wwPDB EM Validation Summary Report

Nov 11, 2024 – 06:40 PM JST

PDB ID	:	7ETJ
EMDB ID	:	EMD-31298
Title	:	C5 portal vertex in the partially-enveloped virion capsid
Authors	:	Li, Z.; Yu, X.
Deposited on	:	2021-05-13
Resolution	:	4.00 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 ⓘ 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 ⓘ) were used in the production of this report:

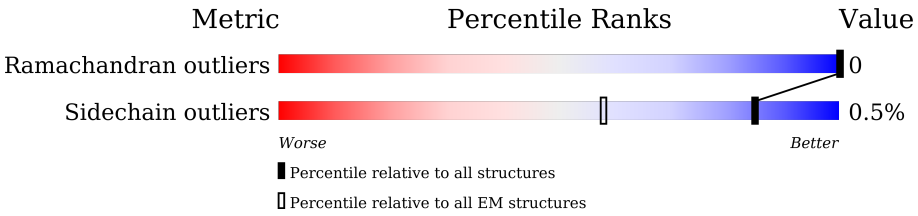
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	I	306	11% 98%
1	h	306	11% 98%
1	n	306	95%
1	o	306	6% 94% 6%
2	H	2241	99%
2	P	2241	99%
3	g	290	23% 78% 22%
3	m	290	99%
4	M	594	6% 78% 21%

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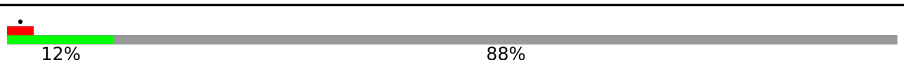
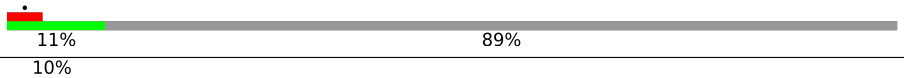
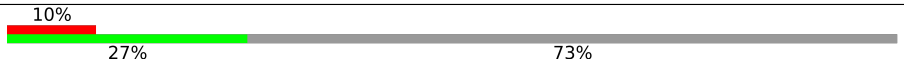
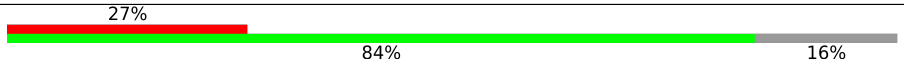
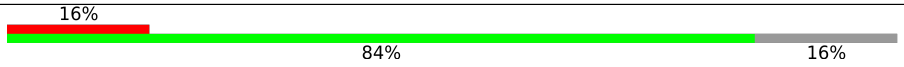
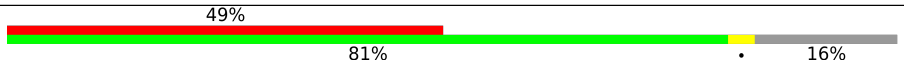
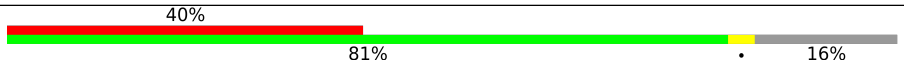
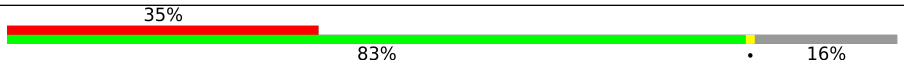
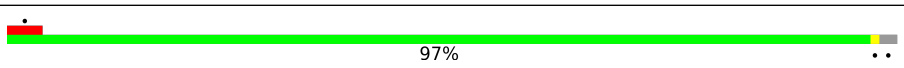
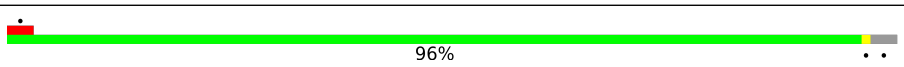
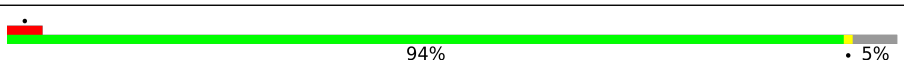
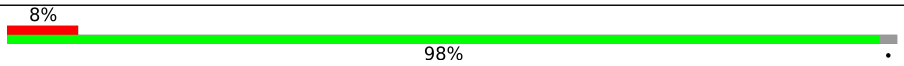
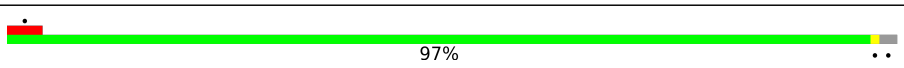
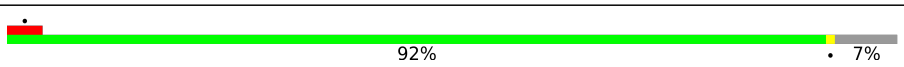
Mol	Chain	Length	Quality of chain
5	N	642	
5	O	642	
6	1	1048	
7	R	75	
7	S	75	
7	T	75	
7	i	75	
7	j	75	
8	B	1370	
8	C	1370	
8	D	1370	
8	Y	1370	
8	Z	1370	
8	a	1370	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 86613 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	300	Total	C	N	O	S	0	0
			2384	1528	415	424	17		
1	I	301	Total	C	N	O	S	0	0
			2389	1531	417	424	17		
1	n	294	Total	C	N	O	S	0	0
			2329	1499	401	410	19		
1	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

- Molecule 2 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
2	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	227	Total	C	N	O	S	0	0
			1822	1171	319	321	11		
3	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	76	Total	C	N	O	S	0	0
			648	408	127	109	4		
5	O	69	Total	C	N	O	S	0	0
			589	371	113	102	3		

- Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	T	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	i	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	j	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 8 is a protein called Major capsid protein.

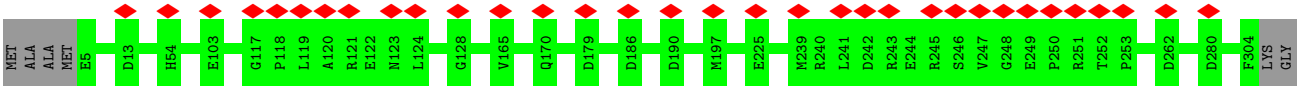
Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1275	Total	C	N	O	S	0	0
			10079	6410	1756	1855	58		
8	B	1339	Total	C	N	O	S	0	0
			10617	6762	1838	1956	61		
8	C	1331	Total	C	N	O	S	0	0
			10536	6711	1827	1938	60		
8	D	1297	Total	C	N	O	S	0	0
			10269	6538	1785	1887	59		
8	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
8	Z	1337	Total	C	N	O	S	0	0
			10582	6740	1831	1952	59		

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.

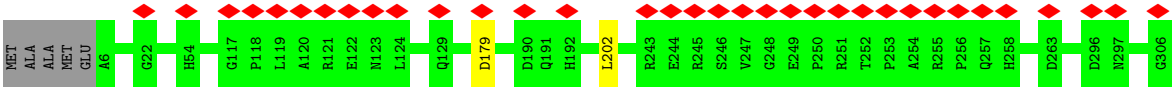
• Molecule 1: Triplex capsid protein 2

Chain h:



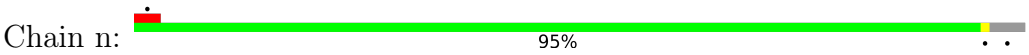
• Molecule 1: Triplex capsid protein 2

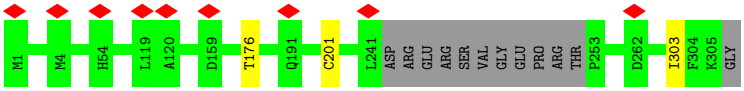
Chain I:



• Molecule 1: Triplex capsid protein 2

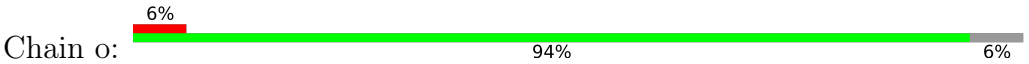
Chain n:

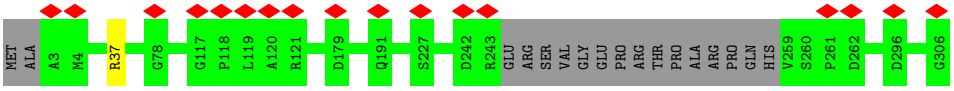




• Molecule 1: Triplex capsid protein 2

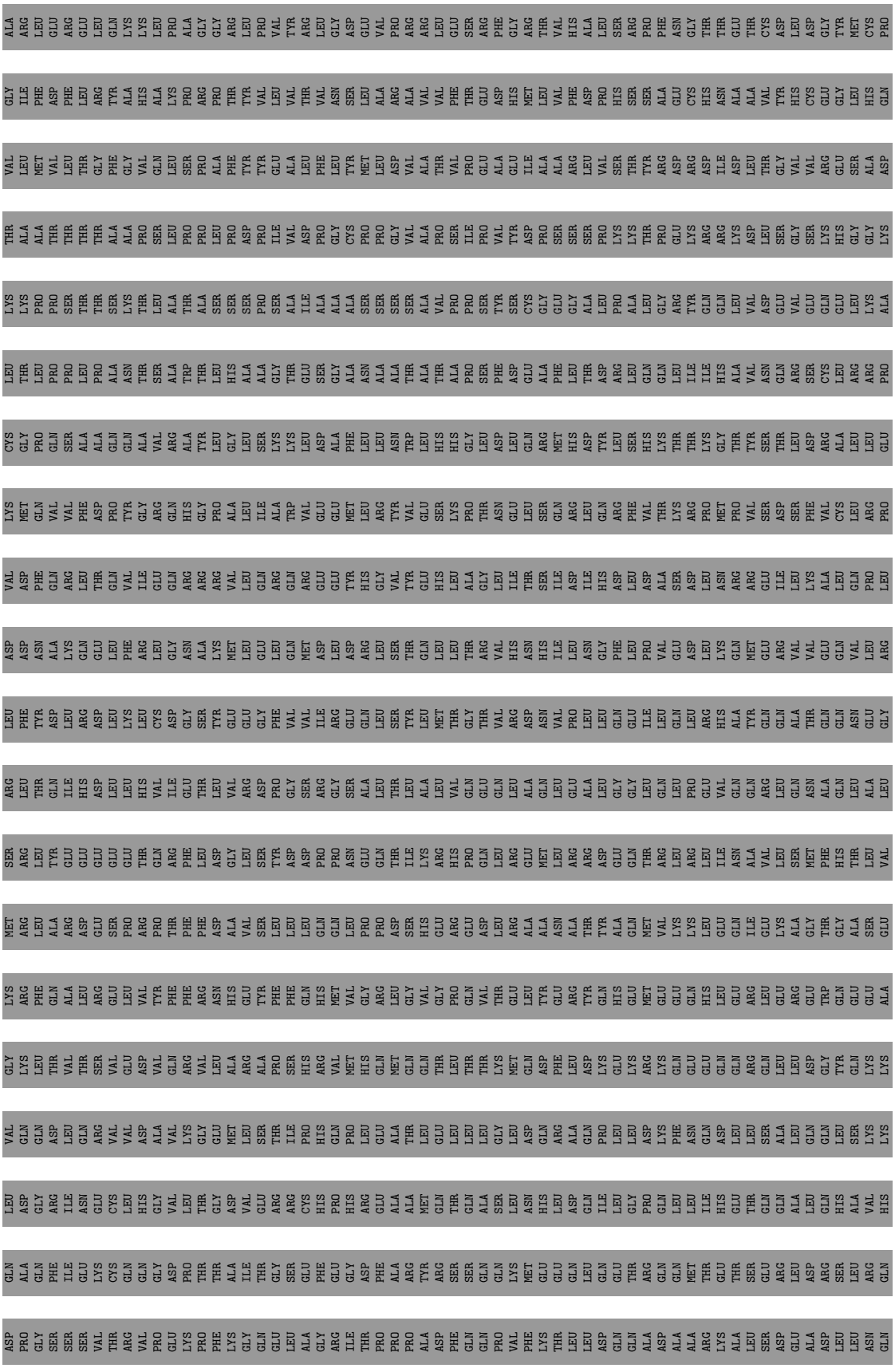
Chain o:





• Molecule 2: Large tegument protein deneddylase

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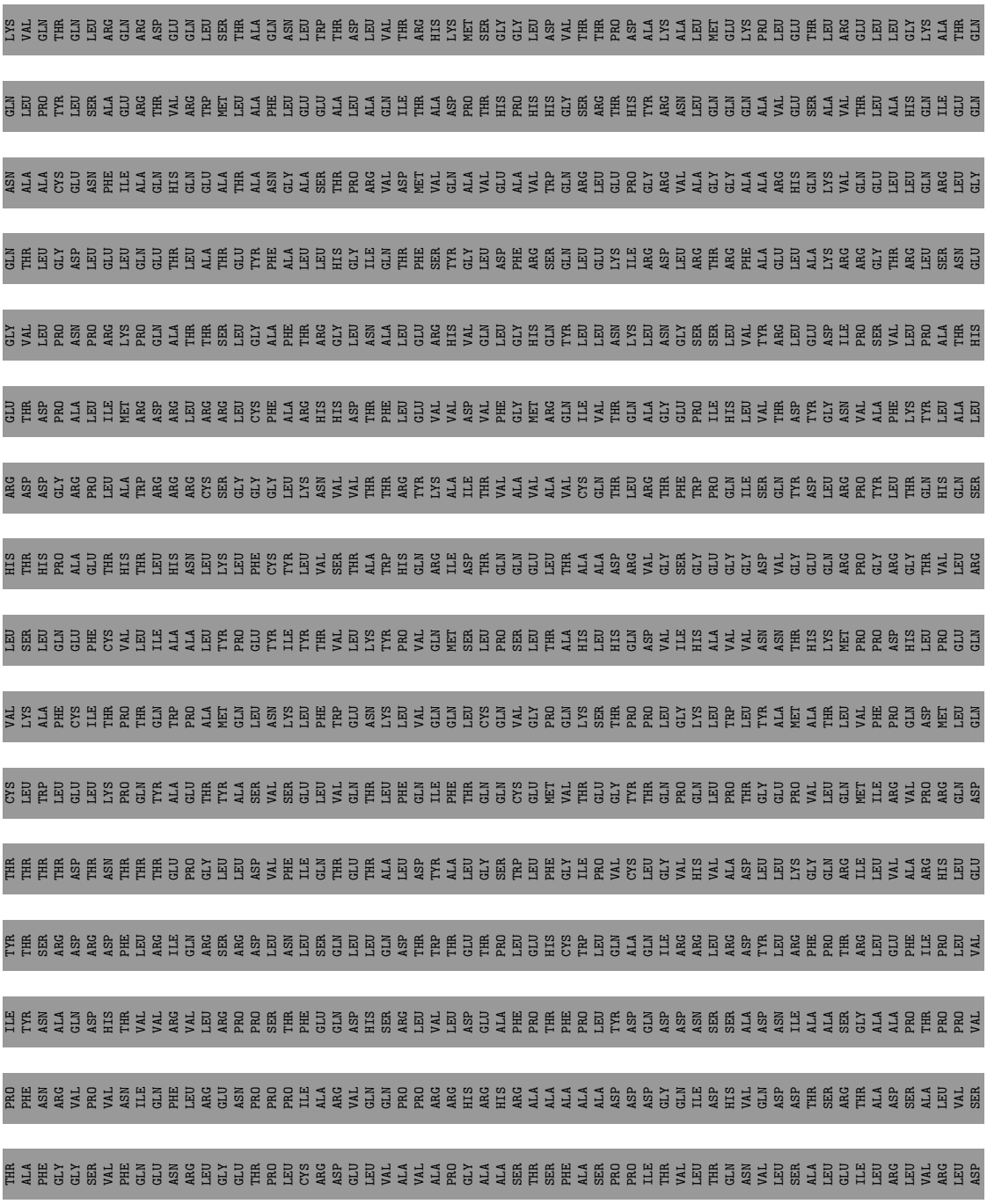
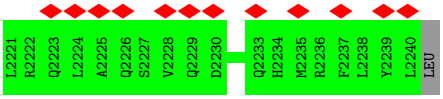
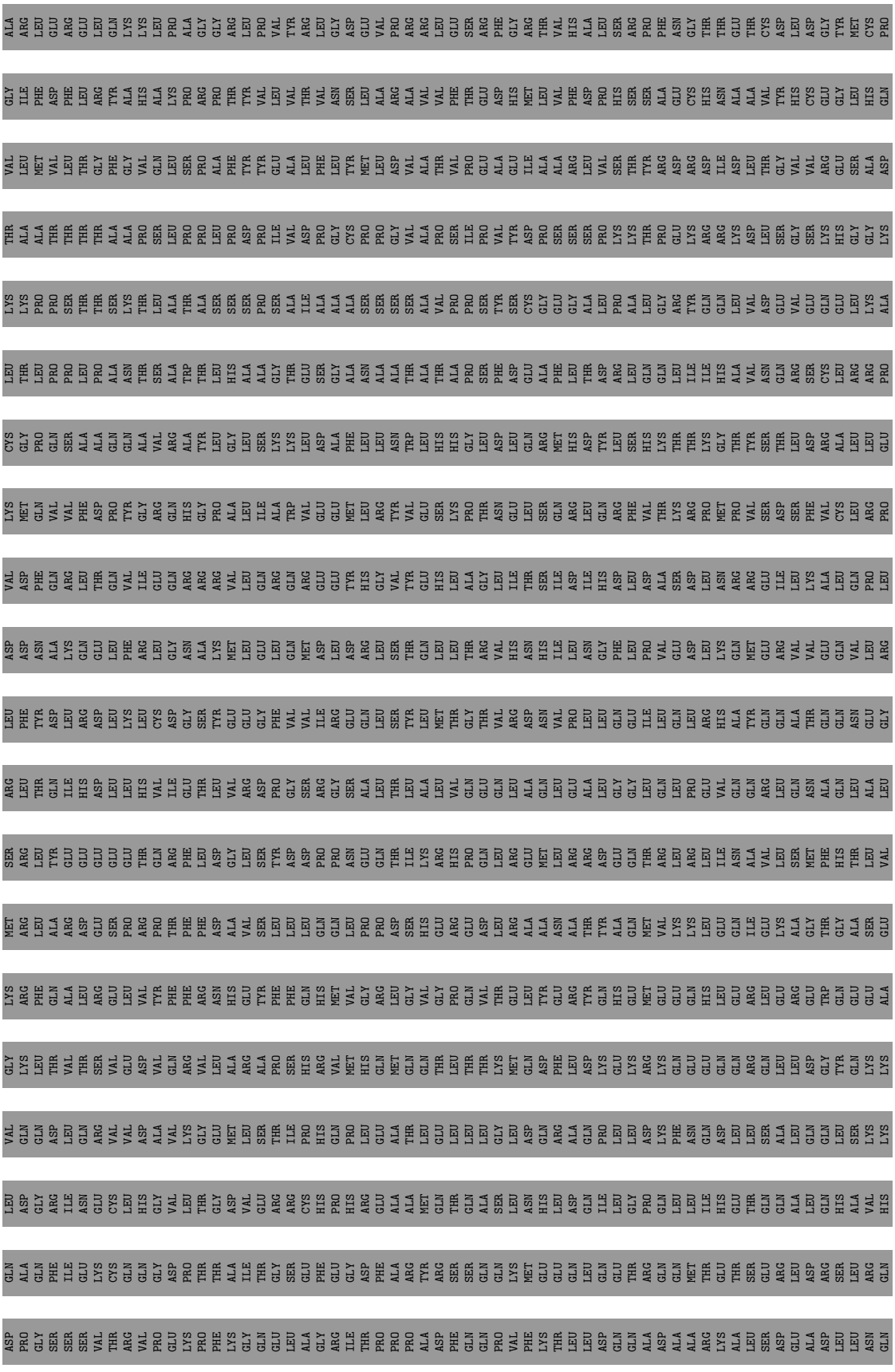
GLY LYS LEU THR VAL GLU ASP VAL GLN ARG VAL LEU HIS ARG VAL MET HIS GLN MET GLN GLN THR LEU THR THR LYS MET GLN ASP PHE LEU ASP LYS GLU LYS ARG LYS GLN GLN GLU GLN LEU LEU ASP GLY TYR GLN LYS LYS
VAL GLN GLN ASP LEU GLN ARG VAL ALA VAL LYS GLY GLU MET LEU SER THR ILE PRO HIS GLN PRO LEU GLU ALA THR LEU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





