



Full wwPDB EM Validation Report ⓘ

Jun 30, 2025 – 12:51 PM JST

PDB ID : 9M5R / pdb_00009m5r
EMDB ID : EMD-63648
Title : ES-type (short pitch) amyloid fibril (40) of Tottori (D7N) mutant
Authors : Burton-Smith, R.N.; Murata, K.
Deposited on : 2025-03-06
Resolution : 3.60 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

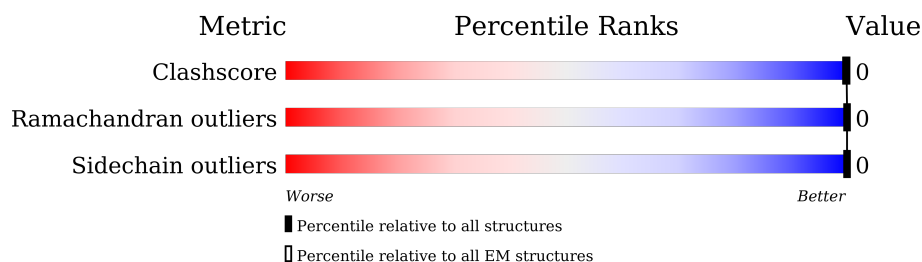
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



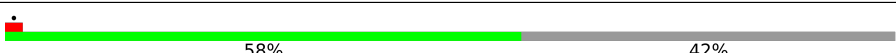
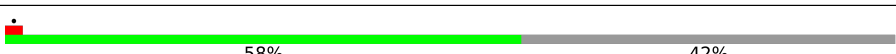
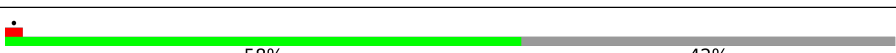
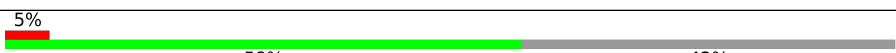
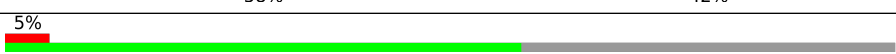
The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	40	
1	1	40	
1	2	40	
1	3	40	
1	4	40	
1	5	40	
1	6	40	
1	7	40	






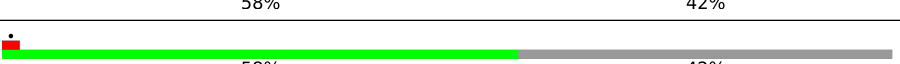
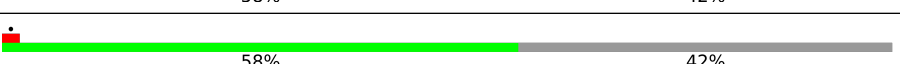
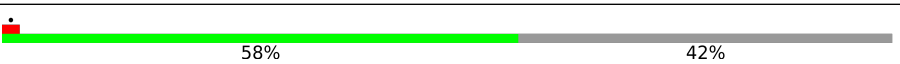


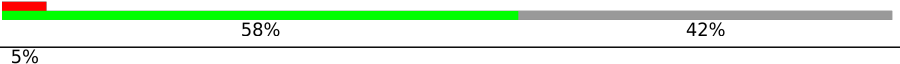
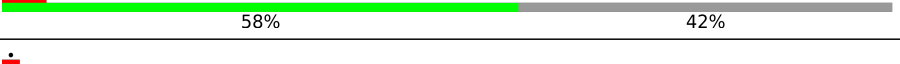

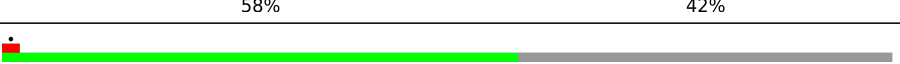
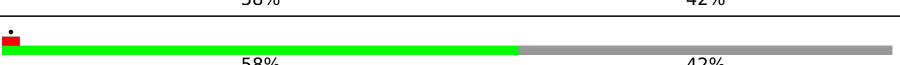










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Mol	Chain	Length	Quality of chain
1	8	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	9	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A0	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A1	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A2	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A3	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A4	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A5	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A6	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A7	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A8	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	A9	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AA	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AB	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AC	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AD	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AE	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AF	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AG	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AH	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AI	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AJ	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AK	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	AL	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>

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Mol	Chain	Length	Quality of chain	
1	AM	40		
1	AN	40		
1	AO	40		
1	AP	40		
1	AQ	40		
1	AR	40		
1	AS	40		
1	AT	40		
1	AU	40		
1	AV	40		
1	AW	40		
1	AX	40		
1	AY	40		
1	AZ	40		
1	Aa	40		
1	Ab	40		
1	Ac	40		
1	Ad	40		
1	Ae	40		
1	Af	40		
1	Ag	40		
1	Ah	40		
1	Ai	40		
1	Aj	40		
1	Ak	40		




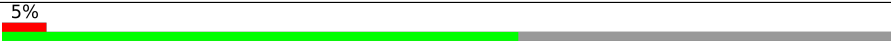

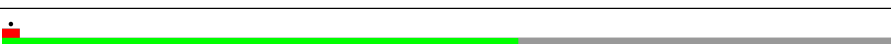
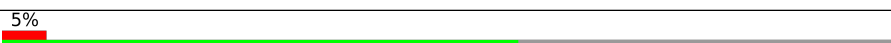

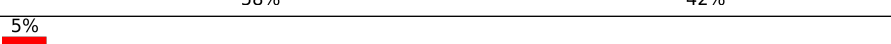
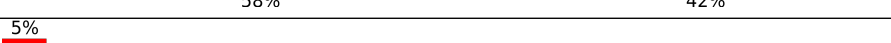
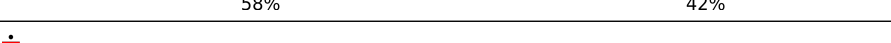

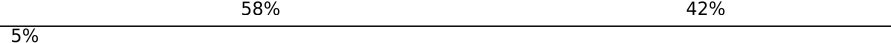
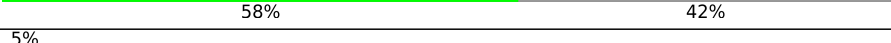











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Mol	Chain	Length	Quality of chain
1	Al	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Am	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	An	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Ao	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Ap	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Aq	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Ar	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	As	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	At	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Au	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Av	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Aw	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Ax	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Ay	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	Az	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	B	40	<div> <div>58%</div> <div>58%</div> <div>42%</div> </div>
1	BA	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BB	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BC	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BD	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BE	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BF	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BG	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BH	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	BI	40	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>




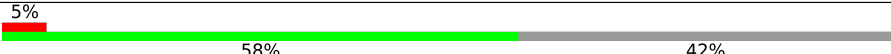
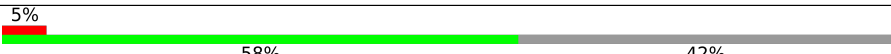
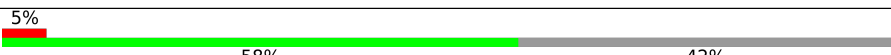
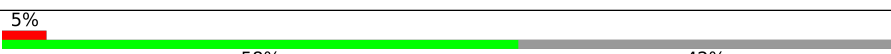
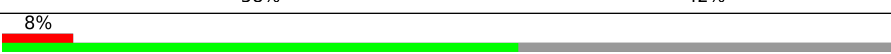

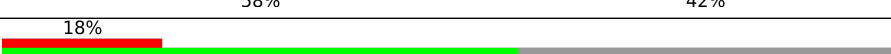
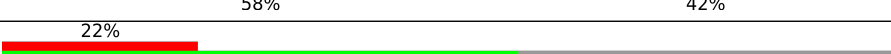
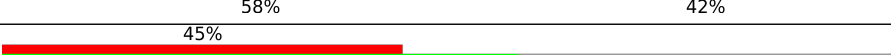







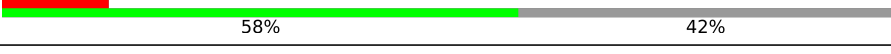

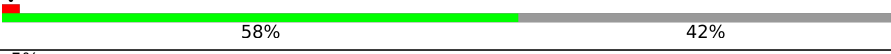



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Mol	Chain	Length	Quality of chain	
1	BJ	40	5% 	58% 42%
1	BK	40	5% 	58% 42%
1	BL	40	• 	58% 42%
1	BM	40	5% 	58% 42%
1	BN	40	• 	58% 42%
1	BO	40	• 	58% 42%
1	BP	40	5% 	58% 42%
1	BQ	40	5% 	58% 42%
1	BR	40	5% 	58% 42%
1	BS	40	5% 	58% 42%
1	BT	40	• 	58% 42%
1	BU	40	• 	58% 42%
1	BV	40	5% 	58% 42%
1	BW	40	5% 	58% 42%
1	BX	40	5% 	58% 42%
1	BY	40	5% 	58% 42%
1	BZ	40	5% 	58% 42%
1	Ba	40	• 	58% 42%
1	Bb	40	• 	58% 42%
1	Bc	40	• 	58% 42%
1	Bd	40	5% 	58% 42%
1	Be	40	5% 	58% 42%
1	Bf	40	5% 	58% 42%
1	Bg	40	5% 	58% 42%
1	Bh	40	• 	58% 42%





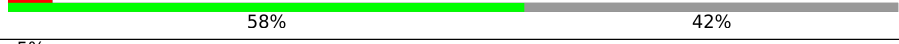


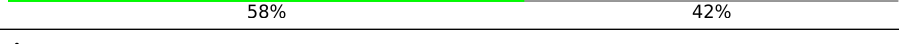
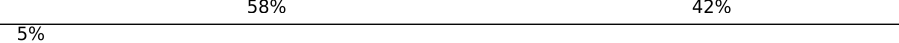
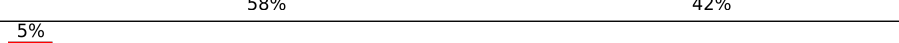
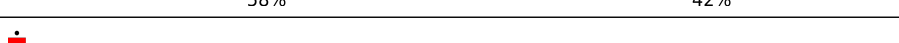











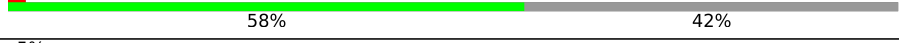


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Mol	Chain	Length	Quality of chain
1	Bi	40	
1	Bj	40	
1	Bk	40	
1	Bl	40	
1	Bm	40	
1	Bn	40	
1	Bo	40	
1	Bp	40	
1	Bq	40	
1	Br	40	
1	Bs	40	
1	Bt	40	
1	Bu	40	
1	Bv	40	
1	C	40	
1	D	40	
1	E	40	
1	F	40	
1	G	40	
1	H	40	
1	I	40	
1	J	40	
1	K	40	
1	L	40	
1	M	40	

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Mol	Chain	Length	Quality of chain
1	N	40	
1	O	40	
1	P	40	
1	Q	40	
1	R	40	
1	S	40	
1	T	40	
1	U	40	
1	V	40	
1	W	40	
1	X	40	
1	Y	40	
1	Z	40	
1	a	40	
1	b	40	
1	c	40	
1	d	40	
1	e	40	
1	f	40	
1	g	40	
1	h	40	
1	i	40	
1	j	40	
1	k	40	
1	l	40	

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Mol	Chain	Length	Quality of chain	
1	m	40		
1	n	40		
1	o	40		
1	p	40		
1	q	40		
1	r	40		
1	s	40		
1	t	40		
1	u	40		
1	v	40		
1	w	40		
1	x	40		
1	y	40		
1	z	40		

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 56072 atoms, of which 28552 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 Amyloid-beta protein 40.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	B	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	C	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	D	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	E	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	F	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	G	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	H	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	I	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	J	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	K	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	L	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	M	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	N	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	O	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	P	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Q	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	R	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	S	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	T	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	U	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	V	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	W	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	X	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Y	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Z	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	a	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	b	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	c	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	d	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	e	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	f	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	g	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	h	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	i	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	j	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	k	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	l	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	m	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	n	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	o	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	p	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	q	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	r	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	s	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	t	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	u	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	v	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	w	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	x	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	y	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	z	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	1	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	2	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	3	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	4	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	5	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	6	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	7	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	8	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	9	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AA	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AB	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AC	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AD	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AE	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AF	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AG	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AH	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AI	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AJ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AK	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AL	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AM	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AN	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AO	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AP	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AQ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AR	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	AS	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AT	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AU	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AV	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AW	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AX	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AY	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	AZ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Aa	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ab	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ac	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ad	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ae	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Af	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ag	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ah	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ai	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Aj	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ak	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Al	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Am	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	An	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ao	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ap	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Aq	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ar	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	As	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	At	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Au	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Av	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Aw	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ax	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ay	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Az	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A0	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A1	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A2	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A3	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A4	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A5	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A6	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A7	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	A8	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	A9	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BA	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BB	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BC	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BD	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BE	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BF	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BG	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BH	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BI	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BJ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BK	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BL	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BM	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BN	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BO	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BP	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BQ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BR	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BS	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	BT	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BU	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BV	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BW	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BX	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BY	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	BZ	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Ba	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bb	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bc	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bd	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Be	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bf	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bg	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bh	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bi	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bj	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bk	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bl	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bm	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0
1	Bn	23	Total 326	C 105	H 166	N 25	O 29	S 1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Bo	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bp	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bq	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Br	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bs	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bt	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bu	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		
1	Bv	23	Total	C	H	N	O	S	0	0
			326	105	166	25	29	1		

