



## wwPDB EM Validation Summary Report i

Sep 18, 2023 – 10:40 am BST

PDB ID : 8ODN  
EMDB ID : EMD-16810  
Title : RcpA-TadD with C13 symmetry from the *Pseudomonas aeruginosa* Tight Adherence Secretion System  
Authors : Tassinari, M.; Low, H.H.  
Deposited on : 2023-03-09  
Resolution : 2.70 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

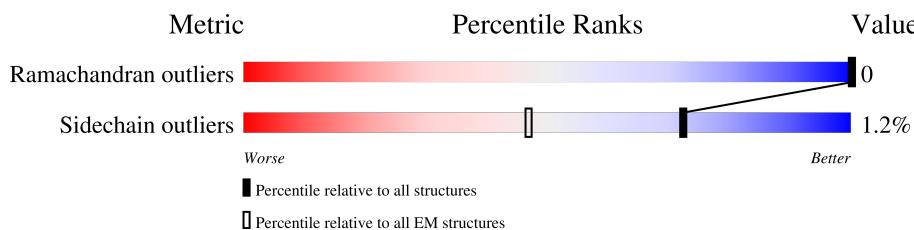
EMDB validation analysis : 0.0.1.dev50  
MolProbit : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

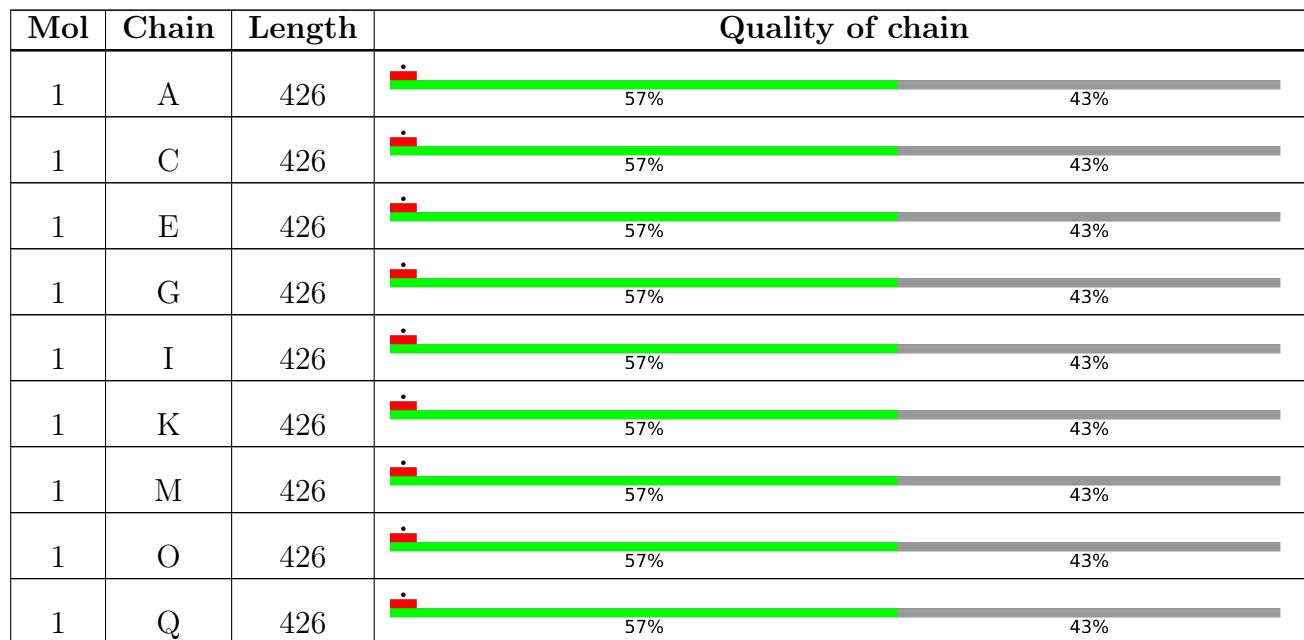
The reported resolution of this entry is 2.70 Å.

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.



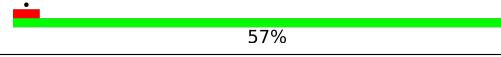
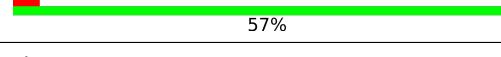
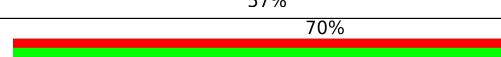
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.



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Mol	Chain	Length	Quality of chain		
1	S	426		57%	43%
1	V	426		57%	43%
1	X	426		57%	43%
1	Z	426		57%	43%
2	B	255		70%	71%
2	D	255		70%	71%
2	F	255		69%	71%
2	H	255		70%	71%
2	J	255		70%	71%
2	L	255		70%	71%
2	N	255		70%	71%
2	P	255		69%	71%
2	R	255		70%	71%
2	T	255		71%	71%
2	W	255		69%	71%
2	Y	255		70%	71%
2	a	255		70%	71%

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 85033 atoms, of which 42445 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 RcpA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	C	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	E	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	G	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	I	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	K	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	M	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	O	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	Q	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	S	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	V	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	X	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		
1	Z	244	Total	C	H	N	O	S	0	0
			3640	1153	1822	313	347	5		

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	SER	-	expression tag	UNP Q9HW96
A	418	ALA	-	expression tag	UNP Q9HW96
A	419	TRP	-	expression tag	UNP Q9HW96
A	420	SER	-	expression tag	UNP Q9HW96

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Chain	Residue	Modelled	Actual	Comment	Reference
A	421	HIS	-	expression tag	UNP Q9HW96
A	422	PRO	-	expression tag	UNP Q9HW96
A	423	GLN	-	expression tag	UNP Q9HW96
A	424	PHE	-	expression tag	UNP Q9HW96
A	425	GLU	-	expression tag	UNP Q9HW96
A	426	LYS	-	expression tag	UNP Q9HW96
C	417	SER	-	expression tag	UNP Q9HW96
C	418	ALA	-	expression tag	UNP Q9HW96
C	419	TRP	-	expression tag	UNP Q9HW96
C	420	SER	-	expression tag	UNP Q9HW96
C	421	HIS	-	expression tag	UNP Q9HW96
C	422	PRO	-	expression tag	UNP Q9HW96
C	423	GLN	-	expression tag	UNP Q9HW96
C	424	PHE	-	expression tag	UNP Q9HW96
C	425	GLU	-	expression tag	UNP Q9HW96
C	426	LYS	-	expression tag	UNP Q9HW96
E	417	SER	-	expression tag	UNP Q9HW96
E	418	ALA	-	expression tag	UNP Q9HW96
E	419	TRP	-	expression tag	UNP Q9HW96
E	420	SER	-	expression tag	UNP Q9HW96
E	421	HIS	-	expression tag	UNP Q9HW96
E	422	PRO	-	expression tag	UNP Q9HW96
E	423	GLN	-	expression tag	UNP Q9HW96
E	424	PHE	-	expression tag	UNP Q9HW96
E	425	GLU	-	expression tag	UNP Q9HW96
E	426	LYS	-	expression tag	UNP Q9HW96
G	417	SER	-	expression tag	UNP Q9HW96
G	418	ALA	-	expression tag	UNP Q9HW96
G	419	TRP	-	expression tag	UNP Q9HW96
G	420	SER	-	expression tag	UNP Q9HW96
G	421	HIS	-	expression tag	UNP Q9HW96
G	422	PRO	-	expression tag	UNP Q9HW96
G	423	GLN	-	expression tag	UNP Q9HW96
G	424	PHE	-	expression tag	UNP Q9HW96
G	425	GLU	-	expression tag	UNP Q9HW96
G	426	LYS	-	expression tag	UNP Q9HW96
I	417	SER	-	expression tag	UNP Q9HW96
I	418	ALA	-	expression tag	UNP Q9HW96
I	419	TRP	-	expression tag	UNP Q9HW96
I	420	SER	-	expression tag	UNP Q9HW96
I	421	HIS	-	expression tag	UNP Q9HW96
I	422	PRO	-	expression tag	UNP Q9HW96

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Chain	Residue	Modelled	Actual	Comment	Reference
I	423	GLN	-	expression tag	UNP Q9HW96
I	424	PHE	-	expression tag	UNP Q9HW96
I	425	GLU	-	expression tag	UNP Q9HW96
I	426	LYS	-	expression tag	UNP Q9HW96
K	417	SER	-	expression tag	UNP Q9HW96
K	418	ALA	-	expression tag	UNP Q9HW96
K	419	TRP	-	expression tag	UNP Q9HW96
K	420	SER	-	expression tag	UNP Q9HW96
K	421	HIS	-	expression tag	UNP Q9HW96
K	422	PRO	-	expression tag	UNP Q9HW96
K	423	GLN	-	expression tag	UNP Q9HW96
K	424	PHE	-	expression tag	UNP Q9HW96
K	425	GLU	-	expression tag	UNP Q9HW96
K	426	LYS	-	expression tag	UNP Q9HW96
M	417	SER	-	expression tag	UNP Q9HW96
M	418	ALA	-	expression tag	UNP Q9HW96
M	419	TRP	-	expression tag	UNP Q9HW96
M	420	SER	-	expression tag	UNP Q9HW96
M	421	HIS	-	expression tag	UNP Q9HW96
M	422	PRO	-	expression tag	UNP Q9HW96
M	423	GLN	-	expression tag	UNP Q9HW96
M	424	PHE	-	expression tag	UNP Q9HW96
M	425	GLU	-	expression tag	UNP Q9HW96
M	426	LYS	-	expression tag	UNP Q9HW96
O	417	SER	-	expression tag	UNP Q9HW96
O	418	ALA	-	expression tag	UNP Q9HW96
O	419	TRP	-	expression tag	UNP Q9HW96
O	420	SER	-	expression tag	UNP Q9HW96
O	421	HIS	-	expression tag	UNP Q9HW96
O	422	PRO	-	expression tag	UNP Q9HW96
O	423	GLN	-	expression tag	UNP Q9HW96
O	424	PHE	-	expression tag	UNP Q9HW96
O	425	GLU	-	expression tag	UNP Q9HW96
O	426	LYS	-	expression tag	UNP Q9HW96
Q	417	SER	-	expression tag	UNP Q9HW96
Q	418	ALA	-	expression tag	UNP Q9HW96
Q	419	TRP	-	expression tag	UNP Q9HW96
Q	420	SER	-	expression tag	UNP Q9HW96
Q	421	HIS	-	expression tag	UNP Q9HW96
Q	422	PRO	-	expression tag	UNP Q9HW96
Q	423	GLN	-	expression tag	UNP Q9HW96
Q	424	PHE	-	expression tag	UNP Q9HW96

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	425	GLU	-	expression tag	UNP Q9HW96
Q	426	LYS	-	expression tag	UNP Q9HW96
S	417	SER	-	expression tag	UNP Q9HW96
S	418	ALA	-	expression tag	UNP Q9HW96
S	419	TRP	-	expression tag	UNP Q9HW96
S	420	SER	-	expression tag	UNP Q9HW96
S	421	HIS	-	expression tag	UNP Q9HW96
S	422	PRO	-	expression tag	UNP Q9HW96
S	423	GLN	-	expression tag	UNP Q9HW96
S	424	PHE	-	expression tag	UNP Q9HW96
S	425	GLU	-	expression tag	UNP Q9HW96
S	426	LYS	-	expression tag	UNP Q9HW96
V	417	SER	-	expression tag	UNP Q9HW96
V	418	ALA	-	expression tag	UNP Q9HW96
V	419	TRP	-	expression tag	UNP Q9HW96
V	420	SER	-	expression tag	UNP Q9HW96
V	421	HIS	-	expression tag	UNP Q9HW96
V	422	PRO	-	expression tag	UNP Q9HW96
V	423	GLN	-	expression tag	UNP Q9HW96
V	424	PHE	-	expression tag	UNP Q9HW96
V	425	GLU	-	expression tag	UNP Q9HW96
V	426	LYS	-	expression tag	UNP Q9HW96
X	417	SER	-	expression tag	UNP Q9HW96
X	418	ALA	-	expression tag	UNP Q9HW96
X	419	TRP	-	expression tag	UNP Q9HW96
X	420	SER	-	expression tag	UNP Q9HW96
X	421	HIS	-	expression tag	UNP Q9HW96
X	422	PRO	-	expression tag	UNP Q9HW96
X	423	GLN	-	expression tag	UNP Q9HW96
X	424	PHE	-	expression tag	UNP Q9HW96
X	425	GLU	-	expression tag	UNP Q9HW96
X	426	LYS	-	expression tag	UNP Q9HW96
Z	417	SER	-	expression tag	UNP Q9HW96
Z	418	ALA	-	expression tag	UNP Q9HW96
Z	419	TRP	-	expression tag	UNP Q9HW96
Z	420	SER	-	expression tag	UNP Q9HW96
Z	421	HIS	-	expression tag	UNP Q9HW96
Z	422	PRO	-	expression tag	UNP Q9HW96
Z	423	GLN	-	expression tag	UNP Q9HW96
Z	424	PHE	-	expression tag	UNP Q9HW96
Z	425	GLU	-	expression tag	UNP Q9HW96
Z	426	LYS	-	expression tag	UNP Q9HW96

