



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 10:07 PM EDT

PDB ID : 9N4V / pdb\_00009n4v  
EMDB ID : EMD-48906  
Title : Azotobacter vinelandii extended type VI secretion system sheath tube complex  
Authors : Warmack, R.A.  
Deposited on : 2025-02-03  
Resolution : 1.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 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 ⓘ](#)) were used in the production of this report:

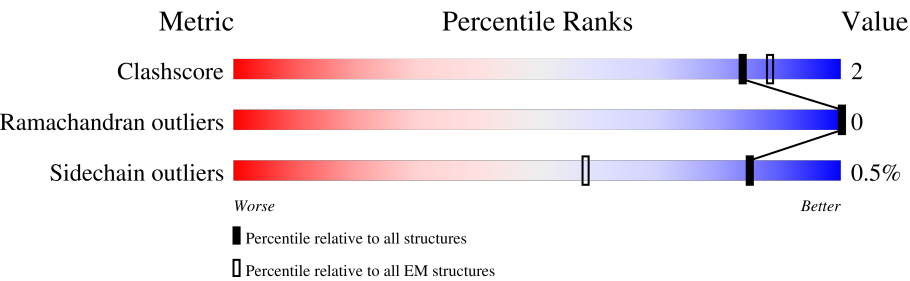
EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.85 Å.

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









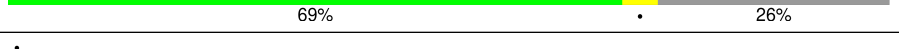
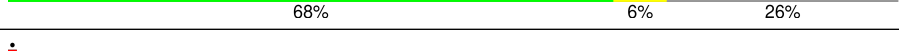
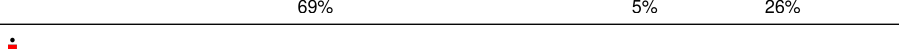
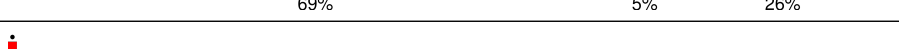
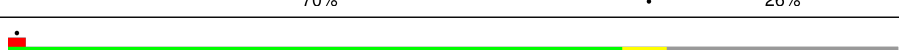

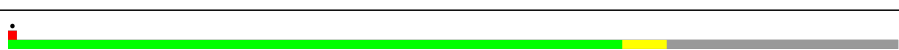

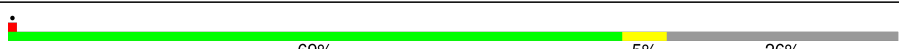










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	493	<div><div></div><div>70%</div><div>26%</div></div>
1	C	493	<div><div></div><div>70%</div><div>26%</div></div>
1	E	493	<div><div></div><div>69%</div><div>5%</div><div>26%</div></div>
1	G	493	<div><div></div><div>69%</div><div>26%</div></div>
1	I	493	<div><div></div><div>68%</div><div>6%</div><div>26%</div></div>
1	K	493	<div><div></div><div>69%</div><div>26%</div></div>
1	M	493	<div><div></div><div>69%</div><div>5%</div><div>26%</div></div>
1	O	493	<div><div></div><div>69%</div><div>26%</div></div>

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Mol	Chain	Length	Quality of chain
1	Q	493	
1	S	493	
1	U	493	
1	W	493	
1	Y	493	
1	a	493	
1	c	493	
1	e	493	
1	g	493	
1	i	493	
1	k	493	
1	m	493	
1	o	493	
1	q	493	
1	s	493	
1	u	493	
2	B	187	
2	D	187	
2	F	187	
2	H	187	
2	J	187	
2	L	187	
2	N	187	
2	P	187	
2	R	187	

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Mol	Chain	Length	Quality of chain
2	T	187	 34% 66%
2	V	187	 33% 66%
2	X	187	 33% 66%
2	Z	187	 33% 66%
2	b	187	 33% 66%
2	d	187	 33% 66%
2	f	187	 34% 66%
2	h	187	 34% 66%
2	j	187	 34% 66%
2	l	187	 33% 66%
2	n	187	 33% 66%
2	p	187	 33% 66%
2	r	187	 34% 66%
2	t	187	 33% 66%
2	v	187	 34% 66%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 88086 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 DUF877 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	C	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	E	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	G	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	I	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	K	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	M	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	O	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	Q	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	S	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	U	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	W	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	Y	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	a	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	c	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	e	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	g	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	k	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	m	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	o	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	q	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	s	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		
1	u	365	Total	C	N	O	S	0	0
			2898	1858	511	521	8		

- Molecule 2 is a protein called Type VI secretion system contractile sheath small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	D	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	F	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	H	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	J	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	L	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	N	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	P	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	R	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	T	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	V	64	Total	C	N	O	S	0	0
			516	324	93	98	1		
2	X	64	Total	C	N	O	S	0	0
			516	324	93	98	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	b	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	d	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	f	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	h	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	j	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	l	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	n	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	p	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	r	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	t	64	Total 516	C 324	N 93	O 98	S 1	0	0
2	v	64	Total 516	C 324	N 93	O 98	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	232	Total 232	O 232	0
3	B	33	Total 33	O 33	0
3	C	250	Total 250	O 250	0
3	D	50	Total 50	O 50	0
3	E	192	Total 192	O 192	0
3	F	27	Total 27	O 27	0
3	G	230	Total 230	O 230	0

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Mol	Chain	Residues	Atoms		AltConf
3	H	36	Total 36	O 36	0
3	I	202	Total 202	O 202	0
3	J	31	Total 31	O 31	0
3	K	249	Total 249	O 249	0
3	L	50	Total 50	O 50	0
3	M	196	Total 196	O 196	0
3	N	27	Total 27	O 27	0
3	O	197	Total 197	O 197	0
3	P	24	Total 24	O 24	0
3	Q	223	Total 223	O 223	0
3	R	36	Total 36	O 36	0
3	S	208	Total 208	O 208	0
3	T	31	Total 31	O 31	0
3	U	250	Total 250	O 250	0
3	V	48	Total 48	O 48	0
3	W	194	Total 194	O 194	0
3	X	27	Total 27	O 27	0
3	Y	231	Total 231	O 231	0
3	Z	36	Total 36	O 36	0
3	a	205	Total 205	O 205	0
3	b	31	Total 31	O 31	0

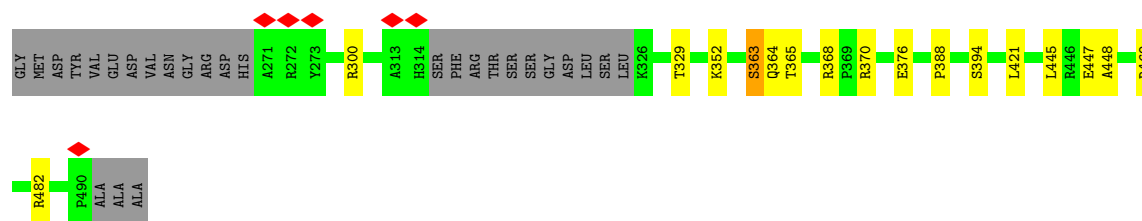
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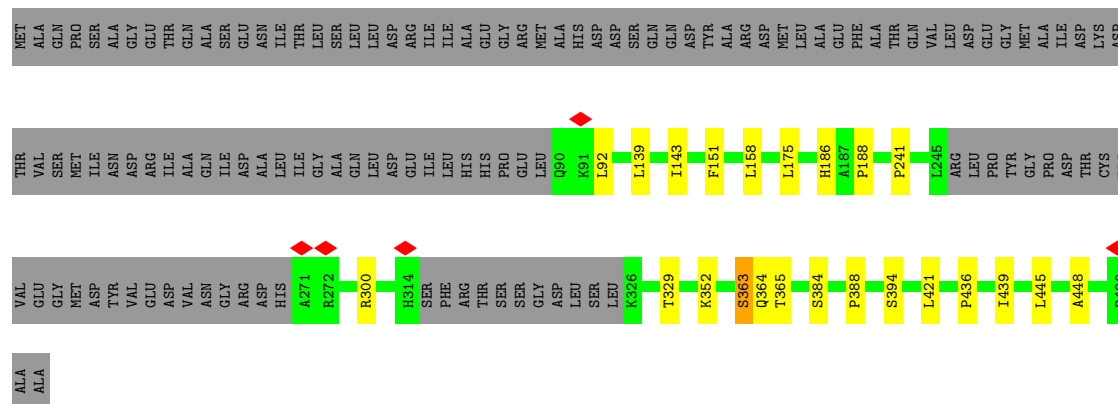
Mol	Chain	Residues	Atoms		AltConf
3	c	253	Total 253	O 253	0
3	d	50	Total 50	O 50	0
3	e	195	Total 195	O 195	0
3	f	27	Total 27	O 27	0
3	g	231	Total 231	O 231	0
3	h	32	Total 32	O 32	0
3	i	206	Total 206	O 206	0
3	j	31	Total 31	O 31	0
3	k	268	Total 268	O 268	0
3	l	44	Total 44	O 44	0
3	m	195	Total 195	O 195	0
3	n	24	Total 24	O 24	0
3	o	223	Total 223	O 223	0
3	p	36	Total 36	O 36	0
3	q	207	Total 207	O 207	0
3	r	31	Total 31	O 31	0
3	s	269	Total 269	O 269	0
3	t	44	Total 44	O 44	0
3	u	208	Total 208	O 208	0
3	v	30	Total 30	O 30	0





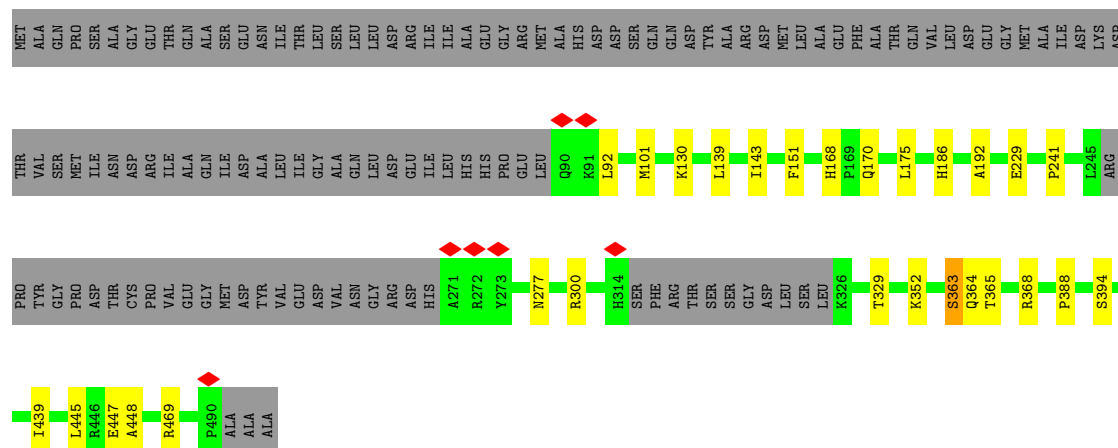
- Molecule 1: DUF877 family protein

Chain G: 69% 26%



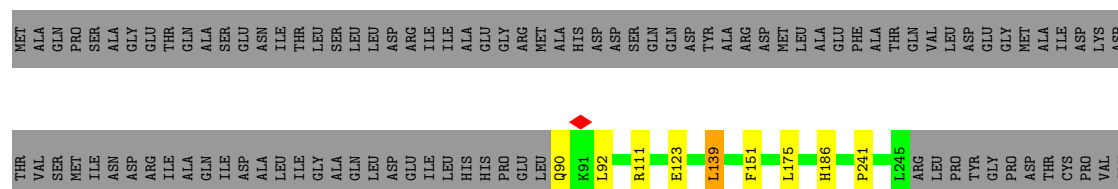
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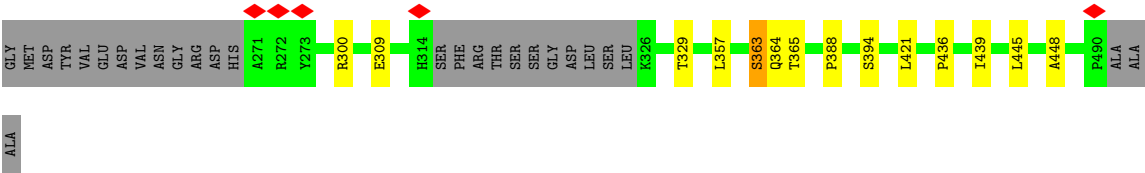
Chain I: 68% 6% 26%



