



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2022 – 10:08 am BST

PDB ID : 7O0I  
EMDB ID : EMD-12676  
Title : Vibrio vulnificus stressosome  
Authors : Kaltwasser, S.; Heinz, V.; Madej, M.G.; Pane-Farre, J.; Ziegler, C.  
Deposited on : 2021-03-26  
Resolution : 8.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

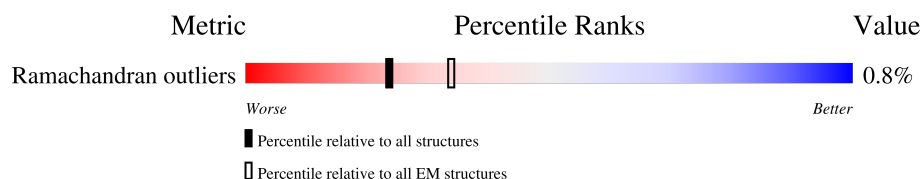
EMDB validation analysis : 0.0.0.dev97  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 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 8.30 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)
Ramachandran outliers	154571	4023

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  $\geq 3$ , 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	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
1	D	115	<div> <div>5%</div> <div>97%</div> <div>..</div> </div>
1	O	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
1	P	115	<div> <div>9%</div> <div>97%</div> <div>..</div> </div>
1	a	115	<div> <div>6%</div> <div>97%</div> <div>..</div> </div>
1	b	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
1	e	115	<div> <div>.</div> <div>97%</div> <div>..</div> </div>
1	f	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
1	g	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
1	t	115	<div> <div>7%</div> <div>97%</div> <div>..</div> </div>
1	u	115	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>




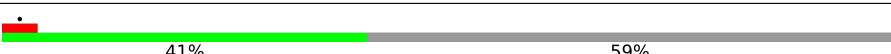
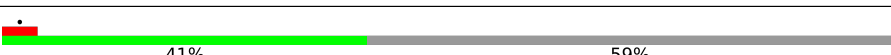
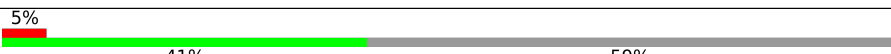
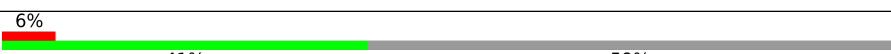


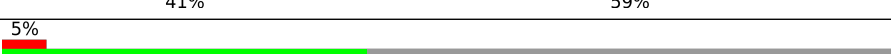


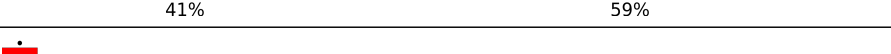











Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	v	115	
2	1	306	
2	2	306	
2	4	306	
2	5	306	
2	6	306	
2	7	306	
2	8	306	
2	9	306	
2	B	306	
2	C	306	
2	E	306	
2	F	306	
2	G	306	
2	H	306	
2	I	306	
2	J	306	
2	K	306	
2	L	306	
2	M	306	
2	N	306	
2	Q	306	
2	R	306	
2	S	306	
2	T	306	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	U	306		
2	V	306		
2	W	306		
2	X	306		
2	Y	306		
2	Z	306		
2	c	306		
2	d	306		
2	h	306		
2	i	306		
2	j	306		
2	k	306		
2	l	306		
2	m	306		
2	n	306		
2	o	306		
2	p	306		
2	q	306		
2	r	306		
2	s	306		
2	w	306		
2	x	306		
2	y	306		
2	z	306		

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36384 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 RsbS, negative regulator of sigma-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	a	113	Total 556	C 330	N 113	O 113	0	0
1	b	113	Total 556	C 330	N 113	O 113	0	0
1	A	113	Total 556	C 330	N 113	O 113	0	0
1	D	113	Total 556	C 330	N 113	O 113	0	0
1	O	113	Total 556	C 330	N 113	O 113	0	0
1	P	113	Total 556	C 330	N 113	O 113	0	0
1	e	113	Total 556	C 330	N 113	O 113	0	0
1	f	113	Total 556	C 330	N 113	O 113	0	0
1	g	113	Total 556	C 330	N 113	O 113	0	0
1	t	113	Total 556	C 330	N 113	O 113	0	0
1	u	113	Total 556	C 330	N 113	O 113	0	0
1	v	113	Total 556	C 330	N 113	O 113	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	SER	ARG	conflict	UNP A0A2S3QZH9
b	63	SER	ARG	conflict	UNP A0A2S3QZH9
A	63	SER	ARG	conflict	UNP A0A2S3QZH9
D	63	SER	ARG	conflict	UNP A0A2S3QZH9
O	63	SER	ARG	conflict	UNP A0A2S3QZH9
P	63	SER	ARG	conflict	UNP A0A2S3QZH9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
e	63	SER	ARG	conflict	UNP A0A2S3QZH9
f	63	SER	ARG	conflict	UNP A0A2S3QZH9
g	63	SER	ARG	conflict	UNP A0A2S3QZH9
t	63	SER	ARG	conflict	UNP A0A2S3QZH9
u	63	SER	ARG	conflict	UNP A0A2S3QZH9
v	63	SER	ARG	conflict	UNP A0A2S3QZH9

- Molecule 2 is a protein called Anti-anti-sigma factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	125	Total 619	C 369	N 125	O 125	0	0
2	C	125	Total 619	C 369	N 125	O 125	0	0
2	E	125	Total 619	C 369	N 125	O 125	0	0
2	F	125	Total 619	C 369	N 125	O 125	0	0
2	G	125	Total 619	C 369	N 125	O 125	0	0
2	H	125	Total 619	C 369	N 125	O 125	0	0
2	I	125	Total 619	C 369	N 125	O 125	0	0
2	J	125	Total 619	C 369	N 125	O 125	0	0
2	K	125	Total 619	C 369	N 125	O 125	0	0
2	L	125	Total 619	C 369	N 125	O 125	0	0
2	M	125	Total 619	C 369	N 125	O 125	0	0
2	N	125	Total 619	C 369	N 125	O 125	0	0
2	Q	125	Total 619	C 369	N 125	O 125	0	0
2	R	125	Total 619	C 369	N 125	O 125	0	0
2	S	125	Total 619	C 369	N 125	O 125	0	0
2	T	125	Total 619	C 369	N 125	O 125	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	125	Total 619	C 369	N 125	O 125	0	0
2	V	125	Total 619	C 369	N 125	O 125	0	0
2	W	125	Total 619	C 369	N 125	O 125	0	0
2	X	125	Total 619	C 369	N 125	O 125	0	0
2	Y	125	Total 619	C 369	N 125	O 125	0	0
2	Z	125	Total 619	C 369	N 125	O 125	0	0
2	c	125	Total 619	C 369	N 125	O 125	0	0
2	d	125	Total 619	C 369	N 125	O 125	0	0
2	h	125	Total 619	C 369	N 125	O 125	0	0
2	i	125	Total 619	C 369	N 125	O 125	0	0
2	j	125	Total 619	C 369	N 125	O 125	0	0
2	k	125	Total 619	C 369	N 125	O 125	0	0
2	l	125	Total 619	C 369	N 125	O 125	0	0
2	m	125	Total 619	C 369	N 125	O 125	0	0
2	n	125	Total 619	C 369	N 125	O 125	0	0
2	o	125	Total 619	C 369	N 125	O 125	0	0
2	p	125	Total 619	C 369	N 125	O 125	0	0
2	q	125	Total 619	C 369	N 125	O 125	0	0
2	r	125	Total 619	C 369	N 125	O 125	0	0
2	s	125	Total 619	C 369	N 125	O 125	0	0
2	w	125	Total 619	C 369	N 125	O 125	0	0

*Continued on next page...*

*Continued from previous page...*

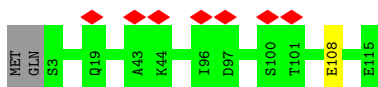
Mol	Chain	Residues	Atoms				AltConf	Trace
2	x	125	Total 619	C 369	N 125	O 125	0	0
2	y	125	Total 619	C 369	N 125	O 125	0	0
2	z	125	Total 619	C 369	N 125	O 125	0	0
2	1	125	Total 619	C 369	N 125	O 125	0	0
2	2	125	Total 619	C 369	N 125	O 125	0	0
2	4	125	Total 619	C 369	N 125	O 125	0	0
2	5	125	Total 619	C 369	N 125	O 125	0	0
2	6	125	Total 619	C 369	N 125	O 125	0	0
2	7	125	Total 619	C 369	N 125	O 125	0	0
2	8	125	Total 619	C 369	N 125	O 125	0	0
2	9	125	Total 619	C 369	N 125	O 125	0	0



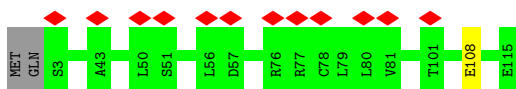
### 3 Residue-property plots [i](#)

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.