- Molecule 2 is a protein called TPR repeat-containing protein PA4299.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	D	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	F	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	H	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	J	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	L	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	N	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	P	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	R	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	T	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	W	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	Y	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		
2	a	185	Total	C	H	N	O	S	0	0
			2901	895	1443	289	268	6		

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	246	GLY	-	expression tag	UNP Q9HWA1
B	247	SER	-	expression tag	UNP Q9HWA1
B	248	ASP	-	expression tag	UNP Q9HWA1
B	249	TYR	-	expression tag	UNP Q9HWA1
B	250	LYS	-	expression tag	UNP Q9HWA1
B	251	ASP	-	expression tag	UNP Q9HWA1
B	252	ASP	-	expression tag	UNP Q9HWA1
B	253	ASP	-	expression tag	UNP Q9HWA1
B	254	ASP	-	expression tag	UNP Q9HWA1
B	255	LYS	-	expression tag	UNP Q9HWA1
D	246	GLY	-	expression tag	UNP Q9HWA1
D	247	SER	-	expression tag	UNP Q9HWA1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	248	ASP	-	expression tag	UNP Q9HWA1
D	249	TYR	-	expression tag	UNP Q9HWA1
D	250	LYS	-	expression tag	UNP Q9HWA1
D	251	ASP	-	expression tag	UNP Q9HWA1
D	252	ASP	-	expression tag	UNP Q9HWA1
D	253	ASP	-	expression tag	UNP Q9HWA1
D	254	ASP	-	expression tag	UNP Q9HWA1
D	255	LYS	-	expression tag	UNP Q9HWA1
F	246	GLY	-	expression tag	UNP Q9HWA1
F	247	SER	-	expression tag	UNP Q9HWA1
F	248	ASP	-	expression tag	UNP Q9HWA1
F	249	TYR	-	expression tag	UNP Q9HWA1
F	250	LYS	-	expression tag	UNP Q9HWA1
F	251	ASP	-	expression tag	UNP Q9HWA1
F	252	ASP	-	expression tag	UNP Q9HWA1
F	253	ASP	-	expression tag	UNP Q9HWA1
F	254	ASP	-	expression tag	UNP Q9HWA1
F	255	LYS	-	expression tag	UNP Q9HWA1
H	246	GLY	-	expression tag	UNP Q9HWA1
H	247	SER	-	expression tag	UNP Q9HWA1
H	248	ASP	-	expression tag	UNP Q9HWA1
H	249	TYR	-	expression tag	UNP Q9HWA1
H	250	LYS	-	expression tag	UNP Q9HWA1
H	251	ASP	-	expression tag	UNP Q9HWA1
H	252	ASP	-	expression tag	UNP Q9HWA1
H	253	ASP	-	expression tag	UNP Q9HWA1
H	254	ASP	-	expression tag	UNP Q9HWA1
H	255	LYS	-	expression tag	UNP Q9HWA1
J	246	GLY	-	expression tag	UNP Q9HWA1
J	247	SER	-	expression tag	UNP Q9HWA1
J	248	ASP	-	expression tag	UNP Q9HWA1
J	249	TYR	-	expression tag	UNP Q9HWA1
J	250	LYS	-	expression tag	UNP Q9HWA1
J	251	ASP	-	expression tag	UNP Q9HWA1
J	252	ASP	-	expression tag	UNP Q9HWA1
J	253	ASP	-	expression tag	UNP Q9HWA1
J	254	ASP	-	expression tag	UNP Q9HWA1
J	255	LYS	-	expression tag	UNP Q9HWA1
L	246	GLY	-	expression tag	UNP Q9HWA1
L	247	SER	-	expression tag	UNP Q9HWA1
L	248	ASP	-	expression tag	UNP Q9HWA1
L	249	TYR	-	expression tag	UNP Q9HWA1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	250	LYS	-	expression tag	UNP Q9HWA1
L	251	ASP	-	expression tag	UNP Q9HWA1
L	252	ASP	-	expression tag	UNP Q9HWA1
L	253	ASP	-	expression tag	UNP Q9HWA1
L	254	ASP	-	expression tag	UNP Q9HWA1
L	255	LYS	-	expression tag	UNP Q9HWA1
N	246	GLY	-	expression tag	UNP Q9HWA1
N	247	SER	-	expression tag	UNP Q9HWA1
N	248	ASP	-	expression tag	UNP Q9HWA1
N	249	TYR	-	expression tag	UNP Q9HWA1
N	250	LYS	-	expression tag	UNP Q9HWA1
N	251	ASP	-	expression tag	UNP Q9HWA1
N	252	ASP	-	expression tag	UNP Q9HWA1
N	253	ASP	-	expression tag	UNP Q9HWA1
N	254	ASP	-	expression tag	UNP Q9HWA1
N	255	LYS	-	expression tag	UNP Q9HWA1
P	246	GLY	-	expression tag	UNP Q9HWA1
P	247	SER	-	expression tag	UNP Q9HWA1
P	248	ASP	-	expression tag	UNP Q9HWA1
P	249	TYR	-	expression tag	UNP Q9HWA1
P	250	LYS	-	expression tag	UNP Q9HWA1
P	251	ASP	-	expression tag	UNP Q9HWA1
P	252	ASP	-	expression tag	UNP Q9HWA1
P	253	ASP	-	expression tag	UNP Q9HWA1
P	254	ASP	-	expression tag	UNP Q9HWA1
P	255	LYS	-	expression tag	UNP Q9HWA1
R	246	GLY	-	expression tag	UNP Q9HWA1
R	247	SER	-	expression tag	UNP Q9HWA1
R	248	ASP	-	expression tag	UNP Q9HWA1
R	249	TYR	-	expression tag	UNP Q9HWA1
R	250	LYS	-	expression tag	UNP Q9HWA1
R	251	ASP	-	expression tag	UNP Q9HWA1
R	252	ASP	-	expression tag	UNP Q9HWA1
R	253	ASP	-	expression tag	UNP Q9HWA1
R	254	ASP	-	expression tag	UNP Q9HWA1
R	255	LYS	-	expression tag	UNP Q9HWA1
T	246	GLY	-	expression tag	UNP Q9HWA1
T	247	SER	-	expression tag	UNP Q9HWA1
T	248	ASP	-	expression tag	UNP Q9HWA1
T	249	TYR	-	expression tag	UNP Q9HWA1
T	250	LYS	-	expression tag	UNP Q9HWA1
T	251	ASP	-	expression tag	UNP Q9HWA1

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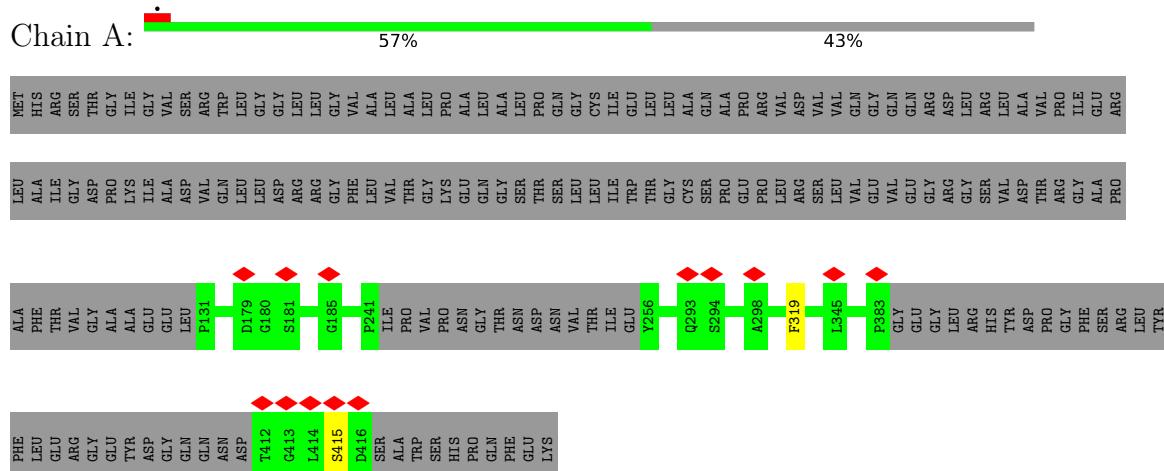
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Chain	Residue	Modelled	Actual	Comment	Reference
T	252	ASP	-	expression tag	UNP Q9HWA1
T	253	ASP	-	expression tag	UNP Q9HWA1
T	254	ASP	-	expression tag	UNP Q9HWA1
T	255	LYS	-	expression tag	UNP Q9HWA1
W	246	GLY	-	expression tag	UNP Q9HWA1
W	247	SER	-	expression tag	UNP Q9HWA1
W	248	ASP	-	expression tag	UNP Q9HWA1
W	249	TYR	-	expression tag	UNP Q9HWA1
W	250	LYS	-	expression tag	UNP Q9HWA1
W	251	ASP	-	expression tag	UNP Q9HWA1
W	252	ASP	-	expression tag	UNP Q9HWA1
W	253	ASP	-	expression tag	UNP Q9HWA1
W	254	ASP	-	expression tag	UNP Q9HWA1
W	255	LYS	-	expression tag	UNP Q9HWA1
Y	246	GLY	-	expression tag	UNP Q9HWA1
Y	247	SER	-	expression tag	UNP Q9HWA1
Y	248	ASP	-	expression tag	UNP Q9HWA1
Y	249	TYR	-	expression tag	UNP Q9HWA1
Y	250	LYS	-	expression tag	UNP Q9HWA1
Y	251	ASP	-	expression tag	UNP Q9HWA1
Y	252	ASP	-	expression tag	UNP Q9HWA1
Y	253	ASP	-	expression tag	UNP Q9HWA1
Y	254	ASP	-	expression tag	UNP Q9HWA1
Y	255	LYS	-	expression tag	UNP Q9HWA1
a	246	GLY	-	expression tag	UNP Q9HWA1
a	247	SER	-	expression tag	UNP Q9HWA1
a	248	ASP	-	expression tag	UNP Q9HWA1
a	249	TYR	-	expression tag	UNP Q9HWA1
a	250	LYS	-	expression tag	UNP Q9HWA1
a	251	ASP	-	expression tag	UNP Q9HWA1
a	252	ASP	-	expression tag	UNP Q9HWA1
a	253	ASP	-	expression tag	UNP Q9HWA1
a	254	ASP	-	expression tag	UNP Q9HWA1
a	255	LYS	-	expression tag	UNP Q9HWA1

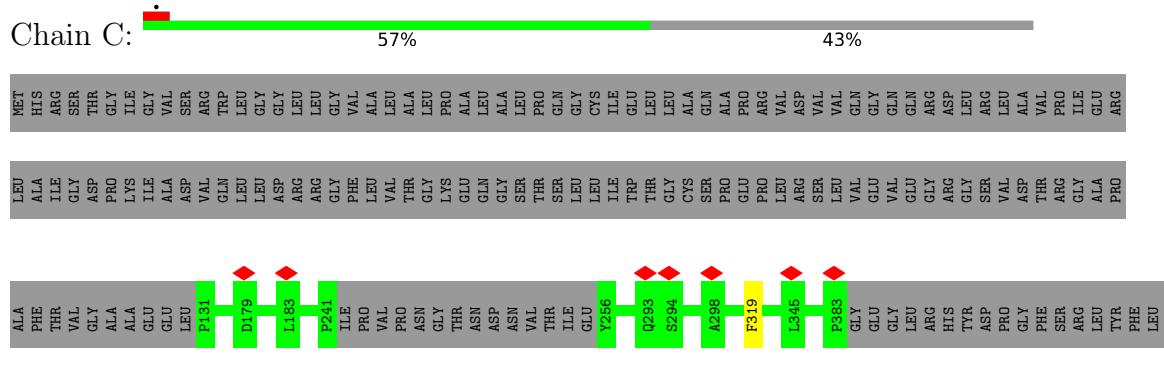
### 3 Residue-property plots [\(i\)](#)

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.

