



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:01 PM UTC

PDB ID : 9BGM / pdb_00009bgm
EMDB ID : EMD-44517
Title : Pseudomonas phage DEV neck and tail (portal, head-to-tail and tail tube proteins)
Authors : Iglesias, S.M.; Hou, C.-F.D.; Li, F.; Cingolani, G.
Deposited on : 2024-04-19
Resolution : 3.10 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

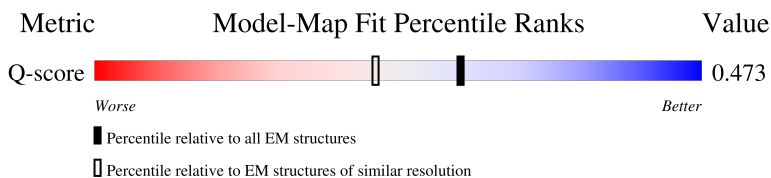
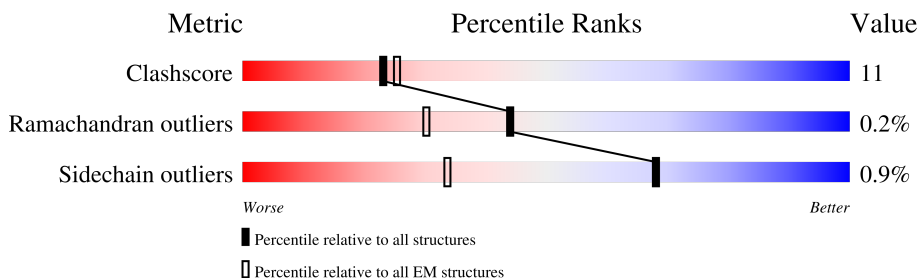
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	
1	D	321	
1	G	321	
1	J	321	

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Mol	Chain	Length	Quality of chain
1	M	321	
1	P	321	
1	S	321	
1	W	321	
1	Z	321	
1	a	321	
1	f	321	
1	i	321	
2	B	244	
2	E	244	
2	H	244	
2	K	244	
2	N	244	
2	Q	244	
2	T	244	
2	X	244	
2	b	244	
2	d	244	
2	g	244	
2	j	244	
3	C	726	
3	F	726	
3	I	726	
3	L	726	
3	O	726	

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Mol	Chain	Length	Quality of chain
3	R	726	23% 74% 22% ..
3	V	726	25% 73% 23% ..
3	Y	726	24% 71% 25% ..
3	c	726	24% 72% 24% ..
3	e	726	23% 71% 25% ..
3	h	726	24% 72% 24% ..
3	k	726	24% 72% 24% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 102552 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 gp75 tail tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	A	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	D	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	G	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	J	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	M	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	P	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	S	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	W	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	Z	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	f	157	Total 1071	C 670	N 190	O 210	S 1	0	0
1	i	157	Total 1071	C 670	N 190	O 210	S 1	0	0

- Molecule 2 is a protein called gp83 head-to-tail.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	B	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	E	243	Total 1955	C 1247	N 335	O 365	S 8	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	K	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	N	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	Q	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	T	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	X	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	d	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	g	243	Total 1955	C 1247	N 335	O 365	S 8	1	0
2	j	243	Total 1955	C 1247	N 335	O 365	S 8	1	0

- Molecule 3 is a protein called gp80 portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	C	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	F	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	I	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	L	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	O	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	R	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	V	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	Y	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0
3	e	701	Total 5520	C 3434	N 976	O 1084	S 26	0	0

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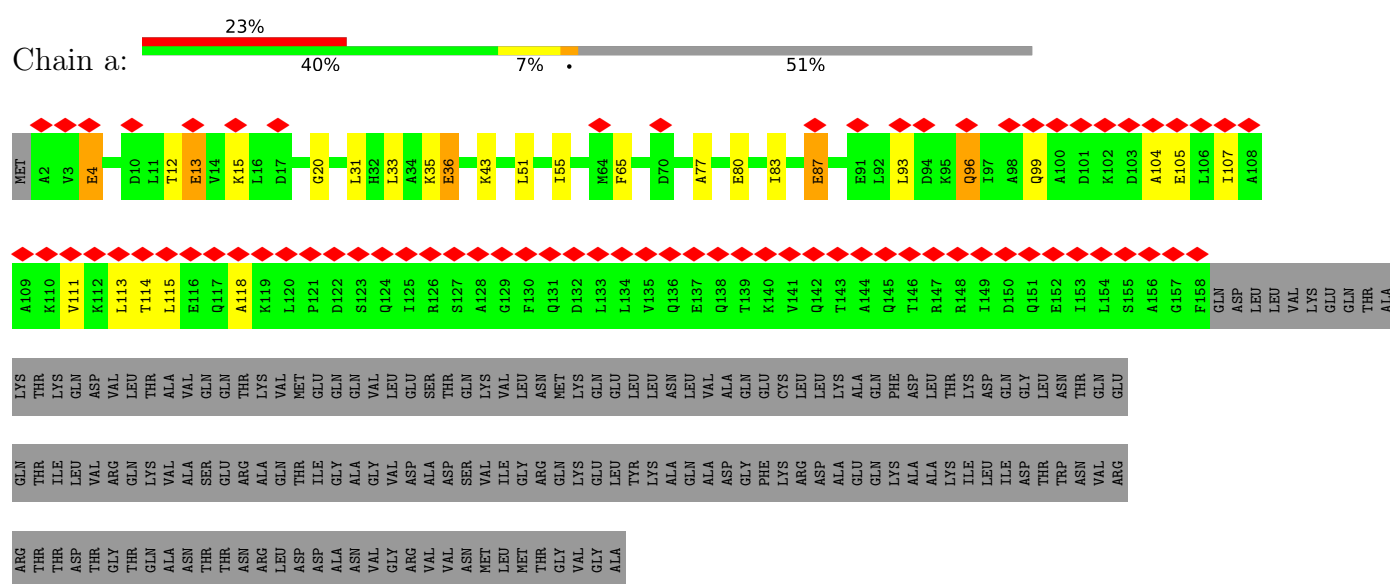
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	701	Total	C	N	O	S	0	0
			5520	3434	976	1084	26		
3	k	701	Total	C	N	O	S	0	0
			5520	3434	976	1084	26		

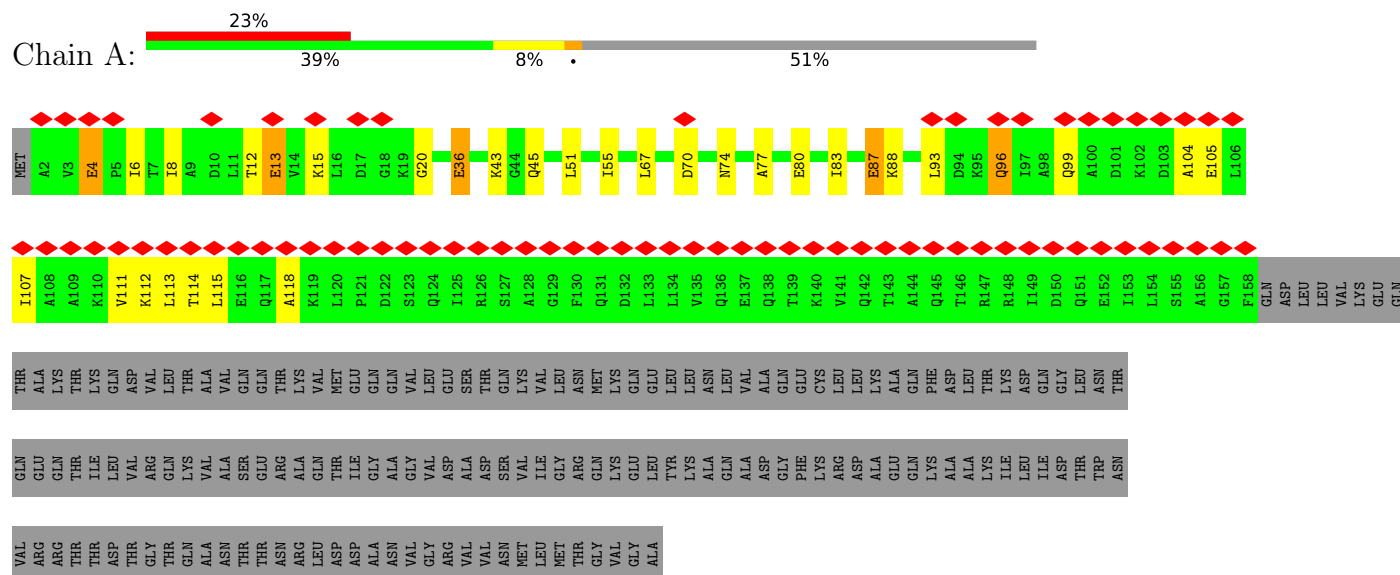
3 Residue-property plots [i](#)

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: gp75 tail tube



- Molecule 1: gp75 tail tube



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

THR
THR
ASP
THR
GLY
THR
GLN
ALA
ASN
THR
THR
ASN
ARG
LEU
ASP
ASP
ASN
VAL
GLY
ARG
VAL
VAL
ASP
ASN
MET
LEU
MET
THR
GLY
VAL
GLY
ALA

• Molecule 1: gp75 tail tube

Chain M: 23% 40% 7% 51%

MET
A2
V3
E4
D10
T11
E13
V14
K15
L16
D17
G20
D23
E36
K43
L51
I55
F65
D70
A77
L78
V79
E80
I83
E87
E91
L92
L93
D94
K95
Q96
I97
A98
Q99
A100
D101
K102
D103
A104
E105
L106
I107
A108
A109
K110
V111
K112
L113
T114
L115
E116
A118
K119
P121
D122
S123
I124
I125
R126
S127
G129
F130
Q131
D132
L133
L134
V135
Q136
E137
Q138
T139
K140
V141
Q142
T143
A144
Q145
T146
R147
R148
I149
D150
Q151
E152
I153
L154
S155
A156
G157
F158
GLN
ASP
LEU
LEU
VAL
LYS
GLU
THR
ALA
LYS
THR
LYS

GLN
ASP
VAL
LEU
THR
ALA
VAL
GLN
THR
LYS
VAL
MET
GLU
GLN
GLN
VAL
LEU
ASN
MET
GLY
D132
L133
L134
V135
Q136
E137
Q138
T139
K140
V141
Q142
T143
A144
Q145
T146
R147
R148
I149
D150
Q151
E152
I153
L154
S155
A156
G157
F158
GLN
ASP
LEU
LEU
VAL
LYS
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ALA
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LEU
VAL
ARG
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ALA
SER
GLU
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VAL
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ALA
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VAL
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LEU
TYR
LYS
ALA
GLN
ALA
ASP
GLY
PHE
LYS
ARG
ASP
GLU
LYS
PHE
ASP
LEU
ILE
ASP
TRP
ASN
VAL
ARG
ARG
THR
THR

ASP
THR
GLY
THR
GLN
ALA
ASN
THR
THR
ASN
ARG
LEU
ASP
ASP
ALA
ASN
VAL
ARG
VAL
VAL
ASP
SER
MET
MET
THR
GLY
VAL
GLY
ALA

• Molecule 1: gp75 tail tube

Chain P: 24% 40% 7% 51%

MET
A2
V3
E4
P5
T8
A9
D10
L11
T12
E13
V14
K15
L16
D17
G20
L33
E36
K43
L51
I55
K69
D70
A77
E80
I83
E87
E91
L92
L93
D94
K95
Q96
I97
A98
Q99
A100
D101
K102
D103
A104
E105
L106
I107
A108
A109
K110
V111
K112
L113
T114
L115
E116
A118
K119
P121
D122
S123
I124
I125
R126
S127
G129
F130
Q131
D132
L133
L134
V135
Q136
E137
Q138
T139
K140
V141
Q142
T143
A144
Q145
T146
R147
R148
I149
D150
Q151
E152
I153
L154
S155
A156
G157
F158
GLN
ASP
LEU
LEU
VAL
LYS
GLU
THR
ALA
LYS
THR
LYS

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

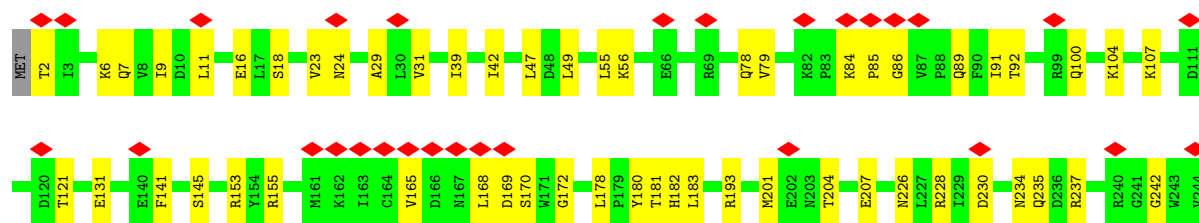
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ASP
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GLU
ARG
VAL
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ASP
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THR
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VAL
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ALA

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ASN
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THR
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ARG
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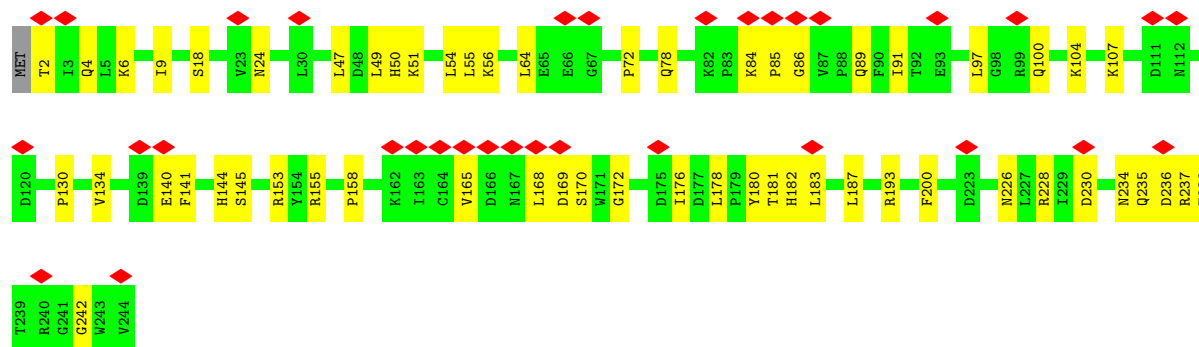
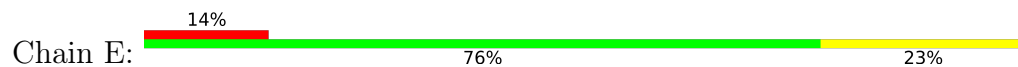
• Molecule 1: gp75 tail tube