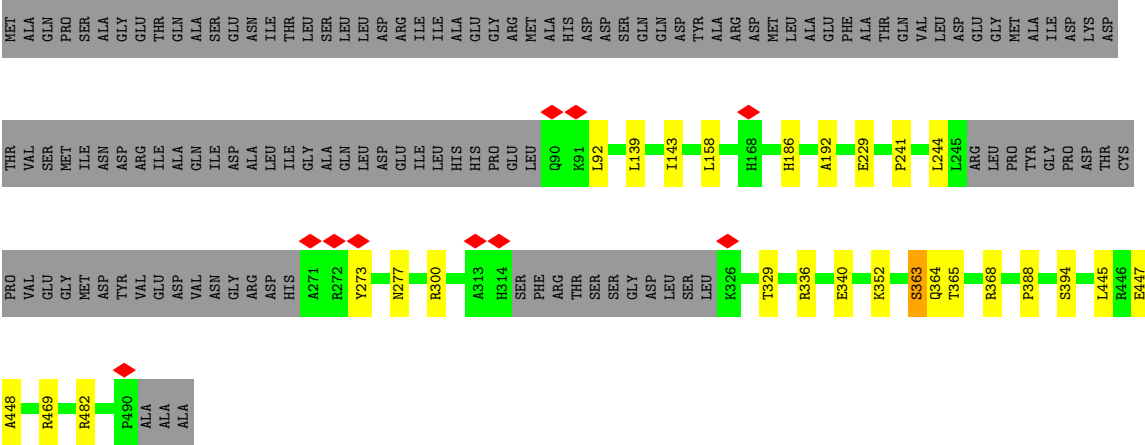
- Molecule 1: DUF877 family protein

Chain K: 69% 26%

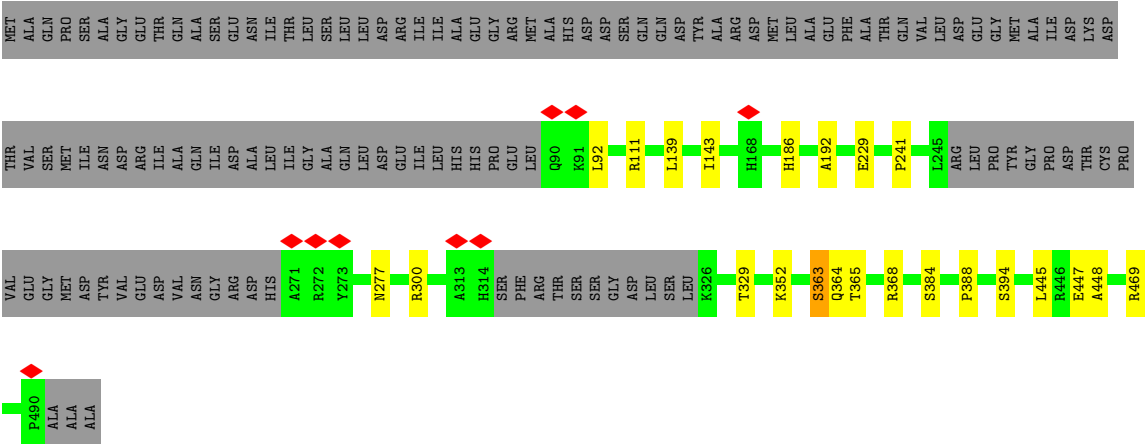




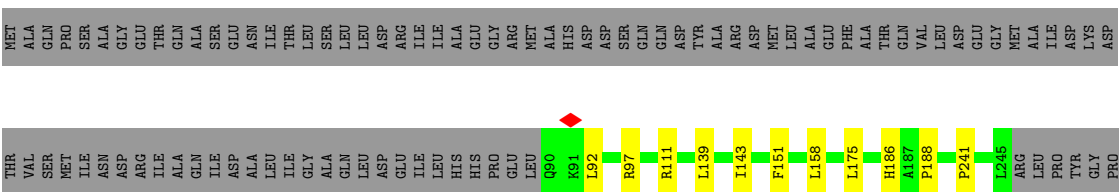
• Molecule 1: DUF877 family protein



• Molecule 1: DUF877 family protein



• Molecule 1: DUF877 family protein



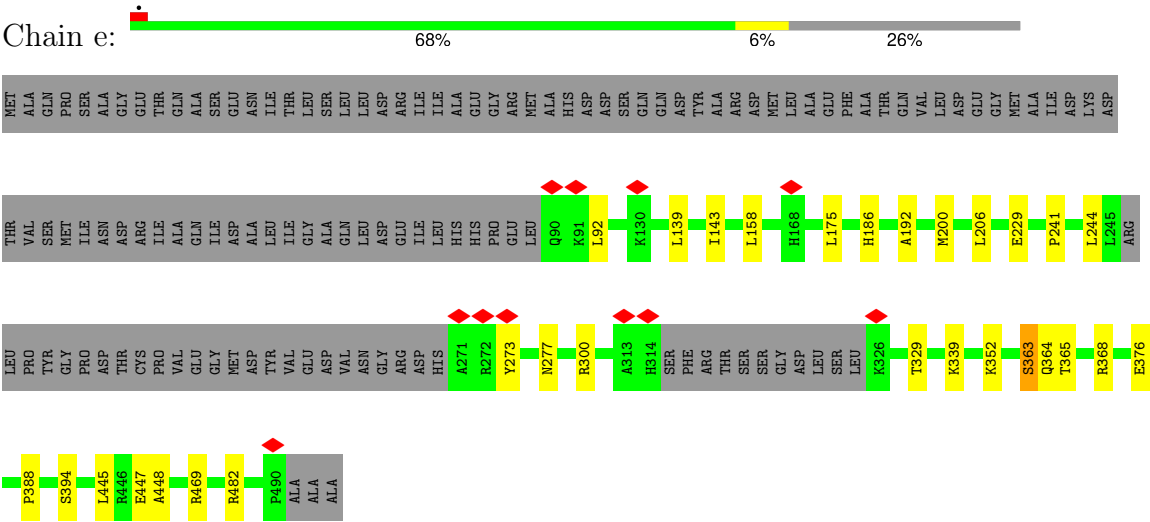




ALA

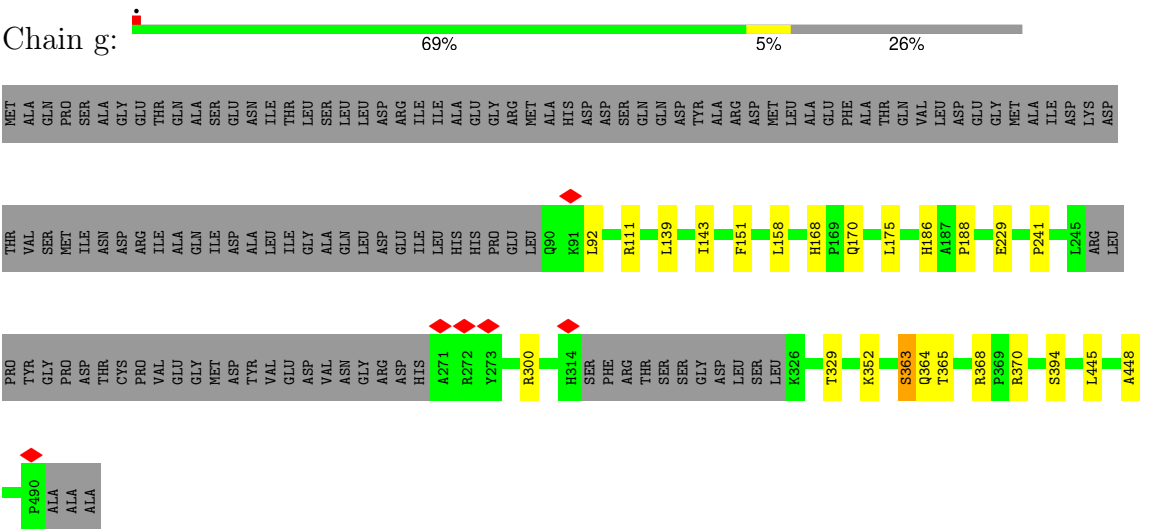
• Molecule 1: DUF877 family protein

Chain e:



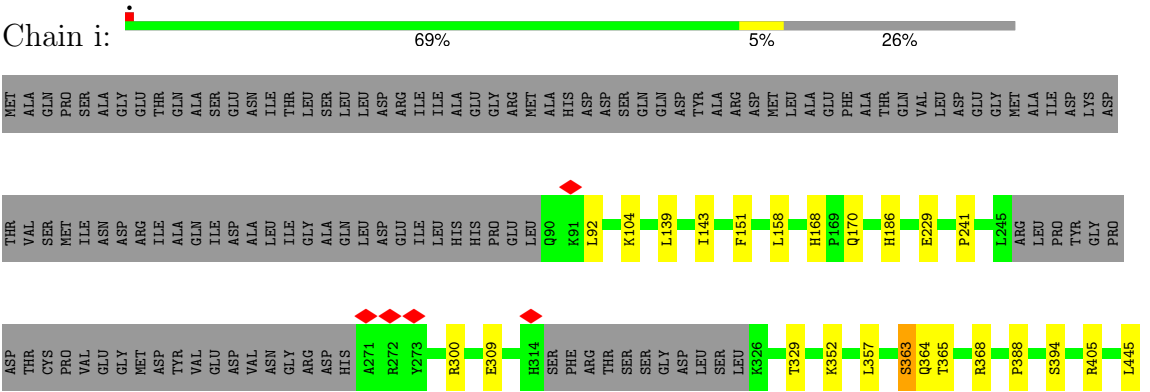
• Molecule 1: DUF877 family protein

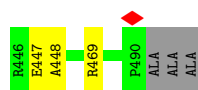
Chain g:



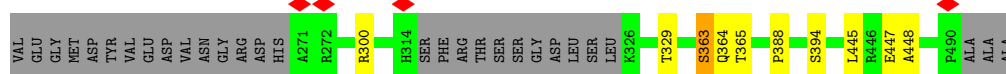
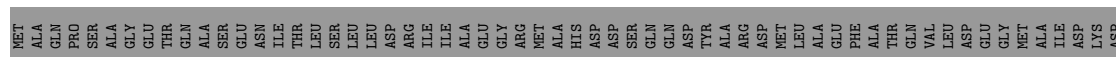
• Molecule 1: DUF877 family protein

Chain i:

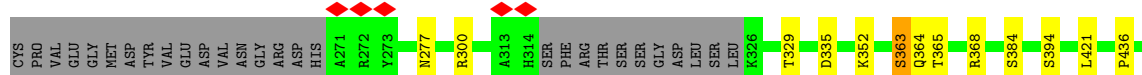
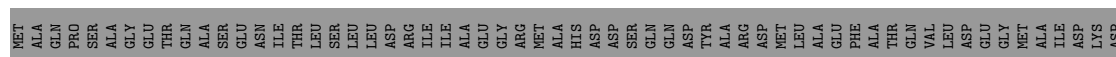




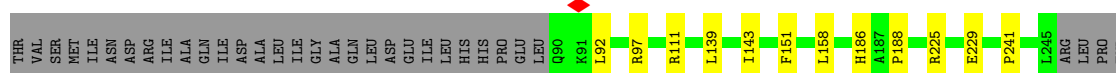
- Molecule 1: DUF877 family protein



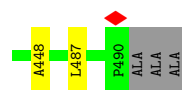
- Molecule 1: DUF877 family protein



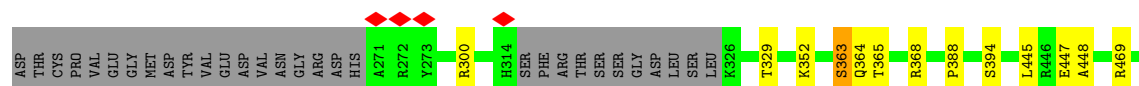
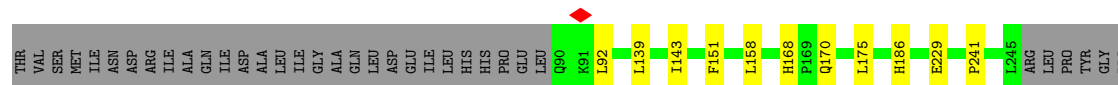
- Molecule 1: DUF877 family protein



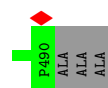
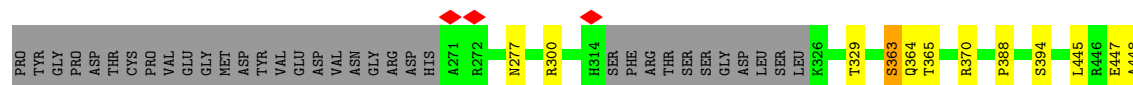
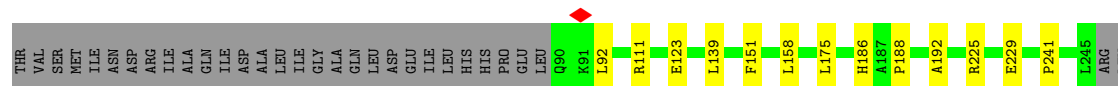
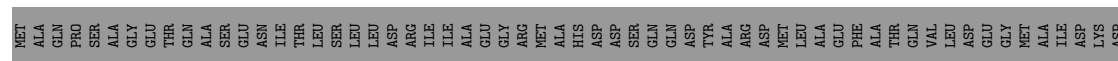




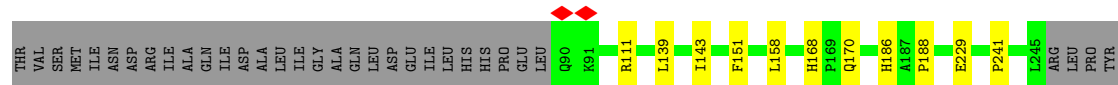
- Molecule 1: DUF877 family protein

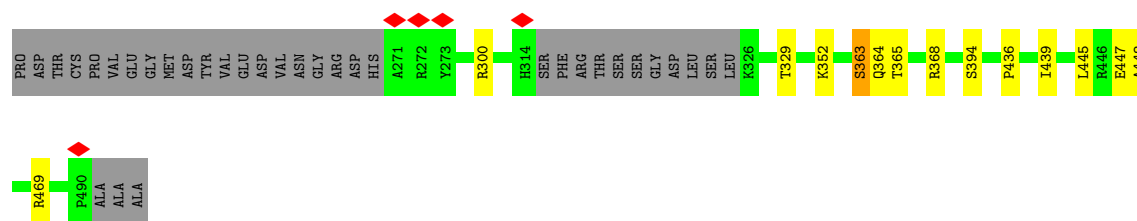


- Molecule 1: DUF877 family protein



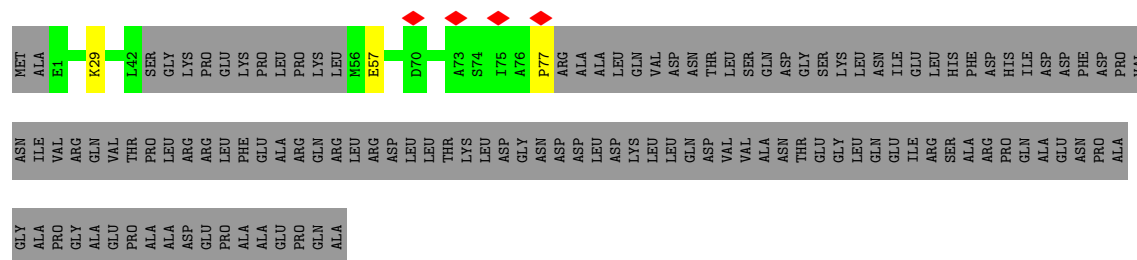
- Molecule 1: DUF877 family protein





- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain B: 33% 66%



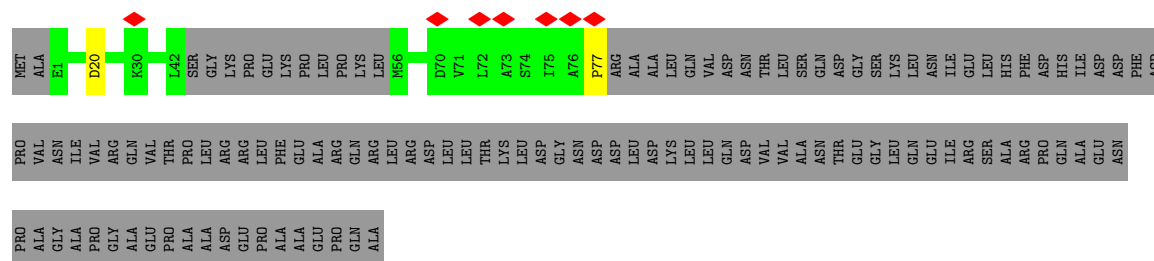
- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain D: 32% 66%



- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain F: 33% 66%



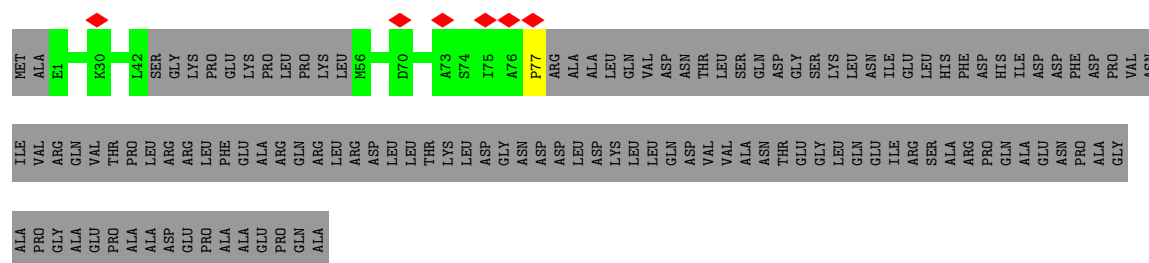
- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain H: 32% 66%