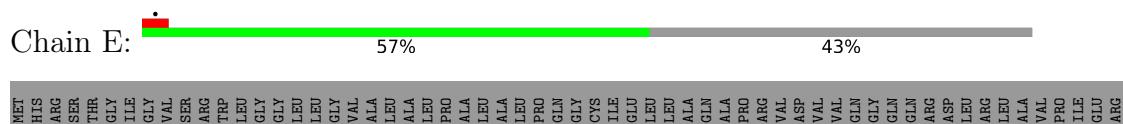
- Molecule 1: RcpA

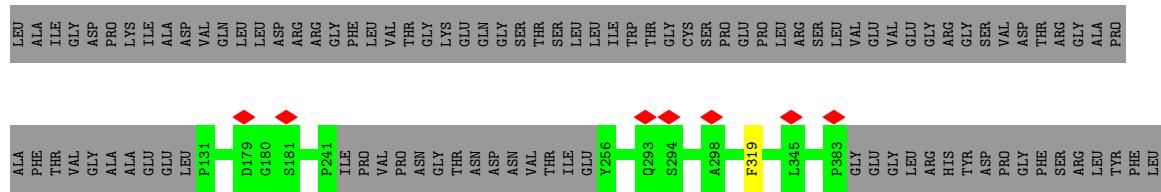


- Molecule 1: RcpA



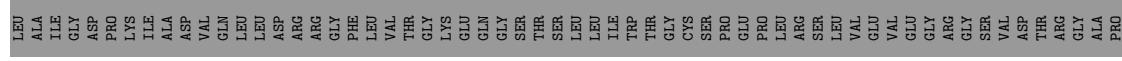
- Molecule 1: RcpA





- Molecule 1: RcpA

Chain G:  57% 43%

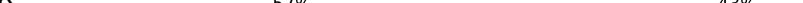


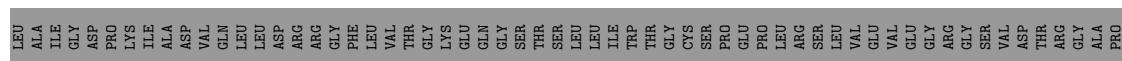
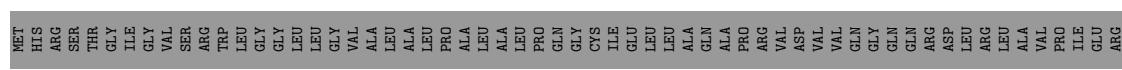
- Molecule 1: RcpA

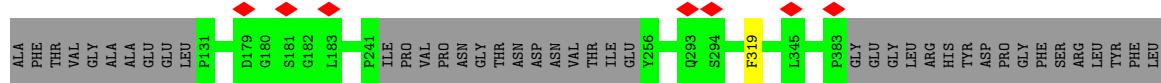
Chain I:  57% 43%



- Molecule 1: RcpA

Chain K:  57% 43%

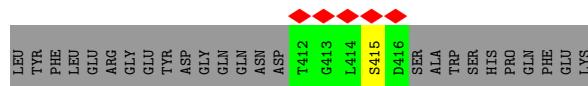
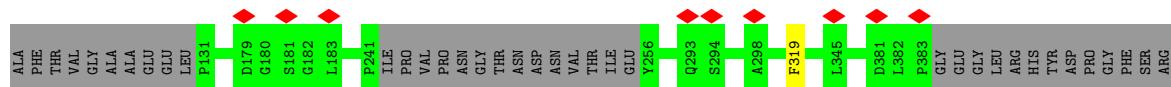
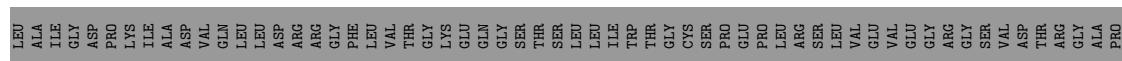
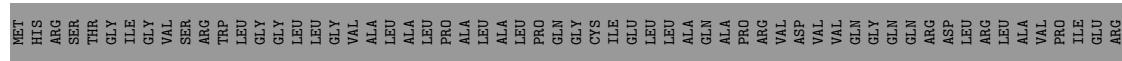




- Molecule 1: RcpA

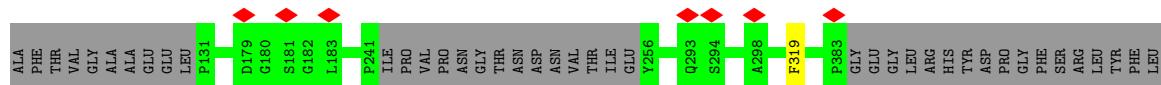
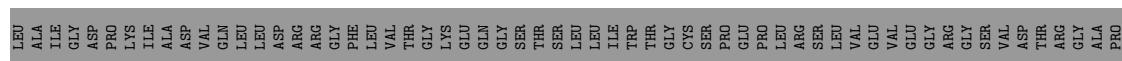
Chain M: 57% 43%

A horizontal progress bar for 'Chain M'. The bar is divided into two segments: a green segment representing 57% completion and a grey segment representing 43% completion. The percentage values are displayed in white text inside their respective segments.



- Molecule 1: RcpA

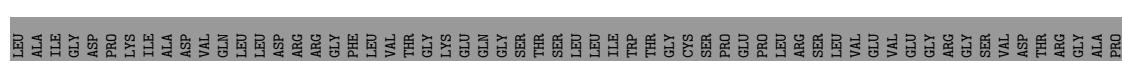
Chain O:  57% 43%



- Molecule 1: RcpA

Chain Q: 57% 43%

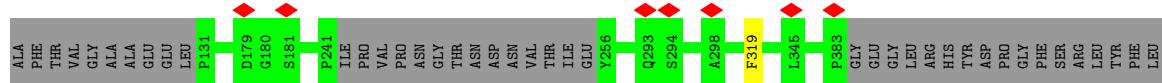
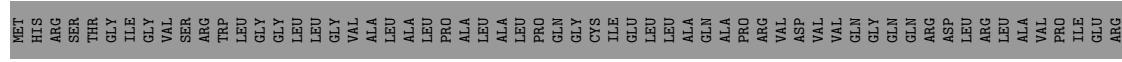
A horizontal progress bar for 'Chain Q'. The bar is green and spans most of the width of the container. A red dot is positioned near the left end of the bar. To the right of the bar, the text '57%' is displayed above the number '43%', indicating the completion percentage.





- Molecule 1: RcpA

Chain S:  57% 43%



- Molecule 1: RcpA

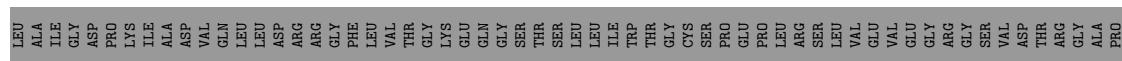
A horizontal progress bar representing the completion of Chain V. The bar is divided into three segments: a small red segment on the left, a long green segment in the middle labeled '57%', and a grey segment on the right labeled '43%'. The total length of the bar is approximately 80%.

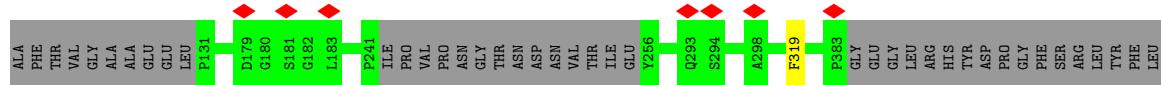


- Molecule 1: RcpA

Chain X: 57% 43%

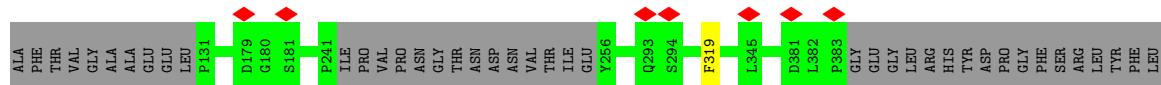
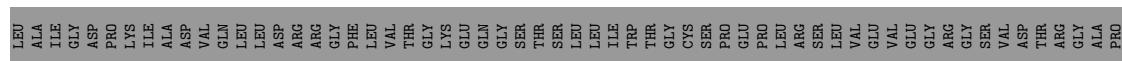
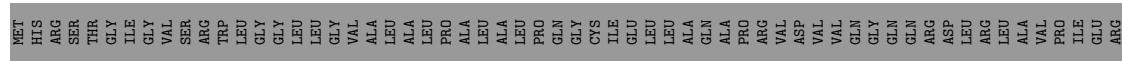
A horizontal progress bar for 'Chain X'. The bar is mostly grey, with a green segment representing 57% completion. A red segment is at the far left end. To the right of the bar, '57%' is written above the grey part, and '43%' is written below the grey part.





- Molecule 1: RcpA

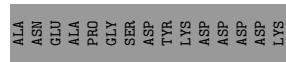
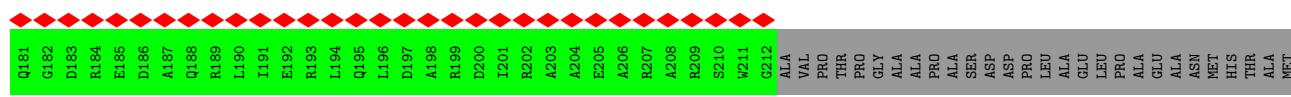
Chain Z:  57% 43%



- Molecule 2: TPR repeat-containing protein PA4299

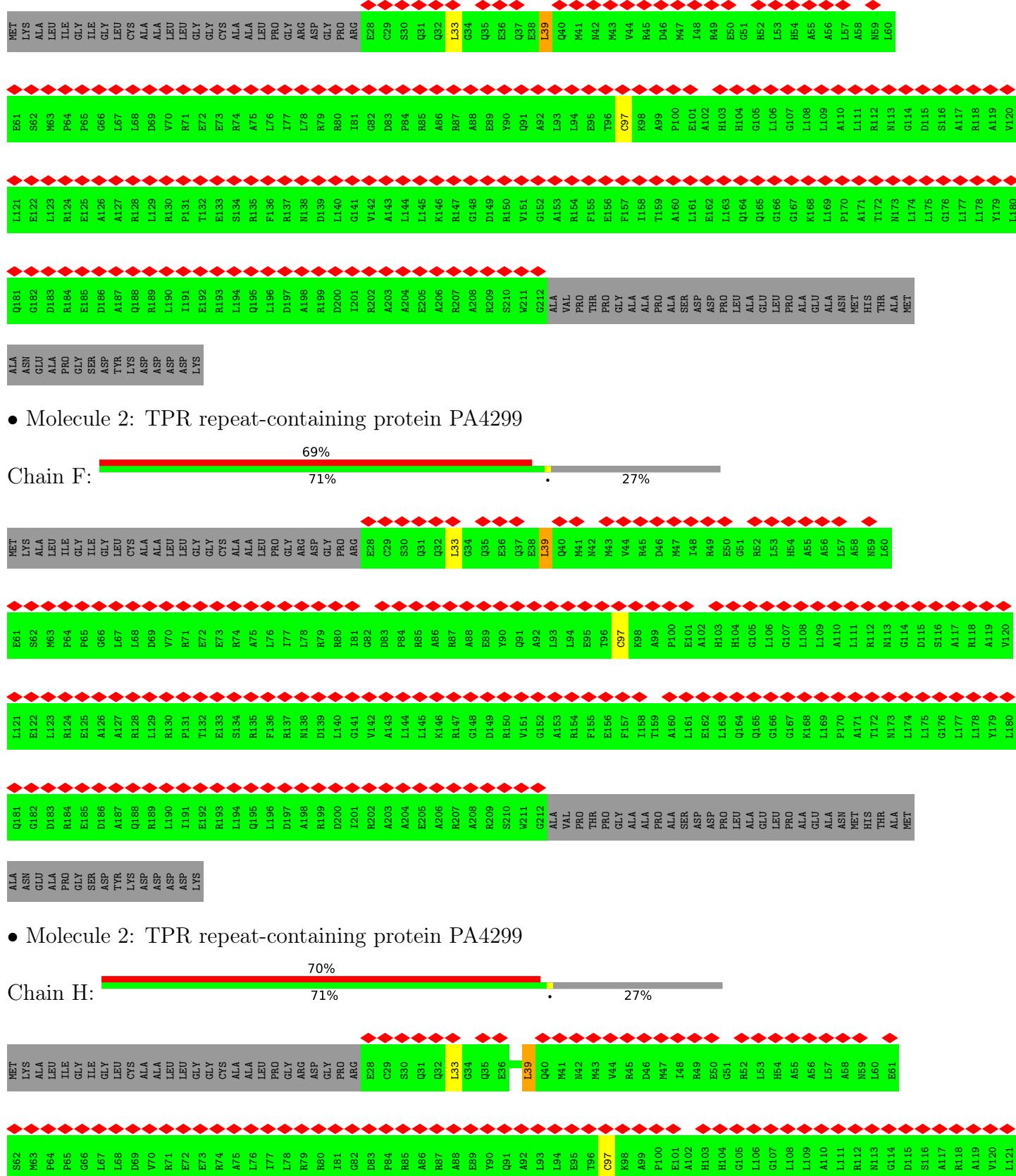
A horizontal bar chart comparing the percentage of Chain B across three categories. The categories are represented by colored bars: red, green, and grey. The red bar reaches 70%, the green bar reaches 71%, and the grey bar reaches 27%. The bars are positioned side-by-side, with their respective percentages labeled above them.