• Molecule 2: Large tegument protein deneddylase

Chain P: 99%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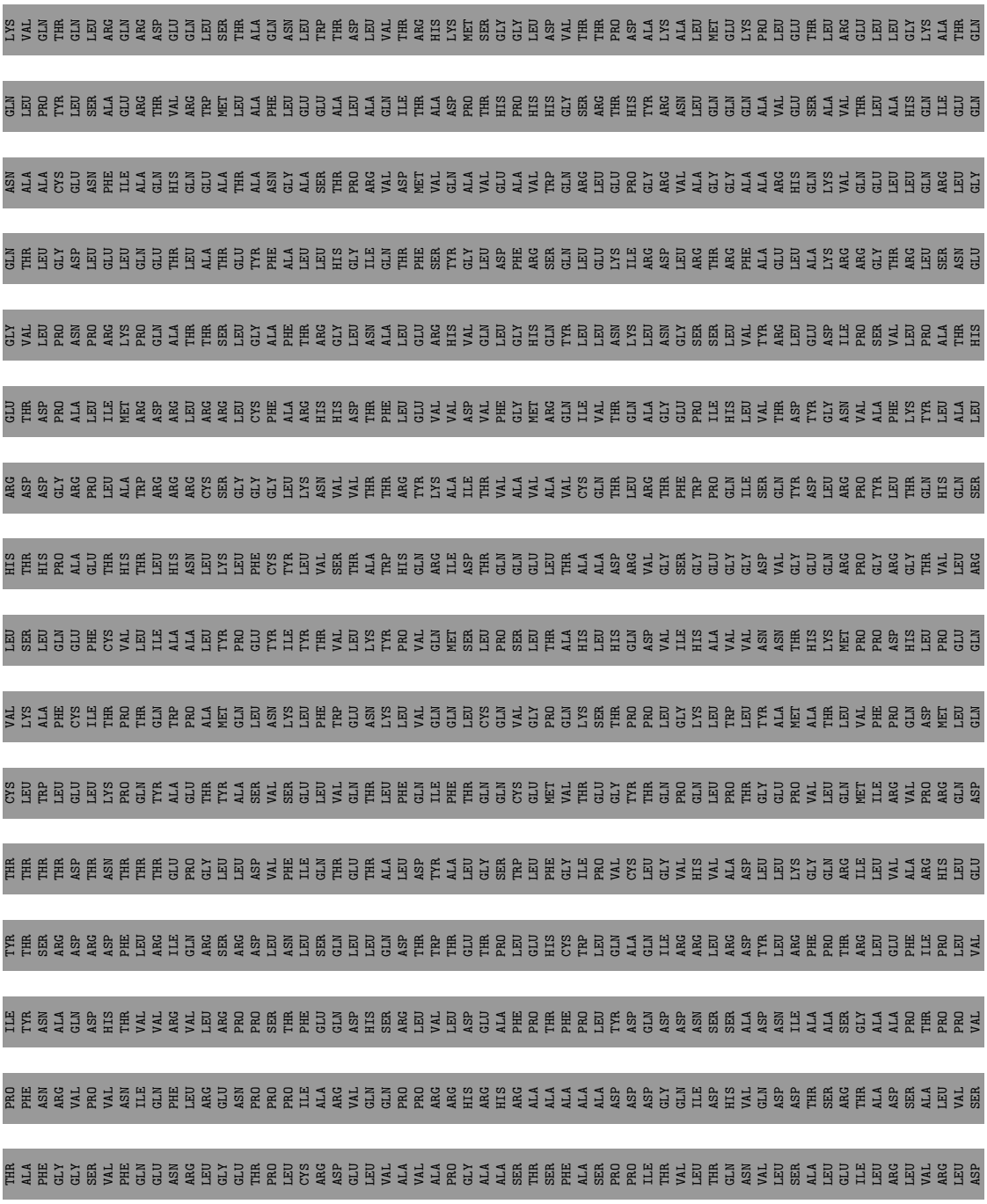
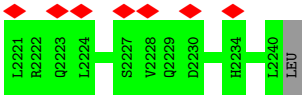
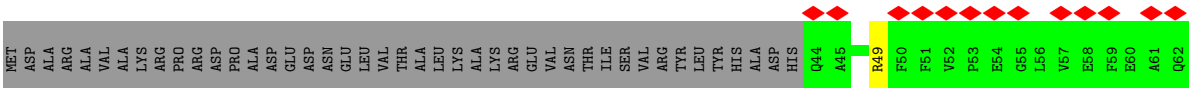
GLY ILE PHE ASP PHE LEU ARG TYR ALA HIS ALA LYS PRO ARG PRO THR TYR VAL LEU VAL THR VAL ASN SER LEU ALA ARG ALA VAL VAL PHE THR GLU ASP HIS MET LEU VAL PHE ASP PRO HIS SER SER ALA GLU CYS HIS ASN ALA ALA LEU VAL TYR HIS CYS GLU GLY LEU HIS GLN
VAL LEU MET VAL LEU THR GLY PHE GLY VAL GLN LEU SER PRO ALA PHE TYR TYR GLU ALA LEU PHE LEU TYR MET LEU ASP VAL ALA THR VAL PRO GLU ALA ILE ASP LEU THR GLY VAL VAL ARG GLU SER ALA ASP
THR ALA ALA THR THR THR THR ALA ALA ALA PRO SER LEU PRO PRO LEU PRO ASP PRO ILE VAL ASP PRO GLY CYS PRO PRO GLY VAL ALA PRO SER ILE PRO VAL TYR ASP PRO SER GLY SER LYS HIS GLY GLY LYS
LYS LYS PRO PRO SER THR THR SER LYS THR LEU ALA THR ALA ILE ALA ALA ALA SER SER SER SER ALA LEU GLY ARG TYR GLN LEU LEU VAL ASP GLU VAL GLU GLN LEU LYS
LEU THR LEU PRO PRO LEU PRO ALA ASN THR SER ALA TRP THR HIS ALA ALA GLY THR ALA ALA ALA THR ALA ALA THR ALA PRO SER PRO ALA ASP ARG LEU ILE HIS ALA VAL ASN GLN ARG SER CYS LEU ARG ARG
CYS GLY PRO GLN SER ALA ALA GLN GLN GLN ALA VAL ARG ALA TYR LEU GLY LEU ALA ALA PHE LEU ASN TRP LEU HIS HIS GLY LEU ASP GLU LEU GLN ARG MET HIS ASP TYR LEU SER HIS LYS THR THR LYS GLY THR TYR SER THR LEU ASP SER ASP THR LEU LEU LEU
LYS MET GLN VAL VAL PHE ASP PRO TYR GLY ARG GLN HIS GLY PRO ALA LEU ILE ALA TRP VAL GLU GLU MET LEU ARG TYR VAL GLU SER LYS PRO THR ASN GLU LEU GLN ARG MET HIS ASP TYR LEU GLN ARG PHE VAL THR LYS ARG PRO MET PRO VAL SER ASP SER PHE VAL CYS LEU LEU ARG PRO
VAL ASP PHE GLN ARG LEU THR GLN VAL GLU GLN ARG ARG ARG VAL LEU GLN ARG GLN ARG GLU GLU TYR HIS GLY VAL TYR GLU HIS LEU ALA GLY LEU ILE THR SER ILE ASP ILE HIS ASP LEU ASP ALA SER ASP LEU ASN ARG ARG GLU ILE LEU LYS ALA LEU GLN PRO LEU
ASP ASP ASN ALA LYS GLN LEU MET LEU GLU LEU GLU ASP ARG LEU LEU THR ARG VAL HIS ASN HIS ILE LEU ASN GLY PHE LEU PRO VAL GLU ASP LEU LYS GLN MET GLU ARG VAL VAL GLU GLN VAL LEU ARG
LEU PHE TYR ASP LEU ARG ASP LEU LYS LEU GLU GLY PHE VAL VAL ILE ARG GLU GLN LEU SER TYR LEU MET THR GLY THR VAL ARG ASP ASN VAL PRO LEU LEU GLN LEU GLU ILE LEU GLN LEU ARG ALA THR GLN GLN ASN GLU GLY
ARG LEU THR GLN ILE HIS ASP LEU LEU LEU GLU VAL ARG ASP PRO GLY SER ARG GLY SER ALA LEU THR LEU ALA LEU VAL GLN GLU ILE GLU ARG ALA LEU GLY GLY LEU GLN LEU PRO PRO GLU VAL GLN GLN ARG ARG LEU VAL ALA
SER ARG LEU TYR GLU GLU GLU GLU THR GLN ARG PHE LEU ASP GLY LEU SER TYR ASP ASP PRO PRO ASN GLU GLN THR ILE LYS ARG HIS PRO GLN LEU ARG ARG ASP GLU GLN THR ARG LEU ARG ARG LEU ILE ASN ALA VAL LEU GLN GLN ARG LEU VAL
MET ARG LEU ALA ARG ASP GLU SER PRO THR PHE PHE ASP ALA VAL SER LEU LEU LEU GLN LEU PRO PRO ASP SER HIS GLU ARG GLU ASP LEU ARG ALA ALA ASN ALA THR TYR ALA GLN MET VAL LYS LYS LEU GLU GLN ILE GLU LYS ALA GLY THR HIS GLY ALA SER GLU
LYS ARG PHE GLN ALA GLU LEU VAL TYR PHE PHE ARG ASN HIS GLU MET VAL GLY ARG LEU GLY VAL GLY PRO GLN VAL THR GLU LEU TYR PHE PHE PHE GLN HIS MET GLU GLU ARG TYR GLN HIS GLU MET GLU GLU GLN HIS LEU GLU ARG LEU GLU GLU ARG GLU TRP GLN GLU GLU ALA
GLY LYS LEU THR VAL ASP VAL GLU LEU GLN VAL ARG ARG VAL LEU GLN ARG PRO SER HIS ARG VAL MET HIS GLN MET GLN GLN THR LEU THR THR LYS MET GLN ASP PHE LEU ASP LYS GLU LYS ARG LYS GLN GLU GLU LEU ASP GLY TYR GLN LYS LYS
VAL GLN GLN ASP LEU GLN ARG VAL SER THR ILE PRO HIS GLN PRO LEU GLU ALA THR LEU GLU LEU LEU LEU GLY LEU ASP GLN PRO LEU LEU ASP ASP LYS PHE ASN GLN ASP LEU GLN LEU LEU SER LEU GLN LEU SER LYS LYS
LEU ASP GLY ARG ILE ASN GLY VAL LEU THR GLY ASP VAL GLU ARG CYS HIS PRO HIS ARG GLU ALA ALA MET GLN THR GLN ALA SER LEU ASN HIS LEU ASP LEU GLY PRO GLN LEU LEU ILE HIS GLU THR GLN GLN GLN ALA LEU GLN GLN HIS ALA VAL HIS
GLN ALA GLN PHE ILE PHE GLU GLY ASP PRO THR THR GLY LYS MET GLU GLU GLN GLN PRO VAL PHE LYS THR LEU LEU ASP GLN GLU THR ARG GLN GLN ALA ASP ALA ALA ARG THR LYS ALA LEU GLU GLU ARG LEU ASP ARG SER LEU ARG GLN
ASP PRO GLY SER LEU GLN GLY GLN GLN PRO GLN ALA ASP PHE GLN GLN ILE THR PRO PRO ALA ASP PHE GLN GLN GLY ALA ASP ALA ALA ARG LYS ALA ASP GLU ALA ASP LEU ASP SER GLN

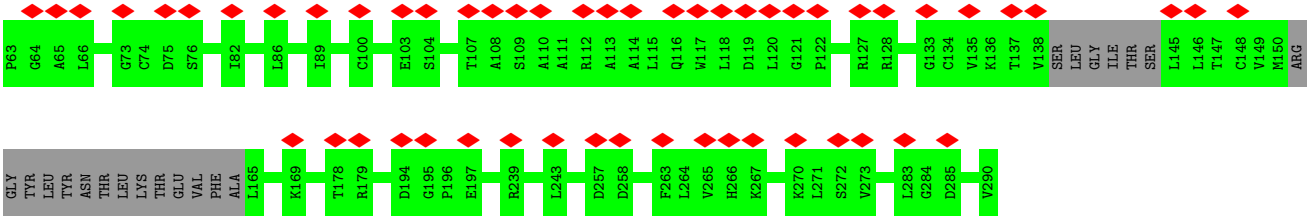




• Molecule 3: Triplex capsid protein 1

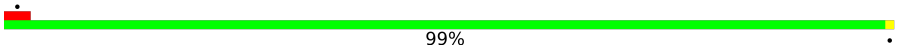
Chain g:

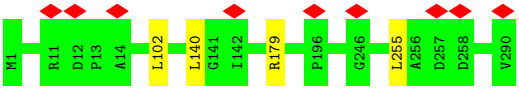




• Molecule 3: Triplex capsid protein 1

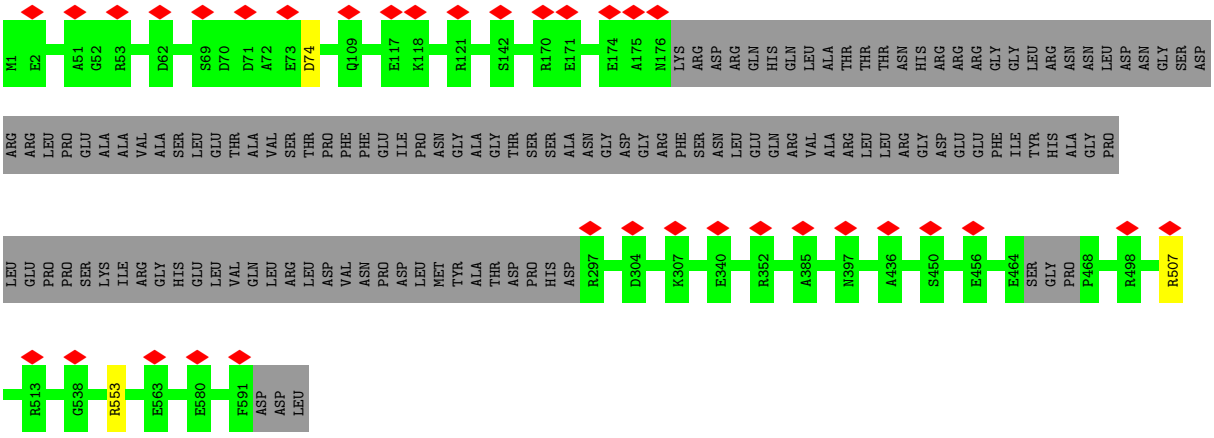
Chain m:





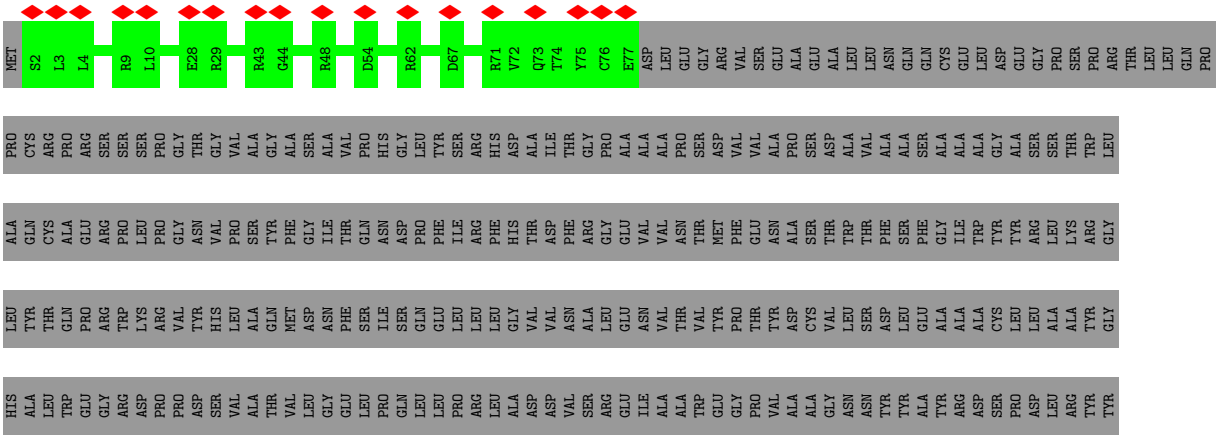
• Molecule 4: Capsid vertex component 1

Chain M:



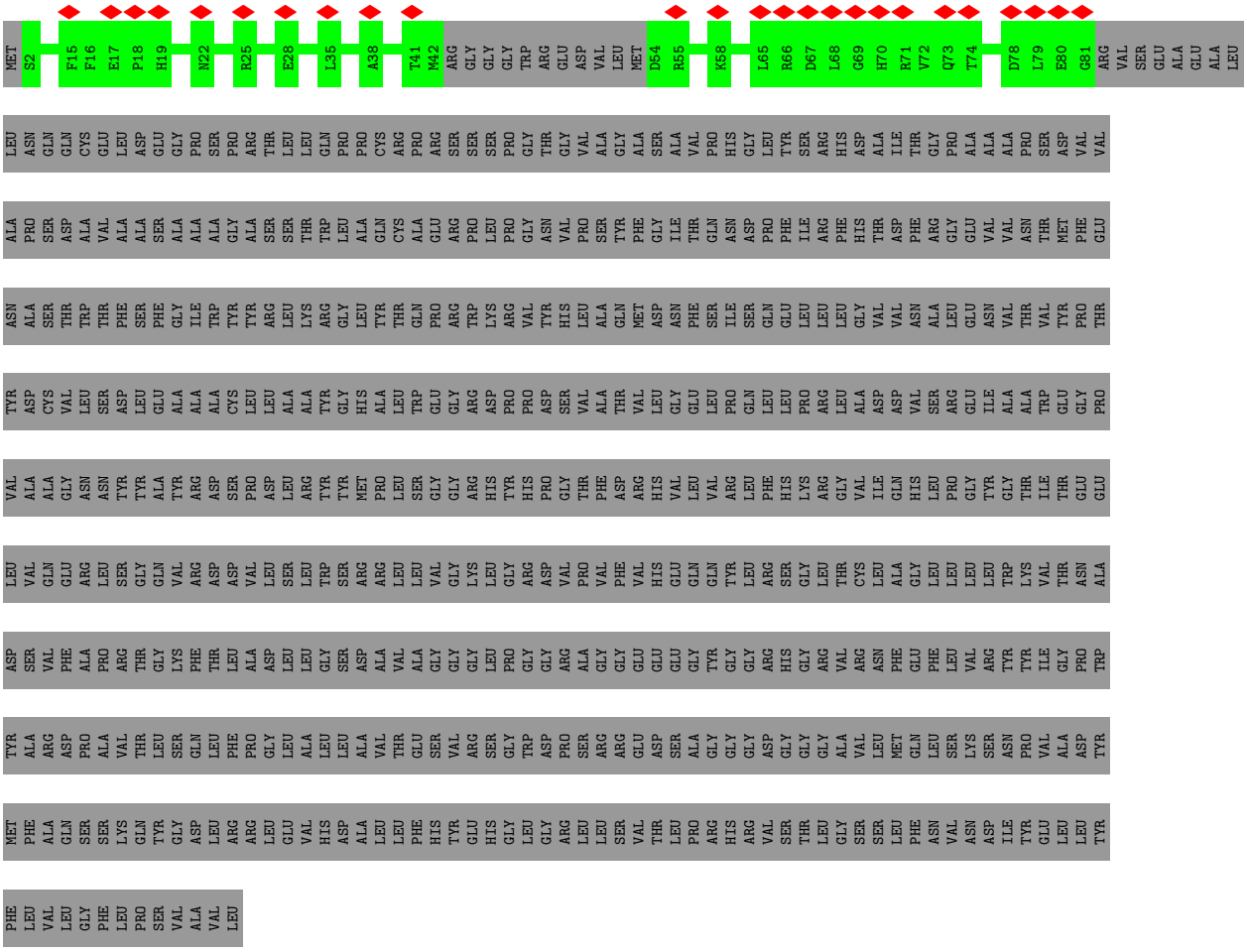
• Molecule 5: Capsid vertex component 2

Chain N:



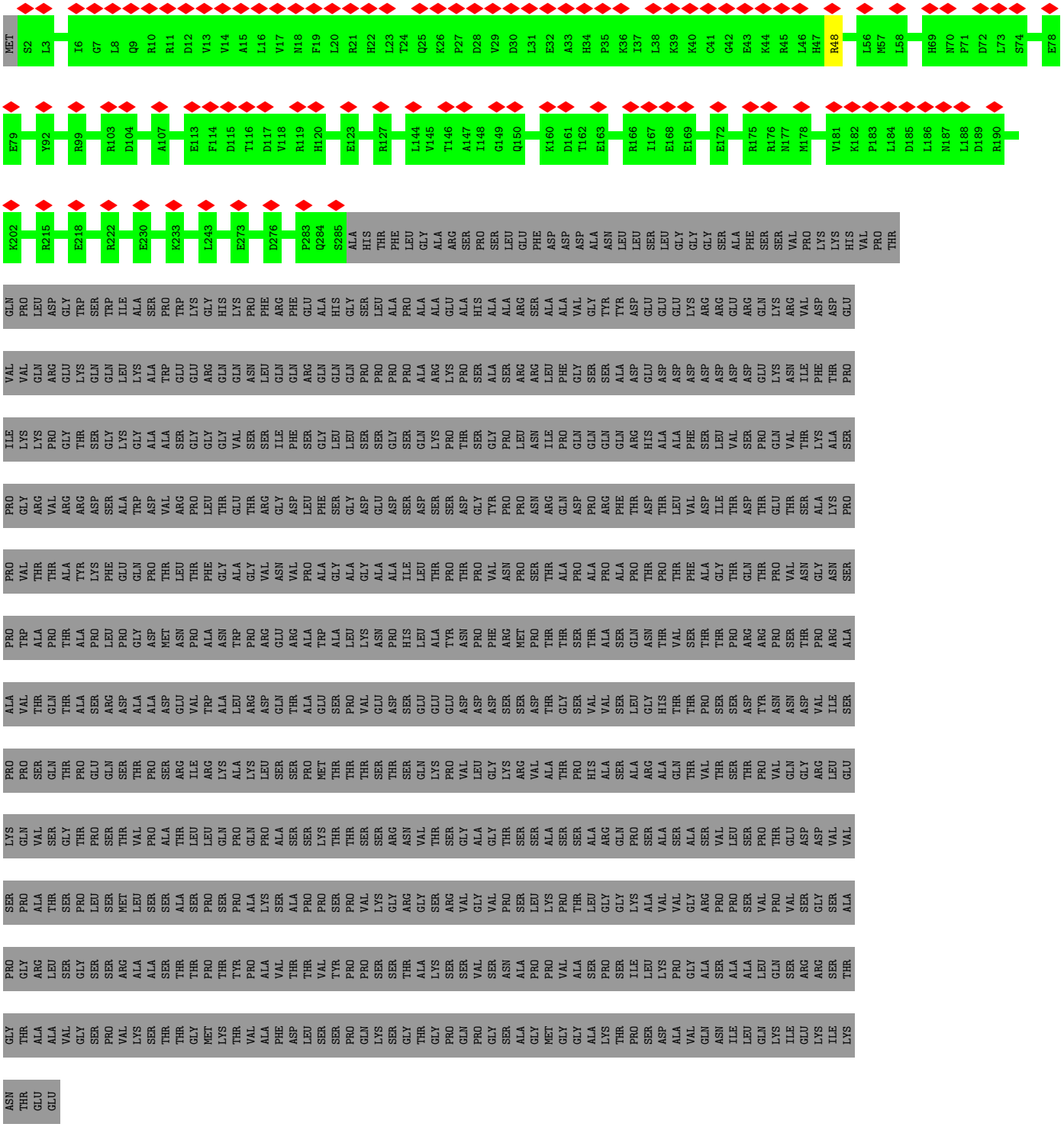
• Molecule 5: Capsid vertex component 2

Chain O:

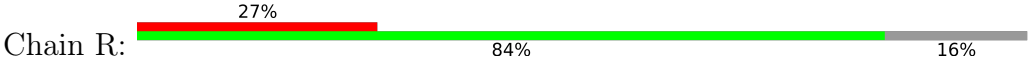


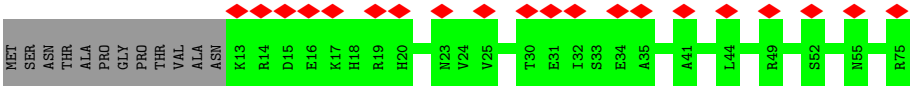
• Molecule 6: ORFL92C_UL32

Chain 1:



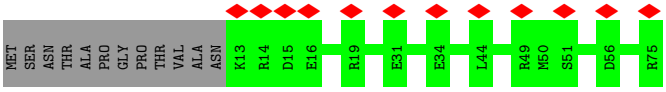
• Molecule 7: Small capsomere-interacting protein





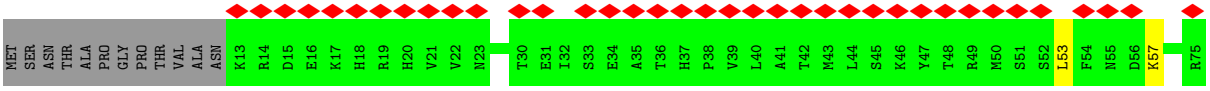
• Molecule 7: Small capsomere-interacting protein

Chain S:



• Molecule 7: Small capsomere-interacting protein

Chain T:

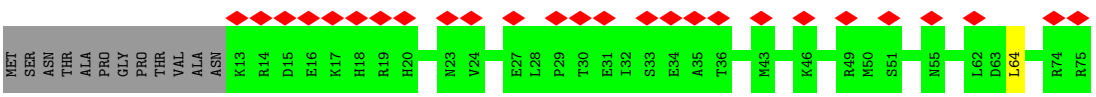


• Molecule 7: Small capsomere-interacting protein

Chain i:

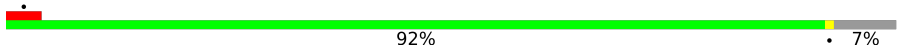
• Molecule 7: Small capsomere-interacting protein

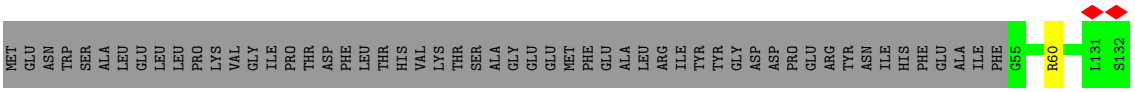
Chain j:

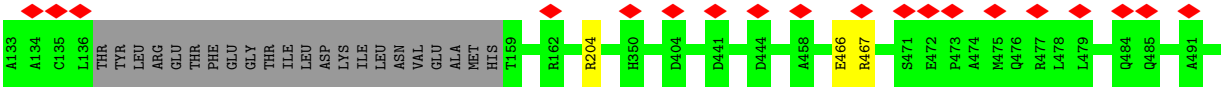


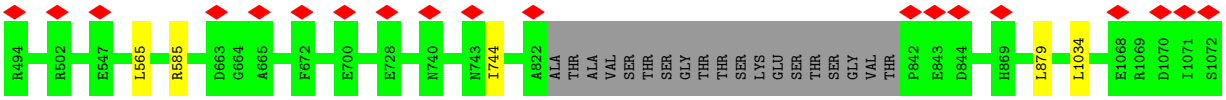
• Molecule 8: Major capsid protein

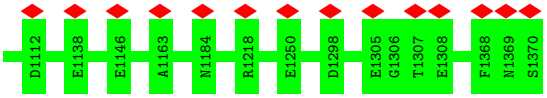
Chain a:





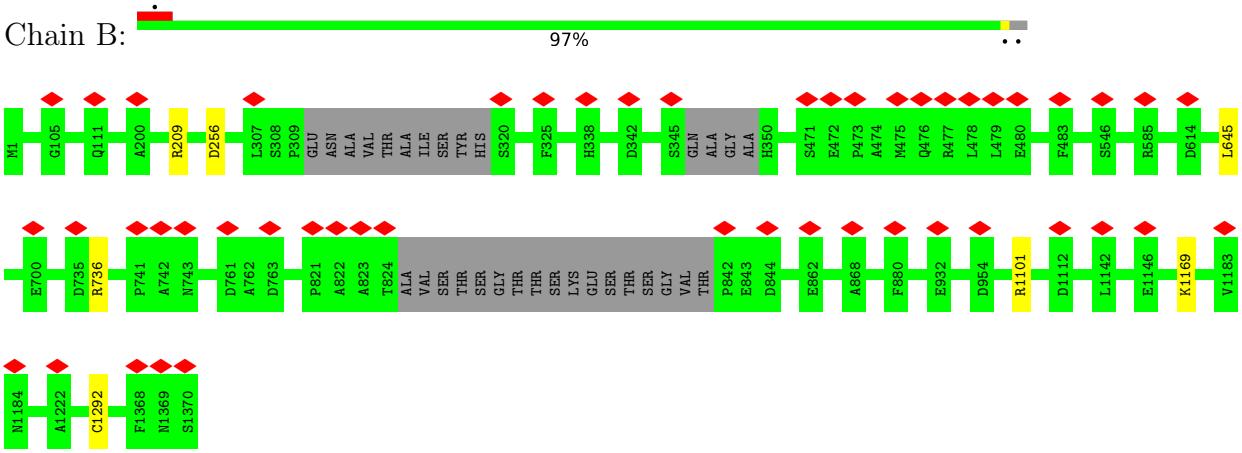






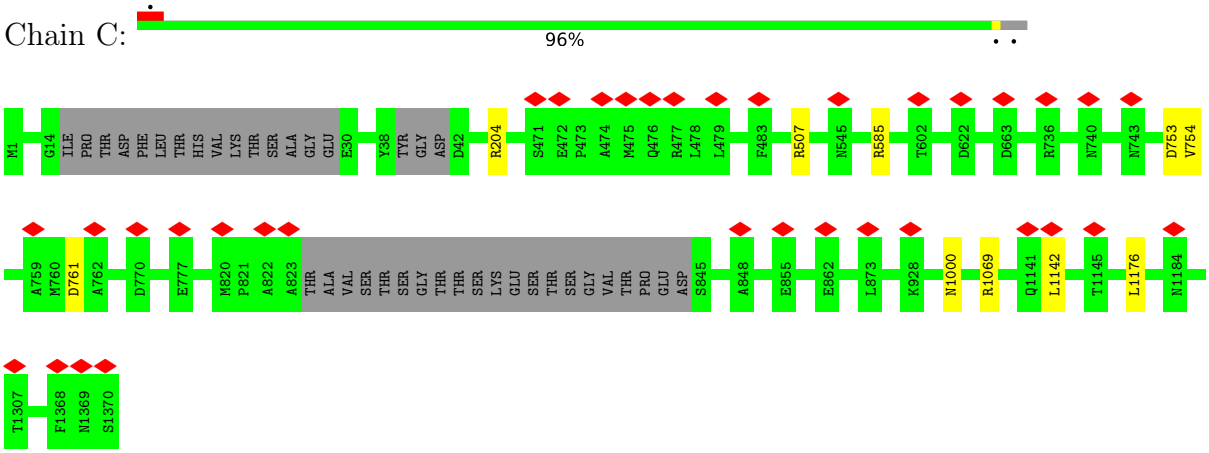
• Molecule 8: Major capsid protein

Chain B:



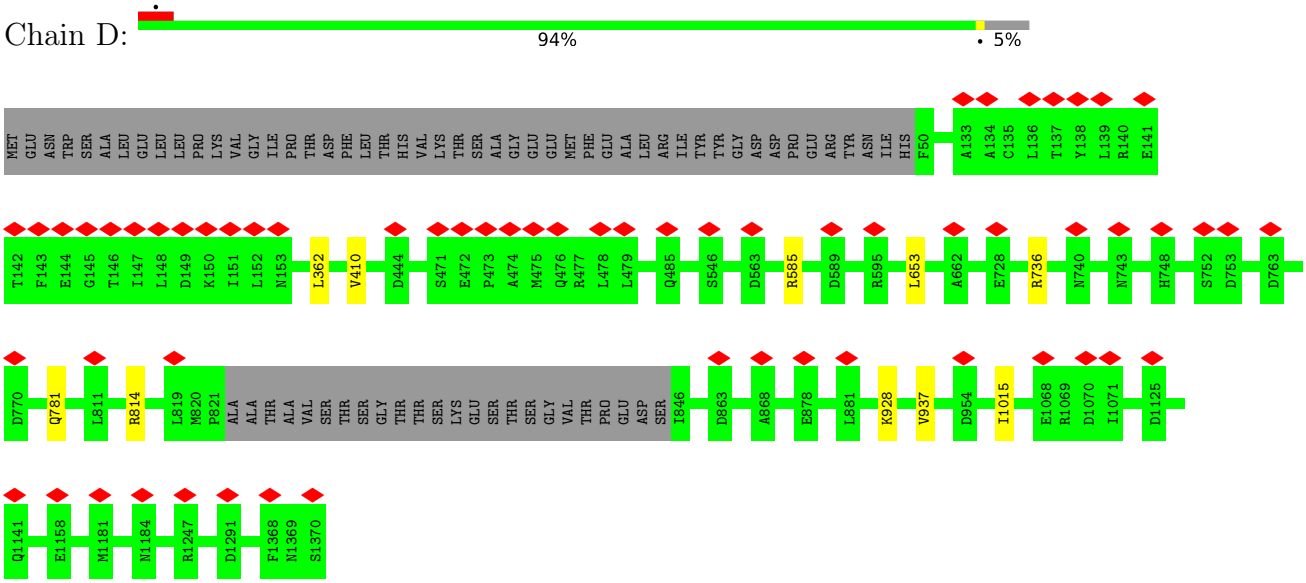
• Molecule 8: Major capsid protein

Chain C:



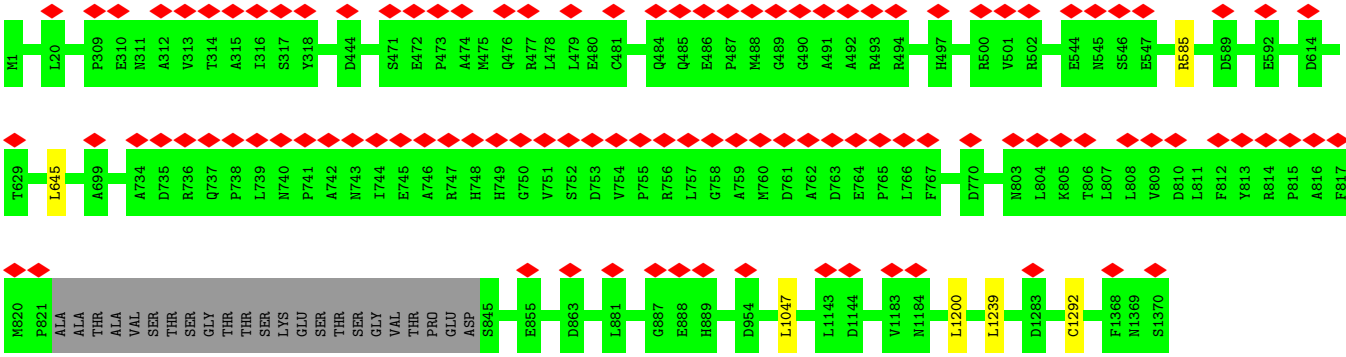
• Molecule 8: Major capsid protein

Chain D:



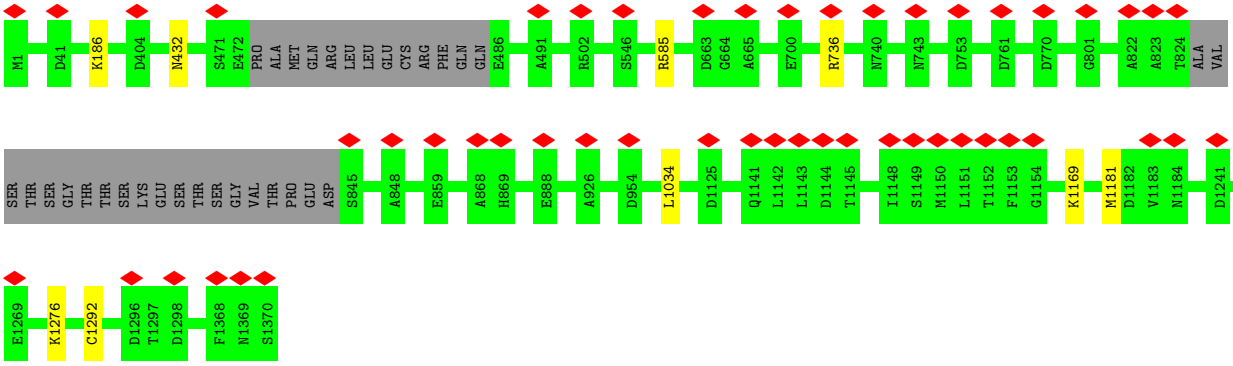
• Molecule 8: Major capsid protein

Chain Y:



• Molecule 8: Major capsid protein

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42849	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	Depositor