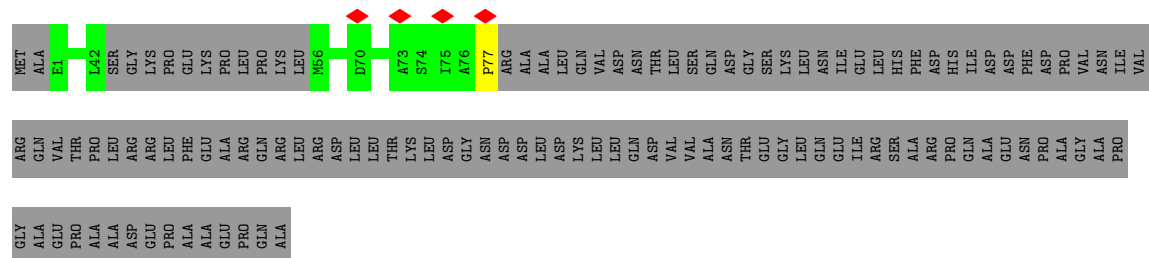






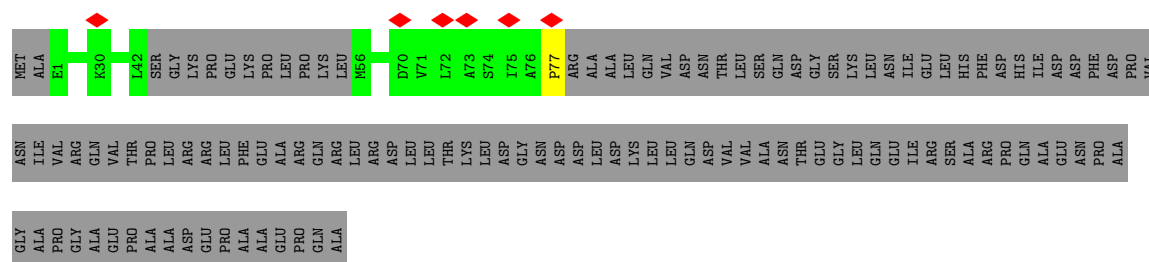
- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain h: 34% 66%



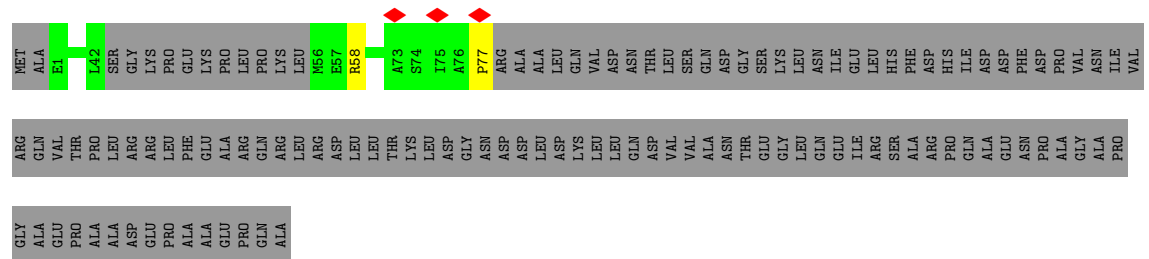
- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain j: 34% 66%



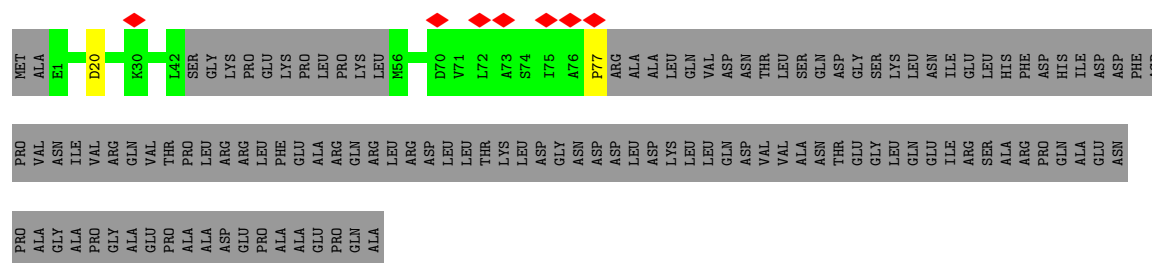
- Molecule 2: Type VI secretion system contractile sheath small subunit

Chain l: 33% 66%



- Molecule 2: Type VI secretion system contractile sheath small subunit

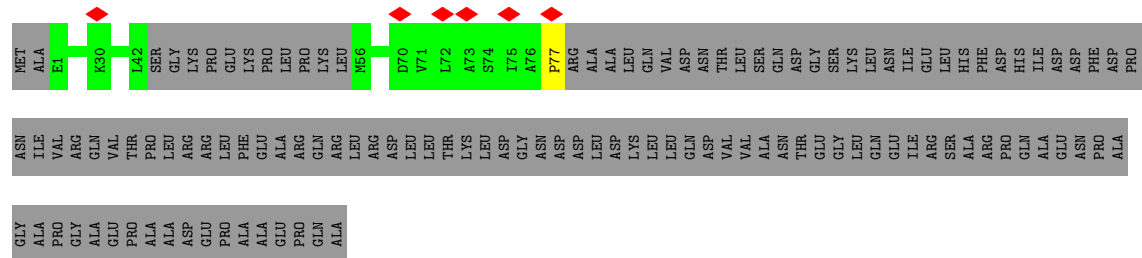
Chain n: 33% 66%



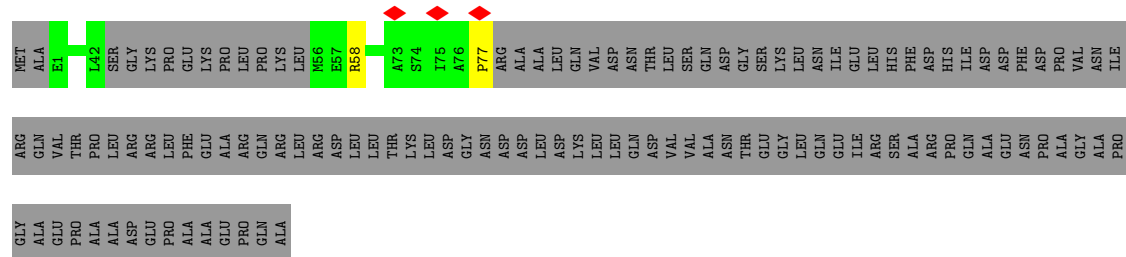
- Molecule 2: Type VI secretion system contractile sheath small subunit



- Molecule 2: Type VI secretion system contractile sheath small subunit

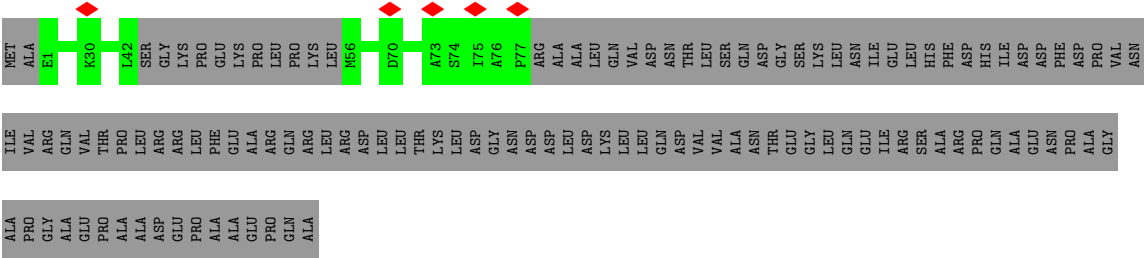


- Molecule 2: Type VI secretion system contractile sheath small subunit



- Molecule 2: Type VI secretion system contractile sheath small subunit







## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=22.12°, rise=30.58 Å, axial sym=C6	Depositor
Number of segments used	265571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	60	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	3.276	Depositor
Minimum map value	-1.676	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.736	Depositor
Map size (Å)	561.6, 561.6, 561.6	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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	0.17	0/2964	0.33	0/4018
1	C	0.18	0/2964	0.33	0/4018
1	E	0.17	0/2964	0.33	0/4018
1	G	0.18	0/2964	0.35	0/4018
1	I	0.17	0/2964	0.34	0/4018
1	K	0.18	0/2964	0.34	0/4018
1	M	0.17	0/2964	0.33	0/4018
1	O	0.16	0/2964	0.33	0/4018
1	Q	0.17	0/2964	0.34	0/4018
1	S	0.17	0/2964	0.34	0/4018
1	U	0.18	0/2964	0.33	0/4018
1	W	0.17	0/2964	0.33	0/4018
1	Y	0.17	0/2964	0.34	0/4018
1	a	0.17	0/2964	0.33	0/4018
1	c	0.18	0/2964	0.33	0/4018
1	e	0.17	0/2964	0.33	0/4018
1	g	0.17	0/2964	0.33	0/4018
1	i	0.17	0/2964	0.33	0/4018
1	k	0.17	0/2964	0.34	0/4018
1	m	0.16	0/2964	0.33	0/4018
1	o	0.17	0/2964	0.34	0/4018
1	q	0.17	0/2964	0.33	0/4018
1	s	0.18	0/2964	0.34	0/4018
1	u	0.17	0/2964	0.34	0/4018
2	B	0.16	0/522	0.32	0/705
2	D	0.18	0/522	0.33	0/705
2	F	0.16	0/522	0.30	0/705
2	H	0.16	0/522	0.31	0/705
2	J	0.16	0/522	0.32	0/705
2	L	0.17	0/522	0.31	0/705
2	N	0.15	0/522	0.30	0/705
2	P	0.15	0/522	0.30	0/705
2	R	0.16	0/522	0.32	0/705
2	T	0.16	0/522	0.31	0/705

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	V	0.17	0/522	0.31	0/705
2	X	0.16	0/522	0.30	0/705
2	Z	0.16	0/522	0.31	0/705
2	b	0.16	0/522	0.32	0/705
2	d	0.17	0/522	0.31	0/705
2	f	0.15	0/522	0.30	0/705
2	h	0.16	0/522	0.31	0/705
2	j	0.16	0/522	0.32	0/705
2	l	0.17	0/522	0.33	0/705
2	n	0.15	0/522	0.30	0/705
2	p	0.16	0/522	0.32	0/705
2	r	0.16	0/522	0.32	0/705
2	t	0.17	0/522	0.33	0/705
2	v	0.16	0/522	0.31	0/705
All	All	0.17	0/83664	0.33	0/113352