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	7	ASN	ASP	variant	UNP P05067
A	7	ASN	ASP	variant	UNP P05067
B	7	ASN	ASP	variant	UNP P05067
C	7	ASN	ASP	variant	UNP P05067
D	7	ASN	ASP	variant	UNP P05067
E	7	ASN	ASP	variant	UNP P05067
F	7	ASN	ASP	variant	UNP P05067
G	7	ASN	ASP	variant	UNP P05067
H	7	ASN	ASP	variant	UNP P05067
I	7	ASN	ASP	variant	UNP P05067
J	7	ASN	ASP	variant	UNP P05067
K	7	ASN	ASP	variant	UNP P05067
L	7	ASN	ASP	variant	UNP P05067
M	7	ASN	ASP	variant	UNP P05067
N	7	ASN	ASP	variant	UNP P05067
O	7	ASN	ASP	variant	UNP P05067
P	7	ASN	ASP	variant	UNP P05067
Q	7	ASN	ASP	variant	UNP P05067
R	7	ASN	ASP	variant	UNP P05067
S	7	ASN	ASP	variant	UNP P05067
T	7	ASN	ASP	variant	UNP P05067
U	7	ASN	ASP	variant	UNP P05067
V	7	ASN	ASP	variant	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
W	7	ASN	ASP	variant	UNP P05067
X	7	ASN	ASP	variant	UNP P05067
Y	7	ASN	ASP	variant	UNP P05067
Z	7	ASN	ASP	variant	UNP P05067
a	7	ASN	ASP	variant	UNP P05067
b	7	ASN	ASP	variant	UNP P05067
c	7	ASN	ASP	variant	UNP P05067
d	7	ASN	ASP	variant	UNP P05067
e	7	ASN	ASP	variant	UNP P05067
f	7	ASN	ASP	variant	UNP P05067
g	7	ASN	ASP	variant	UNP P05067
h	7	ASN	ASP	variant	UNP P05067
i	7	ASN	ASP	variant	UNP P05067
j	7	ASN	ASP	variant	UNP P05067
k	7	ASN	ASP	variant	UNP P05067
l	7	ASN	ASP	variant	UNP P05067
m	7	ASN	ASP	variant	UNP P05067
n	7	ASN	ASP	variant	UNP P05067
o	7	ASN	ASP	variant	UNP P05067
p	7	ASN	ASP	variant	UNP P05067
q	7	ASN	ASP	variant	UNP P05067
r	7	ASN	ASP	variant	UNP P05067
s	7	ASN	ASP	variant	UNP P05067
t	7	ASN	ASP	variant	UNP P05067
u	7	ASN	ASP	variant	UNP P05067
v	7	ASN	ASP	variant	UNP P05067
w	7	ASN	ASP	variant	UNP P05067
x	7	ASN	ASP	variant	UNP P05067
y	7	ASN	ASP	variant	UNP P05067
z	7	ASN	ASP	variant	UNP P05067
1	7	ASN	ASP	variant	UNP P05067
2	7	ASN	ASP	variant	UNP P05067
3	7	ASN	ASP	variant	UNP P05067
4	7	ASN	ASP	variant	UNP P05067
5	7	ASN	ASP	variant	UNP P05067
6	7	ASN	ASP	variant	UNP P05067
7	7	ASN	ASP	variant	UNP P05067
8	7	ASN	ASP	variant	UNP P05067
9	7	ASN	ASP	variant	UNP P05067
AA	7	ASN	ASP	variant	UNP P05067
AB	7	ASN	ASP	variant	UNP P05067
AC	7	ASN	ASP	variant	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	7	ASN	ASP	variant	UNP P05067
AE	7	ASN	ASP	variant	UNP P05067
AF	7	ASN	ASP	variant	UNP P05067
AG	7	ASN	ASP	variant	UNP P05067
AH	7	ASN	ASP	variant	UNP P05067
AI	7	ASN	ASP	variant	UNP P05067
AJ	7	ASN	ASP	variant	UNP P05067
AK	7	ASN	ASP	variant	UNP P05067
AL	7	ASN	ASP	variant	UNP P05067
AM	7	ASN	ASP	variant	UNP P05067
AN	7	ASN	ASP	variant	UNP P05067
AO	7	ASN	ASP	variant	UNP P05067
AP	7	ASN	ASP	variant	UNP P05067
AQ	7	ASN	ASP	variant	UNP P05067
AR	7	ASN	ASP	variant	UNP P05067
AS	7	ASN	ASP	variant	UNP P05067
AT	7	ASN	ASP	variant	UNP P05067
AU	7	ASN	ASP	variant	UNP P05067
AV	7	ASN	ASP	variant	UNP P05067
AW	7	ASN	ASP	variant	UNP P05067
AX	7	ASN	ASP	variant	UNP P05067
AY	7	ASN	ASP	variant	UNP P05067
AZ	7	ASN	ASP	variant	UNP P05067
Aa	7	ASN	ASP	variant	UNP P05067
Ab	7	ASN	ASP	variant	UNP P05067
Ac	7	ASN	ASP	variant	UNP P05067
Ad	7	ASN	ASP	variant	UNP P05067
Ae	7	ASN	ASP	variant	UNP P05067
Af	7	ASN	ASP	variant	UNP P05067
Ag	7	ASN	ASP	variant	UNP P05067
Ah	7	ASN	ASP	variant	UNP P05067
Ai	7	ASN	ASP	variant	UNP P05067
Aj	7	ASN	ASP	variant	UNP P05067
Ak	7	ASN	ASP	variant	UNP P05067
Al	7	ASN	ASP	variant	UNP P05067
Am	7	ASN	ASP	variant	UNP P05067
An	7	ASN	ASP	variant	UNP P05067
Ao	7	ASN	ASP	variant	UNP P05067
Ap	7	ASN	ASP	variant	UNP P05067
Aq	7	ASN	ASP	variant	UNP P05067
Ar	7	ASN	ASP	variant	UNP P05067
As	7	ASN	ASP	variant	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
At	7	ASN	ASP	variant	UNP P05067
Au	7	ASN	ASP	variant	UNP P05067
Av	7	ASN	ASP	variant	UNP P05067
Aw	7	ASN	ASP	variant	UNP P05067
Ax	7	ASN	ASP	variant	UNP P05067
Ay	7	ASN	ASP	variant	UNP P05067
Az	7	ASN	ASP	variant	UNP P05067
A0	7	ASN	ASP	variant	UNP P05067
A1	7	ASN	ASP	variant	UNP P05067
A2	7	ASN	ASP	variant	UNP P05067
A3	7	ASN	ASP	variant	UNP P05067
A4	7	ASN	ASP	variant	UNP P05067
A5	7	ASN	ASP	variant	UNP P05067
A6	7	ASN	ASP	variant	UNP P05067
A7	7	ASN	ASP	variant	UNP P05067
A8	7	ASN	ASP	variant	UNP P05067
A9	7	ASN	ASP	variant	UNP P05067
BA	7	ASN	ASP	variant	UNP P05067
BB	7	ASN	ASP	variant	UNP P05067
BC	7	ASN	ASP	variant	UNP P05067
BD	7	ASN	ASP	variant	UNP P05067
BE	7	ASN	ASP	variant	UNP P05067
BF	7	ASN	ASP	variant	UNP P05067
BG	7	ASN	ASP	variant	UNP P05067
BH	7	ASN	ASP	variant	UNP P05067
BI	7	ASN	ASP	variant	UNP P05067
BJ	7	ASN	ASP	variant	UNP P05067
BK	7	ASN	ASP	variant	UNP P05067
BL	7	ASN	ASP	variant	UNP P05067
BM	7	ASN	ASP	variant	UNP P05067
BN	7	ASN	ASP	variant	UNP P05067
BO	7	ASN	ASP	variant	UNP P05067
BP	7	ASN	ASP	variant	UNP P05067
BQ	7	ASN	ASP	variant	UNP P05067
BR	7	ASN	ASP	variant	UNP P05067
BS	7	ASN	ASP	variant	UNP P05067
BT	7	ASN	ASP	variant	UNP P05067
BU	7	ASN	ASP	variant	UNP P05067
BV	7	ASN	ASP	variant	UNP P05067
BW	7	ASN	ASP	variant	UNP P05067
BX	7	ASN	ASP	variant	UNP P05067
BY	7	ASN	ASP	variant	UNP P05067

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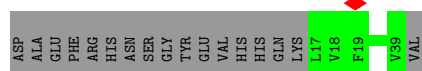
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Chain	Residue	Modelled	Actual	Comment	Reference
BZ	7	ASN	ASP	variant	UNP P05067
Ba	7	ASN	ASP	variant	UNP P05067
Bb	7	ASN	ASP	variant	UNP P05067
Bc	7	ASN	ASP	variant	UNP P05067
Bd	7	ASN	ASP	variant	UNP P05067
Be	7	ASN	ASP	variant	UNP P05067
Bf	7	ASN	ASP	variant	UNP P05067
Bg	7	ASN	ASP	variant	UNP P05067
Bh	7	ASN	ASP	variant	UNP P05067
Bi	7	ASN	ASP	variant	UNP P05067
Bj	7	ASN	ASP	variant	UNP P05067
Bk	7	ASN	ASP	variant	UNP P05067
Bl	7	ASN	ASP	variant	UNP P05067
Bm	7	ASN	ASP	variant	UNP P05067
Bn	7	ASN	ASP	variant	UNP P05067
Bo	7	ASN	ASP	variant	UNP P05067
Bp	7	ASN	ASP	variant	UNP P05067
Bq	7	ASN	ASP	variant	UNP P05067
Br	7	ASN	ASP	variant	UNP P05067
Bs	7	ASN	ASP	variant	UNP P05067
Bt	7	ASN	ASP	variant	UNP P05067
Bu	7	ASN	ASP	variant	UNP P05067
Bv	7	ASN	ASP	variant	UNP P05067

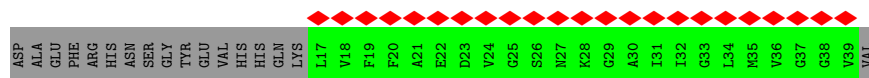
3 Residue-property plots [i](#)

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

- Molecule 1: Amyloid-beta protein 40



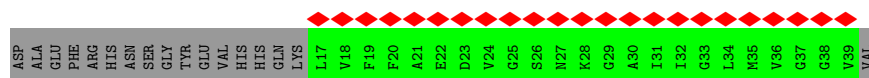
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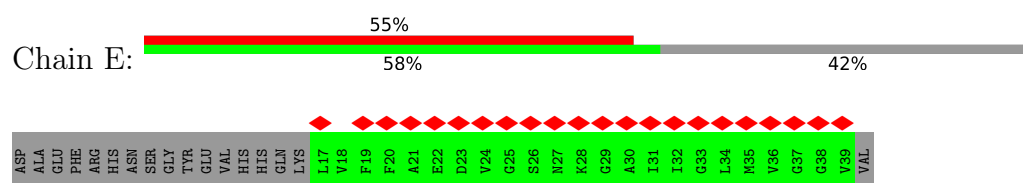
- Molecule 1: Amyloid-beta protein 40



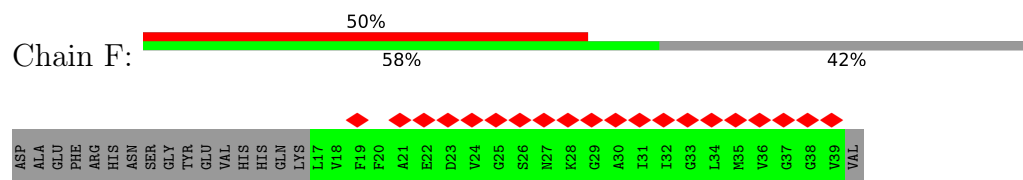
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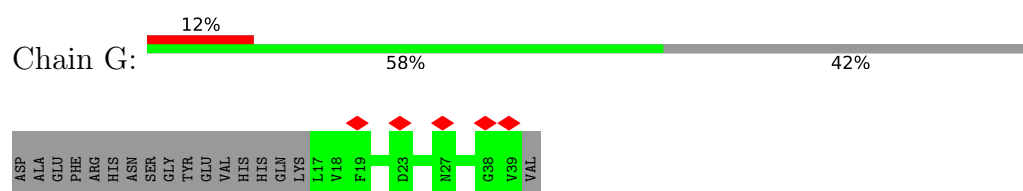
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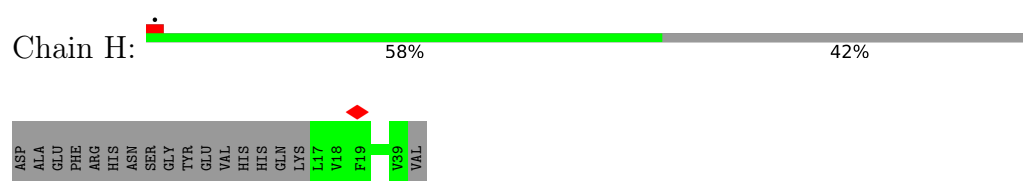
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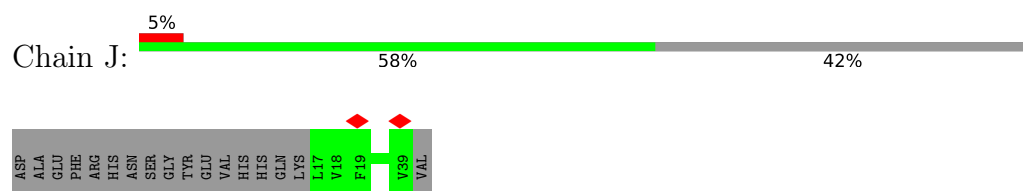
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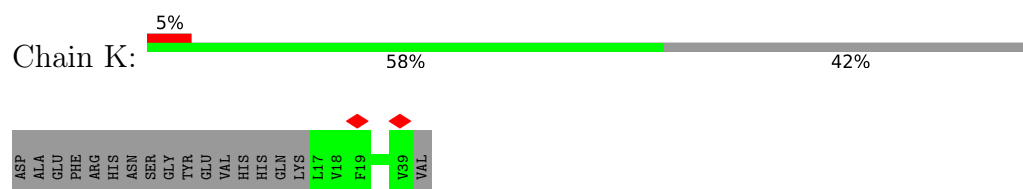
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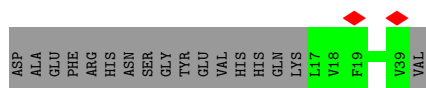
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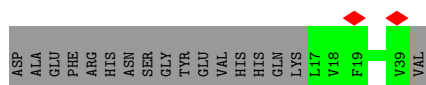
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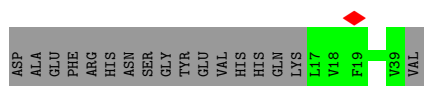
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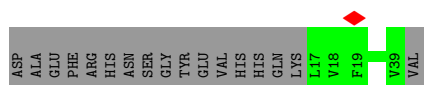
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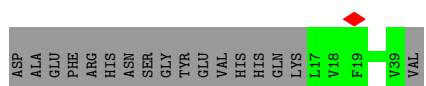
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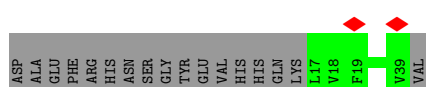
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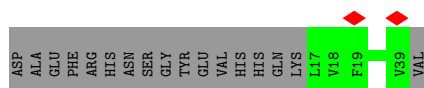


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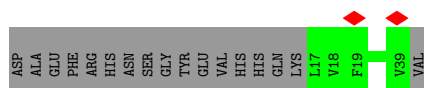


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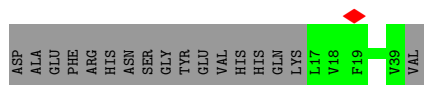




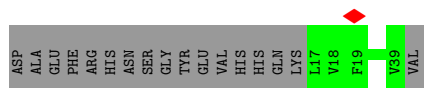
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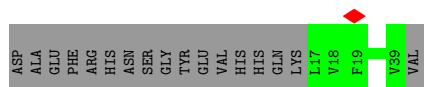
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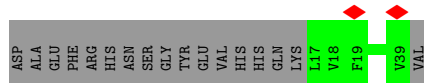
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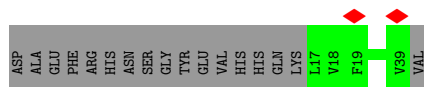
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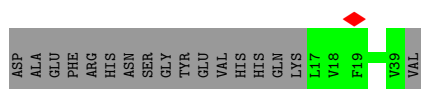
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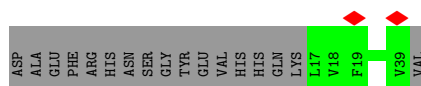
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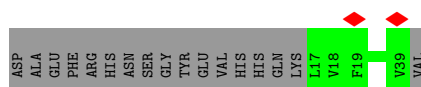
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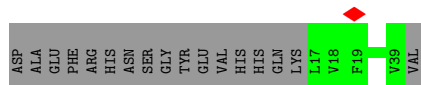
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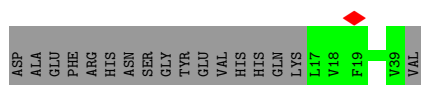
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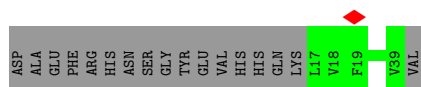
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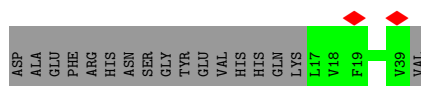
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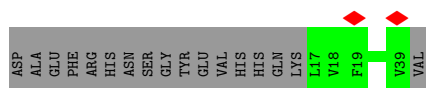
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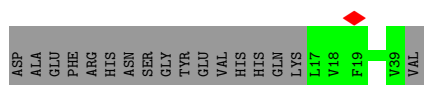
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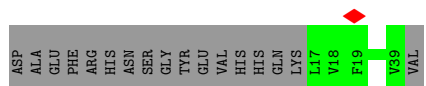
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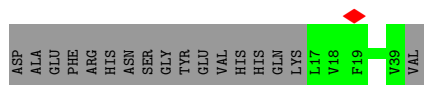
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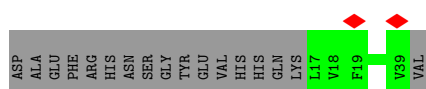
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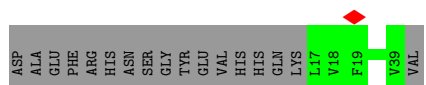
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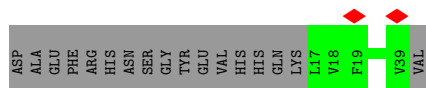


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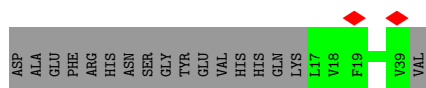


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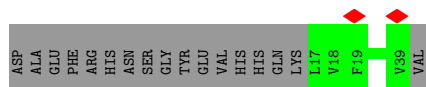