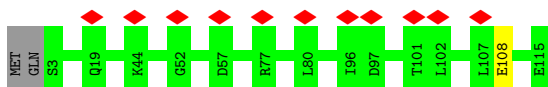
- Molecule 1: RsbS, negative regulator of sigma-B



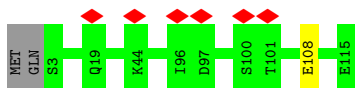
- Molecule 1: RsbS, negative regulator of sigma-B



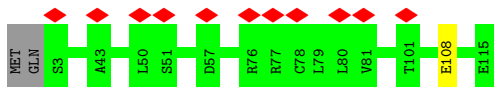
- Molecule 1: RsbS, negative regulator of sigma-B



- Molecule 1: RsbS, negative regulator of sigma-B

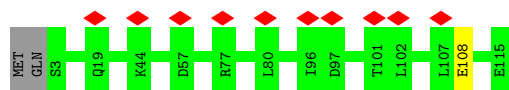


- Molecule 1: RsbS, negative regulator of sigma-B



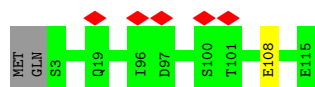
- Molecule 1: RsbS, negative regulator of sigma-B

Chain P:  9% 97% ..



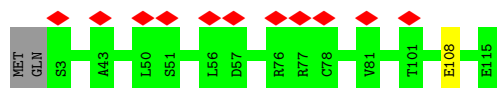
- Molecule 1: RsbS, negative regulator of sigma-B

Chain e:  97% ..



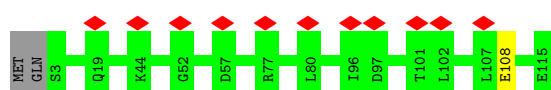
- Molecule 1: RsbS, negative regulator of sigma-B

Chain f:  10% 97% ..



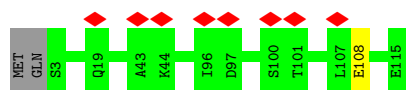
- Molecule 1: RsbS, negative regulator of sigma-B

Chain g:  10% 97% ..



- Molecule 1: RsbS, negative regulator of sigma-B

Chain t:  7% 97% ..



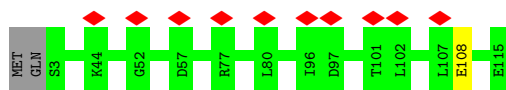
- Molecule 1: RsbS, negative regulator of sigma-B

Chain u:  10% 97% ..



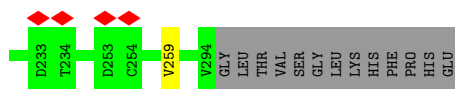
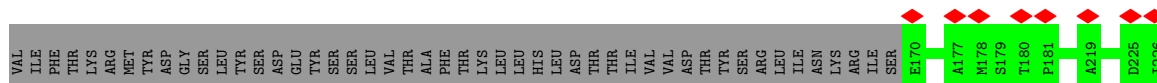
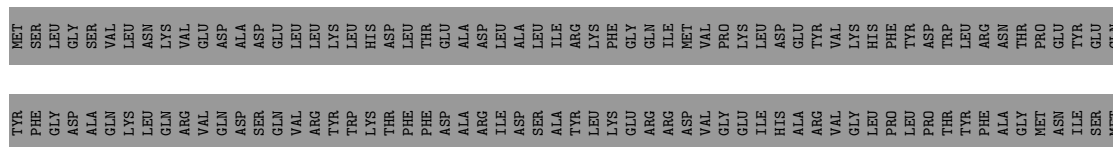
- Molecule 1: RsbS, negative regulator of sigma-B

Chain v:  9% 97% ..



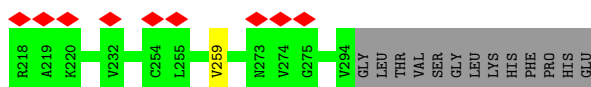
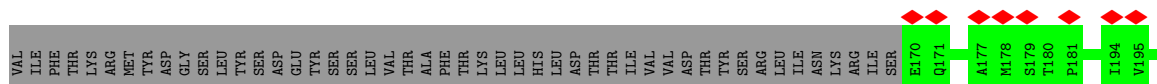
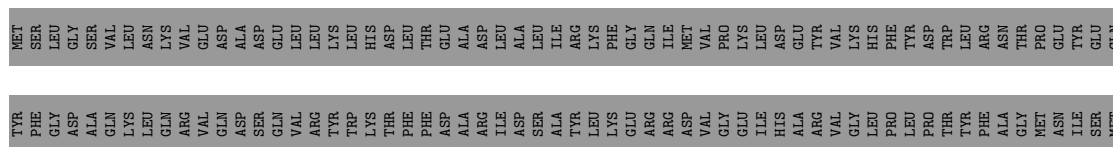
- Molecule 2: Anti-anti-sigma factor

Chain B: 41% 59%



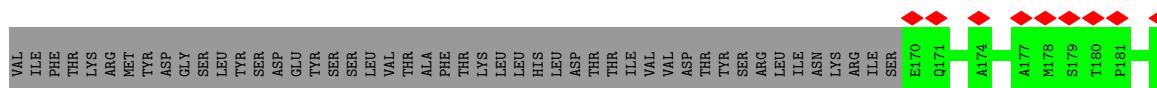
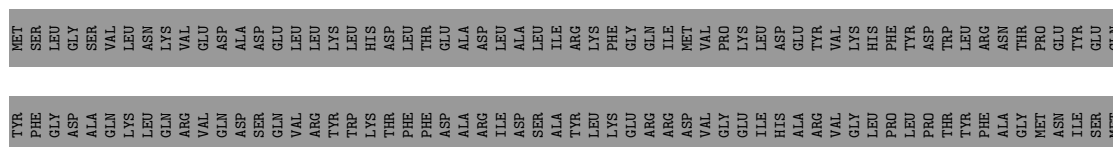
- Molecule 2: Anti-anti-sigma factor

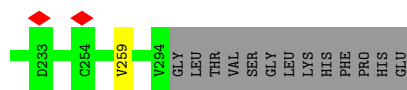
Chain C: 6% 41% 59%



- Molecule 2: Anti-anti-sigma factor

Chain E: 41% 59%



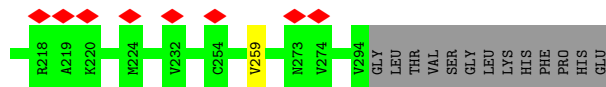
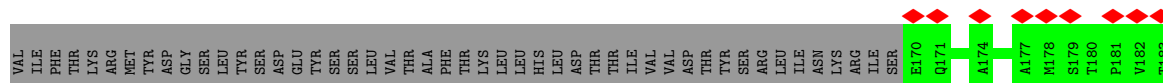


• Molecule 2: Anti-anti-sigma factor



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

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

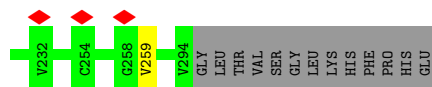
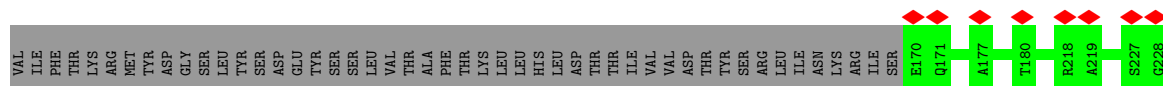


• Molecule 2: Anti-anti-sigma factor

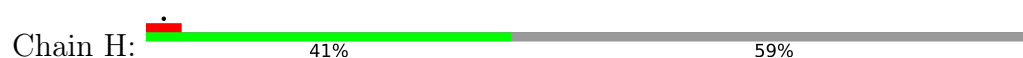


MET SER LEU GLY SER ALA VAL LEU ASN LYS VAL GLU ASP ALA ASP GLU LEU LYS THR LEU HIS THR ASP LEU THR GLU THR ASP ALA ASP LEU ILE ARG TYR LYS PHE GLY GLN ILE ASP MET VAL PRO LYS LYS ASP TYR VAL VAL VAL HIS HIS PHE ASP TYR TRP LEU ARG ASN THR PRO GLU TYR GLN

