



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:01 AM UTC

PDB ID : 7OFQ / pdb_00007ofq
EMDB ID : EMD-12875
Title : The archaellum of Methanocaldococcus villosus
Authors : Isupov, M.; Gambelli, L.; Daum, B.
Deposited on : 2021-05-05
Resolution : 3.08 Å(reported)
Based on initial model : 5O4U

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

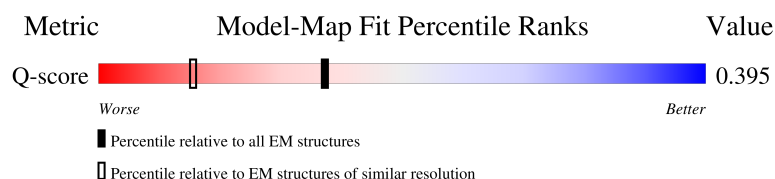
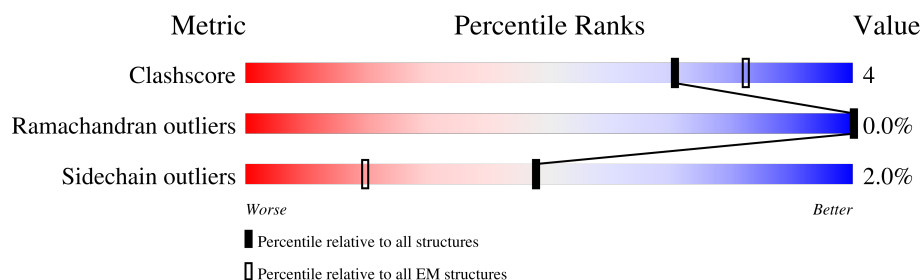
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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

Mol	Chain	Length	Quality of chain
1	A	209	13% 96% .
1	C	209	11% 95% ..
1	E	209	13% 95% ..
1	G	209	11% 95% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	209	14% 95% ..
1	K	209	17% 95% ..
1	M	209	25% 96% .
1	O	209	40% 95% ..
1	Q	209	12% 96% ..
1	S	209	11% 95% ..
1	U	209	12% 96% ..
1	W	209	12% 96% .
1	Y	209	11% 95% ..
1	a	209	15% 96% ..
1	c	209	20% 95% ..
1	e	209	14% 95% ..
1	g	209	11% 95% .
1	i	209	9% 95% ..
1	k	209	10% 94% 5% .
1	m	209	12% 95% ..
1	o	209	11% 95% ..
1	q	209	19% 95% .
1	s	209	49% 96% ..
2	B	213	10% 90% 9% .
2	D	213	9% 90% 8% .
2	F	213	10% 89% 9% .
2	H	213	9% 90% 9% .
2	J	213	12% 90% 8% .
2	L	213	17% 91% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	213	
2	P	213	
2	R	213	
2	T	213	
2	V	213	
2	X	213	
2	Z	213	
2	b	213	
2	d	213	
2	f	213	
2	h	213	
2	j	213	
2	l	213	
2	n	213	
2	p	213	
2	r	213	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	B	302	-	-	X	-
4	UNL	B	310	-	-	X	-
4	UNL	B	311	-	-	X	-
4	UNL	D	302	-	-	X	-
4	UNL	D	310	-	-	X	-
4	UNL	D	311	-	-	X	-
4	UNL	F	302	-	-	X	-
4	UNL	F	310	-	-	X	-
4	UNL	F	311	-	-	X	-
4	UNL	H	302	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	H	310	-	-	X	-
4	UNL	H	311	-	-	X	-
4	UNL	J	302	-	-	X	-
4	UNL	J	310	-	-	X	-
4	UNL	J	311	-	-	X	-
4	UNL	L	302	-	-	X	-
4	UNL	L	310	-	-	X	-
4	UNL	L	311	-	-	X	-
4	UNL	N	302	-	-	X	-
4	UNL	N	310	-	-	X	-
4	UNL	N	311	-	-	X	-
4	UNL	P	302	-	-	X	-
4	UNL	P	310	-	-	X	-
4	UNL	P	311	-	-	X	-
4	UNL	R	302	-	-	X	-
4	UNL	R	310	-	-	X	-
4	UNL	R	311	-	-	X	-
4	UNL	T	302	-	-	X	-
4	UNL	T	310	-	-	X	-
4	UNL	T	311	-	-	X	-
4	UNL	V	302	-	-	X	-
4	UNL	V	310	-	-	X	-
4	UNL	V	311	-	-	X	-
4	UNL	X	302	-	-	X	-
4	UNL	X	310	-	-	X	-
4	UNL	X	311	-	-	X	-
4	UNL	Z	302	-	-	X	-
4	UNL	Z	310	-	-	X	-
4	UNL	Z	311	-	-	X	-
4	UNL	b	302	-	-	X	-
4	UNL	b	310	-	-	X	-
4	UNL	b	311	-	-	X	-
4	UNL	d	302	-	-	X	-
4	UNL	d	310	-	-	X	-
4	UNL	d	311	-	-	X	-
4	UNL	f	302	-	-	X	-
4	UNL	f	310	-	-	X	-
4	UNL	f	311	-	-	X	-
4	UNL	h	302	-	-	X	-
4	UNL	h	310	-	-	X	-
4	UNL	h	311	-	-	X	-
4	UNL	j	302	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	j	310	-	-	X	-
4	UNL	j	311	-	-	X	-
4	UNL	l	302	-	-	X	-
4	UNL	l	306	-	-	X	-
4	UNL	l	310	-	-	X	-
4	UNL	l	311	-	-	X	-
4	UNL	n	302	-	-	X	-
4	UNL	n	310	-	-	X	-
4	UNL	n	311	-	-	X	-
4	UNL	o	302	-	-	X	-
4	UNL	p	302	-	-	X	-
4	UNL	p	310	-	-	X	-
4	UNL	p	311	-	-	X	-
4	UNL	r	302	-	-	X	-
4	UNL	r	310	-	-	X	-
4	UNL	r	311	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 80691 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 Archaeollin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	C	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	E	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	G	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	I	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	K	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	M	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	O	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	Q	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	S	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	U	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	W	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	Y	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	a	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	c	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	e	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	g	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	k	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	m	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	o	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	q	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	s	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		

- Molecule 2 is a protein called Archaeollin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	D	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	F	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	H	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	J	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	L	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	N	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	P	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	R	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	T	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	V	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	X	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	Z	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	d	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	f	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	h	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	j	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	l	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	n	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	p	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	r	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	
3	E	1	Total	Ca	0
			1	1	
3	F	1	Total	Ca	0
			1	1	
3	G	1	Total	Ca	0
			1	1	
3	H	1	Total	Ca	0
			1	1	
3	I	1	Total	Ca	0
			1	1	
3	J	1	Total	Ca	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	K	1	Total 1	Ca 1	0
3	L	1	Total 1	Ca 1	0
3	M	1	Total 1	Ca 1	0
3	N	1	Total 1	Ca 1	0
3	O	1	Total 1	Ca 1	0
3	P	1	Total 1	Ca 1	0
3	Q	1	Total 1	Ca 1	0
3	R	1	Total 1	Ca 1	0
3	S	1	Total 1	Ca 1	0
3	T	1	Total 1	Ca 1	0
3	U	1	Total 1	Ca 1	0
3	V	1	Total 1	Ca 1	0
3	W	1	Total 1	Ca 1	0
3	X	1	Total 1	Ca 1	0
3	Y	1	Total 1	Ca 1	0
3	Z	1	Total 1	Ca 1	0
3	a	1	Total 1	Ca 1	0
3	b	1	Total 1	Ca 1	0
3	c	1	Total 1	Ca 1	0
3	d	1	Total 1	Ca 1	0
3	e	1	Total 1	Ca 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	f	1	Total 1	Ca 1	0
3	g	1	Total 1	Ca 1	0
3	h	1	Total 1	Ca 1	0
3	i	1	Total 1	Ca 1	0
3	j	1	Total 1	Ca 1	0
3	k	1	Total 1	Ca 1	0
3	l	1	Total 1	Ca 1	0
3	m	1	Total 1	Ca 1	0
3	n	1	Total 1	Ca 1	0
3	o	1	Total 1	Ca 1	0
3	p	1	Total 1	Ca 1	0
3	q	1	Total 1	Ca 1	0
3	r	1	Total 1	Ca 1	0
3	s	1	Total 1	Ca 1	0

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
4	A	12	Total 156	C 87	N 6	O 63	0
4	B	24	Total 312	C 174	N 12	O 126	0
4	C	12	Total 156	C 87	N 6	O 63	0
4	D	24	Total 312	C 174	N 12	O 126	0
4	E	12	Total 156	C 87	N 6	O 63	0

Continued on next page...

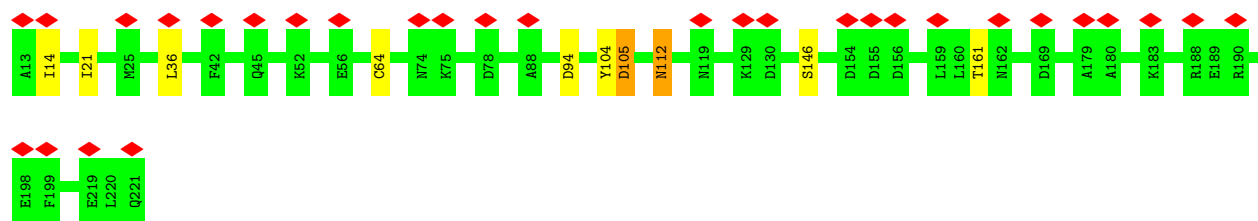
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	F	24	Total	C	N	O	0
			312	174	12	126	
4	G	12	Total	C	N	O	0
			156	87	6	63	
4	H	24	Total	C	N	O	0
			312	174	12	126	
4	I	12	Total	C	N	O	0
			156	87	6	63	
4	J	24	Total	C	N	O	0
			312	174	12	126	
4	K	12	Total	C	N	O	0
			156	87	6	63	
4	L	24	Total	C	N	O	0
			312	174	12	126	
4	M	12	Total	C	N	O	0
			156	87	6	63	
4	N	24	Total	C	N	O	0
			312	174	12	126	
4	O	12	Total	C	N	O	0
			156	87	6	63	
4	P	24	Total	C	N	O	0
			312	174	12	126	
4	Q	12	Total	C	N	O	0
			156	87	6	63	
4	R	24	Total	C	N	O	0
			312	174	12	126	
4	S	12	Total	C	N	O	0
			156	87	6	63	
4	T	24	Total	C	N	O	0
			312	174	12	126	
4	U	12	Total	C	N	O	0
			156	87	6	63	
4	V	24	Total	C	N	O	0
			312	174	12	126	
4	W	12	Total	C	N	O	0
			156	87	6	63	
4	X	24	Total	C	N	O	0
			312	174	12	126	
4	Y	12	Total	C	N	O	0
			156	87	6	63	
4	Z	24	Total	C	N	O	0
			312	174	12	126	

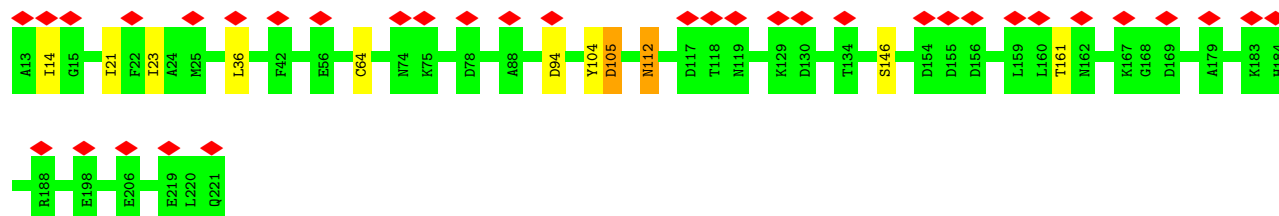
Continued on next page...

Continued from previous page...

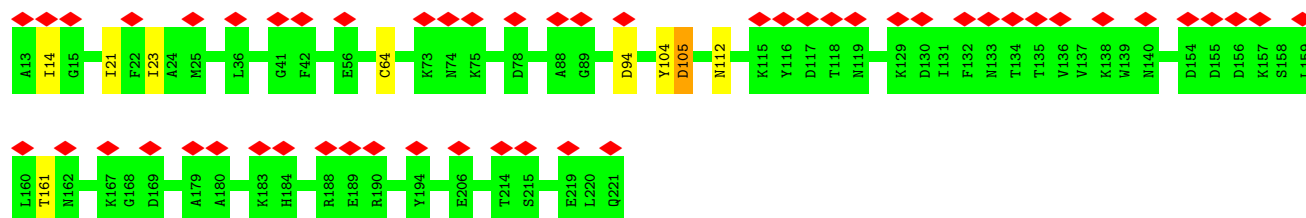
Mol	Chain	Residues	Atoms				AltConf
4	a	13	Total	C	N	O	0
			171	96	6	69	
4	b	23	Total	C	N	O	0
			297	165	12	120	
4	c	12	Total	C	N	O	0
			156	87	6	63	
4	d	24	Total	C	N	O	0
			312	174	12	126	
4	e	12	Total	C	N	O	0
			156	87	6	63	
4	f	24	Total	C	N	O	0
			312	174	12	126	
4	g	12	Total	C	N	O	0
			156	87	6	63	
4	h	24	Total	C	N	O	0
			312	174	12	126	
4	i	12	Total	C	N	O	0
			156	87	6	63	
4	j	24	Total	C	N	O	0
			312	174	12	126	
4	k	12	Total	C	N	O	0
			156	87	6	63	
4	l	24	Total	C	N	O	0
			312	174	12	126	
4	m	12	Total	C	N	O	0
			156	87	6	63	
4	n	24	Total	C	N	O	0
			312	174	12	126	
4	o	12	Total	C	N	O	0
			156	87	6	63	
4	p	24	Total	C	N	O	0
			312	174	12	126	
4	q	12	Total	C	N	O	0
			156	87	6	63	
4	r	24	Total	C	N	O	0
			312	174	12	126	
4	s	12	Total	C	N	O	0
			156	87	6	63	



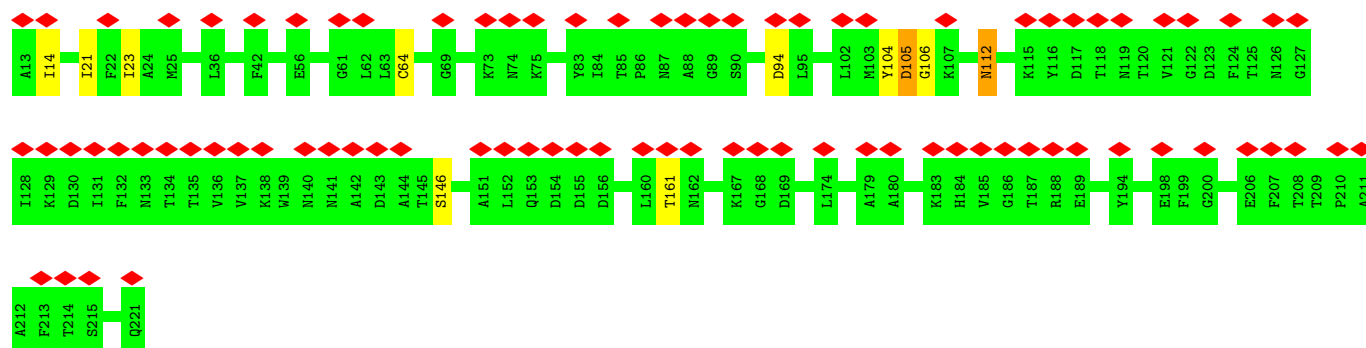
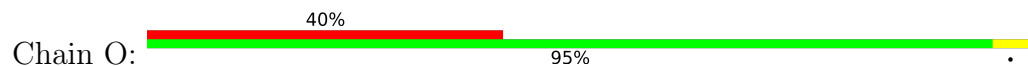
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin

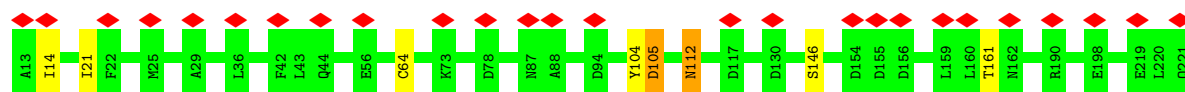


• Molecule 1: Archaeollin

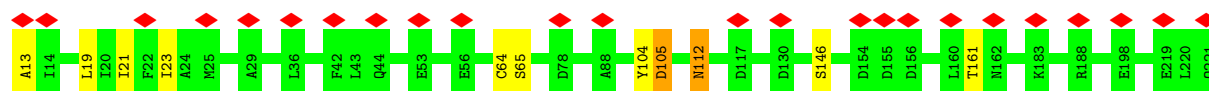


• Molecule 1: Archaeollin

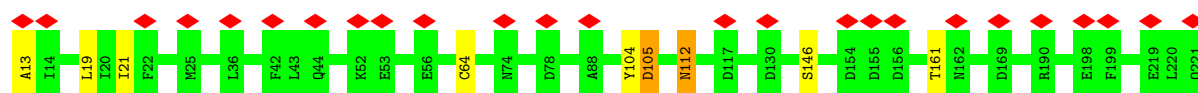




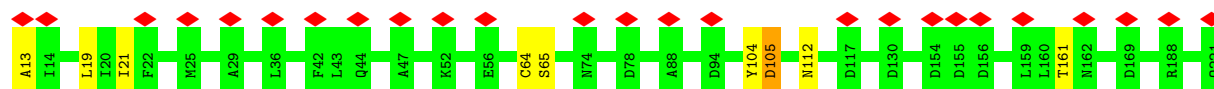
- Molecule 1: Archaeollin



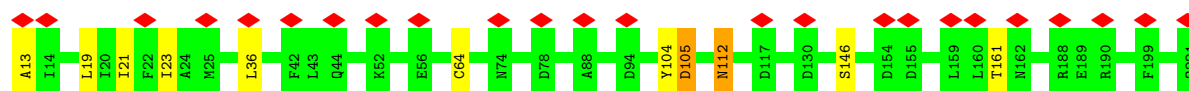
- Molecule 1: Archaeollin



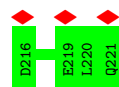
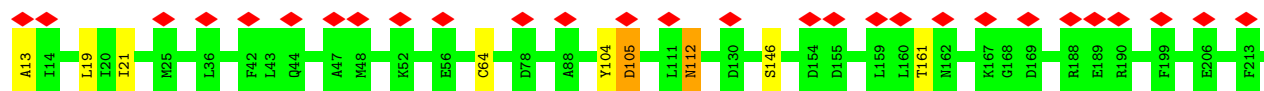
- Molecule 1: Archaeollin