Category	Percentage
Red	70%
Green	71%
Grey	27%



- Molecule 2: TPR repeat-containing protein PA4299

Chain D: 71% : 27%



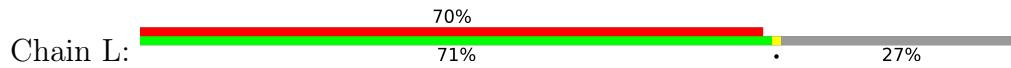
- Molecule 2: TPR repeat-containing protein PA4299



E61	S62	M63	P64	P65	G66	L67	L68	D69	V70	R71	E72	T73	R74	R75	R76	I77	L78	R79	R80	I81	G82	D83	P84	R85	A86	B87	A88	E89	Y90	Q91	A92	L93	I94	E95	T96	C97	K98	A99	P100	E101	A102	H103	H104	L105	L106	G107	L108	L109	A110	L111	L112	N113	G114	D115	S116	A117	R118	A119	V120
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L121 E152 E152 L123 R124 E126 A126 A127 R128 L129 R130 F131 T132 E133 S134 R135 F136 R137 N138 D139 L140 G141 V142 A143 L144 L145 K146 R147 D149 R150 V151 G152 A153 R154 F155 E156 F157 I158 T159 L161 E162 L163 Q164 Q165 C166 C167 K168 L169 P170 A171 T172 M173 L174 L175 G176 L177 L178 Y179 L180

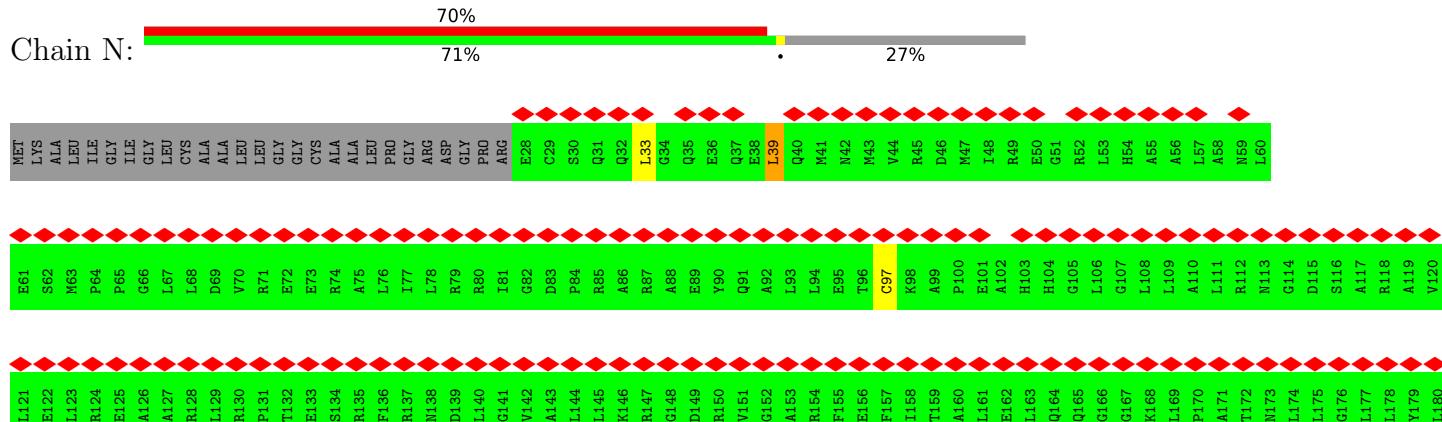
- Molecule 2: TPR repeat-containing protein PA4299



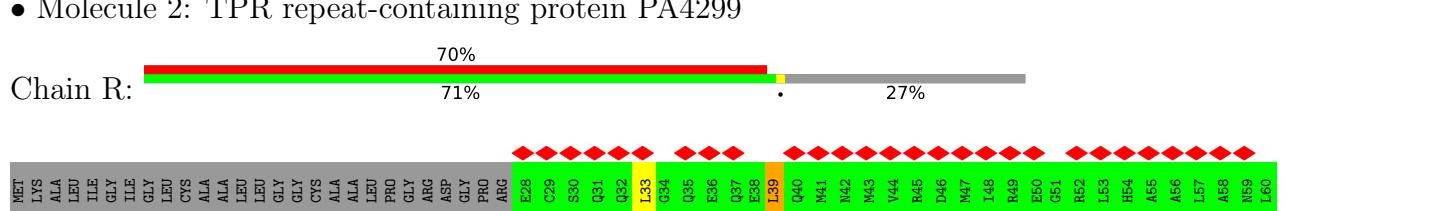
S62	M63	P64	P65	G66	L67	L68	D69	V70	R71	E72	E73	R74	A75	L76	I77	L78	R79	R80	I81	G82	D83	P84	B85	A86	R87	A88	E89	Y90	Q91	A92	L93	L94	E95	T96	C97	K98	A99	P100	E101	A102	H103	H104	G105	L106	G107	L108	L109	A110	L111	R112	M113	G114	D115	S116	A117	R118	A119	V120	L121
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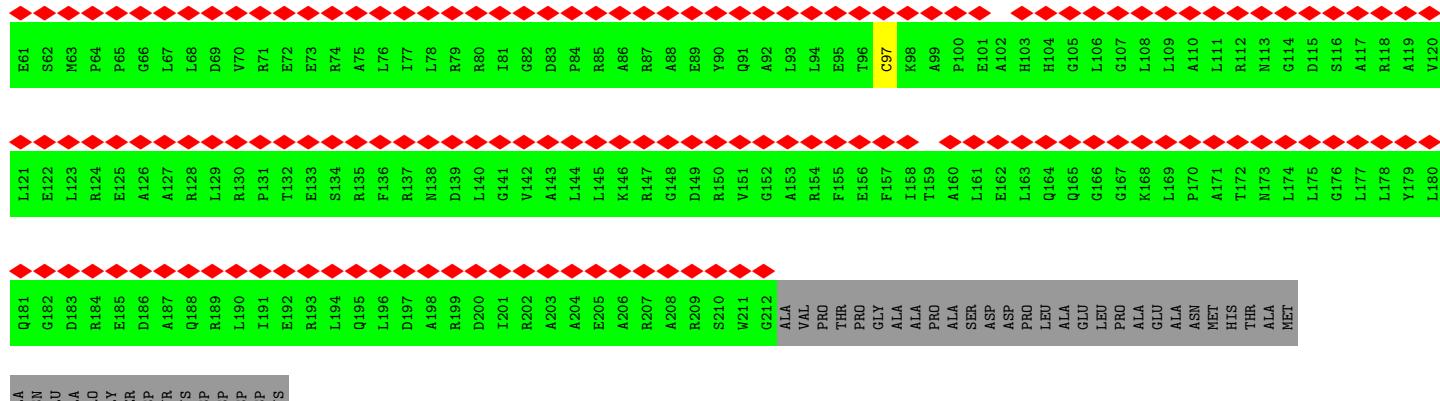
E122	L123	R124	E125	A126	A127	R128	L129	R130	P131	T132	E133	S134	R135	F136	R137	M138	D139	L140	G141	V142	A143	L144	L145	K146	R147	G148	D149	R150	V151	G152	A153	R154	F155	E156	F157	I158	T159	A160	L161	E162	L163	Q164	Q165	G166	G167	K168	L169	P170	A171	T172	N173	L174	L175	G176	L177	L178	Y179	L180	O181
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- Molecule 2: TPR repeat-containing protein PA4299



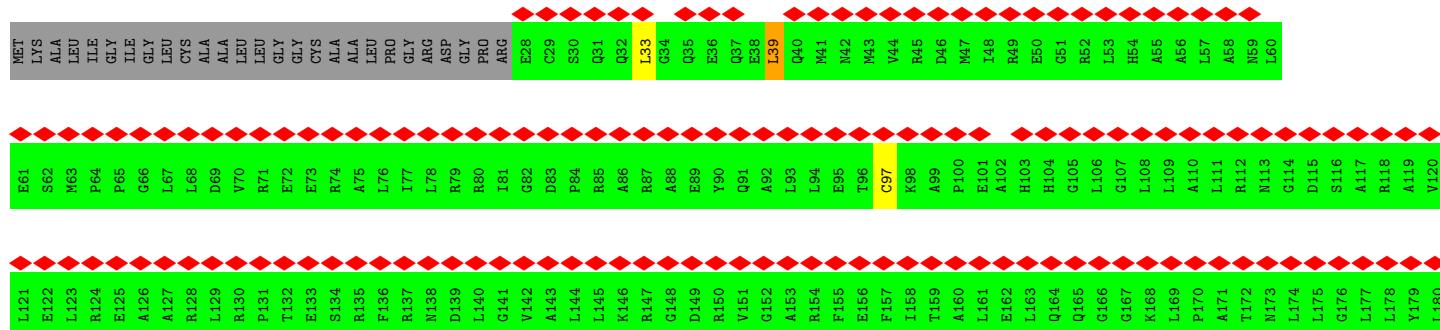
- Molecule 2: TPR repeat-containing protein PA4299





- Molecule 2: TPR repeat-containing protein PA4299

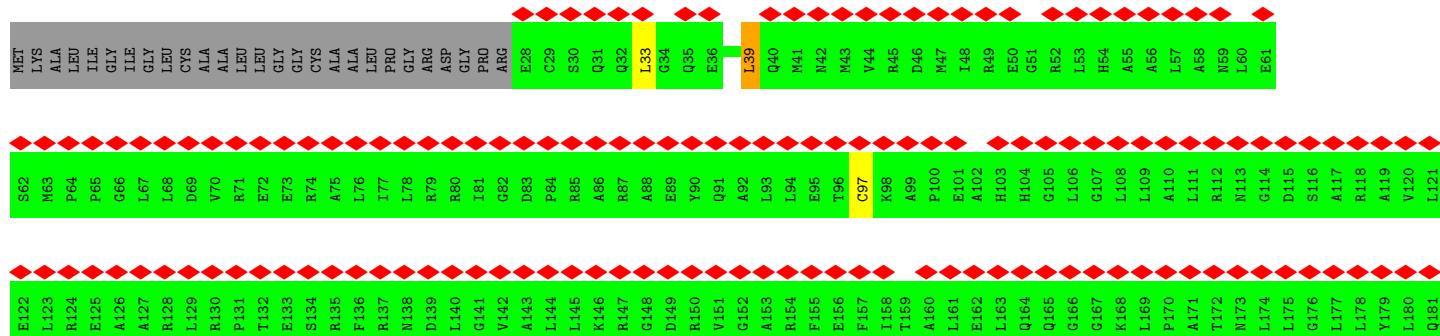
Category	Percentage
Red	71%
Green	71%
Grey	27%



- Molecule 2: TPR repeat-containing protein PA4299

A horizontal bar chart titled "Chain W:" at the top left. The chart consists of three bars of increasing length from left to right. The first bar is red and ends at the 69% mark. The second bar is green and ends at the 71% mark. The third bar is grey and ends at the 27% mark. Each bar has its percentage value labeled above it.

Category	Percentage
Red Bar	69%
Green Bar	71%
Grey Bar	27%



ALA	Q181	L121	E61	G182	S62	S62	S62	MET
ASN	G182	E122	P64	G183	A123	A123	A123	LYS
GLU	D183	L123	P65	E125	A124	R124	R124	GLU
ALA	PRO	R184	R124	E125	G66	R184	P64	ALA
GLY	SER	E185	A125	A126	G67	E185	G65	ALA
ASP	ASP	D186	A126	A127	L67	A126	A126	ALA
TYR	LYS	A187	A127	R128	E72	A187	A127	TYR
ASP	ASP	R188	R128	R129	L68	R188	R128	LYS
ASP	ASP	R189	L129	R130	D69	R189	L129	ASP
ASP	ASP	L190	R135	P131	V70	L190	R130	ASP
ASP	ASP	E192	T132	E72	R71	P131	P131	ASP
LYS	ASP	R193	E133	E73	CYS	R193	E133	ASP
ASP	ASP	L194	S134	H74	CYS	L194	S134	ASP
ASP	ASP	R195	R135	A75	ALA	Q195	R135	ASP
ASP	ASP	D200	L140	R80	ALA	D200	L140	ASP
ASP	ASP	I201	G141	T81	LEU	I201	L140	ASP
ASP	ASP	R202	V142	Q82	PRO	R202	V142	ASP
ASP	ASP	A203	A143	D83	PRO	A203	A143	ASP
ASP	ASP	A204	L144	P84	PRO	A204	L144	ASP
ASP	ASP	E205	L145	R85	PRO	E205	L145	ASP
ASP	ASP	A206	K146	A86	ARG	A206	K146	ASP
ASP	ASP	R207	R147	R87	ARG	R207	R147	ASP
ASP	ASP	A208	G148	A88	ASP	A208	G148	ASP
ASP	ASP	R209	D149	E89	ASP	R209	D149	ASP
ASP	ASP	S210	R150	Y90	ASP	S210	R150	ASP
ASP	ASP	W211	V151	Q91	ASP	W211	V151	ASP
ASP	ASP	G212	G152	A92	ASP	G212	A92	ASP
ASP	ASP	A153	A153	I93	ASP	A153	A153	ASP
VAL	PRO	R154	R154	L94	ASP	R154	R154	ASP
PRO	PRO	F155	D149	E95	ASP	F155	E95	ASP
THR	PRO	E156	E156	T96	ASP	E156	T96	ASP
PRO	PRO	P157	P157	C97	ASP	P157	C97	ASP
PRO	PRO	A158	A158	K98	ASP	A158	K98	ASP
PRO	PRO	T159	T159	A99	ASP	T159	A99	ASP
LEU	LEU	A160	A160	P100	ASP	A160	P100	ASP
ALA	ALA	A161	A161	E101	ASP	A161	E101	ASP
SER	SER	A162	A162	A102	ASP	A162	A102	ASP
ASP	ASP	T163	T163	H103	ASP	T163	H103	ASP
PRO	PRO	L164	L164	H104	ASP	L164	H104	ASP
LEU	LEU	A165	A165	G105	ASP	A165	G105	ASP
GLU	GLU	Q166	Q166	R52	ASP	Q166	R52	ASP
LEU	LEU	G167	G167	G107	ASP	G167	G107	ASP
PRO	PRO	A168	A168	H108	ASP	A168	H108	ASP
ALA	ALA	K169	K169	L109	ASP	K169	L109	ASP
ALA	ALA	A170	A170	A110	ASP	A170	A110	ASP
ASN	ASN	A171	A171	L111	ASP	A171	L111	ASP
MET	MET	H172	H172	R112	ASP	H172	R112	ASP
HIS	HIS	A173	A173	N113	ASP	A173	N113	ASP
THR	THR	M174	M174	G114	ASP	M174	G114	ASP
ALA	ALA	L175	L175	D115	ASP	L175	D115	ASP
MET	MET	G176	G176	S116	ASP	G176	S116	ASP
ALA	ALA	L177	L177	A117	ASP	L177	A117	ASP
ALA	ALA	R118	R118	R118	ASP	R118	R118	ASP
ALA	ALA	Y179	Y179	A119	ASP	Y179	A119	ASP
ALA	ALA	V120	V120	V120	ASP	V120	V120	ASP