5 Model quality

5.1 Standard geometry

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	I	0.31	0/2436	0.65	2/3310 (0.1%)
1	h	0.31	0/2431	0.58	0/3306
1	n	0.30	0/2374	0.52	0/3225
1	o	0.30	0/2333	0.51	0/3167
2	H	0.27	0/174	0.60	0/233
2	P	0.28	0/174	0.51	0/233
3	g	0.31	0/1860	0.57	0/2521
3	m	0.34	0/2374	0.58	2/3221 (0.1%)
4	M	0.34	0/3935	0.57	0/5331
5	N	0.30	0/662	0.62	0/892
5	O	0.27	0/600	0.58	0/808
6	1	0.28	0/2358	0.55	0/3182
7	R	0.28	0/520	0.59	0/697
7	S	0.31	0/520	0.59	0/697
7	T	0.27	0/520	0.62	1/697 (0.1%)
7	i	0.29	0/520	0.74	2/697 (0.3%)
7	j	0.30	0/520	0.64	0/697
8	B	0.34	0/10870	0.58	2/14804 (0.0%)
8	C	0.34	0/10786	0.57	3/14692 (0.0%)
8	D	0.33	0/10513	0.54	1/14322 (0.0%)
8	Y	0.32	0/10932	0.54	3/14892 (0.0%)
8	Z	0.33	0/10835	0.54	1/14762 (0.0%)
8	a	0.34	0/10318	0.57	3/14057 (0.0%)
All	All	0.33	0/88565	0.56	20/120443 (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
8	C	0	1
8	D	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	Y	0	1
8	Z	0	1
8	a	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1142	LEU	CA-CB-CG	8.64	135.16	115.30
1	I	179	ASP	CB-CG-OD2	8.31	125.78	118.30
3	m	140	LEU	CA-CB-CG	6.81	130.96	115.30
7	i	64	LEU	CA-CB-CG	6.66	130.63	115.30
8	C	761	ASP	CB-CG-OD2	6.65	124.28	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	C	585	ARG	Peptide
8	D	585	ARG	Peptide
8	Y	585	ARG	Peptide
8	Z	585	ARG	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	I	299/306 (98%)	287 (96%)	12 (4%)	0	100	100
1	h	298/306 (97%)	283 (95%)	15 (5%)	0	100	100
1	n	290/306 (95%)	273 (94%)	17 (6%)	0	100	100
1	o	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
2	H	18/2241 (1%)	18 (100%)	0	0	100	100
2	P	18/2241 (1%)	18 (100%)	0	0	100	100
3	g	221/290 (76%)	204 (92%)	17 (8%)	0	100	100
3	m	288/290 (99%)	274 (95%)	14 (5%)	0	100	100
4	M	462/594 (78%)	442 (96%)	20 (4%)	0	100	100
5	N	74/642 (12%)	70 (95%)	4 (5%)	0	100	100
5	O	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	1	282/1048 (27%)	269 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	T	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	i	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	j	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
8	B	1331/1370 (97%)	1260 (95%)	71 (5%)	0	100	100
8	C	1323/1370 (97%)	1268 (96%)	55 (4%)	0	100	100
8	D	1293/1370 (94%)	1210 (94%)	83 (6%)	0	100	100
8	Y	1343/1370 (98%)	1267 (94%)	76 (6%)	0	100	100
8	Z	1331/1370 (97%)	1264 (95%)	67 (5%)	0	100	100
8	a	1269/1370 (93%)	1216 (96%)	53 (4%)	0	100	100
All	All	10795/17807 (61%)	10256 (95%)	539 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	I	270/273 (99%)	270 (100%)	0	100	100
1	h	270/273 (99%)	270 (100%)	0	100	100
1	n	263/273 (96%)	260 (99%)	3 (1%)	70	80
1	o	259/273 (95%)	258 (100%)	1 (0%)	89	91
2	H	19/1941 (1%)	19 (100%)	0	100	100
2	P	19/1941 (1%)	19 (100%)	0	100	100
3	g	199/252 (79%)	198 (100%)	1 (0%)	86	89
3	m	252/252 (100%)	250 (99%)	2 (1%)	79	84
4	M	395/500 (79%)	392 (99%)	3 (1%)	79	84
5	N	69/526 (13%)	69 (100%)	0	100	100
5	O	64/526 (12%)	64 (100%)	0	100	100
6	1	255/883 (29%)	254 (100%)	1 (0%)	89	91
7	R	59/68 (87%)	59 (100%)	0	100	100
7	S	59/68 (87%)	59 (100%)	0	100	100
7	T	59/68 (87%)	58 (98%)	1 (2%)	56	72
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	58 (98%)	1 (2%)	56	72
8	B	1169/1192 (98%)	1164 (100%)	5 (0%)	89	91
8	C	1156/1192 (97%)	1150 (100%)	6 (0%)	86	89
8	D	1130/1192 (95%)	1122 (99%)	8 (1%)	81	86
8	Y	1174/1192 (98%)	1172 (100%)	2 (0%)	92	93
8	Z	1163/1192 (98%)	1156 (99%)	7 (1%)	84	88
8	a	1110/1192 (93%)	1105 (100%)	5 (0%)	86	89
All	All	9531/15405 (62%)	9485 (100%)	46 (0%)	85	89

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	1069	ARG
8	D	937	VAL
8	D	410	VAL
8	D	781	GLN
8	Y	1200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157

such sidechains are listed below:

Mol	Chain	Res	Type
8	D	1000	ASN
8	Z	543	GLN
8	D	1166	HIS
8	Y	940	HIS
8	Z	1082	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

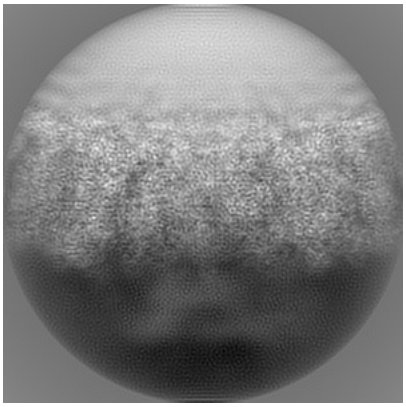
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31298. These allow visual inspection of the internal detail of the map and identification of artifacts.

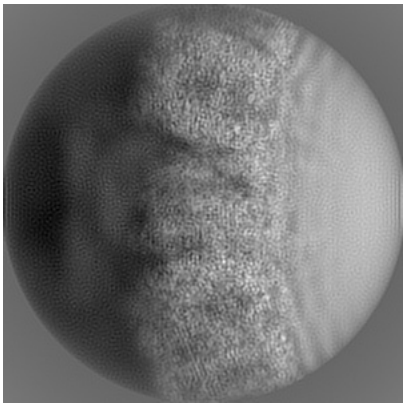
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

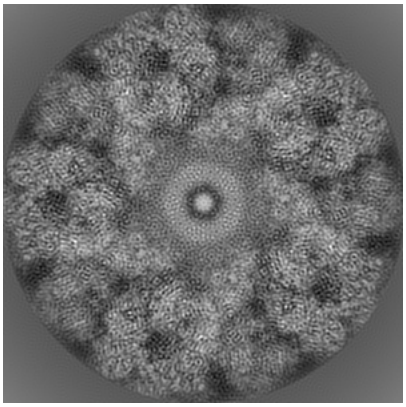
6.1.1 Primary map



X



Y

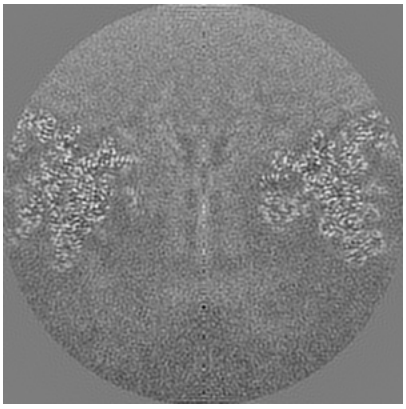


Z

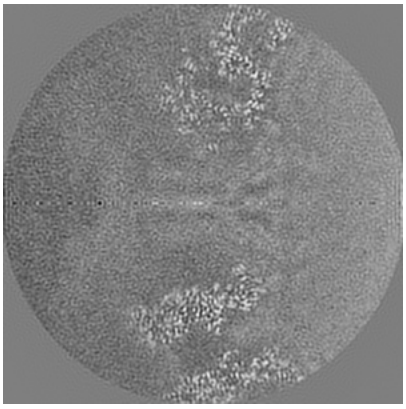
The images above show the map projected in three orthogonal directions.

6.2 Central slices

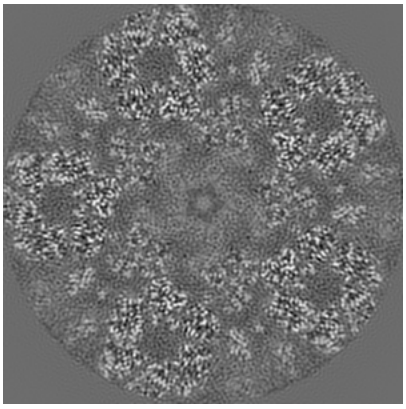
6.2.1 Primary map



X Index: 128



Y Index: 128

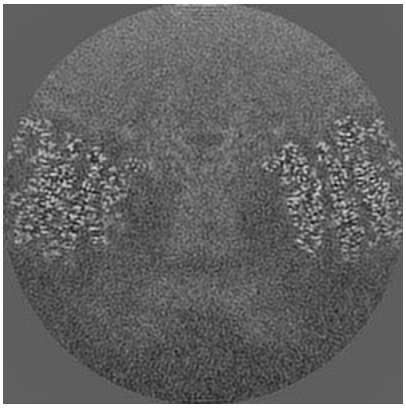


Z Index: 128

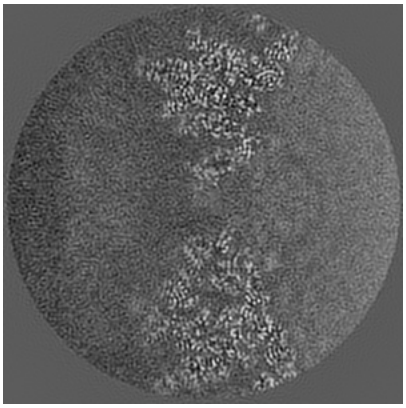
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

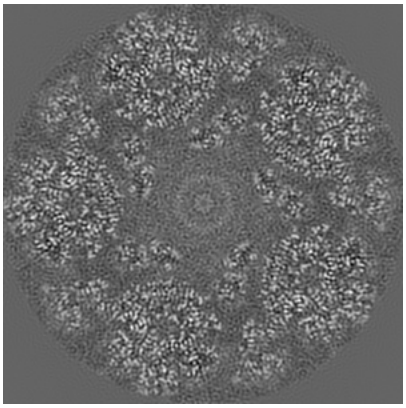
6.3.1 Primary map



X Index: 116



Y Index: 97

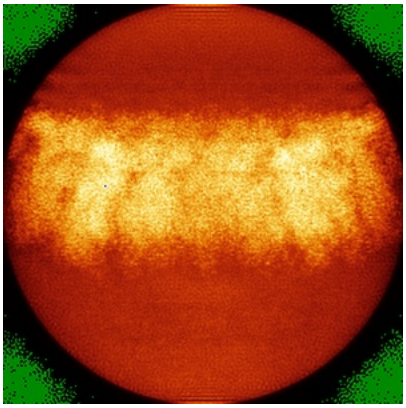


Z Index: 141

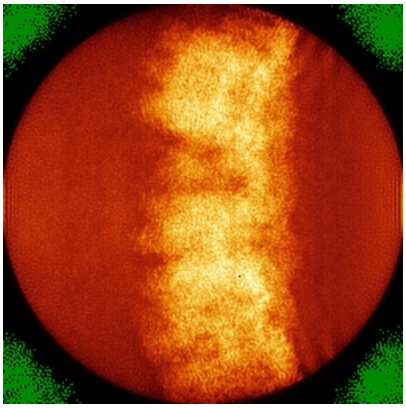
The images above show the largest variance slices of the map in three orthogonal directions.

