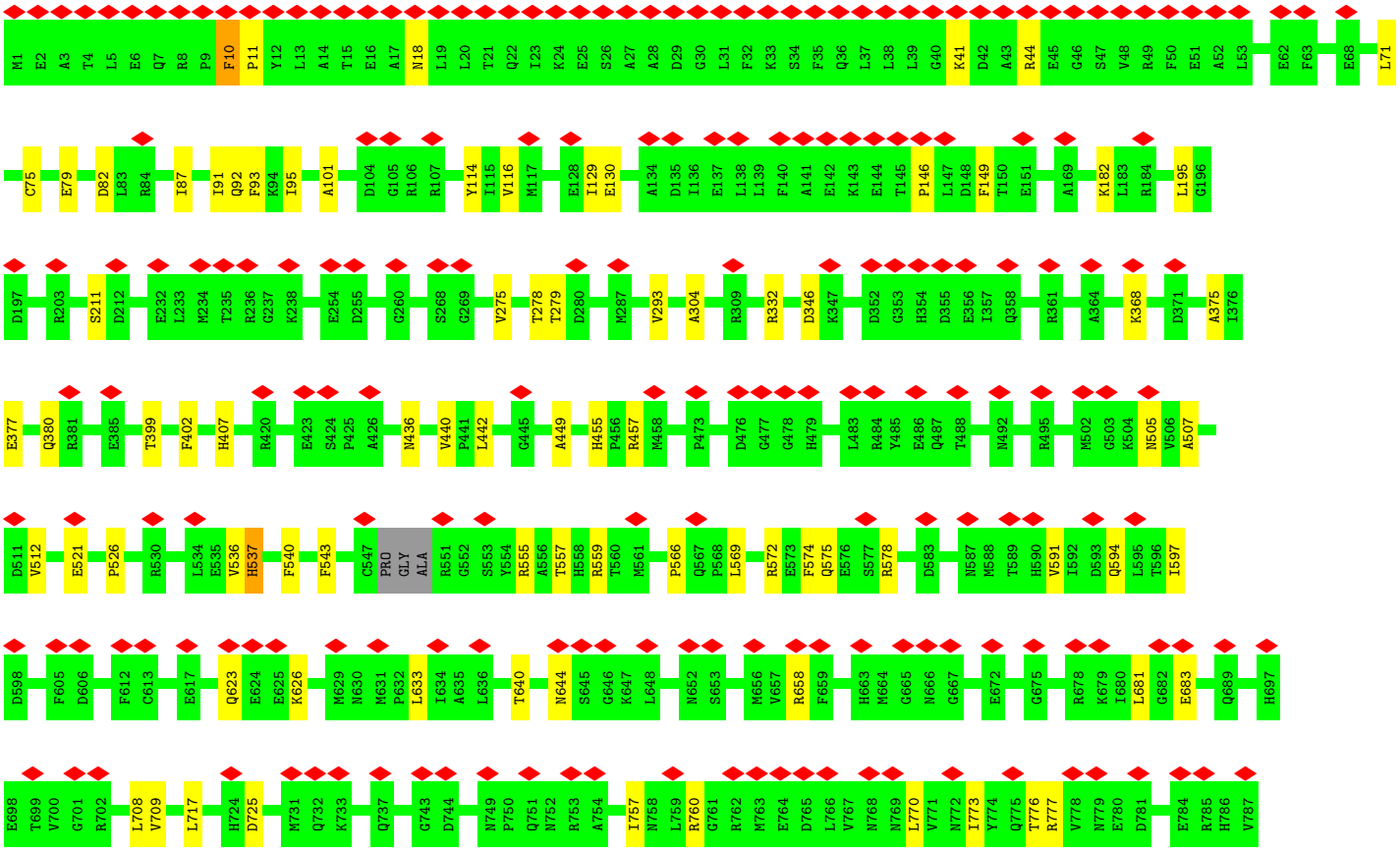
Chain S:

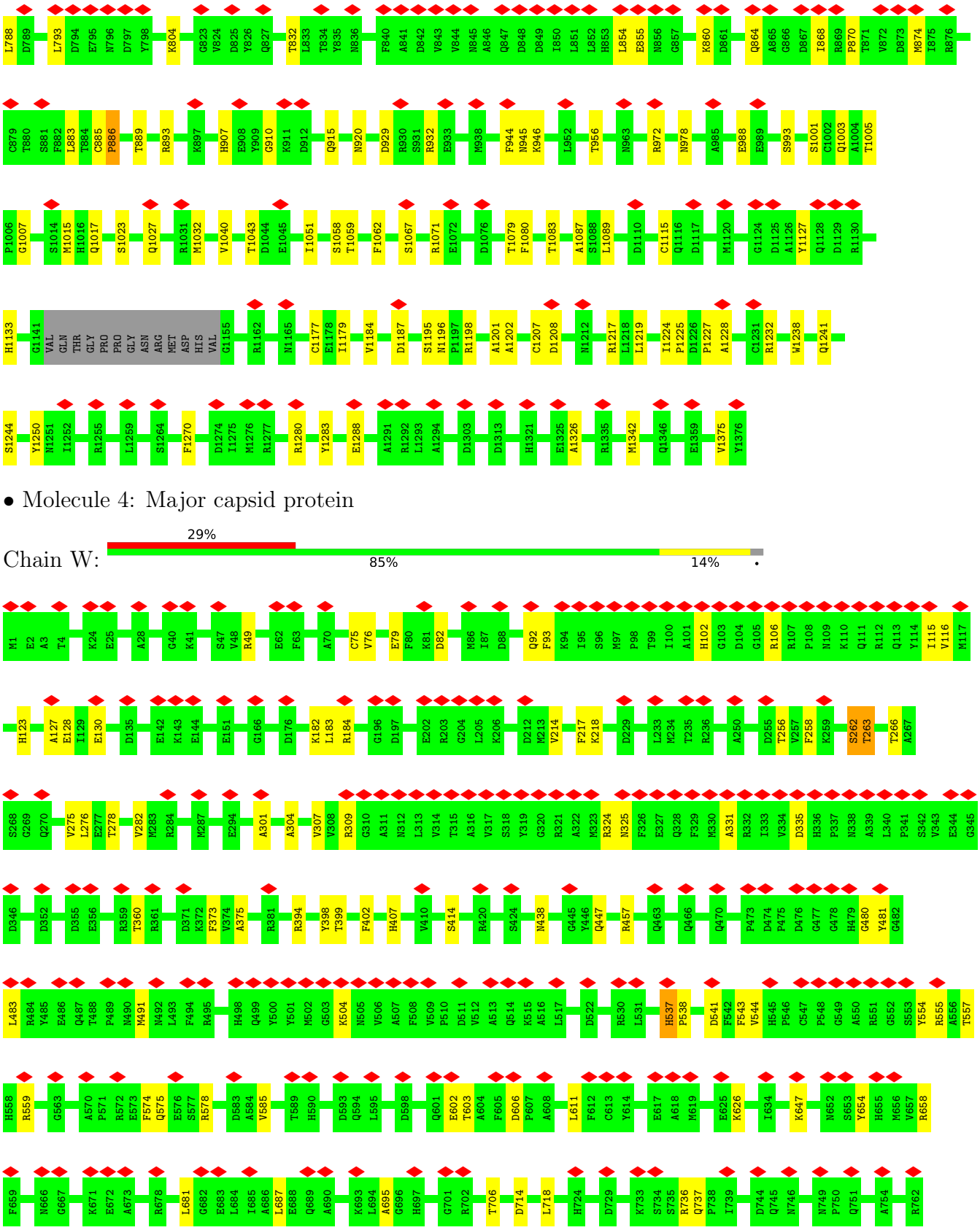




- Molecule 4: Major capsid protein

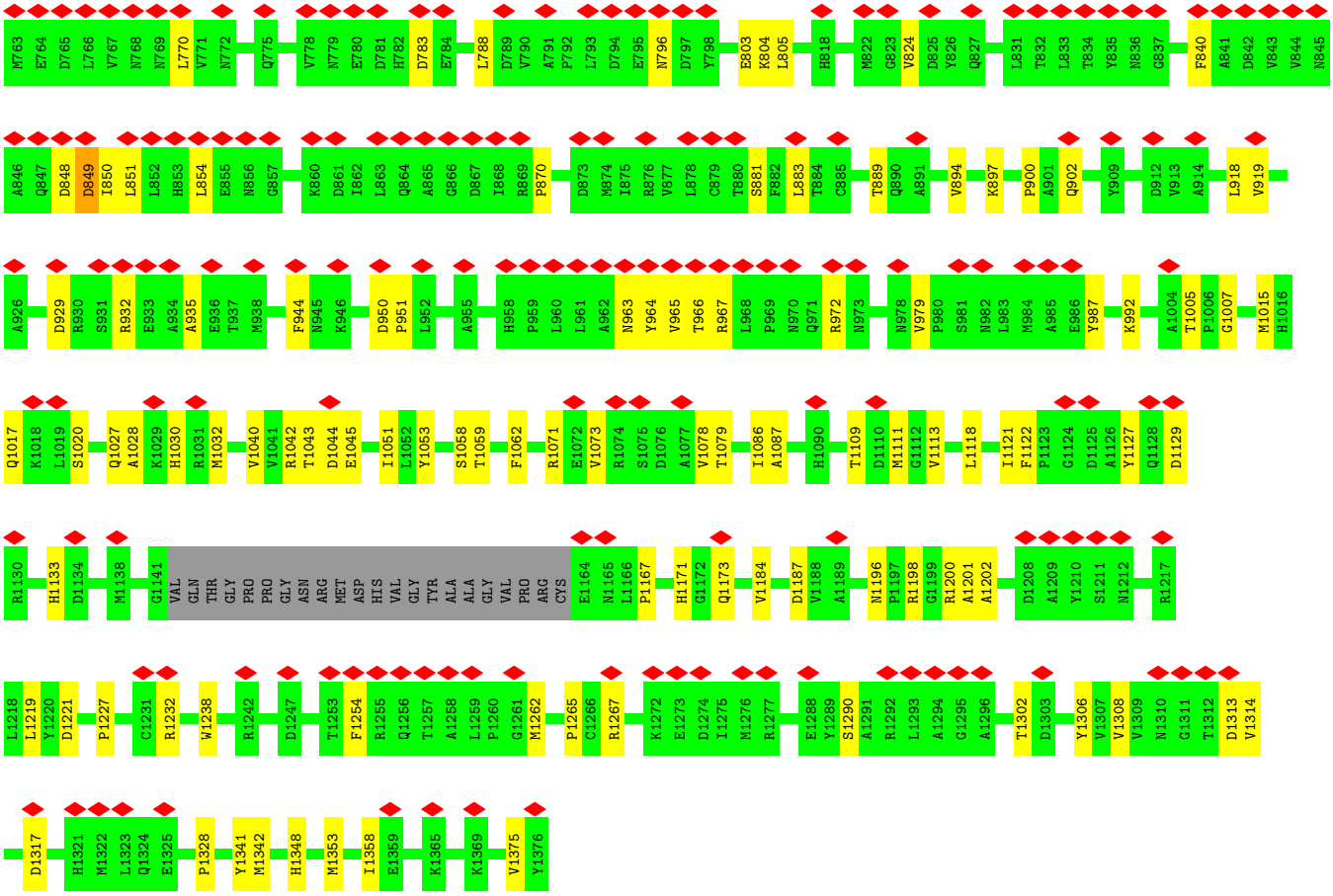
Chain T:





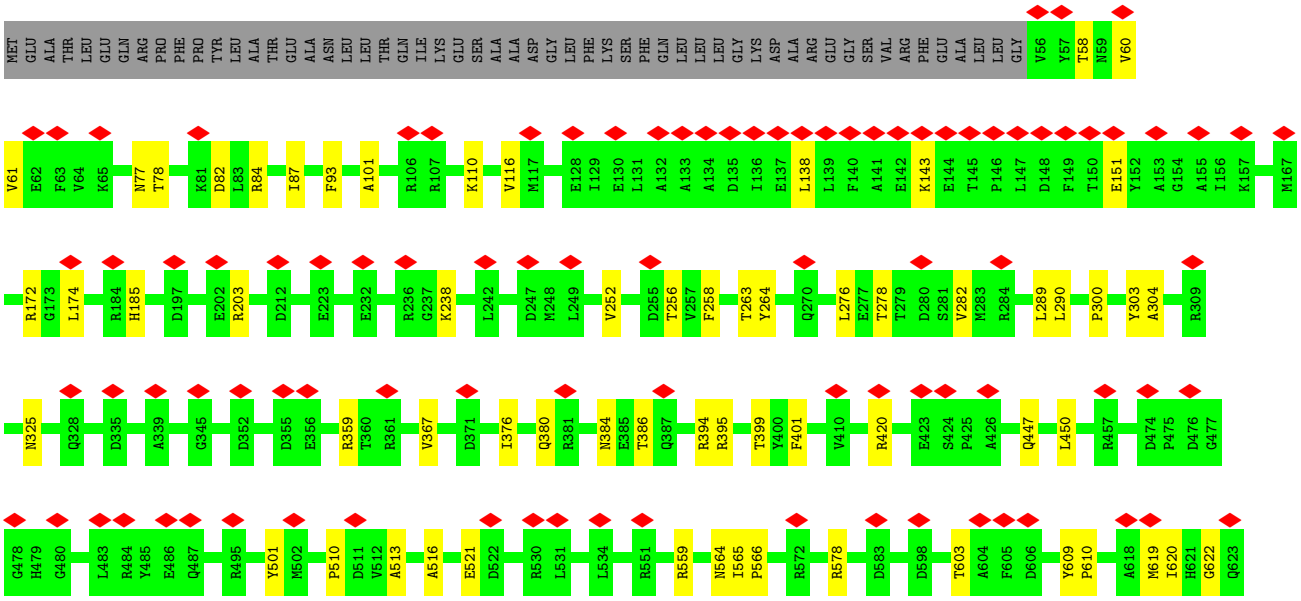
- Molecule 4: Major capsid protein

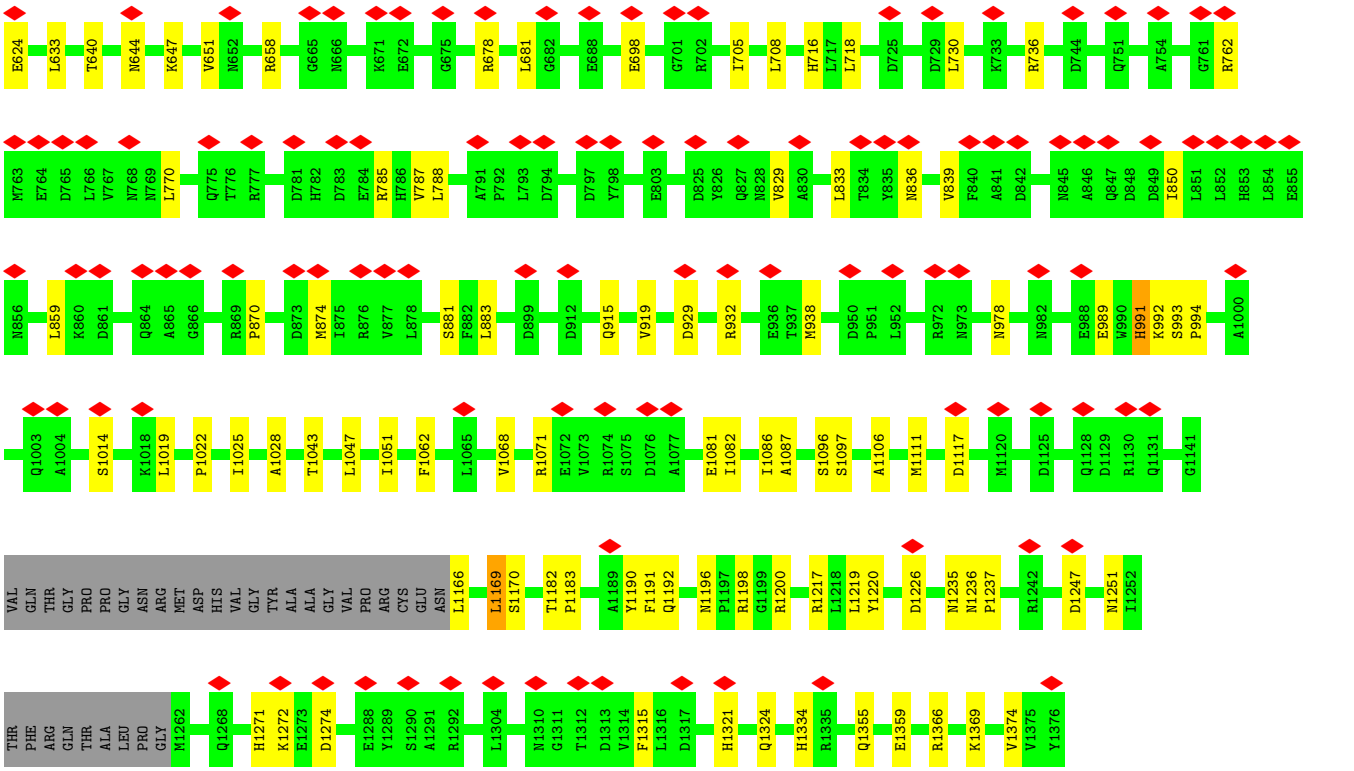
Chain W:



- Molecule 4: Major capsid protein

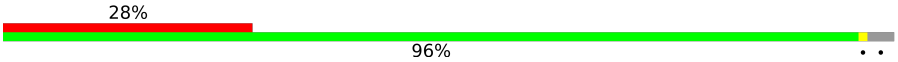
Chain X:

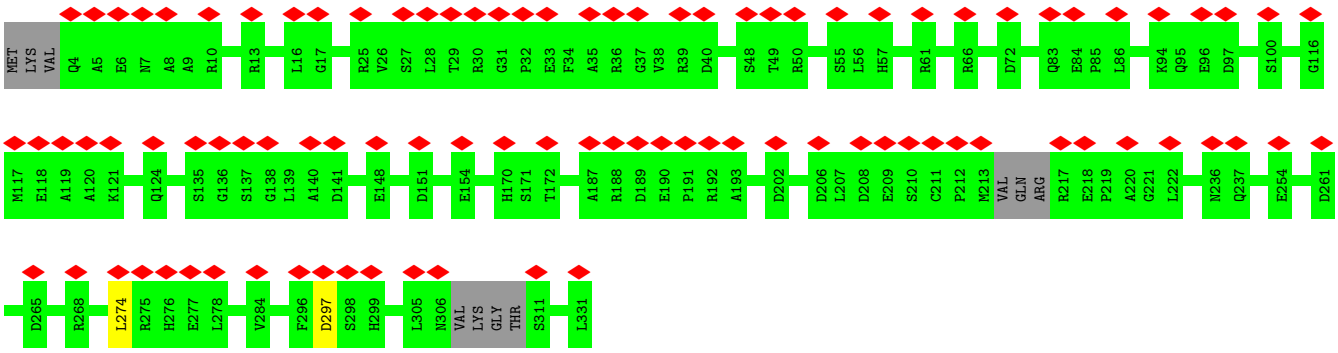




- Molecule 5: Triplex capsid protein 1

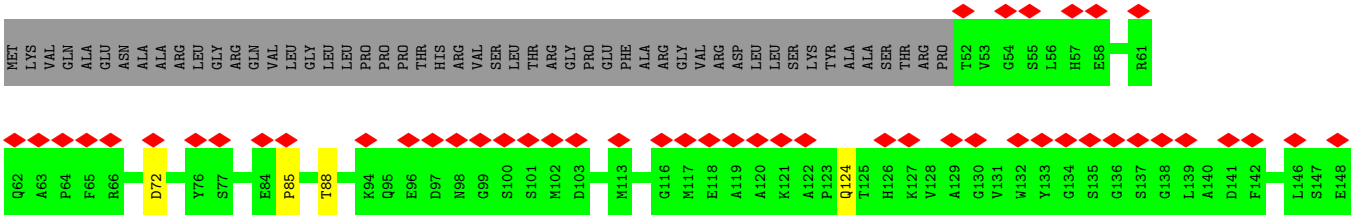
Chain b:

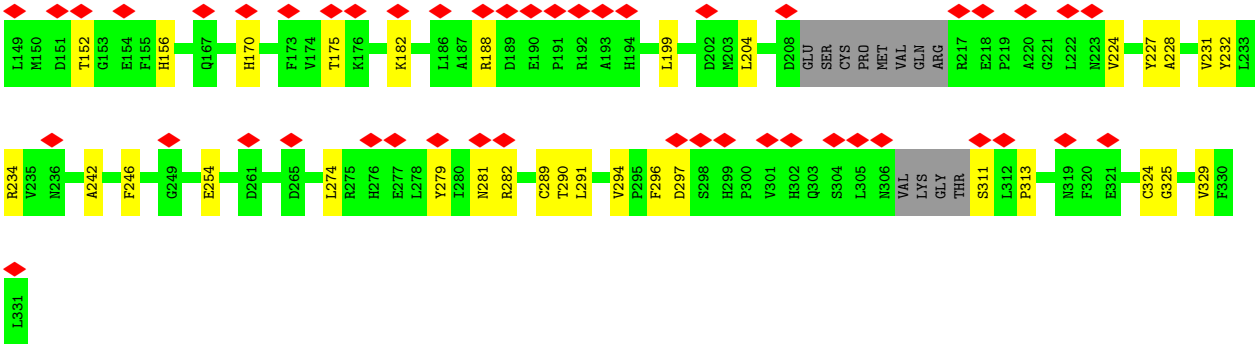




- Molecule 5: Triplex capsid protein 1

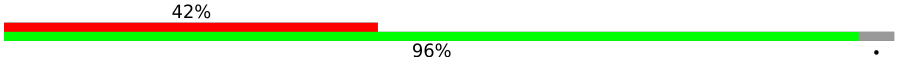
Chain 5:

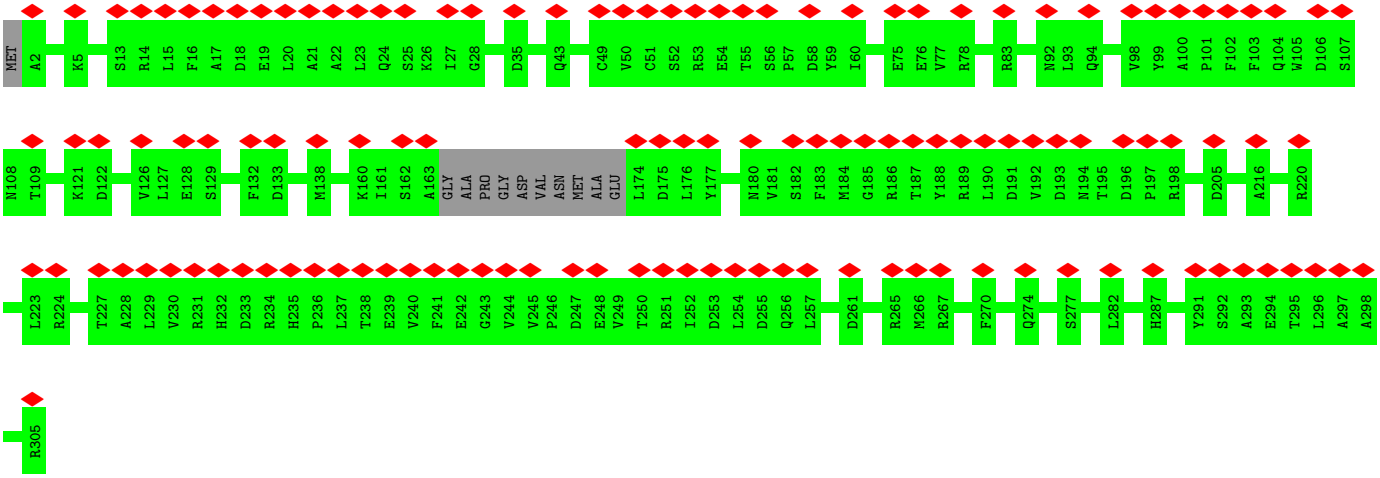




• Molecule 6: Triplex capsid protein 2

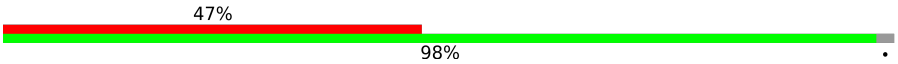
Chain c:

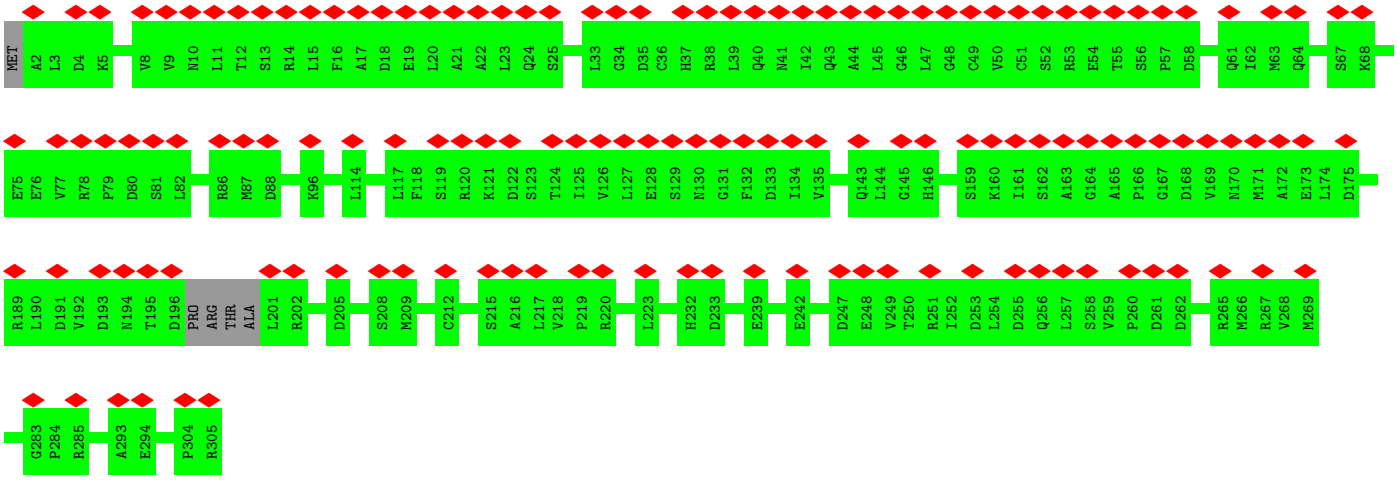




• Molecule 6: Triplex capsid protein 2

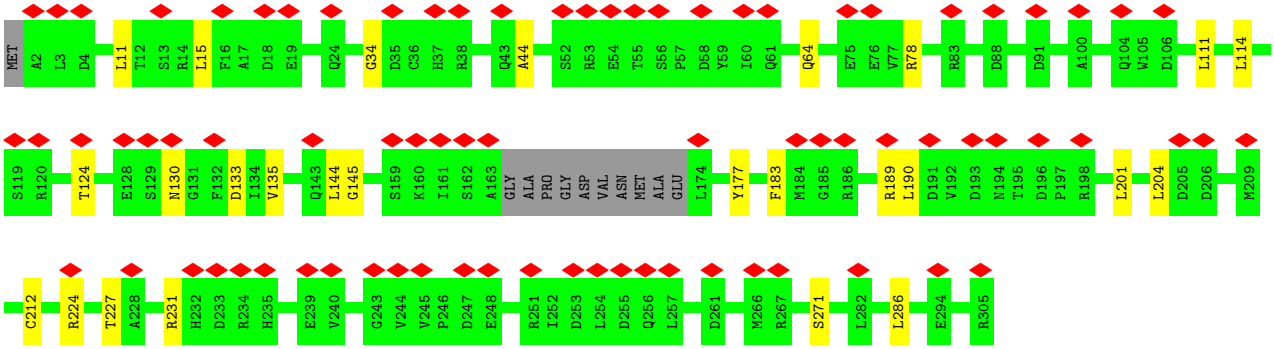
Chain d:





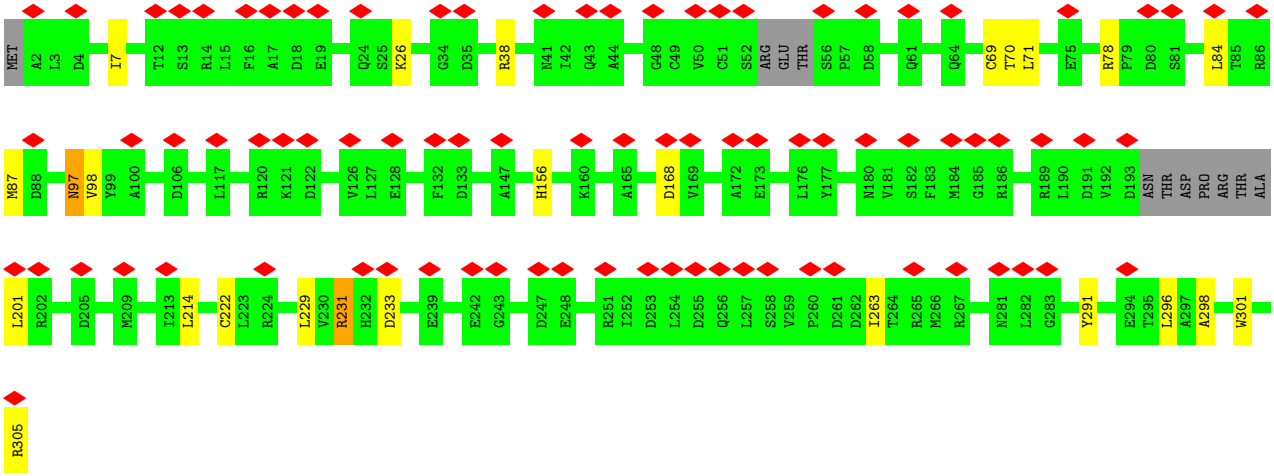
• Molecule 6: Triplex capsid protein 2

Chain 6:



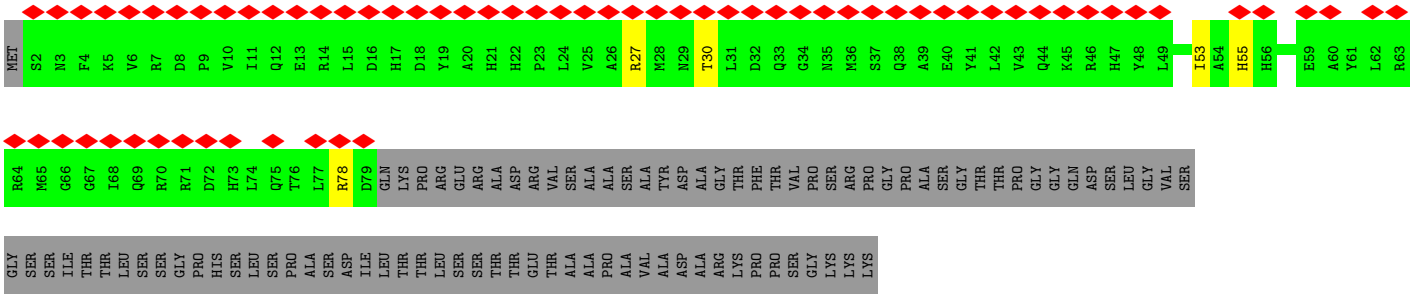
- Molecule 6: Triplex capsid protein 2

Chain 7:



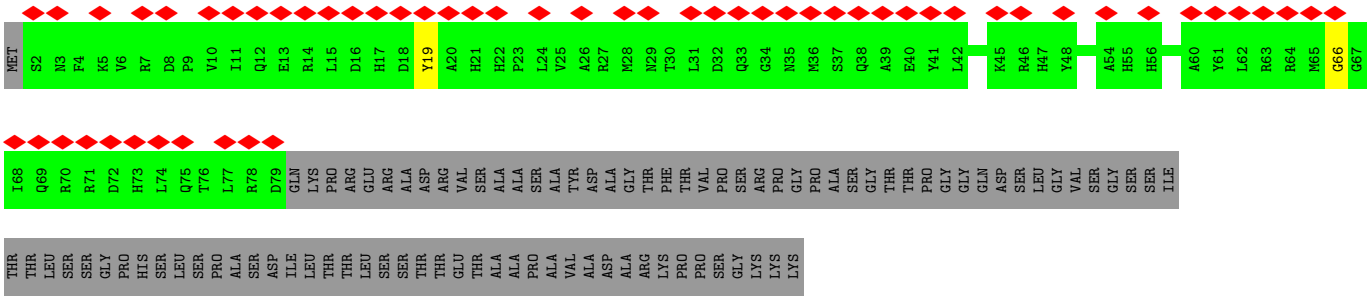
- Molecule 7: Small capsomere-interacting protein

Chain 0:



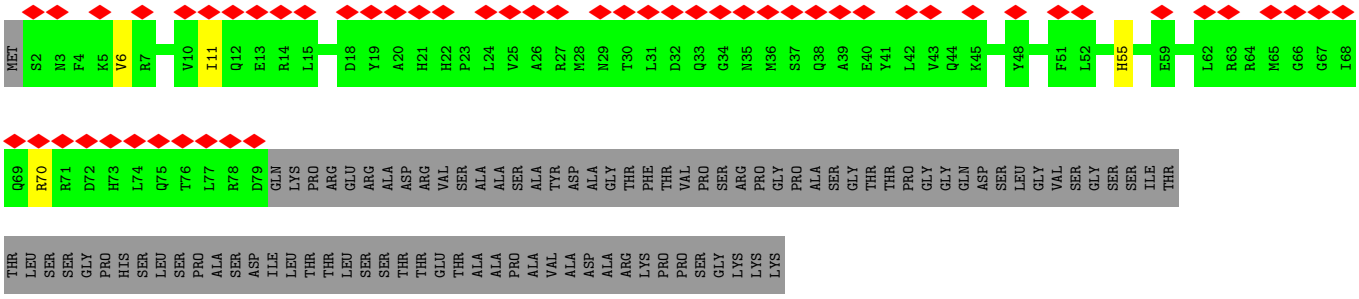
- Molecule 7: Small capsomere-interacting protein

Chain 1:



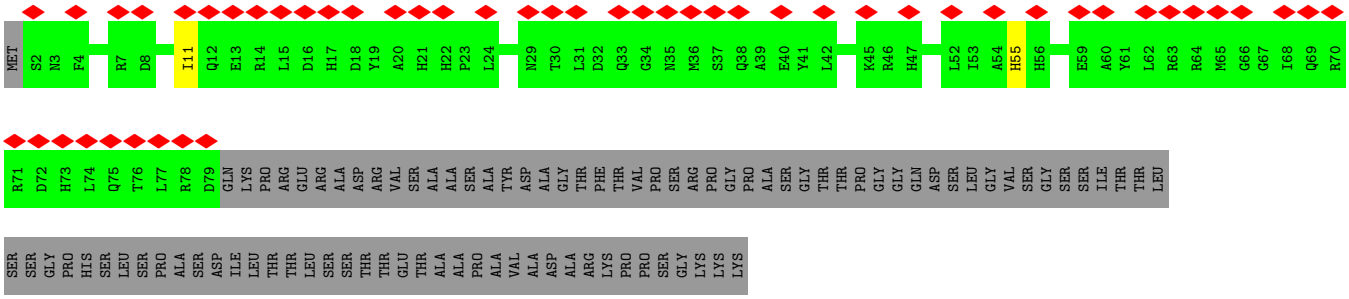
- Molecule 7: Small capsomere-interacting protein

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.

All (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
4	S	992	LYS	C-N-CA	5.23	134.78	121.70
4	W	262	SER	C-N-CA	5.21	134.73	121.70
4	X	1019	LEU	CA-CB-CG	5.21	127.28	115.30
6	7	214	LEU	CA-CB-CG	5.20	127.26	115.30
1	k	89	ASP	CB-CG-OD1	5.12	122.91	118.30
4	S	1019	LEU	CA-CB-CG	5.10	127.03	115.30
4	S	1019	LEU	CB-CG-CD2	-5.09	102.35	111.00

There are no chirality outliers.

All (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
4	T	886	PRO	Peptide
4	T	944	PHE	Peptide
4	W	262	SER	Peptide
4	W	263	THR	Mainchain
4	W	537	HIS	Peptide
4	W	848	ASP	Peptide
4	W	849	ASP	Peptide
4	X	991	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
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.