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

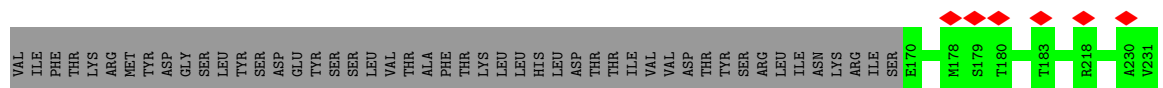


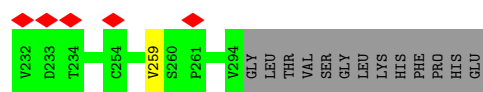
• Molecule 2: Anti-anti-sigma factor



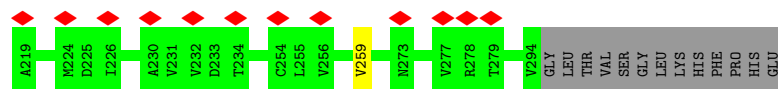
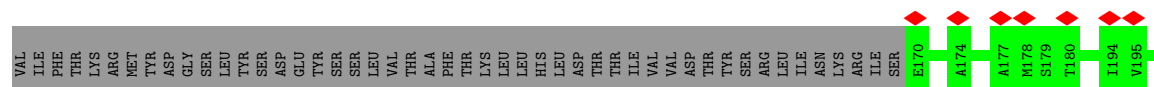
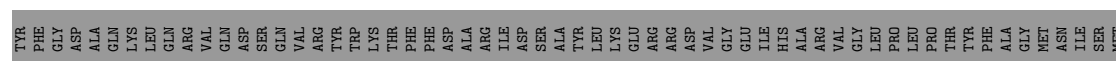
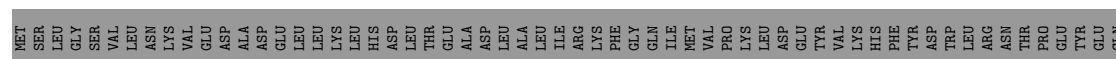
MET SER LEU GLY SER ALA VAL LEU ASN LYS VAL GLU ASP ALA ASP GLU LEU LYS THR LEU HIS THR ASP LEU THR GLU THR ASP ALA ASP LEU ILE ARG TYR LYS PHE GLY GLN ILE ASP MET VAL PRO LYS LYS ASP TYR VAL VAL VAL HIS HIS PHE ASP TYR TRP LEU ARG ASN THR PRO GLU TYR GLN

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

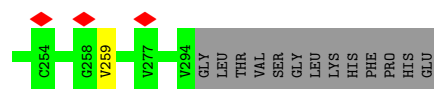
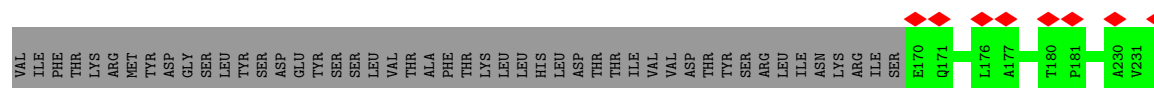
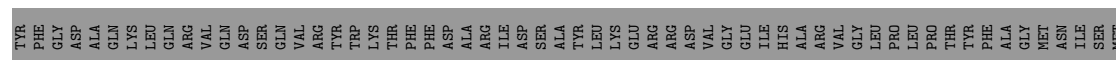
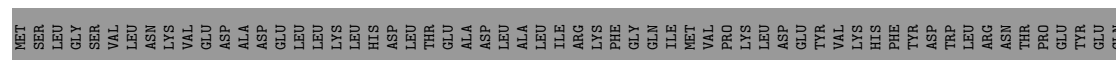




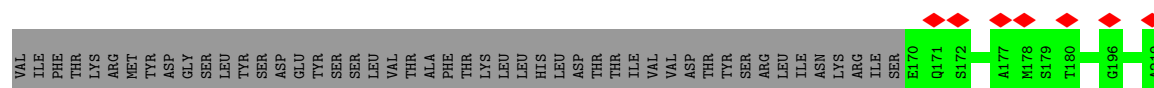
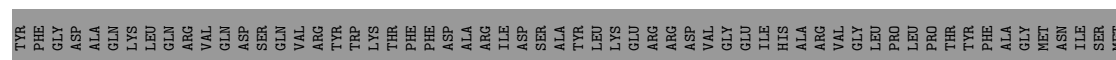
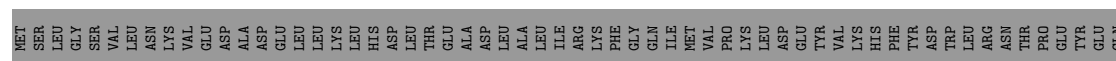
• Molecule 2: Anti-anti-sigma factor

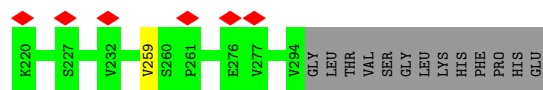


• Molecule 2: Anti-anti-sigma factor



• Molecule 2: Anti-anti-sigma factor



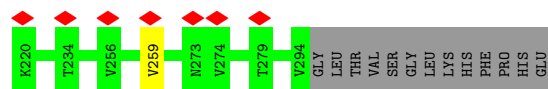
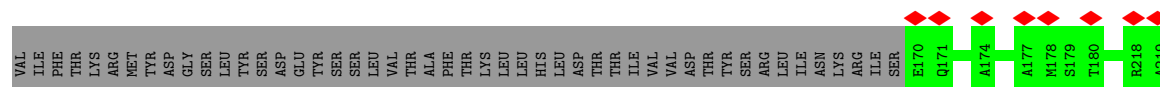


• Molecule 2: Anti-anti-sigma factor



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

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

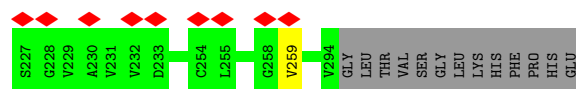
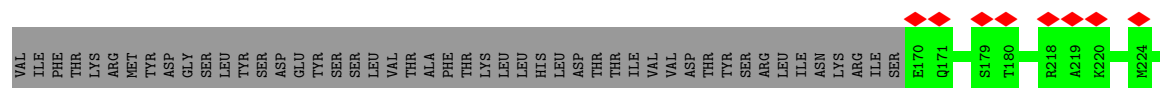


• Molecule 2: Anti-anti-sigma factor



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

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

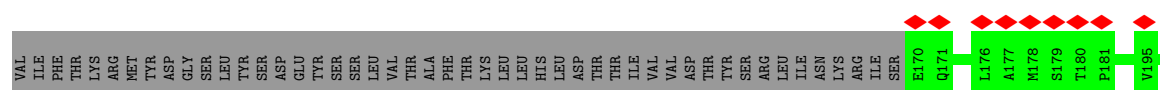


• Molecule 2: Anti-anti-sigma factor

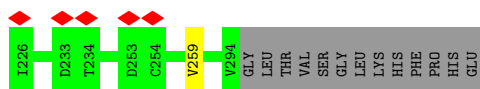
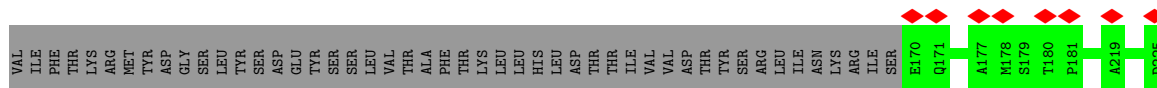
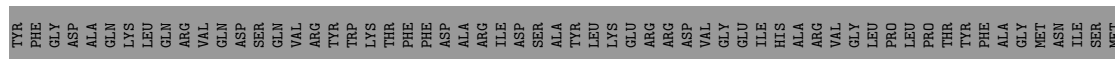


MET SER LEU GLY SER VAL LEU ASN LYS VAL GLU ASP ASP ALA GLU LEU LEU LYS LEU THR LEU VAL SER GLY THR LEU LYS HIS ALA ASP ASP ALA ILE LEU ARG LYS PHE LEU GLN ARG ILE MET VAL PRO GLY LYS LEU ASP TYR TRP LEU THR PHE ARG ASN TRP LEU THR PRO GLN

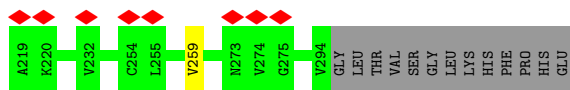
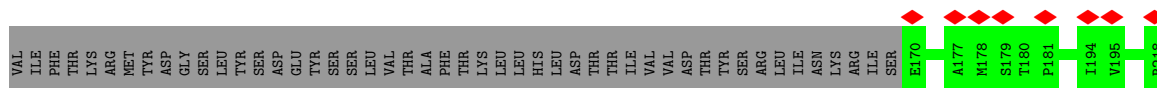
TYR PHE GLY ASP ALA GLN LYS LEU GLN ARG VAL GLN ASP SER GLN VAL ARG TRP LYS THR PHE THR ASP ALA THR ARG ILE SER LEU TYR ARG LYS LEU THR THR THR ILE VAL ARG VAL ASP THR TYR SER ARG ILE ASN VAL ARG VAL LEU PHE LEU PRO THR TYR PHE ARG ALA GLY MET ASN ILE TYR GLN