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

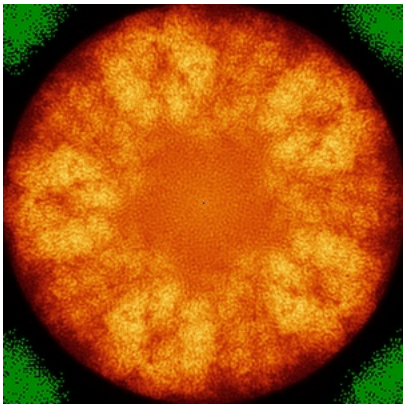
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

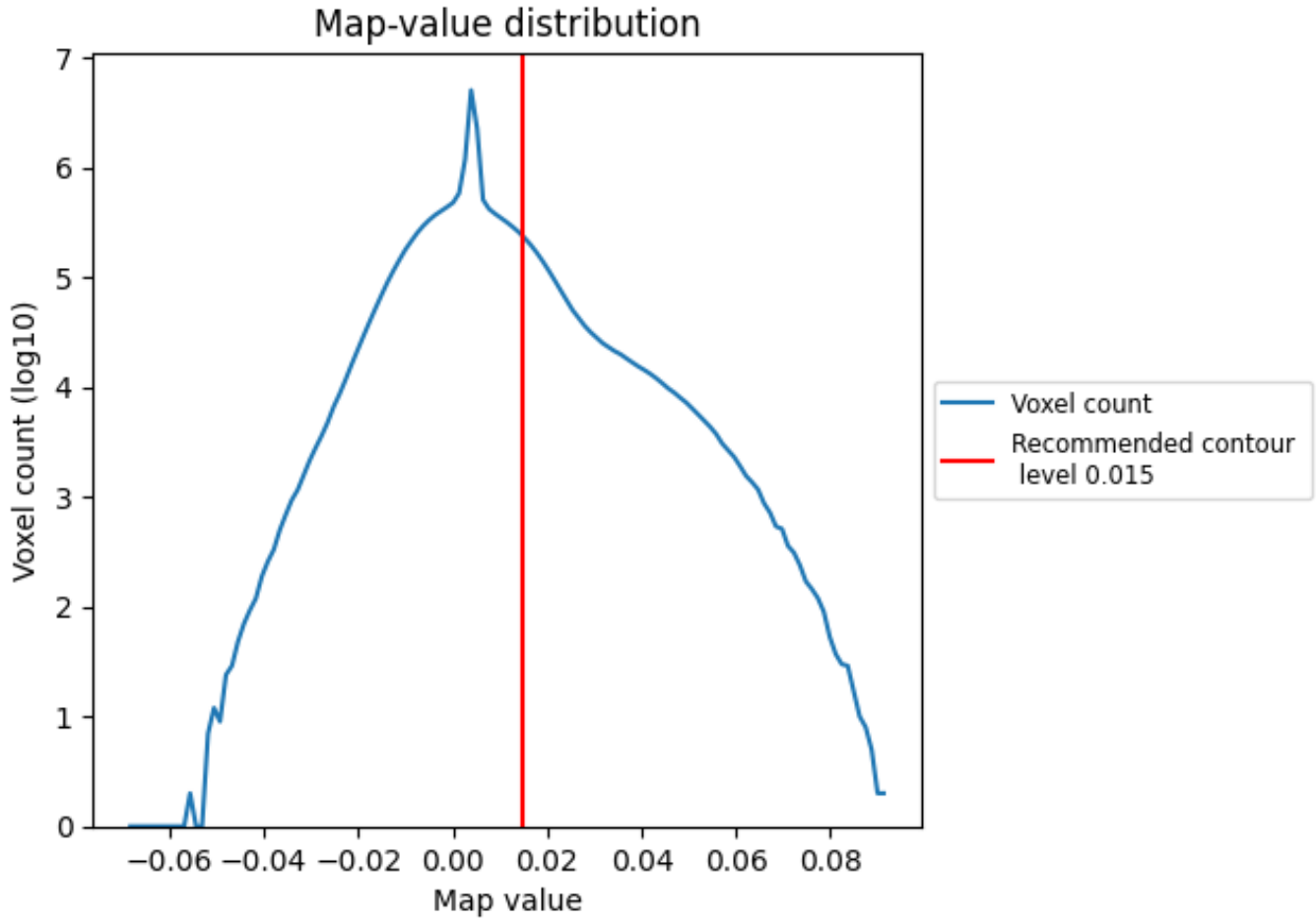
6.6 Mask visualisation (i)

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

7 Map analysis

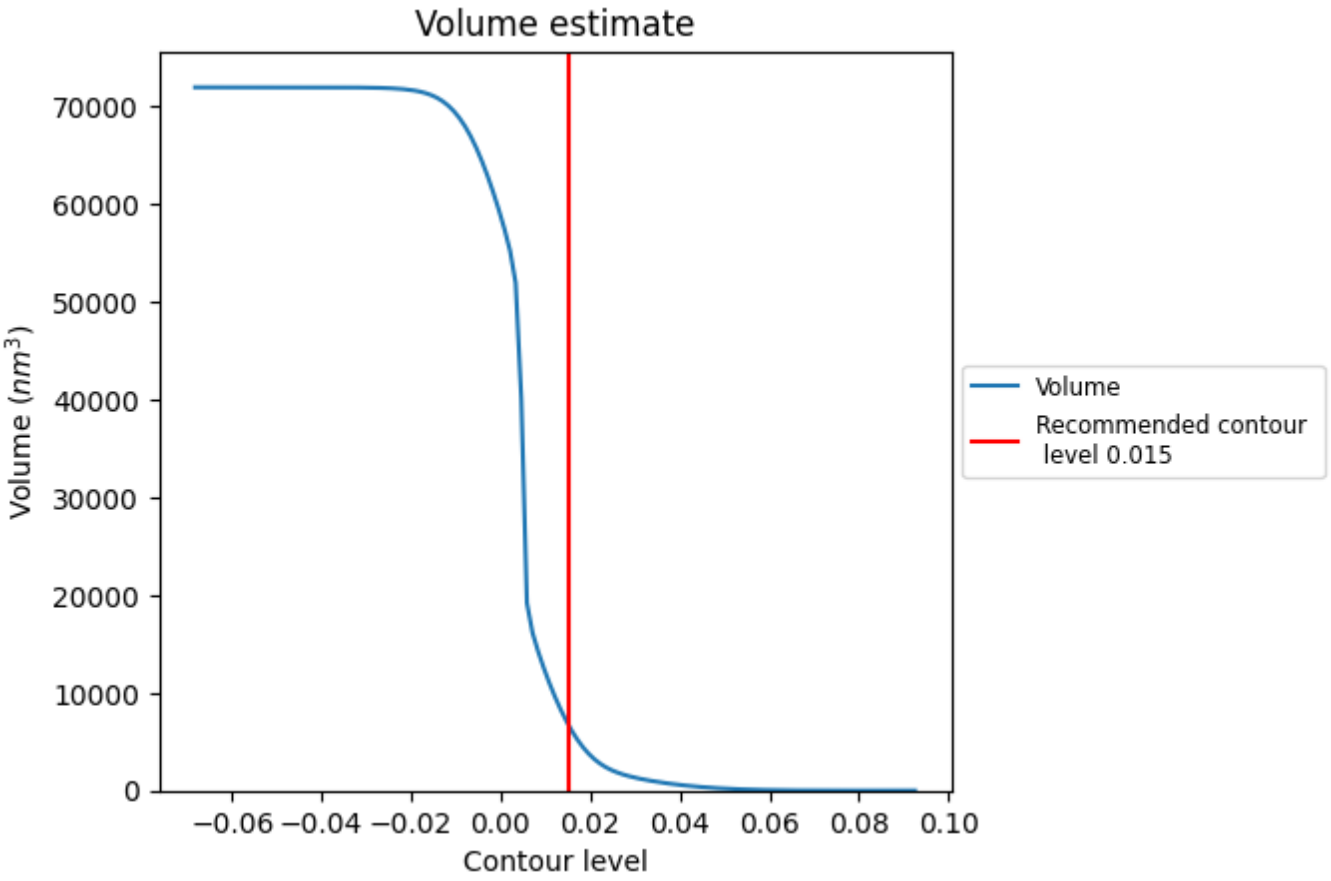
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

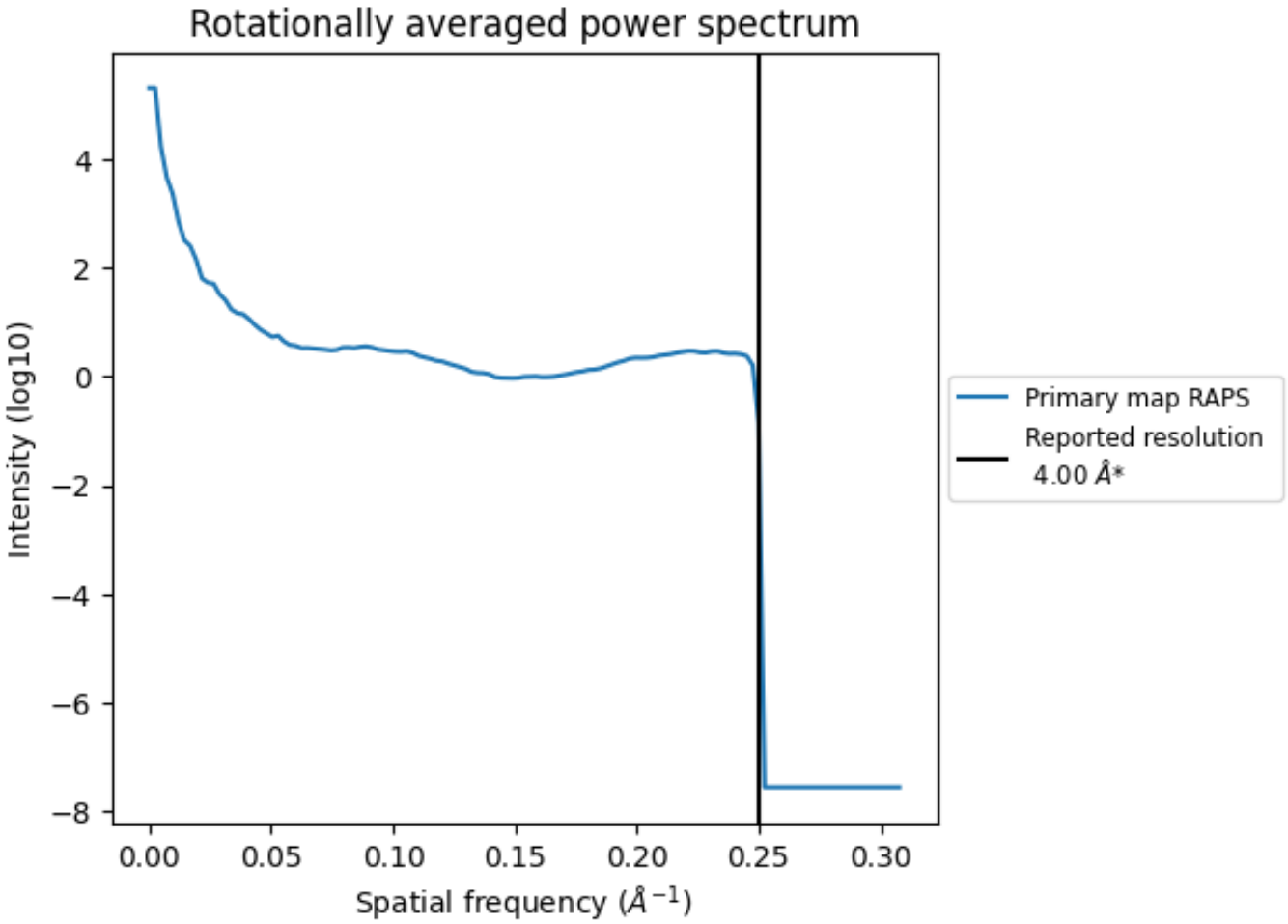
7.2 Volume estimate (i)