- Molecule 1: Archaeollin

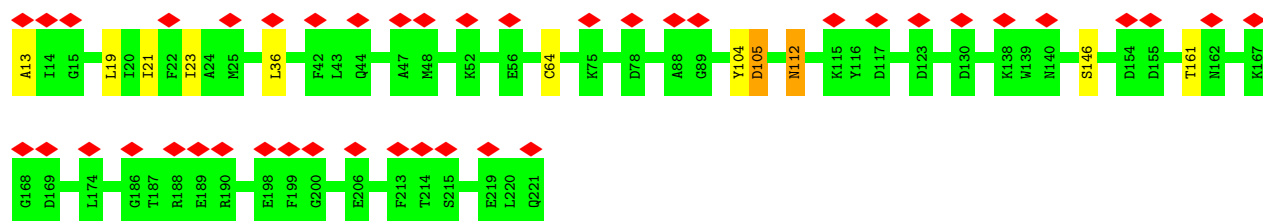


- Molecule 1: Archaeollin

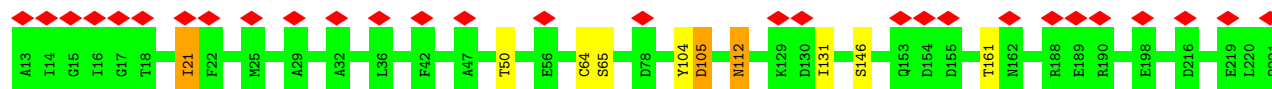


- Molecule 1: Archaeollin





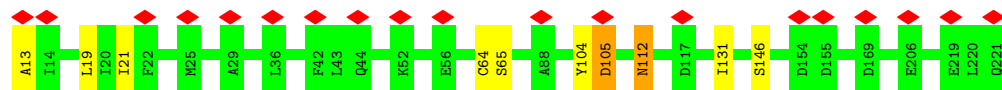
• Molecule 1: Archaeollin



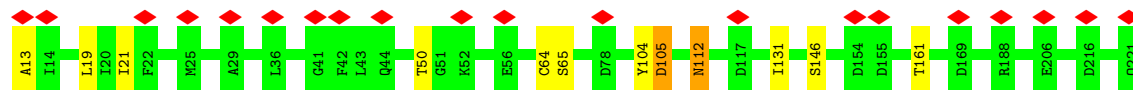
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin



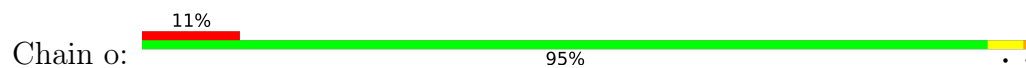
• Molecule 1: Archaeollin

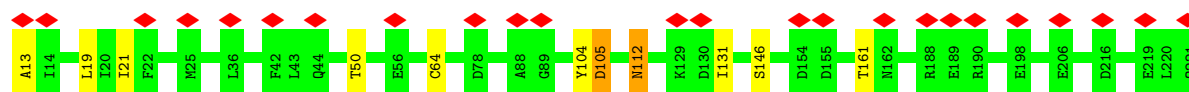


• Molecule 1: Archaeollin

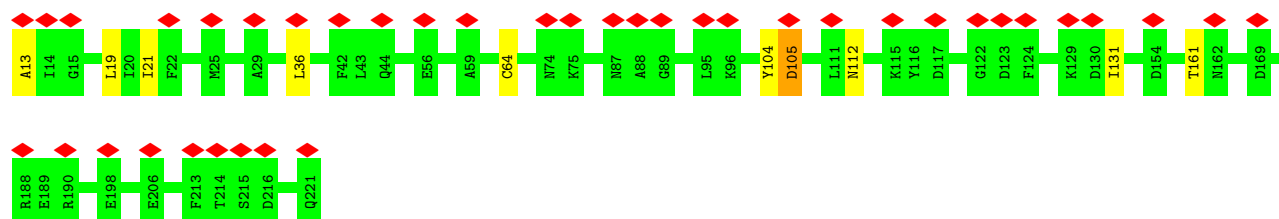


• Molecule 1: Archaeollin

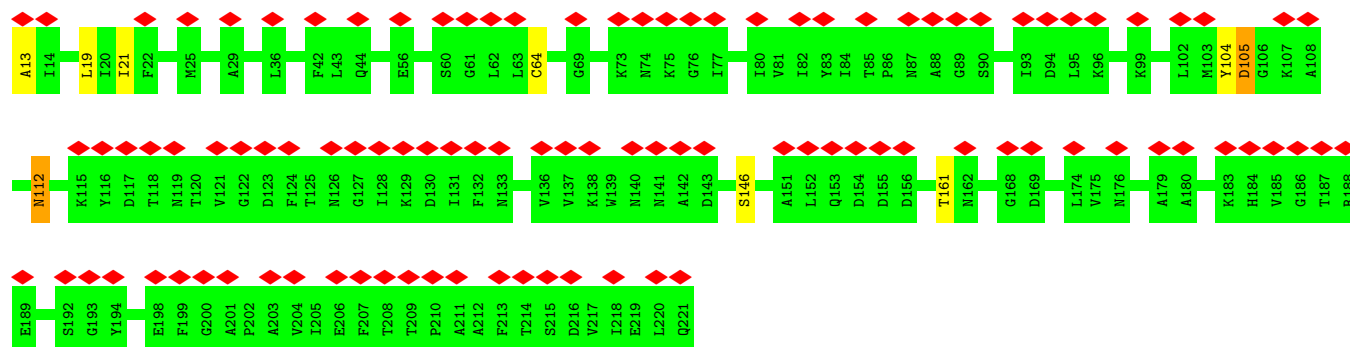




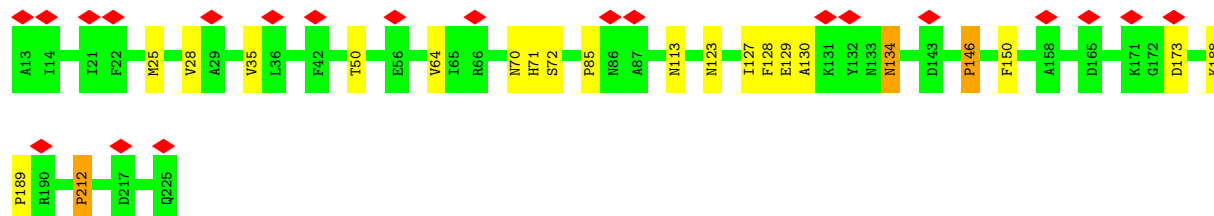
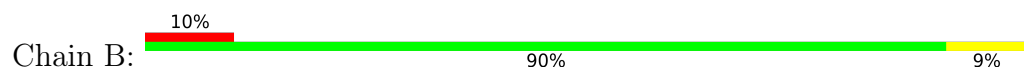
• Molecule 1: Archaeollin



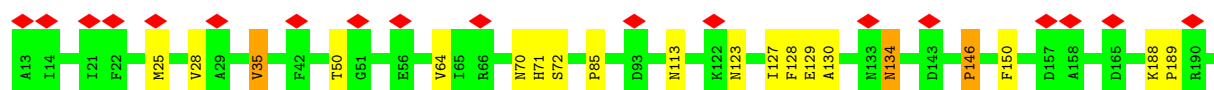
• Molecule 1: Archaeollin

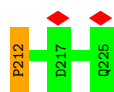


• Molecule 2: Archaeollin

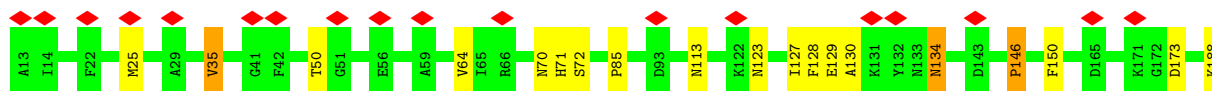
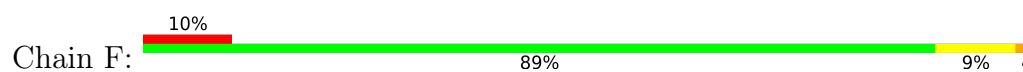


• Molecule 2: Archaeollin

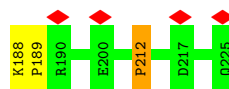
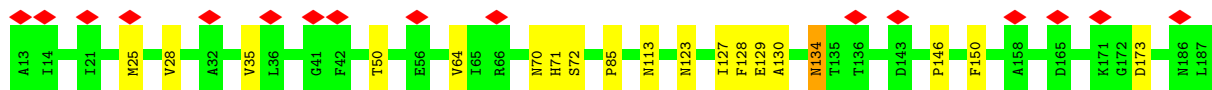
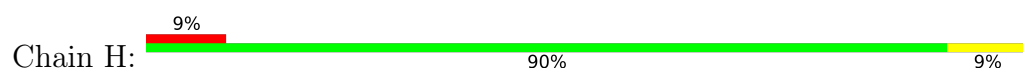




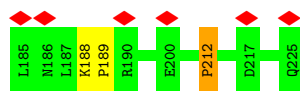
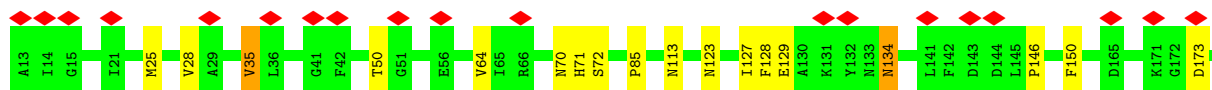
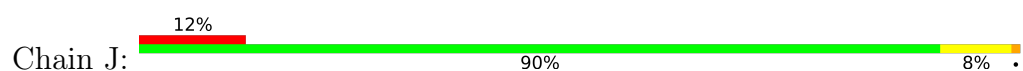
- Molecule 2: Archaeellin



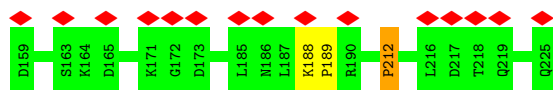
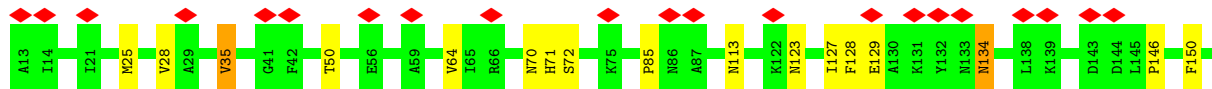
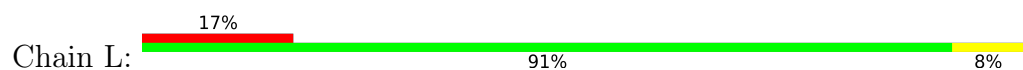
- Molecule 2: Archaeellin



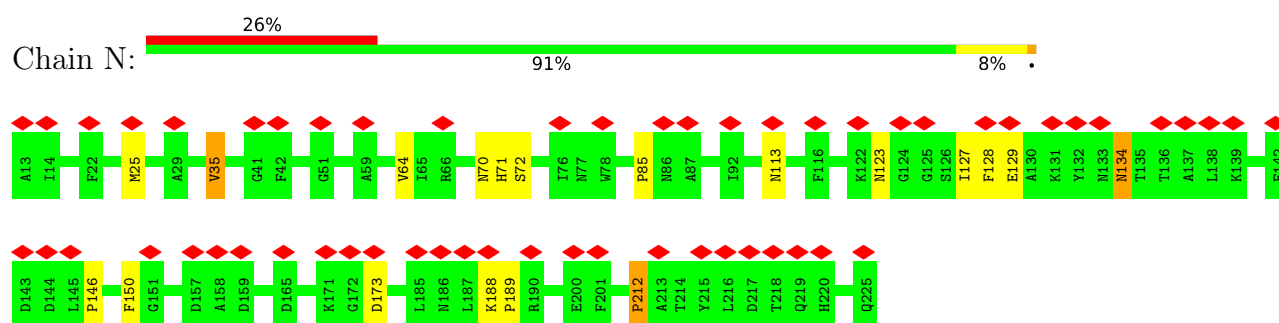
- Molecule 2: Archaeellin



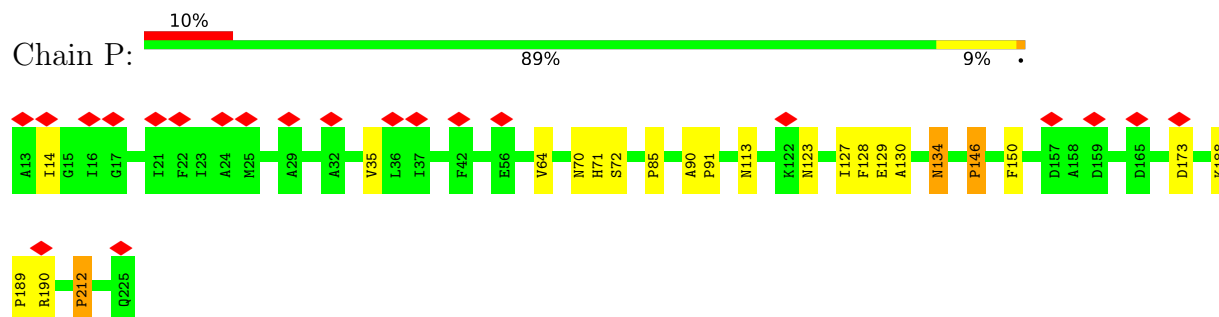
- Molecule 2: Archaeellin



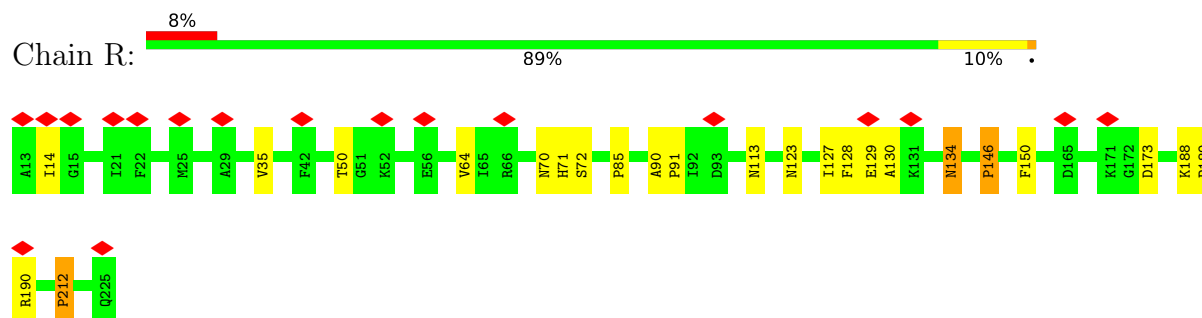
- Molecule 2: Archaeellin



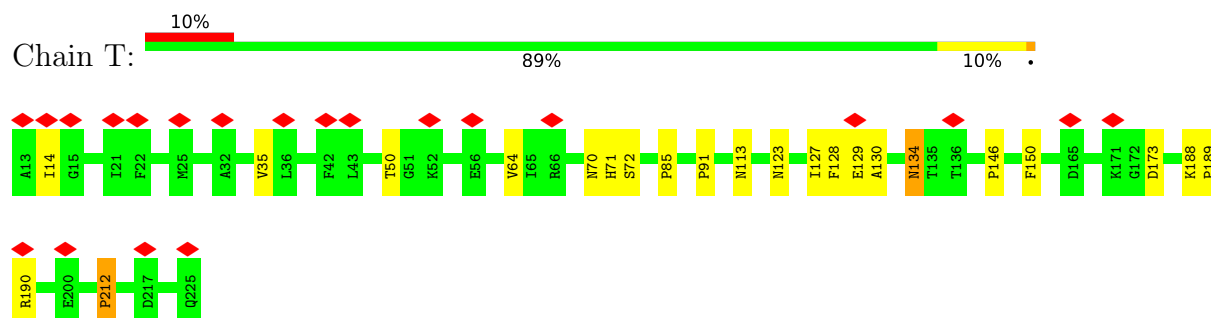
- Molecule 2: Archaeollin



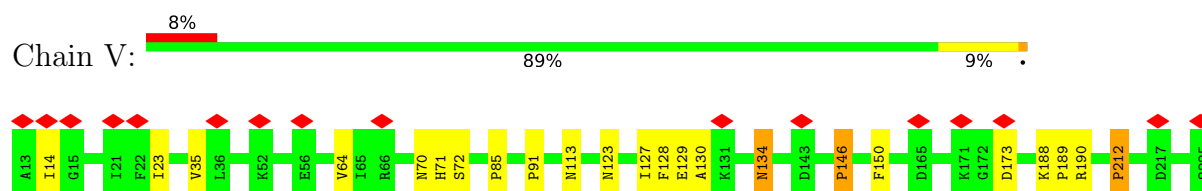
- Molecule 2: Archaeollin



- Molecule 2: Archaeollin

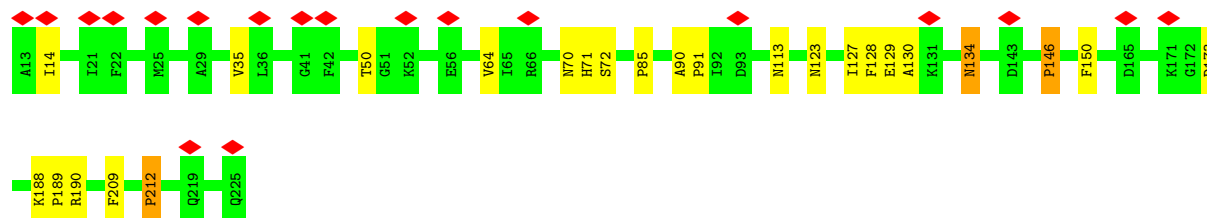


- Molecule 2: Archaeollin



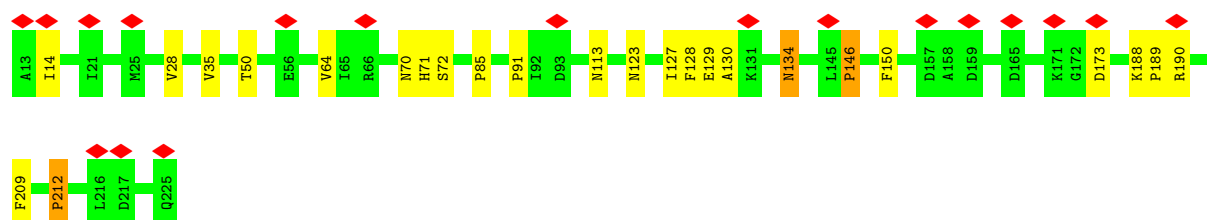
- Molecule 2: Archaeollin

Chain X: 

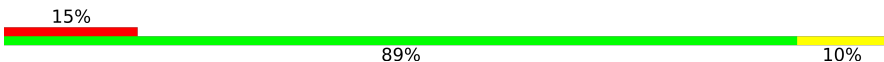


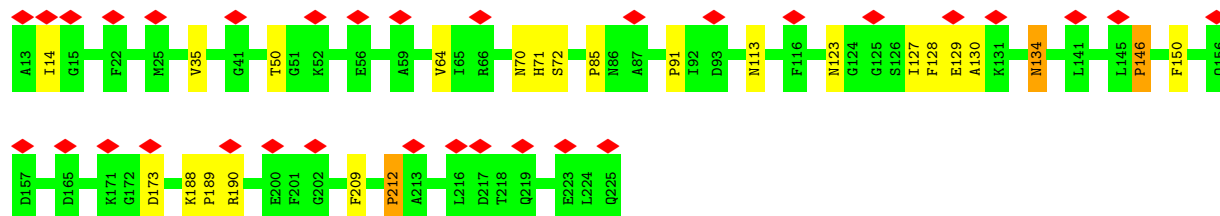
- Molecule 2: Archaeollin

Chain Z: 

