



Full wwPDB EM Validation Report ⓘ

Apr 3, 2023 – 12:18 PM EDT

PDB ID : 7UIT
EMDB ID : EMD-26552
Title : Cryo-EM of pH-controlled and self-assembled fibers, peptide 2
Authors : Wang, F.; Grosvirt-Dramen, A.; Hochbaum, A.I.; Egelman, E.H.
Deposited on : 2022-03-29
Resolution : 3.90 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

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.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

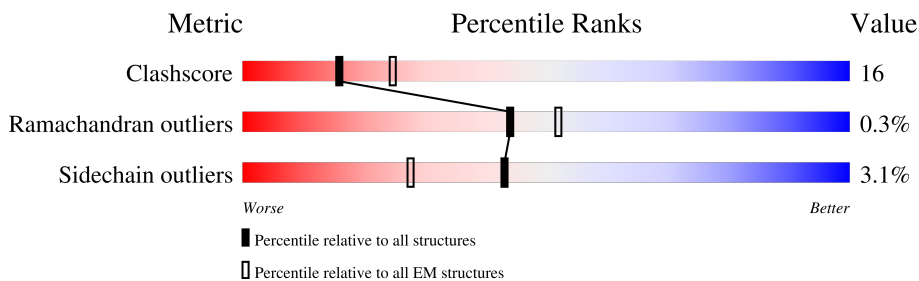
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	30	
1	1	30	
1	2	30	
1	3	30	
1	4	30	
1	5	30	
1	6	30	
1	7	30	

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Mol	Chain	Length	Quality of chain
1	8	30	83% 60% 40%
1	9	30	100% 63% 37%
1	A	30	100% 53% 43%
1	AA	30	100% 77% 23%
1	B	30	17% 63% 33%
1	BA	30	100% 63% 37%
1	C	30	13% 77% 23%
1	CA	30	93% 70% 27%
1	D	30	17% 67% 33%
1	DA	30	93% 67% 33%
1	E	30	13% 67% 33%
1	EA	30	100% 67% 27% 7%
1	F	30	17% 70% 30%
1	FA	30	97% 77% 20%
1	G	30	13% 70% 20% 10%
1	GA	30	97% 43% 50% 7%
1	H	30	77% 50% 47%
1	HA	30	97% 43% 53%
1	I	30	73% 67% 30%
1	IA	30	90% 47% 47% 7%
1	J	30	83% 60% 40%
1	JA	30	100% 43% 53%
1	K	30	73% 50% 47%
1	L	30	87% 63% 37%
1	M	30	93% 80% 13% 7%

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Mol	Chain	Length	Quality of chain
1	N	30	53% 67% 27% 7%
1	O	30	60% 63% 33% .
1	P	30	67% 57% 43%
1	Q	30	53% 67% 30% .
1	R	30	57% 57% 40% .
1	S	30	50% 57% 43%
1	T	30	67% 57% 40% .
1	U	30	90% 63% 33% .
1	V	30	77% 60% 37% .
1	W	30	80% 57% 40% .
1	X	30	70% 70% 27% .
1	Y	30	87% 60% 37% .
1	Z	30	13% 67% 27% 7%
1	a	30	13% 90% 10%
1	b	30	17% 90% 10%
1	c	30	13% 93% 7%
1	d	30	10% 87% 13%
1	e	30	13% 93% 7%
1	f	30	20% 93% 7%
1	g	30	20% 93% 7%
1	h	30	20% 93% 7%
1	i	30	17% 97% .
1	j	30	20% 90% 10%
1	k	30	13% 90% 10%
1	l	30	37% 93% 7%

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Mol	Chain	Length	Quality of chain
1	m	30	
1	n	30	
1	o	30	
1	p	30	
1	q	30	
1	r	30	
1	s	30	
1	t	30	
1	u	30	
1	v	30	
1	w	30	
1	x	30	
1	y	30	
1	z	30	

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
1	PHI	V	5621	-	-	X	-

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17064 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 Peptide 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	I	N	O		
1	B	30	237	159	1	39	38	0	1
1	C	30	237	159	1	39	38	0	1
1	D	30	237	159	1	39	38	0	1
1	E	30	237	159	1	39	38	0	1
1	F	30	237	159	1	39	38	0	1
1	G	30	237	159	1	39	38	0	1
1	H	30	237	159	1	39	38	0	1
1	I	30	237	159	1	39	38	0	1
1	J	30	237	159	1	39	38	0	1
1	K	30	237	159	1	39	38	0	1
1	L	30	237	159	1	39	38	0	1
1	M	30	237	159	1	39	38	0	1
1	N	30	237	159	1	39	38	0	1
1	O	30	237	159	1	39	38	0	1
1	P	30	237	159	1	39	38	0	1
1	Q	30	237	159	1	39	38	0	1
1	R	30	237	159	1	39	38	0	1

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	T	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	U	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	V	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	W	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	X	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	Y	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	Z	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	a	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	b	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	c	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	d	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	e	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	f	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	g	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	h	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	i	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	j	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	k	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	l	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	m	30	Total	C	I	N	O	0	1
			237	159	1	39	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	n	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	o	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	p	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	q	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	r	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	s	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	t	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	u	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	v	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	w	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	x	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	y	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	z	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	0	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	1	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	2	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	3	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	4	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	5	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	6	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	7	30	Total	C	I	N	O	0	1
			237	159	1	39	38		

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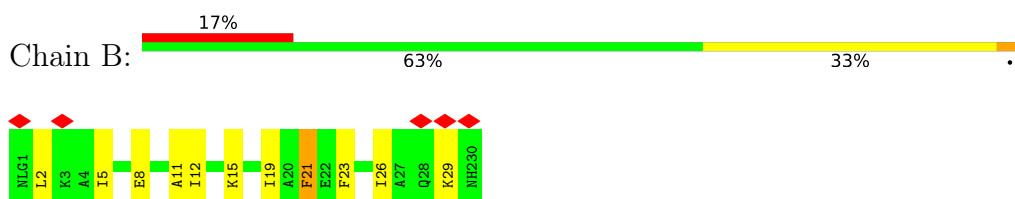
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Mol	Chain	Residues	Atoms				AltConf	Trace	
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			237	159	1	39	38		
1	9	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	AA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	BA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	CA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	DA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	EA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	FA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	A	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	JA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	GA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	HA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		
1	IA	30	Total	C	I	N	O	0	1
			237	159	1	39	38		

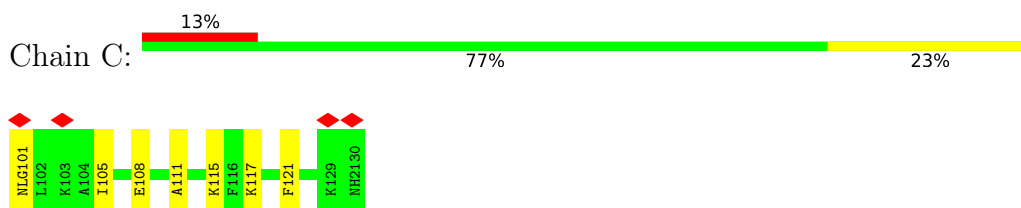
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

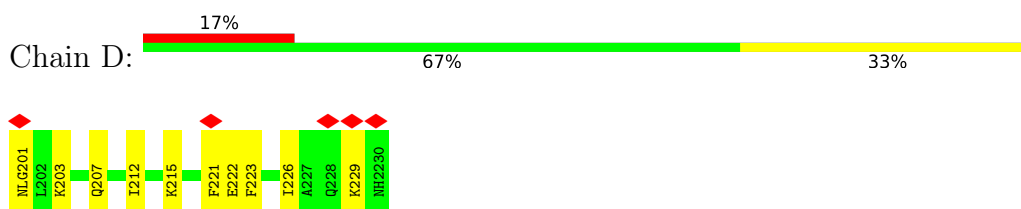
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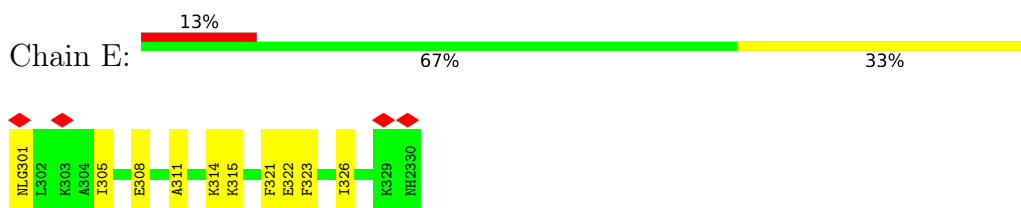
- Molecule 1: Peptide 2



- Molecule 1: Peptide 2

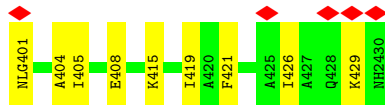


- Molecule 1: Peptide 2



- Molecule 1: Peptide 2

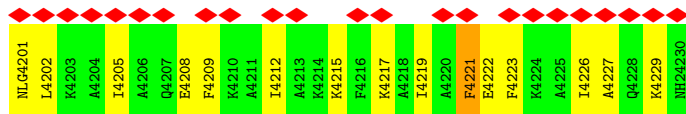
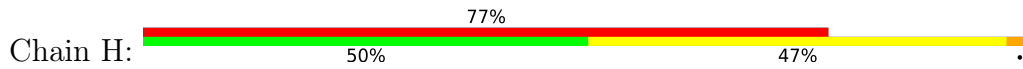




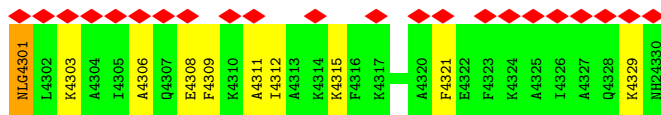
- Molecule 1: Peptide 2



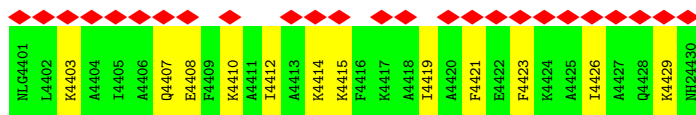
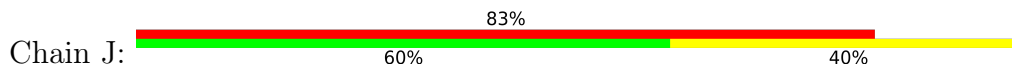
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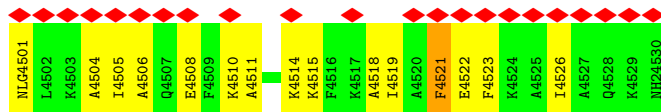
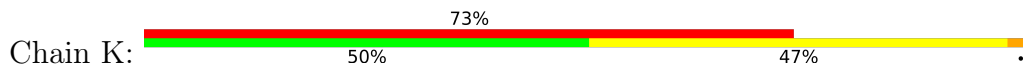
- Molecule 1: Peptide 2



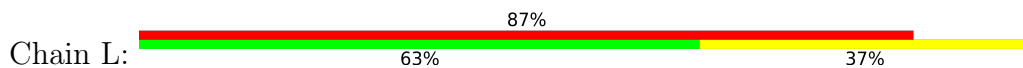
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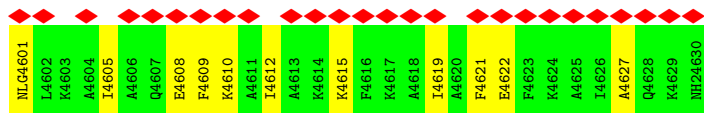


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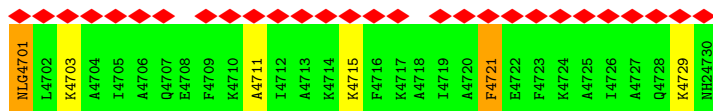
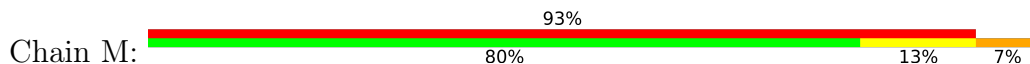


- Molecule 1: Peptide 2

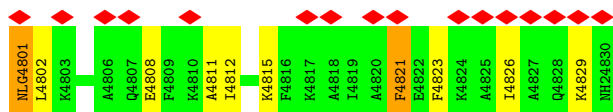




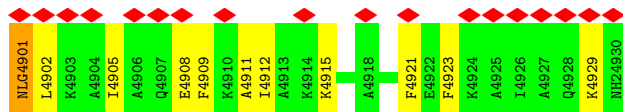
• Molecule 1: Peptide 2



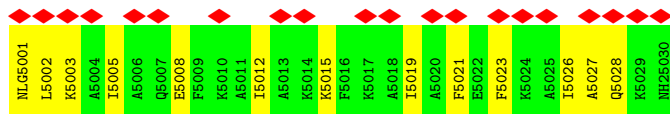
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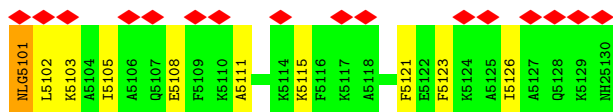
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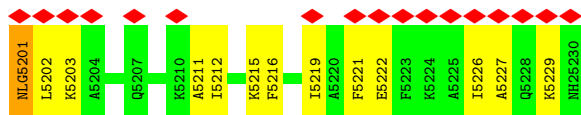


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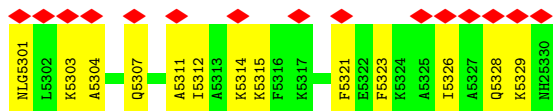


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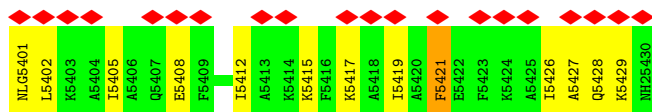




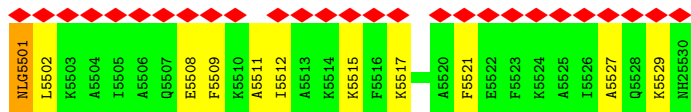
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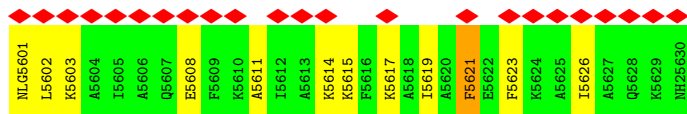
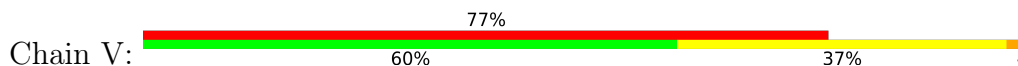
• Molecule 1: Peptide 2



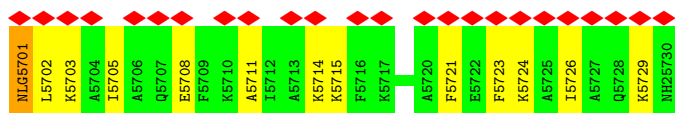
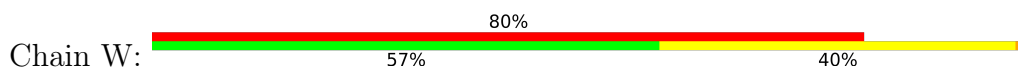
• Molecule 1: Peptide 2



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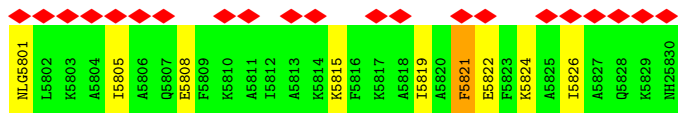


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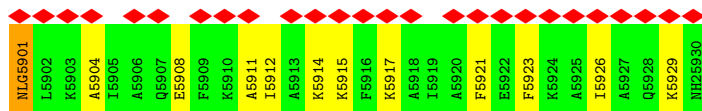
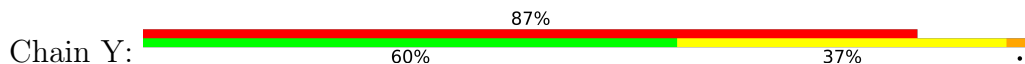


• Molecule 1: Peptide 2





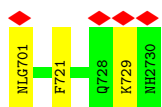
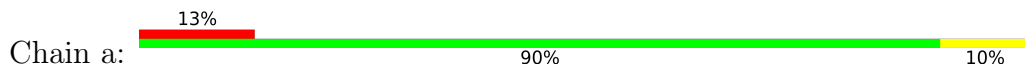
• Molecule 1: Peptide 2



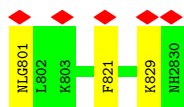
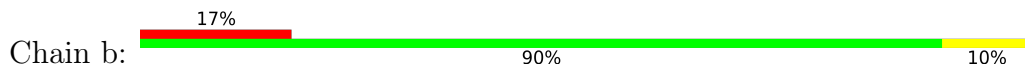
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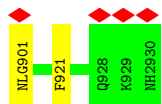
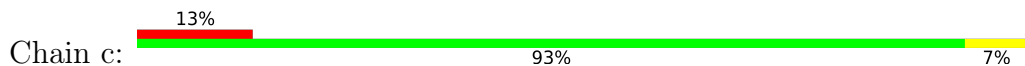
• Molecule 1: Peptide 2



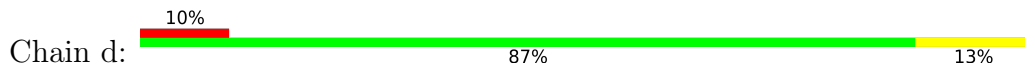
• Molecule 1: Peptide 2

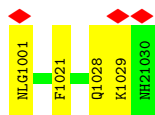


• Molecule 1: Peptide 2

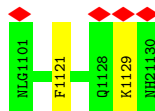


• Molecule 1: Peptide 2

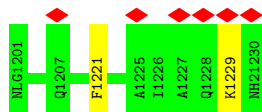
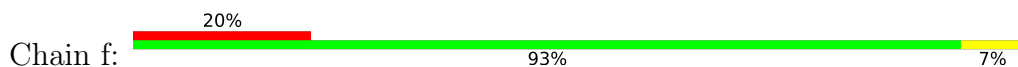




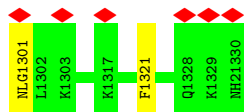
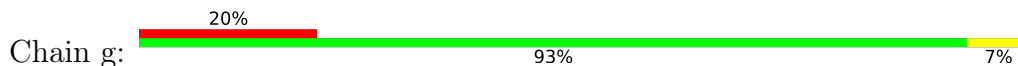
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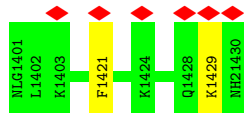
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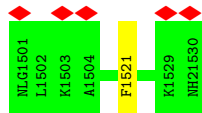
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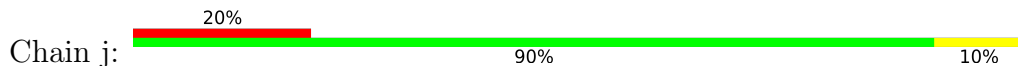
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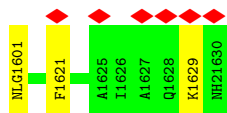


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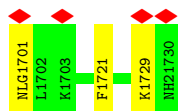
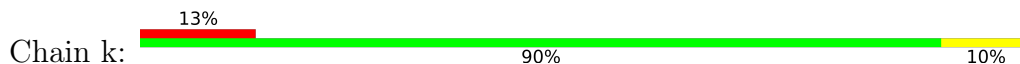


• Molecule 1: Peptide 2

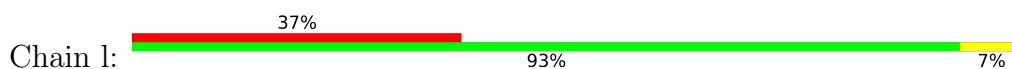




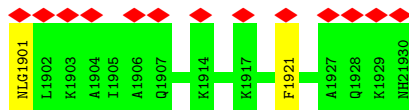
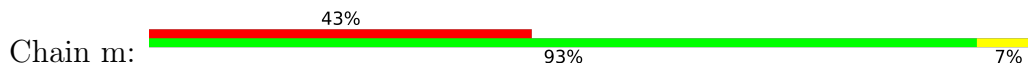
- Molecule 1: Peptide 2