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2898	0	2903	13	0
1	C	2898	0	2903	13	0
1	E	2898	0	2903	16	0
1	G	2898	0	2903	15	0
1	I	2898	0	2903	18	0
1	K	2898	0	2903	16	0
1	M	2898	0	2903	15	0
1	O	2898	0	2903	15	0
1	Q	2898	0	2903	17	0
1	S	2898	0	2903	14	0
1	U	2898	0	2903	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	2898	0	2903	17	0
1	Y	2898	0	2903	14	0
1	a	2898	0	2903	15	0
1	c	2898	0	2903	17	0
1	e	2898	0	2903	19	0
1	g	2898	0	2903	16	0
1	i	2898	0	2903	18	0
1	k	2898	0	2903	12	0
1	m	2898	0	2903	18	0
1	o	2898	0	2903	17	0
1	q	2898	0	2903	16	0
1	s	2898	0	2903	17	0
1	u	2898	0	2903	16	0
2	B	516	0	528	3	0
2	D	516	0	528	3	0
2	F	516	0	528	2	0
2	H	516	0	528	2	0
2	J	516	0	528	2	0
2	L	516	0	528	2	0
2	N	516	0	528	1	0
2	P	516	0	528	2	0
2	R	516	0	528	1	0
2	T	516	0	528	1	0
2	V	516	0	528	2	0
2	X	516	0	528	2	0
2	Z	516	0	528	1	0
2	b	516	0	528	2	0
2	d	516	0	528	2	0
2	f	516	0	528	1	0
2	h	516	0	528	1	0
2	j	516	0	528	1	0
2	l	516	0	528	2	0
2	n	516	0	528	2	0
2	p	516	0	528	2	0
2	r	516	0	528	1	0
2	t	516	0	528	2	0
2	v	516	0	528	0	0
3	A	232	0	0	1	0
3	B	33	0	0	0	0
3	C	250	0	0	0	0
3	D	50	0	0	0	0
3	E	192	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	0	0	0
3	G	230	0	0	1	0
3	H	36	0	0	0	0
3	I	202	0	0	0	0
3	J	31	0	0	0	0
3	K	249	0	0	2	0
3	L	50	0	0	0	0
3	M	196	0	0	0	0
3	N	27	0	0	0	0
3	O	197	0	0	2	0
3	P	24	0	0	0	0
3	Q	223	0	0	1	0
3	R	36	0	0	0	0
3	S	208	0	0	1	0
3	T	31	0	0	0	0
3	U	250	0	0	0	0
3	V	48	0	0	0	0
3	W	194	0	0	1	0
3	X	27	0	0	0	0
3	Y	231	0	0	1	0
3	Z	36	0	0	0	0
3	a	205	0	0	1	0
3	b	31	0	0	0	0
3	c	253	0	0	2	0
3	d	50	0	0	0	0
3	e	195	0	0	0	0
3	f	27	0	0	0	0
3	g	231	0	0	1	0
3	h	32	0	0	0	0
3	i	206	0	0	0	0
3	j	31	0	0	0	0
3	k	268	0	0	0	0
3	l	44	0	0	0	0
3	m	195	0	0	2	0
3	n	24	0	0	0	0
3	o	223	0	0	1	0
3	p	36	0	0	0	0
3	q	207	0	0	0	0
3	r	31	0	0	0	0
3	s	269	0	0	1	0
3	t	44	0	0	0	0
3	u	208	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	v	30	0	0	0	0
All	All	88086	0	82344	364	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (364) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD22	1:C:139:LEU:HD11	1.66	0.77
1:U:124:LEU:HD22	1:U:139:LEU:HD11	1.65	0.76
1:u:447:GLU:OE2	1:u:469:ARG:NH1	2.21	0.72
1:M:447:GLU:OE2	1:M:469:ARG:NH1	2.26	0.65
1:K:90:GLN:N	3:K:503:HOH:O	2.32	0.62
1:c:90:GLN:N	3:c:503:HOH:O	2.32	0.62
1:S:447:GLU:OE2	1:S:469:ARG:NH1	2.32	0.60
1:W:300:ARG:HD2	1:W:363:SER:HB2	1.83	0.59
1:E:300:ARG:HD2	1:E:363:SER:HB2	1.84	0.58
1:O:447:GLU:OE2	1:O:469:ARG:NH1	2.32	0.58
1:M:139:LEU:HG	1:M:143:ILE:HD12	1.86	0.58
1:e:139:LEU:HG	1:e:143:ILE:HD12	1.86	0.57
1:E:364:GLN:HG3	1:E:365:THR:O	2.06	0.56
1:O:300:ARG:HD2	1:O:363:SER:HB2	1.87	0.56
1:Q:364:GLN:HG3	1:Q:365:THR:O	2.06	0.56
1:W:139:LEU:HG	1:W:143:ILE:HD12	1.88	0.56
1:O:139:LEU:HG	1:O:143:ILE:HD12	1.88	0.56
1:o:364:GLN:HG3	1:o:365:THR:O	2.06	0.56
1:u:139:LEU:HG	1:u:143:ILE:HD12	1.88	0.56
1:K:309:GLU:HG2	1:K:357:LEU:HD12	1.88	0.56
1:a:300:ARG:HD2	1:a:363:SER:HB2	1.88	0.56
1:i:447:GLU:OE2	1:i:469:ARG:NH1	2.37	0.56
1:m:139:LEU:HG	1:m:143:ILE:HD12	1.87	0.56
1:U:364:GLN:HG3	1:U:365:THR:O	2.06	0.55
1:O:364:GLN:HG3	1:O:365:THR:O	2.07	0.55
1:W:364:GLN:HG3	1:W:365:THR:O	2.06	0.55
1:C:364:GLN:HG3	1:C:365:THR:O	2.07	0.55
1:S:139:LEU:HG	1:S:143:ILE:HD12	1.88	0.55
1:m:364:GLN:HG3	1:m:365:THR:O	2.07	0.55
1:q:300:ARG:HD2	1:q:363:SER:HB2	1.88	0.55
1:K:364:GLN:HG3	1:K:365:THR:O	2.06	0.55
1:E:139:LEU:HG	1:E:143:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:309:GLU:HG2	1:i:357:LEU:HD12	1.88	0.55
1:M:364:GLN:HG3	1:M:365:THR:O	2.07	0.55
1:c:364:GLN:HG3	1:c:365:THR:O	2.06	0.55
1:i:139:LEU:HG	1:i:143:ILE:HD12	1.89	0.55
1:I:300:ARG:HD2	1:I:363:SER:HB2	1.88	0.55
1:i:300:ARG:HD2	1:i:363:SER:HB2	1.88	0.55
1:m:300:ARG:HD2	1:m:363:SER:HB2	1.87	0.54
1:G:364:GLN:HG3	1:G:365:THR:O	2.07	0.54
1:q:364:GLN:HG3	1:q:365:THR:O	2.07	0.54
1:q:139:LEU:HG	1:q:143:ILE:HD12	1.89	0.54
1:e:364:GLN:HG3	1:e:365:THR:O	2.07	0.54
1:g:364:GLN:HG3	1:g:365:THR:O	2.08	0.54
1:Y:364:GLN:HG3	1:Y:365:THR:O	2.08	0.54
1:C:309:GLU:HG2	1:C:357:LEU:HD12	1.90	0.53
1:u:364:GLN:HG3	1:u:365:THR:O	2.09	0.53
1:S:364:GLN:HG3	1:S:365:THR:O	2.08	0.53
1:o:139:LEU:HG	1:o:143:ILE:HD12	1.90	0.53
1:A:364:GLN:HG3	1:A:365:THR:O	2.08	0.53
1:Q:139:LEU:HG	1:Q:143:ILE:HD12	1.91	0.53
1:S:300:ARG:HD2	1:S:363:SER:HB2	1.91	0.53
1:s:364:GLN:HG3	1:s:365:THR:O	2.09	0.53
2:D:57:GLU:H	2:D:57:GLU:CD	2.16	0.53
1:i:364:GLN:HG3	1:i:365:THR:O	2.08	0.53
1:o:445:LEU:HD13	1:o:448:ALA:HB2	1.91	0.52
1:U:309:GLU:HG2	1:U:357:LEU:HD12	1.92	0.52
1:A:300:ARG:HD2	1:A:363:SER:HB2	1.91	0.52
1:Q:445:LEU:HD13	1:Q:448:ALA:HB2	1.91	0.52
1:U:300:ARG:HD2	1:U:363:SER:HB2	1.92	0.52
1:k:364:GLN:HG3	1:k:365:THR:O	2.09	0.52
1:c:168:HIS:CE1	1:c:170:GLN:NE2	2.78	0.52
1:g:92:LEU:HD21	2:h:77:PRO:HB2	1.91	0.52
1:A:92:LEU:HD21	2:B:77:PRO:HB2	1.91	0.52
1:M:300:ARG:HD2	1:M:363:SER:HB2	1.90	0.52
1:m:92:LEU:HD21	2:n:77:PRO:HB2	1.92	0.52
1:e:300:ARG:HD2	1:e:363:SER:HB2	1.90	0.52
1:E:239:VAL:HB	3:E:511:HOH:O	2.10	0.52
1:i:445:LEU:HD13	1:i:448:ALA:HB2	1.92	0.52
1:o:241:PRO:HG2	1:o:329:THR:O	2.10	0.52
1:G:445:LEU:HD13	1:G:448:ALA:HB2	1.92	0.51
1:e:92:LEU:HD21	2:f:77:PRO:HB2	1.93	0.51
1:u:300:ARG:HD2	1:u:363:SER:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:364:GLN:HG3	1:I:365:THR:O	2.10	0.51
1:g:300:ARG:HD2	1:g:363:SER:HB2	1.91	0.51
1:s:300:ARG:HD2	1:s:363:SER:HB2	1.92	0.51
1:Q:241:PRO:HG2	1:Q:329:THR:O	2.10	0.51
1:g:168:HIS:CE1	1:g:170:GLN:HE21	2.28	0.51
1:a:364:GLN:HG3	1:a:365:THR:O	2.10	0.51
1:W:239:VAL:HB	3:W:511:HOH:O	2.10	0.51
1:s:111:ARG:NH1	3:s:506:HOH:O	2.43	0.51
1:G:139:LEU:HG	1:G:143:ILE:HD12	1.93	0.51
1:K:111:ARG:NH1	3:K:508:HOH:O	2.43	0.51
1:m:186:HIS:O	1:m:394:SER:HB3	2.11	0.51
1:q:447:GLU:OE2	1:q:469:ARG:NH1	2.37	0.51
1:o:436:PRO:HG2	1:o:439:ILE:HG12	1.93	0.51
1:O:92:LEU:HD21	2:P:77:PRO:HB2	1.92	0.51
1:Y:300:ARG:HD2	1:Y:363:SER:HB2	1.93	0.51
1:Y:445:LEU:HD13	1:Y:448:ALA:HB2	1.92	0.51
1:E:447:GLU:HB2	1:E:469:ARG:HD3	1.93	0.50
1:c:111:ARG:NH1	3:c:508:HOH:O	2.43	0.50
1:q:445:LEU:HD13	1:q:448:ALA:HB2	1.92	0.50
1:s:225:ARG:O	1:s:229:GLU:HG2	2.11	0.50
1:k:300:ARG:HD2	1:k:363:SER:HB2	1.92	0.50
1:A:139:LEU:HG	1:A:143:ILE:HD12	1.93	0.50
1:O:445:LEU:HD13	1:O:448:ALA:HB2	1.93	0.50
1:W:376:GLU:CD	1:W:376:GLU:H	2.19	0.50
1:U:241:PRO:HG2	1:U:329:THR:O	2.12	0.50
1:e:186:HIS:O	1:e:394:SER:HB3	2.11	0.50
1:C:241:PRO:HG2	1:C:329:THR:O	2.12	0.50
1:C:300:ARG:HD2	1:C:363:SER:HB2	1.93	0.50
1:W:370:ARG:HG3	1:W:370:ARG:HH11	1.76	0.50
1:g:139:LEU:HG	1:g:143:ILE:HD12	1.93	0.50
1:q:168:HIS:CE1	1:q:170:GLN:HE21	2.29	0.50
1:O:186:HIS:O	1:O:394:SER:HB3	2.11	0.50
1:u:445:LEU:HD13	1:u:448:ALA:HB2	1.94	0.50
1:G:384:SER:HB3	3:G:502:HOH:O	2.12	0.50
1:M:92:LEU:HD21	2:N:77:PRO:HB2	1.93	0.50
1:Q:300:ARG:HD2	1:Q:363:SER:HB2	1.94	0.49
1:k:225:ARG:O	1:k:229:GLU:HG2	2.11	0.49
1:G:241:PRO:HG2	1:G:329:THR:O	2.13	0.49
1:W:447:GLU:HB2	1:W:469:ARG:HD3	1.94	0.49
1:g:186:HIS:O	1:g:394:SER:HB3	2.12	0.49
1:M:186:HIS:O	1:M:394:SER:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:241:PRO:HG2	1:S:329:THR:O	2.13	0.49
1:Y:139:LEU:HG	1:Y:143:ILE:HD12	1.93	0.49
1:c:300:ARG:HD2	1:c:363:SER:HB2	1.94	0.49
1:I:445:LEU:HD13	1:I:448:ALA:HB2	1.94	0.49
1:g:445:LEU:HD13	1:g:448:ALA:HB2	1.93	0.49
1:A:445:LEU:HD13	1:A:448:ALA:HB2	1.93	0.49
1:E:370:ARG:HG3	1:E:370:ARG:HH11	1.76	0.49
1:Y:92:LEU:HD21	2:Z:77:PRO:HB2	1.94	0.49
1:a:241:PRO:HG2	1:a:329:THR:O	2.12	0.49
1:S:229:GLU:OE2	1:S:368:ARG:HD2	2.13	0.49
1:k:92:LEU:HD21	2:l:77:PRO:HB2	1.95	0.49
1:G:300:ARG:HD2	1:G:363:SER:HB2	1.93	0.49
1:I:241:PRO:HG2	1:I:329:THR:O	2.12	0.49
1:g:229:GLU:OE1	1:g:368:ARG:HD2	2.13	0.49
1:m:241:PRO:HG2	1:m:329:THR:O	2.13	0.49
1:q:168:HIS:CE1	1:q:170:GLN:NE2	2.80	0.49
1:E:376:GLU:H	1:E:376:GLU:CD	2.19	0.49
1:U:445:LEU:HD13	1:U:448:ALA:HB2	1.95	0.49
1:a:445:LEU:HD13	1:a:448:ALA:HB2	1.94	0.49
1:m:445:LEU:HD13	1:m:448:ALA:HB2	1.95	0.49
1:q:241:PRO:HG2	1:q:329:THR:O	2.13	0.49
1:s:92:LEU:HD21	2:t:77:PRO:HB2	1.94	0.49
1:Y:241:PRO:HG2	1:Y:329:THR:O	2.13	0.49
1:s:241:PRO:HG2	1:s:329:THR:O	2.13	0.49
1:C:123:GLU:OE2	2:D:58:ARG:NH2	2.36	0.48
1:C:445:LEU:HD13	1:C:448:ALA:HB2	1.94	0.48
1:c:123:GLU:OE2	2:d:58:ARG:NH2	2.35	0.48
1:G:92:LEU:HD21	2:H:77:PRO:HB2	1.95	0.48
1:k:241:PRO:HG2	1:k:329:THR:O	2.13	0.48
1:S:445:LEU:HD13	1:S:448:ALA:HB2	1.95	0.48
1:i:241:PRO:HG2	1:i:329:THR:O	2.13	0.48
1:o:186:HIS:O	1:o:394:SER:HB3	2.13	0.48
1:u:241:PRO:HG2	1:u:329:THR:O	2.13	0.48
1:I:139:LEU:HG	1:I:143:ILE:HD12	1.95	0.48
1:I:229:GLU:OE2	1:I:368:ARG:HD2	2.14	0.48
1:K:186:HIS:O	1:K:394:SER:HB3	2.14	0.48
1:o:300:ARG:HD2	1:o:363:SER:HB2	1.94	0.48
1:C:186:HIS:O	1:C:394:SER:HB3	2.14	0.48
1:Q:436:PRO:HG2	1:Q:439:ILE:HG12	1.95	0.48
1:a:229:GLU:OE2	1:a:368:ARG:HD2	2.14	0.48
1:g:241:PRO:HG2	1:g:329:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:O	1:A:394:SER:HB3	2.13	0.48
1:K:300:ARG:HD2	1:K:363:SER:HB2	1.95	0.48
1:c:241:PRO:HG2	1:c:329:THR:O	2.14	0.48
1:Q:186:HIS:O	1:Q:394:SER:HB3	2.13	0.48
1:i:168:HIS:CE1	1:i:170:GLN:HE21	2.31	0.48
1:m:447:GLU:HB2	1:m:469:ARG:HD3	1.96	0.48
1:O:241:PRO:HG2	1:O:329:THR:O	2.13	0.47
1:A:241:PRO:HG2	1:A:329:THR:O	2.13	0.47
1:K:241:PRO:HG2	1:K:329:THR:O	2.14	0.47
1:c:186:HIS:O	1:c:394:SER:HB3	2.14	0.47
1:Y:384:SER:HB3	3:Y:502:HOH:O	2.12	0.47
1:a:139:LEU:HG	1:a:143:ILE:HD12	1.95	0.47
1:m:384:SER:HB3	3:m:502:HOH:O	2.14	0.47
1:q:229:GLU:OE2	1:q:368:ARG:HD2	2.14	0.47
1:I:186:HIS:O	1:I:394:SER:HB3	2.15	0.47
1:e:447:GLU:OE1	1:e:469:ARG:NH1	2.40	0.47
1:i:168:HIS:CE1	1:i:170:GLN:NE2	2.83	0.47
1:i:229:GLU:OE2	1:i:368:ARG:HD2	2.14	0.47
1:o:92:LEU:HD21	2:p:77:PRO:HB2	1.97	0.47
1:u:186:HIS:O	1:u:394:SER:HB3	2.15	0.47
1:u:229:GLU:OE1	1:u:368:ARG:HD2	2.14	0.47
1:S:168:HIS:CE1	1:S:170:GLN:HE21	2.32	0.47
1:U:186:HIS:O	1:U:394:SER:HB3	2.14	0.47
1:O:384:SER:HB3	3:O:502:HOH:O	2.14	0.47
1:W:186:HIS:O	1:W:394:SER:HB3	2.15	0.47
1:c:92:LEU:HD21	2:d:77:PRO:HB2	1.97	0.47
1:e:445:LEU:HD13	1:e:448:ALA:HB2	1.96	0.47
1:a:186:HIS:O	1:a:394:SER:HB3	2.15	0.46
1:M:445:LEU:HD13	1:M:448:ALA:HB2	1.96	0.46
1:S:186:HIS:O	1:S:394:SER:HB3	2.14	0.46
1:E:186:HIS:O	1:E:394:SER:HB3	2.15	0.46
1:A:225:ARG:O	1:A:229:GLU:HG2	2.16	0.46
1:M:229:GLU:OE1	1:M:368:ARG:HD2	2.15	0.46
1:W:92:LEU:HD21	2:X:77:PRO:HB2	1.97	0.46
1:i:92:LEU:HD21	2:j:77:PRO:HB2	1.97	0.46
1:E:241:PRO:HG2	1:E:329:THR:O	2.16	0.46
1:e:229:GLU:OE2	1:e:368:ARG:HD2	2.16	0.46
1:q:92:LEU:HD21	2:r:77:PRO:HB2	1.97	0.46
1:A:151:PHE:CE2	1:q:352:LYS:HB2	2.51	0.46
1:K:123:GLU:OE2	2:L:58:ARG:NH2	2.36	0.46
1:g:168:HIS:CE1	1:g:170:GLN:NE2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HD21	2:F:77:PRO:HB2	1.98	0.46
1:Y:186:HIS:O	1:Y:394:SER:HB3	2.15	0.46
1:k:186:HIS:O	1:k:394:SER:HB3	2.16	0.46
1:e:241:PRO:HG2	1:e:329:THR:O	2.16	0.46
1:o:111:ARG:NH1	3:o:509:HOH:O	2.47	0.46
1:K:445:LEU:HD13	1:K:448:ALA:HB2	1.98	0.46
1:s:186:HIS:O	1:s:394:SER:HB3	2.15	0.45
2:B:57:GLU:CD	2:B:57:GLU:H	2.24	0.45
1:E:445:LEU:HD13	1:E:448:ALA:HB2	1.98	0.45
1:K:92:LEU:HD21	2:L:77:PRO:HB2	1.97	0.45
1:Q:92:LEU:HD21	2:R:77:PRO:HB2	1.97	0.45
1:Q:363:SER:HB3	1:Q:388:PRO:HD3	1.97	0.45
1:c:168:HIS:ND1	1:c:170:GLN:NE2	2.55	0.45
1:G:186:HIS:O	1:G:394:SER:HB3	2.15	0.45
1:W:445:LEU:HD13	1:W:448:ALA:HB2	1.98	0.45
1:g:151:PHE:CE2	1:i:352:LYS:HB2	2.51	0.45
1:s:123:GLU:OE2	2:t:58:ARG:NH2	2.38	0.45
1:M:241:PRO:HG2	1:M:329:THR:O	2.16	0.45
1:k:445:LEU:HD13	1:k:448:ALA:HB2	1.98	0.45
1:W:241:PRO:HG2	1:W:329:THR:O	2.16	0.45
1:G:363:SER:HB3	1:G:388:PRO:HD3	1.99	0.45
1:U:363:SER:HB3	1:U:388:PRO:HD3	1.98	0.45
1:i:186:HIS:O	1:i:394:SER:HB3	2.17	0.45
1:I:130:LYS:HA	1:I:130:LYS:HD2	1.80	0.45
1:I:363:SER:HB3	1:I:388:PRO:HD3	1.99	0.45
1:g:111:ARG:NH1	3:g:506:HOH:O	2.45	0.45
1:q:186:HIS:O	1:q:394:SER:HB3	2.17	0.45
1:s:363:SER:HB3	1:s:388:PRO:HD3	1.99	0.45
1:I:168:HIS:ND1	1:I:170:GLN:HG2	2.32	0.44
1:c:445:LEU:HD13	1:c:448:ALA:HB2	1.98	0.44
1:O:111:ARG:NH1	3:O:506:HOH:O	2.49	0.44
1:a:363:SER:HB3	1:a:388:PRO:HD3	1.98	0.44
1:K:139:LEU:HD23	1:K:139:LEU:HA	1.83	0.44
1:i:104:LYS:HE2	1:i:104:LYS:HB2	1.87	0.44
1:s:445:LEU:HD13	1:s:448:ALA:HB2	1.98	0.44
1:G:436:PRO:HG2	1:G:439:ILE:HG12	1.99	0.44
1:o:363:SER:HB3	1:o:388:PRO:HD3	1.98	0.44
1:C:363:SER:HB3	1:C:388:PRO:HD3	1.99	0.44
1:I:101:MET:HE2	1:I:101:MET:HA	2.00	0.44
2:p:29:LYS:HD2	2:p:29:LYS:HA	1.86	0.44
1:A:352:LYS:HB2	1:K:151:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:139:LEU:HD12	1:O:139:LEU:HA	1.90	0.44
1:E:363:SER:HB3	1:E:388:PRO:HD3	2.00	0.43
1:Q:97:ARG:HG2	1:Q:97:ARG:HH11	1.82	0.43
2:V:29:LYS:HD2	2:V:29:LYS:HA	1.83	0.43
1:c:151:PHE:CE2	1:g:352:LYS:HB2	2.52	0.43
1:o:97:ARG:HG2	1:o:97:ARG:HH11	1.82	0.43
1:Q:151:PHE:CE2	1:S:352:LYS:HB2	2.54	0.43
1:c:139:LEU:HD23	1:c:139:LEU:HA	1.83	0.43
1:m:229:GLU:OE1	1:m:368:ARG:HD2	2.18	0.43
1:O:229:GLU:OE1	1:O:368:ARG:HD2	2.18	0.43
1:Q:139:LEU:HD12	1:Q:139:LEU:HA	1.89	0.43
1:I:151:PHE:CE2	1:M:352:LYS:HB2	2.53	0.43
1:Y:363:SER:HB3	1:Y:388:PRO:HD3	1.99	0.43
1:a:151:PHE:CE2	1:e:352:LYS:HB2	2.53	0.43
1:k:363:SER:HB3	1:k:388:PRO:HD3	1.99	0.43
1:C:92:LEU:HD21	2:D:77:PRO:HB2	2.00	0.43
1:I:92:LEU:HD21	2:J:77:PRO:HB2	2.00	0.43
1:a:101:MET:HE2	1:a:101:MET:HA	2.00	0.43
1:a:436:PRO:HG2	1:a:439:ILE:HG12	2.01	0.43
1:C:151:PHE:CE2	1:G:352:LYS:HB2	2.54	0.43
1:U:151:PHE:CE2	1:Y:352:LYS:HB2	2.54	0.43
1:Q:111:ARG:NH1	3:Q:509:HOH:O	2.47	0.43
1:Q:352:LYS:HB2	1:s:151:PHE:CE2	2.54	0.43
1:S:139:LEU:HD12	1:S:139:LEU:HA	1.90	0.43
1:U:92:LEU:HD21	2:V:77:PRO:HB2	2.00	0.43
1:I:436:PRO:HG2	1:I:439:ILE:HG12	2.01	0.43
1:W:363:SER:HB3	1:W:388:PRO:HD3	2.00	0.43
1:S:158:LEU:HD12	1:S:188:PRO:O	2.19	0.42
1:E:352:LYS:HB2	1:u:151:PHE:CE2	2.54	0.42
1:o:158:LEU:HD12	1:o:188:PRO:O	2.19	0.42
1:u:139:LEU:HD12	1:u:139:LEU:HA	1.89	0.42
1:S:151:PHE:CE2	1:W:352:LYS:HB2	2.54	0.42
1:Y:151:PHE:CE2	1:a:352:LYS:HB2	2.55	0.42
1:k:151:PHE:CE2	1:o:352:LYS:HB2	2.54	0.42
1:K:175:LEU:HD12	1:K:175:LEU:HA	1.91	0.42
1:Y:436:PRO:HG2	1:Y:439:ILE:HG12	2.01	0.42
1:o:151:PHE:CE2	1:u:352:LYS:HB2	2.53	0.42
1:A:111:ARG:NH1	3:A:505:HOH:O	2.45	0.42
1:S:111:ARG:NH1	3:S:510:HOH:O	2.49	0.42
1:m:111:ARG:NH1	3:m:507:HOH:O	2.49	0.42
2:T:65:ARG:HB2	1:U:132:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:158:LEU:HD12	1:u:188:PRO:O	2.20	0.42
1:m:175:LEU:HD12	1:m:175:LEU:HA	1.90	0.42
1:q:363:SER:HB3	1:q:388:PRO:HD3	2.02	0.42
1:s:158:LEU:HD12	1:s:188:PRO:O	2.20	0.42
2:J:29:LYS:HD2	2:J:29:LYS:HA	1.88	0.42
1:e:175:LEU:HD12	1:e:175:LEU:HA	1.92	0.42
1:k:158:LEU:HD12	1:k:188:PRO:O	2.20	0.42
1:s:175:LEU:HD12	1:s:175:LEU:HA	1.91	0.42
1:e:192:ALA:HB2	1:e:277:ASN:OD1	2.20	0.42
1:i:139:LEU:HD12	1:i:139:LEU:HA	1.93	0.42
1:A:158:LEU:HD12	1:A:188:PRO:O	2.20	0.42
1:E:229:GLU:OE2	1:E:368:ARG:HD2	2.20	0.42
1:G:151:PHE:CE2	1:I:352:LYS:HB2	2.55	0.42
1:O:352:LYS:HB2	1:q:151:PHE:CE2	2.55	0.42
1:m:436:PRO:HG2	1:m:439:ILE:HG12	2.02	0.42
1:K:363:SER:HB3	1:K:388:PRO:HD3	2.02	0.41
1:M:363:SER:HB3	1:M:388:PRO:HD3	2.01	0.41
1:Q:158:LEU:HD12	1:Q:188:PRO:O	2.19	0.41
1:Q:175:LEU:HD12	1:Q:175:LEU:HA	1.94	0.41
2:X:20:ASP:O	1:e:482:ARG:HG2	2.20	0.41
1:e:139:LEU:HD12	1:e:139:LEU:HA	1.92	0.41
1:k:123:GLU:OE2	2:l:58:ARG:NH2	2.38	0.41
2:H:8:ASP:OD1	2:H:16:GLN:NE2	2.49	0.41
1:M:192:ALA:HB2	1:M:277:ASN:OD1	2.20	0.41
1:Q:487:LEU:HD11	1:s:447:GLU:HG2	2.02	0.41
1:U:158:LEU:HD12	1:U:188:PRO:O	2.21	0.41
1:W:229:GLU:OE2	1:W:368:ARG:HD2	2.20	0.41
1:a:111:ARG:NH1	3:a:506:HOH:O	2.45	0.41
1:a:447:GLU:HB2	1:a:469:ARG:HD3	2.02	0.41
1:c:175:LEU:HD12	1:c:175:LEU:HA	1.91	0.41
1:i:405:ARG:NH1	1:m:335:ASP:OD2	2.45	0.41
1:u:111:ARG:NH1	3:u:510:HOH:O	2.49	0.41
1:u:168:HIS:CE1	1:u:170:GLN:NE2	2.88	0.41
1:G:158:LEU:HD12	1:G:188:PRO:O	2.19	0.41
1:i:151:PHE:CE2	1:m:352:LYS:HB2	2.55	0.41
1:k:447:GLU:HG2	1:o:487:LEU:HD11	2.02	0.41
1:o:225:ARG:O	1:o:229:GLU:HG2	2.20	0.41
1:q:139:LEU:HD12	1:q:139:LEU:HA	1.93	0.41
2:P:20:ASP:O	1:W:482:ARG:HG2	2.20	0.41
1:c:363:SER:HB3	1:c:388:PRO:HD3	2.01	0.41
1:E:482:ARG:HG2	2:n:20:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:158:LEU:HD12	1:Y:188:PRO:O	2.19	0.41
1:a:92:LEU:HD21	2:b:77:PRO:HB2	2.03	0.41
2:b:29:LYS:HD2	2:b:29:LYS:HA	1.87	0.41
1:i:363:SER:HB3	1:i:388:PRO:HD3	2.01	0.41
1:U:370:ARG:HH11	1:U:370:ARG:HG3	1.85	0.41
1:e:339:LYS:HA	1:e:339:LYS:HD2	1.90	0.41
1:g:158:LEU:HD12	1:g:188:PRO:O	2.20	0.41
1:g:370:ARG:HG3	1:g:370:ARG:HH11	1.86	0.41
1:u:168:HIS:CE1	1:u:170:GLN:HE21	2.38	0.41
1:o:370:ARG:HG3	1:o:370:ARG:HH11	1.86	0.41
1:u:436:PRO:HG2	1:u:439:ILE:HG12	2.03	0.41
1:O:363:SER:HB3	1:O:388:PRO:HD3	2.03	0.41
1:e:363:SER:HB3	1:e:388:PRO:HD3	2.01	0.41
1:m:421:LEU:HD23	1:m:421:LEU:HA	1.94	0.41
1:s:139:LEU:HD23	1:s:139:LEU:HA	1.84	0.41
2:B:29:LYS:HA	2:B:29:LYS:HD2	1.91	0.41
1:G:175:LEU:HD12	1:G:175:LEU:HA	1.93	0.41
1:M:336:ARG:O	1:M:340:GLU:HG3	2.21	0.41
1:Y:225:ARG:O	1:Y:229:GLU:HG2	2.22	0.41
1:c:436:PRO:HG2	1:c:439:ILE:HG12	2.03	0.41
1:A:145:GLU:O	1:A:150:THR:OG1	2.34	0.40
1:O:192:ALA:HB2	1:O:277:ASN:OD1	2.21	0.40
1:c:370:ARG:HG3	1:c:370:ARG:HH11	1.86	0.40
1:e:376:GLU:H	1:e:376:GLU:CD	2.29	0.40
1:q:175:LEU:HD12	1:q:175:LEU:HA	1.91	0.40
1:G:421:LEU:HD23	1:G:421:LEU:HA	1.91	0.40
1:I:447:GLU:HB2	1:I:469:ARG:HD3	2.02	0.40
1:e:200:MET:HE1	1:e:206:LEU:HA	2.02	0.40
1:C:158:LEU:HD12	1:C:188:PRO:O	2.21	0.40
1:I:175:LEU:HD12	1:I:175:LEU:HA	1.91	0.40
1:K:436:PRO:HG2	1:K:439:ILE:HG12	2.03	0.40
1:W:139:LEU:HD12	1:W:139:LEU:HA	1.93	0.40
1:m:139:LEU:HD12	1:m:139:LEU:HA	1.90	0.40
1:m:192:ALA:HB2	1:m:277:ASN:OD1	2.21	0.40
1:C:370:ARG:HG3	1:C:370:ARG:HH11	1.85	0.40
1:K:421:LEU:HD23	1:K:421:LEU:HA	1.90	0.40
1:M:244:LEU:HD11	1:M:273:TYR:HB3	2.04	0.40
1:W:175:LEU:HD12	1:W:175:LEU:HA	1.90	0.40
1:s:192:ALA:HB2	1:s:277:ASN:OD1	2.22	0.40
1:s:370:ARG:HH11	1:s:370:ARG:HG3	1.87	0.40
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:ASP:O	1:M:482:ARG:HG2	2.20	0.40
1:I:192:ALA:HB2	1:I:277:ASN:OD1	2.22	0.40
1:e:244:LEU:HD11	1:e:273:TYR:HB3	2.04	0.40
1:g:175:LEU:HD12	1:g:175:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	C	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	E	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	G	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	I	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	K	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	M	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	O	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	Q	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	S	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	U	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	W	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	Y	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	a	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	c	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	e	359/493 (73%)	352 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	i	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	k	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	m	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	o	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	q	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	s	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
1	u	359/493 (73%)	352 (98%)	7 (2%)	0	100	100
2	B	60/187 (32%)	60 (100%)	0	0	100	100
2	D	60/187 (32%)	60 (100%)	0	0	100	100
2	F	60/187 (32%)	60 (100%)	0	0	100	100
2	H	60/187 (32%)	60 (100%)	0	0	100	100
2	J	60/187 (32%)	60 (100%)	0	0	100	100
2	L	60/187 (32%)	60 (100%)	0	0	100	100
2	N	60/187 (32%)	60 (100%)	0	0	100	100
2	P	60/187 (32%)	60 (100%)	0	0	100	100
2	R	60/187 (32%)	60 (100%)	0	0	100	100
2	T	60/187 (32%)	60 (100%)	0	0	100	100
2	V	60/187 (32%)	60 (100%)	0	0	100	100
2	X	60/187 (32%)	60 (100%)	0	0	100	100
2	Z	60/187 (32%)	60 (100%)	0	0	100	100
2	b	60/187 (32%)	60 (100%)	0	0	100	100
2	d	60/187 (32%)	60 (100%)	0	0	100	100
2	f	60/187 (32%)	60 (100%)	0	0	100	100
2	h	60/187 (32%)	60 (100%)	0	0	100	100
2	j	60/187 (32%)	60 (100%)	0	0	100	100
2	l	60/187 (32%)	60 (100%)	0	0	100	100
2	n	60/187 (32%)	60 (100%)	0	0	100	100
2	p	60/187 (32%)	60 (100%)	0	0	100	100
2	r	60/187 (32%)	60 (100%)	0	0	100	100
2	t	60/187 (32%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	v	60/187 (32%)	60 (100%)	0	0	100	100
All	All	10056/16320 (62%)	9888 (98%)	168 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	C	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	E	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	G	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	I	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	K	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	M	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	O	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	Q	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	S	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	U	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	W	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	Y	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	a	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	c	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	e	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	g	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	i	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	k	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	m	301/406 (74%)	300 (100%)	1 (0%)	91	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	q	301/406 (74%)	299 (99%)	2 (1%)	81	78
1	s	301/406 (74%)	300 (100%)	1 (0%)	91	90
1	u	301/406 (74%)	300 (100%)	1 (0%)	91	90
2	B	58/160 (36%)	58 (100%)	0	100	100
2	D	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	F	58/160 (36%)	58 (100%)	0	100	100
2	H	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	J	58/160 (36%)	58 (100%)	0	100	100
2	L	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	N	58/160 (36%)	58 (100%)	0	100	100
2	P	58/160 (36%)	58 (100%)	0	100	100
2	R	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	T	58/160 (36%)	58 (100%)	0	100	100
2	V	58/160 (36%)	58 (100%)	0	100	100
2	X	58/160 (36%)	58 (100%)	0	100	100
2	Z	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	b	58/160 (36%)	58 (100%)	0	100	100
2	d	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	f	58/160 (36%)	58 (100%)	0	100	100
2	h	58/160 (36%)	58 (100%)	0	100	100
2	j	58/160 (36%)	58 (100%)	0	100	100
2	l	58/160 (36%)	58 (100%)	0	100	100
2	n	58/160 (36%)	58 (100%)	0	100	100
2	p	58/160 (36%)	57 (98%)	1 (2%)	56	44
2	r	58/160 (36%)	58 (100%)	0	100	100
2	t	58/160 (36%)	58 (100%)	0	100	100
2	v	58/160 (36%)	58 (100%)	0	100	100
All	All	8616/13584 (63%)	8577 (100%)	39 (0%)	85	84