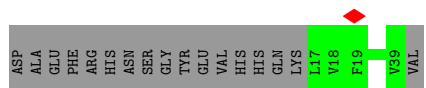
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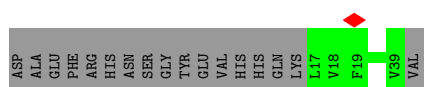
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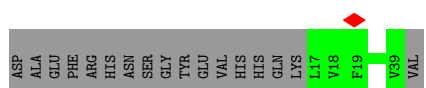
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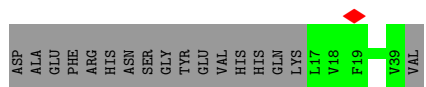
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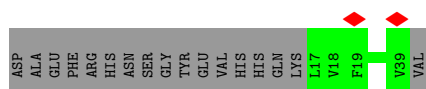
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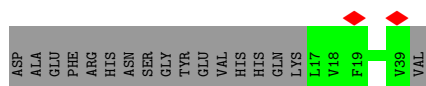
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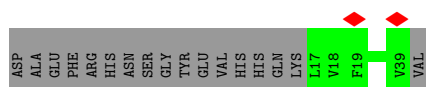
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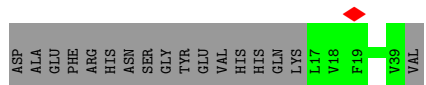
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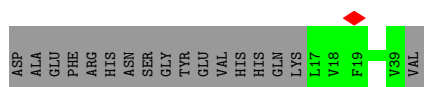
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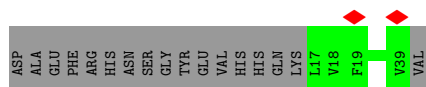
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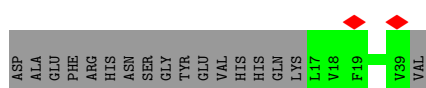
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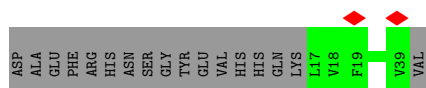
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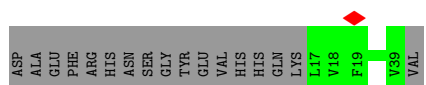
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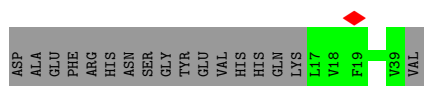
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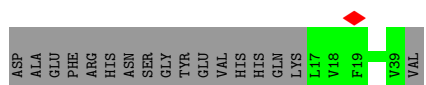
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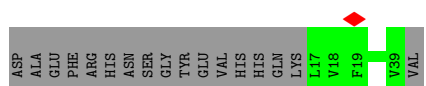
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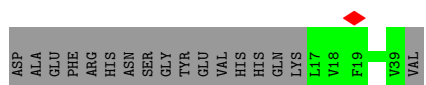
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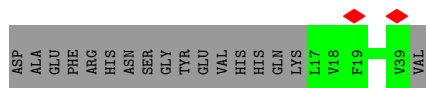


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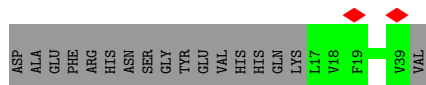


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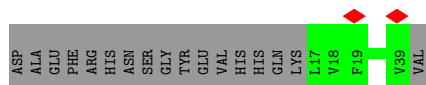




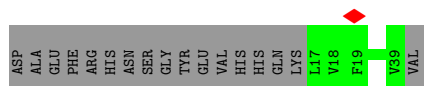
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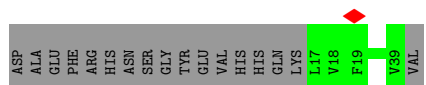
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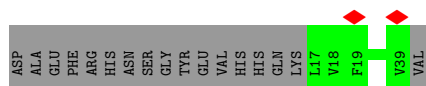
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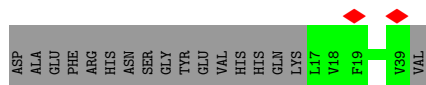
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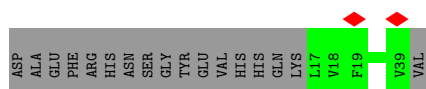
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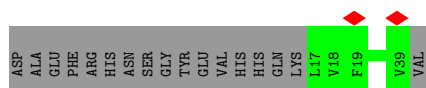
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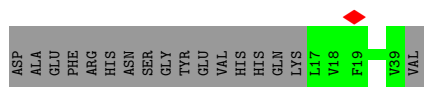
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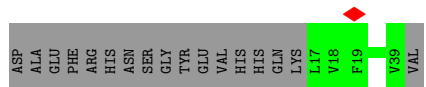
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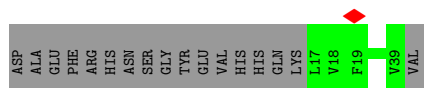
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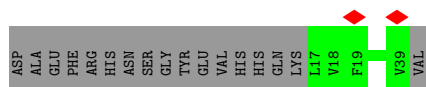
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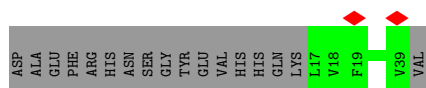
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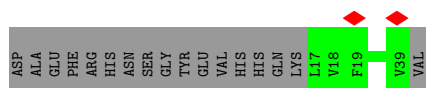
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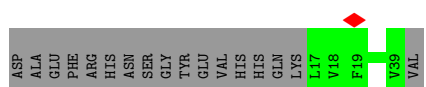
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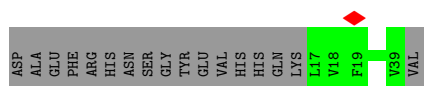
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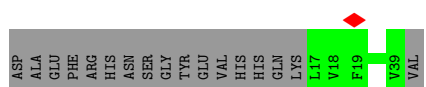
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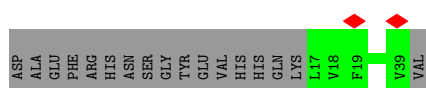
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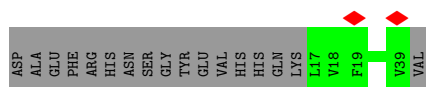
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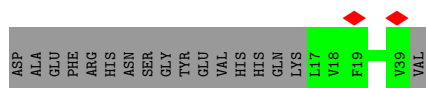


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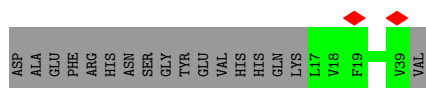


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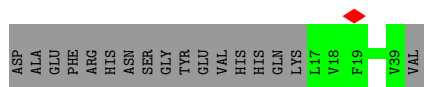




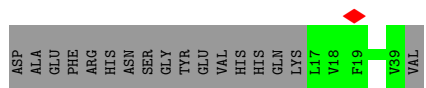
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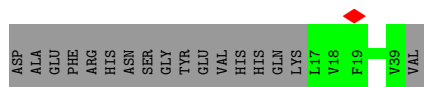
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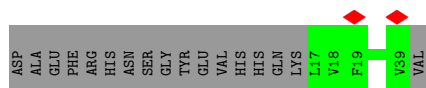
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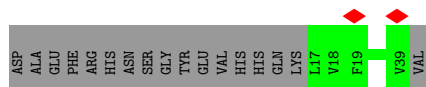
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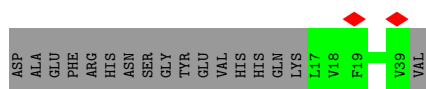
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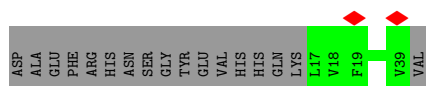
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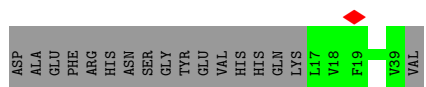
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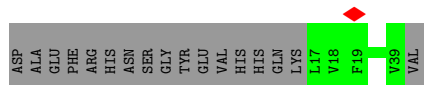
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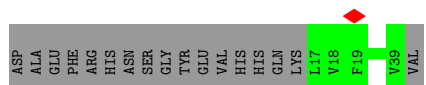
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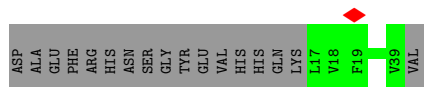
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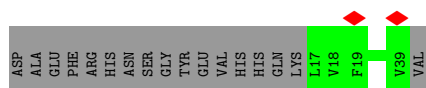
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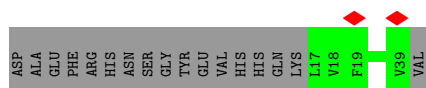
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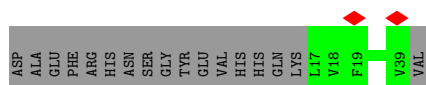
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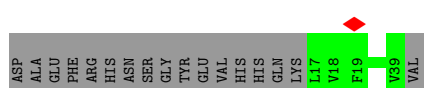
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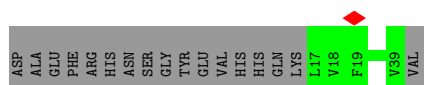
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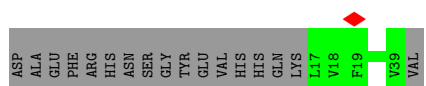
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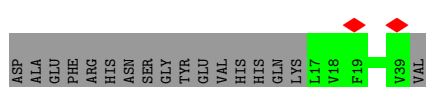
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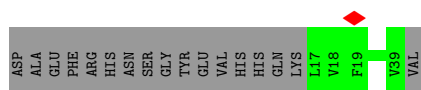


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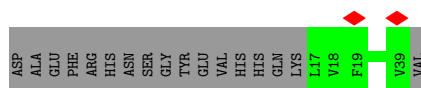


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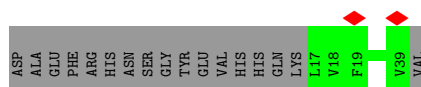




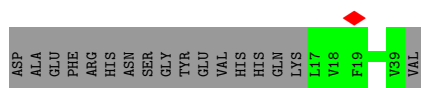
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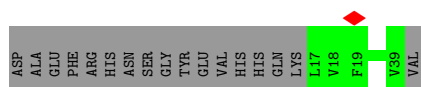
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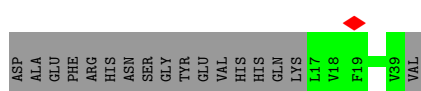
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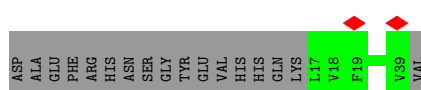
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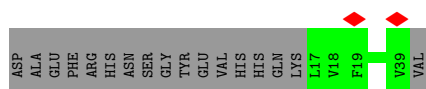
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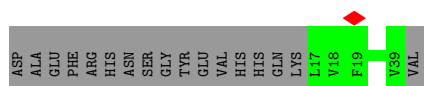
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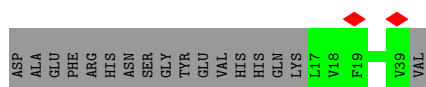
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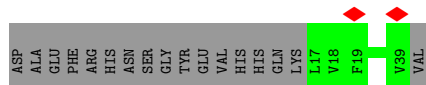
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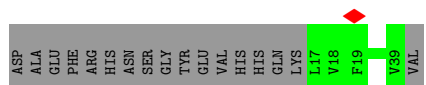
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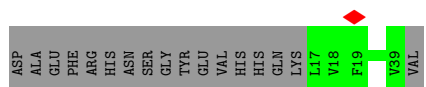
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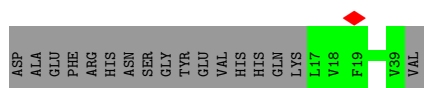
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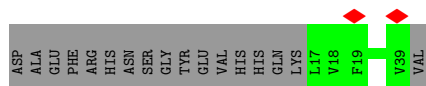
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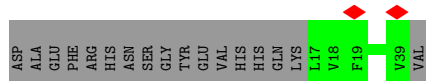
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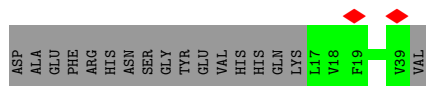
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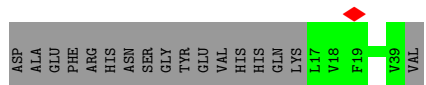
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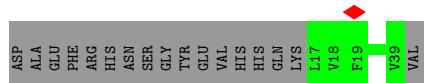
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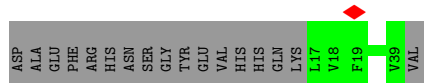
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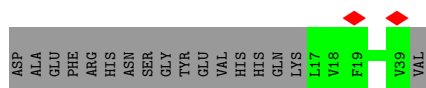


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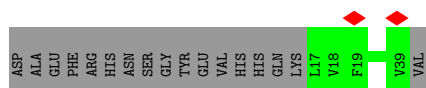


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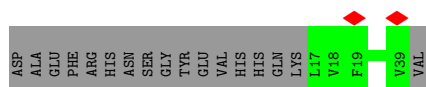




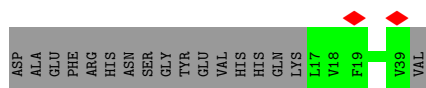
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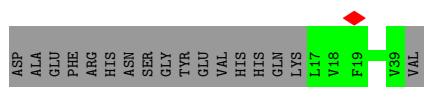
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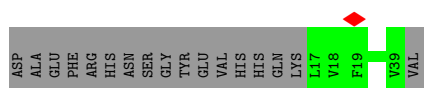
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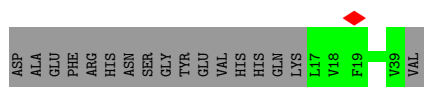
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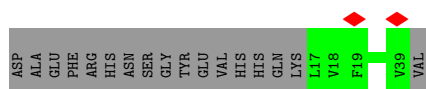
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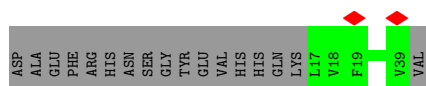
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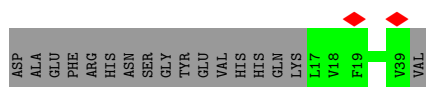
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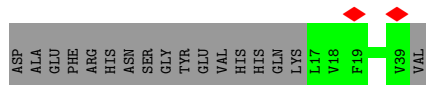
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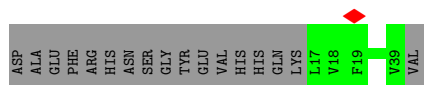
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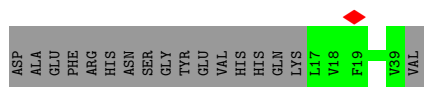
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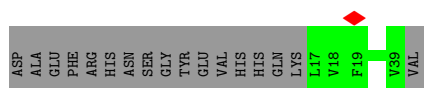
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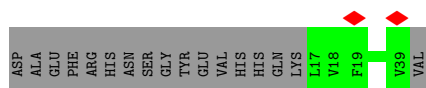
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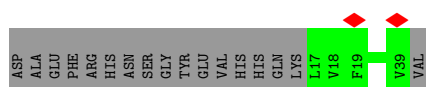
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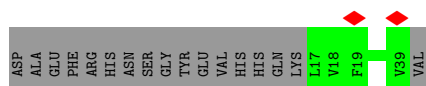
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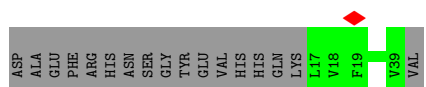
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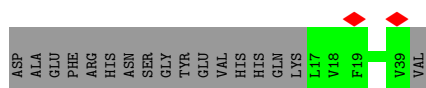
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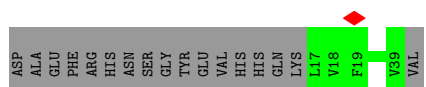
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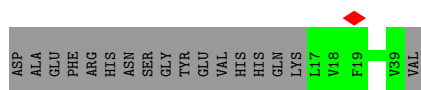