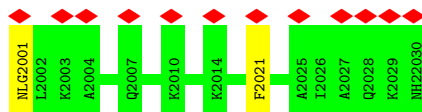
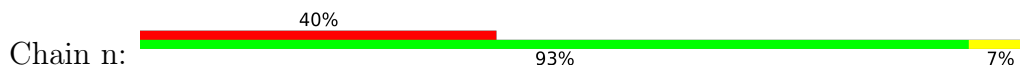
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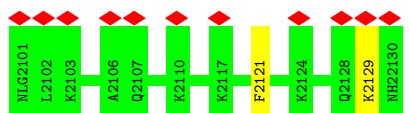
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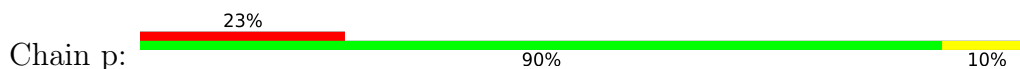
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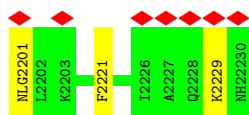


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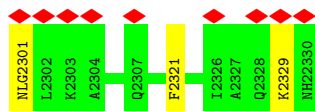
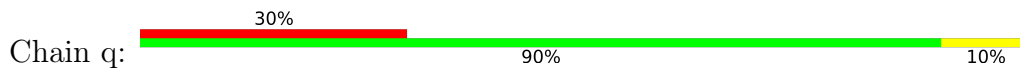


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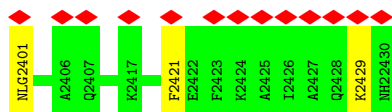
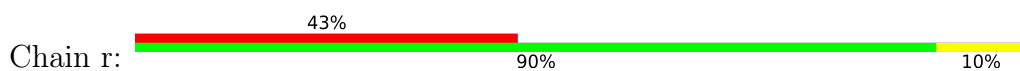




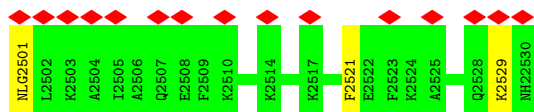
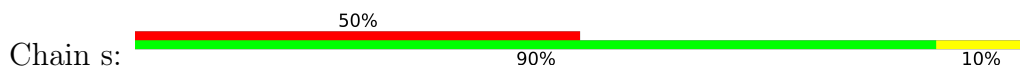
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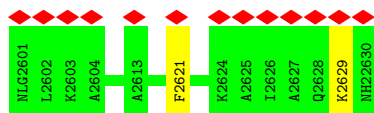
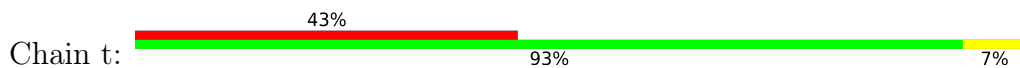
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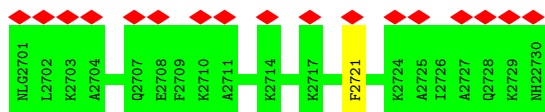
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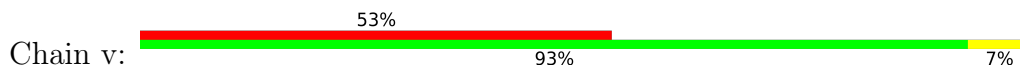
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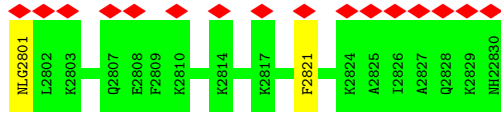


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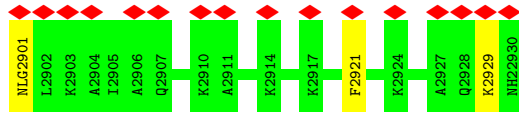
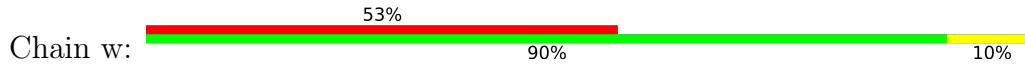


- Molecule 1: Peptide 2

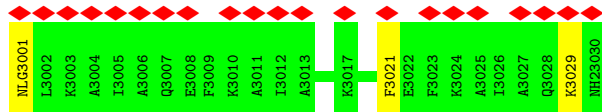
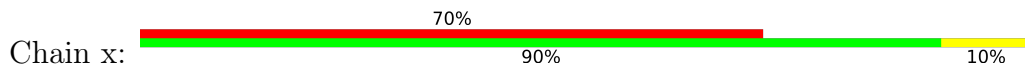




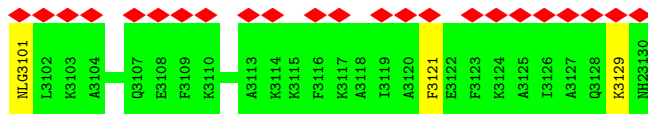
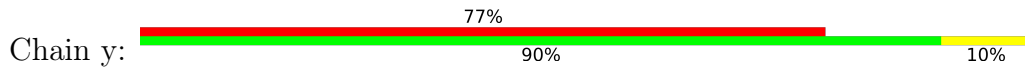
• Molecule 1: Peptide 2



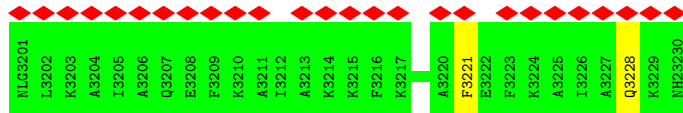
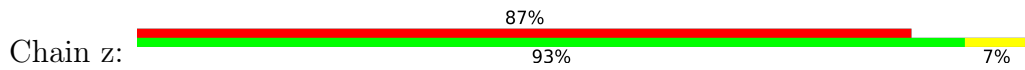
• Molecule 1: Peptide 2



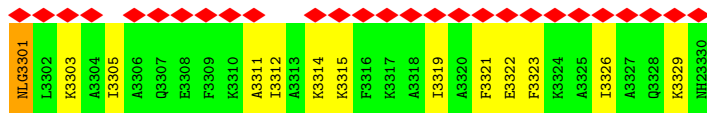
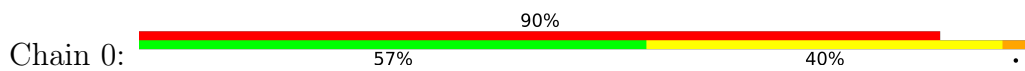
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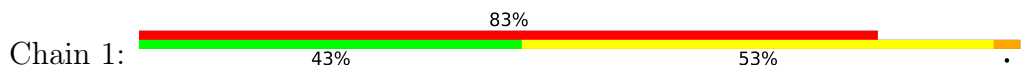
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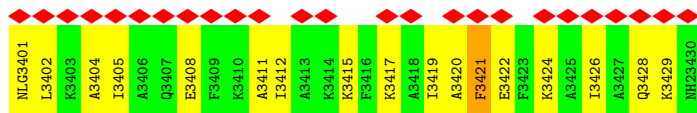


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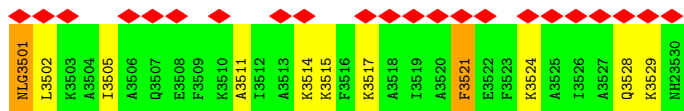


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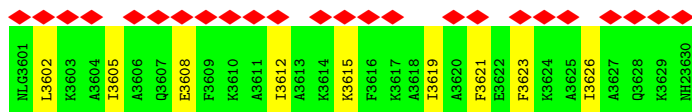
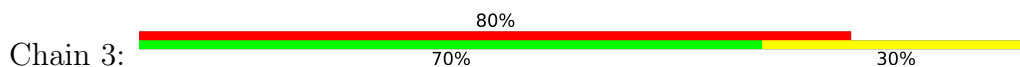




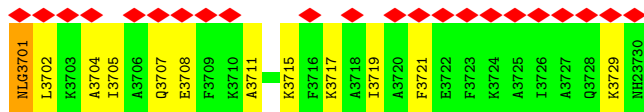
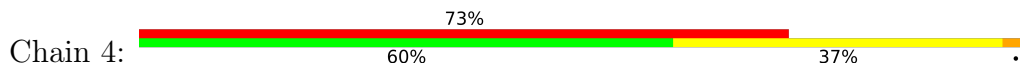
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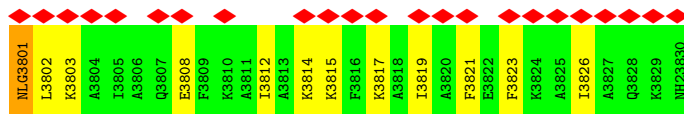
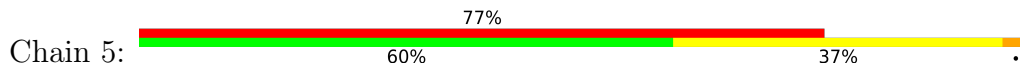
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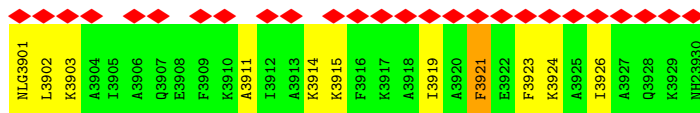
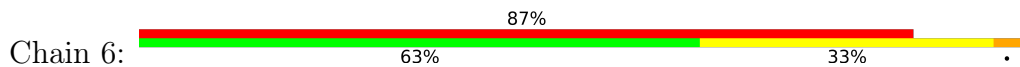
• Molecule 1: Peptide 2



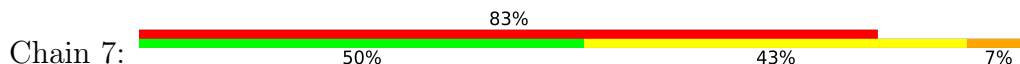
• Molecule 1: Peptide 2



• Molecule 1: Peptide 2

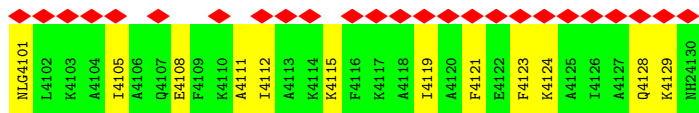
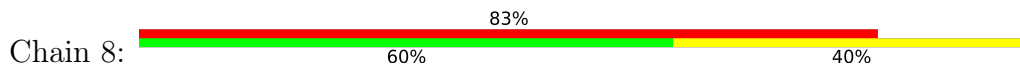


• Molecule 1: Peptide 2

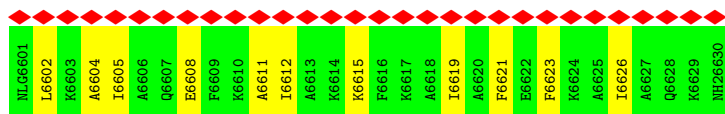




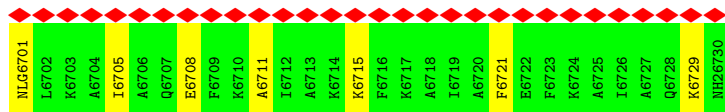
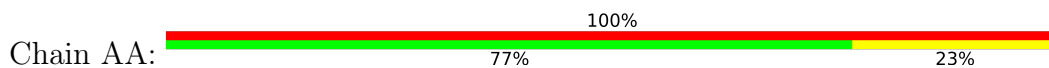
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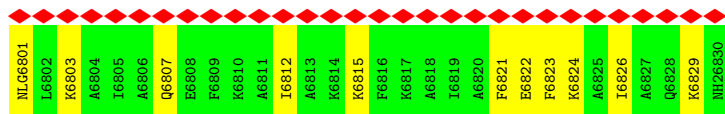
• Molecule 1: Peptide 2



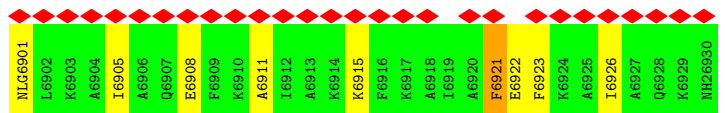
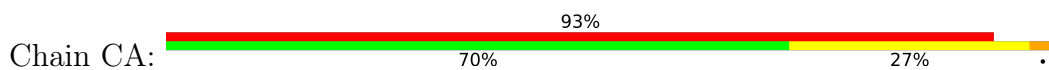
• Molecule 1: Peptide 2



• Molecule 1: Peptide 2

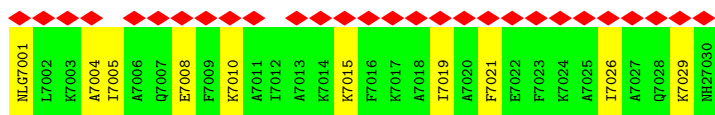


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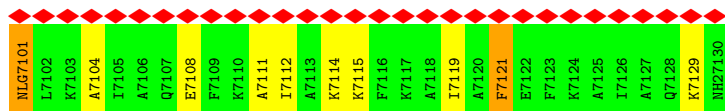


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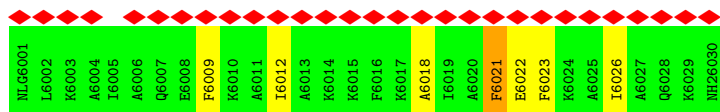
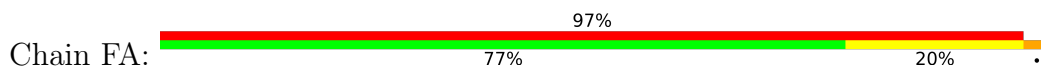




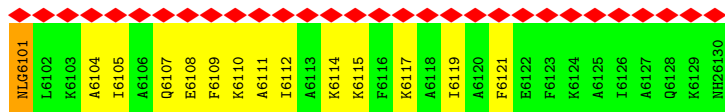
• Molecule 1: Peptide 2



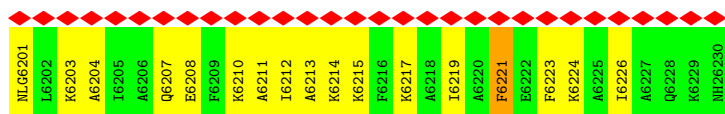
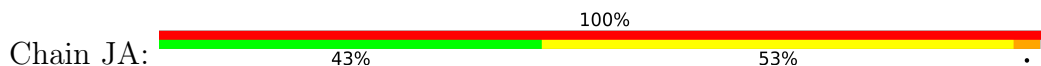
• Molecule 1: Peptide 2



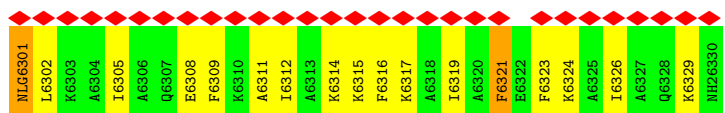
• Molecule 1: Peptide 2



• Molecule 1: Peptide 2

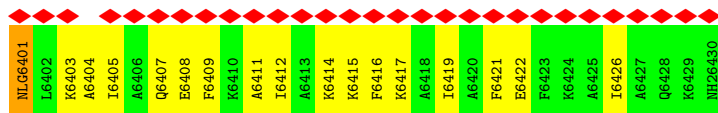


• Molecule 1: Peptide 2

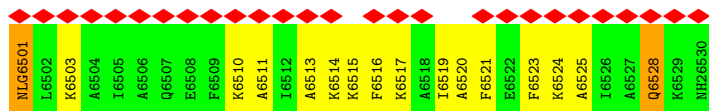
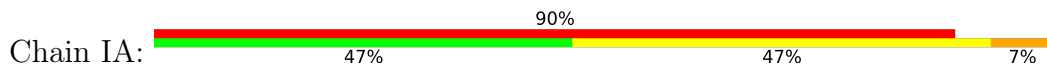


• Molecule 1: Peptide 2





● Molecule 1: Peptide 2



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-58.76°, rise=12.68 Å, axial sym=C1	Depositor
Number of segments used	85453	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.374	Depositor
Minimum map value	-0.576	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	691.2, 691.2, 691.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, NLG, PHI

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	0	0.35	0/213	0.42	0/278
1	1	0.34	0/213	0.47	0/278
1	2	0.33	0/213	0.42	0/278
1	3	0.33	0/213	0.36	0/278
1	4	0.33	0/213	0.42	0/278
1	5	0.33	0/213	0.38	0/278
1	6	0.33	0/213	0.39	0/278
1	7	0.33	0/213	0.40	0/278
1	8	0.33	0/213	0.39	0/278
1	9	0.39	0/213	0.40	0/278
1	A	0.32	0/213	0.38	0/278
1	AA	0.40	0/213	0.45	0/278
1	B	0.39	0/213	0.40	0/278
1	BA	0.42	0/213	0.46	0/278
1	C	0.41	0/213	0.45	0/278
1	CA	0.41	0/213	0.48	0/278
1	D	0.42	0/213	0.46	0/278
1	DA	0.39	0/213	0.40	0/278
1	E	0.41	0/213	0.48	0/278
1	EA	0.40	0/213	0.40	0/278
1	F	0.39	0/213	0.40	0/278
1	FA	0.37	0/213	0.46	0/278
1	G	0.40	0/213	0.40	0/278
1	GA	0.36	0/213	0.66	0/278
1	H	0.34	0/213	0.38	0/278
1	HA	0.42	0/213	0.66	0/278
1	I	0.34	0/213	0.39	0/278
1	IA	0.37	0/213	0.46	0/278
1	J	0.34	0/213	0.38	0/278
1	JA	0.34	0/213	0.53	0/278
1	K	0.43	0/213	0.56	0/278
1	L	0.35	0/213	0.38	0/278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.33	0/213	0.40	0/278
1	N	0.34	0/213	0.42	0/278
1	O	0.39	0/213	0.42	0/278
1	P	0.36	0/213	0.42	0/278
1	Q	0.35	0/213	0.48	0/278
1	R	0.36	0/213	0.40	0/278
1	S	0.34	0/213	0.39	0/278
1	T	0.34	0/213	0.37	0/278
1	U	0.36	0/213	0.41	0/278
1	V	0.34	0/213	0.39	0/278
1	W	0.33	0/213	0.36	0/278
1	X	0.35	0/213	0.42	0/278
1	Y	0.34	0/213	0.42	0/278
1	Z	0.40	0/213	0.46	0/278
1	a	0.39	0/213	0.46	0/278
1	b	0.44	0/213	0.45	0/278
1	c	0.41	0/213	0.48	0/278
1	d	0.40	0/213	0.38	0/278
1	e	0.38	0/213	0.39	0/278
1	f	0.40	0/213	0.41	0/278
1	g	0.41	0/213	0.44	0/278
1	h	0.44	0/213	0.41	0/278
1	i	0.42	0/213	0.50	0/278
1	j	0.38	0/213	0.44	0/278
1	k	0.37	0/213	0.40	0/278
1	l	0.36	0/213	0.43	0/278
1	m	0.40	0/213	0.41	0/278
1	n	0.37	0/213	0.40	0/278
1	o	0.37	0/213	0.53	0/278
1	p	0.35	0/213	0.36	0/278
1	q	0.35	0/213	0.41	0/278
1	r	0.35	0/213	0.42	0/278
1	s	0.34	0/213	0.35	0/278
1	t	0.34	0/213	0.36	0/278
1	u	0.35	0/213	0.36	0/278
1	v	0.35	0/213	0.37	0/278
1	w	0.34	0/213	0.38	0/278
1	x	0.34	0/213	0.38	0/278
1	y	0.32	0/213	0.35	0/278
1	z	0.34	0/213	0.45	0/278
All	All	0.37	0/15336	0.43	0/20016

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
1	2	0	1
1	4	0	1
1	5	0	1
1	7	0	1
1	8	0	1
1	A	0	1
1	AA	0	1
1	C	0	1
1	DA	0	1
1	EA	0	1
1	F	0	1
1	G	0	1
1	GA	0	1
1	H	0	1
1	HA	0	1
1	I	0	1
1	IA	0	1
1	JA	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	U	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	g	0	1
1	j	0	1
1	k	0	1
1	m	0	1
1	n	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	v	0	1
1	w	0	1
1	x	0	1
1	y	0	1
All	All	0	48