Chain S: 24% 40% 8% 51%

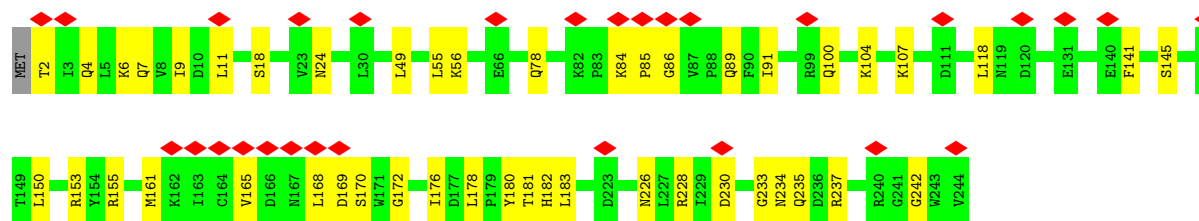
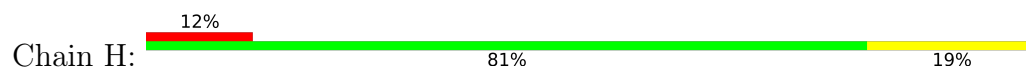
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P5
T8
A9
D10
L11
T12
E13
V14
K15
L16
D17
G20
L26
E36
H37
D38
K43
A48
L51
I55
F65
K69
D70
A77
E80
I83
E87
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I97
A98
Q99
A100
D101
K102
D103
A104



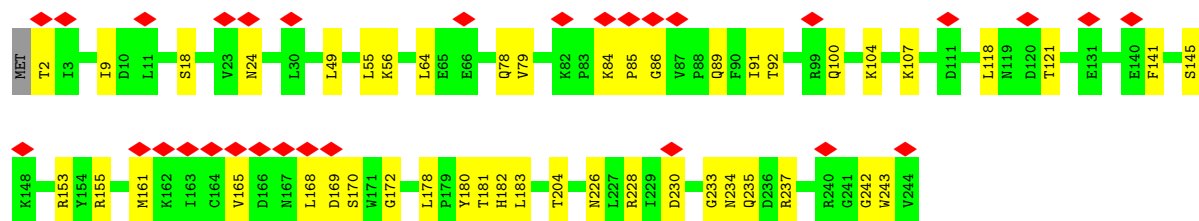
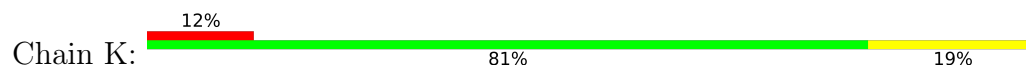
- Molecule 2: gp83 head-to-tail



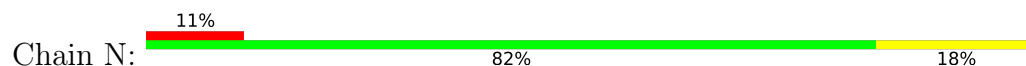
- Molecule 2: gp83 head-to-tail

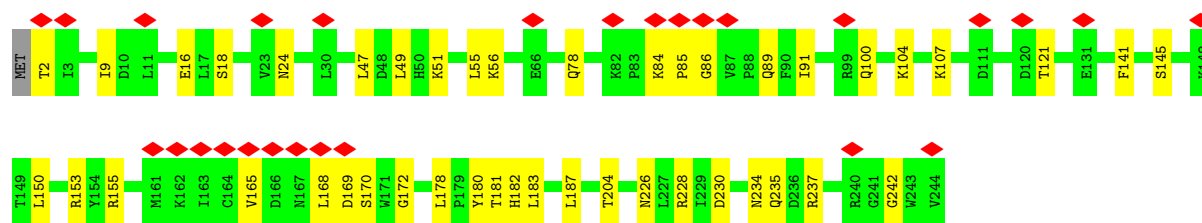


- Molecule 2: gp83 head-to-tail

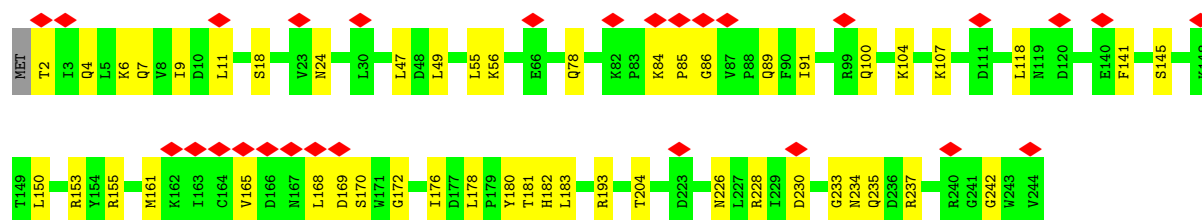
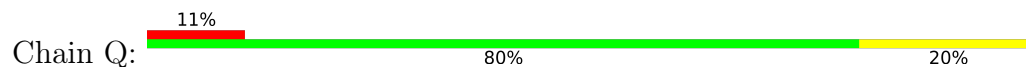


- Molecule 2: gp83 head-to-tail

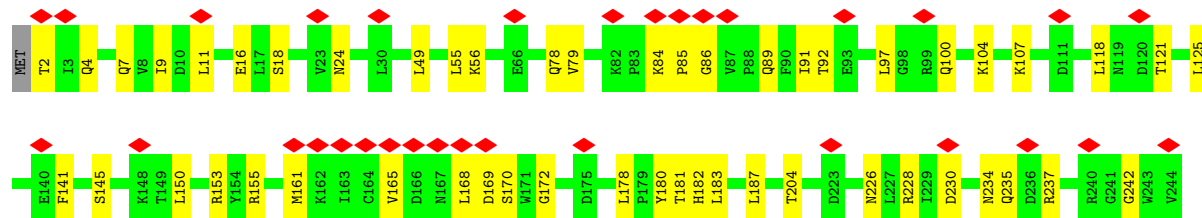
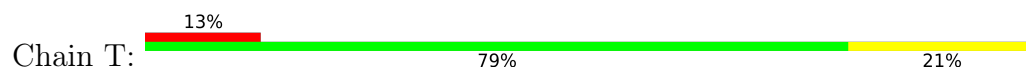




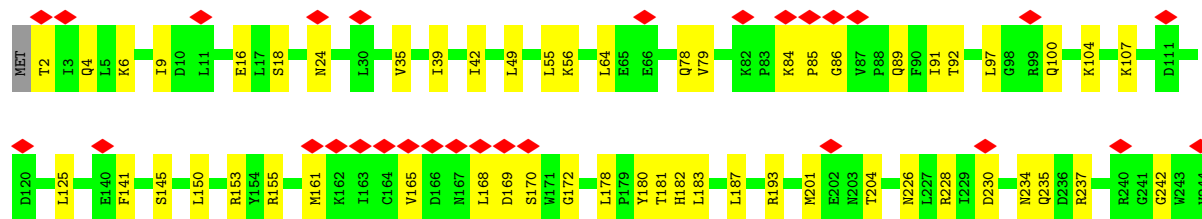
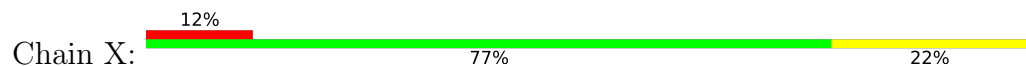
- Molecule 2: gp83 head-to-tail



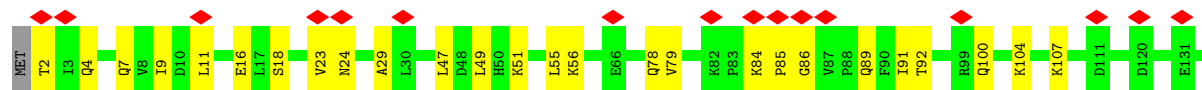
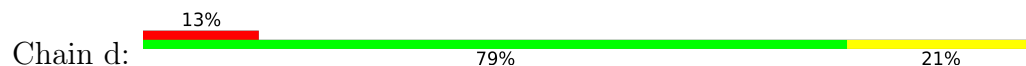
- Molecule 2: gp83 head-to-tail

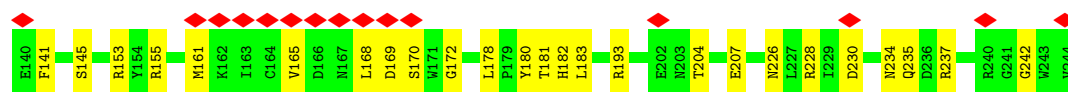


- Molecule 2: gp83 head-to-tail

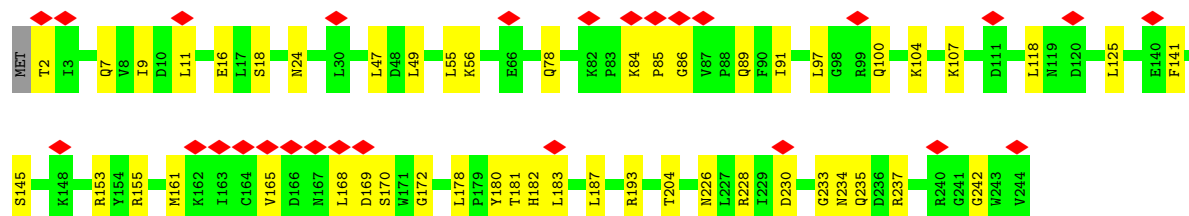
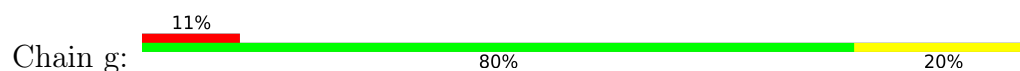


- Molecule 2: gp83 head-to-tail

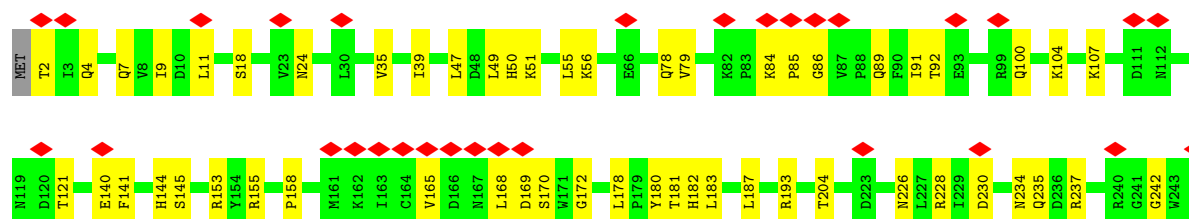
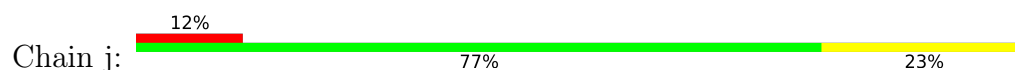