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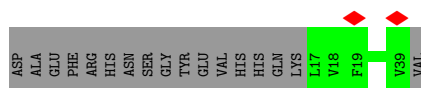


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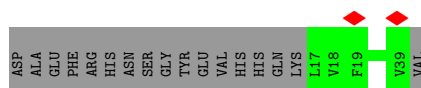




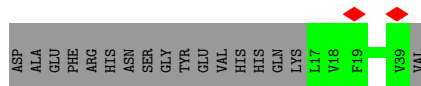
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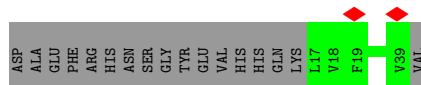
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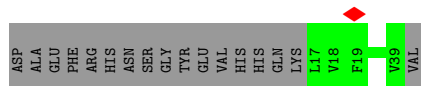
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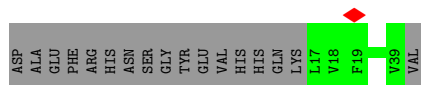
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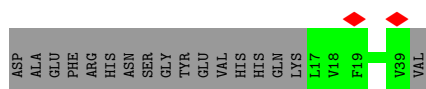
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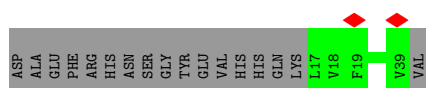
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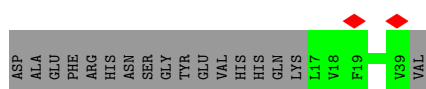
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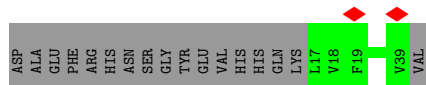
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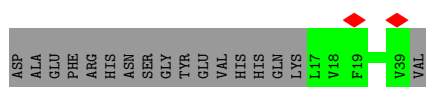
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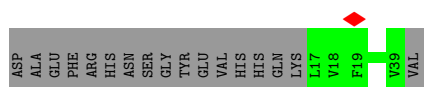
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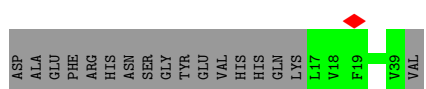
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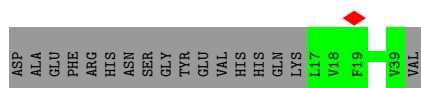
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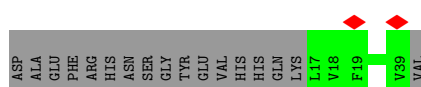
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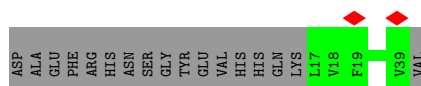
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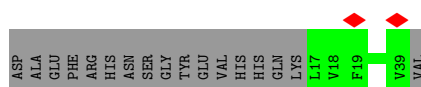
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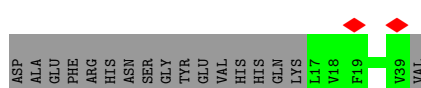
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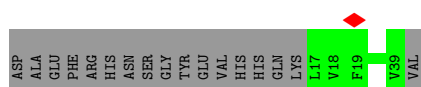
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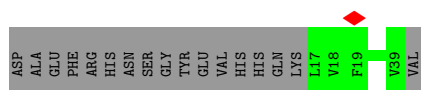


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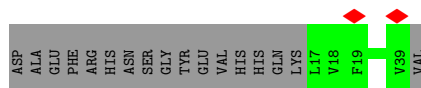


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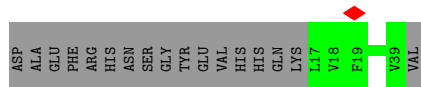




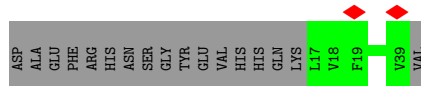
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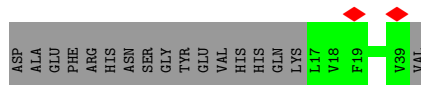
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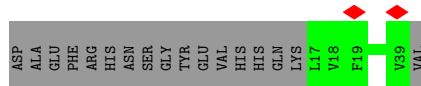
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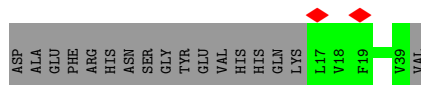
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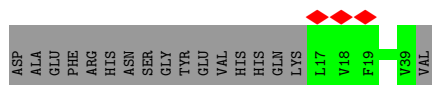
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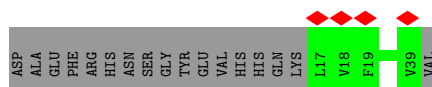
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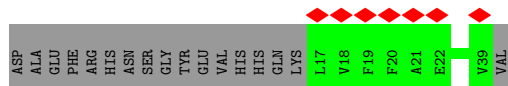
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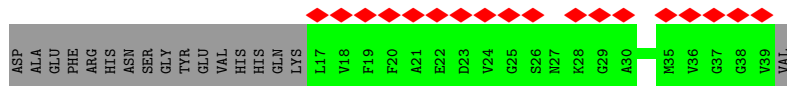
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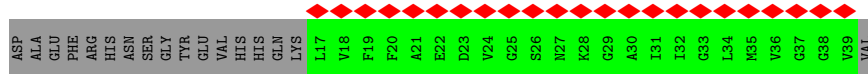
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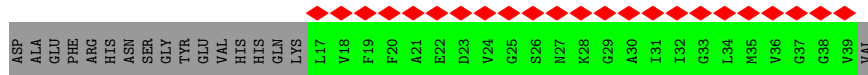
- Molecule 1: Amyloid-beta protein 40



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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=177.573°, rise=2.38205 Å, axial sym=C1	Depositor
Number of segments used	40424	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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	0.52	0/161	0.84	0/215
1	1	0.52	0/161	0.84	0/215
1	2	0.52	0/161	0.84	0/215
1	3	0.52	0/161	0.84	0/215
1	4	0.52	0/161	0.84	0/215
1	5	0.52	0/161	0.84	0/215
1	6	0.52	0/161	0.84	0/215
1	7	0.51	0/161	0.84	0/215
1	8	0.52	0/161	0.84	0/215
1	9	0.52	0/161	0.84	0/215
1	A	0.52	0/161	0.83	0/215
1	A0	0.52	0/161	0.84	0/215
1	A1	0.52	0/161	0.84	0/215
1	A2	0.52	0/161	0.84	0/215
1	A3	0.52	0/161	0.84	0/215
1	A4	0.52	0/161	0.84	0/215
1	A5	0.52	0/161	0.84	0/215
1	A6	0.52	0/161	0.84	0/215
1	A7	0.52	0/161	0.84	0/215
1	A8	0.52	0/161	0.84	0/215
1	A9	0.52	0/161	0.84	0/215
1	AA	0.52	0/161	0.84	0/215
1	AB	0.52	0/161	0.84	0/215
1	AC	0.52	0/161	0.84	0/215
1	AD	0.52	0/161	0.84	0/215
1	AE	0.52	0/161	0.84	0/215
1	AF	0.52	0/161	0.84	0/215
1	AG	0.52	0/161	0.84	0/215
1	AH	0.52	0/161	0.84	0/215
1	AI	0.52	0/161	0.84	0/215
1	AJ	0.52	0/161	0.84	0/215
1	AK	0.52	0/161	0.84	0/215
1	AL	0.52	0/161	0.84	0/215
1	AM	0.52	0/161	0.84	0/215

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AN	0.52	0/161	0.84	0/215
1	AO	0.52	0/161	0.83	0/215
1	AP	0.52	0/161	0.84	0/215
1	AQ	0.52	0/161	0.84	0/215
1	AR	0.52	0/161	0.84	0/215
1	AS	0.52	0/161	0.84	0/215
1	AT	0.52	0/161	0.84	0/215
1	AU	0.52	0/161	0.84	0/215
1	AV	0.52	0/161	0.84	0/215
1	AW	0.52	0/161	0.84	0/215
1	AX	0.52	0/161	0.84	0/215
1	AY	0.52	0/161	0.84	0/215
1	AZ	0.52	0/161	0.84	0/215
1	Aa	0.52	0/161	0.84	0/215
1	Ab	0.52	0/161	0.84	0/215
1	Ac	0.52	0/161	0.84	0/215
1	Ad	0.52	0/161	0.84	0/215
1	Ae	0.52	0/161	0.84	0/215
1	Af	0.52	0/161	0.84	0/215
1	Ag	0.52	0/161	0.84	0/215
1	Ah	0.52	0/161	0.84	0/215
1	Ai	0.52	0/161	0.84	0/215
1	Aj	0.52	0/161	0.84	0/215
1	Ak	0.52	0/161	0.84	0/215
1	Al	0.52	0/161	0.84	0/215
1	Am	0.52	0/161	0.84	0/215
1	An	0.52	0/161	0.84	0/215
1	Ao	0.52	0/161	0.84	0/215
1	Ap	0.52	0/161	0.84	0/215
1	Aq	0.52	0/161	0.83	0/215
1	Ar	0.52	0/161	0.84	0/215
1	As	0.52	0/161	0.84	0/215
1	At	0.52	0/161	0.83	0/215
1	Au	0.52	0/161	0.84	0/215
1	Av	0.52	0/161	0.84	0/215
1	Aw	0.52	0/161	0.83	0/215
1	Ax	0.52	0/161	0.84	0/215
1	Ay	0.52	0/161	0.84	0/215
1	Az	0.52	0/161	0.83	0/215
1	B	0.51	0/161	0.83	0/215
1	BA	0.52	0/161	0.83	0/215
1	BB	0.52	0/161	0.84	0/215
1	BC	0.52	0/161	0.84	0/215

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BD	0.52	0/161	0.84	0/215
1	BE	0.52	0/161	0.84	0/215
1	BF	0.52	0/161	0.84	0/215
1	BG	0.52	0/161	0.84	0/215
1	BH	0.52	0/161	0.84	0/215
1	BI	0.52	0/161	0.84	0/215
1	BJ	0.52	0/161	0.84	0/215
1	BK	0.52	0/161	0.84	0/215
1	BL	0.52	0/161	0.84	0/215
1	BM	0.52	0/161	0.84	0/215
1	BN	0.52	0/161	0.84	0/215
1	BO	0.52	0/161	0.84	0/215
1	BP	0.52	0/161	0.84	0/215
1	BQ	0.52	0/161	0.84	0/215
1	BR	0.52	0/161	0.84	0/215
1	BS	0.52	0/161	0.84	0/215
1	BT	0.52	0/161	0.84	0/215
1	BU	0.52	0/161	0.84	0/215
1	BV	0.52	0/161	0.84	0/215
1	BW	0.52	0/161	0.84	0/215
1	BX	0.52	0/161	0.84	0/215
1	BY	0.51	0/161	0.84	0/215
1	BZ	0.52	0/161	0.84	0/215
1	Ba	0.52	0/161	0.84	0/215
1	Bb	0.52	0/161	0.84	0/215
1	Bc	0.52	0/161	0.84	0/215
1	Bd	0.52	0/161	0.84	0/215
1	Be	0.52	0/161	0.84	0/215
1	Bf	0.52	0/161	0.84	0/215
1	Bg	0.52	0/161	0.84	0/215
1	Bh	0.52	0/161	0.84	0/215
1	Bi	0.52	0/161	0.84	0/215
1	Bj	0.52	0/161	0.84	0/215
1	Bk	0.52	0/161	0.84	0/215
1	Bl	0.52	0/161	0.84	0/215
1	Bm	0.52	0/161	0.84	0/215
1	Bn	0.52	0/161	0.84	0/215
1	Bo	0.52	0/161	0.84	0/215
1	Bp	0.52	0/161	0.84	0/215
1	Bq	0.52	0/161	0.84	0/215
1	Br	0.52	0/161	0.84	0/215
1	Bs	0.52	0/161	0.84	0/215
1	Bt	0.52	0/161	0.84	0/215

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Bu	0.52	0/161	0.84	0/215
1	Bv	0.52	0/161	0.84	0/215
1	C	0.52	0/161	0.84	0/215
1	D	0.52	0/161	0.84	0/215
1	E	0.52	0/161	0.84	0/215
1	F	0.52	0/161	0.84	0/215
1	G	0.52	0/161	0.84	0/215
1	H	0.52	0/161	0.84	0/215
1	I	0.52	0/161	0.84	0/215
1	J	0.52	0/161	0.84	0/215
1	K	0.52	0/161	0.84	0/215
1	L	0.52	0/161	0.84	0/215
1	M	0.52	0/161	0.84	0/215
1	N	0.52	0/161	0.84	0/215
1	O	0.52	0/161	0.84	0/215
1	P	0.52	0/161	0.84	0/215
1	Q	0.52	0/161	0.84	0/215
1	R	0.52	0/161	0.84	0/215
1	S	0.52	0/161	0.84	0/215
1	T	0.52	0/161	0.84	0/215
1	U	0.52	0/161	0.84	0/215
1	V	0.52	0/161	0.84	0/215
1	W	0.52	0/161	0.84	0/215
1	X	0.52	0/161	0.84	0/215
1	Y	0.52	0/161	0.84	0/215
1	Z	0.52	0/161	0.84	0/215
1	a	0.52	0/161	0.84	0/215
1	b	0.52	0/161	0.84	0/215
1	c	0.52	0/161	0.84	0/215
1	d	0.52	0/161	0.84	0/215
1	e	0.52	0/161	0.84	0/215
1	f	0.52	0/161	0.84	0/215
1	g	0.52	0/161	0.84	0/215
1	h	0.52	0/161	0.84	0/215
1	i	0.52	0/161	0.84	0/215
1	j	0.52	0/161	0.83	0/215
1	k	0.52	0/161	0.84	0/215
1	l	0.52	0/161	0.84	0/215
1	m	0.52	0/161	0.84	0/215
1	n	0.52	0/161	0.84	0/215
1	o	0.52	0/161	0.84	0/215
1	p	0.52	0/161	0.84	0/215
1	q	0.52	0/161	0.84	0/215

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	r	0.52	0/161	0.84	0/215
1	s	0.52	0/161	0.84	0/215
1	t	0.52	0/161	0.84	0/215
1	u	0.52	0/161	0.84	0/215
1	v	0.52	0/161	0.83	0/215
1	w	0.52	0/161	0.84	0/215
1	x	0.52	0/161	0.84	0/215
1	y	0.52	0/161	0.84	0/215
1	z	0.52	0/161	0.84	0/215
All	All	0.52	0/27692	0.84	0/36980