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	3301	NLG	Mainchain
1	2	3501	NLG	Mainchain
1	4	3701	NLG	Mainchain
1	5	3801	NLG	Mainchain
1	7	4001	NLG	Mainchain
1	8	4101	NLG	Mainchain
1	A	6101	NLG	Mainchain
1	AA	6701	NLG	Mainchain
1	C	101	NLG	Mainchain
1	DA	7001	NLG	Mainchain
1	EA	7101	NLG	Mainchain
1	F	401	NLG	Mainchain
1	G	501	NLG	Mainchain
1	GA	6301	NLG	Mainchain
1	H	4201	NLG	Mainchain
1	HA	6401	NLG	Mainchain
1	I	4301	NLG	Mainchain
1	IA	6501	NLG	Mainchain
1	JA	6201	NLG	Mainchain
1	K	4501	NLG	Mainchain
1	L	4601	NLG	Mainchain
1	M	4701	NLG	Mainchain
1	N	4801	NLG	Mainchain
1	O	4901	NLG	Mainchain
1	Q	5101	NLG	Mainchain

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Mol	Chain	Res	Type	Group
1	R	5201	NLG	Mainchain
1	S	5301	NLG	Mainchain
1	U	5501	NLG	Mainchain
1	W	5701	NLG	Mainchain
1	X	5801	NLG	Mainchain
1	Y	5901	NLG	Mainchain
1	a	701	NLG	Mainchain
1	b	801	NLG	Mainchain
1	c	901	NLG	Mainchain
1	d	1001	NLG	Mainchain
1	g	1301	NLG	Mainchain
1	j	1601	NLG	Mainchain
1	k	1701	NLG	Mainchain
1	m	1901	NLG	Mainchain
1	n	2001	NLG	Mainchain
1	p	2201	NLG	Mainchain
1	q	2301	NLG	Mainchain
1	r	2401	NLG	Mainchain
1	s	2501	NLG	Mainchain
1	v	2801	NLG	Mainchain
1	w	2901	NLG	Mainchain
1	x	3001	NLG	Mainchain
1	y	3101	NLG	Mainchain

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	0	237	0	258	13	0
1	1	237	0	258	25	0
1	2	237	0	258	7	0
1	3	237	0	258	11	0
1	4	237	0	258	10	0
1	5	237	0	258	10	0
1	6	237	0	258	11	0
1	7	237	0	258	16	0
1	8	237	0	258	11	0
1	9	237	0	258	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	237	0	258	14	0
1	AA	237	0	258	5	0
1	B	237	0	258	11	0
1	BA	237	0	258	12	0
1	C	237	0	258	5	0
1	CA	237	0	258	10	0
1	D	237	0	258	6	0
1	DA	237	0	258	7	0
1	E	237	0	258	7	0
1	EA	237	0	258	9	0
1	F	237	0	258	6	0
1	FA	237	0	258	6	0
1	G	237	0	258	8	0
1	GA	237	0	258	14	0
1	H	237	0	258	11	0
1	HA	237	0	258	14	0
1	I	237	0	258	10	0
1	IA	237	0	258	16	0
1	J	237	0	258	9	0
1	JA	237	0	258	18	0
1	K	237	0	258	11	0
1	L	237	0	258	8	0
1	M	237	0	258	5	0
1	N	237	0	258	8	0
1	O	237	0	258	11	0
1	P	237	0	258	9	0
1	Q	237	0	258	7	0
1	R	237	0	258	13	0
1	S	237	0	258	9	0
1	T	237	0	258	13	0
1	U	237	0	258	8	0
1	V	237	0	258	16	0
1	W	237	0	258	9	0
1	X	237	0	258	8	0
1	Y	237	0	258	9	0
1	Z	237	0	258	7	0
1	a	237	0	258	0	0
1	b	237	0	258	0	0
1	c	237	0	258	0	0
1	d	237	0	258	0	0
1	e	237	0	258	0	0
1	f	237	0	258	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	237	0	258	0	0
1	h	237	0	258	0	0
1	i	237	0	258	0	0
1	j	237	0	258	0	0
1	k	237	0	258	0	0
1	l	237	0	258	0	0
1	m	237	0	258	0	0
1	n	237	0	258	0	0
1	o	237	0	258	0	0
1	p	237	0	258	0	0
1	q	237	0	258	0	0
1	r	237	0	258	0	0
1	s	237	0	258	0	0
1	t	237	0	258	0	0
1	u	237	0	258	0	0
1	v	237	0	258	0	0
1	w	237	0	258	0	0
1	x	237	0	258	0	0
1	y	237	0	258	0	0
1	z	237	0	258	0	0
All	All	17064	0	18576	358	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 16.