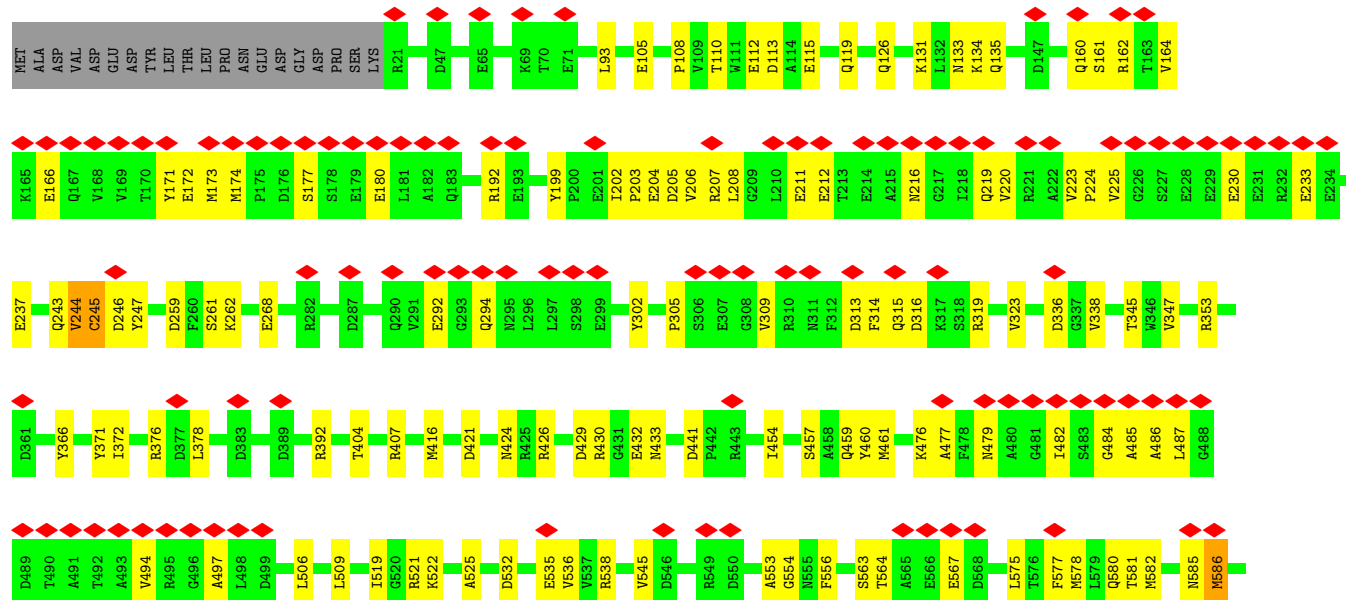
- Molecule 2: gp83 head-to-tail

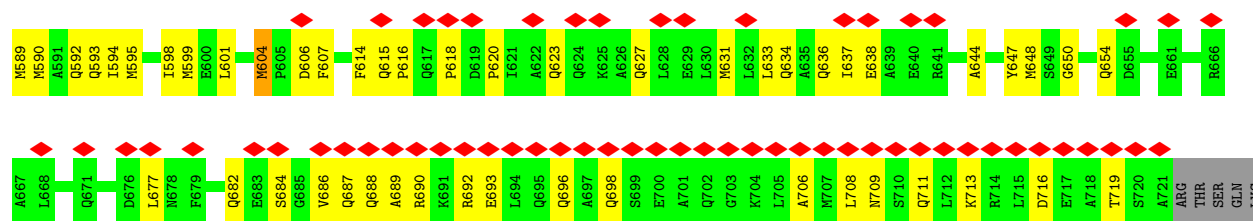


- Molecule 2: gp83 head-to-tail

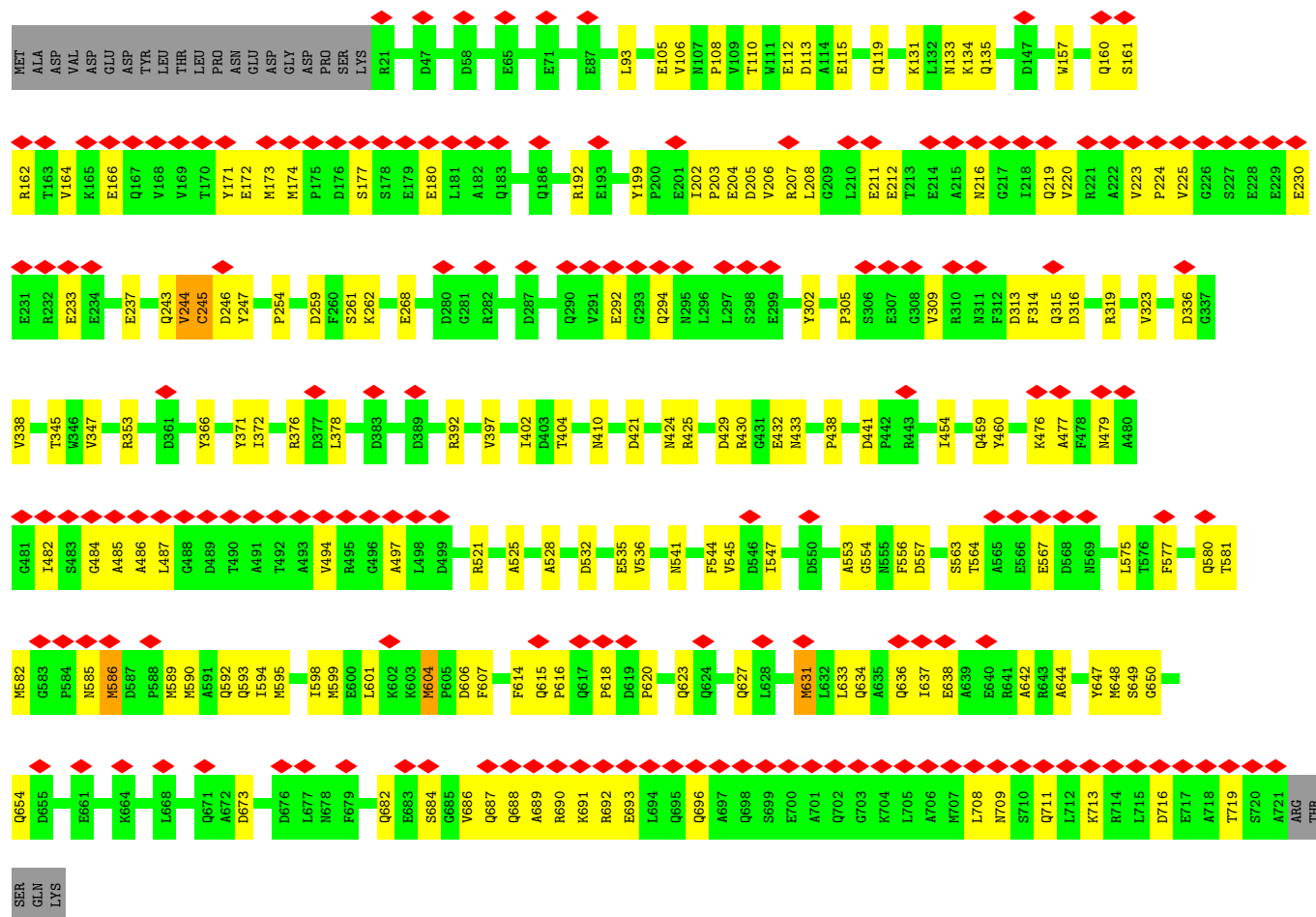
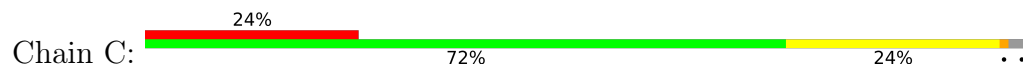


- Molecule 3: gp80 portal protein

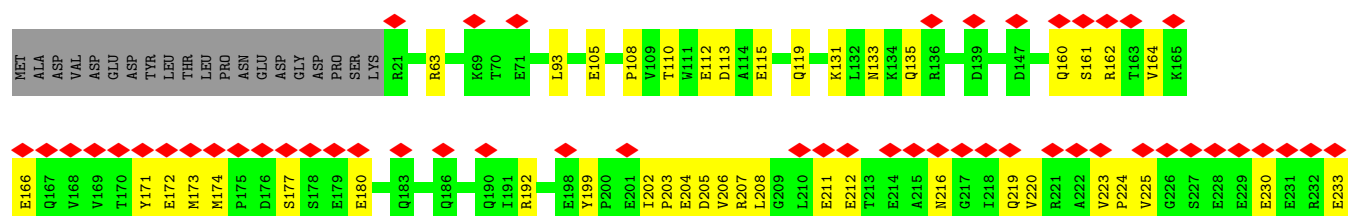
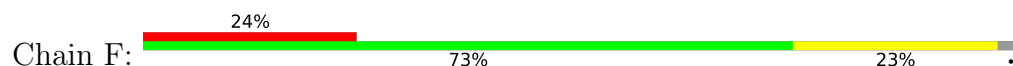


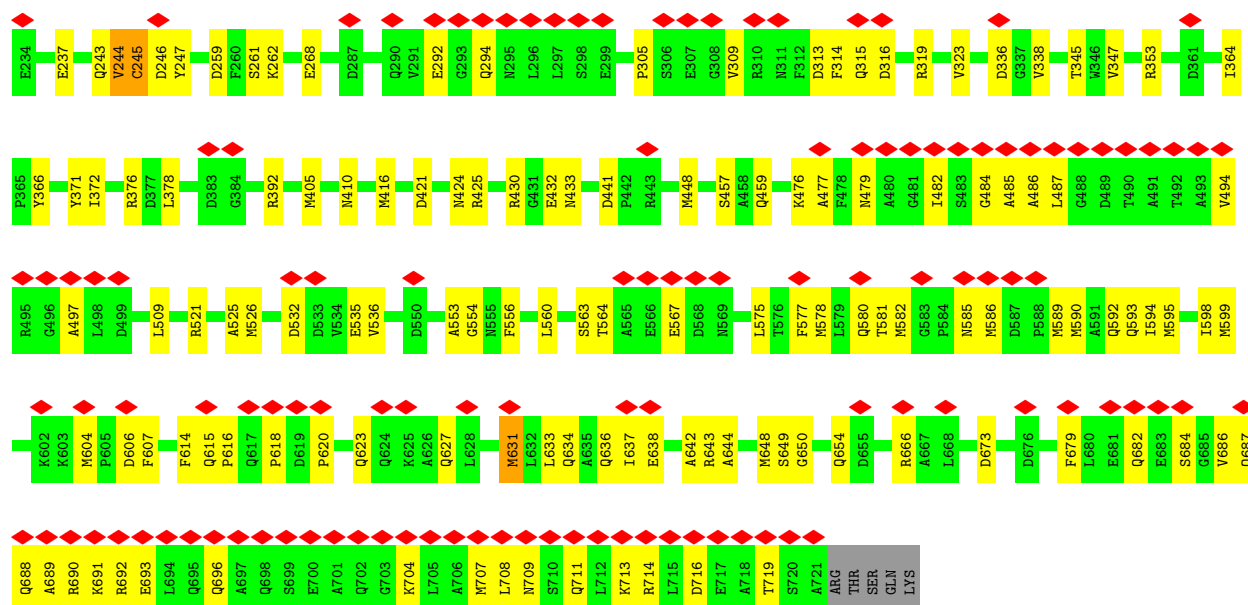


• Molecule 3: gp80 portal protein

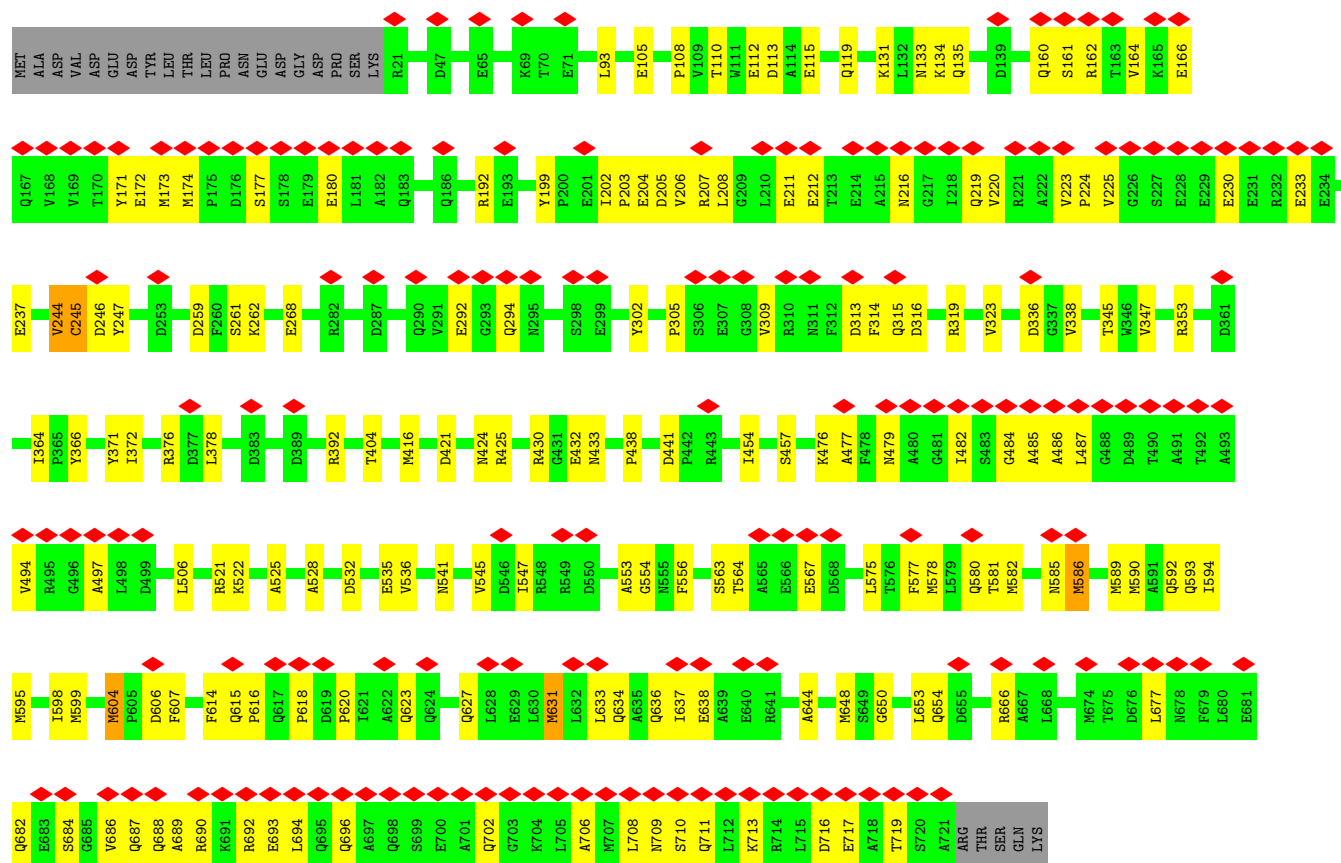


• Molecule 3: gp80 portal protein

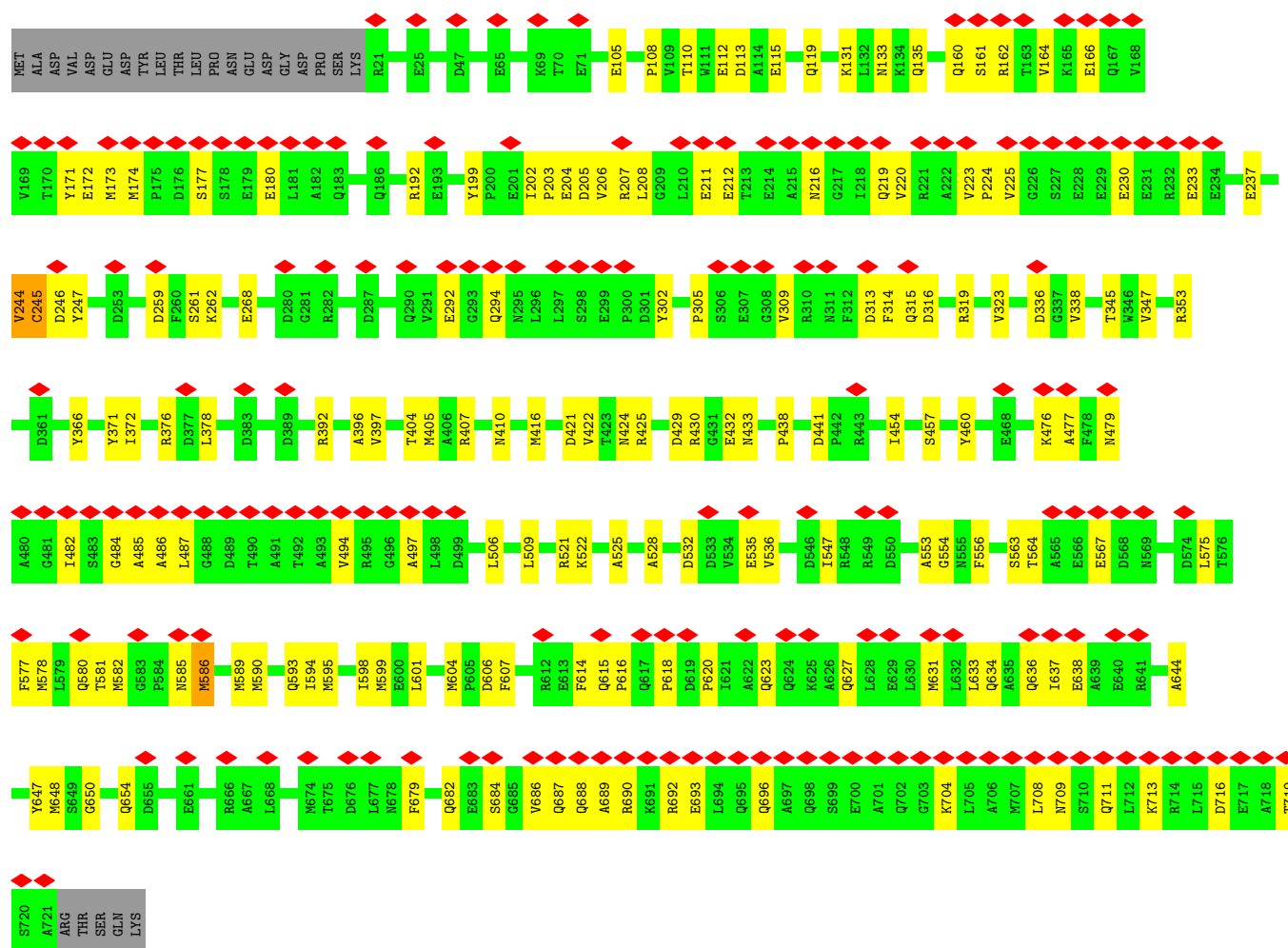
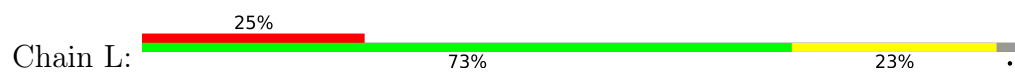