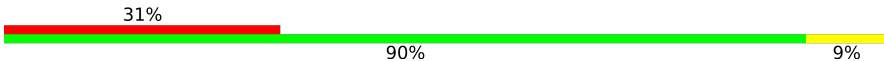


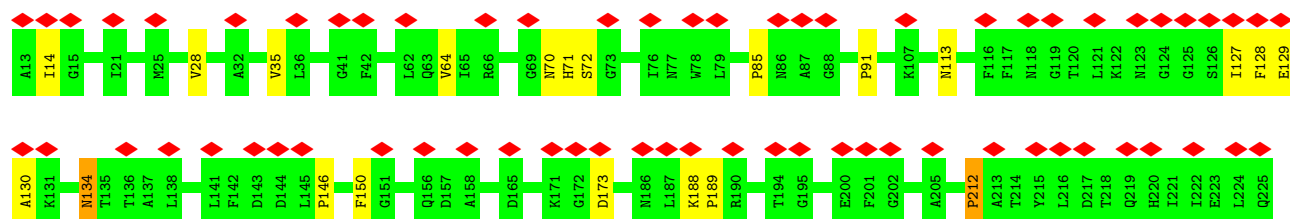
- Molecule 2: Archaeollin

Chain b: 



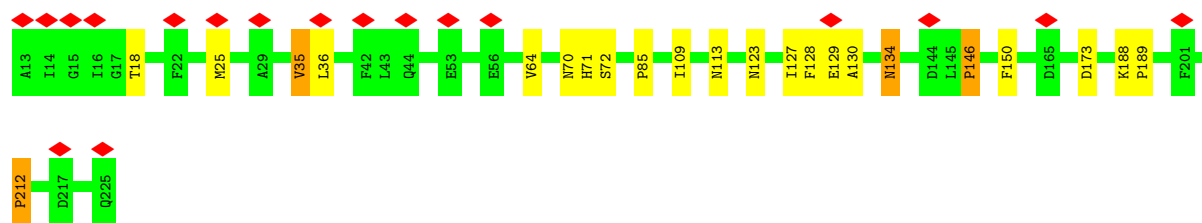
- Molecule 2: Archaeollin

Chain d: 

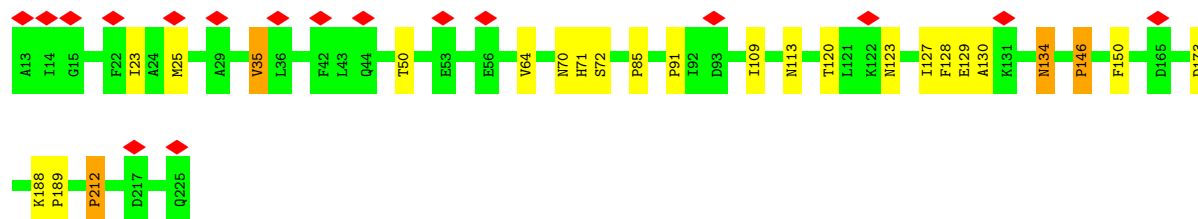
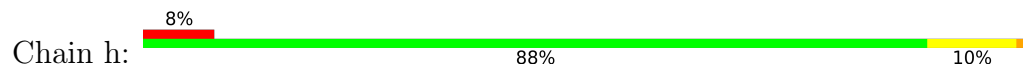


- Molecule 2: Archaeollin

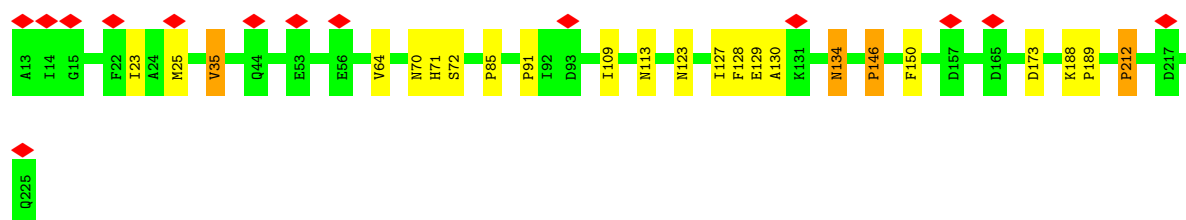
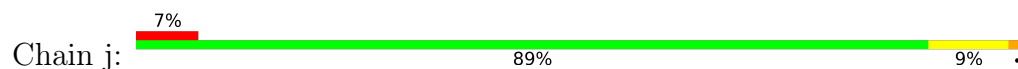
Chain f: 



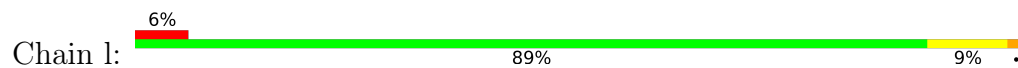
- Molecule 2: Archaelin



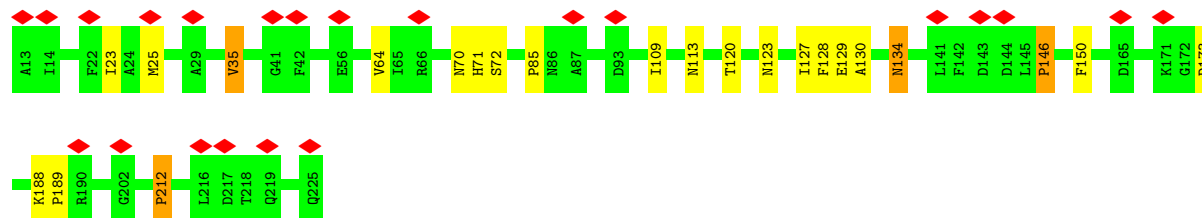
- Molecule 2: Archaelin



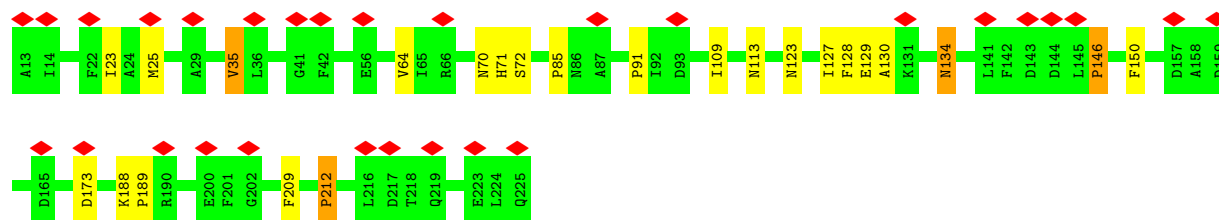
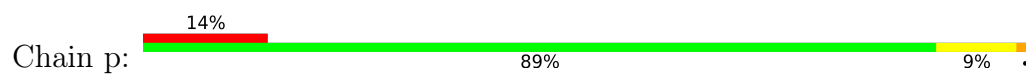
- Molecule 2: Archaelin



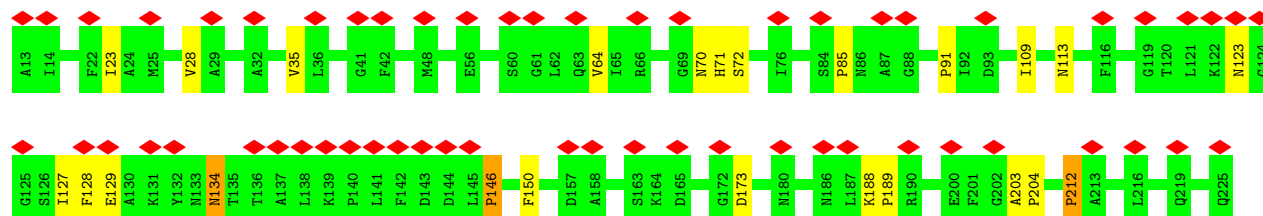
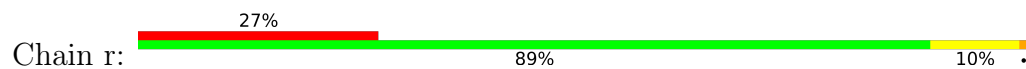
- Molecule 2: Archaelin



- Molecule 2: Archaelin



• Molecule 2: Archaeollin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-71.8°, rise=33.4 Å, axial sym=C1	Depositor
Number of segments used	399178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.073	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, UNL

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	0.67	0/1578	1.25	3/2144 (0.1%)
1	C	0.68	0/1578	1.25	3/2144 (0.1%)
1	E	0.69	0/1578	1.26	3/2144 (0.1%)
1	G	0.68	0/1578	1.25	3/2144 (0.1%)
1	I	0.68	0/1578	1.25	3/2144 (0.1%)
1	K	0.68	0/1578	1.26	3/2144 (0.1%)
1	M	0.66	0/1578	1.26	3/2144 (0.1%)
1	O	0.64	0/1578	1.25	3/2144 (0.1%)
1	Q	0.68	0/1578	1.26	3/2144 (0.1%)
1	S	0.68	0/1578	1.26	4/2144 (0.2%)
1	U	0.68	0/1578	1.25	3/2144 (0.1%)
1	W	0.69	0/1578	1.26	4/2144 (0.2%)
1	Y	0.69	0/1578	1.26	3/2144 (0.1%)
1	a	0.68	0/1578	1.25	3/2144 (0.1%)
1	c	0.66	0/1578	1.25	3/2144 (0.1%)
1	e	0.69	0/1578	1.25	4/2144 (0.2%)
1	g	0.70	0/1578	1.26	4/2144 (0.2%)
1	i	0.70	0/1578	1.26	4/2144 (0.2%)
1	k	0.70	0/1578	1.26	4/2144 (0.2%)
1	m	0.69	0/1578	1.26	4/2144 (0.2%)
1	o	0.69	0/1578	1.25	3/2144 (0.1%)
1	q	0.67	0/1578	1.25	3/2144 (0.1%)
1	s	0.65	0/1578	1.25	3/2144 (0.1%)
2	B	0.71	0/1591	1.27	5/2169 (0.2%)
2	D	0.72	0/1591	1.27	4/2169 (0.2%)
2	F	0.71	0/1591	1.27	5/2169 (0.2%)
2	H	0.71	0/1591	1.27	5/2169 (0.2%)
2	J	0.71	0/1591	1.27	5/2169 (0.2%)
2	L	0.70	0/1591	1.27	4/2169 (0.2%)
2	N	0.67	0/1591	1.26	5/2169 (0.2%)
2	P	0.71	0/1591	1.27	7/2169 (0.3%)
2	R	0.71	0/1591	1.27	7/2169 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	T	0.71	0/1591	1.27	6/2169 (0.3%)
2	V	0.71	0/1591	1.27	6/2169 (0.3%)
2	X	0.71	0/1591	1.27	8/2169 (0.4%)
2	Z	0.71	0/1591	1.27	7/2169 (0.3%)
2	b	0.69	0/1591	1.27	7/2169 (0.3%)
2	d	0.67	0/1591	1.26	6/2169 (0.3%)
2	f	0.71	0/1591	1.27	5/2169 (0.2%)
2	h	0.72	0/1591	1.27	6/2169 (0.3%)
2	j	0.72	0/1591	1.28	6/2169 (0.3%)
2	l	0.72	0/1591	1.28	6/2169 (0.3%)
2	n	0.71	0/1591	1.27	5/2169 (0.2%)
2	p	0.69	0/1591	1.27	7/2169 (0.3%)
2	r	0.67	0/1591	1.26	6/2169 (0.3%)
All	All	0.69	0/71296	1.26	204/97030 (0.2%)

There are no bond length outliers.