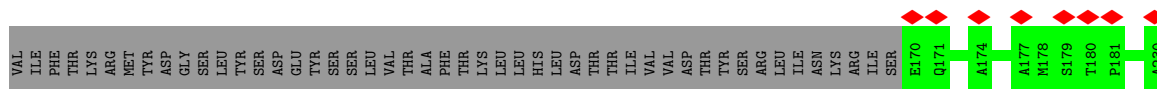
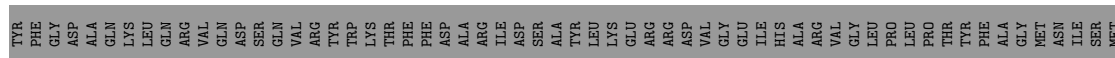
- Molecule 2: Anti-anti-sigma factor

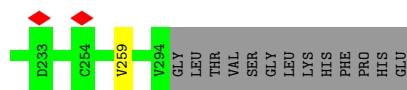


- Molecule 2: Anti-anti-sigma factor



- Molecule 2: Anti-anti-sigma factor





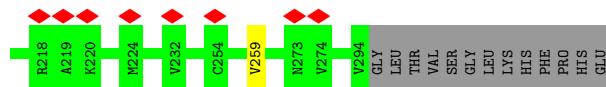
• Molecule 2: Anti-anti-sigma factor



MET SER LEU GLY SER ALA VAL LEU ASN LYS VAL GLU ASP ALA ASP GLU LEU LYS THR LEU HIS THR VAL GLN

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

VAL ILE PHE THR LYS ARG MET TYR ASP GLN SER LEU TYR SER ASP GLU TYR SER LEU VAL THR ALA PHE THR LYS LEU HIS LEU ASP THR THR THR VAL VAL VAL ASP THR TYR SER ARG LEU ILE ILE SER E170 Q171 A174 L175 L176 A177 M178 S179 T180 P181 V182



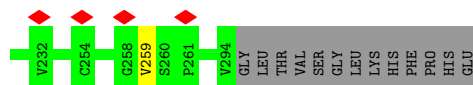
• Molecule 2: Anti-anti-sigma factor



MET SER LEU GLY SER VAL LEU ASN LYS VAL GLU ASP ALA ASP GLU LEU LEU LYS THR LEU THR PHE THR ASP ALA ARG ASP ALA LEU ILE LEU ASP TYR LYS PHE THR LEU LYS THR THR THR VAL VAL VAL ASP THR TYR SER ARG LEU ILE ILE SER E170 Q171 A177 T180 R218 A219 S227 G228

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

VAL ILE PHE THR LYS ARG MET TYR ASP GLN SER LEU TYR SER ASP GLU TYR SER LEU VAL THR ALA PHE THR LYS LEU HIS LEU ASP THR THR THR VAL VAL VAL ASP THR TYR SER ARG LEU ILE ILE SER E170 Q171 A177 T180 R218 A219 S227 G228



• Molecule 2: Anti-anti-sigma factor

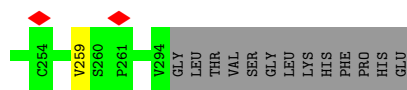


MET SER LEU GLY SER VAL LEU ASN LYS VAL GLU ASP ALA ASP GLU LEU LYS THR LEU HIS THR THR PHE THR ASP ALA ARG ASP ALA LEU ILE LEU ASP TYR LYS PHE THR LEU LYS THR THR THR VAL VAL VAL ASP THR TYR SER ARG LEU ILE ILE SER E170 Q171 A177 T180 R218 A219 S227 G228

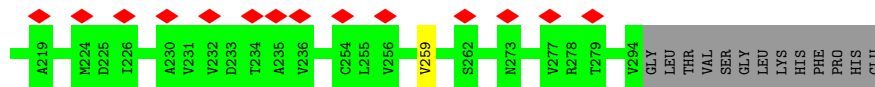
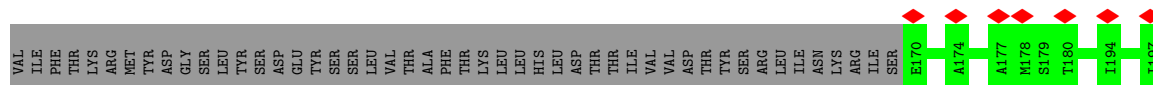
TYR PHE GLY ALA SER LYS LEU GLN ARG VAL GLN ASP SER GLN VAL ARG TYR TRP LYS THR PHE THR ASP ALA ARG ILE LEU SER ALA ILE ARG TYR LYS PHE GLU ARG ILE VAL GLY LYS HIS ARG ILE ILE SER PRO PHE TYR TRP THR PHE ARG ALA MET ASN GLU TYR GLN

VAL ILE PHE THR LYS ARG MET TYR ASP GLN SER LEU TYR SER ASP GLU TYR SER LEU VAL THR ALA PHE THR LYS LEU HIS LEU ASP THR THR THR VAL VAL VAL ASP THR TYR SER ARG LEU ILE ILE SER E170 Q171 A177 T180 R218 A219 S227 G228

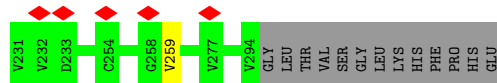
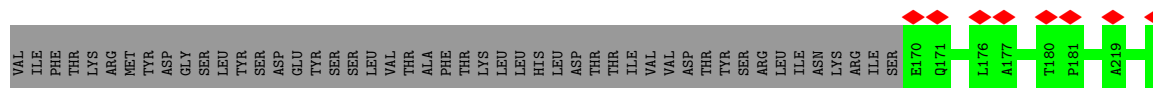
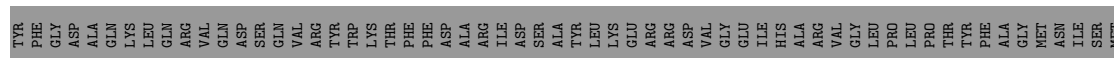
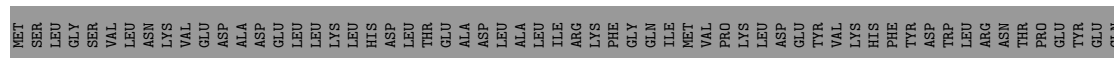




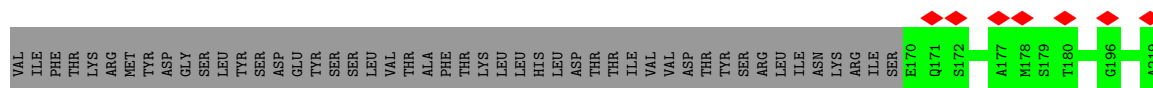
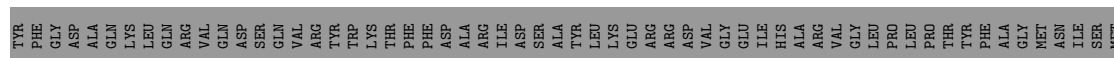
- Molecule 2: Anti-anti-sigma factor



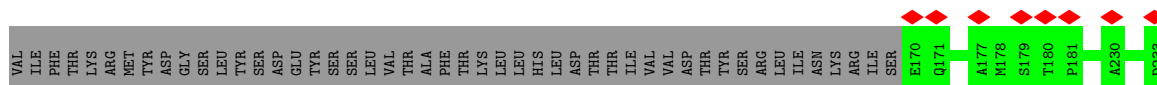
- Molecule 2: Anti-anti-sigma factor



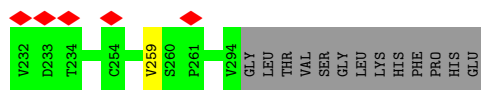
- Molecule 2: Anti-anti-sigma factor



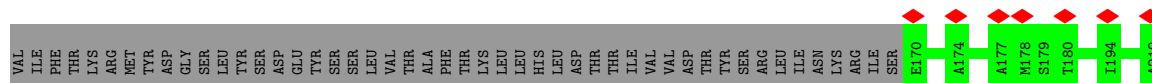




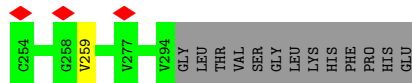
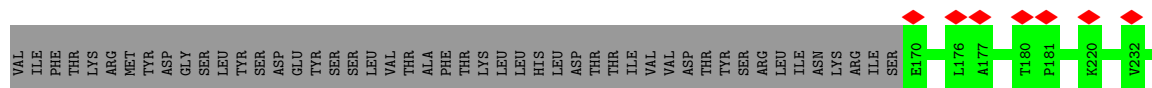
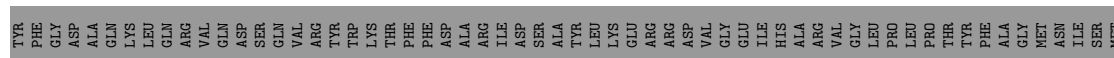
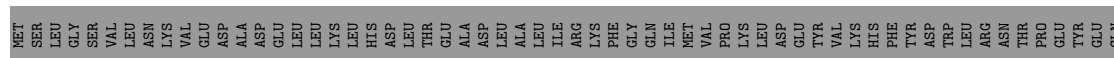