All (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
4:S:1182:THR:HG23	4:S:1236:ASN:HB3	1.78	0.65
4:T:1201:ALA:HB3	4:T:1227:PRO:HG2	1.79	0.65
4:W:602:GLU:HB3	4:W:647:LYS:HE2	1.78	0.64
4:W:658:ARG:HA	4:W:681:LEU:HD11	1.78	0.64
4:W:1200:ARG:NH1	4:W:1221:ASP:O	2.30	0.64
4:T:1187:ASP:OD2	4:T:1232:ARG:NH2	2.32	0.63
4:T:1241:GLN:HB3	4:T:1244:SER:HB3	1.82	0.62
4:X:658:ARG:HA	4:X:681:LEU:HD11	1.81	0.62
4:S:1111:MET:SD	4:S:1366:ARG:NH2	2.72	0.62
4:T:929:ASP:OD1	4:T:932:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:69:CYS:SG	6:7:70:THR:N	2.74	0.61
4:W:796:ASN:OD1	4:X:932:ARG:NH1	2.33	0.61
4:W:278:THR:HG22	4:W:1051:ILE:HG12	1.83	0.61
4:T:1280:ARG:NH2	4:T:1288:GLU:OE1	2.34	0.60
4:S:658:ARG:HA	4:S:681:LEU:HD11	1.83	0.60
6:6:201:LEU:HD13	6:7:231:ARG:HH22	1.66	0.60
5:5:234:ARG:HD3	5:5:274:LEU:HD11	1.82	0.60
4:T:540:PHE:O	4:T:559:ARG:NH1	2.35	0.59
4:S:416:SER:HB3	4:S:1349:ALA:HB2	1.82	0.59
4:T:129:ILE:HB	4:T:1080:PHE:HB2	1.84	0.59
4:T:717:LEU:HA	4:T:915:GLN:HE22	1.66	0.59
4:X:633:LEU:HD12	4:X:874:MET:HB3	1.85	0.59
4:X:1182:THR:HG23	4:X:1236:ASN:HB3	1.85	0.59
4:T:591:VAL:HB	4:T:683:GLU:HB2	1.85	0.59
4:S:259:LYS:HE2	4:X:60:VAL:HB	1.84	0.58
4:S:1047:LEU:HD12	4:S:1106:ALA:HB3	1.85	0.58
4:W:481:TYR:OH	4:W:979:VAL:O	2.20	0.58
4:W:578:ARG:NH2	4:W:1017:GLN:OE1	2.37	0.58
4:S:742:ILE:HG12	4:S:788:LEU:HD22	1.85	0.58
4:T:275:VAL:HG22	4:T:375:ALA:HB3	1.84	0.58
4:S:587:ASN:HB2	4:T:572:ARG:HH22	1.68	0.58
4:W:850:ILE:HD12	4:W:870:PRO:HG2	1.86	0.58
4:S:692:LEU:HD13	4:T:972:ARG:HG2	1.86	0.57
4:X:718:LEU:O	4:X:915:GLN:NE2	2.37	0.57
4:X:1192:GLN:NE2	4:X:1359:GLU:O	2.36	0.57
4:S:603:THR:HG22	4:S:647:LYS:HB3	1.87	0.57
4:W:447:GLN:HB3	4:W:1028:ALA:HB1	1.87	0.57
4:W:182:LYS:NZ	4:W:1058:SER:OG	2.38	0.57
4:W:1313:ASP:OD2	4:X:203:ARG:NH1	2.38	0.56
4:S:447:GLN:NE2	4:T:521:GLU:OE1	2.38	0.56
4:T:946:LYS:HE2	4:T:993:SER:HA	1.86	0.56
5:5:289:CYS:SG	5:5:290:THR:N	2.78	0.56
6:6:189:ARG:NH1	6:6:190:LEU:O	2.38	0.56
4:S:718:LEU:O	4:S:915:GLN:NE2	2.35	0.56
4:W:965:VAL:HG13	4:W:972:ARG:HG2	1.88	0.56
4:X:698:GLU:HG3	4:X:705:ILE:HD12	1.88	0.56
6:6:111:LEU:HB2	6:6:286:LEU:HB2	1.88	0.56
6:7:156:HIS:HD2	6:7:201:LEU:HB2	1.71	0.56
4:T:658:ARG:HA	4:T:681:LEU:HD11	1.88	0.56
4:T:293:VAL:HG21	4:T:368:LYS:HE3	1.88	0.55
6:7:71:LEU:HB2	6:7:87:MET:HE2	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:227:THR:O	6:6:231:ARG:NH1	2.39	0.55
4:S:94:LYS:HB2	4:X:58:THR:HG22	1.89	0.55
4:X:785:ARG:NH1	4:X:787:VAL:O	2.39	0.55
6:7:231:ARG:HG2	6:7:233:ASP:H	1.71	0.55
6:7:7:ILE:HB	6:7:84:LEU:HB2	1.89	0.55
4:W:399:THR:HG22	4:W:1043:THR:HG22	1.87	0.55
4:X:516:ALA:HB2	4:X:994:PRO:HG3	1.89	0.55
4:X:559:ARG:HH11	4:X:565:ILE:HG12	1.72	0.55
4:T:640:THR:O	4:T:644:ASN:ND2	2.39	0.55
4:X:278:THR:HG22	4:X:1051:ILE:HG12	1.89	0.55
4:X:833:LEU:HA	4:X:859:LEU:HD11	1.88	0.54
4:X:559:ARG:O	4:X:564:ASN:ND2	2.35	0.54
4:S:127:ALA:HB2	4:T:101:ALA:HB2	1.89	0.54
4:S:218:LYS:NZ	4:S:1325:GLU:OE1	2.36	0.54
4:T:832:THR:HG22	7:3:11:ILE:HD11	1.88	0.54
4:W:1044:ASP:HA	4:W:1109:THR:HG21	1.87	0.54
4:X:708:LEU:HD21	4:X:1022:PRO:HG2	1.90	0.54
4:T:572:ARG:NH1	4:T:1001:SER:O	2.41	0.54
4:W:93:PHE:HB2	4:W:116:VAL:HB	1.90	0.54
4:T:182:LYS:NZ	4:T:1058:SER:OG	2.41	0.53
4:W:1198:ARG:NH2	4:W:1219:LEU:O	2.40	0.53
5:5:72:ASP:OD1	5:5:188:ARG:NH1	2.40	0.53
4:S:7:GLN:NE2	4:S:36:GLN:OE1	2.41	0.53
4:T:537:HIS:HA	4:T:1238:TRP:CD1	2.42	0.53
4:W:736:ARG:HH21	4:W:900:PRO:HB3	1.74	0.53
4:W:537:HIS:HA	4:W:1238:TRP:CD1	2.44	0.53
6:7:97:ASN:HB3	6:7:296:LEU:HD22	1.90	0.53
4:W:1027:GLN:HB3	4:W:1032:MET:HB2	1.90	0.53
4:W:1045:GLU:N	4:W:1109:THR:OG1	2.40	0.53
4:X:1111:MET:SD	4:X:1366:ARG:NH2	2.79	0.53
4:S:183:LEU:HD13	4:S:394:ARG:HH21	1.72	0.53
4:W:214:VAL:HA	4:W:217:PHE:HD2	1.74	0.53
6:6:224:ARG:NH2	6:7:168:ASP:OD2	2.41	0.53
5:5:254:GLU:HG2	6:6:64:GLN:HE21	1.74	0.53
4:T:93:PHE:HB2	4:T:116:VAL:HB	1.90	0.53
4:W:183:LEU:HD13	4:W:394:ARG:HH21	1.73	0.53
4:W:447:GLN:NE2	4:X:521:GLU:OE1	2.42	0.53
4:X:1183:PRO:HG2	4:X:1237:PRO:HD2	1.91	0.53
4:S:481:TYR:HH	4:S:979:VAL:H	1.56	0.53
5:5:324:CYS:SG	5:5:325:GLY:N	2.81	0.53
4:W:543:PHE:HZ	4:W:555:ARG:HH11	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:770:LEU:HD22	7:2:55:HIS:HD2	1.75	0.52
4:S:1167:PRO:HD3	4:T:1224:ILE:HD13	1.91	0.52
4:T:1071:ARG:O	4:T:1079:THR:OG1	2.25	0.52
4:S:1027:GLN:HB3	4:S:1032:MET:HB2	1.91	0.52
4:W:275:VAL:HG22	4:W:375:ALA:HB3	1.90	0.52
4:S:451:LYS:HB3	4:S:1117:ASP:HB3	1.90	0.52
4:W:1073:VAL:HG13	4:W:1078:VAL:HG22	1.92	0.52
7:0:78:ARG:NH2	7:1:19:TYR:O	2.43	0.52
4:T:770:LEU:HD21	4:T:883:LEU:HD22	1.92	0.52
5:5:228:ALA:HB2	5:5:291:LEU:HD11	1.91	0.52
4:S:49:ARG:HD3	4:T:87:ILE:HD11	1.91	0.52
4:S:623:GLN:HG3	4:S:626:LYS:HD3	1.91	0.52
4:S:725:ASP:HB3	4:S:793:LEU:HD22	1.91	0.52
4:S:1169:LEU:O	4:T:211:SER:OG	2.22	0.52
6:6:212:CYS:N	6:7:222:CYS:SG	2.83	0.52
4:T:1005:THR:HG22	4:T:1007:GLY:H	1.76	0.51
4:W:75:CYS:SG	4:W:1059:THR:OG1	2.68	0.51
4:S:698:GLU:HG3	4:S:705:ILE:HD12	1.92	0.51
4:T:526:PRO:HG3	4:T:1225:PRO:HB3	1.92	0.51
4:X:256:THR:HG22	4:X:258:PHE:H	1.75	0.51
4:S:1344:ASN:ND2	4:S:1347:THR:OG1	2.43	0.51
4:T:854:LEU:HD13	4:T:860:LYS:HG2	1.92	0.51
4:X:624:GLU:HB3	4:X:762:ARG:HH12	1.74	0.51
4:S:1332:ALA:HB1	4:S:1337:MET:HB2	1.92	0.51
4:W:92:GLN:HE22	4:W:115:ILE:HG23	1.76	0.51
4:S:1117:ASP:OD1	4:S:1117:ASP:N	2.44	0.51
4:T:278:THR:HG22	4:T:1051:ILE:HG12	1.93	0.51
4:X:264:TYR:HE1	4:X:300:PRO:HD2	1.76	0.51
4:S:9:PRO:HB3	4:S:45:GLU:HB3	1.93	0.50
4:T:889:THR:HA	4:T:920:ASN:HB3	1.91	0.50
4:W:480:GLY:HA3	4:W:483:LEU:HD11	1.93	0.50
4:T:578:ARG:NH2	4:T:1017:GLN:OE1	2.44	0.50
4:W:851:LEU:HD23	4:W:854:LEU:HD12	1.92	0.50
4:S:1294:ALA:HB3	4:S:1318:GLN:HE21	1.77	0.50
4:T:146:PRO:HA	4:T:149:PHE:HD2	1.77	0.50
4:S:100:ILE:HG12	4:X:172:ARG:HB3	1.93	0.50
4:W:398:TYR:O	4:W:1044:ASP:N	2.44	0.50
4:S:295:SER:HA	4:S:365:SER:HA	1.93	0.50
6:6:11:LEU:HG	6:6:15:LEU:HD23	1.93	0.50
4:S:826:TYR:OH	4:S:920:ASN:O	2.30	0.50
4:W:438:ASN:HD22	4:W:1171:HIS:HD2	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:211:SER:OG	4:X:1169:LEU:O	2.22	0.50
4:T:332:ARG:NH2	4:T:346:ASP:OD1	2.44	0.50
4:T:777:ARG:NH2	4:T:885:CYS:O	2.45	0.50
4:W:695:ALA:HB1	4:W:706:THR:HG22	1.94	0.49
4:W:603:THR:HG22	4:W:647:LYS:HB3	1.94	0.49
4:W:963:ASN:O	4:W:967:ARG:N	2.44	0.49
4:T:717:LEU:HD23	4:T:804:LYS:HD3	1.95	0.49
6:6:114:LEU:HD11	6:6:145:GLY:HA2	1.92	0.49
4:T:868:ILE:HG22	4:T:870:PRO:HD3	1.95	0.49
4:W:606:ASP:OD1	4:W:647:LYS:NZ	2.37	0.49
4:T:757:ILE:HG12	4:T:788:LEU:HD22	1.94	0.49
4:X:1247:ASP:OD1	4:X:1251:ASN:ND2	2.39	0.49
4:T:543:PHE:HE1	4:T:557:THR:HG23	1.76	0.49
4:W:963:ASN:HA	4:W:966:THR:HG22	1.94	0.49
4:S:559:ARG:O	4:S:564:ASN:ND2	2.37	0.49
4:W:824:VAL:H	4:W:889:THR:HG21	1.78	0.49
4:X:619:MET:SD	4:X:881:SER:OG	2.67	0.49
4:T:1198:ARG:NH2	4:T:1219:LEU:O	2.43	0.49
4:X:394:ARG:HD3	4:X:1315:PHE:HB3	1.95	0.49
4:X:1220:TYR:HE2	4:X:1272:LYS:HD3	1.78	0.48
4:W:714:ASP:O	4:W:804:LYS:NZ	2.46	0.48
4:X:380:GLN:HG2	4:X:384:ASN:HD21	1.77	0.48
4:X:447:GLN:HB3	4:X:1028:ALA:HB1	1.95	0.48
4:X:1071:ARG:HH12	4:X:1081:GLU:HB3	1.77	0.48
6:7:26:LYS:HA	6:7:98:VAL:HG21	1.95	0.48
4:X:1190:TYR:OH	4:X:1196:ASN:O	2.25	0.48
4:W:402:PHE:HD2	4:W:1040:VAL:HB	1.78	0.48
4:W:1071:ARG:O	4:W:1079:THR:OG1	2.29	0.48
4:X:578:ARG:NH1	4:X:1014:SER:O	2.43	0.48
4:X:829:VAL:HG22	4:X:938:MET:HE3	1.96	0.48
4:W:266:THR:HG21	4:W:373:PHE:HD2	1.78	0.48
4:W:1042:ARG:NH2	4:W:1111:MET:O	2.47	0.48
4:X:510:PRO:HD2	4:X:513:ALA:HB3	1.96	0.48
4:X:1047:LEU:HD12	4:X:1106:ALA:HB3	1.95	0.48
5:5:152:THR:HA	5:5:281:ASN:HB3	1.95	0.48
4:T:770:LEU:HD11	4:T:883:LEU:HD13	1.96	0.48
4:W:394:ARG:NH1	4:W:1317:ASP:OD2	2.46	0.48
4:W:575:GLN:NE2	4:W:1015:MET:SD	2.87	0.48
4:X:238:LYS:HG2	4:X:289:LEU:HD22	1.96	0.48
4:X:1068:VAL:HG22	4:X:1082:ILE:HG12	1.95	0.48
4:T:402:PHE:HD2	4:T:1040:VAL:HB	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:575:GLN:NE2	4:T:1015:MET:SD	2.87	0.47
4:W:1062:PHE:HB2	4:W:1087:ALA:HB3	1.96	0.47
4:X:450:LEU:HD11	4:X:1025:ILE:HG13	1.94	0.47
5:5:124:GLN:NE2	5:5:311:SER:O	2.47	0.47
4:W:1118:LEU:HD23	4:W:1121:ILE:HD13	1.96	0.47
4:W:1341:TYR:HA	4:W:1348:HIS:HD2	1.77	0.47
4:T:41:LYS:O	4:T:44:ARG:NH1	2.47	0.47
4:W:256:THR:HG22	4:W:258:PHE:H	1.79	0.47
4:S:1043:THR:HG23	4:S:1265:PRO:HB3	1.96	0.47
4:T:399:THR:HG22	4:T:1043:THR:HG22	1.96	0.47
4:X:640:THR:O	4:X:644:ASN:ND2	2.47	0.47
4:X:1062:PHE:HB2	4:X:1087:ALA:HB3	1.96	0.47
5:5:329:VAL:HG21	6:6:271:SER:HB2	1.97	0.47
4:T:1250:TYR:HB2	4:T:1270:PHE:HD2	1.79	0.47
4:W:324:ARG:NH1	4:W:325:ASN:OD1	2.48	0.47
4:S:1334:HIS:HB2	4:S:1355:GLN:HG2	1.95	0.47
4:T:1342:MET:HA	4:T:1375:VAL:HG21	1.97	0.47
4:X:252:VAL:HG13	4:X:1096:SER:HA	1.96	0.47
4:X:929:ASP:OD1	4:X:932:ARG:NH2	2.47	0.47
6:6:133:ASP:OD1	6:6:133:ASP:N	2.47	0.47
4:T:770:LEU:HD22	7:3:55:HIS:HD2	1.80	0.47
4:T:1207:CYS:SG	4:T:1208:ASP:N	2.87	0.47
4:W:214:VAL:HG12	4:W:218:LYS:HE2	1.95	0.47
4:W:407:HIS:HB2	4:W:1184:VAL:HG12	1.96	0.47