All (358) 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:R:5201:NLG:CD	1:R:5201:NLG:H2	1.66	1.05
1:V:5621:PHI:HE2	1:IA:6525:ALA:HA	1.42	0.97
1:7:4017:LYS:O	1:7:4021:PHI:HD1	1.69	0.93
1:V:5621:PHI:I	1:IA:6524:LYS:C	2.77	0.92
1:GA:6314:LYS:HA	1:GA:6317:LYS:HE2	1.58	0.85
1:R:5201:NLG:CD	1:R:5201:NLG:N2	2.41	0.81
1:P:5023:PHE:HA	1:P:5026:ILE:HG12	1.64	0.80
1:7:4017:LYS:HG2	1:7:4021:PHI:HE1	1.62	0.80
1:7:4017:LYS:CG	1:7:4021:PHI:HE1	2.16	0.76
1:A:6107:GLN:NE2	1:A:6108:GLU:OE2	2.20	0.74
1:2:3524:LYS:O	1:2:3528:GLN:NE2	2.21	0.73
1:1:3429:LYS:HZ2	1:BA:6824:LYS:HE3	1.53	0.73
1:0:3326:ILE:HD13	1:1:3401:NLG:HGC2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5201:NLG:N2	1:R:5201:NLG:OE1	2.21	0.72
1:1:3417:LYS:O	1:1:3421:PHI:HD1	1.87	0.72
1:1:3429:LYS:NZ	1:BA:6824:LYS:HE3	2.05	0.72
1:K:4508:GLU:HB2	1:L:4619:ILE:HD11	1.71	0.71
1:1:3429:LYS:HE3	1:BA:6824:LYS:HZ1	1.54	0.71
1:7:4003:LYS:NZ	1:8:4128:GLN:OE1	2.24	0.71
1:7:4024:LYS:CG	1:CA:6921:PHI:I	3.09	0.71
1:JA:6210:LYS:HG2	1:JA:6214:LYS:HZ3	1.57	0.68
1:1:3401:NLG:HBC1	1:1:3402:LEU:HD22	1.75	0.68
1:V:5623:PHE:HA	1:V:5626:ILE:HG22	1.76	0.68
1:2:3511:ALA:O	1:2:3515:LYS:HG2	1.94	0.68
1:7:4001:NLG:H8C2	1:7:4003:LYS:HG2	1.76	0.67
1:CA:6923:PHE:HA	1:CA:6926:ILE:HG22	1.77	0.67
1:1:3420:ALA:O	1:1:3424:LYS:HG3	1.94	0.67
1:M:4711:ALA:O	1:M:4715:LYS:HG2	1.94	0.67
1:E:323:PHE:HA	1:E:326:ILE:HG22	1.76	0.66
1:T:5426:ILE:HD13	1:Y:5901:NLG:HGC2	1.78	0.65
1:BA:6823:PHE:HA	1:BA:6826:ILE:HG22	1.79	0.65
1:GA:6321:PHI:HA	1:GA:6324:LYS:HD2	1.79	0.65
1:0:3323:PHE:HA	1:0:3326:ILE:HG22	1.79	0.64
1:7:4024:LYS:HG3	1:CA:6921:PHI:I	2.66	0.64
1:JA:6211:ALA:HA	1:JA:6214:LYS:HE2	1.78	0.64
1:D:223:PHE:HA	1:D:226:ILE:HG22	1.79	0.64
1:Q:5123:PHE:HA	1:Q:5126:ILE:HG22	1.80	0.64
1:DA:7010:LYS:HE2	1:EA:7121:PHI:I	2.69	0.63
1:J:4403:LYS:O	1:J:4407:GLN:NE2	2.32	0.63
1:T:5401:NLG:HBC2	1:T:5402:LEU:HD22	1.81	0.63
1:GA:6323:PHE:HA	1:GA:6326:ILE:HG12	1.82	0.62
1:5:3823:PHE:HA	1:5:3826:ILE:HG22	1.82	0.62
1:GA:6312:ILE:HG22	1:GA:6316:PHE:HE2	1.63	0.62
1:J:4423:PHE:HA	1:J:4426:ILE:HG22	1.82	0.62
1:IA:6516:PHE:HA	1:IA:6519:ILE:HD12	1.81	0.62
1:T:5419:ILE:HD11	1:Y:5908:GLU:HB3	1.82	0.61
1:7:4017:LYS:HG2	1:7:4021:PHI:CE1	2.30	0.61
1:FA:6009:PHE:HA	1:FA:6012:ILE:HG12	1.81	0.61
1:Q:5105:ILE:HD12	1:R:5219:ILE:HG13	1.83	0.61
1:4:3711:ALA:O	1:4:3715:LYS:HG2	2.00	0.61
1:N:4823:PHE:HA	1:N:4826:ILE:HG22	1.83	0.60
1:S:5311:ALA:O	1:S:5315:LYS:HG2	2.00	0.60
1:A:6111:ALA:O	1:A:6115:LYS:HG2	2.01	0.60
1:AA:6711:ALA:O	1:AA:6715:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:6213:ALA:HB1	1:GA:6317:LYS:HD3	1.83	0.60
1:C:111:ALA:O	1:C:115:LYS:HG2	2.01	0.60
1:JA:6223:PHE:HA	1:JA:6226:ILE:HG22	1.82	0.60
1:O:4911:ALA:O	1:O:4915:LYS:HG2	2.02	0.60
1:9:6608:GLU:O	1:9:6612:ILE:HD12	2.02	0.60
1:H:4202:LEU:HD13	1:H:4205:ILE:HD12	1.83	0.60
1:N:4808:GLU:O	1:N:4812:ILE:HD12	2.02	0.60
1:FA:6023:PHE:HA	1:FA:6026:ILE:HG22	1.84	0.60
1:A:6108:GLU:O	1:A:6112:ILE:HG12	2.01	0.60
1:JA:6210:LYS:HG2	1:JA:6214:LYS:NZ	2.15	0.59
1:Q:5111:ALA:O	1:Q:5115:LYS:HG2	2.02	0.59
1:IA:6511:ALA:O	1:IA:6515:LYS:HG2	2.01	0.59
1:8:4111:ALA:O	1:8:4115:LYS:HG2	2.02	0.59
1:I:4311:ALA:O	1:I:4315:LYS:HG2	2.02	0.59
1:N:4821:PHI:I	1:T:5428:GLN:HG2	2.72	0.59
1:9:6602:LEU:HD13	1:9:6605:ILE:HD12	1.85	0.59
1:3:3602:LEU:HA	1:3:3605:ILE:HD12	1.84	0.59
1:W:5723:PHE:HA	1:W:5726:ILE:HG22	1.84	0.59
1:B:8:GLU:O	1:B:12:ILE:HD12	2.02	0.58
1:6:3921:PHI:HA	1:6:3924:LYS:HZ3	1.68	0.58
1:GA:6312:ILE:HG22	1:GA:6316:PHE:CE2	2.38	0.58
1:R:5201:NLG:HBC2	1:R:5202:LEU:HD22	1.85	0.58
1:8:4124:LYS:O	1:8:4128:GLN:NE2	2.35	0.58
1:Z:608:GLU:O	1:Z:612:ILE:HD12	2.04	0.58
1:AA:6715:LYS:HB2	1:BA:6812:ILE:HD11	1.86	0.58
1:B:2:LEU:HD13	1:B:5:ILE:HD12	1.85	0.58
1:L:4610:LYS:HD3	1:X:5821:PHI:HE2	1.84	0.58
1:O:4902:LEU:HD13	1:O:4905:ILE:HD13	1.84	0.58
1:3:3608:GLU:O	1:3:3612:ILE:HD12	2.04	0.58
1:6:3923:PHE:HA	1:6:3926:ILE:HG22	1.84	0.58
1:GA:6305:ILE:HG23	1:GA:6309:PHE:HE2	1.69	0.58
1:C:115:LYS:HB2	1:D:212:ILE:HD11	1.86	0.57
1:A:6115:LYS:HB2	1:JA:6212:ILE:HD11	1.85	0.57
1:B:19:ILE:HD11	1:G:508:GLU:HG2	1.86	0.57
1:V:5621:PHI:I	1:IA:6528:GLN:HG2	2.74	0.57
1:G:511:ALA:O	1:G:515:LYS:HG2	2.04	0.57
1:T:5402:LEU:HD13	1:T:5405:ILE:HD12	1.87	0.57
1:1:3429:LYS:NZ	1:BA:6824:LYS:CE	2.68	0.57
1:5:3815:LYS:O	1:5:3819:ILE:HG12	2.05	0.56
1:K:4511:ALA:O	1:K:4515:LYS:HG2	2.04	0.56
1:O:4915:LYS:HE2	1:P:5008:GLU:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:7111:ALA:O	1:EA:7115:LYS:HG2	2.04	0.56
1:V:5621:PHI:CE2	1:IA:6525:ALA:HA	2.27	0.56
1:0:3315:LYS:HB2	1:1:3412:ILE:HD11	1.87	0.56
1:GA:6308:GLU:OE2	1:HA:6419:ILE:HG13	2.06	0.56
1:J:4408:GLU:O	1:J:4412:ILE:HG12	2.05	0.56
1:9:6619:ILE:HD11	1:EA:7108:GLU:HG2	1.86	0.56
1:6:3901:NLG:HBC1	1:6:3902:LEU:HD22	1.88	0.56
1:H:4209:PHE:HA	1:H:4212:ILE:HG12	1.88	0.56
1:H:4217:LYS:HD2	1:H:4221:PHI:I	2.76	0.56
1:4:3705:ILE:HD12	1:5:3819:ILE:HD12	1.88	0.56
1:2:3514:LYS:HA	1:2:3517:LYS:HE3	1.88	0.55
1:U:5509:PHE:HA	1:U:5512:ILE:HG12	1.88	0.55
1:V:5601:NLG:H8C2	1:V:5603:LYS:HB2	1.88	0.55
1:N:4801:NLG:HBC2	1:N:4802:LEU:HD22	1.88	0.55
1:IA:6510:LYS:O	1:IA:6514:LYS:HG2	2.07	0.55
1:T:5408:GLU:O	1:T:5412:ILE:HD12	2.06	0.55
1:W:5705:ILE:HD12	1:X:5819:ILE:HG23	1.87	0.55
1:W:5711:ALA:O	1:W:5715:LYS:HG2	2.06	0.55
1:1:3429:LYS:HD2	1:1:3429:LYS:N	2.20	0.55
1:7:4024:LYS:HG2	1:CA:6921:PHI:I	2.77	0.55
1:B:23:PHE:HA	1:B:26:ILE:HG22	1.89	0.55
1:3:3623:PHE:HE1	1:8:4105:ILE:HG12	1.72	0.55
1:DA:7004:ALA:O	1:DA:7008:GLU:HG2	2.07	0.55
1:9:6623:PHE:HA	1:9:6626:ILE:HG22	1.89	0.54
1:O:4901:NLG:HBC1	1:O:4902:LEU:HD22	1.90	0.54
1:Q:5101:NLG:H8C2	1:Q:5103:LYS:HB2	1.89	0.54
1:0:3315:LYS:HG3	1:1:3408:GLU:OE2	2.06	0.54
1:K:4515:LYS:HD2	1:L:4608:GLU:OE2	2.06	0.54
1:FA:6023:PHE:HE2	1:A:6109:PHE:HE2	1.54	0.54
1:1:3415:LYS:O	1:1:3419:ILE:HD12	2.08	0.54
1:X:5815:LYS:O	1:X:5819:ILE:HD12	2.07	0.54
1:HA:6415:LYS:O	1:HA:6419:ILE:HD12	2.08	0.54
1:IA:6519:ILE:HG22	1:IA:6523:PHE:CE2	2.43	0.54
1:B:15:LYS:HB2	1:G:512:ILE:HD11	1.90	0.54
1:O:4902:LEU:HA	1:O:4905:ILE:HD13	1.90	0.54
1:U:5511:ALA:O	1:U:5515:LYS:HG2	2.08	0.54
1:9:6615:LYS:HB2	1:EA:7112:ILE:HD11	1.90	0.54
1:F:404:ALA:O	1:F:408:GLU:HG2	2.07	0.54
1:O:4908:GLU:HG2	1:O:4909:PHE:N	2.23	0.53
1:V:5611:ALA:O	1:V:5615:LYS:HG2	2.08	0.53
1:T:5408:GLU:OE2	1:Y:5915:LYS:HE2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:5621:PHI:HE2	1:IA:6525:ALA:CA	2.29	0.53
1:O:4905:ILE:HA	1:O:4908:GLU:OE1	2.08	0.53
1:K:4514:LYS:HE2	1:K:4514:LYS:HA	1.91	0.53
1:I:4308:GLU:O	1:I:4312:ILE:HG12	2.09	0.53
1:4:3715:LYS:HB2	1:5:3812:ILE:HD11	1.90	0.53
1:HA:6409:PHE:HA	1:HA:6412:ILE:HD12	1.91	0.53
1:B:11:ALA:O	1:B:15:LYS:HG3	2.09	0.53
1:F:415:LYS:O	1:F:419:ILE:HD12	2.09	0.53
1:E:311:ALA:O	1:E:315:LYS:HG2	2.09	0.52
1:K:4523:PHE:HA	1:K:4526:ILE:HG22	1.91	0.52
1:6:3911:ALA:O	1:6:3915:LYS:HG2	2.10	0.52
1:DA:7015:LYS:O	1:DA:7019:ILE:HD12	2.09	0.52
1:I:4315:LYS:HB2	1:J:4412:ILE:HD11	1.90	0.52
1:R:5203:LYS:NZ	1:S:5328:GLN:OE1	2.41	0.52
1:4:3704:ALA:HA	1:4:3707:GLN:NE2	2.25	0.52
1:7:4009:PHE:HD1	1:7:4012:ILE:HD12	1.75	0.52
1:W:5708:GLU:HB3	1:X:5819:ILE:HD11	1.92	0.52
1:0:3323:PHE:HE1	1:1:3405:ILE:HG12	1.74	0.52
1:V:5603:LYS:HZ3	1:W:5724:LYS:HG2	1.74	0.52
1:W:5701:NLG:H8C1	1:W:5703:LYS:HE2	1.91	0.52
1:7:4007:GLN:NE2	1:7:4008:GLU:OE1	2.41	0.52
1:D:201:NLG:H8C2	1:D:203:LYS:HB2	1.92	0.51
1:9:6611:ALA:O	1:9:6615:LYS:HG3	2.09	0.51
1:HA:6405:ILE:O	1:HA:6409:PHE:HD1	1.94	0.51
1:HA:6412:ILE:HG22	1:HA:6416:PHE:CE2	2.45	0.51
1:HA:6416:PHE:HA	1:HA:6419:ILE:HD13	1.92	0.51
1:IA:6520:ALA:O	1:IA:6524:LYS:HG3	2.10	0.51
1:H:4215:LYS:O	1:H:4219:ILE:HG12	2.10	0.51
1:CA:6911:ALA:O	1:CA:6915:LYS:HG2	2.09	0.51
1:T:5417:LYS:HD2	1:T:5421:PHI:I	2.80	0.51
1:Z:629:LYS:HZ3	1:Z:629:LYS:HA	1.74	0.51
1:5:3801:NLG:H8C2	1:5:3803:LYS:HB2	1.93	0.51
1:CA:6908:GLU:HB3	1:DA:7019:ILE:HD11	1.93	0.51
1:C:108:GLU:OE1	1:D:215:LYS:HD2	2.12	0.50
1:E:308:GLU:HB3	1:F:419:ILE:HD11	1.93	0.50
1:BA:6801:NLG:H8C2	1:BA:6803:LYS:HB2	1.92	0.50
1:4:3715:LYS:HE2	1:5:3808:GLU:OE1	2.11	0.50
1:N:4815:LYS:HB2	1:S:5312:ILE:HD11	1.93	0.50
1:R:5216:PHE:HA	1:R:5219:ILE:HG22	1.93	0.50
1:V:5601:NLG:HBC1	1:V:5602:LEU:HD22	1.93	0.50
1:1:3429:LYS:HZ2	1:BA:6824:LYS:CE	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:6305:ILE:HG23	1:GA:6309:PHE:CE2	2.47	0.50
1:HA:6416:PHE:HB2	1:IA:6513:ALA:HB2	1.93	0.50
1:O:4915:LYS:HB2	1:P:5012:ILE:HD11	1.94	0.49
1:U:5501:NLG:HBC1	1:U:5502:LEU:HD12	1.94	0.49
1:O:3311:ALA:HB1	1:O:3315:LYS:NZ	2.27	0.49
1:A:6101:NLG:HGC2	1:JA:6226:ILE:HB	1.93	0.49
1:IA:6501:NLG:H8C2	1:IA:6503:LYS:HD2	1.95	0.49
1:4:3719:ILE:HD11	1:5:3808:GLU:HB2	1.94	0.49
1:6:3921:PHI:HD1	1:6:3924:LYS:NZ	2.27	0.49
1:W:5715:LYS:HB3	1:X:5808:GLU:OE2	2.13	0.49
1:GA:6311:ALA:O	1:GA:6314:LYS:HG2	2.12	0.49
1:H:4226:ILE:HD13	1:M:4701:NLG:HGC2	1.95	0.49
1:3:3623:PHE:HA	1:3:3626:ILE:HG22	1.95	0.49
1:AA:6708:GLU:OE1	1:BA:6815:LYS:HD2	2.12	0.49
1:3:3605:ILE:HD13	1:8:4123:PHE:HE1	1.77	0.49
1:A:6110:LYS:HE2	1:A:6114:LYS:NZ	2.27	0.49
1:Y:5923:PHE:HA	1:Y:5926:ILE:HG22	1.95	0.48
1:M:4721:PHI:I	1:X:5824:LYS:HB3	2.84	0.48
1:HA:6412:ILE:HG22	1:HA:6416:PHE:HE2	1.78	0.48
1:K:4518:ALA:O	1:K:4521:PHI:HB2	2.13	0.48
1:3:3619:ILE:HD11	1:8:4108:GLU:HB3	1.95	0.48
1:N:4812:ILE:HG23	1:S:5312:ILE:HD12	1.95	0.48
1:T:5415:LYS:HB2	1:Y:5912:ILE:HD11	1.96	0.48
1:I:4315:LYS:HE2	1:J:4408:GLU:OE1	2.13	0.48
1:GA:6315:LYS:O	1:GA:6319:ILE:HG13	2.14	0.48
1:HA:6414:LYS:O	1:HA:6417:LYS:HG2	2.14	0.48
1:6:3901:NLG:H8C2	1:6:3903:LYS:HB3	1.96	0.47
1:Z:604:ALA:HA	1:Z:607:GLN:NE2	2.30	0.47
1:O:3301:NLG:H8C2	1:O:3303:LYS:HB3	1.96	0.47
1:7:4024:LYS:HD3	1:CA:6921:PHI:HE2	1.95	0.47
1:D:207:GLN:HA	1:D:207:GLN:OE1	2.15	0.47
1:H:4223:PHE:HB3	1:I:4306:ALA:HB2	1.97	0.47
1:K:4506:ALA:O	1:K:4510:LYS:HG2	2.15	0.47
1:Y:5901:NLG:O	1:Y:5904:ALA:N	2.47	0.47
1:Y:5914:LYS:HG3	1:Y:5917:LYS:NZ	2.29	0.47
1:O:3305:ILE:HD12	1:1:3419:ILE:HG23	1.97	0.47
1:BA:6807:GLN:HA	1:BA:6807:GLN:OE1	2.15	0.47
1:Y:5911:ALA:O	1:Y:5915:LYS:HG2	2.15	0.47
1:6:3921:PHI:HA	1:6:3924:LYS:NZ	2.28	0.47
1:3:3608:GLU:HG2	1:8:4119:ILE:HD11	1.97	0.46
1:O:4923:PHE:HE1	1:P:5005:ILE:HG13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4410:LYS:O	1:J:4414:LYS:HG2	2.14	0.46
1:P:5015:LYS:O	1:P:5019:ILE:HG12	2.16	0.46
1:0:3312:ILE:HG23	1:1:3412:ILE:HD12	1.97	0.46
1:0:3319:ILE:HD11	1:1:3408:GLU:HG2	1.97	0.46
1:JA:6221:PHI:HA	1:JA:6224:LYS:NZ	2.31	0.46
1:I:4312:ILE:HD11	1:J:4415:LYS:HB2	1.98	0.46
1:V:5621:PHI:I	1:IA:6524:LYS:HB3	2.85	0.46
1:A:6109:PHE:HE1	1:JA:6219:ILE:HD13	1.81	0.46
1:GA:6323:PHE:CD1	1:GA:6326:ILE:HD11	2.51	0.46
1:E:322:GLU:OE1	1:F:405:ILE:HD11	2.16	0.46
1:Z:621:PHI:HA	1:Z:621:PHI:HD2	1.57	0.46
1:O:4912:ILE:HG23	1:P:5012:ILE:HD12	1.97	0.46
1:P:5027:ALA:HA	1:Q:5102:LEU:HD12	1.98	0.46
1:H:4208:GLU:OE2	1:M:4715:LYS:HE3	2.16	0.46
1:L:4615:LYS:O	1:L:4619:ILE:HG12	2.16	0.45
1:V:5621:PHI:I	1:IA:6528:GLN:CG	3.34	0.45
1:A:6115:LYS:HE2	1:JA:6208:GLU:OE1	2.17	0.45
1:JA:6204:ALA:O	1:JA:6208:GLU:HG2	2.16	0.45
1:JA:6217:LYS:O	1:JA:6221:PHI:HD1	2.17	0.45
1:H:4227:ALA:HB1	1:I:4303:LYS:HD2	1.98	0.45
1:N:4808:GLU:OE2	1:S:5315:LYS:HE3	2.17	0.45
1:2:3501:NLG:HBC1	1:2:3502:LEU:HD12	1.99	0.45
1:6:3914:LYS:HE2	1:6:3914:LYS:HB2	1.80	0.45
1:H:4223:PHE:HA	1:H:4226:ILE:HG22	1.98	0.45
1:X:5805:ILE:H	1:X:5805:ILE:HD12	1.82	0.45
1:1:3422:GLU:O	1:1:3426:ILE:HG12	2.16	0.45
1:6:3926:ILE:HD13	1:7:4001:NLG:HGC2	1.99	0.45
1:G:501:NLG:O	1:G:504:ALA:N	2.50	0.45
1:4:3708:GLU:HB3	1:5:3819:ILE:HD11	1.98	0.45
1:5:3801:NLG:HBC1	1:5:3802:LEU:HD22	1.98	0.45
1:7:4015:LYS:O	1:7:4019:ILE:HG12	2.16	0.45
1:HA:6401:NLG:H8C2	1:HA:6403:LYS:HB3	1.99	0.45
1:D:222:GLU:HA	1:D:222:GLU:OE1	2.17	0.44
1:L:4627:ALA:HB1	1:M:4703:LYS:HD3	1.98	0.44
1:P:5001:NLG:H8C2	1:P:5003:LYS:HB2	1.98	0.44
1:S:5323:PHE:HA	1:S:5326:ILE:HG22	1.98	0.44
1:GA:6305:ILE:HD13	1:GA:6308:GLU:OE2	2.17	0.44
1:CA:6922:GLU:OE1	1:DA:7005:ILE:HD11	2.16	0.44
1:FA:6018:ALA:HA	1:FA:6021:PHI:HD1	2.00	0.44
1:IA:6515:LYS:O	1:IA:6519:ILE:HG13	2.18	0.44
1:FA:6018:ALA:O	1:FA:6021:PHI:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:6822:GLU:HA	1:BA:6822:GLU:OE1	2.17	0.44
1:GA:6301:NLG:HBC1	1:GA:6302:LEU:HD22	1.99	0.44
1:E:305:ILE:HD12	1:F:419:ILE:HG23	2.00	0.44
1:L:4605:ILE:H	1:L:4605:ILE:HD12	1.83	0.44
1:S:5314:LYS:HE2	1:S:5314:LYS:HB2	1.81	0.44
1:4:3717:LYS:HB2	1:4:3717:LYS:HE3	1.80	0.44
1:N:4811:ALA:O	1:N:4815:LYS:HG3	2.18	0.43
1:4:3701:NLG:HBC2	1:4:3702:LEU:HD12	2.00	0.43
1:CA:6905:ILE:HD12	1:DA:7019:ILE:HG23	2.00	0.43
1:W:5701:NLG:HBC1	1:W:5702:LEU:HD22	2.00	0.43
1:2:3505:ILE:H	1:2:3505:ILE:HD12	1.83	0.43
1:EA:7101:NLG:O	1:EA:7104:ALA:N	2.50	0.43
1:A:6104:ALA:O	1:A:6108:GLU:HG2	2.19	0.43
1:E:314:LYS:HB2	1:E:314:LYS:HE2	1.86	0.43
1:3:3608:GLU:OE2	1:8:4115:LYS:HE3	2.18	0.43
1:W:5714:LYS:HB2	1:W:5714:LYS:HE2	1.79	0.43
1:H:4221:PHI:HD2	1:H:4221:PHI:HA	1.73	0.43
1:G:521:PHI:HA	1:G:521:PHI:HD2	1.56	0.43
1:U:5515:LYS:HE2	1:V:5608:GLU:OE1	2.17	0.43
1:1:3404:ALA:O	1:1:3408:GLU:HB2	2.19	0.43
1:EA:7121:PHI:HD2	1:EA:7121:PHI:HA	1.55	0.43
1:A:6105:ILE:HG12	1:JA:6223:PHE:CE1	2.52	0.43
1:V:5615:LYS:O	1:V:5619:ILE:HG12	2.19	0.43
1:K:4518:ALA:O	1:K:4522:GLU:OE1	2.37	0.43
1:5:3814:LYS:O	1:5:3817:LYS:HG2	2.18	0.43
1:2:3521:PHI:CD2	1:2:3524:LYS:HZ2	2.32	0.43
1:9:6608:GLU:HB2	1:EA:7119:ILE:HD11	2.01	0.43
1:R:5216:PHE:O	1:R:5219:ILE:HG22	2.19	0.42
1:R:5222:GLU:O	1:R:5226:ILE:HG12	2.19	0.42
1:1:3428:GLN:C	1:1:3429:LYS:HD2	2.39	0.42
1:JA:6204:ALA:O	1:JA:6207:GLN:HG3	2.19	0.42
1:HA:6404:ALA:O	1:HA:6408:GLU:OE1	2.37	0.42
1:A:6117:LYS:HE3	1:A:6117:LYS:HB2	1.80	0.42
1:Q:5108:GLU:OE2	1:R:5215:LYS:HD2	2.19	0.42
1:6:3915:LYS:O	1:6:3919:ILE:HG12	2.19	0.42
1:7:4022:GLU:O	1:7:4026:ILE:HG12	2.18	0.42
1:EA:7114:LYS:HE2	1:EA:7114:LYS:HB2	1.79	0.42
1:Z:623:PHE:HA	1:Z:626:ILE:HG22	2.00	0.42
1:1:3408:GLU:O	1:1:3412:ILE:HG12	2.18	0.42
1:3:3602:LEU:HD13	1:3:3605:ILE:HD12	2.00	0.42
1:R:5227:ALA:HB1	1:S:5303:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:5508:GLU:HB3	1:V:5619:ILE:HD11	2.02	0.42
1:B:21:PHI:HD2	1:B:21:PHI:HA	1.54	0.42
1:P:5001:NLG:HBC1	1:P:5002:LEU:HD22	2.01	0.42
1:3:3612:ILE:HG23	1:8:4112:ILE:HD12	2.01	0.42
1:4:3704:ALA:HA	1:4:3707:GLN:CD	2.40	0.42
1:8:4105:ILE:H	1:8:4105:ILE:HD12	1.84	0.42
1:K:4504:ALA:O	1:K:4508:GLU:OE1	2.38	0.42
1:T:5402:LEU:HB3	1:U:5527:ALA:HB2	2.02	0.42
1:9:6619:ILE:HD11	1:EA:7108:GLU:CG	2.50	0.42
1:CA:6901:NLG:HGC1	1:DA:7026:ILE:HD11	2.02	0.42
1:B:19:ILE:HD11	1:G:508:GLU:CG	2.50	0.42
1:I:4309:PHE:CZ	1:J:4419:ILE:HD13	2.55	0.42
1:T:5401:NLG:O	1:T:5405:ILE:HG13	2.20	0.42
1:Y:5914:LYS:HB2	1:Y:5914:LYS:HE2	1.82	0.42
1:C:117:LYS:HE3	1:C:117:LYS:HB2	1.76	0.41
1:Z:611:ALA:O	1:Z:615:LYS:HG3	2.20	0.41
1:1:3429:LYS:CE	1:BA:6824:LYS:HZ1	2.27	0.41
1:E:301:NLG:HGC1	1:F:426:ILE:HD11	2.02	0.41
1:I:4301:NLG:H8C2	1:I:4303:LYS:HD3	2.01	0.41
1:FA:6018:ALA:O	1:FA:6022:GLU:OE1	2.38	0.41
1:B:8:GLU:HB2	1:G:519:ILE:HD11	2.01	0.41
1:K:4505:ILE:HD11	1:L:4622:GLU:HB2	2.02	0.41
1:K:4519:ILE:HG22	1:K:4523:PHE:CE2	2.55	0.41
1:O:4905:ILE:HD12	1:O:4905:ILE:H	1.86	0.41
1:Q:5115:LYS:HB2	1:R:5212:ILE:HD11	2.02	0.41
1:0:3322:GLU:OE2	1:1:3401:NLG:HGC1	2.20	0.41
1:9:6604:ALA:O	1:9:6608:GLU:HG2	2.21	0.41
1:A:6109:PHE:CE1	1:JA:6219:ILE:HD13	2.55	0.41
1:H:4222:GLU:OE2	1:H:4223:PHE:HD1	2.02	0.41
1:IA:6514:LYS:O	1:IA:6517:LYS:HG2	2.21	0.41
1:2:3511:ALA:HA	1:2:3514:LYS:HG2	2.01	0.41
1:3:3615:LYS:HB2	1:8:4112:ILE:HD11	2.03	0.41
1:AA:6705:ILE:HD12	1:AA:6705:ILE:H	1.85	0.41
1:C:105:ILE:HD12	1:C:105:ILE:H	1.85	0.41
1:S:5304:ALA:HA	1:S:5307:GLN:HE21	1.84	0.41
1:AA:6729:LYS:HD2	1:AA:6729:LYS:HA	1.82	0.41
1:T:5427:ALA:HA	1:U:5502:LEU:HD22	2.03	0.41
1:0:3314:LYS:HB2	1:0:3314:LYS:HE2	1.86	0.41
1:0:3315:LYS:CB	1:1:3412:ILE:HD11	2.50	0.41
1:JA:6215:LYS:O	1:JA:6219:ILE:HG13	2.21	0.41
1:HA:6411:ALA:O	1:HA:6414:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HZ3	1:B:29:LYS:HA	1.86	0.41
1:Z:623:PHE:O	1:Z:626:ILE:HG22	2.21	0.41
1:A:6119:ILE:HD11	1:JA:6208:GLU:HB3	2.03	0.41
1:HA:6404:ALA:O	1:HA:6407:GLN:HB3	2.21	0.41
1:HA:6422:GLU:O	1:HA:6426:ILE:HG12	2.21	0.41
1:U:5517:LYS:HE3	1:U:5517:LYS:HB2	1.77	0.40
1:V:5614:LYS:O	1:V:5617:LYS:HG2	2.21	0.40
1:X:5822:GLU:O	1:X:5826:ILE:HG12	2.22	0.40
1:B:29:LYS:HA	1:B:29:LYS:HD2	1.84	0.40
1:R:5211:ALA:O	1:R:5215:LYS:HG2	2.21	0.40
1:T:5421:PHI:HD2	1:T:5421:PHI:HA	1.73	0.40
1:G:529:LYS:HZ3	1:G:529:LYS:HA	1.86	0.40
1:1:3411:ALA:O	1:1:3415:LYS:HG2	2.21	0.40
1:I:4312:ILE:HD11	1:J:4415:LYS:CB	2.52	0.40
1:L:4609:PHE:HA	1:L:4612:ILE:HD12	2.02	0.40
1:6:3923:PHE:HE1	1:7:4005:ILE:HG21	1.86	0.40
1:JA:6210:LYS:C	1:JA:6214:LYS:HZ3	2.24	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	0	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	1	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	2	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	3	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	4	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	5	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	6	27/30 (90%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
1	8	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	9	27/30 (90%)	27 (100%)	0	0	100	100
1	A	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	AA	27/30 (90%)	27 (100%)	0	0	100	100
1	B	27/30 (90%)	27 (100%)	0	0	100	100
1	BA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	C	27/30 (90%)	27 (100%)	0	0	100	100
1	CA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	D	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	DA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	E	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	EA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	F	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	FA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	G	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	GA	27/30 (90%)	27 (100%)	0	0	100	100
1	H	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	HA	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	I	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	IA	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
1	J	27/30 (90%)	27 (100%)	0	0	100	100
1	JA	27/30 (90%)	27 (100%)	0	0	100	100
1	K	27/30 (90%)	27 (100%)	0	0	100	100
1	L	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
1	M	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	N	27/30 (90%)	27 (100%)	0	0	100	100
1	O	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	P	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
1	Q	27/30 (90%)	27 (100%)	0	0	100	100
1	R	27/30 (90%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	T	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	U	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	V	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	W	27/30 (90%)	27 (100%)	0	0	100	100
1	X	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
1	Z	27/30 (90%)	27 (100%)	0	0	100	100
1	a	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	b	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
1	c	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	d	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
1	e	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	f	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	g	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	h	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	i	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	j	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	k	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
1	l	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	m	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	n	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	o	27/30 (90%)	27 (100%)	0	0	100	100
1	p	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	q	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	r	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	s	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
1	t	27/30 (90%)	27 (100%)	0	0	100	100
1	u	27/30 (90%)	27 (100%)	0	0	100	100
1	v	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	w	27/30 (90%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
1	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
1	z	27/30 (90%)	26 (96%)	0	1 (4%)	3	29
All	All	1944/2160 (90%)	1883 (97%)	55 (3%)	6 (0%)	44	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	5028	GLN
1	d	1028	GLN
1	s	2529	LYS
1	z	3228	GLN
1	7	4028	GLN
1	IA	6528	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	1	19/19 (100%)	19 (100%)	0	100	100
1	2	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	3	19/19 (100%)	19 (100%)	0	100	100
1	4	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	5	19/19 (100%)	19 (100%)	0	100	100
1	6	19/19 (100%)	19 (100%)	0	100	100
1	7	19/19 (100%)	19 (100%)	0	100	100
1	8	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	9	19/19 (100%)	19 (100%)	0	100	100
1	A	19/19 (100%)	19 (100%)	0	100	100
1	AA	19/19 (100%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	19/19 (100%)	19 (100%)	0	100	100
1	BA	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	C	19/19 (100%)	19 (100%)	0	100	100
1	CA	19/19 (100%)	19 (100%)	0	100	100
1	D	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	DA	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	E	19/19 (100%)	19 (100%)	0	100	100
1	EA	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	F	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	FA	19/19 (100%)	19 (100%)	0	100	100
1	G	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	GA	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	H	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	HA	19/19 (100%)	19 (100%)	0	100	100
1	I	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	IA	19/19 (100%)	19 (100%)	0	100	100
1	J	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	JA	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	K	19/19 (100%)	19 (100%)	0	100	100
1	L	19/19 (100%)	19 (100%)	0	100	100
1	M	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	N	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	O	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	P	19/19 (100%)	19 (100%)	0	100	100
1	Q	19/19 (100%)	19 (100%)	0	100	100
1	R	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	S	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	T	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	U	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	V	19/19 (100%)	19 (100%)	0	100	100
1	W	19/19 (100%)	18 (95%)	1 (5%)	22	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	19/19 (100%)	19 (100%)	0	100	100
1	Y	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	Z	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	a	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	b	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	c	19/19 (100%)	19 (100%)	0	100	100
1	d	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	e	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	f	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	g	19/19 (100%)	19 (100%)	0	100	100
1	h	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	i	19/19 (100%)	19 (100%)	0	100	100
1	j	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	k	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	l	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	m	19/19 (100%)	19 (100%)	0	100	100
1	n	19/19 (100%)	19 (100%)	0	100	100
1	o	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	p	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	q	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	r	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	s	19/19 (100%)	19 (100%)	0	100	100
1	t	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	u	19/19 (100%)	19 (100%)	0	100	100
1	v	19/19 (100%)	19 (100%)	0	100	100
1	w	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	x	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	y	19/19 (100%)	18 (95%)	1 (5%)	22	52
1	z	19/19 (100%)	19 (100%)	0	100	100
All	All	1368/1368 (100%)	1326 (97%)	42 (3%)	43	64