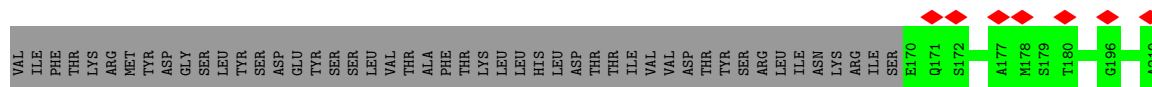
• Molecule 2: Anti-anti-sigma factor

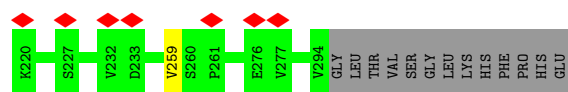


• Molecule 2: Anti-anti-sigma factor

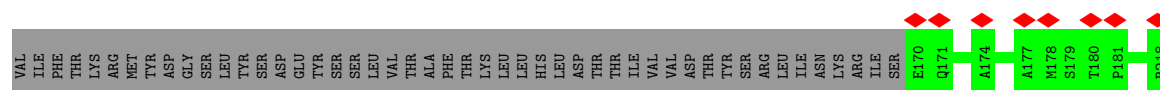
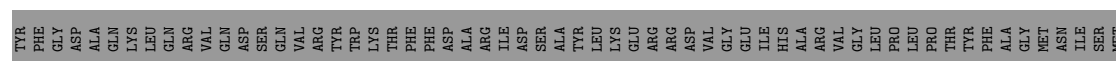
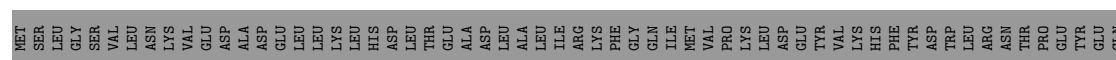


• Molecule 2: Anti-anti-sigma factor

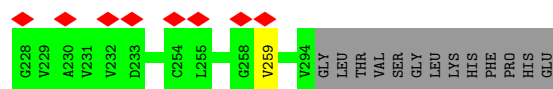
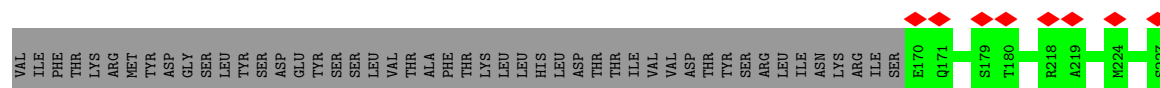
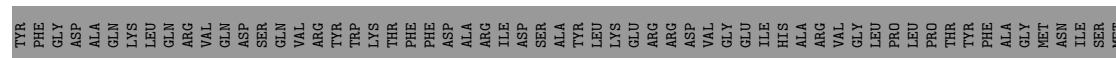
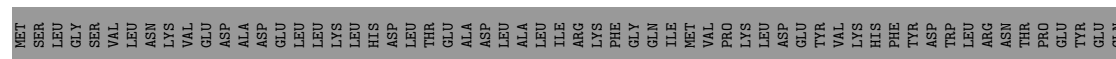




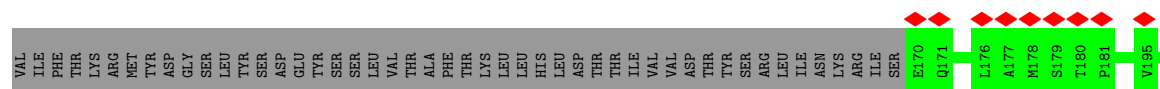
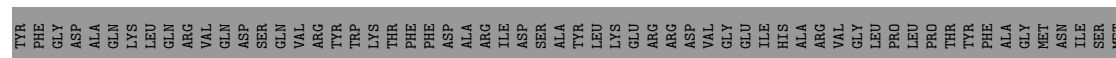
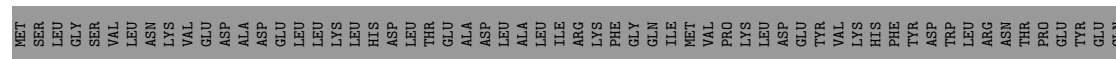
- Molecule 2: Anti-anti-sigma factor

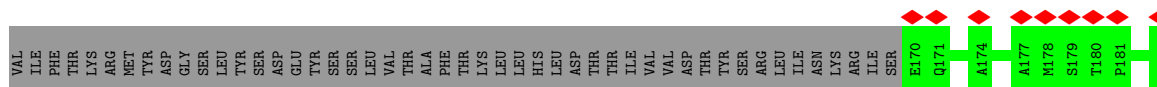


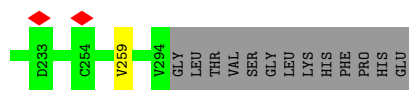
- Molecule 2: Anti-anti-sigma factor



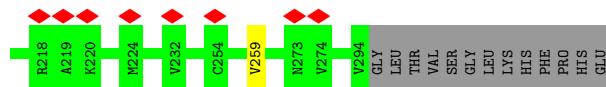
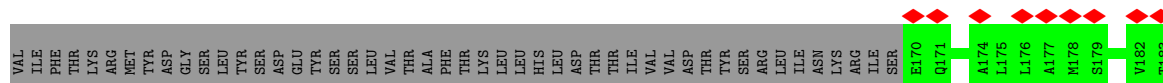
- Molecule 2: Anti-anti-sigma factor



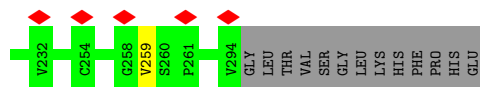
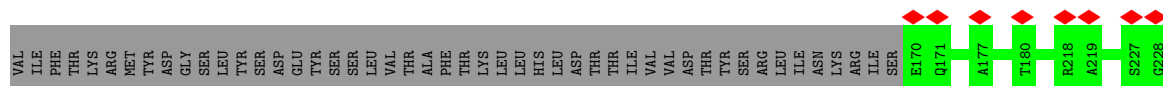
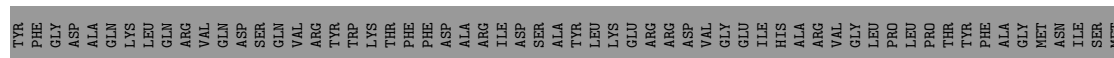
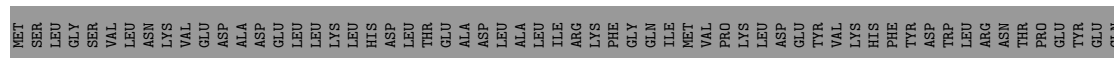




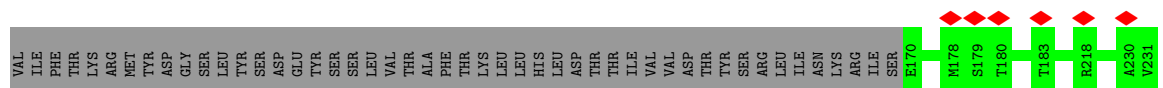
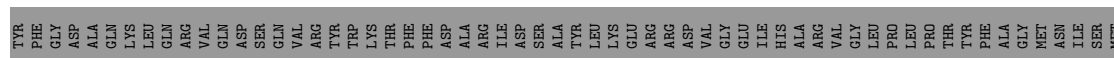
- Molecule 2: Anti-anti-sigma factor