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	146	PRO	CB-CA-C	-8.30	100.41	111.12
2	p	146	PRO	CB-CA-C	-8.17	100.58	111.12
2	l	146	PRO	CB-CA-C	-8.17	100.58	111.12
2	j	146	PRO	CB-CA-C	-8.15	100.61	111.12
2	b	146	PRO	CB-CA-C	-8.13	100.63	111.12
2	D	146	PRO	CB-CA-C	-8.10	100.68	111.12
2	R	146	PRO	CB-CA-C	-8.09	100.69	111.12
2	h	146	PRO	CB-CA-C	-8.07	100.71	111.12
2	r	146	PRO	CB-CA-C	-8.01	100.78	111.12
2	f	146	PRO	CB-CA-C	-8.00	100.80	111.12
2	Z	146	PRO	CB-CA-C	-7.99	100.82	111.12
2	V	146	PRO	CB-CA-C	-7.95	100.87	111.12
2	n	146	PRO	CB-CA-C	-7.95	100.87	111.12
2	X	146	PRO	CB-CA-C	-7.93	100.89	111.12
2	P	146	PRO	CB-CA-C	-7.92	100.90	111.12
2	B	146	PRO	CB-CA-C	-7.80	101.06	111.12
2	N	146	PRO	CB-CA-C	-7.71	101.18	111.12
2	L	146	PRO	CB-CA-C	-7.68	101.21	111.12
2	d	146	PRO	CB-CA-C	-7.63	101.28	111.12
2	J	146	PRO	CB-CA-C	-7.58	101.34	111.12
2	T	146	PRO	CB-CA-C	-7.54	101.39	111.12
2	H	146	PRO	CB-CA-C	-7.32	101.68	111.12
2	J	150	PHE	CA-CB-CG	6.96	120.75	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	150	PHE	CA-CB-CG	6.94	120.74	113.80
2	N	150	PHE	CA-CB-CG	6.92	120.72	113.80
2	H	150	PHE	CA-CB-CG	6.86	120.66	113.80
2	r	150	PHE	CA-CB-CG	6.84	120.64	113.80
2	T	150	PHE	CA-CB-CG	6.84	120.64	113.80
2	V	150	PHE	CA-CB-CG	6.83	120.63	113.80
2	p	150	PHE	CA-CB-CG	6.81	120.61	113.80
2	F	150	PHE	CA-CB-CG	6.79	120.59	113.80
2	D	150	PHE	CA-CB-CG	6.79	120.59	113.80
2	n	150	PHE	CA-CB-CG	6.78	120.58	113.80
2	B	150	PHE	CA-CB-CG	6.74	120.54	113.80
2	d	150	PHE	CA-CB-CG	6.74	120.54	113.80
2	X	150	PHE	CA-CB-CG	6.71	120.51	113.80
2	l	150	PHE	CA-CB-CG	6.71	120.51	113.80
1	E	112	ASN	CA-CB-CG	6.71	119.31	112.60
2	Z	150	PHE	CA-CB-CG	6.68	120.48	113.80
2	j	150	PHE	CA-CB-CG	6.67	120.47	113.80
2	h	150	PHE	CA-CB-CG	6.65	120.45	113.80
2	R	150	PHE	CA-CB-CG	6.64	120.44	113.80
2	b	150	PHE	CA-CB-CG	6.64	120.44	113.80
2	P	150	PHE	CA-CB-CG	6.64	120.44	113.80
1	M	112	ASN	CA-CB-CG	6.61	119.21	112.60
1	K	112	ASN	CA-CB-CG	6.60	119.20	112.60
1	k	112	ASN	CA-CB-CG	6.60	119.20	112.60
2	f	150	PHE	CA-CB-CG	6.60	120.40	113.80
1	G	112	ASN	CA-CB-CG	6.59	119.19	112.60
1	I	112	ASN	CA-CB-CG	6.58	119.18	112.60
1	c	112	ASN	CA-CB-CG	6.52	119.12	112.60
1	g	112	ASN	CA-CB-CG	6.51	119.11	112.60
1	a	112	ASN	CA-CB-CG	6.50	119.10	112.60
1	m	112	ASN	CA-CB-CG	6.50	119.10	112.60
1	i	112	ASN	CA-CB-CG	6.49	119.09	112.60
1	q	112	ASN	CA-CB-CG	6.49	119.09	112.60
1	O	112	ASN	CA-CB-CG	6.49	119.09	112.60
1	s	112	ASN	CA-CB-CG	6.45	119.05	112.60
1	C	112	ASN	CA-CB-CG	6.45	119.05	112.60
1	Y	112	ASN	CA-CB-CG	6.39	118.99	112.60
1	o	112	ASN	CA-CB-CG	6.38	118.98	112.60
1	Q	112	ASN	CA-CB-CG	6.38	118.98	112.60
1	S	112	ASN	CA-CB-CG	6.38	118.98	112.60
1	W	112	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	112	ASN	CA-CB-CG	6.32	118.92	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	112	ASN	CA-CB-CG	6.28	118.88	112.60
1	e	112	ASN	CA-CB-CG	6.27	118.87	112.60
1	s	105	ASP	CA-CB-CG	6.04	118.64	112.60
1	Q	105	ASP	CA-CB-CG	5.97	118.57	112.60
2	j	212	PRO	CB-CA-C	-5.96	101.73	111.56
1	a	105	ASP	CA-CB-CG	5.91	118.51	112.60
1	Y	105	ASP	CA-CB-CG	5.91	118.51	112.60
1	O	105	ASP	CA-CB-CG	5.90	118.50	112.60
2	p	212	PRO	CB-CA-C	-5.87	101.88	111.56
1	i	105	ASP	CA-CB-CG	5.84	118.44	112.60
1	e	105	ASP	CA-CB-CG	5.84	118.44	112.60
1	c	105	ASP	CA-CB-CG	5.83	118.43	112.60
1	U	105	ASP	CA-CB-CG	5.82	118.42	112.60
1	E	105	ASP	CA-CB-CG	5.82	118.42	112.60
2	h	212	PRO	CB-CA-C	-5.81	101.97	111.56
1	q	105	ASP	CA-CB-CG	5.80	118.40	112.60
2	l	212	PRO	CB-CA-C	-5.79	102.00	111.56
1	g	105	ASP	CA-CB-CG	5.79	118.39	112.60
2	f	212	PRO	CB-CA-C	-5.78	102.03	111.56
1	k	105	ASP	CA-CB-CG	5.75	118.35	112.60
1	M	105	ASP	CA-CB-CG	5.75	118.35	112.60
1	W	105	ASP	CA-CB-CG	5.73	118.33	112.60
2	n	212	PRO	CB-CA-C	-5.73	102.11	111.56
2	Z	212	PRO	CB-CA-C	-5.72	102.13	111.56
1	m	105	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	105	ASP	CA-CB-CG	5.70	118.30	112.60
1	S	105	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	105	ASP	CA-CB-CG	5.69	118.29	112.60
1	G	105	ASP	CA-CB-CG	5.69	118.29	112.60
1	o	105	ASP	CA-CB-CG	5.68	118.28	112.60
1	I	105	ASP	CA-CB-CG	5.67	118.27	112.60
2	P	212	PRO	CB-CA-C	-5.65	102.24	111.56
2	T	212	PRO	CB-CA-C	-5.64	102.25	111.56
2	R	212	PRO	CB-CA-C	-5.61	102.30	111.56
2	X	212	PRO	CB-CA-C	-5.61	102.30	111.56
1	K	105	ASP	CA-CB-CG	5.59	118.19	112.60
2	V	212	PRO	CB-CA-C	-5.56	102.38	111.56
2	b	212	PRO	CB-CA-C	-5.56	102.39	111.56
2	L	212	PRO	CB-CA-C	-5.56	102.39	111.56
2	J	212	PRO	CB-CA-C	-5.54	102.41	111.56
2	L	85	PRO	CB-CA-C	-5.53	103.71	110.95
2	D	212	PRO	CB-CA-C	-5.52	102.46	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	85	PRO	CB-CA-C	-5.48	103.77	110.95
1	M	64	CYS	CB-CA-C	-5.47	100.28	109.53
1	c	64	CYS	CB-CA-C	-5.47	100.29	109.53
1	K	64	CYS	CB-CA-C	-5.46	100.30	109.53
1	m	64	CYS	CB-CA-C	-5.45	100.32	109.53
2	N	212	PRO	CB-CA-C	-5.44	102.58	111.56
1	e	64	CYS	CB-CA-C	-5.42	100.36	109.53
1	Q	64	CYS	CB-CA-C	-5.41	100.38	109.53
2	b	85	PRO	CB-CA-C	-5.41	103.86	110.95
2	N	85	PRO	CB-CA-C	-5.40	103.87	110.95
2	H	212	PRO	CB-CA-C	-5.40	102.65	111.56
1	a	64	CYS	CB-CA-C	-5.40	100.40	109.53
2	D	85	PRO	CB-CA-C	-5.40	103.88	110.95
2	r	212	PRO	CB-CA-C	-5.39	102.66	111.56
2	B	212	PRO	CB-CA-C	-5.39	102.67	111.56
1	q	64	CYS	CB-CA-C	-5.39	100.42	109.53
2	B	85	PRO	CB-CA-C	-5.39	103.89	110.95
1	i	64	CYS	CB-CA-C	-5.39	100.43	109.53
2	J	85	PRO	CB-CA-C	-5.38	103.90	110.95
2	d	212	PRO	CB-CA-C	-5.37	102.70	111.56
1	o	64	CYS	CB-CA-C	-5.37	100.46	109.53
2	Z	85	PRO	CB-CA-C	-5.36	103.93	110.95
2	p	85	PRO	CB-CA-C	-5.36	103.93	110.95
1	Y	64	CYS	CB-CA-C	-5.35	100.48	109.53
1	g	64	CYS	CB-CA-C	-5.35	100.48	109.53
2	F	85	PRO	CB-CA-C	-5.35	103.94	110.95
2	F	212	PRO	CB-CA-C	-5.35	102.73	111.56
1	O	64	CYS	CB-CA-C	-5.35	100.50	109.53
2	P	85	PRO	CB-CA-C	-5.34	103.95	110.95
1	k	64	CYS	CB-CA-C	-5.34	100.51	109.53
1	W	64	CYS	CB-CA-C	-5.33	100.53	109.53
1	S	64	CYS	CB-CA-C	-5.33	100.53	109.53
1	I	64	CYS	CB-CA-C	-5.32	100.53	109.53
2	H	85	PRO	CB-CA-C	-5.32	103.98	110.95
2	R	91	PRO	N-CA-CB	-5.32	98.39	103.34
2	d	85	PRO	CB-CA-C	-5.32	103.98	110.95
2	j	85	PRO	CB-CA-C	-5.31	103.99	110.95
2	n	85	PRO	CB-CA-C	-5.31	104.00	110.95
1	E	64	CYS	CB-CA-C	-5.31	100.56	109.53
1	U	64	CYS	CB-CA-C	-5.30	100.56	109.53
2	V	85	PRO	CB-CA-C	-5.30	104.00	110.95
1	A	64	CYS	CB-CA-C	-5.30	100.58	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	64	CYS	CB-CA-C	-5.30	100.58	109.53
2	f	85	PRO	CB-CA-C	-5.29	104.02	110.95
2	h	85	PRO	CB-CA-C	-5.29	104.02	110.95
2	P	91	PRO	N-CA-CB	-5.28	98.43	103.34
1	s	64	CYS	CB-CA-C	-5.28	100.61	109.53
2	l	85	PRO	CB-CA-C	-5.28	104.04	110.95
2	r	85	PRO	CB-CA-C	-5.27	104.04	110.95
2	h	91	PRO	N-CA-CB	-5.27	98.72	103.36
2	T	85	PRO	CB-CA-C	-5.27	104.05	110.95
1	C	64	CYS	CB-CA-C	-5.25	100.66	109.53
2	d	91	PRO	N-CA-CB	-5.24	98.75	103.36
2	r	91	PRO	N-CA-CB	-5.24	98.75	103.36
2	P	90	ALA	N-CA-C	-5.23	103.36	110.36
2	R	85	PRO	CB-CA-C	-5.22	104.11	110.95
2	Z	91	PRO	N-CA-CB	-5.20	98.51	103.34
2	h	173	ASP	CA-CB-CG	5.20	117.80	112.60
2	T	173	ASP	CA-CB-CG	5.19	117.79	112.60
2	p	91	PRO	N-CA-CB	-5.19	98.79	103.36
2	R	173	ASP	CA-CB-CG	5.18	117.78	112.60
2	f	173	ASP	CA-CB-CG	5.17	117.77	112.60
2	V	173	ASP	CA-CB-CG	5.16	117.76	112.60
2	R	90	ALA	N-CA-C	-5.16	103.45	110.36
2	X	173	ASP	CA-CB-CG	5.15	117.75	112.60
1	i	65	SER	N-CA-C	-5.15	107.54	113.88
2	Z	173	ASP	CA-CB-CG	5.15	117.75	112.60
2	P	173	ASP	CA-CB-CG	5.15	117.75	112.60
2	j	173	ASP	CA-CB-CG	5.13	117.73	112.60
2	T	91	PRO	N-CA-CB	-5.13	98.57	103.34
1	W	65	SER	N-CA-C	-5.12	107.58	113.88
2	V	91	PRO	N-CA-CB	-5.12	98.58	103.34
2	X	91	PRO	N-CA-CB	-5.11	98.59	103.34
2	d	173	ASP	CA-CB-CG	5.11	117.71	112.60
1	k	65	SER	N-CA-C	-5.11	107.60	113.88
2	b	91	PRO	N-CA-CB	-5.10	98.59	103.34
1	S	65	SER	N-CA-C	-5.10	107.61	113.88
2	r	173	ASP	CA-CB-CG	5.10	117.70	112.60
2	b	209	PHE	CA-CB-CG	5.09	118.89	113.80
2	Z	209	PHE	CA-CB-CG	5.08	118.88	113.80
2	l	173	ASP	CA-CB-CG	5.06	117.66	112.60
2	b	173	ASP	CA-CB-CG	5.06	117.66	112.60
1	g	65	SER	N-CA-C	-5.06	107.66	113.88
2	n	173	ASP	CA-CB-CG	5.05	117.65	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	91	PRO	N-CA-CB	-5.05	98.64	103.34
2	N	173	ASP	CA-CB-CG	5.04	117.64	112.60
2	X	90	ALA	N-CA-C	-5.03	103.62	110.36
2	X	209	PHE	CA-CB-CG	5.03	118.83	113.80
1	m	65	SER	N-CA-C	-5.03	107.70	113.88
2	p	173	ASP	CA-CB-CG	5.02	117.62	112.60
1	e	65	SER	N-CA-C	-5.02	107.71	113.88
2	l	91	PRO	N-CA-CB	-5.01	98.68	103.34
2	B	173	ASP	CA-CB-CG	5.00	117.60	112.60
2	F	173	ASP	CA-CB-CG	5.00	117.60	112.60
2	H	173	ASP	CA-CB-CG	5.00	117.60	112.60
2	J	173	ASP	CA-CB-CG	5.00	117.60	112.60
2	p	209	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1554	0	1578	4	0
1	C	1554	0	1578	7	0
1	E	1554	0	1578	8	0
1	G	1554	0	1578	7	0
1	I	1554	0	1578	9	0
1	K	1554	0	1578	9	0
1	M	1554	0	1578	7	0
1	O	1554	0	1578	8	0
1	Q	1554	0	1578	3	0
1	S	1554	0	1578	5	0
1	U	1554	0	1578	4	0
1	W	1554	0	1578	3	0
1	Y	1554	0	1578	6	0
1	a	1554	0	1578	4	0
1	c	1554	0	1578	7	0
1	e	1554	0	1578	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	1554	0	1578	4	0
1	i	1554	0	1578	5	0
1	k	1554	0	1578	6	0
1	m	1554	0	1578	4	0
1	o	1554	0	1578	7	0
1	q	1554	0	1578	5	0
1	s	1554	0	1578	4	0
2	B	1566	0	1610	19	0
2	D	1566	0	1610	18	0
2	F	1566	0	1610	18	0
2	H	1566	0	1610	17	0
2	J	1566	0	1610	17	0
2	L	1566	0	1610	17	0
2	N	1566	0	1610	15	0
2	P	1566	0	1610	18	0
2	R	1566	0	1610	19	0
2	T	1566	0	1609	19	0
2	V	1566	0	1610	19	0
2	X	1566	0	1610	20	0
2	Z	1566	0	1610	22	0
2	b	1566	0	1610	20	0
2	d	1566	0	1610	17	0
2	f	1566	0	1609	20	0
2	h	1566	0	1610	20	0
2	j	1566	0	1609	18	0
2	l	1566	0	1608	20	0
2	n	1566	0	1609	19	0
2	p	1566	0	1610	19	0
2	r	1566	0	1610	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
3	e	1	0	0	0	0
3	f	1	0	0	0	0
3	g	1	0	0	0	0
3	h	1	0	0	0	0
3	i	1	0	0	0	0
3	j	1	0	0	0	0
3	k	1	0	0	0	0
3	l	1	0	0	0	0
3	m	1	0	0	0	0
3	n	1	0	0	0	0
3	o	1	0	0	0	0
3	p	1	0	0	0	0
3	q	1	0	0	0	0
3	r	1	0	0	0	0
3	s	1	0	0	0	0
4	A	156	0	0	0	0
4	B	312	0	0	10	0
4	C	156	0	0	1	0
4	D	312	0	0	10	0
4	E	156	0	0	1	0
4	F	312	0	0	10	0
4	G	156	0	0	1	0
4	H	312	0	0	10	0
4	I	156	0	0	1	0
4	J	312	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	156	0	0	1	0
4	L	312	0	0	9	0
4	M	156	0	0	1	0
4	N	312	0	0	9	0
4	O	156	0	0	1	0
4	P	312	0	0	10	0
4	Q	156	0	0	1	0
4	R	312	0	0	10	0
4	S	156	0	0	1	0
4	T	312	0	0	10	0
4	U	156	0	0	1	0
4	V	312	0	0	10	0
4	W	156	0	0	1	0
4	X	312	0	0	10	0
4	Y	156	0	0	1	0
4	Z	312	0	0	10	0
4	a	171	0	0	1	0
4	b	297	0	0	10	0
4	c	156	0	0	1	0
4	d	312	0	0	10	0
4	e	156	0	0	0	0
4	f	312	0	0	10	0
4	g	156	0	0	1	0
4	h	312	0	0	11	0
4	i	156	0	0	1	0
4	j	312	0	0	10	0
4	k	156	0	0	1	0
4	l	312	0	0	12	0
4	m	156	0	0	1	0
4	n	312	0	0	11	0
4	o	156	0	0	2	0
4	p	312	0	0	10	0
4	q	156	0	0	1	0
4	r	312	0	0	9	0
4	s	156	0	0	1	0
All	All	80691	0	71708	533	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 4.