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	SER
1	C	363	SER
2	D	29	LYS
1	E	363	SER
1	G	363	SER
2	H	31	GLU
1	I	363	SER
1	K	139	LEU
1	K	363	SER
2	L	29	LYS
1	M	158	LEU
1	M	363	SER
1	O	363	SER
1	Q	363	SER
2	R	31	GLU
1	S	363	SER
1	U	357	LEU
1	U	363	SER
1	W	363	SER
1	Y	326	LYS
1	Y	363	SER
2	Z	31	GLU
1	a	363	SER
1	c	139	LEU
1	c	363	SER
2	d	29	LYS
1	e	158	LEU
1	e	363	SER
1	g	363	SER
1	i	158	LEU
1	i	363	SER
1	k	363	SER
1	m	363	SER
1	o	363	SER
2	p	31	GLU
1	q	158	LEU
1	q	363	SER
1	s	363	SER
1	u	363	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	C	136	GLN
1	E	170	GLN
1	E	354	ASN
1	E	471	HIS
1	G	170	GLN
1	I	354	ASN
1	K	136	GLN
1	K	170	GLN
1	M	354	ASN
1	O	170	GLN
1	O	354	ASN
1	S	136	GLN
1	S	170	GLN
1	U	136	GLN
1	W	170	GLN
1	W	354	ASN
1	W	471	HIS
1	Y	170	GLN
1	Y	180	ASN
1	a	354	ASN
1	c	136	GLN
1	c	170	GLN
1	c	242	HIS
1	e	471	HIS
1	g	170	GLN
1	g	423	ASN
1	i	170	GLN
1	k	136	GLN
1	q	170	GLN
1	s	136	GLN
1	u	136	GLN
1	u	170	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