- Molecule 2: Anti-anti-sigma factor



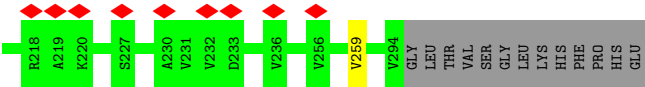
- Molecule 2: Anti-anti-sigma factor











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	35647	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	72	Depositor
Minimum defocus (nm)	-1700	Depositor
Maximum defocus (nm)	-5500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.446	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	442.5, 442.5, 442.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.77, 1.77, 1.77	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.75	0/555	1.12	0/770
1	D	0.75	0/555	1.12	0/770
1	O	0.75	0/555	1.12	0/770
1	P	0.75	0/555	1.12	0/770
1	a	0.75	0/555	1.12	0/770
1	b	0.75	0/555	1.12	0/770
1	e	0.75	0/555	1.12	0/770
1	f	0.75	0/555	1.12	0/770
1	g	0.75	0/555	1.12	0/770
1	t	0.75	0/555	1.12	0/770
1	u	0.75	0/555	1.12	0/770
1	v	0.75	0/555	1.12	0/770
2	1	0.77	0/618	1.12	0/860
2	2	0.76	0/618	1.09	0/860
2	4	0.76	0/618	1.12	0/860
2	5	0.76	0/618	1.09	0/860
2	6	0.77	0/618	1.12	0/860
2	7	0.76	0/618	1.12	0/860
2	8	0.76	0/618	1.12	0/860
2	9	0.76	0/618	1.09	0/860
2	B	0.76	0/618	1.11	0/860
2	C	0.76	0/618	1.12	0/860
2	E	0.76	0/618	1.12	0/860
2	F	0.76	0/618	1.12	0/860
2	G	0.76	0/618	1.12	0/860
2	H	0.76	0/618	1.09	0/860
2	I	0.77	0/618	1.12	0/860
2	J	0.76	0/618	1.08	0/860
2	K	0.76	0/618	1.12	0/860
2	L	0.76	0/618	1.12	0/860
2	M	0.77	0/618	1.12	0/860
2	N	0.76	0/618	1.09	0/860
2	Q	0.76	0/618	1.12	0/860
2	R	0.76	0/618	1.12	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	S	0.76	0/618	1.12	0/860
2	T	0.76	0/618	1.12	0/860
2	U	0.76	0/618	1.12	0/860
2	V	0.76	0/618	1.10	0/860
2	W	0.76	0/618	1.12	0/860
2	X	0.76	0/618	1.09	0/860
2	Y	0.76	0/618	1.12	0/860
2	Z	0.76	0/618	1.12	0/860
2	c	0.76	0/618	1.12	0/860
2	d	0.76	0/618	1.09	0/860
2	h	0.76	0/618	1.12	0/860
2	i	0.76	0/618	1.12	0/860
2	j	0.77	0/618	1.12	0/860
2	k	0.76	0/618	1.12	0/860
2	l	0.76	0/618	1.12	0/860
2	m	0.76	0/618	1.10	0/860
2	n	0.76	0/618	1.12	0/860
2	o	0.76	0/618	1.09	0/860
2	p	0.76	0/618	1.12	0/860
2	q	0.76	0/618	1.12	0/860
2	r	0.76	0/618	1.12	0/860
2	s	0.76	0/618	1.09	0/860
2	w	0.76	0/618	1.12	0/860
2	x	0.76	0/618	1.12	0/860
2	y	0.76	0/618	1.12	0/860
2	z	0.76	0/618	1.12	0/860
All	All	0.76	0/36324	1.11	0/50520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

## 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	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
1	D	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	O	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	P	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	a	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	b	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
1	e	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	f	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
1	g	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
1	t	111/115 (96%)	104 (94%)	6 (5%)	1 (1%)	17	57
1	u	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
1	v	111/115 (96%)	103 (93%)	7 (6%)	1 (1%)	17	57
2	1	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	2	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	4	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	5	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	6	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	7	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	8	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	9	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	B	123/306 (40%)	108 (88%)	14 (11%)	1 (1%)	19	60
2	C	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	E	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	F	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	G	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	I	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	J	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	K	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	L	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	M	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	N	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	Q	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	R	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	S	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	T	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	U	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	V	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	W	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	X	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	Y	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	Z	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	c	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	d	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	h	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	i	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	j	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	k	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	l	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	m	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	n	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	o	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	p	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	q	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	r	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	s	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	w	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	x	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	y	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
2	z	123/306 (40%)	107 (87%)	15 (12%)	1 (1%)	19	60
All	All	7236/16068 (45%)	6379 (88%)	797 (11%)	60 (1%)	24	60

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	108	GLU
1	b	108	GLU
1	A	108	GLU
1	D	108	GLU
1	O	108	GLU

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.

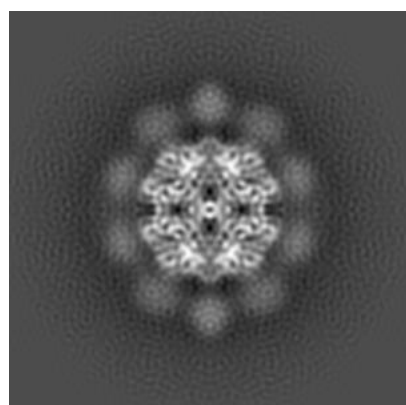
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12676. These allow visual inspection of the internal detail of the map and identification of artifacts.

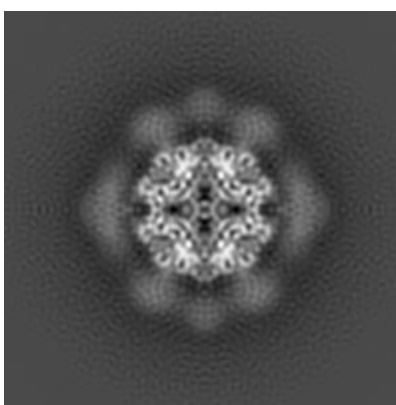
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

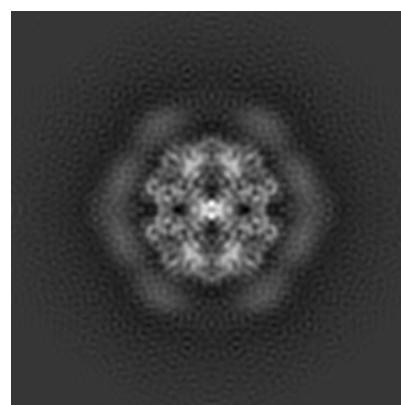
#### 6.1.1 Primary map



X



Y

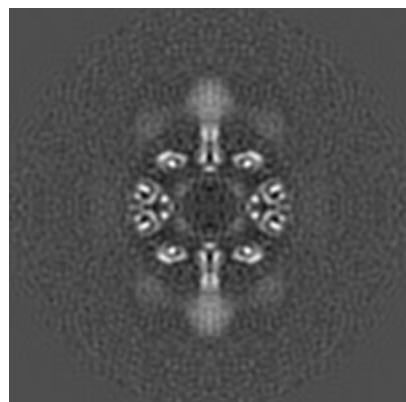


Z

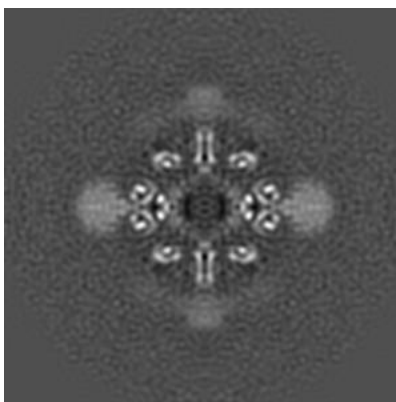
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

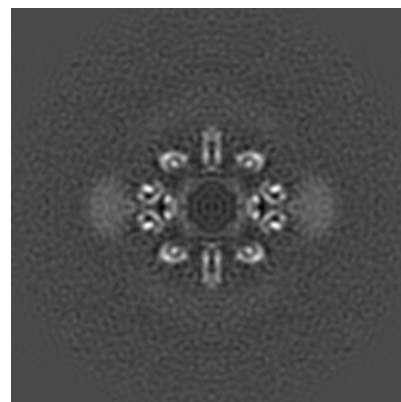
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

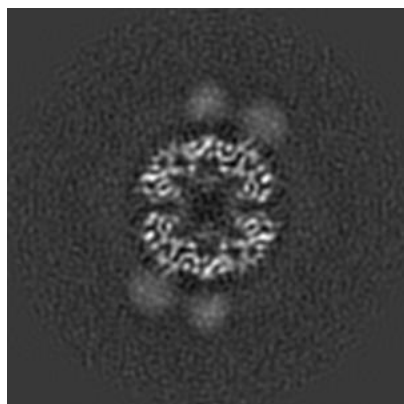


Z Index: 125

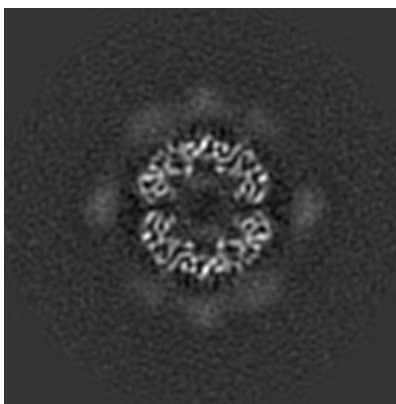
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