All (533) 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)
2:j:72:SER:HB2	4:j:302:UNL:O4	1.53	1.09
1:C:94:ASP:OD2	2:P:190:ARG:NH1	1.88	1.06
1:I:94:ASP:OD2	2:V:190:ARG:NH1	1.90	1.04
1:G:94:ASP:OD2	2:T:190:ARG:NH1	1.91	1.04
1:M:94:ASP:OD2	2:Z:190:ARG:NH1	1.91	1.03
1:E:94:ASP:OD2	2:R:190:ARG:NH1	1.89	1.03
2:l:72:SER:HB2	4:l:302:UNL:O4	1.57	1.03
1:K:94:ASP:OD2	2:X:190:ARG:NH1	1.91	1.02
1:O:94:ASP:OD2	2:b:190:ARG:NH1	1.92	1.00
2:n:72:SER:HB2	4:n:302:UNL:O4	1.63	0.97
2:j:72:SER:CB	4:j:302:UNL:O4	2.10	0.97
2:h:72:SER:HB2	4:h:302:UNL:O4	1.62	0.97
2:l:72:SER:CB	4:l:302:UNL:O4	2.13	0.95
2:f:72:SER:HB2	4:f:302:UNL:O4	1.66	0.95
2:X:72:SER:HB2	4:X:302:UNL:O4	1.64	0.95
2:Z:72:SER:HB2	4:Z:302:UNL:O4	1.69	0.93
2:V:72:SER:HB2	4:V:302:UNL:O4	1.68	0.92
2:n:72:SER:CB	4:n:302:UNL:O4	2.17	0.92
2:X:72:SER:CB	4:X:302:UNL:O4	2.17	0.92
2:h:72:SER:CB	4:h:302:UNL:O4	2.17	0.92
2:P:72:SER:HB2	4:P:302:UNL:O4	1.71	0.91
2:D:72:SER:HB2	4:D:302:UNL:O4	1.71	0.91
2:f:72:SER:CB	4:f:302:UNL:O4	2.19	0.91
2:T:72:SER:HB2	4:T:302:UNL:O4	1.71	0.90
2:Z:72:SER:CB	4:Z:302:UNL:O4	2.20	0.90
2:D:72:SER:CB	4:D:302:UNL:O4	2.20	0.90
2:B:72:SER:HB2	4:B:302:UNL:O4	1.71	0.90
2:V:72:SER:CB	4:V:302:UNL:O4	2.20	0.89
2:B:72:SER:CB	4:B:302:UNL:O4	2.21	0.88
2:R:72:SER:HB2	4:R:302:UNL:O4	1.72	0.88
2:b:72:SER:HB2	4:b:302:UNL:O4	1.72	0.88
2:F:72:SER:HB2	4:F:302:UNL:O4	1.73	0.88
2:R:72:SER:CB	4:R:302:UNL:O4	2.22	0.88
2:F:72:SER:CB	4:F:302:UNL:O4	2.21	0.88
2:P:72:SER:CB	4:P:302:UNL:O4	2.22	0.88
2:b:72:SER:CB	4:b:302:UNL:O4	2.21	0.87
2:T:72:SER:CB	4:T:302:UNL:O4	2.23	0.87
2:p:72:SER:HB2	4:p:302:UNL:O4	1.75	0.86
2:L:72:SER:CB	4:L:302:UNL:O4	2.26	0.83
2:p:72:SER:CB	4:p:302:UNL:O4	2.27	0.83
2:L:72:SER:HB2	4:L:302:UNL:O4	1.80	0.81
2:H:72:SER:HB2	4:H:302:UNL:O4	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:72:SER:CB	4:J:302:UNL:O4	2.29	0.80
2:H:72:SER:CB	4:H:302:UNL:O4	2.30	0.79
2:J:72:SER:HB2	4:J:302:UNL:O4	1.82	0.78
2:r:72:SER:HB2	4:r:302:UNL:O4	1.83	0.78
2:X:72:SER:HB2	4:X:302:UNL:C4	2.16	0.76
2:B:72:SER:HB2	4:B:302:UNL:C4	2.16	0.75
2:j:72:SER:HB2	4:j:302:UNL:C4	2.16	0.75
2:l:72:SER:HB2	4:l:302:UNL:C4	2.17	0.75
2:b:72:SER:HB2	4:b:302:UNL:C4	2.17	0.75
2:F:72:SER:HB2	4:F:302:UNL:C4	2.17	0.75
2:L:72:SER:HB2	4:L:302:UNL:C4	2.16	0.75
2:n:130:ALA:HA	4:n:310:UNL:C6	2.17	0.75
2:D:72:SER:HB2	4:D:302:UNL:C4	2.16	0.75
2:h:72:SER:HB2	4:h:302:UNL:C4	2.17	0.75
2:D:123:ASN:HB3	4:E:302:UNL:C6	2.17	0.75
2:d:72:SER:HB2	4:d:302:UNL:O4	1.86	0.75
2:N:72:SER:HB2	4:N:302:UNL:O4	1.87	0.74
2:R:72:SER:HB2	4:R:302:UNL:C4	2.18	0.73
2:n:72:SER:HB2	4:n:302:UNL:C4	2.18	0.73
2:B:123:ASN:HB3	4:C:302:UNL:C6	2.18	0.73
2:r:72:SER:CB	4:r:302:UNL:O4	2.36	0.73
2:l:130:ALA:HA	4:l:310:UNL:C6	2.17	0.73
2:V:72:SER:HB2	4:V:302:UNL:C4	2.18	0.73
2:Z:72:SER:HB2	4:Z:302:UNL:C4	2.18	0.73
2:N:72:SER:CB	4:N:302:UNL:O4	2.37	0.72
2:d:72:SER:CB	4:d:302:UNL:O4	2.38	0.72
2:f:72:SER:HB2	4:f:302:UNL:C4	2.19	0.72
2:f:130:ALA:HA	4:f:310:UNL:C6	2.20	0.72
2:l:113:ASN:OD1	4:l:306:UNL:C5	2.38	0.72
2:J:72:SER:HB2	4:J:302:UNL:C4	2.20	0.71
2:P:72:SER:HB2	4:P:302:UNL:C4	2.20	0.71
1:K:14:ILE:HG12	2:Z:14:ILE:HD11	1.71	0.70
2:F:123:ASN:HB3	4:G:302:UNL:C6	2.22	0.69
2:j:113:ASN:OD1	4:j:306:UNL:C5	2.41	0.69
1:E:14:ILE:HG12	2:T:14:ILE:HD11	1.72	0.69
2:L:123:ASN:HB3	4:M:302:UNL:C6	2.22	0.69
2:r:123:ASN:HB3	4:s:302:UNL:C6	2.23	0.69
2:p:123:ASN:HB3	4:q:302:UNL:C6	2.24	0.68
2:T:72:SER:HB2	4:T:302:UNL:C4	2.23	0.68
2:H:72:SER:HB2	4:H:302:UNL:C4	2.24	0.68
2:p:72:SER:HB2	4:p:302:UNL:C4	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:72:SER:HB3	4:j:302:UNL:O4	1.94	0.68
2:P:123:ASN:HB3	4:Q:302:UNL:C6	2.24	0.68
2:N:123:ASN:HB3	4:O:302:UNL:C6	2.24	0.67
1:A:14:ILE:HG12	2:P:14:ILE:HD11	1.76	0.67
2:H:123:ASN:HB3	4:I:302:UNL:C6	2.24	0.67
2:b:72:SER:HB3	4:b:302:UNL:O4	1.95	0.67
2:l:72:SER:HB3	4:l:302:UNL:O4	1.94	0.66
2:X:72:SER:HB3	4:X:302:UNL:O4	1.95	0.66
2:F:72:SER:HB3	4:F:302:UNL:O4	1.94	0.66
1:C:14:ILE:HG12	2:R:14:ILE:HD11	1.76	0.66
2:h:72:SER:HB3	4:h:302:UNL:O4	1.96	0.65
1:q:104:TYR:CG	1:q:105:ASP:N	2.65	0.65
2:D:72:SER:HB3	4:D:302:UNL:O4	1.95	0.65
2:R:72:SER:HB3	4:R:302:UNL:O4	1.95	0.65
1:U:104:TYR:CG	1:U:105:ASP:N	2.65	0.65
2:j:130:ALA:HA	4:j:310:UNL:C6	2.27	0.65
2:J:123:ASN:HB3	4:K:302:UNL:C6	2.27	0.65
1:I:104:TYR:CG	1:I:105:ASP:N	2.65	0.65
1:e:104:TYR:CG	1:e:105:ASP:N	2.65	0.65
1:S:104:TYR:CG	1:S:105:ASP:N	2.65	0.64
2:l:123:ASN:HB3	4:m:302:UNL:C6	2.27	0.64
1:o:104:TYR:CG	1:o:105:ASP:N	2.65	0.64
2:Z:72:SER:HB3	4:Z:302:UNL:O4	1.97	0.64
2:Z:113:ASN:OD1	4:Z:306:UNL:C5	2.45	0.64
2:T:130:ALA:HA	4:T:310:UNL:C6	2.27	0.64
2:Z:123:ASN:HB3	4:a:302:UNL:C6	2.28	0.64
1:G:104:TYR:CG	1:G:105:ASP:N	2.65	0.64
2:V:72:SER:HB3	4:V:302:UNL:O4	1.97	0.64
2:f:72:SER:HB3	4:f:302:UNL:O4	1.97	0.64
2:B:72:SER:HB3	4:B:302:UNL:O4	1.96	0.64
1:m:104:TYR:CG	1:m:105:ASP:N	2.65	0.63
2:L:72:SER:HB3	4:L:302:UNL:O4	1.97	0.63
2:p:130:ALA:HA	4:p:310:UNL:C6	2.29	0.63
2:H:25:MET:SD	1:m:13:ALA:N	2.72	0.63
2:D:113:ASN:OD1	4:D:306:UNL:C5	2.46	0.63
1:Q:104:TYR:CG	1:Q:105:ASP:N	2.65	0.63
2:B:25:MET:SD	1:g:13:ALA:N	2.72	0.63
2:F:25:MET:SD	1:k:13:ALA:N	2.72	0.63
1:G:14:ILE:HG12	2:V:14:ILE:HD11	1.79	0.63
2:P:72:SER:HB3	4:P:302:UNL:O4	1.98	0.63
2:T:113:ASN:OD1	4:T:306:UNL:C5	2.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:72:SER:HB2	4:N:302:UNL:C4	2.29	0.63
1:S:13:ALA:N	2:f:25:MET:SD	2.72	0.63
1:E:104:TYR:CG	1:E:105:ASP:N	2.65	0.62
2:h:130:ALA:HA	4:h:310:UNL:C6	2.30	0.62
2:D:25:MET:SD	1:i:13:ALA:N	2.73	0.62
1:M:104:TYR:CG	1:M:105:ASP:N	2.65	0.62
1:s:104:TYR:CG	1:s:105:ASP:N	2.65	0.62
1:Y:104:TYR:CG	1:Y:105:ASP:N	2.65	0.62
2:Z:130:ALA:HA	4:Z:310:UNL:C6	2.29	0.62
1:a:104:TYR:CG	1:a:105:ASP:N	2.65	0.62
2:f:113:ASN:OD1	4:f:306:UNL:C5	2.48	0.62
1:k:104:TYR:CG	1:k:105:ASP:N	2.65	0.62
1:i:104:TYR:CG	1:i:105:ASP:N	2.65	0.62
1:C:104:TYR:CG	1:C:105:ASP:N	2.65	0.62
2:h:113:ASN:OD1	4:h:306:UNL:C5	2.48	0.62
1:I:14:ILE:HG12	2:X:14:ILE:HD11	1.82	0.62
2:X:113:ASN:OD1	4:X:306:UNL:C5	2.47	0.61
1:O:104:TYR:CG	1:O:105:ASP:N	2.65	0.61
2:b:123:ASN:HB3	4:c:302:UNL:C6	2.30	0.61
2:J:72:SER:HB3	4:J:302:UNL:O4	2.00	0.61
2:T:72:SER:HB3	4:T:302:UNL:O4	2.00	0.61
2:n:113:ASN:OD1	4:n:306:UNL:C5	2.49	0.61
2:n:72:SER:HB3	4:n:302:UNL:O4	1.98	0.61
2:p:113:ASN:OD1	4:p:306:UNL:C5	2.50	0.60
4:V:310:UNL:O4	4:V:311:UNL:C1	2.50	0.60
4:T:310:UNL:O4	4:T:311:UNL:C1	2.50	0.59
4:f:310:UNL:O4	4:f:311:UNL:C1	2.50	0.59
4:p:310:UNL:O4	4:p:311:UNL:C1	2.50	0.59
4:B:310:UNL:O4	4:B:311:UNL:C1	2.51	0.59
2:r:72:SER:HB2	4:r:302:UNL:C4	2.32	0.59
2:J:25:MET:SD	1:o:13:ALA:N	2.76	0.59
4:J:310:UNL:O4	4:J:311:UNL:C1	2.50	0.59
1:M:14:ILE:HG12	2:b:14:ILE:HD11	1.84	0.59
4:n:310:UNL:O4	4:n:311:UNL:C1	2.50	0.59
4:H:310:UNL:O4	4:H:311:UNL:C1	2.50	0.59
4:L:310:UNL:O4	4:L:311:UNL:C1	2.51	0.59
4:X:310:UNL:O4	4:X:311:UNL:C1	2.51	0.59
4:d:310:UNL:O4	4:d:311:UNL:C1	2.50	0.59
4:h:310:UNL:O4	4:h:311:UNL:C1	2.50	0.59
2:p:72:SER:HB3	4:p:302:UNL:O4	2.02	0.59
2:R:130:ALA:HA	4:R:310:UNL:C6	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:72:SER:HB2	4:d:302:UNL:C4	2.33	0.59
4:D:310:UNL:O4	4:D:311:UNL:C1	2.50	0.58
4:R:310:UNL:O4	4:R:311:UNL:C1	2.50	0.58
1:W:13:ALA:N	2:j:25:MET:SD	2.76	0.58
4:r:310:UNL:O4	4:r:311:UNL:C1	2.51	0.58
4:P:310:UNL:O4	4:P:311:UNL:C1	2.51	0.58
2:V:130:ALA:HA	4:V:310:UNL:C6	2.33	0.58
4:Z:310:UNL:O4	4:Z:311:UNL:C1	2.51	0.58
4:b:310:UNL:O4	4:b:311:UNL:C1	2.50	0.58
2:f:123:ASN:HB3	4:g:302:UNL:C6	2.33	0.58
2:j:123:ASN:HB3	4:k:302:UNL:C6	2.33	0.58
4:N:310:UNL:O4	4:N:311:UNL:C1	2.50	0.58
4:F:310:UNL:O4	4:F:311:UNL:C1	2.50	0.58
2:H:72:SER:HB3	4:H:302:UNL:O4	2.04	0.58
1:O:14:ILE:HG12	2:d:14:ILE:HD11	1.85	0.58
2:P:113:ASN:OD1	4:P:306:UNL:C5	2.51	0.58
4:l:310:UNL:O4	4:l:311:UNL:C1	2.50	0.58
1:U:13:ALA:N	2:h:25:MET:SD	2.77	0.57
2:h:123:ASN:HB3	4:i:302:UNL:C6	2.34	0.57
2:B:113:ASN:OD1	4:B:306:UNL:C5	2.52	0.57
1:K:14:ILE:HG12	2:Z:14:ILE:CD1	2.34	0.57
4:j:310:UNL:O4	4:j:311:UNL:C1	2.51	0.57
2:R:123:ASN:HB3	4:S:302:UNL:C6	2.35	0.56
2:V:123:ASN:HB3	4:W:302:UNL:C6	2.35	0.56
2:X:123:ASN:HB3	4:Y:302:UNL:C6	2.35	0.56
2:b:130:ALA:HA	4:b:310:UNL:C6	2.35	0.56
1:Y:13:ALA:N	2:l:25:MET:SD	2.79	0.56
2:P:130:ALA:HA	4:P:310:UNL:C6	2.35	0.56
2:F:113:ASN:OD1	4:F:306:UNL:C5	2.53	0.56
1:K:104:TYR:CG	1:K:105:ASP:N	2.65	0.56
1:W:104:TYR:CG	1:W:105:ASP:N	2.65	0.56
2:b:113:ASN:OD1	4:b:306:UNL:C5	2.54	0.55
2:r:113:ASN:OD1	4:r:306:UNL:C5	2.55	0.55
2:H:113:ASN:OD1	4:H:306:UNL:C5	2.54	0.55
2:T:123:ASN:HB3	4:U:302:UNL:C6	2.36	0.55
2:N:25:MET:SD	1:s:13:ALA:N	2.79	0.55
2:V:113:ASN:OD1	4:V:306:UNL:C5	2.55	0.55
1:g:104:TYR:CG	1:g:105:ASP:N	2.65	0.54
1:A:104:TYR:CG	1:A:105:ASP:N	2.65	0.54
1:a:13:ALA:N	2:n:25:MET:SD	2.81	0.54
2:R:113:ASN:OD1	4:R:306:UNL:C5	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:ASN:OD1	2:F:134:ASN:O	2.26	0.54
2:X:134:ASN:OD1	2:X:134:ASN:O	2.26	0.54
2:b:134:ASN:OD1	2:b:134:ASN:O	2.26	0.54
1:c:104:TYR:CG	1:c:105:ASP:N	2.65	0.54
2:R:134:ASN:OD1	2:R:134:ASN:O	2.26	0.54
2:j:134:ASN:OD1	2:j:134:ASN:O	2.26	0.54
2:B:134:ASN:OD1	2:B:134:ASN:O	2.26	0.53
2:H:134:ASN:OD1	2:H:134:ASN:O	2.26	0.53
2:N:113:ASN:OD1	4:N:306:UNL:C5	2.56	0.53
2:T:134:ASN:OD1	2:T:134:ASN:O	2.26	0.53
2:d:113:ASN:OD1	4:d:306:UNL:C5	2.56	0.53
2:d:134:ASN:OD1	2:d:134:ASN:O	2.26	0.53
2:h:134:ASN:OD1	2:h:134:ASN:O	2.26	0.53
2:L:70:ASN:OD1	2:L:71:HIS:N	2.42	0.53
2:L:134:ASN:OD1	2:L:134:ASN:O	2.26	0.53
2:n:134:ASN:OD1	2:n:134:ASN:O	2.26	0.53
2:r:134:ASN:O	2:r:134:ASN:OD1	2.26	0.53
2:p:70:ASN:OD1	2:p:71:HIS:N	2.42	0.53
2:H:70:ASN:OD1	2:H:71:HIS:N	2.42	0.53
2:V:134:ASN:OD1	2:V:134:ASN:O	2.26	0.53
2:d:70:ASN:OD1	2:d:71:HIS:N	2.42	0.53
2:J:70:ASN:OD1	2:J:71:HIS:N	2.41	0.53
2:V:134:ASN:OD1	2:V:134:ASN:C	2.52	0.53
2:T:70:ASN:OD1	2:T:71:HIS:N	2.42	0.53
2:Z:134:ASN:OD1	2:Z:134:ASN:O	2.26	0.53
2:b:70:ASN:OD1	2:b:71:HIS:N	2.42	0.53
2:f:70:ASN:OD1	2:f:71:HIS:N	2.42	0.53
2:n:70:ASN:OD1	2:n:71:HIS:N	2.42	0.53
2:r:70:ASN:OD1	2:r:71:HIS:N	2.42	0.53
2:D:134:ASN:OD1	2:D:134:ASN:O	2.26	0.53
2:J:134:ASN:OD1	2:J:134:ASN:O	2.26	0.53
2:N:70:ASN:OD1	2:N:71:HIS:N	2.41	0.53
2:P:134:ASN:OD1	2:P:134:ASN:O	2.26	0.53
2:X:134:ASN:OD1	2:X:134:ASN:C	2.52	0.53
2:N:134:ASN:OD1	2:N:134:ASN:O	2.26	0.53
2:X:70:ASN:OD1	2:X:71:HIS:N	2.42	0.53
2:p:134:ASN:OD1	2:p:134:ASN:O	2.26	0.53
2:B:70:ASN:OD1	2:B:71:HIS:N	2.42	0.53
2:B:134:ASN:OD1	2:B:134:ASN:C	2.52	0.53
2:F:70:ASN:OD1	2:F:71:HIS:N	2.42	0.53
2:J:113:ASN:OD1	4:J:306:UNL:C5	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:134:ASN:OD1	2:J:134:ASN:C	2.52	0.53
2:f:134:ASN:O	2:f:134:ASN:OD1	2.26	0.53
2:l:134:ASN:OD1	2:l:134:ASN:O	2.26	0.53
2:F:130:ALA:HA	4:F:310:UNL:C6	2.39	0.52
2:R:134:ASN:OD1	2:R:134:ASN:C	2.52	0.52
2:V:70:ASN:OD1	2:V:71:HIS:N	2.42	0.52
1:E:94:ASP:CG	2:R:190:ARG:HH12	2.07	0.52
2:F:50:THR:HG21	2:l:23:ILE:HG23	1.92	0.52
2:R:70:ASN:OD1	2:R:71:HIS:N	2.42	0.52
2:h:70:ASN:OD1	2:h:71:HIS:N	2.42	0.52
2:j:70:ASN:OD1	2:j:71:HIS:N	2.42	0.52
2:j:134:ASN:OD1	2:j:134:ASN:C	2.52	0.52
2:L:134:ASN:OD1	2:L:134:ASN:C	2.52	0.52
2:F:134:ASN:OD1	2:F:134:ASN:C	2.52	0.52
2:b:134:ASN:OD1	2:b:134:ASN:C	2.52	0.52
1:c:13:ALA:N	2:p:25:MET:SD	2.83	0.52
2:r:134:ASN:OD1	2:r:134:ASN:C	2.52	0.52
1:K:14:ILE:CD1	2:Z:14:ILE:HD11	2.40	0.52
2:N:35:VAL:HG11	1:s:19:LEU:CD2	2.40	0.52
2:Z:70:ASN:OD1	2:Z:71:HIS:N	2.42	0.52
2:h:134:ASN:OD1	2:h:134:ASN:C	2.52	0.52
2:D:70:ASN:OD1	2:D:71:HIS:N	2.42	0.52
4:Z:314:UNL:C6	4:Z:314:UNL:C2	2.87	0.52
2:h:70:ASN:OD1	2:h:70:ASN:C	2.53	0.52
2:p:70:ASN:OD1	2:p:70:ASN:C	2.53	0.52
2:r:70:ASN:OD1	2:r:70:ASN:C	2.53	0.52
2:T:70:ASN:OD1	2:T:70:ASN:C	2.53	0.52
2:f:134:ASN:OD1	2:f:134:ASN:C	2.52	0.52
2:l:70:ASN:OD1	2:l:71:HIS:N	2.42	0.52
2:Z:70:ASN:OD1	2:Z:70:ASN:C	2.53	0.52
4:r:314:UNL:C6	4:r:314:UNL:C2	2.87	0.52
2:H:50:THR:HG21	2:n:23:ILE:HG23	1.91	0.52
1:K:14:ILE:CG1	2:Z:14:ILE:HD11	2.37	0.52
2:N:70:ASN:OD1	2:N:70:ASN:C	2.53	0.52
2:b:70:ASN:OD1	2:b:70:ASN:C	2.53	0.52
2:f:70:ASN:OD1	2:f:70:ASN:C	2.53	0.52
2:j:70:ASN:OD1	2:j:70:ASN:C	2.53	0.52
2:H:70:ASN:OD1	2:H:70:ASN:C	2.53	0.52
2:H:134:ASN:OD1	2:H:134:ASN:C	2.52	0.52
2:P:70:ASN:OD1	2:P:70:ASN:C	2.53	0.52
2:P:70:ASN:OD1	2:P:71:HIS:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:70:ASN:OD1	2:R:70:ASN:C	2.53	0.52
2:T:134:ASN:OD1	2:T:134:ASN:C	2.52	0.52
2:d:70:ASN:OD1	2:d:70:ASN:C	2.53	0.52
2:d:134:ASN:OD1	2:d:134:ASN:C	2.52	0.52
2:F:70:ASN:OD1	2:F:70:ASN:C	2.53	0.51
2:p:134:ASN:OD1	2:p:134:ASN:C	2.52	0.51
2:D:70:ASN:OD1	2:D:70:ASN:C	2.53	0.51
2:n:70:ASN:OD1	2:n:70:ASN:C	2.53	0.51
2:X:70:ASN:OD1	2:X:70:ASN:C	2.53	0.51
2:l:134:ASN:OD1	2:l:134:ASN:C	2.52	0.51