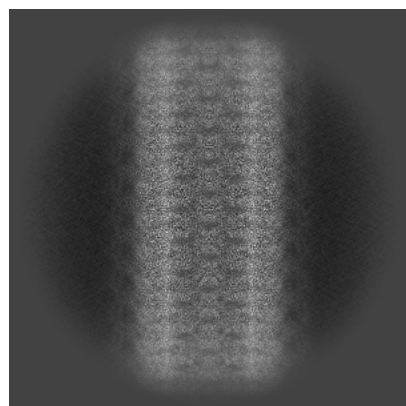
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48906. These allow visual inspection of the internal detail of the map and identification of artifacts.

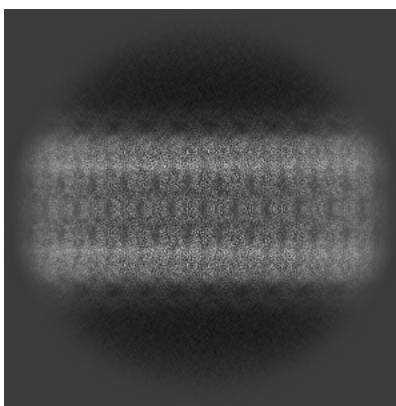
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

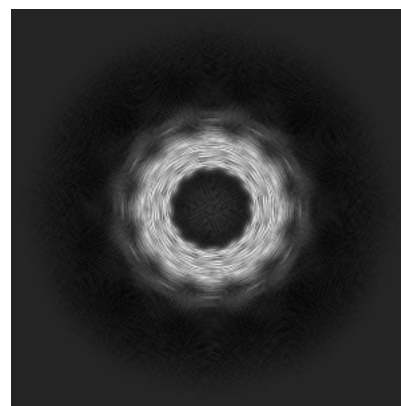
#### 6.1.1 Primary map



X

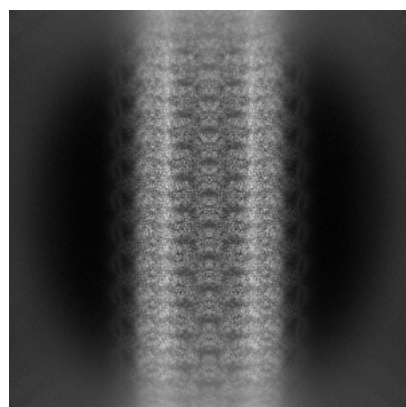


Y

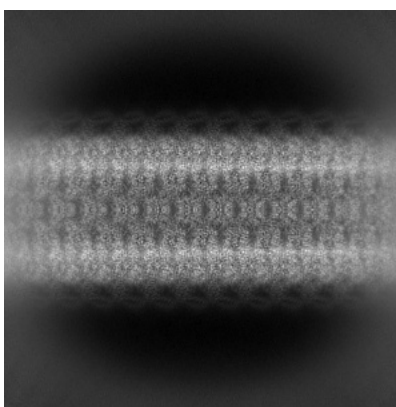


Z

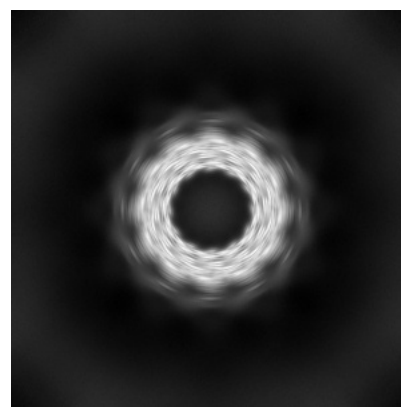
#### 6.1.2 Raw map



X



Y

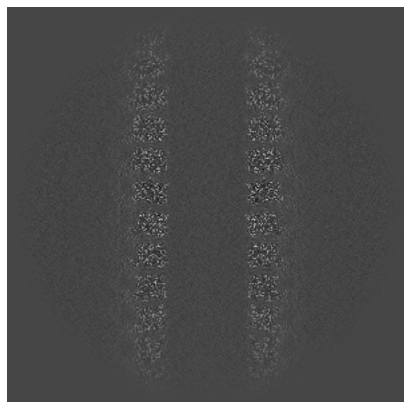


Z

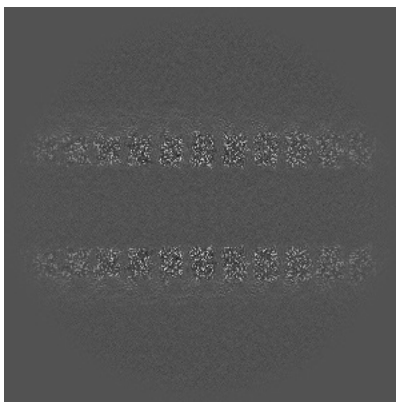
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