4:X:716:HIS:HD2	4:X:736:ARG:HH21	1.61	0.47
4:X:1198:ARG:NH2	4:X:1219:LEU:O	2.42	0.47
4:S:1200:ARG:HG2	4:S:1226:ASP:HB3	1.96	0.47
4:T:82:ASP:OD1	4:T:82:ASP:N	2.46	0.47
4:T:1067:SER:OG	4:T:1083:THR:OG1	2.33	0.47
4:X:77:ASN:HB3	4:X:303:TYR:HD1	1.78	0.47
4:X:1271:HIS:ND1	4:X:1274:ASP:OD2	2.47	0.47
4:W:276:LEU:HA	4:W:1053:TYR:HA	1.97	0.47
4:X:620:ILE:HG22	4:X:622:GLY:H	1.80	0.47
4:W:491:MET:HB2	4:W:783:ASP:HA	1.96	0.47
4:S:488:THR:OG1	4:S:982:ASN:ND2	2.34	0.46
4:S:526:PRO:HB3	4:S:1233:SER:HB2	1.97	0.46
4:T:893:ARG:NH2	4:T:988:GLU:OE1	2.47	0.46
4:X:716:HIS:CD2	4:X:736:ARG:HE	2.33	0.46
4:S:100:ILE:HG13	4:X:386:THR:HG21	1.97	0.46
4:S:394:ARG:NH1	4:S:1317:ASP:OD2	2.49	0.46
4:S:1173:GLN:HE21	4:S:1305:GLN:HA	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:1062:PHE:HB2	4:T:1087:ALA:HB3	1.97	0.46
4:T:773:ILE:O	4:T:776:THR:OG1	2.33	0.46
4:W:1254:PHE:HB2	4:W:1267:ARG:HH22	1.79	0.46
4:X:401:PHE:HE2	4:X:1191:PHE:HD1	1.62	0.46
5:5:224:VAL:HG13	5:5:294:VAL:HB	1.97	0.46
4:W:79:GLU:N	4:W:304:ALA:O	2.49	0.46
4:X:138:LEU:HD13	4:X:151:GLU:HG3	1.97	0.46
4:X:718:LEU:HD21	4:X:730:LEU:HD12	1.97	0.46
4:S:1067:SER:OG	4:S:1083:THR:OG1	2.33	0.46
4:T:91:ILE:HD12	4:T:1089:LEU:HD21	1.97	0.46
4:T:860:LYS:O	4:T:864:GLN:N	2.47	0.46
4:T:1195:SER:O	4:T:1326:ALA:N	2.47	0.46
4:W:1005:THR:HG22	4:W:1007:GLY:H	1.79	0.46
4:S:98:PRO:HG3	4:X:61:VAL:HG11	1.97	0.46
4:W:918:LEU:HD22	4:W:944:PHE:HZ	1.80	0.46
4:X:1321:HIS:O	4:X:1324:GLN:NE2	2.46	0.46
4:S:1190:TYR:OH	4:S:1196:ASN:O	2.30	0.46
4:T:95:ILE:HB	4:T:114:TYR:HB2	1.98	0.46
4:X:84:ARG:O	6:6:78:ARG:NH2	2.48	0.46
4:W:718:LEU:HD12	4:W:894:VAL:HG21	1.98	0.45
4:W:1308:VAL:HG21	4:W:1314:VAL:HG21	1.97	0.45
4:X:399:THR:HG22	4:X:1043:THR:HG22	1.97	0.45
4:X:1369:LYS:HG2	4:X:1374:VAL:HG22	1.98	0.45
4:S:633:LEU:HG	4:S:874:MET:HE2	1.98	0.45
4:X:276:LEU:HB3	4:X:376:ILE:HG12	1.97	0.45
4:T:1115:CYS:HA	4:T:1177:CYS:HB2	1.98	0.45
4:X:82:ASP:OD1	4:X:82:ASP:N	2.48	0.45
4:S:898:ARG:HE	4:S:913:VAL:HB	1.81	0.45
4:W:1201:ALA:HB3	4:W:1227:PRO:HG2	1.99	0.45
4:S:1227:PRO:O	4:X:1170:SER:OG	2.31	0.45
4:X:1200:ARG:HG2	4:X:1226:ASP:HB3	1.99	0.45
4:S:71:LEU:N	4:S:377:GLU:OE2	2.48	0.45
4:X:603:THR:HG22	4:X:647:LYS:HB3	1.99	0.45
4:S:1236:ASN:OD1	4:S:1236:ASN:N	2.49	0.45
4:T:623:GLN:HB2	4:T:626:LYS:HB2	1.99	0.45
4:W:1173:GLN:NE2	4:W:1302:THR:O	2.50	0.45
4:W:130:GLU:HG3	4:X:110:LYS:HD2	1.98	0.45
4:T:725:ASP:HB3	4:T:793:LEU:HG	1.99	0.45
4:W:276:LEU:HB3	4:W:1053:TYR:HD1	1.82	0.45
4:X:788:LEU:HD12	4:X:919:VAL:HG11	1.99	0.45
4:S:1183:PRO:HG2	4:S:1237:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:130:GLU:HG2	4:T:1079:THR:HG22	1.98	0.45
4:S:245:LEU:HD22	4:S:369:ILE:HD13	1.99	0.44
4:S:1005:THR:HG22	4:S:1007:GLY:H	1.82	0.44
4:T:555:ARG:HE	4:T:907:HIS:CD2	2.34	0.44
4:W:611:LEU:HD13	4:W:935:ALA:HB1	1.98	0.44
4:W:902:GLN:NE2	4:W:1020:SER:OG	2.43	0.44
4:W:987:TYR:O	4:W:992:LYS:NZ	2.50	0.44
4:W:504:LYS:HG2	4:W:964:TYR:HE1	1.82	0.44
4:X:501:TYR:OH	4:X:978:ASN:O	2.31	0.44
6:7:291:TYR:HD1	6:7:298:ALA:HB2	1.82	0.44
4:S:423:GLU:OE2	4:X:420:ARG:NH2	2.51	0.44
4:S:811:MET:O	4:S:815:SER:OG	2.26	0.44
4:W:128:GLU:OE1	4:X:110:LYS:NZ	2.37	0.44
4:W:278:THR:HB	4:W:282:VAL:HB	2.00	0.44
5:5:85:PRO:O	5:5:88:THR:OG1	2.27	0.44
4:W:788:LEU:HD11	4:W:919:VAL:HG21	1.99	0.44
4:T:566:PRO:HG2	4:T:569:LEU:HD12	2.00	0.44
4:X:185:HIS:O	4:X:1097:SER:OG	2.36	0.44
4:S:591:VAL:N	4:S:683:GLU:OE1	2.50	0.44
4:S:1169:LEU:H	4:S:1169:LEU:HG	1.47	0.44
4:W:184:ARG:O	4:W:1290:SER:OG	2.33	0.44
5:5:227:TYR:HB2	5:5:246:PHE:HB2	1.99	0.44
4:S:56:VAL:HG22	4:T:92:GLN:HB3	2.00	0.44
4:S:93:PHE:HE1	4:S:257:VAL:HG21	1.82	0.44
4:S:578:ARG:NH1	4:S:1014:SER:OG	2.50	0.44
4:S:773:ILE:O	4:S:776:THR:OG1	2.30	0.44
4:W:585:VAL:HG11	4:W:1030:HIS:HB3	1.99	0.43
4:S:711:ALA:HB3	4:S:1016:HIS:HB3	2.00	0.43
4:T:407:HIS:HB2	4:T:1184:VAL:HG12	1.99	0.43
4:T:436:ASN:HD21	4:T:442:LEU:HG	1.82	0.43
4:W:626:LYS:NZ	4:W:881:SER:O	2.44	0.43
4:T:75:CYS:SG	4:T:1059:THR:OG1	2.74	0.43
4:T:79:GLU:N	4:T:304:ALA:O	2.51	0.43
4:W:770:LEU:HD22	7:0:55:HIS:HD2	1.82	0.43
4:X:850:ILE:HG13	4:X:870:PRO:HG2	2.01	0.43
4:W:737:GLN:HE21	4:W:897:LYS:HD2	1.84	0.43
4:X:174:LEU:HD23	4:X:1086:ILE:HD11	2.00	0.43
4:X:290:LEU:HB3	4:X:367:VAL:HG21	2.01	0.43
4:T:760:ARG:HH22	4:T:886:PRO:HA	1.83	0.43
4:W:1342:MET:HA	4:W:1375:VAL:HG21	2.00	0.43
4:X:1334:HIS:HB2	4:X:1355:GLN:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:124:THR:HG22	6:6:135:VAL:HG13	2.00	0.43
4:S:969:PRO:HB2	4:S:972:ARG:NH2	2.33	0.43
4:W:414:SER:HB2	4:W:1353:MET:HG3	2.00	0.43
4:X:263:THR:O	4:X:359:ARG:NH1	2.43	0.43
4:X:1166:LEU:HD11	4:X:1169:LEU:HD23	1.99	0.43
4:S:825:ASP:HB2	7:2:6:VAL:HG21	2.00	0.43
4:T:633:LEU:HD12	4:T:874:MET:HB3	2.00	0.43
4:W:407:HIS:CE1	4:W:574:PHE:HB2	2.54	0.43
4:X:836:ASN:HD22	4:X:839:VAL:HG23	1.84	0.43
4:X:1169:LEU:H	4:X:1169:LEU:HG	1.56	0.43
4:S:661:CYS:HB2	4:S:681:LEU:HD12	2.01	0.43
4:T:1027:GLN:HB3	4:T:1032:MET:HB2	2.00	0.43
4:W:49:ARG:HD3	4:X:87:ILE:HD11	2.00	0.43
4:W:1043:THR:HG23	4:W:1265:PRO:HB3	2.01	0.43
4:W:1196:ASN:ND2	4:W:1202:ALA:H	2.17	0.43
4:W:1262:MET:HA	4:W:1306:TYR:HA	2.00	0.43
5:5:279:TYR:HB2	5:5:282:ARG:HG2	2.01	0.43
6:6:144:LEU:HD11	6:6:183:PHE:HB2	2.01	0.43
4:S:619:MET:SD	4:S:881:SER:OG	2.72	0.42
4:W:127:ALA:HB2	4:X:101:ALA:HB2	2.01	0.42
4:T:455:HIS:ND1	4:T:457:ARG:HG2	2.34	0.42
4:W:123:HIS:HB2	4:W:1086:ILE:HB	2.00	0.42
4:X:93:PHE:HB2	4:X:116:VAL:HB	2.00	0.42
4:T:512:VAL:HG12	4:T:993:SER:HB3	2.02	0.42
5:5:182:LYS:HD2	6:7:301:TRP:CG	2.55	0.42
4:S:82:ASP:OD1	4:S:82:ASP:N	2.52	0.42
4:W:1328:PRO:HB2	4:W:1358:ILE:HG21	2.02	0.42
4:S:587:ASN:OD1	4:T:1003:GLN:NE2	2.53	0.42
4:S:623:GLN:HB2	4:S:626:LYS:HB2	2.01	0.42
4:W:950:ASP:HA	4:W:951:PRO:HD3	1.86	0.42
4:W:1127:TYR:H	4:W:1133:HIS:CD2	2.38	0.42
4:W:1187:ASP:OD2	4:W:1232:ARG:NH1	2.52	0.42
4:S:1321:HIS:O	4:S:1324:GLN:NE2	2.52	0.42
4:T:932:ARG:HH21	4:T:956:THR:HG23	1.83	0.42
4:T:1196:ASN:ND2	4:T:1202:ALA:H	2.18	0.42
4:W:82:ASP:OD1	4:W:82:ASP:N	2.46	0.42
4:W:438:ASN:HD22	4:W:1171:HIS:CD2	2.36	0.42
6:6:204:LEU:HB3	6:7:229:LEU:HD11	2.00	0.42
4:S:1046:VAL:HG13	4:S:1104:VAL:HG23	2.01	0.42
4:T:855:GLU:HG2	7:2:70:ARG:HE	1.84	0.42
4:W:102:HIS:HE1	4:W:106:ARG:HD2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:78:THR:HG22	4:X:304:ALA:HB3	2.02	0.42
6:6:201:LEU:HD23	6:6:204:LEU:HD12	2.01	0.42
4:T:407:HIS:CE1	4:T:574:PHE:HB2	2.55	0.42
4:W:541:ASP:N	4:W:557:THR:O	2.52	0.42
4:S:529:HIS:O	4:S:533:ARG:N	2.48	0.42
4:T:279:THR:HB	4:T:380:GLN:HE21	1.84	0.42
4:S:394:ARG:HD3	4:S:1315:PHE:HB3	2.01	0.41
4:S:520:THR:HG22	4:S:568:PRO:HA	2.02	0.41
4:S:902:GLN:NE2	4:S:1020:SER:OG	2.47	0.41
4:X:770:LEU:HD21	4:X:883:LEU:HD22	2.01	0.41
4:S:832:THR:HG22	7:2:11:ILE:HD11	2.02	0.41
4:T:195:LEU:HD23	4:T:1283:TYR:HE1	1.86	0.41
4:W:331:ALA:HA	4:W:335:ASP:HB2	2.02	0.41
4:W:538:PRO:O	4:W:559:ARG:NH1	2.53	0.41
4:S:399:THR:HG22	4:S:1043:THR:HG22	2.01	0.41
4:T:709:VAL:HG22	4:T:1023:SER:HA	2.02	0.41
4:X:565:ILE:HA	4:X:566:PRO:HD3	1.94	0.41
5:5:124:GLN:HG2	5:5:313:PRO:HD2	2.01	0.41
4:T:1127:TYR:H	4:T:1133:HIS:CD2	2.39	0.41
6:6:34:GLY:H	6:6:44:ALA:HB1	1.84	0.41
4:S:192:LEU:HD13	4:S:1098:VAL:HG22	2.01	0.41
4:W:76:VAL:HG21	4:W:258:PHE:HD2	1.86	0.41
4:W:457:ARG:HG3	4:W:1122:PHE:HD2	1.86	0.41
4:X:278:THR:HB	4:X:282:VAL:HB	2.02	0.41
4:X:1071:ARG:NH1	4:X:1081:GLU:HB3	2.36	0.41
5:5:199:LEU:HD12	5:5:204:LEU:HD12	2.01	0.41
5:5:231:VAL:O	5:5:242:ALA:N	2.53	0.41
4:S:447:GLN:HB3	4:S:1028:ALA:HB1	2.02	0.41
6:6:177:TYR:HB3	6:7:263:ILE:HG21	2.02	0.41
4:W:1167:PRO:HG3	4:X:1217:ARG:HB2	2.03	0.41
4:S:192:LEU:O	4:S:196:GLY:N	2.50	0.41
4:S:1043:THR:OG1	4:S:1305:GLN:NE2	2.53	0.41
4:T:436:ASN:ND2	4:T:440:VAL:O	2.54	0.41
4:T:449:ALA:HB1	4:T:1179:ILE:HG12	2.03	0.41
4:T:907:HIS:HB2	4:T:910:GLY:N	2.36	0.41
4:W:687:LEU:HD23	4:W:805:LEU:HD22	2.02	0.41
4:X:989:GLU:HG2	4:X:991:HIS:H	1.86	0.41
4:X:1117:ASP:N	4:X:1117:ASP:OD1	2.44	0.41
4:S:1171:HIS:HE1	4:T:1228:ALA:HA	1.86	0.41
4:S:606:ASP:OD1	4:X:678:ARG:NH1	2.53	0.40
4:S:614:TYR:HE2	4:S:927:VAL:HG22	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:71:LEU:N	4:T:377:GLU:OE2	2.54	0.40
5:5:170:HIS:HA	5:5:175:THR:HG23	2.03	0.40
4:T:946:LYS:HD2	4:T:946:LYS:HA	1.92	0.40
4:W:301:ALA:HB2	4:W:360:THR:HB	2.03	0.40
4:S:252:VAL:HG13	4:S:1096:SER:HA	2.02	0.40
4:T:507:ALA:HB1	4:T:978:ASN:ND2	2.37	0.40
4:X:609:TYR:HA	4:X:610:PRO:HD3	1.97	0.40
5:5:156:HIS:H	5:5:232:TYR:HH	1.69	0.40
7:0:27:ARG:O	7:0:30:THR:OG1	2.31	0.40
4:S:799:ASN:OD1	4:S:799:ASN:N	2.55	0.40
4:T:594:GLN:HA	4:T:597:ILE:HD12	2.03	0.40
4:T:1217:ARG:HH21	4:T:1224:ILE:HD11	1.85	0.40
4:W:307:VAL:HB	4:W:309:ARG:HH11	1.86	0.40
4:W:736:ARG:NH2	4:W:1129:ASP:OD2	2.54	0.40
4:S:856:ASN:ND2	7:1:66:GLY:O	2.55	0.40
4:T:18:ASN:OD1	4:T:18:ASN:N	2.54	0.40
4:W:544:VAL:HG22	4:W:554:TYR:HE1	1.85	0.40
4:W:654:TYR:CD2	4:W:803:GLU:HG2	2.57	0.40
4:W:840:PHE:CE1	7:0:53:ILE:HD13	2.56	0.40
4:X:395:ARG:HG2	4:X:1047:LEU:HD23	2.04	0.40