2:L:70:ASN:OD1	2:L:70:ASN:C	2.53	0.51
2:V:70:ASN:OD1	2:V:70:ASN:C	2.53	0.51
4:d:314:UNL:C6	4:d:314:UNL:C2	2.87	0.51
2:n:134:ASN:OD1	2:n:134:ASN:C	2.52	0.51
1:E:14:ILE:HG12	2:T:14:ILE:CD1	2.39	0.51
2:N:134:ASN:OD1	2:N:134:ASN:C	2.52	0.51
2:P:134:ASN:OD1	2:P:134:ASN:C	2.52	0.51
2:Z:134:ASN:OD1	2:Z:134:ASN:C	2.52	0.51
4:j:314:UNL:C6	4:j:314:UNL:C2	2.87	0.51
4:n:314:UNL:C6	4:n:314:UNL:C2	2.87	0.51
2:B:70:ASN:OD1	2:B:70:ASN:C	2.53	0.51
2:J:70:ASN:OD1	2:J:70:ASN:C	2.53	0.51
4:L:314:UNL:C6	4:L:314:UNL:C2	2.87	0.51
2:D:134:ASN:OD1	2:D:134:ASN:C	2.52	0.51
2:l:70:ASN:OD1	2:l:70:ASN:C	2.53	0.51
2:n:120:THR:HG23	4:n:310:UNL:C7	2.42	0.50
1:i:131:ILE:HD11	2:j:109:ILE:CD1	2.41	0.50
2:L:113:ASN:OD1	4:L:306:UNL:C5	2.60	0.50
1:O:94:ASP:CG	2:b:190:ARG:HH12	2.09	0.50
4:H:314:UNL:C6	4:H:314:UNL:C2	2.87	0.50
1:c:19:LEU:CD2	2:p:35:VAL:HG11	2.42	0.49
2:L:35:VAL:HG11	1:q:19:LEU:CD2	2.42	0.49
4:b:314:UNL:C6	4:b:314:UNL:C2	2.87	0.49
4:f:314:UNL:C6	4:f:314:UNL:C2	2.87	0.49
4:B:314:UNL:C6	4:B:314:UNL:C2	2.87	0.49
2:B:25:MET:HE1	2:f:18:THR:CG2	2.43	0.49
2:J:50:THR:HG21	2:p:23:ILE:HG23	1.95	0.49
4:F:314:UNL:C6	4:F:314:UNL:C2	2.87	0.49
4:T:314:UNL:C6	4:T:314:UNL:C2	2.87	0.49
2:l:120:THR:HG23	4:l:310:UNL:C7	2.43	0.49
2:d:72:SER:HB3	4:d:302:UNL:O4	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:72:SER:HB3	4:r:302:UNL:O4	2.13	0.49
1:C:14:ILE:HG12	2:R:14:ILE:CD1	2.41	0.49
2:D:50:THR:HG21	2:j:23:ILE:HG23	1.95	0.49
2:N:72:SER:HB3	4:N:302:UNL:O4	2.10	0.49
2:D:130:ALA:HA	4:D:310:UNL:C6	2.43	0.48
4:J:314:UNL:C6	4:J:314:UNL:C2	2.87	0.48
4:N:314:UNL:C6	4:N:314:UNL:C2	2.87	0.48
1:k:131:ILE:HD11	2:l:109:ILE:CD1	2.44	0.48
1:A:14:ILE:HG12	2:P:14:ILE:CD1	2.44	0.48
4:h:314:UNL:C6	4:h:314:UNL:C2	2.87	0.48
4:l:314:UNL:C6	4:l:314:UNL:C2	2.87	0.48
4:R:314:UNL:C6	4:R:314:UNL:C2	2.87	0.48
2:L:50:THR:HG21	2:r:23:ILE:HG23	1.94	0.47
2:J:35:VAL:HG11	1:o:19:LEU:CD2	2.44	0.47
4:V:314:UNL:C2	4:V:314:UNL:C6	2.87	0.47
4:X:314:UNL:C6	4:X:314:UNL:C2	2.87	0.47
2:l:113:ASN:CG	4:l:306:UNL:C5	2.86	0.47
2:n:123:ASN:HB3	4:o:302:UNL:C6	2.44	0.47
1:I:94:ASP:CG	2:V:190:ARG:HH12	2.08	0.47
1:G:14:ILE:HG12	2:V:14:ILE:CD1	2.45	0.47
4:d:310:UNL:O4	4:d:311:UNL:C2	2.63	0.47
4:H:310:UNL:O4	4:H:311:UNL:C2	2.63	0.47
2:j:127:ILE:HG22	2:j:128:PHE:N	2.30	0.47
4:J:310:UNL:O4	4:J:311:UNL:C2	2.63	0.47
4:R:310:UNL:O4	4:R:311:UNL:C2	2.63	0.47
4:V:310:UNL:O4	4:V:311:UNL:C2	2.63	0.47
1:M:14:ILE:HG12	2:b:14:ILE:CD1	2.45	0.46
4:T:310:UNL:O4	4:T:311:UNL:C2	2.63	0.46
4:f:310:UNL:O4	4:f:311:UNL:C2	2.63	0.46
1:m:131:ILE:HD11	2:n:109:ILE:CD1	2.45	0.46
1:E:14:ILE:CG1	2:T:14:ILE:HD11	2.44	0.46
4:b:310:UNL:O4	4:b:311:UNL:C2	2.63	0.46
4:n:310:UNL:O4	4:n:311:UNL:C2	2.64	0.46
2:B:25:MET:HE1	2:f:18:THR:HG23	1.96	0.46
2:P:127:ILE:HG22	2:P:128:PHE:N	2.31	0.46
2:f:127:ILE:HG22	2:f:128:PHE:N	2.30	0.46
4:l:310:UNL:O4	4:l:311:UNL:C2	2.63	0.46
4:p:310:UNL:O4	4:p:311:UNL:C2	2.64	0.46
4:F:310:UNL:O4	4:F:311:UNL:C2	2.64	0.46
1:O:14:ILE:HG12	2:d:14:ILE:CD1	2.46	0.46
1:g:131:ILE:HD11	2:h:109:ILE:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:127:ILE:HG22	2:l:128:PHE:N	2.30	0.46
1:K:23:ILE:HG23	2:X:50:THR:HG21	1.98	0.46
4:P:310:UNL:O4	4:P:311:UNL:C2	2.63	0.46
4:X:310:UNL:O4	4:X:311:UNL:C2	2.64	0.46
4:Z:310:UNL:O4	4:Z:311:UNL:C2	2.63	0.46
2:d:130:ALA:HA	4:d:310:UNL:C6	2.46	0.46
4:B:310:UNL:O4	4:B:311:UNL:C2	2.64	0.46
2:Z:127:ILE:HG22	2:Z:128:PHE:N	2.31	0.46
2:d:127:ILE:HG22	2:d:128:PHE:N	2.31	0.46
4:r:310:UNL:O4	4:r:311:UNL:C2	2.64	0.46
1:C:94:ASP:CG	2:P:190:ARG:HH12	2.07	0.46
2:T:127:ILE:HG22	2:T:128:PHE:N	2.31	0.46
4:h:310:UNL:O4	4:h:311:UNL:C2	2.63	0.46
4:r:310:UNL:O4	4:r:310:UNL:O6	2.34	0.46
4:J:310:UNL:O4	4:J:310:UNL:O6	2.34	0.46
4:N:310:UNL:O4	4:N:310:UNL:O6	2.34	0.46
1:e:131:ILE:HD11	2:f:109:ILE:CD1	2.46	0.46
2:h:127:ILE:HG22	2:h:128:PHE:N	2.30	0.46
2:n:127:ILE:HG22	2:n:128:PHE:N	2.31	0.46
1:Q:14:ILE:HG22	1:e:21:ILE:HG12	1.97	0.46
2:V:127:ILE:HG22	2:V:128:PHE:N	2.31	0.46
2:X:130:ALA:HA	4:X:310:UNL:C6	2.46	0.46
4:D:310:UNL:O4	4:D:311:UNL:C2	2.63	0.45
4:D:314:UNL:C6	4:D:314:UNL:C2	2.87	0.45
1:G:23:ILE:HG23	2:T:50:THR:HG21	1.98	0.45
4:L:310:UNL:O4	4:L:311:UNL:C2	2.63	0.45
4:N:310:UNL:O4	4:N:311:UNL:C2	2.64	0.45
2:p:127:ILE:HG22	2:p:128:PHE:N	2.31	0.45
4:P:314:UNL:C6	4:P:314:UNL:C2	2.87	0.45
2:b:127:ILE:HG22	2:b:128:PHE:N	2.31	0.45
4:j:310:UNL:O4	4:j:311:UNL:C2	2.64	0.45
2:N:127:ILE:HG22	2:N:128:PHE:N	2.32	0.45
4:T:310:UNL:O4	4:T:310:UNL:O6	2.34	0.45
4:f:310:UNL:O4	4:f:310:UNL:O6	2.34	0.45
4:B:310:UNL:O4	4:B:310:UNL:O6	2.34	0.45
4:H:310:UNL:O4	4:H:310:UNL:O6	2.34	0.45
4:X:310:UNL:O4	4:X:310:UNL:O6	2.34	0.45
4:n:310:UNL:O4	4:n:310:UNL:O6	2.34	0.45
4:D:310:UNL:O4	4:D:310:UNL:O6	2.34	0.45
2:X:127:ILE:HG22	2:X:128:PHE:N	2.31	0.45
2:n:188:LYS:HB2	2:n:189:PRO:CD	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HB3	2:B:28:VAL:HG21	1.99	0.45
2:R:127:ILE:HG22	2:R:128:PHE:N	2.31	0.45
4:R:310:UNL:O4	4:R:310:UNL:O6	2.34	0.45
4:d:310:UNL:O4	4:d:310:UNL:O6	2.34	0.45
4:j:310:UNL:O4	4:j:310:UNL:O6	2.34	0.45
2:H:130:ALA:HA	4:H:310:UNL:C6	2.46	0.45
4:b:310:UNL:O4	4:b:310:UNL:O6	2.34	0.45
4:l:310:UNL:O4	4:l:310:UNL:O6	2.34	0.45
1:O:23:ILE:HG23	2:b:50:THR:HG21	1.99	0.45
2:T:188:LYS:HB2	2:T:189:PRO:CD	2.47	0.45
4:V:310:UNL:O4	4:V:310:UNL:O6	2.34	0.45
2:F:188:LYS:HB2	2:F:189:PRO:CD	2.47	0.45
1:I:14:ILE:HG12	2:X:14:ILE:CD1	2.45	0.45
4:L:310:UNL:O4	4:L:310:UNL:O6	2.34	0.45
2:R:188:LYS:HB2	2:R:189:PRO:CD	2.47	0.45
2:Z:188:LYS:HB2	2:Z:189:PRO:CD	2.47	0.45
4:h:310:UNL:O4	4:h:310:UNL:O6	2.34	0.45
4:F:310:UNL:O4	4:F:310:UNL:O6	2.34	0.44
2:b:188:LYS:HB2	2:b:189:PRO:CD	2.47	0.44
2:r:127:ILE:HG22	2:r:128:PHE:N	2.31	0.44
2:L:25:MET:SD	1:q:13:ALA:N	2.90	0.44
2:N:188:LYS:HB2	2:N:189:PRO:CD	2.47	0.44
2:d:188:LYS:HB2	2:d:189:PRO:CD	2.47	0.44
2:r:188:LYS:HB2	2:r:189:PRO:CD	2.47	0.44
1:M:23:ILE:HG23	2:Z:50:THR:HG21	1.98	0.44
2:D:127:ILE:HG22	2:D:128:PHE:N	2.33	0.44
2:H:127:ILE:HG22	2:H:128:PHE:N	2.33	0.44
2:H:188:LYS:HB2	2:H:189:PRO:CD	2.47	0.44
2:P:188:LYS:HB2	2:P:189:PRO:CD	2.47	0.44
2:h:188:LYS:HB2	2:h:189:PRO:CD	2.47	0.44
4:p:310:UNL:O4	4:p:310:UNL:O6	2.34	0.44
2:D:188:LYS:HB2	2:D:189:PRO:CD	2.47	0.44
2:X:188:LYS:HB2	2:X:189:PRO:CD	2.47	0.44
4:Z:310:UNL:O4	4:Z:310:UNL:O6	2.34	0.44
2:j:188:LYS:HB2	2:j:189:PRO:CD	2.47	0.44
4:p:314:UNL:C6	4:p:314:UNL:C2	2.87	0.44
4:P:310:UNL:O4	4:P:310:UNL:O6	2.34	0.44
2:L:127:ILE:HG22	2:L:128:PHE:N	2.32	0.44
2:L:188:LYS:HB2	2:L:189:PRO:CD	2.47	0.44
2:B:188:LYS:HB2	2:B:189:PRO:CD	2.47	0.44
2:J:188:LYS:HB2	2:J:189:PRO:CD	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:94:ASP:CG	2:Z:190:ARG:HH12	2.08	0.43
2:h:120:THR:HG23	4:h:310:UNL:C7	2.48	0.43
2:B:127:ILE:HG22	2:B:128:PHE:N	2.32	0.43
1:E:23:ILE:HG23	2:R:50:THR:HG21	1.99	0.43
2:l:188:LYS:HB2	2:l:189:PRO:CD	2.47	0.43
2:F:127:ILE:HG22	2:F:128:PHE:N	2.33	0.43
2:J:127:ILE:HG22	2:J:128:PHE:N	2.33	0.43
2:V:188:LYS:HB2	2:V:189:PRO:CD	2.47	0.43
1:c:36:LEU:HB3	2:d:28:VAL:HG21	2.00	0.43
2:f:188:LYS:HB2	2:f:189:PRO:CD	2.47	0.43
2:p:188:LYS:HB2	2:p:189:PRO:CD	2.47	0.43
1:c:23:ILE:HG23	1:o:50:THR:HG21	2.00	0.43
1:O:14:ILE:CD1	2:d:14:ILE:HD11	2.48	0.43
2:f:36:LEU:CD1	1:g:25:MET:HE1	2.48	0.43
2:n:127:ILE:C	2:n:129:GLU:H	2.27	0.43
1:I:14:ILE:CD1	2:X:14:ILE:HD11	2.49	0.43
1:a:19:LEU:CD2	2:n:35:VAL:HG11	2.49	0.43
2:R:127:ILE:C	2:R:129:GLU:H	2.27	0.42
2:T:127:ILE:C	2:T:129:GLU:H	2.28	0.42
2:d:127:ILE:C	2:d:129:GLU:H	2.28	0.42
1:S:19:LEU:CD2	2:f:35:VAL:HG11	2.49	0.42
1:Y:19:LEU:CD2	2:l:35:VAL:HG11	2.49	0.42
1:c:19:LEU:HD22	2:p:35:VAL:HG11	2.01	0.42
2:j:127:ILE:C	2:j:129:GLU:H	2.27	0.42
2:p:127:ILE:C	2:p:129:GLU:H	2.27	0.42
1:C:36:LEU:HB3	2:D:28:VAL:HG21	2.02	0.42
2:l:127:ILE:C	2:l:129:GLU:H	2.27	0.42
2:H:127:ILE:C	2:H:129:GLU:H	2.28	0.42
2:f:127:ILE:C	2:f:129:GLU:H	2.27	0.42
2:F:127:ILE:C	2:F:129:GLU:H	2.28	0.42
2:P:127:ILE:C	2:P:129:GLU:H	2.28	0.42
2:V:127:ILE:C	2:V:129:GLU:H	2.27	0.42
2:B:50:THR:HG21	2:h:23:ILE:HG23	2.01	0.41
2:B:130:ALA:HA	4:B:310:UNL:C6	2.50	0.41
2:D:127:ILE:C	2:D:129:GLU:H	2.28	0.41
2:b:127:ILE:C	2:b:129:GLU:H	2.28	0.41
2:B:127:ILE:C	2:B:129:GLU:H	2.28	0.41
2:J:127:ILE:C	2:J:129:GLU:H	2.28	0.41
1:S:23:ILE:HG23	1:e:50:THR:HG21	2.03	0.41
1:W:19:LEU:CD2	2:j:35:VAL:HG11	2.50	0.41
1:o:131:ILE:HD11	2:p:109:ILE:CD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:VAL:HG11	1:i:19:LEU:CD2	2.50	0.41
1:M:14:ILE:CD1	2:b:14:ILE:HD11	2.50	0.41
2:X:127:ILE:C	2:X:129:GLU:H	2.28	0.41
2:Z:127:ILE:C	2:Z:129:GLU:H	2.28	0.41
2:N:127:ILE:C	2:N:129:GLU:H	2.28	0.41
1:o:112:ASN:HD22	4:o:302:UNL:C7	2.33	0.41
1:I:14:ILE:CG1	2:X:14:ILE:HD11	2.49	0.41
1:q:131:ILE:HD11	2:r:109:ILE:CD1	2.51	0.41
2:r:127:ILE:C	2:r:129:GLU:H	2.28	0.41
1:I:36:LEU:HB3	2:J:28:VAL:HG21	2.03	0.41
1:U:112:ASN:O	1:U:146:SER:HB2	2.21	0.41
1:Y:23:ILE:HG23	1:k:50:THR:HG21	2.02	0.41
1:c:112:ASN:O	1:c:146:SER:HB2	2.21	0.41
2:h:127:ILE:C	2:h:129:GLU:H	2.27	0.41
1:k:112:ASN:O	1:k:146:SER:HB2	2.21	0.41
1:s:112:ASN:O	1:s:146:SER:HB2	2.21	0.41
1:G:112:ASN:O	1:G:146:SER:HB2	2.21	0.41
1:I:112:ASN:O	1:I:146:SER:HB2	2.21	0.41
1:O:112:ASN:O	1:O:146:SER:HB2	2.21	0.41
1:i:112:ASN:O	1:i:146:SER:HB2	2.21	0.41
1:q:36:LEU:HB3	2:r:28:VAL:HG21	2.03	0.41
2:L:127:ILE:C	2:L:129:GLU:H	2.28	0.40
1:a:112:ASN:O	1:a:146:SER:HB2	2.21	0.40
1:E:112:ASN:O	1:E:146:SER:HB2	2.21	0.40
1:G:36:LEU:HB3	2:H:28:VAL:HG21	2.03	0.40
1:S:112:ASN:O	1:S:146:SER:HB2	2.21	0.40
1:U:19:LEU:CD2	2:h:35:VAL:HG11	2.51	0.40
2:V:23:ILE:HG23	2:h:50:THR:HG21	2.02	0.40
1:o:112:ASN:O	1:o:146:SER:HB2	2.21	0.40
1:K:36:LEU:HB3	2:L:28:VAL:HG21	2.03	0.40
1:Q:112:ASN:O	1:Q:146:SER:HB2	2.21	0.40
1:e:112:ASN:O	1:e:146:SER:HB2	2.21	0.40
1:m:112:ASN:O	1:m:146:SER:HB2	2.21	0.40
2:r:203:ALA:HA	2:r:204:PRO:HD3	1.93	0.40
2:F:35:VAL:HG11	1:k:19:LEU:CD2	2.52	0.40
2:F:203:ALA:HA	2:F:204:PRO:HD3	1.94	0.40
1:K:112:ASN:O	1:K:146:SER:HB2	2.21	0.40
1:Y:36:LEU:HB3	2:Z:28:VAL:HG21	2.03	0.40
1:Y:112:ASN:O	1:Y:146:SER:HB2	2.21	0.40
1:C:112:ASN:O	1:C:146:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	C	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	E	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	G	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	K	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	M	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	O	207/209 (99%)	199 (96%)	7 (3%)	1 (0%)	24	54
1	Q	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	S	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	U	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	W	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	Y	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	a	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	c	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	e	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	g	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	i	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	k	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	m	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	o	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	q	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
1	s	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
2	B	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	D	211/213 (99%)	198 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	H	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	J	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	L	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	N	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	P	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	R	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	T	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	V	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	X	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	Z	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	b	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	d	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	f	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	h	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	j	211/213 (99%)	199 (94%)	12 (6%)	0	100	100
2	l	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	n	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	p	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	r	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
All	All	9403/9493 (99%)	8933 (95%)	469 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	106	GLY