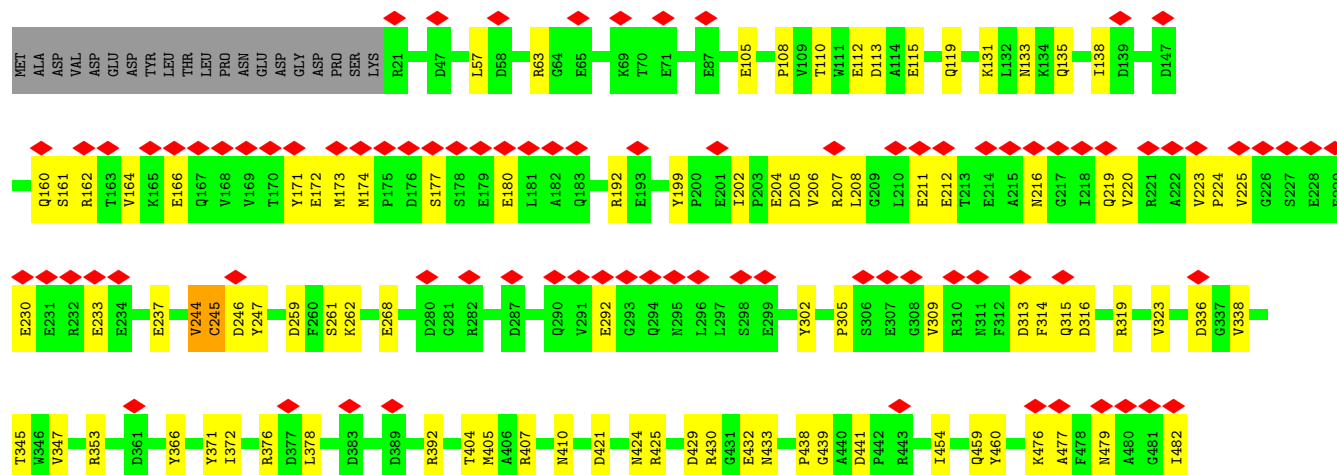
• Molecule 3: gp80 portal protein

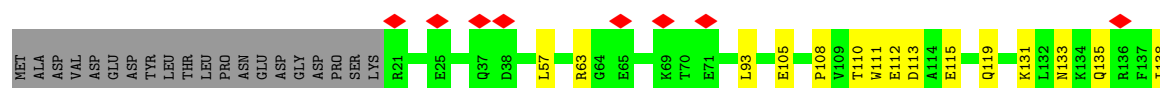


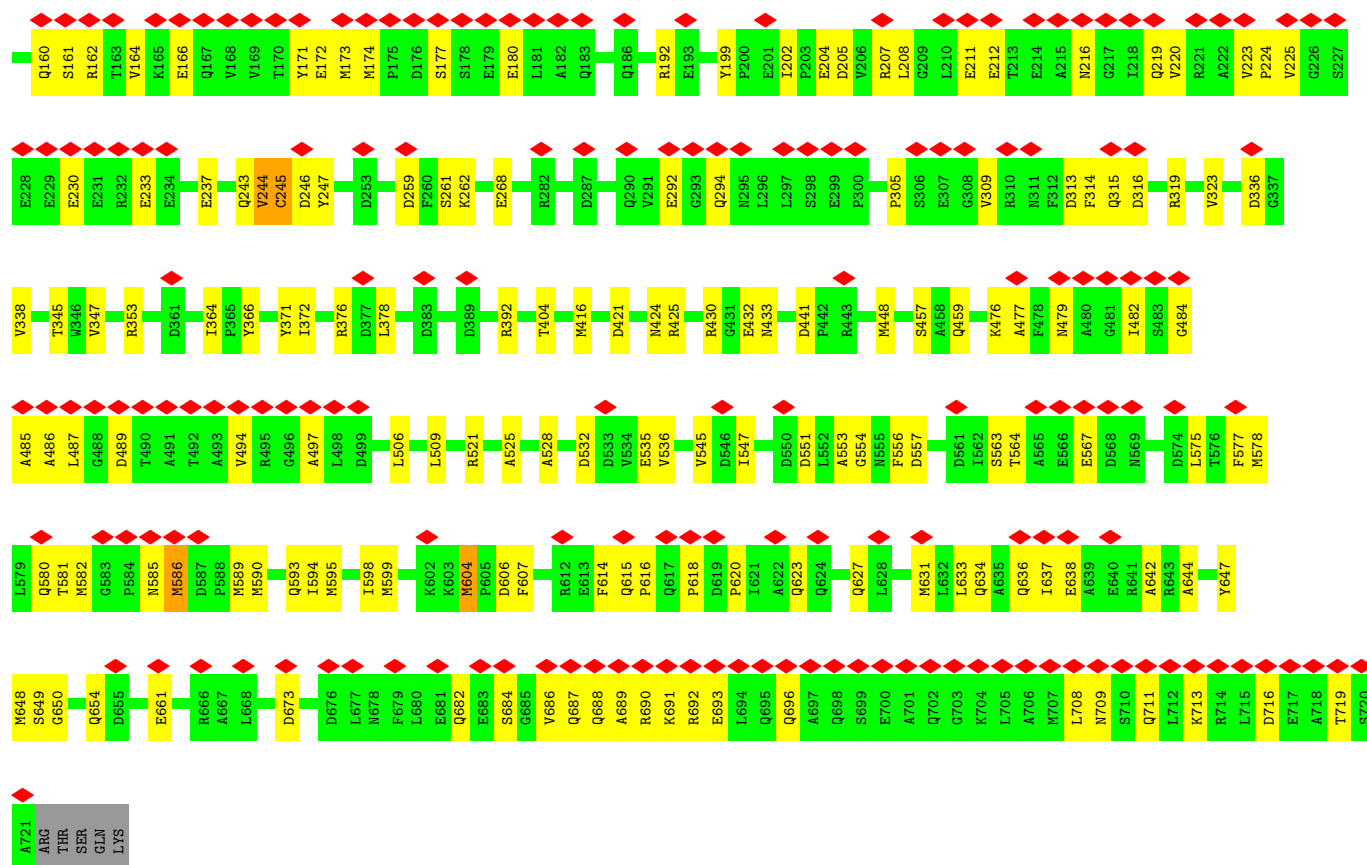
• Molecule 3: gp80 portal protein



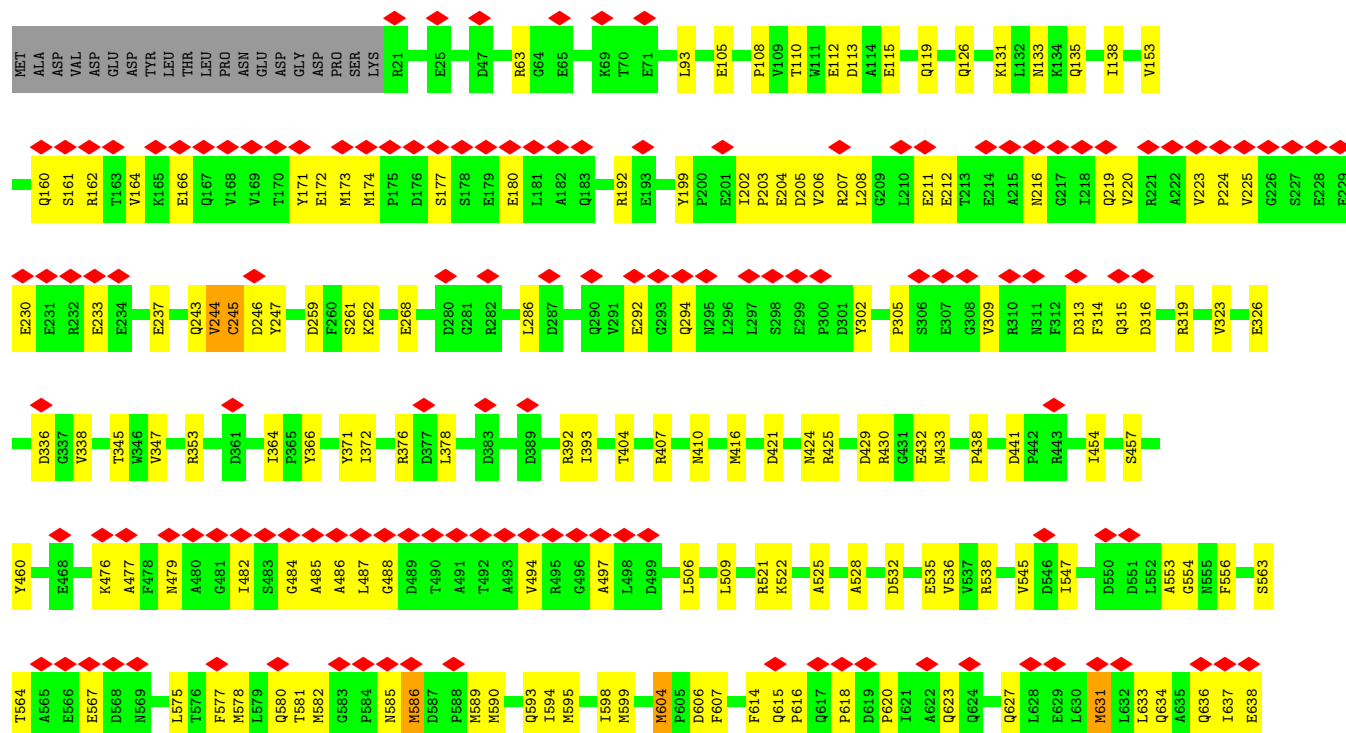
• Molecule 3: gp80 portal protein

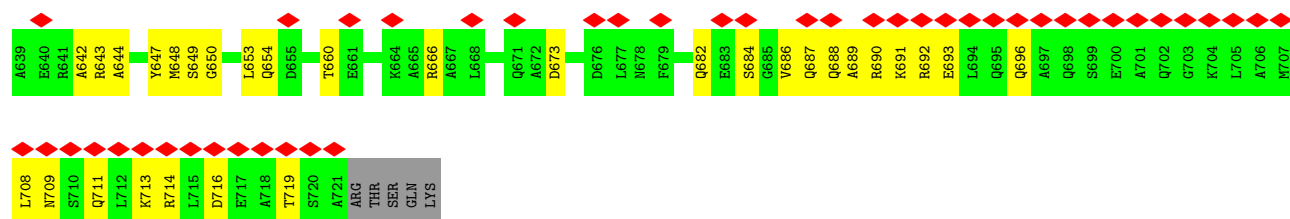




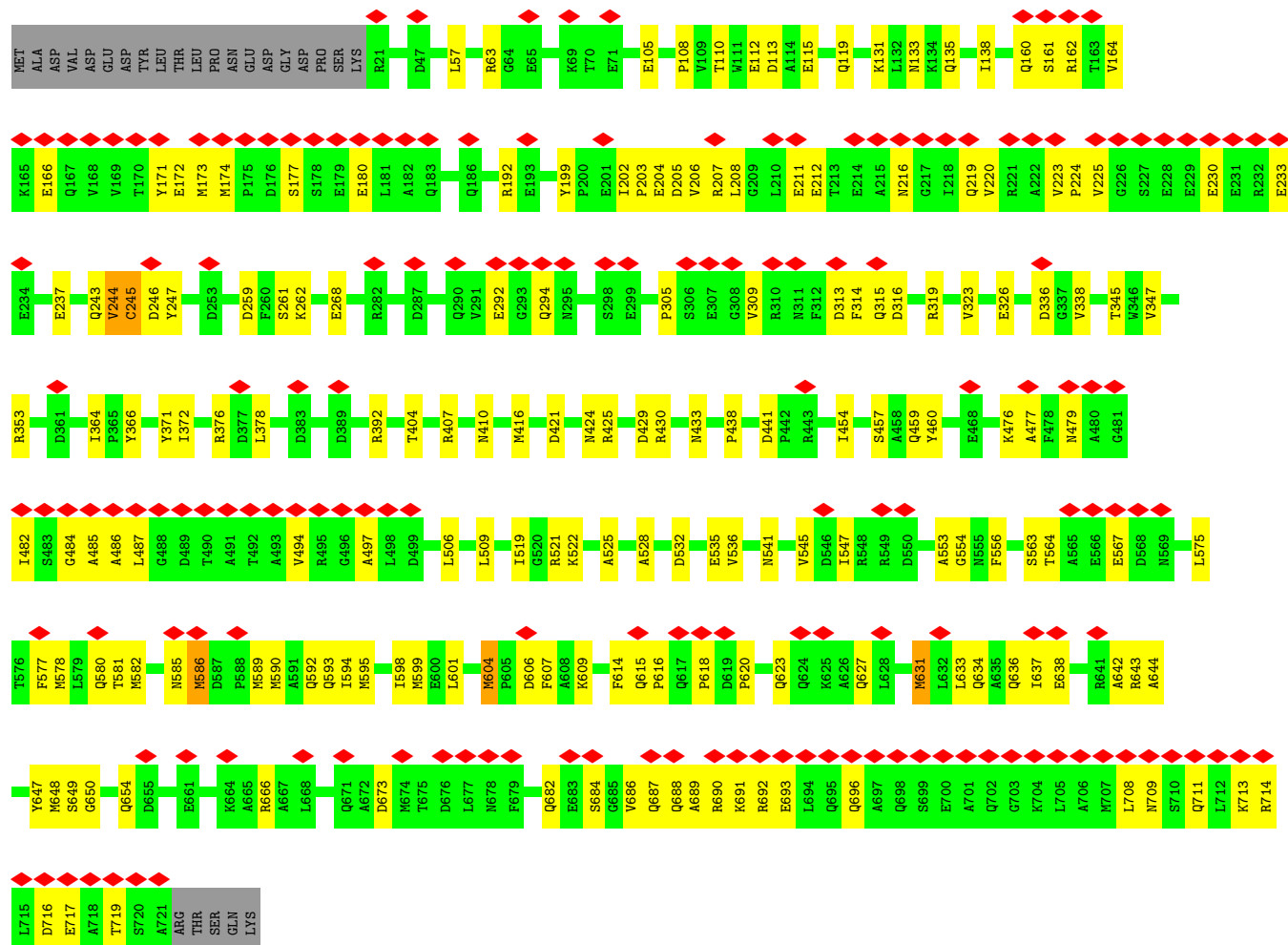


• Molecule 3: gp80 portal protein

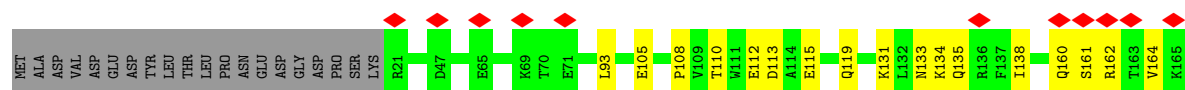
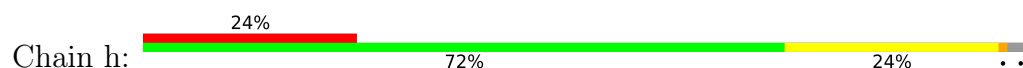