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	229	LYS
1	F	429	LYS
1	G	529	LYS
1	H	4229	LYS
1	I	4329	LYS
1	J	4429	LYS
1	M	4729	LYS
1	N	4829	LYS
1	O	4929	LYS
1	R	5229	LYS
1	S	5329	LYS
1	T	5429	LYS
1	U	5529	LYS
1	W	5729	LYS
1	Y	5929	LYS
1	Z	629	LYS
1	a	729	LYS
1	b	829	LYS
1	d	1029	LYS
1	e	1129	LYS
1	f	1229	LYS
1	h	1429	LYS
1	j	1629	LYS
1	k	1729	LYS
1	l	1829	LYS
1	o	2129	LYS
1	p	2229	LYS
1	q	2329	LYS
1	r	2429	LYS
1	t	2629	LYS
1	w	2929	LYS
1	x	3029	LYS
1	y	3129	LYS
1	0	3329	LYS
1	2	3529	LYS
1	4	3729	LYS
1	8	4129	LYS
1	BA	6829	LYS
1	DA	7029	LYS
1	EA	7129	LYS
1	JA	6203	LYS
1	GA	6329	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	J	4407	GLN
1	W	5728	GLN
1	y	3128	GLN
1	3	3628	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

72 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PHI	t	2621	1	11,12,13	1.17	1 (9%)	12,15,17	1.01	2 (16%)
1	PHI	S	5321	1	11,12,13	1.18	1 (9%)	12,15,17	1.03	2 (16%)
1	PHI	n	2021	1	11,12,13	1.19	1 (9%)	12,15,17	1.08	2 (16%)
1	PHI	V	5621	1	11,12,13	1.18	1 (9%)	12,15,17	0.95	1 (8%)
1	PHI	H	4221	1	11,12,13	1.18	1 (9%)	12,15,17	1.02	2 (16%)
1	PHI	O	4921	1	11,12,13	1.19	1 (9%)	12,15,17	0.96	1 (8%)
1	PHI	a	721	1	11,12,13	1.18	1 (9%)	12,15,17	1.03	2 (16%)
1	PHI	c	921	1	11,12,13	1.20	1 (9%)	12,15,17	0.81	0
1	PHI	R	5221	1	11,12,13	1.19	1 (9%)	12,15,17	0.96	1 (8%)
1	PHI	Z	621	1	11,12,13	1.14	1 (9%)	12,15,17	1.10	2 (16%)
1	PHI	G	521	1	11,12,13	1.17	1 (9%)	12,15,17	1.13	2 (16%)
1	PHI	l	1821	1	11,12,13	1.20	1 (9%)	12,15,17	0.92	1 (8%)
1	PHI	1	3421	1	11,12,13	1.20	1 (9%)	12,15,17	0.93	1 (8%)
1	PHI	3	3621	1	11,12,13	1.19	1 (9%)	12,15,17	0.98	1 (8%)
1	PHI	u	2721	1	11,12,13	1.22	1 (9%)	12,15,17	1.27	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PHI	I	4321	1	11,12,13	1.19	1 (9%)	12,15,17	0.93	1 (8%)
1	PHI	0	3321	1	11,12,13	1.19	1 (9%)	12,15,17	0.74	0
1	PHI	Q	5121	1	11,12,13	1.20	1 (9%)	12,15,17	0.71	0
1	PHI	N	4821	1	11,12,13	1.19	1 (9%)	12,15,17	0.93	1 (8%)
1	PHI	J	4421	1	11,12,13	1.18	1 (9%)	12,15,17	0.87	1 (8%)
1	PHI	d	1021	1	11,12,13	1.21	1 (9%)	12,15,17	1.58	2 (16%)
1	PHI	j	1621	1	11,12,13	1.19	1 (9%)	12,15,17	1.22	2 (16%)
1	PHI	b	821	1	11,12,13	1.20	1 (9%)	12,15,17	1.19	2 (16%)
1	PHI	z	3221	1	11,12,13	1.18	1 (9%)	12,15,17	0.92	1 (8%)
1	PHI	6	3921	1	11,12,13	1.20	1 (9%)	12,15,17	0.61	0
1	PHI	s	2521	1	11,12,13	1.19	1 (9%)	12,15,17	0.77	0
1	PHI	HA	6421	1	11,12,13	1.19	1 (9%)	12,15,17	0.96	1 (8%)
1	PHI	e	1121	1	11,12,13	1.18	1 (9%)	12,15,17	1.08	2 (16%)
1	PHI	DA	7021	1	11,12,13	1.20	1 (9%)	12,15,17	1.16	2 (16%)
1	PHI	JA	6221	1	11,12,13	1.19	1 (9%)	12,15,17	1.03	2 (16%)
1	PHI	U	5521	1	11,12,13	1.21	1 (9%)	12,15,17	0.76	0
1	PHI	Y	5921	1	11,12,13	1.22	1 (9%)	12,15,17	1.04	1 (8%)
1	PHI	f	1221	1	11,12,13	1.19	1 (9%)	12,15,17	1.06	2 (16%)
1	PHI	x	3021	1	11,12,13	1.20	1 (9%)	12,15,17	0.93	1 (8%)
1	PHI	FA	6021	1	11,12,13	1.21	1 (9%)	12,15,17	1.05	2 (16%)
1	PHI	EA	7121	1	11,12,13	1.16	1 (9%)	12,15,17	1.14	2 (16%)
1	PHI	B	21	1	11,12,13	1.17	1 (9%)	12,15,17	1.10	2 (16%)
1	PHI	r	2421	1	11,12,13	1.18	1 (9%)	12,15,17	0.91	1 (8%)
1	PHI	w	2921	1	11,12,13	1.19	1 (9%)	12,15,17	0.99	1 (8%)
1	PHI	K	4521	1	11,12,13	1.18	1 (9%)	12,15,17	0.83	1 (8%)
1	PHI	X	5821	1	11,12,13	1.19	1 (9%)	12,15,17	0.96	1 (8%)
1	PHI	o	2121	1	11,12,13	1.21	1 (9%)	12,15,17	0.62	0
1	PHI	P	5021	1	11,12,13	1.16	1 (9%)	12,15,17	0.91	1 (8%)
1	PHI	m	1921	1	11,12,13	1.18	1 (9%)	12,15,17	0.99	1 (8%)
1	PHI	F	421	1	11,12,13	1.19	1 (9%)	12,15,17	1.17	2 (16%)
1	PHI	i	1521	1	11,12,13	1.20	1 (9%)	12,15,17	0.76	1 (8%)
1	PHI	7	4021	1	11,12,13	1.16	1 (9%)	12,15,17	0.90	1 (8%)
1	PHI	A	6121	1	11,12,13	1.20	1 (9%)	12,15,17	1.12	2 (16%)
1	PHI	9	6621	1	11,12,13	1.18	1 (9%)	12,15,17	1.10	2 (16%)
1	PHI	2	3521	1	11,12,13	1.19	1 (9%)	12,15,17	0.90	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PHI	L	4621	1	11,12,13	1.19	1 (9%)	12,15,17	1.04	2 (16%)
1	PHI	y	3121	1	11,12,13	1.19	1 (9%)	12,15,17	0.98	1 (8%)
1	PHI	8	4121	1	11,12,13	1.19	1 (9%)	12,15,17	1.18	2 (16%)
1	PHI	E	321	1	11,12,13	1.19	1 (9%)	12,15,17	0.84	1 (8%)
1	PHI	4	3721	1	11,12,13	1.19	1 (9%)	12,15,17	1.04	2 (16%)
1	PHI	k	1721	1	11,12,13	1.18	1 (9%)	12,15,17	1.12	2 (16%)
1	PHI	W	5721	1	11,12,13	1.21	1 (9%)	12,15,17	0.73	0
1	PHI	T	5421	1	11,12,13	1.20	1 (9%)	12,15,17	0.93	1 (8%)
1	PHI	IA	6521	1	11,12,13	1.21	1 (9%)	12,15,17	0.90	1 (8%)
1	PHI	C	121	1	11,12,13	1.19	1 (9%)	12,15,17	0.77	0
1	PHI	D	221	1	11,12,13	1.17	1 (9%)	12,15,17	1.20	2 (16%)
1	PHI	h	1421	1	11,12,13	1.19	1 (9%)	12,15,17	1.04	1 (8%)
1	PHI	p	2221	1	11,12,13	1.20	1 (9%)	12,15,17	1.05	2 (16%)
1	PHI	AA	6721	1	11,12,13	1.19	1 (9%)	12,15,17	0.78	0
1	PHI	5	3821	1	11,12,13	1.19	1 (9%)	12,15,17	1.44	2 (16%)
1	PHI	M	4721	1	11,12,13	1.19	1 (9%)	12,15,17	1.20	1 (8%)
1	PHI	CA	6921	1	11,12,13	1.19	1 (9%)	12,15,17	0.85	1 (8%)
1	PHI	GA	6321	1	11,12,13	1.22	1 (9%)	12,15,17	0.91	1 (8%)
1	PHI	q	2321	1	11,12,13	1.17	1 (9%)	12,15,17	0.95	1 (8%)
1	PHI	v	2821	1	11,12,13	1.19	1 (9%)	12,15,17	1.16	2 (16%)
1	PHI	BA	6821	1	11,12,13	1.18	1 (9%)	12,15,17	1.18	2 (16%)
1	PHI	g	1321	1	11,12,13	1.20	1 (9%)	12,15,17	1.47	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHI	t	2621	1	-	4/5/6/8	0/1/1/1
1	PHI	S	5321	1	-	1/5/6/8	0/1/1/1
1	PHI	n	2021	1	-	2/5/6/8	0/1/1/1
1	PHI	V	5621	1	-	2/5/6/8	0/1/1/1
1	PHI	H	4221	1	-	2/5/6/8	0/1/1/1
1	PHI	O	4921	1	-	0/5/6/8	0/1/1/1
1	PHI	a	721	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHI	c	921	1	-	2/5/6/8	0/1/1/1
1	PHI	R	5221	1	-	2/5/6/8	0/1/1/1
1	PHI	Z	621	1	-	4/5/6/8	0/1/1/1
1	PHI	G	521	1	-	3/5/6/8	0/1/1/1
1	PHI	l	1821	1	-	4/5/6/8	0/1/1/1
1	PHI	1	3421	1	-	2/5/6/8	0/1/1/1
1	PHI	3	3621	1	-	2/5/6/8	0/1/1/1
1	PHI	u	2721	1	-	0/5/6/8	0/1/1/1
1	PHI	I	4321	1	-	0/5/6/8	0/1/1/1
1	PHI	0	3321	1	-	2/5/6/8	0/1/1/1
1	PHI	Q	5121	1	-	2/5/6/8	0/1/1/1
1	PHI	N	4821	1	-	3/5/6/8	0/1/1/1
1	PHI	J	4421	1	-	2/5/6/8	0/1/1/1
1	PHI	d	1021	1	-	2/5/6/8	0/1/1/1
1	PHI	j	1621	1	-	2/5/6/8	0/1/1/1
1	PHI	b	821	1	-	2/5/6/8	0/1/1/1
1	PHI	z	3221	1	-	2/5/6/8	0/1/1/1
1	PHI	6	3921	1	-	0/5/6/8	0/1/1/1
1	PHI	s	2521	1	-	0/5/6/8	0/1/1/1
1	PHI	HA	6421	1	-	2/5/6/8	0/1/1/1
1	PHI	e	1121	1	-	3/5/6/8	0/1/1/1
1	PHI	DA	7021	1	-	2/5/6/8	0/1/1/1
1	PHI	JA	6221	1	-	2/5/6/8	0/1/1/1
1	PHI	U	5521	1	-	1/5/6/8	0/1/1/1
1	PHI	Y	5921	1	-	2/5/6/8	0/1/1/1
1	PHI	f	1221	1	-	5/5/6/8	0/1/1/1
1	PHI	x	3021	1	-	2/5/6/8	0/1/1/1
1	PHI	FA	6021	1	-	2/5/6/8	0/1/1/1
1	PHI	EA	7121	1	-	3/5/6/8	0/1/1/1
1	PHI	B	21	1	-	4/5/6/8	0/1/1/1
1	PHI	r	2421	1	-	2/5/6/8	0/1/1/1
1	PHI	w	2921	1	-	3/5/6/8	0/1/1/1
1	PHI	K	4521	1	-	0/5/6/8	0/1/1/1
1	PHI	X	5821	1	-	2/5/6/8	0/1/1/1
1	PHI	o	2121	1	-	2/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHI	P	5021	1	-	2/5/6/8	0/1/1/1
1	PHI	m	1921	1	-	0/5/6/8	0/1/1/1
1	PHI	F	421	1	-	2/5/6/8	0/1/1/1
1	PHI	i	1521	1	-	2/5/6/8	0/1/1/1
1	PHI	7	4021	1	-	2/5/6/8	0/1/1/1
1	PHI	A	6121	1	-	0/5/6/8	0/1/1/1
1	PHI	9	6621	1	-	5/5/6/8	0/1/1/1
1	PHI	2	3521	1	-	3/5/6/8	0/1/1/1
1	PHI	L	4621	1	-	2/5/6/8	0/1/1/1
1	PHI	y	3121	1	-	2/5/6/8	0/1/1/1
1	PHI	8	4121	1	-	3/5/6/8	0/1/1/1
1	PHI	E	321	1	-	0/5/6/8	0/1/1/1
1	PHI	4	3721	1	-	0/5/6/8	0/1/1/1
1	PHI	k	1721	1	-	3/5/6/8	0/1/1/1
1	PHI	W	5721	1	-	1/5/6/8	0/1/1/1
1	PHI	T	5421	1	-	2/5/6/8	0/1/1/1
1	PHI	IA	6521	1	-	2/5/6/8	0/1/1/1
1	PHI	C	121	1	-	0/5/6/8	0/1/1/1
1	PHI	D	221	1	-	4/5/6/8	0/1/1/1
1	PHI	h	1421	1	-	4/5/6/8	0/1/1/1
1	PHI	p	2221	1	-	5/5/6/8	0/1/1/1
1	PHI	AA	6721	1	-	0/5/6/8	0/1/1/1
1	PHI	5	3821	1	-	0/5/6/8	0/1/1/1
1	PHI	M	4721	1	-	3/5/6/8	0/1/1/1
1	PHI	CA	6921	1	-	0/5/6/8	0/1/1/1
1	PHI	GA	6321	1	-	0/5/6/8	0/1/1/1
1	PHI	q	2321	1	-	2/5/6/8	0/1/1/1
1	PHI	v	2821	1	-	2/5/6/8	0/1/1/1
1	PHI	BA	6821	1	-	4/5/6/8	0/1/1/1
1	PHI	g	1321	1	-	0/5/6/8	0/1/1/1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	6921	PHI	CZ-I	-3.24	2.02	2.10
1	p	2221	PHI	CZ-I	-3.24	2.02	2.10
1	E	321	PHI	CZ-I	-3.23	2.02	2.10
1	i	1521	PHI	CZ-I	-3.21	2.02	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	GA	6321	PHI	CZ-I	-3.21	2.02	2.10
1	AA	6721	PHI	CZ-I	-3.20	2.02	2.10
1	C	121	PHI	CZ-I	-3.20	2.02	2.10
1	u	2721	PHI	CZ-I	-3.19	2.02	2.10
1	Q	5121	PHI	CZ-I	-3.19	2.02	2.10
1	Y	5921	PHI	CZ-I	-3.18	2.02	2.10
1	d	1021	PHI	CZ-I	-3.18	2.02	2.10
1	B	21	PHI	CZ-I	-3.18	2.02	2.10
1	DA	7021	PHI	CZ-I	-3.18	2.02	2.10
1	5	3821	PHI	CZ-I	-3.17	2.02	2.10
1	b	821	PHI	CZ-I	-3.17	2.02	2.10
1	k	1721	PHI	CZ-I	-3.16	2.02	2.10
1	G	521	PHI	CZ-I	-3.16	2.02	2.10
1	g	1321	PHI	CZ-I	-3.16	2.02	2.10
1	JA	6221	PHI	CZ-I	-3.16	2.02	2.10
1	e	1121	PHI	CZ-I	-3.16	2.02	2.10
1	x	3021	PHI	CZ-I	-3.16	2.02	2.10
1	9	6621	PHI	CZ-I	-3.16	2.02	2.10
1	W	5721	PHI	CZ-I	-3.16	2.02	2.10
1	N	4821	PHI	CZ-I	-3.15	2.02	2.10
1	I	4321	PHI	CZ-I	-3.15	2.02	2.10
1	U	5521	PHI	CZ-I	-3.14	2.02	2.10
1	m	1921	PHI	CZ-I	-3.14	2.02	2.10
1	F	421	PHI	CZ-I	-3.14	2.02	2.10
1	O	4921	PHI	CZ-I	-3.14	2.02	2.10
1	IA	6521	PHI	CZ-I	-3.14	2.02	2.10
1	h	1421	PHI	CZ-I	-3.14	2.02	2.10
1	l	1821	PHI	CZ-I	-3.14	2.02	2.10
1	y	3121	PHI	CZ-I	-3.13	2.02	2.10
1	EA	7121	PHI	CZ-I	-3.13	2.02	2.10
1	A	6121	PHI	CZ-I	-3.13	2.02	2.10
1	c	921	PHI	CZ-I	-3.13	2.02	2.10
1	V	5621	PHI	CZ-I	-3.13	2.02	2.10
1	Z	621	PHI	CZ-I	-3.13	2.02	2.10
1	a	721	PHI	CZ-I	-3.13	2.02	2.10
1	M	4721	PHI	CZ-I	-3.13	2.02	2.10
1	f	1221	PHI	CZ-I	-3.13	2.02	2.10
1	0	3321	PHI	CZ-I	-3.13	2.02	2.10
1	j	1621	PHI	CZ-I	-3.12	2.02	2.10
1	l	3421	PHI	CZ-I	-3.12	2.02	2.10
1	o	2121	PHI	CZ-I	-3.12	2.02	2.10
1	v	2821	PHI	CZ-I	-3.12	2.02	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	5821	PHI	CZ-I	-3.12	2.02	2.10
1	n	2021	PHI	CZ-I	-3.11	2.02	2.10
1	H	4221	PHI	CZ-I	-3.11	2.02	2.10
1	BA	6821	PHI	CZ-I	-3.11	2.02	2.10
1	S	5321	PHI	CZ-I	-3.11	2.02	2.10
1	w	2921	PHI	CZ-I	-3.11	2.02	2.10
1	T	5421	PHI	CZ-I	-3.11	2.02	2.10
1	3	3621	PHI	CZ-I	-3.11	2.02	2.10
1	8	4121	PHI	CZ-I	-3.11	2.02	2.10
1	R	5221	PHI	CZ-I	-3.11	2.02	2.10
1	r	2421	PHI	CZ-I	-3.11	2.02	2.10
1	J	4421	PHI	CZ-I	-3.10	2.02	2.10
1	P	5021	PHI	CZ-I	-3.10	2.02	2.10
1	4	3721	PHI	CZ-I	-3.10	2.02	2.10
1	D	221	PHI	CZ-I	-3.10	2.02	2.10
1	6	3921	PHI	CZ-I	-3.10	2.02	2.10
1	FA	6021	PHI	CZ-I	-3.10	2.02	2.10
1	t	2621	PHI	CZ-I	-3.09	2.02	2.10
1	z	3221	PHI	CZ-I	-3.09	2.02	2.10
1	q	2321	PHI	CZ-I	-3.09	2.02	2.10
1	s	2521	PHI	CZ-I	-3.08	2.02	2.10
1	HA	6421	PHI	CZ-I	-3.08	2.02	2.10
1	K	4521	PHI	CZ-I	-3.07	2.02	2.10
1	L	4621	PHI	CZ-I	-3.06	2.02	2.10
1	2	3521	PHI	CZ-I	-3.06	2.02	2.10
1	7	4021	PHI	CZ-I	-3.00	2.02	2.10