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	160	166	165	0	0
1	1	160	166	165	0	0
1	2	160	166	165	0	0
1	3	160	166	165	0	0
1	4	160	166	165	0	0
1	5	160	166	165	0	0
1	6	160	166	165	0	0
1	7	160	166	165	0	0
1	8	160	166	165	0	0
1	9	160	166	165	0	0
1	A	160	166	165	0	0
1	A0	160	166	165	0	0
1	A1	160	166	165	0	0
1	A2	160	166	165	0	0
1	A3	160	166	165	0	0
1	A4	160	166	165	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A5	160	166	165	0	0
1	A6	160	166	165	0	0
1	A7	160	166	165	0	0
1	A8	160	166	165	0	0
1	A9	160	166	165	0	0
1	AA	160	166	165	0	0
1	AB	160	166	165	0	0
1	AC	160	166	165	0	0
1	AD	160	166	165	0	0
1	AE	160	166	165	0	0
1	AF	160	166	165	0	0
1	AG	160	166	165	0	0
1	AH	160	166	165	0	0
1	AI	160	166	165	0	0
1	AJ	160	166	165	0	0
1	AK	160	166	165	0	0
1	AL	160	166	165	0	0
1	AM	160	166	165	0	0
1	AN	160	166	165	0	0
1	AO	160	166	165	0	0
1	AP	160	166	165	0	0
1	AQ	160	166	165	0	0
1	AR	160	166	165	0	0
1	AS	160	166	165	0	0
1	AT	160	166	165	0	0
1	AU	160	166	165	0	0
1	AV	160	166	165	0	0
1	AW	160	166	165	0	0
1	AX	160	166	165	0	0
1	AY	160	166	165	0	0
1	AZ	160	166	165	0	0
1	Aa	160	166	165	0	0
1	Ab	160	166	165	0	0
1	Ac	160	166	165	0	0
1	Ad	160	166	165	0	0
1	Ae	160	166	165	0	0
1	Af	160	166	165	0	0
1	Ag	160	166	165	0	0
1	Ah	160	166	165	0	0
1	Ai	160	166	165	0	0
1	Aj	160	166	165	0	0
1	Ak	160	166	165	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Al	160	166	165	0	0
1	Am	160	166	165	0	0
1	An	160	166	165	0	0
1	Ao	160	166	165	0	0
1	Ap	160	166	165	0	0
1	Aq	160	166	165	0	0
1	Ar	160	166	165	0	0
1	As	160	166	165	0	0
1	At	160	166	165	0	0
1	Au	160	166	165	0	0
1	Av	160	166	165	0	0
1	Aw	160	166	165	0	0
1	Ax	160	166	165	0	0
1	Ay	160	166	165	0	0
1	Az	160	166	165	0	0
1	B	160	166	165	0	0
1	BA	160	166	165	0	0
1	BB	160	166	165	0	0
1	BC	160	166	165	0	0
1	BD	160	166	165	0	0
1	BE	160	166	165	0	0
1	BF	160	166	165	0	0
1	BG	160	166	165	0	0
1	BH	160	166	165	0	0
1	BI	160	166	165	0	0
1	BJ	160	166	165	0	0
1	BK	160	166	165	0	0
1	BL	160	166	165	0	0
1	BM	160	166	165	0	0
1	BN	160	166	165	0	0
1	BO	160	166	165	0	0
1	BP	160	166	165	0	0
1	BQ	160	166	165	0	0
1	BR	160	166	165	0	0
1	BS	160	166	165	0	0
1	BT	160	166	165	0	0
1	BU	160	166	165	0	0
1	BV	160	166	165	0	0
1	BW	160	166	165	0	0
1	BX	160	166	165	0	0
1	BY	160	166	165	0	0
1	BZ	160	166	165	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ba	160	166	165	0	0
1	Bb	160	166	165	0	0
1	Bc	160	166	165	0	0
1	Bd	160	166	165	0	0
1	Be	160	166	165	0	0
1	Bf	160	166	165	0	0
1	Bg	160	166	165	0	0
1	Bh	160	166	165	0	0
1	Bi	160	166	165	0	0
1	Bj	160	166	165	0	0
1	Bk	160	166	165	0	0
1	Bl	160	166	165	0	0
1	Bm	160	166	165	0	0
1	Bn	160	166	165	0	0
1	Bo	160	166	165	0	0
1	Bp	160	166	165	0	0
1	Bq	160	166	165	0	0
1	Br	160	166	165	0	0
1	Bs	160	166	165	0	0
1	Bt	160	166	165	0	0
1	Bu	160	166	165	0	0
1	Bv	160	166	165	0	0
1	C	160	166	165	0	0
1	D	160	166	165	0	0
1	E	160	166	165	0	0
1	F	160	166	165	0	0
1	G	160	166	165	0	0
1	H	160	166	165	0	0
1	I	160	166	165	0	0
1	J	160	166	165	0	0
1	K	160	166	165	0	0
1	L	160	166	165	0	0
1	M	160	166	165	0	0
1	N	160	166	165	0	0
1	O	160	166	165	0	0
1	P	160	166	165	0	0
1	Q	160	166	165	0	0
1	R	160	166	165	0	0
1	S	160	166	165	0	0
1	T	160	166	165	0	0
1	U	160	166	165	0	0
1	V	160	166	165	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	160	166	165	0	0
1	X	160	166	165	0	0
1	Y	160	166	165	0	0
1	Z	160	166	165	0	0
1	a	160	166	165	0	0
1	b	160	166	165	0	0
1	c	160	166	165	0	0
1	d	160	166	165	0	0
1	e	160	166	165	0	0
1	f	160	166	165	0	0
1	g	160	166	165	0	0
1	h	160	166	165	0	0
1	i	160	166	165	0	0
1	j	160	166	165	0	0
1	k	160	166	165	0	0
1	l	160	166	165	0	0
1	m	160	166	165	0	0
1	n	160	166	165	0	0
1	o	160	166	165	0	0
1	p	160	166	165	0	0
1	q	160	166	165	0	0
1	r	160	166	165	0	0
1	s	160	166	165	0	0
1	t	160	166	165	0	0
1	u	160	166	165	0	0
1	v	160	166	165	0	0
1	w	160	166	165	0	0
1	x	160	166	165	0	0
1	y	160	166	165	0	0
1	z	160	166	165	0	0
All	All	27520	28552	28380	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	1	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	2	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	3	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	4	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	5	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	6	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	7	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	8	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	9	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A0	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A1	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A2	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A3	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A4	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A5	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A6	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A7	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A8	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	A9	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AA	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AB	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AC	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AD	21/40 (52%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AE	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AF	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AG	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AH	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AI	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AJ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AK	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AL	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AM	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AN	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AO	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AP	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AQ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AR	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AS	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AT	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AU	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AV	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AW	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AX	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AY	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	AZ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Aa	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ab	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ac	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ad	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ae	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Af	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ag	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ah	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ai	21/40 (52%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aj	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ak	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Al	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Am	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	An	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ao	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ap	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Aq	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ar	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	As	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	At	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Au	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Av	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Aw	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ax	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ay	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Az	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	B	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BA	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BB	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BC	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BD	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BE	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BF	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BG	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BH	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BI	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BJ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BK	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BL	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BM	21/40 (52%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BN	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BO	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BP	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BQ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BR	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BS	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BT	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BU	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BV	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BW	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BX	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BY	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	BZ	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Ba	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bb	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bc	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bd	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Be	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bf	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bg	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bh	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bi	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bj	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bk	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bl	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bm	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bn	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bo	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bp	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bq	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Br	21/40 (52%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bs	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bt	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bu	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Bv	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	C	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	D	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	E	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	F	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	G	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	H	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	I	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	J	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	K	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	L	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	M	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	N	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	O	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	P	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Q	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	R	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	S	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	T	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	U	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	V	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	W	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	X	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Y	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	Z	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	a	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	b	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	c	21/40 (52%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	e	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	f	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	g	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	h	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	i	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	j	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	k	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	l	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	m	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	n	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	o	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	p	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	q	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	r	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	s	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	t	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	u	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	v	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	w	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	x	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	y	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
1	z	21/40 (52%)	18 (86%)	3 (14%)	0	100	100
All	All	3612/6880 (52%)	3096 (86%)	516 (14%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	16/31 (52%)	16 (100%)	0	100	100
1	1	16/31 (52%)	16 (100%)	0	100	100
1	2	16/31 (52%)	16 (100%)	0	100	100
1	3	16/31 (52%)	16 (100%)	0	100	100
1	4	16/31 (52%)	16 (100%)	0	100	100
1	5	16/31 (52%)	16 (100%)	0	100	100
1	6	16/31 (52%)	16 (100%)	0	100	100
1	7	16/31 (52%)	16 (100%)	0	100	100
1	8	16/31 (52%)	16 (100%)	0	100	100
1	9	16/31 (52%)	16 (100%)	0	100	100
1	A	16/31 (52%)	16 (100%)	0	100	100
1	A0	16/31 (52%)	16 (100%)	0	100	100
1	A1	16/31 (52%)	16 (100%)	0	100	100
1	A2	16/31 (52%)	16 (100%)	0	100	100
1	A3	16/31 (52%)	16 (100%)	0	100	100
1	A4	16/31 (52%)	16 (100%)	0	100	100
1	A5	16/31 (52%)	16 (100%)	0	100	100
1	A6	16/31 (52%)	16 (100%)	0	100	100
1	A7	16/31 (52%)	16 (100%)	0	100	100
1	A8	16/31 (52%)	16 (100%)	0	100	100
1	A9	16/31 (52%)	16 (100%)	0	100	100
1	AA	16/31 (52%)	16 (100%)	0	100	100
1	AB	16/31 (52%)	16 (100%)	0	100	100
1	AC	16/31 (52%)	16 (100%)	0	100	100
1	AD	16/31 (52%)	16 (100%)	0	100	100
1	AE	16/31 (52%)	16 (100%)	0	100	100
1	AF	16/31 (52%)	16 (100%)	0	100	100
1	AG	16/31 (52%)	16 (100%)	0	100	100
1	AH	16/31 (52%)	16 (100%)	0	100	100
1	AI	16/31 (52%)	16 (100%)	0	100	100
1	AJ	16/31 (52%)	16 (100%)	0	100	100
1	AK	16/31 (52%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AL	16/31 (52%)	16 (100%)	0	100	100
1	AM	16/31 (52%)	16 (100%)	0	100	100
1	AN	16/31 (52%)	16 (100%)	0	100	100
1	AO	16/31 (52%)	16 (100%)	0	100	100
1	AP	16/31 (52%)	16 (100%)	0	100	100
1	AQ	16/31 (52%)	16 (100%)	0	100	100
1	AR	16/31 (52%)	16 (100%)	0	100	100
1	AS	16/31 (52%)	16 (100%)	0	100	100
1	AT	16/31 (52%)	16 (100%)	0	100	100
1	AU	16/31 (52%)	16 (100%)	0	100	100
1	AV	16/31 (52%)	16 (100%)	0	100	100
1	AW	16/31 (52%)	16 (100%)	0	100	100
1	AX	16/31 (52%)	16 (100%)	0	100	100
1	AY	16/31 (52%)	16 (100%)	0	100	100
1	AZ	16/31 (52%)	16 (100%)	0	100	100
1	Aa	16/31 (52%)	16 (100%)	0	100	100
1	Ab	16/31 (52%)	16 (100%)	0	100	100
1	Ac	16/31 (52%)	16 (100%)	0	100	100
1	Ad	16/31 (52%)	16 (100%)	0	100	100
1	Ae	16/31 (52%)	16 (100%)	0	100	100
1	Af	16/31 (52%)	16 (100%)	0	100	100
1	Ag	16/31 (52%)	16 (100%)	0	100	100
1	Ah	16/31 (52%)	16 (100%)	0	100	100
1	Ai	16/31 (52%)	16 (100%)	0	100	100
1	Aj	16/31 (52%)	16 (100%)	0	100	100
1	Ak	16/31 (52%)	16 (100%)	0	100	100
1	Al	16/31 (52%)	16 (100%)	0	100	100
1	Am	16/31 (52%)	16 (100%)	0	100	100
1	An	16/31 (52%)	16 (100%)	0	100	100
1	Ao	16/31 (52%)	16 (100%)	0	100	100
1	Ap	16/31 (52%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aq	16/31 (52%)	16 (100%)	0	100	100
1	Ar	16/31 (52%)	16 (100%)	0	100	100
1	As	16/31 (52%)	16 (100%)	0	100	100
1	At	16/31 (52%)	16 (100%)	0	100	100
1	Au	16/31 (52%)	16 (100%)	0	100	100
1	Av	16/31 (52%)	16 (100%)	0	100	100
1	Aw	16/31 (52%)	16 (100%)	0	100	100
1	Ax	16/31 (52%)	16 (100%)	0	100	100
1	Ay	16/31 (52%)	16 (100%)	0	100	100
1	Az	16/31 (52%)	16 (100%)	0	100	100
1	B	16/31 (52%)	16 (100%)	0	100	100
1	BA	16/31 (52%)	16 (100%)	0	100	100
1	BB	16/31 (52%)	16 (100%)	0	100	100
1	BC	16/31 (52%)	16 (100%)	0	100	100
1	BD	16/31 (52%)	16 (100%)	0	100	100
1	BE	16/31 (52%)	16 (100%)	0	100	100
1	BF	16/31 (52%)	16 (100%)	0	100	100
1	BG	16/31 (52%)	16 (100%)	0	100	100
1	BH	16/31 (52%)	16 (100%)	0	100	100
1	BI	16/31 (52%)	16 (100%)	0	100	100
1	BJ	16/31 (52%)	16 (100%)	0	100	100
1	BK	16/31 (52%)	16 (100%)	0	100	100
1	BL	16/31 (52%)	16 (100%)	0	100	100
1	BM	16/31 (52%)	16 (100%)	0	100	100
1	BN	16/31 (52%)	16 (100%)	0	100	100
1	BO	16/31 (52%)	16 (100%)	0	100	100
1	BP	16/31 (52%)	16 (100%)	0	100	100
1	BQ	16/31 (52%)	16 (100%)	0	100	100
1	BR	16/31 (52%)	16 (100%)	0	100	100
1	BS	16/31 (52%)	16 (100%)	0	100	100
1	BT	16/31 (52%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BU	16/31 (52%)	16 (100%)	0	100	100
1	BV	16/31 (52%)	16 (100%)	0	100	100
1	BW	16/31 (52%)	16 (100%)	0	100	100
1	BX	16/31 (52%)	16 (100%)	0	100	100
1	BY	16/31 (52%)	16 (100%)	0	100	100
1	BZ	16/31 (52%)	16 (100%)	0	100	100
1	Ba	16/31 (52%)	16 (100%)	0	100	100
1	Bb	16/31 (52%)	16 (100%)	0	100	100
1	Bc	16/31 (52%)	16 (100%)	0	100	100
1	Bd	16/31 (52%)	16 (100%)	0	100	100
1	Be	16/31 (52%)	16 (100%)	0	100	100
1	Bf	16/31 (52%)	16 (100%)	0	100	100
1	Bg	16/31 (52%)	16 (100%)	0	100	100
1	Bh	16/31 (52%)	16 (100%)	0	100	100
1	Bi	16/31 (52%)	16 (100%)	0	100	100
1	Bj	16/31 (52%)	16 (100%)	0	100	100
1	Bk	16/31 (52%)	16 (100%)	0	100	100
1	Bl	16/31 (52%)	16 (100%)	0	100	100
1	Bm	16/31 (52%)	16 (100%)	0	100	100
1	Bn	16/31 (52%)	16 (100%)	0	100	100
1	Bo	16/31 (52%)	16 (100%)	0	100	100
1	Bp	16/31 (52%)	16 (100%)	0	100	100
1	Bq	16/31 (52%)	16 (100%)	0	100	100
1	Br	16/31 (52%)	16 (100%)	0	100	100
1	Bs	16/31 (52%)	16 (100%)	0	100	100
1	Bt	16/31 (52%)	16 (100%)	0	100	100
1	Bu	16/31 (52%)	16 (100%)	0	100	100
1	Bv	16/31 (52%)	16 (100%)	0	100	100
1	C	16/31 (52%)	16 (100%)	0	100	100
1	D	16/31 (52%)	16 (100%)	0	100	100
1	E	16/31 (52%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	16/31 (52%)	16 (100%)	0	100	100
1	G	16/31 (52%)	16 (100%)	0	100	100
1	H	16/31 (52%)	16 (100%)	0	100	100
1	I	16/31 (52%)	16 (100%)	0	100	100
1	J	16/31 (52%)	16 (100%)	0	100	100
1	K	16/31 (52%)	16 (100%)	0	100	100
1	L	16/31 (52%)	16 (100%)	0	100	100
1	M	16/31 (52%)	16 (100%)	0	100	100
1	N	16/31 (52%)	16 (100%)	0	100	100
1	O	16/31 (52%)	16 (100%)	0	100	100
1	P	16/31 (52%)	16 (100%)	0	100	100
1	Q	16/31 (52%)	16 (100%)	0	100	100
1	R	16/31 (52%)	16 (100%)	0	100	100
1	S	16/31 (52%)	16 (100%)	0	100	100
1	T	16/31 (52%)	16 (100%)	0	100	100
1	U	16/31 (52%)	16 (100%)	0	100	100
1	V	16/31 (52%)	16 (100%)	0	100	100
1	W	16/31 (52%)	16 (100%)	0	100	100
1	X	16/31 (52%)	16 (100%)	0	100	100
1	Y	16/31 (52%)	16 (100%)	0	100	100
1	Z	16/31 (52%)	16 (100%)	0	100	100
1	a	16/31 (52%)	16 (100%)	0	100	100
1	b	16/31 (52%)	16 (100%)	0	100	100
1	c	16/31 (52%)	16 (100%)	0	100	100
1	d	16/31 (52%)	16 (100%)	0	100	100
1	e	16/31 (52%)	16 (100%)	0	100	100
1	f	16/31 (52%)	16 (100%)	0	100	100
1	g	16/31 (52%)	16 (100%)	0	100	100
1	h	16/31 (52%)	16 (100%)	0	100	100
1	i	16/31 (52%)	16 (100%)	0	100	100
1	j	16/31 (52%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	16/31 (52%)	16 (100%)	0	100	100
1	l	16/31 (52%)	16 (100%)	0	100	100
1	m	16/31 (52%)	16 (100%)	0	100	100
1	n	16/31 (52%)	16 (100%)	0	100	100
1	o	16/31 (52%)	16 (100%)	0	100	100
1	p	16/31 (52%)	16 (100%)	0	100	100
1	q	16/31 (52%)	16 (100%)	0	100	100
1	r	16/31 (52%)	16 (100%)	0	100	100
1	s	16/31 (52%)	16 (100%)	0	100	100
1	t	16/31 (52%)	16 (100%)	0	100	100
1	u	16/31 (52%)	16 (100%)	0	100	100
1	v	16/31 (52%)	16 (100%)	0	100	100
1	w	16/31 (52%)	16 (100%)	0	100	100
1	x	16/31 (52%)	16 (100%)	0	100	100
1	y	16/31 (52%)	16 (100%)	0	100	100
1	z	16/31 (52%)	16 (100%)	0	100	100
All	All	2752/5332 (52%)	2752 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

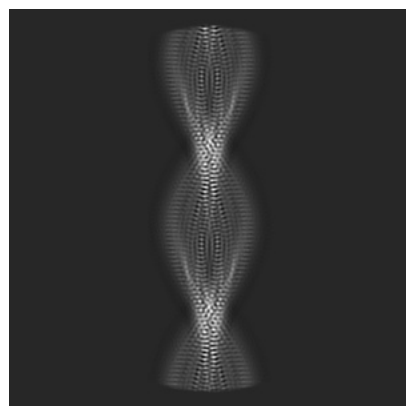
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63648. These allow visual inspection of the internal detail of the map and identification of artifacts.