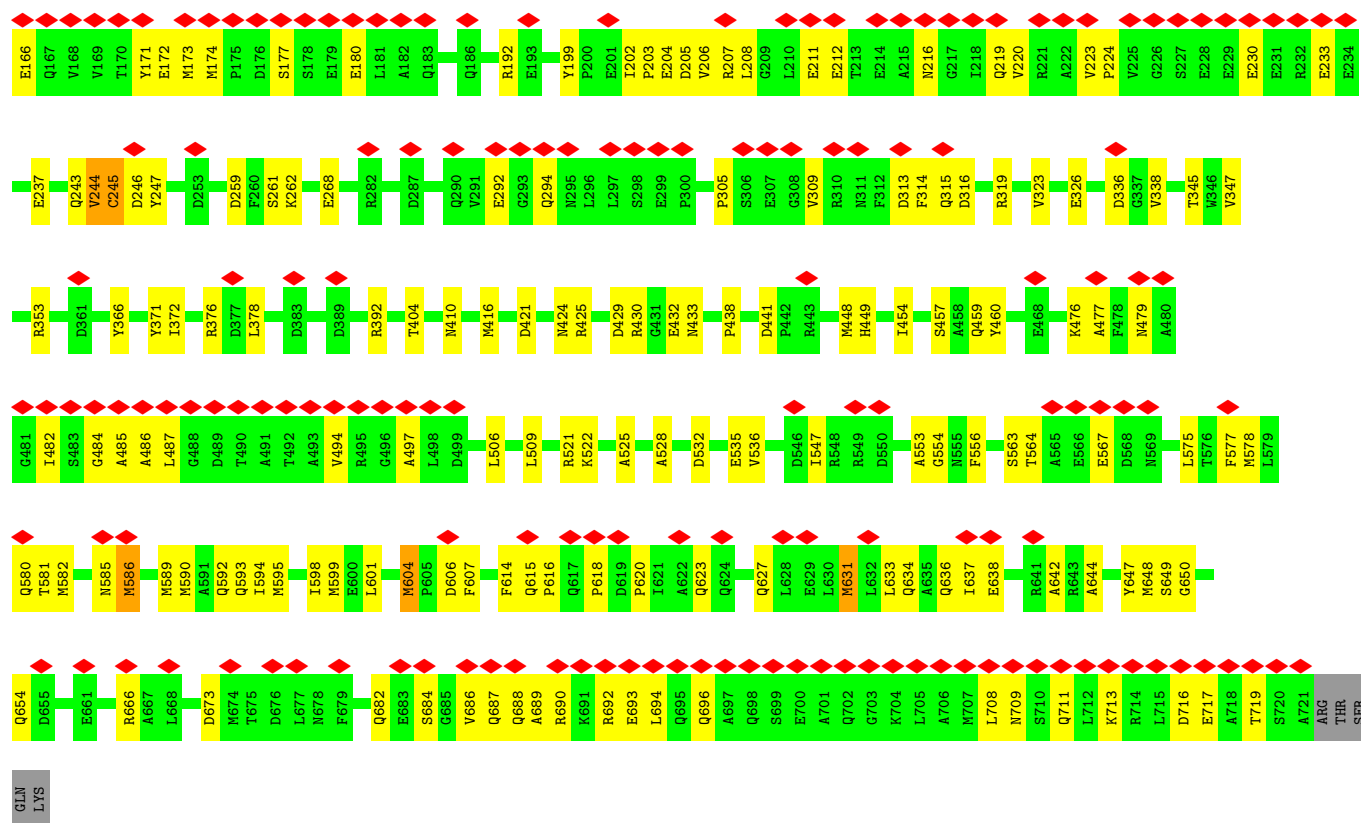


• Molecule 3: gp80 portal protein

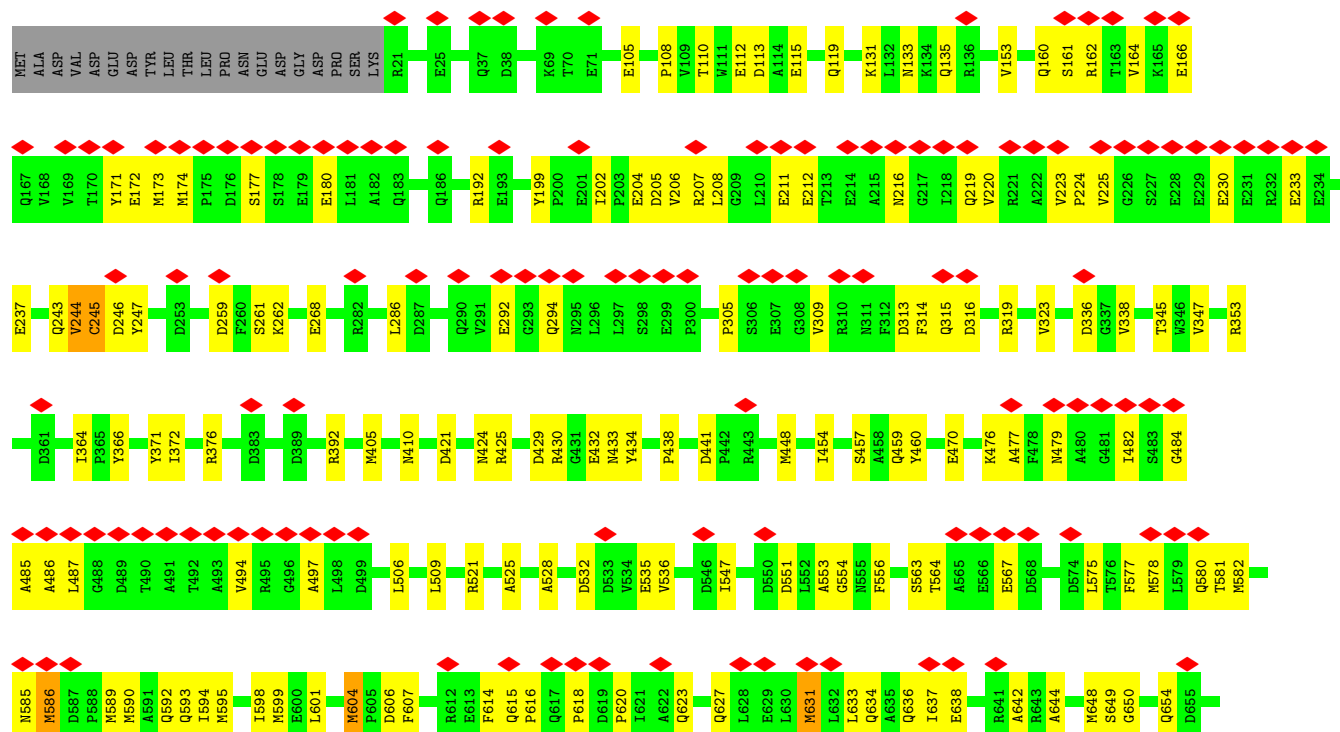


• Molecule 3: gp80 portal protein





• Molecule 3: gp80 portal protein



R666	A667	L668	D673	D676	L677	N678	F679	L680	E681	Q682	E683	S684	Q685	V686	Q687	Q688	A689	R690	K691	R692	E693	L694	Q695	Q696	A697	Q698	S699	E700	A701	Q702	G703	K704	L705	A706	M707	L708	N709	S710	Q711	L712	K713	R714	L715	D716	E717	A718	T719	S720	A721	ARG	THR	SER	GLN	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	3228	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.12, 1.12, 1.12	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	A	0.28	0/1075	0.49	0/1459
1	D	0.28	0/1075	0.49	0/1459
1	G	0.28	0/1075	0.49	0/1459
1	J	0.28	0/1075	0.49	0/1459
1	M	0.28	0/1075	0.49	0/1459
1	P	0.28	0/1075	0.49	0/1459
1	S	0.28	0/1075	0.49	0/1459
1	W	0.28	0/1075	0.49	0/1459
1	Z	0.28	0/1075	0.49	0/1459
1	a	0.28	0/1075	0.49	0/1459
1	f	0.28	0/1075	0.49	0/1459
1	i	0.28	0/1075	0.49	0/1459
2	B	0.35	0/1995	0.45	0/2704
2	E	0.35	0/1995	0.45	0/2704
2	H	0.33	0/1995	0.44	0/2704
2	K	0.33	0/1995	0.44	0/2704
2	N	0.33	0/1995	0.44	0/2704
2	Q	0.34	0/1995	0.43	0/2704
2	T	0.34	0/1995	0.44	0/2704
2	X	0.34	0/1995	0.44	0/2704
2	b	0.34	0/1995	0.44	0/2704
2	d	0.34	0/1995	0.44	0/2704
2	g	0.34	0/1995	0.44	0/2704
2	j	0.34	0/1995	0.44	0/2704
3	C	0.30	0/5614	0.45	2/7584 (0.0%)
3	F	0.29	0/5614	0.45	2/7584 (0.0%)
3	I	0.29	0/5614	0.45	2/7584 (0.0%)
3	L	0.29	0/5614	0.45	2/7584 (0.0%)
3	O	0.29	0/5614	0.45	2/7584 (0.0%)
3	R	0.30	0/5614	0.45	2/7584 (0.0%)
3	V	0.30	0/5614	0.45	2/7584 (0.0%)
3	Y	0.29	0/5614	0.45	2/7584 (0.0%)
3	c	0.29	0/5614	0.45	2/7584 (0.0%)
3	e	0.29	0/5614	0.45	2/7584 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	h	0.29	0/5614	0.45	2/7584 (0.0%)
3	k	0.29	0/5614	0.45	2/7584 (0.0%)
All	All	0.30	0/104208	0.46	24/140964 (0.0%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	620	PRO	N-CA-CB	6.73	110.32	103.25
3	F	620	PRO	N-CA-CB	6.72	110.31	103.25
3	C	620	PRO	N-CA-CB	6.71	110.29	103.25
3	L	620	PRO	N-CA-CB	6.70	110.29	103.25
3	Y	620	PRO	N-CA-CB	6.70	110.29	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1071	0	1010	35	0
1	D	1071	0	1010	31	0
1	G	1071	0	1010	24	0
1	J	1071	0	1010	25	0
1	M	1071	0	1010	23	0
1	P	1071	0	1010	26	0
1	S	1071	0	1010	33	0
1	W	1071	0	1010	35	0
1	Z	1071	0	1010	22	0
1	a	1071	0	1010	28	0
1	f	1071	0	1010	30	0
1	i	1071	0	1010	35	0
2	B	1955	0	1959	50	0
2	E	1955	0	1959	47	0
2	H	1955	0	1959	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1955	0	1959	39	0
2	N	1955	0	1959	38	0
2	Q	1955	0	1959	43	0
2	T	1955	0	1959	44	0
2	X	1955	0	1959	50	0
2	b	1955	0	1959	48	0
2	d	1955	0	1959	45	0
2	g	1955	0	1959	45	0
2	j	1955	0	1959	46	0
3	C	5520	0	5400	157	0
3	F	5520	0	5400	170	0
3	I	5520	0	5400	155	0
3	L	5520	0	5400	151	0
3	O	5520	0	5400	154	0
3	R	5520	0	5400	137	0
3	V	5520	0	5400	149	0
3	Y	5520	0	5400	159	0
3	c	5520	0	5400	152	0
3	e	5520	0	5400	161	0
3	h	5520	0	5400	158	0
3	k	5520	0	5400	153	0
All	All	102552	0	100428	2248	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 11.

The worst 5 of 2248 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)
3:h:119:GLN:HE21	3:k:536:VAL:HG11	1.35	0.92
3:F:691:LYS:HG3	3:I:690:ARG:HH21	1.34	0.91
3:C:476:LYS:HB2	3:F:482:ILE:HD11	1.53	0.89
3:I:119:GLN:HE21	3:L:536:VAL:HG11	1.36	0.89
3:R:119:GLN:HE21	3:V:536:VAL:HG11	1.36	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	D	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	G	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	J	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	M	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	P	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	S	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	W	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	Z	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	a	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	f	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
1	i	155/321 (48%)	149 (96%)	6 (4%)	0	100	100
2	B	242/244 (99%)	219 (90%)	23 (10%)	0	100	100
2	E	242/244 (99%)	218 (90%)	24 (10%)	0	100	100
2	H	242/244 (99%)	219 (90%)	23 (10%)	0	100	100
2	K	242/244 (99%)	220 (91%)	22 (9%)	0	100	100
2	N	242/244 (99%)	221 (91%)	21 (9%)	0	100	100
2	Q	242/244 (99%)	220 (91%)	22 (9%)	0	100	100
2	T	242/244 (99%)	220 (91%)	22 (9%)	0	100	100
2	X	242/244 (99%)	220 (91%)	22 (9%)	0	100	100
2	b	242/244 (99%)	219 (90%)	23 (10%)	0	100	100
2	d	242/244 (99%)	219 (90%)	23 (10%)	0	100	100
2	g	242/244 (99%)	218 (90%)	24 (10%)	0	100	100
2	j	242/244 (99%)	218 (90%)	24 (10%)	0	100	100
3	C	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	699/726 (96%)	640 (92%)	57 (8%)	2 (0%)	36	67
3	I	699/726 (96%)	640 (92%)	57 (8%)	2 (0%)	36	67
3	L	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	O	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	R	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	V	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	Y	699/726 (96%)	640 (92%)	57 (8%)	2 (0%)	36	67
3	c	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	e	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	h	699/726 (96%)	641 (92%)	56 (8%)	2 (0%)	36	67
3	k	699/726 (96%)	640 (92%)	57 (8%)	2 (0%)	36	67
All	All	13152/15492 (85%)	12107 (92%)	1021 (8%)	24 (0%)	44	73