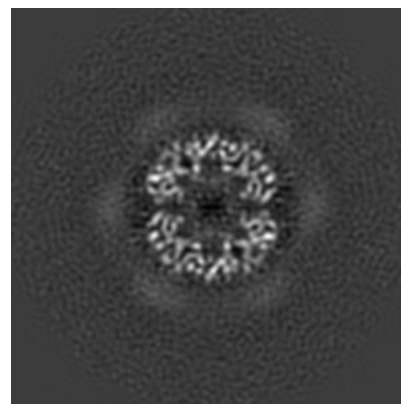
### 6.3.1 Primary map



X Index: 136



Y Index: 136



Z Index: 136

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

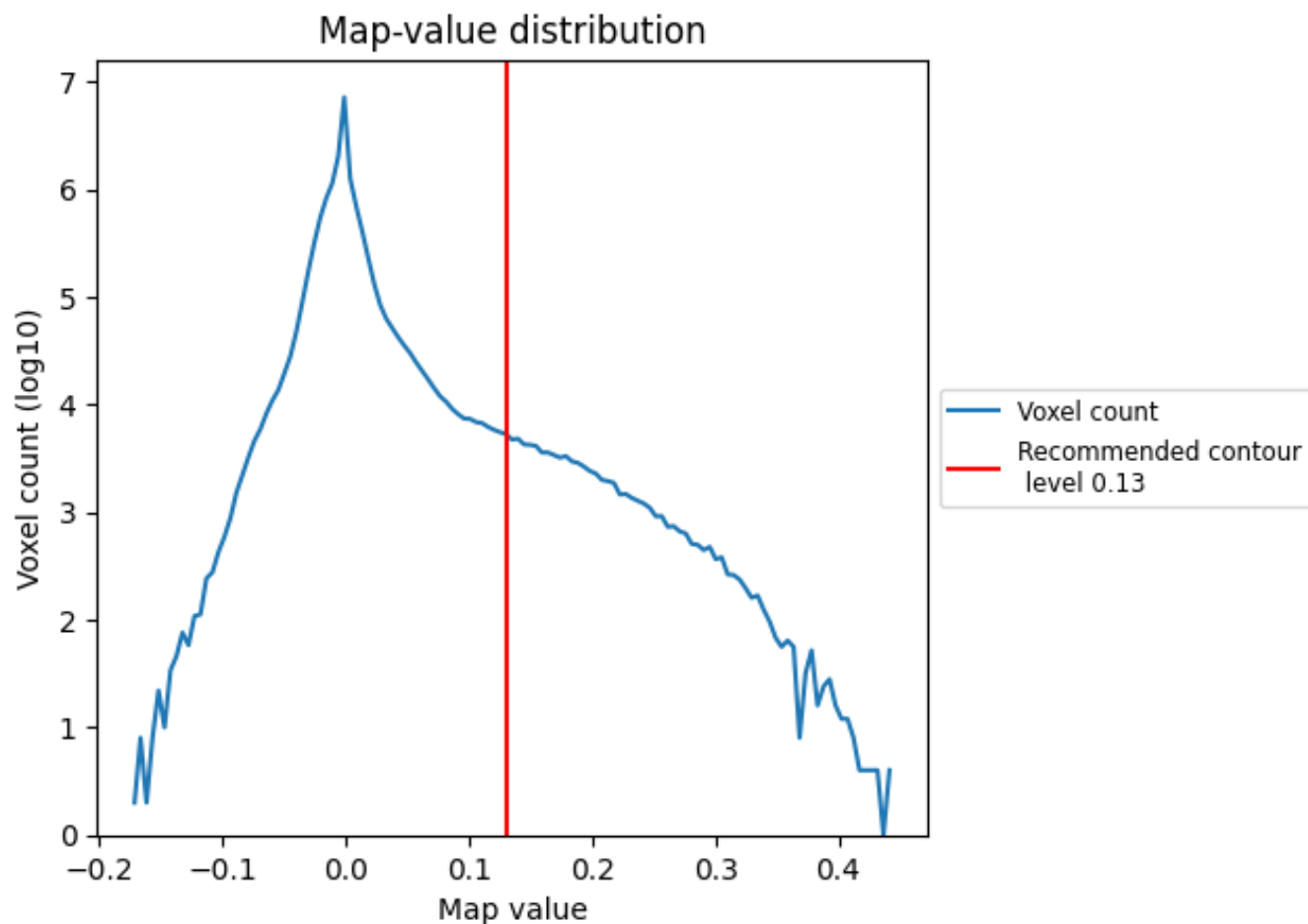
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

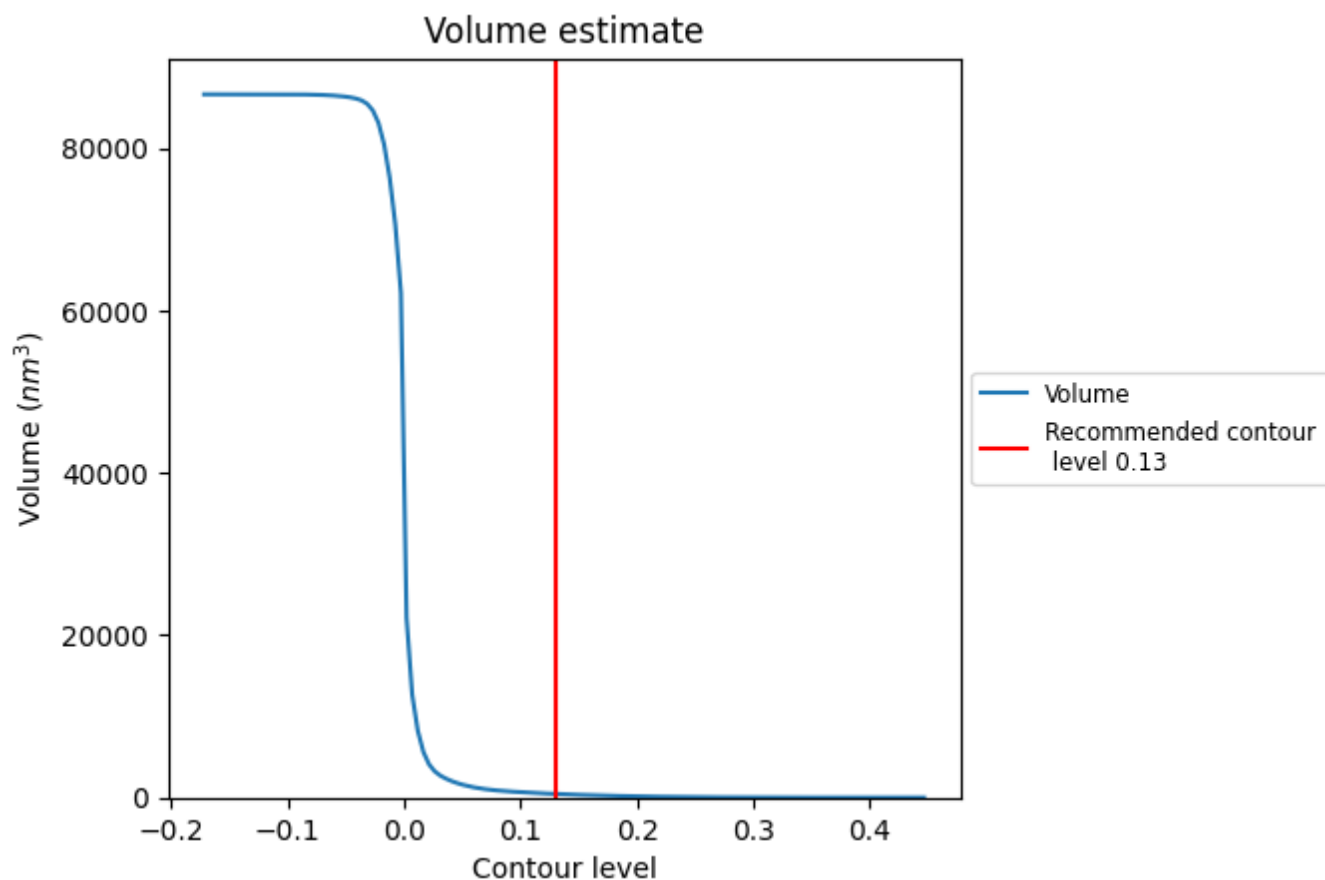
This section contains the results of statistical analysis of the map.