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	o	38/2635 (1%)	38 (100%)	0	0	100	100
4	S	1273/1376 (92%)	1179 (93%)	92 (7%)	2 (0%)	47	81
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

All (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
4	T	945	ASN
4	X	993	SER
4	W	849	ASP
4	T	11	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	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
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

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S	41	LYS
4	S	106	ARG
4	S	110	LYS
4	S	143	LYS
4	S	651	VAL
4	S	736	ARG
4	S	1169	LEU
4	S	1235	ASN
4	W	1113	VAL
4	X	143	LYS
4	X	325	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	X	651	VAL
4	X	1169	LEU
4	X	1235	ASN
6	6	130	ASN
6	7	38	ARG
6	7	78	ARG
6	7	97	ASN
6	7	231	ARG
6	7	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	16	HIS
1	k	91	ASN
2	l	30	ASN
2	l	77	HIS
2	l	97	ASN
2	m	52	GLN
4	S	575	GLN
4	S	587	ASN
4	S	630	ASN
4	S	746	ASN
4	S	1133	HIS
4	S	1171	HIS
4	S	1173	GLN
4	S	1235	ASN
4	S	1318	GLN
4	S	1344	ASN
4	T	113	GLN
4	T	436	ASN
4	T	492	ASN
4	T	674	HIS
4	T	707	HIS
4	T	746	ASN
4	T	907	HIS
4	T	915	GLN
4	T	1003	GLN
4	T	1133	HIS
4	T	1196	ASN
4	T	1241	GLN
4	T	1305	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	1344	ASN
4	W	92	GLN
4	W	102	HIS
4	W	312	ASN
4	W	438	ASN
4	W	537	HIS
4	W	674	HIS
4	W	716	HIS
4	W	737	GLN
4	W	746	ASN
4	W	816	ASN
4	W	978	ASN
4	W	1090	HIS
4	W	1133	HIS
4	W	1196	ASN
4	X	102	HIS
4	X	312	ASN
4	X	325	ASN
4	X	384	ASN
4	X	428	GLN
4	X	447	GLN
4	X	630	ASN
4	X	716	HIS
4	X	746	ASN
4	X	1084	HIS
4	X	1171	HIS
4	X	1235	ASN
4	X	1344	ASN
5	b	124	GLN
5	b	262	HIS
6	c	40	GLN
6	c	130	ASN
6	c	146	HIS
6	c	150	GLN
6	c	281	ASN
6	d	94	GLN
6	d	146	HIS
6	d	150	GLN
6	d	194	ASN
6	d	274	GLN
5	5	145	ASN
6	6	64	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	6	110	GLN
6	6	150	GLN
6	6	151	GLN
6	6	232	HIS
6	6	281	ASN
6	7	97	ASN
6	7	143	GLN
6	7	281	ASN
7	0	38	GLN
7	0	55	HIS
7	1	38	GLN
7	1	55	HIS
7	2	38	GLN
7	2	55	HIS
7	3	38	GLN
7	3	55	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.

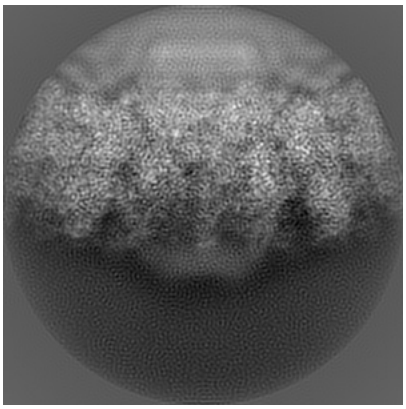
6 Map visualisation (i)

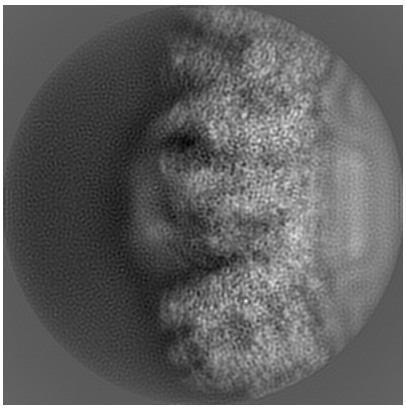
This section contains visualisations of the EMDB entry EMD-20432. These allow visual inspection of the internal detail of the map and identification of artifacts.

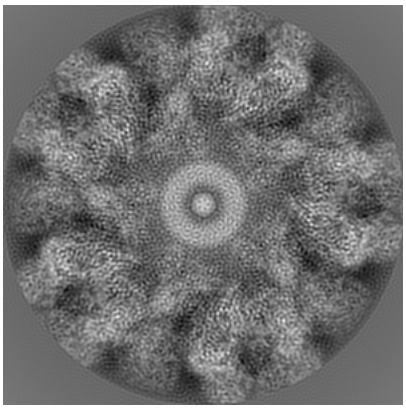
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

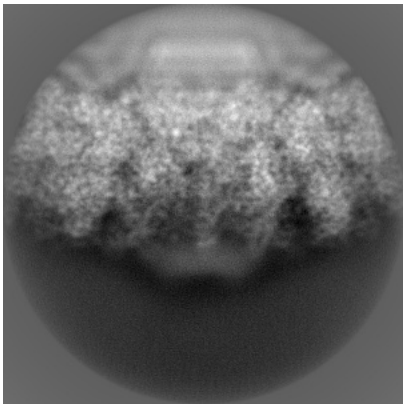
6.1.1 Primary map

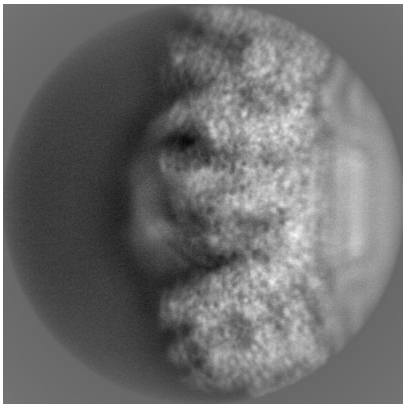

X

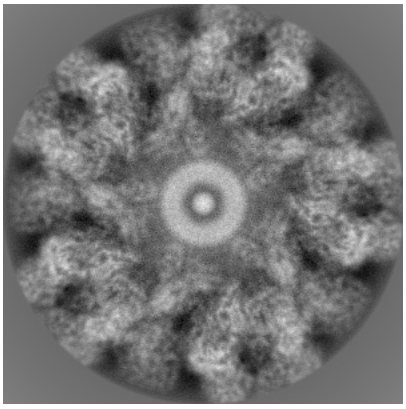

Y


Z

6.1.2 Raw map


X

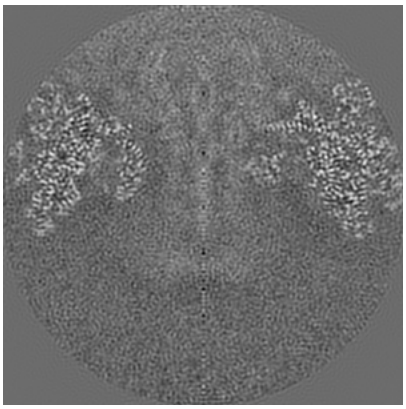

Y

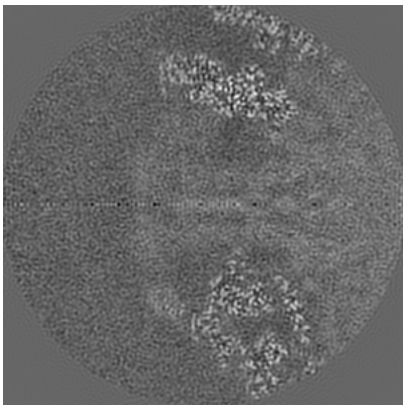

Z

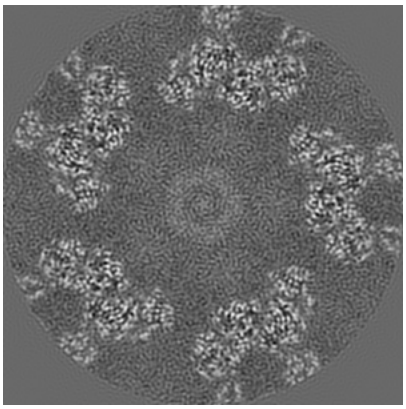
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

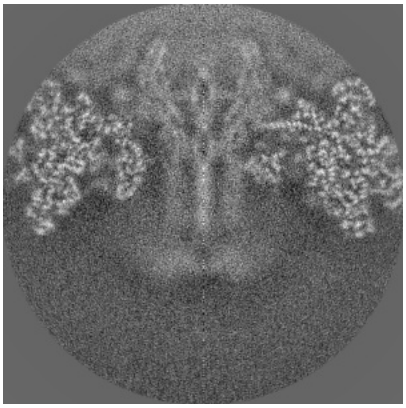
6.2.1 Primary map

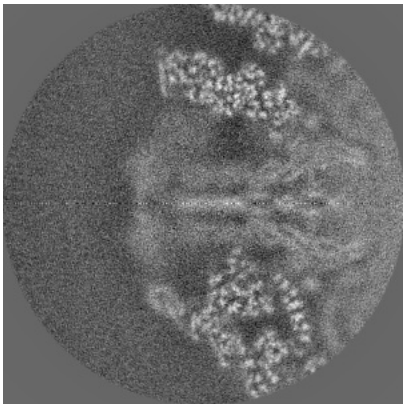

X Index: 192

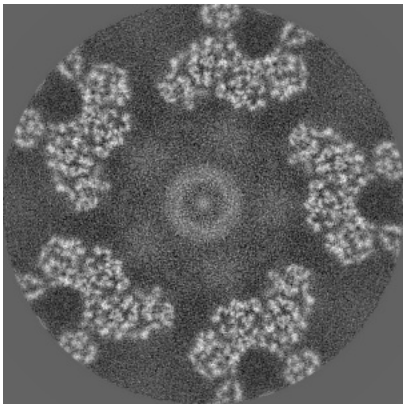

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

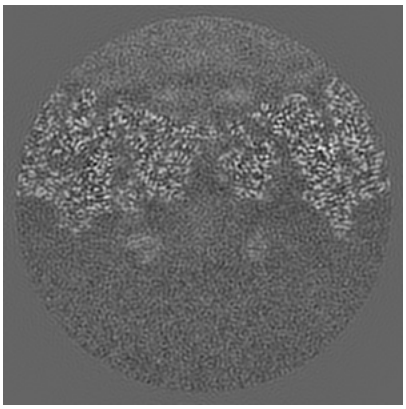

Y Index: 192


Z Index: 192

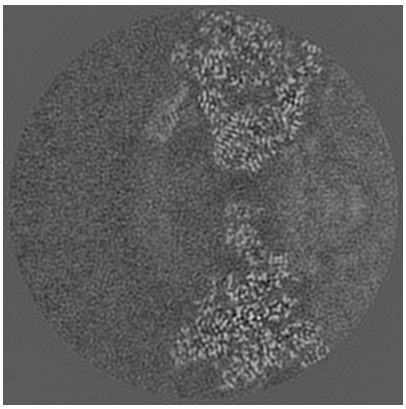
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