- Molecule 2: TPR repeat-containing protein PA4299



ALA	Q181	L121	E61	G182	S62	S62	S62	MET
ASN	G182	E122	P64	G183	A122	R124	R124	LYS
GLU	D183	L123	P65	E125	A123	R124	P64	GLY
ALA	PRO	R184	R124	E125	G66	E125	P65	GLY
GLY	SER	E185	A125	A126	G67	A126	A126	SER
ASP	ASP	D186	A126	A127	L67	A127	A127	ASP
ASP	ASP	A187	A127	R128	E72	A187	A127	ASP
TYR	LYS	R188	R128	R129	L68	R188	R128	ASP
ASP	ASP	R189	L129	R130	D69	R189	L129	ASP
ASP	ASP	L190	R135	P131	V70	L190	R130	ASP
ASP	ASP	E192	T132	E72	R71	P131	P131	ASP
LYS	ASP	R193	E133	E73	CYS	R193	E133	ASP
ASP	ASP	L194	S134	H74	CYS	L194	S134	ASP
ASP	ASP	R195	R135	A75	ALA	Q195	R135	ASP
ASP	ASP	D200	L140	R80	ALA	D200	L140	ASP
ASP	ASP	I201	G141	T81	LEU	I201	L140	ASP
ASP	ASP	R202	V142	Q82	PRO	R202	V142	ASP
ASP	ASP	A203	A143	D83	PRO	A203	A143	ASP
ASP	ASP	A204	L144	P84	PRO	A204	L144	ASP
ASP	ASP	E205	L145	R85	PRO	E205	L145	ASP
ASP	ASP	A206	K146	A86	ARG	A206	K146	ASP
ASP	ASP	R207	R147	R87	ARG	R207	R147	ASP
ASP	ASP	A208	G148	A88	ASP	A208	G148	ASP
ASP	ASP	R209	D149	E89	ASP	R209	D149	ASP
ASP	ASP	S210	R150	Y90	ASP	S210	R150	ASP
ASP	ASP	W211	V151	Q91	ASP	W211	V151	ASP
ASP	ASP	G212	G152	A92	ASP	G212	A92	ASP
ASP	ASP	A153	A153	I93	ASP	A153	A153	ASP
VAL	PRO	R154	R154	L94	ASP	R154	R154	ASP
PRO	PRO	F155	D149	E95	ASP	F155	E95	ASP
THR	PRO	E156	E156	T96	ASP	E156	T96	ASP
PRO	PRO	P157	P157	C97	ASP	P157	C97	ASP
PRO	PRO	A158	A158	K98	ASP	A158	K98	ASP
PRO	PRO	T159	T159	A99	ASP	T159	A99	ASP
LEU	LEU	A160	A160	P100	ASP	A160	P100	ASP
ALA	ALA	A161	A161	E101	ASP	A161	E101	ASP
SER	SER	A162	A162	A102	ASP	A162	A102	ASP
ASP	ASP	T163	T163	H103	ASP	T163	H103	ASP
PRO	PRO	L164	L164	H104	ASP	L164	H104	ASP
LEU	LEU	A165	A165	G105	ASP	A165	G105	ASP
GLU	GLU	Q166	Q166	R52	ASP	Q166	R52	ASP
LEU	LEU	G167	G167	G107	ASP	G167	G107	ASP
PRO	PRO	A168	A168	H108	ASP	A168	H108	ASP
ALA	ALA	K169	K169	L109	ASP	K169	L109	ASP
ALA	ALA	A170	A170	A110	ASP	A170	A110	ASP
ASN	ASN	A171	A171	L111	ASP	A171	L111	ASP
MET	MET	H172	H172	R112	ASP	H172	R112	ASP
HIS	HIS	A173	A173	N113	ASP	A173	N113	ASP
ALA	ALA	R118	R118	R118	ASP	R118	R118	ASP
ALA	ALA	Y179	Y179	A119	ASP	Y179	A119	ASP
ALA	ALA	V120	V120	V120	ASP	V120	V120	ASP

- Molecule 2: TPR repeat-containing protein PA4299



ALA	Q181	L121	E61	G182	S62	S62	S62	MET
ASN	G182	E122	P64	G183	A122	R124	R124	LYS
GLU	D183	L123	P65	E125	A123	R124	P64	GLY
ALA	PRO	R184	R124	E125	G66	E125	P65	GLY
GLY	SER	E185	A125	A126	G67	A126	A126	SER
ASP	ASP	D186	A126	A127	L67	A127	A127	ASP
ASP	ASP	A187	A127	R128	E72	A187	A127	ASP
TYR	LYS	R188	R128	R129	L68	R188	R128	ASP
ASP	ASP	R189	L129	R130	D69	R189	L129	ASP
ASP	ASP	L190	R135	P131	V70	L190	R130	ASP
ASP	ASP	E192	T132	E72	R71	P131	P131	ASP
LYS	ASP	R193	E133	E73	CYS	R193	E133	ASP
ASP	ASP	L194	S134	H74	CYS	L194	S134	ASP
ASP	ASP	R195	R135	A75	ALA	Q195	R135	ASP
ASP	ASP	D200	L140	R80	ALA	D200	L140	ASP
ASP	ASP	I201	G141	T81	LEU	I201	L140	ASP
ASP	ASP	R202	V142	Q82	PRO	R202	V142	ASP
ASP	ASP	A203	A143	D83	PRO	A203	A143	ASP
ASP	ASP	A204	L144	P84	PRO	A204	L144	ASP
ASP	ASP	E205	L145	R85	PRO	E205	L145	ASP
ASP	ASP	A206	K146	A86	ARG	A206	K146	ASP
ASP	ASP	R207	R147	R87	ARG	R207	R147	ASP
ASP	ASP	A208	G148	A88	ASP	A208	G148	ASP
ASP	ASP	R209	D149	E89	ASP	R209	D149	ASP
ASP	ASP	S210	R150	Y90	ASP	S210	R150	ASP
ASP	ASP	W211	V151	Q91	ASP	W211	V151	ASP
ASP	ASP	G212	G152	A92	ASP	G212	A92	ASP
ASP	ASP	A153	A153	I93	ASP	A153	A153	ASP
VAL	PRO	R154	R154	L94	ASP	R154	R154	ASP
PRO	PRO	F155	D149	E95	ASP	F155	E95	ASP
THR	PRO	E156	E156	T96	ASP	E156	T96	ASP
PRO	PRO	P157	P157	C97	ASP	P157	C97	ASP
LEU	LEU	A158	A158	K98	ASP	A158	K98	ASP
PRO	PRO	T159	T159	A99	ASP	T159	A99	ASP
LEU	LEU	A160	A160	P100	E50	A160	P100	E50
ALA	ALA	A161	A161	E101	D46	A161	E101	D46
SER	SER	A162	A162	A102	M47	A162	E102	R49
ASP	ASP	T159	T159	H103	E49	T159	H103	E49
PRO	PRO	L163	L163	H104	E50	L163	H104	E50
LEU	LEU	A164	A164	A104	G51	A164	G	

## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	119534	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.26	0/1852	0.54	1/2506 (0.0%)
1	C	0.26	0/1852	0.54	1/2506 (0.0%)
1	E	0.26	0/1852	0.54	1/2506 (0.0%)
1	G	0.26	0/1852	0.55	1/2506 (0.0%)
1	I	0.26	0/1852	0.54	1/2506 (0.0%)
1	K	0.26	0/1852	0.55	1/2506 (0.0%)
1	M	0.26	0/1852	0.55	1/2506 (0.0%)
1	O	0.26	0/1852	0.54	1/2506 (0.0%)
1	Q	0.26	0/1852	0.54	1/2506 (0.0%)
1	S	0.26	0/1852	0.54	1/2506 (0.0%)
1	V	0.26	0/1852	0.54	1/2506 (0.0%)
1	X	0.26	0/1852	0.54	1/2506 (0.0%)
1	Z	0.26	0/1852	0.54	1/2506 (0.0%)
2	B	0.25	0/1473	0.60	1/1978 (0.1%)
2	D	0.25	0/1473	0.60	1/1978 (0.1%)
2	F	0.25	0/1473	0.60	1/1978 (0.1%)
2	H	0.25	0/1473	0.60	1/1978 (0.1%)
2	J	0.25	0/1473	0.60	1/1978 (0.1%)
2	L	0.25	0/1473	0.60	1/1978 (0.1%)
2	N	0.25	0/1473	0.60	1/1978 (0.1%)
2	P	0.25	0/1473	0.60	1/1978 (0.1%)
2	R	0.25	0/1473	0.60	1/1978 (0.1%)
2	T	0.25	0/1473	0.60	1/1978 (0.1%)
2	W	0.25	0/1473	0.59	1/1978 (0.1%)
2	Y	0.25	0/1473	0.60	1/1978 (0.1%)
2	a	0.25	0/1473	0.60	1/1978 (0.1%)
All	All	0.25	0/43225	0.57	26/58292 (0.0%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	Z	415	SER	C-N-CA	7.17	139.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	415	SER	C-N-CA	7.16	139.61	121.70
1	X	415	SER	C-N-CA	7.16	139.61	121.70
1	A	415	SER	C-N-CA	7.16	139.60	121.70
1	E	415	SER	C-N-CA	7.16	139.60	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	C	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	E	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	G	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	I	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	K	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	M	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	O	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	Q	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	S	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	V	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
1	X	238/426 (56%)	233 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Z	238/426 (56%)	233 (98%)	5 (2%)	0	100 100
2	B	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	D	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	F	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	H	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	J	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	L	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	N	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	P	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	R	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	T	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
2	W	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	Y	183/255 (72%)	177 (97%)	6 (3%)	0	100 100
2	a	183/255 (72%)	178 (97%)	5 (3%)	0	100 100
All	All	5473/8853 (62%)	5337 (98%)	136 (2%)	0	100 100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	C	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	E	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	G	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	I	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	K	196/342 (57%)	195 (100%)	1 (0%)	88 96
1	M	196/342 (57%)	195 (100%)	1 (0%)	88 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	196/342 (57%)	195 (100%)	1 (0%)	88	96
1	Q	196/342 (57%)	195 (100%)	1 (0%)	88	96
1	S	196/342 (57%)	195 (100%)	1 (0%)	88	96
1	V	196/342 (57%)	195 (100%)	1 (0%)	88	96
1	X	196/342 (57%)	195 (100%)	1 (0%)	88	96
1	Z	196/342 (57%)	195 (100%)	1 (0%)	88	96
2	B	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	D	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	F	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	H	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	J	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	L	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	N	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	P	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	R	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	T	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	W	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	Y	146/193 (76%)	143 (98%)	3 (2%)	53	80
2	a	146/193 (76%)	143 (98%)	3 (2%)	53	80
All	All	4446/6955 (64%)	4394 (99%)	52 (1%)	72	88

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	319	PHE
2	R	97	CYS
2	a	33	LEU
2	P	33	LEU
1	Q	319	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	173	ASN

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Mol	Chain	Res	Type
1	S	133	GLN
2	a	173	ASN
2	R	173	ASN
2	T	173	ASN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

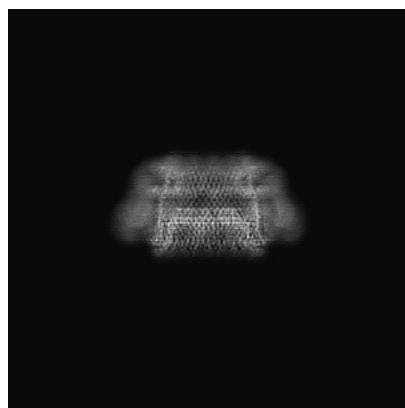
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16810. These allow visual inspection of the internal detail of the map and identification of artifacts.