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	1021	PHI	CG-CB-CA	-4.40	105.19	114.10
1	5	3821	PHI	CG-CB-CA	-3.86	106.28	114.10
1	g	1321	PHI	CG-CB-CA	-3.83	106.35	114.10
1	M	4721	PHI	CG-CB-CA	-3.27	107.47	114.10
1	u	2721	PHI	CG-CB-CA	-3.22	107.59	114.10
1	EA	7121	PHI	CG-CB-CA	-3.01	108.00	114.10
1	G	521	PHI	CG-CB-CA	-3.00	108.02	114.10
1	b	821	PHI	CB-CA-C	-2.90	106.03	111.47
1	HA	6421	PHI	CB-CA-C	-2.90	106.03	111.47
1	k	1721	PHI	CG-CB-CA	-2.82	108.39	114.10
1	D	221	PHI	CG-CB-CA	-2.78	108.48	114.10
1	A	6121	PHI	CG-CB-CA	-2.76	108.51	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	3021	PHI	CB-CA-C	-2.76	106.29	111.47
1	l	1821	PHI	CB-CA-C	-2.76	106.29	111.47
1	j	1621	PHI	CG-CB-CA	-2.75	108.53	114.10
1	5	3821	PHI	CB-CA-C	-2.74	106.33	111.47
1	8	4121	PHI	CG-CB-CA	-2.73	108.58	114.10
1	j	1621	PHI	CB-CA-C	-2.72	106.37	111.47
1	Y	5921	PHI	CB-CA-C	-2.72	106.37	111.47
1	BA	6821	PHI	CG-CB-CA	-2.69	108.64	114.10
1	g	1321	PHI	CB-CA-C	-2.69	106.42	111.47
1	h	1421	PHI	CB-CA-C	-2.68	106.44	111.47
1	P	5021	PHI	CB-CA-C	-2.68	106.45	111.47
1	v	2821	PHI	CG-CB-CA	-2.67	108.69	114.10
1	D	221	PHI	CB-CA-C	-2.67	106.47	111.47
1	DA	7021	PHI	CB-CA-C	-2.67	106.47	111.47
1	F	421	PHI	CB-CA-C	-2.66	106.47	111.47
1	BA	6821	PHI	CB-CA-C	-2.64	106.52	111.47
1	q	2321	PHI	CB-CA-C	-2.63	106.54	111.47
1	d	1021	PHI	CB-CA-C	-2.62	106.55	111.47
1	Z	621	PHI	CG-CB-CA	-2.62	108.79	114.10
1	u	2721	PHI	CB-CA-C	-2.61	106.58	111.47
1	B	21	PHI	CG-CB-CA	-2.60	108.84	114.10
1	v	2821	PHI	CB-CA-C	-2.59	106.62	111.47
1	9	6621	PHI	CG-CB-CA	-2.58	108.87	114.10
1	r	2421	PHI	CB-CA-C	-2.56	106.67	111.47
1	w	2921	PHI	CB-CA-C	-2.56	106.67	111.47
1	8	4121	PHI	CB-CA-C	-2.54	106.70	111.47
1	l	3421	PHI	CB-CA-C	-2.54	106.71	111.47
1	F	421	PHI	CG-CB-CA	-2.54	108.96	114.10
1	p	2221	PHI	CB-CA-C	-2.53	106.72	111.47
1	e	1121	PHI	CG-CB-CA	-2.53	108.97	114.10
1	b	821	PHI	CG-CB-CA	-2.52	109.00	114.10
1	m	1921	PHI	CB-CA-C	-2.52	106.75	111.47
1	DA	7021	PHI	CG-CB-CA	-2.52	109.00	114.10
1	f	1221	PHI	CG-CB-CA	-2.51	109.02	114.10
1	n	2021	PHI	CB-CA-C	-2.51	106.76	111.47
1	X	5821	PHI	CB-CA-C	-2.49	106.80	111.47
1	4	3721	PHI	CB-CA-C	-2.48	106.81	111.47
1	R	5221	PHI	CB-CA-C	-2.48	106.81	111.47
1	JA	6221	PHI	CG-CB-CA	-2.48	109.09	114.10
1	FA	6021	PHI	CB-CA-C	-2.46	106.86	111.47
1	t	2621	PHI	CG-CB-CA	-2.43	109.19	114.10
1	J	4421	PHI	CB-CA-C	-2.42	106.92	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	3121	PHI	CG-CB-CA	-2.41	109.23	114.10
1	9	6621	PHI	CB-CA-C	-2.40	106.98	111.47
1	O	4921	PHI	CB-CA-C	-2.39	106.99	111.47
1	3	3621	PHI	CB-CA-C	-2.38	107.01	111.47
1	B	21	PHI	CB-CA-C	-2.38	107.01	111.47
1	L	4621	PHI	CB-CA-C	-2.36	107.04	111.47
1	IA	6521	PHI	CB-CA-C	-2.35	107.06	111.47
1	a	721	PHI	CB-CA-C	-2.33	107.11	111.47
1	L	4621	PHI	CG-CB-CA	-2.32	109.40	114.10
1	z	3221	PHI	CB-CA-C	-2.31	107.13	111.47
1	S	5321	PHI	CG-CB-CA	-2.31	109.41	114.10
1	e	1121	PHI	CB-CA-C	-2.29	107.17	111.47
1	H	4221	PHI	CG-CB-CA	-2.29	109.47	114.10
1	n	2021	PHI	CG-CB-CA	-2.27	109.51	114.10
1	7	4021	PHI	CB-CA-C	-2.26	107.23	111.47
1	A	6121	PHI	CB-CA-C	-2.26	107.23	111.47
1	GA	6321	PHI	CB-CA-C	-2.26	107.24	111.47
1	Z	621	PHI	CB-CA-C	-2.25	107.25	111.47
1	p	2221	PHI	CG-CB-CA	-2.23	109.58	114.10
1	V	5621	PHI	CB-CA-C	-2.23	107.29	111.47
1	f	1221	PHI	CB-CA-C	-2.22	107.30	111.47
1	N	4821	PHI	CB-CA-C	-2.21	107.33	111.47
1	H	4221	PHI	CB-CA-C	-2.20	107.34	111.47
1	S	5321	PHI	CB-CA-C	-2.20	107.35	111.47
1	a	721	PHI	CG-CB-CA	-2.19	109.67	114.10
1	4	3721	PHI	CG-CB-CA	-2.17	109.70	114.10
1	FA	6021	PHI	CG-CB-CA	-2.17	109.70	114.10
1	I	4321	PHI	CB-CA-C	-2.16	107.41	111.47
1	2	3521	PHI	CB-CA-C	-2.15	107.44	111.47
1	T	5421	PHI	CB-CA-C	-2.14	107.45	111.47
1	i	1521	PHI	CB-CA-C	-2.13	107.48	111.47
1	JA	6221	PHI	CB-CA-C	-2.13	107.48	111.47
1	k	1721	PHI	CB-CA-C	-2.11	107.50	111.47
1	EA	7121	PHI	CB-CA-C	-2.08	107.56	111.47
1	K	4521	PHI	CB-CA-C	-2.07	107.59	111.47
1	t	2621	PHI	CB-CA-C	-2.06	107.60	111.47
1	E	321	PHI	CB-CA-C	-2.06	107.61	111.47
1	CA	6921	PHI	CB-CA-C	-2.05	107.63	111.47
1	G	521	PHI	CB-CA-C	-2.03	107.66	111.47

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	21	PHI	C-CA-CB-CG
1	D	221	PHI	C-CA-CB-CG
1	F	421	PHI	N-CA-CB-CG
1	F	421	PHI	C-CA-CB-CG
1	J	4421	PHI	C-CA-CB-CG
1	L	4621	PHI	N-CA-CB-CG
1	L	4621	PHI	C-CA-CB-CG
1	M	4721	PHI	C-CA-CB-CG
1	M	4721	PHI	O-C-CA-CB
1	N	4821	PHI	O-C-CA-CB
1	P	5021	PHI	C-CA-CB-CG
1	R	5221	PHI	N-CA-CB-CG
1	R	5221	PHI	C-CA-CB-CG
1	U	5521	PHI	O-C-CA-CB
1	V	5621	PHI	C-CA-CB-CG
1	X	5821	PHI	C-CA-CB-CG
1	Z	621	PHI	O-C-CA-CB
1	b	821	PHI	C-CA-CB-CG
1	c	921	PHI	N-CA-CB-CG
1	c	921	PHI	C-CA-CB-CG
1	d	1021	PHI	C-CA-CB-CG
1	f	1221	PHI	C-CA-CB-CG
1	f	1221	PHI	O-C-CA-CB
1	h	1421	PHI	C-CA-CB-CG
1	j	1621	PHI	N-CA-CB-CG
1	j	1621	PHI	C-CA-CB-CG
1	l	1821	PHI	C-CA-CB-CG
1	n	2021	PHI	C-CA-CB-CG
1	p	2221	PHI	O-C-CA-CB
1	r	2421	PHI	C-CA-CB-CG
1	t	2621	PHI	C-CA-CB-CG
1	v	2821	PHI	N-CA-CB-CG
1	v	2821	PHI	C-CA-CB-CG
1	w	2921	PHI	C-CA-CB-CG
1	w	2921	PHI	O-C-CA-CB
1	z	3221	PHI	C-CA-CB-CG
1	1	3421	PHI	C-CA-CB-CG
1	2	3521	PHI	O-C-CA-CB
1	3	3621	PHI	C-CA-CB-CG
1	7	4021	PHI	C-CA-CB-CG
1	9	6621	PHI	C-CA-CB-CG
1	9	6621	PHI	O-C-CA-CB
1	BA	6821	PHI	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	DA	7021	PHI	N-CA-CB-CG
1	DA	7021	PHI	C-CA-CB-CG
1	JA	6221	PHI	C-CA-CB-CG
1	HA	6421	PHI	C-CA-CB-CG
1	IA	6521	PHI	C-CA-CB-CG
1	q	2321	PHI	CA-CB-CG-CD2
1	f	1221	PHI	CA-CB-CG-CD2
1	Z	621	PHI	CA-CB-CG-CD2
1	q	2321	PHI	CA-CB-CG-CD1
1	f	1221	PHI	CA-CB-CG-CD1
1	B	21	PHI	N-CA-CB-CG
1	D	221	PHI	N-CA-CB-CG
1	J	4421	PHI	N-CA-CB-CG
1	M	4721	PHI	N-CA-CB-CG
1	P	5021	PHI	N-CA-CB-CG
1	Y	5921	PHI	N-CA-CB-CG
1	Z	621	PHI	CA-CB-CG-CD1
1	b	821	PHI	N-CA-CB-CG
1	d	1021	PHI	N-CA-CB-CG
1	f	1221	PHI	N-CA-CB-CG
1	h	1421	PHI	N-CA-CB-CG
1	n	2021	PHI	N-CA-CB-CG
1	p	2221	PHI	N-CA-CB-CG
1	y	3121	PHI	N-CA-CB-CG
1	z	3221	PHI	N-CA-CB-CG
1	1	3421	PHI	N-CA-CB-CG
1	3	3621	PHI	N-CA-CB-CG
1	7	4021	PHI	N-CA-CB-CG
1	9	6621	PHI	N-CA-CB-CG
1	BA	6821	PHI	N-CA-CB-CG
1	HA	6421	PHI	N-CA-CB-CG
1	IA	6521	PHI	N-CA-CB-CG
1	B	21	PHI	CA-CB-CG-CD2
1	p	2221	PHI	CA-CB-CG-CD2
1	9	6621	PHI	CA-CB-CG-CD2
1	B	21	PHI	CA-CB-CG-CD1
1	l	1821	PHI	CA-CB-CG-CD2
1	9	6621	PHI	CA-CB-CG-CD1
1	G	521	PHI	CA-CB-CG-CD2
1	2	3521	PHI	CA-CB-CG-CD2
1	EA	7121	PHI	CA-CB-CG-CD2
1	p	2221	PHI	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	2	3521	PHI	CA-CB-CG-CD1
1	G	521	PHI	CA-CB-CG-CD1
1	l	1821	PHI	CA-CB-CG-CD1
1	EA	7121	PHI	CA-CB-CG-CD1
1	k	1721	PHI	CA-CB-CG-CD1
1	t	2621	PHI	CA-CB-CG-CD1
1	t	2621	PHI	CA-CB-CG-CD2
1	T	5421	PHI	CA-CB-CG-CD1
1	T	5421	PHI	CA-CB-CG-CD2
1	e	1121	PHI	CA-CB-CG-CD1
1	H	4221	PHI	CA-CB-CG-CD2
1	k	1721	PHI	CA-CB-CG-CD2
1	H	4221	PHI	CA-CB-CG-CD1
1	e	1121	PHI	CA-CB-CG-CD2
1	Q	5121	PHI	C-CA-CB-CG
1	Y	5921	PHI	C-CA-CB-CG
1	p	2221	PHI	C-CA-CB-CG
1	y	3121	PHI	C-CA-CB-CG
1	0	3321	PHI	C-CA-CB-CG
1	FA	6021	PHI	C-CA-CB-CG
1	h	1421	PHI	CA-CB-CG-CD2
1	h	1421	PHI	CA-CB-CG-CD1
1	x	3021	PHI	CA-CB-CG-CD2
1	Q	5121	PHI	N-CA-CB-CG
1	V	5621	PHI	N-CA-CB-CG
1	X	5821	PHI	N-CA-CB-CG
1	l	1821	PHI	N-CA-CB-CG
1	r	2421	PHI	N-CA-CB-CG
1	t	2621	PHI	N-CA-CB-CG
1	w	2921	PHI	N-CA-CB-CG
1	FA	6021	PHI	N-CA-CB-CG
1	JA	6221	PHI	N-CA-CB-CG
1	8	4121	PHI	CA-CB-CG-CD2
1	x	3021	PHI	CA-CB-CG-CD1
1	8	4121	PHI	CA-CB-CG-CD1
1	N	4821	PHI	CA-CB-CG-CD2
1	BA	6821	PHI	CA-CB-CG-CD2
1	D	221	PHI	CA-CB-CG-CD2
1	N	4821	PHI	CA-CB-CG-CD1
1	G	521	PHI	C-CA-CB-CG
1	W	5721	PHI	C-CA-CB-CG
1	Z	621	PHI	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	e	1121	PHI	C-CA-CB-CG
1	i	1521	PHI	C-CA-CB-CG
1	k	1721	PHI	C-CA-CB-CG
1	o	2121	PHI	C-CA-CB-CG
1	8	4121	PHI	C-CA-CB-CG
1	EA	7121	PHI	C-CA-CB-CG
1	i	1521	PHI	N-CA-CB-CG
1	o	2121	PHI	N-CA-CB-CG
1	0	3321	PHI	N-CA-CB-CG
1	D	221	PHI	CA-CB-CG-CD1
1	BA	6821	PHI	CA-CB-CG-CD1
1	S	5321	PHI	CA-CB-CG-CD2

There are no ring outliers.

19 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	V	5621	PHI	7	0
1	H	4221	PHI	2	0
1	Z	621	PHI	1	0
1	G	521	PHI	1	0
1	1	3421	PHI	1	0
1	N	4821	PHI	1	0
1	6	3921	PHI	3	0
1	JA	6221	PHI	2	0
1	FA	6021	PHI	2	0
1	EA	7121	PHI	2	0
1	B	21	PHI	1	0
1	K	4521	PHI	1	0
1	X	5821	PHI	1	0
1	7	4021	PHI	4	0
1	2	3521	PHI	1	0
1	T	5421	PHI	2	0
1	M	4721	PHI	1	0
1	CA	6921	PHI	4	0
1	GA	6321	PHI	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

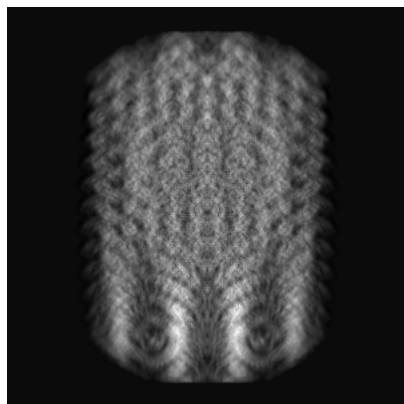
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26552. These allow visual inspection of the internal detail of the map and identification of artifacts.