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	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	C	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	E	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	G	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	I	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	K	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	M	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	O	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	Q	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	S	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	U	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	W	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	Y	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	a	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	c	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	e	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	g	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	i	167/167 (100%)	166 (99%)	1 (1%)	78	81
1	k	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	m	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	o	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	q	167/167 (100%)	165 (99%)	2 (1%)	63	75
1	s	167/167 (100%)	165 (99%)	2 (1%)	63	75
2	B	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	D	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	F	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	H	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	J	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	L	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	N	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	P	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	R	171/171 (100%)	166 (97%)	5 (3%)	37	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	V	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	X	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	Z	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	b	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	d	171/171 (100%)	167 (98%)	4 (2%)	44	67
2	f	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	h	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	j	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	l	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	n	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	p	171/171 (100%)	166 (97%)	5 (3%)	37	63
2	r	171/171 (100%)	166 (97%)	5 (3%)	37	63
All	All	7603/7603 (100%)	7454 (98%)	149 (2%)	48	69

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	161	THR
2	B	35	VAL
2	B	64	VAL
2	B	134	ASN
2	B	146	PRO
2	B	212	PRO
1	C	21	ILE
1	C	161	THR
2	D	35	VAL
2	D	64	VAL
2	D	134	ASN
2	D	146	PRO
2	D	212	PRO
1	E	21	ILE
1	E	161	THR
2	F	35	VAL
2	F	64	VAL
2	F	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	146	PRO
2	F	212	PRO
1	G	21	ILE
1	G	161	THR
2	H	35	VAL
2	H	64	VAL
2	H	134	ASN
2	H	212	PRO
1	I	21	ILE
1	I	161	THR
2	J	35	VAL
2	J	64	VAL
2	J	134	ASN
2	J	212	PRO
1	K	21	ILE
1	K	161	THR
2	L	35	VAL
2	L	64	VAL
2	L	134	ASN
2	L	212	PRO
1	M	21	ILE
1	M	161	THR
2	N	35	VAL
2	N	64	VAL
2	N	134	ASN
2	N	212	PRO
1	O	21	ILE
1	O	161	THR
2	P	35	VAL
2	P	64	VAL
2	P	134	ASN
2	P	146	PRO
2	P	212	PRO
1	Q	21	ILE
1	Q	161	THR
2	R	35	VAL
2	R	64	VAL
2	R	134	ASN
2	R	146	PRO
2	R	212	PRO
1	S	21	ILE
1	S	161	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	35	VAL
2	T	64	VAL
2	T	134	ASN
2	T	212	PRO
1	U	21	ILE
1	U	161	THR
2	V	35	VAL
2	V	64	VAL
2	V	134	ASN
2	V	146	PRO
2	V	212	PRO
1	W	21	ILE
1	W	161	THR
2	X	35	VAL
2	X	64	VAL
2	X	134	ASN
2	X	146	PRO
2	X	212	PRO
1	Y	21	ILE
1	Y	161	THR
2	Z	35	VAL
2	Z	64	VAL
2	Z	134	ASN
2	Z	146	PRO
2	Z	212	PRO
1	a	21	ILE
1	a	161	THR
2	b	35	VAL
2	b	64	VAL
2	b	134	ASN
2	b	146	PRO
2	b	212	PRO
1	c	21	ILE
1	c	161	THR
2	d	35	VAL
2	d	64	VAL
2	d	134	ASN
2	d	212	PRO
1	e	21	ILE
1	e	161	THR
2	f	35	VAL
2	f	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	f	134	ASN
2	f	146	PRO
2	f	212	PRO
1	g	21	ILE
1	g	161	THR
2	h	35	VAL
2	h	64	VAL
2	h	134	ASN
2	h	146	PRO
2	h	212	PRO
1	i	21	ILE
2	j	35	VAL
2	j	64	VAL
2	j	134	ASN
2	j	146	PRO
2	j	212	PRO
1	k	21	ILE
1	k	161	THR
2	l	35	VAL
2	l	64	VAL
2	l	134	ASN
2	l	146	PRO
2	l	212	PRO
1	m	21	ILE
1	m	161	THR
2	n	35	VAL
2	n	64	VAL
2	n	134	ASN
2	n	146	PRO
2	n	212	PRO
1	o	21	ILE
1	o	161	THR
2	p	35	VAL
2	p	64	VAL
2	p	134	ASN
2	p	146	PRO
2	p	212	PRO
1	q	21	ILE
1	q	161	THR
2	r	35	VAL
2	r	64	VAL
2	r	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	r	146	PRO
2	r	212	PRO
1	s	21	ILE
1	s	161	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
2	B	183	ASN
1	C	57	GLN
1	E	44	GLN
1	E	57	GLN
1	G	44	GLN
1	G	57	GLN
2	H	183	ASN
1	I	44	GLN
2	J	220	HIS
2	N	183	ASN
2	P	183	ASN
1	Q	44	GLN
1	Q	97	GLN
1	Q	153	GLN
2	R	183	ASN
1	S	97	GLN
2	T	183	ASN
1	U	97	GLN
2	V	183	ASN
1	W	97	GLN
2	X	183	ASN
1	Y	97	GLN
2	Z	183	ASN
1	a	97	GLN
2	b	183	ASN
1	c	97	GLN
2	d	183	ASN
2	d	220	HIS
1	e	44	GLN
1	e	97	GLN
2	f	183	ASN
1	g	97	GLN
1	i	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	153	GLN
2	j	183	ASN
1	k	97	GLN
1	m	97	GLN
2	n	183	ASN
2	n	220	HIS
1	o	97	GLN
2	p	183	ASN
1	q	97	GLN
2	r	183	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 849 ligands modelled in this entry, 45 are monoatomic and 804 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

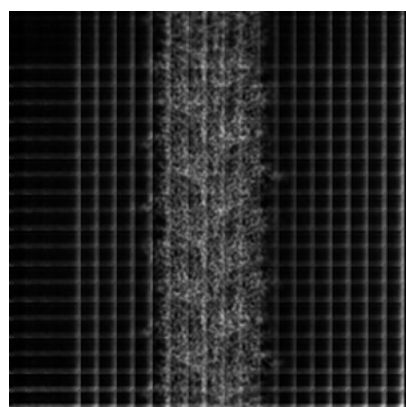
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12875. These allow visual inspection of the internal detail of the map and identification of artifacts.

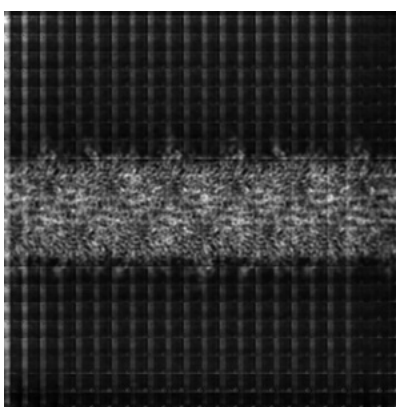
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

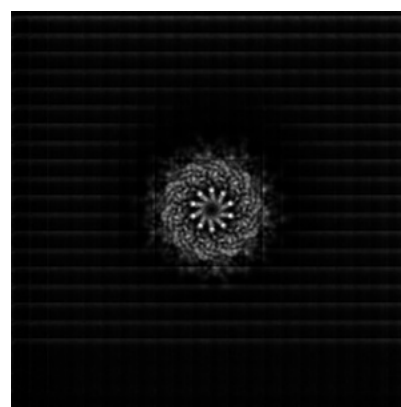
6.1.1 Primary map



X



Y

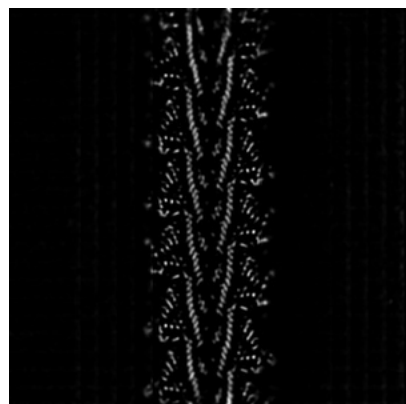


Z

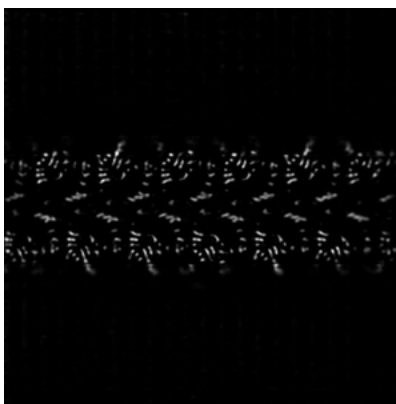
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

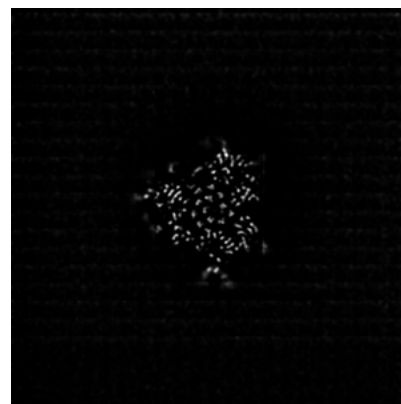
6.2.1 Primary map



X Index: 128



Y Index: 128

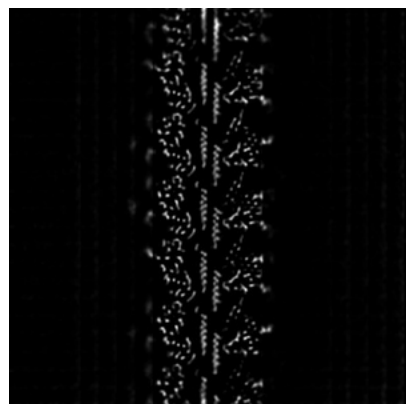


Z Index: 128

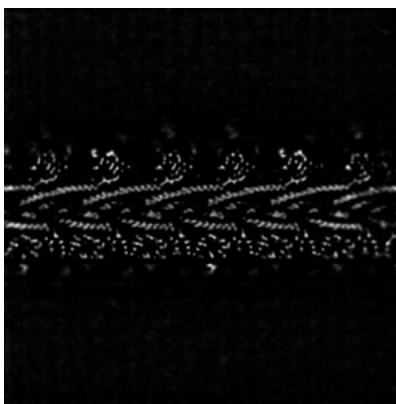
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

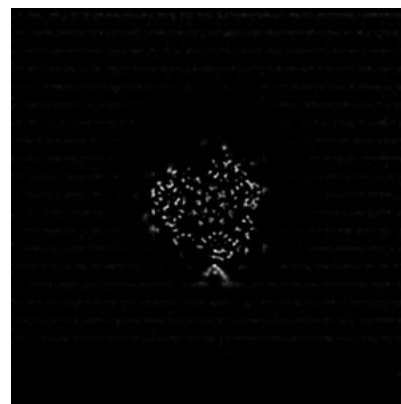
6.3.1 Primary map



X Index: 140



Y Index: 124

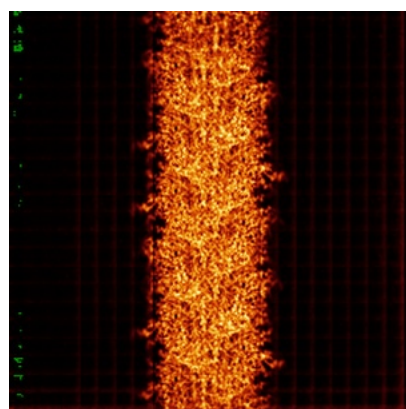


Z Index: 130

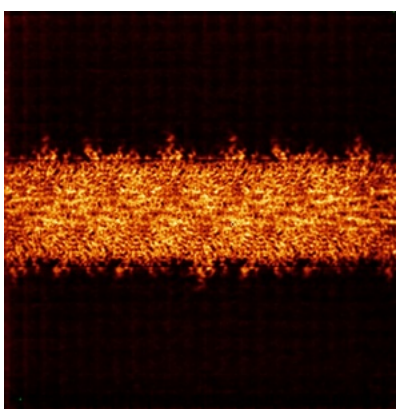
The images above show the largest variance slices of the map in three orthogonal directions.

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

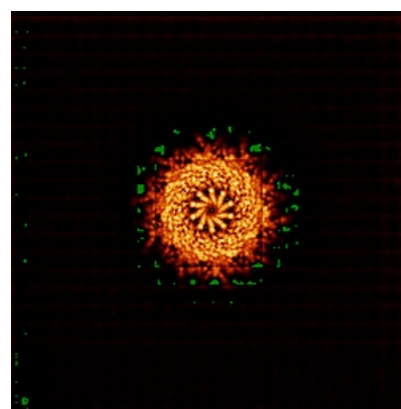
6.4.1 Primary map



X



Y

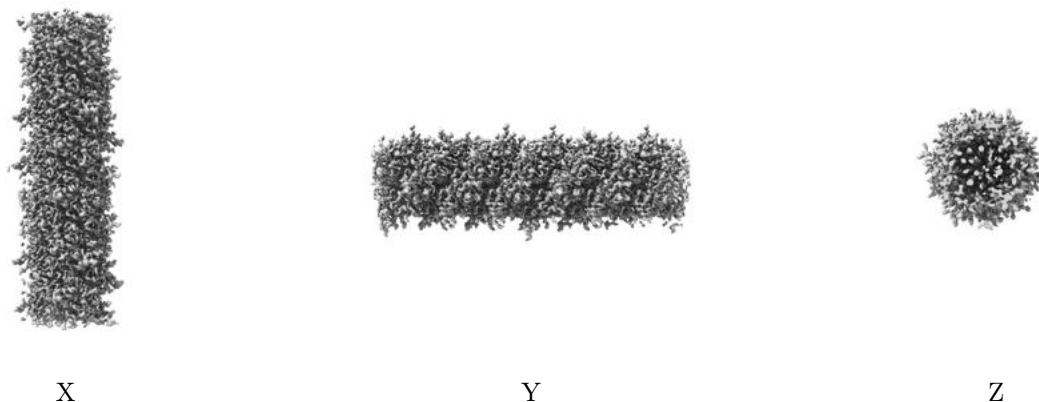


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

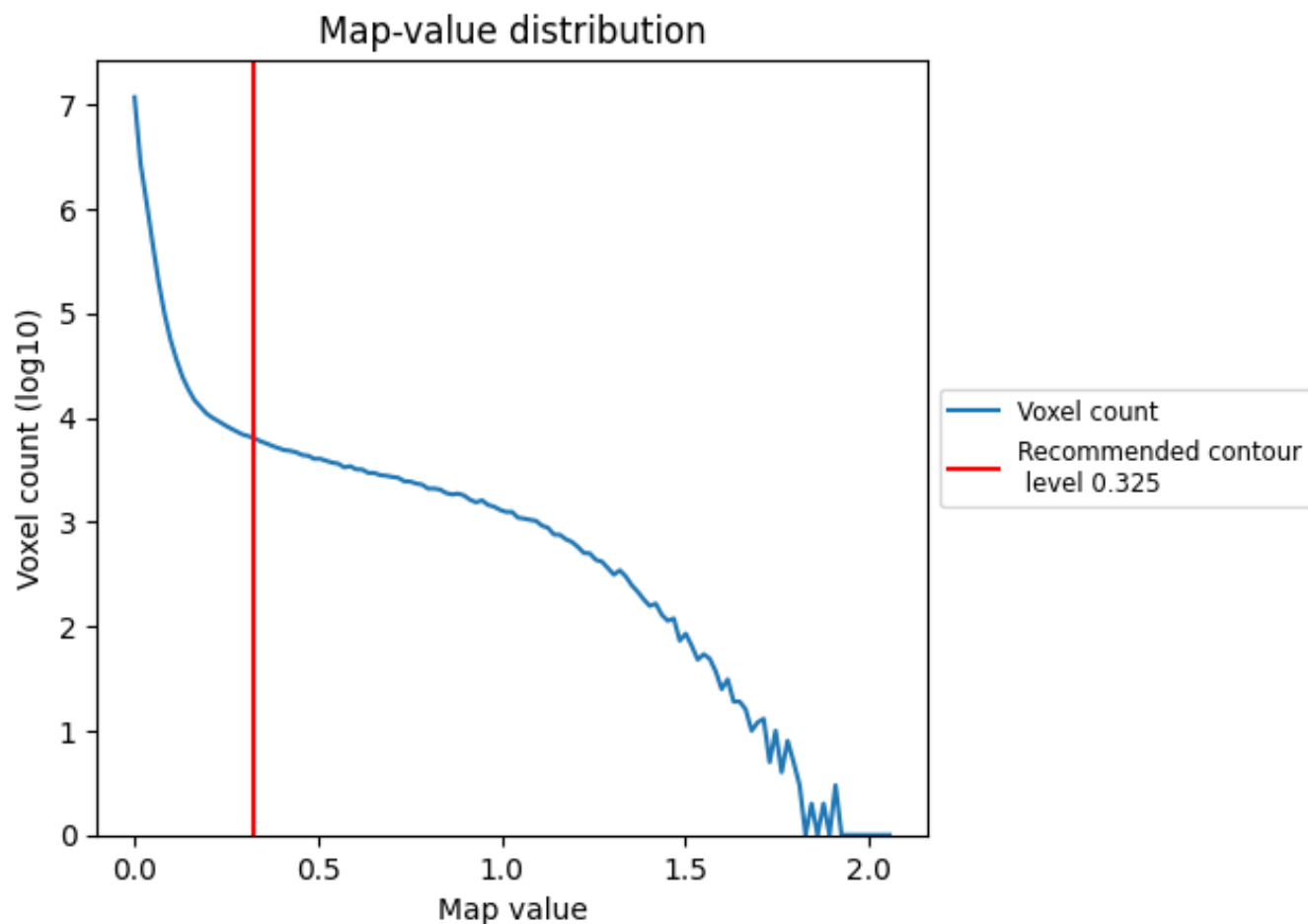
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

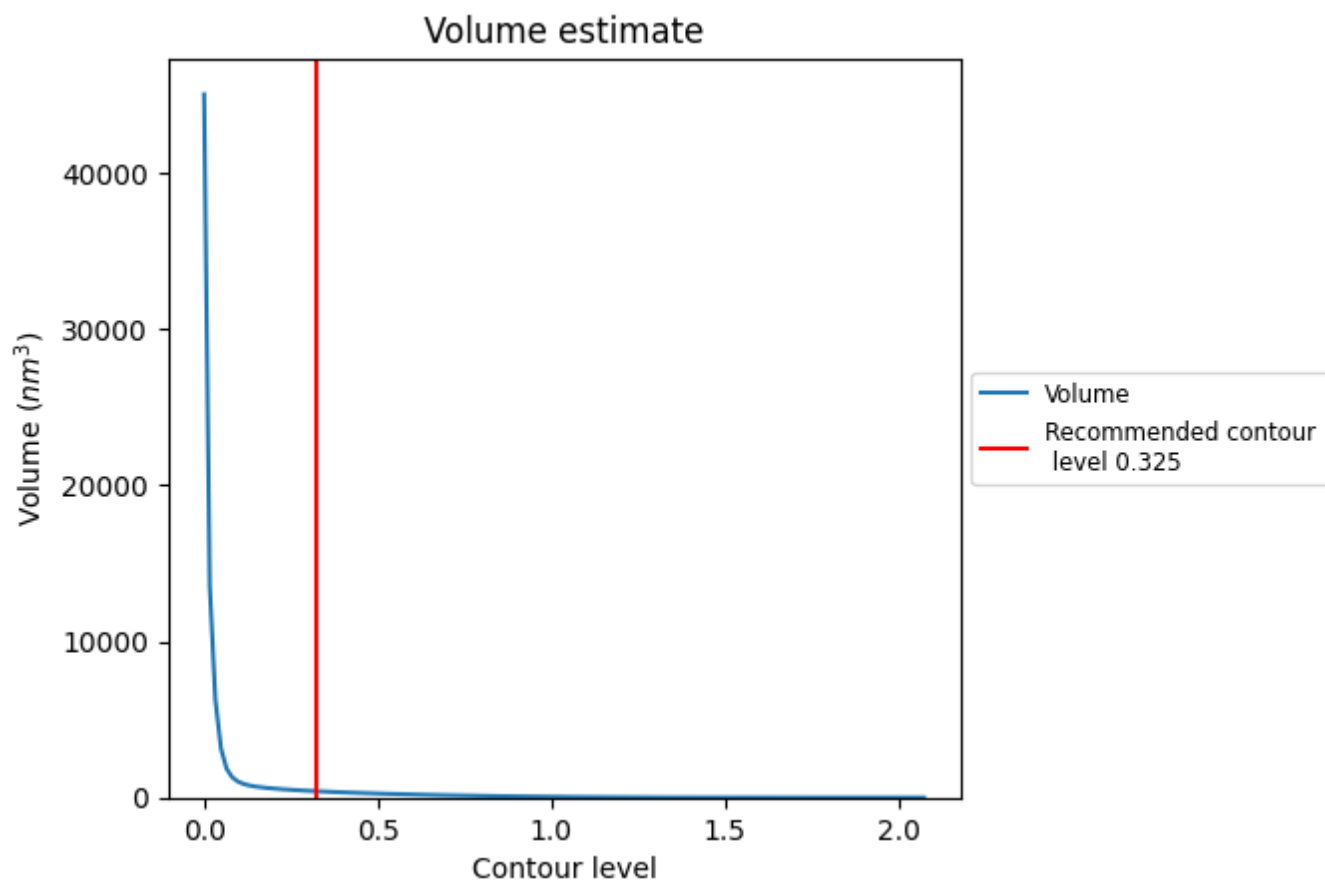
This section contains the results of statistical analysis of the map.