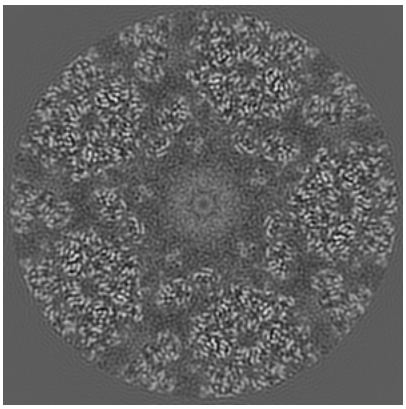
6.3.1 Primary map



X Index: 262

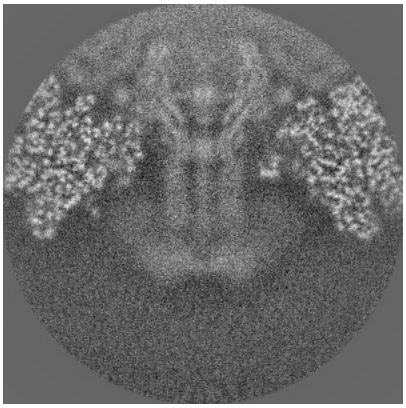


Y Index: 242

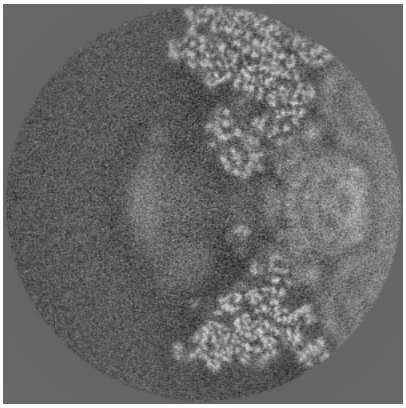


Z Index: 246

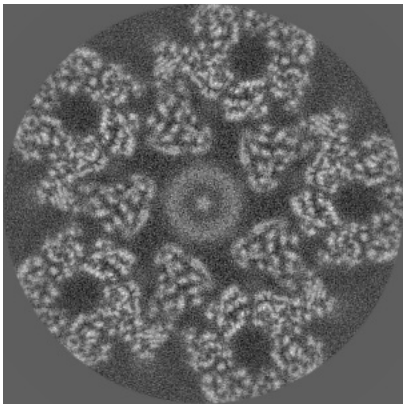
6.3.2 Raw map



X Index: 199



Y Index: 154

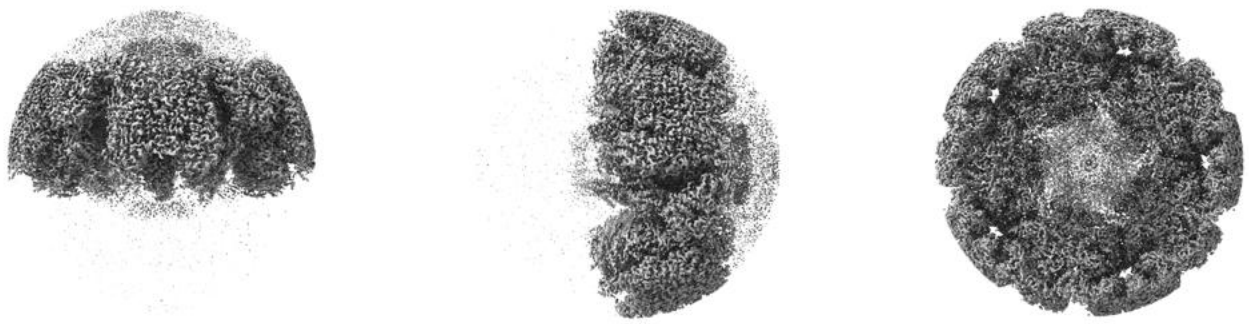


Z Index: 216

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.

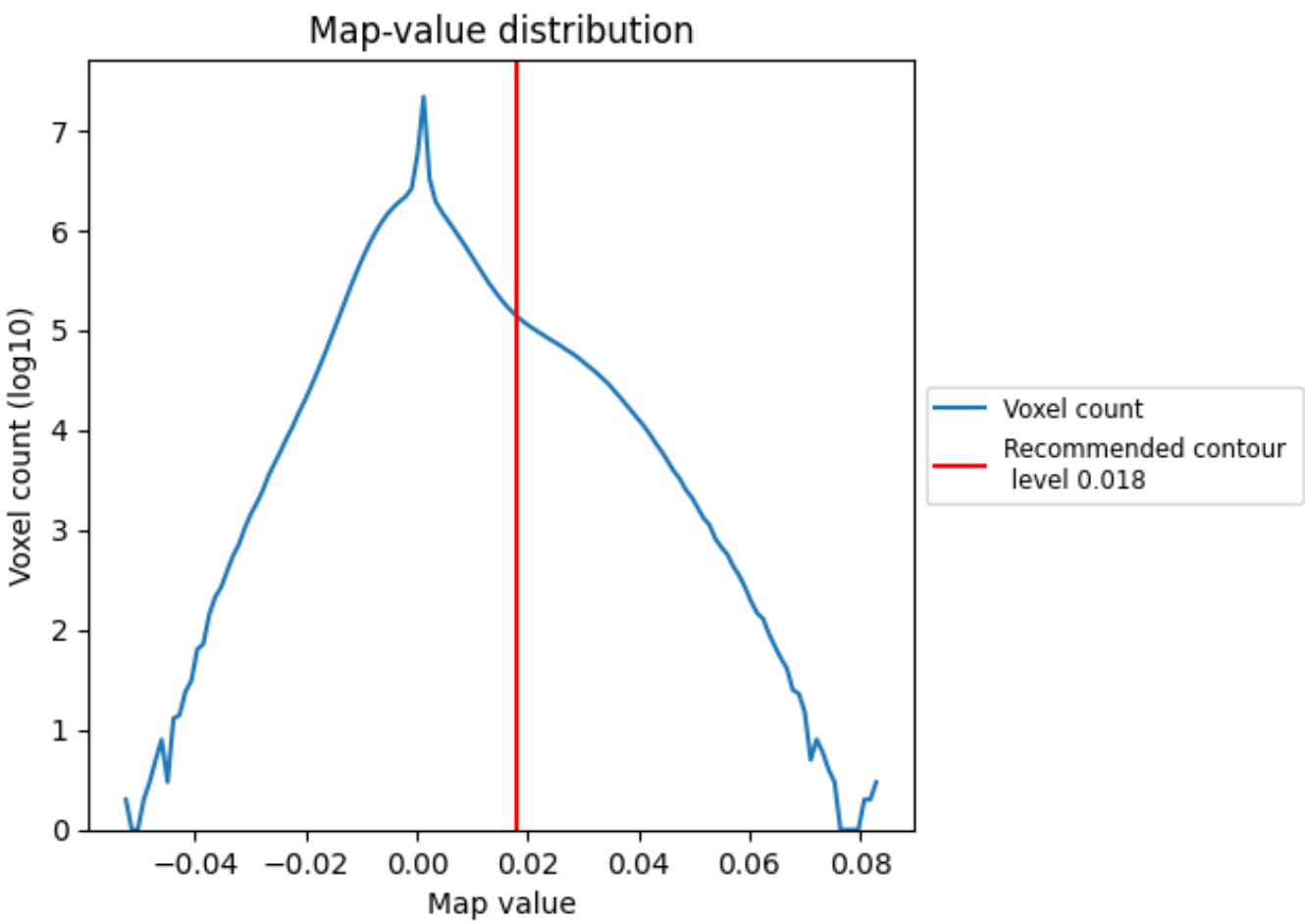
6.5 Mask visualisation (i)

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

7 Map analysis (i)

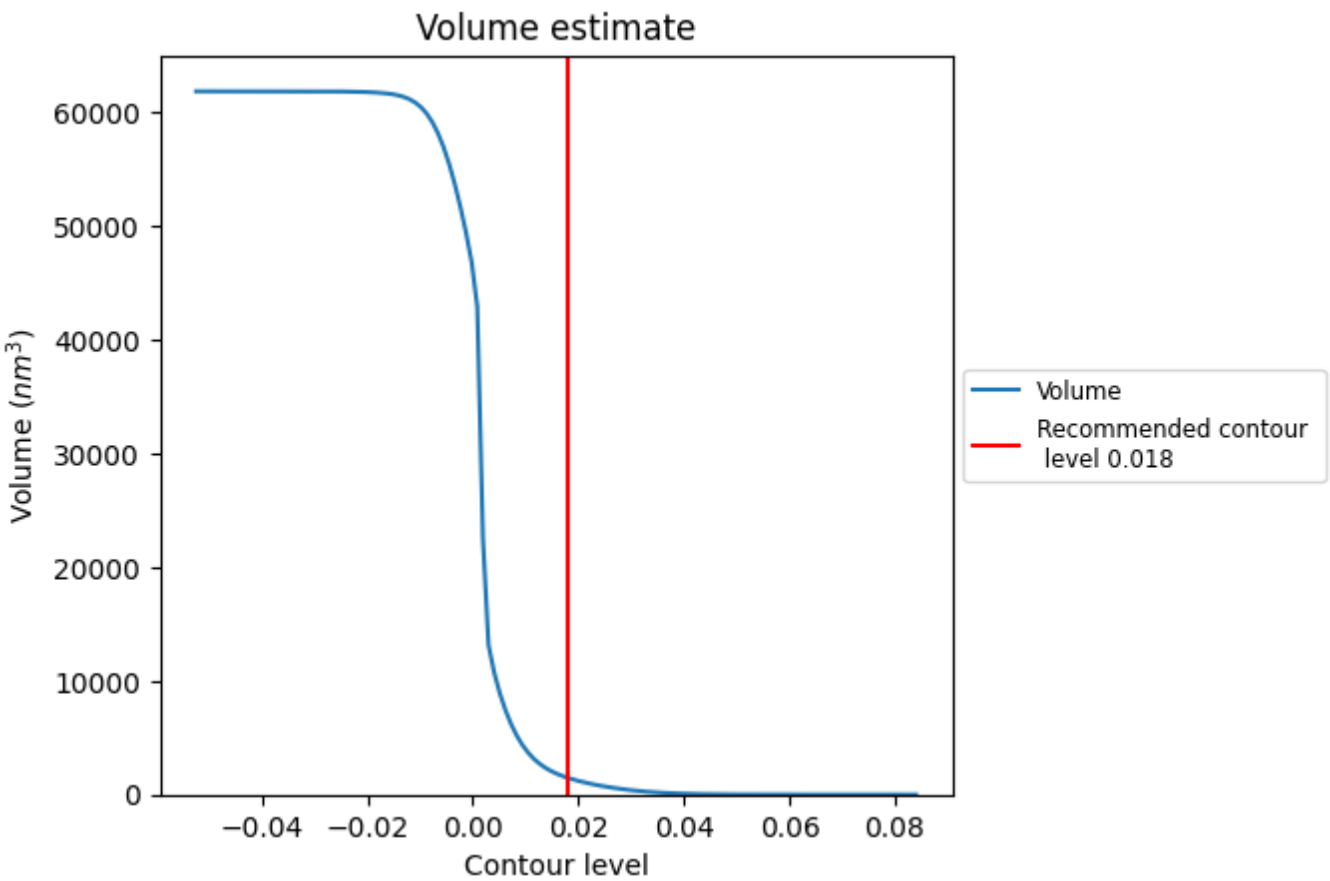
This section contains the results of statistical analysis of the map.

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.

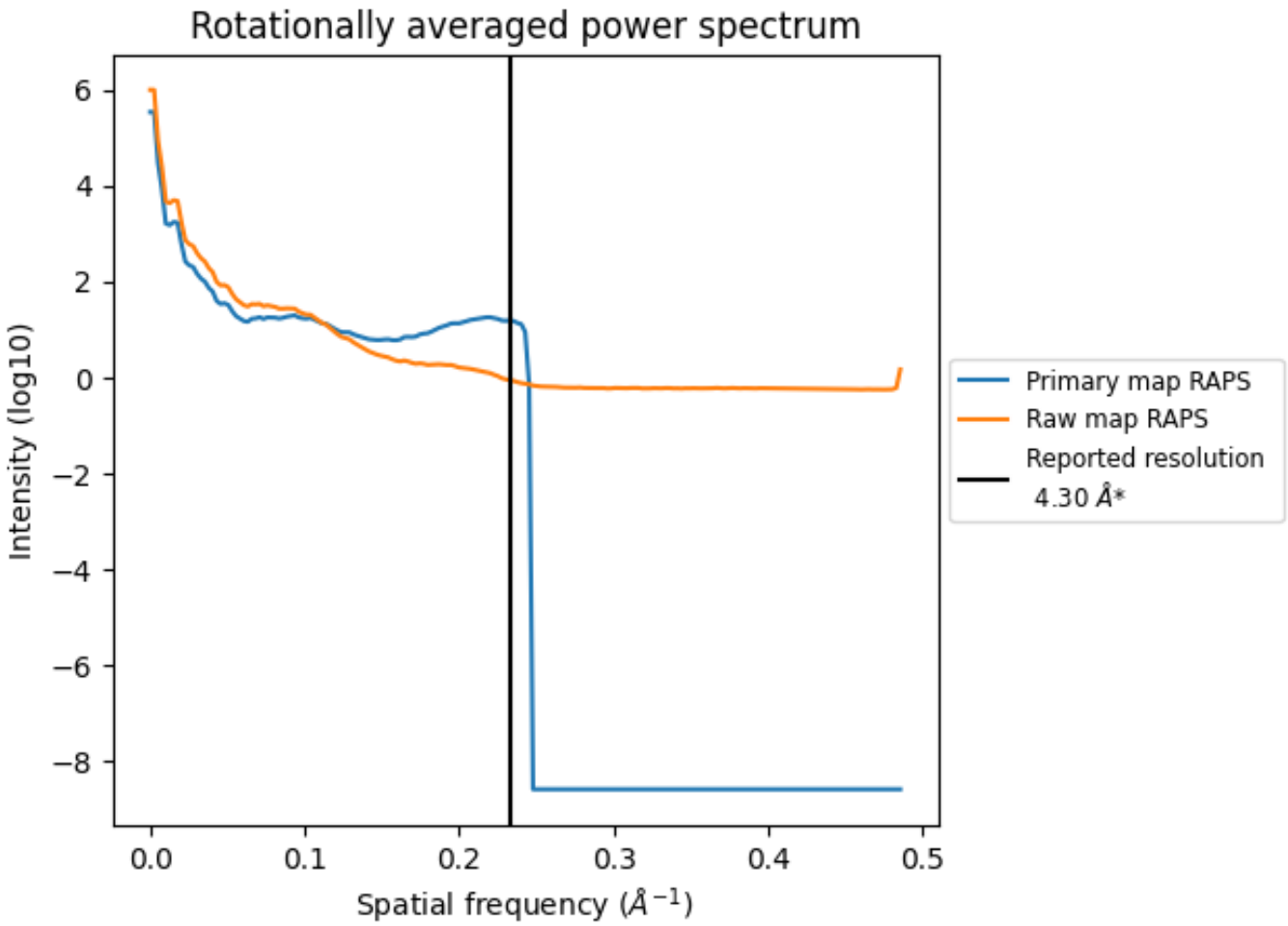
7.2 Volume estimate (i)