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	245	CYS
3	C	245	CYS
3	F	245	CYS
3	I	245	CYS
3	L	245	CYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	D	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	G	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	J	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	M	88/264 (33%)	83 (94%)	5 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	S	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	W	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	Z	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	a	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	f	88/264 (33%)	83 (94%)	5 (6%)	18	49
1	i	88/264 (33%)	83 (94%)	5 (6%)	18	49
2	B	215/216 (100%)	215 (100%)	0	100	100
2	E	215/216 (100%)	215 (100%)	0	100	100
2	H	215/216 (100%)	215 (100%)	0	100	100
2	K	215/216 (100%)	215 (100%)	0	100	100
2	N	215/216 (100%)	215 (100%)	0	100	100
2	Q	215/216 (100%)	215 (100%)	0	100	100
2	T	215/216 (100%)	215 (100%)	0	100	100
2	X	215/216 (100%)	215 (100%)	0	100	100
2	b	215/216 (100%)	215 (100%)	0	100	100
2	d	215/216 (100%)	215 (100%)	0	100	100
2	g	215/216 (100%)	215 (100%)	0	100	100
2	j	215/216 (100%)	215 (100%)	0	100	100
3	C	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	F	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	I	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	L	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	O	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	R	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	V	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	Y	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	c	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	e	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	h	586/615 (95%)	583 (100%)	3 (0%)	81	85
3	k	586/615 (95%)	583 (100%)	3 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10668/13140 (81%)	10572 (99%)	96 (1%)	68 80

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	13	GLU
3	Y	631	MET
1	S	87	GLU
1	W	13	GLU
1	Z	87	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	37	GLN
3	h	183	GLN
3	R	391	GLN
3	h	119	GLN
2	j	95	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

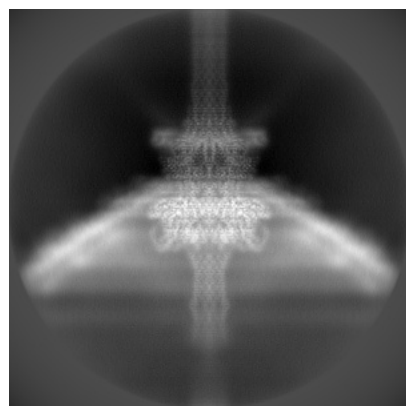
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44517. These allow visual inspection of the internal detail of the map and identification of artifacts.

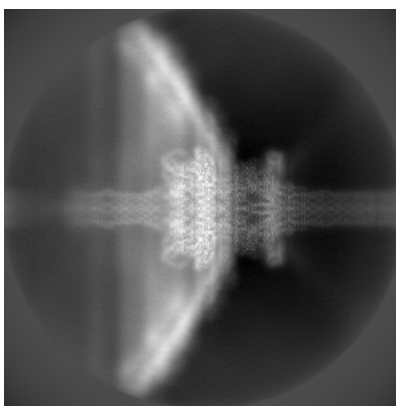
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

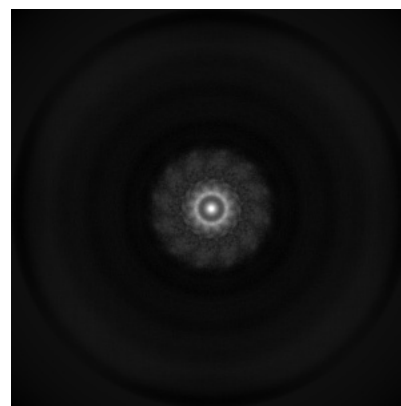
6.1.1 Primary map



X

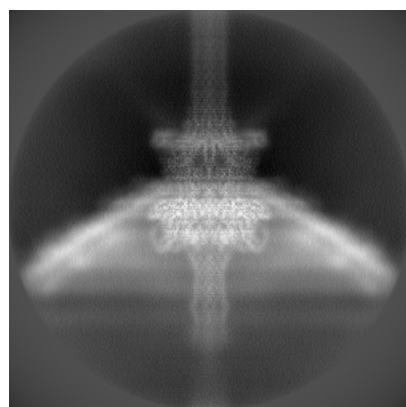


Y

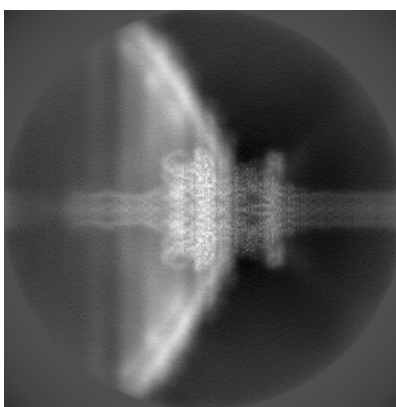


Z

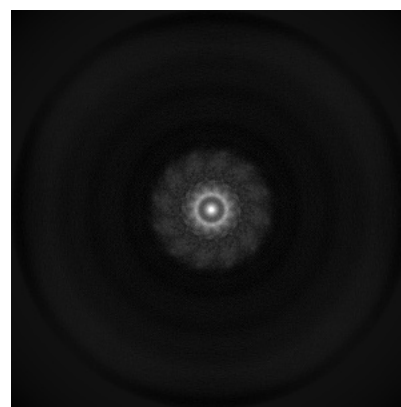
6.1.2 Raw map



X



Y

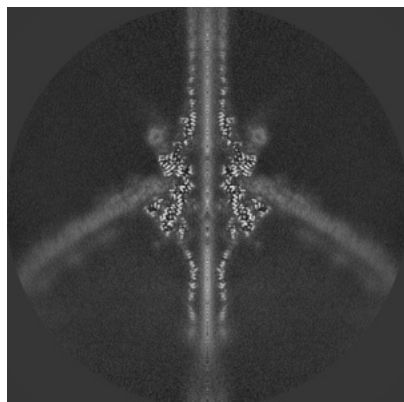


Z

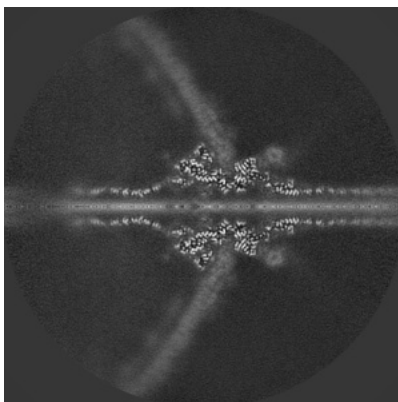
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

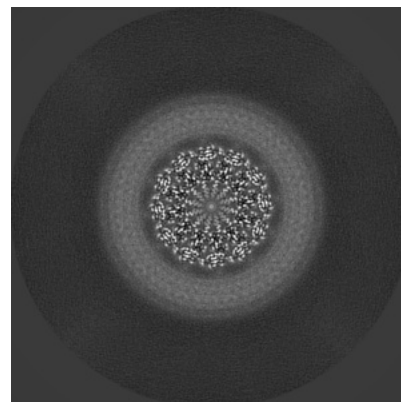
6.2.1 Primary map



X Index: 256

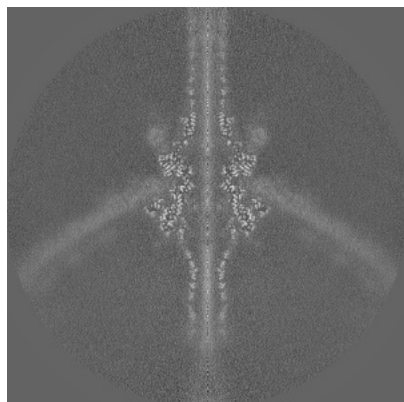


Y Index: 256

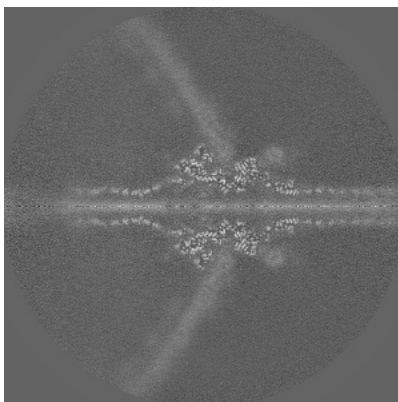


Z Index: 256

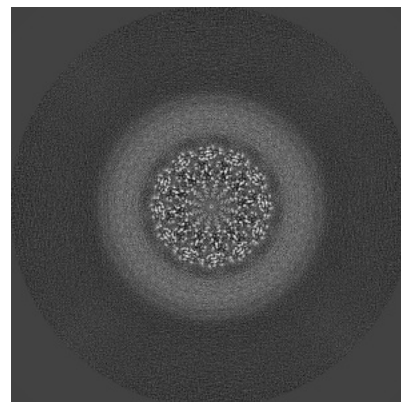
6.2.2 Raw map



X Index: 256



Y Index: 256

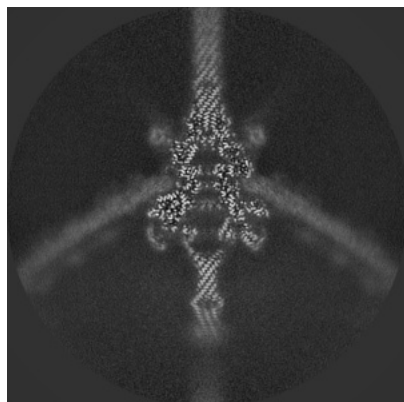


Z Index: 256

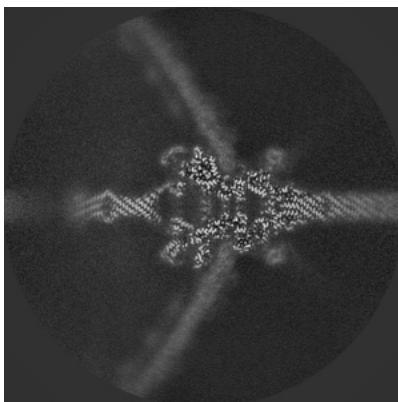
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

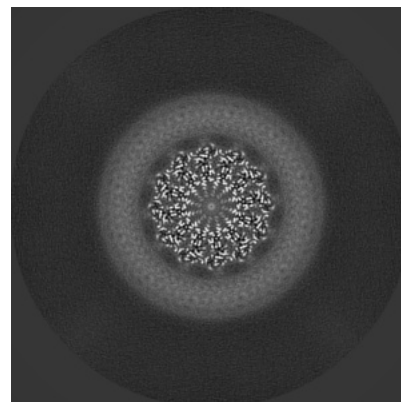
6.3.1 Primary map



X Index: 238

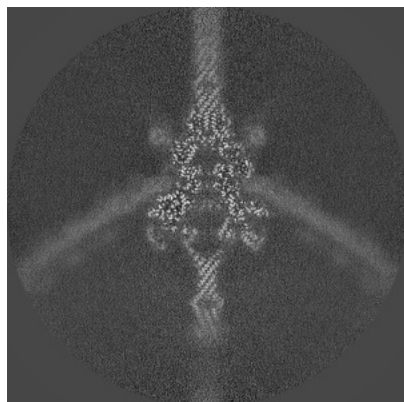


Y Index: 238

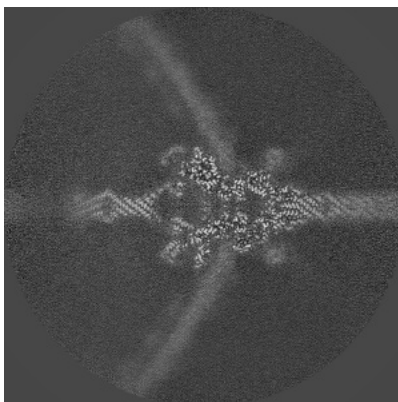


Z Index: 254

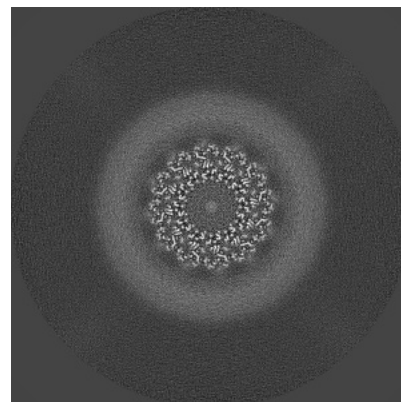
6.3.2 Raw map



X Index: 238



Y Index: 238

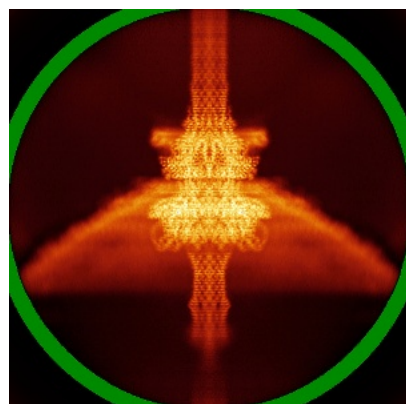


Z Index: 251

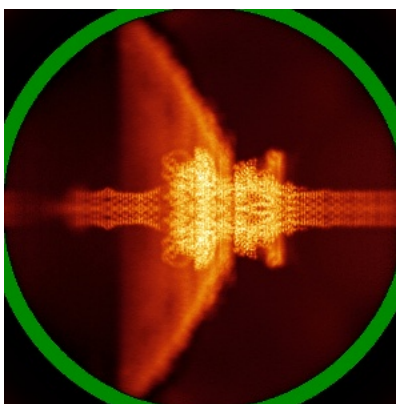
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