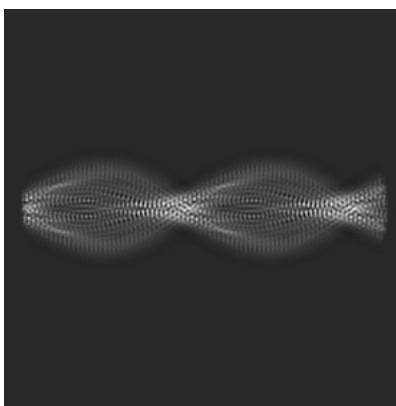
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

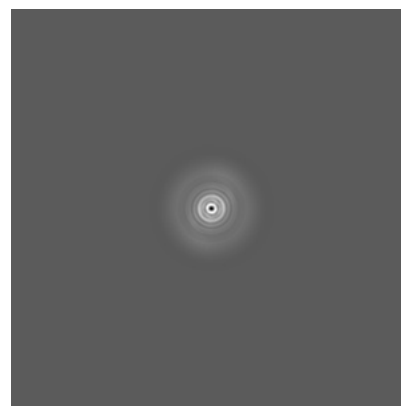
6.1.1 Primary map



X

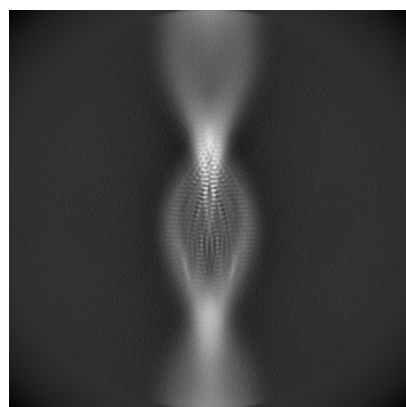


Y

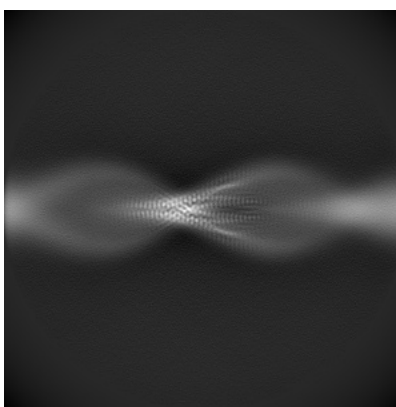


Z

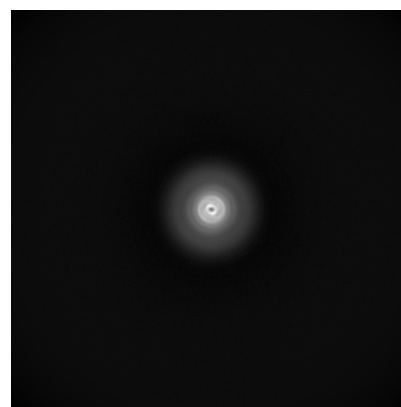
6.1.2 Raw map



X



Y

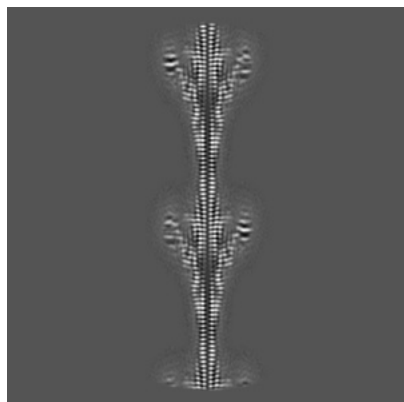


Z

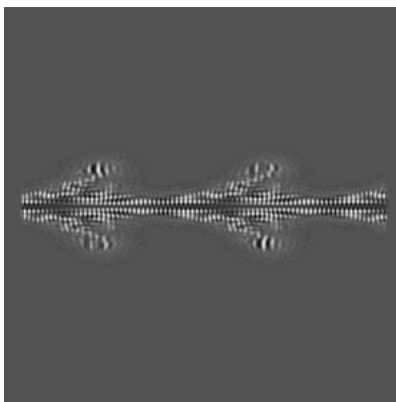
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192

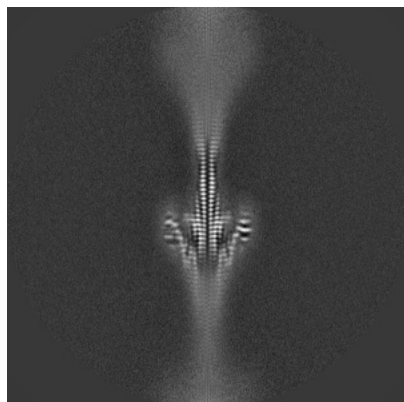


Y Index: 192

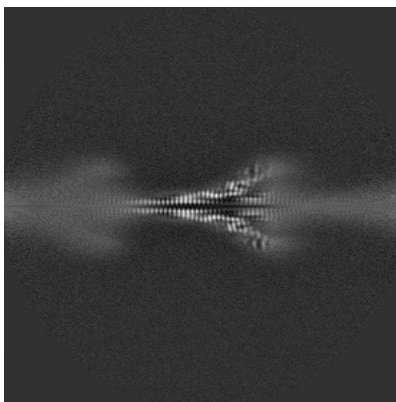


Z Index: 192

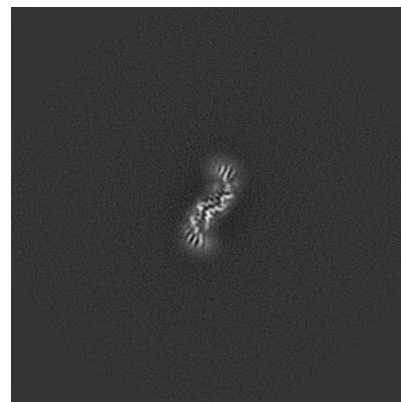
6.2.2 Raw map



X Index: 192



Y Index: 192

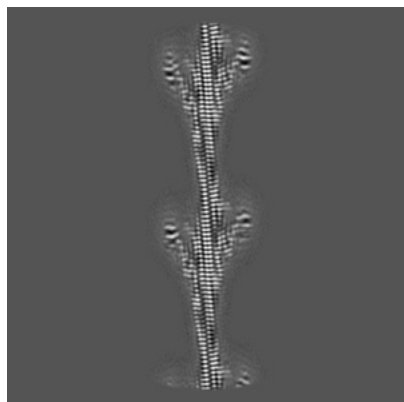


Z Index: 192

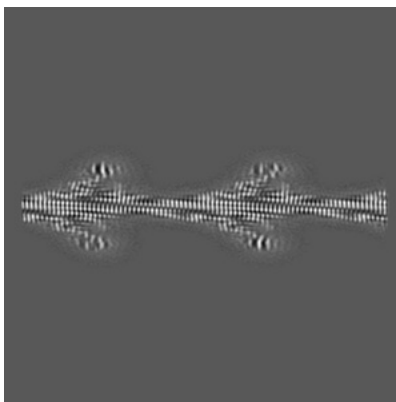
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

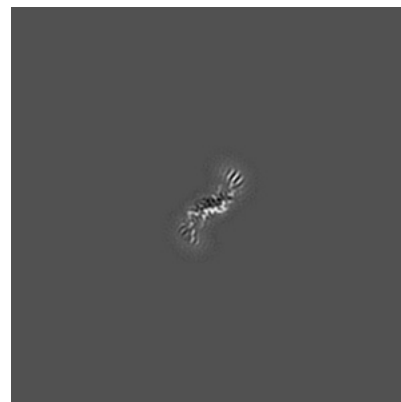
6.3.1 Primary map



X Index: 196

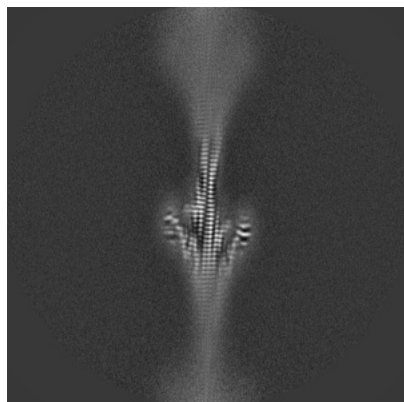


Y Index: 189

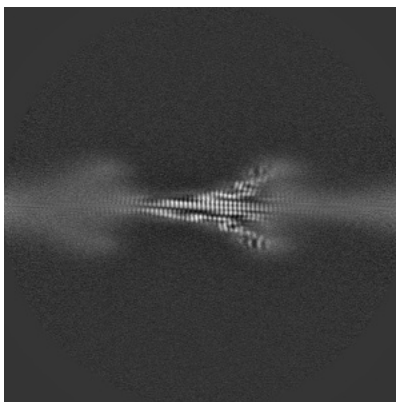


Z Index: 204

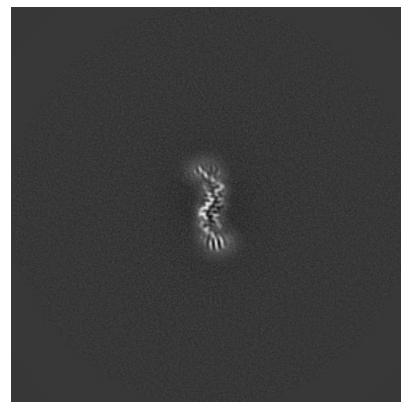
6.3.2 Raw map



X Index: 189



Y Index: 189

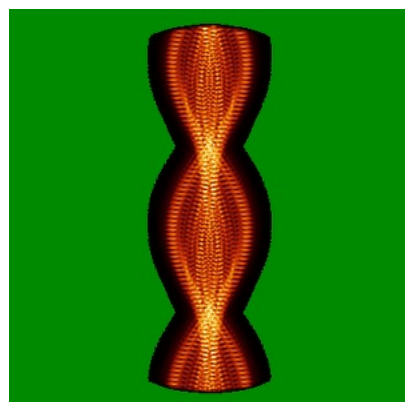


Z Index: 163

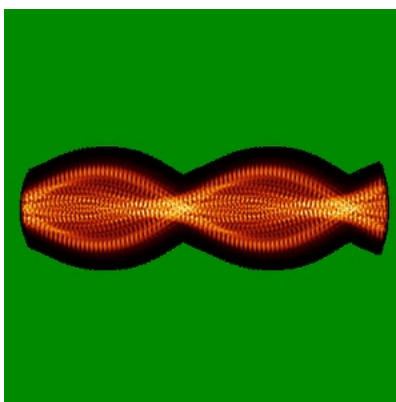
The images above show the largest variance slices of the map in three orthogonal directions.

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

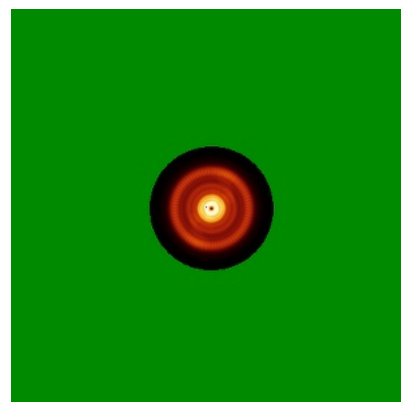
6.4.1 Primary map



X

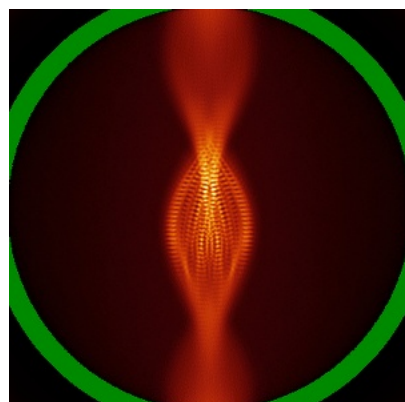


Y

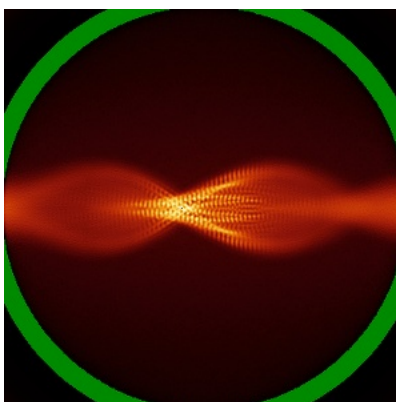


Z

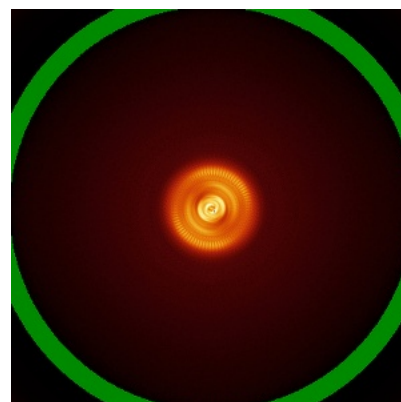
6.4.2 Raw map



X



Y

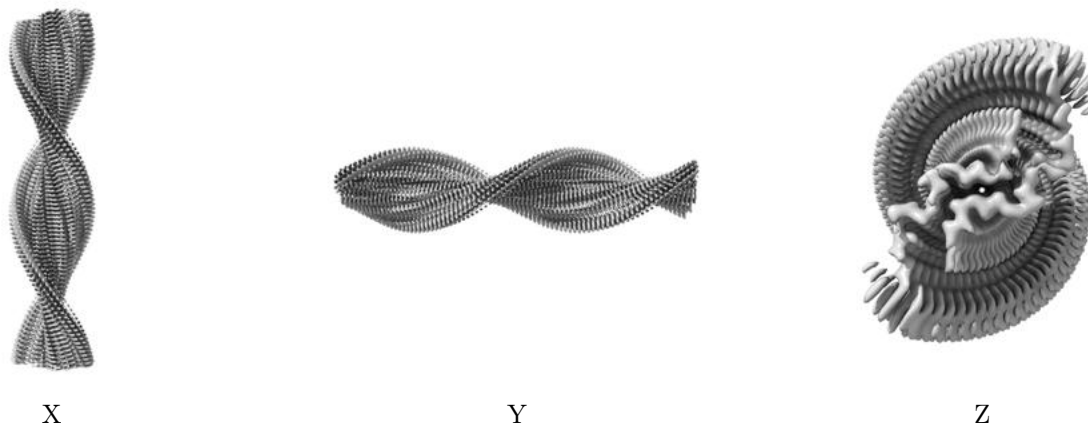


Z

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.