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)

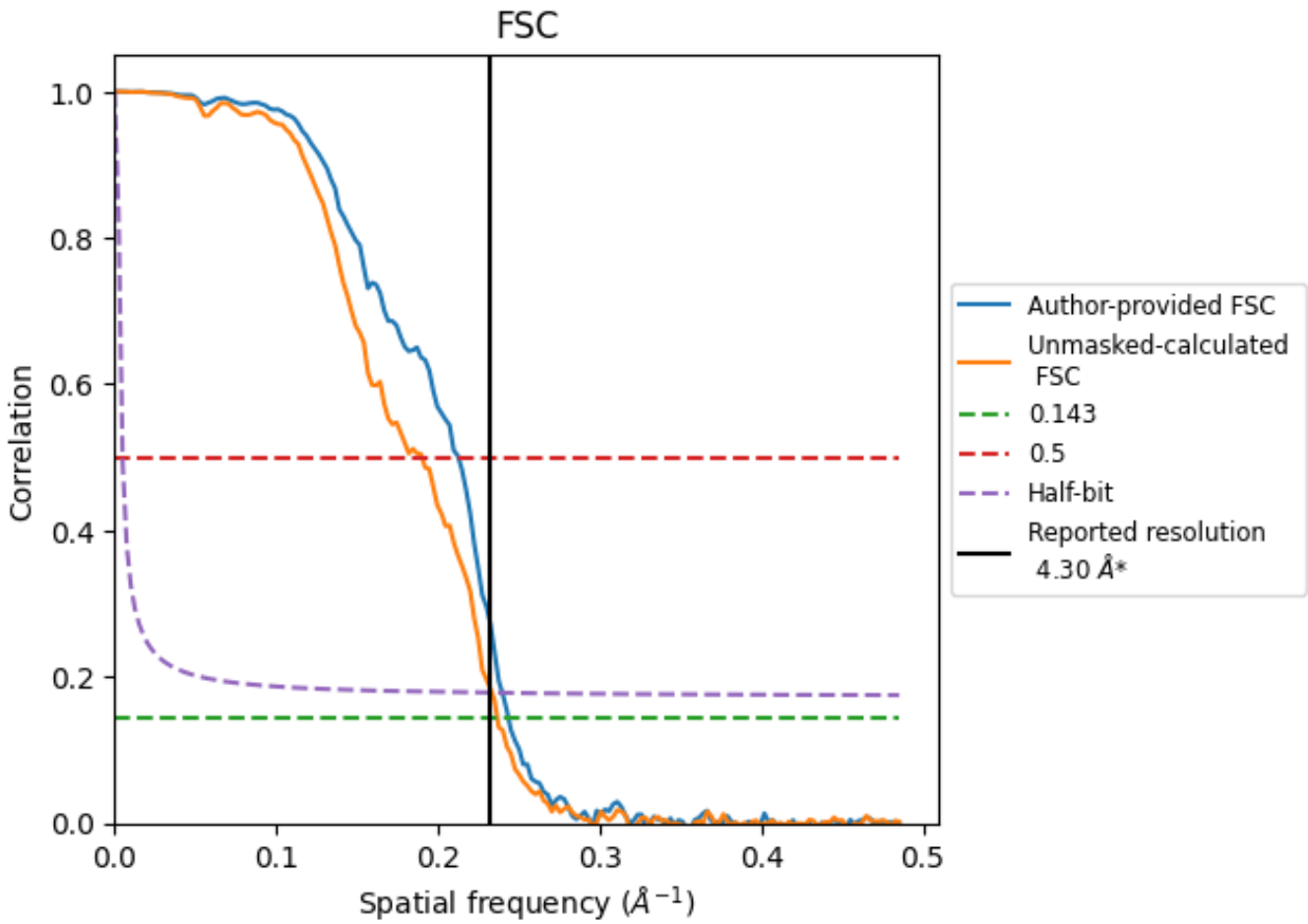


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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)

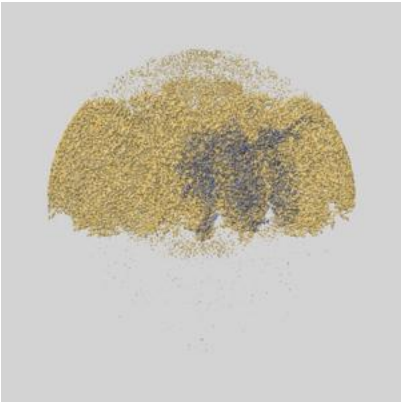
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.10	4.70	4.17
Unmasked-calculated*	4.22	5.26	4.28

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

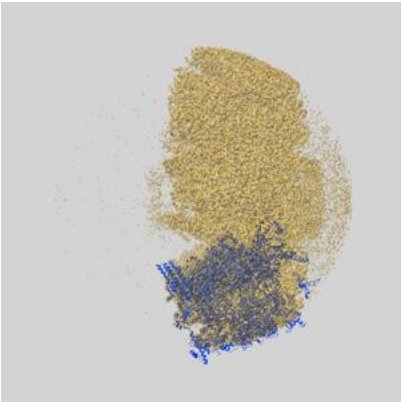
9 Map-model fit (i)

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.

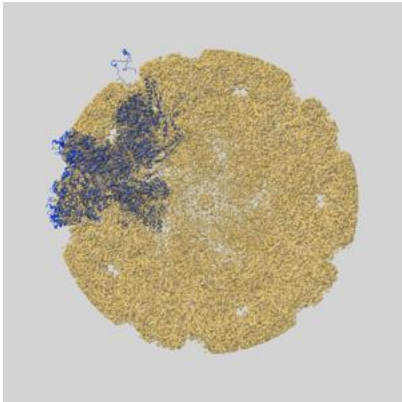
9.1 Map-model overlay (i)



X



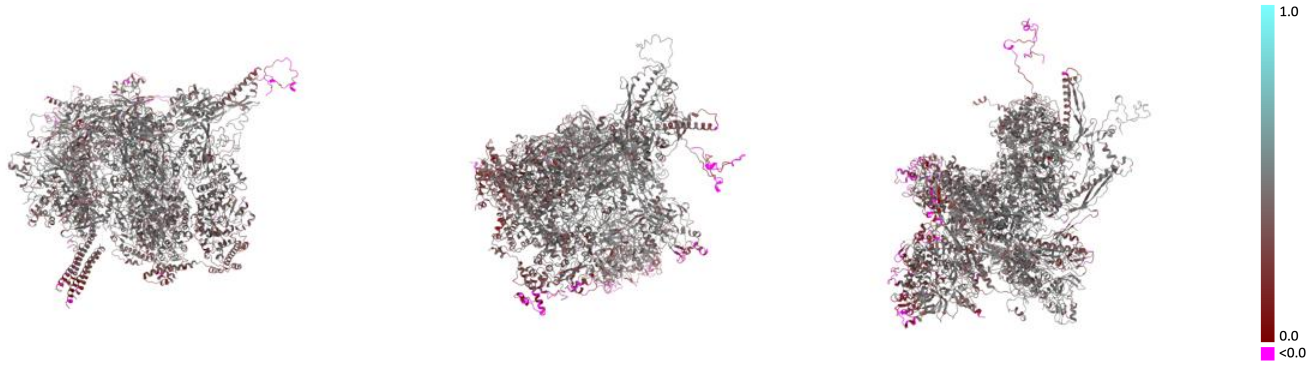
Y



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.

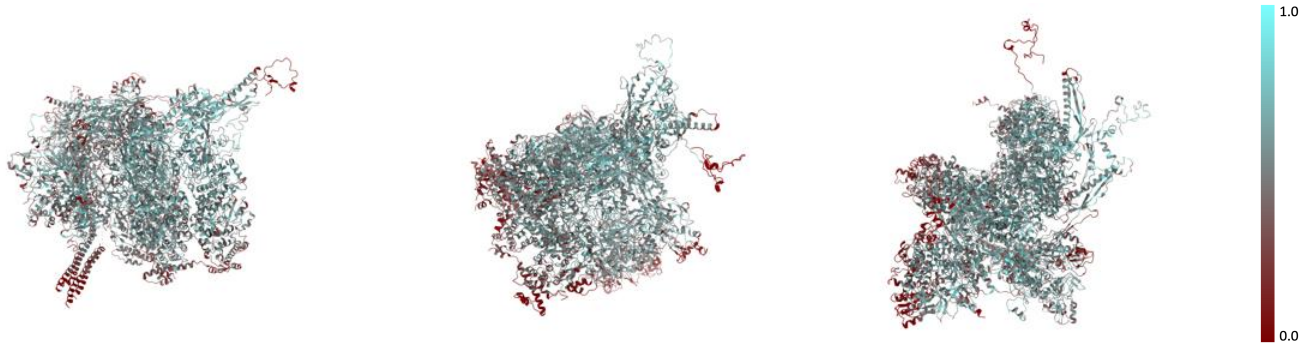
9.2 Q-score mapped to coordinate model (i)



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.

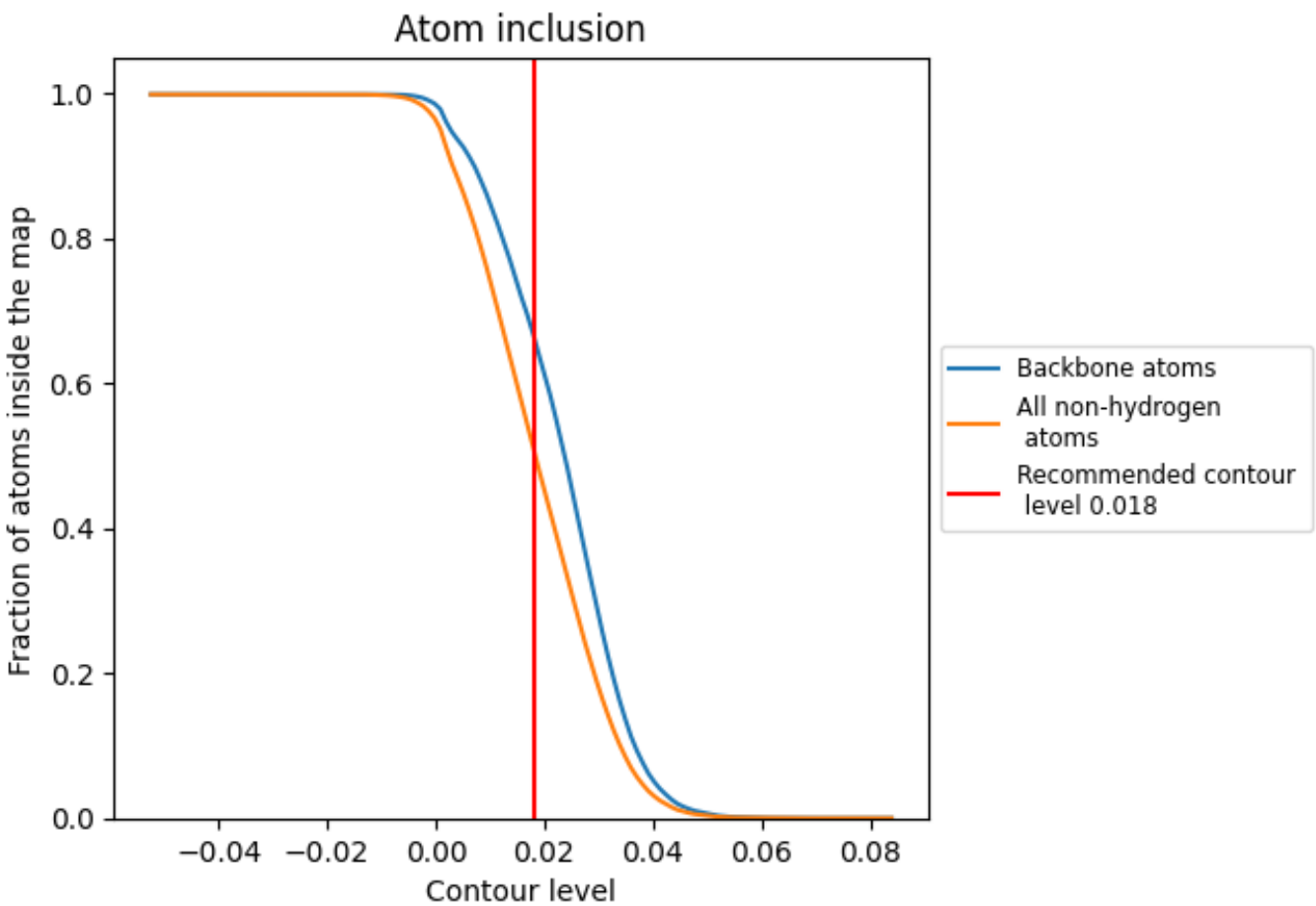
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

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