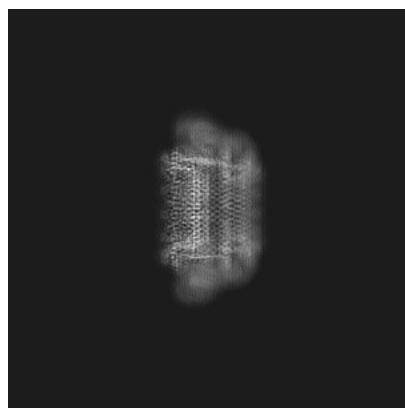
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

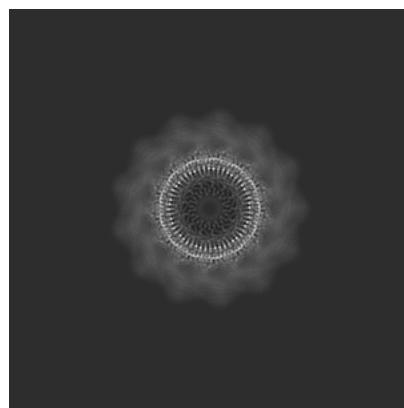
#### 6.1.1 Primary map



X

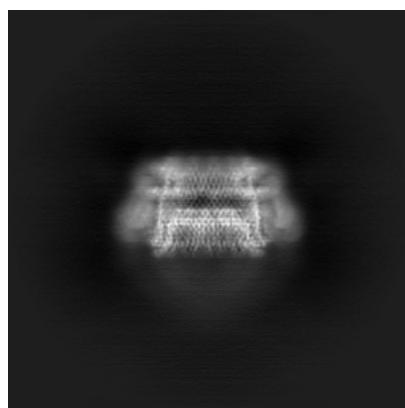


Y

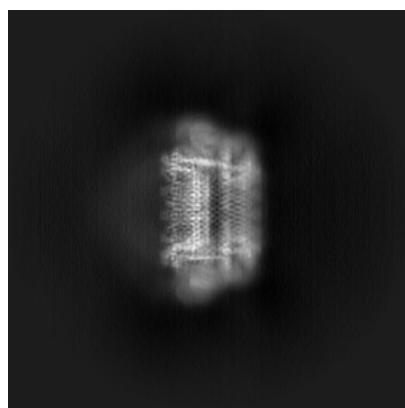


Z

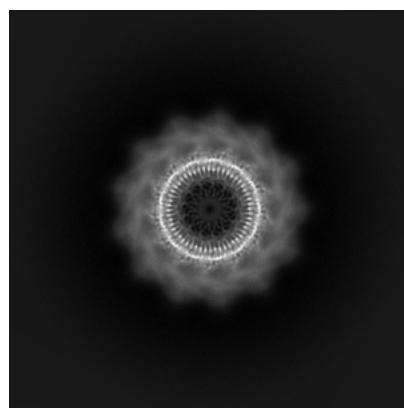
#### 6.1.2 Raw map



X



Y



Z

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

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

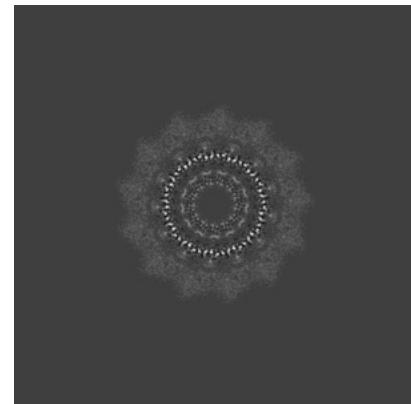
### 6.2.1 Primary map



X Index: 180

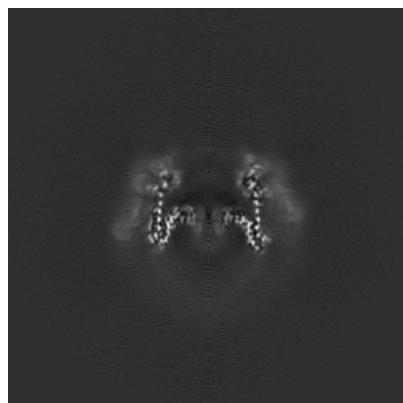


Y Index: 180

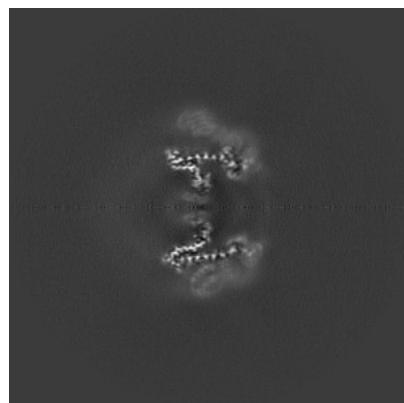


Z Index: 180

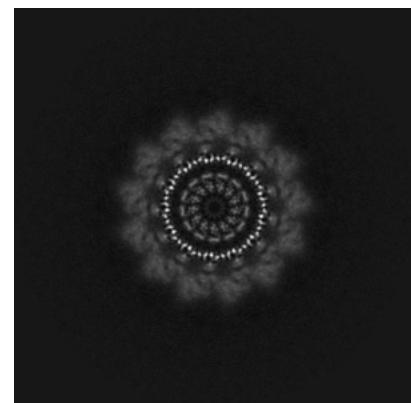
### 6.2.2 Raw map



X Index: 180



Y Index: 180

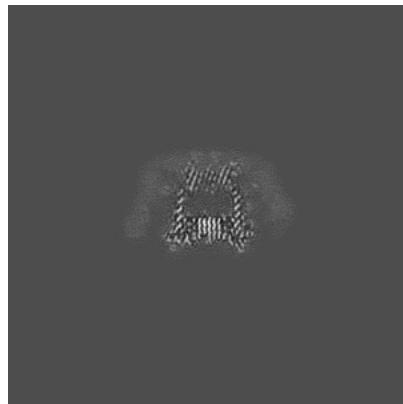


Z Index: 180

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

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

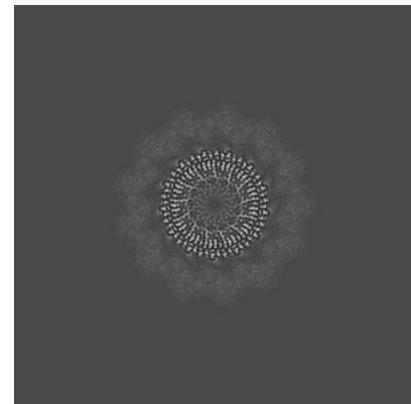
### 6.3.1 Primary map



X Index: 216

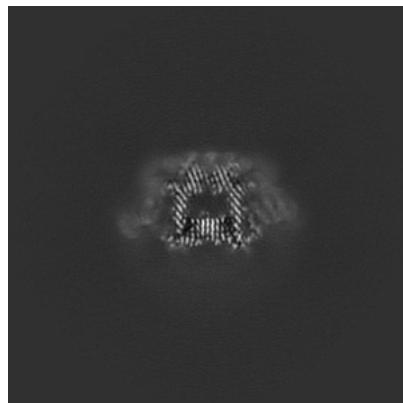


Y Index: 216

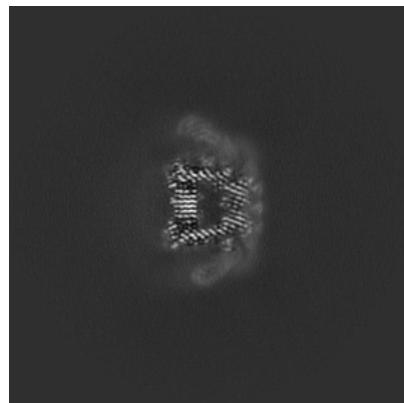


Z Index: 167

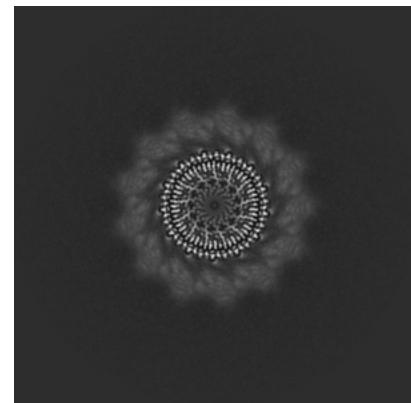
### 6.3.2 Raw map



X Index: 144



Y Index: 216

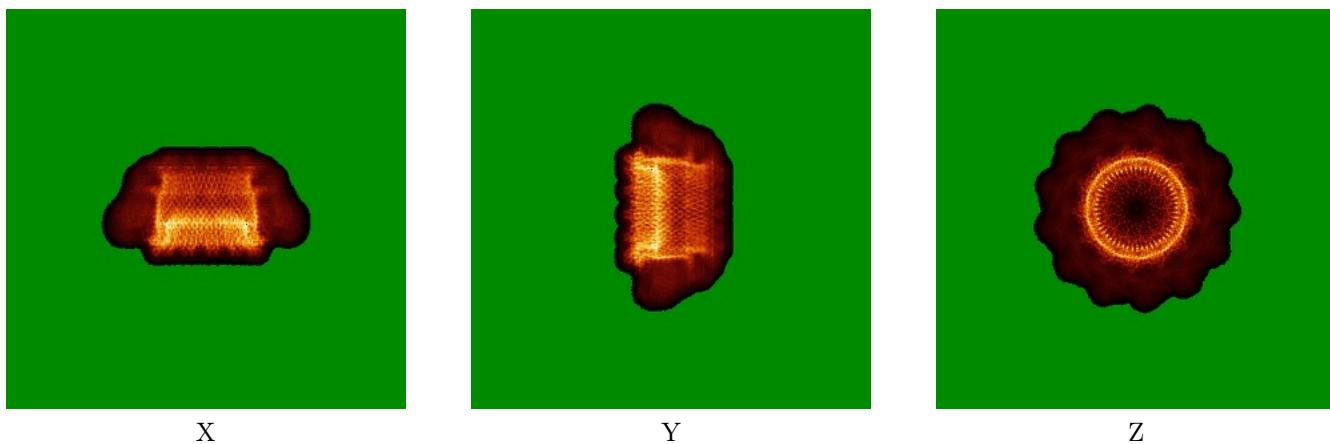


Z Index: 167

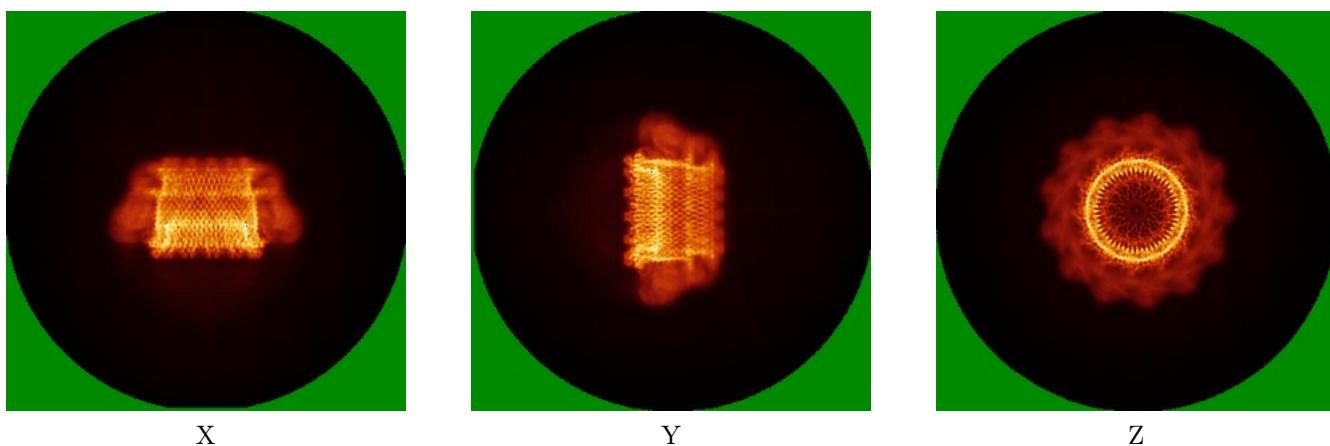
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



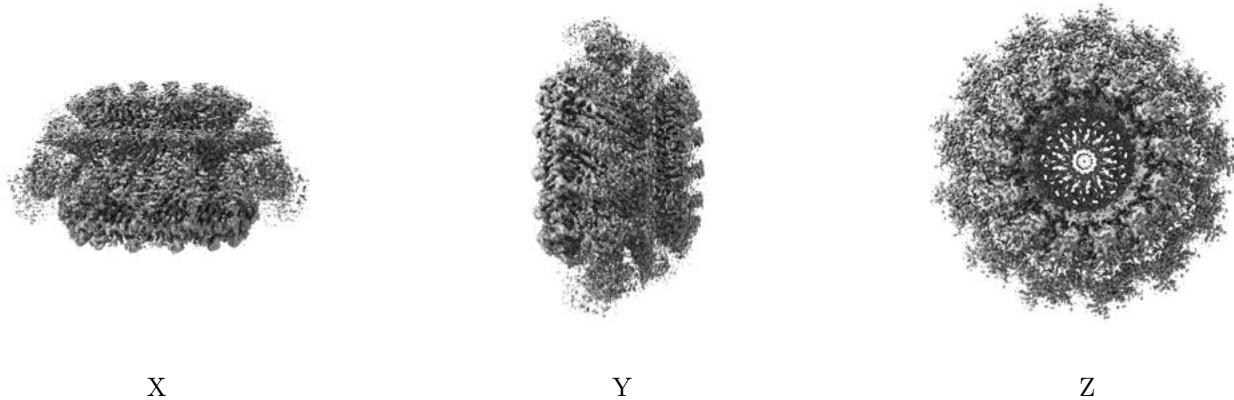
### 6.4.2 Raw map



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.