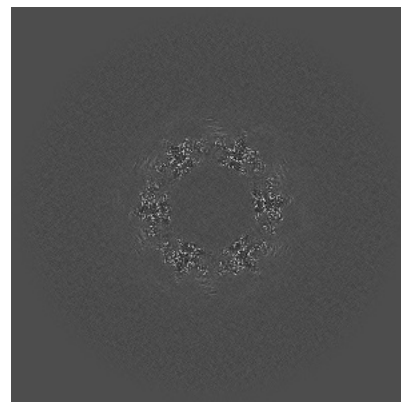
### 6.2.1 Primary map



X Index: 432

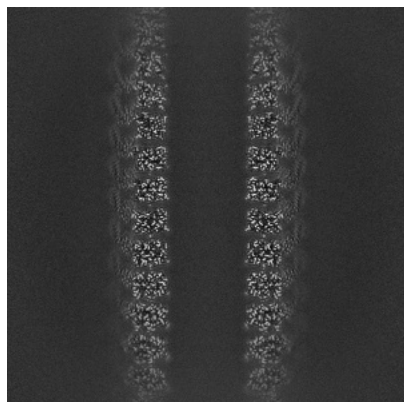


Y Index: 432

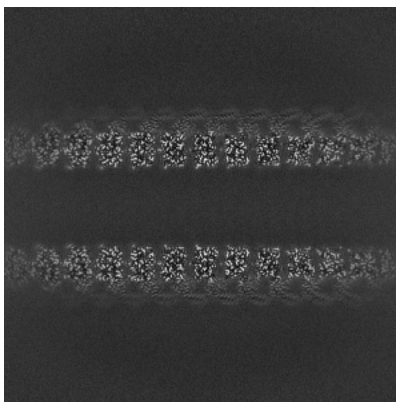


Z Index: 432

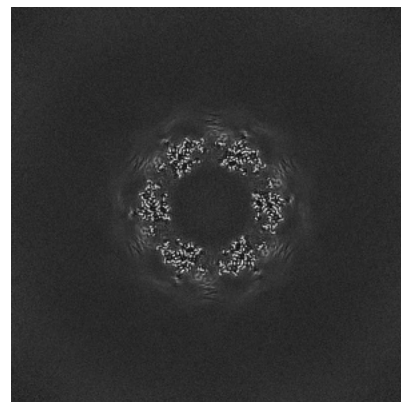
### 6.2.2 Raw map



X Index: 432



Y Index: 432



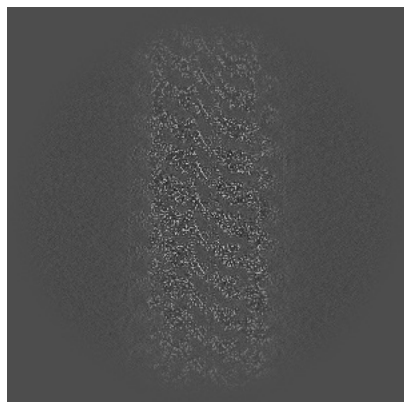
Z Index: 432

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

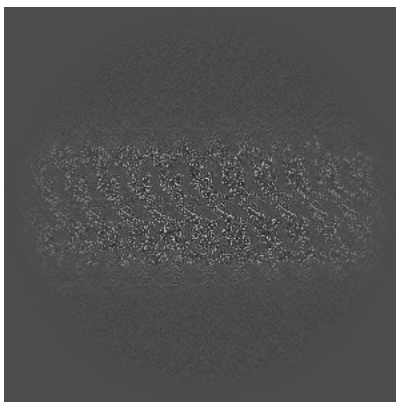


## 6.3 Largest variance slices [i](#)

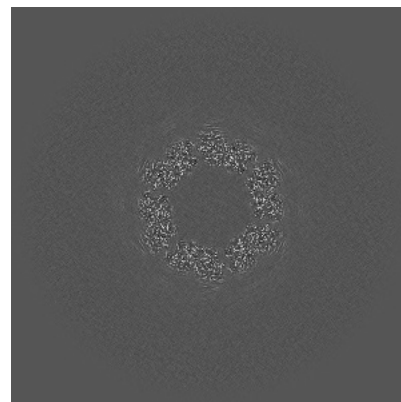
### 6.3.1 Primary map



X Index: 339

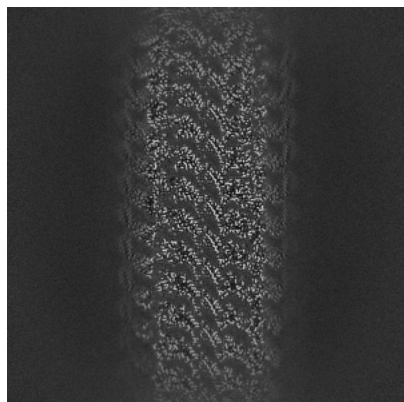


Y Index: 525

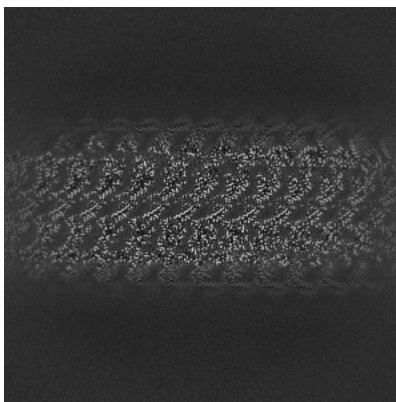


Z Index: 449

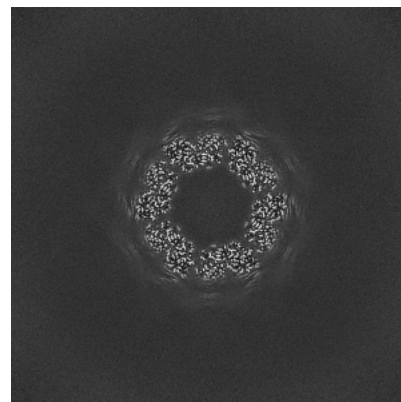
### 6.3.2 Raw map



X Index: 525



Y Index: 525



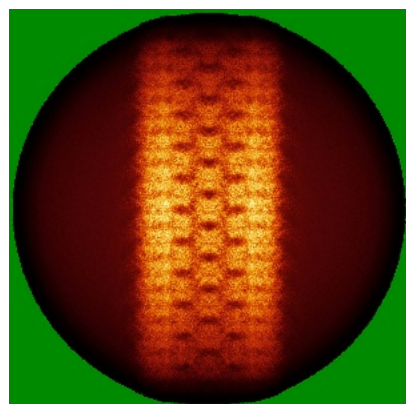
Z Index: 448

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

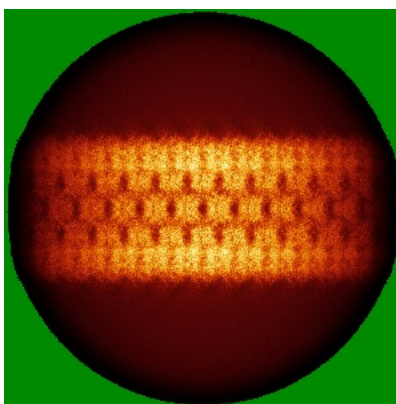


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

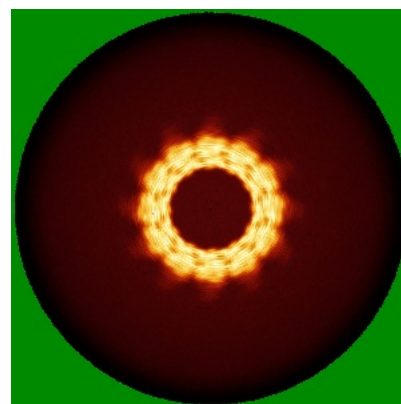
### 6.4.1 Primary map



X

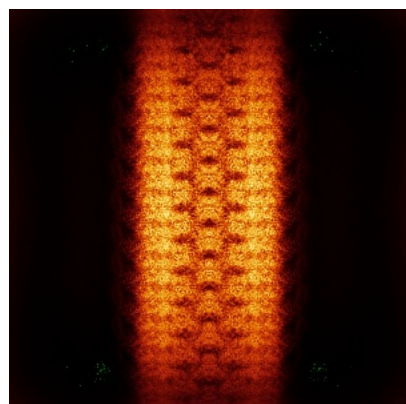


Y

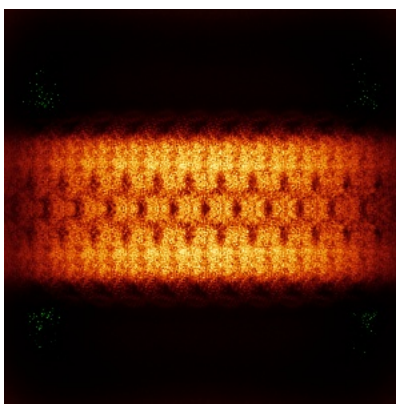


Z

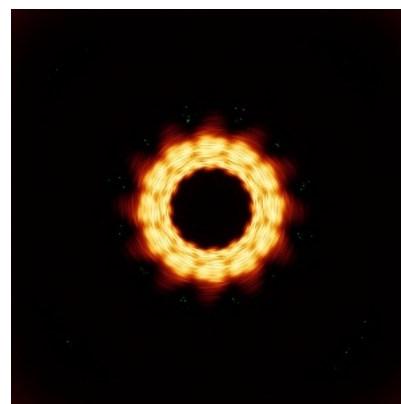
### 6.4.2 Raw map



X



Y

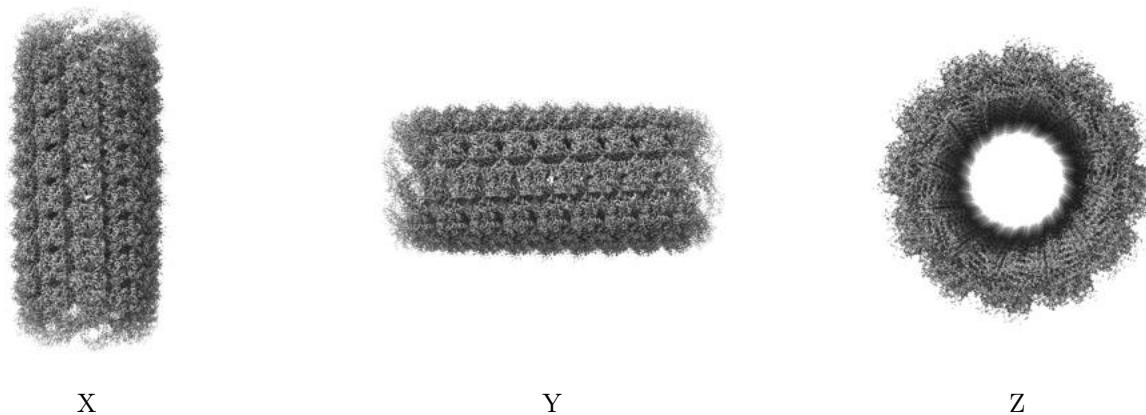


Z

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

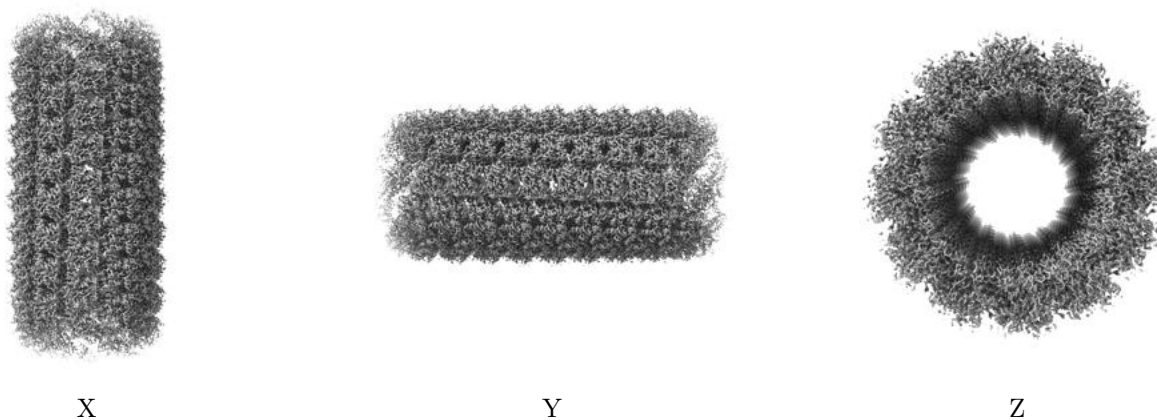
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.736. 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.

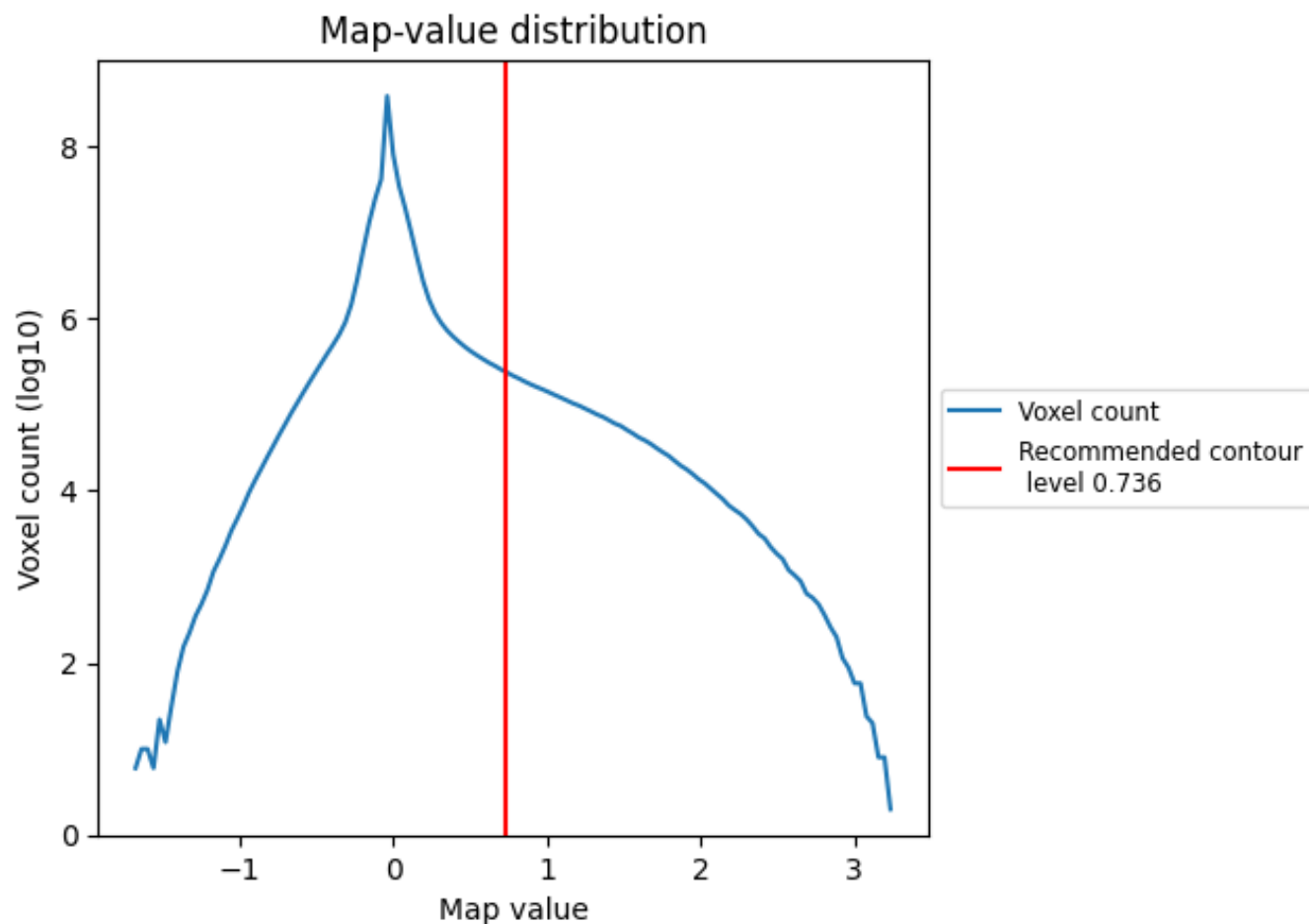
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

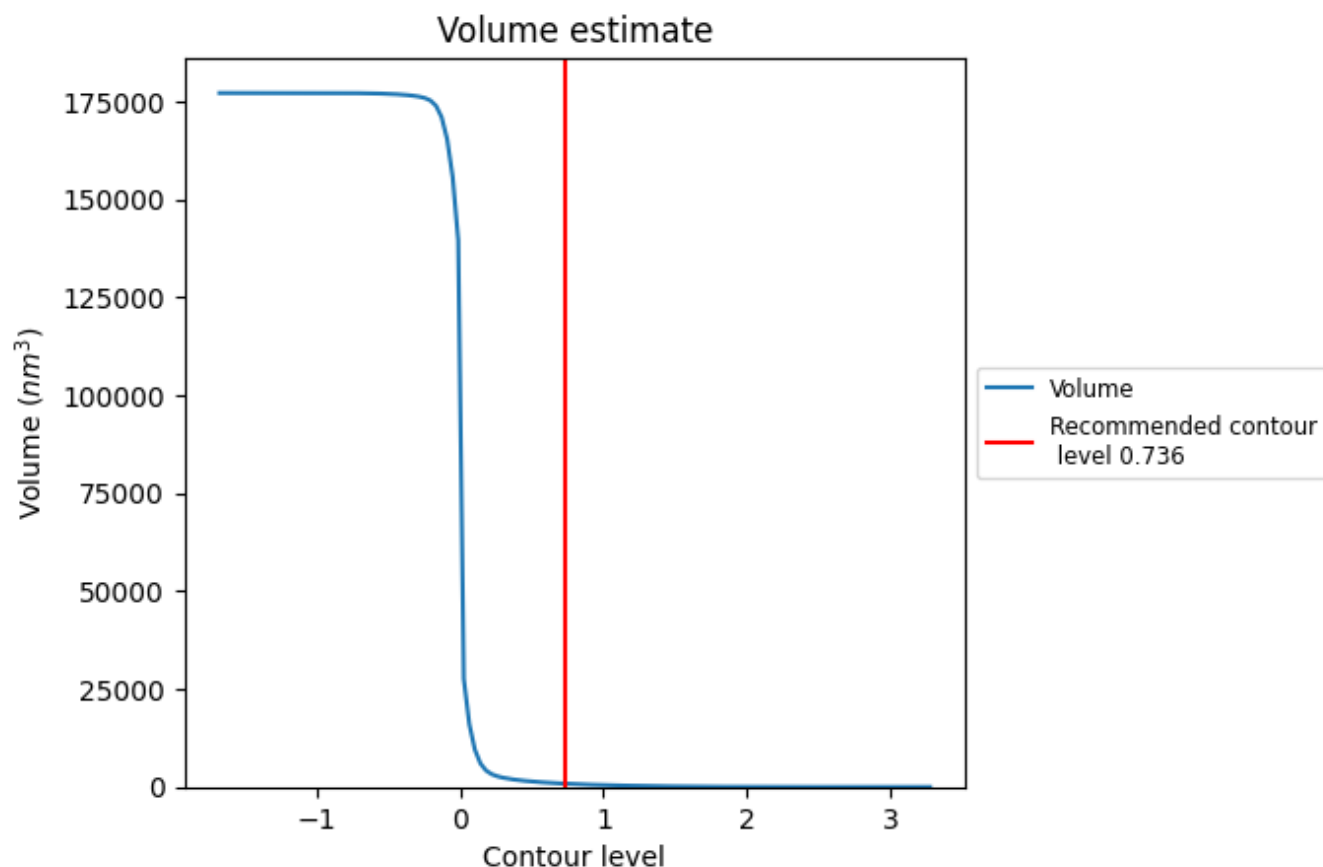
This section contains the results of statistical analysis of the map.

### 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.

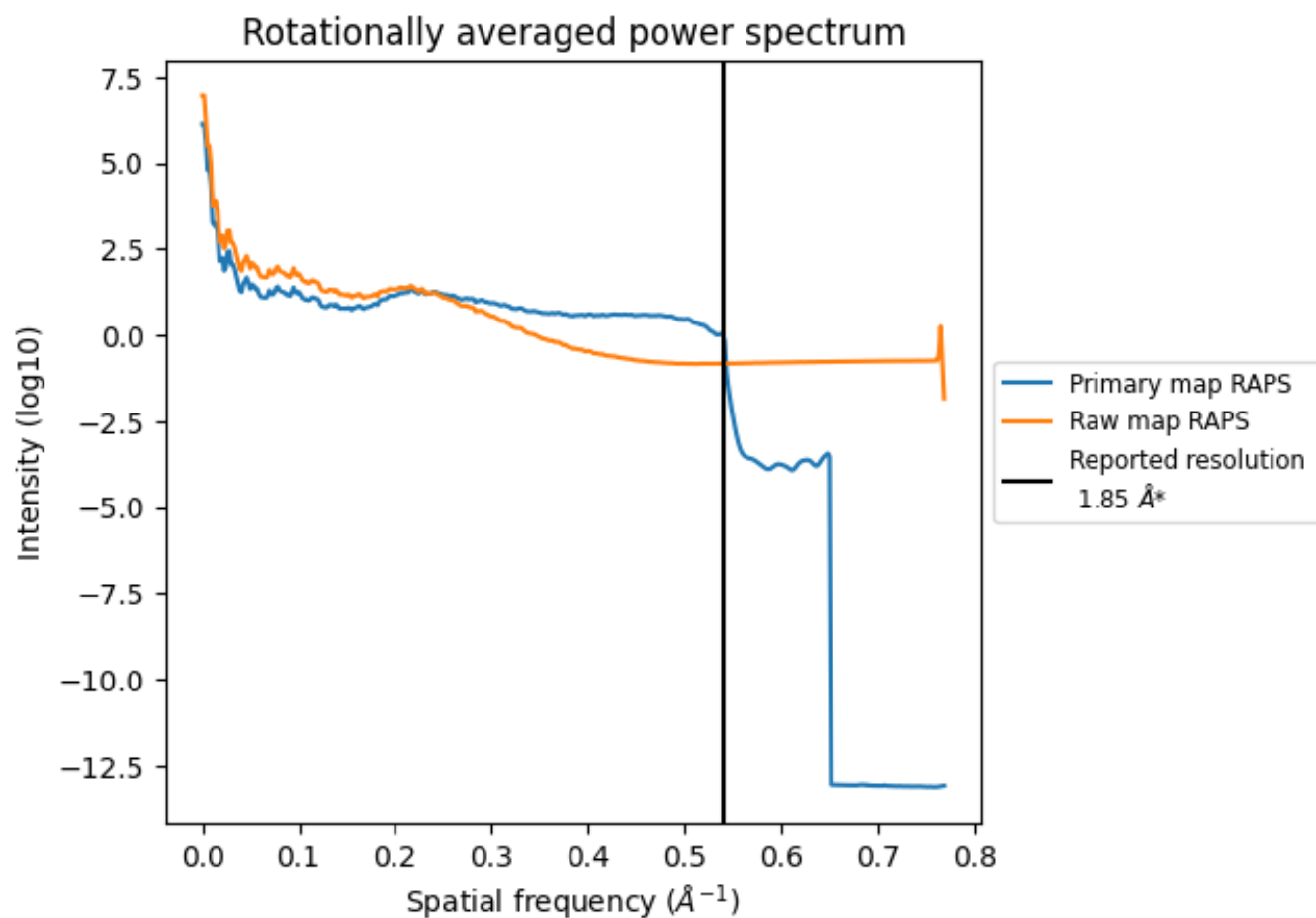
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836  $\text{nm}^3$ ; this corresponds to an approximate mass of 755 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 ⓘ