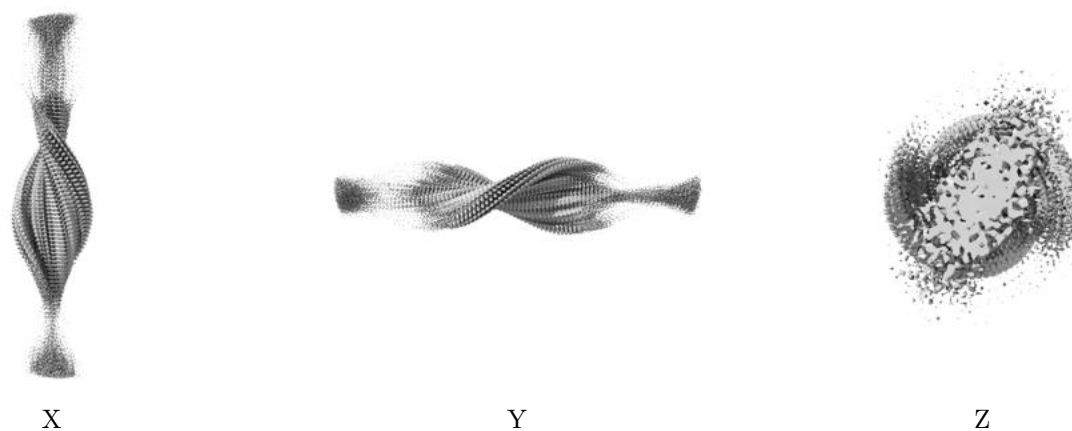
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

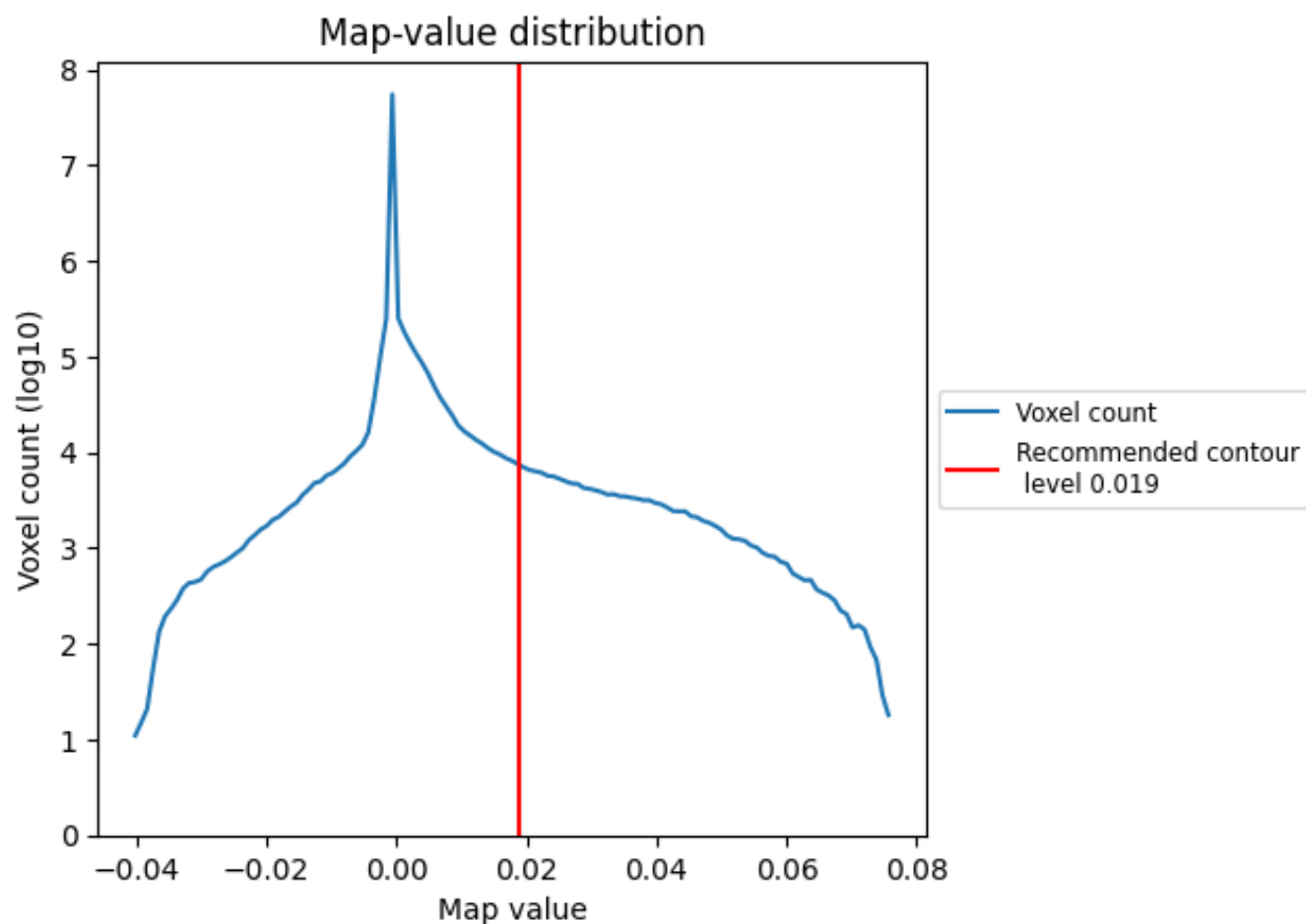
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

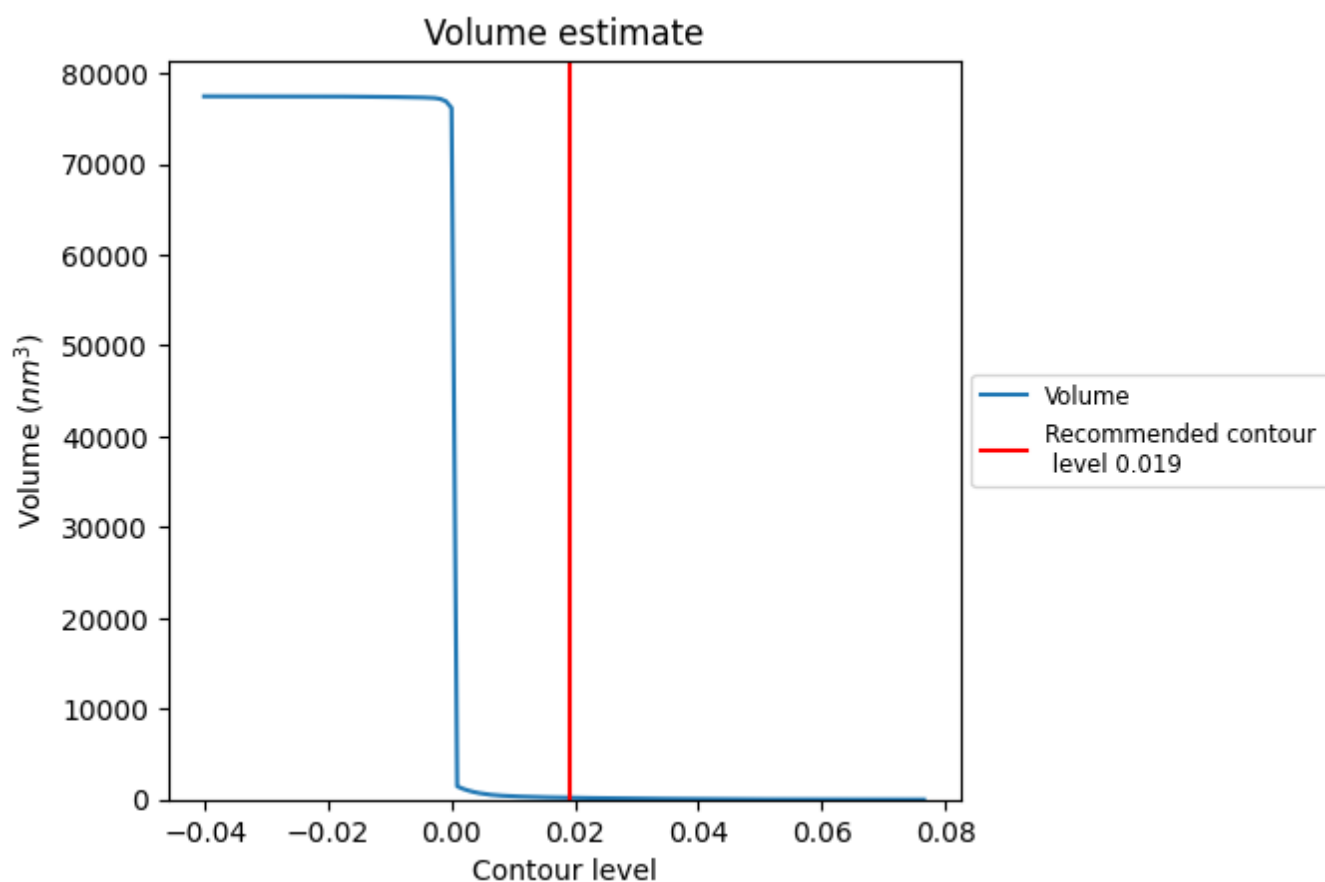
This section contains the results of statistical analysis of the map.

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.

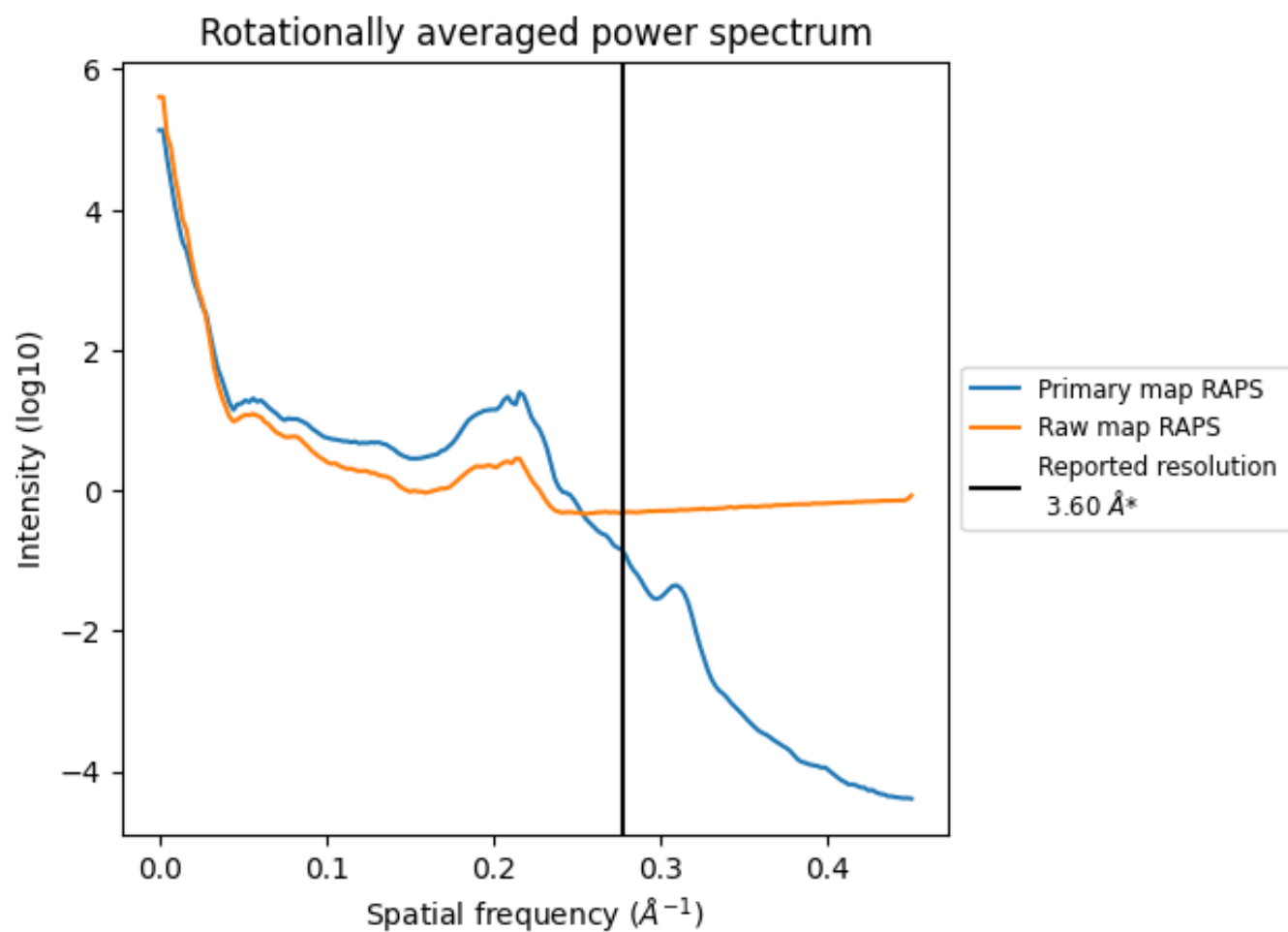
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 182 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