The volume at the recommended contour level is 6849 nm^3; this corresponds to an approximate mass of 6187 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 0.250 Å^{-1}

8 Fourier-Shell correlation (i)

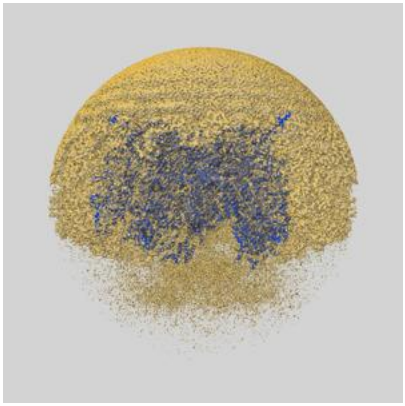
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

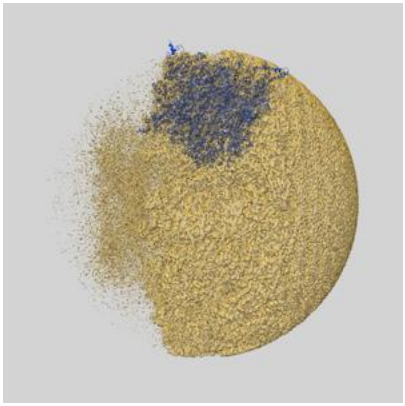
This section contains information regarding the fit between EMDB map EMD-31298 and PDB model 7ETJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

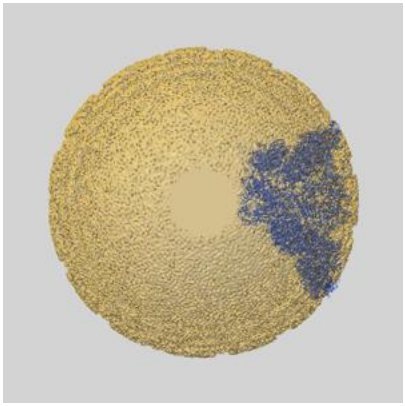
9.1.1 Map-model overlay



X

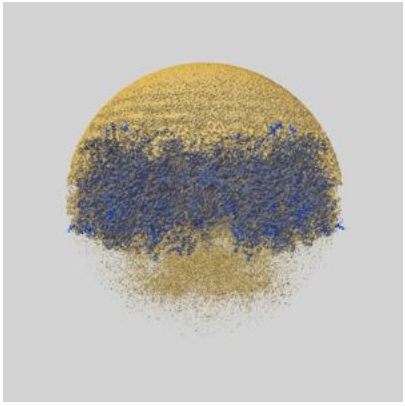


Y

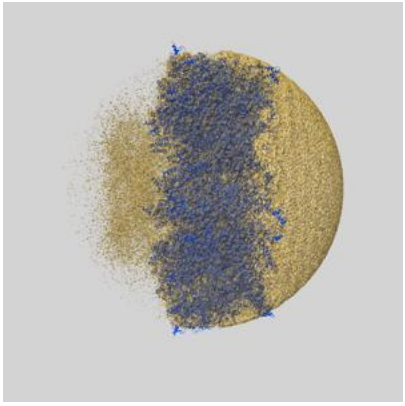


Z

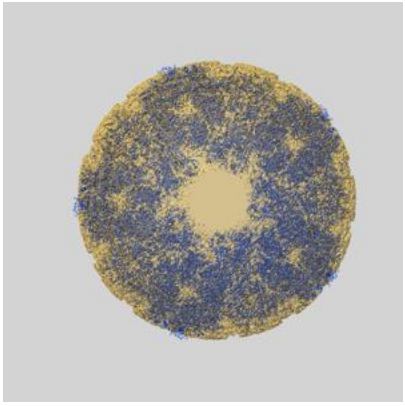
9.1.2 Map-model assembly overlay



X



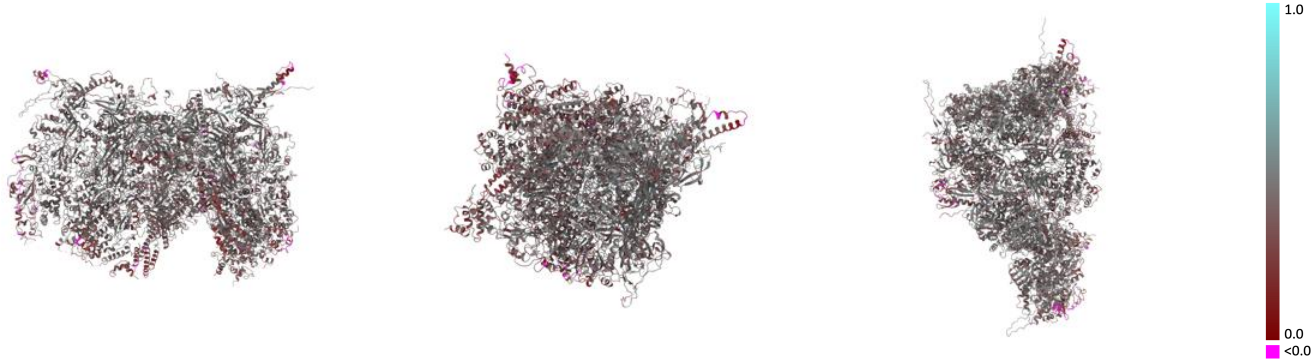
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

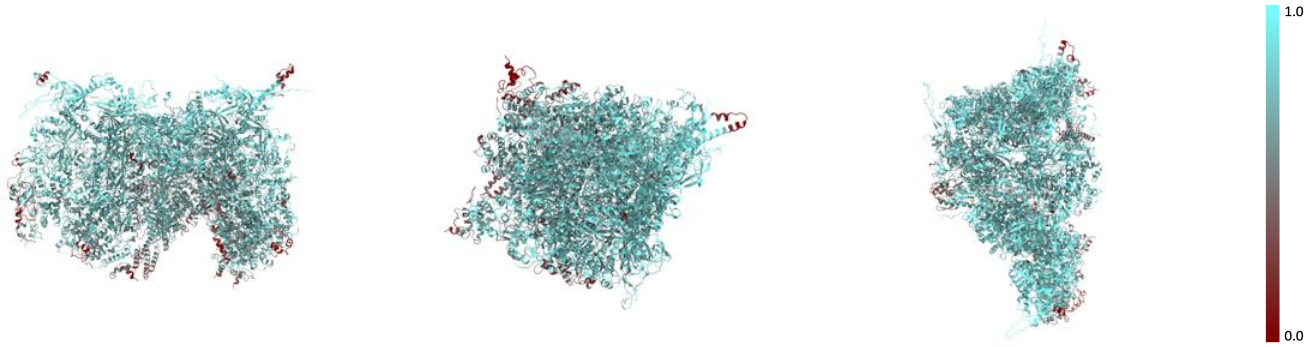
9.2 Q-score mapped to coordinate model



X Y Z

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

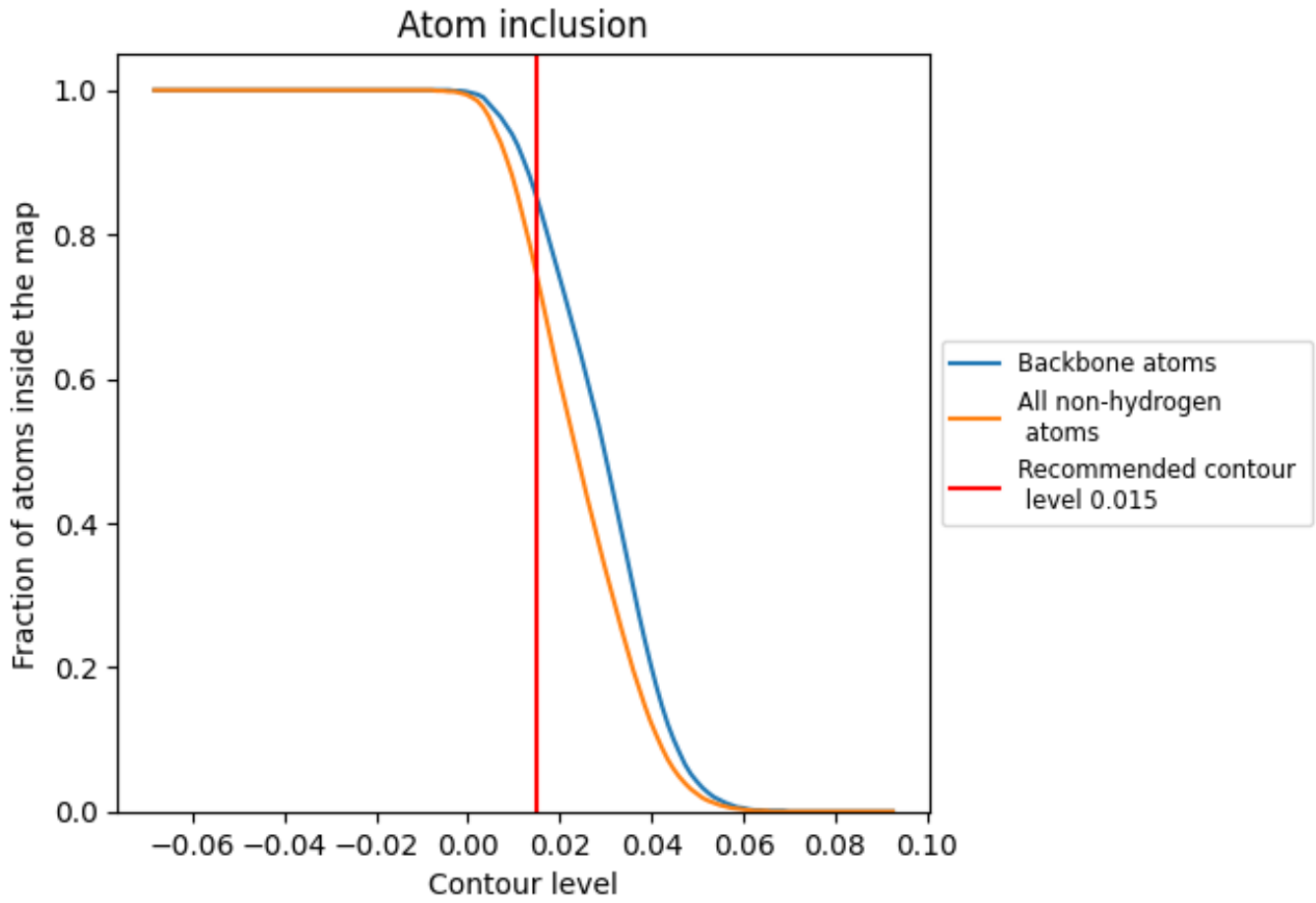
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4060
1	0.5070	0.3130
B	0.7710	0.4180
C	0.7890	0.4290
D	0.7800	0.4160
H	0.4130	0.2030
I	0.6930	0.3800
M	0.7210	0.4020
N	0.6100	0.3640
O	0.5020	0.2500
P	0.5330	0.2810
R	0.5060	0.3220
S	0.5960	0.3500
T	0.3030	0.2460
Y	0.7570	0.4060
Z	0.7860	0.4280
a	0.7770	0.4250
g	0.5520	0.3090
h	0.6850	0.3930
i	0.3860	0.2820
j	0.4480	0.3160
m	0.7790	0.4300
n	0.7740	0.4140
o	0.7690	0.4100