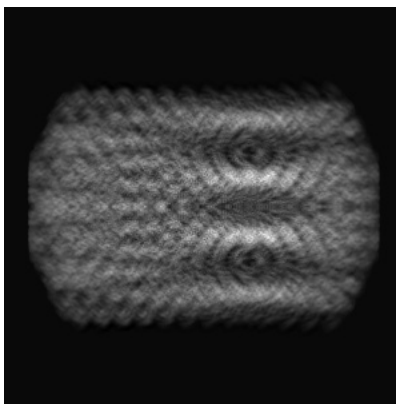
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

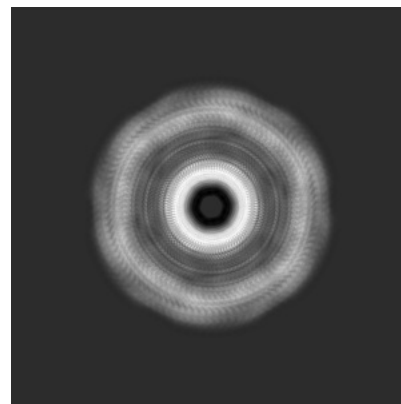
6.1.1 Primary map



X

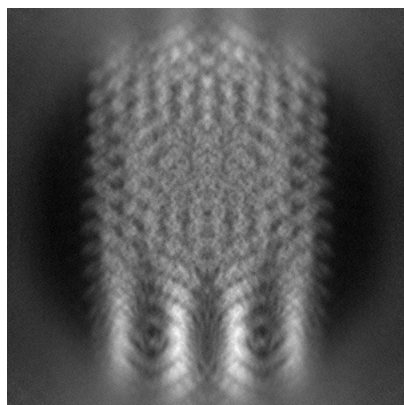


Y

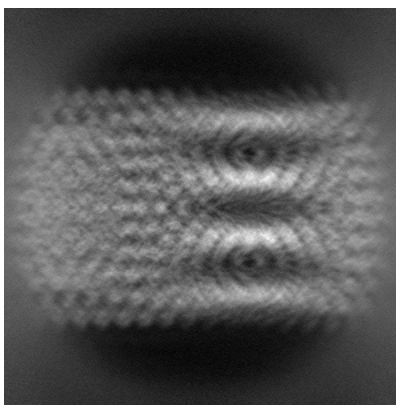


Z

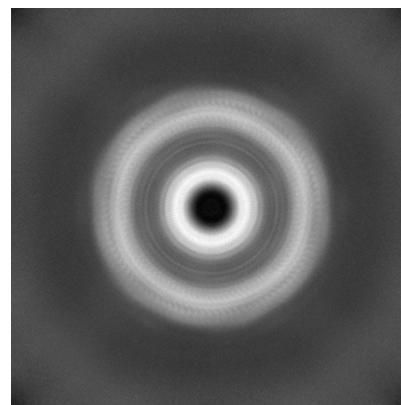
6.1.2 Raw map



X



Y

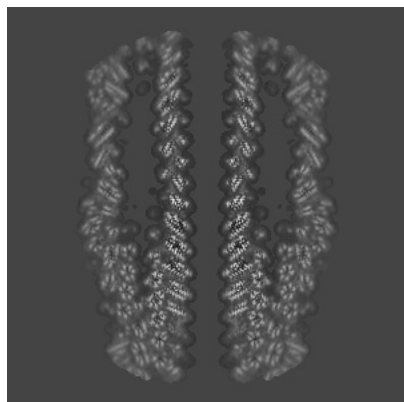


Z

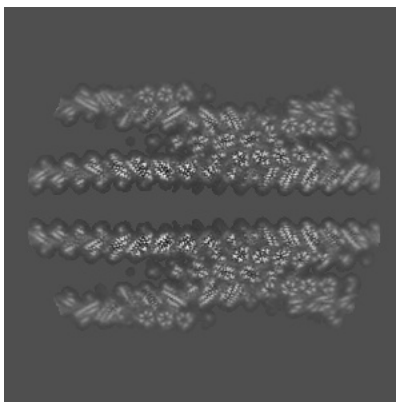
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

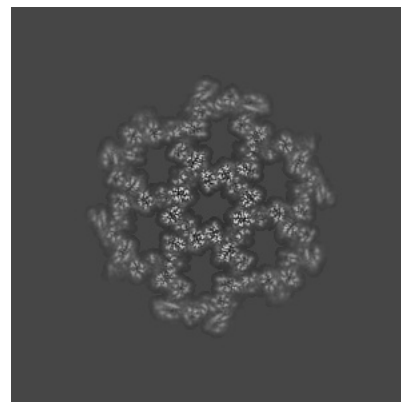
6.2.1 Primary map



X Index: 320

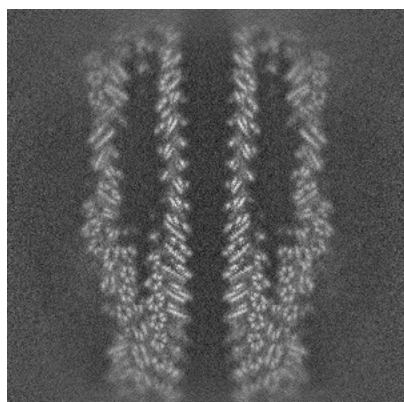


Y Index: 320

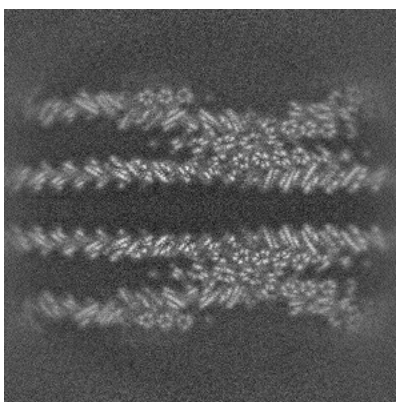


Z Index: 320

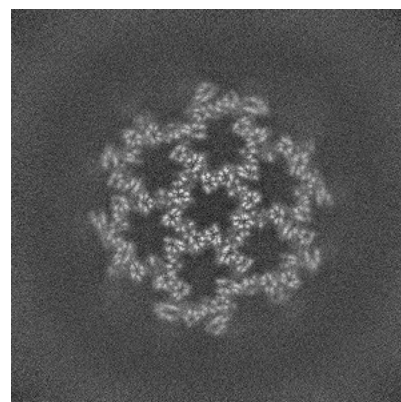
6.2.2 Raw map



X Index: 320



Y Index: 320

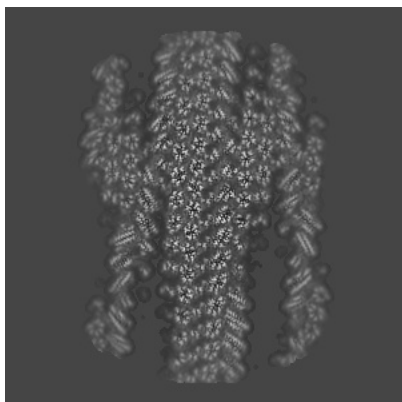


Z Index: 320

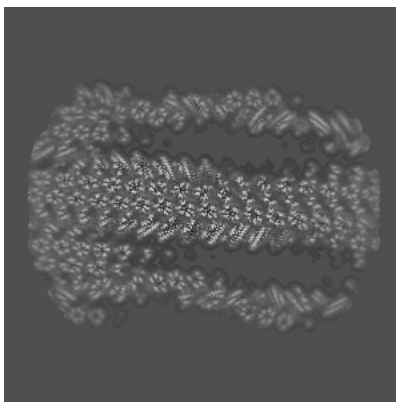
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

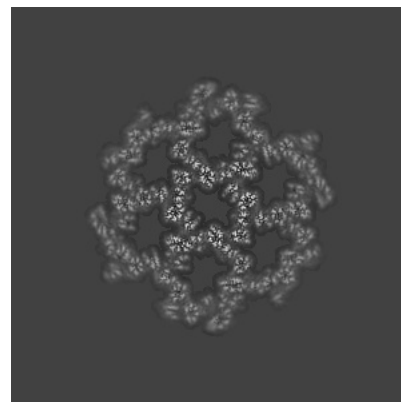
6.3.1 Primary map



X Index: 365

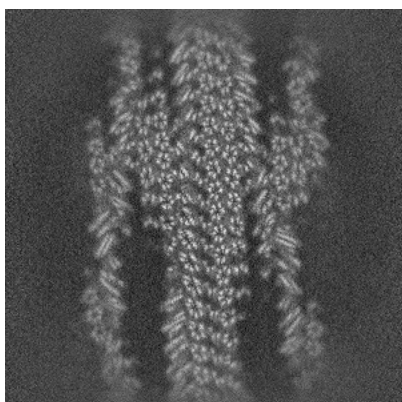


Y Index: 368

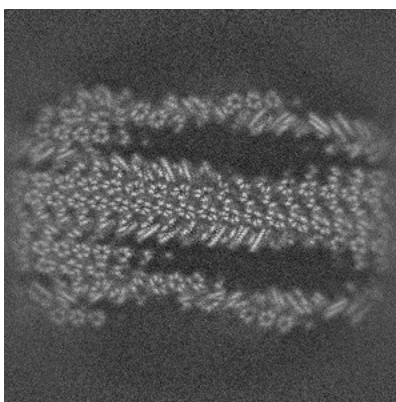


Z Index: 327

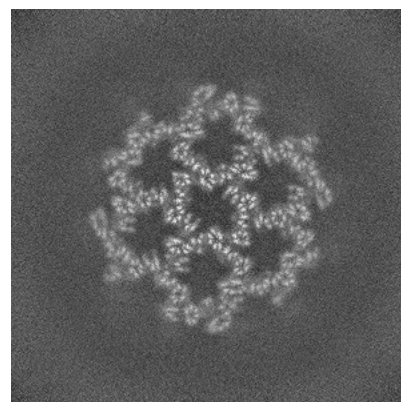
6.3.2 Raw map



X Index: 275



Y Index: 368

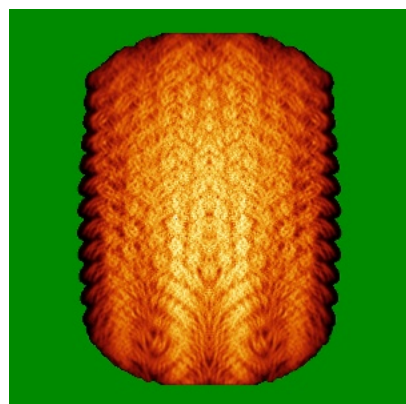


Z Index: 327

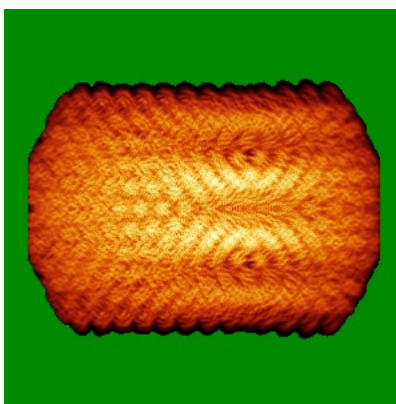
The images above show the largest variance slices of the map in three orthogonal directions.

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

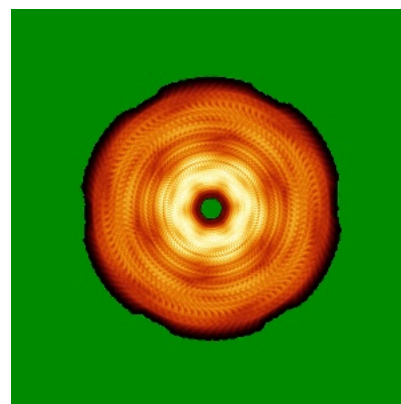
6.4.1 Primary map



X

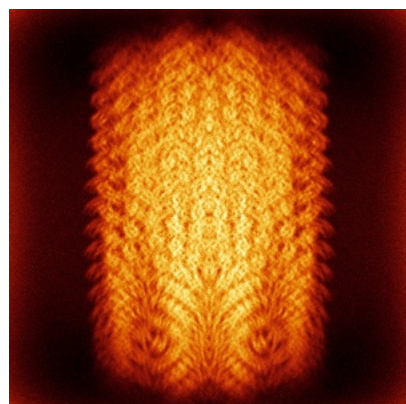


Y

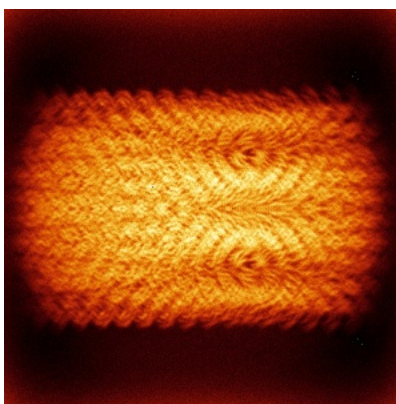


Z

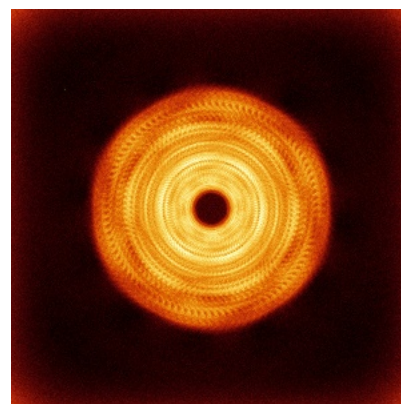
6.4.2 Raw map



X



Y

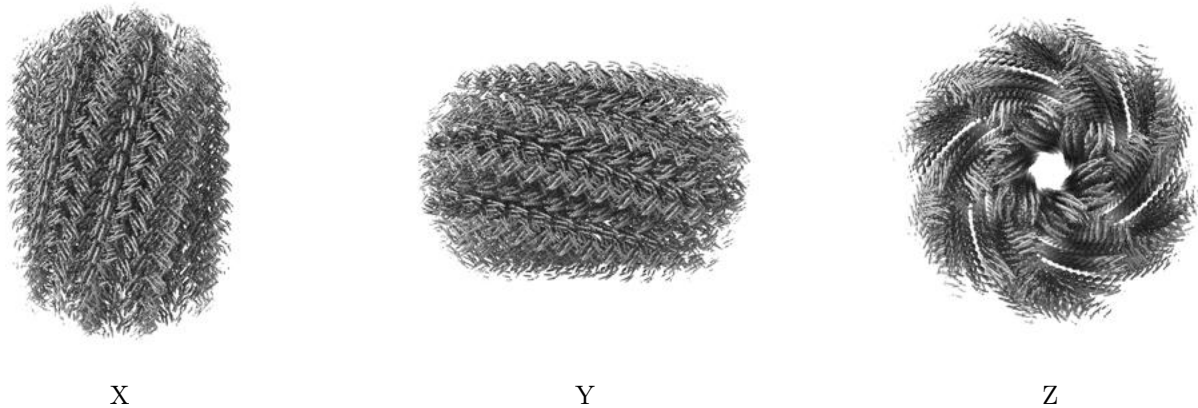


Z

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.

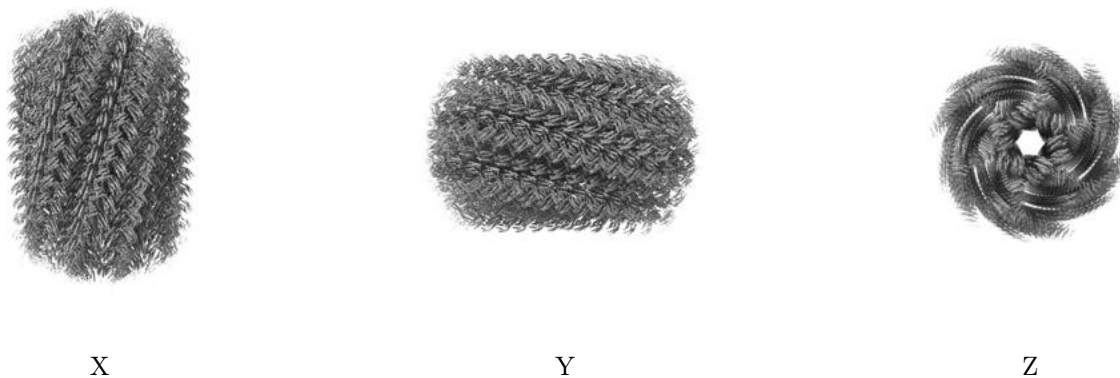
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

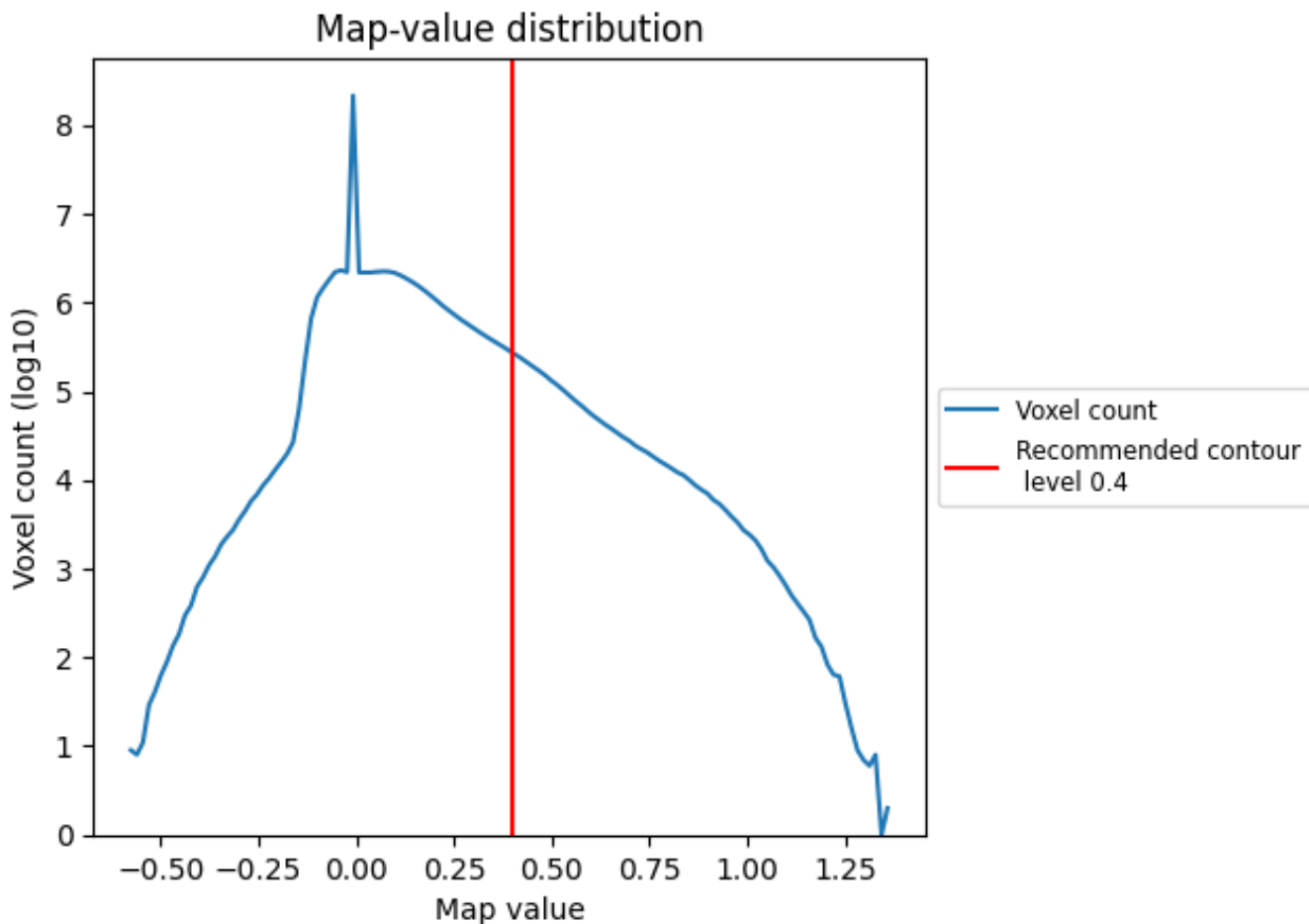
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

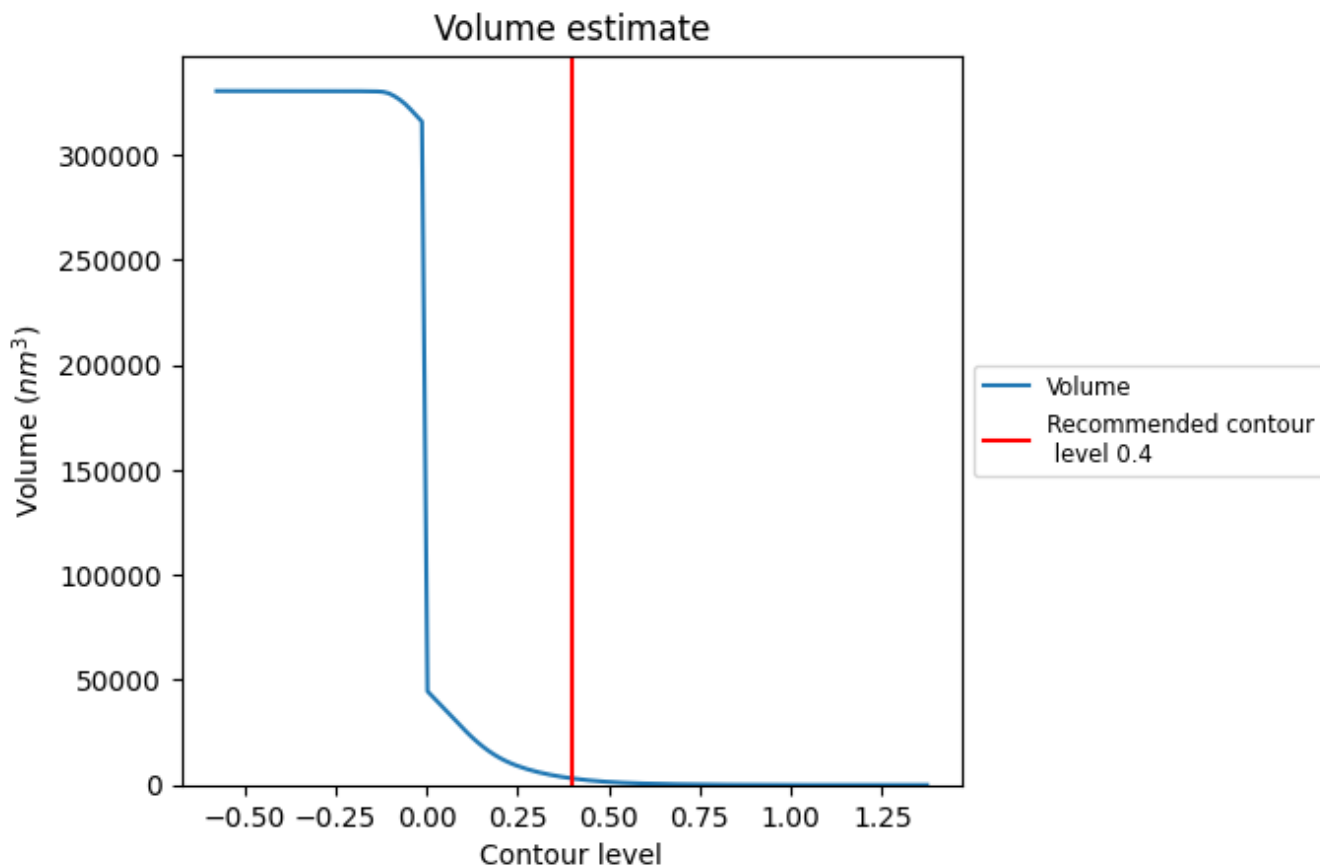
This section contains the results of statistical analysis of the map.