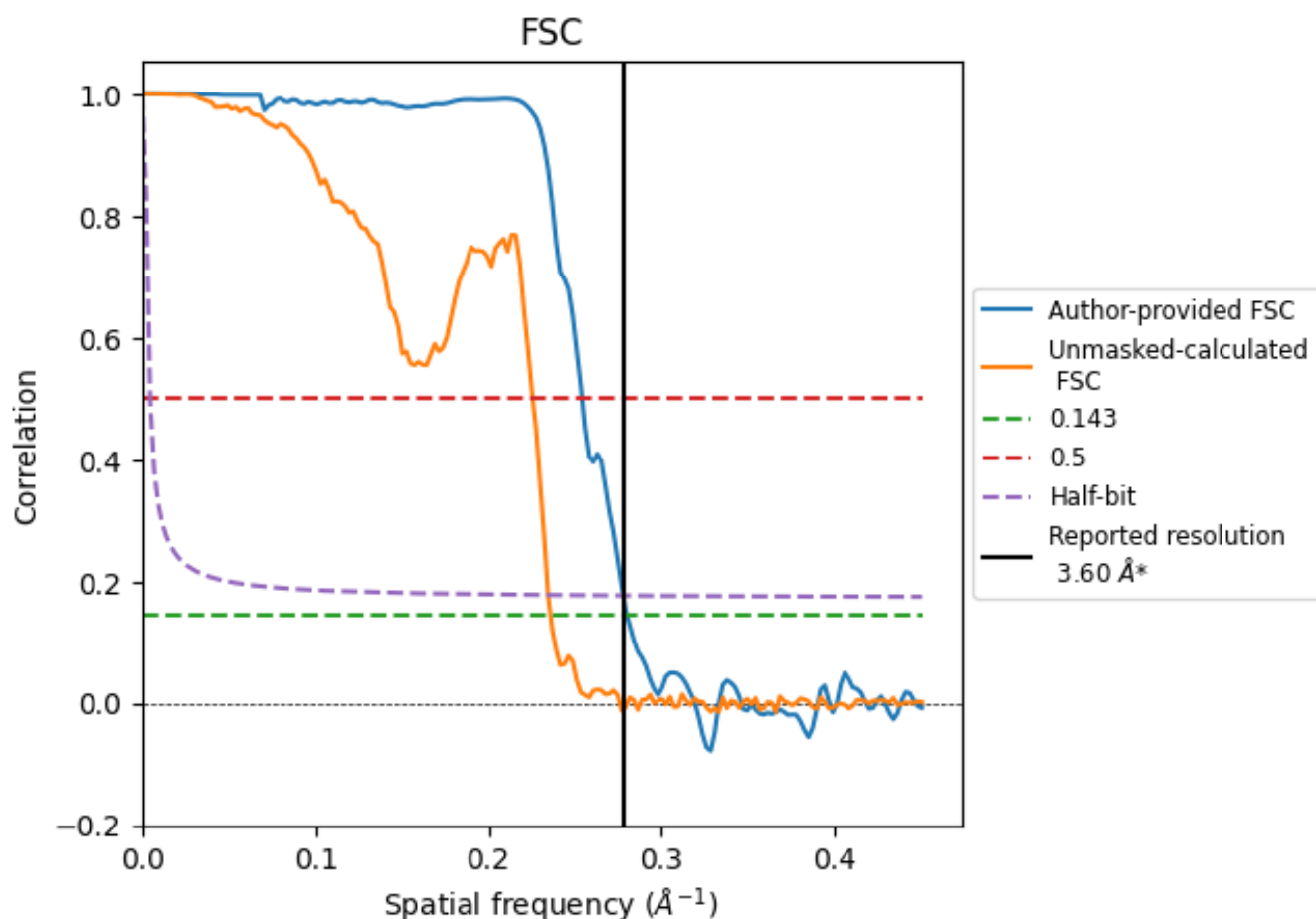


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

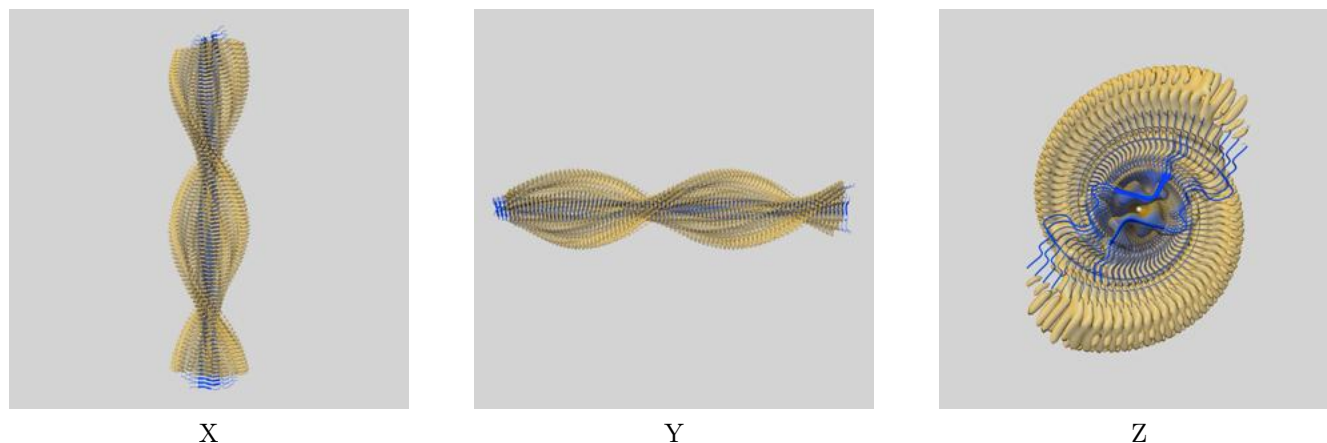
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	3.94	3.60
Unmasked-calculated*	4.24	4.43	4.26

*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 4.24 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

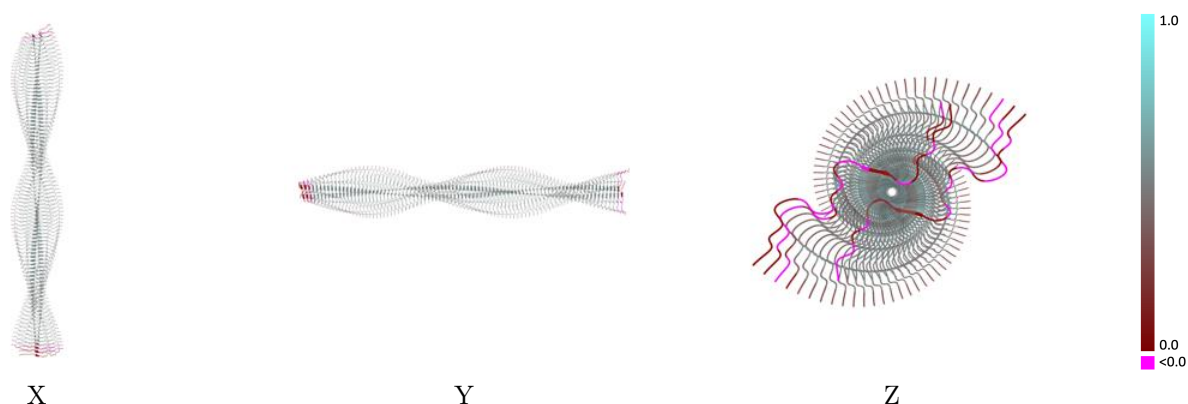
This section contains information regarding the fit between EMDB map EMD-63648 and PDB model 9M5R. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



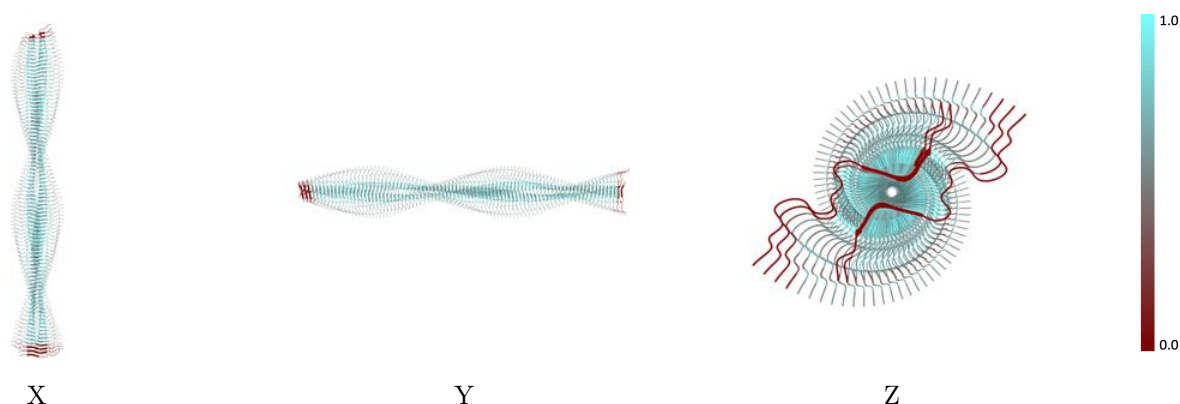
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



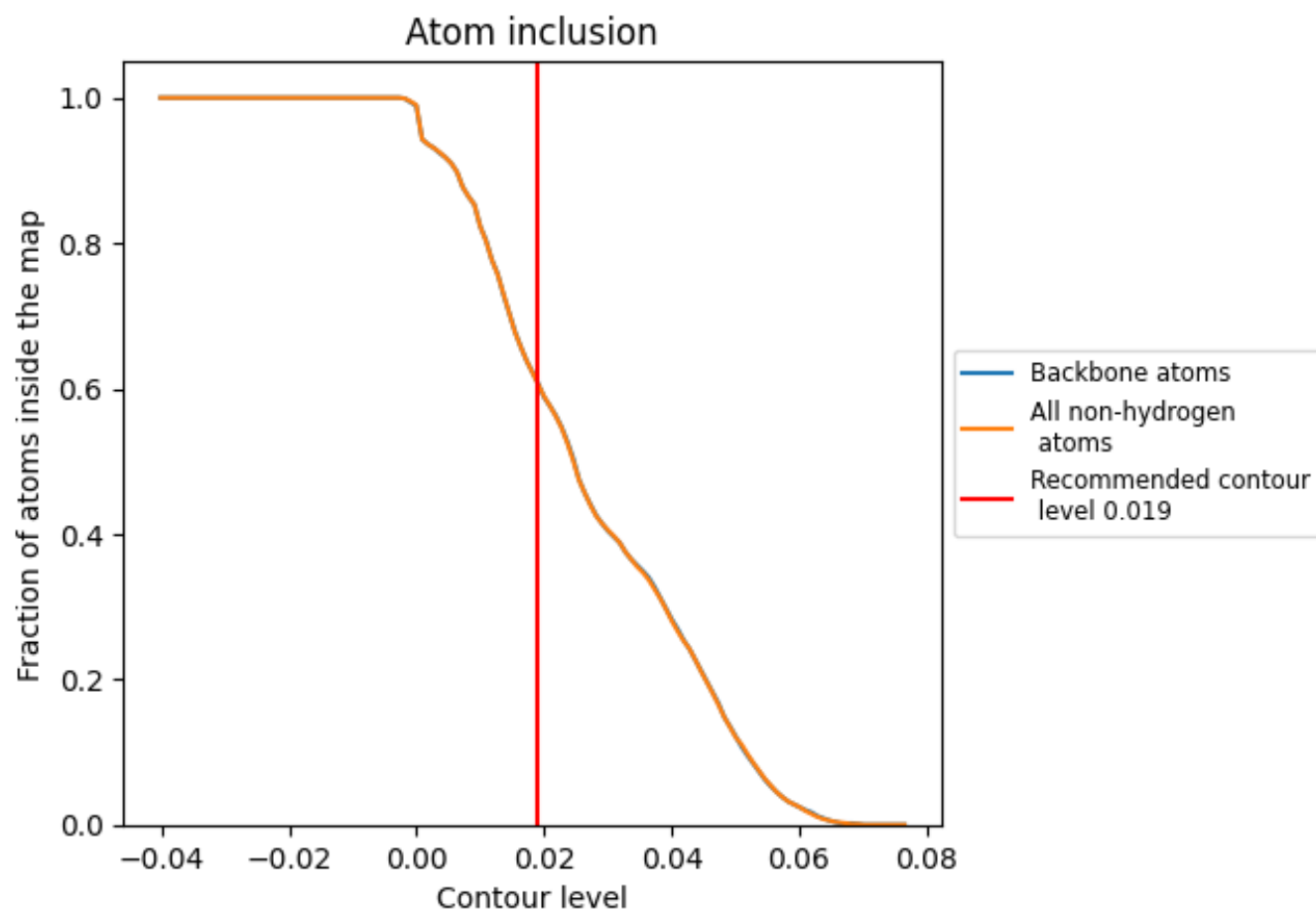
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6080	 0.4560
0	 0.6370	 0.4880
1	 0.6370	 0.4870
2	 0.6620	 0.4770
3	 0.6560	 0.4840
4	 0.6500	 0.4790
5	 0.6370	 0.4870
6	 0.6370	 0.4770
7	 0.6310	 0.4880
8	 0.6500	 0.4730
9	 0.6620	 0.4860
A	 0.0000	 0.0010
A0	 0.6310	 0.4840
A1	 0.6560	 0.4750
A2	 0.6620	 0.4830
A3	 0.6620	 0.4810
A4	 0.6310	 0.4830
A5	 0.6310	 0.4840
A6	 0.6310	 0.4850
A7	 0.6310	 0.4820
A8	 0.6620	 0.4820
A9	 0.6440	 0.4760
AA	 0.6500	 0.4770
AB	 0.6440	 0.4880
AC	 0.6310	 0.4780
AD	 0.6370	 0.4860
AE	 0.6440	 0.4790
AF	 0.6500	 0.4810
AG	 0.6560	 0.4750
AH	 0.6620	 0.4830
AI	 0.6500	 0.4770
AJ	 0.6310	 0.4830
AK	 0.6500	 0.4790
AL	 0.6560	 0.4820
AM	 0.6500	 0.4690























































































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Chain	Atom inclusion	Q-score
AN	 0.6500	 0.4810
AO	 0.6440	 0.4700
AP	 0.6560	 0.4790
AQ	 0.6440	 0.4760
AR	 0.6310	 0.4810
AS	 0.6440	 0.4770
AT	 0.6560	 0.4820
AU	 0.6560	 0.4760
AV	 0.6370	 0.4770
AW	 0.6440	 0.4770
AX	 0.6310	 0.4840
AY	 0.6190	 0.4770
AZ	 0.6560	 0.4820
Aa	 0.6620	 0.4740
Ab	 0.6500	 0.4820
Ac	 0.6500	 0.4750
Ad	 0.6440	 0.4840
Ae	 0.6370	 0.4780
Af	 0.6250	 0.4820
Ag	 0.6440	 0.4790
Ah	 0.6560	 0.4760
Ai	 0.6500	 0.4740
Aj	 0.6440	 0.4730
Ak	 0.6560	 0.4760
Al	 0.6250	 0.4790
Am	 0.6370	 0.4820
An	 0.6440	 0.4750
Ao	 0.6500	 0.4820
Ap	 0.6500	 0.4760
Aq	 0.6440	 0.4810
Ar	 0.6440	 0.4760
As	 0.6560	 0.4890
At	 0.6310	 0.4750
Au	 0.6370	 0.4860
Av	 0.6620	 0.4770
Aw	 0.6500	 0.4840
Ax	 0.6370	 0.4730
Ay	 0.6370	 0.4850
Az	 0.6250	 0.4760
B	 0.0000	 -0.0020
BA	 0.6560	 0.4830
BB	 0.6440	 0.4800





















































































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Chain	Atom inclusion	Q-score
BC	 0.6370	 0.4890
BD	 0.6250	 0.4800
BE	 0.6440	 0.4890
BF	 0.6560	 0.4780
BG	 0.6500	 0.4860
BH	 0.6560	 0.4770
BI	 0.6440	 0.4860
BJ	 0.6440	 0.4820
BK	 0.6440	 0.4870
BL	 0.6500	 0.4740
BM	 0.6560	 0.4880
BN	 0.6500	 0.4760
BO	 0.6560	 0.4830
BP	 0.6370	 0.4810
BQ	 0.6370	 0.4870
BR	 0.6370	 0.4770
BS	 0.6440	 0.4840
BT	 0.6620	 0.4770
BU	 0.6500	 0.4800
BV	 0.6370	 0.4740
BW	 0.6500	 0.4840
BX	 0.6370	 0.4790
BY	 0.6310	 0.4780
BZ	 0.6440	 0.4740
Ba	 0.6560	 0.4780
Bb	 0.6500	 0.4700
Bc	 0.6560	 0.4810
Bd	 0.6250	 0.4760
Be	 0.6440	 0.4850
Bf	 0.6310	 0.4770
Bg	 0.6440	 0.4830
Bh	 0.6620	 0.4730
Bi	 0.6440	 0.4840
Bj	 0.6500	 0.4760
Bk	 0.6310	 0.4820
Bl	 0.6440	 0.4790
Bm	 0.6310	 0.4830
Bn	 0.6500	 0.4750
Bo	 0.6310	 0.4810
Bp	 0.6190	 0.4570
Bq	 0.5620	 0.4300
Br	 0.4940	 0.4020

























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Chain	Atom inclusion	Q-score
Bs	 0.3810	 0.3320
Bt	 0.1750	 0.1980
Bu	 0.0000	 0.0270
Bv	 0.0000	 0.0060
C	 0.0000	 -0.0080
D	 0.0060	 0.0070
E	 0.0440	 0.0250
F	 0.1190	 0.2200
G	 0.5060	 0.4390
H	 0.6440	 0.4730
I	 0.6500	 0.4840
J	 0.6310	 0.4740
K	 0.6440	 0.4850
L	 0.6370	 0.4780
M	 0.6310	 0.4820
N	 0.6620	 0.4700
O	 0.6560	 0.4810
P	 0.6500	 0.4750
Q	 0.6310	 0.4830
R	 0.6500	 0.4790
S	 0.6370	 0.4800
T	 0.6560	 0.4770
U	 0.6620	 0.4760
V	 0.6620	 0.4730
W	 0.6500	 0.4760
X	 0.6440	 0.4740
Y	 0.6500	 0.4800
Z	 0.6370	 0.4810
a	 0.6500	 0.4750
b	 0.6560	 0.4800
c	 0.6560	 0.4760
d	 0.6560	 0.4840
e	 0.6310	 0.4740
f	 0.6310	 0.4880
g	 0.6500	 0.4770
h	 0.6560	 0.4850
i	 0.6500	 0.4760
j	 0.6500	 0.4860
k	 0.6370	 0.4770
l	 0.6250	 0.4840
m	 0.6310	 0.4780
n	 0.6370	 0.4830

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Chain	Atom inclusion	Q-score
o	 0.6560	 0.4740
p	 0.6500	 0.4840
q	 0.6500	 0.4780
r	 0.6620	 0.4850
s	 0.6310	 0.4830
t	 0.6250	 0.4900
u	 0.6440	 0.4780
v	 0.6560	 0.4850
w	 0.6500	 0.4790
x	 0.6440	 0.4820
y	 0.6370	 0.4810
z	 0.6370	 0.4800