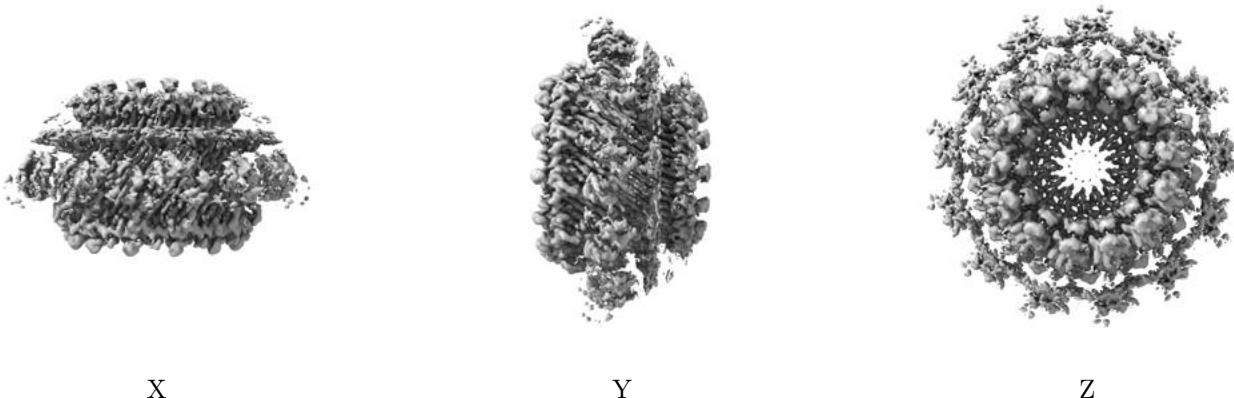
## 6.5 Orthogonal surface views [\(i\)](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

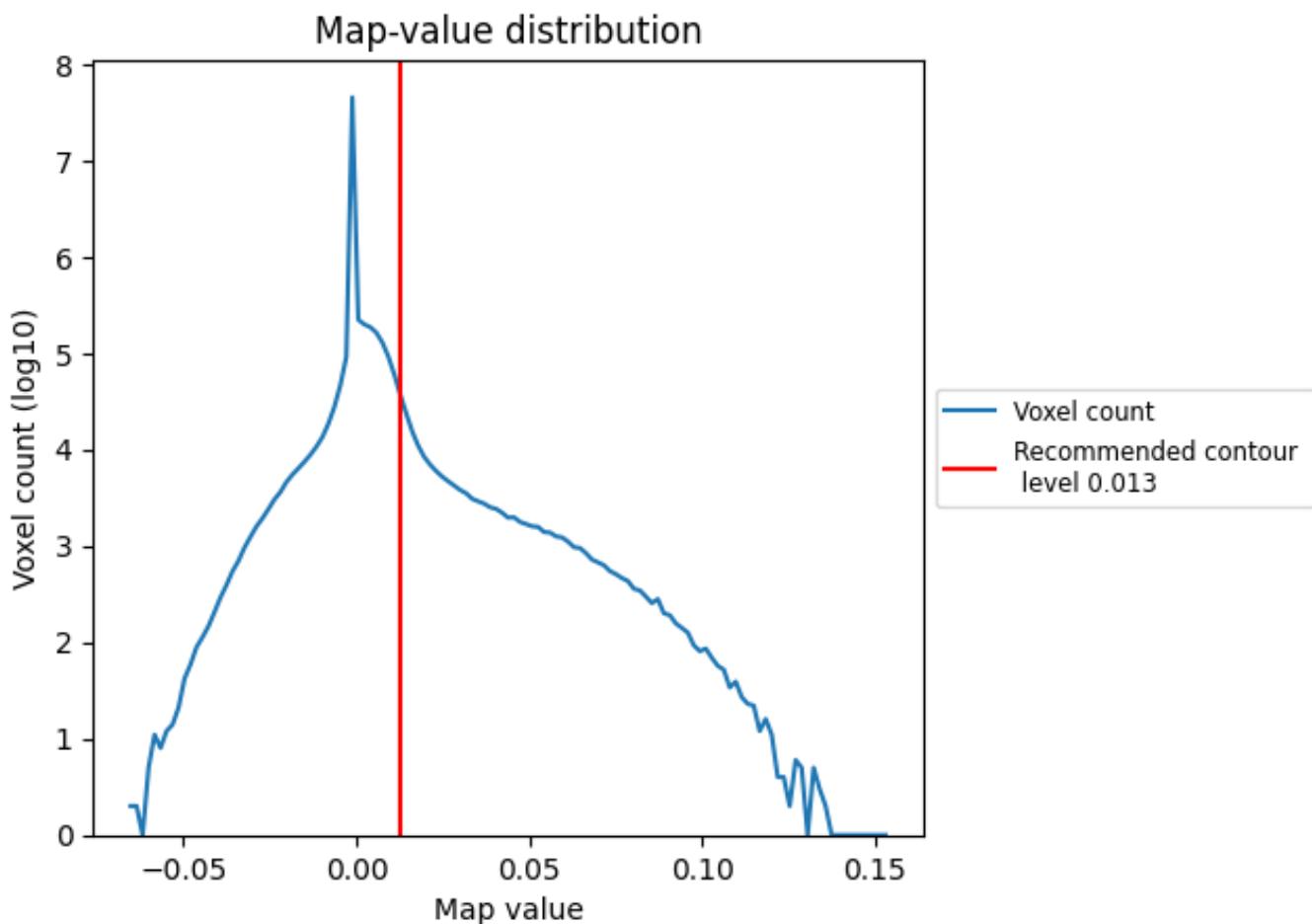
## 6.6 Mask visualisation [\(i\)](#)

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

## 7 Map analysis (i)

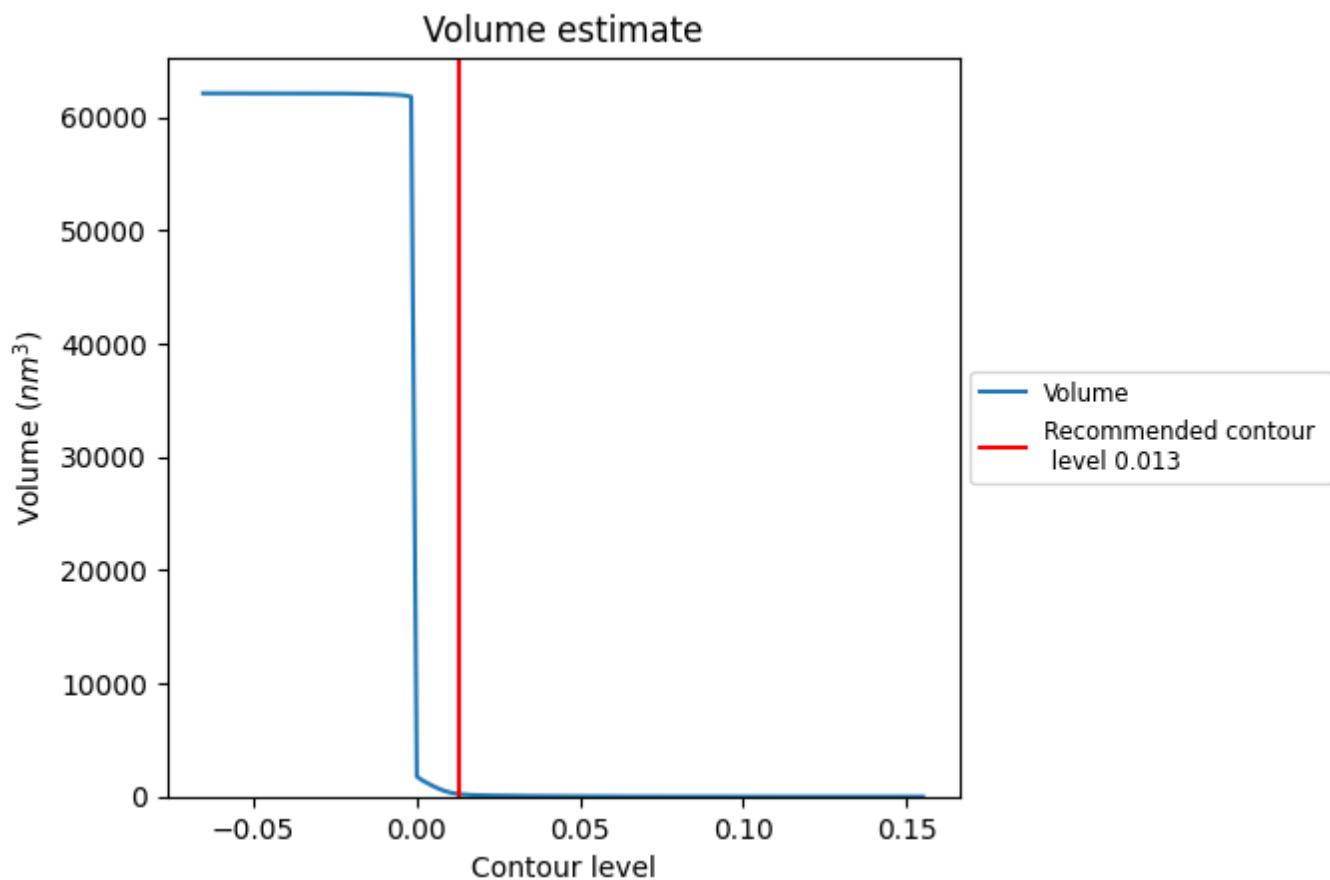
This section contains the results of statistical analysis of the map.

### 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.

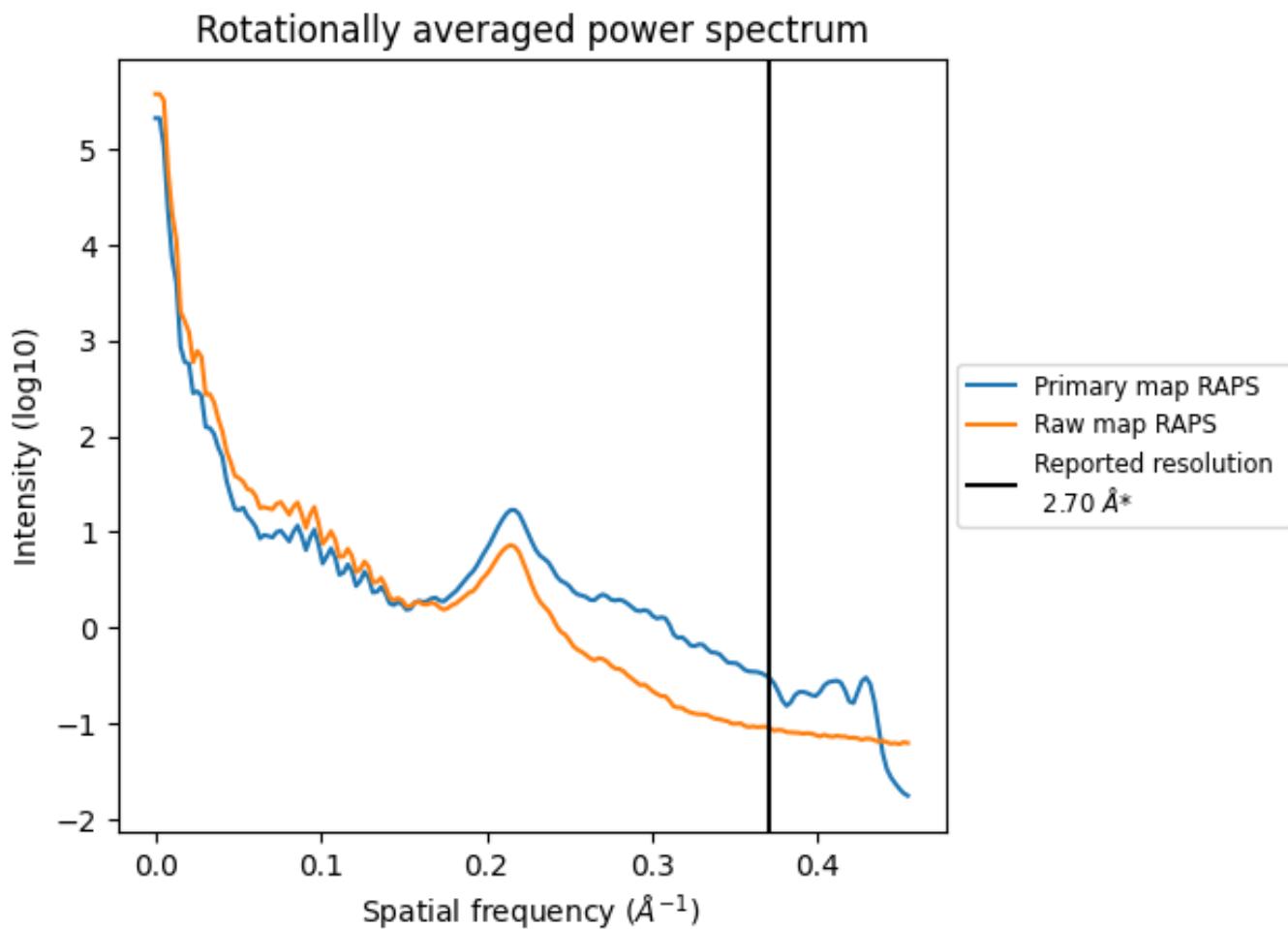
## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $225 \text{ nm}^3$ ; this corresponds to an approximate mass of 203 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