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.

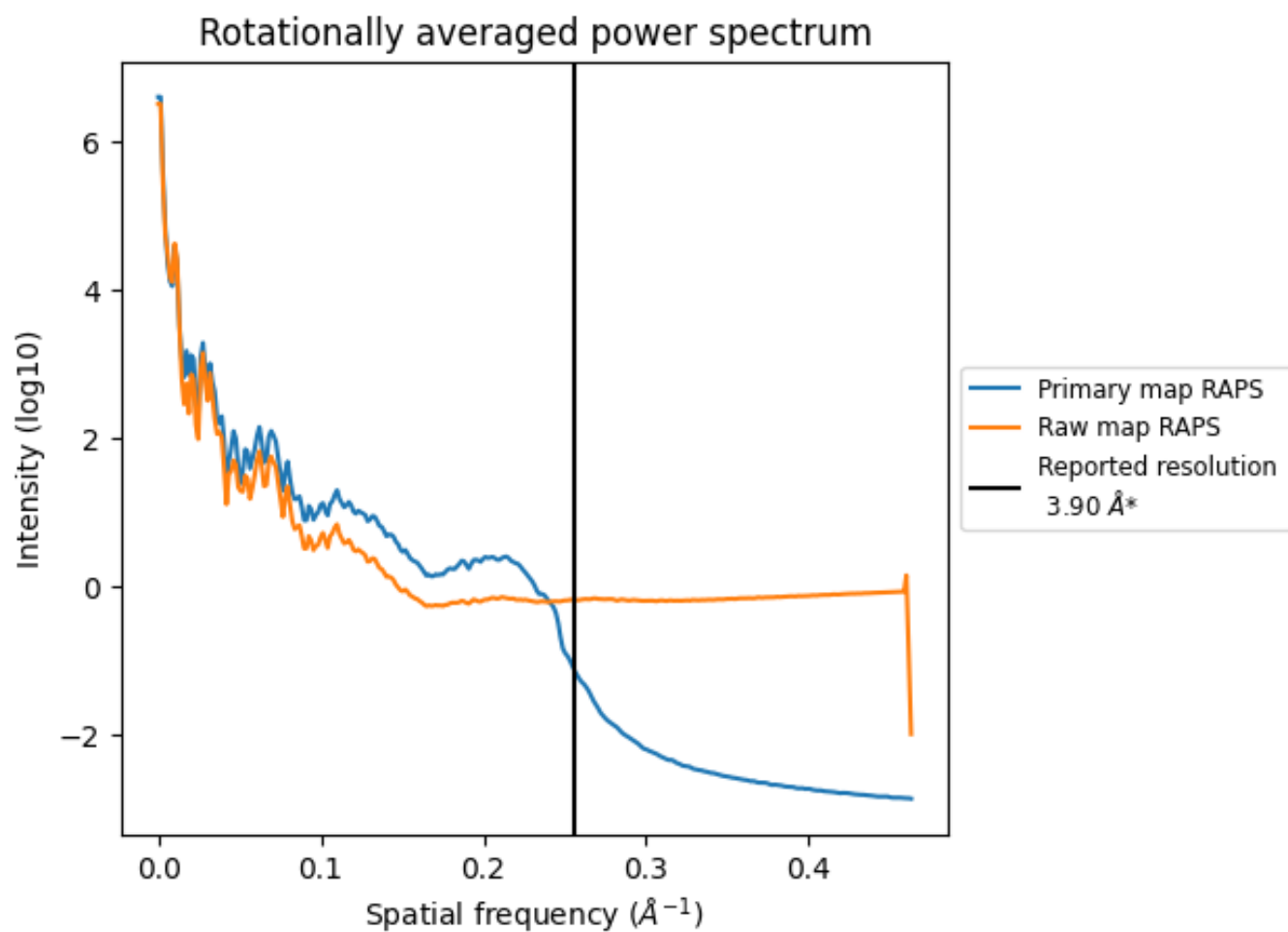
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3123 nm^3 ; this corresponds to an approximate mass of 2821 kDa.

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

7.3 Rotationally averaged power spectrum i

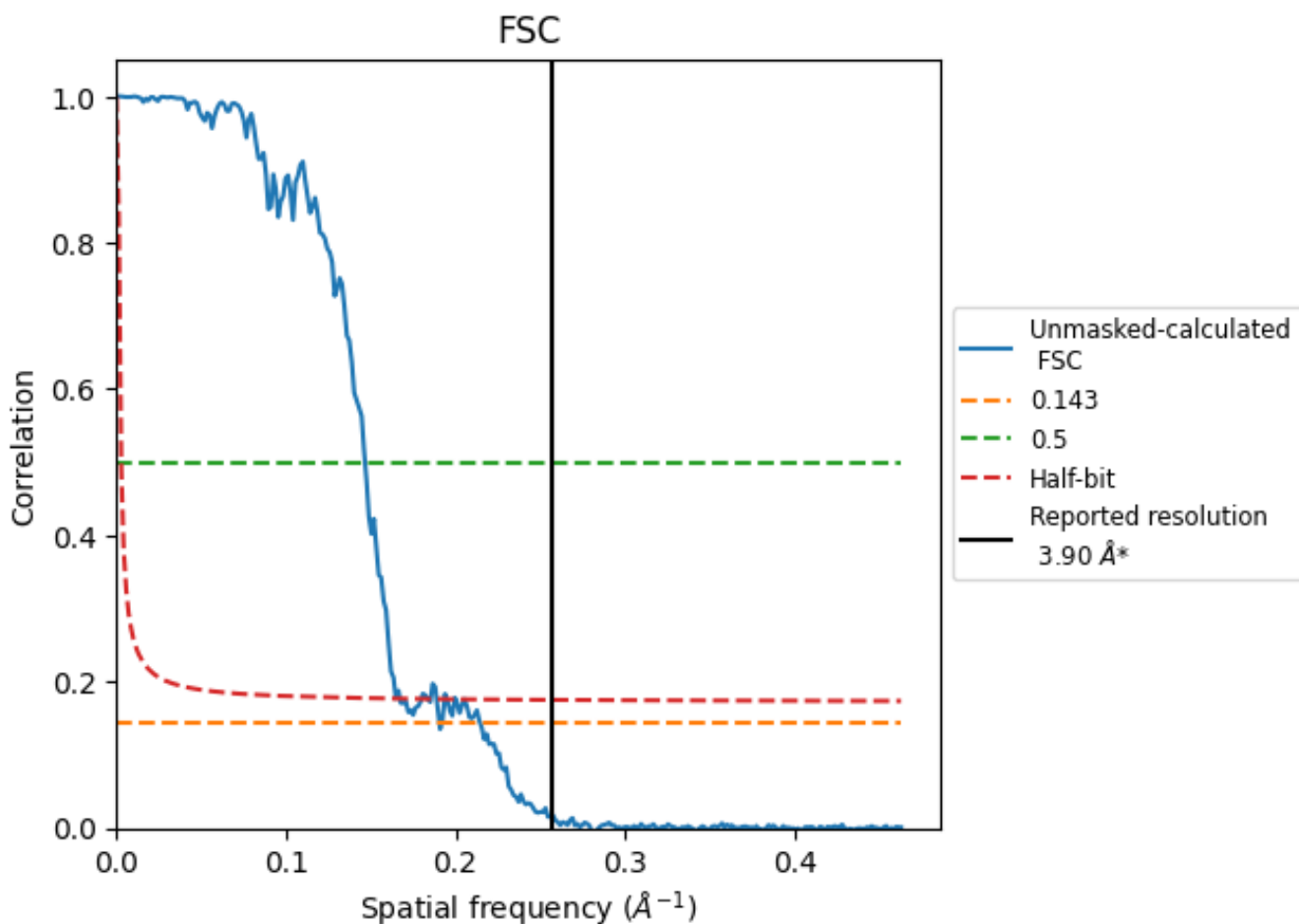


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

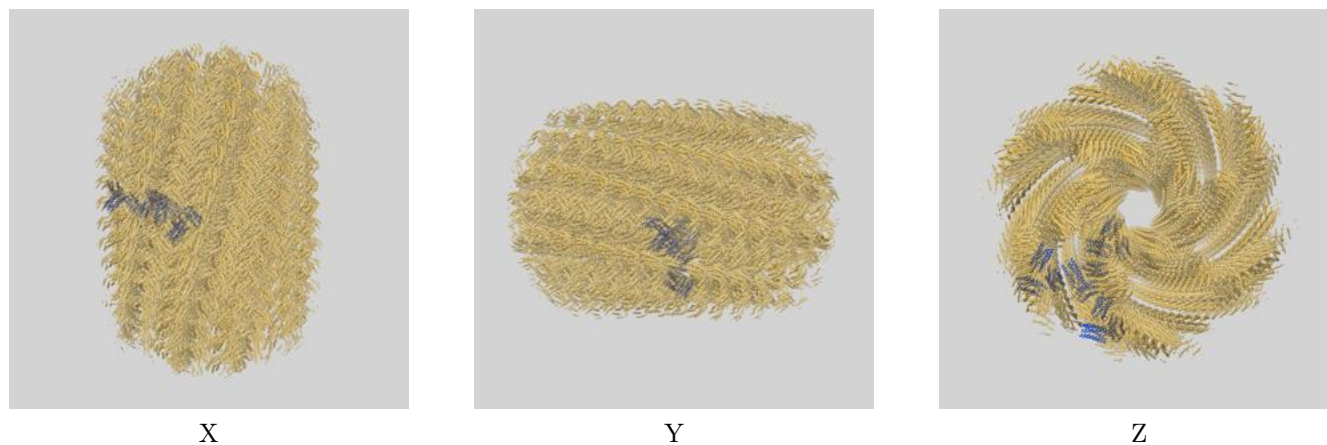
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.25	6.82	6.06

*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 5.25 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

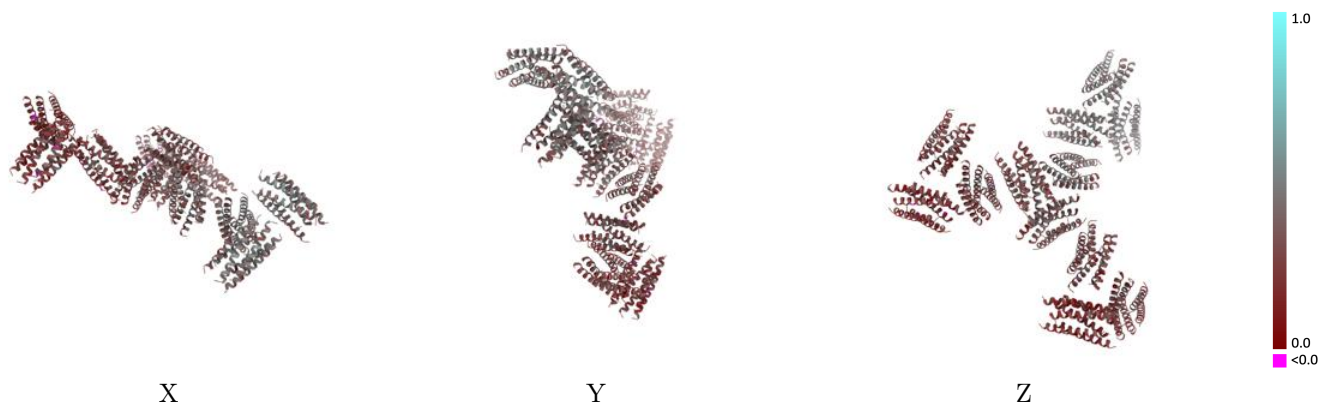
This section contains information regarding the fit between EMDB map EMD-26552 and PDB model 7UIT. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



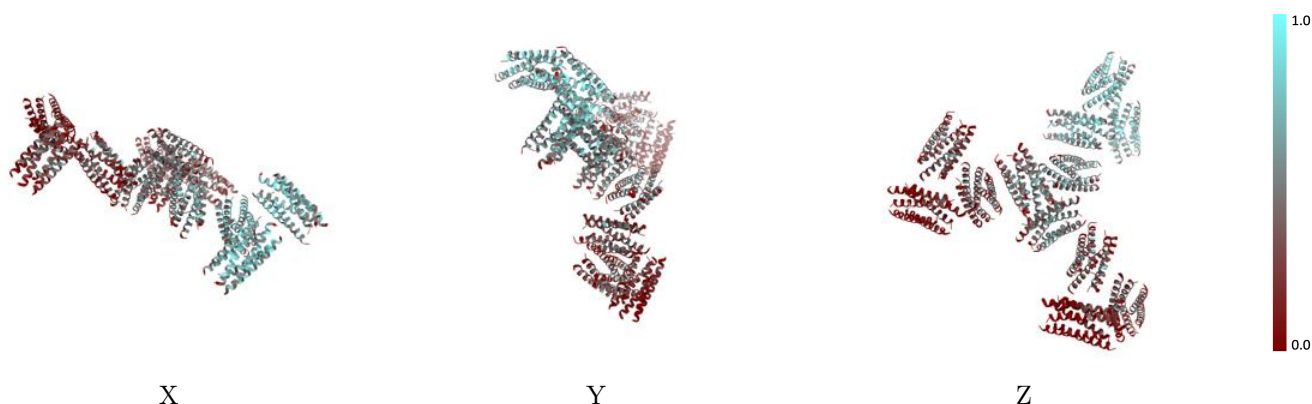
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



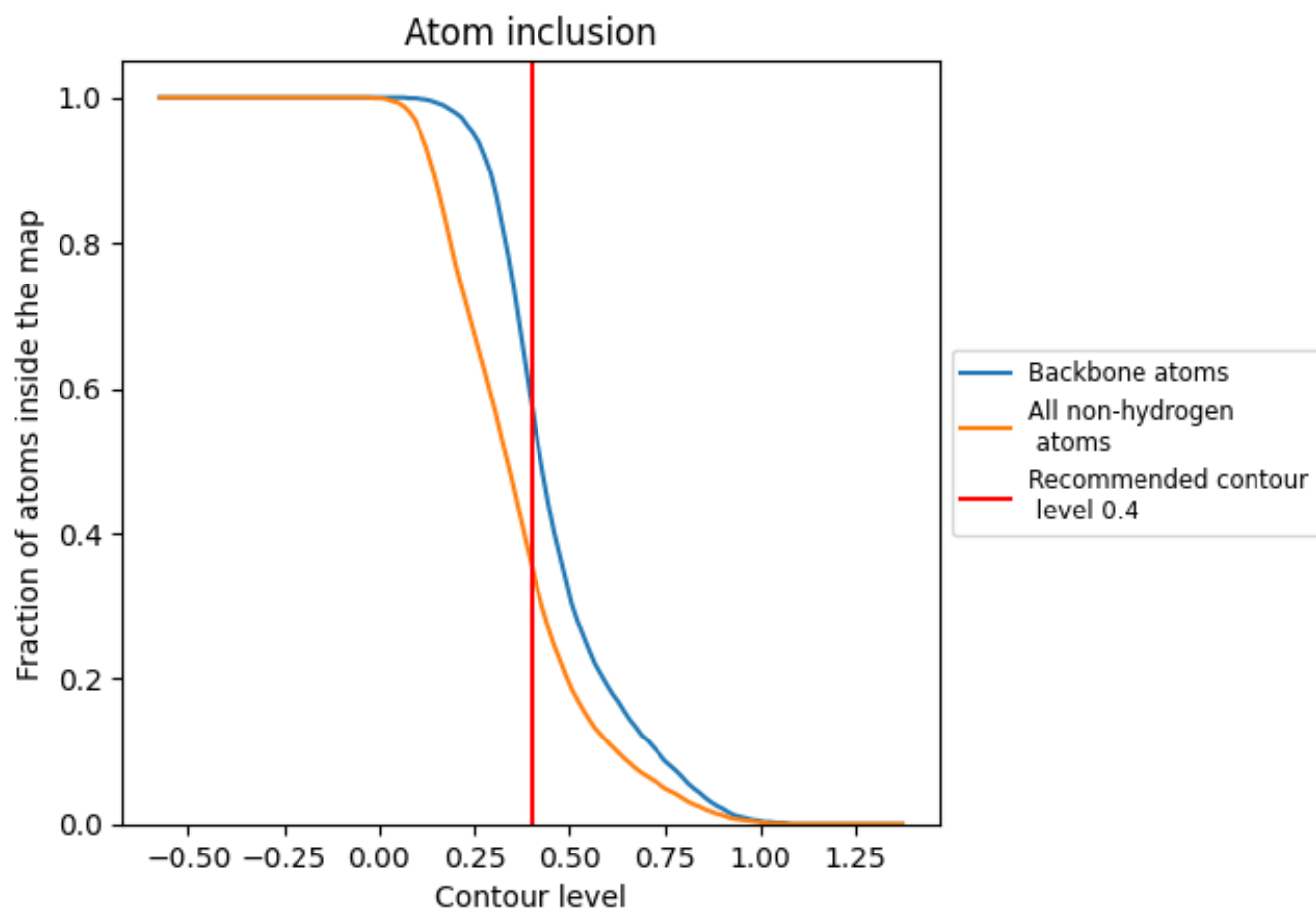
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 36% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3550	 0.3170
0	 0.2400	 0.3110
1	 0.2280	 0.2600
2	 0.2530	 0.2760
3	 0.2360	 0.2530
4	 0.2660	 0.2610
5	 0.2790	 0.3010
6	 0.2490	 0.2550
7	 0.2400	 0.2810
8	 0.2360	 0.2660
9	 0.0130	 0.2050
A	 0.0930	 0.2200
AA	 0.0380	 0.1880
B	 0.6410	 0.4290
BA	 0.0590	 0.1970
C	 0.6370	 0.4390
CA	 0.1270	 0.2160
D	 0.6410	 0.4060
DA	 0.1100	 0.2030
E	 0.6460	 0.4180
EA	 0.0760	 0.2180
F	 0.5780	 0.4150
FA	 0.1010	 0.2240
G	 0.6410	 0.4400
GA	 0.0680	 0.1830
H	 0.2660	 0.2650
HA	 0.0800	 0.1800
I	 0.3120	 0.2740
IA	 0.1390	 0.2110
J	 0.2660	 0.2960
JA	 0.0250	 0.2180
K	 0.2570	 0.2620
L	 0.2360	 0.2690
M	 0.2320	 0.2900
N	 0.3420	 0.3130



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Chain	Atom inclusion	Q-score
O	0.3630	0.3160
P	0.3590	0.3150
Q	0.3840	0.3240
R	0.3670	0.3080
S	0.3840	0.3270
T	0.3120	0.2990
U	0.2400	0.2870
V	0.2490	0.2650
W	0.2660	0.2770
X	0.3080	0.2790
Y	0.2660	0.2840
Z	0.6250	0.4260
a	0.6080	0.4110
b	0.6370	0.4170
c	0.6030	0.4160
d	0.5950	0.4230
e	0.6370	0.4400
f	0.5650	0.4000
g	0.5780	0.3910
h	0.5870	0.3890
i	0.5740	0.4000
j	0.5610	0.4060
k	0.6120	0.4280
l	0.4470	0.3520
m	0.4470	0.3810
n	0.4600	0.3620
o	0.4520	0.3640
p	0.4980	0.3900
q	0.4560	0.3830
r	0.3970	0.3400
s	0.4050	0.3290
t	0.4180	0.3330
u	0.4050	0.3290
v	0.4350	0.3260
w	0.3880	0.3300
x	0.2950	0.3150
y	0.2910	0.3040
z	0.2190	0.2770