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.

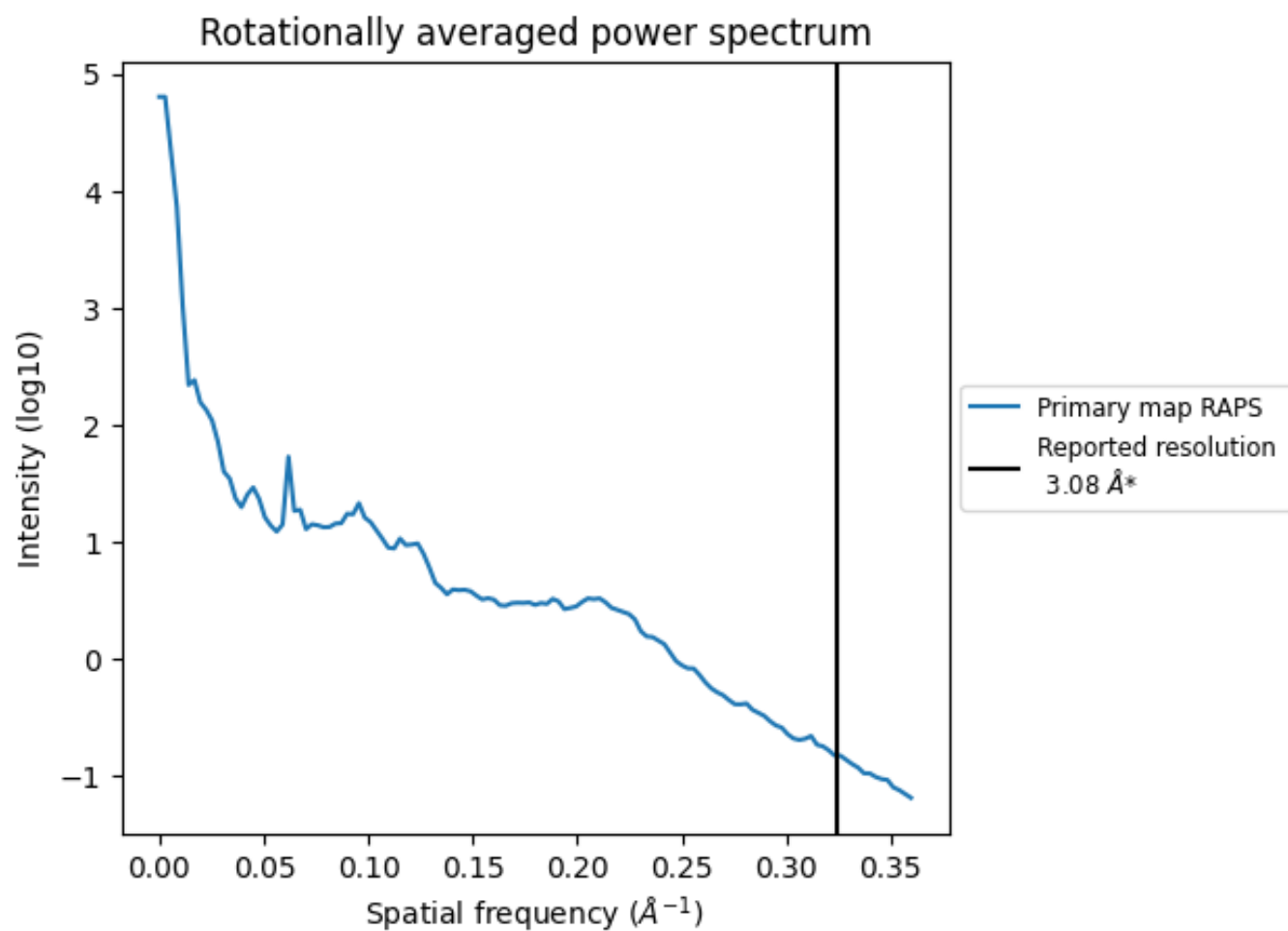
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403 nm³; this corresponds to an approximate mass of 364 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 ⓘ

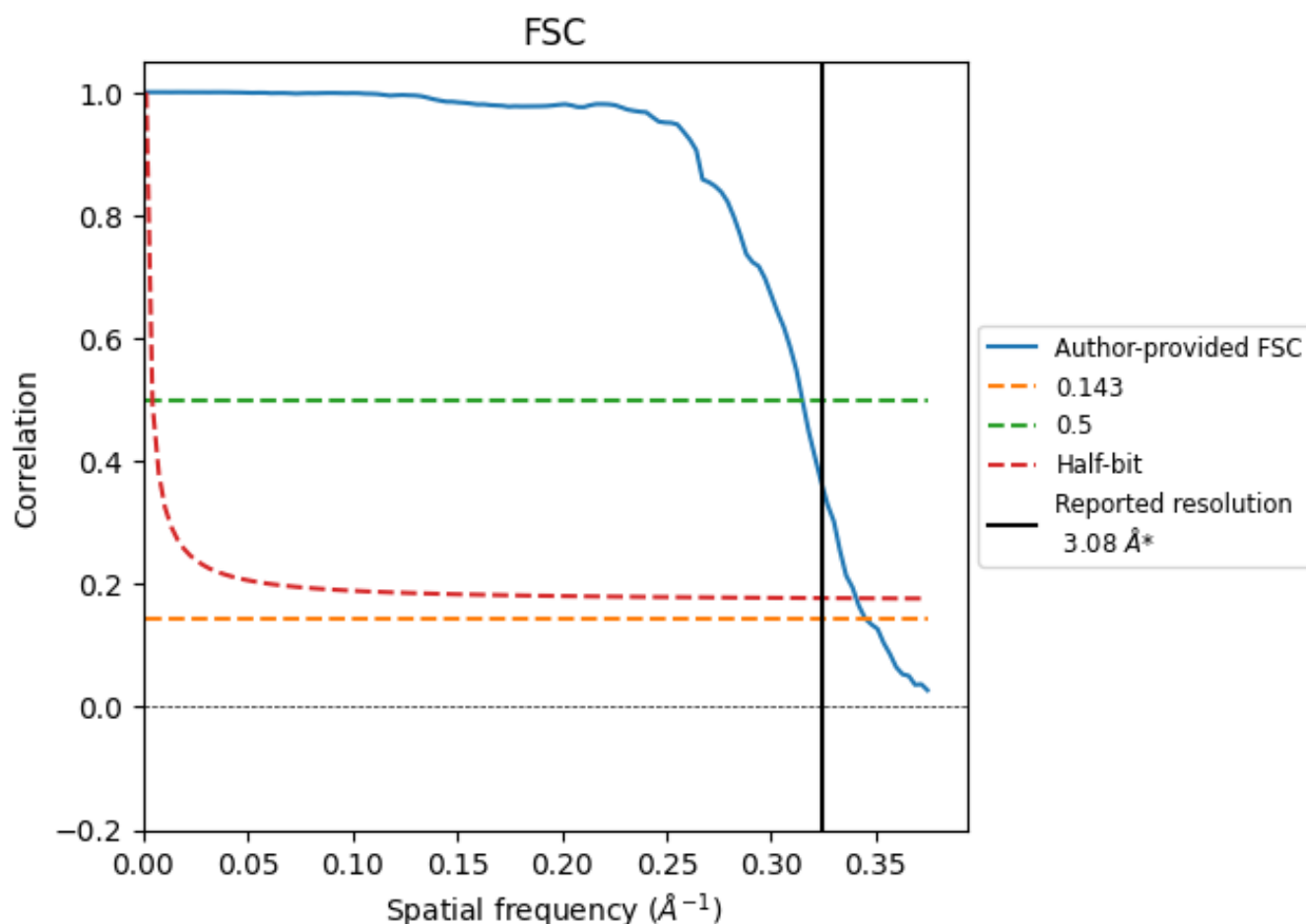


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

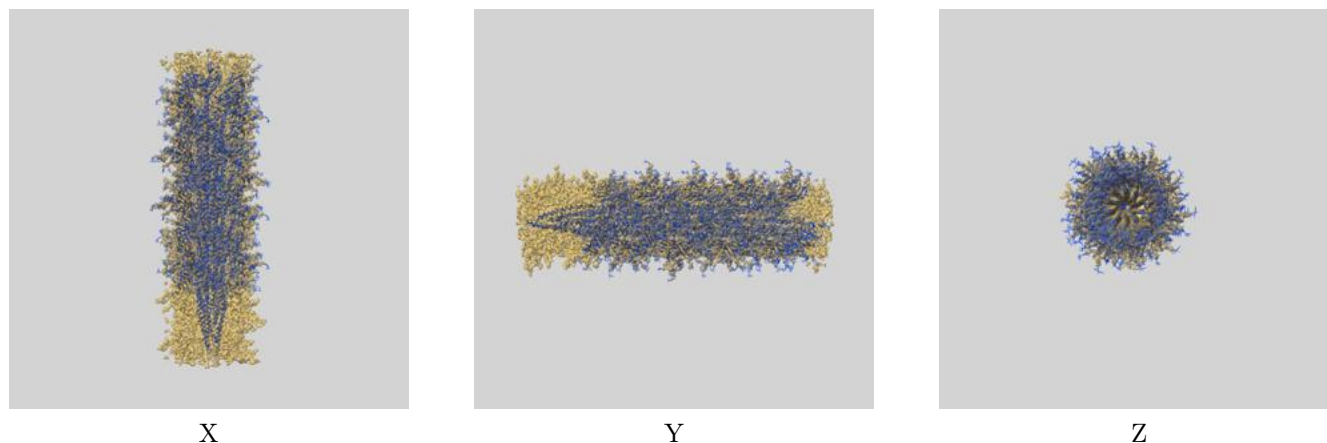
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	2.90	3.18	2.94
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

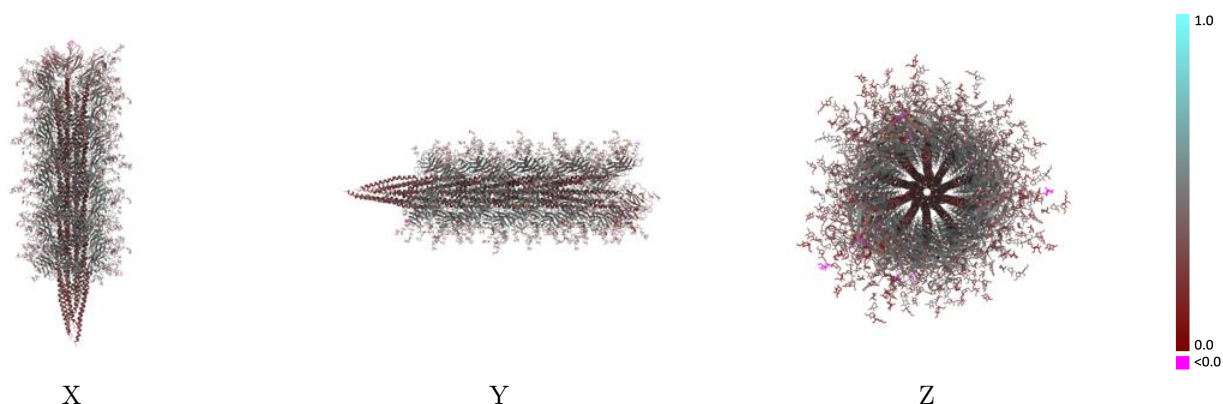
This section contains information regarding the fit between EMDB map EMD-12875 and PDB model 7OFQ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



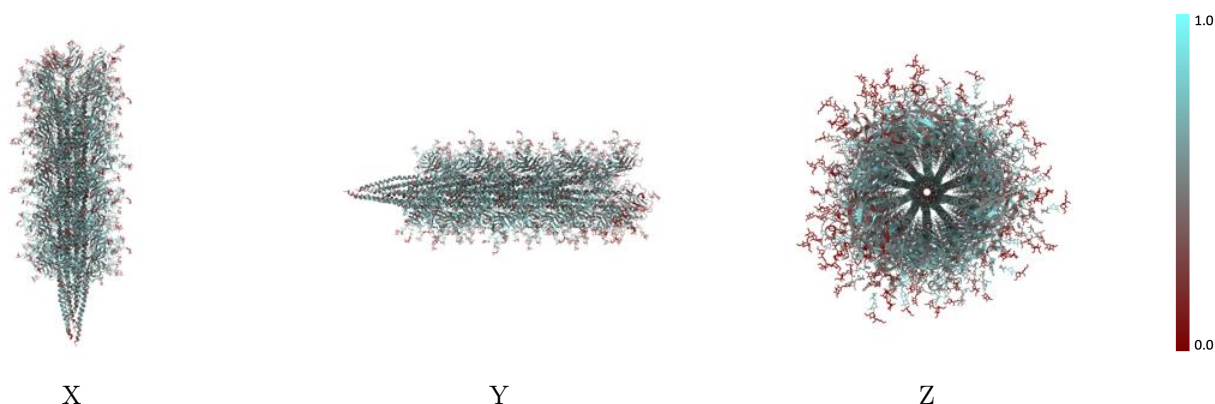
The images above show the 3D surface view of the map at the recommended contour level 0.325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



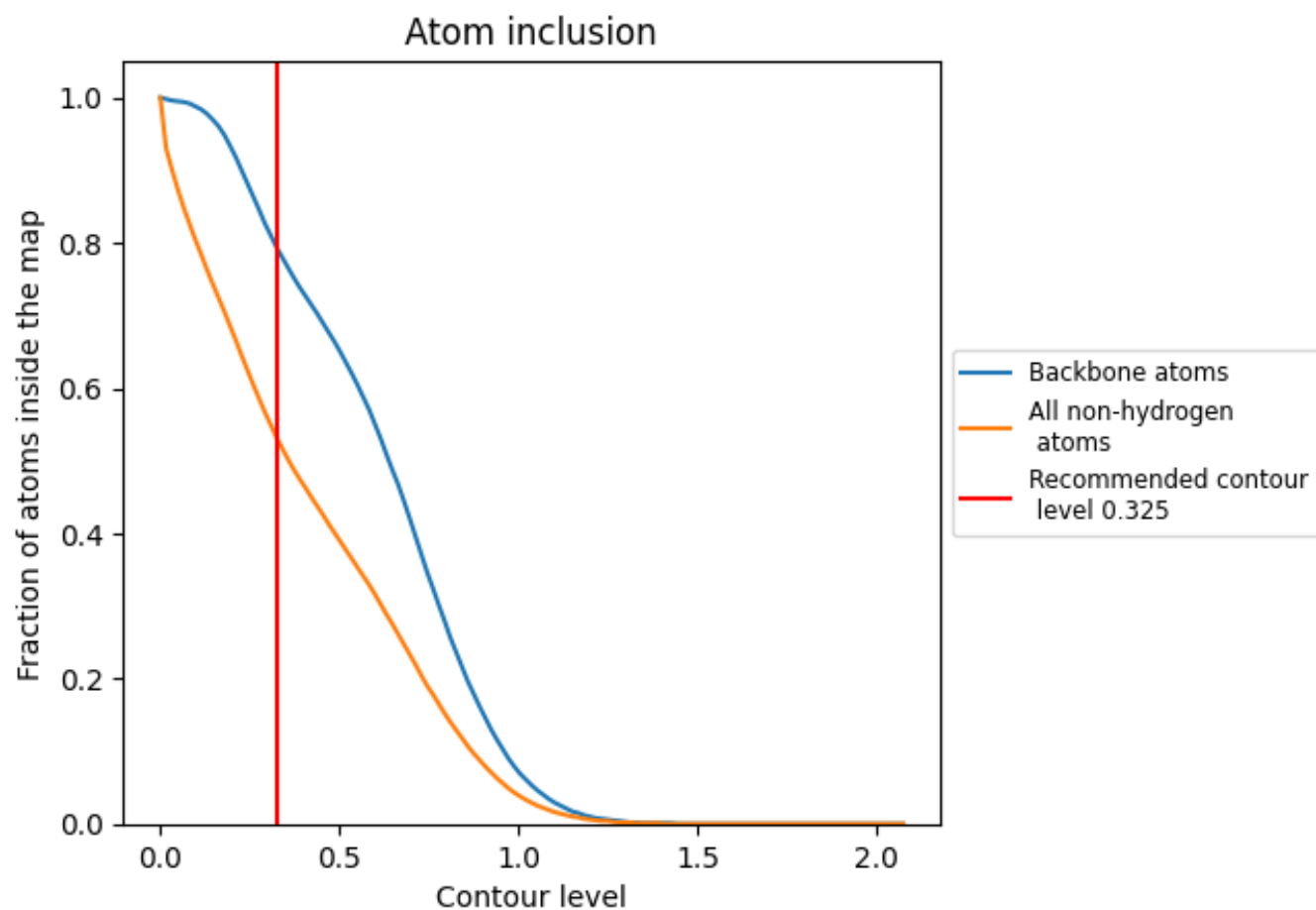
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.325).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 53% 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 (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5310	 0.3950
A	 0.5300	 0.3890
B	 0.5320	 0.4000
C	 0.5660	 0.4120
D	 0.5420	 0.4170
E	 0.5670	 0.4170
F	 0.5350	 0.4190
G	 0.5490	 0.4200
H	 0.5260	 0.4120
I	 0.5310	 0.4100
J	 0.5210	 0.4010
K	 0.5120	 0.3910
L	 0.4840	 0.3780
M	 0.4770	 0.3640
N	 0.4280	 0.3420
O	 0.4040	 0.3090
P	 0.5290	 0.3860
Q	 0.5640	 0.3980
R	 0.5480	 0.4040
S	 0.5660	 0.4130
T	 0.5480	 0.4140
U	 0.5590	 0.4170
V	 0.5470	 0.4160
W	 0.5570	 0.4160
X	 0.5500	 0.4140
Y	 0.5710	 0.4080
Z	 0.5420	 0.4050
a	 0.5440	 0.3900
b	 0.5230	 0.3840
c	 0.5030	 0.3620
d	 0.4510	 0.3330
e	 0.5550	 0.3980
f	 0.5580	 0.4080
g	 0.5720	 0.4140
h	 0.5640	 0.4180



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5750	 0.4210
j	 0.5880	 0.4260
k	 0.5760	 0.4210
l	 0.5760	 0.4210
m	 0.5630	 0.4130
n	 0.5470	 0.4080
o	 0.5530	 0.3970
p	 0.5290	 0.3860
q	 0.5130	 0.3690
r	 0.4630	 0.3460
s	 0.3810	 0.2970