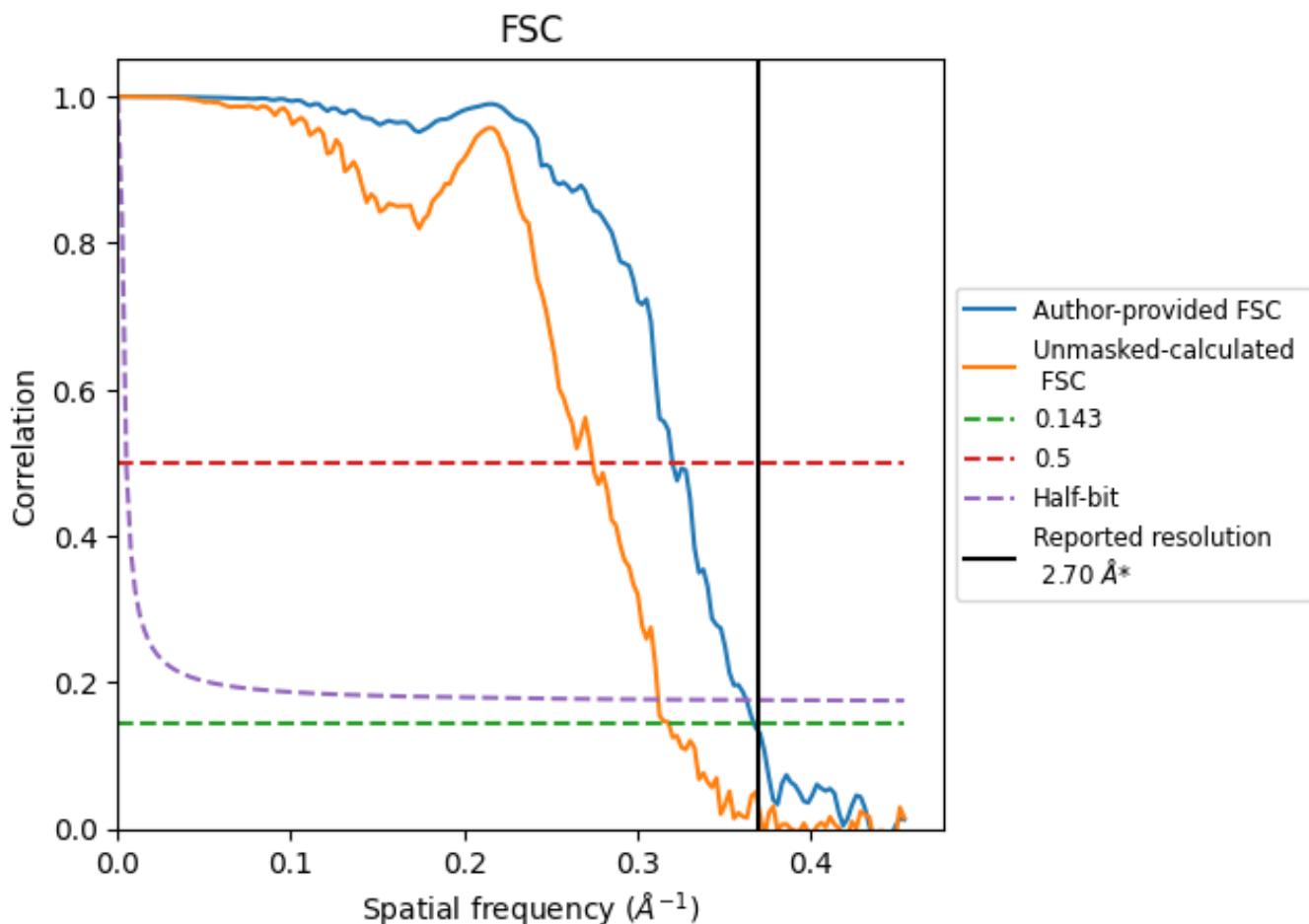


\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

## 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 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [\(i\)](#)

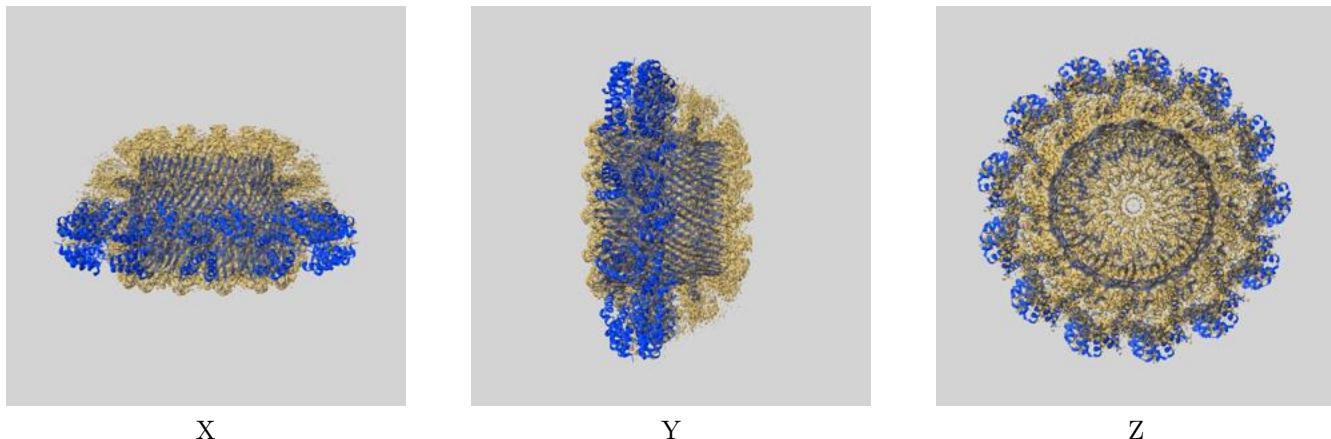
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.12	2.75
Unmasked-calculated*	3.14	3.64	3.20

\*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 3.14 differs from the reported value 2.7 by more than 10 %

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

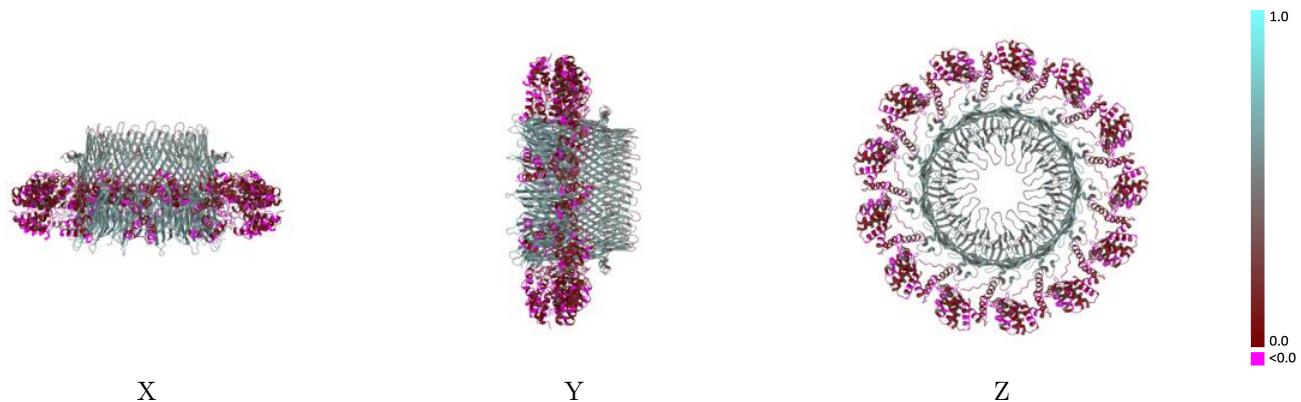
This section contains information regarding the fit between EMDB map EMD-16810 and PDB model 8ODN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



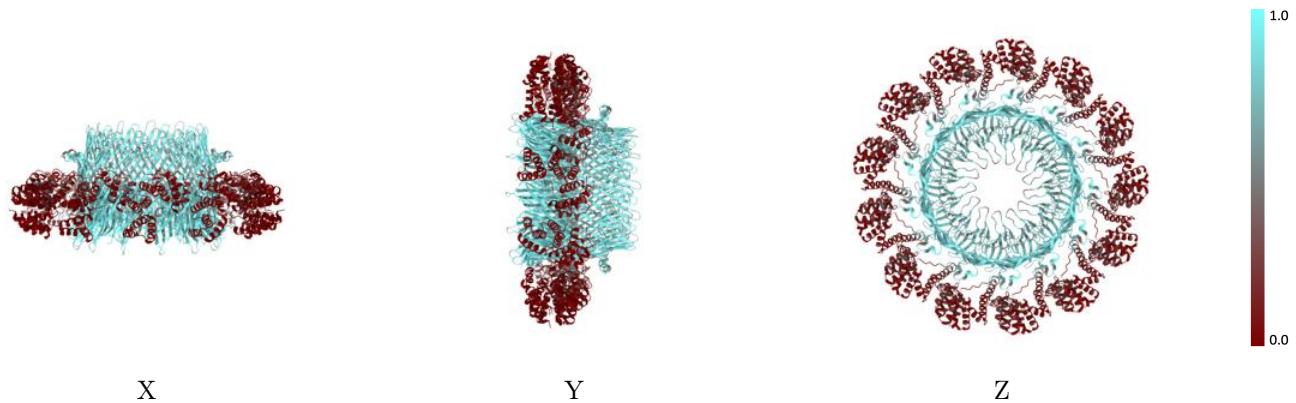
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



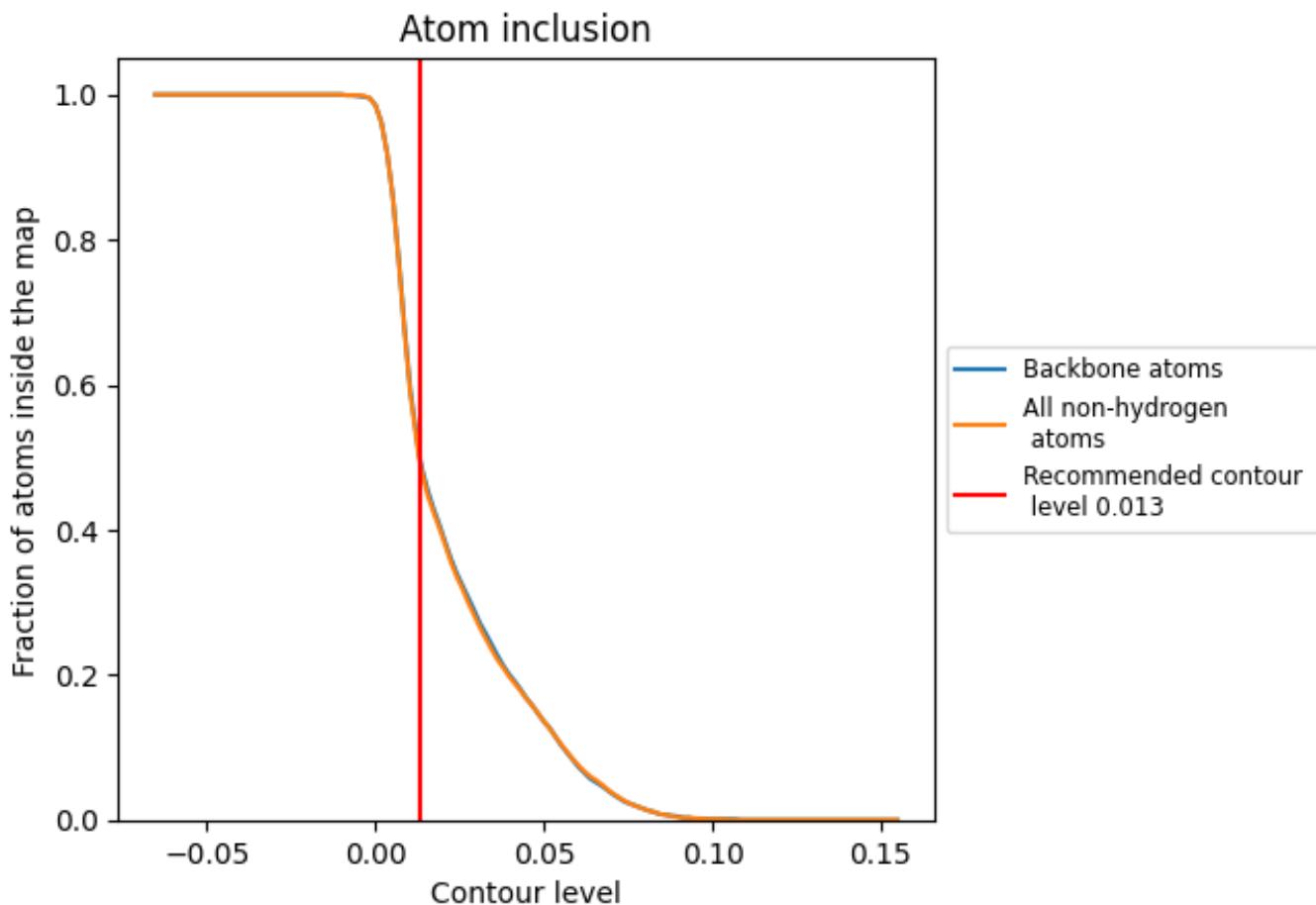
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4990	0.3360
A	0.8400	0.5340
B	0.0760	0.0880
C	0.8390	0.5340
D	0.0730	0.0840
E	0.8370	0.5300
F	0.0800	0.0920
G	0.8380	0.5350
H	0.0770	0.0850
I	0.8360	0.5360
J	0.0800	0.0890
K	0.8380	0.5340
L	0.0730	0.0890
M	0.8410	0.5340
N	0.0770	0.0830
O	0.8410	0.5350
P	0.0780	0.0880
Q	0.8390	0.5340
R	0.0760	0.0880
S	0.8400	0.5340
T	0.0710	0.0890
V	0.8390	0.5320
W	0.0780	0.0960
X	0.8380	0.5330
Y	0.0760	0.0930
Z	0.8420	0.5330
a	0.0730	0.0900