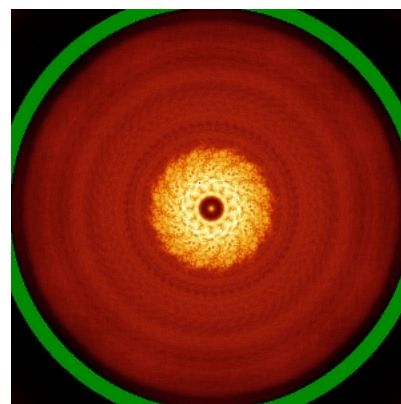
6.4.1 Primary map



X

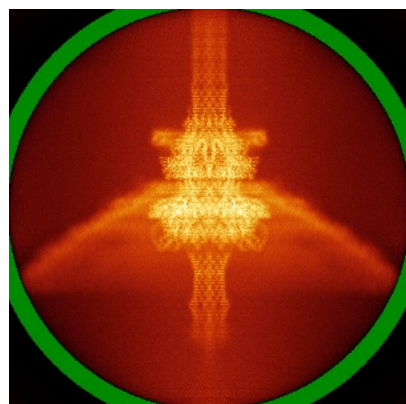


Y

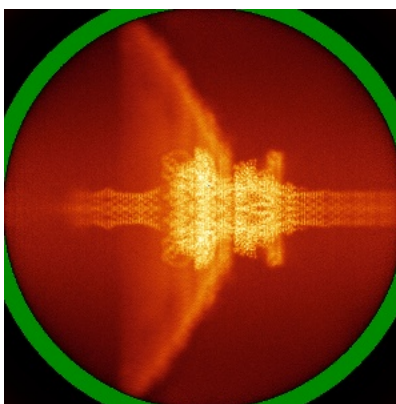


Z

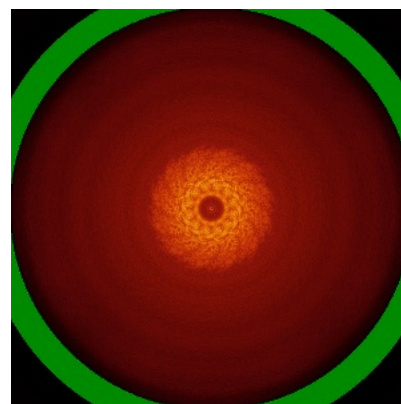
6.4.2 Raw map



X



Y

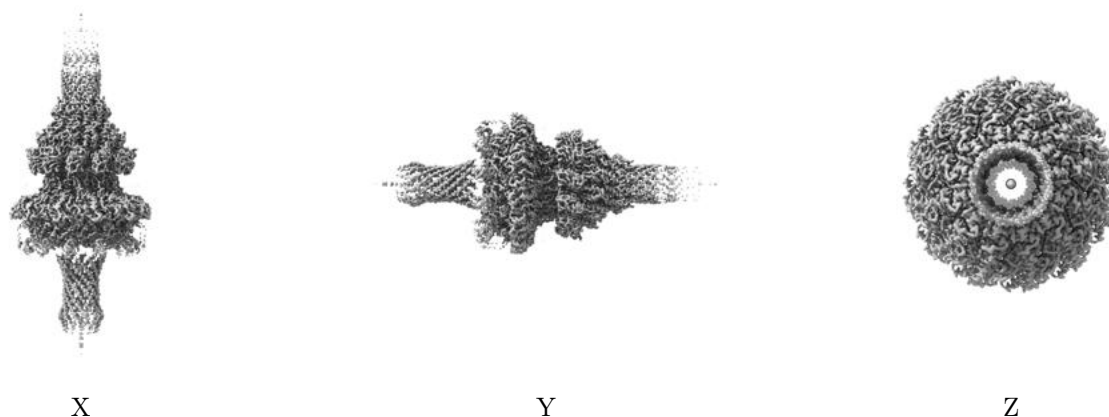


Z

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.

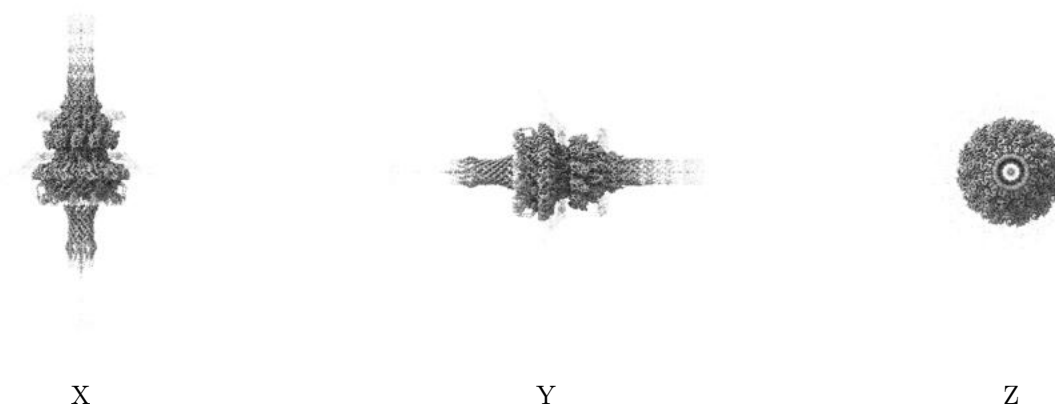
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

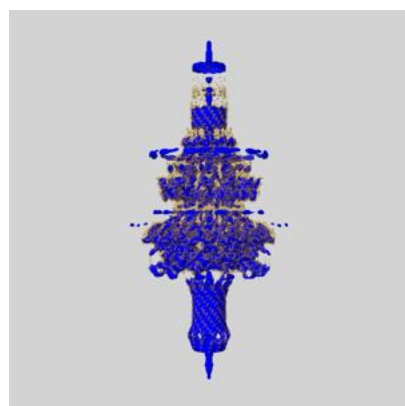
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

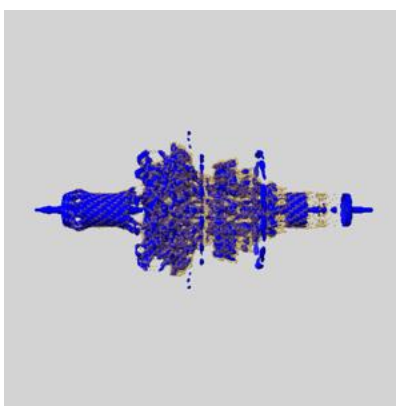
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

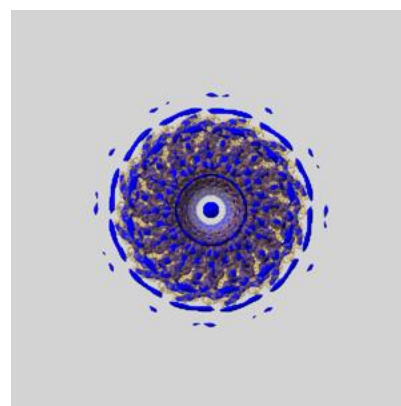
6.6.1 emd_44517_msk_1.map [i](#)



X



Y

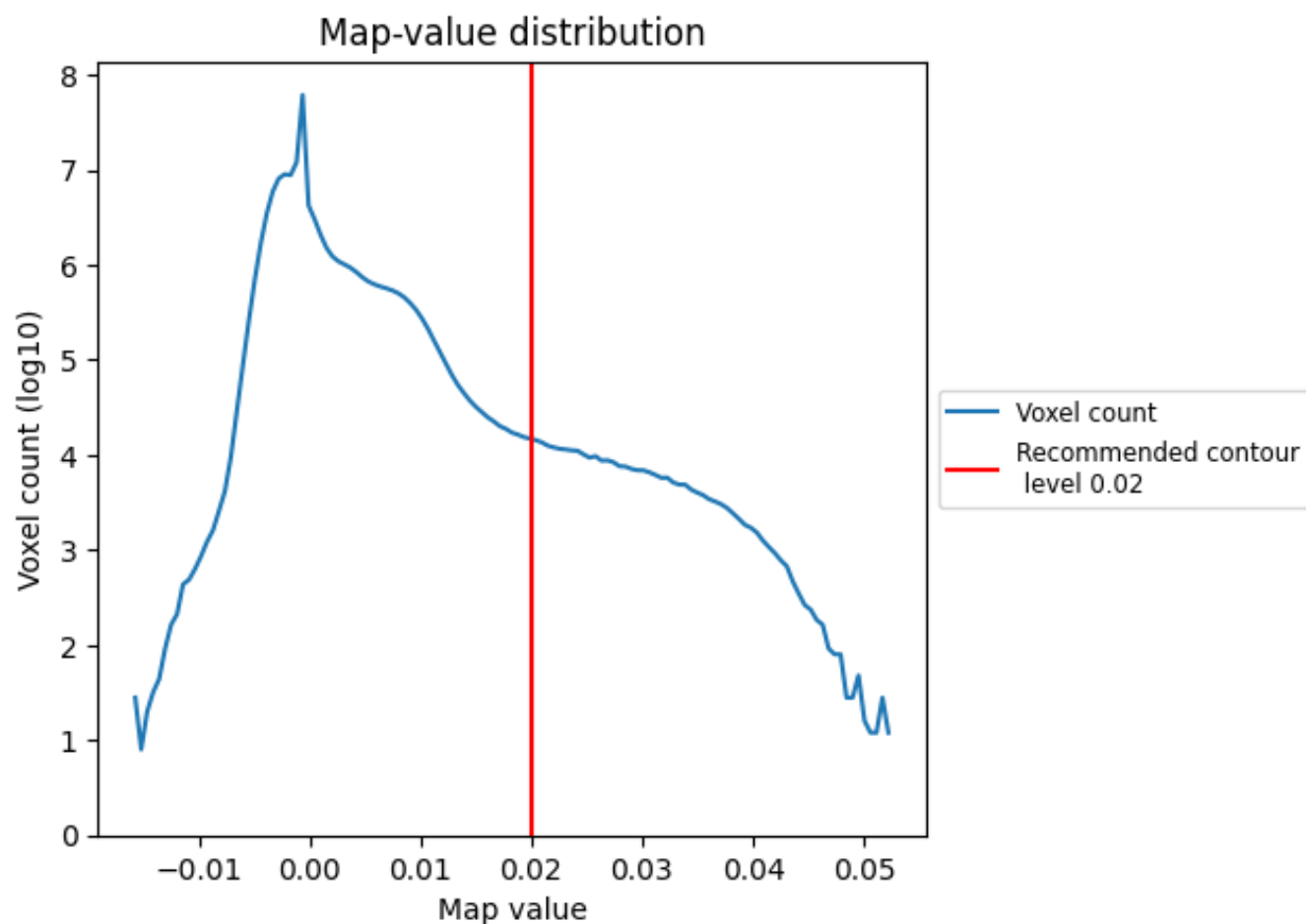


Z

7 Map analysis [i](#)

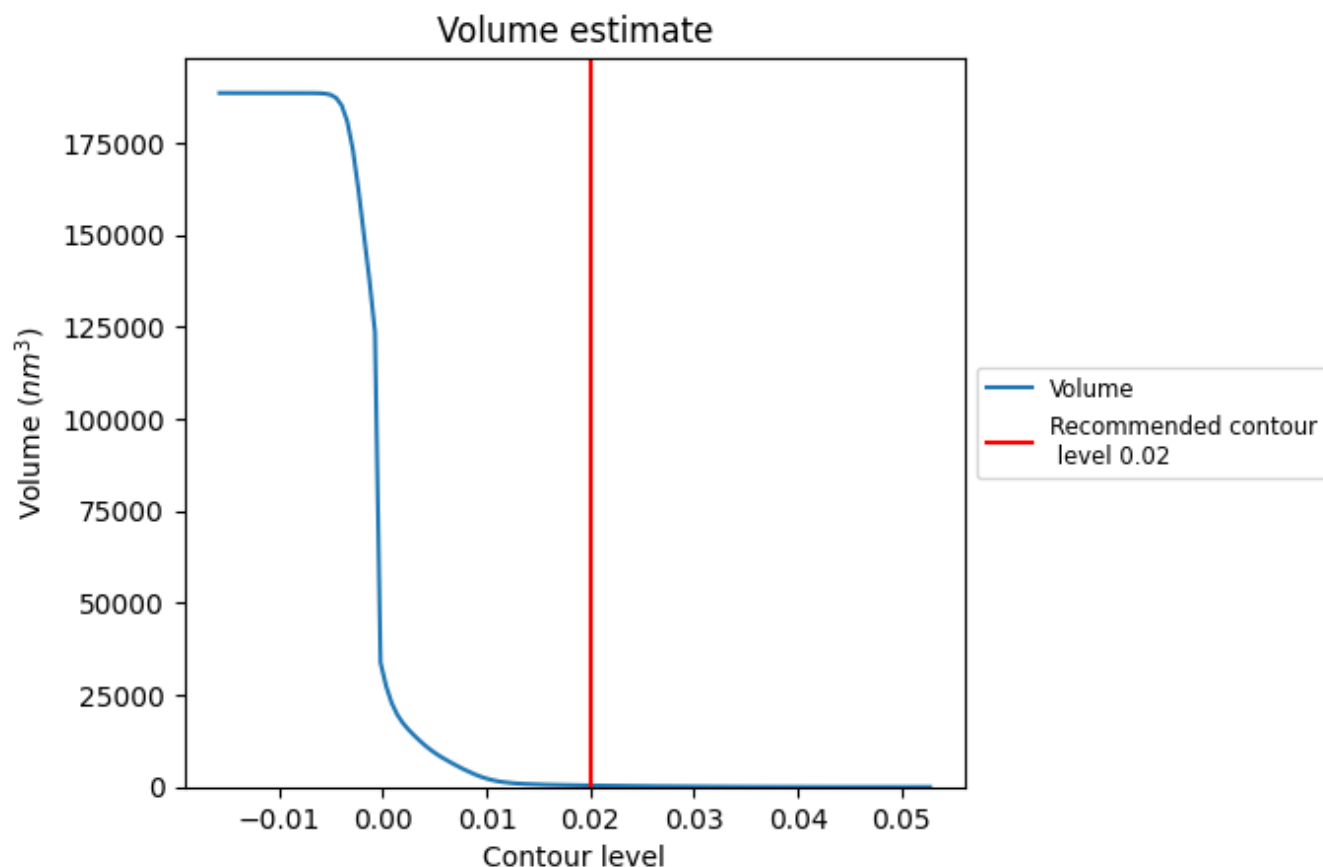
This section contains the results of statistical analysis of the map.

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.