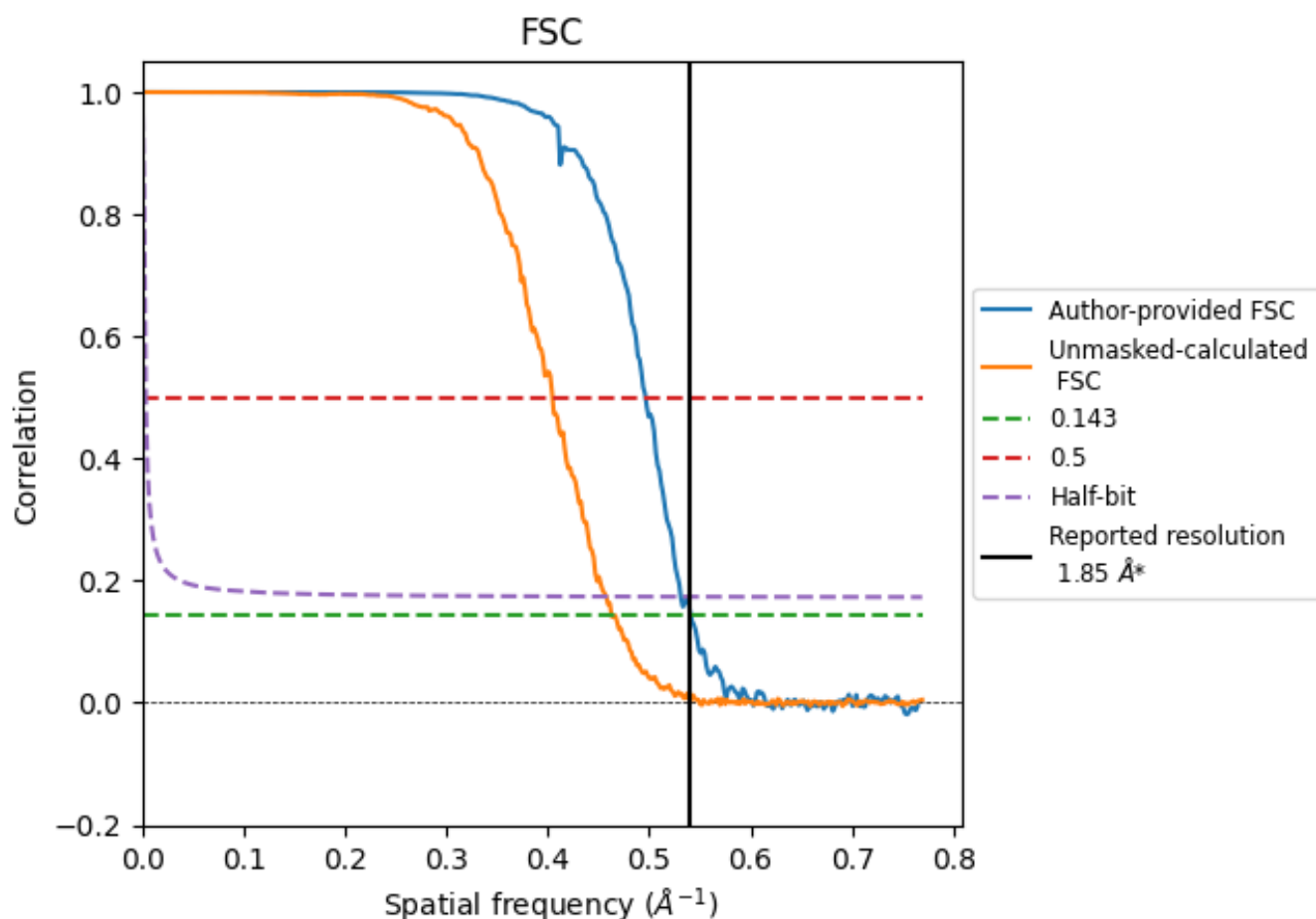


\*Reported resolution corresponds to spatial frequency of 0.541  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

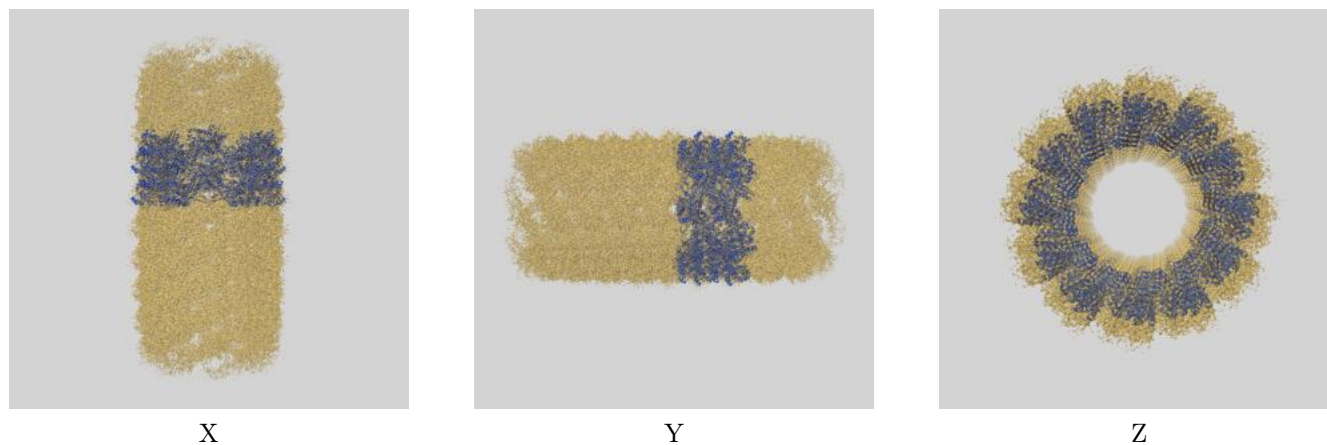
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.85	-	-
Author-provided FSC curve	1.85	2.01	1.88
Unmasked-calculated*	2.16	2.47	2.18

\*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 2.16 differs from the reported value 1.85 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-48906 and PDB model 9N4V. Per-residue inclusion information can be found in section [3](#) on page [10](#).

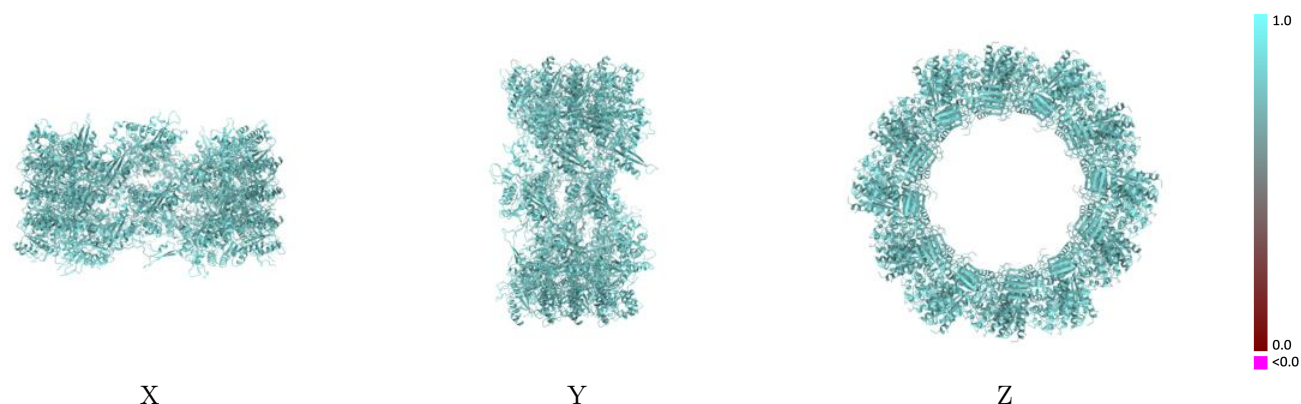
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.736 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.

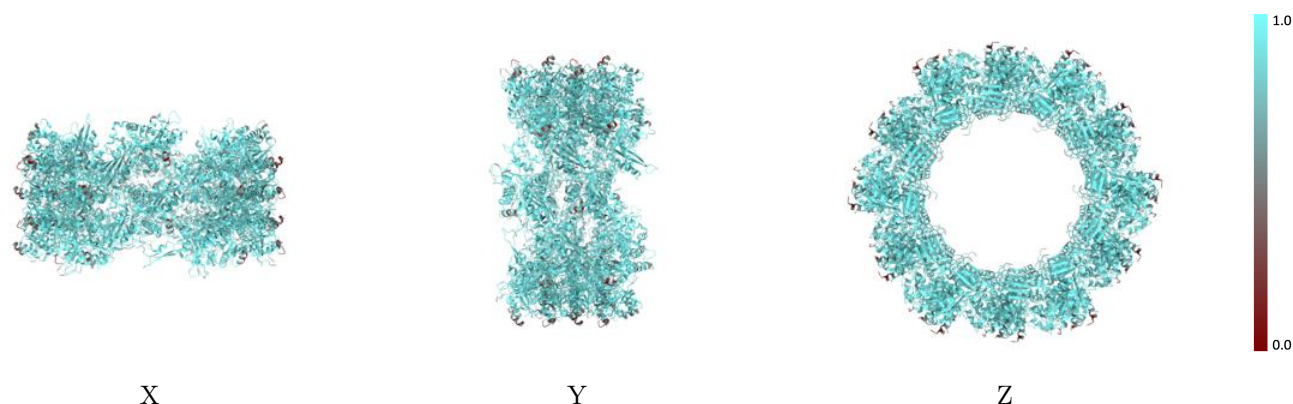


## 9.2 Q-score mapped to coordinate model [i](#)



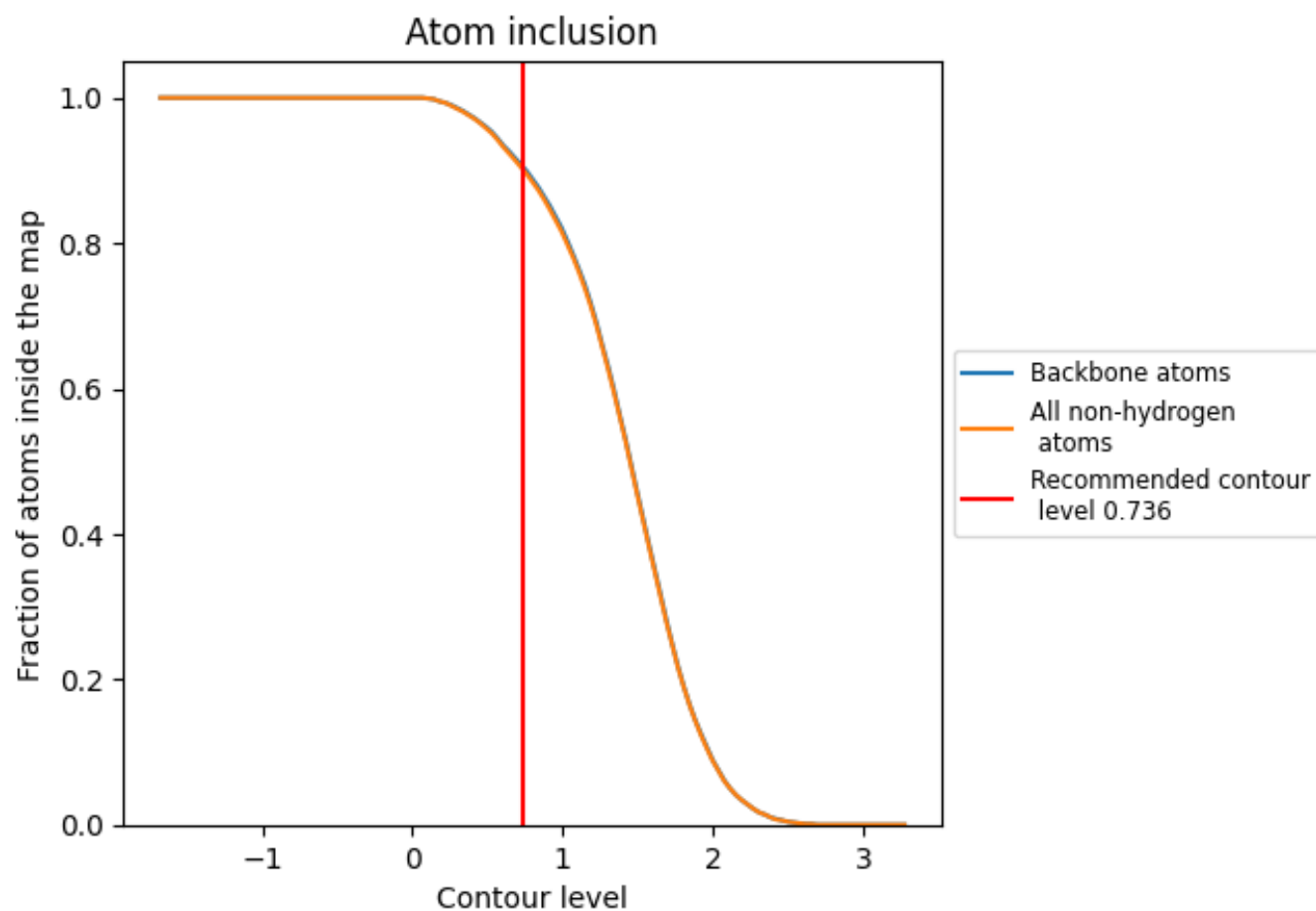
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.736).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.736) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.8070
A	 0.9220	 0.8130
B	 0.8410	 0.7880
C	 0.9260	 0.8140
D	 0.8450	 0.7880
E	 0.9060	 0.8070
F	 0.8130	 0.7840
G	 0.9240	 0.8130
H	 0.8390	 0.7900
I	 0.9190	 0.8100
J	 0.8230	 0.7880
K	 0.9270	 0.8140
L	 0.8530	 0.7890
M	 0.9040	 0.8060
N	 0.8090	 0.7830
O	 0.9060	 0.8060
P	 0.8150	 0.7850
Q	 0.9210	 0.8130
R	 0.8350	 0.7900
S	 0.9160	 0.8110
T	 0.8270	 0.7870
U	 0.9260	 0.8140
V	 0.8470	 0.7910
W	 0.9050	 0.8070
X	 0.8110	 0.7830
Y	 0.9240	 0.8130
Z	 0.8390	 0.7900
a	 0.9190	 0.8110
b	 0.8250	 0.7870
c	 0.9270	 0.8140
d	 0.8530	 0.7890
e	 0.9030	 0.8070
f	 0.8110	 0.7840
g	 0.9230	 0.8130
h	 0.8390	 0.7890



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Chain	Atom inclusion	Q-score
i	 0.9170	 0.8110
j	 0.8270	 0.7870
k	 0.9270	 0.8140
l	 0.8450	 0.7890
m	 0.9060	 0.8070
n	 0.8150	 0.7840
o	 0.9210	 0.8130
p	 0.8350	 0.7900
q	 0.9160	 0.8100
r	 0.8270	 0.7860
s	 0.9270	 0.8130
t	 0.8450	 0.7870
u	 0.9180	 0.8110
v	 0.8270	 0.7870