### 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.

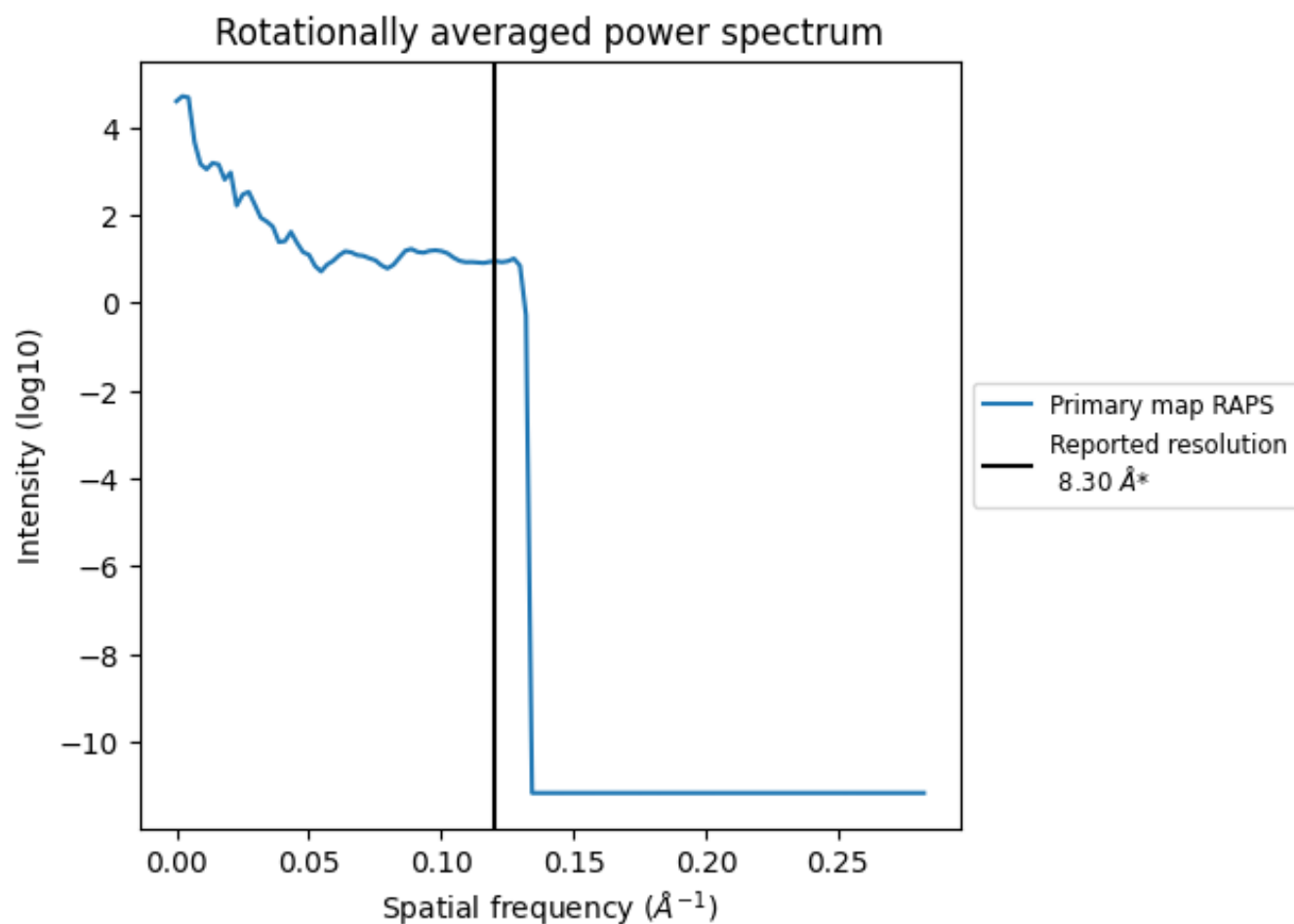
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm<sup>3</sup>; this corresponds to an approximate mass of 404 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  $0.120 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation

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

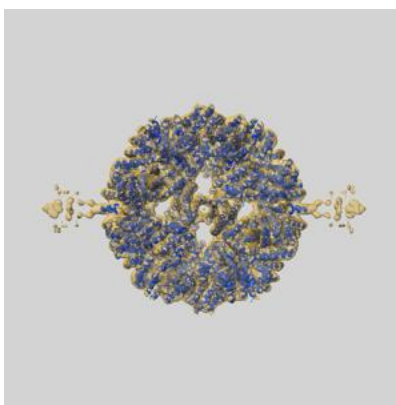
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12676 and PDB model 7O0I. Per-residue inclusion information can be found in section 3 on page 9.

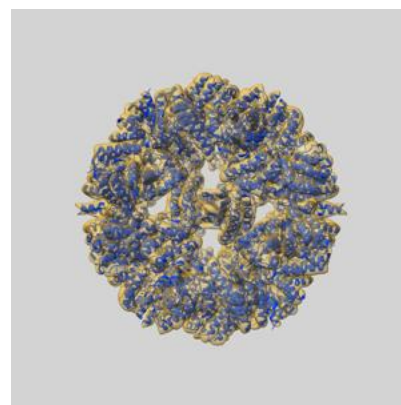
### 9.1 Map-model overlay [i](#)



X



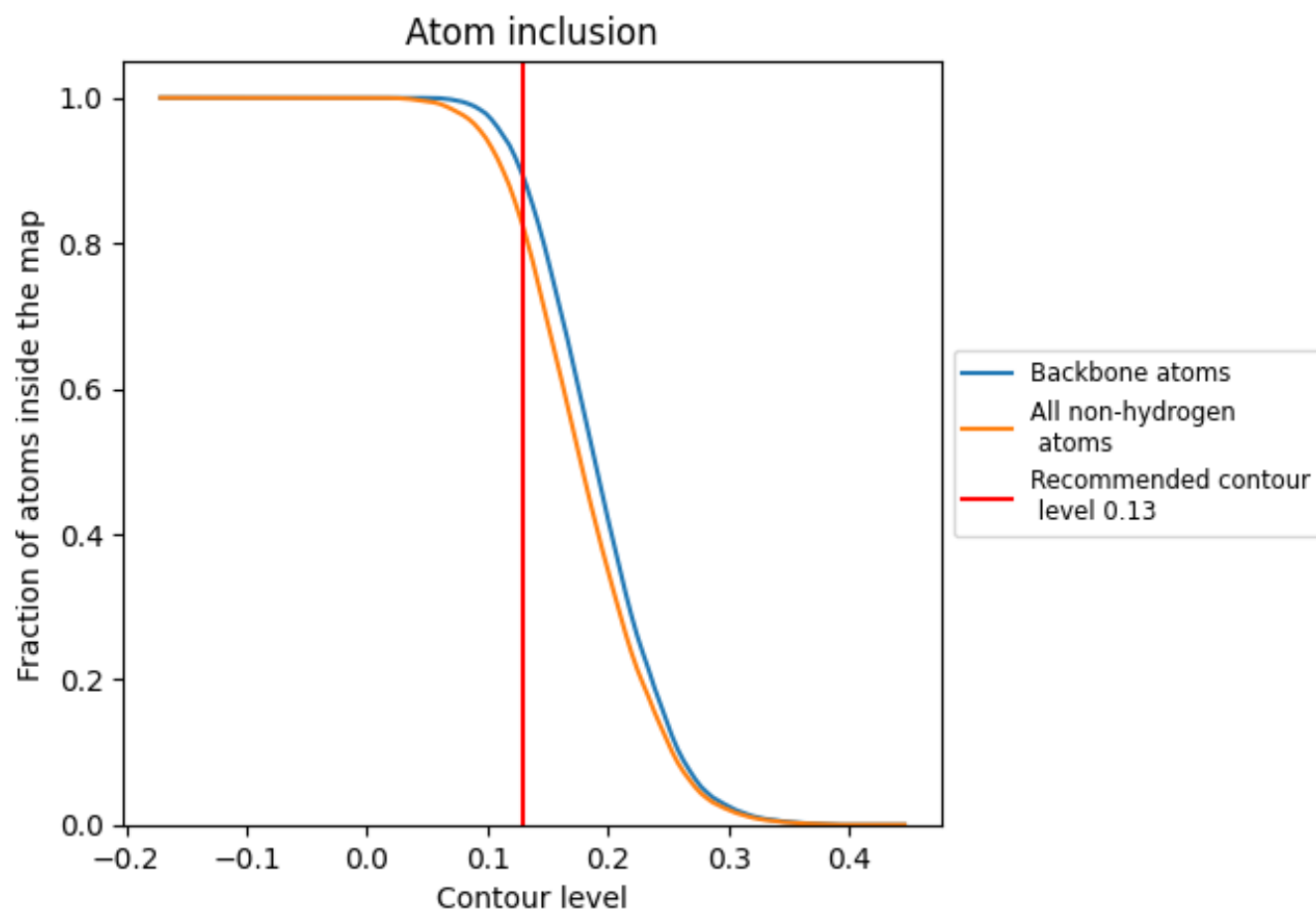
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.