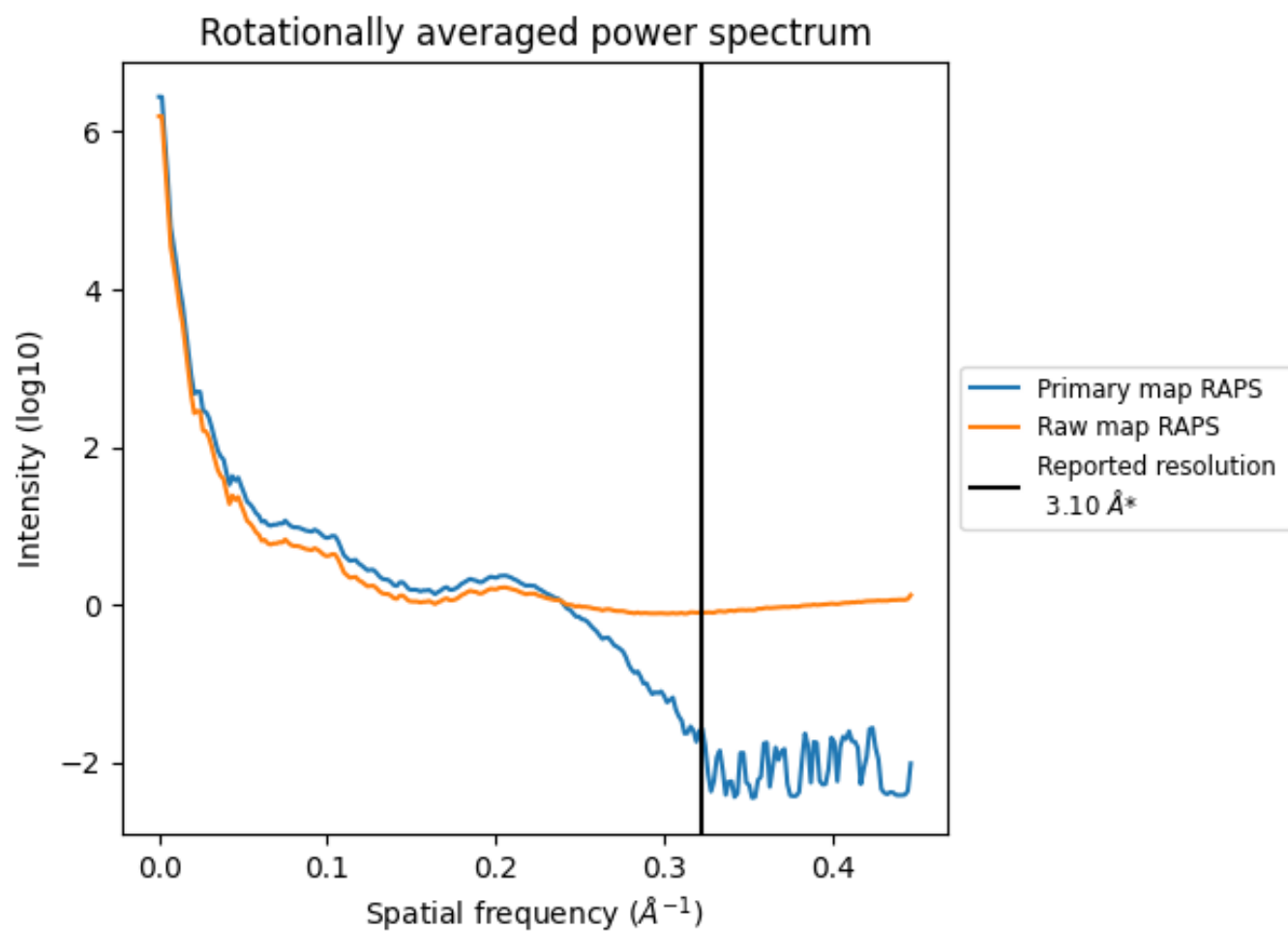
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm³; this corresponds to an approximate mass of 356 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 ⓘ

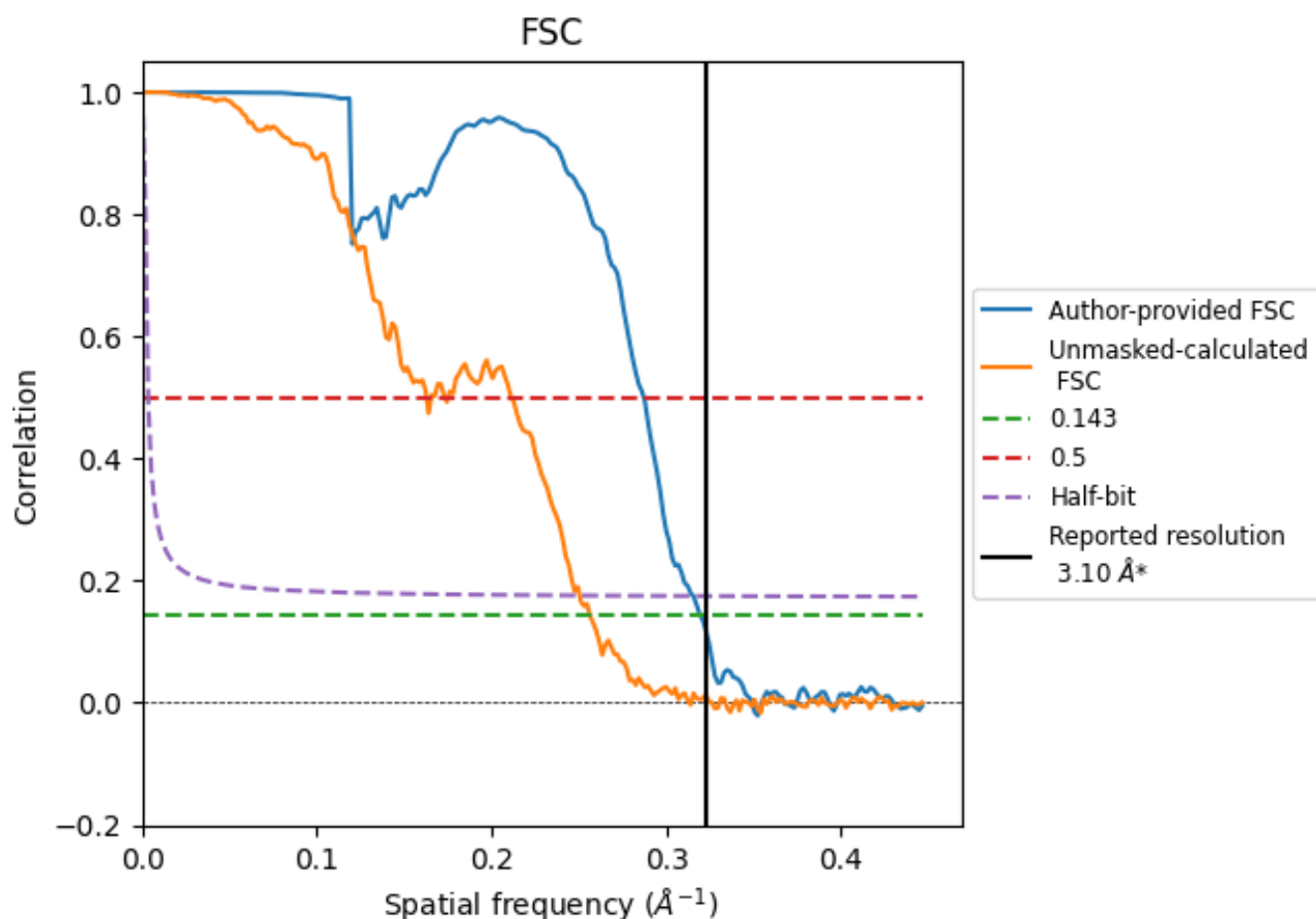


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.48	3.17
Unmasked-calculated*	3.90	6.15	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.1 by more than 10 %

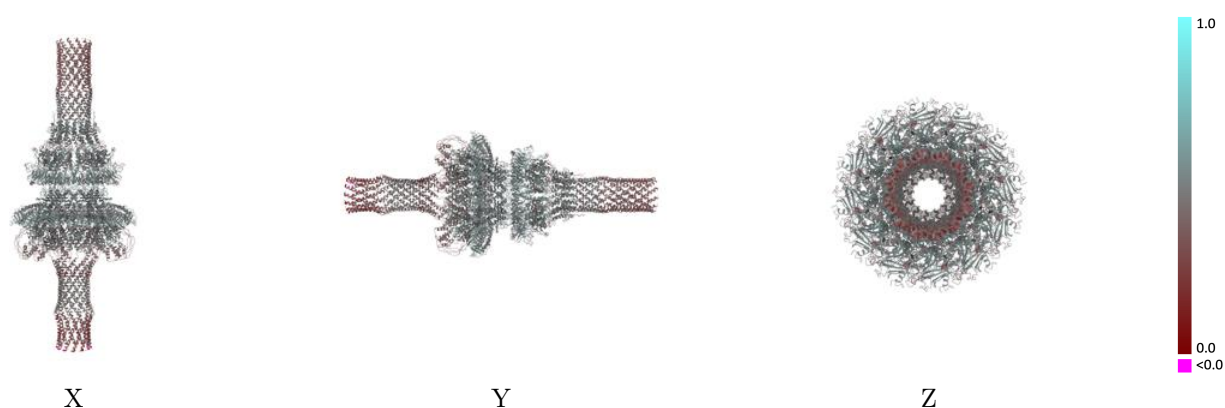
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44517 and PDB model 9BGM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

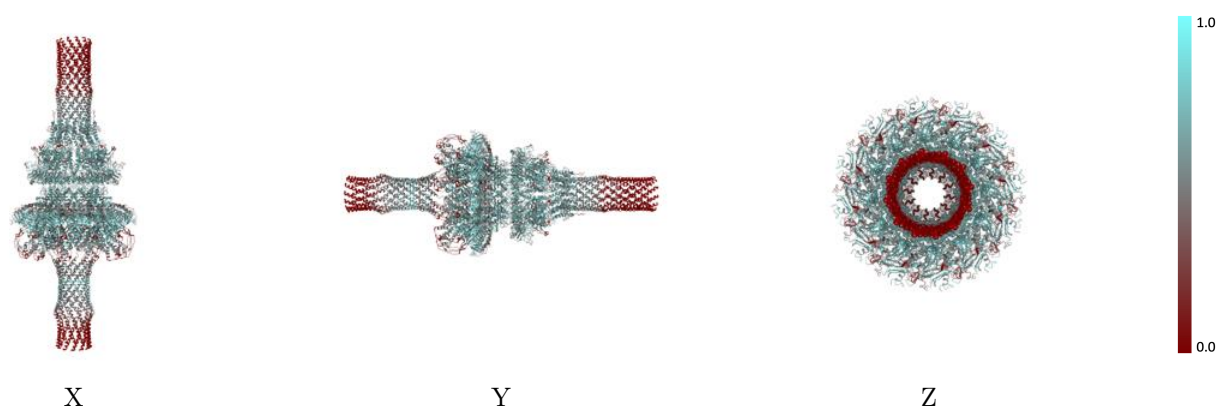
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



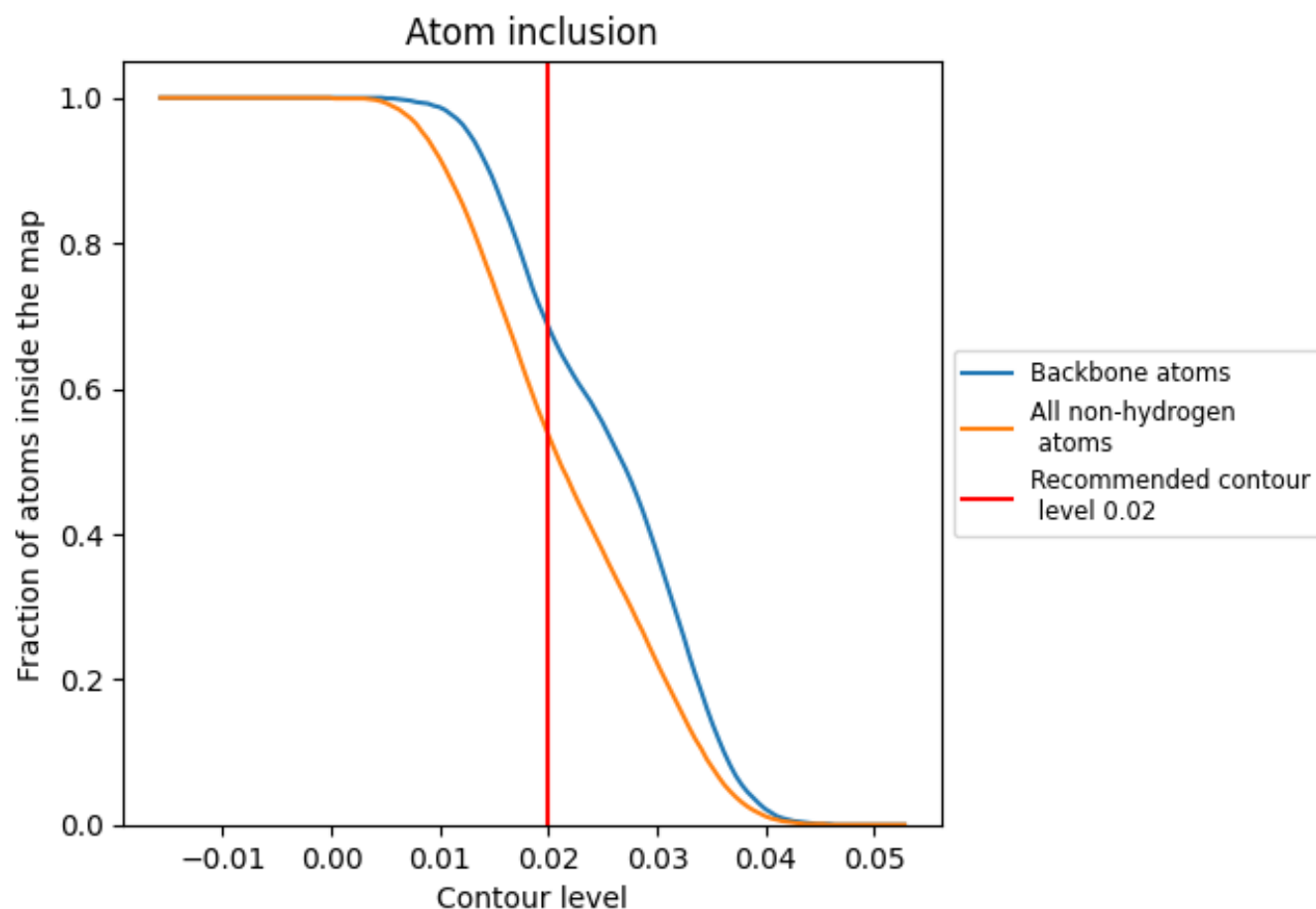
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5350	 0.4730
A	 0.3880	 0.4380
B	 0.5980	 0.5020
C	 0.5400	 0.4710
D	 0.3960	 0.4270
E	 0.6010	 0.4920
F	 0.5440	 0.4640
G	 0.4000	 0.4430
H	 0.6000	 0.5030
I	 0.5410	 0.4720
J	 0.3970	 0.4450
K	 0.5910	 0.5020
L	 0.5380	 0.4710
M	 0.3940	 0.4340
N	 0.5960	 0.5030
O	 0.5380	 0.4690
P	 0.3990	 0.4420
Q	 0.6010	 0.5010
R	 0.5400	 0.4710
S	 0.3930	 0.4410
T	 0.5960	 0.4970
V	 0.5420	 0.4680
W	 0.3900	 0.4380
X	 0.6010	 0.5010
Y	 0.5390	 0.4700
Z	 0.4000	 0.4390
a	 0.3940	 0.4400
b	 0.5970	 0.5040
c	 0.5440	 0.4700
d	 0.5970	 0.5030
e	 0.5410	 0.4730
f	 0.4020	 0.4410
g	 0.5950	 0.5010
h	 0.5390	 0.4730
i	 0.3940	 0.4350



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Chain	Atom inclusion	Q-score
j	 0.6010	 0.4970
k	 0.5420	 0.4680